



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:36 PM UTC

PDB ID : 1LSH / pdb_00001lsh
Title : LIPID-PROTEIN INTERACTIONS IN LIPOVITELLIN
Authors : Thompson, J.R.; Banaszak, L.J.
Deposited on : 2002-05-17
Resolution : 1.90 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

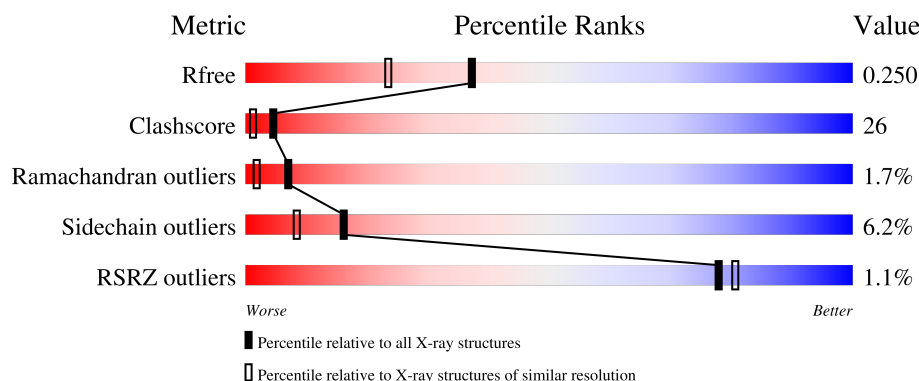
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1056	59% 28% • 10%
2	B	319	24% 25% 5% • 45%

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	PLD	A	2001[A]	X	-	-	-
3	PLD	A	2001[B]	X	-	-	-
3	PLD	A	2005[A]	X	-	-	-
3	PLD	A	2005[B]	X	-	-	-
3	PLD	A	2006	X	-	-	-
3	PLD	A	2007[A]	X	-	-	-
3	PLD	A	2007[B]	X	-	-	-
4	UPL	A	2008	X	-	-	-
4	UPL	A	2009	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10935 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 LIPOVITELLIN (LV-1N, LV-1C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	955	Total	C	N	O	S	15	65	0
			7781	4960	1362	1418	41			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLY	ALA	conflict	UNP Q91062
A	396	ALA	TYR	conflict	UNP Q91062
A	417	ASN	HIS	conflict	UNP Q91062
A	469	LYS	ASP	conflict	UNP Q91062
A	782	GLY	ARG	conflict	UNP Q91062
A	834	SER	HIS	conflict	UNP Q91062
A	?	-	GLN	deletion	UNP Q91062
A	1013	SER	HIS	conflict	UNP Q91062
A	1064	THR	GLN	conflict	UNP Q91062

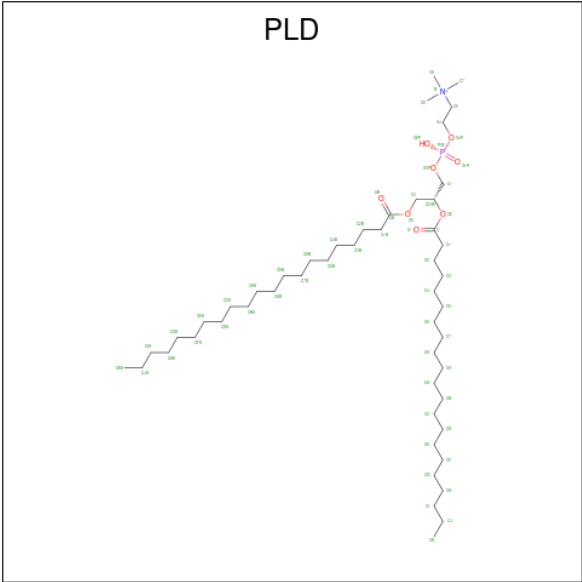
- Molecule 2 is a protein called LIPOVITELLIN (LV-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	3	4	0
			1375	886	250	231	8			

There are 2 discrepancies between the modelled and reference sequences:

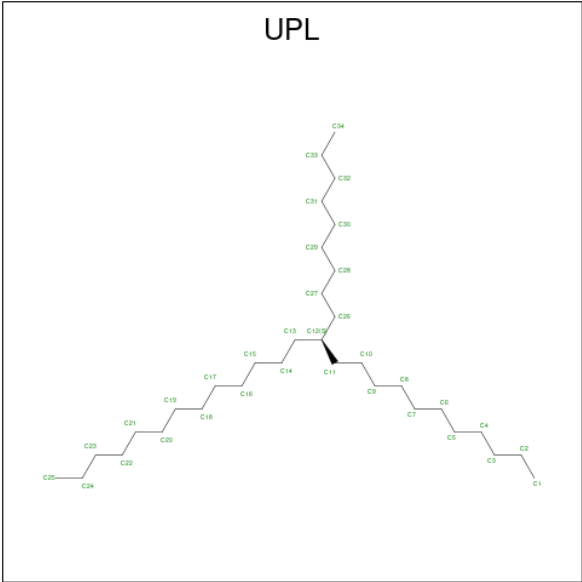
Chain	Residue	Modelled	Actual	Comment	Reference
B	1473	GLY	LYS	conflict	UNP Q91062
B	1489	ALA	LYS	conflict	UNP Q91062

- Molecule 3 is di-heneicosanoyl phosphatidyl choline (CCD ID: PLD) (formula: C₅₀H₁₀₁NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			57	47	1	8	1		
3	A	1	Total	C	O	P		0	0
			35	26	8	1			
3	A	1	Total	C	O	P		0	0
			34	25	8	1			
3	A	1	Total	C	O	P		0	1
			53	44	8	1			
3	A	1	Total	C	O	P		0	0
			34	25	8	1			
3	A	1	Total	C	O	P		0	1
			40	31	8	1			
3	B	1	Total	C	N	O	P	0	0
			31	21	1	8	1		

- Molecule 4 is UNKNOWN BRANCHED FRAGMENT OF PHOSPHOLIPID (CCD ID: UPL) (formula: C₃₄H₇₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 17 17	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C 19 19	0	0
4	A	1	Total C 17 17	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 8 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 8 8	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 6 6	0	0
4	B	1	Total C 14 14	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 7 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 7 7	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 5 5	0	0
4	B	1	Total C 6 6	0	0

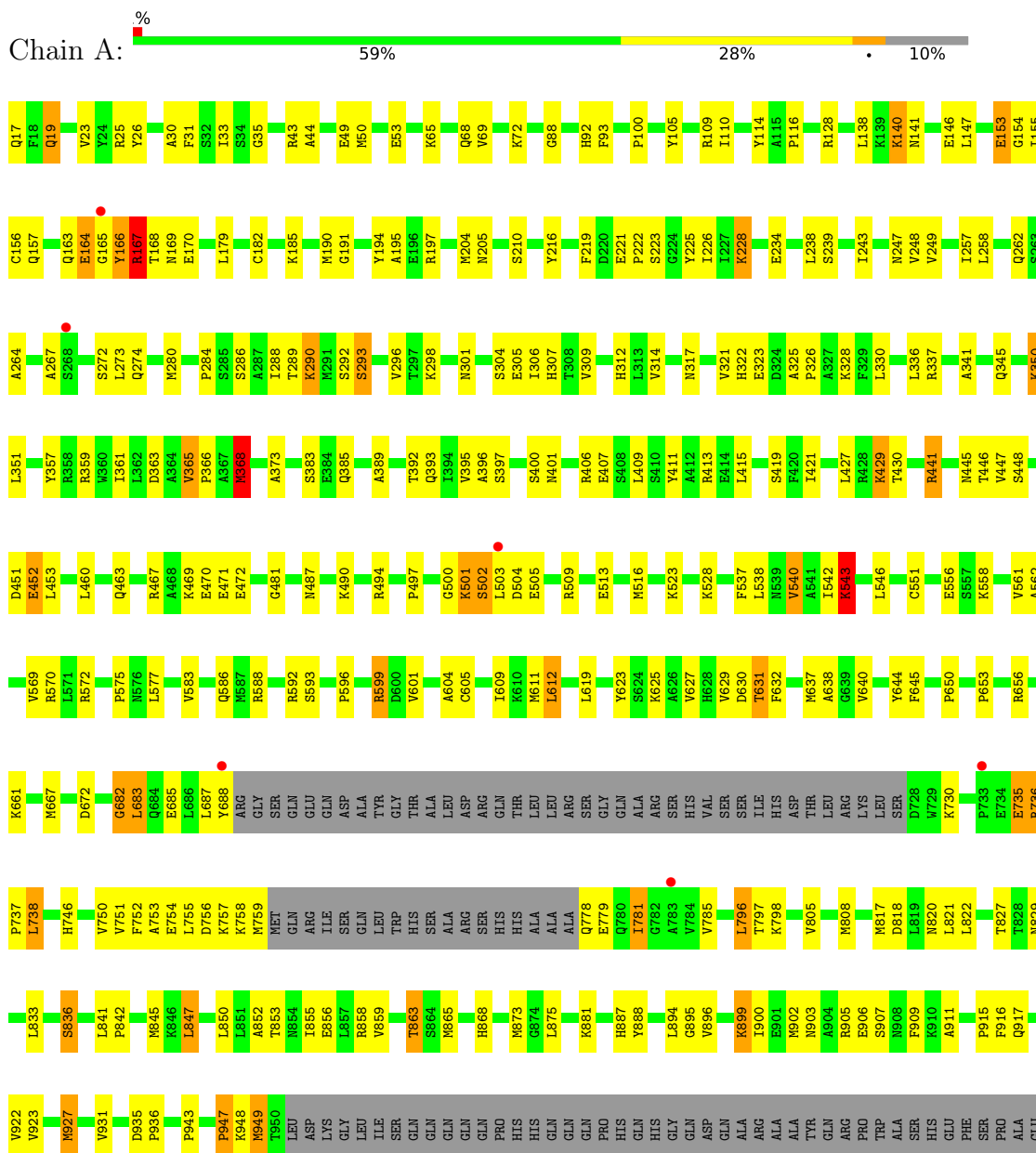
- Molecule 5 is water.

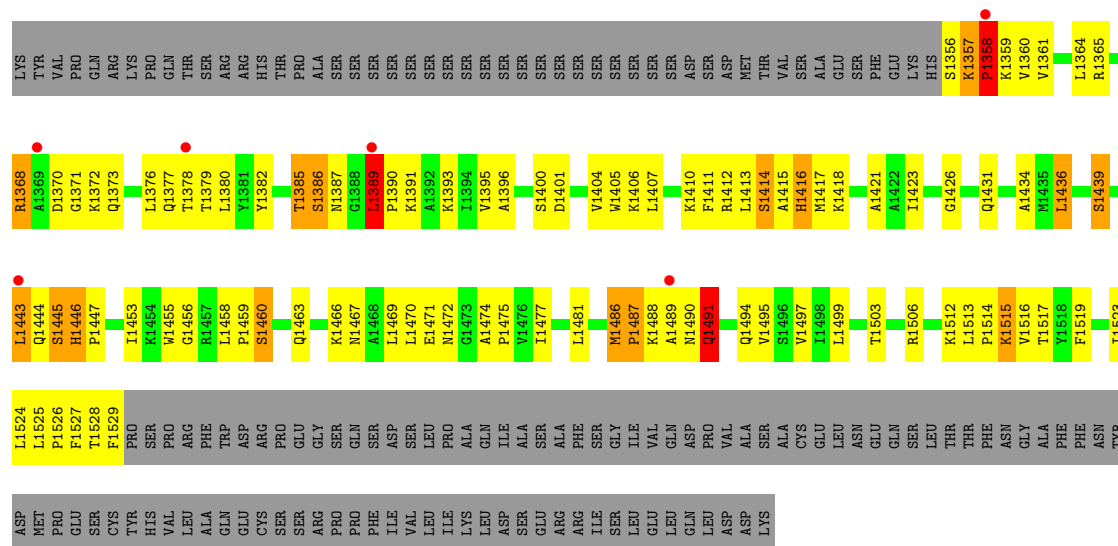
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1002	Total O 1002 1002	0	1
5	B	120	Total O 120 120	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: LIPOVITELLIN (LV-1N, LV-1C)





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.17Å 84.52Å 89.53Å 90.00° 100.39° 90.00°	Depositor
Resolution (Å)	21.60 – 1.90 21.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	74.3 (21.60-1.90) 74.4 (21.60-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.255 0.208 , 0.250	Depositor DCC
R_{free} test set	983 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 140.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10935	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: PCA, UPL, PLD

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	1.05	2/8093 (0.0%)	1.35	33/10921 (0.3%)
2	B	0.72	0/1412	1.24	11/1901 (0.6%)
All	All	1.01	2/9505 (0.0%)	1.33	44/12822 (0.3%)

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	A	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	PRO	CA-C	8.08	1.56	1.51
1	A	365	VAL	CA-CB	7.14	1.58	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	PRO	N-CA-C	-7.53	104.45	113.86
1	A	257	ILE	CB-CA-C	-7.24	100.28	110.12
2	B	1456	GLY	N-CA-C	-6.92	102.85	112.13
1	A	350[A]	LYS	CA-C-N	-6.58	111.73	121.99
1	A	350[A]	LYS	C-N-CA	-6.58	111.73	121.99
1	A	350[B]	LYS	CA-C-N	-6.58	111.73	121.99
1	A	350[B]	LYS	C-N-CA	-6.58	111.73	121.99
1	A	1004	ALA	N-CA-C	-6.14	105.36	112.92
1	A	1055	GLN	CA-C-N	6.13	127.51	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1055	GLN	C-N-CA	6.13	127.51	119.84
2	B	1459	PRO	N-CA-C	-5.99	101.80	111.03
1	A	441	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	875	LEU	CA-CB-CG	-5.90	95.65	116.30
1	A	88	GLY	N-CA-C	5.86	120.57	112.37
1	A	395	VAL	O-C-N	5.83	127.83	121.83
2	B	1414	SER	N-CA-C	5.80	118.03	110.43
2	B	1389	LEU	CA-C-N	5.80	125.81	119.89
2	B	1389	LEU	C-N-CA	5.80	125.81	119.89
1	A	290[A]	LYS	CA-C-N	-5.75	114.77	122.42
1	A	290[A]	LYS	C-N-CA	-5.75	114.77	122.42
1	A	290[B]	LYS	CA-C-N	-5.75	114.77	122.42
1	A	290[B]	LYS	C-N-CA	-5.75	114.77	122.42
2	B	1446	HIS	CA-C-N	-5.73	113.86	119.76
2	B	1446	HIS	C-N-CA	-5.73	113.86	119.76
1	A	682	GLY	N-CA-C	-5.65	105.95	112.50
1	A	481	GLY	N-CA-C	-5.63	105.83	112.64
1	A	593	SER	CA-C-N	-5.62	113.63	122.79
1	A	593	SER	C-N-CA	-5.62	113.63	122.79
2	B	1486	MET	CA-C-N	5.42	125.50	119.32
2	B	1486	MET	C-N-CA	5.42	125.50	119.32
1	A	738	LEU	N-CA-C	-5.41	104.78	111.33
1	A	1049	VAL	CB-CA-C	-5.31	102.90	110.12
2	B	1487	PRO	N-CA-C	5.29	121.63	113.75
1	A	735	GLU	N-CA-C	-5.29	101.53	109.15
2	B	1371	GLY	N-CA-C	-5.27	108.04	115.32
1	A	543	LYS	CA-C-N	5.27	127.66	120.54
1	A	543	LYS	C-N-CA	5.27	127.66	120.54
1	A	273	LEU	N-CA-C	-5.16	105.71	112.41
1	A	368	MET	N-CA-CB	5.14	117.78	110.06
1	A	451	ASP	N-CA-C	5.11	116.53	111.07
1	A	656	ARG	N-CA-C	-5.08	105.83	111.36
1	A	128	ARG	N-CA-C	-5.06	105.95	111.82
1	A	153	GLU	CA-CB-CG	-5.06	103.98	114.10
1	A	216	TYR	N-CA-C	5.00	117.55	109.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	SER	Mainchain
1	A	631	THR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	796	LEU	Mainchain
1	A	820	ASN	Mainchain
1	A	863	THR	Mainchain

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	7781	0	8167	356	0
2	B	1375	0	1488	104	0
3	A	253	0	205	51	0
3	B	31	0	33	8	0
4	A	273	0	494	46	0
4	B	100	0	179	19	0
5	A	1002	0	0	63	0
5	B	120	0	0	11	0
All	All	10935	0	10566	527	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 26.

All (527) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LYS:HE3	1:A:543:LYS:H	1.09	1.11
3:A:2004:PLD:H2A2	3:A:2004:PLD:H32	1.35	1.05
1:A:785:VAL:HG21	1:A:845:MET:HE1	1.36	1.04
1:A:1011:LYS:HD3	1:A:1012:GLN:H	1.25	1.01
3:A:2005[B]:PLD:H5'1	3:A:2007[B]:PLD:H8A1	1.46	0.97
1:A:588:ARG:HD2	1:A:609[A]:ILE:HD13	1.46	0.95
1:A:469:LYS:HE3	1:A:471:GLU:HB2	1.46	0.95
1:A:366:PRO:HB3	1:A:397:SER:HB3	1.49	0.94
1:A:543:LYS:H	1:A:543:LYS:CE	1.82	0.93
2:B:1490:ASN:HD22	2:B:1491:GLN:H	0.97	0.92
1:A:543:LYS:HE3	1:A:543:LYS:N	1.85	0.91
1:A:856:GLU:HG2	1:A:858[A]:ARG:HH12	1.32	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805[B]:VAL:HG12	1:A:821:LEU:HB3	1.52	0.90
2:B:1436:LEU:HD12	2:B:1453:ILE:HG12	1.53	0.90
1:A:907:SER:HB2	1:A:1071:GLN:HG2	1.55	0.88
2:B:1489:ALA:HB2	2:B:1517:THR:OG1	1.74	0.87
1:A:368:MET:HG3	1:A:373:ALA:HB2	1.54	0.87
1:A:317:ASN:ND2	1:A:322[A]:HIS:H	1.73	0.86
1:A:317:ASN:ND2	1:A:322[B]:HIS:H	1.73	0.86
2:B:1490:ASN:ND2	2:B:1491:GLN:H	1.74	0.85
1:A:194:TYR:HB2	5:A:2910:HOH:O	1.76	0.84
1:A:751:VAL:HG23	5:A:2684:HOH:O	1.76	0.83
4:A:2015:UPL:H62	4:B:2016:UPL:H12	1.58	0.83
2:B:1490:ASN:HD22	2:B:1491:GLN:N	1.74	0.82
1:A:219:PHE:HD2	1:A:226:ILE:HD11	1.44	0.82
3:B:2003:PLD:H5A1	4:B:2046:UPL:C5	2.10	0.81
2:B:1389:LEU:HD12	2:B:1389:LEU:H	1.46	0.81
4:A:2009:UPL:H142	4:A:2009:UPL:H271	1.63	0.80
1:A:948:LYS:HA	1:A:1005[A]:ARG:NH1	1.96	0.79
1:A:1011:LYS:HD3	1:A:1012:GLN:N	1.98	0.79
1:A:1054:VAL:HG21	4:A:2012:UPL:H131	1.62	0.79
3:A:2006:PLD:H5A2	4:A:2018:UPL:H52	1.63	0.78
1:A:592:ARG:NH1	3:B:2003:PLD:H52	1.96	0.78
3:A:2002:PLD:OB	3:A:2002:PLD:H11	1.84	0.78
4:A:2011:UPL:H62	4:A:2011:UPL:H12	1.64	0.78
2:B:1373:GLN:HG2	2:B:1400:SER:HA	1.64	0.78
1:A:23:VAL:HG23	1:A:264:ALA:HB2	1.66	0.78
2:B:1506:ARG:HD2	5:B:107:HOH:O	1.83	0.78
1:A:317:ASN:HD22	1:A:321:VAL:HA	1.49	0.77
1:A:543:LYS:HE2	5:A:2056:HOH:O	1.86	0.75
2:B:1385:THR:HG22	2:B:1386:SER:N	2.02	0.74
3:A:2004:PLD:H32	3:A:2004:PLD:C2B	2.15	0.73
1:A:561[B]:VAL:HG12	1:A:604:ALA:HA	1.70	0.73
1:A:469:LYS:C	1:A:469:LYS:HD2	2.13	0.73
1:A:366:PRO:CB	1:A:397:SER:HB3	2.18	0.72
1:A:599:ARG:HG3	1:A:599:ARG:HH11	1.53	0.72
2:B:1373:GLN:CG	2:B:1400:SER:HA	2.20	0.72
1:A:1005[A]:ARG:HH22	1:A:1031:ARG:HH21	1.38	0.71
1:A:856:GLU:CG	1:A:858[A]:ARG:HH12	2.03	0.71
1:A:415:LEU:HG	1:A:421:ILE:CD1	2.21	0.70
2:B:1385:THR:HG22	2:B:1386:SER:H	1.57	0.70
1:A:856:GLU:HG2	1:A:858[A]:ARG:NH1	2.07	0.69
2:B:1488:LYS:HA	2:B:1516:VAL:HA	1.72	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HG2	5:A:2131:HOH:O	1.93	0.69
1:A:735:GLU:O	1:A:737:PRO:HD3	1.93	0.69
2:B:1416:HIS:HB2	2:B:1418:LYS:HE2	1.73	0.69
1:A:1068:LEU:HD21	2:B:1360:VAL:HG13	1.74	0.69
1:A:948:LYS:HA	1:A:1005[A]:ARG:HH12	1.57	0.68
1:A:900:ILE:HD11	4:A:2013:UPL:C12	2.23	0.68
1:A:330:LEU:HD11	5:A:2902:HOH:O	1.93	0.68
1:A:730[B]:LYS:HD2	5:A:2938:HOH:O	1.92	0.68
2:B:1423:ILE:HD13	4:B:2021:UPL:H13	1.76	0.67
1:A:494:ARG:HD2	5:A:2756:HOH:O	1.94	0.67
1:A:219:PHE:CD2	1:A:226:ILE:HD11	2.30	0.67
1:A:1070:LEU:CD2	1:A:1071:GLN:H	2.07	0.67
2:B:1370:ASP:OD1	2:B:1372:LYS:HG3	1.93	0.67
1:A:592:ARG:HD2	2:B:1524:LEU:HB3	1.75	0.67
1:A:888:TYR:CE1	1:A:927:MET:HG3	2.30	0.67
3:A:2004:PLD:H2A2	3:A:2004:PLD:C3	2.20	0.67
1:A:661[B]:LYS:HE2	5:A:2104:HOH:O	1.94	0.66
1:A:368:MET:HG3	1:A:373:ALA:CB	2.23	0.66
1:A:936[B]:PRO:HD2	5:A:2680:HOH:O	1.95	0.66
4:A:2011:UPL:H12	4:A:2011:UPL:C6	2.26	0.66
1:A:661[B]:LYS:HD3	5:A:2749:HOH:O	1.96	0.66
1:A:1068:LEU:HD23	1:A:1069:GLU:N	2.11	0.66
1:A:166:TYR:C	1:A:167:ARG:O	2.36	0.65
1:A:1070:LEU:HD22	1:A:1071:GLN:H	1.62	0.65
1:A:1020:LEU:HD21	2:B:1364:LEU:HD21	1.79	0.65
1:A:33[B]:ILE:HD11	1:A:43[B]:ARG:HB2	1.78	0.65
3:A:2002:PLD:H4A2	3:A:2002:PLD:H32	1.78	0.65
3:A:2006:PLD:H1'2	3:A:2006:PLD:C3	2.26	0.64
1:A:441:ARG:NH1	1:A:441:ARG:HG2	2.12	0.64
2:B:1529:PHE:HB2	5:B:1032:HOH:O	1.97	0.64
4:B:2010:UPL:H102	4:B:2049:UPL:H11	1.79	0.64
1:A:286:SER:HB3	1:A:290[A]:LYS:HD3	1.78	0.64
1:A:558:LYS:HA	1:A:601[A]:VAL:CG2	2.28	0.64
1:A:65:LYS:HG3	1:A:100:PRO:HG3	1.81	0.63
4:A:2015:UPL:H62	4:B:2016:UPL:C1	2.27	0.63
1:A:501:LYS:O	1:A:502:SER:HB3	1.97	0.63
2:B:1443:LEU:HD11	5:B:922:HOH:O	1.98	0.63
1:A:540[A]:VAL:HG11	1:A:575:PRO:HG3	1.80	0.63
3:A:2006:PLD:H4A1	4:A:2018:UPL:H71	1.79	0.63
1:A:858[B]:ARG:HD2	1:A:899:LYS:HG2	1.80	0.63
1:A:164:GLU:HG2	5:A:2512:HOH:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1491:GLN:HE21	2:B:1494:GLN:HB2	1.64	0.62
1:A:558:LYS:HA	1:A:601[A]:VAL:HG21	1.81	0.62
2:B:1486:MET:HG3	2:B:1519:PHE:HE2	1.64	0.62
4:A:2008:UPL:C27	4:A:2008:UPL:H101	2.29	0.62
2:B:1436:LEU:HB2	4:B:2033:UPL:H13	1.80	0.62
1:A:389:ALA:O	1:A:393:GLN:HG3	2.00	0.62
1:A:469:LYS:HZ2	1:A:471:GLU:HG2	1.64	0.62
4:A:2009:UPL:H142	4:A:2009:UPL:C27	2.26	0.62
1:A:441:ARG:NE	5:A:3009:HOH:O	2.33	0.61
1:A:881:LYS:NZ	5:A:2283:HOH:O	2.32	0.61
2:B:1389:LEU:HD13	5:B:766:HOH:O	2.00	0.61
1:A:463:GLN:O	1:A:467[B]:ARG:HG2	2.00	0.61
1:A:561[A]:VAL:HG23	5:A:2138:HOH:O	1.99	0.61
1:A:357:TYR:O	1:A:361:ILE:HG13	2.01	0.61
3:A:2006:PLD:H1'2	3:A:2006:PLD:O3	2.01	0.61
2:B:1469:LEU:HD11	4:B:2023:UPL:H11	1.82	0.61
1:A:805[B]:VAL:CG1	1:A:821:LEU:HB3	2.30	0.61
1:A:190:MET:HE1	1:A:289:THR:HG22	1.83	0.60
1:A:469:LYS:NZ	1:A:471:GLU:HG2	2.16	0.60
1:A:542:ILE:HA	1:A:543:LYS:HE3	1.82	0.60
1:A:833:LEU:HD23	1:A:859:VAL:HG22	1.82	0.60
3:A:2001[A]:PLD:HB'2	3:A:2002:PLD:H1A2	1.83	0.60
1:A:138:LEU:HD12	1:A:225:TYR:CD2	2.36	0.60
1:A:141:ASN:HB2	5:A:2219:HOH:O	2.01	0.60
1:A:1031:ARG:HB3	1:A:1047[B]:ASP:OD1	2.01	0.60
2:B:1385:THR:OG1	2:B:1391:LYS:HD3	2.01	0.60
1:A:166:TYR:O	1:A:167:ARG:C	2.43	0.60
2:B:1389:LEU:HD23	2:B:1415:ALA:N	2.16	0.60
1:A:168:THR:O	1:A:169:ASN:HB2	2.01	0.60
1:A:551:CYS:SG	1:A:586[A]:GLN:NE2	2.74	0.60
1:A:35:GLY:HA3	1:A:43[B]:ARG:HD3	1.83	0.59
1:A:753:ALA:HB2	4:A:2011:UPL:H52	1.83	0.59
1:A:855:ILE:HG21	4:A:2024:UPL:H21	1.82	0.59
1:A:935:ASP:HB2	1:A:936[A]:PRO:HD2	1.84	0.59
1:A:949:MET:HE1	5:A:2586:HOH:O	2.02	0.59
1:A:1011:LYS:O	1:A:1012:GLN:HB2	2.03	0.59
2:B:1385:THR:CG2	2:B:1386:SER:H	2.15	0.59
1:A:1054:VAL:CG2	4:A:2012:UPL:H131	2.33	0.59
2:B:1490:ASN:ND2	2:B:1491:GLN:N	2.44	0.59
1:A:407:GLU:HG3	1:A:411:TYR:CZ	2.38	0.59
1:A:1043:LYS:HE2	5:A:2185:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HG2	1:A:223:SER:HB2	1.85	0.59
2:B:1455:TRP:HB2	2:B:1458:LEU:HD11	1.83	0.59
4:A:2012:UPL:H61	4:A:2029:UPL:C9	2.33	0.58
1:A:301:ASN:OD1	1:A:301:ASN:N	2.32	0.58
1:A:314:VAL:HG11	1:A:357:TYR:CE1	2.37	0.58
1:A:25:ARG:HH12	1:A:262:GLN:NE2	2.02	0.58
1:A:1005[A]:ARG:NH2	1:A:1031:ARG:HH21	1.99	0.58
1:A:947:PRO:O	1:A:1005[A]:ARG:NH2	2.37	0.58
2:B:1443:LEU:O	2:B:1444:GLN:HG2	2.03	0.58
1:A:500:GLY:C	1:A:502:SER:H	2.12	0.58
2:B:1423:ILE:HG22	2:B:1434:ALA:O	2.03	0.58
1:A:248[B]:VAL:HG23	1:A:873:MET:SD	2.44	0.58
1:A:640[B]:VAL:HG23	3:A:2002:PLD:H2'2	1.86	0.58
4:A:2008:UPL:C19	4:A:2008:UPL:H151	2.34	0.58
1:A:630:ASP:O	4:A:2009:UPL:H141	2.04	0.57
2:B:1389:LEU:CD2	2:B:1414:SER:HA	2.35	0.57
1:A:592:ARG:HH12	3:B:2003:PLD:H52	1.68	0.57
1:A:638:ALA:HB2	3:A:2002:PLD:H3A1	1.86	0.57
1:A:630:ASP:O	4:A:2009:UPL:H111	2.05	0.57
1:A:25:ARG:NH1	1:A:262:GLN:CD	2.62	0.57
1:A:1006:PRO:HG2	1:A:1031:ARG:NH2	2.18	0.57
1:A:366:PRO:HB3	1:A:397:SER:CB	2.30	0.57
1:A:415:LEU:HG	1:A:421:ILE:HD13	1.86	0.57
1:A:469:LYS:HD3	5:A:2877:HOH:O	2.05	0.57
1:A:503:LEU:O	1:A:505:GLU:HG2	2.04	0.57
1:A:911:ALA:O	1:A:1065:LYS:HA	2.04	0.57
2:B:1389:LEU:HD22	2:B:1414:SER:HA	1.87	0.57
1:A:653:PRO:HD2	1:A:688:TYR:CZ	2.40	0.57
2:B:1385:THR:CG2	2:B:1386:SER:N	2.68	0.57
1:A:35:GLY:HA3	1:A:43[B]:ARG:CD	2.35	0.56
1:A:588:ARG:HD2	1:A:609[A]:ILE:CD1	2.27	0.56
1:A:1031:ARG:NH1	5:A:2640:HOH:O	2.37	0.56
1:A:605:CYS:O	1:A:609[A]:ILE:HG13	2.05	0.56
3:A:2001[A]:PLD:HB'2	3:A:2002:PLD:C1B	2.36	0.56
1:A:746[B]:HIS:CD2	5:A:2910:HOH:O	2.58	0.56
3:A:2004:PLD:H2'2	2:B:1527:PHE:CE1	2.41	0.56
4:A:2011:UPL:H62	4:A:2011:UPL:C1	2.36	0.56
2:B:1523:ILE:HG23	3:B:2003:PLD:H11	1.88	0.56
1:A:779:GLU:HG2	5:A:2605:HOH:O	2.04	0.56
1:A:516:MET:HE2	5:A:2818:HOH:O	2.06	0.56
1:A:661[A]:LYS:NZ	5:A:2098:HOH:O	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:VAL:O	1:A:1024:VAL:HG13	2.05	0.55
2:B:1405:TRP:CH2	2:B:1407:LEU:HB2	2.41	0.55
2:B:1410:LYS:O	2:B:1421:ALA:HA	2.06	0.55
1:A:238:LEU:HB3	1:A:248[B]:VAL:HG23	1.87	0.55
1:A:286:SER:HB3	1:A:290[B]:LYS:HD3	1.88	0.55
2:B:1486:MET:HG3	2:B:1519:PHE:CE2	2.42	0.55
4:B:2010:UPL:C16	4:B:2021:UPL:H11	2.36	0.55
4:B:2023:UPL:H52	4:B:2023:UPL:H13	1.88	0.55
3:B:2003:PLD:H4A2	4:B:2027:UPL:H42	1.87	0.55
1:A:756:ASP:HB3	1:A:757:LYS:HE2	1.89	0.55
2:B:1460:SER:O	2:B:1463:GLN:HB3	2.07	0.55
1:A:141:ASN:HB3	5:A:2218:HOH:O	2.07	0.55
1:A:204:MET:HE1	5:A:2591:HOH:O	2.06	0.55
2:B:1470[B]:LEU:HD11	2:B:1514:PRO:HD2	1.89	0.55
1:A:286:SER:HB3	1:A:290[B]:LYS:CD	2.37	0.54
1:A:317:ASN:HD21	1:A:322[B]:HIS:H	1.53	0.54
4:A:2009:UPL:H121	3:B:2003:PLD:H4'1	1.89	0.54
2:B:1389:LEU:HD12	2:B:1389:LEU:N	2.18	0.54
1:A:317:ASN:HD21	1:A:322[A]:HIS:H	1.53	0.54
1:A:923:VAL:HB	1:A:1052:VAL:HB	1.90	0.54
4:A:2009:UPL:H271	4:A:2009:UPL:C14	2.37	0.54
1:A:239:SER:OG	1:A:247:ASN:ND2	2.41	0.54
1:A:469:LYS:HD2	1:A:470:GLU:N	2.23	0.54
3:A:2004:PLD:HDA2	4:A:2034:UPL:H51	1.89	0.54
1:A:1005[A]:ARG:NH1	1:A:1005[A]:ARG:HB2	2.23	0.54
1:A:1058:SER:C	1:A:1060:LYS:H	2.14	0.54
2:B:1477:ILE:O	2:B:1481:LEU:HG	2.08	0.53
1:A:205:ASN:HD21	1:A:243:ILE:H	1.55	0.53
1:A:219:PHE:HB2	1:A:226:ILE:HG13	1.90	0.53
1:A:638:ALA:HB1	3:A:2002:PLD:H1'1	1.90	0.53
1:A:1068:LEU:HD23	1:A:1069:GLU:H	1.73	0.53
2:B:1416:HIS:CB	2:B:1418:LYS:HE2	2.39	0.53
1:A:293[B]:SER:HB2	1:A:818:ASP:OD2	2.08	0.53
1:A:467[A]:ARG:NE	1:A:469:LYS:HB2	2.23	0.53
2:B:1416:HIS:O	2:B:1418:LYS:HG3	2.09	0.53
2:B:1490:ASN:O	2:B:1491:GLN:HB2	2.07	0.53
1:A:682:GLY:O	1:A:683:LEU:C	2.52	0.53
1:A:778:GLN:HG2	1:A:781:ILE:HG22	1.91	0.53
1:A:829:ASN:HB3	3:A:2006:PLD:H6'1	1.91	0.53
1:A:447:VAL:HG13	1:A:448:SER:N	2.22	0.52
2:B:1386:SER:HB2	2:B:1412:ARG:HH22	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577[B]:LEU:HD23	1:A:623:TYR:CE1	2.44	0.52
1:A:836:SER:HB2	1:A:858[A]:ARG:NH2	2.24	0.52
2:B:1444:GLN:O	2:B:1445:SER:HB2	2.08	0.52
1:A:195:ALA:HB2	5:A:2687:HOH:O	2.08	0.52
1:A:798:LYS:HB3	1:A:827:THR:HG22	1.92	0.52
4:B:2010:UPL:H162	4:B:2021:UPL:H11	1.92	0.52
1:A:392[A]:THR:HG23	5:A:2514:HOH:O	2.09	0.52
1:A:936[A]:PRO:CD	5:A:2680:HOH:O	2.58	0.52
2:B:1356:SER:O	2:B:1357:LYS:HB3	2.09	0.52
1:A:497:PRO:HB2	1:A:542:ILE:HD13	1.92	0.52
2:B:1411:PHE:CD1	2:B:1412:ARG:N	2.78	0.52
1:A:833:LEU:CD2	1:A:859:VAL:HG22	2.40	0.51
3:A:2001[A]:PLD:CD'	3:A:2002:PLD:H1A2	2.39	0.51
1:A:441:ARG:HG2	1:A:441:ARG:HH11	1.76	0.51
1:A:672:ASP:O	1:A:746[A]:HIS:HA	2.10	0.51
3:A:2006:PLD:H2A1	4:A:2013:UPL:H42	1.93	0.51
1:A:305:GLU:O	1:A:309:VAL:HG12	2.09	0.51
1:A:543:LYS:H	1:A:543:LYS:CD	2.23	0.51
1:A:1058:SER:C	1:A:1060:LYS:N	2.69	0.51
4:A:2042:UPL:H31	4:A:2047:UPL:H11	1.93	0.51
1:A:168:THR:C	1:A:170[A]:GLU:H	2.18	0.51
1:A:467[A]:ARG:HE	1:A:469:LYS:HB2	1.74	0.51
2:B:1455:TRP:CZ2	2:B:1466:LYS:HD2	2.45	0.51
2:B:1515:LYS:HB2	2:B:1515:LYS:NZ	2.26	0.51
1:A:429[A]:LYS:HD2	1:A:752:PHE:CZ	2.45	0.51
4:B:2027:UPL:C7	4:B:2028:UPL:H41	2.41	0.51
1:A:49:GLU:OE2	1:A:72[A]:LYS:HE3	2.11	0.51
1:A:900:ILE:HD11	4:A:2013:UPL:C13	2.41	0.51
4:A:2013:UPL:H32	4:A:2017:UPL:H32	1.92	0.51
2:B:1356:SER:O	2:B:1358:PRO:HD3	2.10	0.51
3:A:2002:PLD:H11	3:A:2002:PLD:CB	2.41	0.51
1:A:588:ARG:HA	1:A:609[A]:ILE:HD11	1.93	0.50
1:A:363:ASP:O	1:A:366:PRO:HD2	2.12	0.50
1:A:409:LEU:HD13	1:A:453:LEU:HD22	1.93	0.50
1:A:35:GLY:CA	1:A:43[B]:ARG:HD3	2.41	0.50
2:B:1356:SER:HB2	2:B:1382:TYR:HE1	1.77	0.50
2:B:1474:ALA:HB3	2:B:1475:PRO:HD3	1.93	0.50
1:A:312:HIS:CE1	1:A:328:LYS:HE2	2.46	0.50
1:A:672:ASP:O	1:A:746[B]:HIS:HA	2.11	0.50
2:B:1467:ASN:O	2:B:1471:GLU:HB3	2.11	0.50
1:A:856:GLU:O	1:A:858[A]:ARG:NH2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HZ2	1:A:471:GLU:H	1.60	0.50
3:A:2006:PLD:HA'1	4:A:2026:UPL:H13	1.93	0.50
1:A:756:ASP:CG	1:A:757:LYS:HE2	2.37	0.50
1:A:301:ASN:HB2	5:A:2574:HOH:O	2.11	0.49
1:A:165:GLY:HA2	5:A:2791:HOH:O	2.11	0.49
1:A:392[B]:THR:OG1	1:A:427[B]:LEU:HD21	2.13	0.49
1:A:490[A]:LYS:HE2	5:A:2862:HOH:O	2.12	0.49
1:A:900:ILE:HD11	4:A:2013:UPL:H131	1.94	0.49
1:A:290[B]:LYS:HE2	1:A:337:ARG:O	2.10	0.49
2:B:1472:ASN:O	2:B:1475:PRO:HD2	2.13	0.49
1:A:738:LEU:HB2	1:A:755:LEU:O	2.12	0.49
3:A:2005[B]:PLD:C5'	3:A:2007[B]:PLD:H8A1	2.28	0.49
1:A:168:THR:C	1:A:170[B]:GLU:H	2.20	0.49
1:A:888:TYR:CD1	1:A:927:MET:HG3	2.47	0.49
1:A:1016[A]:LYS:NZ	1:A:1016[A]:LYS:H	2.10	0.49
1:A:292:SER:O	1:A:881:LYS:HE3	2.12	0.49
4:A:2013:UPL:H151	4:A:2026:UPL:H11	1.94	0.49
1:A:902:MET:HG2	1:A:903:ASN:N	2.28	0.49
1:A:687:LEU:HG	1:A:688:TYR:CE1	2.48	0.49
1:A:847:LEU:O	1:A:850:LEU:HB2	2.13	0.49
3:A:2001[A]:PLD:CE'	3:A:2002:PLD:H1A2	2.43	0.49
2:B:1524:LEU:H	3:B:2003:PLD:H51	1.78	0.48
1:A:836:SER:HB2	1:A:858[A]:ARG:HH22	1.78	0.48
1:A:943:PRO:HG3	1:A:947:PRO:HD3	1.95	0.48
2:B:1368:ARG:CZ	5:B:845:HOH:O	2.62	0.48
1:A:441:ARG:NH2	5:A:2359:HOH:O	2.46	0.48
1:A:1029[A]:ARG:NH1	5:A:2811:HOH:O	2.37	0.48
1:A:509[A]:ARG:H	1:A:736:ARG:HH22	1.61	0.48
4:A:2022:UPL:H52	4:A:2048:UPL:H11	1.96	0.48
1:A:306:ILE:HD13	1:A:336:LEU:HD23	1.96	0.48
1:A:359:ARG:HD3	5:A:2334:HOH:O	2.14	0.48
1:A:586[B]:GLN:HE22	1:A:645:PHE:HE1	1.61	0.48
1:A:737:PRO:O	1:A:738:LEU:C	2.56	0.48
1:A:205:ASN:HD21	1:A:243:ILE:N	2.12	0.47
2:B:1512:LYS:NZ	5:B:118:HOH:O	2.47	0.47
1:A:509[B]:ARG:H	1:A:736:ARG:HH22	1.61	0.47
1:A:157:GLN:HG2	5:A:2233:HOH:O	2.13	0.47
4:A:2036:UPL:H13	2:B:1364:LEU:HD11	1.96	0.47
2:B:1361:VAL:HG22	2:B:1379:THR:HG22	1.95	0.47
1:A:935:ASP:CB	1:A:936[A]:PRO:HD2	2.44	0.47
4:A:2008:UPL:H151	4:A:2008:UPL:H191	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:THR:O	1:A:1058:SER:CB	2.61	0.47
1:A:288:ILE:CD1	1:A:808:MET:HG3	2.45	0.47
1:A:296:VAL:HG11	1:A:936[B]:PRO:HG3	1.97	0.47
1:A:629:VAL:HG22	3:A:2004:PLD:H8A1	1.96	0.47
1:A:644:TYR:CE1	3:A:2004:PLD:C1B	2.98	0.47
1:A:798:LYS:NZ	5:A:2571:HOH:O	2.47	0.47
1:A:936[A]:PRO:HD3	5:A:2680:HOH:O	2.14	0.47
4:A:2050:UPL:H22	4:A:2050:UPL:H52	1.58	0.47
2:B:1378:THR:HA	2:B:1395:VAL:O	2.15	0.47
2:B:1385:THR:O	2:B:1387:ASN:N	2.47	0.47
1:A:288:ILE:HD12	1:A:808:MET:HG3	1.97	0.47
2:B:1470[B]:LEU:CD1	2:B:1514:PRO:HD2	2.45	0.47
1:A:154:GLY:HA2	1:A:280[A]:MET:SD	2.54	0.47
1:A:392[B]:THR:OG1	1:A:427[B]:LEU:CD2	2.64	0.47
1:A:441:ARG:CD	5:A:3009:HOH:O	2.62	0.47
1:A:537:PHE:CE1	1:A:583:VAL:HG21	2.50	0.47
1:A:542:ILE:CA	1:A:543:LYS:HE3	2.45	0.47
1:A:33[B]:ILE:HD11	1:A:43[B]:ARG:CB	2.42	0.46
1:A:153:GLU:OE2	1:A:234:GLU:OE2	2.33	0.46
1:A:612:LEU:N	1:A:612:LEU:HD12	2.29	0.46
2:B:1444:GLN:O	2:B:1445:SER:CB	2.63	0.46
1:A:406:ARG:HD2	5:A:2372:HOH:O	2.15	0.46
1:A:469:LYS:NZ	1:A:471:GLU:CG	2.79	0.46
1:A:916:PHE:CD2	1:A:1054:VAL:HG11	2.50	0.46
2:B:1469:LEU:N	2:B:1469:LEU:HD23	2.30	0.46
1:A:922:VAL:CG2	1:A:1052:VAL:HG12	2.45	0.46
1:A:205:ASN:ND2	1:A:243:ILE:H	2.12	0.46
1:A:503:LEU:HA	1:A:503:LEU:HD12	1.74	0.46
1:A:197:ARG:NH2	5:A:2649:HOH:O	2.48	0.46
3:A:2002:PLD:HBA2	3:A:2002:PLD:HTA2	1.75	0.46
1:A:43[B]:ARG:HA	1:A:931:VAL:HG11	1.97	0.45
1:A:441:ARG:HH11	1:A:441:ARG:CG	2.28	0.45
1:A:644:TYR:CD1	3:A:2004:PLD:H1A1	2.52	0.45
1:A:1065:LYS:HD2	2:B:1365:ARG:HD2	1.98	0.45
3:A:2006:PLD:CD'	4:A:2026:UPL:H13	2.47	0.45
1:A:23:VAL:CG2	1:A:264:ALA:HB2	2.40	0.45
1:A:469:LYS:HG3	1:A:472:GLU:HB2	1.98	0.45
1:A:625:LYS:HB2	3:A:2004:PLD:OB	2.17	0.45
1:A:627:VAL:HG21	3:A:2004:PLD:H3A1	1.99	0.45
1:A:631:THR:OG1	4:A:2009:UPL:H272	2.17	0.45
4:A:2030:UPL:H32	4:A:2030:UPL:H62	1.69	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1370:ASP:CG	2:B:1372:LYS:HG3	2.42	0.45
2:B:1387:ASN:H	2:B:1389:LEU:HD11	1.80	0.45
2:B:1389:LEU:HA	2:B:1390:PRO:HD3	1.83	0.45
1:A:528:LYS:HE3	5:A:2389:HOH:O	2.17	0.45
1:A:556:GLU:HG3	5:A:2104:HOH:O	2.16	0.45
1:A:561[A]:VAL:HA	1:A:604:ALA:HB1	1.98	0.45
1:A:599:ARG:HG3	1:A:599:ARG:NH1	2.27	0.45
1:A:26:TYR:CZ	1:A:258:LEU:HD13	2.52	0.45
4:A:2038:UPL:H52	2:B:1360:VAL:HG11	1.98	0.45
2:B:1466:LYS:HG3	4:B:2021:UPL:C9	2.47	0.45
2:B:1488:LYS:N	5:B:957:HOH:O	2.50	0.45
2:B:1487:PRO:HB2	5:B:957:HOH:O	2.16	0.44
2:B:1376:LEU:HD21	4:B:2010:UPL:H82	1.99	0.44
2:B:1406:LYS:HE3	2:B:1406:LYS:HB2	1.55	0.44
1:A:109:ARG:NH1	5:A:2272:HOH:O	2.50	0.44
1:A:341:ALA:O	1:A:345:GLN:HG3	2.16	0.44
1:A:797:THR:HA	1:A:827:THR:O	2.17	0.44
1:A:1058:SER:HA	5:A:2333:HOH:O	2.16	0.44
1:A:301:ASN:ND2	1:A:304[A]:SER:HB3	2.32	0.44
1:A:325:ALA:N	1:A:326:PRO:CD	2.80	0.44
1:A:1016[A]:LYS:H	1:A:1016[A]:LYS:HZ1	1.64	0.44
1:A:1070:LEU:O	1:A:1071:GLN:HG3	2.17	0.44
1:A:25:ARG:HH12	1:A:262:GLN:CD	2.25	0.44
1:A:166:TYR:O	1:A:167:ARG:O	2.35	0.44
4:A:2022:UPL:H52	4:A:2048:UPL:C1	2.47	0.44
2:B:1503:THR:HG21	2:B:1506:ARG:NH1	2.32	0.44
2:B:1523:ILE:HD13	3:B:2003:PLD:H1A1	1.99	0.44
1:A:345:GLN:HB3	5:A:2482:HOH:O	2.18	0.44
1:A:25:ARG:NH1	1:A:262:GLN:OE1	2.51	0.44
1:A:796:LEU:HA	1:A:796:LEU:HD12	1.78	0.44
1:A:781:ILE:HG13	5:A:2573:HOH:O	2.18	0.44
1:A:146:GLU:CD	1:A:157:GLN:HE22	2.26	0.43
1:A:105:TYR:CD1	1:A:110:ILE:HD13	2.53	0.43
1:A:429[A]:LYS:NZ	5:A:2684:HOH:O	2.51	0.43
1:A:538:LEU:HD22	1:A:570:ARG:HG3	2.00	0.43
3:A:2002:PLD:H5'2	3:A:2002:PLD:H2'1	1.59	0.43
4:A:2015:UPL:H111	4:A:2015:UPL:H81	1.49	0.43
4:A:2038:UPL:C6	2:B:1380:LEU:HD22	2.48	0.43
1:A:248[B]:VAL:HG13	1:A:1041:LEU:HD21	1.99	0.43
1:A:445:ASN:OD1	1:A:446:THR:HG23	2.18	0.43
1:A:644:TYR:CE1	3:A:2004:PLD:H1A1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ASN:ND2	1:A:863:THR:OG1	2.51	0.43
1:A:850:LEU:C	1:A:852:ALA:H	2.26	0.43
3:A:2004:PLD:H2A2	3:A:2004:PLD:O'	2.18	0.43
1:A:383:SER:OG	1:A:385:GLN:HG3	2.18	0.43
1:A:917:GLN:O	1:A:1056:PRO:HG2	2.18	0.43
1:A:226:ILE:HG12	5:A:2445:HOH:O	2.18	0.43
1:A:543:LYS:HD2	1:A:546:LEU:HD12	1.99	0.43
1:A:596:PRO:HD2	1:A:632:PHE:CG	2.54	0.43
2:B:1506:ARG:HG2	2:B:1524:LEU:HD23	2.01	0.43
1:A:93:PHE:CD1	4:A:2014:UPL:H41	2.54	0.43
1:A:350[B]:LYS:HG3	1:A:351:LEU:HG	2.01	0.43
1:A:43[A]:ARG:HA	1:A:931:VAL:HG11	2.00	0.43
2:B:1439:SER:HB3	5:B:1037:HOH:O	2.18	0.43
1:A:537:PHE:CE2	1:A:538:LEU:HD23	2.54	0.43
1:A:561[B]:VAL:HG23	1:A:562:ALA:N	2.34	0.43
1:A:730[B]:LYS:CD	5:A:2938:HOH:O	2.60	0.43
1:A:896:VAL:HG11	4:A:2013:UPL:H112	2.00	0.43
2:B:1455:TRP:CE2	2:B:1466:LYS:HD2	2.54	0.43
2:B:1525:LEU:HA	2:B:1526:PRO:HD3	1.88	0.43
1:A:156[A]:CYS:HA	1:A:182[A]:CYS:HA	2.00	0.42
1:A:894:LEU:HG	1:A:895:GLY:N	2.34	0.42
2:B:1415:ALA:C	2:B:1417:MET:H	2.23	0.42
1:A:822:LEU:HD21	5:A:2289:HOH:O	2.18	0.42
1:A:947:PRO:HA	1:A:1031:ARG:HH22	1.85	0.42
1:A:1030:LEU:HD21	4:A:2025:UPL:H62	2.02	0.42
1:A:537:PHE:HE1	1:A:583:VAL:HG21	1.85	0.42
1:A:572[B]:ARG:HG2	5:A:2498:HOH:O	2.20	0.42
1:A:509[B]:ARG:NH1	1:A:513[B]:GLU:OE1	2.53	0.42
1:A:868:HIS:ND1	1:A:887:HIS:HE1	2.17	0.42
3:A:2002:PLD:H3'2	5:A:2541:HOH:O	2.19	0.42
2:B:1373:GLN:CD	2:B:1373:GLN:H	2.26	0.42
1:A:179:LEU:O	1:A:182[A]:CYS:SG	2.78	0.42
2:B:1411:PHE:CE1	2:B:1413:LEU:HD13	2.54	0.42
1:A:50:MET:HA	1:A:68:GLN:O	2.20	0.42
1:A:156[B]:CYS:HA	1:A:182[B]:CYS:HA	2.02	0.42
1:A:447:VAL:CG1	1:A:448:SER:N	2.82	0.42
1:A:561[B]:VAL:HA	1:A:604:ALA:HB1	2.01	0.42
1:A:401:ASN:HB2	5:A:2355:HOH:O	2.19	0.42
1:A:922:VAL:HG23	1:A:1052:VAL:HG12	2.02	0.42
1:A:301:ASN:HD22	1:A:304[A]:SER:CB	2.33	0.42
2:B:1513:LEU:N	2:B:1513:LEU:HD23	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ALA:CB	3:A:2002:PLD:H3A1	2.49	0.42
1:A:841:LEU:HD12	1:A:842:PRO:HD2	2.02	0.42
1:A:947:PRO:HA	1:A:1031:ARG:NH2	2.35	0.42
1:A:31:PHE:CD1	1:A:31:PHE:C	2.98	0.41
1:A:114:TYR:HA	1:A:274:GLN:O	2.20	0.41
1:A:523:LYS:NZ	5:A:2697:HOH:O	2.40	0.41
2:B:1377:GLN:O	2:B:1396:ALA:HA	2.20	0.41
1:A:204:MET:HB2	1:A:637:MET:HE1	2.01	0.41
1:A:899:LYS:HB3	1:A:899:LYS:HE2	1.70	0.41
1:A:1008:MET:HE2	5:A:2754:HOH:O	2.20	0.41
4:B:2010:UPL:C10	4:B:2049:UPL:H11	2.46	0.41
1:A:1058:SER:O	1:A:1060:LYS:N	2.53	0.41
1:A:1063:ILE:HG22	1:A:1064:THR:N	2.35	0.41
2:B:1393:LYS:HE2	2:B:1393:LYS:HB3	1.93	0.41
1:A:301:ASN:HD22	1:A:304[A]:SER:HB3	1.86	0.41
1:A:509[A]:ARG:HH22	1:A:754:GLU:CD	2.28	0.41
2:B:1368:ARG:NH2	5:B:845:HOH:O	2.53	0.41
2:B:1443:LEU:HD12	2:B:1443:LEU:HA	1.60	0.41
4:B:2010:UPL:H91	4:B:2049:UPL:H11	2.03	0.41
3:A:2002:PLD:H7A2	5:A:2688:HOH:O	2.20	0.41
4:A:2015:UPL:H82	4:B:2044:UPL:H12	2.01	0.41
2:B:1417:MET:HG3	2:B:1417:MET:O	2.20	0.41
2:B:1426:GLY:HA3	2:B:1431:GLN:HB3	2.03	0.41
1:A:572[A]:ARG:HD2	1:A:611:MET:O	2.20	0.41
1:A:927:MET:HE3	1:A:927:MET:HB3	1.95	0.41
1:A:289:THR:OG1	1:A:290[B]:LYS:NZ	2.53	0.41
1:A:452:GLU:CD	1:A:452:GLU:H	2.29	0.41
2:B:1387:ASN:H	2:B:1389:LEU:CD1	2.34	0.41
1:A:25:ARG:HG2	1:A:53:GLU:HG2	2.03	0.41
1:A:30:ALA:HB3	4:A:2014:UPL:C16	2.50	0.41
1:A:155:ILE:O	1:A:182[B]:CYS:HB3	2.21	0.41
1:A:272:SER:N	5:A:2423:HOH:O	2.50	0.41
1:A:469:LYS:CE	1:A:471:GLU:HB2	2.34	0.41
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.86	0.41
1:A:644:TYR:CE1	3:A:2004:PLD:H1A2	2.56	0.41
1:A:935:ASP:HB2	1:A:936[A]:PRO:CD	2.49	0.41
2:B:1389:LEU:HD21	5:B:113:HOH:O	2.21	0.41
1:A:569:VAL:HG13	1:A:572[B]:ARG:HD2	2.02	0.41
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.95	0.41
1:A:781:ILE:O	1:A:781:ILE:HG12	2.20	0.41
3:A:2006:PLD:H1'2	3:A:2006:PLD:H32	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:GLN:HA	1:A:1026:PHE:O	2.21	0.40
2:B:1446:HIS:O	2:B:1447:PRO:C	2.59	0.40
1:A:243:ILE:HD12	5:A:2709:HOH:O	2.19	0.40
1:A:471:GLU:HG2	1:A:735:GLU:HG3	2.04	0.40
1:A:936[B]:PRO:HG3	5:A:2508:HOH:O	2.21	0.40
1:A:92[B]:HIS:CE1	5:A:2674:HOH:O	2.73	0.40
1:A:185:LYS:HE2	5:A:2171:HOH:O	2.22	0.40
1:A:365:VAL:O	1:A:368:MET:HG2	2.20	0.40
1:A:1057:THR:O	1:A:1058:SER:HB2	2.22	0.40
2:B:1495:VAL:HG11	4:B:2045:UPL:H31	2.02	0.40
1:A:44:ALA:HB2	1:A:931:VAL:HB	2.03	0.40
1:A:756:ASP:CB	1:A:757:LYS:HE2	2.49	0.40
1:A:865:MET:HE2	4:A:2019:UPL:H71	2.03	0.40
2:B:1497:VAL:HG11	4:B:2046:UPL:H21	2.02	0.40
2:B:1515:LYS:NZ	2:B:1515:LYS:CB	2.85	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	1012/1056 (96%)	959 (95%)	42 (4%)	11 (1%)	11	4
2	B	176/319 (55%)	153 (87%)	15 (8%)	8 (4%)	2	0
All	All	1188/1375 (86%)	1112 (94%)	57 (5%)	19 (2%)	7	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
1	A	1058	SER
2	B	1357	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1385	THR
2	B	1386	SER
1	A	1012	GLN
1	A	1056	PRO
1	A	1057	THR
2	B	1491	GLN
1	A	140	LYS
1	A	504	ASP
1	A	1059	SER
2	B	1416	HIS
2	B	1460	SER
1	A	167	ARG
2	B	1445	SER
1	A	502	SER
1	A	1071	GLN
2	B	1358	PRO

5.3.2 Protein sidechains ⓘ

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	881/900 (98%)	826 (94%)	55 (6%)	16	9
2	B	148/277 (53%)	136 (92%)	12 (8%)	11	5
All	All	1029/1177 (87%)	962 (94%)	67 (6%)	16	8

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	69	VAL
1	A	140	LYS
1	A	147	LEU
1	A	164	GLU
1	A	166	TYR
1	A	167	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	221	GLU
1	A	222	PRO
1	A	228[A]	LYS
1	A	228[B]	LYS
1	A	249	VAL
1	A	284	PRO
1	A	293[A]	SER
1	A	293[B]	SER
1	A	298	LYS
1	A	307	HIS
1	A	323[A]	GLU
1	A	323[B]	GLU
1	A	368	MET
1	A	413[A]	ARG
1	A	413[B]	ARG
1	A	419	SER
1	A	429[A]	LYS
1	A	429[B]	LYS
1	A	430	THR
1	A	452	GLU
1	A	460	LEU
1	A	487	ASN
1	A	501	LYS
1	A	540[A]	VAL
1	A	540[B]	VAL
1	A	543	LYS
1	A	599	ARG
1	A	612	LEU
1	A	683	LEU
1	A	685	GLU
1	A	736	ARG
1	A	781	ILE
1	A	817	MET
1	A	836	SER
1	A	847	LEU
1	A	853	THR
1	A	899	LYS
1	A	905	ARG
1	A	906	GLU
1	A	915	PRO
1	A	927	MET
1	A	947	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	949	MET
1	A	1011	LYS
1	A	1016[A]	LYS
1	A	1016[B]	LYS
1	A	1057	THR
1	A	1071	GLN
2	B	1358	PRO
2	B	1359	LYS
2	B	1368	ARG
2	B	1389	LEU
2	B	1401	ASP
2	B	1436	LEU
2	B	1439	SER
2	B	1443	LEU
2	B	1491	GLN
2	B	1499	LEU
2	B	1515	LYS
2	B	1528	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	59	HIS
1	A	169	ASN
1	A	205	ASN
1	A	247	ASN
1	A	262	GLN
1	A	317	ASN
1	A	402	GLN
1	A	423	ASN
1	A	455	GLN
1	A	780	GLN
1	A	809	GLN
1	A	829	ASN
1	A	887	HIS
2	B	1428	ASN
2	B	1430	GLN
2	B	1442	ASN
2	B	1463	GLN
2	B	1467	ASN
2	B	1490	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1491	GLN
2	B	1493	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	A	17	1	7,8,9	2.13	1 (14%)	9,10,12	2.48	5 (55%)

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
1	PCA	A	17	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	PCA	CB-CG	-5.41	1.40	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	PCA	OE-CD-CG	-3.56	120.37	126.72
1	A	17	PCA	CB-CG-CD	-3.46	99.06	104.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	PCA	CG-CD-N	3.13	116.06	108.39
1	A	17	PCA	CA-N-CD	-3.05	103.15	113.58
1	A	17	PCA	CB-CA-C	-2.73	108.92	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

53 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLD	A	2007[B]	-	36,36,59	10.12	7 (19%)	39,41,67	2.44	10 (25%)
4	UPL	B	2010	-	13,13,33	0.63	0	13,13,33	0.88	1 (7%)
4	UPL	A	2009	-	14,14,33	0.82	0	14,14,33	1.04	1 (7%)
3	PLD	B	2003	-	30,30,59	1.24	3 (10%)	33,35,67	2.41	17 (51%)
4	UPL	B	2045	-	4,4,33	0.39	0	3,3,33	0.65	0
4	UPL	A	2038	-	5,5,33	0.53	0	4,4,33	0.62	0
4	UPL	B	2016	-	12,12,33	0.50	0	11,11,33	0.74	0
3	PLD	A	2004	-	33,33,59	1.75	5 (15%)	36,38,67	2.16	14 (38%)
4	UPL	A	2032	-	5,5,33	0.48	0	4,4,33	0.51	0
3	PLD	A	2001[A]	-	52,52,59	1.19	6 (11%)	58,60,67	2.18	13 (22%)
3	PLD	A	2001[B]	-	52,52,59	12.55	7 (13%)	58,60,67	3.01	15 (25%)
4	UPL	A	2047	-	4,4,33	0.31	0	3,3,33	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UPL	A	2050	-	5,5,33	0.35	0	4,4,33	0.52	0
4	UPL	A	2022	-	5,5,33	0.49	0	4,4,33	0.25	0
4	UPL	A	2017	-	10,10,33	0.51	0	9,9,33	0.57	0
4	UPL	A	2019	-	9,9,33	0.44	0	8,8,33	0.77	0
4	UPL	A	2020	-	5,5,33	0.54	0	4,4,33	0.29	0
4	UPL	A	2039	-	4,4,33	0.58	0	3,3,33	0.32	0
4	UPL	A	2012	-	16,16,33	0.38	0	15,15,33	0.76	0
4	UPL	B	2049	-	5,5,33	0.38	0	4,4,33	0.52	0
3	PLD	A	2005[A]	-	45,45,59	1.34	6 (13%)	48,50,67	2.24	10 (20%)
3	PLD	A	2005[B]	-	45,45,59	1.31	6 (13%)	48,50,67	2.22	10 (20%)
4	UPL	B	2033	-	5,5,33	0.47	0	4,4,33	0.36	0
4	UPL	A	2024	-	5,5,33	0.45	0	4,4,33	0.62	0
4	UPL	B	2021	-	8,8,33	0.20	0	7,7,33	0.57	0
4	UPL	B	2028	-	6,6,33	0.32	0	5,5,33	0.36	0
4	UPL	A	2014	-	15,15,33	0.65	0	14,14,33	1.77	2 (14%)
4	UPL	A	2025	-	7,7,33	0.70	0	6,6,33	0.24	0
4	UPL	A	2013	-	15,15,33	0.63	0	14,14,33	0.76	0
4	UPL	A	2011	-	18,18,33	0.70	0	17,17,33	0.81	0
4	UPL	A	2026	-	7,7,33	1.02	0	6,6,33	0.64	0
4	UPL	A	2040	-	4,4,33	0.86	0	3,3,33	0.77	0
4	UPL	A	2036	-	5,5,33	0.32	0	4,4,33	0.46	0
3	PLD	A	2006	-	33,33,59	1.22	4 (12%)	36,38,67	2.18	9 (25%)
4	UPL	B	2044	-	6,6,33	0.61	0	5,5,33	0.44	0
4	UPL	A	2042	-	4,4,33	0.57	0	3,3,33	0.28	0
4	UPL	A	2048	-	9,9,33	0.70	0	8,8,33	0.84	0
4	UPL	A	2015	-	12,12,33	0.44	0	11,11,33	0.54	0
4	UPL	A	2018	-	11,11,33	0.68	0	10,10,33	0.62	0
4	UPL	A	2030	-	6,6,33	0.82	0	5,5,33	0.94	0
4	UPL	A	2041	-	4,4,33	0.42	0	3,3,33	0.56	0
4	UPL	A	2029	-	8,8,33	0.55	0	7,7,33	0.76	0
4	UPL	B	2043	-	4,4,33	0.24	0	3,3,33	0.41	0
4	UPL	A	2008	-	16,16,33	1.14	0	16,16,33	1.51	2 (12%)
4	UPL	A	2034	-	5,5,33	0.57	0	4,4,33	0.30	0
3	PLD	A	2002	-	34,34,59	1.52	6 (17%)	37,39,67	1.85	8 (21%)
4	UPL	A	2037	-	4,4,33	0.58	0	3,3,33	0.88	0
4	UPL	B	2046	-	4,4,33	0.40	0	3,3,33	0.39	0
4	UPL	B	2031	-	6,6,33	0.47	0	5,5,33	0.62	0
4	UPL	B	2023	-	8,8,33	0.63	0	7,7,33	0.51	0
4	UPL	B	2027	-	6,6,33	0.40	0	5,5,33	0.61	0
4	UPL	A	2035	-	6,6,33	0.51	0	5,5,33	0.13	0
3	PLD	A	2007[A]	-	36,36,59	1.60	5 (13%)	39,41,67	1.81	9 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLD	A	2007[B]	-	1/1/4/5	20/38/38/63	-
4	UPL	B	2010	-	-	9/12/12/33	-
4	UPL	A	2009	-	1/1/1/1	5/14/14/33	-
3	PLD	B	2003	-	-	19/34/34/63	-
4	UPL	B	2045	-	-	2/2/2/33	-
4	UPL	A	2038	-	-	2/3/3/33	-
4	UPL	B	2016	-	-	5/10/10/33	-
3	PLD	A	2004	-	-	17/35/35/63	-
4	UPL	A	2032	-	-	2/3/3/33	-
3	PLD	A	2001[A]	-	1/1/5/5	19/56/56/63	-
3	PLD	A	2001[B]	-	1/1/5/5	23/56/56/63	-
4	UPL	A	2047	-	-	2/2/2/33	-
4	UPL	A	2050	-	-	3/3/3/33	-
4	UPL	A	2022	-	-	1/3/3/33	-
4	UPL	A	2017	-	-	5/8/8/33	-
4	UPL	A	2019	-	-	4/7/7/33	-
4	UPL	A	2020	-	-	1/3/3/33	-
4	UPL	A	2039	-	-	1/2/2/33	-
4	UPL	A	2012	-	-	8/14/14/33	-
4	UPL	B	2049	-	-	3/3/3/33	-
3	PLD	A	2005[A]	-	1/1/4/5	27/47/47/63	-
3	PLD	A	2005[B]	-	1/1/4/5	26/47/47/63	-
4	UPL	B	2033	-	-	2/3/3/33	-
4	UPL	A	2024	-	-	0/3/3/33	-
4	UPL	B	2021	-	-	4/6/6/33	-
4	UPL	B	2028	-	-	2/4/4/33	-
4	UPL	A	2014	-	-	7/13/13/33	-
4	UPL	A	2025	-	-	5/5/5/33	-
4	UPL	A	2013	-	-	8/13/13/33	-
4	UPL	A	2011	-	-	13/16/16/33	-
4	UPL	A	2026	-	-	2/5/5/33	-
4	UPL	A	2040	-	-	0/2/2/33	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UPL	A	2036	-	-	2/3/3/33	-
3	PLD	A	2006	-	1/1/4/5	21/35/35/63	-
4	UPL	B	2044	-	-	3/4/4/33	-
4	UPL	A	2042	-	-	2/2/2/33	-
4	UPL	A	2048	-	-	4/7/7/33	-
4	UPL	A	2015	-	-	7/10/10/33	-
4	UPL	A	2018	-	-	5/9/9/33	-
4	UPL	A	2030	-	-	2/4/4/33	-
4	UPL	A	2041	-	-	0/2/2/33	-
4	UPL	A	2029	-	-	3/6/6/33	-
4	UPL	B	2043	-	-	1/2/2/33	-
4	UPL	A	2008	-	1/1/1/1	8/16/16/33	-
4	UPL	A	2034	-	-	1/3/3/33	-
3	PLD	A	2002	-	-	26/36/36/63	-
4	UPL	A	2037	-	-	2/2/2/33	-
4	UPL	B	2046	-	-	1/2/2/33	-
4	UPL	B	2031	-	-	2/4/4/33	-
4	UPL	B	2023	-	-	3/6/6/33	-
4	UPL	B	2027	-	-	3/4/4/33	-
4	UPL	A	2035	-	-	3/4/4/33	-
3	PLD	A	2007[A]	-	1/1/4/5	21/38/38/63	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001[B]	PLD	CG'-CF'	90.10	6.00	1.51
3	A	2007[B]	PLD	C9B-C8B	59.63	5.19	1.51
3	A	2007[B]	PLD	C6B-C5B	6.45	1.83	1.51
3	A	2002	PLD	O3-CB	5.47	1.49	1.33
3	A	2004	PLD	P-O4P	5.21	1.74	1.54
3	A	2007[A]	PLD	O3-CB	5.05	1.48	1.33
3	A	2007[B]	PLD	O3-CB	5.05	1.48	1.33
3	A	2004	PLD	O3-CB	5.05	1.48	1.33
3	A	2002	PLD	C3-C2	3.84	1.62	1.50
3	A	2005[A]	PLD	C1-C2	3.82	1.62	1.50
3	A	2005[B]	PLD	C1-C2	3.82	1.62	1.50
3	B	2003	PLD	O2-C'	3.70	1.44	1.34
3	A	2007[A]	PLD	P-O4P	3.66	1.68	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2007[B]	PLD	P-O4P	3.66	1.68	1.54
3	A	2004	PLD	P-O2P	-3.47	1.41	1.54
3	A	2007[A]	PLD	P-O3P	3.29	1.70	1.60
3	A	2007[B]	PLD	P-O3P	3.29	1.70	1.60
3	A	2006	PLD	P-O4P	3.27	1.67	1.54
3	A	2001[A]	PLD	C2B-C1B	3.27	1.64	1.52
3	A	2001[B]	PLD	C2B-C1B	3.27	1.64	1.52
3	A	2007[A]	PLD	C1B-CB	2.99	1.59	1.50
3	A	2007[B]	PLD	C1B-CB	2.99	1.59	1.50
3	A	2005[A]	PLD	O3-CB	2.94	1.41	1.33
3	A	2005[B]	PLD	O3-CB	2.94	1.41	1.33
3	A	2005[A]	PLD	C3B-C2B	2.90	1.66	1.51
3	A	2005[B]	PLD	C3B-C2B	2.90	1.66	1.51
3	A	2004	PLD	O2-C'	2.64	1.41	1.34
3	A	2001[A]	PLD	C5-N	-2.62	1.43	1.51
3	A	2001[B]	PLD	C5-N	-2.62	1.43	1.51
3	A	2006	PLD	P-O3P	2.47	1.68	1.60
3	A	2006	PLD	O2-C'	2.44	1.41	1.34
3	A	2007[A]	PLD	C1'-C'	2.34	1.57	1.50
3	A	2007[B]	PLD	C1'-C'	2.34	1.57	1.50
3	A	2002	PLD	O2-C'	2.33	1.40	1.34
3	B	2003	PLD	C1B-CB	2.29	1.57	1.50
3	A	2006	PLD	C1B-CB	2.23	1.57	1.50
3	A	2005[A]	PLD	C6'-C5'	2.20	1.62	1.51
3	A	2001[A]	PLD	C1B-CB	2.18	1.57	1.50
3	A	2001[B]	PLD	C1B-CB	2.18	1.57	1.50
3	A	2002	PLD	C1'-C'	2.13	1.56	1.50
3	A	2005[B]	PLD	C6'-C5'	2.13	1.62	1.51
3	A	2001[A]	PLD	C4B-C3B	-2.12	1.41	1.51
3	A	2001[B]	PLD	C4B-C3B	-2.12	1.41	1.51
3	A	2001[A]	PLD	P-O4P	2.11	1.67	1.59
3	A	2001[B]	PLD	P-O4P	2.11	1.67	1.59
3	A	2002	PLD	O3-C3	2.11	1.49	1.45
3	A	2002	PLD	P-O4P	2.10	1.62	1.54
3	A	2005[A]	PLD	C5B-C4B	2.07	1.62	1.51
3	A	2005[B]	PLD	C5B-C4B	2.07	1.62	1.51
3	B	2003	PLD	C1-C2	2.06	1.57	1.50
3	A	2004	PLD	P-O3P	2.03	1.66	1.60
3	A	2005[A]	PLD	P-O4P	2.02	1.62	1.54
3	A	2005[B]	PLD	P-O4P	2.02	1.62	1.54
3	A	2001[A]	PLD	P-O1P	-2.01	1.43	1.50
3	A	2001[B]	PLD	P-O1P	-2.01	1.43	1.50

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001[B]	PLD	CG'-CF'-CE'	-15.07	38.20	114.37
3	A	2001[A]	PLD	C2-O2-C'	9.89	141.47	117.80
3	A	2001[B]	PLD	C2-O2-C'	9.89	141.47	117.80
3	A	2007[B]	PLD	C9B-C8B-C7B	-9.73	29.93	115.25
3	A	2005[A]	PLD	C2-O2-C'	8.82	138.89	117.80
3	A	2005[B]	PLD	C2-O2-C'	8.82	138.89	117.80
3	A	2006	PLD	C2-O2-C'	7.19	134.99	117.80
3	A	2004	PLD	O2-C'-C1'	5.50	123.38	111.48
3	A	2005[A]	PLD	O2-C'-C1'	5.43	123.22	111.48
3	A	2005[B]	PLD	O2-C'-C1'	5.43	123.22	111.48
3	A	2005[A]	PLD	C3B-C2B-C1B	5.42	133.04	113.13
3	A	2005[B]	PLD	C3B-C2B-C1B	5.42	133.04	113.13
3	A	2001[A]	PLD	C5'-C4'-C3'	-5.25	87.82	114.37
3	A	2001[B]	PLD	C5'-C4'-C3'	-5.25	87.82	114.37
3	A	2002	PLD	C2-O2-C'	5.13	130.08	117.80
4	A	2014	UPL	C13-C12-C11	-5.07	88.73	114.37
3	A	2001[A]	PLD	C6B-C5B-C4B	-4.97	89.25	114.37
3	A	2001[B]	PLD	C6B-C5B-C4B	-4.97	89.25	114.37
3	A	2005[A]	PLD	C2B-C1B-CB	-4.94	95.60	113.69
3	A	2005[B]	PLD	C2B-C1B-CB	-4.94	95.60	113.69
3	B	2003	PLD	O4P-C4-C5	4.86	126.96	109.17
3	A	2006	PLD	C5'-C4'-C3'	-4.75	90.34	114.37
3	A	2001[A]	PLD	O3-C3-C2	4.68	121.88	108.40
3	A	2001[B]	PLD	O3-C3-C2	4.68	121.88	108.40
3	A	2001[B]	PLD	CH'-CG'-CF'	-4.45	76.24	115.25
3	A	2002	PLD	O2-C2-C3	4.34	123.90	108.34
3	A	2007[A]	PLD	C5'-C4'-C3'	-4.22	93.03	114.37
3	A	2007[B]	PLD	C5'-C4'-C3'	-4.22	93.03	114.37
3	A	2004	PLD	O2P-P-O3P	4.16	117.53	106.67
3	A	2001[A]	PLD	O2-C2-C3	4.14	123.20	108.34
3	A	2001[B]	PLD	O2-C2-C3	4.14	123.20	108.34
3	B	2003	PLD	O4P-P-O1P	-4.08	92.77	108.94
3	A	2007[B]	PLD	CAA-C9B-C8B	3.91	139.78	113.36
3	A	2007[A]	PLD	C2-O2-C'	3.91	127.15	117.80
3	A	2007[B]	PLD	C2-O2-C'	3.91	127.15	117.80
3	A	2007[A]	PLD	O2-C2-C3	3.88	122.27	108.34
3	A	2007[B]	PLD	O2-C2-C3	3.88	122.27	108.34
3	A	2006	PLD	O2-C'-C1'	3.88	119.86	111.48
3	A	2004	PLD	O2-C2-C3	3.81	122.03	108.34
3	A	2002	PLD	O2-C'-C1'	3.73	119.56	111.48
3	A	2001[A]	PLD	C3-C2-C1	-3.73	103.09	111.78
3	A	2001[B]	PLD	C3-C2-C1	-3.73	103.09	111.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	PLD	C3'-C2'-C1'	-3.73	99.43	113.13
4	A	2008	UPL	C13-C12-C11	-3.67	94.75	113.91
3	B	2003	PLD	C3B-C2B-C1B	-3.50	100.26	113.13
3	B	2003	PLD	O2-C'-C1'	3.48	119.00	111.48
3	A	2004	PLD	O3-C3-C2	3.41	118.22	108.40
3	A	2006	PLD	O2-C2-C1	3.39	120.52	108.34
3	B	2003	PLD	P-O4P-C4	-3.30	105.56	121.26
3	B	2003	PLD	O2P-P-O3P	3.26	122.33	107.57
3	B	2003	PLD	O2-C2-C3	3.15	119.63	108.34
3	A	2007[A]	PLD	C4'-C3'-C2'	-3.13	98.56	114.37
3	A	2007[B]	PLD	C4'-C3'-C2'	-3.13	98.56	114.37
3	B	2003	PLD	O3-C3-C2	3.13	117.41	108.40
3	A	2006	PLD	O3-C3-C2	3.11	117.36	108.40
3	A	2004	PLD	O4P-P-O3P	-3.10	98.58	106.67
3	A	2006	PLD	C3-C2-C1	-3.09	104.58	111.78
3	A	2001[A]	PLD	O2-C2-C1	3.08	119.39	108.34
3	A	2001[B]	PLD	O2-C2-C1	3.08	119.39	108.34
3	A	2005[A]	PLD	C2'-C1'-C'	-2.97	102.82	113.69
3	A	2005[B]	PLD	C2'-C1'-C'	-2.97	102.82	113.69
3	A	2006	PLD	O2-C2-C3	2.96	118.96	108.34
3	A	2002	PLD	O3-CB-C1B	2.96	120.85	111.83
3	A	2006	PLD	C4'-C3'-C2'	-2.96	99.42	114.37
3	A	2005[A]	PLD	O2-C2-C3	2.95	118.94	108.34
3	A	2005[B]	PLD	O2-C2-C3	2.95	118.94	108.34
3	A	2004	PLD	C7B-C6B-C5B	-2.94	99.50	114.37
3	B	2003	PLD	O2P-P-O4P	2.93	120.84	107.57
3	A	2002	PLD	O3-C3-C2	2.90	116.75	108.40
3	A	2004	PLD	O2-C2-C1	2.90	118.73	108.34
3	A	2007[A]	PLD	O3-C3-C2	2.86	116.65	108.40
3	A	2007[B]	PLD	O3-C3-C2	2.86	116.65	108.40
3	B	2003	PLD	C3-C2-C1	-2.77	105.33	111.78
3	B	2003	PLD	O2-C2-C1	2.76	118.26	108.34
3	A	2006	PLD	C3'-C2'-C1'	-2.75	103.01	113.13
3	A	2004	PLD	C5B-C4B-C3B	-2.75	100.47	114.37
3	B	2003	PLD	C2-O2-C'	2.72	124.31	117.80
3	A	2001[A]	PLD	C7'-C6'-C5'	-2.69	100.75	114.37
3	A	2001[B]	PLD	C7'-C6'-C5'	-2.69	100.75	114.37
3	A	2007[A]	PLD	C2B-C1B-CB	2.65	123.41	113.69
3	A	2007[B]	PLD	C2B-C1B-CB	2.65	123.41	113.69
3	B	2003	PLD	O2P-P-O1P	-2.65	100.11	112.44
3	B	2003	PLD	C5'-C4'-C3'	-2.65	95.50	113.36
3	A	2001[A]	PLD	O2P-P-O4P	2.64	119.53	107.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001[B]	PLD	O2P-P-O4P	2.64	119.53	107.57
3	A	2004	PLD	C2B-C1B-CB	2.64	123.35	113.69
3	A	2002	PLD	OB-CB-C1B	-2.62	113.52	123.78
3	A	2005[A]	PLD	O3-CB-C1B	2.57	119.68	111.83
3	A	2005[B]	PLD	O3-CB-C1B	2.57	119.68	111.83
3	A	2004	PLD	O3P-P-O1P	2.55	113.34	106.44
3	A	2005[A]	PLD	O3-C3-C2	2.47	115.51	108.40
3	A	2005[B]	PLD	O3-C3-C2	2.47	115.51	108.40
4	A	2014	UPL	C9-C8-C7	-2.46	101.94	114.37
3	A	2002	PLD	C6B-C5B-C4B	-2.44	102.05	114.37
3	A	2005[A]	PLD	CB'-CA'-C9'	2.43	126.67	114.37
4	A	2009	UPL	C9-C8-C7	-2.41	102.17	114.37
3	A	2004	PLD	O'-C'-C1'	-2.37	114.51	123.78
3	A	2001[A]	PLD	CAA-C9B-C8B	-2.32	102.64	114.37
3	A	2001[B]	PLD	CAA-C9B-C8B	-2.32	102.64	114.37
3	A	2005[B]	PLD	CB'-CA'-C9'	-2.32	102.66	114.37
3	A	2007[A]	PLD	C8B-C7B-C6B	-2.29	102.81	114.37
3	B	2003	PLD	C5B-C4B-C3B	-2.26	102.96	114.37
3	A	2004	PLD	OB-CB-C1B	-2.25	114.98	123.78
3	A	2007[A]	PLD	C2'-C1'-C'	-2.20	105.61	113.69
3	A	2007[B]	PLD	C2'-C1'-C'	-2.20	105.61	113.69
4	A	2008	UPL	C9-C10-C11	2.19	121.88	113.62
3	A	2004	PLD	CBA-CAA-C9B	-2.18	103.36	114.37
3	A	2001[A]	PLD	C9B-C8B-C7B	2.13	125.16	114.37
3	A	2001[B]	PLD	C9B-C8B-C7B	2.13	125.16	114.37
3	A	2007[A]	PLD	C5B-C4B-C3B	-2.12	103.67	114.37
3	A	2007[B]	PLD	C5B-C4B-C3B	-2.12	103.67	114.37
4	B	2010	UPL	C10-C11-C12	-2.11	108.94	115.97
3	A	2001[A]	PLD	C6'-C5'-C4'	-2.09	103.78	114.37
3	A	2001[B]	PLD	C6'-C5'-C4'	-2.09	103.78	114.37
3	B	2003	PLD	O'-C'-C1'	-2.04	115.78	123.78
3	A	2005[A]	PLD	O2-C2-C1	2.03	115.61	108.34
3	A	2005[B]	PLD	O2-C2-C1	2.03	115.61	108.34
3	A	2001[A]	PLD	O3-CB-C1B	2.03	118.01	111.83
3	A	2001[B]	PLD	O3-CB-C1B	2.03	118.01	111.83
3	A	2002	PLD	C2B-C1B-CB	-2.02	106.30	113.69
3	A	2004	PLD	O4P-P-O2P	-2.01	100.26	107.80

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2001[A]	PLD	C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	A	2001[B]	PLD	C2
3	A	2005[A]	PLD	C2
3	A	2005[B]	PLD	C2
3	A	2006	PLD	C2
3	A	2007[A]	PLD	C2
3	A	2007[B]	PLD	C2
4	A	2008	UPL	C12
4	A	2009	UPL	C12

All (367) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001[A]	PLD	C3-C2-O2-C'
3	A	2001[A]	PLD	C4-O4P-P-O2P
3	A	2001[A]	PLD	C4-O4P-P-O3P
3	A	2001[B]	PLD	C3-C2-O2-C'
3	A	2001[B]	PLD	C4-O4P-P-O2P
3	A	2001[B]	PLD	C4-O4P-P-O3P
3	A	2002	PLD	C3-C2-O2-C'
3	A	2002	PLD	C1'-C'-O2-C2
3	A	2002	PLD	O'-C'-O2-C2
3	A	2002	PLD	C1-O3P-P-O1P
3	A	2002	PLD	C1-O3P-P-O2P
3	A	2002	PLD	C1-O3P-P-O4P
3	A	2004	PLD	C3-C2-O2-C'
3	A	2005[A]	PLD	C2-C1-O3P-P
3	A	2005[A]	PLD	C3-C2-O2-C'
3	A	2005[A]	PLD	C1'-C'-O2-C2
3	A	2005[A]	PLD	O'-C'-O2-C2
3	A	2005[B]	PLD	C2-C1-O3P-P
3	A	2005[B]	PLD	C3-C2-O2-C'
3	A	2005[B]	PLD	C1'-C'-O2-C2
3	A	2005[B]	PLD	O'-C'-O2-C2
3	A	2006	PLD	C3-C2-O2-C'
3	A	2006	PLD	C1'-C'-O2-C2
3	A	2006	PLD	O'-C'-O2-C2
3	A	2007[A]	PLD	C3-C2-O2-C'
3	A	2007[A]	PLD	C1-O3P-P-O2P
3	A	2007[A]	PLD	C1-O3P-P-O4P
3	A	2007[B]	PLD	C3-C2-O2-C'
3	A	2007[B]	PLD	C1-O3P-P-O2P
3	A	2007[B]	PLD	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	2003	PLD	C3-C2-O2-C'
3	B	2003	PLD	C1'-C'-O2-C2
3	B	2003	PLD	C1-O3P-P-O4P
3	B	2003	PLD	C4-O4P-P-O2P
3	A	2004	PLD	OB-CB-O3-C3
3	A	2005[A]	PLD	OB-CB-O3-C3
3	A	2005[B]	PLD	OB-CB-O3-C3
3	A	2004	PLD	C1B-CB-O3-C3
3	A	2005[A]	PLD	C1B-CB-O3-C3
3	A	2005[B]	PLD	C1B-CB-O3-C3
3	B	2003	PLD	O'-C'-O2-C2
3	A	2006	PLD	C1B-CB-O3-C3
3	A	2002	PLD	C1B-CB-O3-C3
3	A	2006	PLD	OB-CB-O3-C3
3	A	2002	PLD	OB-CB-O3-C3
3	A	2007[A]	PLD	C5'-C6'-C7'-C8'
3	A	2007[B]	PLD	C5'-C6'-C7'-C8'
3	A	2001[A]	PLD	C1B-CB-O3-C3
3	A	2001[B]	PLD	C1B-CB-O3-C3
4	A	2025	UPL	C2-C3-C4-C5
4	A	2050	UPL	C2-C3-C4-C5
3	A	2002	PLD	C2'-C3'-C4'-C5'
4	A	2030	UPL	C3-C4-C5-C6
3	A	2001[A]	PLD	OB-CB-O3-C3
3	A	2001[B]	PLD	OB-CB-O3-C3
3	A	2002	PLD	C1B-C2B-C3B-C4B
3	A	2005[A]	PLD	C5B-C6B-C7B-C8B
3	A	2005[B]	PLD	C5B-C6B-C7B-C8B
3	A	2005[A]	PLD	C2'-C3'-C4'-C5'
3	A	2007[B]	PLD	C6B-C7B-C8B-C9B
4	A	2015	UPL	C11-C10-C9-C8
4	B	2023	UPL	C2-C3-C4-C5
3	A	2002	PLD	CAA-CBA-CCA-CDA
3	A	2004	PLD	C7B-C8B-C9B-CAA
4	B	2027	UPL	C3-C4-C5-C6
3	A	2006	PLD	O3P-C1-C2-O2
3	A	2006	PLD	CB-C1B-C2B-C3B
4	A	2008	UPL	C16-C17-C18-C19
3	A	2005[B]	PLD	C3'-C4'-C5'-C6'
4	A	2011	UPL	C9-C10-C11-C12
3	A	2001[A]	PLD	C6B-C7B-C8B-C9B
3	A	2001[B]	PLD	C6B-C7B-C8B-C9B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	2003	PLD	CB-C1B-C2B-C3B
4	B	2010	UPL	C9-C10-C11-C12
4	A	2014	UPL	C11-C10-C9-C8
4	A	2008	UPL	C7-C8-C9-C10
3	A	2005[A]	PLD	C7B-C8B-C9B-CAA
3	A	2005[B]	PLD	C7B-C8B-C9B-CAA
4	A	2015	UPL	C3-C4-C5-C6
3	A	2004	PLD	CDA-CEA-CFA-CGA
4	A	2011	UPL	C6-C7-C8-C9
3	A	2001[B]	PLD	CE'-CF'-CG'-CH'
3	A	2002	PLD	C7B-C8B-C9B-CAA
4	A	2013	UPL	C12-C13-C14-C15
3	A	2007[A]	PLD	C2'-C3'-C4'-C5'
3	A	2007[A]	PLD	C9'-CA'-CB'-CC'
3	A	2007[B]	PLD	C2'-C3'-C4'-C5'
3	A	2007[B]	PLD	C9'-CA'-CB'-CC'
4	A	2015	UPL	C6-C7-C8-C9
3	A	2001[A]	PLD	CBA-CCA-CDA-CEA
3	A	2001[B]	PLD	CBA-CCA-CDA-CEA
3	A	2007[A]	PLD	C2B-C3B-C4B-C5B
3	A	2007[B]	PLD	C2B-C3B-C4B-C5B
3	A	2002	PLD	C3B-C4B-C5B-C6B
3	A	2004	PLD	CB-C1B-C2B-C3B
3	A	2007[A]	PLD	C4B-C5B-C6B-C7B
4	A	2025	UPL	C4-C5-C6-C7
3	A	2007[A]	PLD	C3B-C4B-C5B-C6B
4	A	2011	UPL	C15-C16-C17-C18
3	A	2007[B]	PLD	C3B-C4B-C5B-C6B
4	A	2019	UPL	C5-C6-C7-C8
4	B	2016	UPL	C7-C8-C9-C10
3	B	2003	PLD	C3B-C4B-C5B-C6B
4	B	2033	UPL	C2-C3-C4-C5
4	A	2011	UPL	C12-C13-C14-C15
4	A	2038	UPL	C2-C3-C4-C5
4	A	2012	UPL	C4-C5-C6-C7
3	A	2001[A]	PLD	C2'-C3'-C4'-C5'
3	A	2001[B]	PLD	C2'-C3'-C4'-C5'
3	A	2005[A]	PLD	C6'-C7'-C8'-C9'
4	B	2021	UPL	C2-C3-C4-C5
4	B	2021	UPL	C3-C4-C5-C6
3	A	2005[A]	PLD	C1'-C2'-C3'-C4'
3	A	2006	PLD	C4'-C5'-C6'-C7'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2006	PLD	C3B-C4B-C5B-C6B
4	A	2014	UPL	C10-C11-C12-C13
4	A	2029	UPL	C1-C2-C3-C4
4	A	2009	UPL	C13-C14-C15-C16
4	A	2012	UPL	C2-C3-C4-C5
4	A	2012	UPL	C11-C12-C13-C14
3	A	2001[B]	PLD	CD'-CE'-CF'-CG'
3	A	2007[A]	PLD	C5B-C6B-C7B-C8B
3	A	2002	PLD	CBA-CCA-CDA-CEA
3	B	2003	PLD	C5B-C6B-C7B-C8B
3	A	2004	PLD	C3B-C4B-C5B-C6B
4	A	2013	UPL	C2-C3-C4-C5
4	A	2018	UPL	C6-C7-C8-C9
4	B	2010	UPL	C6-C7-C8-C9
4	B	2016	UPL	C2-C3-C4-C5
4	A	2009	UPL	C5-C6-C7-C8
4	B	2010	UPL	C14-C15-C16-C17
3	A	2004	PLD	C1'-C'-O2-C2
4	B	2021	UPL	C5-C6-C7-C8
3	A	2004	PLD	O'-C'-O2-C2
4	A	2017	UPL	C7-C8-C9-C10
3	A	2005[B]	PLD	C1'-C2'-C3'-C4'
4	A	2029	UPL	C2-C3-C4-C5
3	A	2007[A]	PLD	C4'-C5'-C6'-C7'
3	A	2007[B]	PLD	C4'-C5'-C6'-C7'
4	B	2016	UPL	C3-C4-C5-C6
3	A	2001[A]	PLD	O3P-C1-C2-O2
3	A	2001[B]	PLD	O3P-C1-C2-O2
3	A	2001[B]	PLD	C9'-CA'-CB'-CC'
3	A	2005[A]	PLD	C9'-CA'-CB'-CC'
4	A	2011	UPL	C14-C15-C16-C17
4	A	2012	UPL	C5-C6-C7-C8
3	A	2002	PLD	C1'-C2'-C3'-C4'
4	A	2012	UPL	C9-C10-C11-C12
4	A	2048	UPL	C5-C6-C7-C8
3	A	2005[A]	PLD	C4'-C5'-C6'-C7'
3	A	2006	PLD	C1B-C2B-C3B-C4B
4	A	2034	UPL	C3-C4-C5-C6
3	A	2006	PLD	C7'-C8'-C9'-CA'
4	A	2012	UPL	C7-C8-C9-C10
4	A	2048	UPL	C4-C5-C6-C7
4	A	2019	UPL	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2004	PLD	O3P-C1-C2-C3
3	A	2005[A]	PLD	O3P-C1-C2-C3
3	A	2005[B]	PLD	O3P-C1-C2-C3
3	A	2007[A]	PLD	C6'-C7'-C8'-C9'
3	A	2007[B]	PLD	C6'-C7'-C8'-C9'
3	B	2003	PLD	C1'-C2'-C3'-C4'
4	A	2008	UPL	C9-C10-C11-C12
3	A	2005[A]	PLD	C5'-C6'-C7'-C8'
3	A	2007[A]	PLD	CA'-CB'-CC'-CD'
3	A	2007[B]	PLD	CA'-CB'-CC'-CD'
3	A	2002	PLD	C9B-CAA-CBA-CCA
4	A	2017	UPL	C6-C7-C8-C9
3	A	2007[A]	PLD	C1-O3P-P-O1P
3	A	2007[B]	PLD	C1-O3P-P-O1P
4	A	2022	UPL	C2-C3-C4-C5
3	A	2005[A]	PLD	C9B-CAA-CBA-CCA
3	A	2005[B]	PLD	C9B-CAA-CBA-CCA
3	A	2001[A]	PLD	C6'-C7'-C8'-C9'
3	A	2001[B]	PLD	C6'-C7'-C8'-C9'
3	A	2005[A]	PLD	CC'-CD'-CE'-CF'
3	A	2005[B]	PLD	CC'-CD'-CE'-CF'
3	A	2006	PLD	C6'-C7'-C8'-C9'
4	A	2013	UPL	C3-C4-C5-C6
3	A	2005[B]	PLD	C5'-C6'-C7'-C8'
4	A	2032	UPL	C1-C2-C3-C4
4	B	2049	UPL	C1-C2-C3-C4
4	B	2031	UPL	C4-C5-C6-C7
3	A	2005[A]	PLD	CD'-CE'-CF'-CG'
3	A	2005[B]	PLD	CD'-CE'-CF'-CG'
4	A	2011	UPL	C13-C14-C15-C16
4	A	2038	UPL	C1-C2-C3-C4
3	A	2001[A]	PLD	CE'-CF'-CG'-CH'
4	A	2015	UPL	C7-C8-C9-C10
4	A	2018	UPL	C7-C8-C9-C10
4	A	2017	UPL	C11-C10-C9-C8
4	B	2028	UPL	C1-C2-C3-C4
4	A	2039	UPL	C1-C2-C3-C4
4	A	2018	UPL	C3-C4-C5-C6
4	B	2027	UPL	C4-C5-C6-C7
4	B	2044	UPL	C4-C5-C6-C7
4	A	2036	UPL	C1-C2-C3-C4
4	B	2016	UPL	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2050	UPL	C1-C2-C3-C4
4	A	2012	UPL	C6-C7-C8-C9
3	A	2007[A]	PLD	C7'-C8'-C9'-CA'
3	A	2007[B]	PLD	C7'-C8'-C9'-CA'
4	A	2014	UPL	C5-C6-C7-C8
4	A	2042	UPL	C1-C2-C3-C4
3	A	2005[A]	PLD	C3'-C4'-C5'-C6'
3	A	2002	PLD	C6B-C7B-C8B-C9B
4	A	2011	UPL	C1-C2-C3-C4
4	A	2037	UPL	C1-C2-C3-C4
3	A	2001[A]	PLD	O3P-C1-C2-C3
3	A	2001[B]	PLD	O3P-C1-C2-C3
4	A	2015	UPL	C10-C11-C12-C13
4	B	2043	UPL	C2-C3-C4-C5
3	A	2005[B]	PLD	C6'-C7'-C8'-C9'
4	A	2030	UPL	C4-C5-C6-C7
3	A	2002	PLD	CCA-CDA-CEA-CFA
4	B	2031	UPL	C3-C4-C5-C6
3	A	2004	PLD	C1'-C2'-C3'-C4'
4	B	2010	UPL	C5-C6-C7-C8
4	B	2045	UPL	C1-C2-C3-C4
3	A	2001[A]	PLD	C1-C2-C3-O3
3	A	2001[B]	PLD	C1-C2-C3-O3
3	A	2007[A]	PLD	C1-C2-C3-O3
3	A	2007[B]	PLD	C1-C2-C3-O3
3	B	2003	PLD	C1-C2-C3-O3
3	A	2004	PLD	C6B-C7B-C8B-C9B
4	A	2013	UPL	C11-C10-C9-C8
4	A	2011	UPL	C16-C17-C18-C19
4	B	2046	UPL	C1-C2-C3-C4
4	B	2049	UPL	C2-C3-C4-C5
4	A	2011	UPL	C11-C10-C9-C8
4	B	2044	UPL	C3-C4-C5-C6
4	A	2048	UPL	C7-C8-C9-C10
3	A	2005[A]	PLD	C2B-C3B-C4B-C5B
3	A	2005[B]	PLD	C2B-C3B-C4B-C5B
4	A	2017	UPL	C5-C6-C7-C8
3	A	2002	PLD	C2B-C3B-C4B-C5B
4	B	2044	UPL	C2-C3-C4-C5
4	A	2020	UPL	C2-C3-C4-C5
4	B	2010	UPL	C11-C10-C9-C8
4	A	2017	UPL	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	2023	UPL	C6-C7-C8-C9
4	B	2045	UPL	C2-C3-C4-C5
4	B	2023	UPL	C1-C2-C3-C4
3	A	2005[B]	PLD	C9'-CA'-CB'-CC'
3	A	2001[B]	PLD	CB'-CC'-CD'-CE'
3	B	2003	PLD	C4B-C5B-C6B-C7B
4	A	2015	UPL	C9-C10-C11-C12
4	A	2025	UPL	C1-C2-C3-C4
3	A	2006	PLD	O3P-C1-C2-C3
3	A	2006	PLD	C5'-C6'-C7'-C8'
3	A	2007[A]	PLD	C1'-C2'-C3'-C4'
3	A	2007[B]	PLD	C1'-C2'-C3'-C4'
3	A	2001[B]	PLD	CF'-CG'-CH'-CI'
4	A	2013	UPL	C13-C14-C15-C16
4	B	2049	UPL	C3-C4-C5-C6
3	A	2001[B]	PLD	CA'-CB'-CC'-CD'
3	A	2004	PLD	O3P-C1-C2-O2
3	A	2007[A]	PLD	O3P-C1-C2-O2
3	A	2007[B]	PLD	O3P-C1-C2-O2
3	A	2005[A]	PLD	C1-C2-C3-O3
3	A	2005[B]	PLD	C1-C2-C3-O3
4	A	2009	UPL	C11-C10-C9-C8
3	A	2007[A]	PLD	O2-C2-C3-O3
3	A	2007[B]	PLD	O2-C2-C3-O3
3	A	2001[A]	PLD	C2B-C3B-C4B-C5B
3	A	2001[B]	PLD	C2B-C3B-C4B-C5B
4	A	2013	UPL	C11-C12-C13-C14
3	A	2005[A]	PLD	C4B-C5B-C6B-C7B
3	A	2005[B]	PLD	C4B-C5B-C6B-C7B
3	A	2006	PLD	C9'-CA'-CB'-CC'
3	A	2007[A]	PLD	C3'-C4'-C5'-C6'
3	A	2007[B]	PLD	C3'-C4'-C5'-C6'
4	A	2019	UPL	C6-C7-C8-C9
4	A	2042	UPL	C2-C3-C4-C5
4	B	2028	UPL	C4-C5-C6-C7
4	A	2035	UPL	C3-C4-C5-C6
4	A	2012	UPL	C3-C4-C5-C6
3	B	2003	PLD	C2B-C1B-CB-O3
3	A	2002	PLD	O3P-C1-C2-C3
3	A	2002	PLD	C3'-C4'-C5'-C6'
4	A	2019	UPL	C2-C3-C4-C5
4	B	2021	UPL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2005[A]	PLD	CAA-CBA-CCA-CDA
3	A	2005[B]	PLD	CAA-CBA-CCA-CDA
3	A	2005[B]	PLD	C8'-C9'-CA'-CB'
3	A	2006	PLD	C2'-C3'-C4'-C5'
4	A	2035	UPL	C4-C5-C6-C7
3	A	2002	PLD	O3P-C1-C2-O2
3	A	2005[A]	PLD	O3P-C1-C2-O2
3	A	2005[B]	PLD	O3P-C1-C2-O2
4	A	2013	UPL	C4-C5-C6-C7
3	A	2004	PLD	O2-C2-C3-O3
4	A	2035	UPL	C1-C2-C3-C4
3	A	2002	PLD	C1-C2-C3-O3
4	A	2008	UPL	C12-C13-C14-C15
4	A	2015	UPL	C5-C6-C7-C8
3	B	2003	PLD	C1-O3P-P-O1P
3	B	2003	PLD	C4-O4P-P-O1P
3	B	2003	PLD	C4-O4P-P-O3P
3	B	2003	PLD	C2'-C3'-C4'-C5'
4	A	2025	UPL	C5-C6-C7-C8
3	A	2007[A]	PLD	C1B-C2B-C3B-C4B
3	A	2007[B]	PLD	C1B-C2B-C3B-C4B
4	B	2010	UPL	C13-C14-C15-C16
4	B	2016	UPL	C4-C5-C6-C7
4	A	2008	UPL	C10-C11-C12-C13
4	A	2026	UPL	C1-C2-C3-C4
3	A	2002	PLD	C2-C1-O3P-P
3	A	2001[A]	PLD	C5B-C6B-C7B-C8B
3	A	2001[B]	PLD	C5B-C6B-C7B-C8B
3	B	2003	PLD	O2-C2-C3-O3
4	A	2048	UPL	C6-C7-C8-C9
3	A	2004	PLD	C2B-C1B-CB-O3
3	A	2001[A]	PLD	CD'-CE'-CF'-CG'
3	A	2001[A]	PLD	C5'-C6'-C7'-C8'
3	A	2001[B]	PLD	C5'-C6'-C7'-C8'
3	A	2002	PLD	C5B-C6B-C7B-C8B
4	A	2011	UPL	C2-C3-C4-C5
4	A	2037	UPL	C2-C3-C4-C5
4	A	2011	UPL	C5-C6-C7-C8
4	B	2010	UPL	C10-C11-C12-C26
4	A	2050	UPL	C3-C4-C5-C6
3	A	2004	PLD	C4B-C5B-C6B-C7B
4	A	2014	UPL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2014	UPL	C13-C14-C15-C16
4	A	2008	UPL	C10-C11-C12-C26
4	A	2025	UPL	C3-C4-C5-C6
3	A	2005[A]	PLD	CCA-CDA-CEA-CFA
3	A	2005[B]	PLD	CCA-CDA-CEA-CFA
3	A	2005[A]	PLD	O2-C2-C3-O3
3	A	2005[B]	PLD	O2-C2-C3-O3
4	A	2009	UPL	C10-C11-C12-C26
3	A	2005[A]	PLD	C8B-C9B-CAA-CBA
3	A	2005[B]	PLD	C8B-C9B-CAA-CBA
4	B	2027	UPL	C2-C3-C4-C5
3	B	2003	PLD	O2-C'-C1'-C2'
4	B	2010	UPL	C12-C13-C14-C15
4	A	2014	UPL	C1-C2-C3-C4
4	A	2029	UPL	C3-C4-C5-C6
4	A	2018	UPL	C5-C6-C7-C8
3	A	2006	PLD	C3'-C4'-C5'-C6'
3	A	2006	PLD	C1-O3P-P-O2P
4	A	2009	UPL	C10-C11-C12-C13
4	A	2047	UPL	C1-C2-C3-C4
4	A	2011	UPL	C3-C4-C5-C6
4	A	2011	UPL	C7-C8-C9-C10
3	A	2002	PLD	C2-C3-O3-CB
3	A	2006	PLD	C4B-C5B-C6B-C7B
4	A	2018	UPL	C4-C5-C6-C7
4	B	2010	UPL	C10-C11-C12-C13
4	A	2047	UPL	C2-C3-C4-C5
4	B	2033	UPL	C3-C4-C5-C6
3	A	2001[A]	PLD	CCA-CDA-CEA-CFA
3	A	2001[B]	PLD	CCA-CDA-CEA-CFA
4	A	2008	UPL	C11-C10-C9-C8
4	A	2026	UPL	C5-C6-C7-C8
3	A	2006	PLD	O2-C'-C1'-C2'
4	A	2036	UPL	C3-C4-C5-C6
3	B	2003	PLD	C2B-C1B-CB-OB
4	A	2013	UPL	C10-C11-C12-C13
4	A	2014	UPL	C2-C3-C4-C5
3	A	2006	PLD	O'-C'-C1'-C2'
4	A	2032	UPL	C3-C4-C5-C6
3	A	2001[A]	PLD	C2-C3-O3-CB
3	A	2001[B]	PLD	C2-C3-O3-CB
4	A	2008	UPL	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2004	PLD	O'-C'-C1'-C2'

There are no ring outliers.

41 monomers are involved in 112 short contacts:

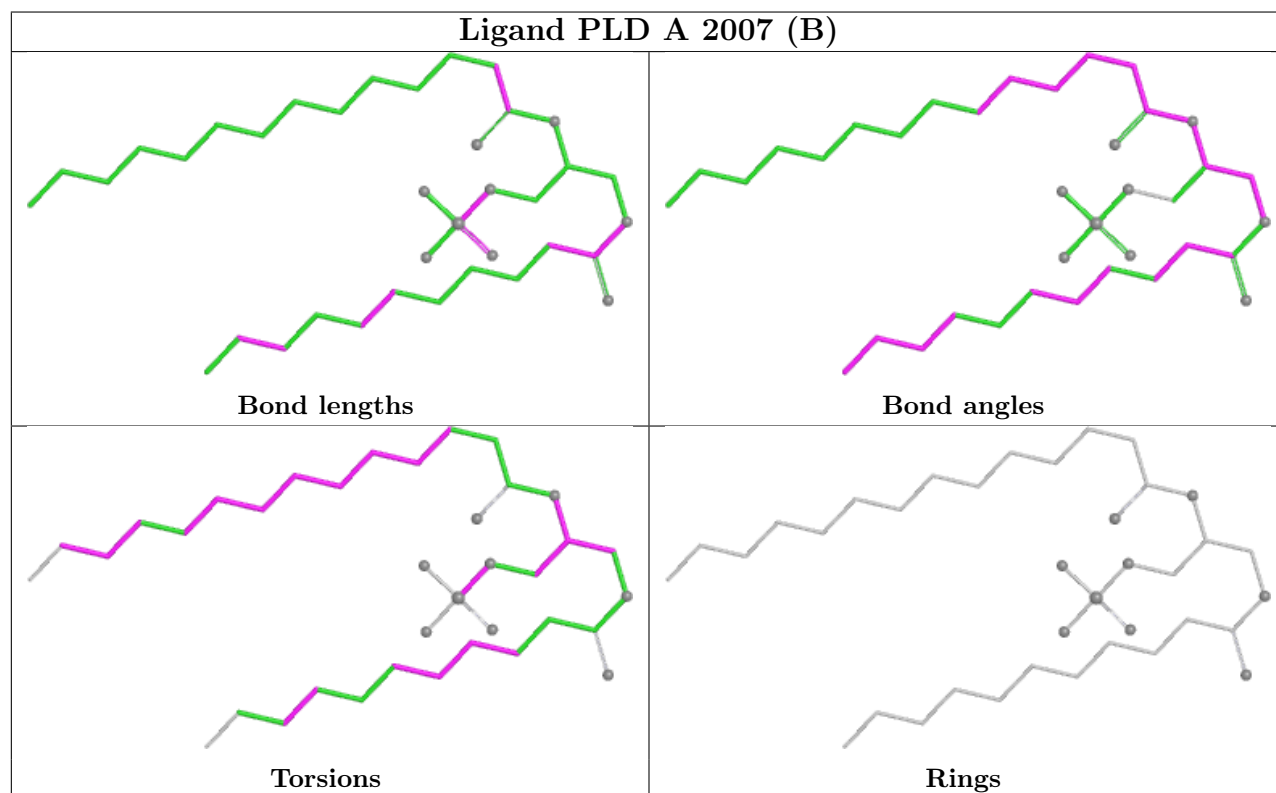
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2007[B]	PLD	10	0
4	B	2010	UPL	6	0
4	A	2009	UPL	7	0
3	B	2003	PLD	8	0
4	B	2045	UPL	1	0
4	A	2038	UPL	2	0
4	B	2016	UPL	2	0
3	A	2004	PLD	13	0
3	A	2001[A]	PLD	4	0
4	A	2047	UPL	1	0
4	A	2050	UPL	1	0
4	A	2022	UPL	2	0
4	A	2017	UPL	1	0
4	A	2019	UPL	1	0
4	A	2012	UPL	3	0
4	B	2049	UPL	3	0
3	A	2005[B]	PLD	5	0
4	B	2033	UPL	1	0
4	A	2024	UPL	1	0
4	B	2021	UPL	4	0
4	B	2028	UPL	1	0
4	A	2014	UPL	2	0
4	A	2025	UPL	1	0
4	A	2013	UPL	7	0
4	A	2011	UPL	4	0
4	A	2026	UPL	3	0
4	A	2036	UPL	1	0
3	A	2006	PLD	9	0
4	B	2044	UPL	1	0
4	A	2042	UPL	1	0
4	A	2048	UPL	2	0
4	A	2015	UPL	4	0
4	A	2018	UPL	2	0
4	A	2030	UPL	1	0
4	A	2029	UPL	1	0
4	A	2008	UPL	3	0

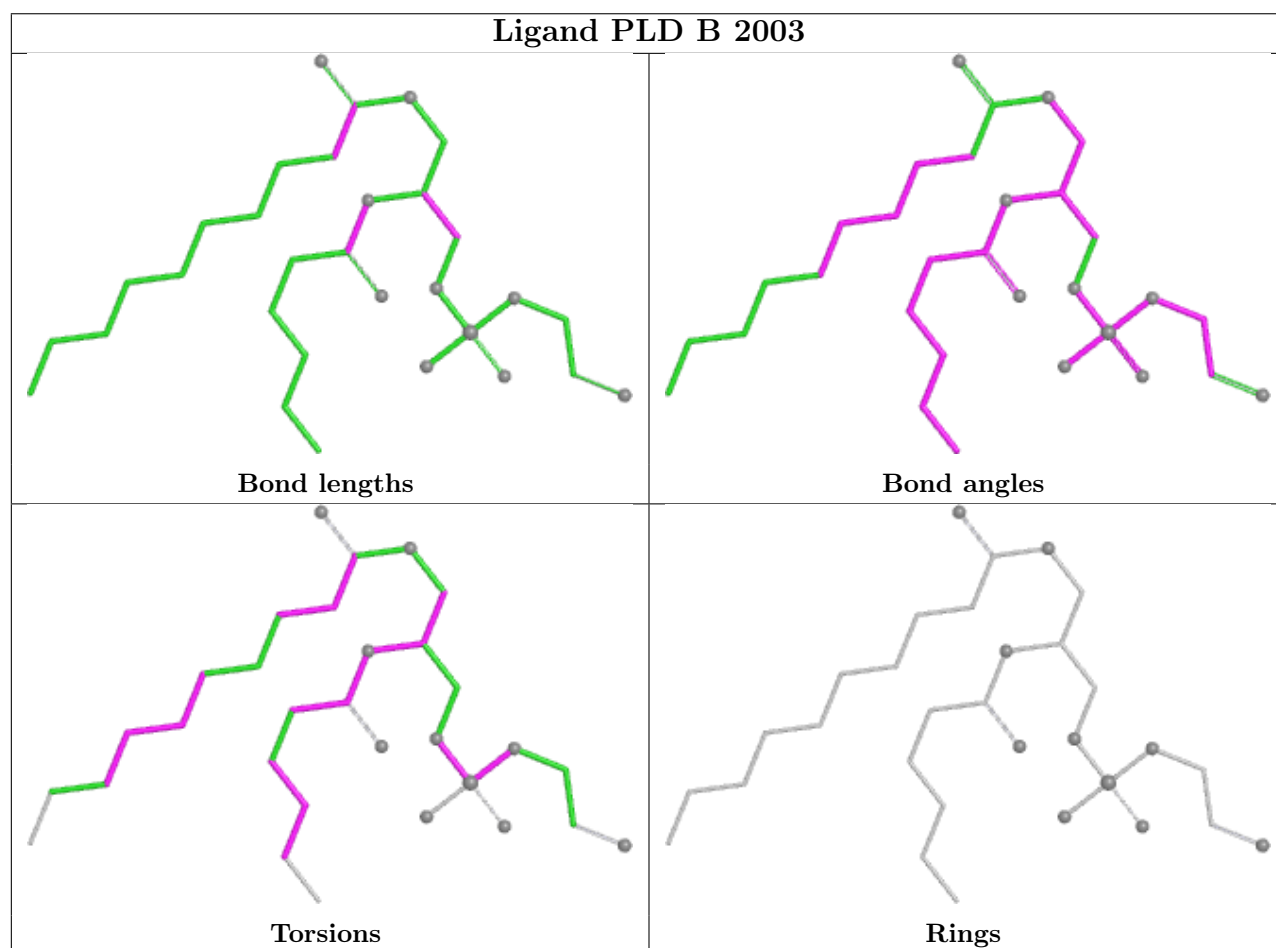
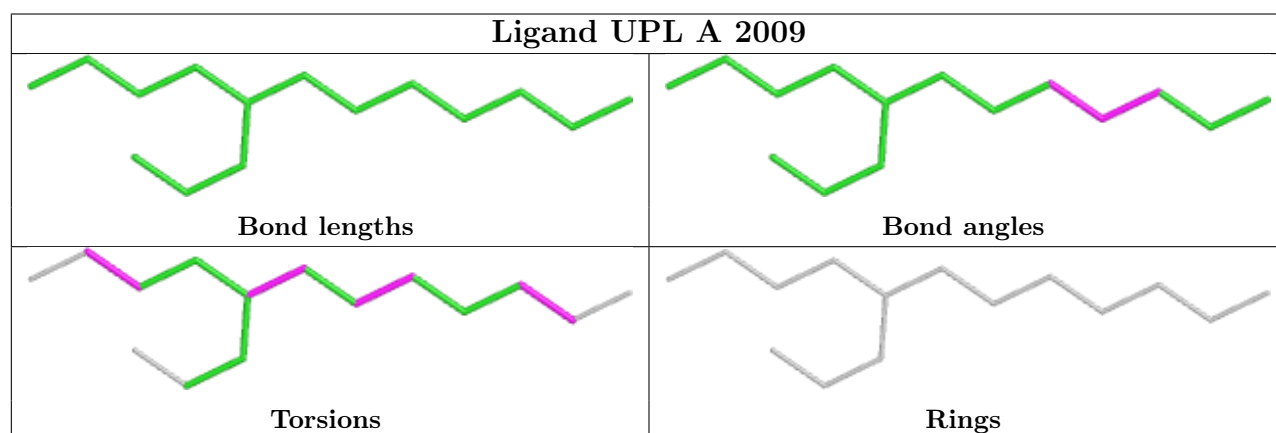
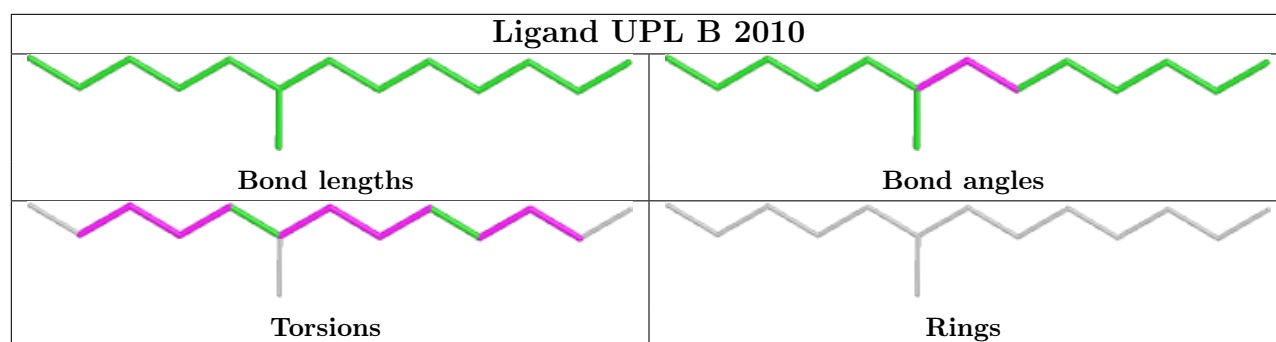
Continued on next page...

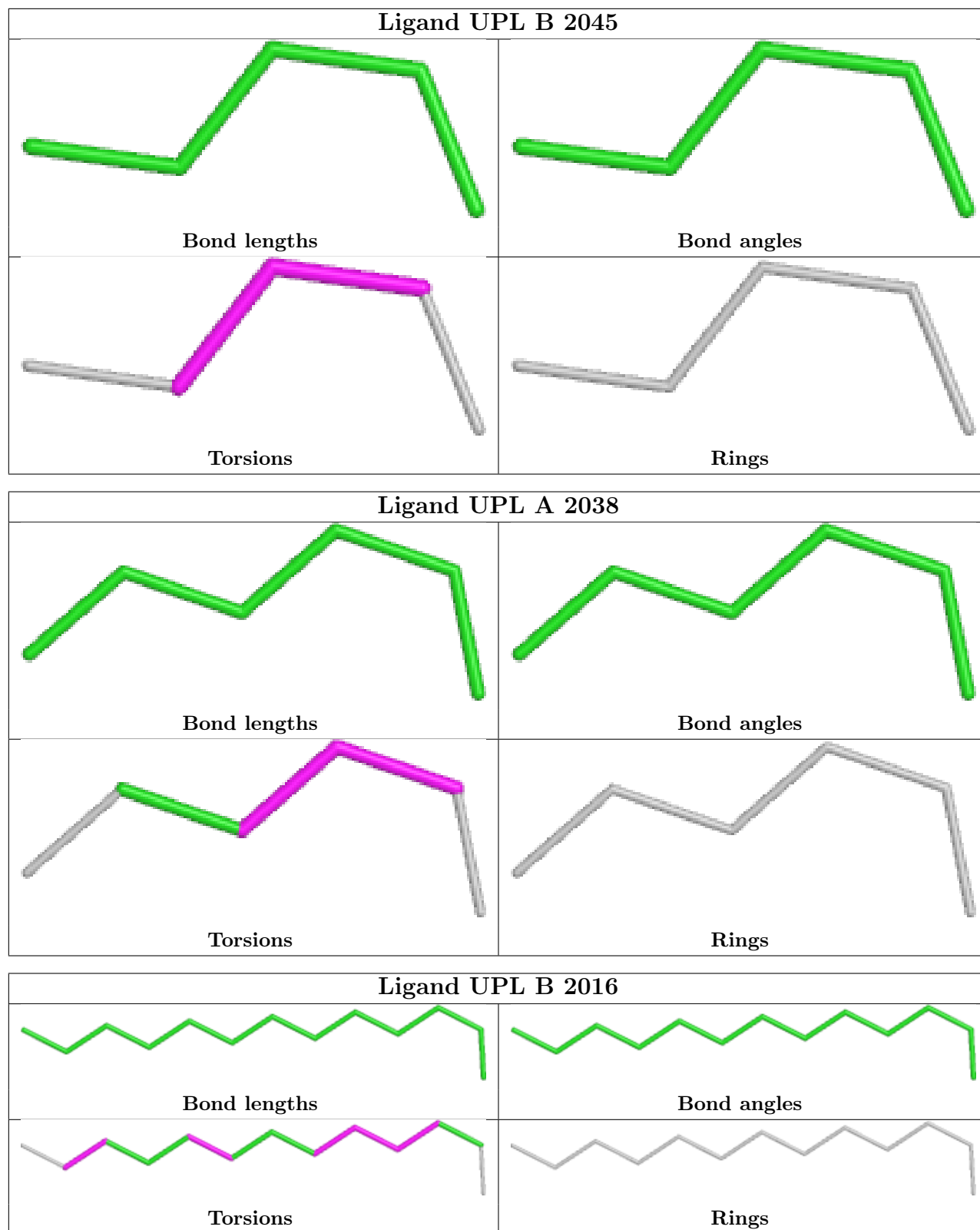
Continued from previous page...

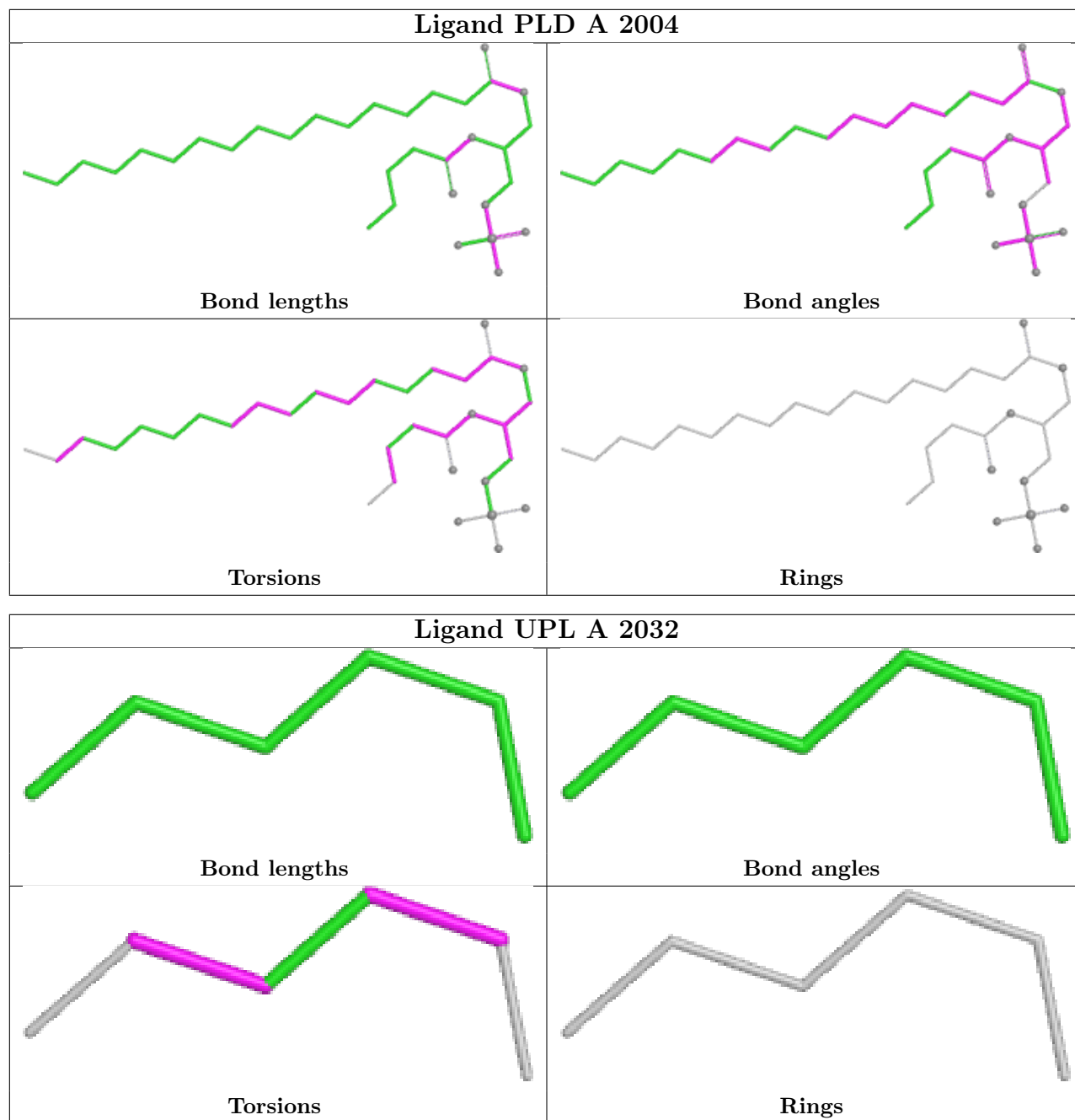
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2034	UPL	1	0
3	A	2002	PLD	16	0
4	B	2046	UPL	2	0
4	B	2023	UPL	2	0
4	B	2027	UPL	2	0

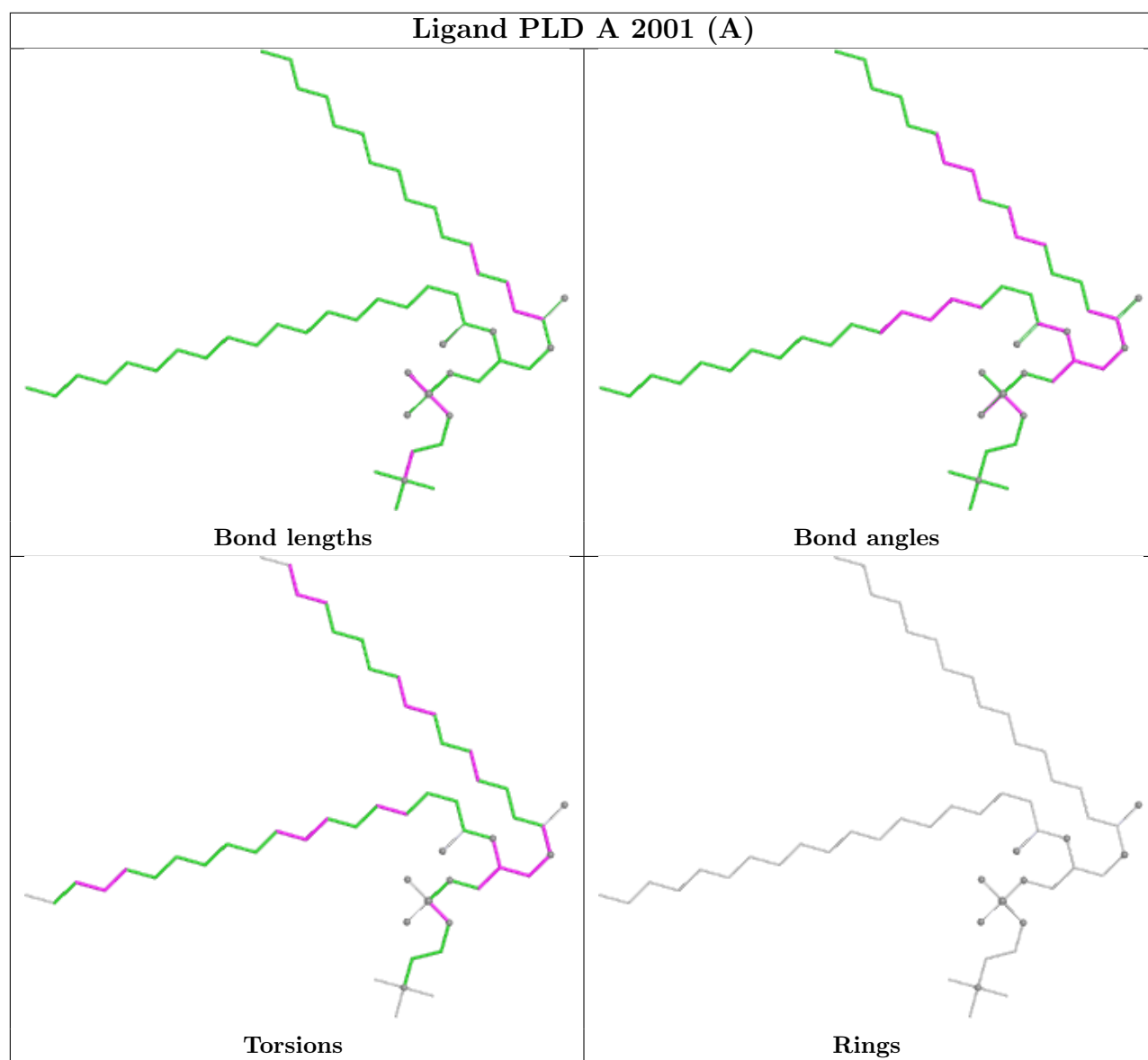
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

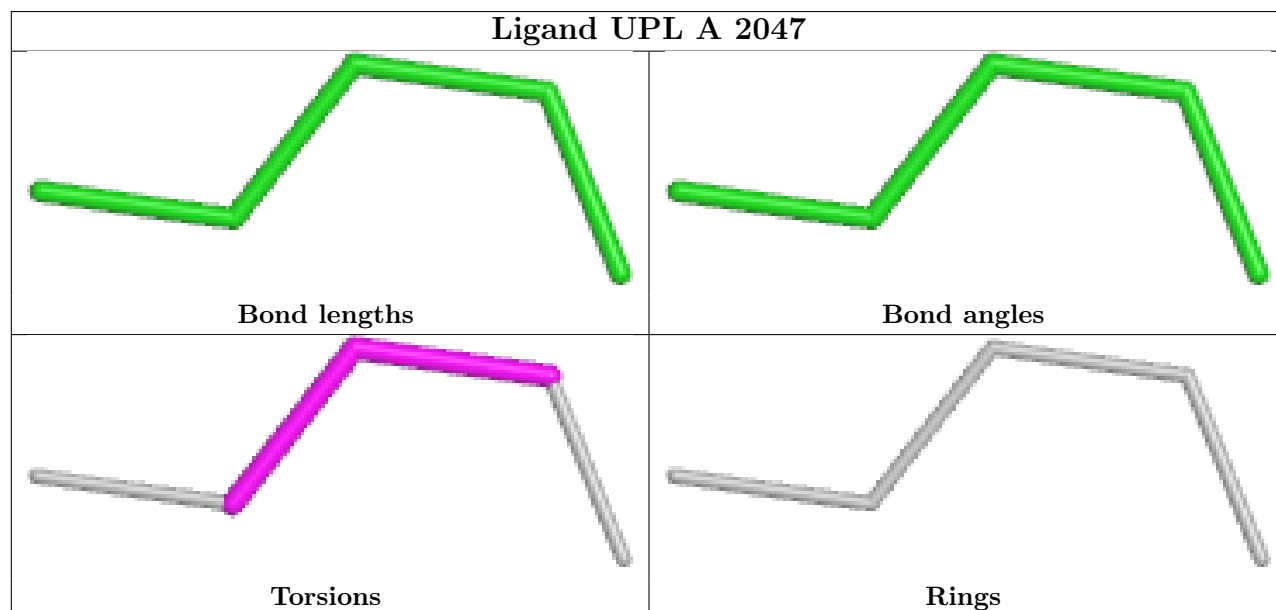
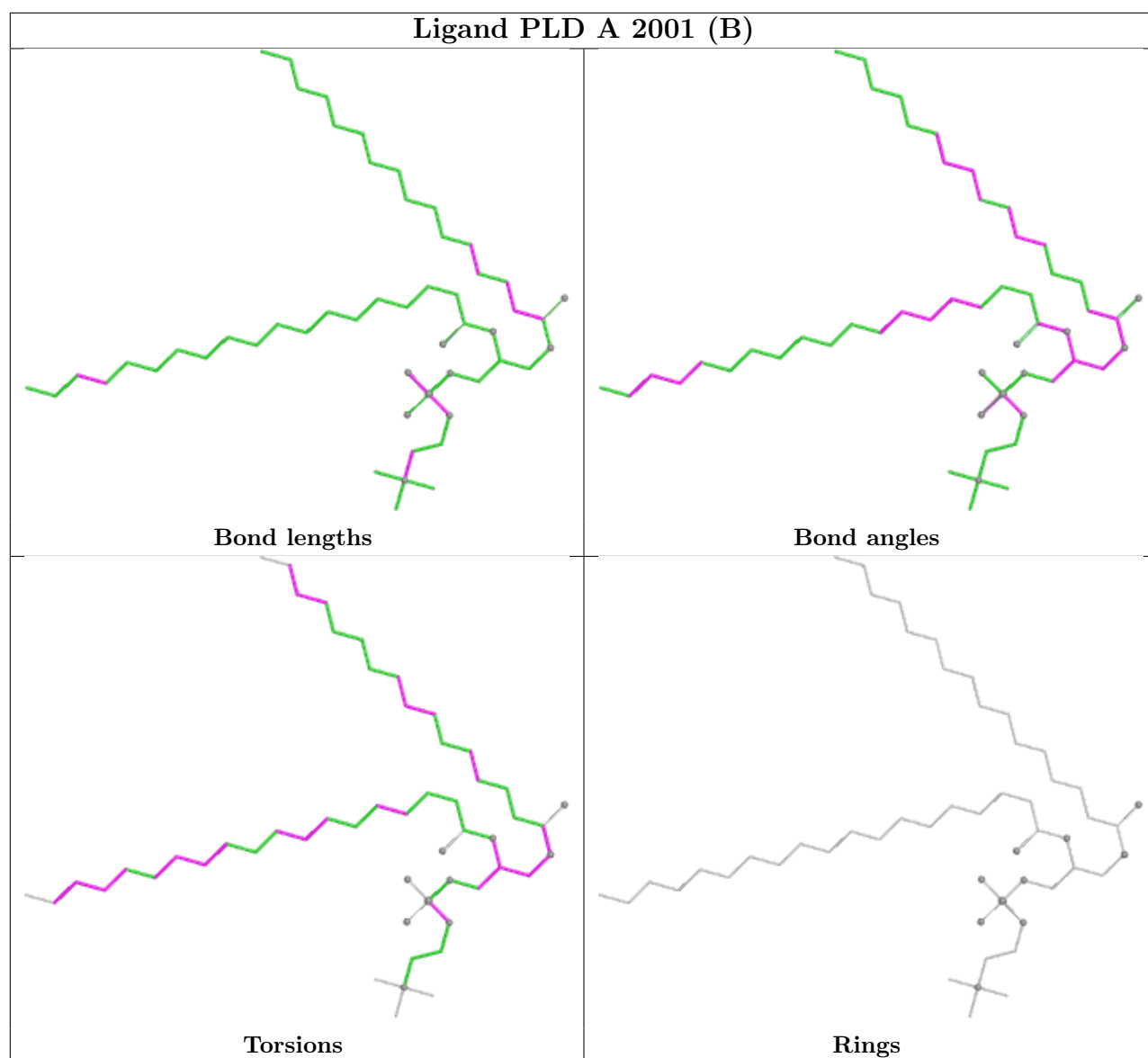


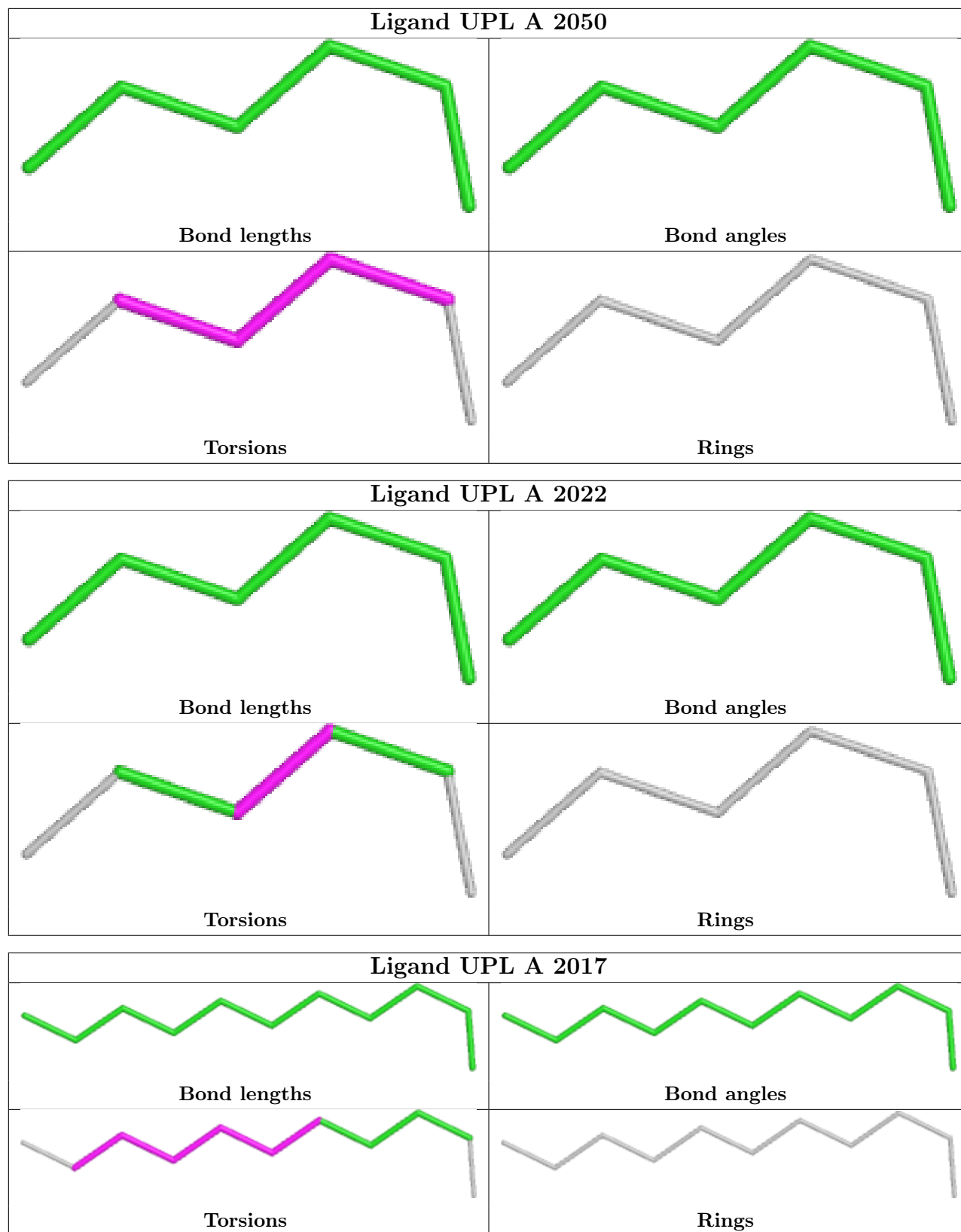


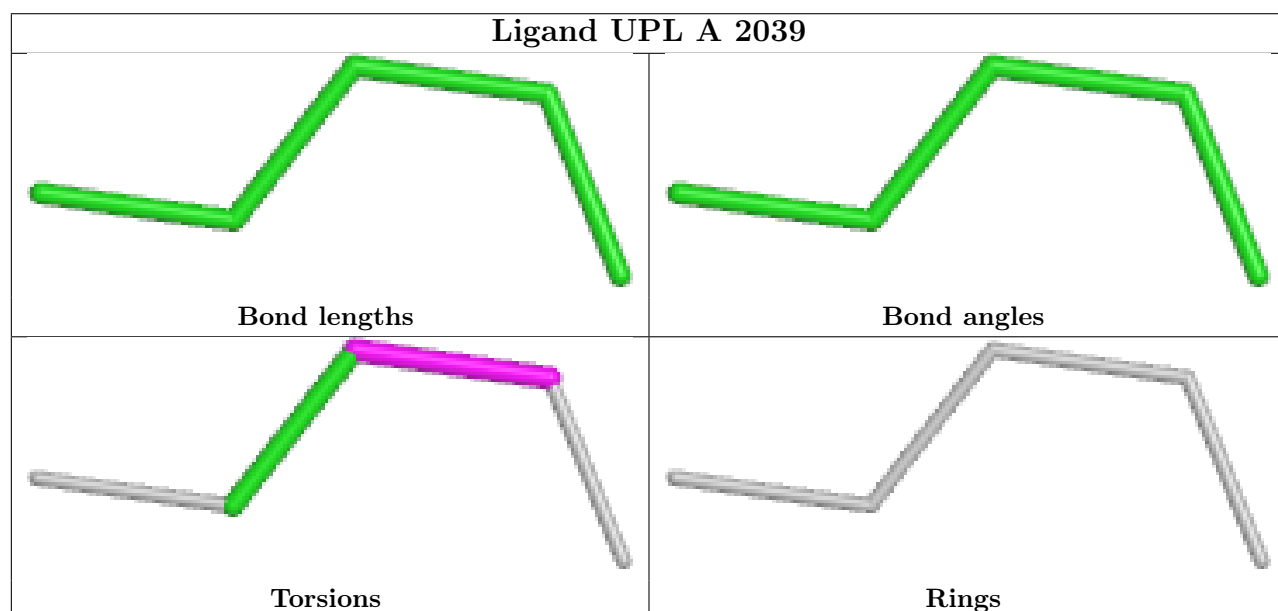
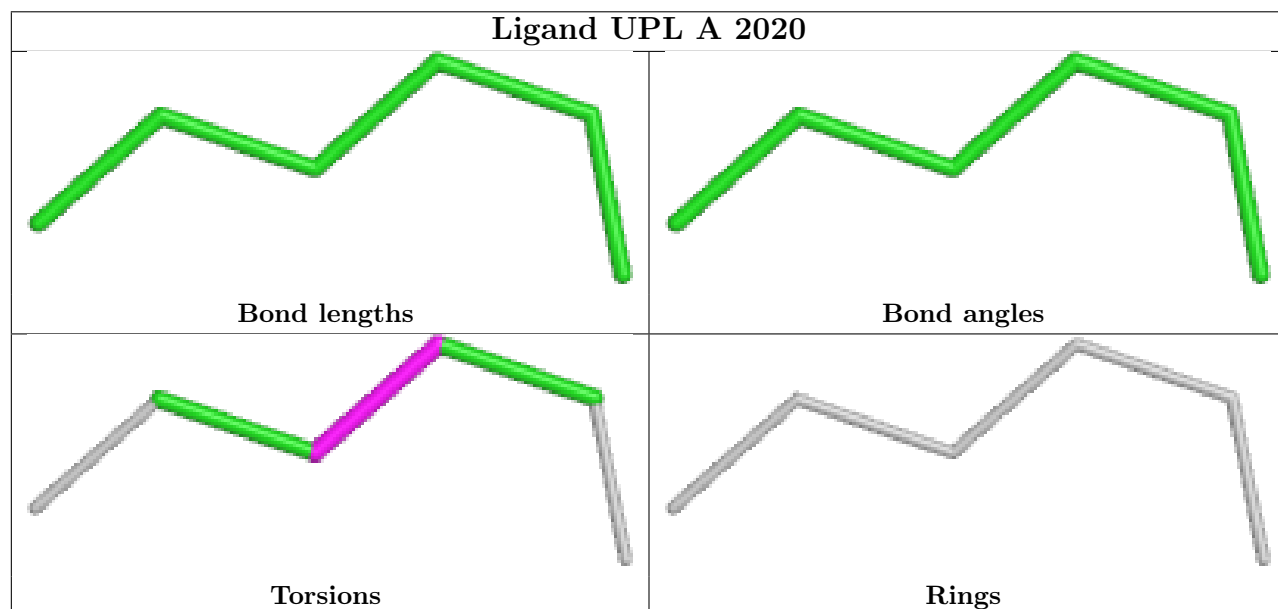
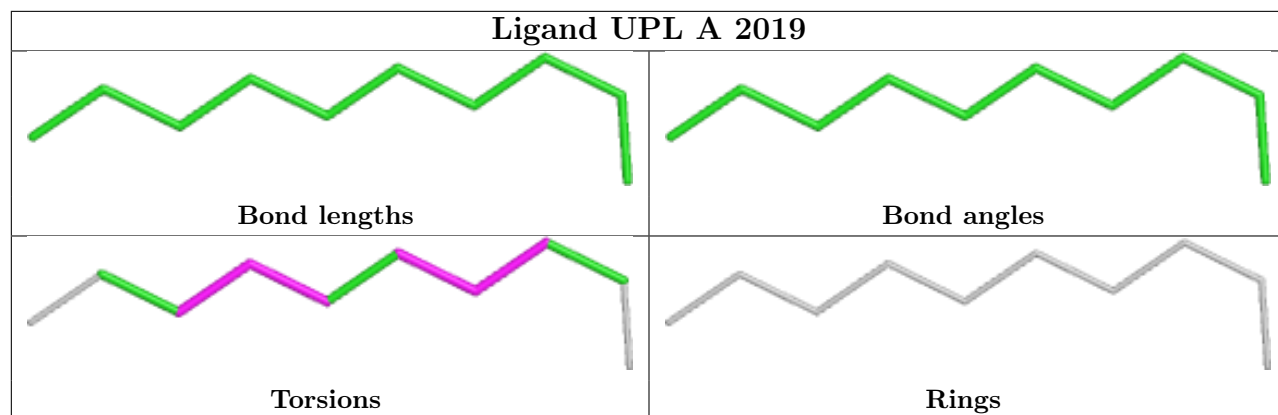


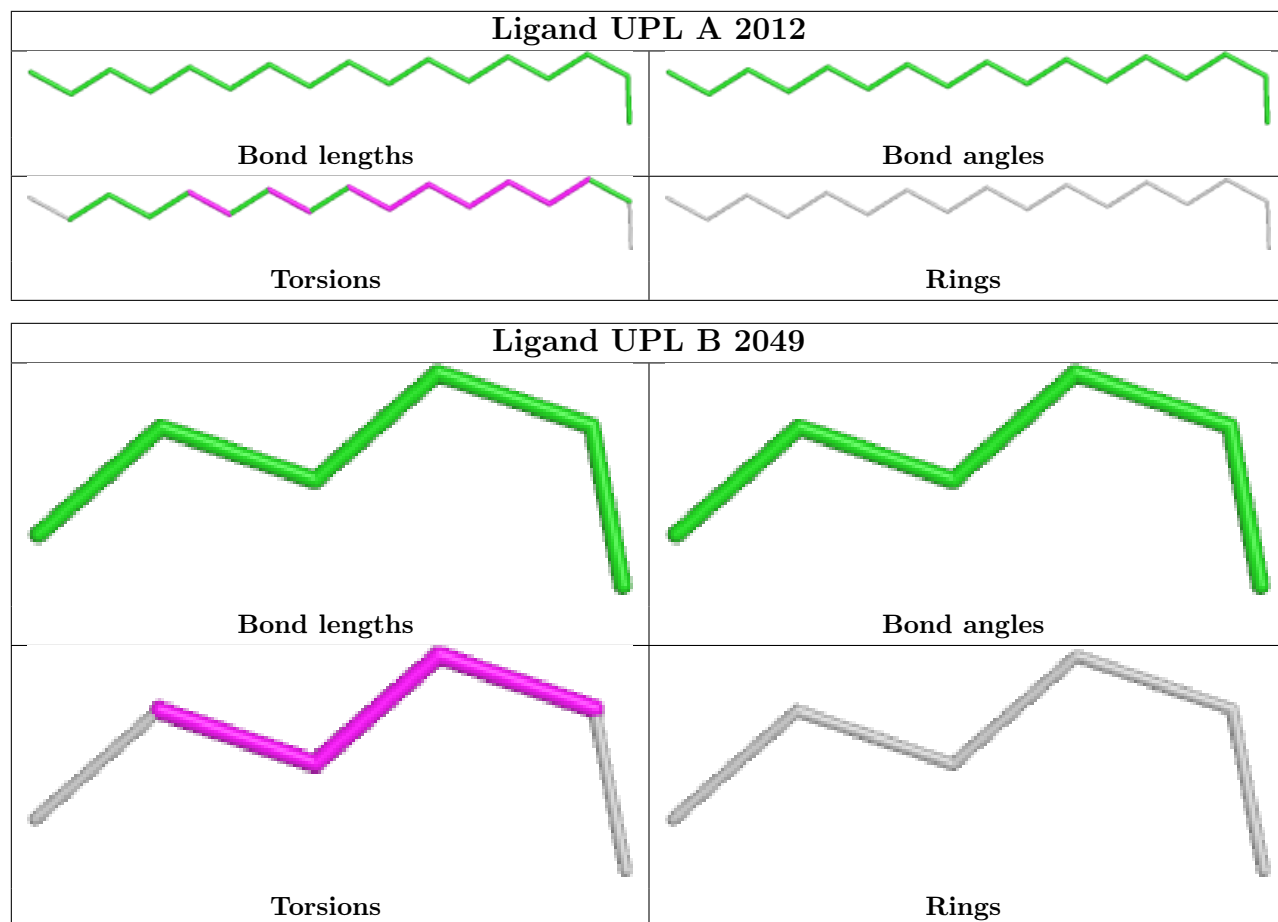


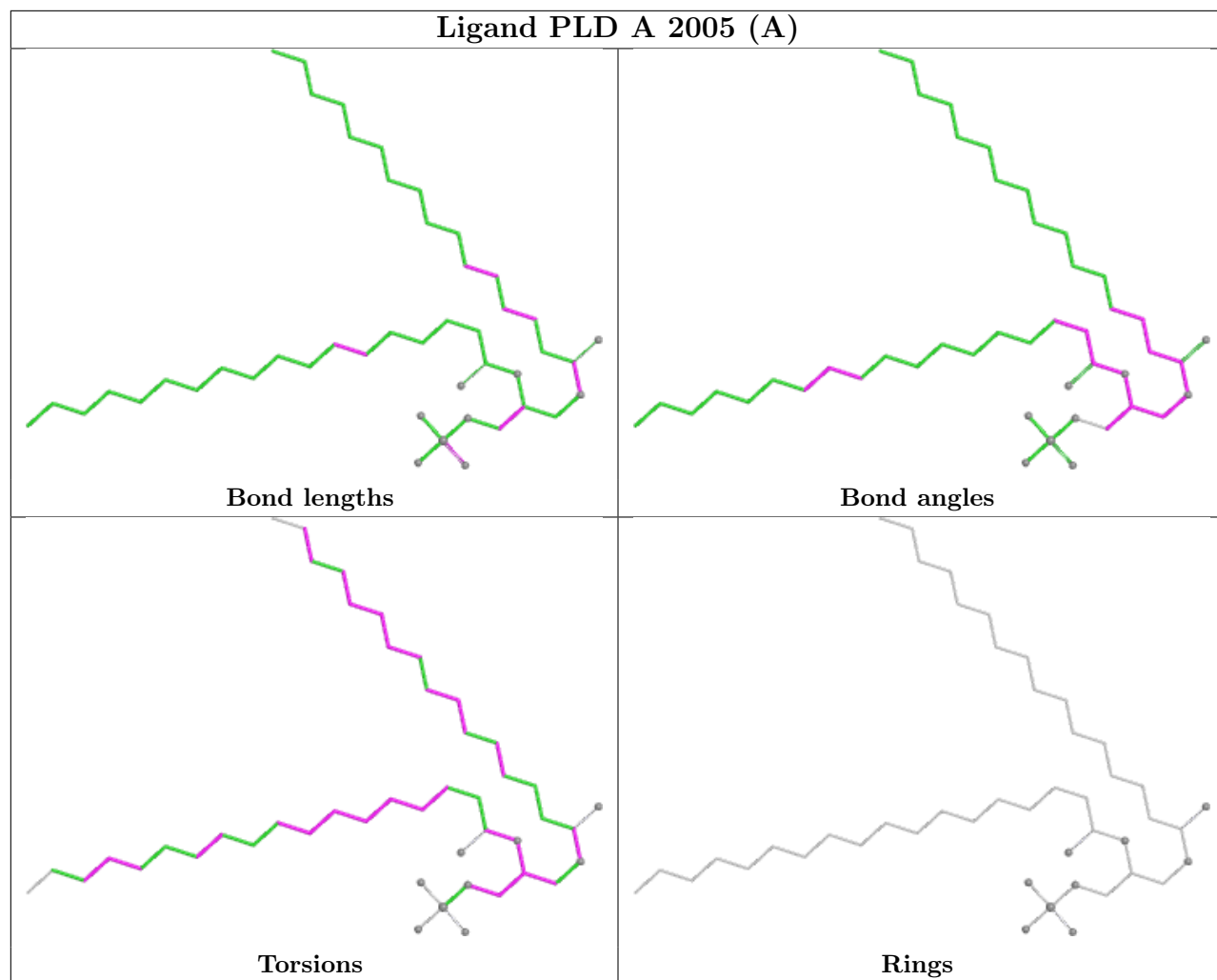


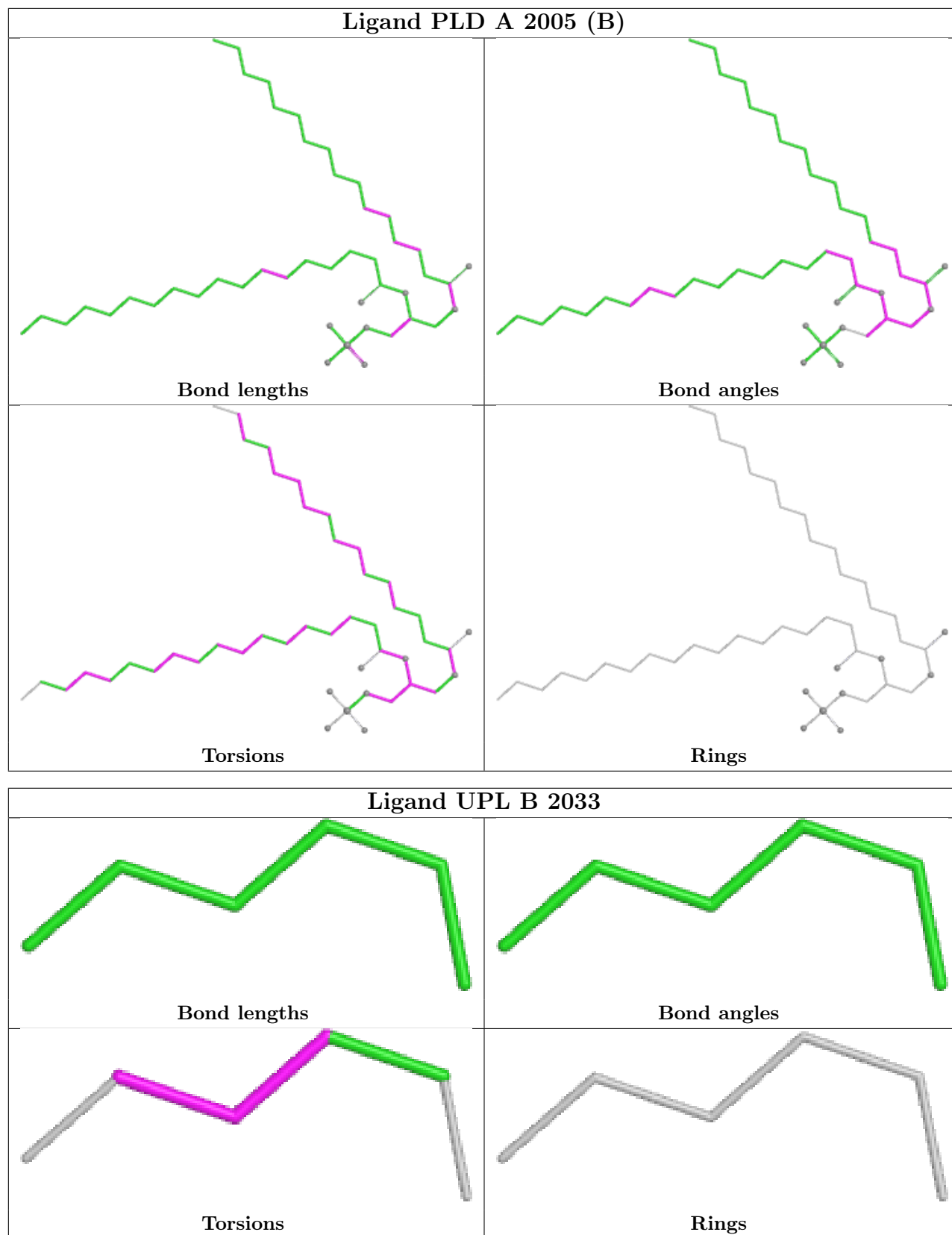


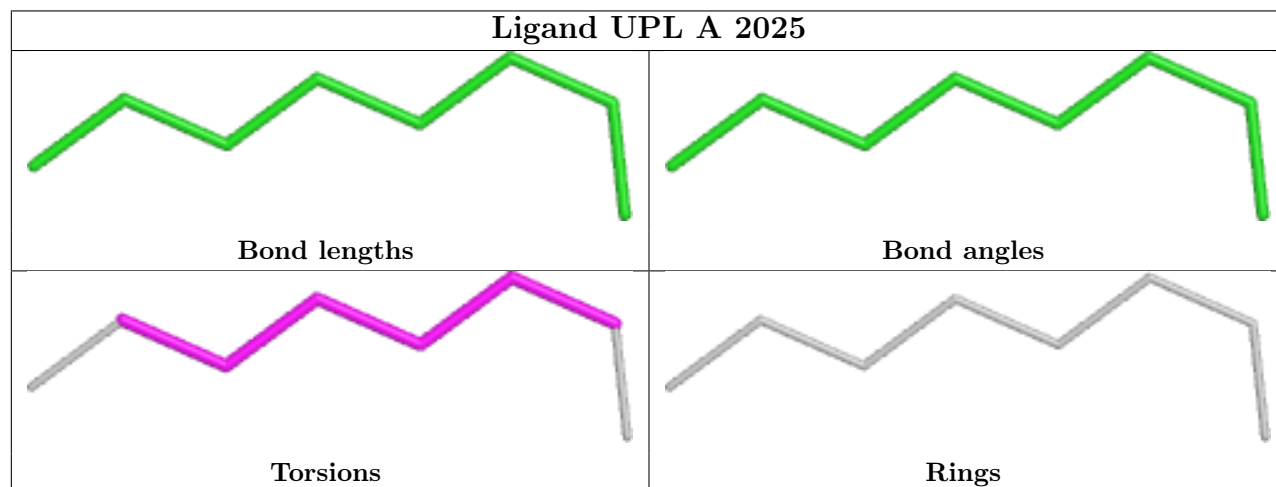
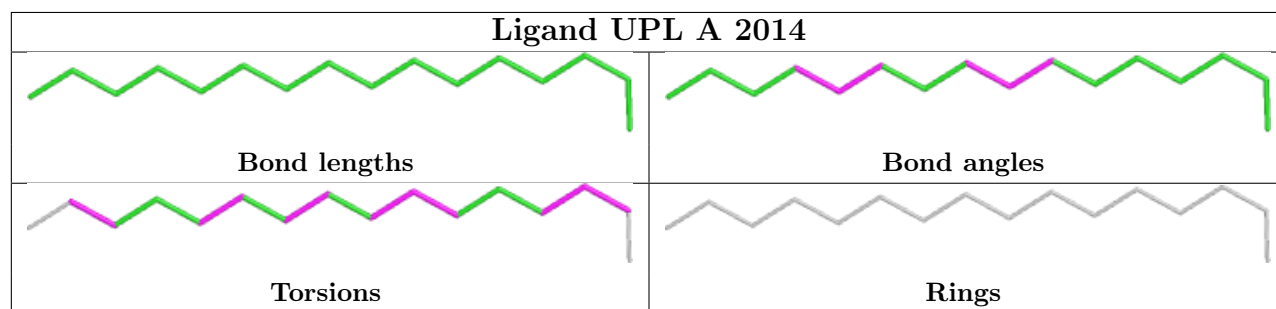
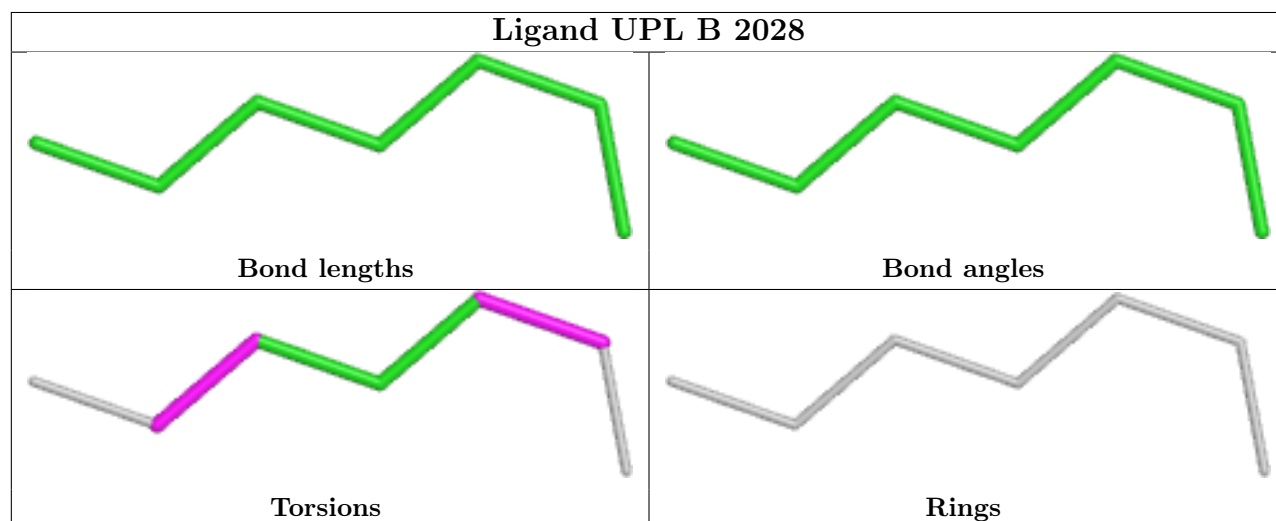
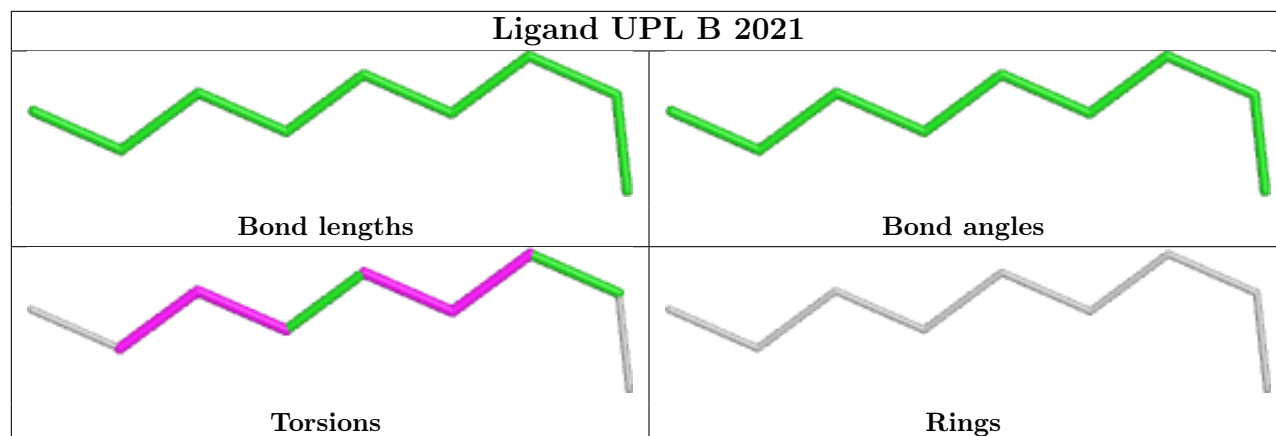


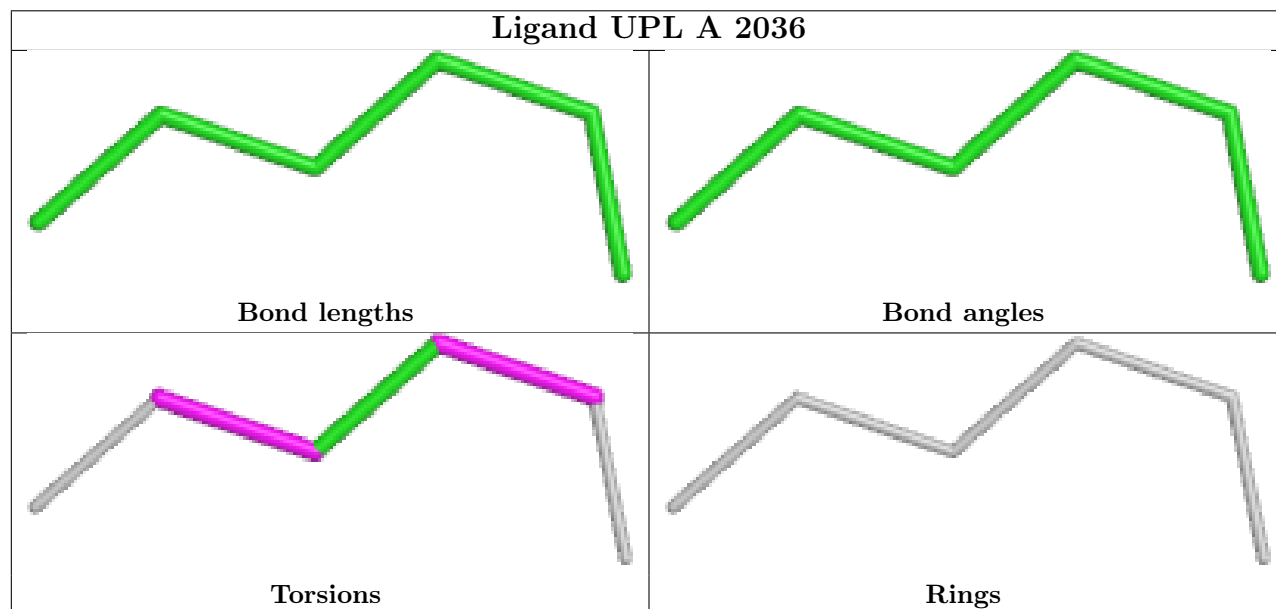
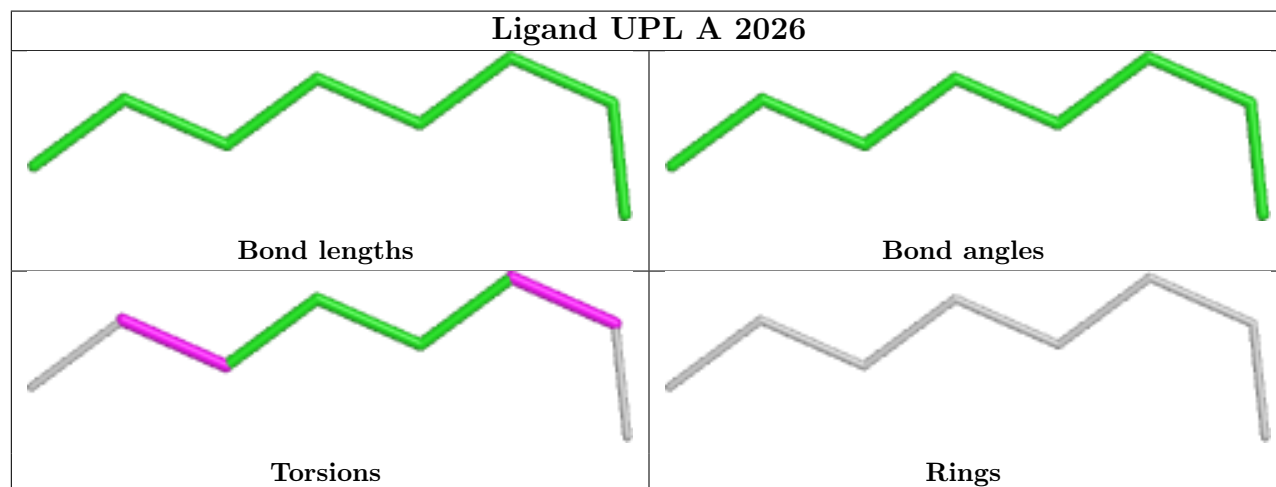
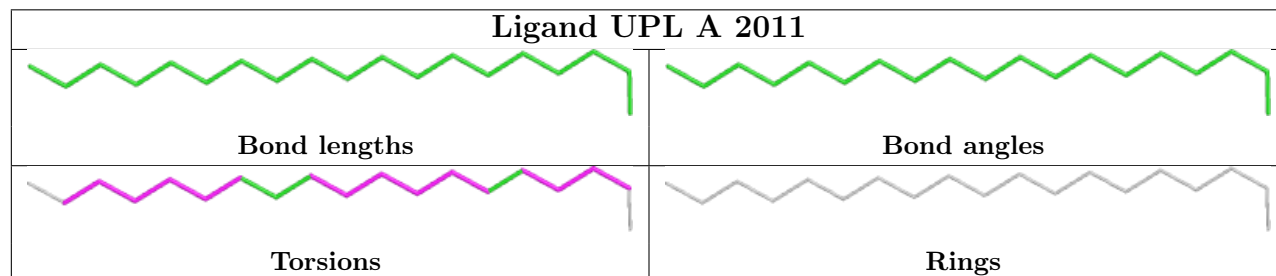
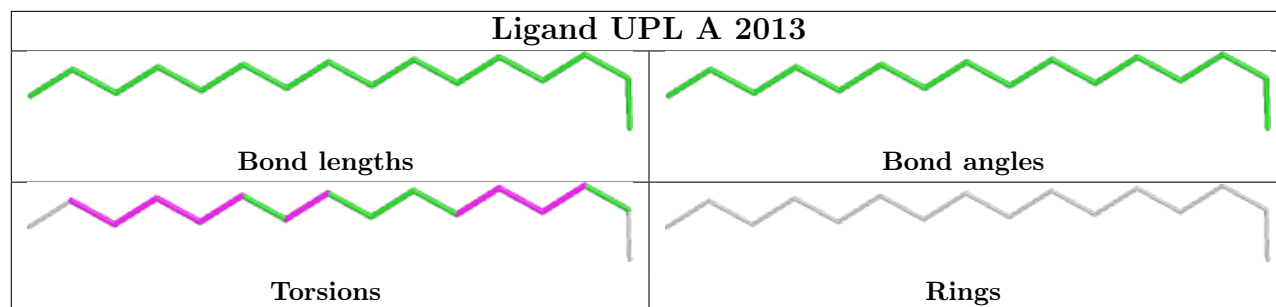


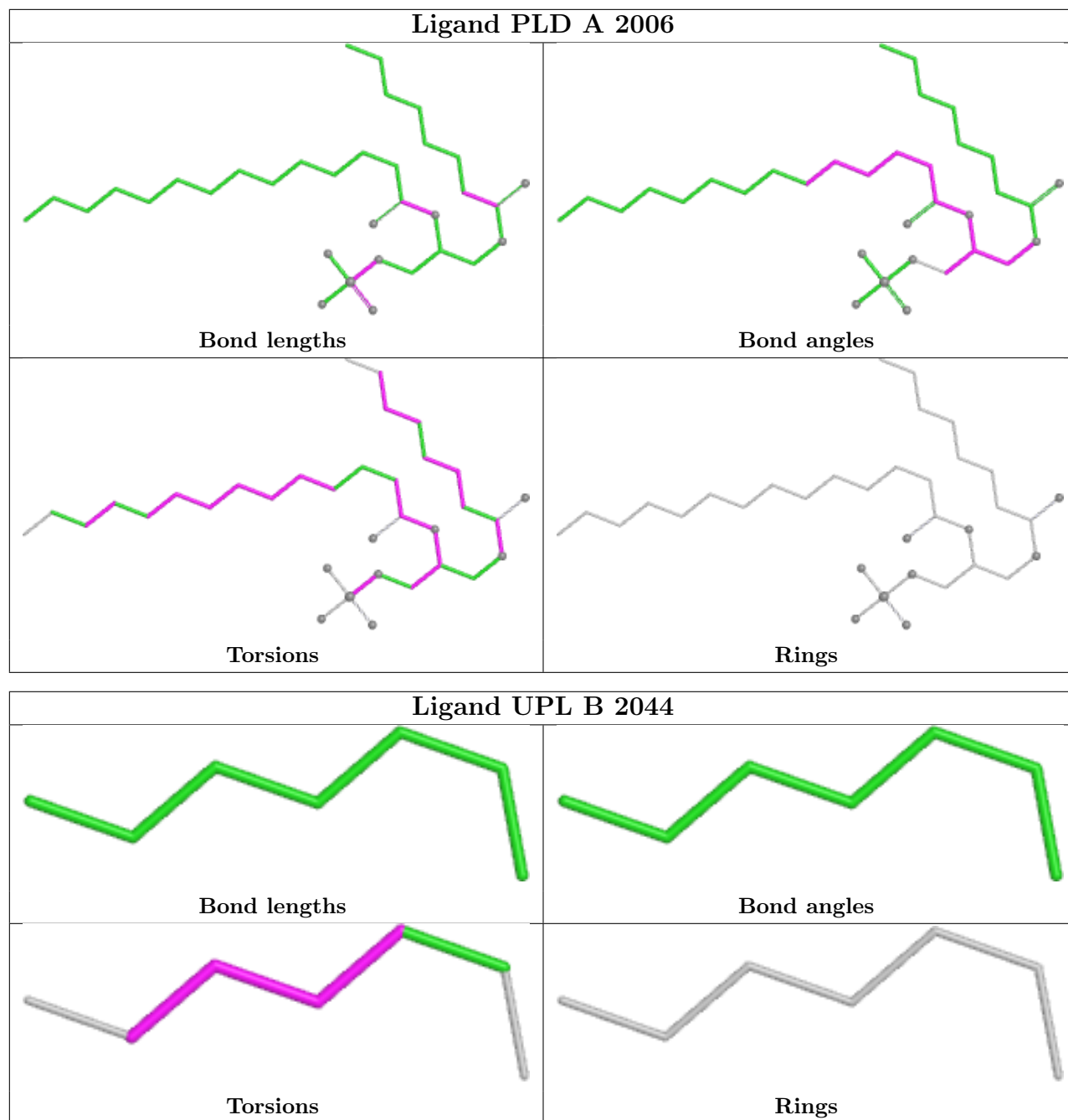


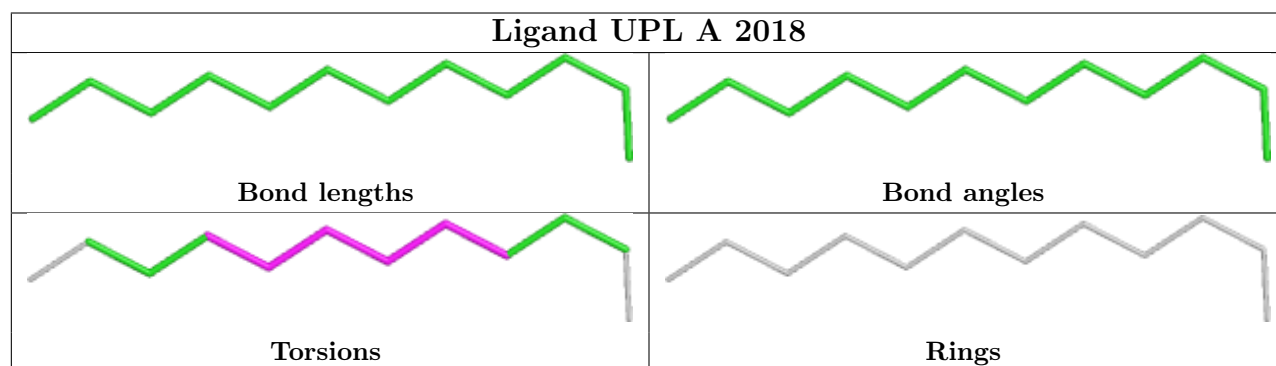
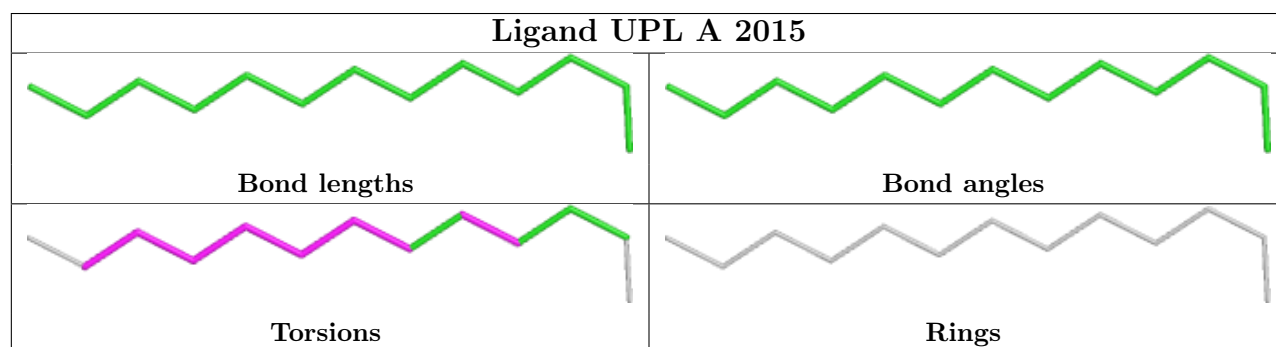
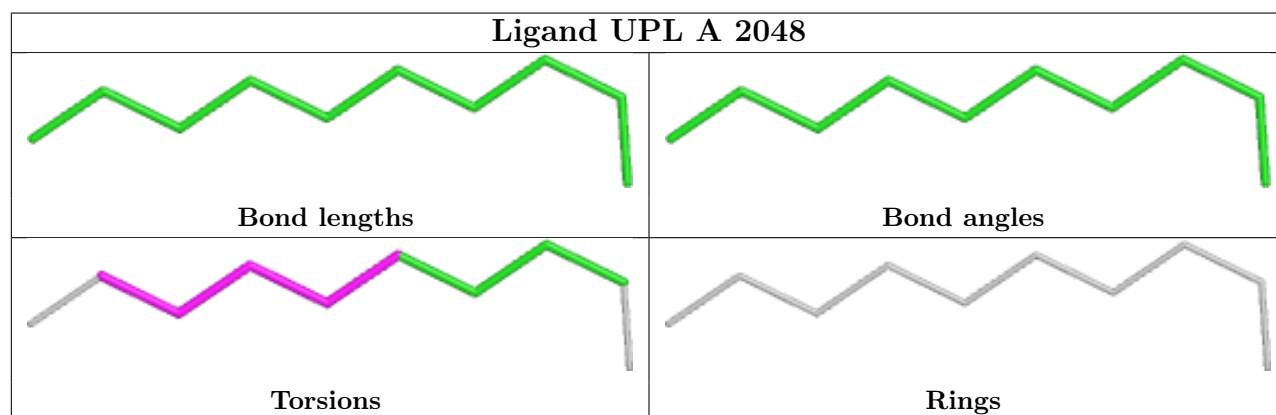
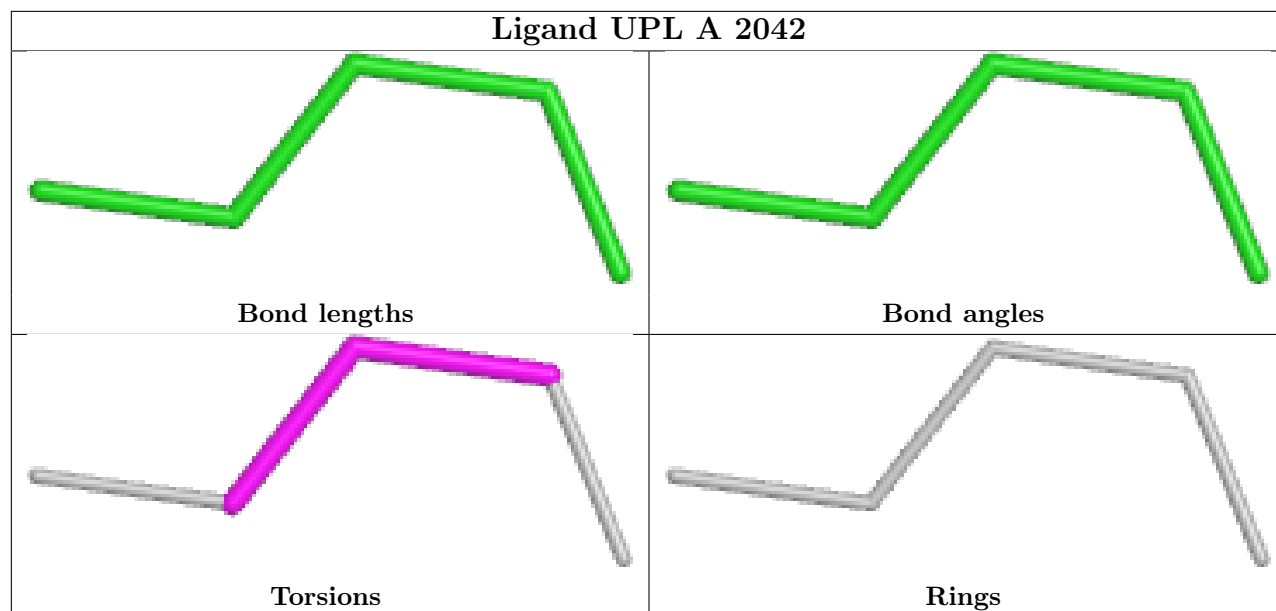


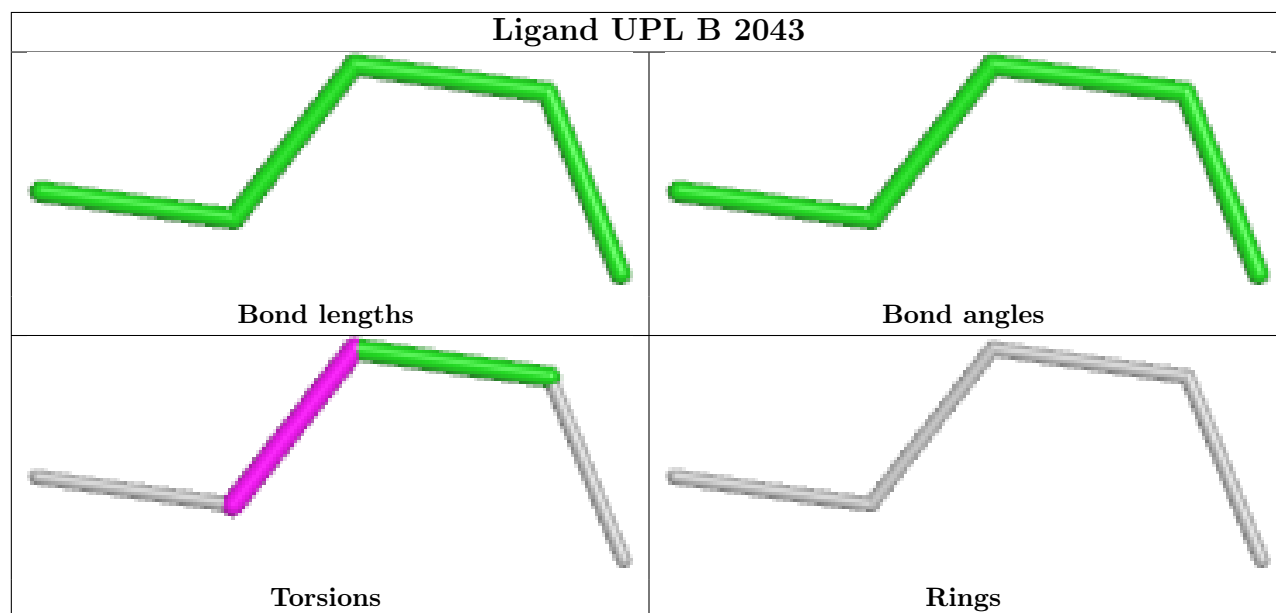
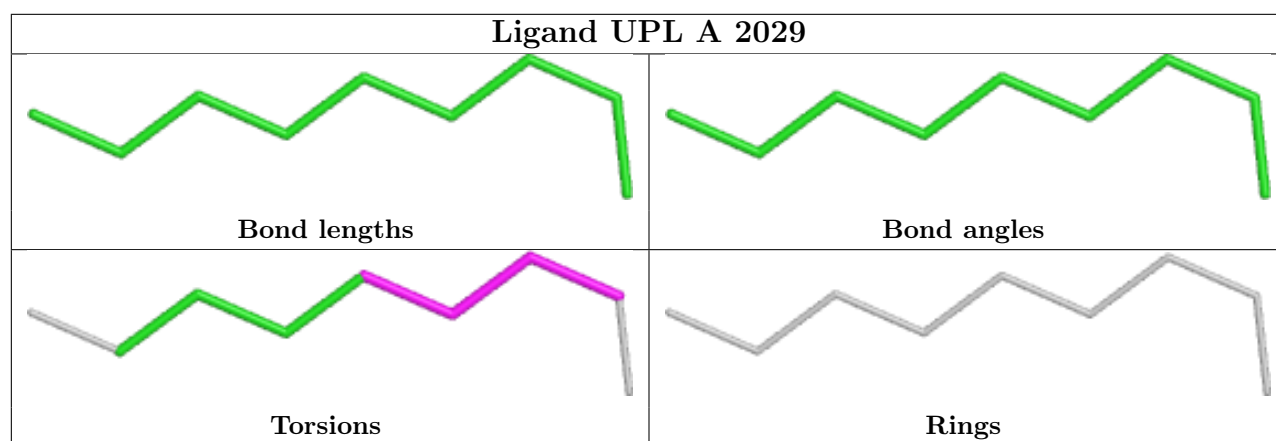
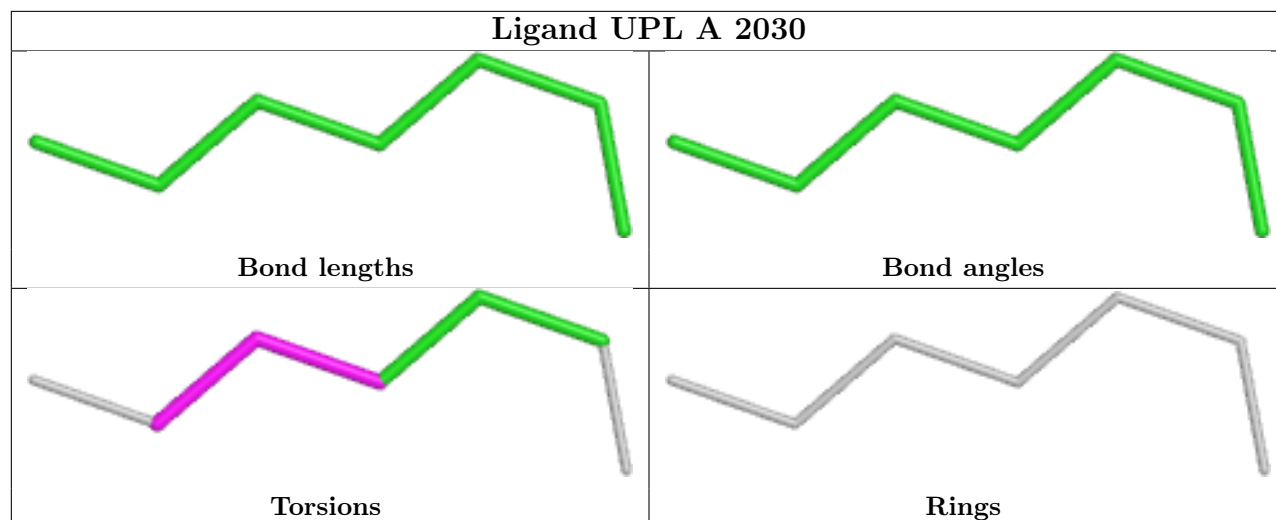


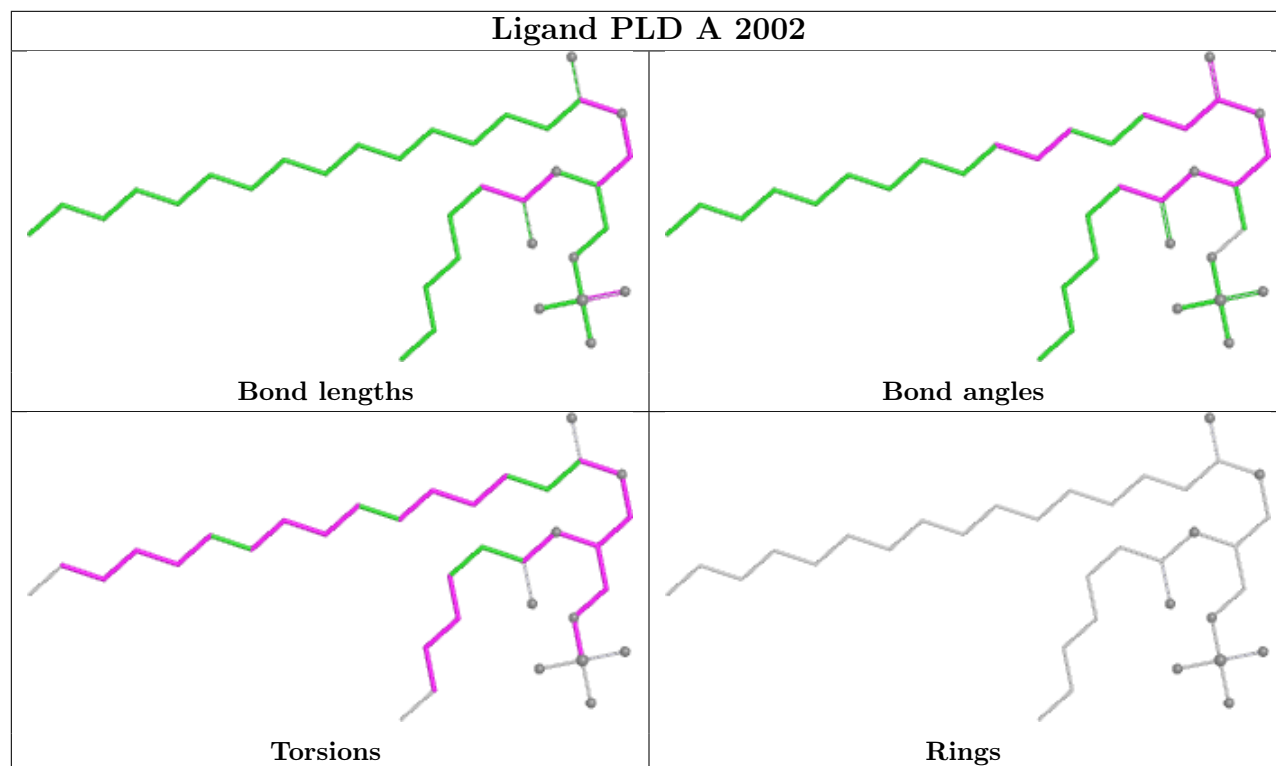
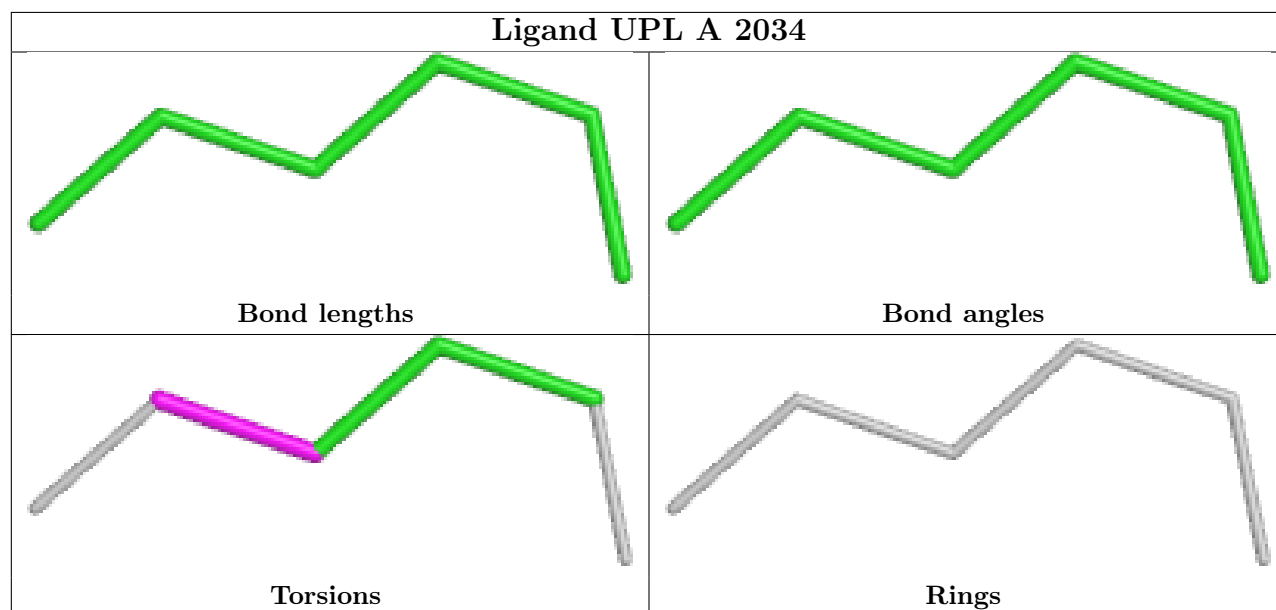
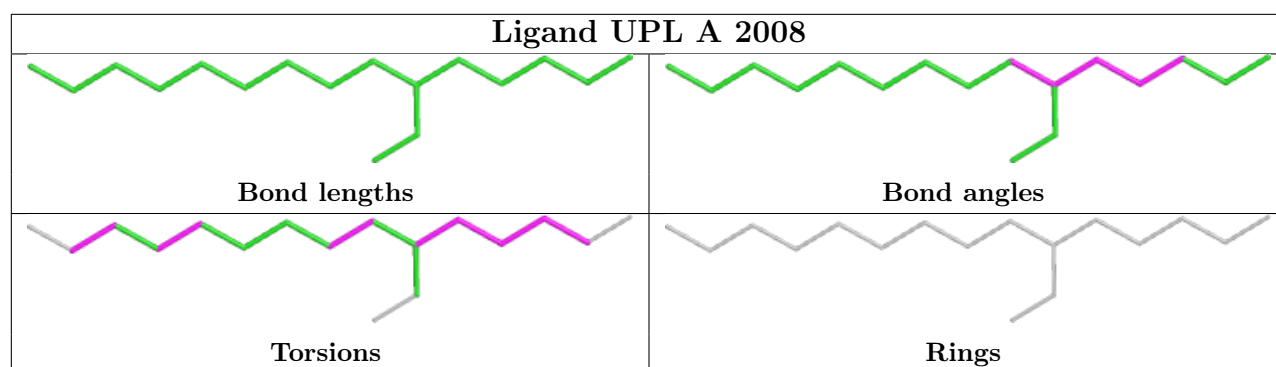


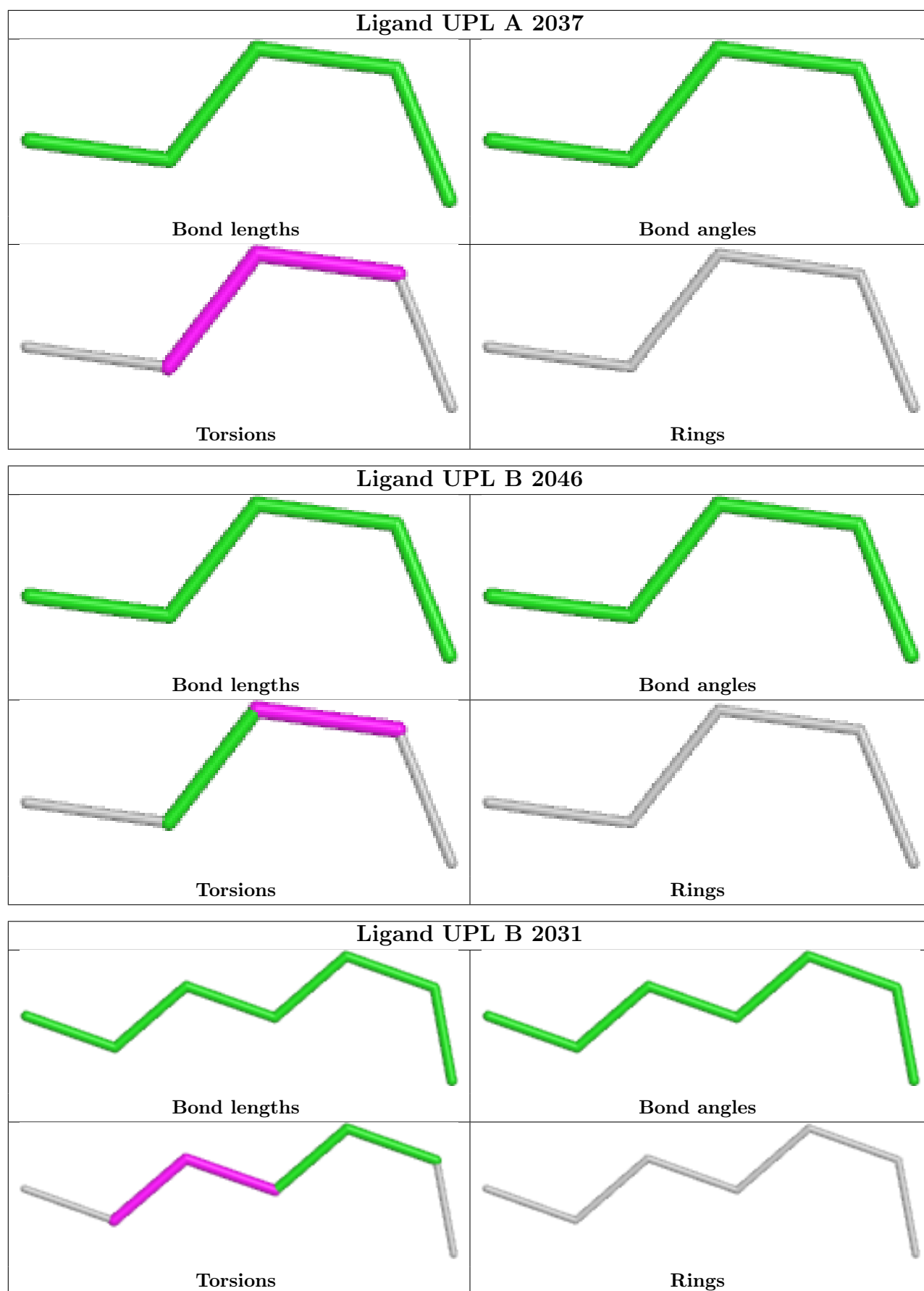


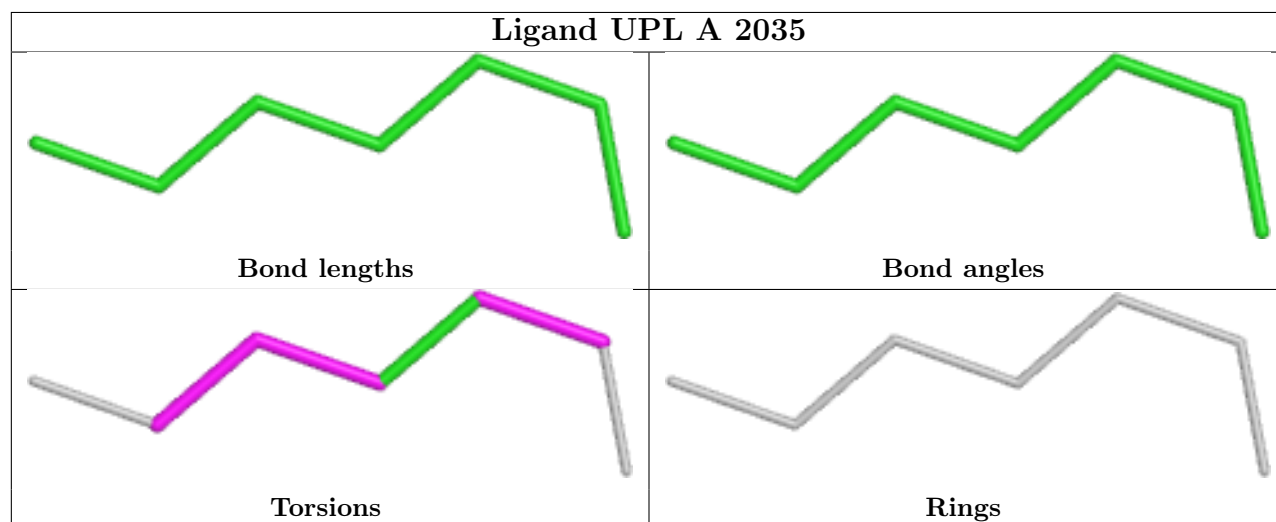
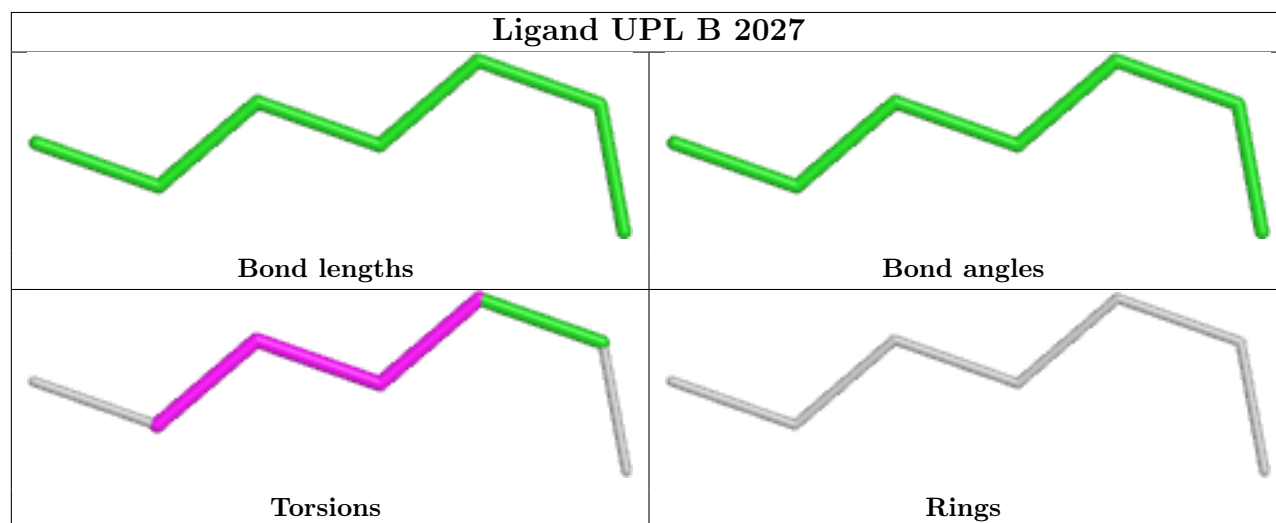
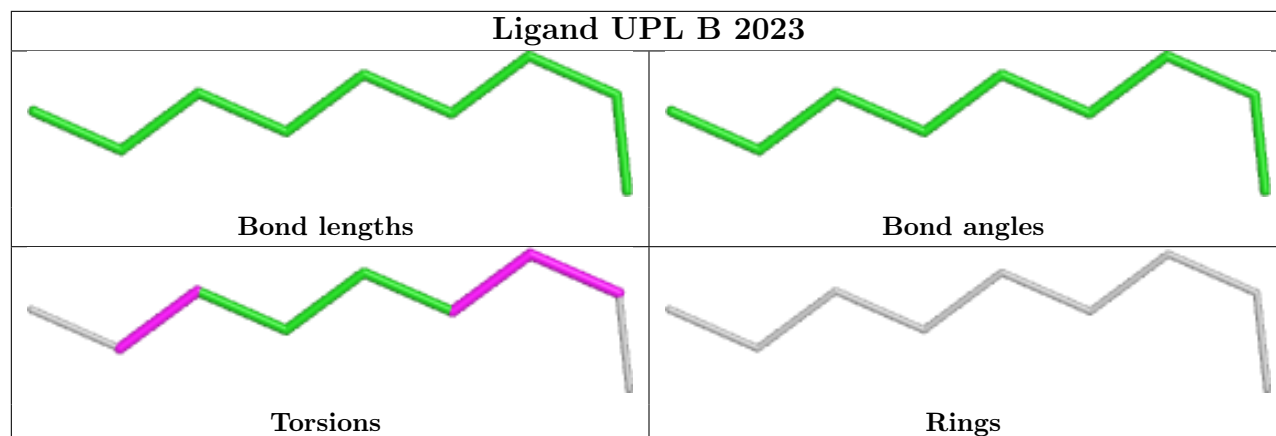


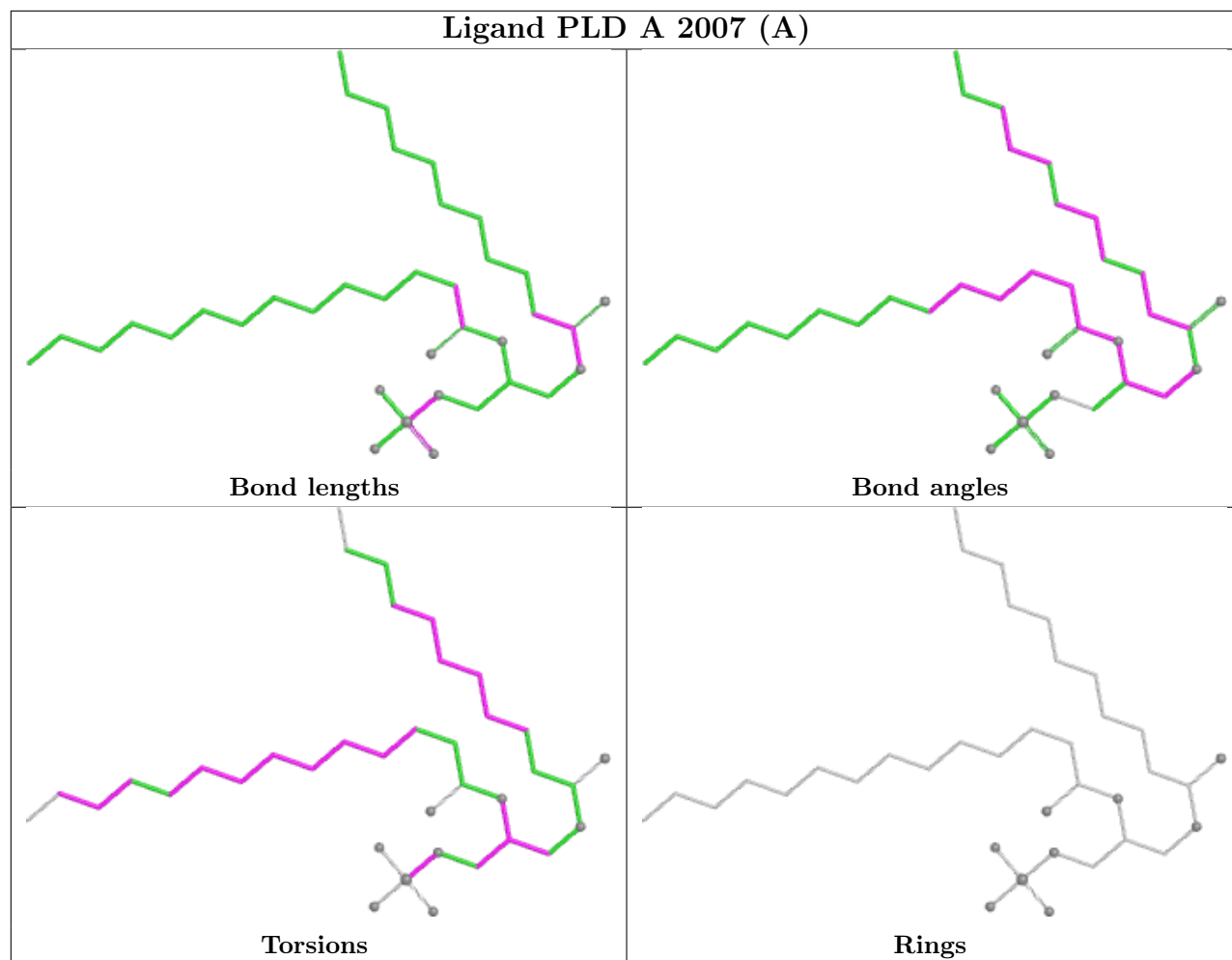












5.7 Other polymers [i](#)

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	954/1056 (90%)	-0.29	6 (0%) 85 87	11, 34, 76, 100	68 (7%)
2	B	174/319 (54%)	0.54	6 (3%) 48 51	33, 66, 96, 100	5 (2%)
All	All	1128/1375 (82%)	-0.16	12 (1%) 78 80	11, 37, 85, 100	73 (6%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1489	ALA	4.2
2	B	1358	PRO	3.0
2	B	1369	ALA	2.8
2	B	1389	LEU	2.3
2	B	1378	THR	2.3
2	B	1443	LEU	2.2
1	A	503	LEU	2.2
1	A	268	SER	2.1
1	A	783	ALA	2.1
1	A	165	GLY	2.1
1	A	688	TYR	2.0
1	A	733	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	A	17	8/9	0.95	0.06	35,44,51,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	UPL	A	2029	9/34	0.72	0.12	89,91,96,97	0
4	UPL	A	2047	5/34	0.73	0.07	84,90,94,95	0
4	UPL	B	2031	7/34	0.73	0.11	81,82,85,85	0
4	UPL	A	2036	6/34	0.74	0.10	87,89,90,91	0
4	UPL	A	2020	6/34	0.74	0.08	70,77,80,82	0
4	UPL	A	2008	17/34	0.74	0.14	86,91,100,100	0
4	UPL	A	2042	5/34	0.75	0.09	68,81,83,84	0
4	UPL	A	2050	6/34	0.76	0.09	88,89,91,91	0
4	UPL	A	2038	6/34	0.77	0.12	81,85,87,92	0
4	UPL	B	2044	7/34	0.78	0.09	75,81,82,82	0
3	PLD	A	2006	34/60	0.79	0.11	62,88,99,100	0
4	UPL	A	2048	10/34	0.79	0.12	77,82,87,89	0
3	PLD	A	2005[A]	46/60	0.79	0.17	31,85,99,100	7
4	UPL	B	2016	13/34	0.79	0.09	71,86,91,95	0
3	PLD	A	2005[B]	46/60	0.79	0.17	31,85,99,100	7
4	UPL	A	2022	6/34	0.79	0.09	87,88,94,94	0
4	UPL	B	2049	6/34	0.79	0.09	90,92,100,100	0
4	UPL	B	2027	7/34	0.80	0.10	81,85,89,90	0
4	UPL	A	2024	6/34	0.80	0.13	75,89,95,95	0
4	UPL	A	2037	5/34	0.80	0.09	52,60,62,69	0
4	UPL	B	2023	9/34	0.80	0.10	52,68,71,72	0
4	UPL	A	2039	5/34	0.82	0.10	58,62,73,78	0
4	UPL	A	2040	5/34	0.82	0.08	56,58,71,71	0
4	UPL	B	2045	5/34	0.82	0.11	73,78,84,85	0
3	PLD	B	2003	31/60	0.82	0.12	63,84,90,93	2
4	UPL	A	2026	8/34	0.83	0.08	43,71,84,85	0
4	UPL	B	2028	7/34	0.83	0.08	87,92,93,93	0
4	UPL	A	2009	15/34	0.85	0.10	55,68,78,85	0
4	UPL	A	2013	16/34	0.85	0.10	75,85,90,91	0
3	PLD	A	2007[A]	37/60	0.85	0.11	51,92,100,100	3
3	PLD	A	2007[B]	37/60	0.85	0.11	51,92,100,100	3
4	UPL	A	2015	13/34	0.86	0.10	75,80,89,92	0

Continued on next page...

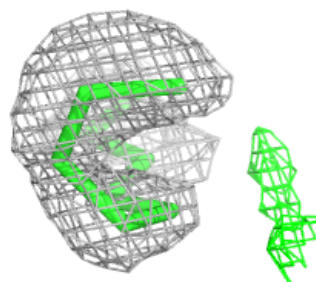
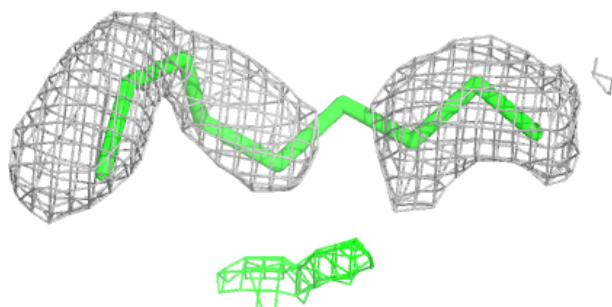
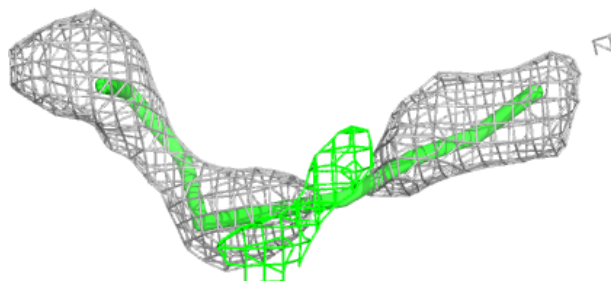
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UPL	A	2017	11/34	0.86	0.10	44,67,94,97	0
4	UPL	B	2010	14/34	0.87	0.09	62,78,81,85	0
4	UPL	A	2034	6/34	0.87	0.11	59,62,65,65	0
4	UPL	A	2041	5/34	0.87	0.11	87,90,95,96	0
4	UPL	A	2018	12/34	0.88	0.09	60,73,81,82	0
4	UPL	A	2035	7/34	0.88	0.10	55,78,94,95	0
4	UPL	B	2033	6/34	0.88	0.10	78,83,87,89	0
4	UPL	B	2043	5/34	0.88	0.09	78,81,82,84	0
4	UPL	B	2021	9/34	0.88	0.09	63,75,79,82	0
3	PLD	A	2002	35/60	0.88	0.12	49,79,90,94	0
4	UPL	A	2032	6/34	0.88	0.09	77,82,88,91	0
4	UPL	A	2011	19/34	0.89	0.09	41,68,85,87	0
4	UPL	A	2030	7/34	0.89	0.08	37,58,72,73	0
4	UPL	B	2046	5/34	0.89	0.10	75,80,82,84	0
4	UPL	A	2012	17/34	0.89	0.07	68,77,89,90	0
4	UPL	A	2025	8/34	0.90	0.11	73,77,79,84	0
4	UPL	A	2019	10/34	0.90	0.10	66,75,81,86	0
3	PLD	A	2004	34/60	0.91	0.09	53,69,86,87	0
3	PLD	A	2001[A]	53/60	0.95	0.09	27,44,74,83	4
4	UPL	A	2014	16/34	0.95	0.06	36,46,57,60	0
3	PLD	A	2001[B]	53/60	0.95	0.09	24,43,74,83	4

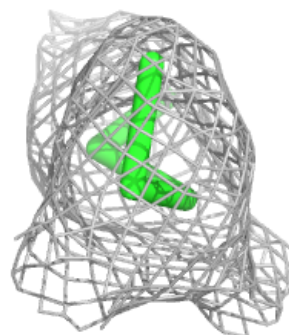
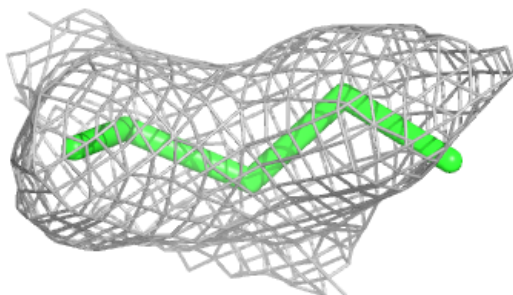
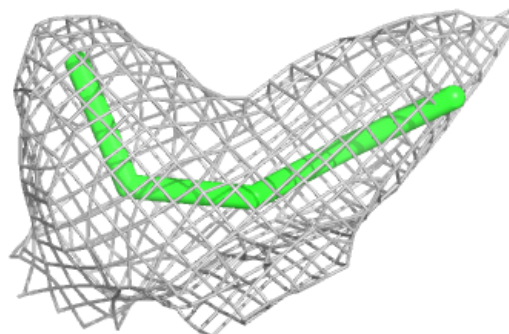
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UPL A 2029:

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

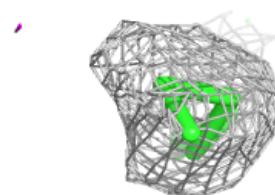
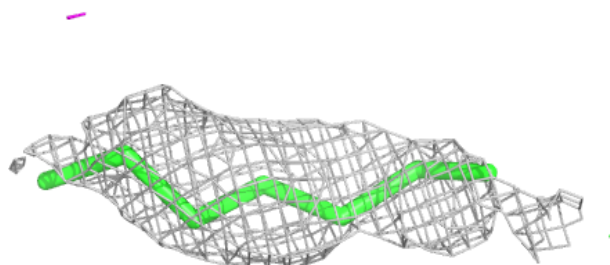
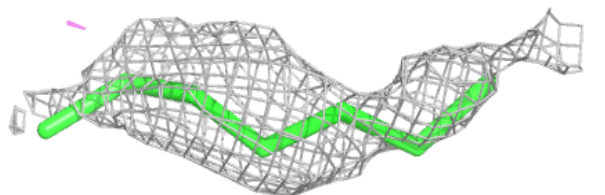
**Electron density around UPL A 2047:**

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

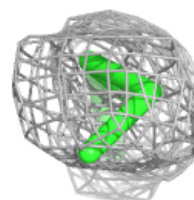
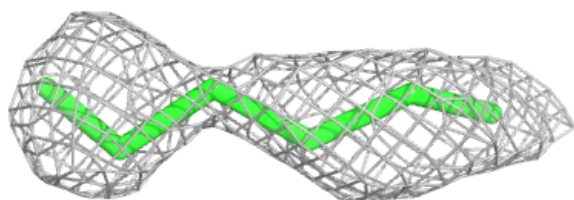
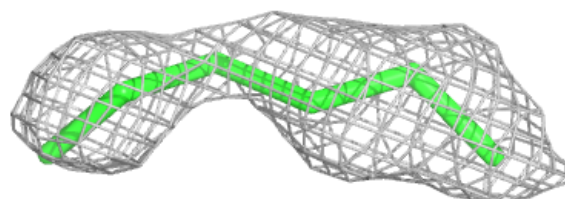


Electron density around UPL B 2031:

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

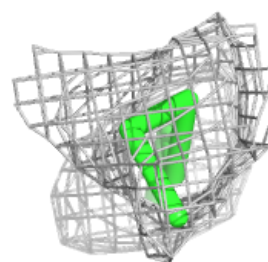
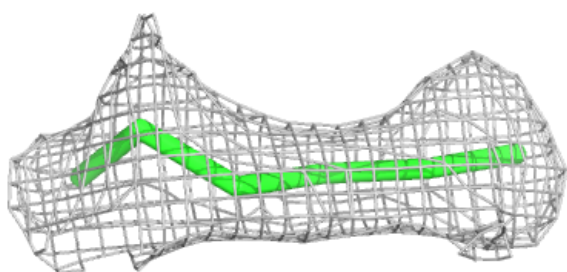
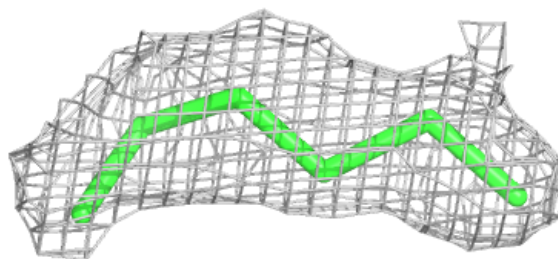
**Electron density around UPL A 2036:**

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

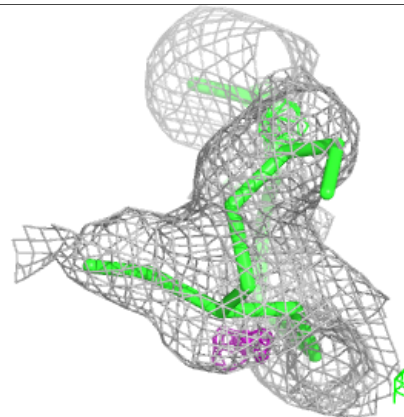
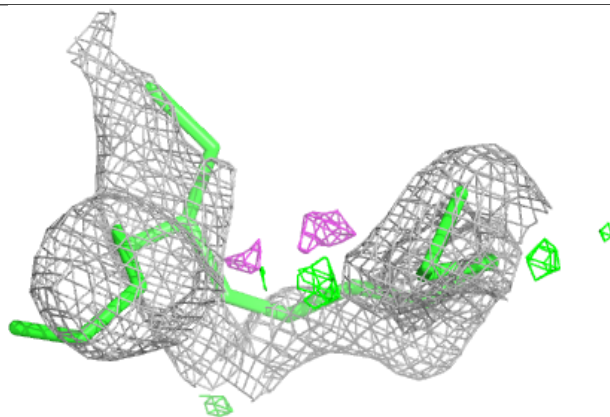
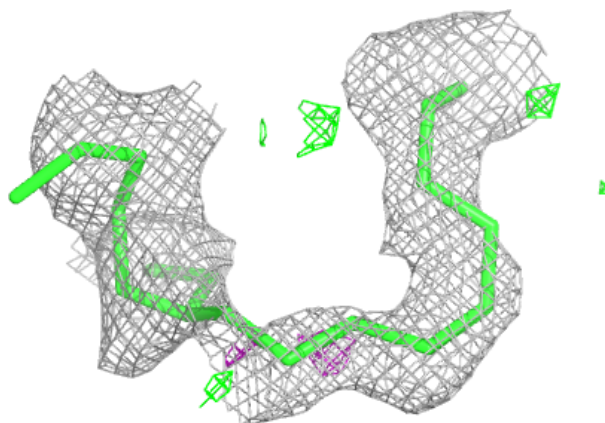


Electron density around UPL A 2020:

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

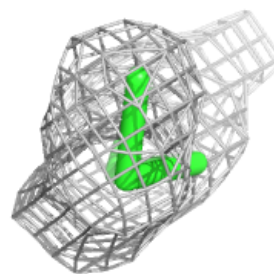
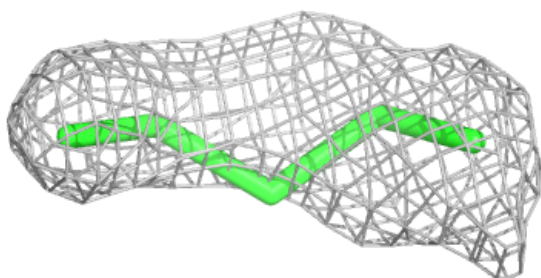
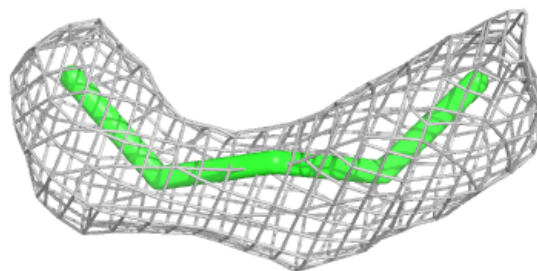
**Electron density around UPL A 2008:**

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

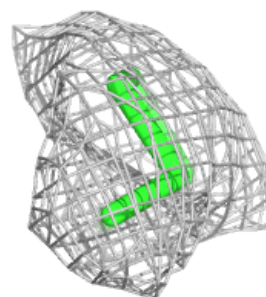
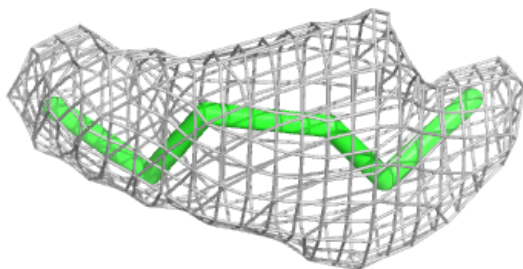
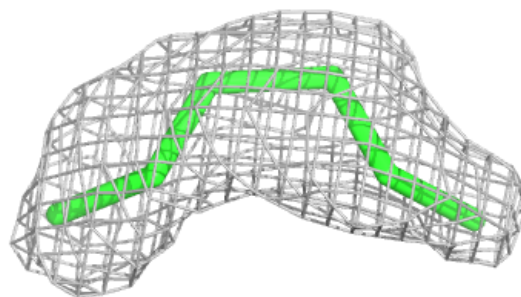


Electron density around UPL A 2042:

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

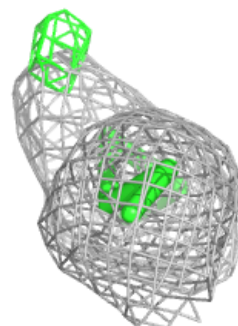
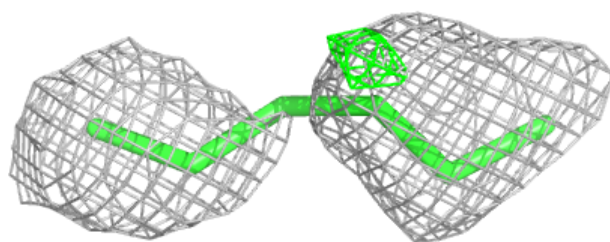
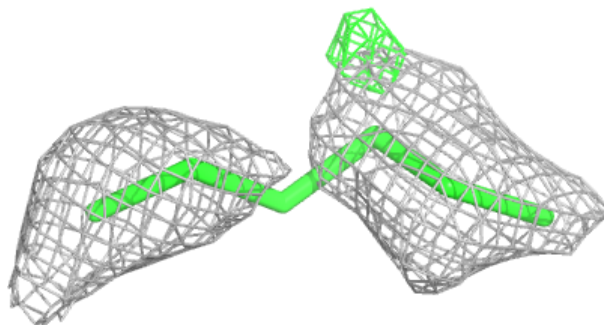
**Electron density around UPL A 2050:**

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

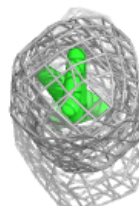
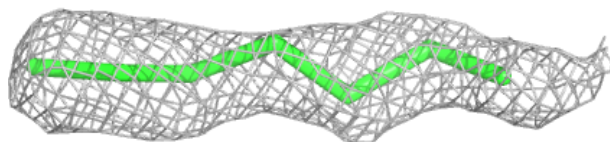
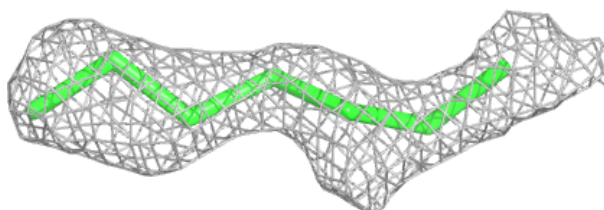


Electron density around UPL A 2038:

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

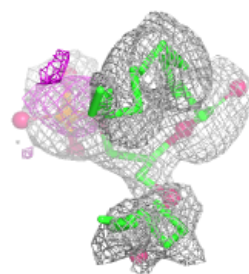
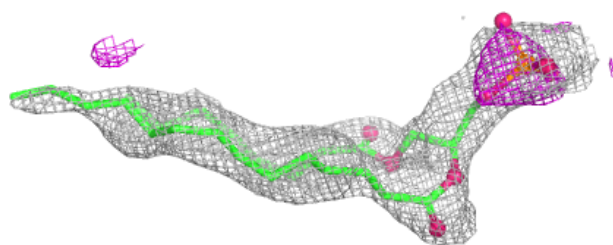
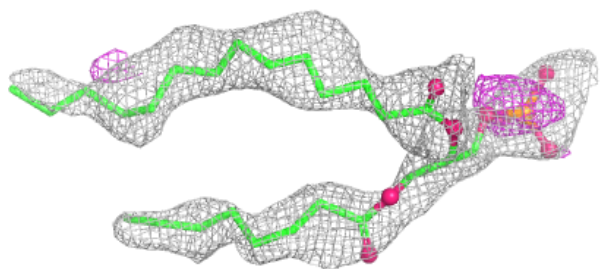
**Electron density around UPL B 2044:**

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

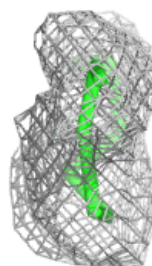
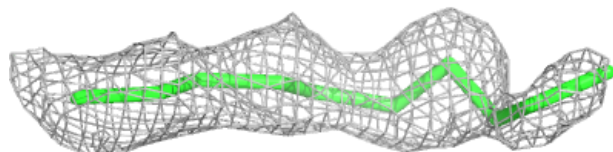
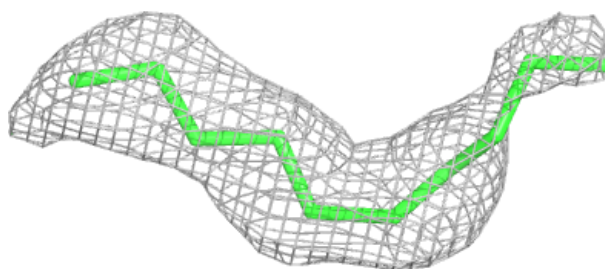


Electron density around PLD A 2006:

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

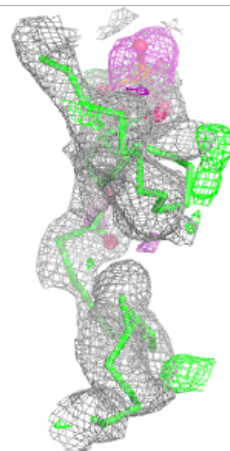
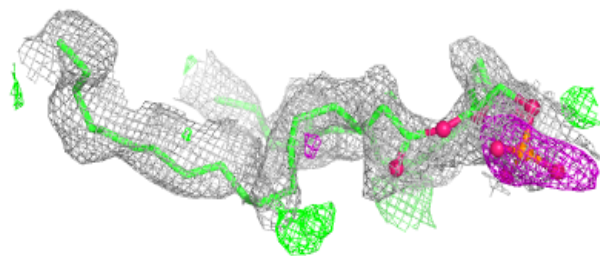
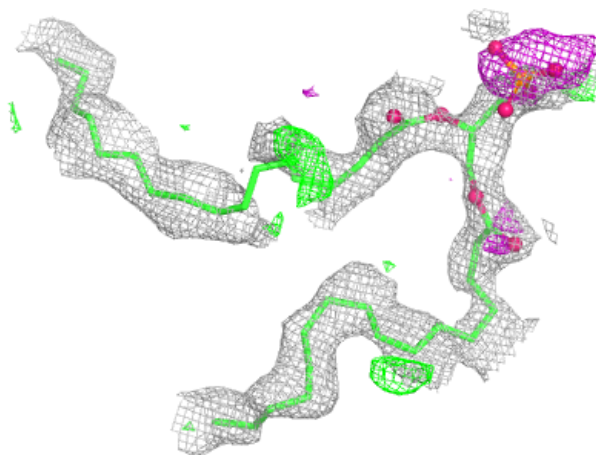
**Electron density around UPL A 2048:**

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



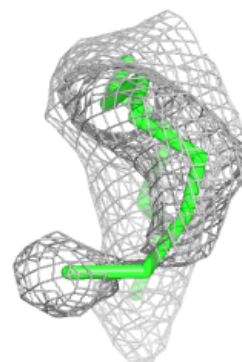
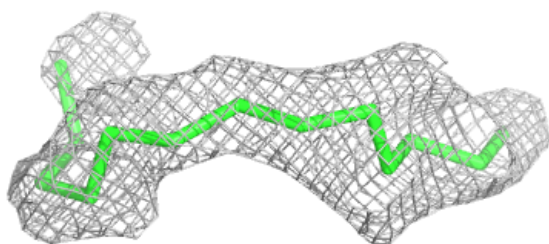
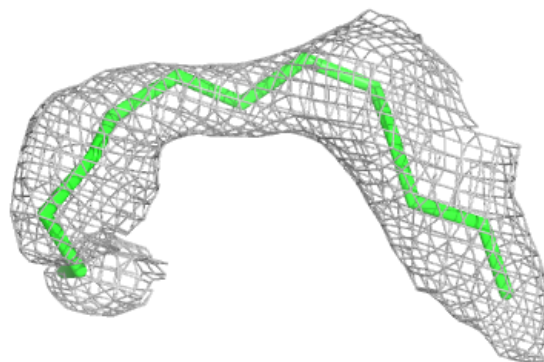
Electron density around PLD A 2005 (A):

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



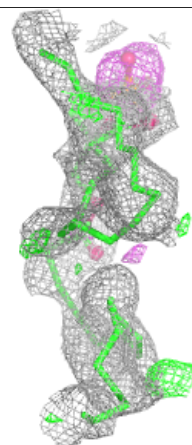
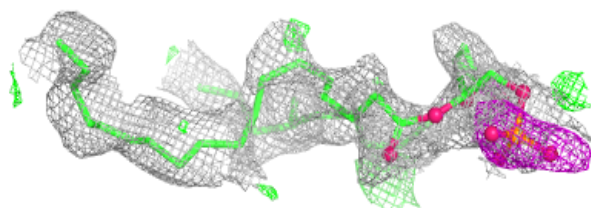
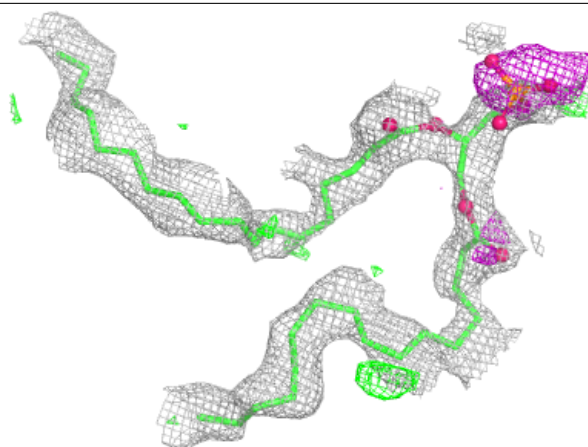
Electron density around UPL B 2016:

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



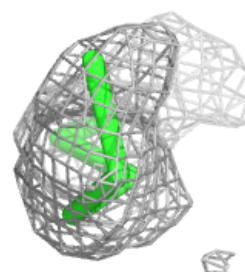
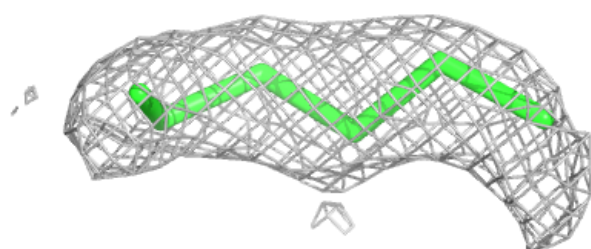
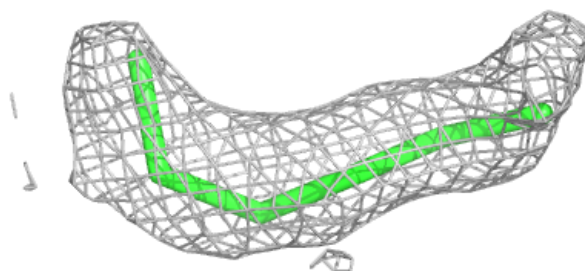
Electron density around PLD A 2005 (B):

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

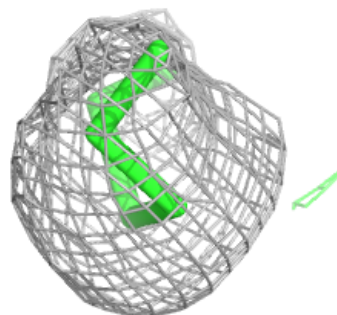
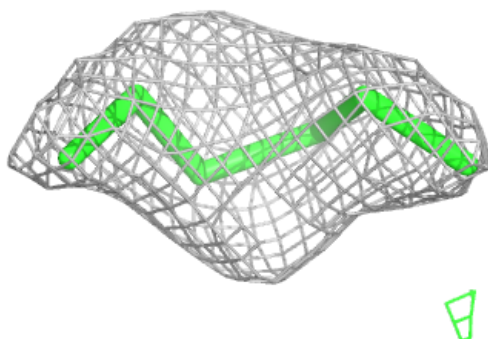
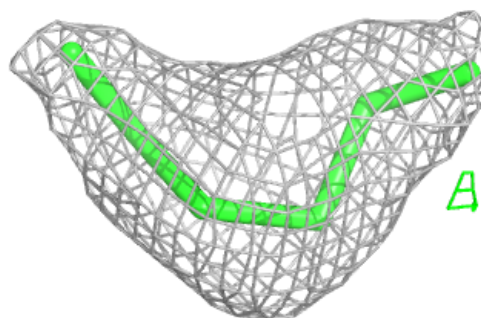


Electron density around UPL A 2022:

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

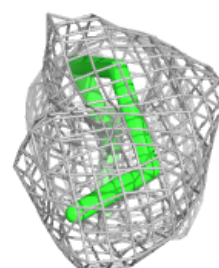
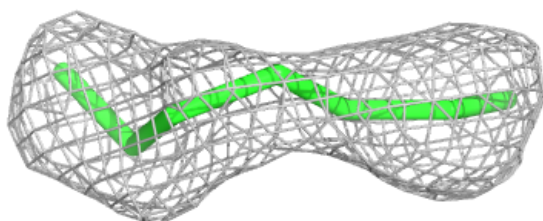
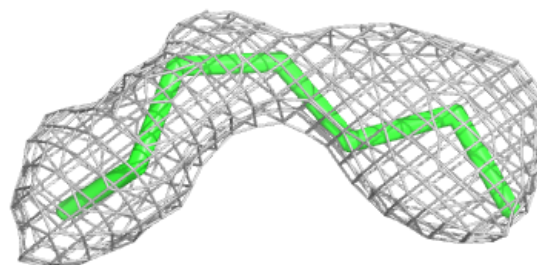
**Electron density around UPL B 2049:**

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

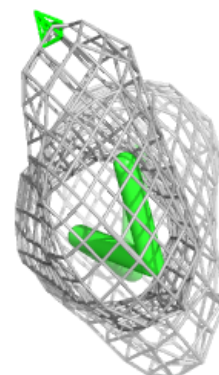
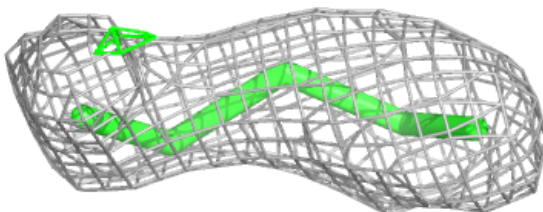
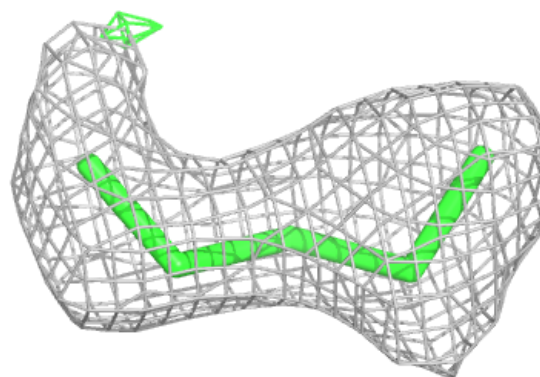


Electron density around UPL B 2027:

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

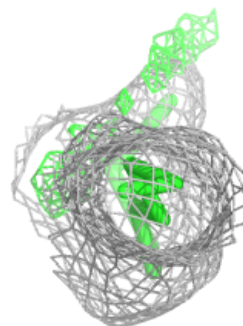
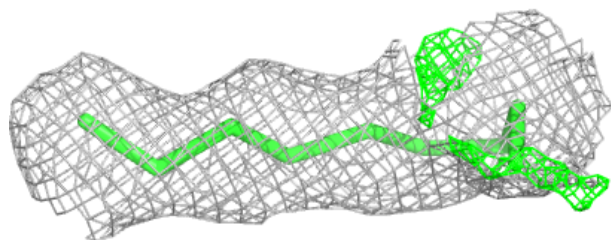
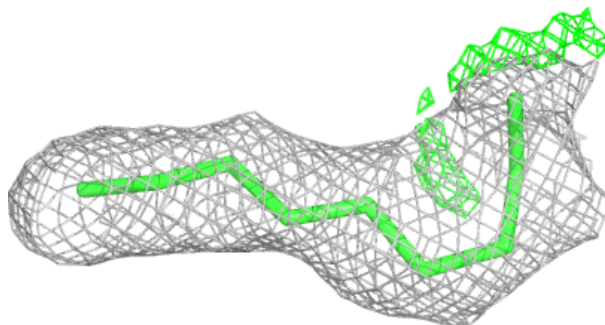
**Electron density around UPL A 2037:**

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



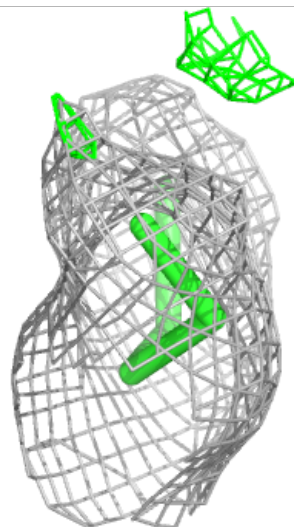
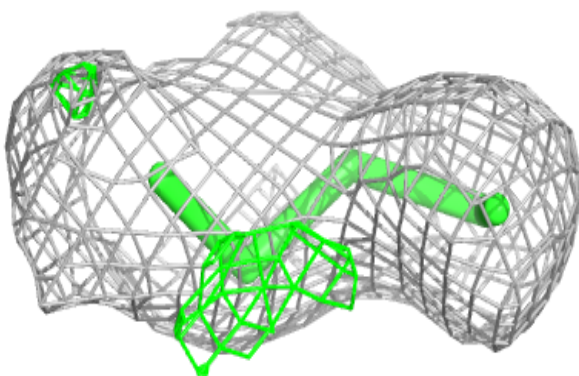
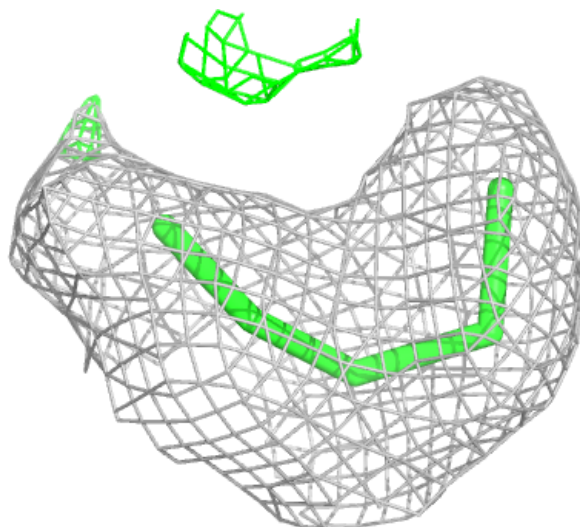
Electron density around UPL B 2023:

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



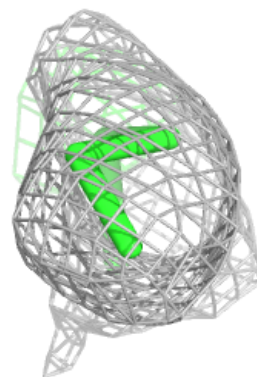
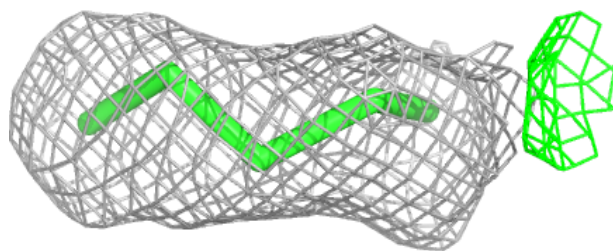
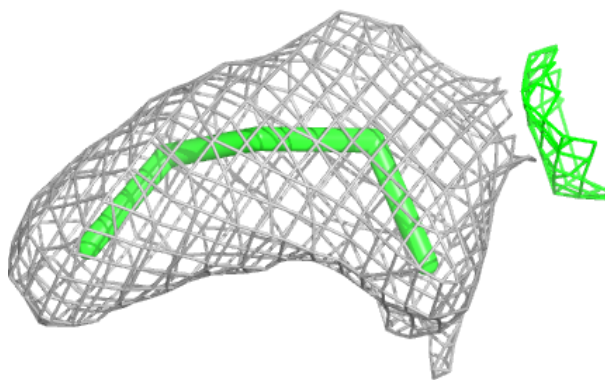
Electron density around UPL A 2039:

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

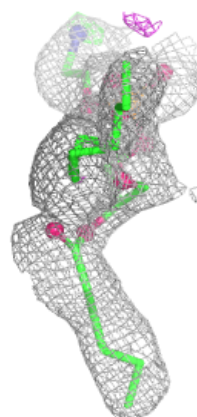
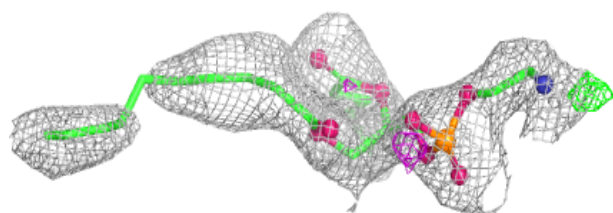
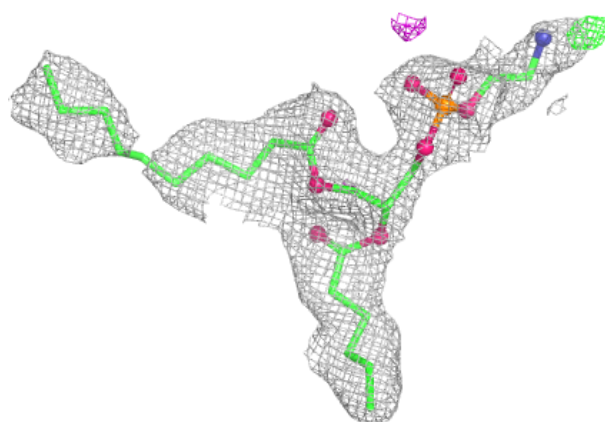


Electron density around UPL B 2045:

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

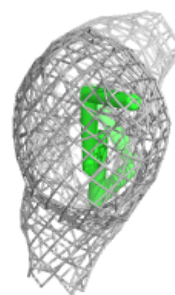
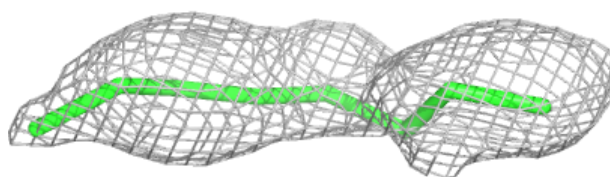
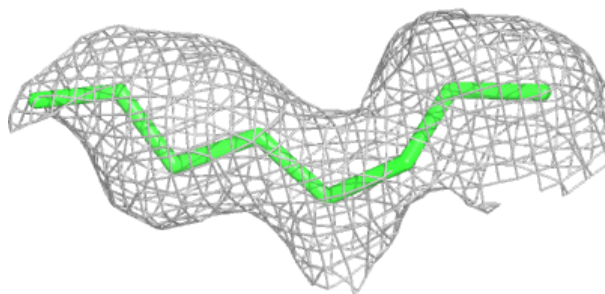
**Electron density around PLD B 2003:**

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

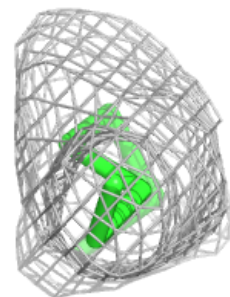
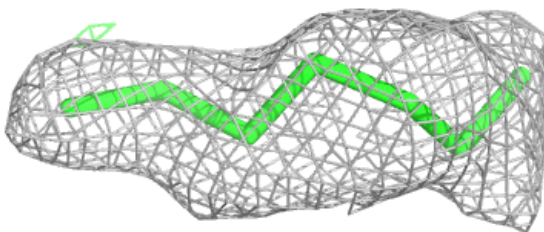
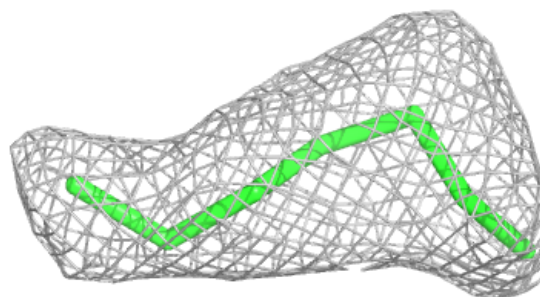


Electron density around UPL A 2026:

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

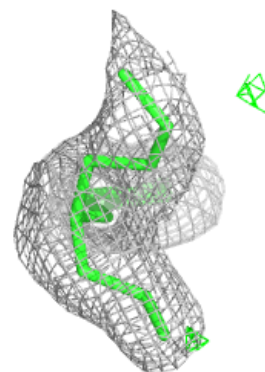
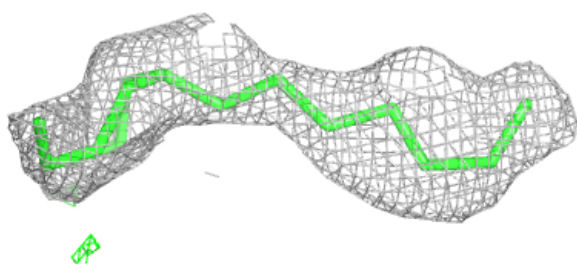
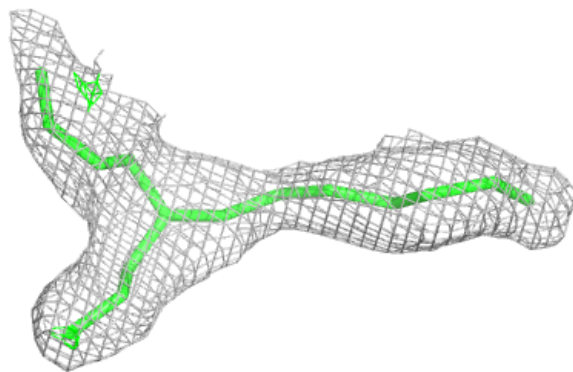
**Electron density around UPL B 2028:**

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

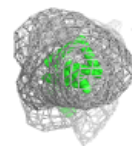
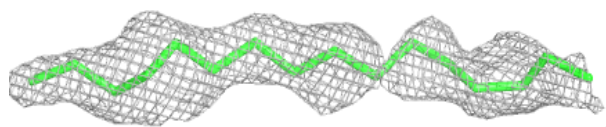
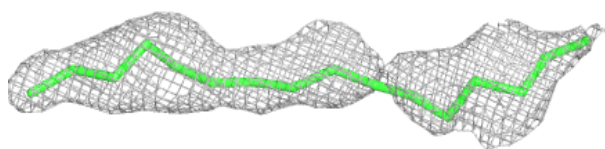


Electron density around UPL A 2009:

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

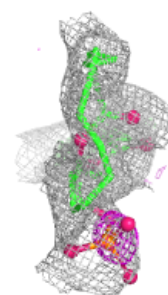
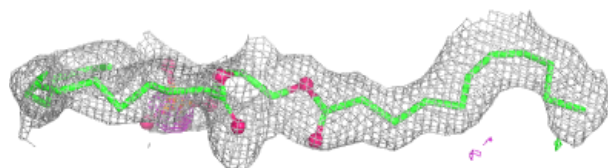
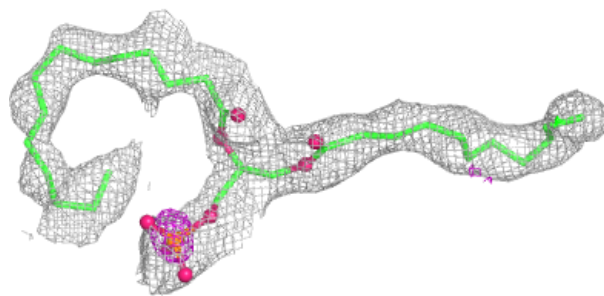
**Electron density around UPL A 2013:**

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

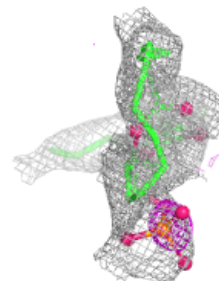
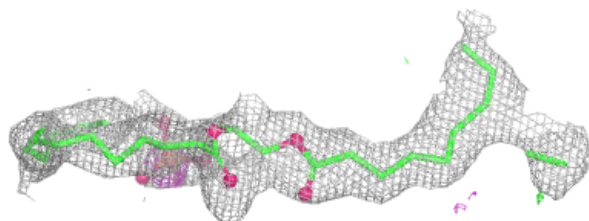
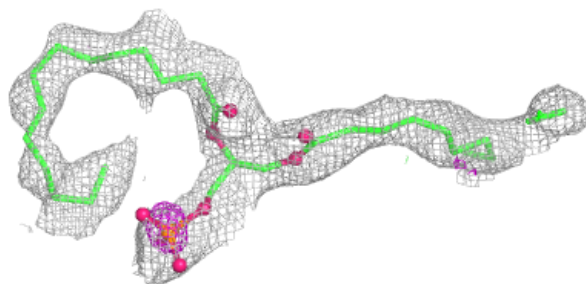


Electron density around PLD A 2007 (A):

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

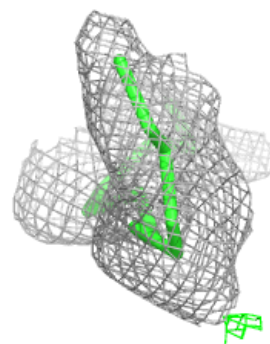
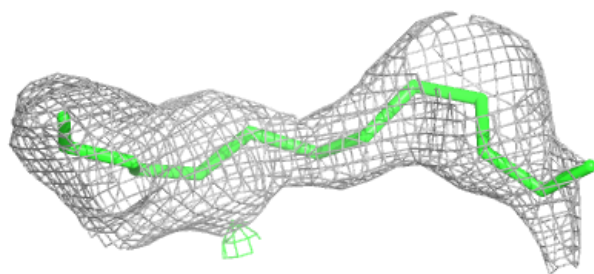
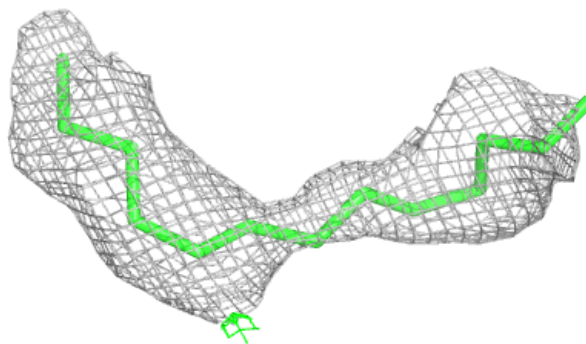
**Electron density around PLD A 2007 (B):**

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

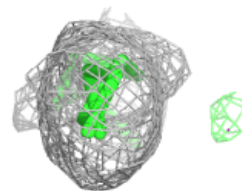
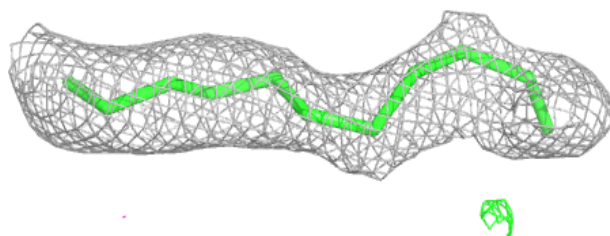
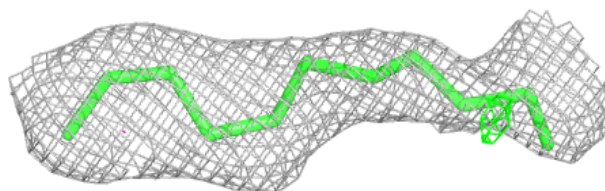


Electron density around UPL A 2015:

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

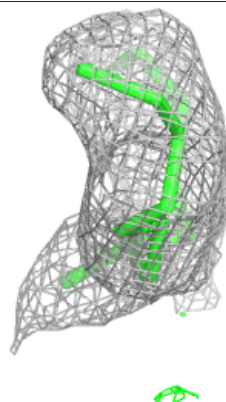
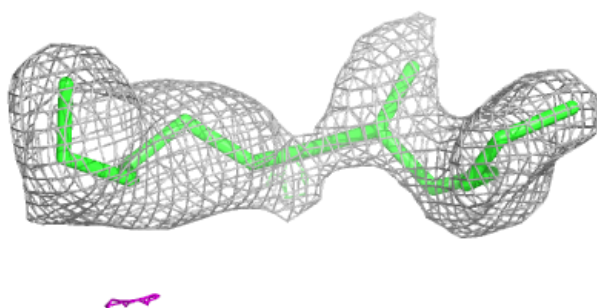
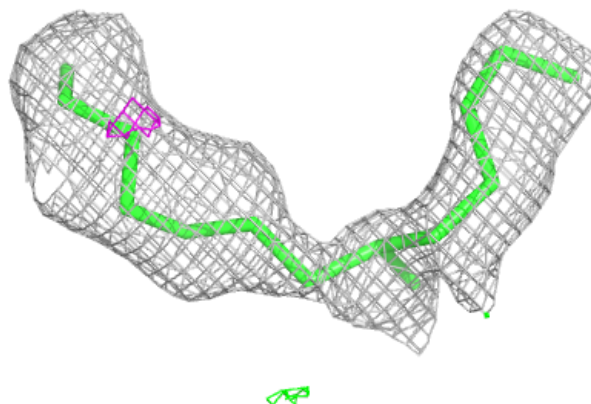
**Electron density around UPL A 2017:**

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

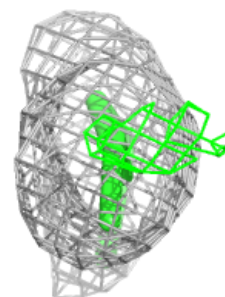
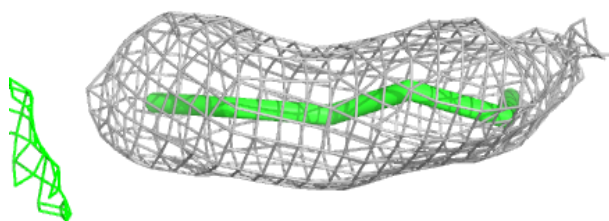
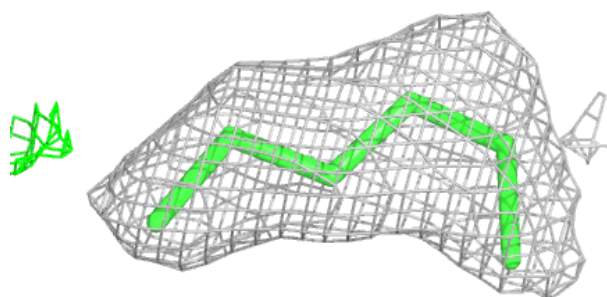


Electron density around UPL B 2010:

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

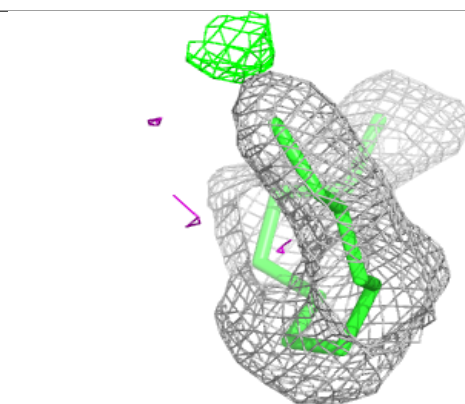
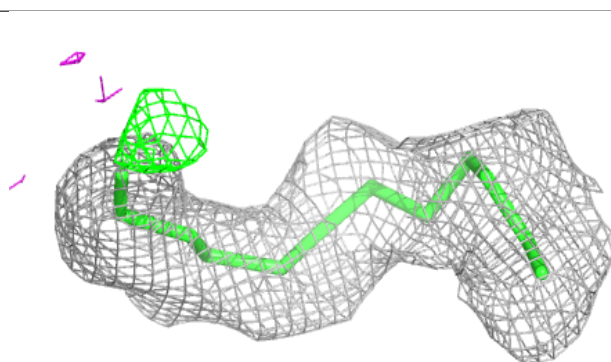
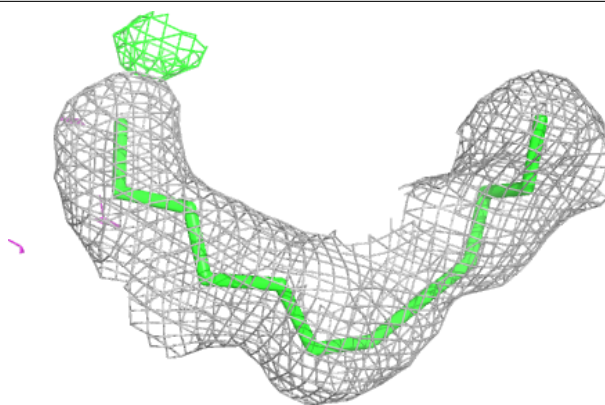
**Electron density around UPL A 2034:**

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

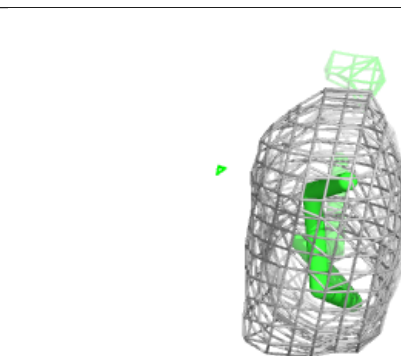
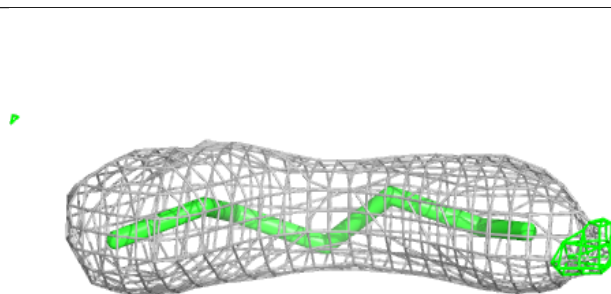
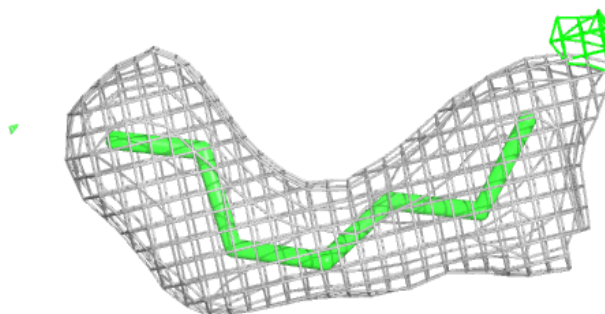


Electron density around UPL A 2018:

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

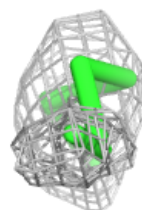
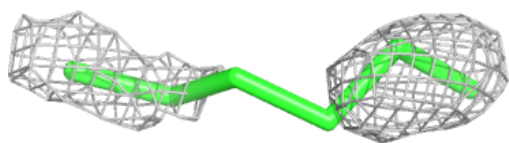
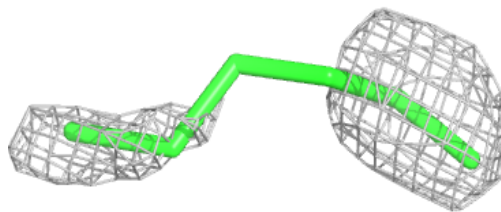
**Electron density around UPL A 2035:**

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

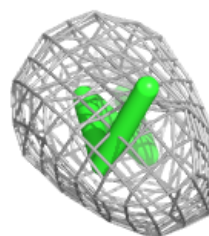
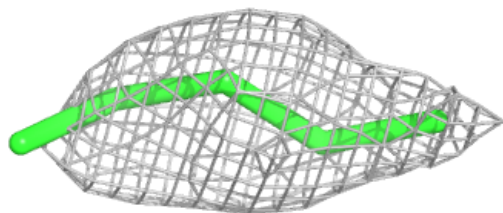
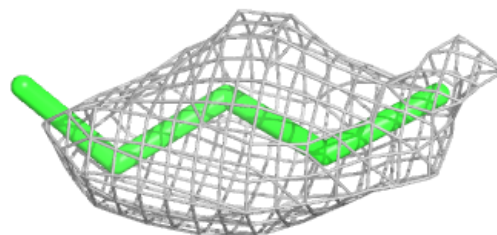


Electron density around UPL B 2033:

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

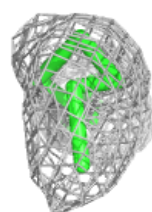
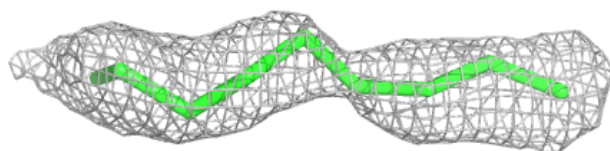
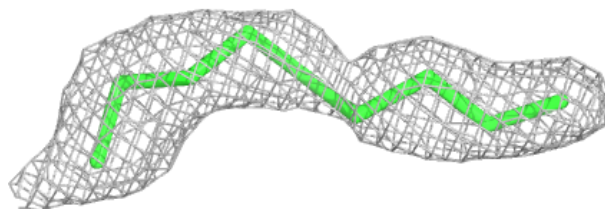
**Electron density around UPL B 2043:**

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

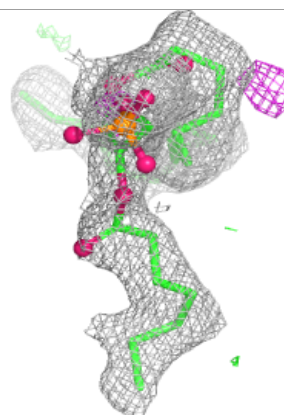
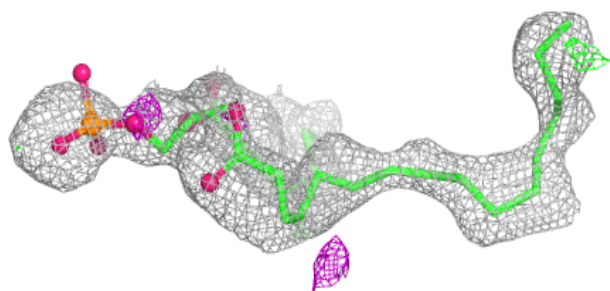
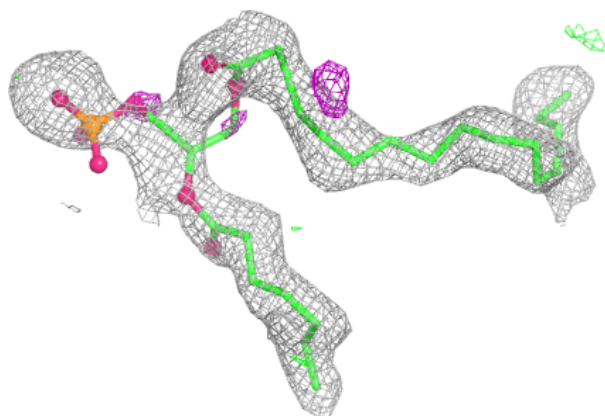


Electron density around UPL B 2021:

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

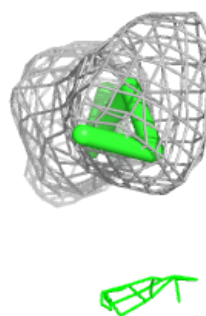
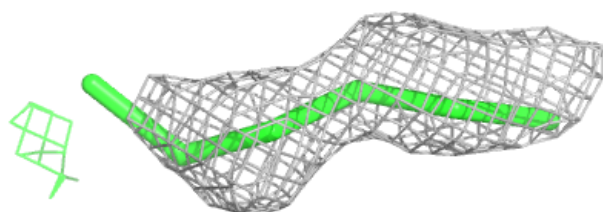
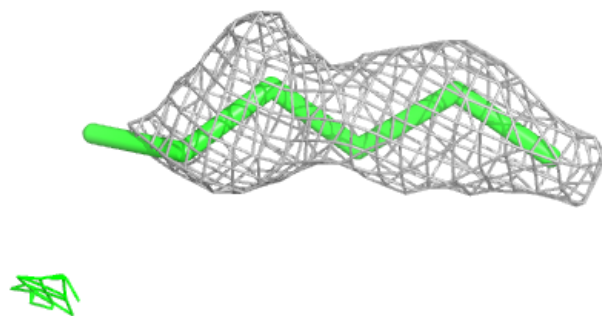
**Electron density around PLD A 2002:**

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

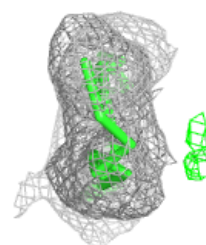
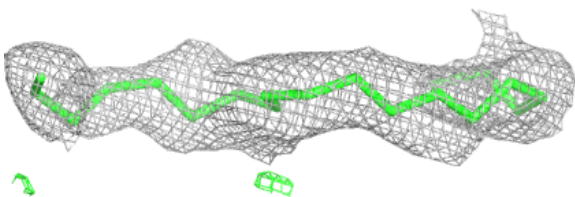
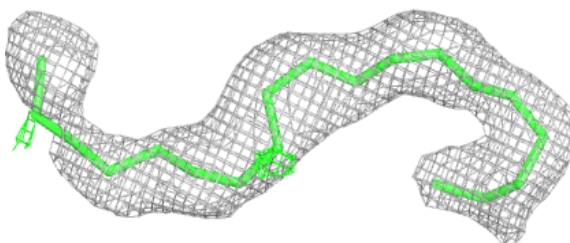


Electron density around UPL A 2032:

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

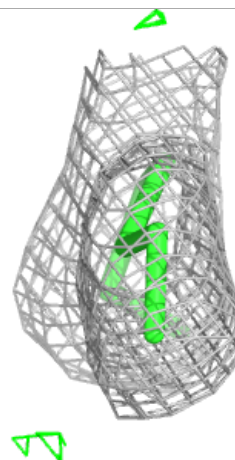
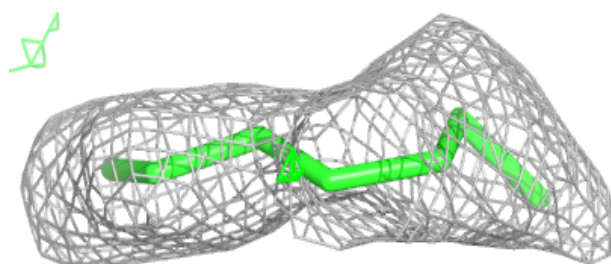
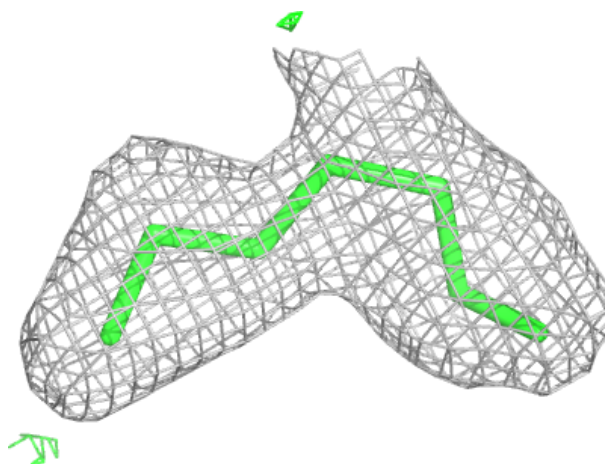
**Electron density around UPL A 2011:**

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



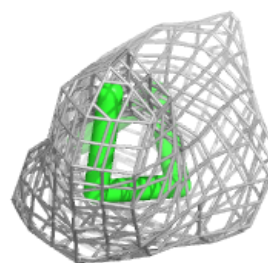
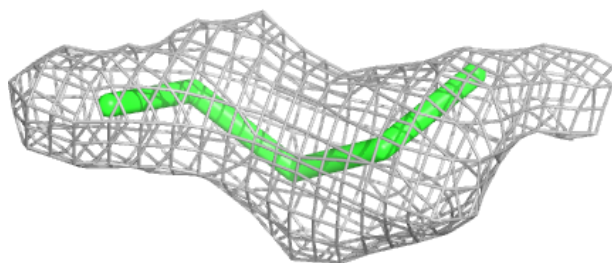
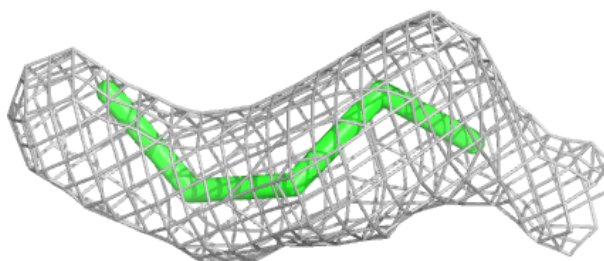
Electron density around UPL A 2030:

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

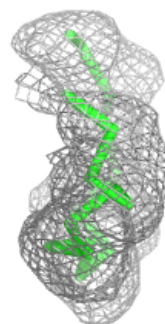
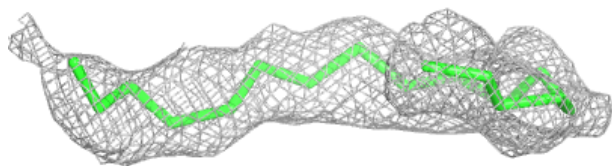
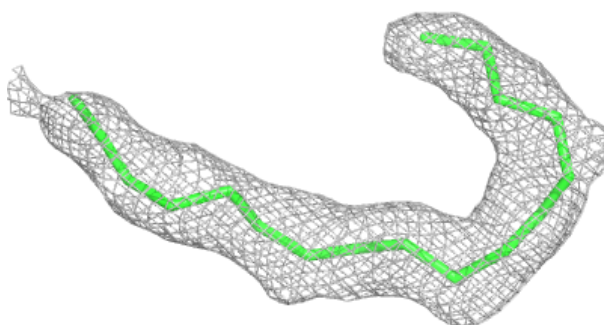


Electron density around UPL B 2046:

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

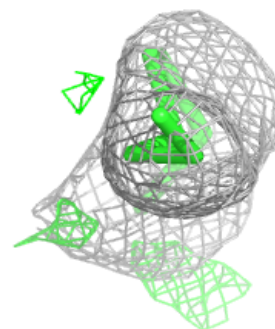
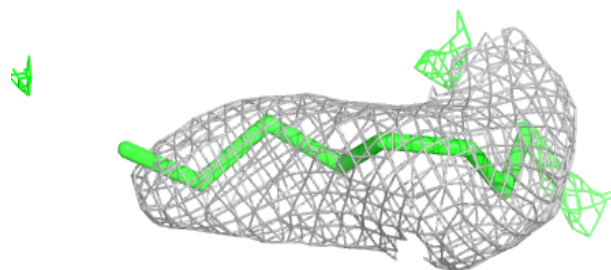
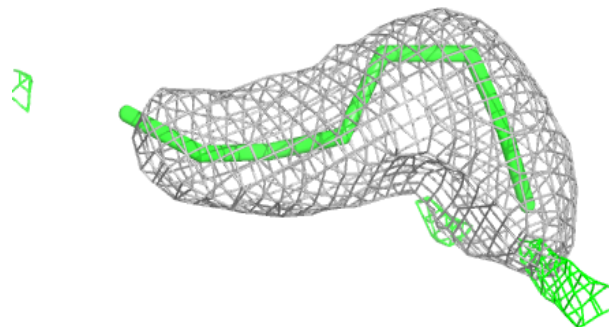
**Electron density around UPL A 2012:**

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

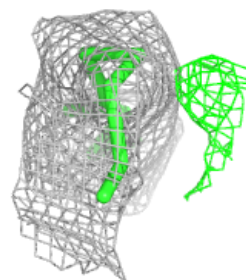
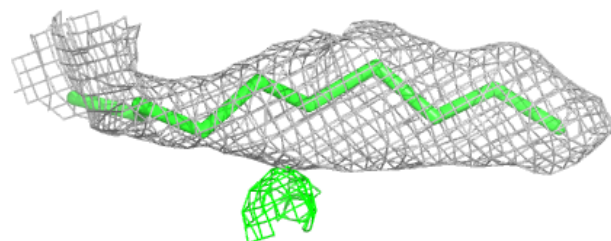
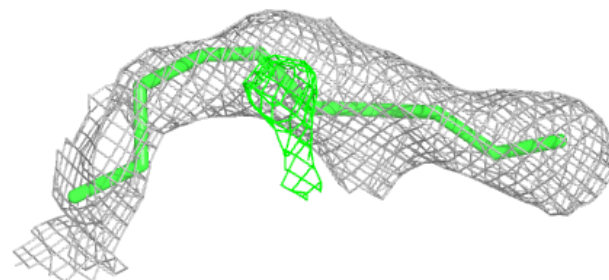


Electron density around UPL A 2025:

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

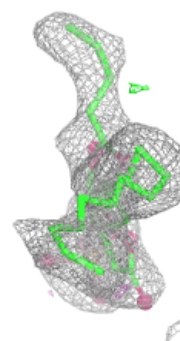
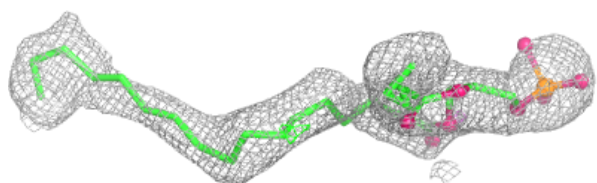
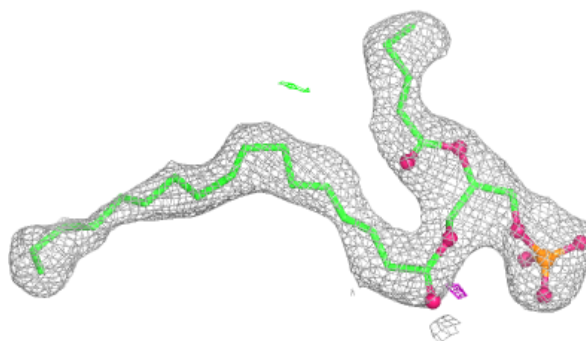
**Electron density around UPL A 2019:**

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

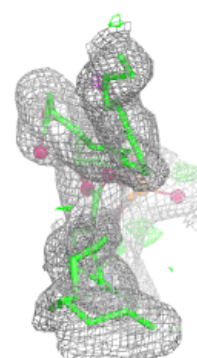
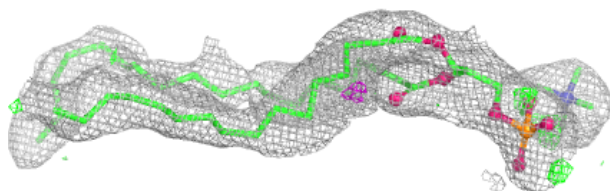
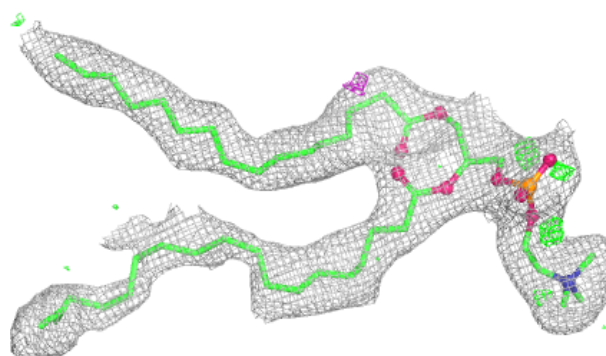


Electron density around PLD A 2004:

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

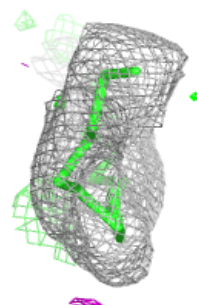
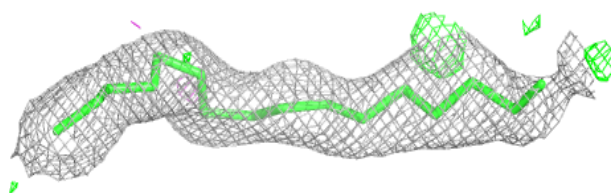
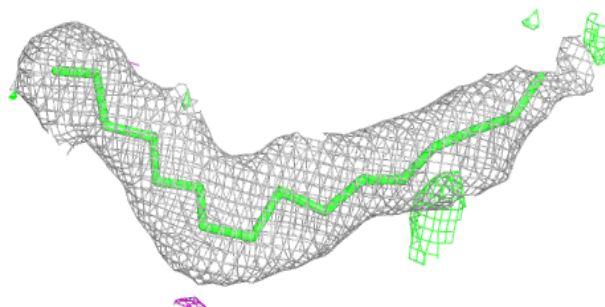
**Electron density around PLD A 2001 (A):**

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

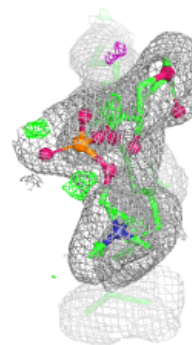
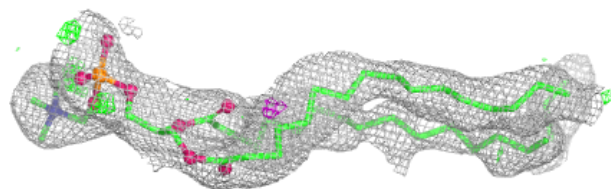
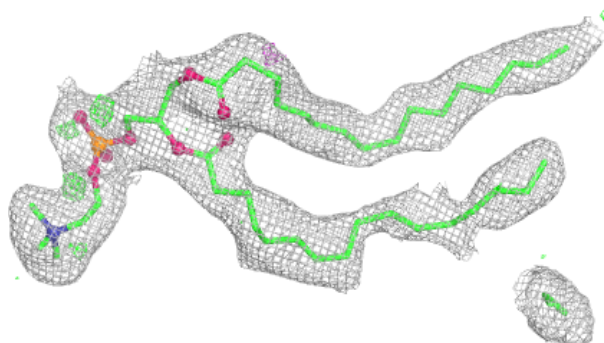


Electron density around UPL A 2014:

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

**Electron density around PLD A 2001 (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.