



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 11:34 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 wwPDB EM Validation Summary 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

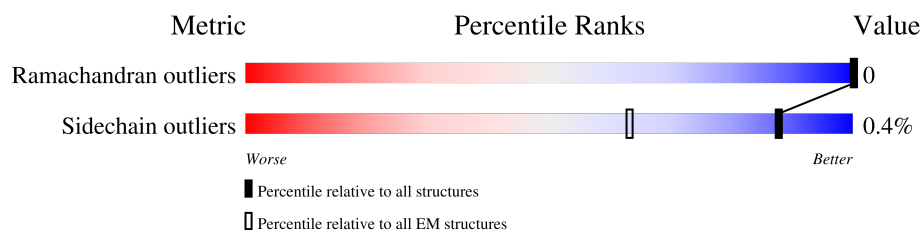
1 Overall quality at a glance

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	
12	Z	175	
13	k	355	
14	l	106	
15	m	84	
16	n	98	
17	o	122	
18	p	130	
19	q	144	
20	r	128	
21	s	137	
22	t	179	
23	u	108	
24	v	186	
25	w	154	
26	x	76	
27	y	58	
28	z	70	
29	4	463	

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		

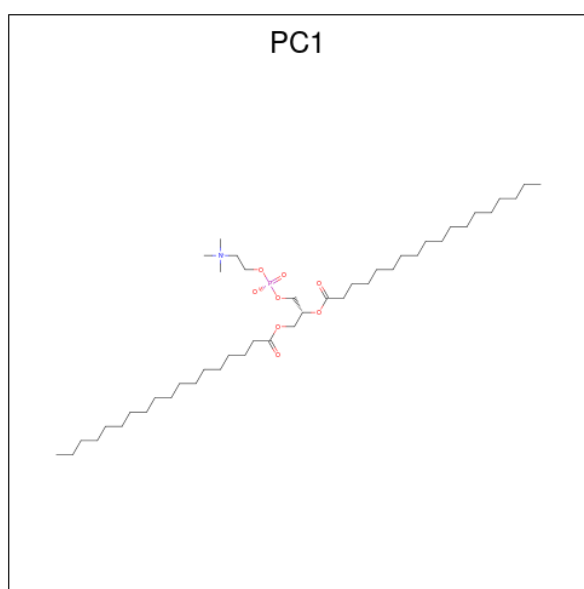
- Molecule 28 is a protein called Mitochondrial complex I, MWFE subunit.

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.

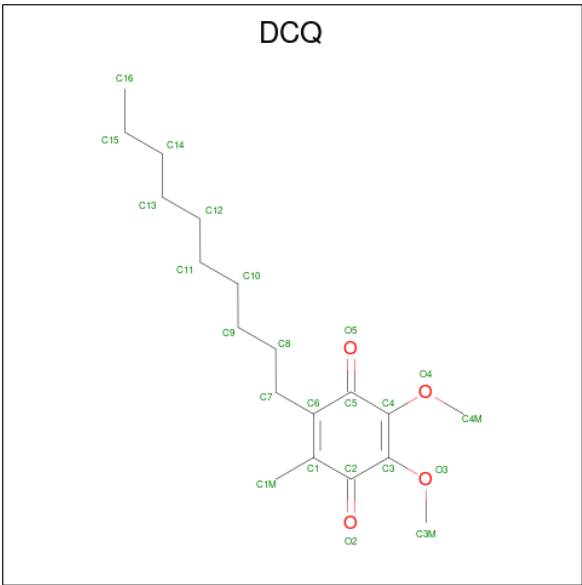
Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	40	Total	C	N	O	S	0	0
			334	217	56	60	1		

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



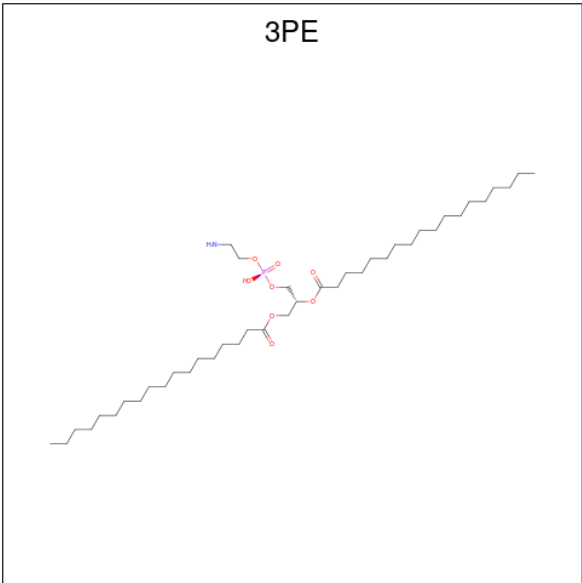
Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
30	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
30	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

- 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: $C_{41}H_{82}NO_8P$).



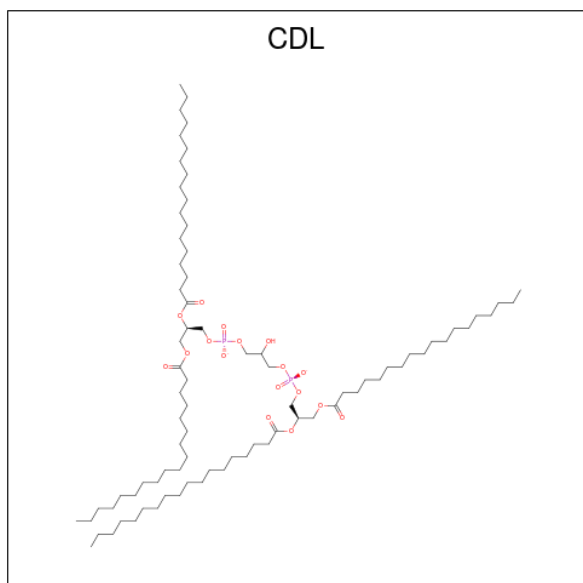
Mol	Chain	Residues	Atoms					AltConf
32	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
32	K	1	Total	C	N	O	P	0
			40	30	1	8	1	

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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: $C_{81}H_{156}O_{17}P_2$).



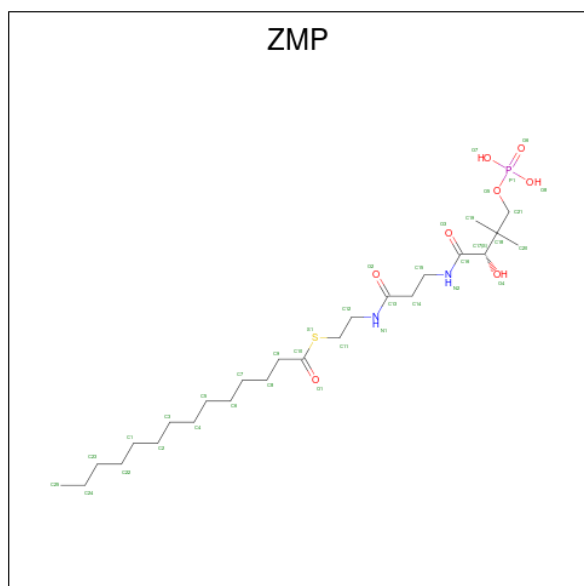
Mol	Chain	Residues	Atoms				AltConf
33	L	1	Total	C	O	P	0
			100	81	17	2	

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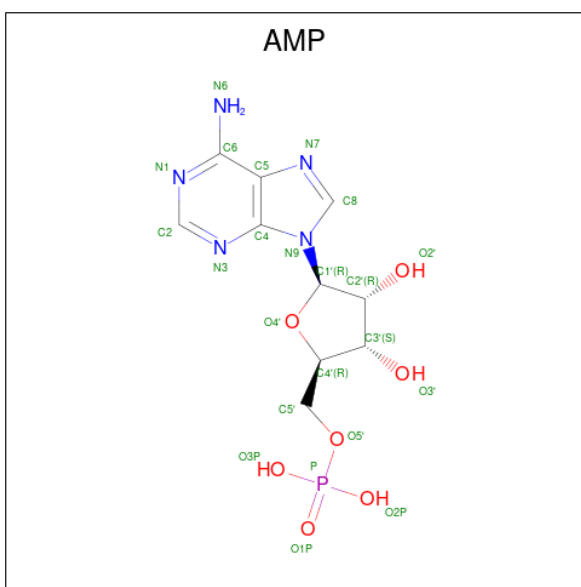
Mol	Chain	Residues	Atoms				AltConf
33	M	1	Total	C	O	P	0
			90	71	17	2	
33	V	1	Total	C	O	P	0
			94	75	17	2	
33	V	1	Total	C	O	P	0
			85	66	17	2	
33	W	1	Total	C	O	P	0
			100	81	17	2	
33	Y	1	Total	C	O	P	0
			100	81	17	2	
33	o	1	Total	C	O	P	0
			75	56	17	2	

- 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).



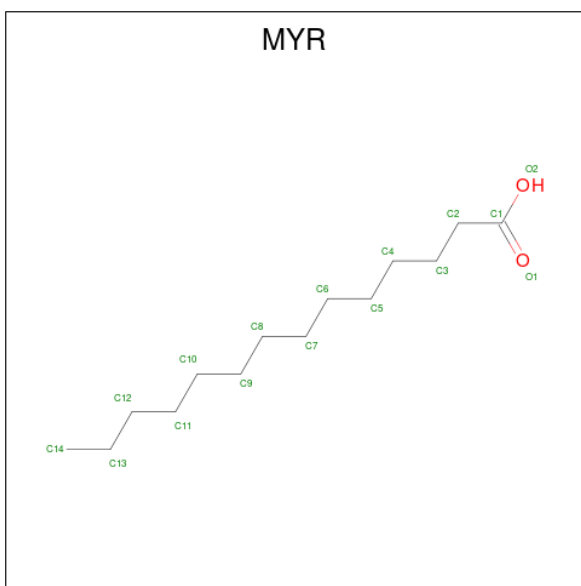
Mol	Chain	Residues	Atoms						AltConf
34	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

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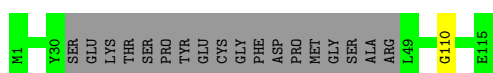
Mol	Chain	Residues	Atoms		AltConf
37	u	1	Total 1	O 1	0
37	v	41	Total 41	O 41	0
37	w	41	Total 41	O 41	0
37	x	6	Total 6	O 6	0
37	y	21	Total 21	O 21	0
37	z	18	Total 18	O 18	0
37	4	24	Total 24	O 24	0

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%



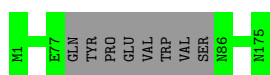
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

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%



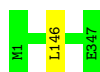
- Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain M:  99%



- Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N: 100%



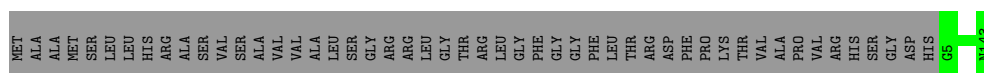
- Molecule 8: Mitochondrial complex I, B14.7 subunit

Chain V: 98%



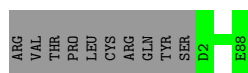
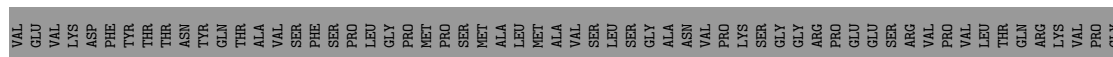
- Molecule 9: NADH:ubiquinone oxidoreductase subunit B5

Chain W: 74% 26%



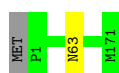
- Molecule 10: Acyl carrier protein

Chain X: 55% 45%



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

Chain Y: 99%




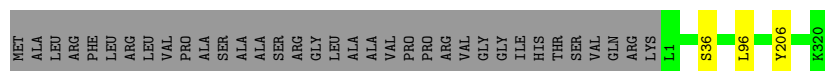
- Molecule 12: Mitochondrial complex I, PDSW subunit

Chain Z: 98%



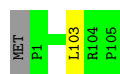
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:  89% 10%



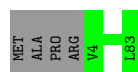
- Molecule 14: NADH:ubiquinone oxidoreductase subunit S5

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%



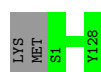
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:  98% .



- Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

Chain p:  98% .




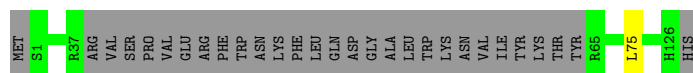
- Molecule 19: Mitochondrial complex I, B16.6 subunit

Chain q:  95% ..




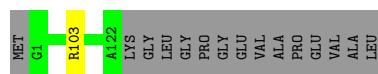
- Molecule 20: Mitochondrial complex I, B17 subunit

Chain r:  77% 23%



- Molecule 21: NADH:ubiquinone oxidoreductase subunit B7

Chain s:  88% 11%



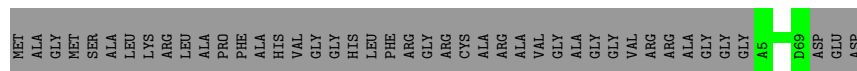
- Molecule 22: NADH:ubiquinone oxidoreductase subunit B9

Chain t:  98% ..




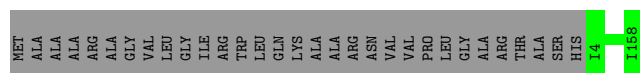
- Molecule 23: NADH:ubiquinone oxidoreductase subunit B2

Chain u:  60% 40%



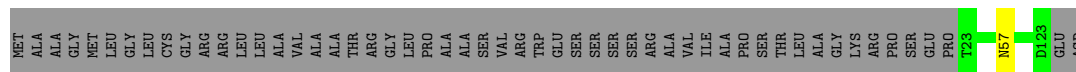
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:  83% 17%



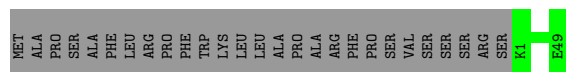
- Molecule 25: Mitochondrial complex I, ESSS subunit

Chain w:  65% 34%



- Molecule 26: Mitochondrial complex I, KFYI subunit

Chain x:  64% 36%



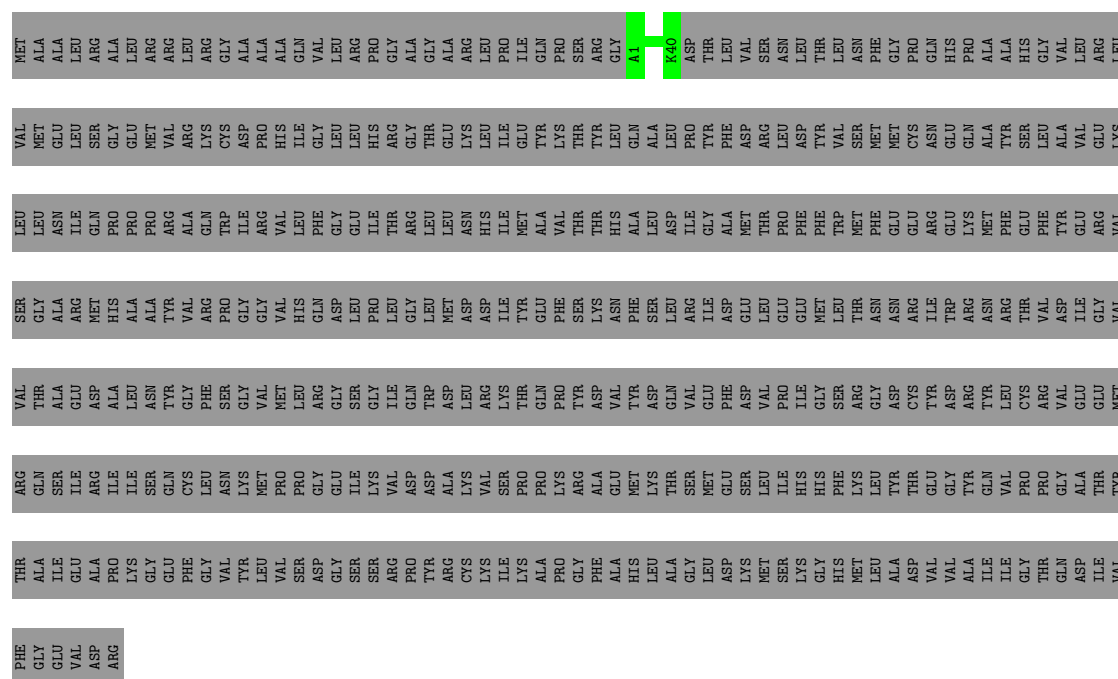
- Molecule 27: Mitochondrial complex I, MNLL subunit

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

The worst 5 of 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

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
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

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

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	s	103	ARG
25	w	57	ASN
5	L	541	ASN
6	M	138	ASN
6	M	144	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
17	o	61	GLN
19	q	23	ASN
19	q	53	ASN
7	N	144	GLN
12	Z	106	GLN

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

The worst 5 of 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
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

There are no chirality outliers.

5 of 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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-
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

The worst 5 of 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

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

5 of 449 torsion outliers are listed below:

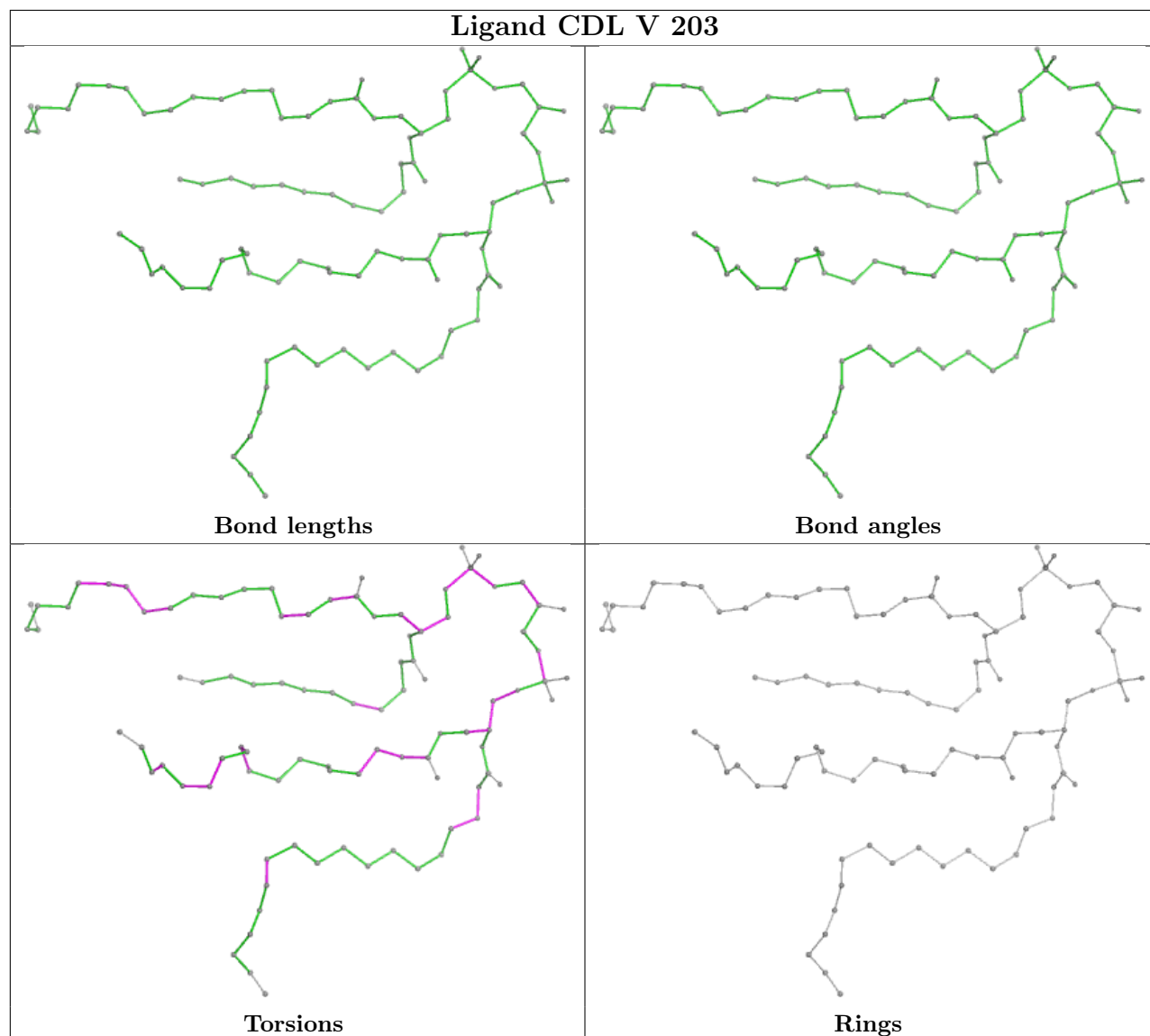
Mol	Chain	Res	Type	Atoms
30	H	503	PC1	C11-O13-P-O14
30	L	703	PC1	C1-O11-P-O12
30	M	502	PC1	C1-O11-P-O12
30	w	801	PC1	C11-O13-P-O14
30	w	801	PC1	O13-C11-C12-N

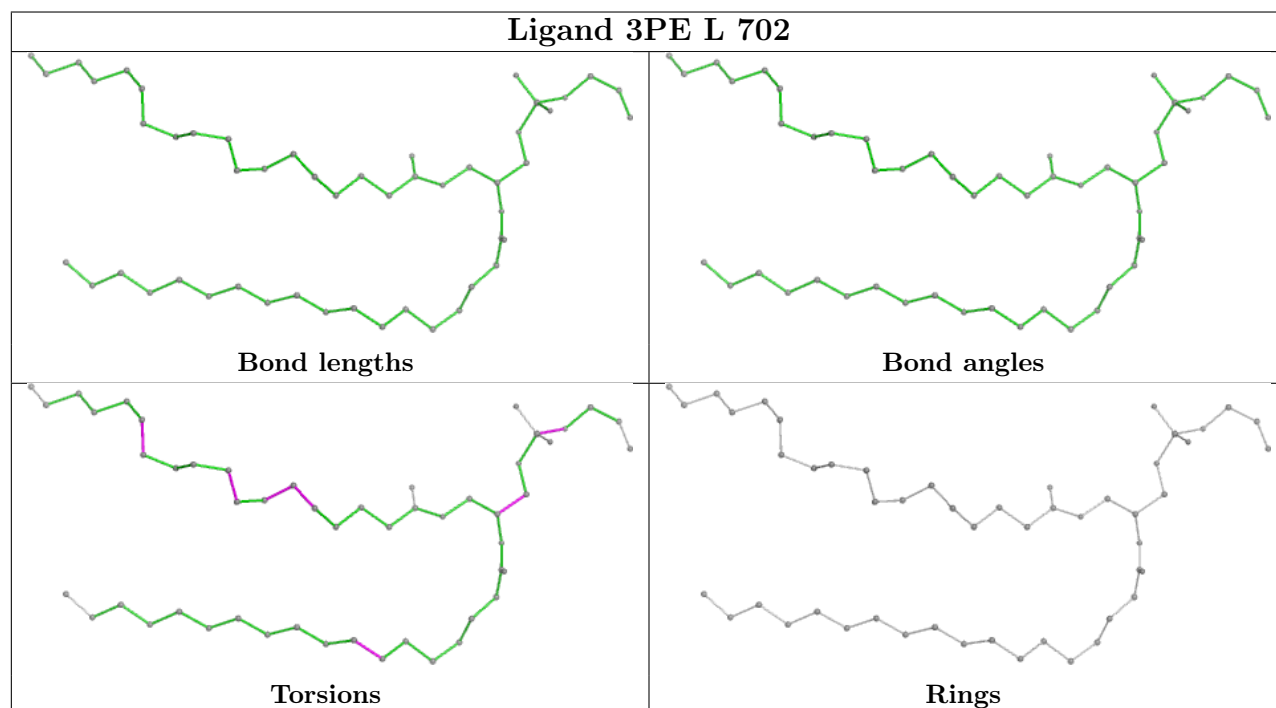
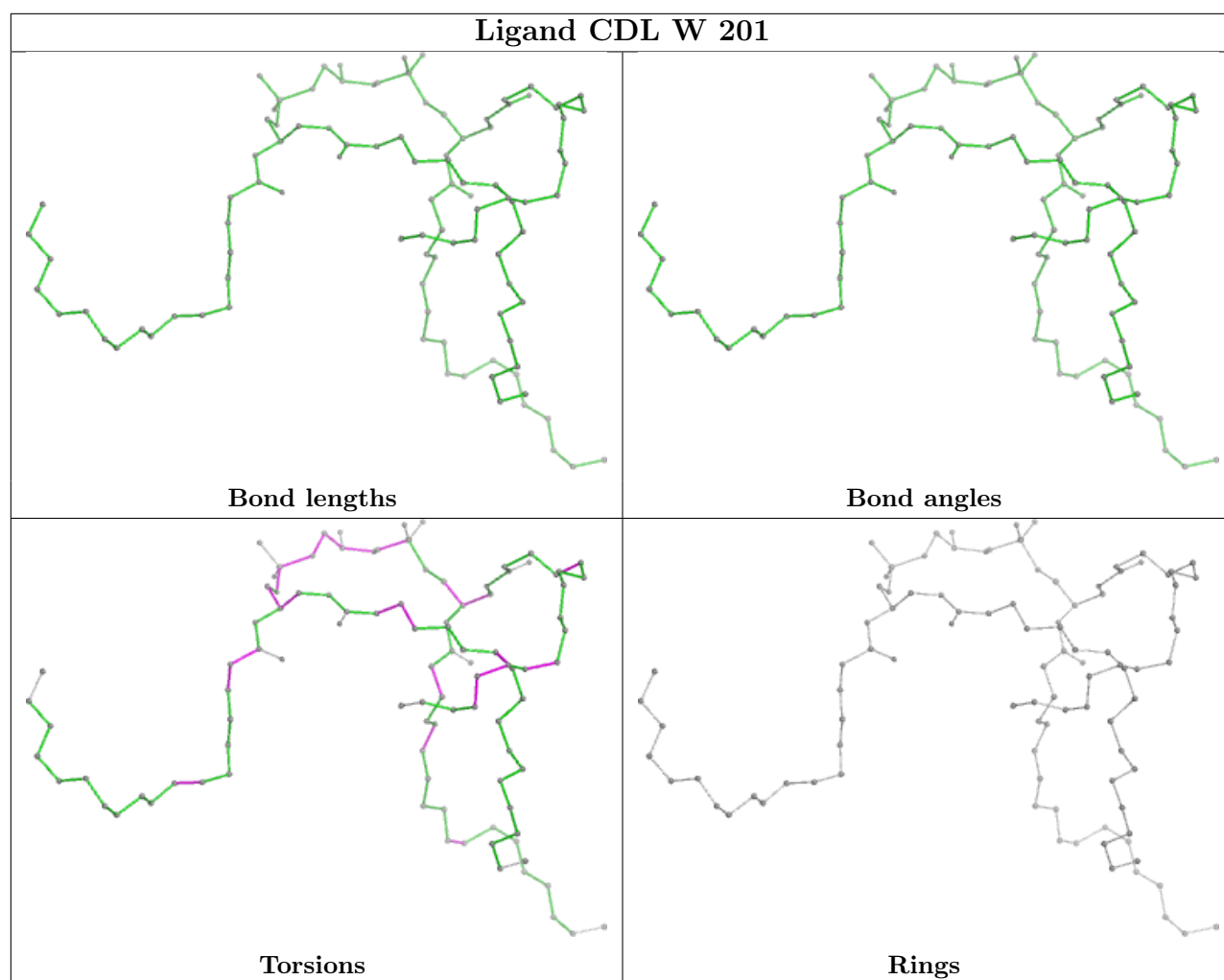
There are no ring outliers.

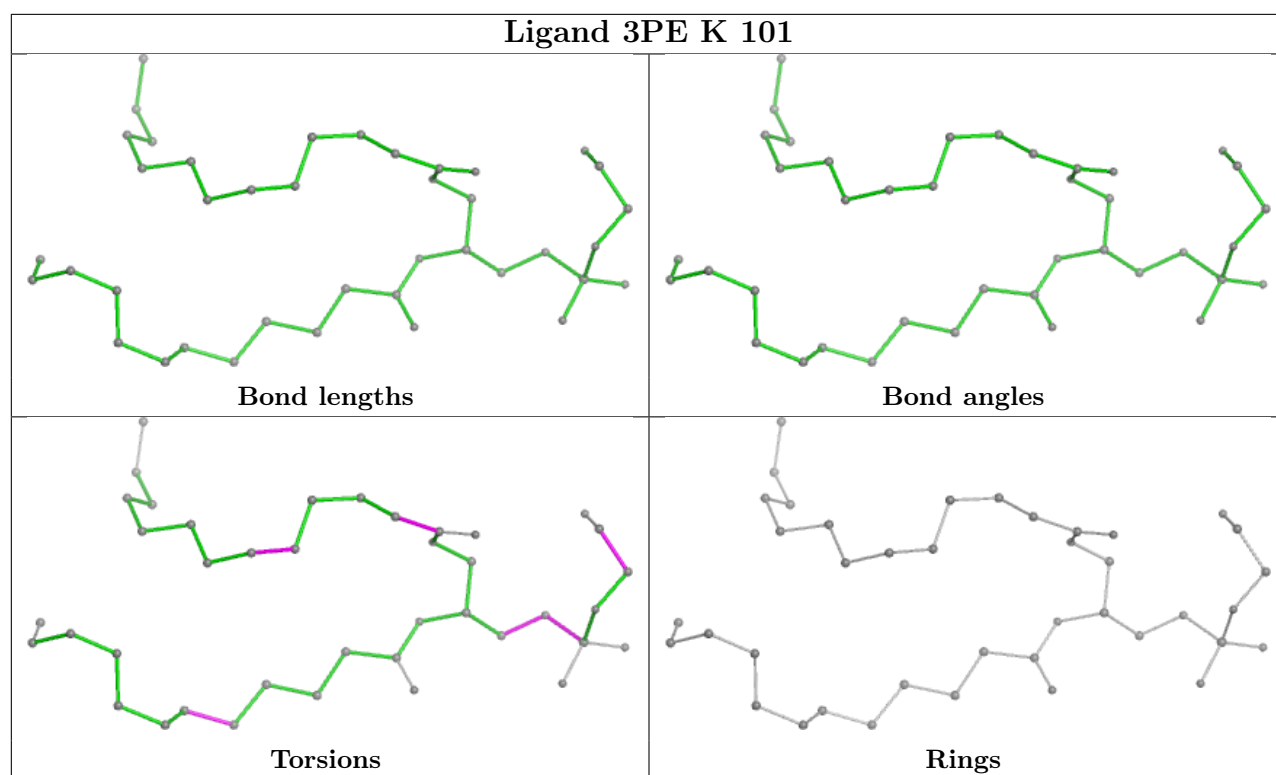
No monomer is involved in short contacts.

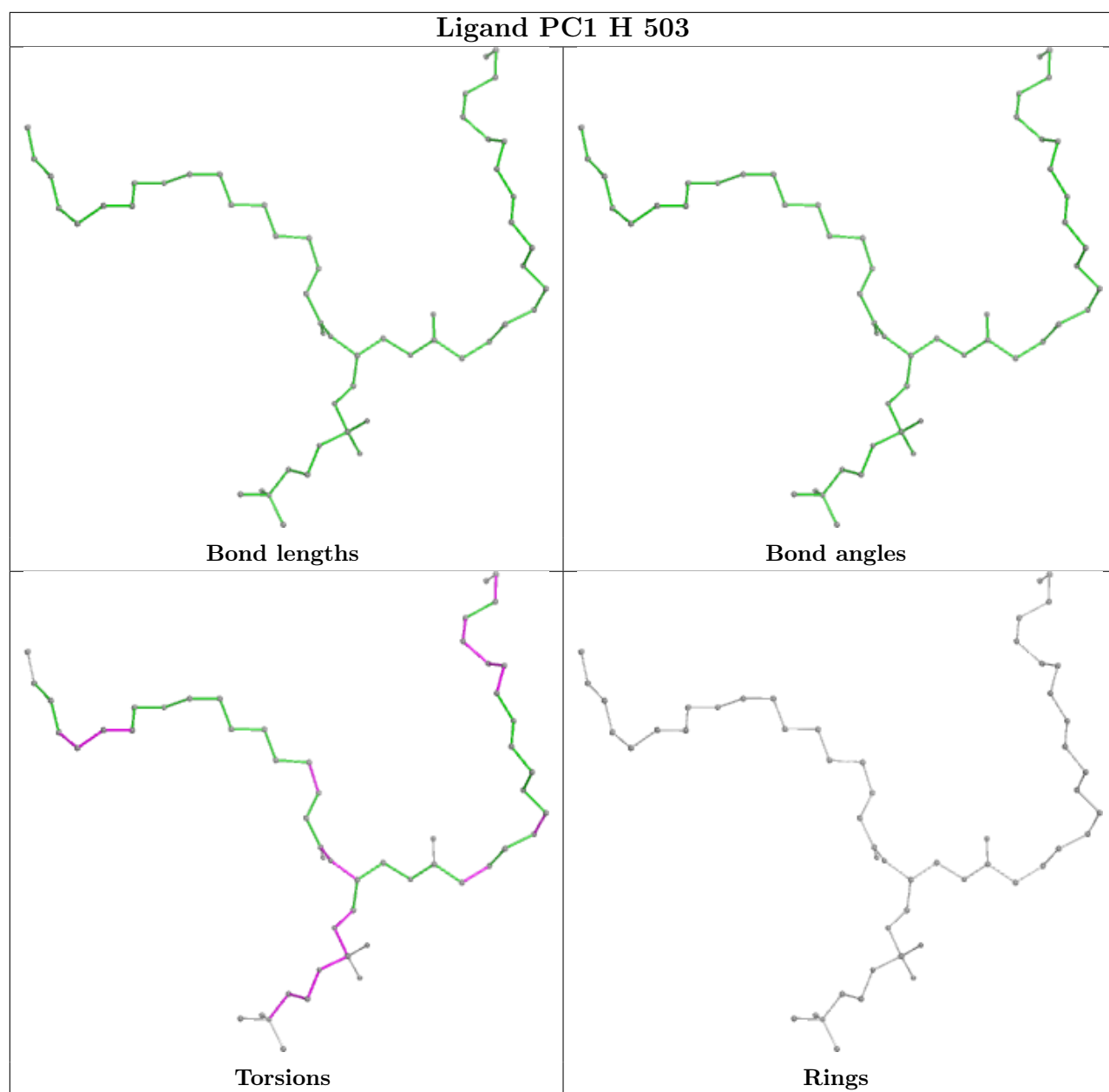
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

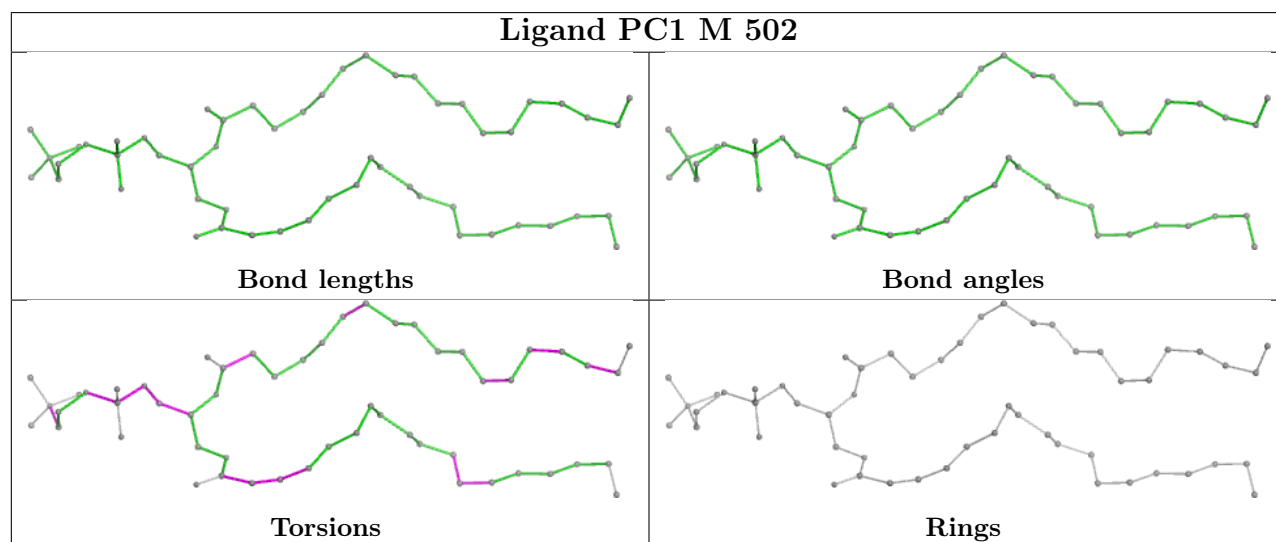
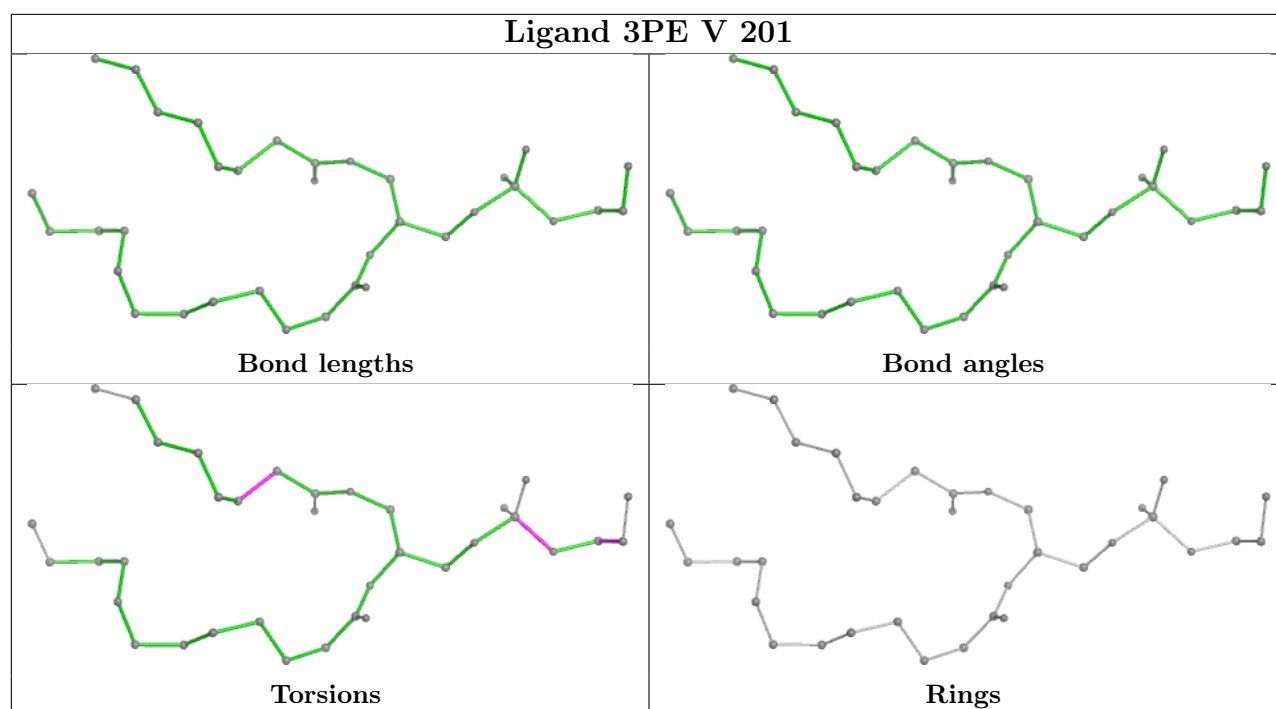
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

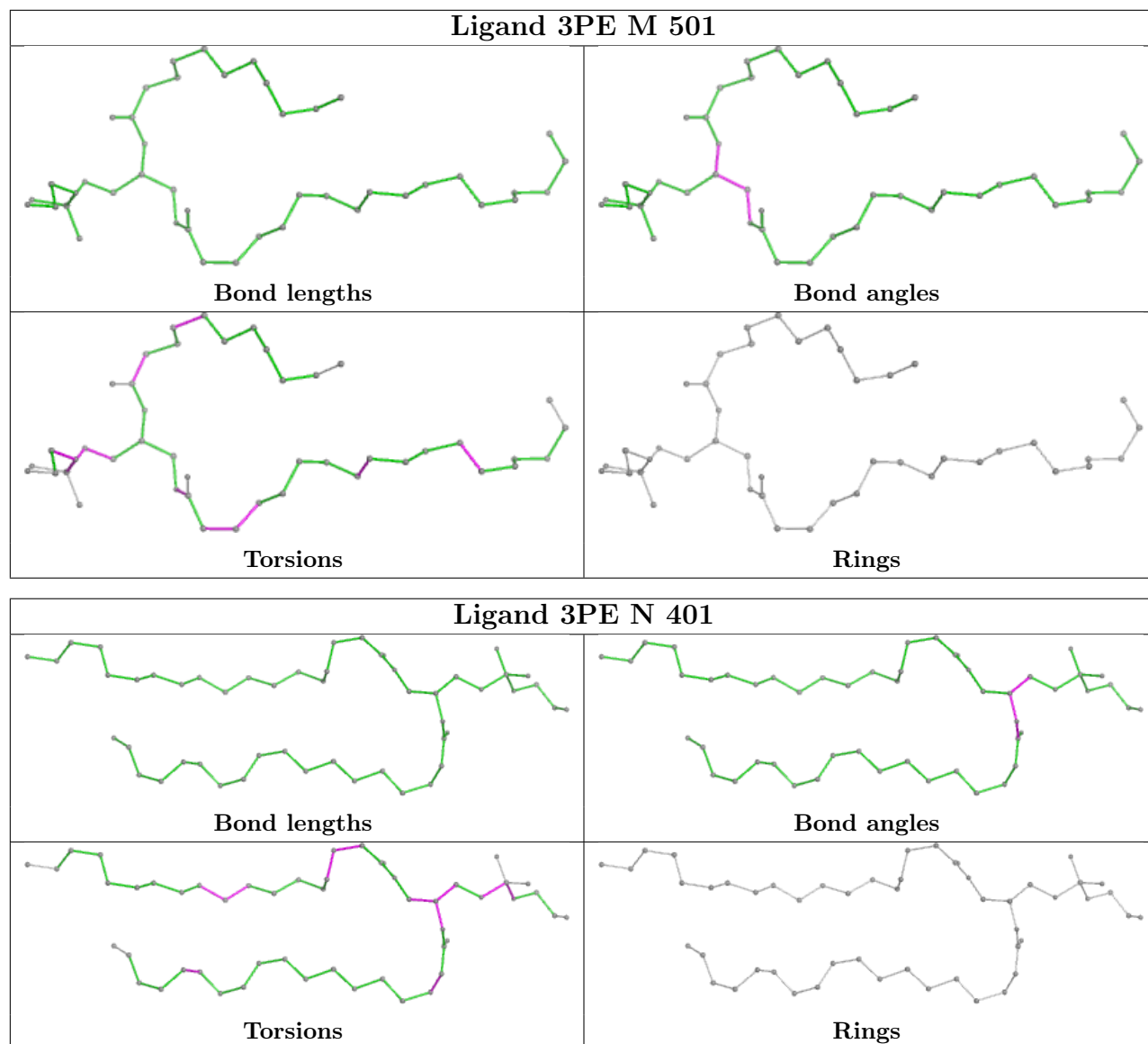


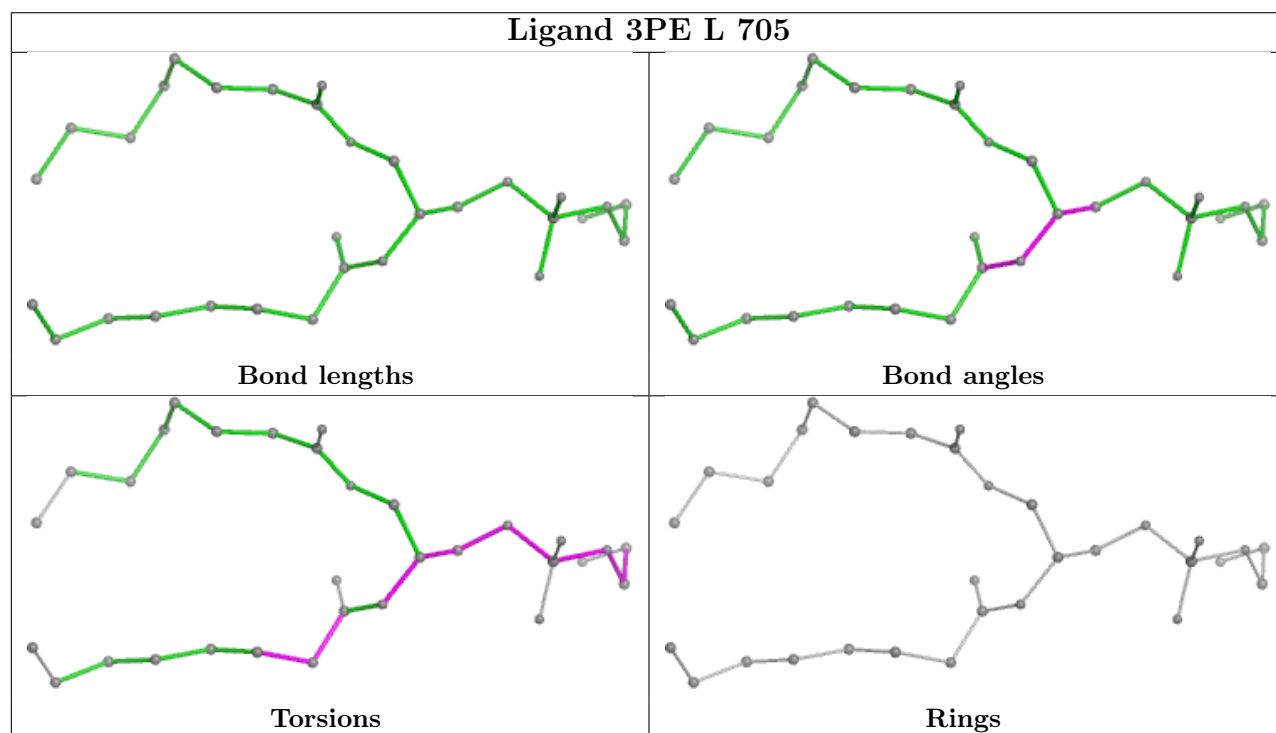
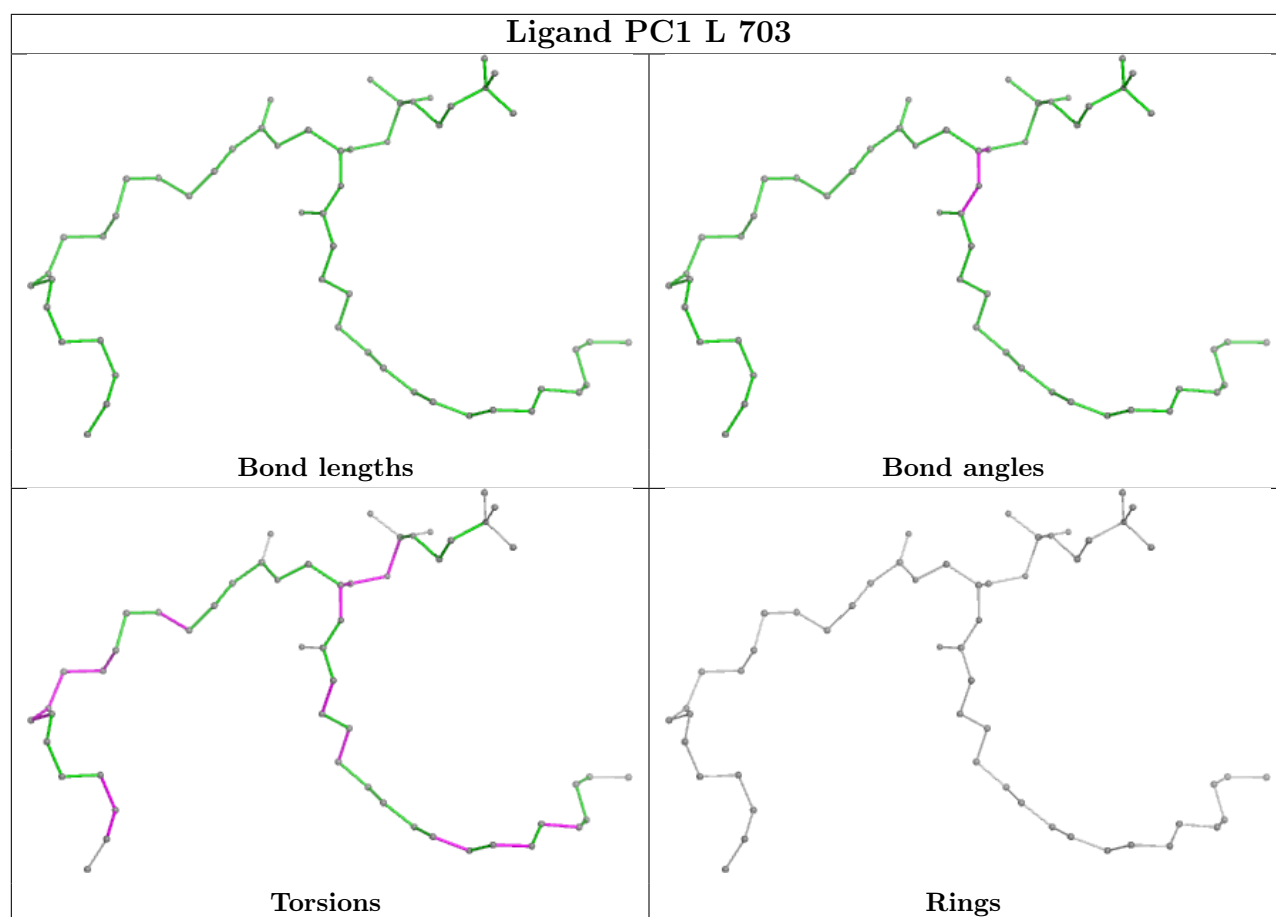


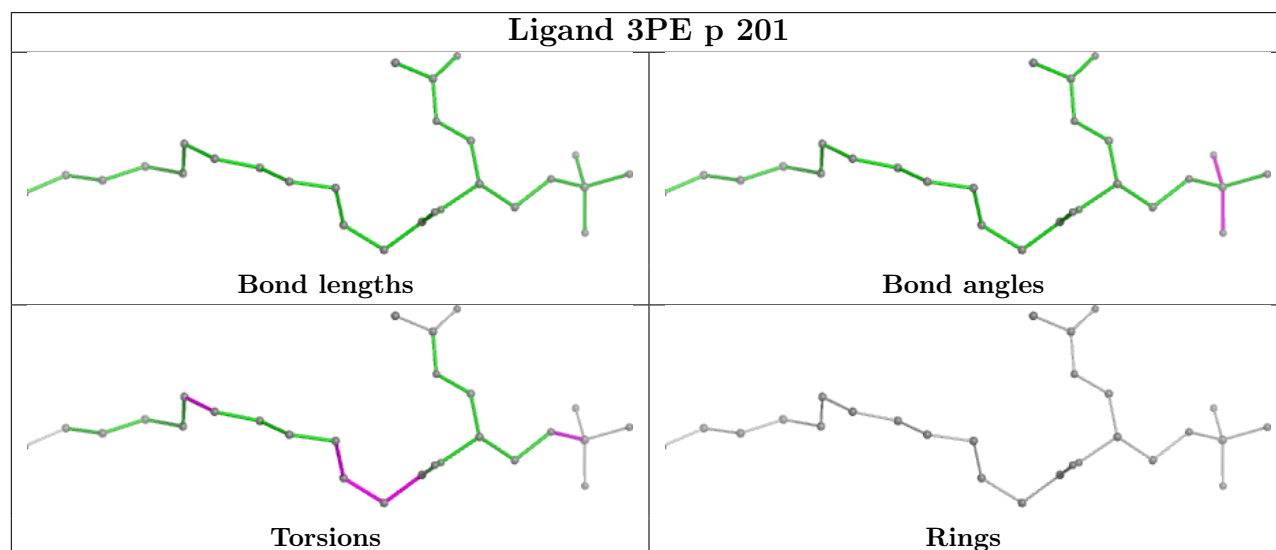
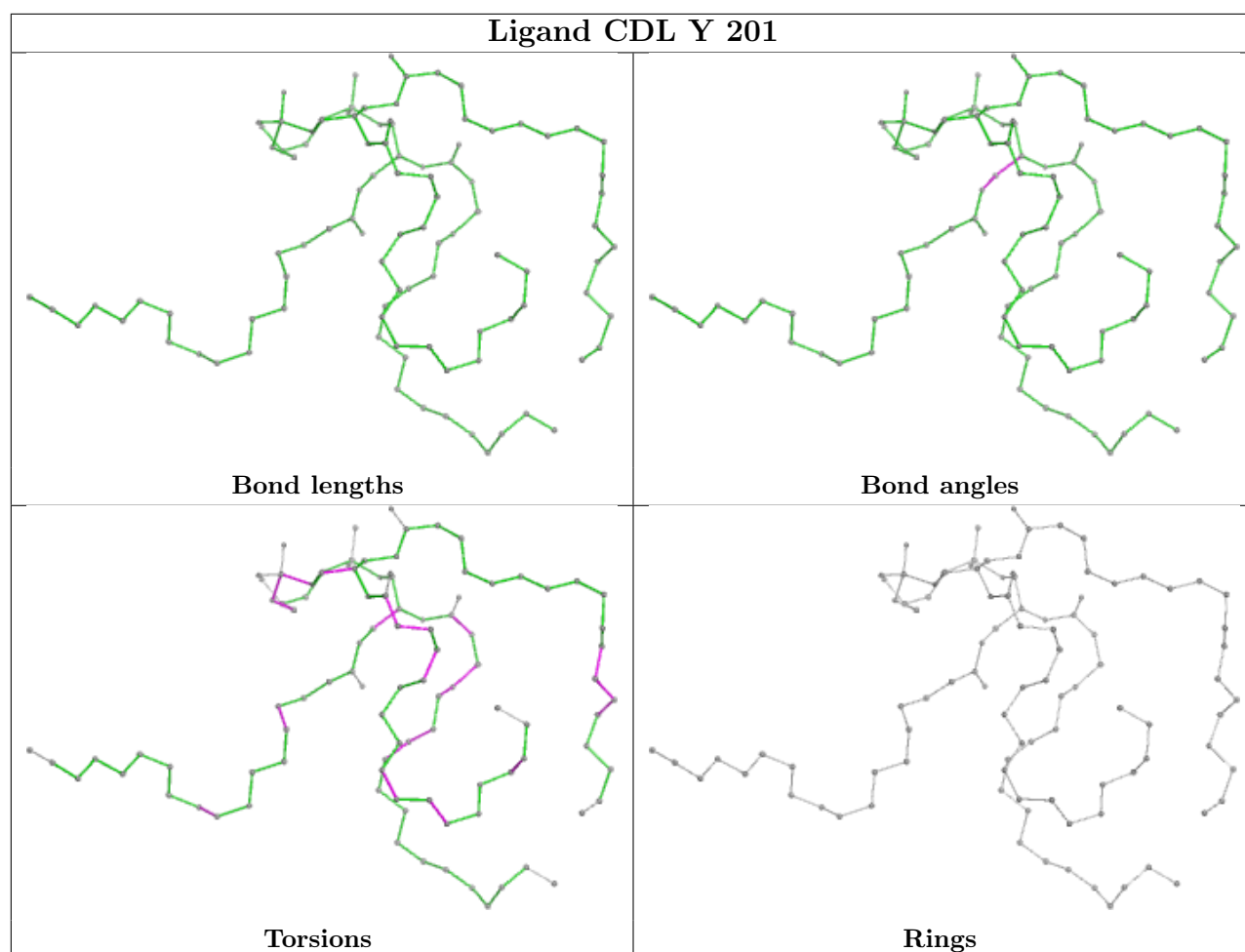


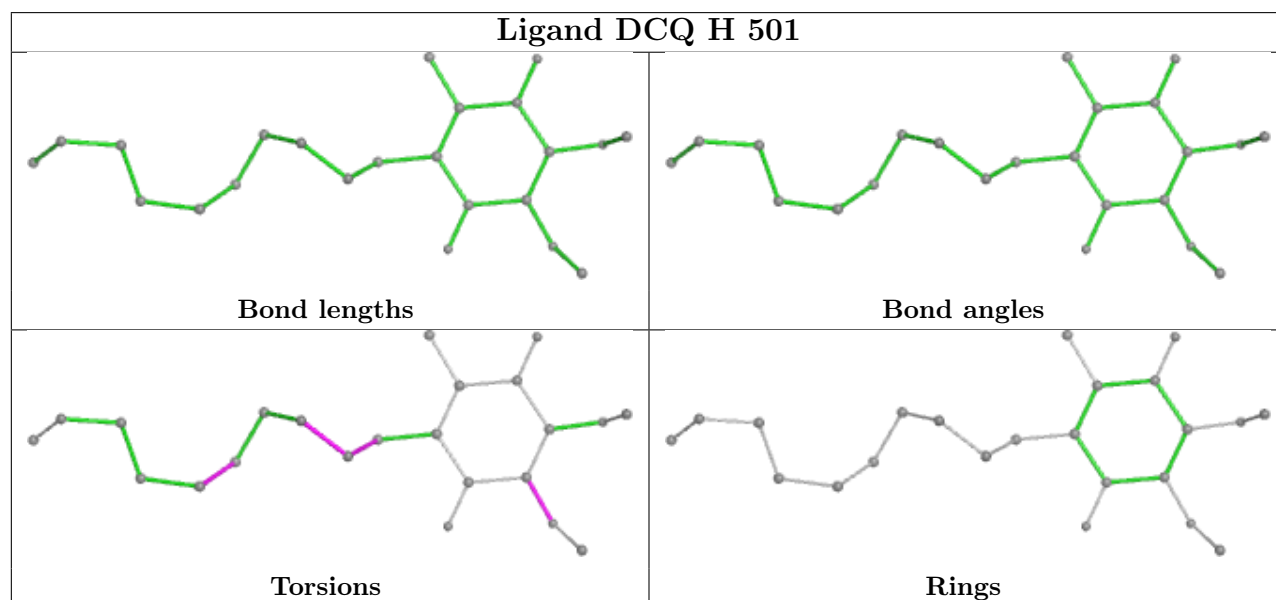
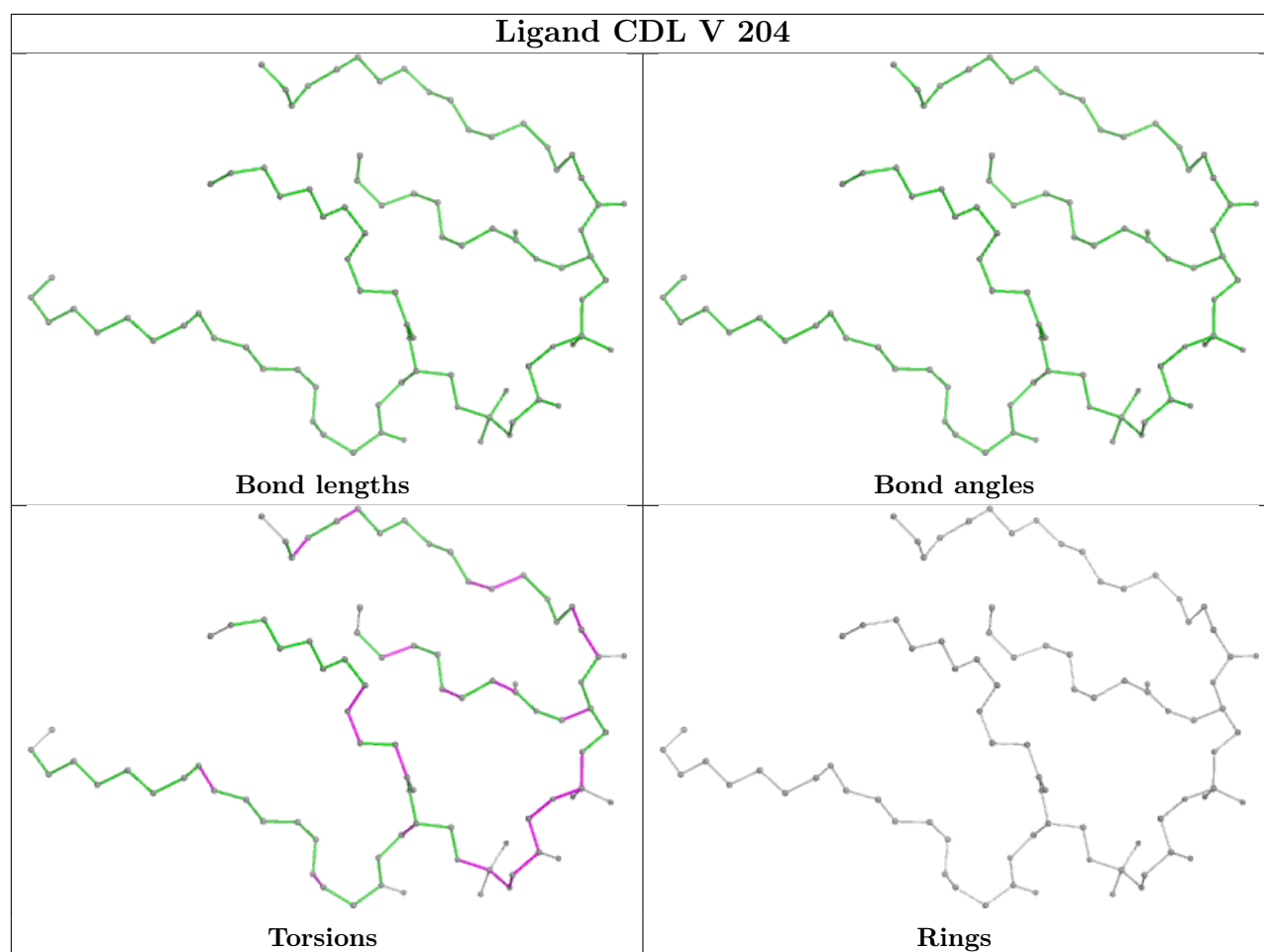


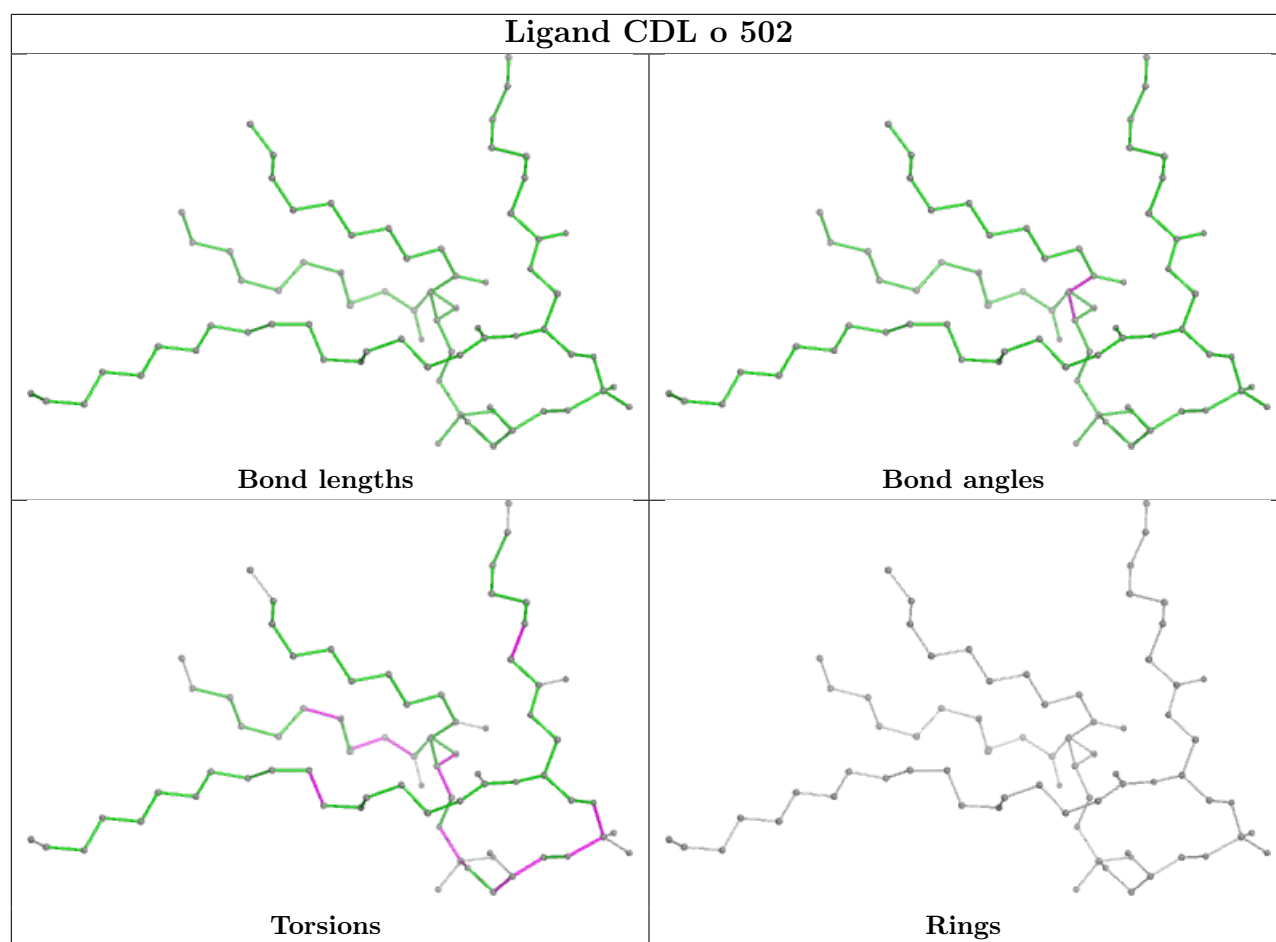


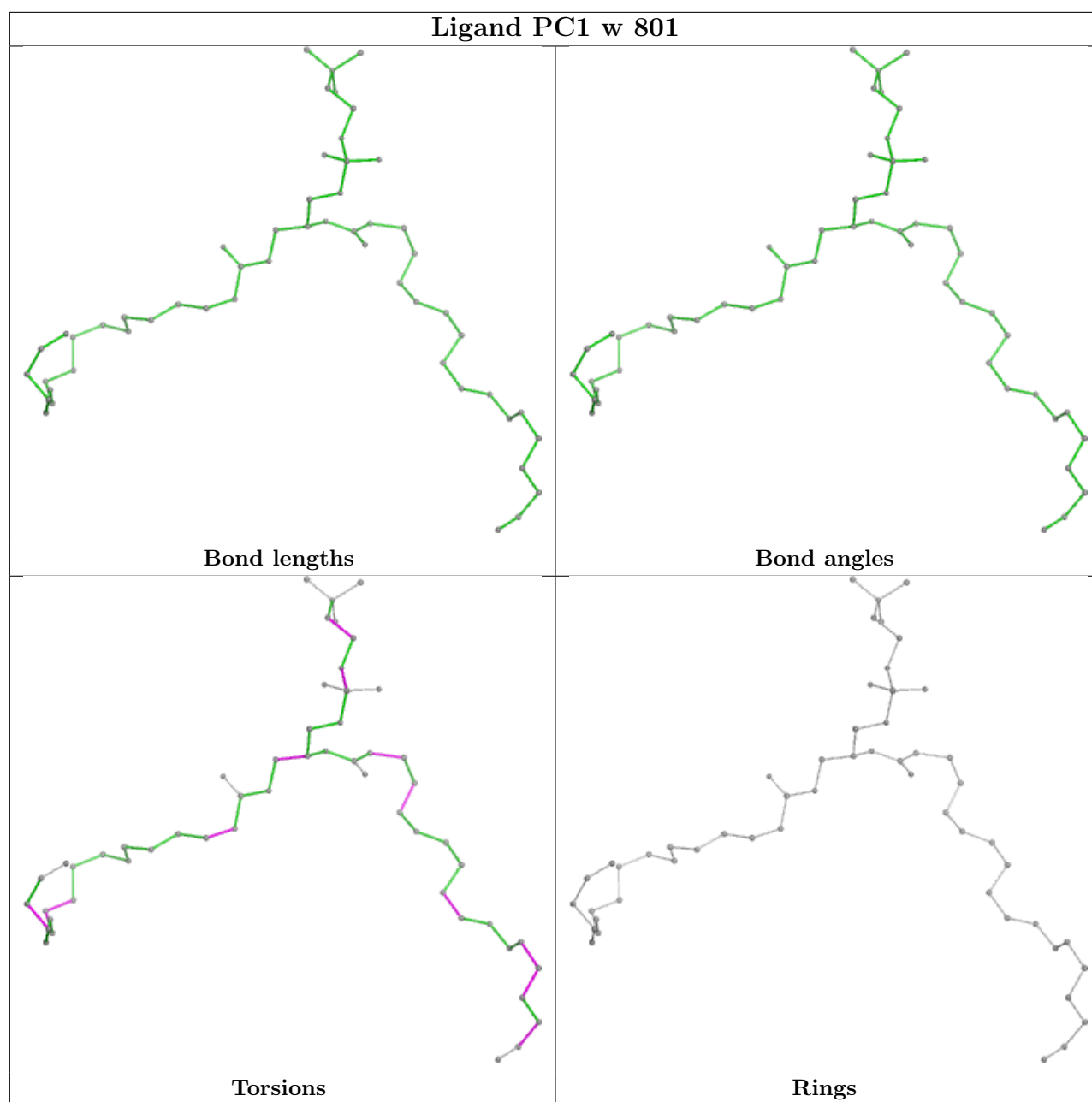




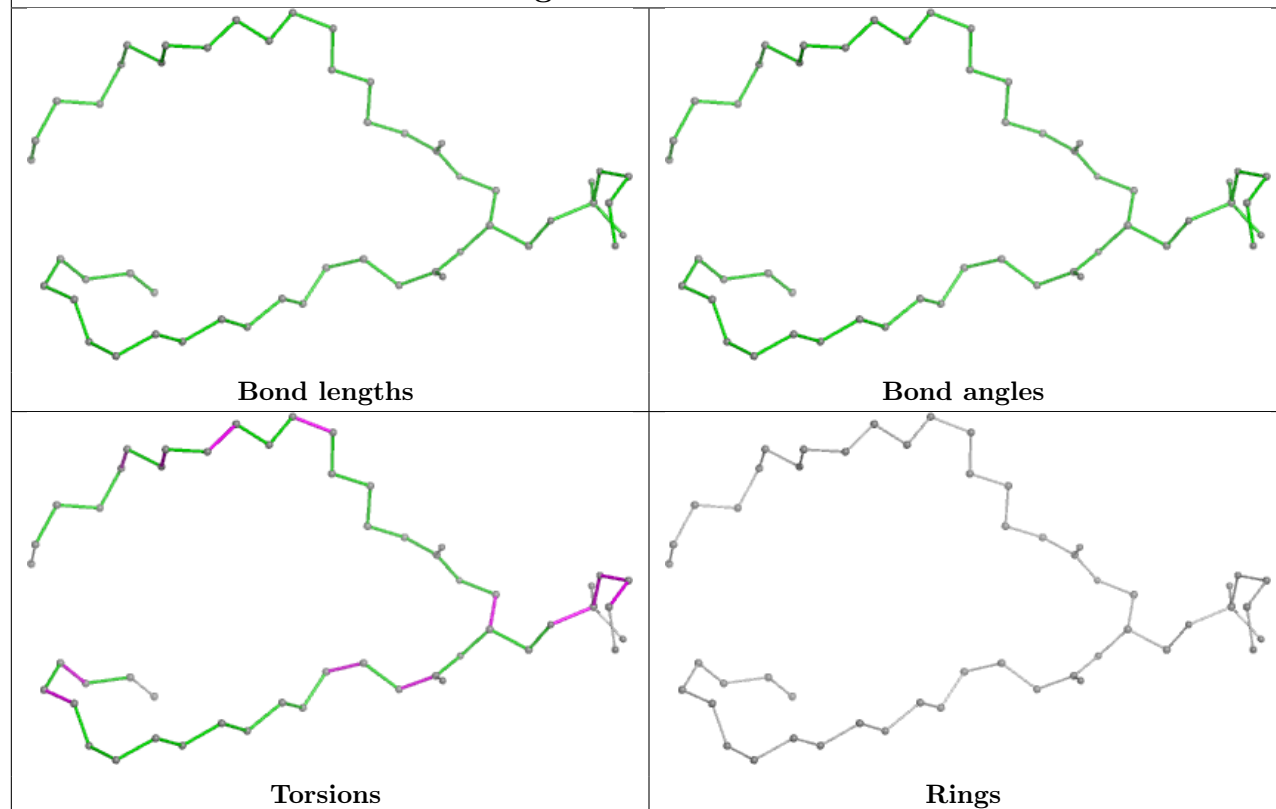




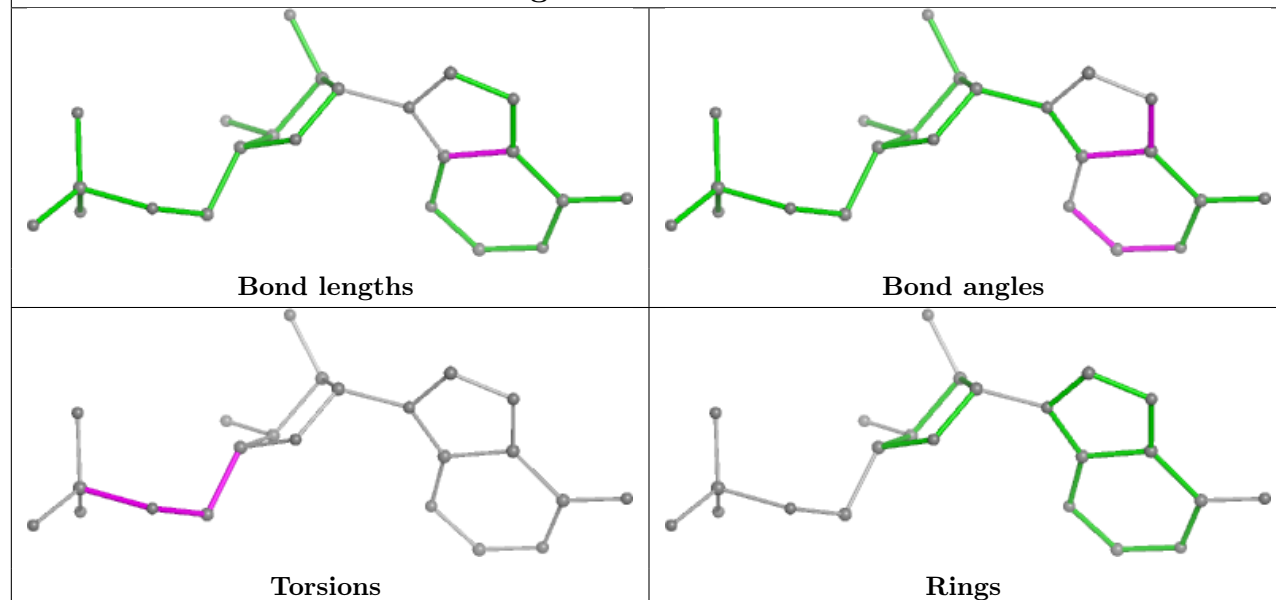


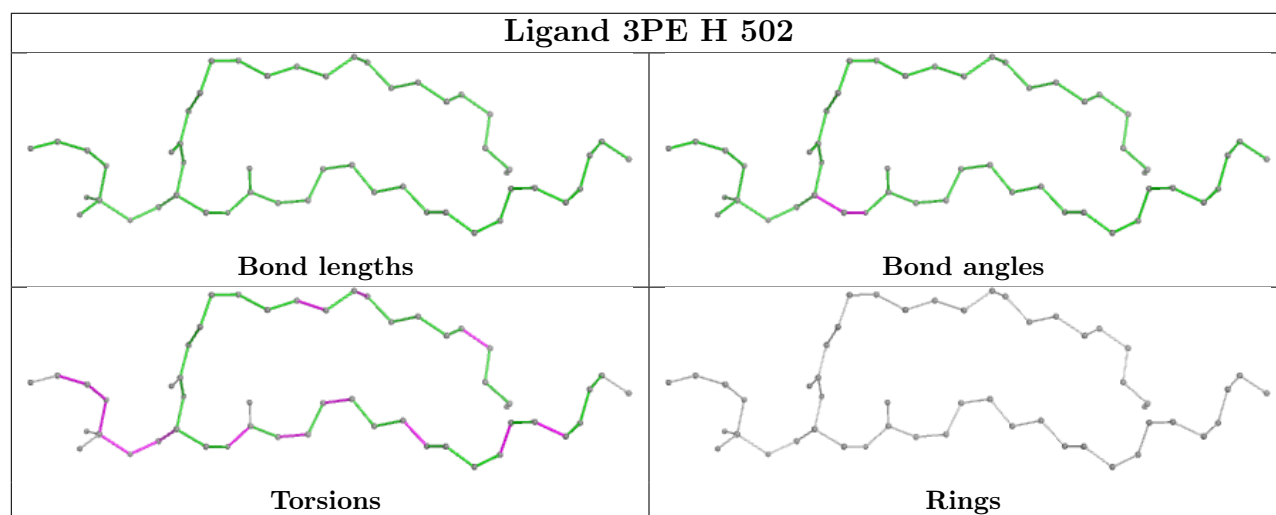
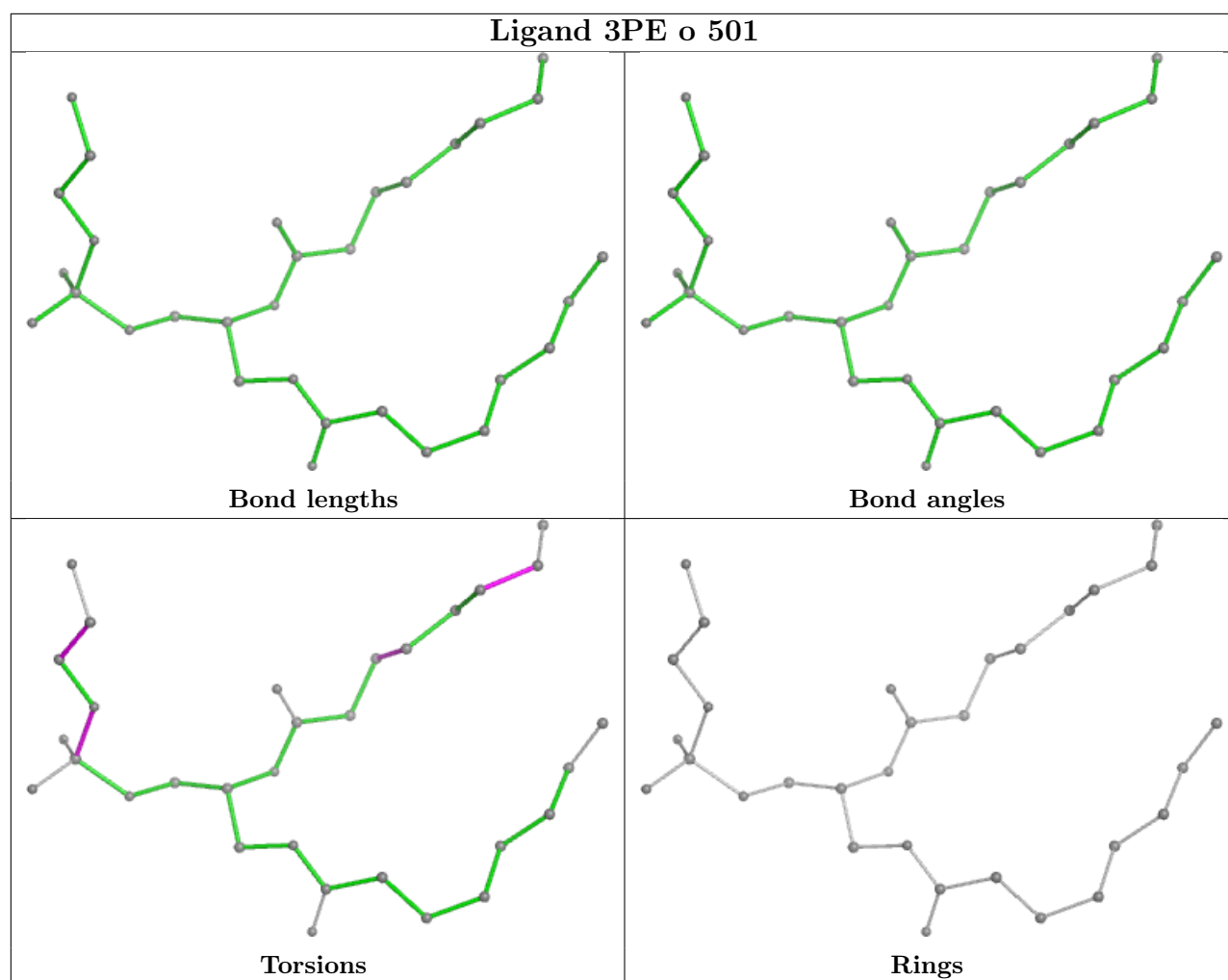


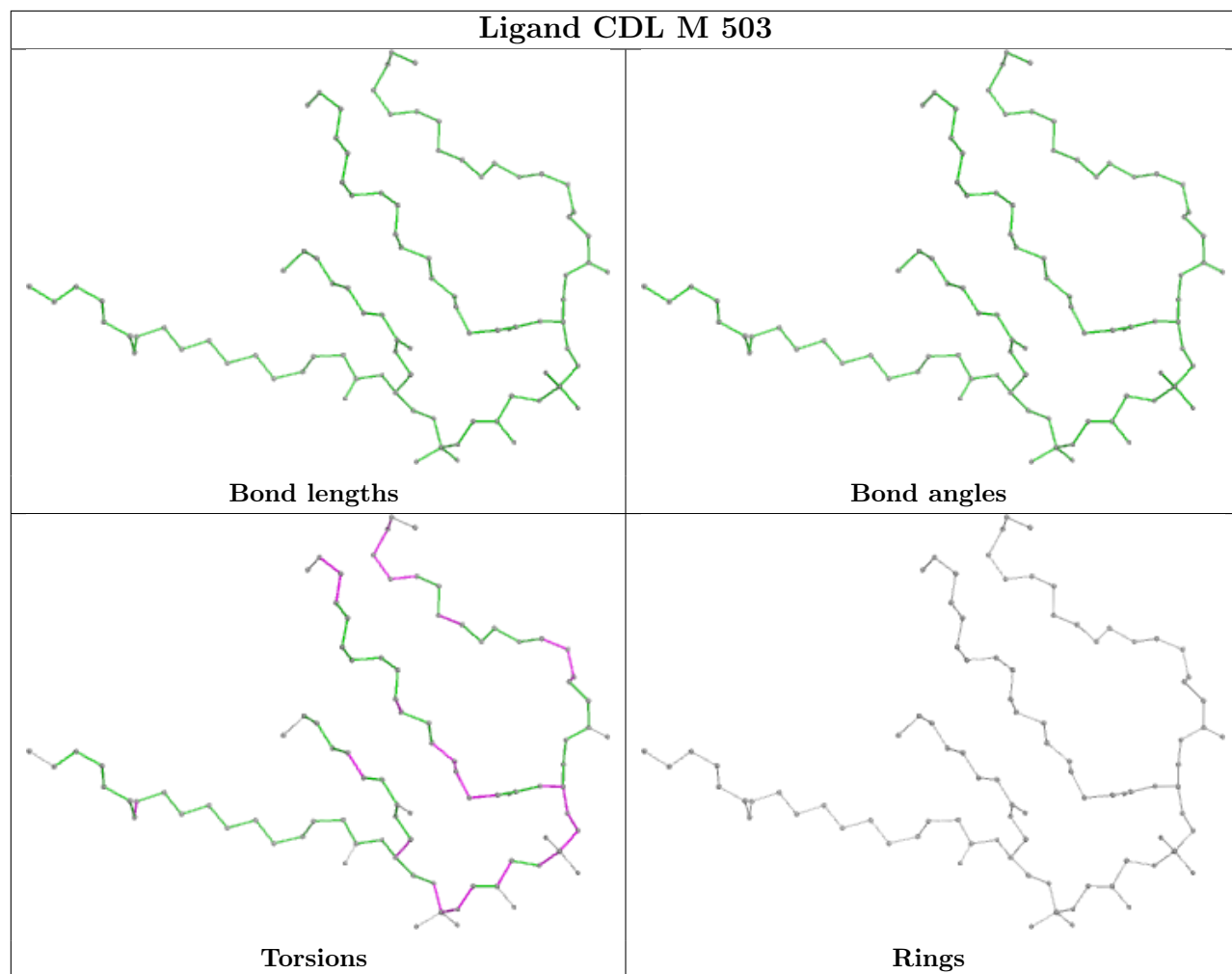
Ligand 3PE m 101

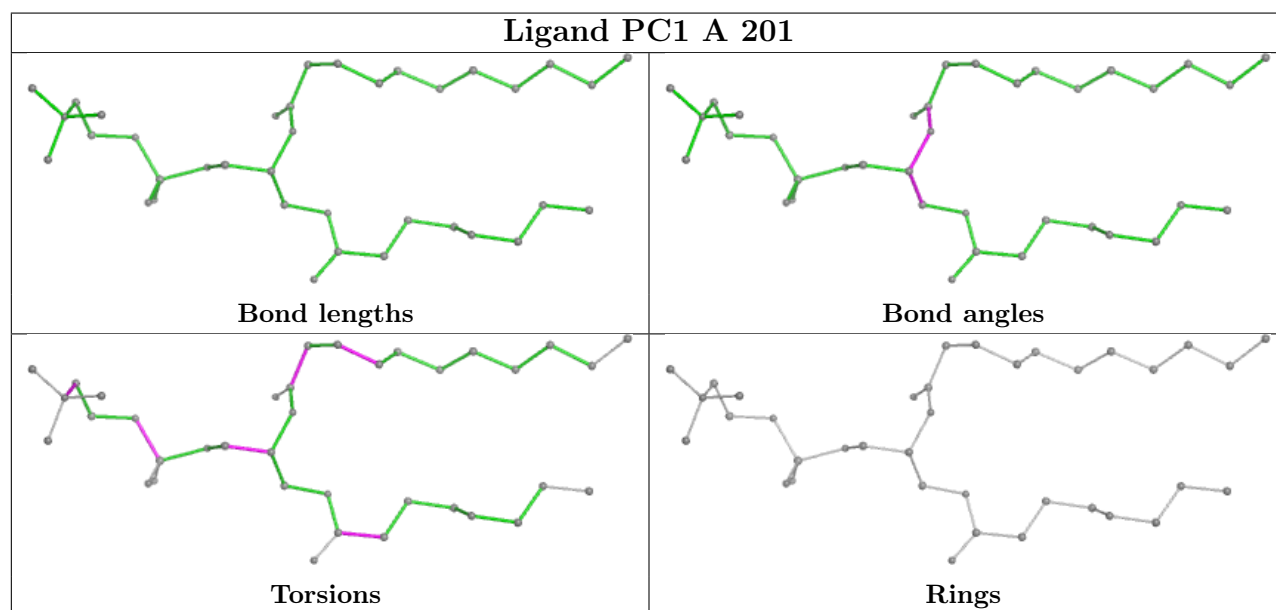
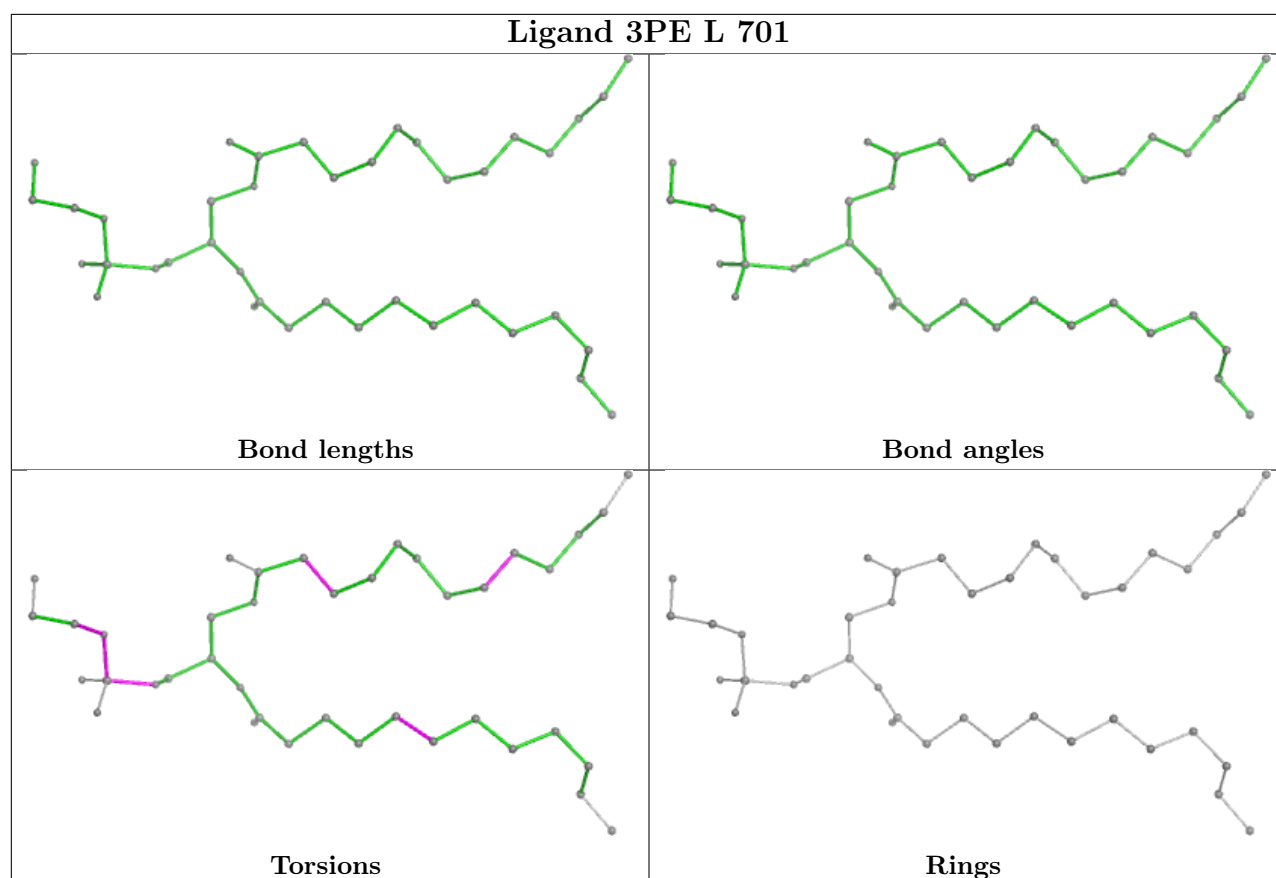


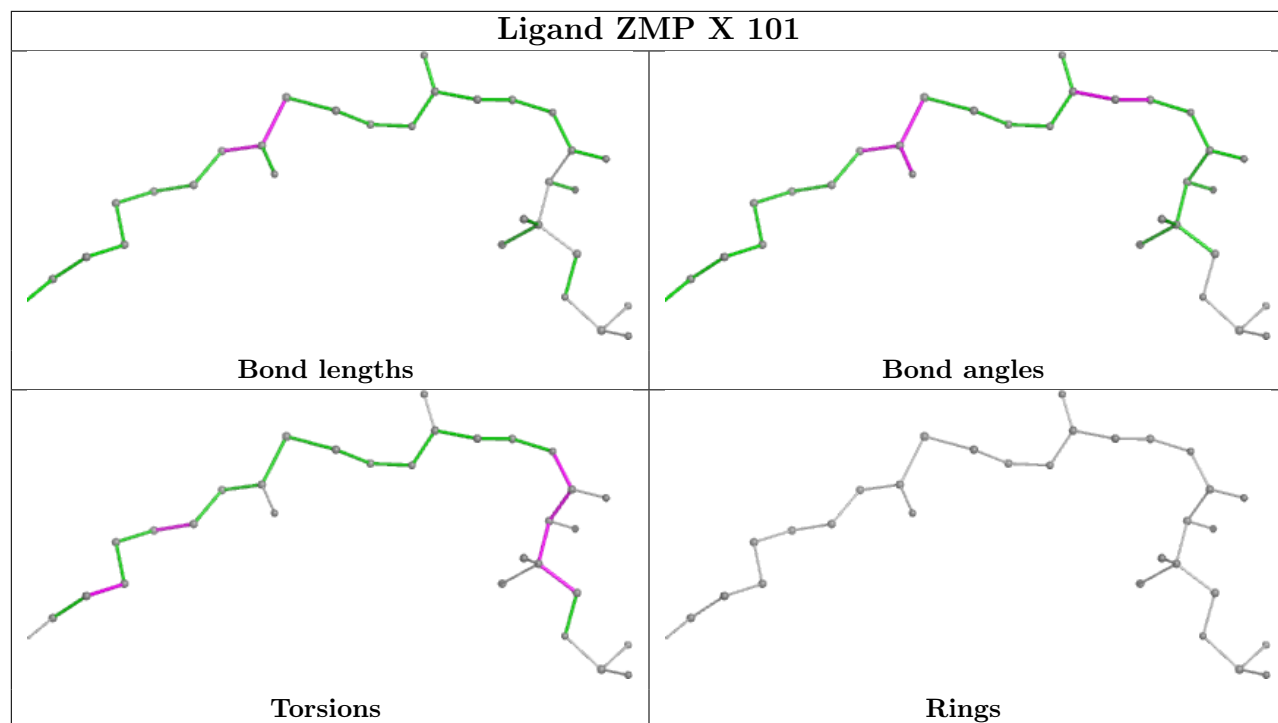
Ligand AMP k 501

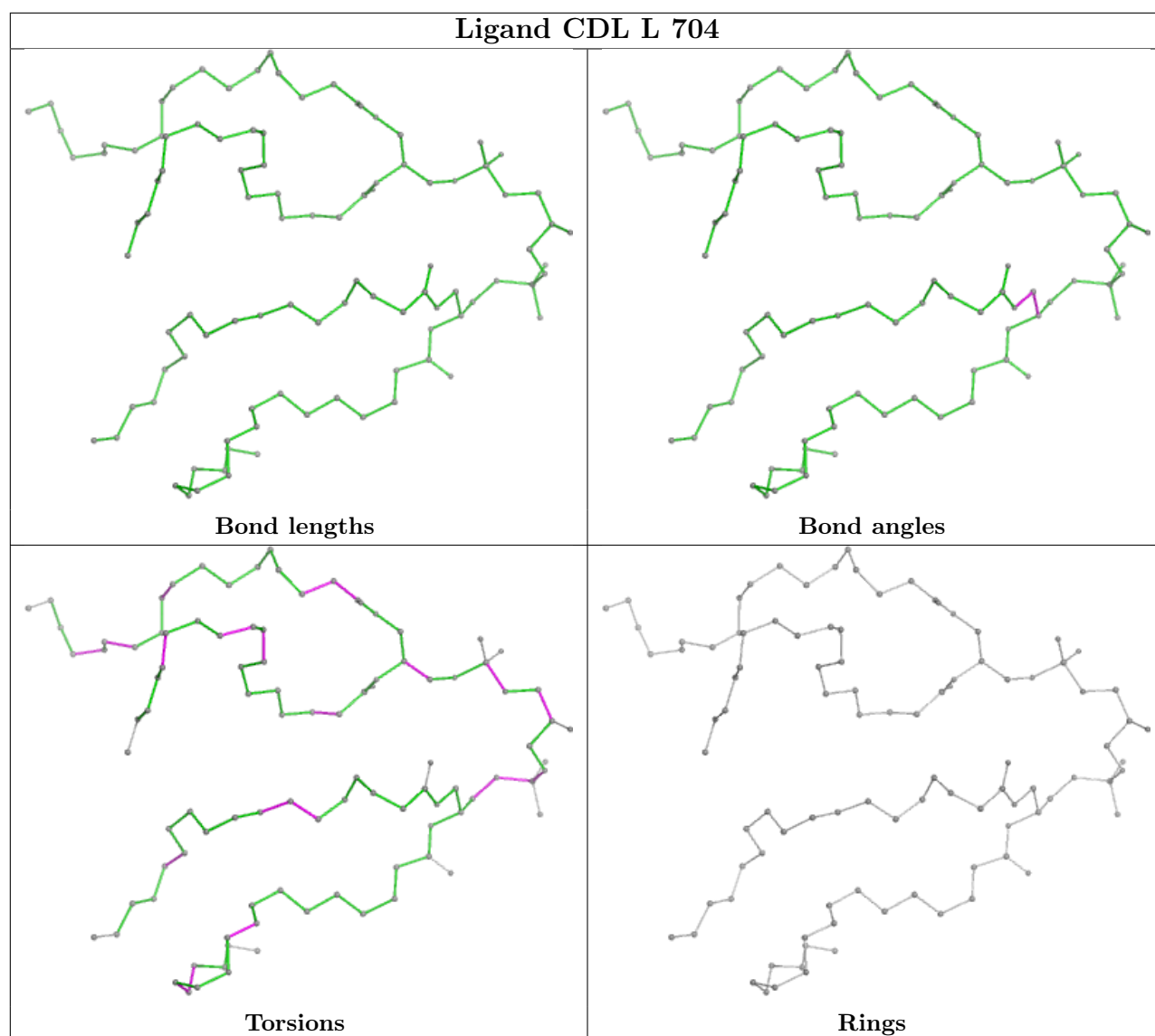


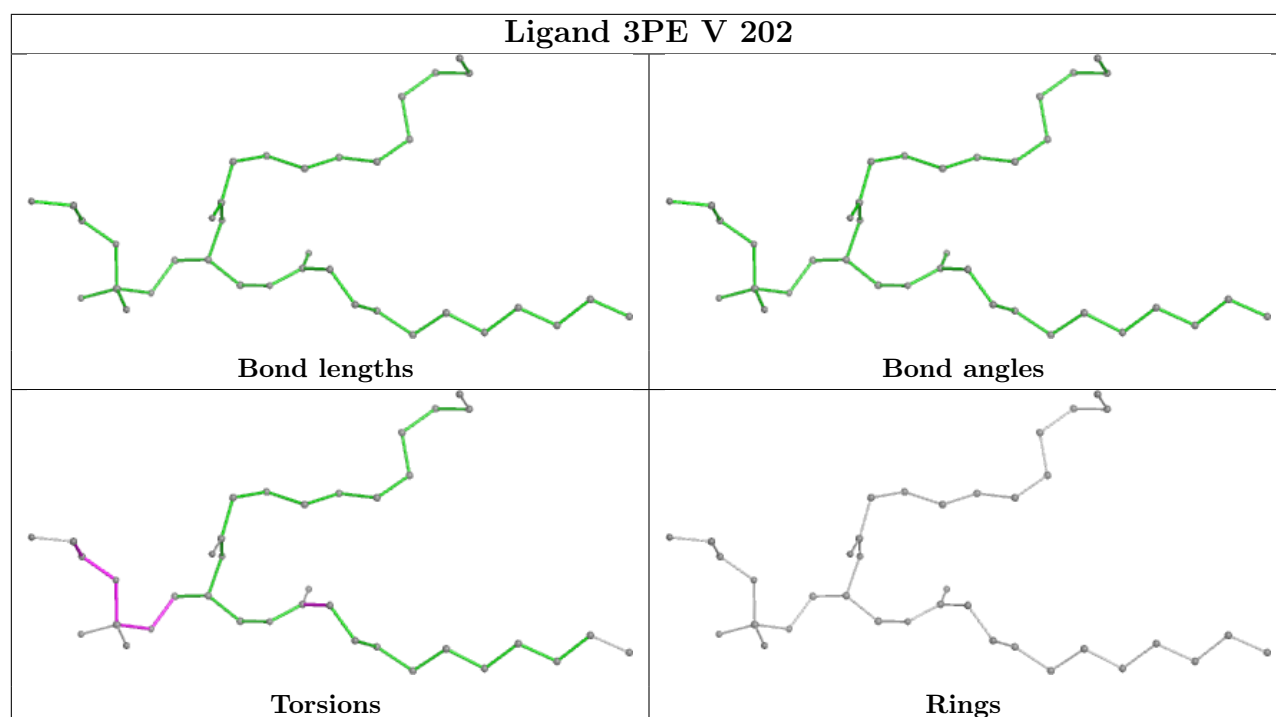












5.7 Other polymers [i](#)

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.