



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 11:36 pm BST

PDB ID : 6ZKA / pdb_00006zka
EMDB ID : EMD-11242
Title : Membrane domain of open complex I during turnover
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.50 Å (reported)
Based on initial model : 5LNK

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

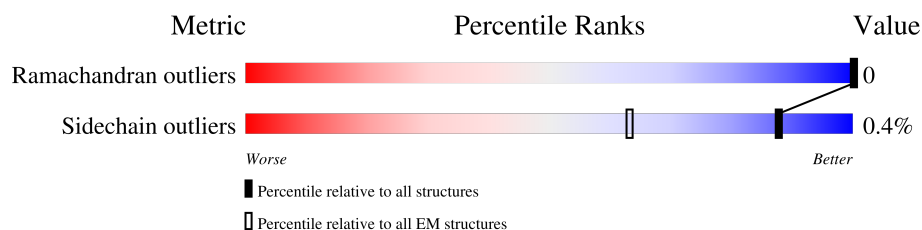
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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.



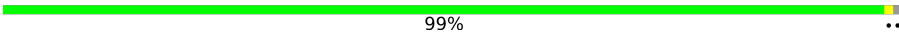
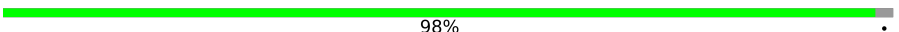

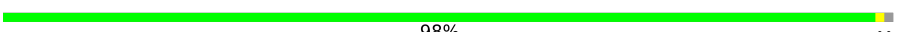
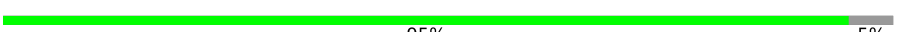







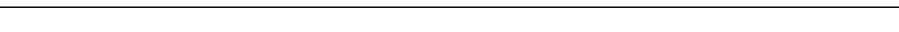

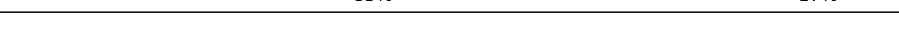



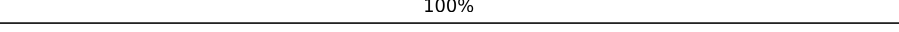
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	115	83% 16%
2	H	318	97% ..
3	J	175	95% 5%
4	K	98	98% .
5	L	606	99% .
6	M	459	99% .
7	N	347	100%
8	V	141	98% ..
9	W	189	74% 26%
10	X	157	55% 45%

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Mol	Chain	Length	Quality of chain
11	Y	172	 99% ..
12	Z	175	 98% .
13	k	355	 89% . 10%
14	l	106	 98% ..
15	m	84	 95% 5%
16	n	98	 81% 19%
17	o	122	 98% .
18	p	130	 98% .
19	q	144	 95% . .
20	r	128	 77% . 23%
21	s	137	 88% . 11%
22	t	179	 98% ..
23	u	108	 60% 40%
24	v	186	 83% 17%
25	w	154	 65% . 34%
26	x	76	 64% 36%
27	y	58	 86% 14%
28	z	70	 100%
29	4	463	 9% 91%

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
33	CDL	L	704	X	-	-	-
33	CDL	V	204	X	-	-	-
33	CDL	Y	201	X	-	-	-
33	CDL	o	502	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 40800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			787	539	111	132	5		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	313	Total	C	N	O	S	0	0
			2494	1683	379	413	19		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	167	Total	C	N	O	S	0	0
			1273	856	182	222	13		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 8 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 9 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 12 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 19 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 20 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 22 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 25 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 26 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	x	49	Total	C	N	O	0	0
			412	271	70	71		

- Molecule 27 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	y	50	Total	C	N	O	0	0
			436	287	77	72		

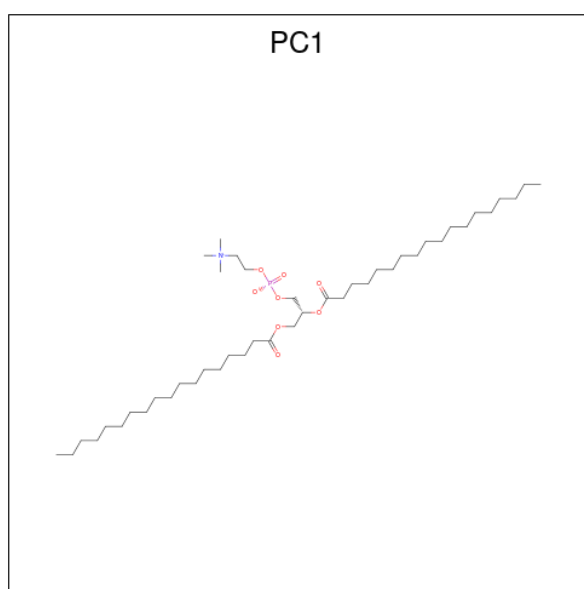
- Molecule 28 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 29 is a protein called Mitochondrial complex I, ND4L subunit.

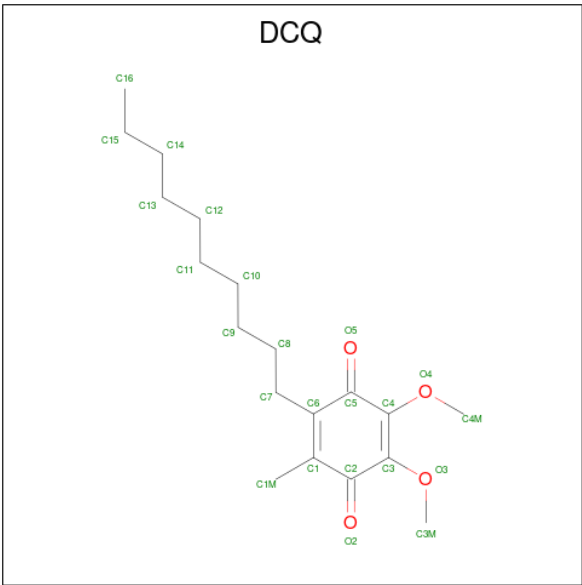
Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	40	Total	C	N	O	S	0	0
			334	217	56	60	1		

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



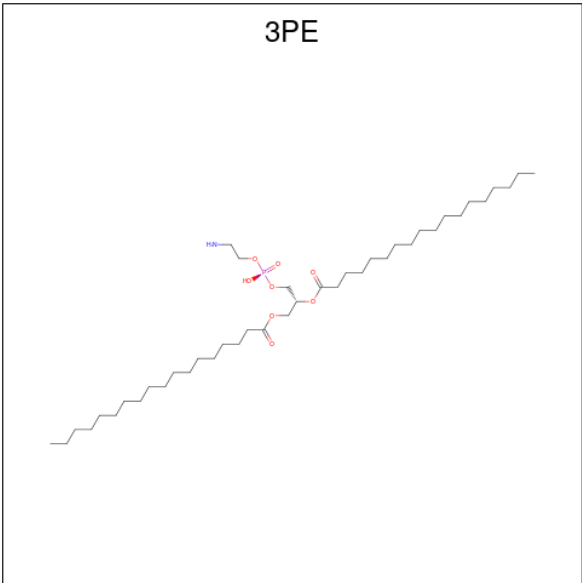
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
30	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 31 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$).



Mol	Chain	Residues	Atoms			AltConf
31	H	1	Total	C	O	0
			23	19	4	

- Molecule 32 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



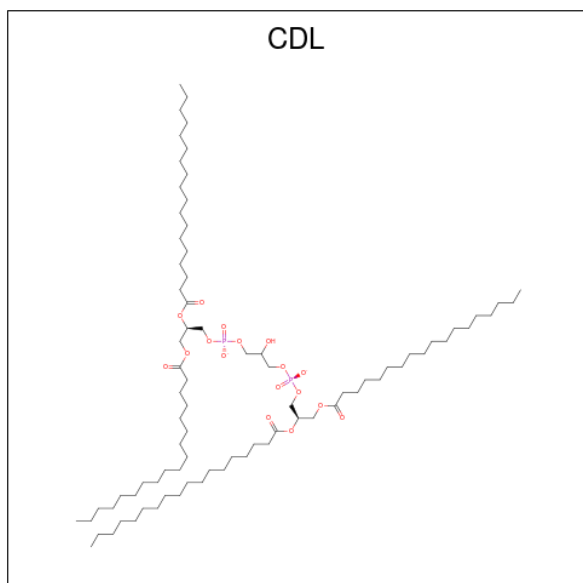
Mol	Chain	Residues	Atoms					AltConf
32	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	K	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
32	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
32	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
32	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
32	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
32	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
32	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	o	1	Total	C	N	O	P	0
			31	21	1	8	1	
32	p	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 33 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



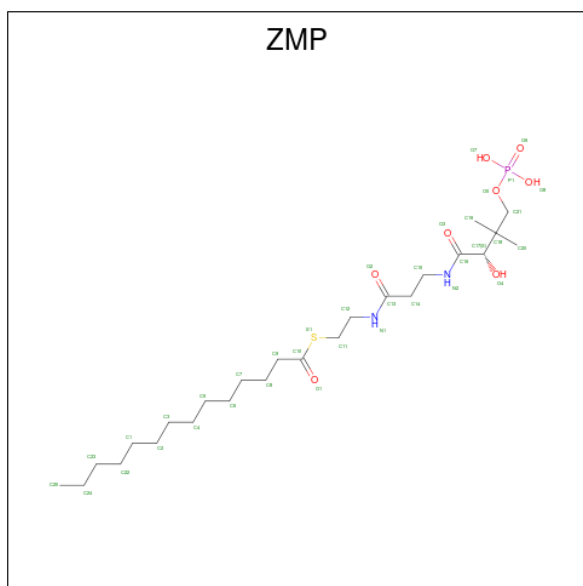
Mol	Chain	Residues	Atoms				AltConf
33	L	1	Total	C	O	P	0
			100	81	17	2	

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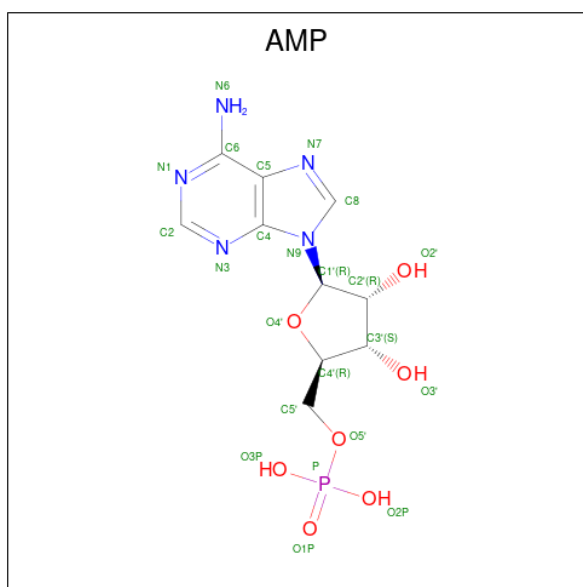
Mol	Chain	Residues	Atoms				AltConf
33	M	1	Total	C	O	P	0
			90	71	17	2	
33	V	1	Total	C	O	P	0
			94	75	17	2	
33	V	1	Total	C	O	P	0
			85	66	17	2	
33	W	1	Total	C	O	P	0
			100	81	17	2	
33	Y	1	Total	C	O	P	0
			100	81	17	2	
33	o	1	Total	C	O	P	0
			75	56	17	2	

- Molecule 34 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



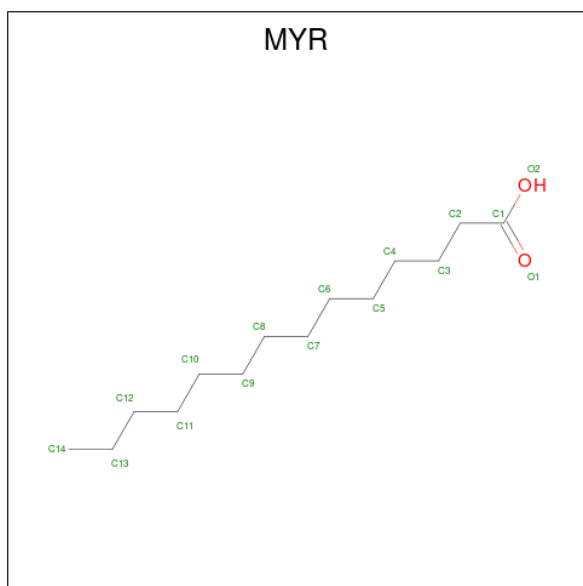
Mol	Chain	Residues	Atoms						AltConf
34	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 35 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					AltConf
35	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 36 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
36	s	1	Total	C	O	0
			15	14	1	

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	A	22	Total 22	O 22	0
37	H	53	Total 53	O 53	0
37	J	44	Total 44	O 44	0
37	K	23	Total 23	O 23	0
37	L	156	Total 156	O 156	0
37	M	184	Total 184	O 184	0
37	N	133	Total 133	O 133	0
37	V	4	Total 4	O 4	0
37	W	75	Total 75	O 75	0
37	X	17	Total 17	O 17	0
37	Y	46	Total 46	O 46	0
37	Z	67	Total 67	O 67	0
37	k	43	Total 43	O 43	0
37	l	45	Total 45	O 45	0
37	m	8	Total 8	O 8	0
37	n	3	Total 3	O 3	0
37	o	59	Total 59	O 59	0
37	p	40	Total 40	O 40	0
37	q	46	Total 46	O 46	0
37	r	20	Total 20	O 20	0
37	s	9	Total 9	O 9	0
37	t	44	Total 44	O 44	0

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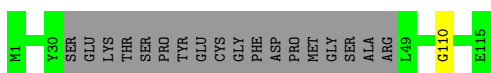
Mol	Chain	Residues	Atoms		AltConf
37	u	1	Total 1	O 1	0
37	v	41	Total 41	O 41	0
37	w	41	Total 41	O 41	0
37	x	6	Total 6	O 6	0
37	y	21	Total 21	O 21	0
37	z	18	Total 18	O 18	0
37	4	24	Total 24	O 24	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

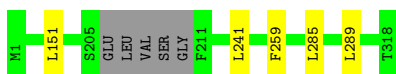
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:  83% 16%



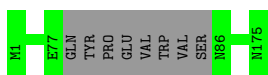
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

Chain H:  97%



- Molecule 3: NADH-ubiquinone oxidoreductase chain 6

Chain J:  95% 5%



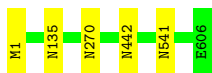
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  98%



- Molecule 5: NADH-ubiquinone oxidoreductase chain 5

Chain L:  99%



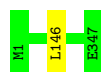
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain M:  99%



- Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N: 100%



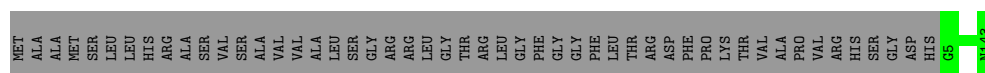
- Molecule 8: Mitochondrial complex I, B14.7 subunit

Chain V: 98%



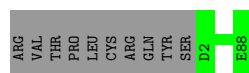
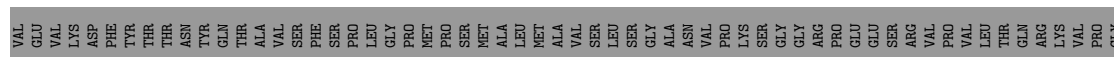
- Molecule 9: NADH:ubiquinone oxidoreductase subunit B5

Chain W: 74% 26%



- Molecule 10: Acyl carrier protein

Chain X: 55% 45%



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y: 99%




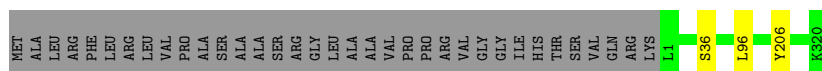
- Molecule 12: Mitochondrial complex I, PDSW subunit

Chain Z: 98%



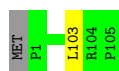
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:  89% • 10%



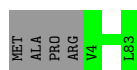
- Molecule 14: NADH:ubiquinone oxidoreductase subunit S5

Chain l:  98% ..




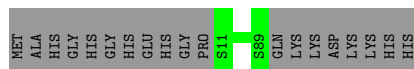
- Molecule 15: NADH:ubiquinone oxidoreductase subunit A3

Chain m:  95% 5%



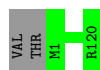
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B3

Chain n:  81% 19%



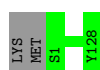
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:  98% .



- Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

Chain p:  98% .




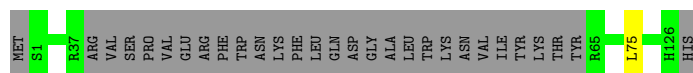
- Molecule 19: Mitochondrial complex I, B16.6 subunit

Chain q:  95% ..




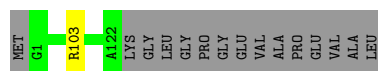
- Molecule 20: Mitochondrial complex I, B17 subunit

Chain r:  77% 23%



- Molecule 21: NADH:ubiquinone oxidoreductase subunit B7

Chain s:  88% 11%



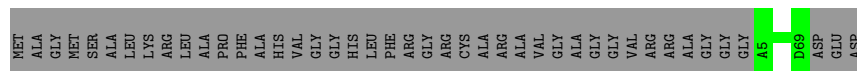
- Molecule 22: NADH:ubiquinone oxidoreductase subunit B9

Chain t:  98% ..




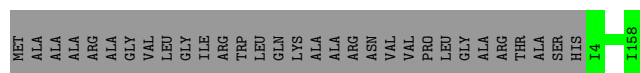
- Molecule 23: NADH:ubiquinone oxidoreductase subunit B2

Chain u:  60% 40%



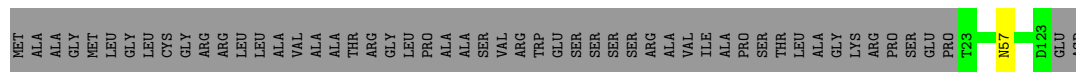
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:  83% 17%



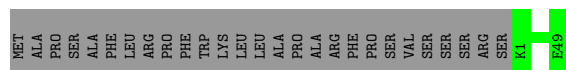
- Molecule 25: Mitochondrial complex I, ESSS subunit

Chain w:  65% 34%



- Molecule 26: Mitochondrial complex I, KFYI subunit

Chain x:  64% 36%



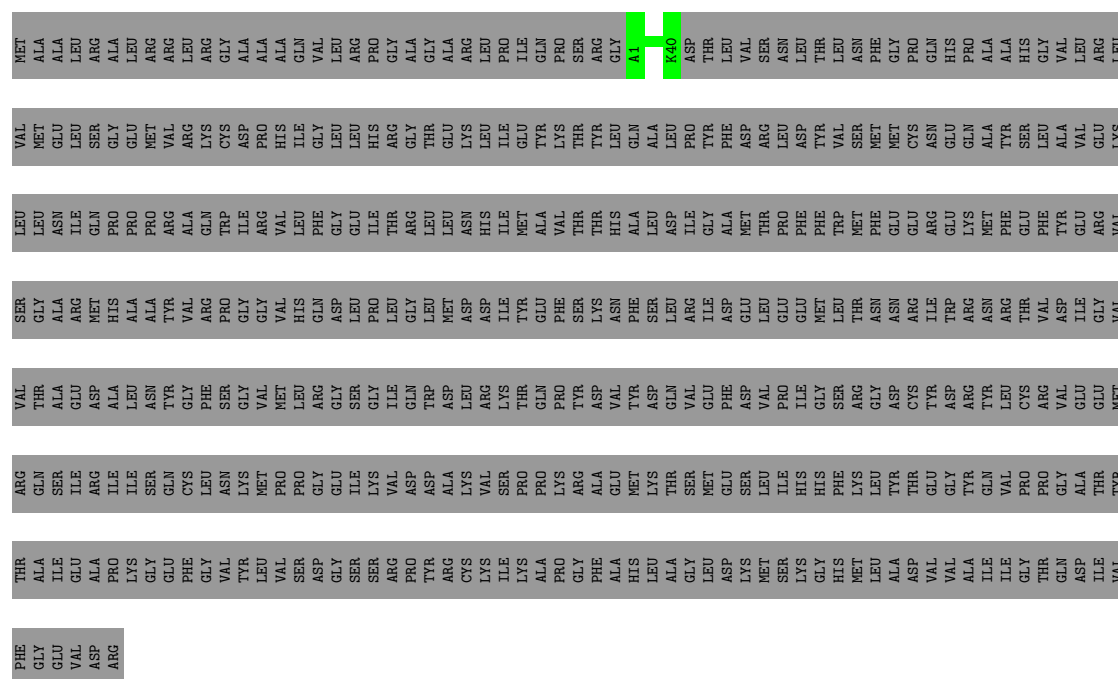
- Molecule 27: Mitochondrial complex I, MNLL subunit

MET
MET
ASN
LEU
LEU
GLN
VAL
VAL
R8
K57

- Chain z: 100%

- Molecule 29: Mitochondrial complex I, ND4L subunit

Chain 4: 9% 91%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	315484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AYA, FME, CDL, MYR, PC1, AMP, 3PE, SEP, DCQ, ZMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	1/807 (0.1%)	0.62	0/1106
2	H	0.41	0/2568	0.64	2/3512 (0.1%)
3	J	0.41	0/1302	0.63	0/1760
4	K	0.41	0/749	0.67	1/1014 (0.1%)
5	L	0.39	0/4924	0.59	0/6698
6	M	0.42	0/3731	0.64	1/5085 (0.0%)
7	N	0.40	0/2787	0.61	1/3795 (0.0%)
8	V	0.28	0/1041	0.51	1/1412 (0.1%)
9	W	0.40	0/1188	0.52	0/1607
10	X	0.36	0/713	0.52	0/963
11	Y	0.38	0/1440	0.53	0/1942
12	Z	0.39	0/1475	0.51	0/1989
13	k	0.37	0/2646	0.50	1/3579 (0.0%)
14	l	0.41	0/896	0.57	1/1200 (0.1%)
15	m	0.32	0/647	0.49	0/890
16	n	0.33	0/653	0.46	0/882
17	o	0.42	0/1035	0.52	0/1398
18	p	0.34	0/1085	0.50	0/1467
19	q	0.35	0/1171	0.50	0/1579
20	r	0.37	0/874	0.55	1/1188 (0.1%)
21	s	0.33	0/1072	0.47	0/1436
22	t	0.38	0/1573	0.52	0/2130
23	u	0.32	0/590	0.45	0/810
24	v	0.37	0/1361	0.52	0/1861
25	w	0.40	0/872	0.56	0/1185
26	x	0.32	0/425	0.42	0/576
27	y	0.35	0/449	0.50	0/605
28	z	0.41	0/591	0.56	0/795
29	4	0.36	0/351	0.46	0/485
All	All	0.38	1/39016 (0.0%)	0.56	9/52949 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLY	C-N	-5.78	1.20	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	289	LEU	CA-CB-CG	-6.11	101.26	115.30
6	M	458	LEU	CA-CB-CG	6.11	129.34	115.30
7	N	146	LEU	CA-CB-CG	6.08	129.28	115.30
20	r	75	LEU	CA-CB-CG	5.57	128.12	115.30
8	V	87	LEU	CA-CB-CG	5.57	128.11	115.30
2	H	151	LEU	CA-CB-CG	5.27	127.42	115.30
13	k	96	LEU	CA-CB-CG	5.18	127.21	115.30
4	K	19	LEU	CA-CB-CG	5.05	126.91	115.30
14	l	103	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	93/115 (81%)	89 (96%)	4 (4%)	0	100	100
2	H	309/318 (97%)	304 (98%)	5 (2%)	0	100	100
3	J	163/175 (93%)	156 (96%)	7 (4%)	0	100	100
4	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	604/606 (100%)	583 (96%)	21 (4%)	0	100	100
6	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
7	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
8	V	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
9	W	137/189 (72%)	137 (100%)	0	0	100	100
10	X	85/157 (54%)	83 (98%)	2 (2%)	0	100	100
11	Y	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
12	Z	169/175 (97%)	167 (99%)	2 (1%)	0	100	100
13	k	317/355 (89%)	309 (98%)	8 (2%)	0	100	100
14	l	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
15	m	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
16	n	77/98 (79%)	76 (99%)	1 (1%)	0	100	100
17	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
18	p	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
19	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
20	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
21	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
22	t	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
23	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
24	v	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
25	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
26	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
27	y	48/58 (83%)	48 (100%)	0	0	100	100
28	z	68/70 (97%)	68 (100%)	0	0	100	100
29	4	38/463 (8%)	36 (95%)	2 (5%)	0	100	100
All	All	4627/5550 (83%)	4511 (98%)	116 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM

entries.

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	88/103 (85%)	88 (100%)	0	100	100
2	H	274/278 (99%)	271 (99%)	3 (1%)	70	87
3	J	136/144 (94%)	136 (100%)	0	100	100
4	K	86/86 (100%)	85 (99%)	1 (1%)	67	86
5	L	538/538 (100%)	534 (99%)	4 (1%)	81	93
6	M	411/411 (100%)	409 (100%)	2 (0%)	86	95
7	N	315/315 (100%)	315 (100%)	0	100	100
8	V	101/102 (99%)	101 (100%)	0	100	100
9	W	122/160 (76%)	122 (100%)	0	100	100
10	X	80/141 (57%)	80 (100%)	0	100	100
11	Y	154/155 (99%)	153 (99%)	1 (1%)	84	94
12	Z	155/157 (99%)	155 (100%)	0	100	100
13	k	283/309 (92%)	282 (100%)	1 (0%)	89	96
14	l	94/95 (99%)	94 (100%)	0	100	100
15	m	69/72 (96%)	69 (100%)	0	100	100
16	n	61/76 (80%)	61 (100%)	0	100	100
17	o	107/109 (98%)	107 (100%)	0	100	100
18	p	114/116 (98%)	114 (100%)	0	100	100
19	q	119/122 (98%)	117 (98%)	2 (2%)	56	79
20	r	95/122 (78%)	95 (100%)	0	100	100
21	s	110/120 (92%)	109 (99%)	1 (1%)	75	90
22	t	159/161 (99%)	158 (99%)	1 (1%)	84	94
23	u	59/84 (70%)	59 (100%)	0	100	100
24	v	140/160 (88%)	140 (100%)	0	100	100
25	w	92/130 (71%)	91 (99%)	1 (1%)	70	87
26	x	44/67 (66%)	44 (100%)	0	100	100
27	y	46/54 (85%)	46 (100%)	0	100	100
28	z	59/59 (100%)	59 (100%)	0	100	100
29	4	34/392 (9%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4145/4838 (86%)	4128 (100%)	17 (0%)	88	96

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	241	LEU
2	H	259	PHE
2	H	285	LEU
4	K	50	ASN
5	L	135	ASN
5	L	270	ASN
5	L	442	ASN
5	L	541	ASN
6	M	138	ASN
6	M	144	ASN
11	Y	63	ASN
13	k	206	TYR
19	q	23	ASN
19	q	67	ARG
21	s	103	ARG
22	t	128	ARG
25	w	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
5	L	446	ASN
6	M	81	GLN
6	M	144	ASN
7	N	144	GLN
12	Z	106	GLN
13	k	180	GLN
14	l	6	GLN
17	o	61	GLN
19	q	23	ASN
19	q	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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
5	FME	L	1	5	8,9,10	0.92	0	7,9,11	1.47	2 (28%)
8	AYA	V	1	8	6,7,8	1.27	1 (16%)	5,8,10	1.92	2 (40%)
13	SEP	k	36	13	8,9,10	1.55	1 (12%)	8,12,14	1.43	2 (25%)
4	FME	K	1	4	8,9,10	0.94	0	7,9,11	0.81	0
6	FME	M	1	6	8,9,10	0.97	0	7,9,11	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FME	L	1	5	-	3/7/9/11	-
8	AYA	V	1	8	-	2/4/6/8	-
13	SEP	k	36	13	-	3/5/8/10	-
4	FME	K	1	4	-	3/7/9/11	-
6	FME	M	1	6	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	k	36	SEP	P-O1P	3.39	1.61	1.50
8	V	1	AYA	CA-N	-2.37	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	V	1	AYA	CB-CA-N	2.97	112.92	109.61
13	k	36	SEP	P-OG-CB	-2.81	110.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1	FME	C-CA-N	2.70	114.61	109.73
8	V	1	AYA	CA-N-CT	2.63	125.35	121.52
5	L	1	FME	CA-N-CN	2.41	126.53	122.82
13	k	36	SEP	OG-CB-CA	2.22	110.31	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	O1-CN-N-CA
6	M	1	FME	C-CA-CB-CG
13	k	36	SEP	CB-OG-P-O1P
13	k	36	SEP	CB-OG-P-O2P
13	k	36	SEP	CB-OG-P-O3P
5	L	1	FME	CA-CB-CG-SD
8	V	1	AYA	OT-CT-N-CA
8	V	1	AYA	CM-CT-N-CA
4	K	1	FME	CA-CB-CG-SD
5	L	1	FME	N-CA-CB-CG
6	M	1	FME	N-CA-CB-CG
5	L	1	FME	CB-CG-SD-CE
4	K	1	FME	CB-CG-SD-CE
6	M	1	FME	CB-CA-N-CN

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](#)

28 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	$\# Z > 2$
33	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.27	0
33	CDL	W	201	-	99,99,99	0.30	0	105,111,111	0.35	0
32	3PE	L	702	-	50,50,50	0.31	0	53,55,55	0.37	0
32	3PE	K	101	-	39,39,50	0.35	0	42,44,55	0.42	0
30	PC1	H	503	-	53,53,53	0.31	0	59,61,61	0.50	0
32	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.30	0
30	PC1	M	502	-	53,53,53	0.31	0	59,61,61	0.39	0
32	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.57	2 (4%)
32	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.52	2 (3%)
30	PC1	L	703	-	53,53,53	0.32	0	59,61,61	0.62	2 (3%)
32	3PE	L	705	-	30,30,50	0.41	0	33,35,55	0.79	2 (6%)
33	CDL	Y	201	-	99,99,99	0.28	0	105,111,111	0.40	1 (0%)
32	3PE	p	201	-	26,26,50	0.47	0	30,31,55	0.50	1 (3%)
33	CDL	V	204	-	84,84,99	0.28	0	90,96,111	0.29	0
31	DCQ	H	501	-	23,23,23	0.15	0	26,29,29	0.67	0
33	CDL	o	502	-	74,74,99	0.34	0	80,86,111	0.52	1 (1%)
30	PC1	w	801	-	53,53,53	0.31	0	59,61,61	0.38	0
32	3PE	m	101	-	50,50,50	0.31	0	53,55,55	0.42	0
35	AMP	k	501	-	22,25,25	0.89	1 (4%)	25,38,38	1.19	2 (8%)
32	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.46	0
32	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.43	1 (1%)
33	CDL	M	503	-	89,89,99	0.31	0	95,101,111	0.41	0
32	3PE	L	701	-	39,39,50	0.34	0	42,44,55	0.35	0
30	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.62	2 (4%)
34	ZMP	X	101	10	24,30,36	0.86	2 (8%)	29,37,45	1.04	3 (10%)
36	MYR	s	201	21	14,14,15	0.20	0	13,13,15	0.20	0
33	CDL	L	704	-	99,99,99	0.29	0	105,111,111	0.40	1 (0%)
32	3PE	V	202	-	36,36,50	0.34	0	39,41,55	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CDL	V	203	-	-	37/104/104/110	-
33	CDL	W	201	-	-	30/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	3PE	L	702	-	-	8/54/54/54	-
32	3PE	K	101	-	-	8/43/43/54	-
30	PC1	H	503	-	-	22/57/57/57	-
32	3PE	V	201	-	-	3/38/38/54	-
30	PC1	M	502	-	-	20/57/57/57	-
32	3PE	M	501	-	-	17/47/47/54	-
32	3PE	N	401	-	-	15/54/54/54	-
30	PC1	L	703	-	-	20/57/57/57	-
32	3PE	L	705	-	-	13/34/34/54	-
33	CDL	Y	201	-	1/1/9/9	27/110/110/110	-
32	3PE	p	201	-	-	7/27/27/54	-
33	CDL	V	204	-	1/1/9/9	34/95/95/110	-
33	CDL	o	502	-	2/2/9/9	18/85/85/110	-
31	DCQ	H	501	-	-	5/14/38/38	0/1/1/1
30	PC1	w	801	-	-	15/57/57/57	-
32	3PE	m	101	-	-	16/54/54/54	-
35	AMP	k	501	-	-	6/6/26/26	0/3/3/3
32	3PE	o	501	-	-	5/34/34/54	-
32	3PE	H	502	-	-	19/54/54/54	-
33	CDL	M	503	-	-	34/100/100/110	-
32	3PE	L	701	-	-	9/43/43/54	-
30	PC1	A	201	-	-	9/40/40/57	-
34	ZMP	X	101	10	-	11/35/37/43	-
36	MYR	s	201	21	-	2/11/12/13	-
33	CDL	L	704	-	1/1/9/9	28/110/110/110	-
32	3PE	V	202	-	-	11/40/40/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	101	ZMP	C9-C10	2.60	1.53	1.50
35	k	501	AMP	C5-C4	2.57	1.47	1.40
34	X	101	ZMP	C10-S1	-2.07	1.71	1.76

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	k	501	AMP	N3-C2-N1	-3.21	123.65	128.68
30	L	703	PC1	C2-O21-C21	2.68	124.38	117.79
32	L	705	3PE	C2-O21-C21	2.40	123.70	117.79
34	X	101	ZMP	O1-C10-C9	-2.40	121.16	123.99
30	A	201	PC1	O21-C2-C3	2.37	116.98	108.40
32	M	501	3PE	O21-C2-C3	-2.30	100.07	108.40
33	Y	201	CDL	OA8-CA6-CA4	2.26	115.02	108.43
34	X	101	ZMP	C9-C10-S1	2.25	116.08	113.46
32	H	502	3PE	O31-C3-C2	2.22	114.88	108.43
30	L	703	PC1	O21-C2-C1	2.20	116.35	108.40
30	A	201	PC1	C2-O21-C21	2.18	123.16	117.79
32	p	201	3PE	O12-P-O14	2.12	119.00	110.68
35	k	501	AMP	C4-C5-N7	-2.12	107.19	109.40
32	N	401	3PE	O21-C2-C1	2.11	116.03	108.40
32	M	501	3PE	O31-C3-C2	2.10	114.55	108.43
32	N	401	3PE	C2-O21-C21	2.09	122.94	117.79
32	L	705	3PE	O21-C2-C1	2.08	115.93	108.40
33	L	704	CDL	OA8-CA6-CA4	-2.04	102.50	108.43
34	X	101	ZMP	C15-C14-C13	-2.03	108.98	112.36
33	o	502	CDL	CB4-OB6-CB5	2.01	122.74	117.79

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	L	704	CDL	CB4
33	V	204	CDL	CB4
33	Y	201	CDL	CB4
33	o	502	CDL	CB4
33	o	502	CDL	CA4

All (449) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	H	503	PC1	C11-O13-P-O14
30	L	703	PC1	C1-O11-P-O12
30	M	502	PC1	C1-O11-P-O12
30	w	801	PC1	C11-O13-P-O14
30	w	801	PC1	O13-C11-C12-N
32	H	502	3PE	C11-O13-P-O12
32	H	502	3PE	C11-O13-P-O14
32	H	502	3PE	O13-C11-C12-N
32	K	101	3PE	C1-O11-P-O12
32	K	101	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
32	K	101	3PE	C1-O11-P-O14
32	L	701	3PE	C1-O11-P-O12
32	L	701	3PE	C11-O13-P-O12
32	L	705	3PE	C1-O11-P-O12
32	L	705	3PE	C1-O11-P-O13
32	L	705	3PE	C1-O11-P-O14
32	L	705	3PE	C11-O13-P-O12
32	L	705	3PE	O13-C11-C12-N
32	M	501	3PE	C1-O11-P-O14
32	M	501	3PE	C11-O13-P-O11
32	M	501	3PE	C11-O13-P-O12
32	M	501	3PE	C11-O13-P-O14
32	N	401	3PE	C1-O11-P-O12
32	N	401	3PE	C1-O11-P-O14
32	V	201	3PE	O13-C11-C12-N
32	V	202	3PE	C1-O11-P-O12
32	V	202	3PE	C1-O11-P-O13
32	V	202	3PE	C11-O13-P-O11
32	V	202	3PE	C11-O13-P-O12
32	V	202	3PE	C11-O13-P-O14
32	V	202	3PE	O13-C11-C12-N
32	m	101	3PE	C11-O13-P-O12
32	m	101	3PE	C11-O13-P-O14
32	o	501	3PE	O13-C11-C12-N
32	p	201	3PE	C1-O11-P-O12
32	p	201	3PE	C1-O11-P-O13
33	L	704	CDL	CA2-C1-CB2-OB2
33	L	704	CDL	CA2-OA2-PA1-OA3
33	L	704	CDL	CA3-OA5-PA1-OA2
33	L	704	CDL	CA3-OA5-PA1-OA4
33	L	704	CDL	CB2-OB2-PB2-OB3
33	L	704	CDL	CB2-OB2-PB2-OB5
33	M	503	CDL	O1-C1-CB2-OB2
33	M	503	CDL	C1-CA2-OA2-PA1
33	M	503	CDL	CA2-OA2-PA1-OA3
33	M	503	CDL	CA3-OA5-PA1-OA2
33	M	503	CDL	CA3-OA5-PA1-OA3
33	M	503	CDL	CB2-OB2-PB2-OB3
33	M	503	CDL	CB3-OB5-PB2-OB3
33	V	203	CDL	CB2-OB2-PB2-OB4
33	V	203	CDL	CB3-OB5-PB2-OB2
33	V	203	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
33	V	203	CDL	CB3-OB5-PB2-OB4
33	V	204	CDL	O1-C1-CB2-OB2
33	V	204	CDL	CA2-OA2-PA1-OA3
33	V	204	CDL	CA2-OA2-PA1-OA4
33	V	204	CDL	CA2-OA2-PA1-OA5
33	V	204	CDL	CB2-OB2-PB2-OB3
33	V	204	CDL	CB3-OB5-PB2-OB3
33	Y	201	CDL	O1-C1-CB2-OB2
33	Y	201	CDL	CB3-OB5-PB2-OB2
33	Y	201	CDL	CB3-OB5-PB2-OB3
33	o	502	CDL	O1-C1-CB2-OB2
34	X	101	ZMP	C17-C18-C21-O5
34	X	101	ZMP	C16-C17-C18-C21
34	X	101	ZMP	C17-C16-N2-C15
35	k	501	AMP	C5'-O5'-P-O2P
35	k	501	AMP	C5'-O5'-P-O3P
36	s	201	MYR	C1-C2-C3-C4
31	H	501	DCQ	C6-C7-C8-C9
34	X	101	ZMP	O3-C16-N2-C15
35	k	501	AMP	C3'-C4'-C5'-O5'
33	M	503	CDL	CA2-C1-CB2-OB2
33	W	201	CDL	CB2-C1-CA2-OA2
33	W	201	CDL	CA2-C1-CB2-OB2
33	o	502	CDL	CA2-C1-CB2-OB2
30	M	502	PC1	C11-C12-N-C14
33	W	201	CDL	O1-C1-CA2-OA2
33	W	201	CDL	O1-C1-CB2-OB2
33	L	704	CDL	CB5-C51-C52-C53
33	L	704	CDL	CB7-C71-C72-C73
32	V	201	3PE	C31-C32-C33-C34
30	M	502	PC1	C11-C12-N-C15
30	w	801	PC1	C21-C22-C23-C24
33	M	503	CDL	C82-C83-C84-C85
33	L	704	CDL	O1-C1-CB2-OB2
33	Y	201	CDL	CB5-C51-C52-C53
30	H	503	PC1	C11-O13-P-O11
30	M	502	PC1	C11-O13-P-O11
32	H	502	3PE	C11-O13-P-O11
32	L	701	3PE	C11-O13-P-O11
32	M	501	3PE	C1-O11-P-O13
32	N	401	3PE	C1-O11-P-O13
32	m	101	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
33	M	503	CDL	CA2-OA2-PA1-OA5
33	M	503	CDL	CB2-OB2-PB2-OB5
33	V	203	CDL	CB2-OB2-PB2-OB5
33	V	204	CDL	CB3-OB5-PB2-OB2
33	V	204	CDL	CA2-C1-CB2-OB2
33	M	503	CDL	C78-C79-C80-C81
33	L	704	CDL	C21-C22-C23-C24
34	X	101	ZMP	C19-C18-C21-O5
34	X	101	ZMP	C20-C18-C21-O5
32	m	101	3PE	C38-C39-C3A-C3B
33	L	704	CDL	C56-C57-C58-C59
33	L	704	CDL	C77-C78-C79-C80
33	V	203	CDL	C52-C53-C54-C55
33	W	201	CDL	C72-C73-C74-C75
32	N	401	3PE	C21-C22-C23-C24
32	K	101	3PE	C24-C25-C26-C27
33	V	204	CDL	C71-C72-C73-C74
33	Y	201	CDL	C63-C64-C65-C66
32	L	705	3PE	C2-C1-O11-P
33	Y	201	CDL	C11-C12-C13-C14
33	Y	201	CDL	C52-C53-C54-C55
32	N	401	3PE	C32-C33-C34-C35
33	V	203	CDL	C20-C21-C22-C23
33	V	203	CDL	CA7-C31-C32-C33
30	L	703	PC1	C37-C38-C39-C3A
33	L	704	CDL	C41-C42-C43-C44
33	V	203	CDL	C40-C41-C42-C43
33	W	201	CDL	C35-C36-C37-C38
33	W	201	CDL	CA5-C11-C12-C13
30	w	801	PC1	C2D-C2E-C2F-C2G
31	H	501	DCQ	C10-C11-C12-C13
32	L	702	3PE	C3B-C3C-C3D-C3E
33	L	704	CDL	C17-C18-C19-C20
33	V	203	CDL	C31-C32-C33-C34
33	Y	201	CDL	C80-C81-C82-C83
33	V	203	CDL	C79-C80-C81-C82
33	W	201	CDL	CB5-C51-C52-C53
30	H	503	PC1	C3C-C3D-C3E-C3F
30	H	503	PC1	C3B-C3C-C3D-C3E
30	L	703	PC1	C38-C39-C3A-C3B
32	K	101	3PE	C34-C35-C36-C37
33	V	203	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
33	V	204	CDL	C14-C15-C16-C17
33	Y	201	CDL	C14-C15-C16-C17
30	w	801	PC1	C3A-C3B-C3C-C3D
32	m	101	3PE	C2C-C2D-C2E-C2F
32	m	101	3PE	C2E-C2F-C2G-C2H
33	W	201	CDL	C82-C83-C84-C85
33	L	704	CDL	C82-C83-C84-C85
33	Y	201	CDL	C15-C16-C17-C18
30	L	703	PC1	C33-C34-C35-C36
33	M	503	CDL	C51-C52-C53-C54
33	V	204	CDL	C34-C35-C36-C37
30	L	703	PC1	C36-C37-C38-C39
33	L	704	CDL	C34-C35-C36-C37
33	L	704	CDL	C35-C36-C37-C38
33	M	503	CDL	C56-C57-C58-C59
30	M	502	PC1	C31-C32-C33-C34
33	Y	201	CDL	C81-C82-C83-C84
32	L	705	3PE	C21-C22-C23-C24
33	o	502	CDL	CA7-C31-C32-C33
33	Y	201	CDL	C37-C38-C39-C40
32	N	401	3PE	O11-C1-C2-O21
33	W	201	CDL	C31-C32-C33-C34
33	V	203	CDL	OB6-CB4-CB6-OB8
30	w	801	PC1	C39-C3A-C3B-C3C
33	M	503	CDL	C73-C74-C75-C76
30	M	502	PC1	C11-C12-N-C13
33	Y	201	CDL	C12-C13-C14-C15
35	k	501	AMP	O4'-C4'-C5'-O5'
33	L	704	CDL	C22-C23-C24-C25
33	V	204	CDL	C51-C52-C53-C54
30	H	503	PC1	C22-C21-O21-C2
32	L	701	3PE	C1-O11-P-O13
33	L	704	CDL	CA2-OA2-PA1-OA5
33	M	503	CDL	C64-C65-C66-C67
30	L	703	PC1	C2-C1-O11-P
33	V	204	CDL	C1-CA2-OA2-PA1
32	H	502	3PE	O11-C1-C2-C3
33	L	704	CDL	OB5-CB3-CB4-CB6
33	V	203	CDL	OA5-CA3-CA4-CA6
33	W	201	CDL	OA5-CA3-CA4-CA6
33	M	503	CDL	C81-C82-C83-C84
32	L	702	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	Y	201	CDL	CA2-C1-CB2-OB2
33	Y	201	CDL	C79-C80-C81-C82
33	M	503	CDL	C53-C54-C55-C56
33	Y	201	CDL	CA3-CA4-CA6-OA8
32	H	502	3PE	C33-C34-C35-C36
30	w	801	PC1	C3E-C3F-C3G-C3H
33	W	201	CDL	CA7-C31-C32-C33
34	X	101	ZMP	O3-C16-C17-O4
30	L	703	PC1	C3F-C3G-C3H-C3I
30	w	801	PC1	C23-C24-C25-C26
30	L	703	PC1	C21-C22-C23-C24
32	L	701	3PE	C31-C32-C33-C34
33	V	204	CDL	C52-C53-C54-C55
30	A	201	PC1	C22-C23-C24-C25
30	M	502	PC1	C3B-C3C-C3D-C3E
33	V	204	CDL	OA6-CA4-CA6-OA8
32	L	702	3PE	C37-C38-C39-C3A
32	p	201	3PE	C22-C23-C24-C25
32	H	502	3PE	C2D-C2E-C2F-C2G
32	N	401	3PE	C31-C32-C33-C34
33	V	204	CDL	C15-C16-C17-C18
30	L	703	PC1	O11-C1-C2-C3
30	M	502	PC1	O11-C1-C2-C3
32	N	401	3PE	O11-C1-C2-C3
32	K	101	3PE	O13-C11-C12-N
33	V	203	CDL	C11-C12-C13-C14
33	M	503	CDL	C19-C20-C21-C22
33	V	204	CDL	C1-CB2-OB2-PB2
35	k	501	AMP	C4'-C5'-O5'-P
30	M	502	PC1	C3A-C3B-C3C-C3D
33	V	203	CDL	CB3-CB4-CB6-OB8
33	W	201	CDL	CA3-CA4-CA6-OA8
33	o	502	CDL	CB3-CB4-CB6-OB8
30	H	503	PC1	O22-C21-O21-C2
32	H	502	3PE	C28-C29-C2A-C2B
30	w	801	PC1	C11-O13-P-O11
32	H	502	3PE	C1-O11-P-O13
33	o	502	CDL	CA3-OA5-PA1-OA2
30	H	503	PC1	C2D-C2E-C2F-C2G
33	L	704	CDL	OB5-CB3-CB4-OB6
33	V	203	CDL	OA5-CA3-CA4-OA6
33	V	203	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
33	W	201	CDL	OA5-CA3-CA4-OA6
32	M	501	3PE	C3B-C3C-C3D-C3E
33	V	204	CDL	OB6-CB4-CB6-OB8
33	W	201	CDL	OA6-CA4-CA6-OA8
33	L	704	CDL	C61-C62-C63-C64
32	L	702	3PE	C35-C36-C37-C38
32	L	701	3PE	C37-C38-C39-C3A
32	H	502	3PE	C2-C1-O11-P
32	V	202	3PE	C2-C1-O11-P
33	L	704	CDL	CA4-CA3-OA5-PA1
30	M	502	PC1	C32-C33-C34-C35
30	L	703	PC1	C3A-C3B-C3C-C3D
34	X	101	ZMP	N2-C16-C17-O4
33	Y	201	CDL	C59-C60-C61-C62
33	o	502	CDL	C71-C72-C73-C74
33	M	503	CDL	C71-C72-C73-C74
33	Y	201	CDL	C57-C58-C59-C60
32	p	201	3PE	C21-C22-C23-C24
30	M	502	PC1	C2-C1-O11-P
30	w	801	PC1	C1-C2-C3-O31
33	M	503	CDL	CB4-CB3-OB5-PB2
33	V	204	CDL	CB3-CB4-CB6-OB8
30	A	201	PC1	O11-C1-C2-O21
30	L	703	PC1	O11-C1-C2-O21
30	L	703	PC1	C23-C24-C25-C26
33	M	503	CDL	C72-C73-C74-C75
33	M	503	CDL	C83-C84-C85-C86
32	N	401	3PE	O21-C2-C3-O31
33	L	704	CDL	C58-C59-C60-C61
30	H	503	PC1	C2B-C2C-C2D-C2E
34	X	101	ZMP	C6-C7-C8-C9
30	L	703	PC1	C1-O11-P-O13
33	o	502	CDL	CB2-OB2-PB2-OB5
30	L	703	PC1	C2A-C2B-C2C-C2D
32	K	101	3PE	C2-C1-O11-P
33	W	201	CDL	C1-CA2-OA2-PA1
30	H	503	PC1	C11-O13-P-O12
30	L	703	PC1	C1-O11-P-O14
30	M	502	PC1	C11-O13-P-O14
32	L	701	3PE	C1-O11-P-O14
32	M	501	3PE	C1-O11-P-O12
32	V	202	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
33	L	704	CDL	CA3-OA5-PA1-OA3
33	M	503	CDL	CA2-OA2-PA1-OA4
33	M	503	CDL	CB2-OB2-PB2-OB4
33	V	203	CDL	CB2-OB2-PB2-OB3
33	V	204	CDL	CB3-OB5-PB2-OB4
33	o	502	CDL	C15-C16-C17-C18
32	o	501	3PE	C25-C26-C27-C28
32	N	401	3PE	C38-C39-C3A-C3B
32	o	501	3PE	C22-C23-C24-C25
30	H	503	PC1	C12-C11-O13-P
32	H	502	3PE	C12-C11-O13-P
32	L	701	3PE	C12-C11-O13-P
30	w	801	PC1	C28-C29-C2A-C2B
36	s	201	MYR	C11-C10-C9-C8
33	o	502	CDL	CB2-C1-CA2-OA2
30	M	502	PC1	O11-C1-C2-O21
32	H	502	3PE	O11-C1-C2-O21
32	L	702	3PE	O11-C1-C2-O21
32	L	705	3PE	O11-C1-C2-O21
33	o	502	CDL	OB5-CB3-CB4-OB6
30	A	201	PC1	C11-C12-N-C13
32	H	502	3PE	C31-C32-C33-C34
30	H	503	PC1	O13-C11-C12-N
33	V	204	CDL	CA3-CA4-CA6-OA8
30	w	801	PC1	O21-C2-C3-O31
33	V	203	CDL	C77-C78-C79-C80
30	L	703	PC1	C39-C3A-C3B-C3C
30	M	502	PC1	C2D-C2E-C2F-C2G
33	V	203	CDL	C41-C42-C43-C44
31	H	501	DCQ	C5-C4-O4-C4M
32	N	401	3PE	C37-C38-C39-C3A
33	Y	201	CDL	C32-C33-C34-C35
33	W	201	CDL	C81-C82-C83-C84
32	L	702	3PE	O11-C1-C2-C3
33	V	203	CDL	OB5-CB3-CB4-CB6
30	H	503	PC1	C22-C23-C24-C25
33	M	503	CDL	CB5-C51-C52-C53
30	M	502	PC1	C2B-C2C-C2D-C2E
32	M	501	3PE	C2-C1-O11-P
33	W	201	CDL	C79-C80-C81-C82
33	V	204	CDL	C23-C24-C25-C26
33	M	503	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
33	V	203	CDL	OA6-CA4-CA6-OA8
33	W	201	CDL	OB6-CB4-CB6-OB8
33	Y	201	CDL	OA6-CA4-CA6-OA8
30	L	703	PC1	C3E-C3F-C3G-C3H
30	A	201	PC1	C11-O13-P-O11
30	H	503	PC1	C1-O11-P-O13
32	L	702	3PE	C11-O13-P-O11
32	N	401	3PE	C11-O13-P-O11
32	V	201	3PE	C11-O13-P-O11
32	m	101	3PE	C1-O11-P-O13
32	o	501	3PE	C11-O13-P-O11
33	V	203	CDL	CA2-OA2-PA1-OA5
33	V	204	CDL	CA3-OA5-PA1-OA2
33	W	201	CDL	CA2-OA2-PA1-OA5
33	o	502	CDL	CA2-OA2-PA1-OA5
33	M	503	CDL	C63-C64-C65-C66
33	o	502	CDL	CB7-C71-C72-C73
30	M	502	PC1	C2F-C2G-C2H-C2I
32	H	502	3PE	C3A-C3B-C3C-C3D
32	H	502	3PE	C32-C31-O31-C3
30	A	201	PC1	O31-C31-C32-C33
32	M	501	3PE	C32-C31-O31-C3
32	M	501	3PE	C32-C33-C34-C35
32	M	501	3PE	C31-C32-C33-C34
33	V	204	CDL	CA5-C11-C12-C13
32	m	101	3PE	O13-C11-C12-N
33	V	204	CDL	C21-C22-C23-C24
33	V	203	CDL	O1-C1-CB2-OB2
30	H	503	PC1	C2C-C2D-C2E-C2F
30	H	503	PC1	C2-C1-O11-P
30	M	502	PC1	C25-C26-C27-C28
30	A	201	PC1	C11-C12-N-C14
33	L	704	CDL	C80-C81-C82-C83
33	M	503	CDL	CA3-CA4-CA6-OA8
33	V	203	CDL	CA2-C1-CB2-OB2
32	H	502	3PE	C36-C37-C38-C39
33	W	201	CDL	C53-C54-C55-C56
30	H	503	PC1	C3-C2-O21-C21
30	L	703	PC1	C1-C2-O21-C21
32	L	705	3PE	C1-C2-O21-C21
32	N	401	3PE	C3-C2-O21-C21
32	N	401	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
30	A	201	PC1	C11-C12-N-C15
33	V	203	CDL	CA5-C11-C12-C13
33	W	201	CDL	OB5-CB3-CB4-OB6
33	M	503	CDL	OB5-CB3-CB4-CB6
34	X	101	ZMP	C3-C4-C5-C6
33	V	203	CDL	C78-C79-C80-C81
31	H	501	DCQ	C7-C8-C9-C10
33	V	203	CDL	C37-C38-C39-C40
32	m	101	3PE	C35-C36-C37-C38
30	w	801	PC1	C2C-C2D-C2E-C2F
33	o	502	CDL	O1-C1-CA2-OA2
30	w	801	PC1	C2F-C2G-C2H-C2I
30	A	201	PC1	O21-C21-C22-C23
30	M	502	PC1	O21-C21-C22-C23
30	M	502	PC1	O31-C31-C32-C33
30	L	703	PC1	C28-C29-C2A-C2B
33	W	201	CDL	C58-C59-C60-C61
33	V	203	CDL	C71-C72-C73-C74
32	K	101	3PE	O31-C31-C32-C33
30	L	703	PC1	C2C-C2D-C2E-C2F
32	M	501	3PE	O32-C31-O31-C3
33	V	203	CDL	C32-C31-CA7-OA8
33	V	203	CDL	CA4-CA3-OA5-PA1
33	Y	201	CDL	C12-C11-CA5-OA6
30	w	801	PC1	C31-C32-C33-C34
32	V	202	3PE	O31-C31-C32-C33
30	H	503	PC1	C3A-C3B-C3C-C3D
33	V	204	CDL	C31-C32-C33-C34
33	W	201	CDL	C15-C16-C17-C18
33	M	503	CDL	C84-C85-C86-C87
33	M	503	CDL	CB3-CB4-OB6-CB5
30	H	503	PC1	C34-C35-C36-C37
32	m	101	3PE	C3A-C3B-C3C-C3D
33	V	203	CDL	C72-C71-CB7-OB8
33	V	204	CDL	C52-C51-CB5-OB6
32	H	502	3PE	O32-C31-O31-C3
32	L	705	3PE	O21-C21-C22-C23
32	L	701	3PE	C24-C25-C26-C27
32	L	702	3PE	C34-C35-C36-C37
32	N	401	3PE	C1-C2-C3-O31
33	W	201	CDL	CB3-CB4-CB6-OB8
35	k	501	AMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
33	V	204	CDL	C77-C78-C79-C80
33	V	204	CDL	CB2-C1-CA2-OA2
34	X	101	ZMP	C16-C17-C18-C20
33	V	204	CDL	C32-C31-CA7-OA8
30	H	503	PC1	C3D-C3E-C3F-C3G
33	W	201	CDL	OB5-CB3-CB4-CB6
33	Y	201	CDL	OB5-CB3-CB4-CB6
32	m	101	3PE	O21-C21-C22-C23
32	m	101	3PE	O21-C2-C3-O31
33	o	502	CDL	C72-C71-CB7-OB8
33	M	503	CDL	C52-C53-C54-C55
32	M	501	3PE	O21-C21-C22-C23
33	V	203	CDL	C72-C71-CB7-OB9
33	o	502	CDL	C73-C74-C75-C76
32	p	201	3PE	O21-C21-C22-C23
33	Y	201	CDL	C12-C11-CA5-OA7
30	H	503	PC1	C31-C32-C33-C34
33	V	204	CDL	C32-C31-CA7-OA9
33	V	204	CDL	C52-C51-CB5-OB7
33	Y	201	CDL	C52-C51-CB5-OB6
33	W	201	CDL	CB2-OB2-PB2-OB5
32	V	202	3PE	O32-C31-C32-C33
33	V	203	CDL	C32-C31-CA7-OA9
32	p	201	3PE	C26-C27-C28-C29
33	Y	201	CDL	C1-CB2-OB2-PB2
32	M	501	3PE	O22-C21-C22-C23
32	H	502	3PE	C3C-C3D-C3E-C3F
30	A	201	PC1	C11-O13-P-O14
30	H	503	PC1	C11-C12-N-C14
30	M	502	PC1	C1-O11-P-O14
32	L	705	3PE	C11-O13-P-O14
32	o	501	3PE	C11-O13-P-O14
33	W	201	CDL	CA3-OA5-PA1-OA3
33	Y	201	CDL	CB2-OB2-PB2-OB3
33	o	502	CDL	CA2-OA2-PA1-OA3
33	o	502	CDL	CB3-OB5-PB2-OB3
30	H	503	PC1	C3F-C3G-C3H-C3I
32	m	101	3PE	C22-C23-C24-C25
32	L	705	3PE	O22-C21-C22-C23
32	M	501	3PE	C37-C38-C39-C3A
33	V	204	CDL	C12-C11-CA5-OA6
32	L	705	3PE	C12-C11-O13-P

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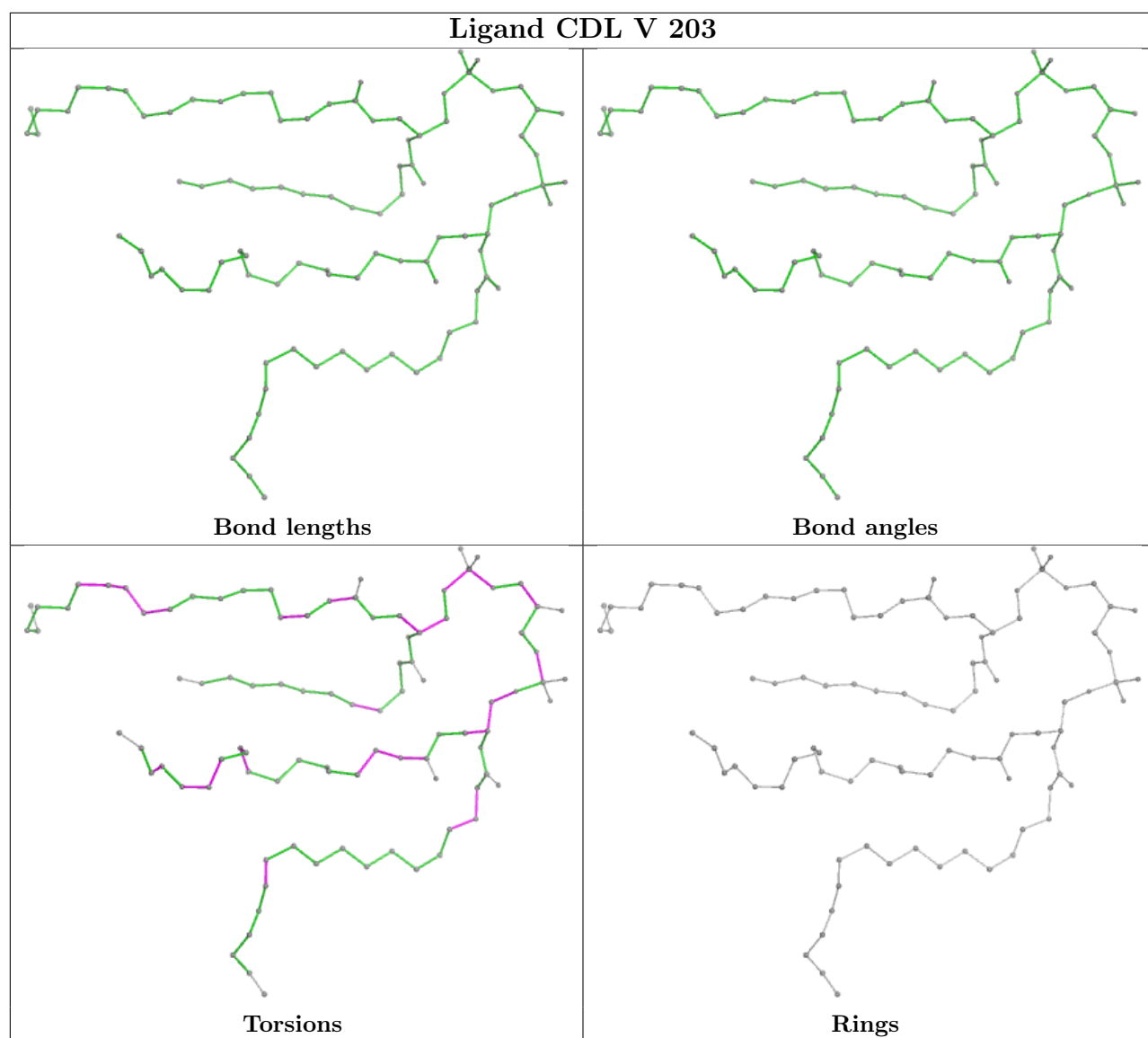
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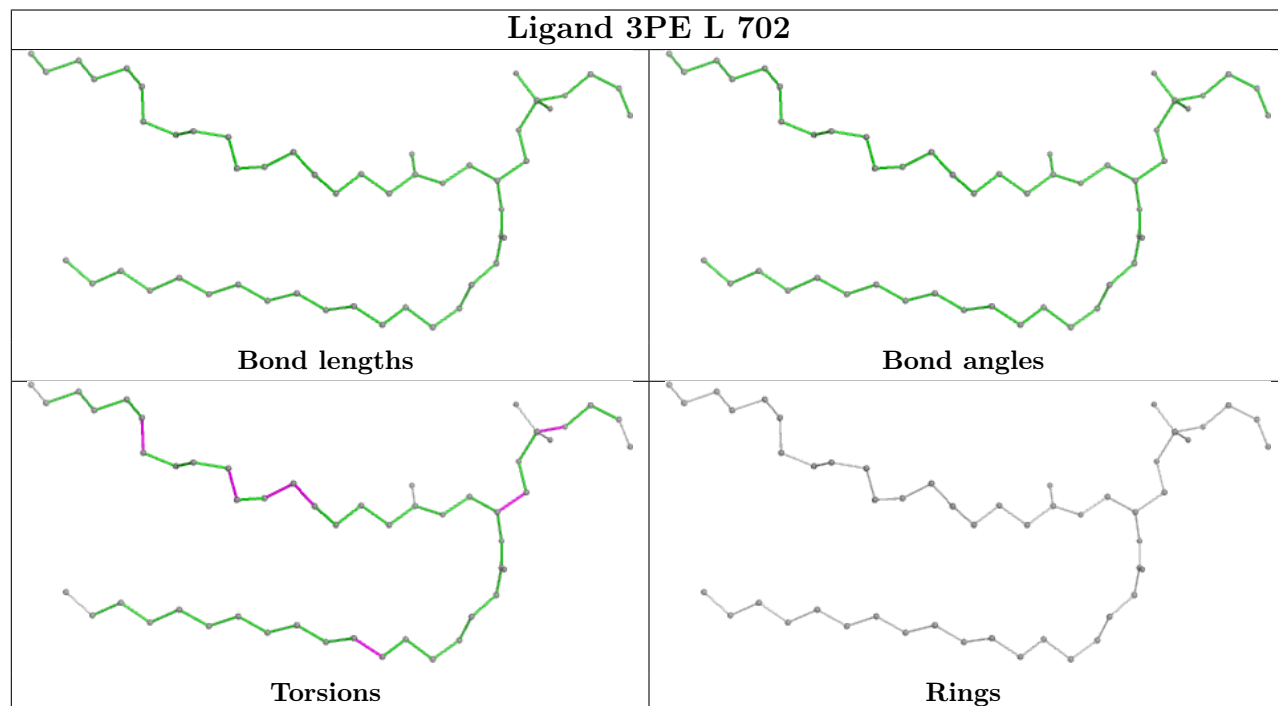
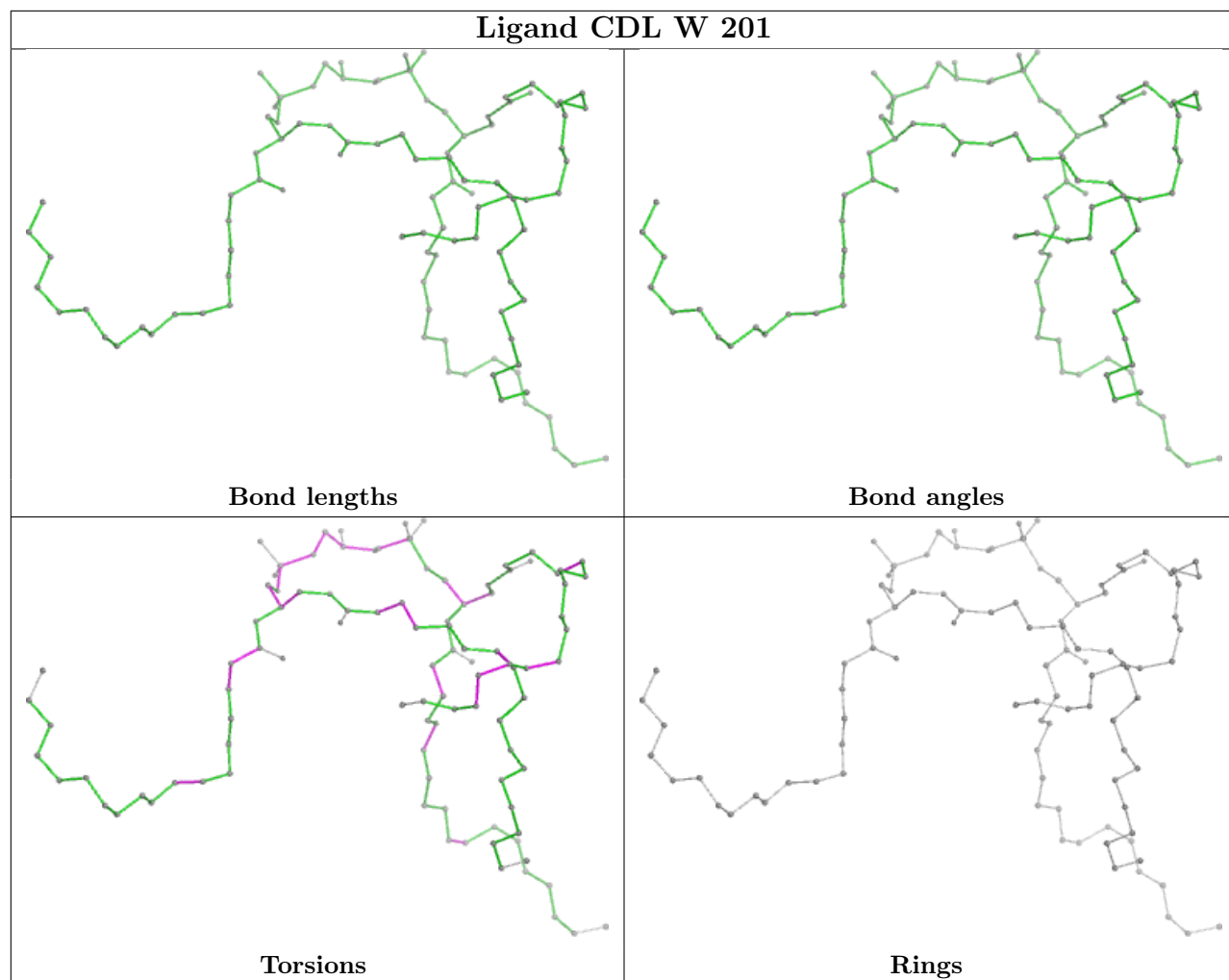
Mol	Chain	Res	Type	Atoms
32	M	501	3PE	C12-C11-O13-P
32	V	202	3PE	C12-C11-O13-P
32	m	101	3PE	C12-C11-O13-P
32	M	501	3PE	C23-C24-C25-C26
33	M	503	CDL	C31-C32-C33-C34
32	H	502	3PE	C26-C27-C28-C29
33	L	704	CDL	C72-C71-CB7-OB8
33	W	201	CDL	C12-C11-CA5-OA6
32	m	101	3PE	O22-C21-C22-C23
33	Y	201	CDL	C52-C51-CB5-OB7
33	o	502	CDL	C72-C71-CB7-OB9
33	V	203	CDL	C80-C81-C82-C83
33	V	203	CDL	C43-C44-C45-C46
31	H	501	DCQ	C3-C4-O4-C4M
32	p	201	3PE	O22-C21-C22-C23
32	m	101	3PE	C3C-C3D-C3E-C3F
33	V	204	CDL	C12-C11-CA5-OA7
33	W	201	CDL	C12-C11-CA5-OA7
33	L	704	CDL	C72-C71-CB7-OB9

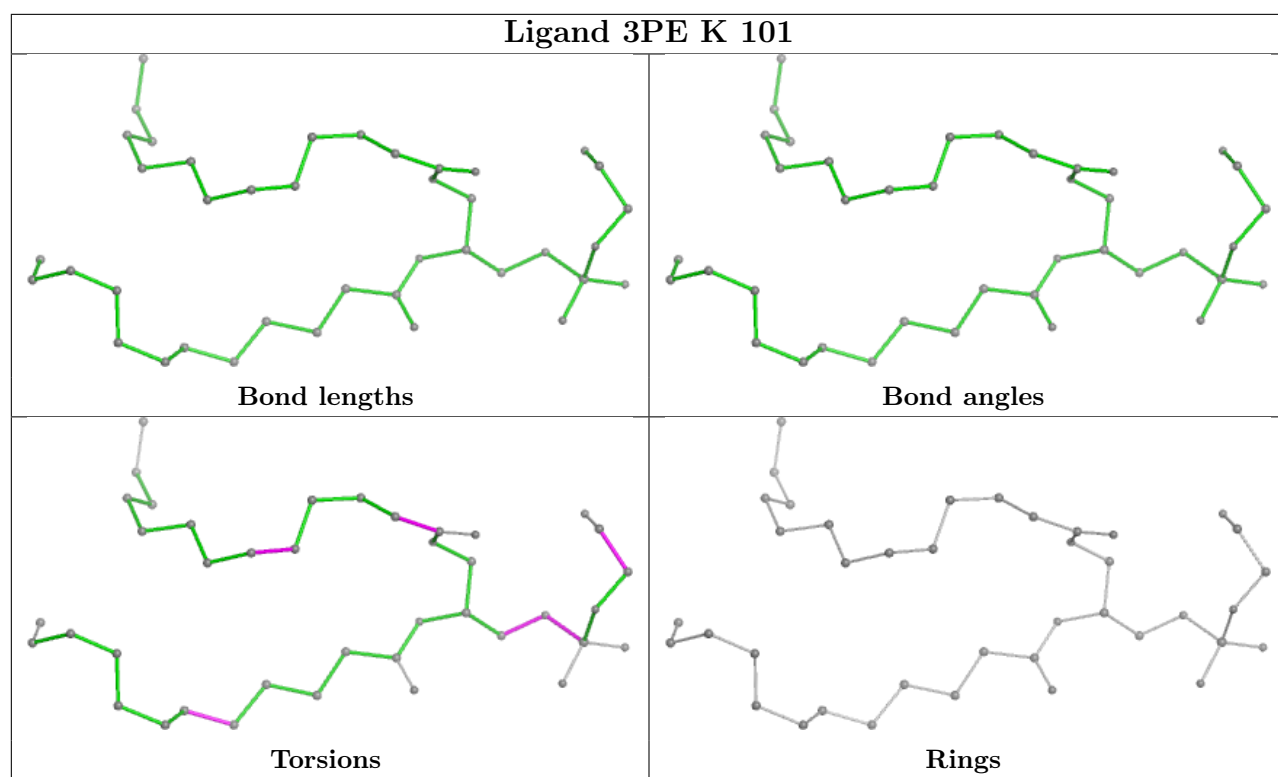
There are no ring outliers.

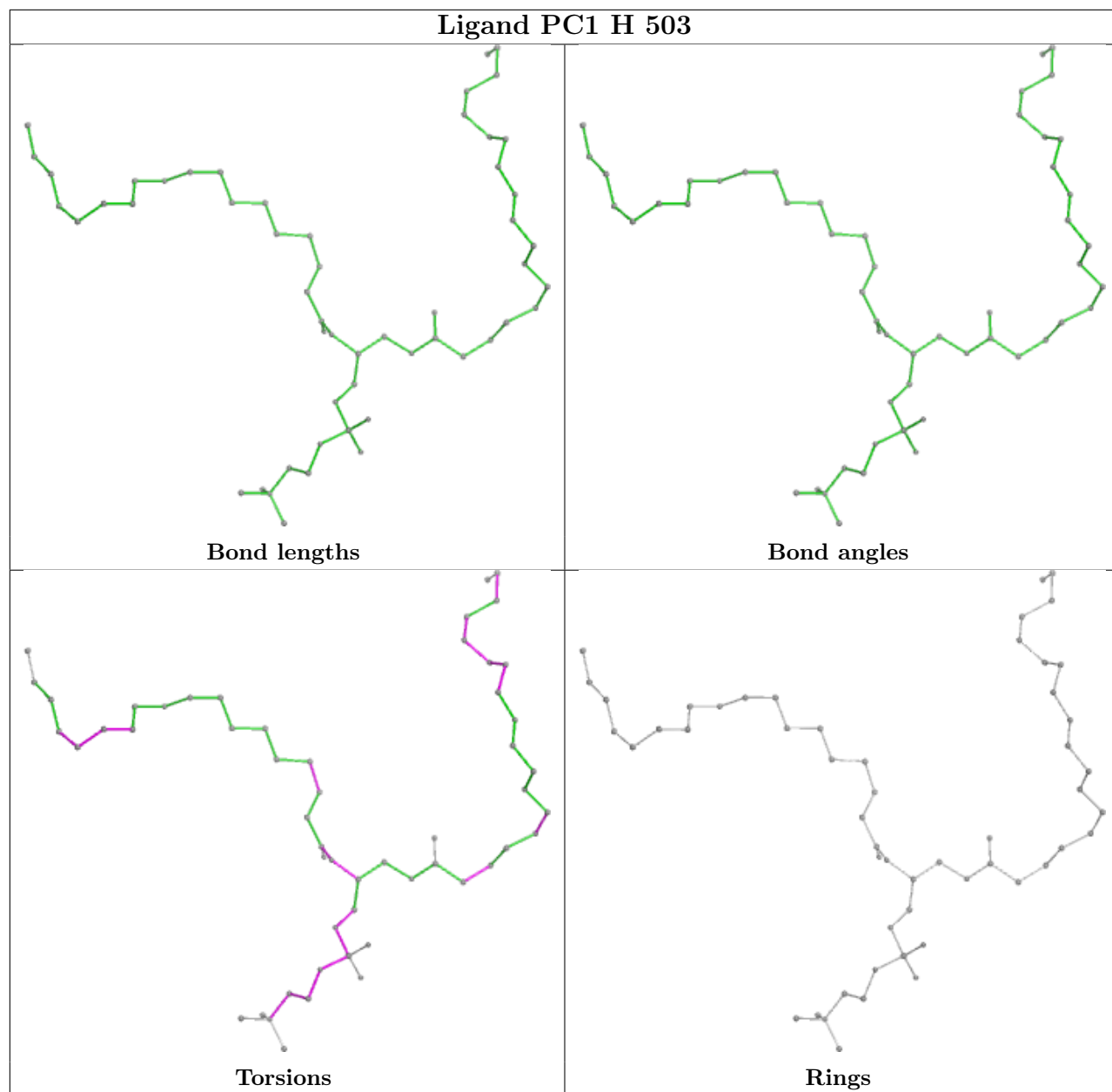
No monomer is involved in short contacts.

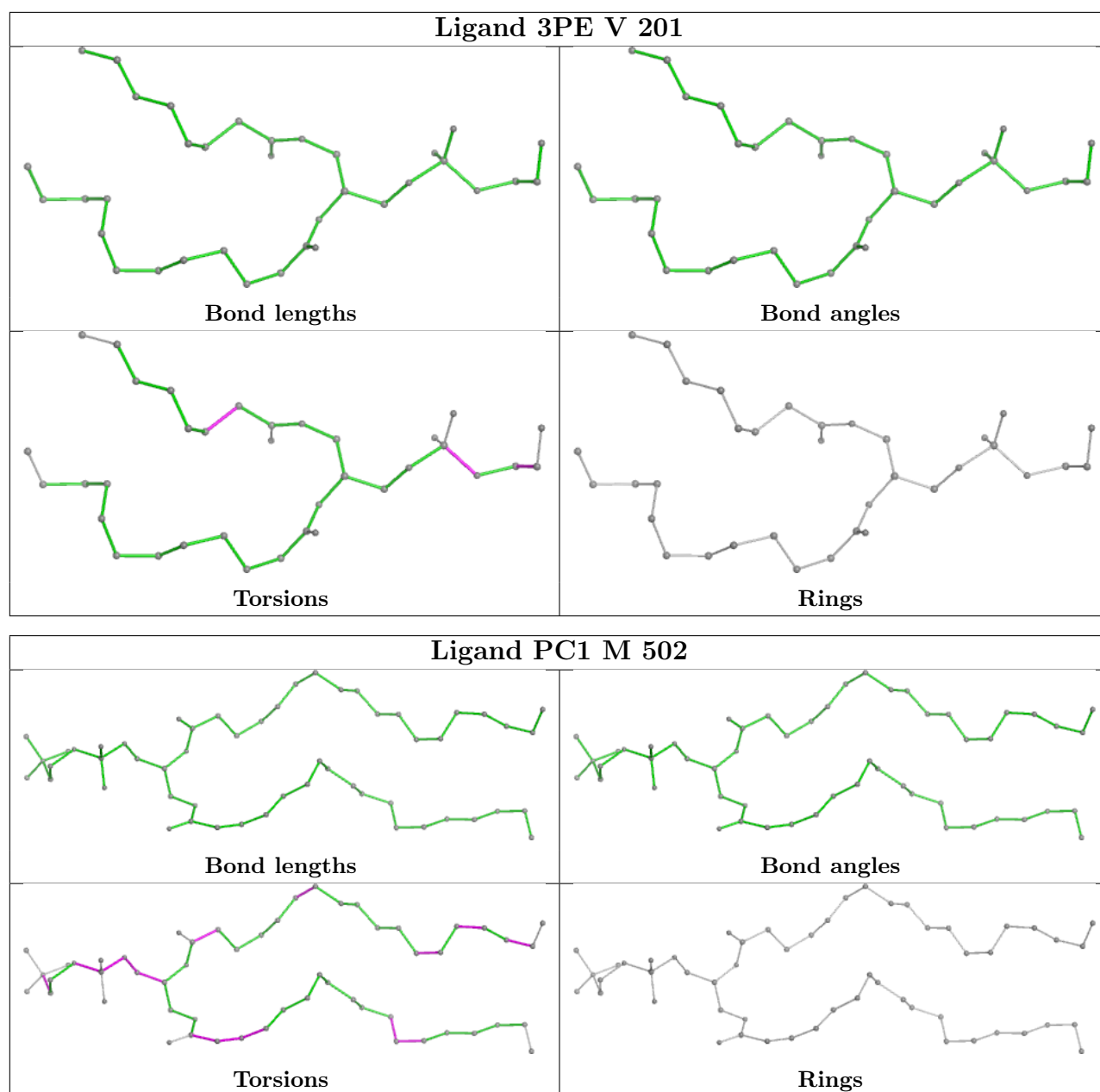
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

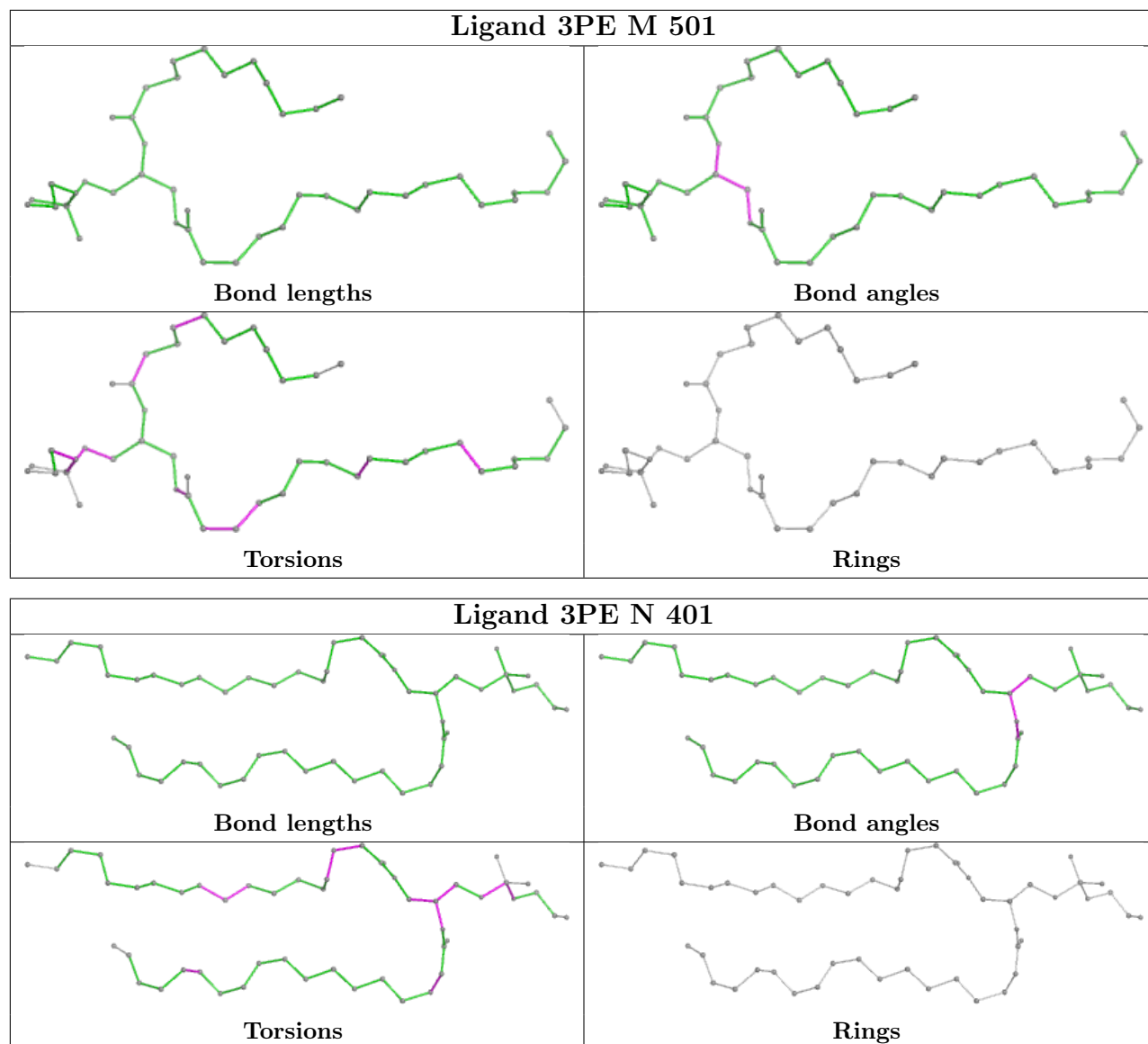


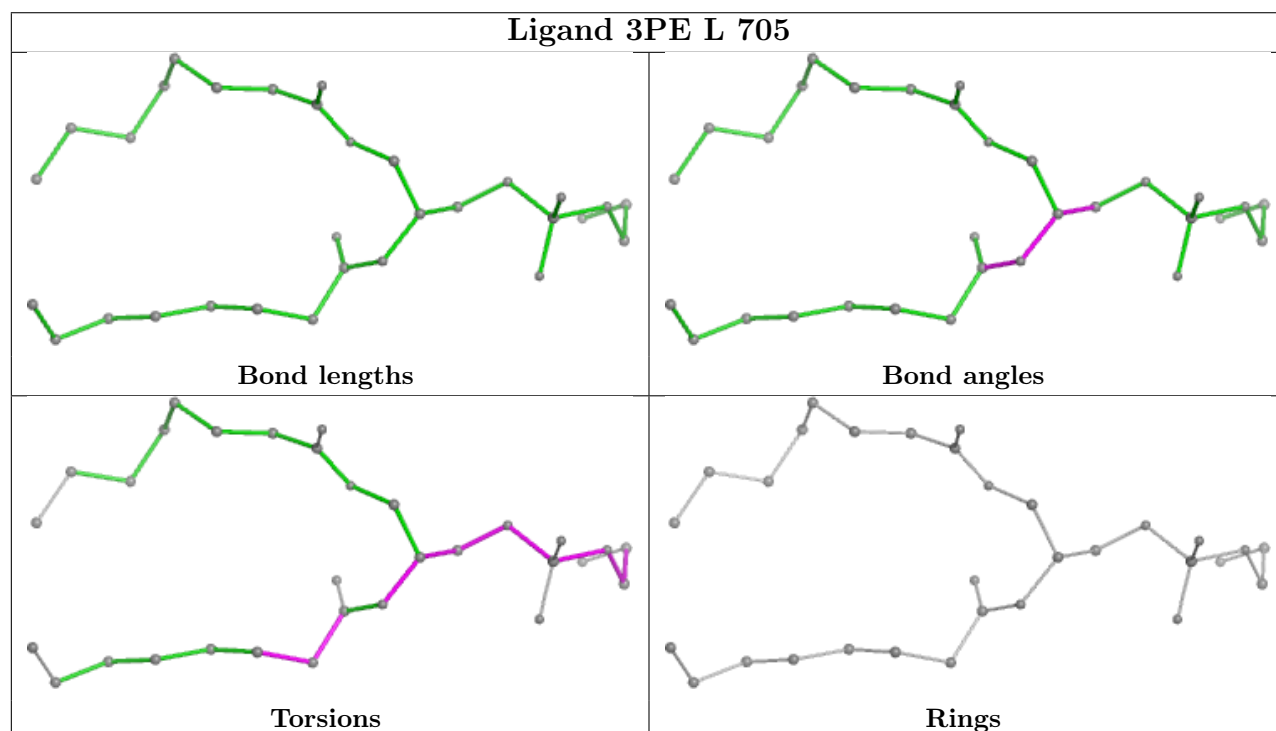
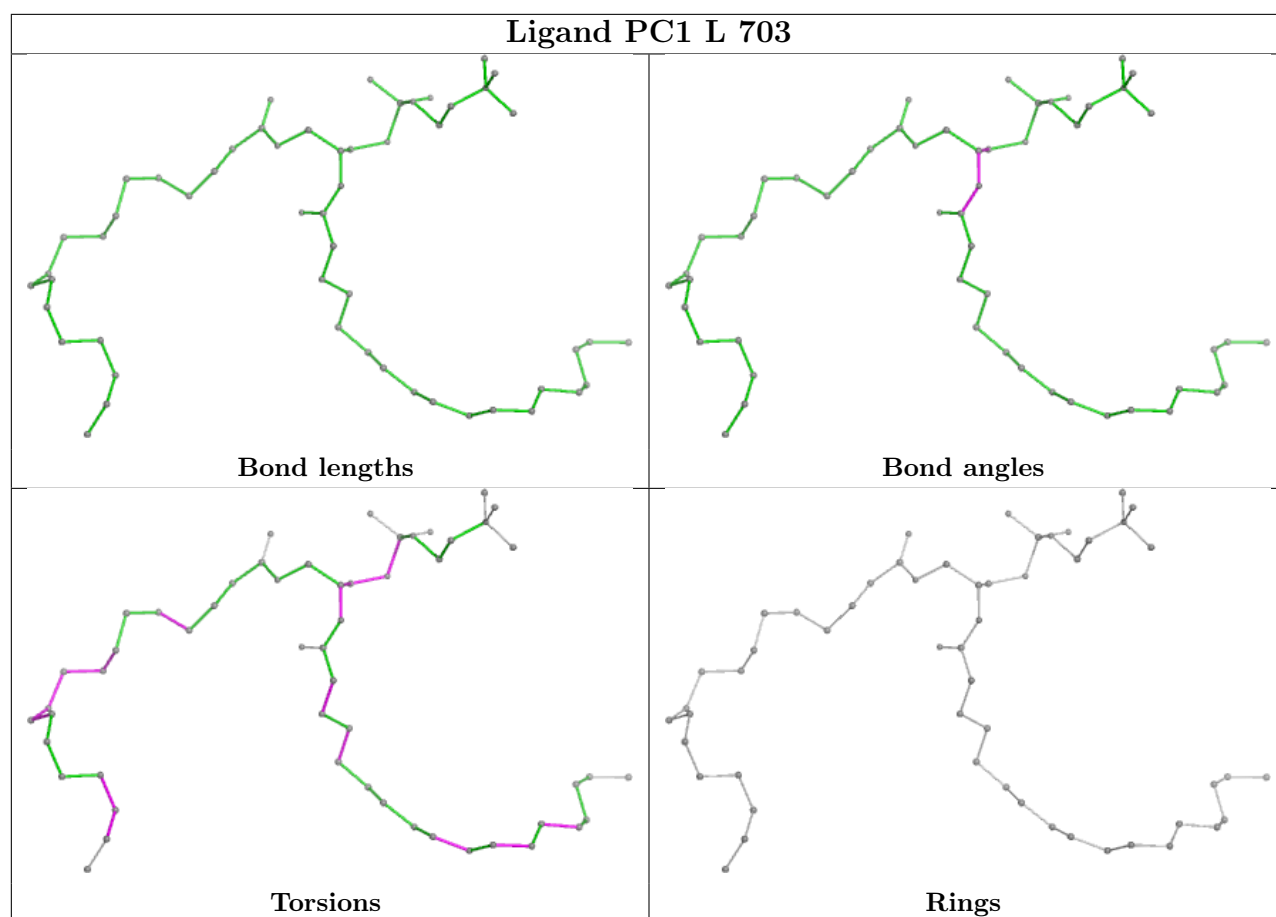


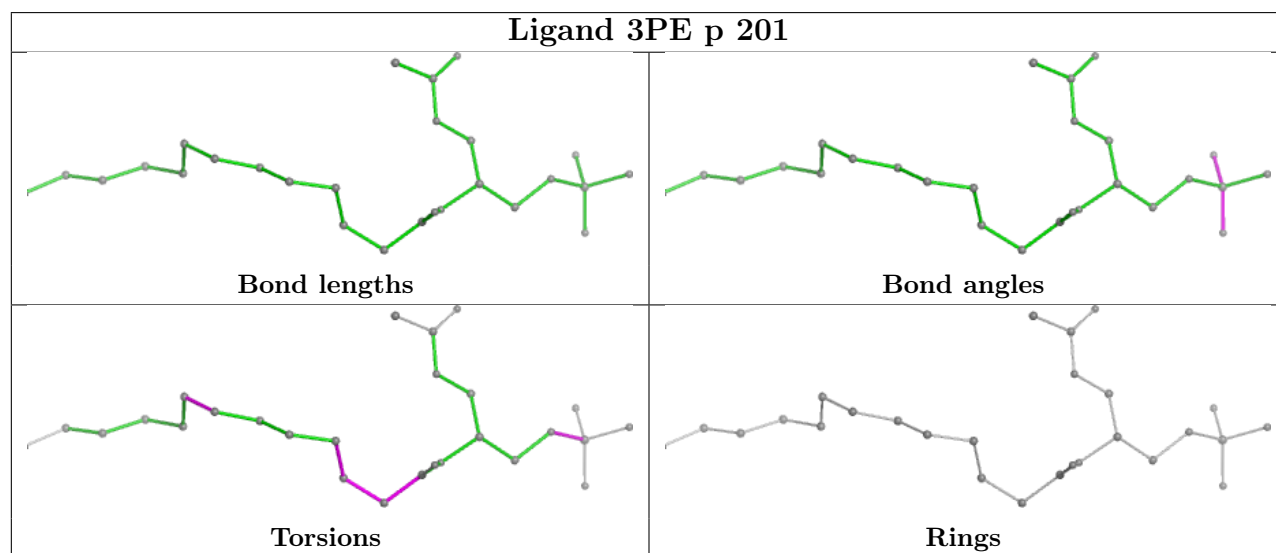
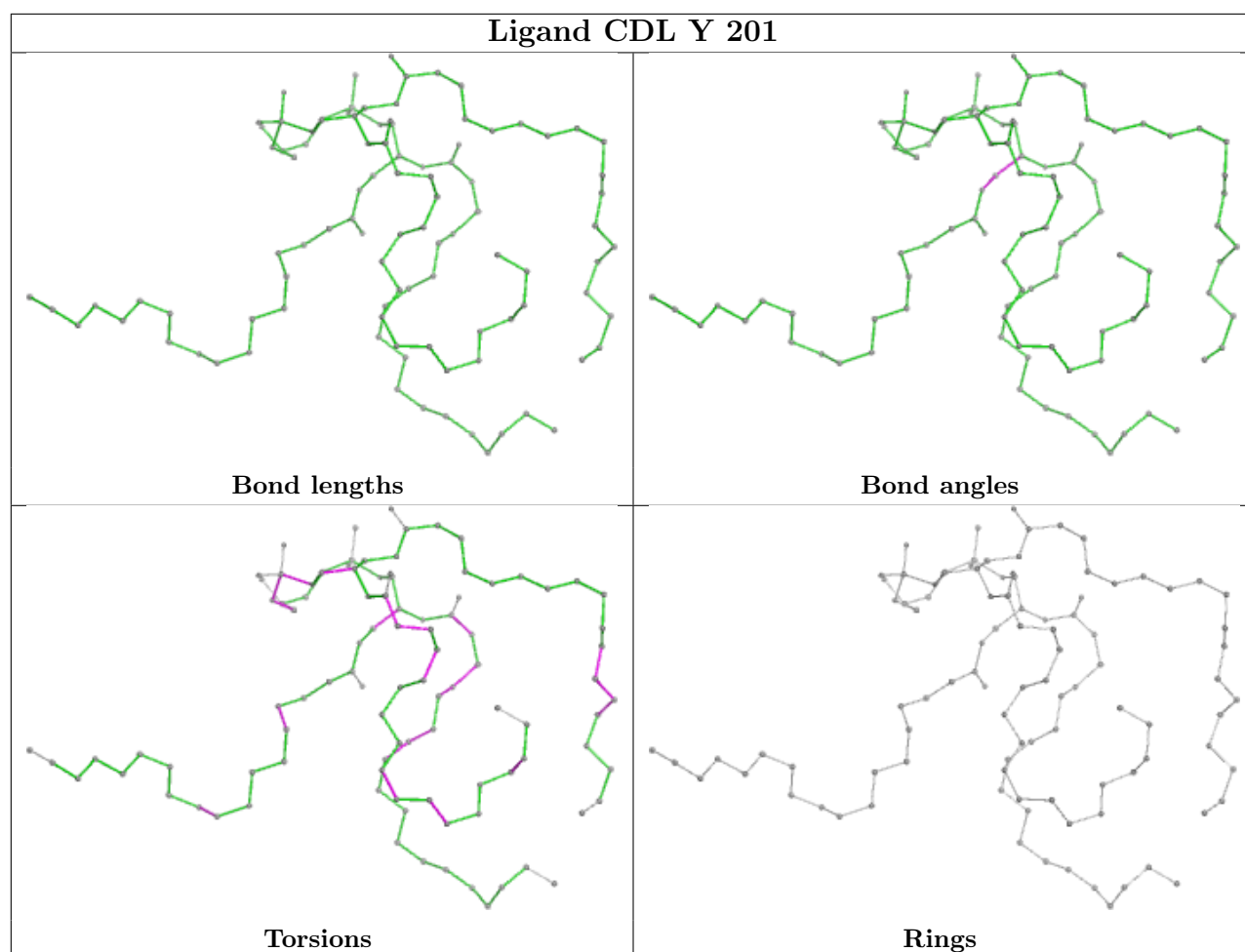


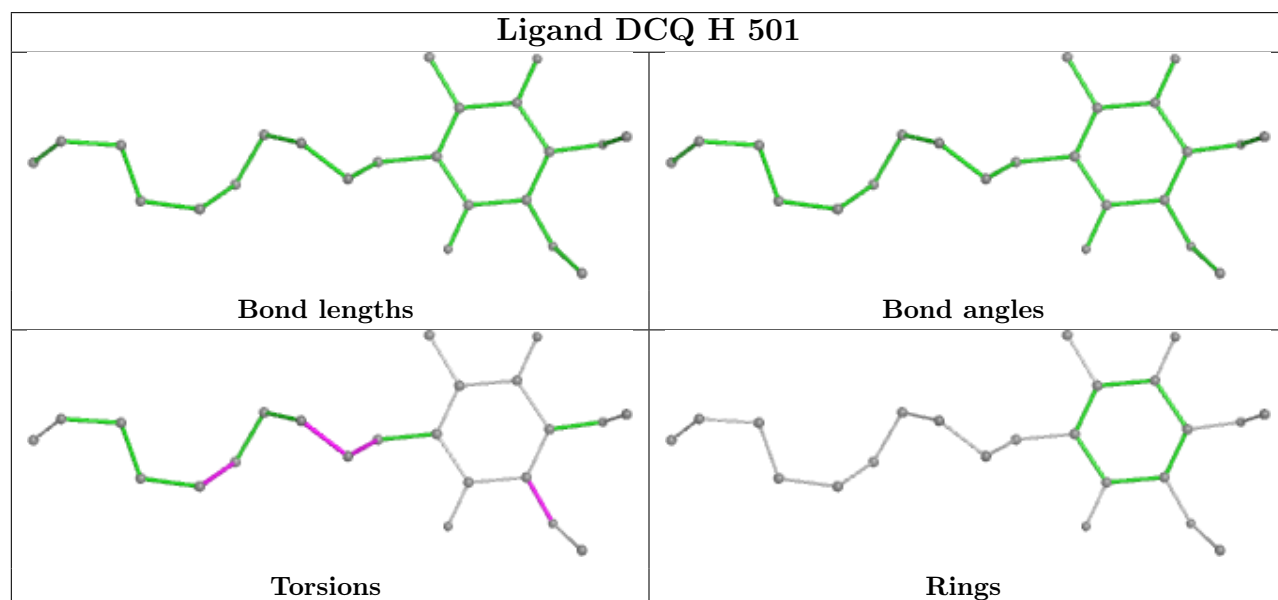
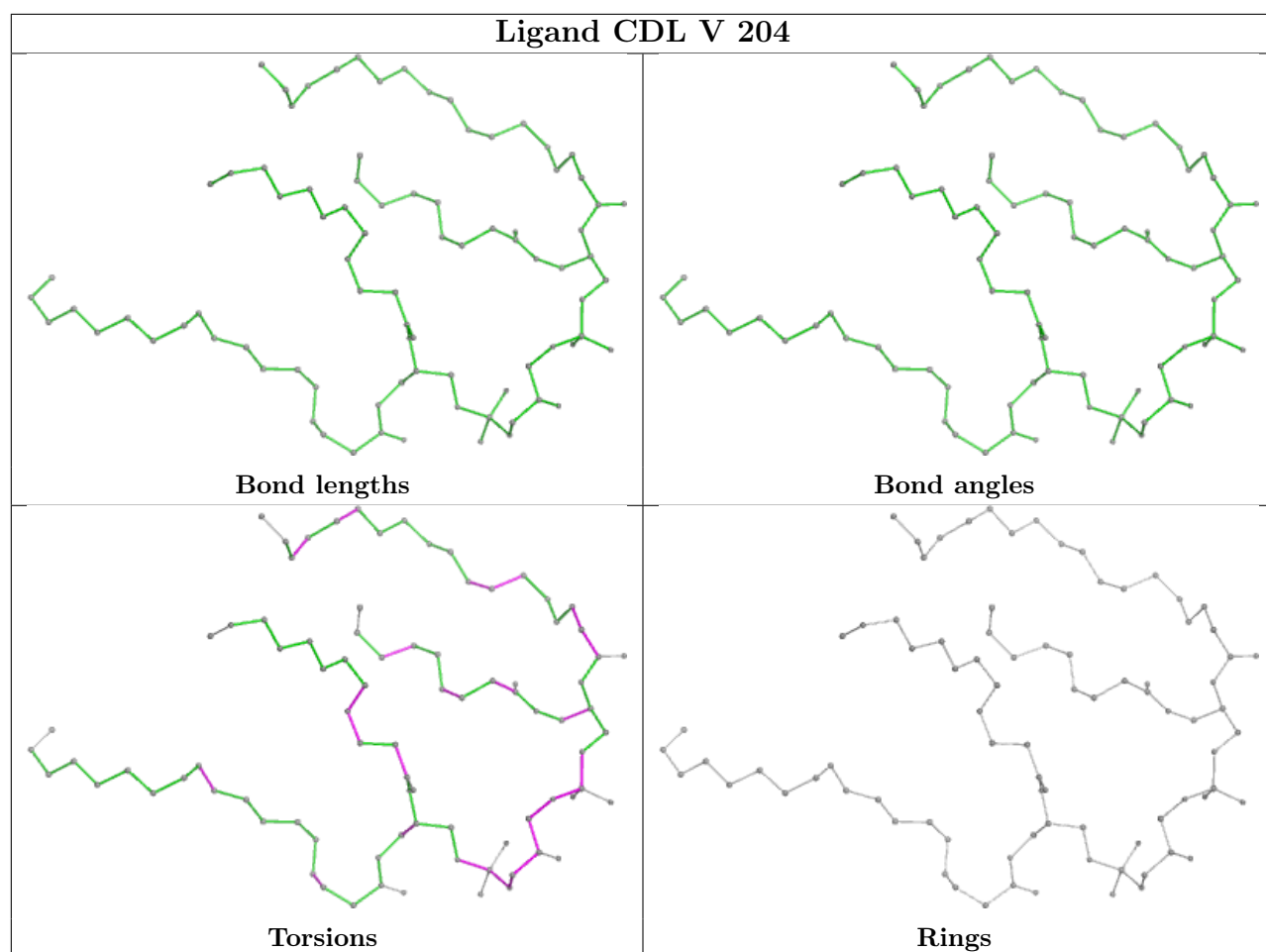


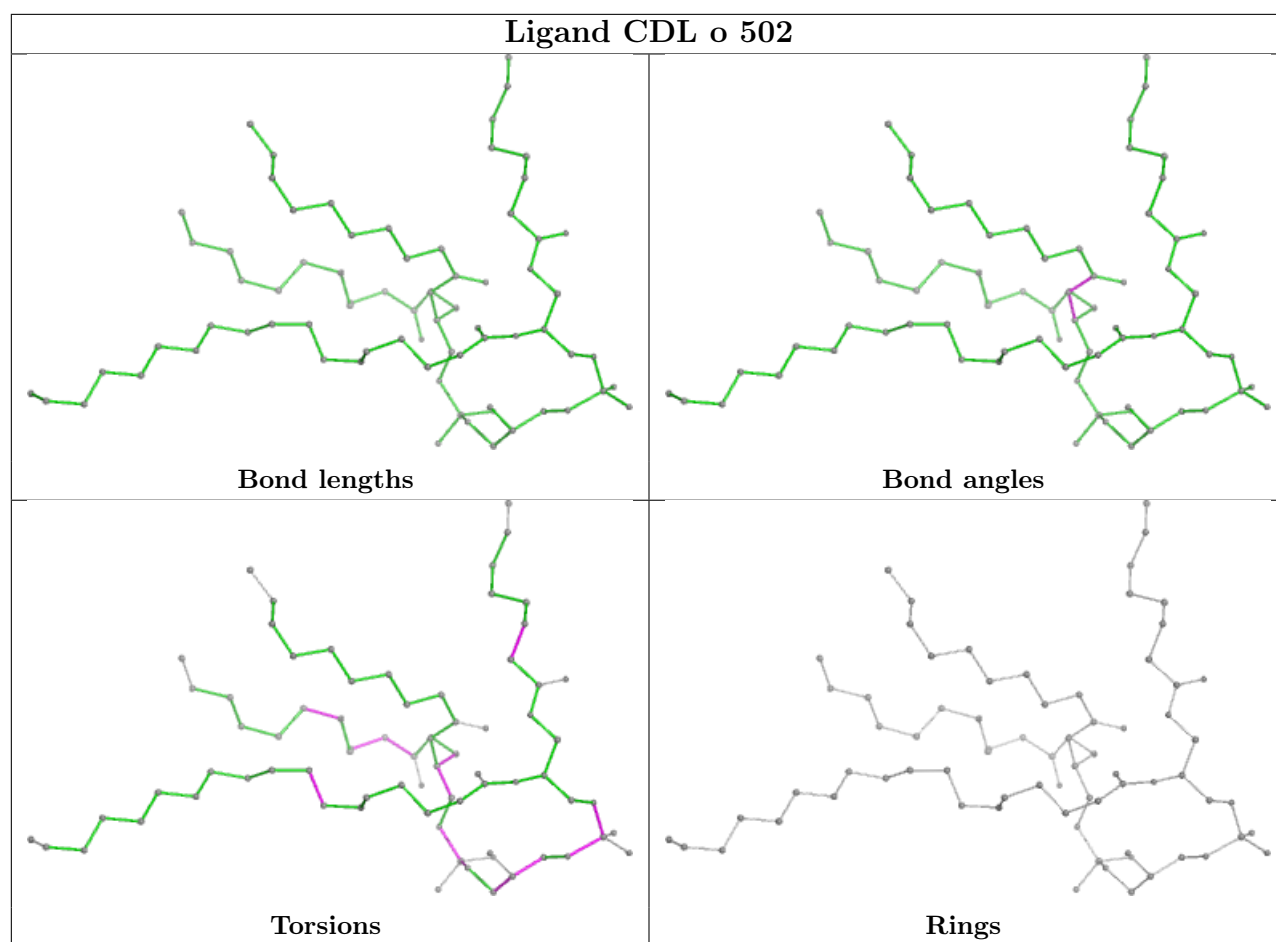


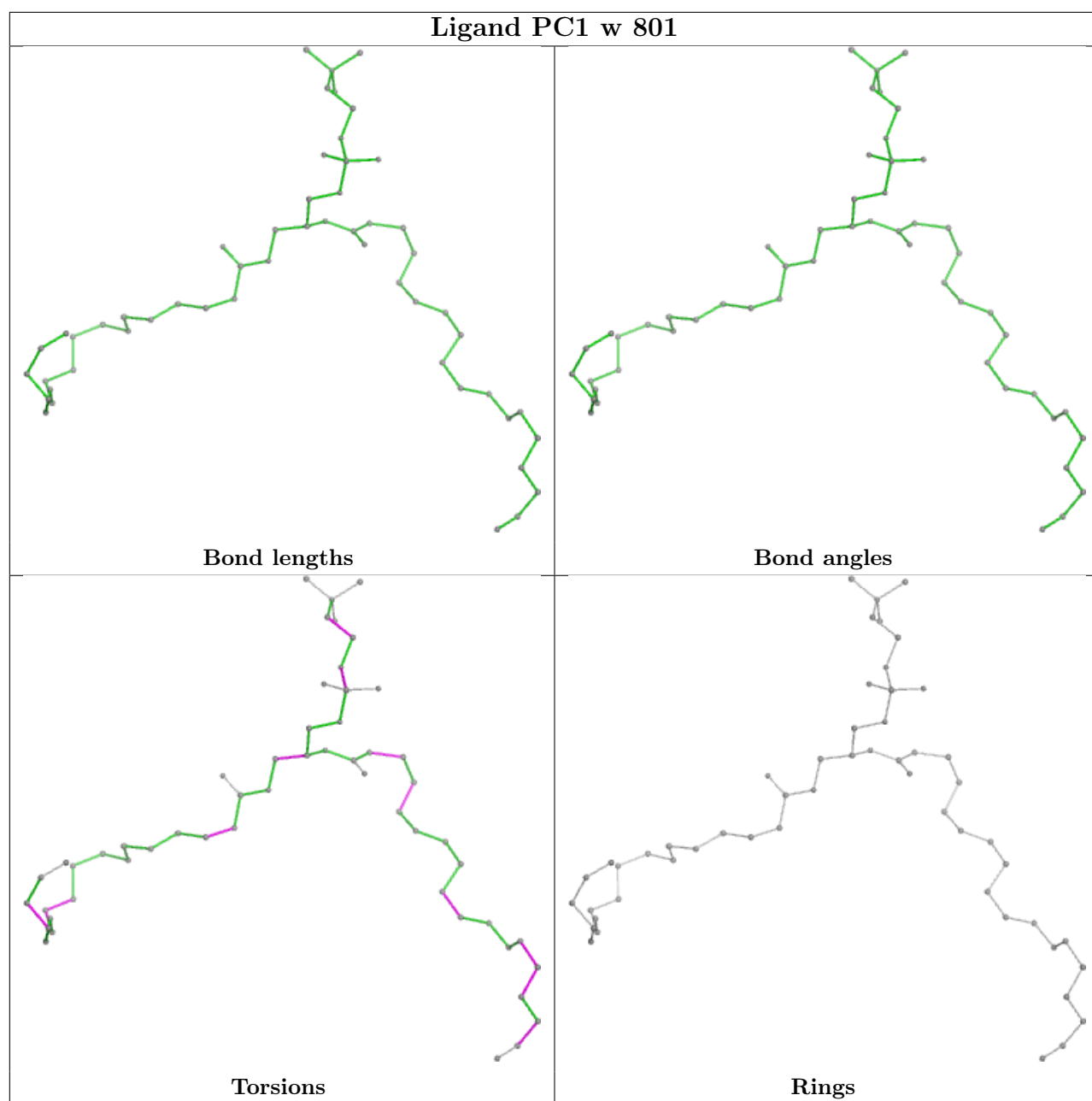




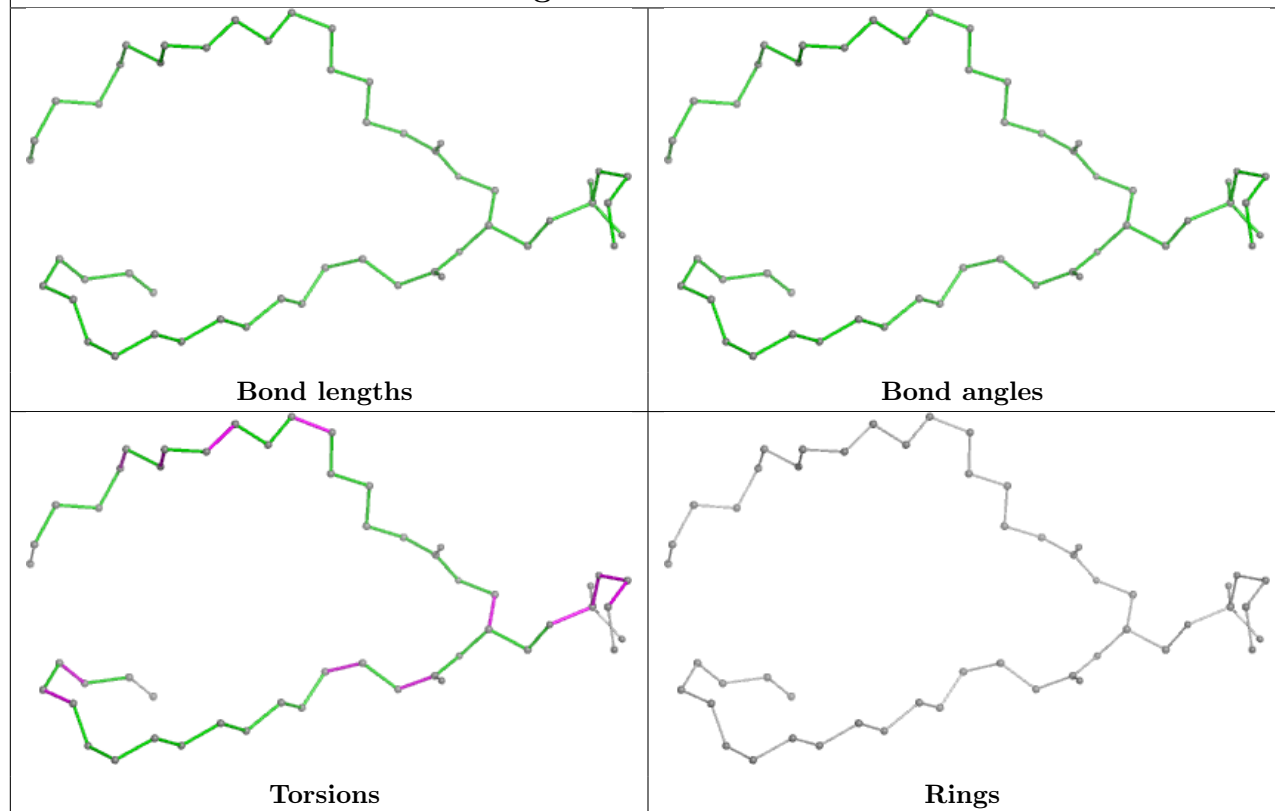




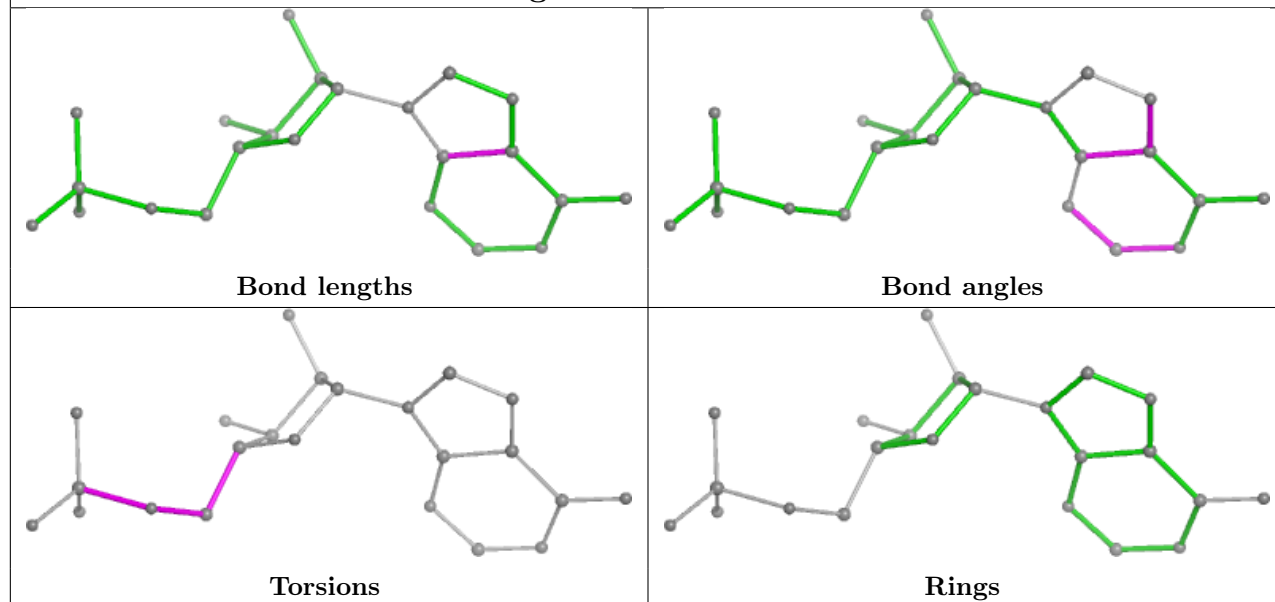


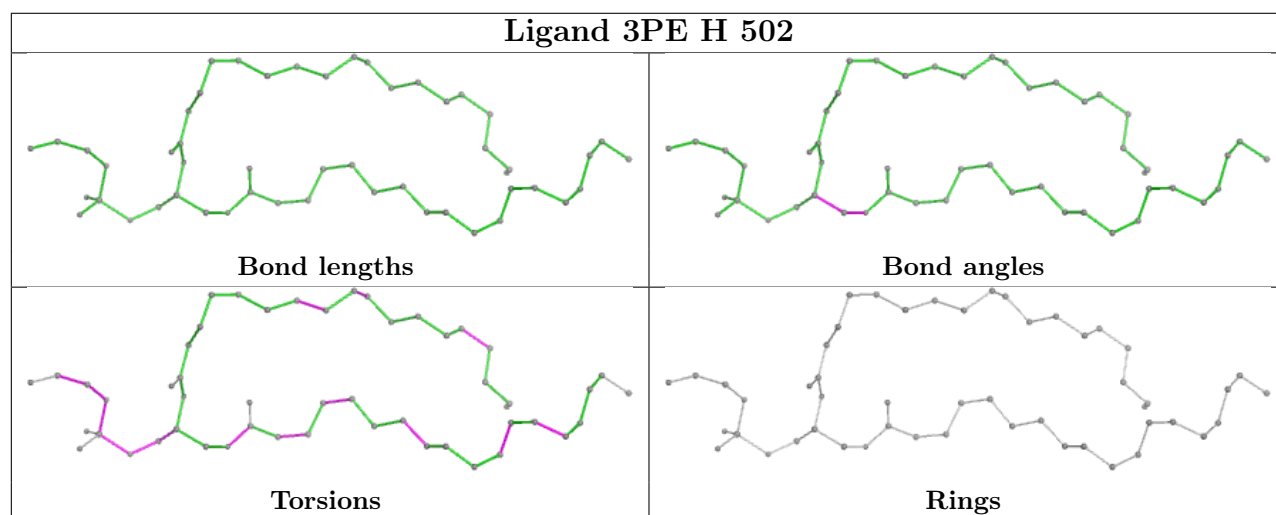
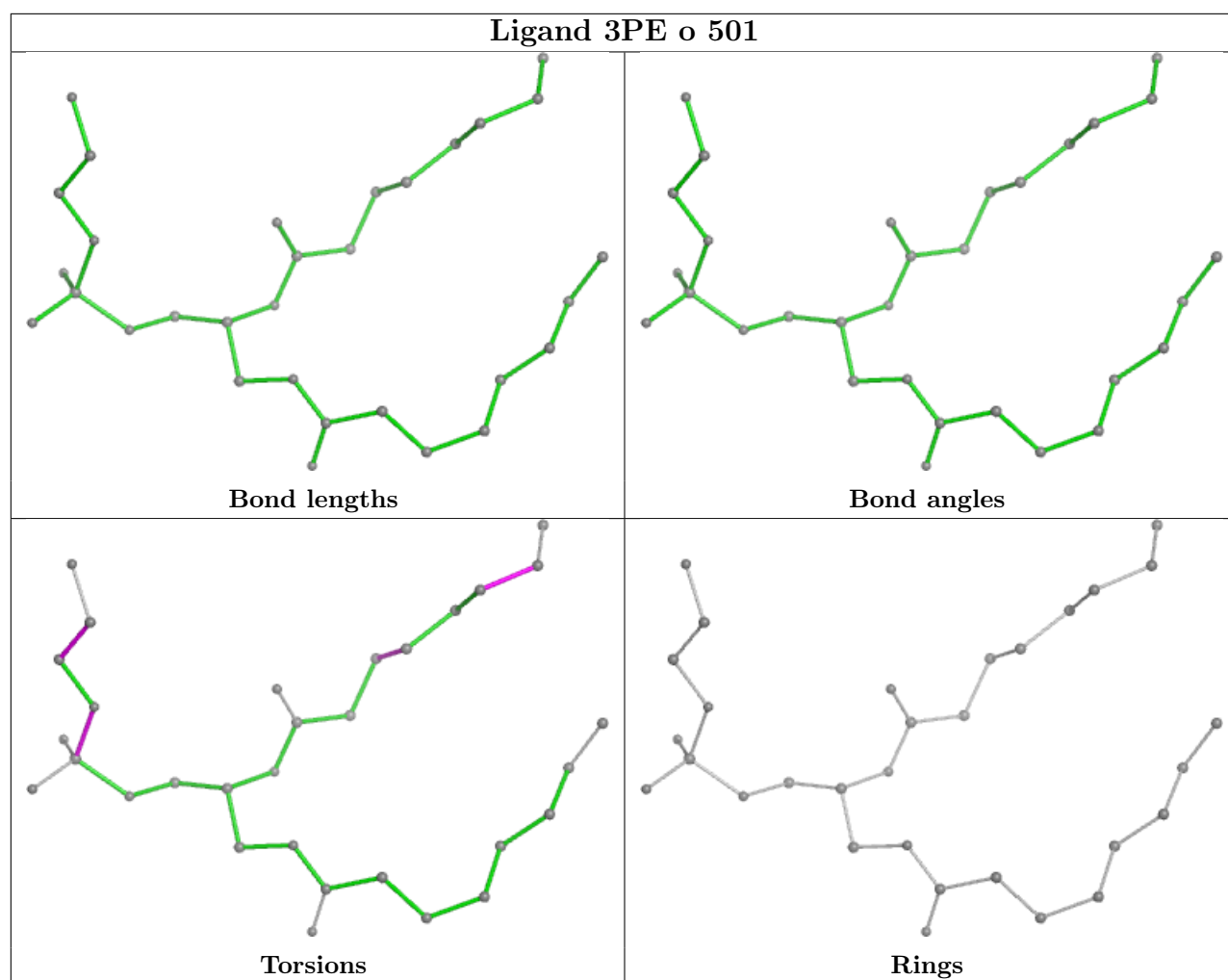


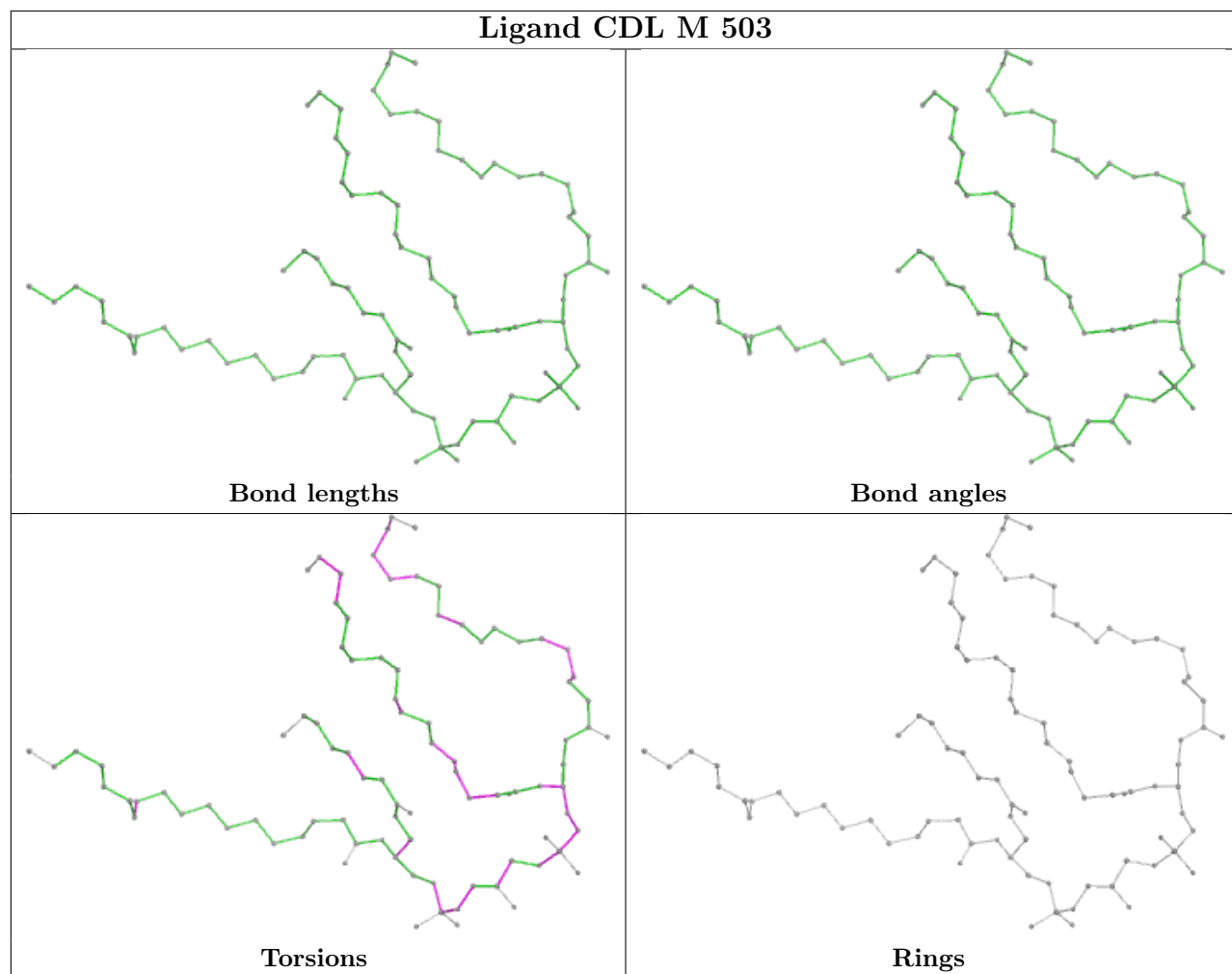
Ligand 3PE m 101

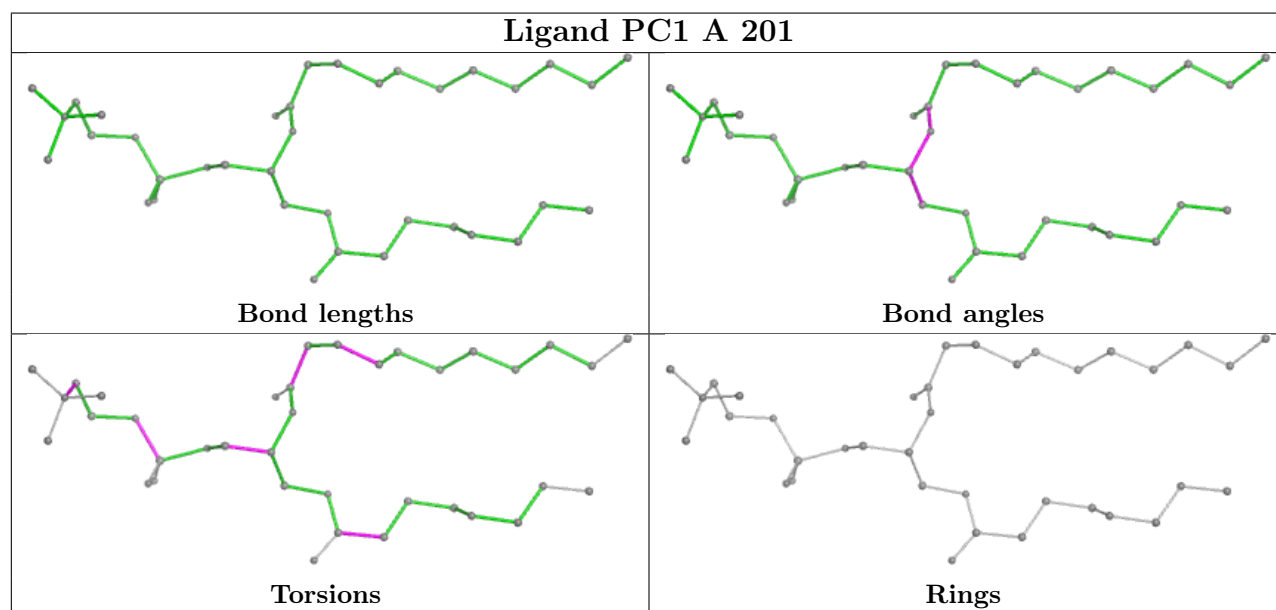
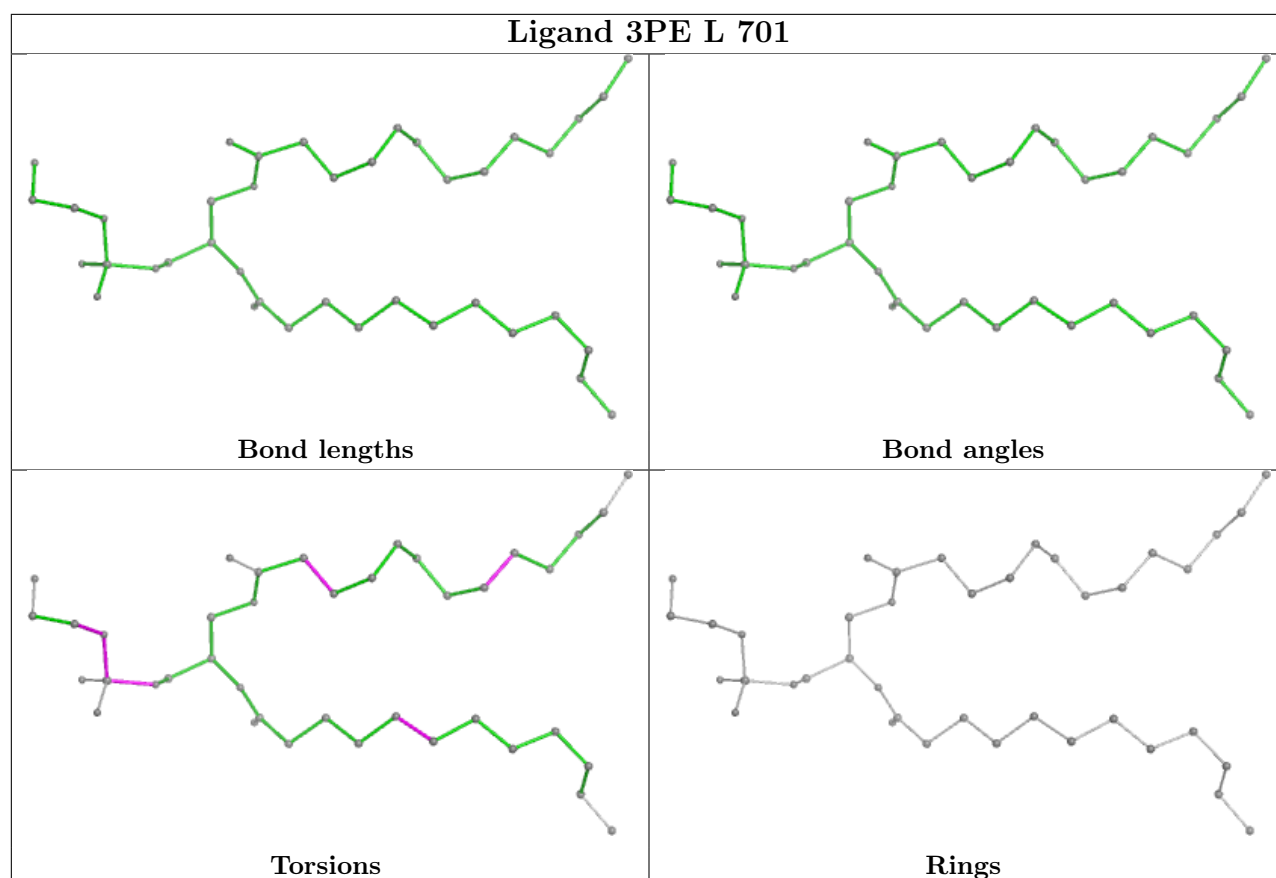


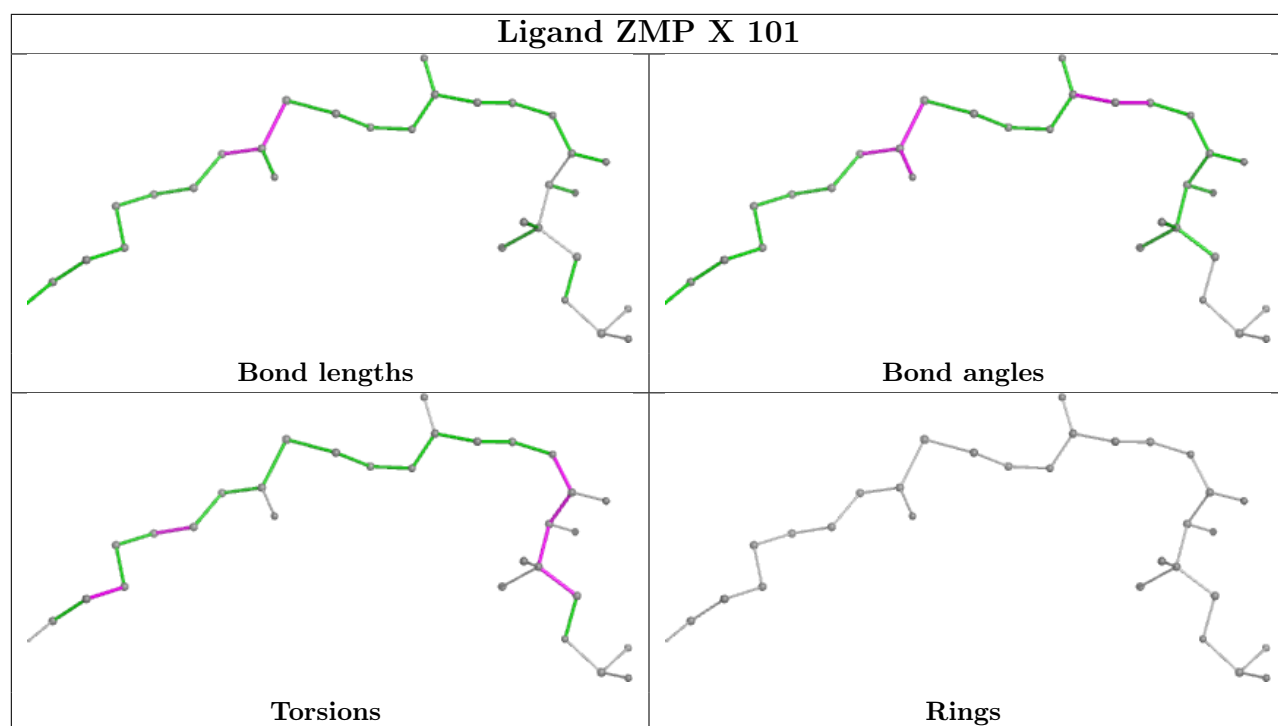
Ligand AMP k 501

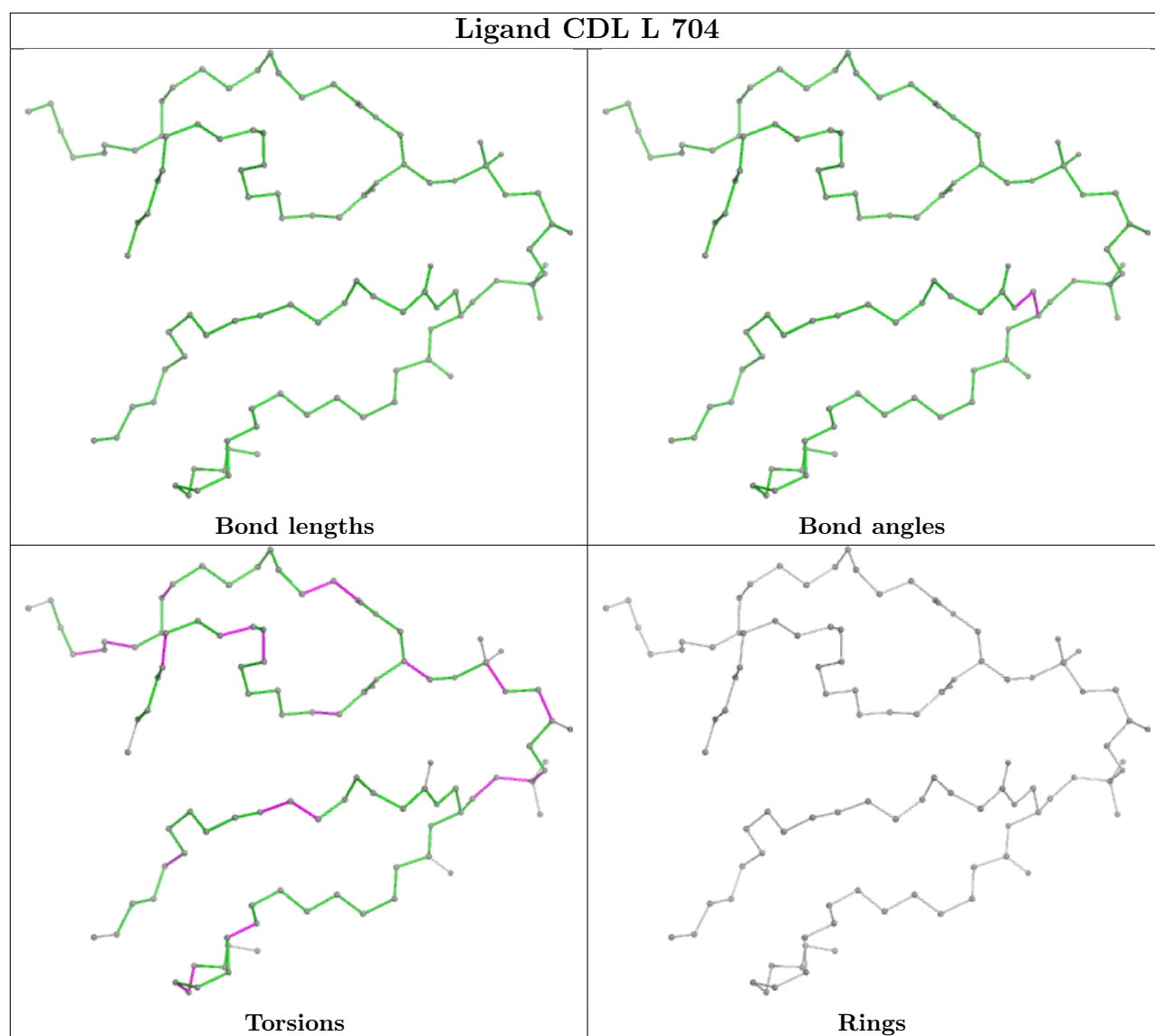


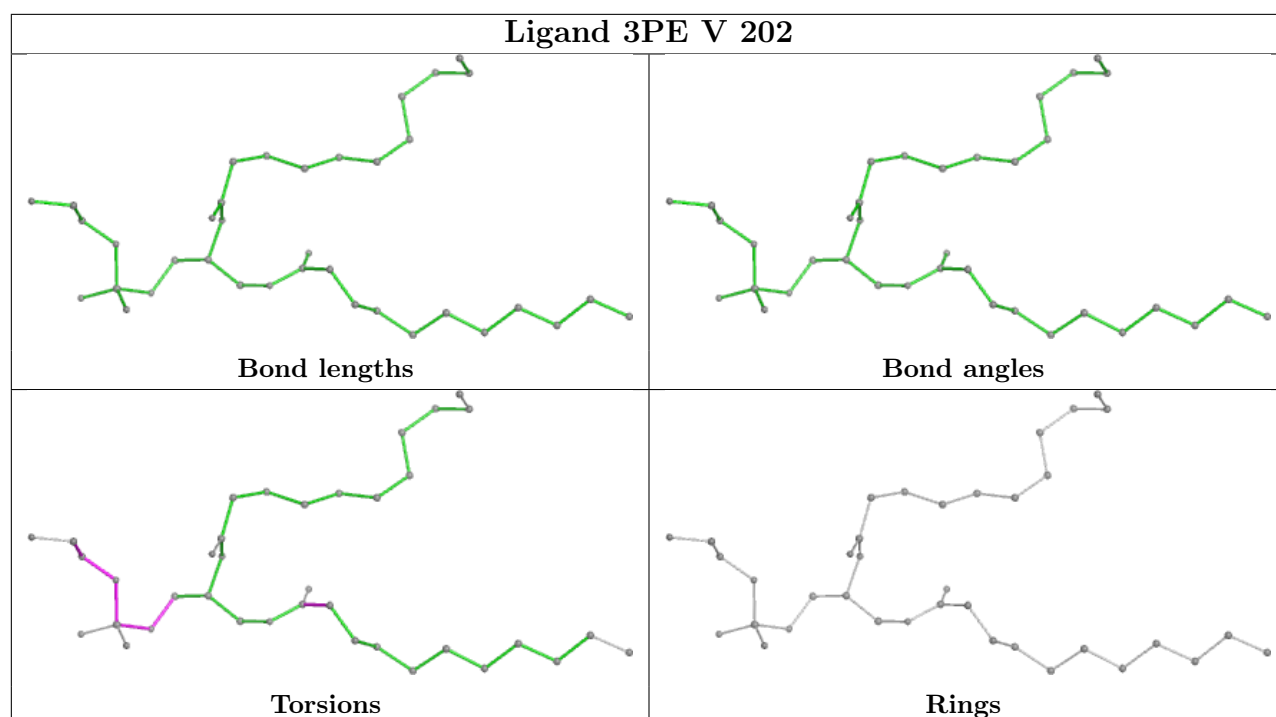












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11242. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.