



Full wwPDB EM Validation Report ⓘ

May 29, 2024 – 04:27 pm BST

PDB ID : 8Q25
EMDB ID : EMD-18069
Title : Outward-facing, open1 proteoliposome complex I at 2.8 Å, after deactivation treatment. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-01
Resolution : 2.80 Å (reported)
Based on initial model : 7QSN

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:

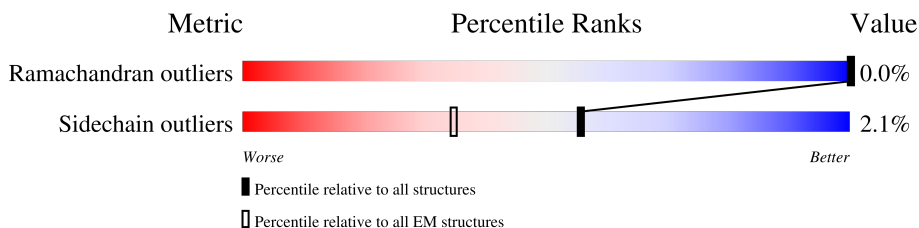
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.80 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	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	 97%
2	B	216	 69% 28%
3	C	266	 78% 22%
4	D	463	 89% 10%
5	E	249	 83% 14%
6	F	464	 91% 7%
7	G	727	 94% 5%
8	H	318	 98%
9	I	212	 83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	175	98%
11	K	98	95% 5%
12	L	606	97%
13	M	459	99%
14	N	347	99%
15	O	343	92% 7%
16	P	380	87% 11%
17	Q	175	73% 26%
18	R	124	77% 23%
19	S	99	85% 13% 5%
20	T	156	53% 44% 10%
20	U	156	56% 44% 9%
21	V	116	97%
22	W	128	90% 9%
23	X	172	99%
24	Y	141	96%
25	Z	144	98%
26	a	70	97%
27	b	84	96%
28	c	76	64% 36%
29	d	120	97%
30	e	106	90% 8%
31	f	57	98% 21%
32	g	154	63% 34%
33	h	189	71% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition i

There are 60 unique types of molecules in this entry. The entry contains 69693 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
			Total	C	N	O	S		
1	A	115	921	622	133	159	7	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	795	225	213	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	419	3377	2159	580	613	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1659	1059	278	312	10	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	432	3326	2096	594	616	20	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	691	5298	3318	925	1016	39	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	318	2509	1681	385	420	23	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	176	1414	889	243	270	12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	175	1345	906	191	236	12	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	98	745	486	112	131	16	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4802	3195	737	827	43	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3654	2436	570	609	39	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	347	2733	1817	416	457	43	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	339	2728	1765	484	474	5	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	129	1049	659	188	199	3	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	96	740	454	140	143	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	86	691	434	129	126	2	0	0

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	88	707	454	104	144	5	0	0
20	U	88	707	454	104	144	5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	114	923	597	156	167	3	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	116	982	628	182	168	4	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	171	1402	887	253	252	10	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	140	1030	657	176	191	6	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	142	1157	743	202	203	9	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	70	569	365	104	95	5	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	83	654	427	109	116	2	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	49	414	273	70	71	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	120	999	650	172	172	5	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	98	825	521	157	141	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	57	492	322	86	82	2	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	101	846	544	140	158	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1154	759	196	197	2	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	127	1097	722	191	183	1	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	71	597	390	99	107	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	81	653	427	110	114	2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	156	1314	850	216	240	8	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	128	1070	686	188	196		0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	171	1487	952	272	256	7	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	122	1048	653	201	185	9	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	174	1458	913	269	268	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	145	1212	780	216	211	5	0	0

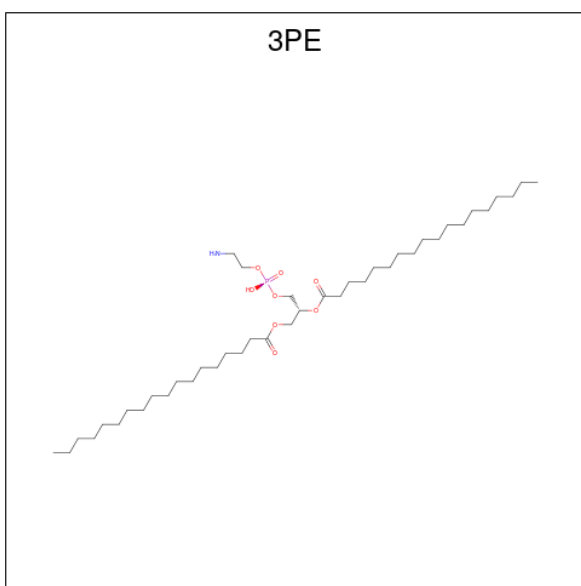
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	95	776	490	144	139	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	44	371	233	66	71	1	0	0

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	A	1	40	30	1	8	1	0
45	A	1	42	32	1	8	1	0
45	I	1	37	27	1	8	1	0
45	J	1	37	27	1	8	1	0
45	J	1	44	34	1	8	1	0
45	L	1	45	35	1	8	1	0
45	L	1	34	24	1	8	1	0

Continued on next page...

Continued from previous page...

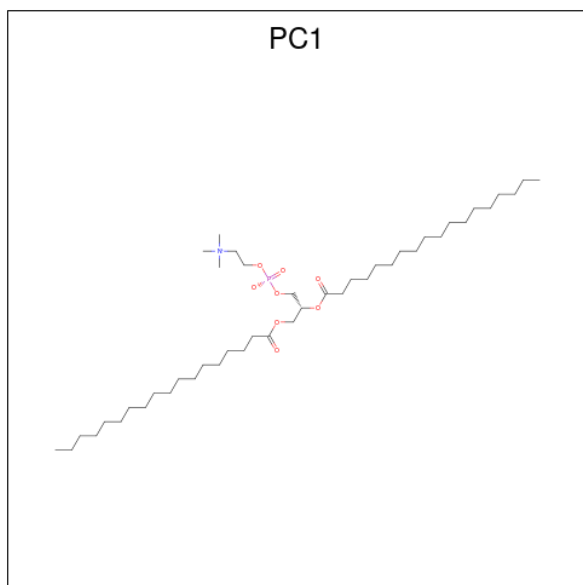
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	L	1	Total 41	C 31	N 1	O 8	P 1	0
45	M	1	Total 50	C 40	N 1	O 8	P 1	0
45	M	1	Total 45	C 35	N 1	O 8	P 1	0
45	N	1	Total 49	C 39	N 1	O 8	P 1	0
45	P	1	Total 38	C 28	N 1	O 8	P 1	0
45	Y	1	Total 41	C 31	N 1	O 8	P 1	0
45	Y	1	Total 27	C 17	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 45	C 35	N 1	O 8	P 1	0
45	Y	1	Total 36	C 26	N 1	O 8	P 1	0
45	Z	1	Total 42	C 32	N 1	O 8	P 1	0
45	a	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 47	C 37	N 1	O 8	P 1	0
45	d	1	Total 49	C 39	N 1	O 8	P 1	0
45	f	1	Total 24	C 14	N 1	O 8	P 1	0
45	g	1	Total 29	C 19	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0
45	q	1	Total 51	C 41	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	r	1	30	20	1	8	1	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



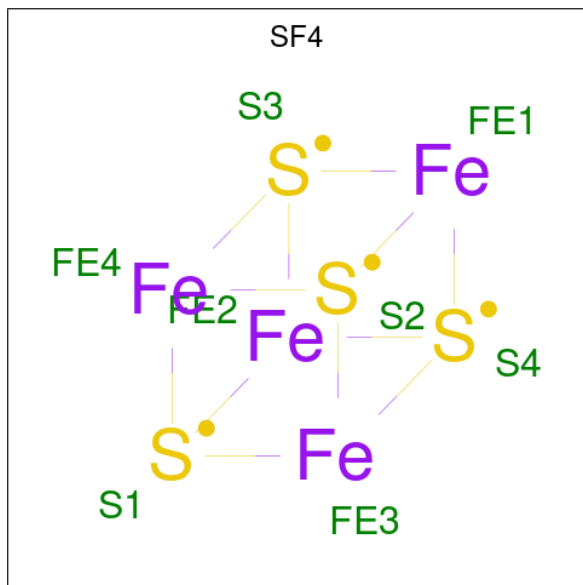
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	35	25	1	8	1	0
46	A	1	33	23	1	8	1	0
46	B	1	46	36	1	8	1	0
46	B	1	48	38	1	8	1	0
46	H	1	48	38	1	8	1	0
46	H	1	41	31	1	8	1	0
46	H	1	47	37	1	8	1	0
46	I	1	54	44	1	8	1	0
46	J	1	35	25	1	8	1	0
46	M	1	44	34	1	8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	M	1	Total 35	C 25	N 1	O 8	P 1	0
46	Z	1	Total 44	C 34	N 1	O 8	P 1	0
46	d	1	Total 39	C 29	N 1	O 8	P 1	0
46	h	1	Total 38	C 28	N 1	O 8	P 1	0
46	l	1	Total 47	C 37	N 1	O 8	P 1	0
46	m	1	Total 41	C 31	N 1	O 8	P 1	0
46	q	1	Total 49	C 39	N 1	O 8	P 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



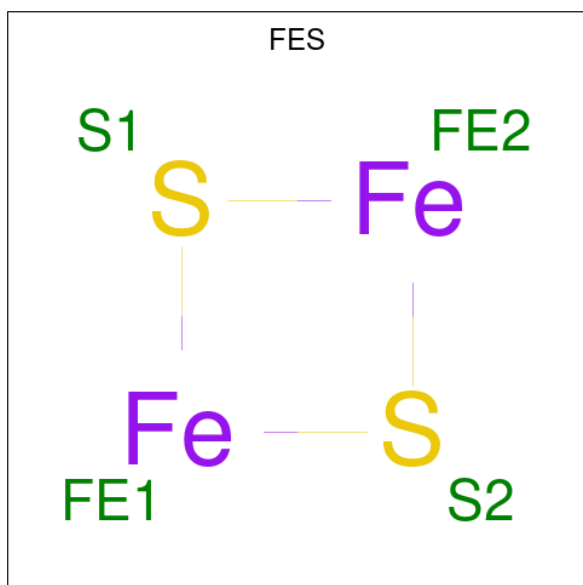
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	Total 8	Fe 4	S 4	0
47	F	1	Total 8	Fe 4	S 4	0
47	G	1	Total 8	Fe 4	S 4	0
47	G	1	Total 8	Fe 4	S 4	0

Continued on next page...

Continued from previous page...

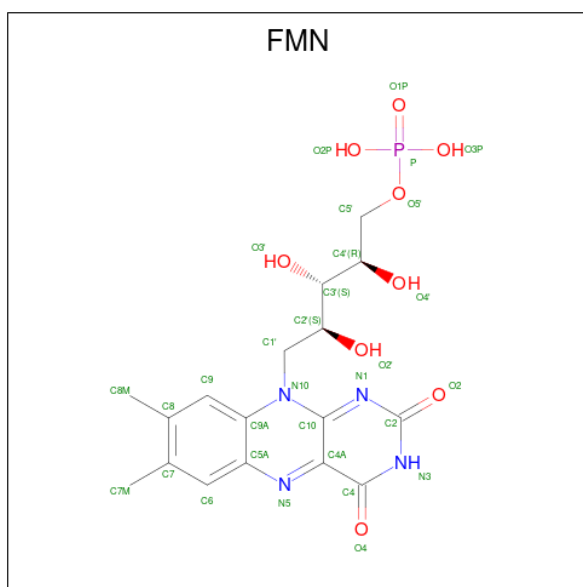
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	E	1	4	2	2	0
48	G	1	4	2	2	0

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

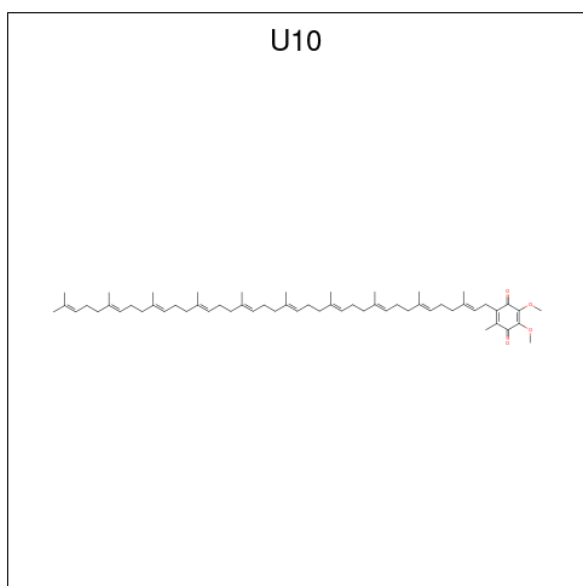


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

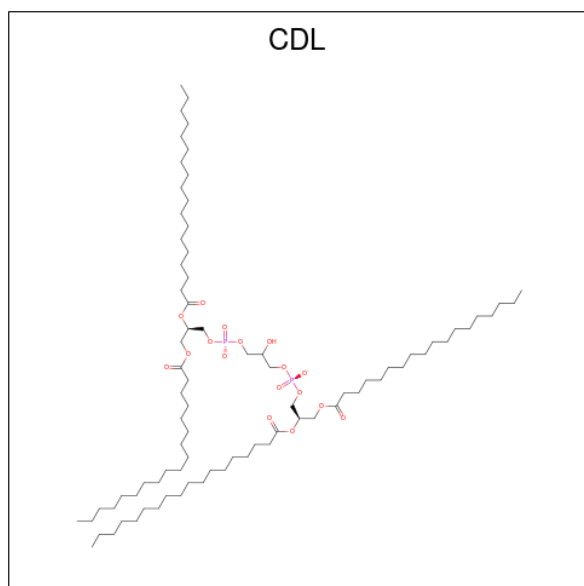
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



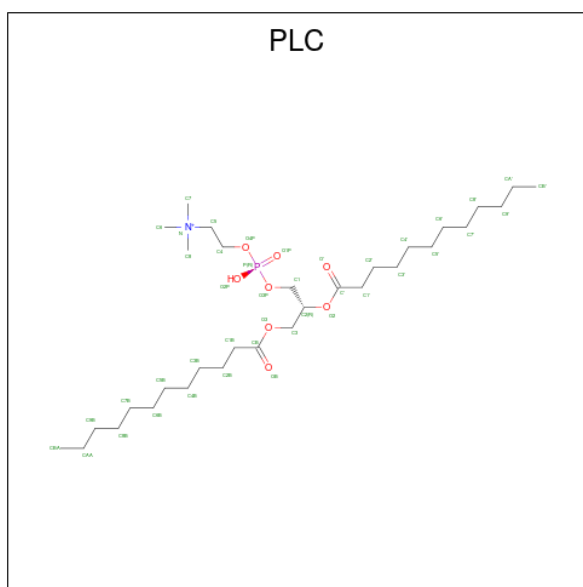
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
51	H	1	34	30	4	0

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	H	1	58	39	17	2	0
52	L	1	100	81	17	2	0
52	M	1	100	81	17	2	0
52	N	1	94	75	17	2	0
52	d	1	65	46	17	2	0
52	d	1	87	68	17	2	0
52	i	1	76	57	17	2	0
52	r	1	61	42	17	2	0

- Molecule 53 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	J	1	Total 35	C 25	N 1	O 8	P 1	0
53	L	1	Total 36	C 26	N 1	O 8	P 1	0
53	M	1	Total 34	C 24	N 1	O 8	P 1	0
53	O	1	Total 31	C 21	N 1	O 8	P 1	0
53	O	1	Total 31	C 21	N 1	O 8	P 1	0
53	Y	1	Total 42	C 32	N 1	O 8	P 1	0
53	Z	1	Total 36	C 26	N 1	O 8	P 1	0
53	b	1	Total 38	C 28	N 1	O 8	P 1	0
53	g	1	Total 42	C 32	N 1	O 8	P 1	0

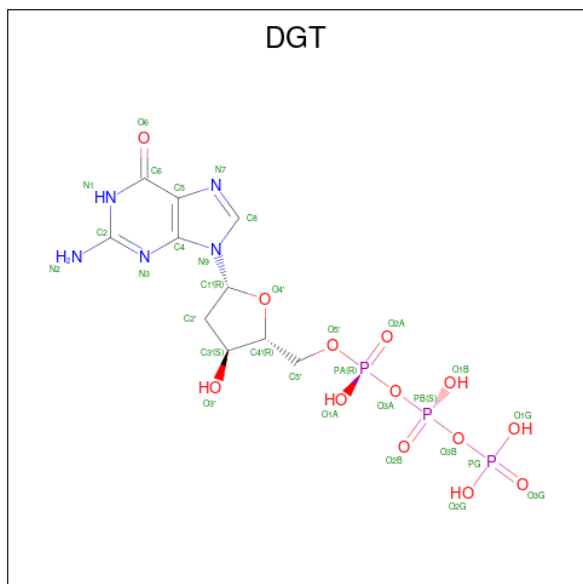
- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	M	1	Total 1	Zn 1	0
54	R	1	Total 1	Zn 1	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

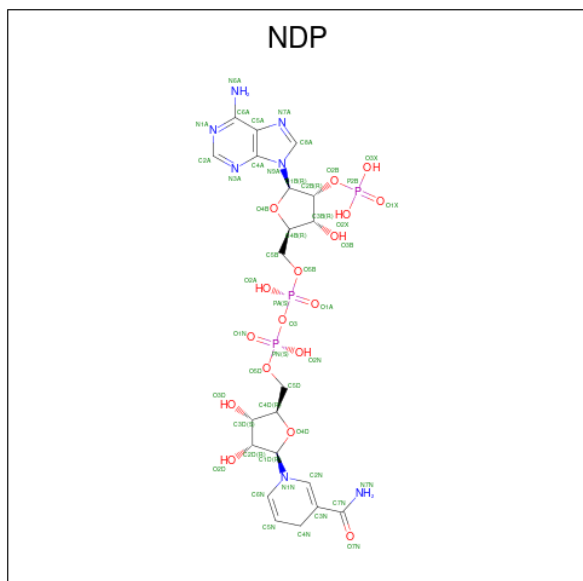
Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total	Mg	0
			1	1	

- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



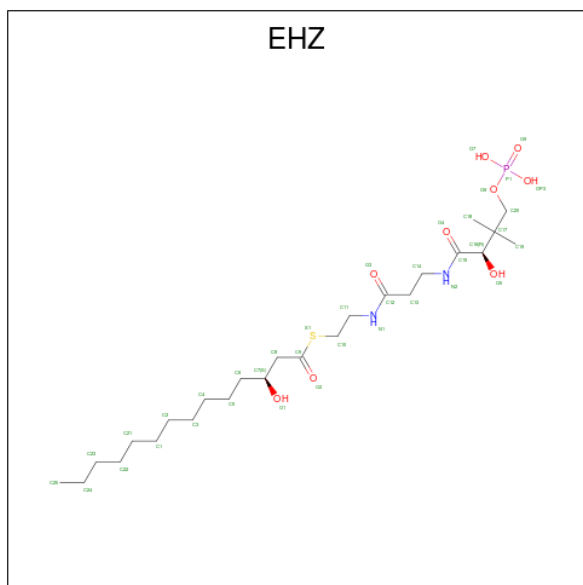
Mol	Chain	Residues	Atoms				AltConf	
56	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



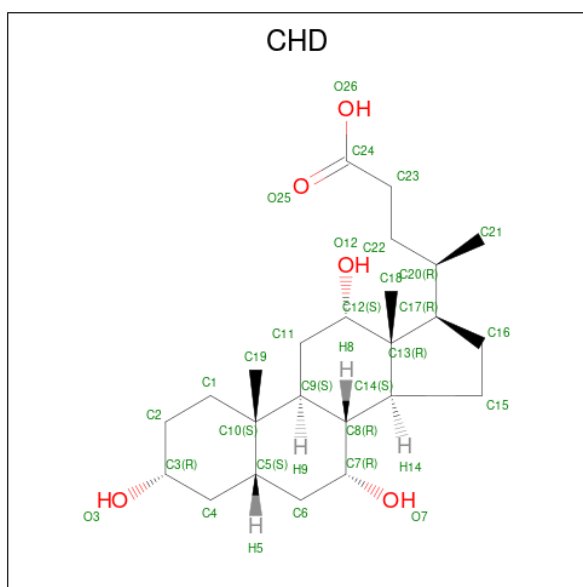
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	P	1	48	21	7	17	3	0

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



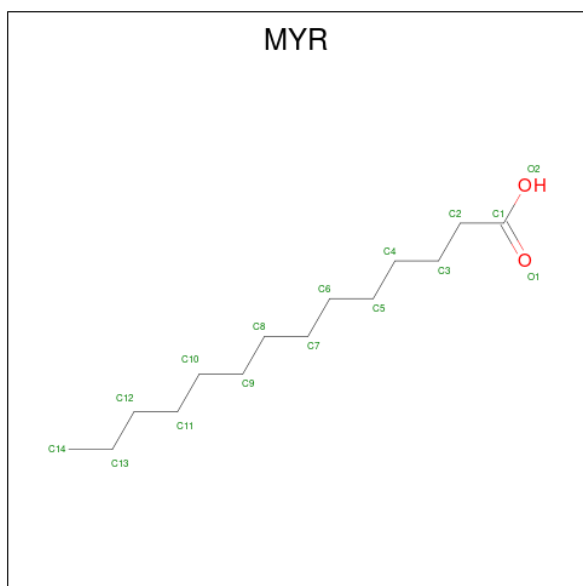
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	T	1	37	25	2	8	1	1	0
58	U	1	37	25	2	8	1	1	0

- Molecule 59 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).

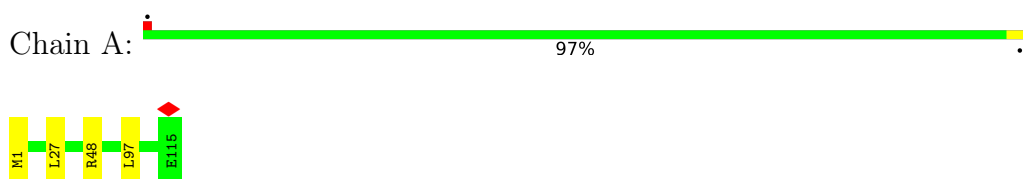


Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

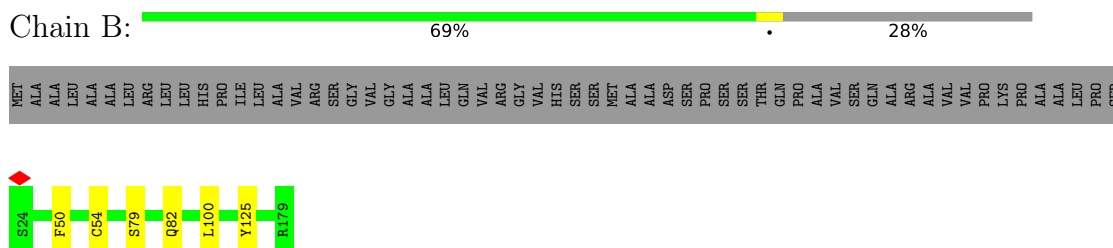
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

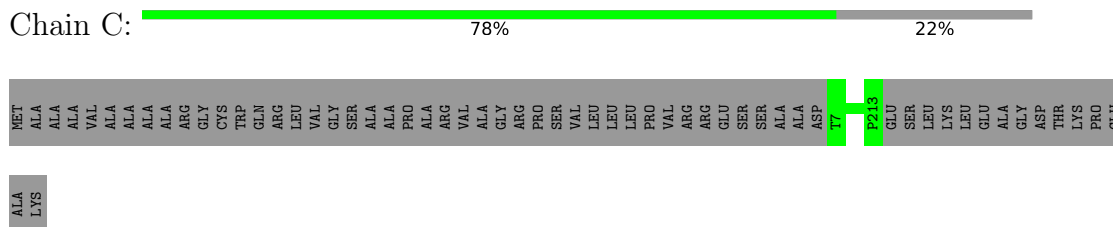
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



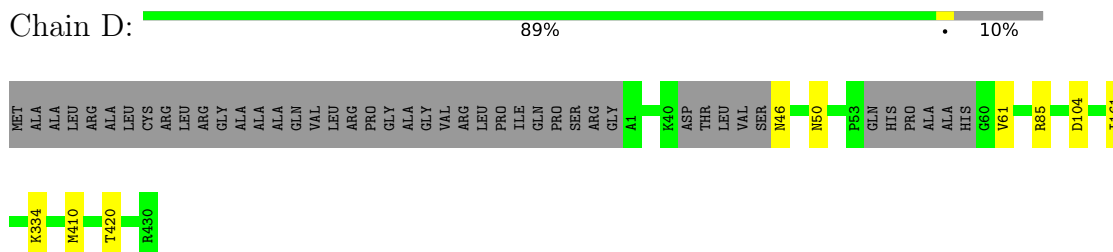
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



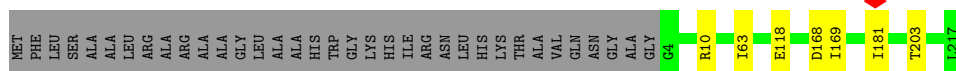
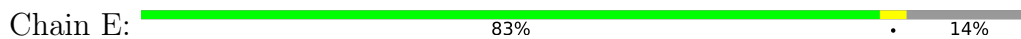
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



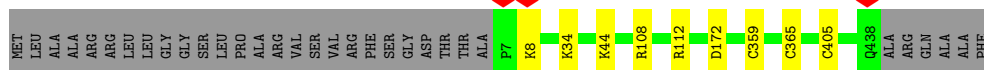
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



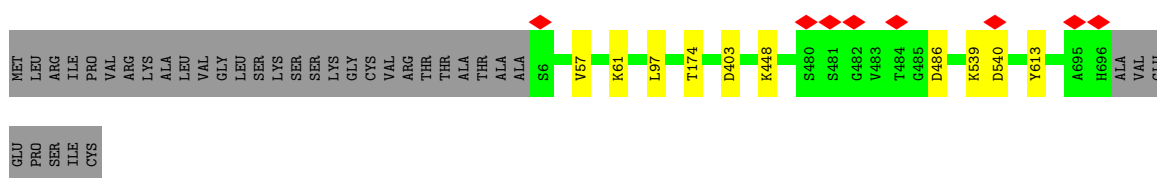
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



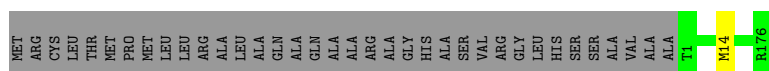
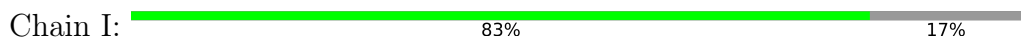
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



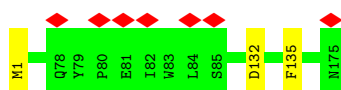
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



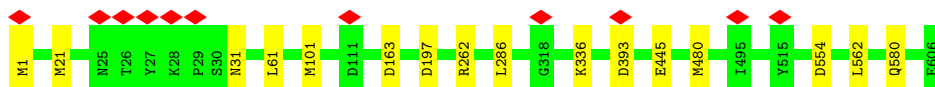
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L





- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 97%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 99%



- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 99%



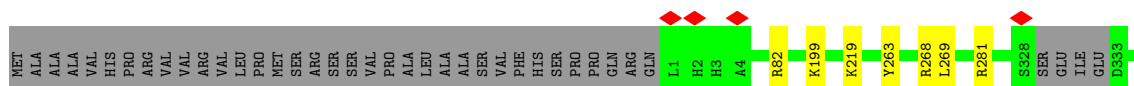
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 92% 7%



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 87% 11%

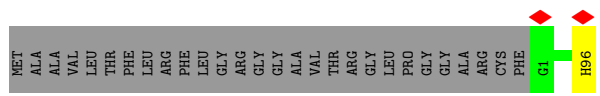
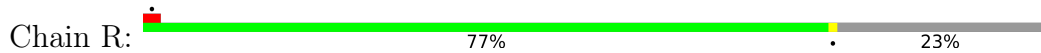


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

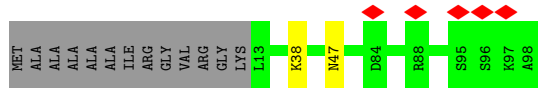
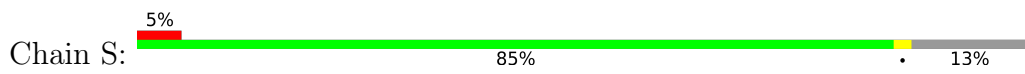
Chain Q: 73% 26%



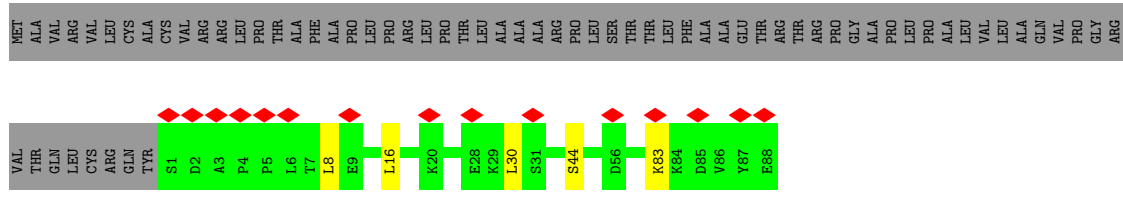
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



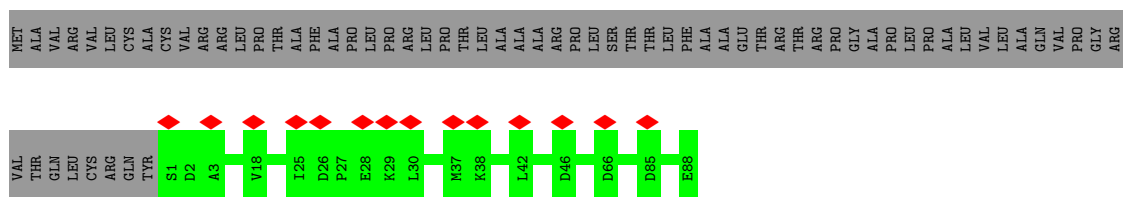
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



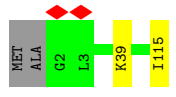
• Molecule 20: Acyl carrier protein, mitochondrial



• Molecule 20: Acyl carrier protein, mitochondrial

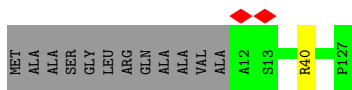


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

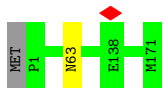


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6





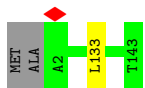
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



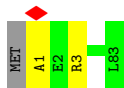
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



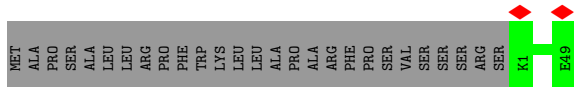
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

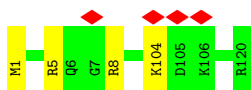


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial




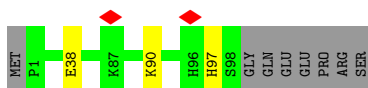
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  97%



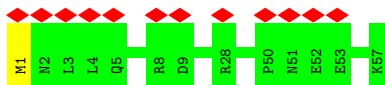
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  90% 8%



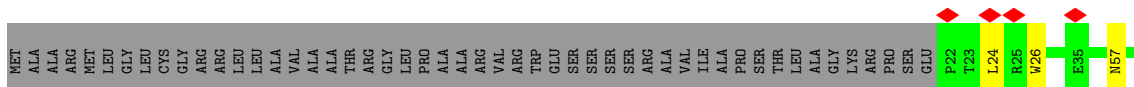
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  21% 98%



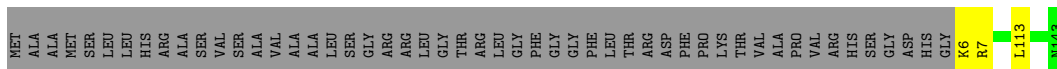
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:  63% 34%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:  71% 27%

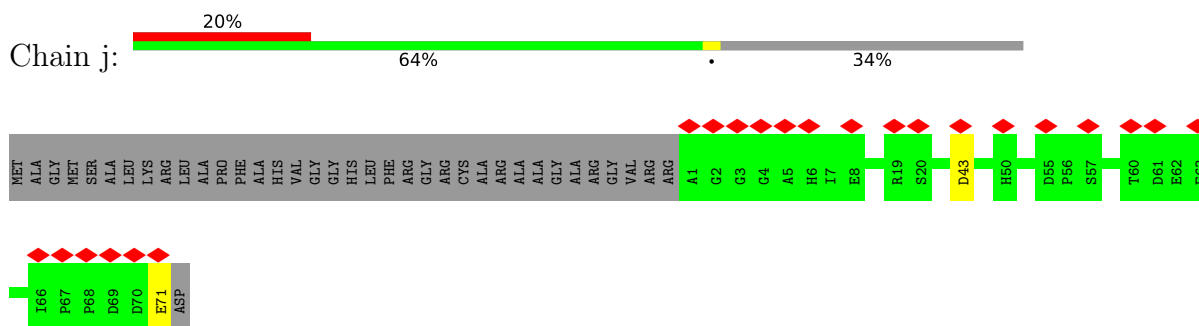


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

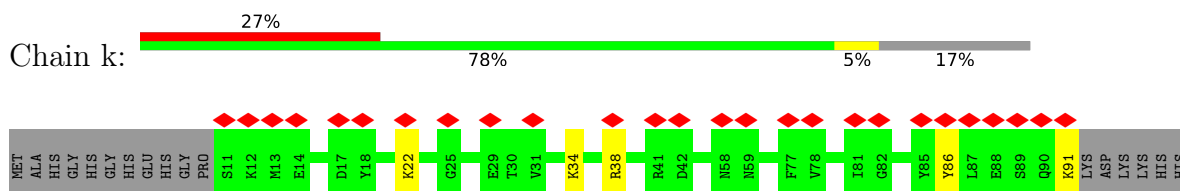
Chain i:  30% 95%



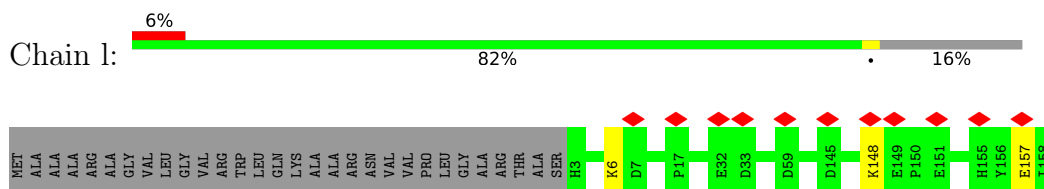
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



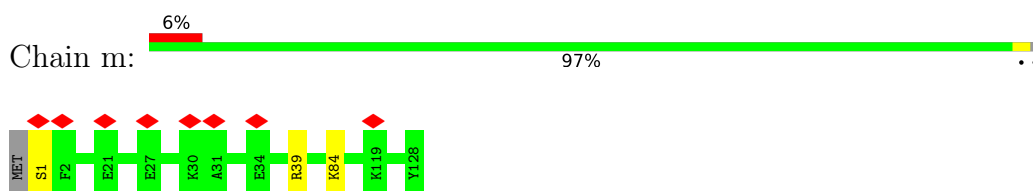
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



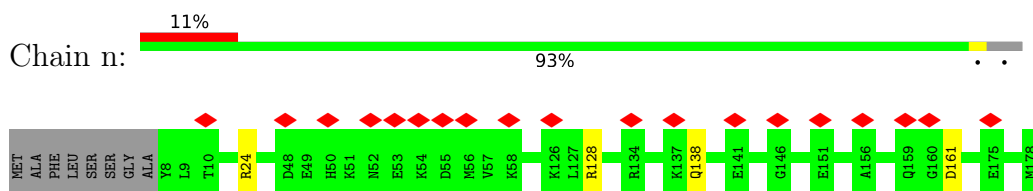
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



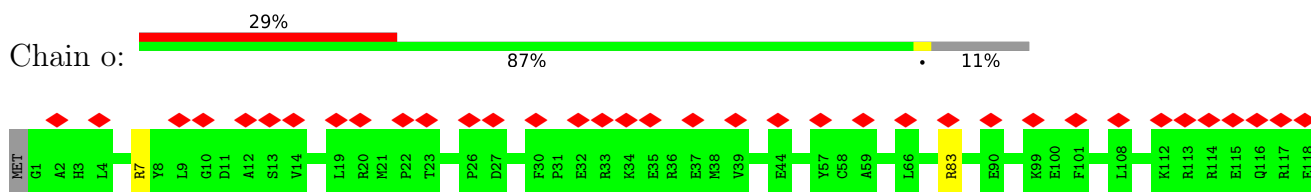
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

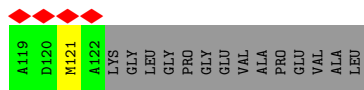


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

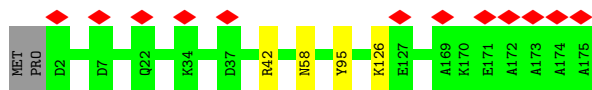


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

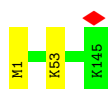




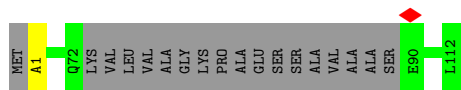
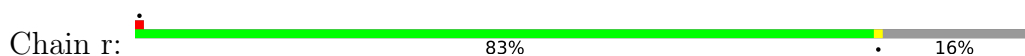
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



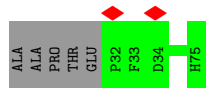
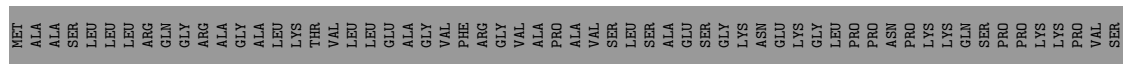
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45912	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 ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.382	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CDL, DGT, 2MR, NDP, EHZ, AME, AYA, U10, SF4, PLC, MG, FME, CHD, MYR, ZN, 3PE, FES, FMN, PC1, SAC

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	0.26	0/936	0.40	0/1281
2	B	0.32	0/1278	0.53	0/1728
3	C	0.30	0/1772	0.51	0/2413
4	D	0.30	0/3450	0.49	0/4670
5	E	0.27	0/1699	0.47	0/2312
6	F	0.26	0/3401	0.50	0/4595
7	G	0.27	0/5387	0.51	0/7301
8	H	0.28	0/2571	0.44	0/3513
9	I	0.31	0/1445	0.53	0/1956
10	J	0.28	0/1370	0.42	0/1859
11	K	0.26	0/745	0.42	0/1008
12	L	0.25	0/4920	0.41	0/6694
13	M	0.25	0/3738	0.42	0/5097
14	N	0.26	0/2792	0.42	0/3800
15	O	0.26	0/2651	0.42	0/3587
16	P	0.26	0/2804	0.50	0/3803
17	Q	0.26	0/1072	0.51	0/1449
18	R	0.28	0/753	0.51	0/1014
19	S	0.25	0/702	0.52	0/945
20	T	0.25	0/719	0.39	0/971
20	U	0.25	0/719	0.40	0/971
21	V	0.25	0/943	0.41	0/1277
22	W	0.25	0/1006	0.50	0/1352
23	X	0.25	0/1439	0.48	0/1942
24	Y	0.25	0/1042	0.47	0/1414
25	Z	0.27	0/1186	0.50	0/1599
26	a	0.28	0/584	0.50	0/786
27	b	0.26	0/667	0.44	0/916
28	c	0.26	0/427	0.40	0/579
29	d	0.28	0/1018	0.48	0/1375
30	e	0.24	0/846	0.49	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.26	0/505	0.47	0/681
32	g	0.26	0/873	0.46	0/1186
33	h	0.26	0/1188	0.47	0/1607
34	i	0.24	0/1127	0.46	0/1534
35	j	0.24	0/624	0.43	0/855
36	k	0.25	0/672	0.43	0/906
37	l	0.25	0/1369	0.44	0/1873
38	m	0.26	0/1088	0.51	0/1472
39	n	0.24	0/1540	0.48	0/2085
40	o	0.25	0/1073	0.52	0/1437
41	p	0.25	0/1491	0.48	0/2011
42	q	0.28	0/1242	0.49	0/1688
43	r	0.28	0/789	0.51	0/1068
44	s	0.26	0/383	0.49	0/518
All	All	0.26	0/68046	0.47	0/92259

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	154/216 (71%)	148 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	412/463 (89%)	399 (97%)	13 (3%)	0	100	100
5	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
6	F	430/464 (93%)	412 (96%)	18 (4%)	0	100	100
7	G	689/727 (95%)	668 (97%)	21 (3%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
11	K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	15	44
12	L	604/606 (100%)	577 (96%)	26 (4%)	1 (0%)	47	78
13	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
14	N	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	335/380 (88%)	327 (98%)	8 (2%)	0	100	100
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	89 (95%)	5 (5%)	0	100	100
19	S	84/99 (85%)	84 (100%)	0	0	100	100
20	T	86/156 (55%)	79 (92%)	7 (8%)	0	100	100
20	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
21	V	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
22	W	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
32	g	99/154 (64%)	93 (94%)	6 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	i	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
35	j	69/108 (64%)	66 (96%)	3 (4%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	m	126/129 (98%)	123 (98%)	3 (2%)	0	100	100
39	n	169/179 (94%)	161 (95%)	8 (5%)	0	100	100
40	o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	p	172/176 (98%)	167 (97%)	5 (3%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8173/9213 (89%)	7927 (97%)	244 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
11	K	2	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	100/100 (100%)	97 (97%)	3 (3%)	41	75
2	B	132/175 (75%)	126 (96%)	6 (4%)	27	60
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	361/392 (92%)	353 (98%)	8 (2%)	52	83
5	E	183/205 (89%)	176 (96%)	7 (4%)	33	67
6	F	346/368 (94%)	337 (97%)	9 (3%)	46	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	579/608 (95%)	569 (98%)	10 (2%)	60	87
8	H	274/274 (100%)	269 (98%)	5 (2%)	59	86
9	I	151/175 (86%)	150 (99%)	1 (1%)	84	95
10	J	141/141 (100%)	139 (99%)	2 (1%)	67	90
11	K	85/85 (100%)	82 (96%)	3 (4%)	36	70
12	L	533/533 (100%)	519 (97%)	14 (3%)	46	79
13	M	412/412 (100%)	407 (99%)	5 (1%)	71	92
14	N	315/315 (100%)	312 (99%)	3 (1%)	76	93
15	O	283/303 (93%)	278 (98%)	5 (2%)	59	86
16	P	293/327 (90%)	286 (98%)	7 (2%)	49	81
17	Q	116/153 (76%)	114 (98%)	2 (2%)	60	87
18	R	79/97 (81%)	78 (99%)	1 (1%)	69	91
19	S	76/82 (93%)	74 (97%)	2 (3%)	46	79
20	T	81/135 (60%)	76 (94%)	5 (6%)	18	47
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	99 (98%)	2 (2%)	55	84
22	W	108/114 (95%)	107 (99%)	1 (1%)	78	94
23	X	154/155 (99%)	153 (99%)	1 (1%)	86	96
24	Y	101/102 (99%)	97 (96%)	4 (4%)	31	65
25	Z	120/121 (99%)	119 (99%)	1 (1%)	81	94
26	a	59/59 (100%)	57 (97%)	2 (3%)	37	71
27	b	71/72 (99%)	70 (99%)	1 (1%)	67	90
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	102 (97%)	3 (3%)	42	76
30	e	89/96 (93%)	86 (97%)	3 (3%)	37	71
31	f	54/54 (100%)	53 (98%)	1 (2%)	57	85
32	g	92/131 (70%)	88 (96%)	4 (4%)	29	62
33	h	121/158 (77%)	118 (98%)	3 (2%)	47	80
34	i	120/121 (99%)	116 (97%)	4 (3%)	38	72
35	j	61/84 (73%)	59 (97%)	2 (3%)	38	72
36	k	63/76 (83%)	58 (92%)	5 (8%)	12	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	l	140/159 (88%)	137 (98%)	3 (2%)	53	84
38	m	113/114 (99%)	111 (98%)	2 (2%)	59	86
39	n	156/161 (97%)	152 (97%)	4 (3%)	46	79
40	o	110/120 (92%)	107 (97%)	3 (3%)	44	78
41	p	155/157 (99%)	151 (97%)	4 (3%)	46	79
42	q	130/130 (100%)	129 (99%)	1 (1%)	81	94
43	r	85/97 (88%)	85 (100%)	0	100	100
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7205/7891 (91%)	7053 (98%)	152 (2%)	56	84

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	48	ARG
1	A	97	LEU
2	B	50	PHE
2	B	54	CYS
2	B	79	SER
2	B	82	GLN
2	B	100	LEU
2	B	125	TYR
4	D	46	ASN
4	D	50	ASN
4	D	61	VAL
4	D	104	ASP
4	D	161	ILE
4	D	334	LYS
4	D	410	MET
4	D	420	THR
5	E	10	ARG
5	E	63	ILE
5	E	118	GLU
5	E	168	ASP
5	E	169	ILE
5	E	181	ILE
5	E	203	THR
6	F	8	LYS
6	F	34	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	44	LYS
6	F	108	ARG
6	F	112	ARG
6	F	172	ASP
6	F	359	CYS
6	F	365	CYS
6	F	405	CYS
7	G	57	VAL
7	G	61	LYS
7	G	97	LEU
7	G	174	THR
7	G	403	ASP
7	G	448	LYS
7	G	486	ASP
7	G	539	LYS
7	G	540	ASP
7	G	613	TYR
8	H	5	ASN
8	H	126	LYS
8	H	234	MET
8	H	237	PHE
8	H	310	LEU
9	I	14	MET
10	J	132	ASP
10	J	135	PHE
11	K	34	GLU
11	K	37	MET
11	K	53	PHE
12	L	21	MET
12	L	31	ASN
12	L	61	LEU
12	L	101	MET
12	L	163	ASP
12	L	197	ASP
12	L	262	ARG
12	L	286	LEU
12	L	336	LYS
12	L	393	ASP
12	L	445	GLU
12	L	480	MET
12	L	554	ASP
12	L	580	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	57	PHE
13	M	86	LYS
13	M	207	MET
13	M	220	HIS
13	M	413	MET
14	N	40	ILE
14	N	46	LYS
14	N	322	LYS
15	O	12	GLU
15	O	81	LYS
15	O	157	LYS
15	O	214	MET
15	O	242	LYS
16	P	82	ARG
16	P	199	LYS
16	P	219	LYS
16	P	263	TYR
16	P	268	ARG
16	P	269	LEU
16	P	281	ARG
17	Q	16	LYS
17	Q	31	LYS
18	R	96	HIS
19	S	38	LYS
19	S	47	ASN
20	T	8	LEU
20	T	16	LEU
20	T	30	LEU
20	T	44	SER
20	T	83	LYS
21	V	39	LYS
21	V	115	ILE
22	W	40	ARG
23	X	63	ASN
24	Y	2	LYS
24	Y	50	GLU
24	Y	85	ASP
24	Y	114	CYS
25	Z	133	LEU
26	a	1	MET
26	a	69	ILE
27	b	3	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	d	5	ARG
29	d	8	ARG
29	d	104	LYS
30	e	38	GLU
30	e	90	LYS
30	e	97	HIS
31	f	1	MET
32	g	24	LEU
32	g	26	TRP
32	g	57	ASN
32	g	117	LYS
33	h	6	LYS
33	h	7	ARG
33	h	113	LEU
34	i	38	ARG
34	i	48	LYS
34	i	66	HIS
34	i	119	MET
35	j	43	ASP
35	j	71	GLU
36	k	22	LYS
36	k	34	LYS
36	k	38	ARG
36	k	86	TYR
36	k	91	LYS
37	l	6	LYS
37	l	148	LYS
37	l	157	GLU
38	m	39	ARG
38	m	84	LYS
39	n	24	ARG
39	n	128	ARG
39	n	138	GLN
39	n	161	ASP
40	o	7	ARG
40	o	83	ARG
40	o	121	MET
41	p	42	ARG
41	p	58	ASN
41	p	95	TYR
41	p	126	LYS
42	q	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
13	M	220	HIS
35	j	21	GLN
39	n	11	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

15 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
12	FME	L	1	12	8,9,10	1.50	1 (12%)	7,9,11	1.65	2 (28%)
1	FME	A	1	1	8,9,10	1.50	1 (12%)	7,9,11	1.67	1 (14%)
24	AYA	Y	1	24	6,7,8	1.80	2 (33%)	5,8,10	1.41	1 (20%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	7,9,11	1.67	3 (42%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.19	1 (20%)
13	FME	M	1	13	8,9,10	1.50	1 (12%)	7,9,11	1.67	1 (14%)
8	FME	H	1	8	8,9,10	1.49	1 (12%)	7,9,11	1.76	3 (42%)
27	AYA	b	1	27	6,7,8	1.81	1 (16%)	5,8,10	1.31	1 (20%)
34	SAC	i	1	34	7,8,9	1.65	1 (14%)	8,9,11	1.43	1 (12%)
38	SAC	m	1	38	7,8,9	1.66	1 (14%)	8,9,11	1.33	1 (12%)
29	AME	d	1	29	9,10,11	1.46	1 (11%)	9,11,13	1.48	2 (22%)
42	AME	q	1	42	9,10,11	1.44	1 (11%)	9,11,13	1.63	2 (22%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	7,9,11	1.71	2 (28%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	7,9,11	1.64	2 (28%)
4	2MR	D	85	4	10,12,13	2.37	2 (20%)	5,13,15	1.35	1 (20%)

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
12	FME	L	1	12	-	2/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
11	FME	K	1	11	-	4/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
13	FME	M	1	13	-	2/7/9/11	-
8	FME	H	1	8	-	0/7/9/11	-
27	AYA	b	1	27	-	0/4/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
38	SAC	m	1	38	-	1/7/8/10	-
29	AME	d	1	29	-	5/9/10/12	-
42	AME	q	1	42	-	4/9/10/12	-
10	FME	J	1	10	-	1/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.12	1.44	1.33
4	D	85	2MR	CZ-NE	5.07	1.45	1.34
10	J	1	FME	CN-N	3.65	1.45	1.33
12	L	1	FME	CN-N	3.64	1.45	1.33
13	M	1	FME	CN-N	3.63	1.45	1.33
1	A	1	FME	CN-N	3.63	1.45	1.33
11	K	1	FME	CN-N	3.61	1.45	1.33
14	N	1	FME	CN-N	3.61	1.45	1.33
8	H	1	FME	CN-N	3.55	1.45	1.33
27	b	1	AYA	CT-N	3.32	1.45	1.34
34	i	1	SAC	C1A-N	3.32	1.45	1.34
38	m	1	SAC	C1A-N	3.29	1.45	1.34
29	d	1	AME	CT1-N	3.25	1.45	1.34
24	Y	1	AYA	CT-N	3.23	1.45	1.34
43	r	1	AYA	CT-N	3.18	1.45	1.34
42	q	1	AME	CT1-N	3.18	1.45	1.34
43	r	1	AYA	OT-CT	-2.06	1.18	1.23
24	Y	1	AYA	OT-CT	-2.00	1.18	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	q	1	AME	CE-SD-CG	2.94	110.50	100.40
34	i	1	SAC	C2A-C1A-N	2.82	120.88	116.10
29	d	1	AME	CE-SD-CG	2.82	110.09	100.40
8	H	1	FME	CE-SD-CG	2.82	110.08	100.40
1	A	1	FME	CE-SD-CG	2.74	109.81	100.40
10	J	1	FME	CE-SD-CG	2.71	109.70	100.40
13	M	1	FME	CE-SD-CG	2.69	109.66	100.40
12	L	1	FME	CE-SD-CG	2.59	109.28	100.40
11	K	1	FME	CE-SD-CG	2.51	109.02	100.40
14	N	1	FME	CE-SD-CG	2.50	108.97	100.40
24	Y	1	AYA	CM-CT-N	2.46	120.27	116.10
42	q	1	AME	CT2-CT1-N	2.36	120.10	116.10
38	m	1	SAC	C2A-C1A-N	2.33	120.04	116.10
27	b	1	AYA	CM-CT-N	2.29	119.98	116.10
4	D	85	2MR	CD-NE-CZ	-2.25	119.19	123.41
8	H	1	FME	CA-N-CN	-2.18	119.47	122.82
43	r	1	AYA	CM-CT-N	2.13	119.71	116.10
12	L	1	FME	O1-CN-N	-2.12	119.70	125.27
29	d	1	AME	CT2-CT1-N	2.11	119.67	116.10
8	H	1	FME	O1-CN-N	-2.09	119.76	125.27
10	J	1	FME	O1-CN-N	-2.08	119.79	125.27
11	K	1	FME	O1-CN-N	-2.06	119.85	125.27
14	N	1	FME	O1-CN-N	-2.06	119.85	125.27
11	K	1	FME	CA-N-CN	-2.00	119.75	122.82

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
29	d	1	AME	C-CA-CB-CG
42	q	1	AME	C-CA-CB-CG
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
10	J	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CG-SD-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
42	q	1	AME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
29	d	1	AME	N-CA-CB-CG
42	q	1	AME	N-CA-CB-CG
42	q	1	AME	CA-CB-CG-SD
29	d	1	AME	CB-CA-N-CT1
12	L	1	FME	N-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
14	N	1	FME	CB-CG-SD-CE
38	m	1	SAC	C-CA-CB-OG
11	K	1	FME	N-CA-CB-CG
29	d	1	AME	C-CA-N-CT1
11	K	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 4 are monoatomic - leaving 79 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	B	201	2	0,12,12	-	-	-		
48	FES	E	301	5	0,4,4	-	-	-		
46	PC1	d	204	-	38,38,53	1.09	3 (7%)	44,46,61	1.03	2 (4%)
46	PC1	J	203	-	34,34,53	1.15	4 (11%)	40,42,61	1.07	2 (5%)
45	3PE	L	702	-	44,44,50	0.91	4 (9%)	47,49,55	1.05	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	Y	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.11	2 (4%)
46	PC1	B	203	-	47,47,53	0.99	4 (8%)	53,55,61	1.07	2 (3%)
46	PC1	A	203	-	34,34,53	1.15	4 (11%)	40,42,61	1.04	2 (5%)
46	PC1	A	204	-	32,32,53	1.20	4 (12%)	38,40,61	1.04	2 (5%)
46	PC1	M	606	-	34,34,53	1.15	4 (11%)	40,42,61	1.08	2 (5%)
52	CDL	H	402	-	57,57,99	1.09	7 (12%)	63,69,111	1.18	3 (4%)
45	3PE	r	202	-	29,29,50	1.11	4 (13%)	32,34,55	1.20	2 (6%)
52	CDL	r	201	-	60,60,99	1.11	8 (13%)	66,72,111	1.12	4 (6%)
45	3PE	I	203	-	36,36,50	1.00	4 (11%)	39,41,55	1.08	2 (5%)
45	3PE	d	203	-	48,48,50	0.88	4 (8%)	51,53,55	1.03	2 (3%)
56	DGT	O	402	55	26,33,33	2.66	8 (30%)	32,52,52	1.75	11 (34%)
45	3PE	N	402	-	48,48,50	0.87	4 (8%)	51,53,55	1.06	2 (3%)
58	EHZ	T	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.70	7 (20%)
45	3PE	m	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.14	2 (4%)
45	3PE	Z	201	-	41,41,50	0.94	4 (9%)	44,46,55	1.05	2 (4%)
52	CDL	M	602	-	99,99,99	0.87	7 (7%)	105,111,111	1.10	4 (3%)
45	3PE	A	201	-	39,39,50	0.97	4 (10%)	42,44,55	1.04	2 (4%)
46	PC1	l	701	-	46,46,53	1.00	4 (8%)	52,54,61	0.96	2 (3%)
53	PLC	Y	208	-	41,41,41	0.50	0	47,49,49	0.50	0
46	PC1	H	404	-	40,40,53	1.07	4 (10%)	46,48,61	1.00	2 (4%)
52	CDL	L	701	-	99,99,99	0.87	8 (8%)	105,111,111	1.05	4 (3%)
45	3PE	q	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.05	2 (3%)
53	PLC	O	403	-	30,30,41	0.54	0	34,37,49	0.58	0
53	PLC	b	103	-	37,37,41	0.54	0	43,45,49	0.51	0
47	SF4	I	202	9	0,12,12	-	-	-	-	-
47	SF4	I	201	9	0,12,12	-	-	-	-	-
46	PC1	m	202	-	40,40,53	1.06	4 (10%)	46,48,61	1.00	2 (4%)
45	3PE	P	502	-	37,37,50	0.98	4 (10%)	40,42,55	1.11	2 (5%)
45	3PE	L	703	-	33,33,50	1.04	4 (12%)	36,38,55	1.15	2 (5%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
52	CDL	d	201	-	64,64,99	1.06	8 (12%)	70,76,111	1.14	4 (5%)
52	CDL	d	202	-	86,86,99	0.92	8 (9%)	92,98,111	1.11	4 (4%)
53	PLC	O	404	-	30,30,41	0.58	0	36,38,49	0.57	0
45	3PE	g	201	-	28,28,50	1.13	4 (14%)	31,33,55	1.32	3 (9%)
57	NDP	P	501	-	45,52,52	4.27	22 (48%)	53,80,80	2.02	5 (9%)
46	PC1	H	405	-	46,46,53	1.00	4 (8%)	52,54,61	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	U10	H	401	-	34,34,63	1.97	15 (44%)	41,44,79	1.74	11 (26%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
58	EHZ	U	101	20	29,36,37	1.68	5 (17%)	35,44,47	1.57	5 (14%)
53	PLC	g	202	-	41,41,41	0.51	0	47,49,49	0.49	0
48	FES	G	803	7	0,4,4	-	-	-	-	-
45	3PE	Y	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
45	3PE	M	604	-	44,44,50	0.91	4 (9%)	47,49,55	1.09	2 (4%)
46	PC1	B	202	-	45,45,53	1.01	4 (8%)	51,53,61	1.02	2 (3%)
45	3PE	M	603	-	49,49,50	0.87	4 (8%)	52,54,55	1.09	2 (3%)
45	3PE	J	202	-	43,43,50	0.92	3 (6%)	46,48,55	1.11	2 (4%)
46	PC1	q	202	-	48,48,53	0.99	4 (8%)	54,56,61	1.01	2 (3%)
45	3PE	b	102	-	46,46,50	0.90	4 (8%)	49,51,55	1.04	2 (4%)
53	PLC	J	204	-	34,34,41	0.55	0	40,42,49	0.55	0
45	3PE	L	704	-	40,40,50	0.96	4 (10%)	43,45,55	1.13	2 (4%)
60	MYR	o	201	40	14,14,15	0.46	0	13,13,15	0.90	0
53	PLC	Z	203	-	35,35,41	0.54	0	41,43,49	0.63	1 (2%)
59	CHD	i	201	-	32,32,32	3.21	11 (34%)	51,51,51	2.38	17 (33%)
46	PC1	H	403	-	47,47,53	1.00	4 (8%)	53,55,61	1.05	2 (3%)
45	3PE	f	101	-	23,23,50	1.23	4 (17%)	26,28,55	1.35	2 (7%)
53	PLC	M	607	-	33,33,41	0.56	0	39,41,49	0.51	0
46	PC1	M	605	-	43,43,53	1.03	4 (9%)	49,51,61	0.99	2 (4%)
45	3PE	Y	205	-	50,50,50	0.85	4 (8%)	53,55,55	1.04	2 (3%)
53	PLC	L	705	-	35,35,41	0.53	0	41,43,49	0.53	0
46	PC1	I	204	-	53,53,53	0.93	4 (7%)	59,61,61	1.03	2 (3%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
52	CDL	i	202	-	75,75,99	0.99	8 (10%)	81,87,111	1.12	4 (4%)
45	3PE	Y	202	-	26,26,50	1.17	4 (15%)	29,31,55	1.14	2 (6%)
45	3PE	Y	207	-	35,35,50	1.01	4 (11%)	38,40,55	1.17	2 (5%)
46	PC1	h	201	-	37,37,53	1.04	3 (8%)	43,45,61	0.95	1 (2%)
46	PC1	Z	202	-	43,43,53	1.03	4 (9%)	49,51,61	1.00	2 (4%)
49	FMN	F	502	-	33,33,33	2.73	10 (30%)	48,50,50	1.74	15 (31%)
45	3PE	Y	206	-	44,44,50	0.91	4 (9%)	47,49,55	1.08	2 (4%)
52	CDL	N	401	-	93,93,99	0.89	8 (8%)	99,105,111	1.08	4 (4%)
45	3PE	J	201	-	36,36,50	1.01	4 (11%)	39,41,55	1.17	2 (5%)
45	3PE	b	101	-	35,35,50	1.01	4 (11%)	38,40,55	1.12	2 (5%)
45	3PE	a	101	-	35,35,50	1.00	4 (11%)	38,40,55	1.07	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	A	202	-	41,41,50	0.94	4 (9%)	44,46,55	1.09	2 (4%)
45	3PE	Y	204	-	50,50,50	0.85	4 (8%)	53,55,55	1.06	2 (3%)

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
47	SF4	B	201	2	-	-	0/6/5/5
48	FES	E	301	5	-	-	0/1/1/1
46	PC1	d	204	-	-	18/42/42/57	-
46	PC1	J	203	-	-	16/38/38/57	-
45	3PE	L	702	-	-	24/48/48/54	-
45	3PE	Y	201	-	-	18/44/44/54	-
46	PC1	B	203	-	-	19/51/51/57	-
46	PC1	A	203	-	-	18/38/38/57	-
46	PC1	A	204	-	-	17/36/36/57	-
46	PC1	M	606	-	-	14/38/38/57	-
52	CDL	H	402	-	-	33/67/67/110	-
45	3PE	r	202	-	-	14/33/33/54	-
52	CDL	r	201	-	-	28/71/71/110	-
45	3PE	I	203	-	-	14/40/40/54	-
45	3PE	d	203	-	-	25/52/52/54	-
56	DGT	O	402	55	-	4/18/34/34	0/3/3/3
45	3PE	N	402	-	-	32/52/52/54	-
58	EHZ	T	101	20	-	8/42/44/45	-
45	3PE	m	201	-	-	14/44/44/54	-
45	3PE	Z	201	-	-	14/45/45/54	-
52	CDL	M	602	-	-	52/110/110/110	-
45	3PE	A	201	-	-	21/43/43/54	-
46	PC1	l	701	-	-	18/50/50/57	-
53	PLC	Y	208	-	-	17/45/45/45	-
46	PC1	H	404	-	-	14/44/44/57	-
52	CDL	L	701	-	-	42/110/110/110	-
45	3PE	q	201	-	-	24/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PLC	O	403	-	-	10/33/33/45	-
53	PLC	b	103	-	-	19/41/41/45	-
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	I	201	9	-	-	0/6/5/5
46	PC1	m	202	-	-	14/44/44/57	-
45	3PE	P	502	-	-	17/41/41/54	-
45	3PE	L	703	-	-	18/37/37/54	-
47	SF4	G	801	7	-	-	0/6/5/5
52	CDL	d	201	-	-	33/75/75/110	-
52	CDL	d	202	-	-	50/97/97/110	-
53	PLC	O	404	-	-	11/34/34/45	-
45	3PE	g	201	-	-	17/31/31/54	-
57	NDP	P	501	-	-	9/30/77/77	0/5/5/5
46	PC1	H	405	-	-	24/50/50/57	-
51	U10	H	401	-	-	10/29/53/87	0/1/1/1
47	SF4	F	501	6	-	-	0/6/5/5
58	EHZ	U	101	20	-	10/42/44/45	-
53	PLC	g	202	-	-	13/45/45/45	-
48	FES	G	803	7	-	-	0/1/1/1
45	3PE	Y	203	-	-	21/54/54/54	-
45	3PE	M	604	-	-	23/48/48/54	-
46	PC1	B	202	-	-	20/49/49/57	-
45	3PE	M	603	-	-	21/53/53/54	-
45	3PE	J	202	-	-	13/47/47/54	-
46	PC1	q	202	-	-	15/52/52/57	-
45	3PE	b	102	-	-	21/50/50/54	-
53	PLC	J	204	-	-	13/38/38/45	-
45	3PE	L	704	-	-	21/44/44/54	-
60	MYR	o	201	40	-	2/11/12/13	-
53	PLC	Z	203	-	-	14/39/39/45	-
59	CHD	i	201	-	-	3/9/74/74	0/4/4/4
46	PC1	H	403	-	-	24/51/51/57	-
45	3PE	f	101	-	-	14/26/26/54	-
53	PLC	M	607	-	-	14/37/37/45	-
46	PC1	M	605	-	-	16/47/47/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Y	205	-	-	22/54/54/54	-
53	PLC	L	705	-	-	14/39/39/45	-
46	PC1	I	204	-	-	16/57/57/57	-
52	CDL	i	202	-	-	39/86/86/110	-
47	SF4	G	802	7	-	-	0/6/5/5
45	3PE	Y	202	-	-	16/30/30/54	-
45	3PE	Y	207	-	-	16/39/39/54	-
46	PC1	h	201	-	-	11/40/40/57	-
46	PC1	Z	202	-	-	19/47/47/57	-
49	FMN	F	502	-	-	2/18/18/18	0/3/3/3
45	3PE	Y	206	-	-	20/48/48/54	-
52	CDL	N	401	-	-	40/104/104/110	-
45	3PE	J	201	-	-	11/40/40/54	-
45	3PE	b	101	-	-	20/39/39/54	-
45	3PE	a	101	-	-	16/39/39/54	-
45	3PE	A	202	-	-	23/45/45/54	-
45	3PE	Y	204	-	-	25/54/54/54	-

All (319) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	O4B-C1B	15.02	1.62	1.41
57	P	501	NDP	C6N-C5N	12.08	1.54	1.33
59	i	201	CHD	C11-C12	8.57	1.67	1.53
56	O	402	DGT	O6-C6	8.32	1.40	1.23
57	P	501	NDP	C7N-N7N	8.31	1.55	1.33
57	P	501	NDP	O4D-C1D	8.17	1.61	1.42
59	i	201	CHD	C16-C15	7.14	1.73	1.54
49	F	502	FMN	C4A-N5	7.13	1.44	1.30
57	P	501	NDP	C2D-C1D	-7.10	1.30	1.53
49	F	502	FMN	C10-N1	6.47	1.46	1.33
57	P	501	NDP	O4D-C4D	-6.44	1.30	1.45
59	i	201	CHD	C20-C17	-5.85	1.44	1.54
59	i	201	CHD	C13-C17	5.46	1.64	1.55
58	U	101	EHZ	C15-N2	5.36	1.45	1.33
57	P	501	NDP	P2B-O2B	5.33	1.69	1.59
58	T	101	EHZ	C15-N2	5.31	1.45	1.33
58	T	101	EHZ	C12-N1	5.30	1.45	1.33
58	U	101	EHZ	C12-N1	5.28	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	i	201	CHD	C8-C9	5.24	1.64	1.53
59	i	201	CHD	O12-C12	-5.20	1.35	1.43
49	F	502	FMN	C5A-N5	5.15	1.49	1.39
57	P	501	NDP	O4B-C4B	-5.06	1.33	1.45
59	i	201	CHD	C6-C5	4.92	1.61	1.53
49	F	502	FMN	C9A-N10	4.90	1.49	1.41
56	O	402	DGT	C2-N2	4.72	1.45	1.34
56	O	402	DGT	C2-N1	4.71	1.49	1.37
49	F	502	FMN	C2-N1	4.70	1.47	1.36
57	P	501	NDP	C2N-C3N	4.68	1.48	1.34
56	O	402	DGT	C2-N3	4.38	1.43	1.33
59	i	201	CHD	C15-C14	4.10	1.62	1.54
49	F	502	FMN	C2-N3	4.08	1.48	1.39
57	P	501	NDP	O7N-C7N	-4.06	1.14	1.24
57	P	501	NDP	O2D-C2D	3.98	1.52	1.43
57	P	501	NDP	C6A-N6A	3.84	1.48	1.34
49	F	502	FMN	C10-N10	3.68	1.45	1.37
49	F	502	FMN	C4-N3	3.65	1.45	1.38
57	P	501	NDP	C5A-C4A	-3.56	1.31	1.40
59	i	201	CHD	C6-C7	3.52	1.58	1.52
51	H	401	U10	C4-C5	-3.30	1.39	1.48
57	P	501	NDP	C4N-C3N	3.16	1.56	1.49
51	H	401	U10	C3-C2	-3.09	1.40	1.48
49	F	502	FMN	O2-C2	-3.08	1.18	1.24
51	H	401	U10	C7-C8	2.95	1.54	1.50
56	O	402	DGT	C5-C6	-2.85	1.41	1.47
51	H	401	U10	C20-C19	2.82	1.57	1.50
51	H	401	U10	C6-C1	2.79	1.40	1.35
57	P	501	NDP	C2A-N3A	2.77	1.36	1.32
57	P	501	NDP	C4N-C5N	2.75	1.56	1.48
51	H	401	U10	C11-C9	2.72	1.56	1.51
49	F	502	FMN	O4-C4	-2.70	1.18	1.23
46	l	701	PC1	O21-C2	-2.70	1.39	1.46
51	H	401	U10	C7-C6	2.68	1.55	1.51
46	d	204	PC1	O21-C2	-2.66	1.39	1.46
56	O	402	DGT	C1'-N9	-2.64	1.41	1.49
45	J	202	3PE	O21-C2	-2.62	1.40	1.46
52	M	602	CDL	OB6-CB4	-2.61	1.40	1.46
52	d	202	CDL	OB6-CB4	-2.61	1.40	1.46
52	H	402	CDL	OB6-CB4	-2.61	1.40	1.46
57	P	501	NDP	O3D-C3D	-2.60	1.36	1.43
57	P	501	NDP	O3B-C3B	-2.59	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	r	201	CDL	OB6-CB4	-2.58	1.40	1.46
52	d	201	CDL	OA6-CA4	-2.58	1.40	1.46
46	A	203	PC1	O21-C2	-2.58	1.40	1.46
52	r	201	CDL	OA6-CA4	-2.57	1.40	1.46
59	i	201	CHD	C13-C12	-2.56	1.50	1.54
45	M	603	3PE	O21-C2	-2.56	1.40	1.46
52	N	401	CDL	OB6-CB4	-2.56	1.40	1.46
52	i	202	CDL	OB6-CB4	-2.56	1.40	1.46
46	I	204	PC1	O21-C2	-2.55	1.40	1.46
46	H	404	PC1	O21-C2	-2.55	1.40	1.46
46	q	202	PC1	O21-C2	-2.55	1.40	1.46
46	J	203	PC1	O21-C2	-2.55	1.40	1.46
46	B	202	PC1	O21-C2	-2.54	1.40	1.46
46	M	606	PC1	O21-C2	-2.54	1.40	1.46
52	H	402	CDL	OA6-CA4	-2.54	1.40	1.46
52	M	602	CDL	OA6-CA4	-2.54	1.40	1.46
46	H	403	PC1	O21-C2	-2.53	1.40	1.46
52	L	701	CDL	OB6-CB4	-2.53	1.40	1.46
45	Y	202	3PE	O21-C2	-2.53	1.40	1.46
52	L	701	CDL	OA6-CA4	-2.53	1.40	1.46
45	a	101	3PE	O21-C2	-2.52	1.40	1.46
46	A	204	PC1	O21-C2	-2.52	1.40	1.46
45	M	604	3PE	O21-C2	-2.51	1.40	1.46
46	H	405	PC1	O21-C2	-2.51	1.40	1.46
52	i	202	CDL	OA6-CA4	-2.51	1.40	1.46
45	I	203	3PE	O21-C2	-2.51	1.40	1.46
45	L	703	3PE	O21-C2	-2.50	1.40	1.46
46	M	605	PC1	O21-C2	-2.50	1.40	1.46
45	N	402	3PE	O21-C2	-2.50	1.40	1.46
52	d	201	CDL	OB6-CB4	-2.50	1.40	1.46
45	g	201	3PE	O21-C2	-2.50	1.40	1.46
52	r	201	CDL	OB8-CB7	2.50	1.40	1.33
45	r	202	3PE	O21-C2	-2.50	1.40	1.46
45	A	201	3PE	O31-C31	2.49	1.40	1.33
45	b	102	3PE	O21-C2	-2.49	1.40	1.46
46	Z	202	PC1	O21-C2	-2.49	1.40	1.46
46	h	201	PC1	O21-C2	-2.49	1.40	1.46
45	d	203	3PE	O21-C2	-2.48	1.40	1.46
46	B	203	PC1	O21-C2	-2.48	1.40	1.46
45	Y	204	3PE	O21-C2	-2.48	1.40	1.46
45	P	502	3PE	O21-C2	-2.47	1.40	1.46
52	L	701	CDL	OB8-CB7	2.47	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	f	101	3PE	O21-C2	-2.46	1.40	1.46
46	m	202	PC1	O21-C2	-2.46	1.40	1.46
46	A	203	PC1	O31-C31	2.46	1.40	1.33
52	d	201	CDL	OB8-CB7	2.45	1.40	1.33
52	i	202	CDL	OB8-CB7	2.45	1.40	1.33
46	H	405	PC1	O31-C31	2.44	1.40	1.33
45	L	704	3PE	O31-C31	2.44	1.40	1.33
45	J	201	3PE	O31-C31	2.44	1.40	1.33
52	d	202	CDL	OA8-CA7	2.44	1.40	1.33
45	Y	203	3PE	O31-C31	2.43	1.40	1.33
45	L	703	3PE	O31-C31	2.43	1.40	1.33
46	m	202	PC1	O31-C31	2.43	1.40	1.33
46	q	202	PC1	O31-C31	2.43	1.40	1.33
45	Y	207	3PE	O21-C2	-2.43	1.40	1.46
45	A	202	3PE	O21-C2	-2.43	1.40	1.46
45	A	201	3PE	O21-C2	-2.43	1.40	1.46
45	b	102	3PE	O31-C31	2.43	1.40	1.33
45	L	704	3PE	O21-C2	-2.43	1.40	1.46
52	i	202	CDL	OA8-CA7	2.42	1.40	1.33
45	d	203	3PE	O31-C31	2.42	1.40	1.33
52	H	402	CDL	OA8-CA7	2.42	1.40	1.33
45	m	201	3PE	O21-C2	-2.42	1.40	1.46
46	Z	202	PC1	O31-C31	2.41	1.40	1.33
45	Y	206	3PE	O21-C2	-2.41	1.40	1.46
45	Z	201	3PE	O31-C31	2.41	1.40	1.33
52	N	401	CDL	OA8-CA7	2.41	1.40	1.33
51	H	401	U10	C15-C14	2.41	1.56	1.50
46	M	606	PC1	O31-C31	2.41	1.40	1.33
45	J	201	3PE	O21-C2	-2.40	1.40	1.46
45	b	101	3PE	O21-C2	-2.40	1.40	1.46
46	A	204	PC1	O31-C31	2.39	1.40	1.33
46	d	204	PC1	O31-C31	2.39	1.40	1.33
52	r	201	CDL	OA8-CA7	2.39	1.40	1.33
46	H	404	PC1	O31-C31	2.39	1.40	1.33
46	M	605	PC1	O31-C31	2.39	1.40	1.33
45	Y	201	3PE	O31-C31	2.38	1.40	1.33
45	Y	202	3PE	O31-C31	2.38	1.40	1.33
45	q	201	3PE	O31-C31	2.38	1.40	1.33
46	H	403	PC1	O31-C31	2.38	1.40	1.33
52	L	701	CDL	OA8-CA7	2.38	1.40	1.33
46	l	701	PC1	O31-C31	2.38	1.40	1.33
45	m	201	3PE	O31-C31	2.38	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	M	602	CDL	OA8-CA7	2.38	1.40	1.33
45	Y	201	3PE	O21-C2	-2.38	1.40	1.46
45	q	201	3PE	O21-C2	-2.38	1.40	1.46
57	P	501	NDP	C6N-N1N	2.38	1.43	1.37
45	b	101	3PE	O31-C31	2.37	1.40	1.33
46	B	202	PC1	O31-C31	2.37	1.40	1.33
46	I	204	PC1	O31-C31	2.37	1.40	1.33
45	Y	207	3PE	O31-C31	2.37	1.40	1.33
52	M	602	CDL	OB8-CB7	2.37	1.40	1.33
45	I	203	3PE	O31-C31	2.36	1.40	1.33
52	d	202	CDL	OA6-CA4	-2.36	1.40	1.46
58	T	101	EHZ	C9-S1	2.35	1.81	1.76
45	f	101	3PE	O31-C31	2.35	1.40	1.33
45	L	702	3PE	O21-C2	-2.35	1.40	1.46
45	L	702	3PE	O31-C31	2.34	1.40	1.33
45	Y	204	3PE	O31-C31	2.34	1.40	1.33
45	M	604	3PE	O31-C31	2.33	1.40	1.33
45	M	603	3PE	O31-C31	2.33	1.40	1.33
45	g	201	3PE	O31-C31	2.33	1.40	1.33
45	A	202	3PE	O31-C31	2.32	1.40	1.33
45	a	101	3PE	O31-C31	2.32	1.40	1.33
45	Y	206	3PE	O31-C31	2.32	1.40	1.33
58	T	101	EHZ	O4-C15	-2.32	1.18	1.23
52	d	201	CDL	OA8-CA6	-2.32	1.39	1.45
58	U	101	EHZ	C9-S1	2.31	1.81	1.76
45	Z	201	3PE	O21-C2	-2.31	1.40	1.46
46	J	203	PC1	O31-C31	2.31	1.40	1.33
45	J	202	3PE	O31-C3	-2.31	1.39	1.45
46	B	203	PC1	O31-C31	2.31	1.40	1.33
51	H	401	U10	C16-C14	2.31	1.56	1.51
57	P	501	NDP	C7N-C3N	2.31	1.53	1.48
52	N	401	CDL	OA6-CA4	-2.30	1.40	1.46
52	N	401	CDL	OB8-CB7	2.30	1.40	1.33
45	Y	203	3PE	O21-C2	-2.30	1.40	1.46
45	Y	205	3PE	O31-C31	2.30	1.40	1.33
45	N	402	3PE	O31-C31	2.29	1.40	1.33
45	r	202	3PE	O31-C3	-2.28	1.39	1.45
45	r	202	3PE	O31-C31	2.28	1.40	1.33
45	Y	206	3PE	O31-C3	-2.28	1.39	1.45
52	d	202	CDL	OB8-CB6	-2.28	1.40	1.45
46	B	203	PC1	O31-C3	-2.27	1.40	1.45
45	P	502	3PE	O31-C31	2.26	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	U	101	EHZ	O4-C15	-2.26	1.18	1.23
58	T	101	EHZ	O3-C12	-2.26	1.18	1.23
45	g	201	3PE	O21-C21	2.25	1.40	1.35
45	f	101	3PE	O21-C21	2.25	1.40	1.35
52	N	401	CDL	OB8-CB6	-2.25	1.40	1.45
46	J	203	PC1	O31-C3	-2.23	1.40	1.45
51	H	401	U10	C6-C5	-2.22	1.40	1.46
45	Y	205	3PE	O21-C2	-2.22	1.41	1.46
45	P	502	3PE	O31-C3	-2.21	1.40	1.45
52	d	201	CDL	OA8-CA7	2.21	1.39	1.33
45	q	201	3PE	O31-C3	-2.21	1.40	1.45
57	P	501	NDP	PA-O5B	2.21	1.68	1.59
46	l	701	PC1	O31-C3	-2.21	1.40	1.45
46	Z	202	PC1	O21-C21	2.21	1.40	1.34
58	U	101	EHZ	O3-C12	-2.20	1.18	1.23
45	Z	201	3PE	O21-C21	2.20	1.40	1.34
46	h	201	PC1	O21-C21	2.20	1.40	1.34
45	Y	205	3PE	O21-C21	2.20	1.40	1.34
51	H	401	U10	C1M-C1	2.19	1.55	1.50
46	H	405	PC1	O21-C21	2.19	1.40	1.34
46	I	204	PC1	O31-C3	-2.19	1.40	1.45
45	Y	203	3PE	O21-C21	2.19	1.40	1.34
45	g	201	3PE	O31-C3	-2.19	1.40	1.45
45	N	402	3PE	O31-C3	-2.18	1.40	1.45
52	N	401	CDL	OA6-CA5	2.18	1.40	1.34
46	m	202	PC1	O21-C21	2.18	1.40	1.34
45	Y	207	3PE	O21-C21	2.18	1.40	1.34
46	B	202	PC1	O31-C3	-2.18	1.40	1.45
52	d	201	CDL	OB6-CB5	2.18	1.40	1.34
45	Y	201	3PE	O21-C21	2.18	1.40	1.34
45	J	202	3PE	O31-C31	2.18	1.39	1.33
45	J	201	3PE	O31-C3	-2.18	1.40	1.45
45	b	101	3PE	O31-C3	-2.17	1.40	1.45
52	L	701	CDL	OB6-CB5	2.17	1.40	1.34
45	Y	202	3PE	O31-C3	-2.17	1.40	1.45
52	M	602	CDL	OA8-CA6	-2.17	1.40	1.45
45	b	102	3PE	O31-C3	-2.17	1.40	1.45
45	d	203	3PE	O21-C21	2.17	1.40	1.34
45	a	101	3PE	O31-C3	-2.17	1.40	1.45
45	A	202	3PE	O31-C3	-2.16	1.40	1.45
56	O	402	DGT	PG-O2G	-2.16	1.46	1.54
45	Y	204	3PE	O31-C3	-2.16	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	204	PC1	O21-C21	2.16	1.40	1.34
45	A	202	3PE	O21-C21	2.16	1.40	1.34
45	L	702	3PE	O31-C3	-2.16	1.40	1.45
46	H	404	PC1	O31-C3	-2.16	1.40	1.45
45	Y	203	3PE	O31-C3	-2.16	1.40	1.45
46	M	605	PC1	O21-C21	2.16	1.40	1.34
52	r	201	CDL	OA6-CA5	2.16	1.40	1.34
45	Y	205	3PE	O31-C3	-2.16	1.40	1.45
45	L	702	3PE	O21-C21	2.15	1.40	1.34
45	m	201	3PE	O21-C21	2.15	1.40	1.34
56	O	402	DGT	PG-O1G	-2.15	1.46	1.54
45	b	102	3PE	O21-C21	2.15	1.40	1.34
46	B	203	PC1	O21-C21	2.15	1.40	1.34
45	Y	201	3PE	O31-C3	-2.15	1.40	1.45
46	M	605	PC1	O31-C3	-2.15	1.40	1.45
46	q	202	PC1	O21-C21	2.15	1.40	1.34
45	M	603	3PE	O31-C3	-2.15	1.40	1.45
52	i	202	CDL	OB8-CB6	-2.14	1.40	1.45
45	b	101	3PE	O21-C21	2.14	1.40	1.34
45	Z	201	3PE	O31-C3	-2.14	1.40	1.45
45	L	704	3PE	O21-C21	2.14	1.40	1.34
45	Y	206	3PE	O21-C21	2.14	1.40	1.34
46	J	203	PC1	O21-C21	2.13	1.40	1.34
45	m	201	3PE	O31-C3	-2.13	1.40	1.45
52	r	201	CDL	OA8-CA6	-2.13	1.40	1.45
45	A	201	3PE	O21-C21	2.13	1.40	1.34
46	d	204	PC1	O31-C3	-2.13	1.40	1.45
52	M	602	CDL	OB8-CB6	-2.13	1.40	1.45
45	f	101	3PE	O31-C3	-2.13	1.40	1.45
46	I	204	PC1	O21-C21	2.13	1.40	1.34
57	P	501	NDP	P2B-O1X	2.13	1.57	1.50
52	d	202	CDL	OA6-CA5	2.13	1.40	1.34
45	J	201	3PE	O21-C21	2.13	1.40	1.34
52	L	701	CDL	OA6-CA5	2.13	1.40	1.34
51	H	401	U10	O3-C3	2.12	1.42	1.36
46	M	606	PC1	O21-C21	2.12	1.40	1.34
52	N	401	CDL	OA8-CA6	-2.12	1.40	1.45
45	r	202	3PE	O21-C21	2.12	1.40	1.34
52	d	201	CDL	OA6-CA5	2.12	1.40	1.34
46	A	204	PC1	O31-C3	-2.12	1.40	1.45
46	B	202	PC1	O21-C21	2.12	1.40	1.34
52	d	202	CDL	OB8-CB7	2.12	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	207	3PE	O31-C3	-2.11	1.40	1.45
45	M	604	3PE	O31-C3	-2.11	1.40	1.45
45	I	203	3PE	O31-C3	-2.11	1.40	1.45
45	I	203	3PE	O21-C21	2.11	1.40	1.34
46	H	403	PC1	O21-C21	2.11	1.40	1.34
45	q	201	3PE	O21-C21	2.11	1.40	1.34
46	h	201	PC1	O31-C3	-2.11	1.40	1.45
51	H	401	U10	O4-C4	2.10	1.42	1.36
45	d	203	3PE	O31-C3	-2.10	1.40	1.45
45	Y	204	3PE	O21-C21	2.10	1.40	1.34
52	i	202	CDL	OA8-CA6	-2.10	1.40	1.45
52	N	401	CDL	OB6-CB5	2.10	1.40	1.34
45	L	704	3PE	O31-C3	-2.10	1.40	1.45
46	H	404	PC1	O21-C21	2.10	1.40	1.34
45	N	402	3PE	O21-C21	2.09	1.40	1.34
52	L	701	CDL	OB8-CB6	-2.09	1.40	1.45
52	d	201	CDL	OB8-CB6	-2.09	1.40	1.45
52	M	602	CDL	OA6-CA5	2.09	1.40	1.34
46	Z	202	PC1	O31-C3	-2.08	1.40	1.45
45	a	101	3PE	O21-C21	2.08	1.40	1.34
52	H	402	CDL	OB8-CB6	-2.08	1.40	1.45
52	r	201	CDL	OB8-CB6	-2.08	1.40	1.45
52	H	402	CDL	OA8-CA6	-2.08	1.40	1.45
45	L	703	3PE	O21-C21	2.07	1.40	1.34
46	q	202	PC1	O31-C3	-2.07	1.40	1.45
52	i	202	CDL	OB6-CB5	2.07	1.40	1.34
52	d	202	CDL	OB6-CB5	2.07	1.40	1.34
45	M	603	3PE	O21-C21	2.07	1.40	1.34
45	P	502	3PE	O21-C21	2.07	1.40	1.34
45	Y	202	3PE	O21-C21	2.06	1.40	1.34
45	L	703	3PE	O31-C3	-2.06	1.40	1.45
46	M	606	PC1	O31-C3	-2.06	1.40	1.45
52	H	402	CDL	OA6-CA5	2.06	1.40	1.34
46	m	202	PC1	O31-C3	-2.06	1.40	1.45
46	l	701	PC1	O21-C21	2.05	1.40	1.34
52	i	202	CDL	OA6-CA5	2.05	1.40	1.34
46	H	405	PC1	O31-C3	-2.05	1.40	1.45
52	L	701	CDL	OA8-CA6	-2.05	1.40	1.45
45	A	201	3PE	O31-C3	-2.04	1.40	1.45
45	M	604	3PE	O21-C21	2.03	1.40	1.34
52	H	402	CDL	OB6-CB5	2.03	1.40	1.34
46	A	203	PC1	O31-C3	-2.03	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	r	201	CDL	OB6-CB5	2.03	1.40	1.34
51	H	401	U10	C1-C2	-2.03	1.40	1.47
46	H	403	PC1	O31-C3	-2.03	1.40	1.45
51	H	401	U10	C25-C24	2.02	1.55	1.50
52	d	202	CDL	OA8-CA6	-2.01	1.40	1.45
46	A	203	PC1	O21-C21	2.01	1.40	1.34
59	i	201	CHD	O7-C7	-2.00	1.39	1.43

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	P	501	NDP	C5A-C6A-N6A	8.67	133.53	120.35
57	P	501	NDP	C1B-N9A-C4A	-6.88	114.55	126.64
59	i	201	CHD	C17-C13-C14	6.53	106.68	100.09
59	i	201	CHD	C13-C17-C20	-6.30	111.98	119.50
57	P	501	NDP	N6A-C6A-N1A	-6.13	105.84	118.57
58	T	101	EHZ	C8-C9-S1	6.06	121.13	113.63
58	U	101	EHZ	C8-C9-S1	5.43	120.34	113.63
57	P	501	NDP	N3A-C2A-N1A	-5.18	120.58	128.68
51	H	401	U10	C10-C9-C11	5.18	123.98	115.27
45	f	101	3PE	O21-C21-C22	4.99	120.27	111.09
45	g	201	3PE	O21-C21-C22	4.82	119.95	111.09
59	i	201	CHD	C17-C13-C12	4.65	121.91	117.67
59	i	201	CHD	C9-C10-C5	4.63	115.09	108.58
49	F	502	FMN	C9-C8-C7	4.62	126.28	119.67
49	F	502	FMN	C7M-C7-C6	4.46	127.72	119.49
45	L	704	3PE	O21-C21-C22	4.45	121.08	111.50
45	m	201	3PE	O21-C21-C22	4.37	120.91	111.50
51	H	401	U10	C7-C8-C9	4.33	134.00	126.79
45	M	604	3PE	O21-C21-C22	4.32	120.81	111.50
45	Y	207	3PE	O21-C21-C22	4.31	120.80	111.50
46	H	403	PC1	O21-C21-C22	4.29	120.75	111.50
46	H	405	PC1	O21-C21-C22	4.27	120.70	111.50
46	M	606	PC1	O21-C21-C22	4.27	120.69	111.50
45	r	202	3PE	O21-C21-C22	4.22	120.60	111.50
46	I	204	PC1	O21-C21-C22	4.19	120.53	111.50
45	Y	201	3PE	O21-C21-C22	4.18	120.52	111.50
52	r	201	CDL	OA6-CA5-C11	4.13	120.41	111.50
52	d	201	CDL	OA6-CA5-C11	4.13	120.39	111.50
52	i	202	CDL	OA6-CA5-C11	4.11	120.37	111.50
46	B	203	PC1	O21-C21-C22	4.09	120.33	111.50
45	J	201	3PE	O21-C21-C22	4.09	120.31	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	b	101	3PE	O21-C21-C22	4.07	120.27	111.50
46	A	204	PC1	O21-C21-C22	4.07	120.27	111.50
45	J	202	3PE	O21-C21-C22	4.06	120.24	111.50
45	A	202	3PE	O21-C21-C22	4.05	120.23	111.50
52	H	402	CDL	OB6-CB5-C51	4.04	120.22	111.50
52	d	202	CDL	OB6-CB5-C51	4.02	120.17	111.50
52	M	602	CDL	OB6-CB5-C51	4.01	120.15	111.50
52	M	602	CDL	OA6-CA5-C11	4.01	120.15	111.50
46	A	203	PC1	O21-C21-C22	4.01	120.14	111.50
45	Y	206	3PE	O21-C21-C22	4.00	120.13	111.50
45	Y	203	3PE	O21-C21-C22	4.00	120.12	111.50
46	q	202	PC1	O21-C21-C22	3.99	120.10	111.50
52	N	401	CDL	OB6-CB5-C51	3.98	120.09	111.50
45	Y	205	3PE	O21-C21-C22	3.98	120.08	111.50
45	L	703	3PE	O21-C21-C22	3.98	120.08	111.50
52	r	201	CDL	OB6-CB5-C51	3.97	120.06	111.50
45	P	502	3PE	O21-C21-C22	3.97	120.05	111.50
52	i	202	CDL	OB6-CB5-C51	3.96	120.03	111.50
45	A	201	3PE	O21-C21-C22	3.95	120.02	111.50
52	d	202	CDL	OA6-CA5-C11	3.95	120.01	111.50
45	Y	204	3PE	O21-C21-C22	3.95	120.00	111.50
45	q	201	3PE	O21-C21-C22	3.95	120.00	111.50
59	i	201	CHD	C14-C13-C12	3.94	111.07	107.40
45	b	102	3PE	O21-C21-C22	3.94	119.98	111.50
52	L	701	CDL	OA6-CA5-C11	3.91	119.93	111.50
45	N	402	3PE	O21-C21-C22	3.90	119.91	111.50
45	Y	202	3PE	O21-C21-C22	3.90	119.91	111.50
59	i	201	CHD	C18-C13-C12	-3.89	105.10	109.07
46	J	203	PC1	O21-C21-C22	3.89	119.87	111.50
52	H	402	CDL	OA6-CA5-C11	3.88	119.87	111.50
45	M	603	3PE	O21-C21-C22	3.86	119.82	111.50
46	B	202	PC1	O21-C21-C22	3.86	119.82	111.50
59	i	201	CHD	C18-C13-C14	-3.85	105.18	111.21
45	Z	201	3PE	O21-C21-C22	3.85	119.80	111.50
46	H	404	PC1	O21-C21-C22	3.82	119.74	111.50
45	d	203	3PE	O21-C21-C22	3.81	119.71	111.50
46	Z	202	PC1	O21-C21-C22	3.80	119.70	111.50
46	m	202	PC1	O21-C21-C22	3.78	119.65	111.50
45	L	702	3PE	O21-C21-C22	3.75	119.59	111.50
46	M	605	PC1	O21-C21-C22	3.74	119.57	111.50
45	I	203	3PE	O21-C21-C22	3.73	119.55	111.50
46	d	204	PC1	O21-C21-C22	3.68	119.44	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	h	201	PC1	O21-C21-C22	3.68	119.44	111.50
52	L	701	CDL	OB6-CB5-C51	3.65	119.36	111.50
51	H	401	U10	C8-C7-C6	3.65	121.88	112.05
59	i	201	CHD	C18-C13-C17	-3.60	105.58	111.21
58	T	101	EHZ	C13-C12-N1	3.57	122.43	116.42
52	N	401	CDL	OA6-CA5-C11	3.52	119.09	111.50
52	d	201	CDL	OB6-CB5-C51	3.44	120.40	110.80
45	a	101	3PE	O21-C21-C22	3.37	120.20	110.80
46	l	701	PC1	O21-C21-C22	3.36	118.73	111.50
49	F	502	FMN	C4-N3-C2	-3.35	119.46	125.64
52	H	402	CDL	OA8-CA7-C31	3.32	120.09	111.38
49	F	502	FMN	C8M-C8-C7	-3.27	114.04	120.74
59	i	201	CHD	C23-C22-C20	-3.26	108.56	114.52
56	O	402	DGT	C5-C6-N1	3.19	119.59	113.95
56	O	402	DGT	C2-N1-C6	-3.15	119.31	125.10
45	Y	207	3PE	O31-C31-C32	3.14	119.61	111.38
56	O	402	DGT	O2G-PG-O3B	3.01	114.72	104.64
52	d	202	CDL	OA8-CA7-C31	2.97	121.22	111.91
56	O	402	DGT	C2'-C3'-C4'	2.96	108.93	102.76
46	l	701	PC1	O31-C31-C32	2.92	121.08	111.91
59	i	201	CHD	C11-C9-C10	-2.91	110.72	113.73
45	J	201	3PE	O31-C31-C32	2.91	121.03	111.91
56	O	402	DGT	PB-O3B-PG	-2.89	122.89	132.83
45	M	603	3PE	O31-C31-C32	2.89	120.99	111.91
46	B	203	PC1	O31-C31-C32	2.89	120.98	111.91
52	L	701	CDL	OA8-CA7-C31	2.85	120.85	111.91
51	H	401	U10	C10-C9-C8	-2.84	116.38	123.68
52	M	602	CDL	OB8-CB7-C71	2.84	120.81	111.91
52	d	202	CDL	OB8-CB7-C71	2.81	120.74	111.91
56	O	402	DGT	O1G-PG-O3B	2.79	113.99	104.64
45	g	201	3PE	O31-C31-C32	2.79	120.66	111.91
49	F	502	FMN	C4A-C10-N10	2.78	120.55	116.48
45	Y	203	3PE	O31-C31-C32	2.74	120.50	111.91
46	H	403	PC1	O31-C31-C32	2.74	120.49	111.91
49	F	502	FMN	C6-C7-C8	-2.73	115.75	119.67
56	O	402	DGT	PA-O3A-PB	-2.73	123.47	132.83
52	i	202	CDL	OB8-CB7-C71	2.73	120.46	111.91
46	B	202	PC1	O31-C31-C32	2.73	120.46	111.91
45	L	704	3PE	O31-C31-C32	2.70	120.38	111.91
59	i	201	CHD	C15-C14-C8	2.67	122.06	118.33
45	N	402	3PE	O31-C31-C32	2.66	120.27	111.91
46	d	204	PC1	O31-C31-C32	2.66	120.26	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	d	201	CDL	OB8-CB7-C71	2.65	120.23	111.91
51	H	401	U10	C20-C19-C21	2.65	119.73	115.27
45	M	604	3PE	O31-C31-C32	2.64	120.19	111.91
45	f	101	3PE	O31-C31-C32	2.64	120.19	111.91
51	H	401	U10	C12-C11-C9	2.63	121.64	112.98
45	m	201	3PE	O31-C31-C32	2.63	120.17	111.91
46	J	203	PC1	O31-C31-C32	2.63	120.15	111.91
45	Z	201	3PE	O31-C31-C32	2.61	120.11	111.91
52	r	201	CDL	OB8-CB7-C71	2.60	120.08	111.91
49	F	502	FMN	C4A-C4-N3	2.60	119.79	113.19
52	N	401	CDL	OB8-CB7-C71	2.60	120.05	111.91
46	q	202	PC1	O31-C31-C32	2.59	120.05	111.91
46	H	405	PC1	O31-C31-C32	2.59	120.03	111.91
45	r	202	3PE	O31-C31-C32	2.58	120.02	111.91
45	L	703	3PE	O31-C31-C32	2.58	119.99	111.91
45	Y	201	3PE	O31-C31-C32	2.58	119.99	111.91
45	Y	205	3PE	O31-C31-C32	2.58	119.99	111.91
45	Y	206	3PE	O31-C31-C32	2.57	119.99	111.91
52	N	401	CDL	OA8-CA7-C31	2.57	119.98	111.91
46	H	404	PC1	O31-C31-C32	2.57	119.98	111.91
45	q	201	3PE	O31-C31-C32	2.57	119.97	111.91
45	I	203	3PE	O31-C31-C32	2.57	119.97	111.91
45	A	202	3PE	O31-C31-C32	2.56	119.95	111.91
52	M	602	CDL	OA8-CA7-C31	2.56	119.95	111.91
59	i	201	CHD	C1-C10-C9	-2.55	107.34	111.35
46	A	203	PC1	O31-C31-C32	2.55	119.91	111.91
59	i	201	CHD	C16-C17-C13	2.54	106.05	103.55
46	M	606	PC1	O31-C31-C32	2.53	119.85	111.91
45	Y	202	3PE	O31-C31-C32	2.53	119.84	111.91
59	i	201	CHD	C19-C10-C9	-2.53	107.70	111.18
46	Z	202	PC1	O31-C31-C32	2.53	119.83	111.91
45	J	202	3PE	O31-C31-C32	2.52	119.83	111.91
45	b	102	3PE	O31-C31-C32	2.52	119.82	111.91
45	L	702	3PE	O31-C31-C32	2.51	119.78	111.91
45	a	101	3PE	O31-C31-C32	2.50	119.76	111.91
49	F	502	FMN	O4-C4-C4A	-2.50	119.98	126.60
46	A	204	PC1	O31-C31-C32	2.49	119.73	111.91
59	i	201	CHD	C4-C3-C2	2.49	113.52	110.55
58	T	101	EHZ	C10-S1-C9	2.48	109.60	101.87
58	T	101	EHZ	C11-N1-C12	-2.48	118.23	122.84
45	Y	204	3PE	O31-C31-C32	2.47	119.66	111.91
58	T	101	EHZ	O2-C9-S1	-2.47	119.41	122.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	P	502	3PE	O31-C31-C32	2.47	119.65	111.91
45	A	201	3PE	O31-C31-C32	2.46	119.64	111.91
45	b	101	3PE	O31-C31-C32	2.44	119.56	111.91
46	M	605	PC1	O31-C31-C32	2.43	119.54	111.91
46	I	204	PC1	O31-C31-C32	2.43	119.53	111.91
52	L	701	CDL	OB8-CB7-C71	2.43	119.53	111.91
52	i	202	CDL	OA8-CA7-C31	2.41	119.48	111.91
52	d	201	CDL	OA8-CA7-C31	2.41	119.47	111.91
45	d	203	3PE	O31-C31-C32	2.41	119.46	111.91
51	H	401	U10	C7-C6-C5	-2.40	115.59	118.48
49	F	502	FMN	C9A-C5A-N5	-2.39	119.83	122.43
46	m	202	PC1	O31-C31-C32	2.39	119.41	111.91
52	r	201	CDL	OA8-CA7-C31	2.37	119.36	111.91
51	H	401	U10	C15-C14-C16	2.34	119.21	115.27
59	i	201	CHD	C9-C11-C12	-2.32	111.24	114.30
58	T	101	EHZ	O3-C12-N1	-2.31	118.65	123.01
58	U	101	EHZ	C13-C12-N1	2.29	120.27	116.42
56	O	402	DGT	O1B-PB-O2B	-2.27	101.00	112.24
49	F	502	FMN	C6-C5A-C9A	2.26	122.14	118.94
51	H	401	U10	C25-C24-C26	2.23	118.54	115.98
56	O	402	DGT	O1A-PA-O2A	-2.23	101.23	112.24
51	H	401	U10	C11-C12-C13	2.22	119.18	111.88
57	P	501	NDP	PN-O3-PA	-2.22	125.20	132.83
49	F	502	FMN	C10-C4A-N5	-2.22	120.16	124.86
58	U	101	EHZ	O2-C9-S1	-2.21	119.74	122.61
56	O	402	DGT	C2'-C1'-N9	-2.21	109.18	114.27
49	F	502	FMN	C5A-C9A-N10	2.18	120.20	117.95
58	U	101	EHZ	C7-C8-C9	-2.17	108.95	113.89
56	O	402	DGT	O6-C6-C5	-2.16	120.16	124.37
51	H	401	U10	C22-C23-C24	-2.14	122.50	127.66
49	F	502	FMN	C4-C4A-C10	2.12	120.35	116.79
49	F	502	FMN	C4A-C10-N1	-2.12	119.82	124.73
53	Z	203	PLC	C3-C2-C1	2.10	116.76	111.79
58	U	101	EHZ	C14-C13-C12	-2.10	108.86	112.36
58	T	101	EHZ	C14-N2-C15	-2.08	118.87	122.59
49	F	502	FMN	C7M-C7-C8	-2.06	116.52	120.74
45	g	201	3PE	C2-O21-C21	-2.05	114.07	117.90
59	i	201	CHD	C1-C2-C3	2.03	113.07	110.47

There are no chirality outliers.

All (1338) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C22-C21-O21-C2
45	A	202	3PE	C1-O11-P-O13
45	A	202	3PE	C1-O11-P-O14
45	A	202	3PE	C11-O13-P-O12
45	A	202	3PE	C11-O13-P-O14
45	A	202	3PE	O22-C21-O21-C2
45	I	203	3PE	O11-C1-C2-O21
45	J	201	3PE	O32-C31-O31-C3
45	L	702	3PE	C1-O11-P-O12
45	L	702	3PE	C1-O11-P-O13
45	L	702	3PE	C1-O11-P-O14
45	L	702	3PE	C22-C21-O21-C2
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	703	3PE	O21-C2-C3-O31
45	L	703	3PE	C22-C21-O21-C2
45	L	704	3PE	C11-O13-P-O14
45	L	704	3PE	O22-C21-O21-C2
45	M	603	3PE	C11-O13-P-O12
45	M	604	3PE	C1-O11-P-O12
45	M	604	3PE	C1-O11-P-O13
45	M	604	3PE	C1-O11-P-O14
45	M	604	3PE	C11-O13-P-O11
45	M	604	3PE	C11-O13-P-O12
45	M	604	3PE	C11-O13-P-O14
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13
45	N	402	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C12-C11-O13-P
45	N	402	3PE	O13-C11-C12-N
45	P	502	3PE	C1-O11-P-O12
45	P	502	3PE	C1-O11-P-O13
45	P	502	3PE	C1-O11-P-O14
45	P	502	3PE	C11-O13-P-O14
45	P	502	3PE	C2-C1-O11-P
45	P	502	3PE	C22-C21-O21-C2
45	Y	201	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	O32-C31-O31-C3
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C11-O13-P-O14
45	Y	203	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O14
45	Y	203	3PE	C22-C21-O21-C2
45	Y	205	3PE	C1-O11-P-O12
45	Y	205	3PE	C1-O11-P-O13
45	Y	205	3PE	C12-C11-O13-P
45	Y	205	3PE	C22-C21-O21-C2
45	Y	206	3PE	C11-O13-P-O11
45	Y	206	3PE	C11-O13-P-O12
45	Y	206	3PE	C11-O13-P-O14
45	Y	207	3PE	C11-O13-P-O12
45	Y	207	3PE	C11-O13-P-O14
45	Y	207	3PE	O22-C21-O21-C2
45	Z	201	3PE	C11-O13-P-O11
45	Z	201	3PE	C11-O13-P-O12
45	Z	201	3PE	C11-O13-P-O14
45	a	101	3PE	C11-O13-P-O12
45	a	101	3PE	O22-C21-O21-C2
45	b	101	3PE	C1-O11-P-O12
45	b	101	3PE	C1-O11-P-O14
45	b	101	3PE	C11-O13-P-O11
45	b	101	3PE	C11-O13-P-O14
45	b	101	3PE	C12-C11-O13-P
45	b	101	3PE	C22-C21-O21-C2
45	b	102	3PE	C11-O13-P-O11
45	b	102	3PE	C11-O13-P-O12
45	b	102	3PE	C11-O13-P-O14
45	b	102	3PE	O21-C2-C3-O31
45	d	203	3PE	C1-O11-P-O12
45	d	203	3PE	C1-O11-P-O14
45	d	203	3PE	O21-C2-C3-O31
45	f	101	3PE	C1-O11-P-O14
45	f	101	3PE	C11-O13-P-O11
45	f	101	3PE	C11-O13-P-O12
45	f	101	3PE	C11-O13-P-O14
45	f	101	3PE	O13-C11-C12-N
45	f	101	3PE	O22-C21-O21-C2
45	f	101	3PE	C22-C21-O21-C2
45	m	201	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	m	201	3PE	O22-C21-O21-C2
45	q	201	3PE	C11-O13-P-O11
45	r	202	3PE	O22-C21-O21-C2
45	r	202	3PE	C22-C21-O21-C2
46	A	203	PC1	C1-O11-P-O12
46	A	203	PC1	C1-O11-P-O14
46	A	203	PC1	C1-O11-P-O13
46	A	203	PC1	O13-C11-C12-N
46	A	204	PC1	C1-O11-P-O12
46	A	204	PC1	C1-O11-P-O14
46	A	204	PC1	O22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C1-O11-P-O14
46	B	203	PC1	C11-O13-P-O12
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C22-C21-O21-C2
46	H	403	PC1	C1-O11-P-O12
46	H	403	PC1	C1-O11-P-O14
46	H	403	PC1	C1-O11-P-O13
46	H	403	PC1	O13-C11-C12-N
46	H	405	PC1	C1-O11-P-O12
46	H	405	PC1	C1-O11-P-O14
46	H	405	PC1	C22-C21-O21-C2
46	I	204	PC1	O13-C11-C12-N
46	J	203	PC1	C1-O11-P-O12
46	J	203	PC1	C1-O11-P-O14
46	J	203	PC1	C22-C21-O21-C2
46	M	605	PC1	C1-O11-P-O12
46	M	606	PC1	C11-O13-P-O12
46	M	606	PC1	C11-O13-P-O14
46	M	606	PC1	C11-O13-P-O11
46	M	606	PC1	C1-O11-P-O12
46	h	201	PC1	C1-O11-P-O12
46	h	201	PC1	C1-O11-P-O14
46	h	201	PC1	C1-O11-P-O13
46	l	701	PC1	C11-O13-P-O12
46	l	701	PC1	C11-O13-P-O14
46	m	202	PC1	C1-O11-P-O12
46	m	202	PC1	C1-O11-P-O14
46	m	202	PC1	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	q	202	PC1	C22-C21-O21-C2
51	H	401	U10	C1-C6-C7-C8
51	H	401	U10	C5-C6-C7-C8
51	H	401	U10	C12-C11-C9-C8
52	H	402	CDL	C1-CA2-OA2-PA1
52	H	402	CDL	C11-CA5-OA6-CA4
52	H	402	CDL	CB3-OB5-PB2-OB3
52	H	402	CDL	C51-CB5-OB6-CB4
52	L	701	CDL	CA3-OA5-PA1-OA3
52	M	602	CDL	O1-C1-CA2-OA2
52	M	602	CDL	CA3-OA5-PA1-OA2
52	M	602	CDL	CA3-OA5-PA1-OA3
52	M	602	CDL	CA3-OA5-PA1-OA4
52	M	602	CDL	C51-CB5-OB6-CB4
52	N	401	CDL	CA2-OA2-PA1-OA3
52	N	401	CDL	OB7-CB5-OB6-CB4
52	d	201	CDL	O1-C1-CA2-OA2
52	d	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	C11-CA5-OA6-CA4
52	d	201	CDL	CB2-OB2-PB2-OB3
52	d	201	CDL	CB2-OB2-PB2-OB5
52	d	201	CDL	OB5-CB3-CB4-OB6
52	d	201	CDL	OB7-CB5-OB6-CB4
52	d	201	CDL	C51-CB5-OB6-CB4
52	d	202	CDL	O1-C1-CA2-OA2
52	d	202	CDL	CA3-OA5-PA1-OA4
52	d	202	CDL	OB7-CB5-OB6-CB4
52	d	202	CDL	C51-CB5-OB6-CB4
52	i	202	CDL	O1-C1-CB2-OB2
52	i	202	CDL	CA3-OA5-PA1-OA3
52	i	202	CDL	CA3-OA5-PA1-OA4
52	i	202	CDL	C51-CB5-OB6-CB4
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CB2-OB2-PB2-OB3
52	r	201	CDL	CB2-OB2-PB2-OB4
53	J	204	PLC	O4P-C4-C5-N
53	J	204	PLC	C1-O3P-P-O1P
53	J	204	PLC	C4-O4P-P-O2P
53	L	705	PLC	O4P-C4-C5-N
53	L	705	PLC	C1-O3P-P-O1P
53	L	705	PLC	C4-O4P-P-O1P
53	O	403	PLC	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	O	403	PLC	O4P-C4-C5-N
53	O	403	PLC	OB-CB-O3-C3
53	O	404	PLC	C1'-C'-O2-C2
53	Y	208	PLC	O4P-C4-C5-N
53	Y	208	PLC	C1-O3P-P-O2P
53	Y	208	PLC	C4-O4P-P-O1P
53	Z	203	PLC	C1'-C'-O2-C2
53	Z	203	PLC	O'-C'-O2-C2
53	Z	203	PLC	C1-O3P-P-O2P
53	Z	203	PLC	C4-O4P-P-O2P
53	b	103	PLC	O3P-C1-C2-O2
53	b	103	PLC	C1-O3P-P-O1P
53	b	103	PLC	C1-O3P-P-O2P
53	b	103	PLC	C1-O3P-P-O4P
53	b	103	PLC	C4-O4P-P-O1P
53	b	103	PLC	C4-O4P-P-O2P
53	g	202	PLC	C1-O3P-P-O4P
57	P	501	NDP	C3B-C4B-C5B-O5B
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	C12-C13-C14-N2
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
45	I	203	3PE	O32-C31-O31-C3
45	Y	205	3PE	O32-C31-O31-C3
46	A	204	PC1	O32-C31-O31-C3
46	d	204	PC1	O32-C31-O31-C3
52	L	701	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OB9-CB7-OB8-CB6
45	Y	205	3PE	C32-C31-O31-C3
46	d	204	PC1	C32-C31-O31-C3
52	M	602	CDL	C71-CB7-OB8-CB6
52	H	402	CDL	OB9-CB7-OB8-CB6
45	A	202	3PE	O32-C31-O31-C3
45	Z	201	3PE	O32-C31-O31-C3
45	a	101	3PE	O32-C31-O31-C3
45	m	201	3PE	O32-C31-O31-C3
45	r	202	3PE	O32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
46	B	203	PC1	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	H	405	PC1	O32-C31-O31-C3
46	l	701	PC1	O32-C31-O31-C3
52	d	201	CDL	OB9-CB7-OB8-CB6
52	d	202	CDL	OA9-CA7-OA8-CA6
52	r	201	CDL	OB9-CB7-OB8-CB6
46	h	201	PC1	O32-C31-O31-C3
52	H	402	CDL	C71-CB7-OB8-CB6
45	A	201	3PE	O22-C21-O21-C2
45	L	702	3PE	O22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
45	Y	205	3PE	O22-C21-O21-C2
45	b	101	3PE	O22-C21-O21-C2
46	B	203	PC1	O22-C21-O21-C2
46	H	405	PC1	O22-C21-O21-C2
46	J	203	PC1	O22-C21-O21-C2
46	m	202	PC1	O22-C21-O21-C2
52	H	402	CDL	OA7-CA5-OA6-CA4
52	H	402	CDL	OB7-CB5-OB6-CB4
52	d	201	CDL	OA7-CA5-OA6-CA4
52	i	202	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	OA7-CA5-OA6-CA4
53	O	404	PLC	O'-C'-O2-C2
45	g	201	3PE	O32-C31-O31-C3
45	g	201	3PE	C22-C21-O21-C2
45	I	203	3PE	C32-C31-O31-C3
45	J	201	3PE	C32-C31-O31-C3
45	Y	201	3PE	C32-C31-O31-C3
45	Z	201	3PE	C32-C31-O31-C3
45	a	101	3PE	C32-C31-O31-C3
45	r	202	3PE	C32-C31-O31-C3
46	A	204	PC1	C32-C31-O31-C3
46	B	203	PC1	C32-C31-O31-C3
46	H	405	PC1	C32-C31-O31-C3
46	l	701	PC1	C32-C31-O31-C3
52	L	701	CDL	C31-CA7-OA8-CA6
52	d	201	CDL	C71-CB7-OB8-CB6
52	r	201	CDL	C71-CB7-OB8-CB6
45	A	202	3PE	C22-C21-O21-C2
45	L	704	3PE	C22-C21-O21-C2
45	Y	207	3PE	C22-C21-O21-C2
45	a	101	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	A	204	PC1	C22-C21-O21-C2
46	m	202	PC1	C22-C21-O21-C2
52	N	401	CDL	C51-CB5-OB6-CB4
51	H	401	U10	C12-C11-C9-C10
51	H	401	U10	C20-C19-C21-C22
45	A	202	3PE	C32-C31-O31-C3
45	g	201	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
52	d	202	CDL	C31-CA7-OA8-CA6
46	h	201	PC1	C32-C31-O31-C3
45	L	703	3PE	O22-C21-O21-C2
45	P	502	3PE	O22-C21-O21-C2
46	q	202	PC1	O22-C21-O21-C2
52	M	602	CDL	OB7-CB5-OB6-CB4
45	N	402	3PE	O32-C31-O31-C3
45	Y	206	3PE	O32-C31-O31-C3
45	f	101	3PE	O32-C31-O31-C3
45	L	704	3PE	C32-C31-O31-C3
45	f	101	3PE	C32-C31-O31-C3
46	J	203	PC1	C32-C31-O31-C3
52	H	402	CDL	C31-CA7-OA8-CA6
52	d	202	CDL	C11-CA5-OA6-CA4
57	P	501	NDP	O4D-C4D-C5D-O5D
57	P	501	NDP	C3D-C4D-C5D-O5D
45	N	402	3PE	C32-C31-O31-C3
45	Y	206	3PE	C32-C31-O31-C3
46	B	203	PC1	C2-C1-O11-P
46	J	203	PC1	O32-C31-O31-C3
45	L	704	3PE	O32-C31-O31-C3
52	H	402	CDL	OA9-CA7-OA8-CA6
51	H	401	U10	C14-C16-C17-C18
52	N	401	CDL	C11-CA5-OA6-CA4
52	M	602	CDL	CB2-C1-CA2-OA2
52	d	201	CDL	CB2-C1-CA2-OA2
52	d	202	CDL	CB2-C1-CA2-OA2
52	d	202	CDL	OA7-CA5-OA6-CA4
45	P	502	3PE	C32-C31-O31-C3
46	q	202	PC1	C32-C31-O31-C3
52	N	401	CDL	C31-CA7-OA8-CA6
52	N	401	CDL	C71-CB7-OB8-CB6
52	i	202	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	M	607	PLC	C1B-CB-O3-C3
53	Z	203	PLC	C1B-CB-O3-C3
53	Z	203	PLC	OB-CB-O3-C3
52	i	202	CDL	OB6-CB4-CB6-OB8
52	i	202	CDL	OB9-CB7-OB8-CB6
51	H	401	U10	C18-C19-C21-C22
45	q	201	3PE	C22-C21-O21-C2
45	Z	201	3PE	C31-C32-C33-C34
46	H	404	PC1	C21-C22-C23-C24
46	I	204	PC1	C21-C22-C23-C24
52	M	602	CDL	CB5-C51-C52-C53
52	d	202	CDL	CA7-C31-C32-C33
52	N	401	CDL	OB9-CB7-OB8-CB6
45	Y	202	3PE	C32-C31-O31-C3
45	I	203	3PE	C21-C22-C23-C24
45	b	102	3PE	C31-C32-C33-C34
45	L	704	3PE	C21-C22-C23-C24
45	Y	204	3PE	C31-C32-C33-C34
45	Y	206	3PE	C31-C32-C33-C34
46	H	403	PC1	C31-C32-C33-C34
46	J	203	PC1	C21-C22-C23-C24
53	Y	208	PLC	CB-C1B-C2B-C3B
57	P	501	NDP	O4B-C4B-C5B-O5B
52	M	602	CDL	C31-CA7-OA8-CA6
45	g	201	3PE	O22-C21-O21-C2
52	r	201	CDL	CB7-C71-C72-C73
52	r	201	CDL	C51-CB5-OB6-CB4
46	q	202	PC1	O32-C31-O31-C3
52	N	401	CDL	OA9-CA7-OA8-CA6
53	M	607	PLC	OB-CB-O3-C3
46	M	606	PC1	C21-C22-C23-C24
52	N	401	CDL	OA7-CA5-OA6-CA4
45	P	502	3PE	O32-C31-O31-C3
45	Y	202	3PE	O32-C31-O31-C3
45	J	202	3PE	C22-C21-O21-C2
46	I	204	PC1	C22-C21-O21-C2
53	g	202	PLC	C1'-C'-O2-C2
45	A	201	3PE	C1-O11-P-O13
45	A	202	3PE	C11-O13-P-O11
45	M	603	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O11
45	Y	202	3PE	C1-O11-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	205	3PE	C11-O13-P-O11
45	Y	207	3PE	C11-O13-P-O11
45	a	101	3PE	C11-O13-P-O11
45	b	101	3PE	C1-O11-P-O13
45	d	203	3PE	C1-O11-P-O13
45	d	203	3PE	C11-O13-P-O11
45	r	202	3PE	C11-O13-P-O11
46	A	204	PC1	C11-O13-P-O11
46	A	204	PC1	C1-O11-P-O13
46	B	203	PC1	C1-O11-P-O13
46	H	405	PC1	C11-O13-P-O11
46	H	405	PC1	C1-O11-P-O13
46	J	203	PC1	C1-O11-P-O13
46	M	605	PC1	C1-O11-P-O13
46	M	606	PC1	C1-O11-P-O13
46	l	701	PC1	C11-O13-P-O11
46	q	202	PC1	C11-O13-P-O11
52	H	402	CDL	CA2-OA2-PA1-OA5
52	L	701	CDL	CA3-OA5-PA1-OA2
52	d	202	CDL	CA2-OA2-PA1-OA5
52	i	202	CDL	CA3-OA5-PA1-OA2
52	r	201	CDL	CA3-OA5-PA1-OA2
52	r	201	CDL	CB2-OB2-PB2-OB5
53	J	204	PLC	C4-O4P-P-O3P
53	L	705	PLC	C4-O4P-P-O3P
53	M	607	PLC	C4-O4P-P-O3P
53	O	404	PLC	C4-O4P-P-O3P
53	Y	208	PLC	C1-O3P-P-O4P
53	Z	203	PLC	C1-O3P-P-O4P
53	Z	203	PLC	C4-O4P-P-O3P
53	b	103	PLC	C4-O4P-P-O3P
45	q	201	3PE	C32-C31-O31-C3
53	g	202	PLC	C1B-CB-O3-C3
52	i	202	CDL	CA2-C1-CB2-OB2
45	J	202	3PE	O22-C21-O21-C2
45	q	201	3PE	O22-C21-O21-C2
46	I	204	PC1	O22-C21-O21-C2
52	r	201	CDL	OB7-CB5-OB6-CB4
53	g	202	PLC	O'-C'-O2-C2
46	Z	202	PC1	C32-C31-O31-C3
45	m	201	3PE	C33-C34-C35-C36
52	d	202	CDL	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	604	3PE	C22-C21-O21-C2
45	L	702	3PE	C24-C25-C26-C27
45	Y	203	3PE	C2A-C2B-C2C-C2D
45	d	203	3PE	C22-C23-C24-C25
52	H	402	CDL	C11-C12-C13-C14
52	i	202	CDL	C35-C36-C37-C38
52	M	602	CDL	OA9-CA7-OA8-CA6
45	M	603	3PE	C3C-C3D-C3E-C3F
45	N	402	3PE	C2A-C2B-C2C-C2D
45	Y	202	3PE	C23-C24-C25-C26
45	Y	205	3PE	C26-C27-C28-C29
45	Y	206	3PE	C28-C29-C2A-C2B
45	b	102	3PE	C33-C34-C35-C36
45	m	201	3PE	C35-C36-C37-C38
46	H	404	PC1	C2B-C2C-C2D-C2E
46	M	605	PC1	C2E-C2F-C2G-C2H
46	Z	202	PC1	C32-C33-C34-C35
46	m	202	PC1	C25-C26-C27-C28
52	i	202	CDL	C31-C32-C33-C34
45	Y	205	3PE	C3-C2-O21-C21
52	N	401	CDL	CA6-CA4-OA6-CA5
45	M	604	3PE	O22-C21-O21-C2
45	Y	201	3PE	C31-C32-C33-C34
45	M	604	3PE	C33-C34-C35-C36
45	Y	204	3PE	C26-C27-C28-C29
45	I	203	3PE	C23-C24-C25-C26
45	Y	204	3PE	C33-C34-C35-C36
45	Y	205	3PE	C36-C37-C38-C39
46	B	202	PC1	C25-C26-C27-C28
52	M	602	CDL	C32-C33-C34-C35
52	M	602	CDL	C62-C63-C64-C65
45	J	201	3PE	C29-C2A-C2B-C2C
45	Y	203	3PE	C35-C36-C37-C38
45	q	201	3PE	C2D-C2E-C2F-C2G
46	A	204	PC1	C22-C23-C24-C25
46	H	404	PC1	C26-C27-C28-C29
46	M	605	PC1	C26-C27-C28-C29
52	N	401	CDL	C16-C17-C18-C19
45	L	702	3PE	C31-C32-C33-C34
45	Y	203	3PE	C21-C22-C23-C24
46	H	404	PC1	O21-C2-C3-O31
45	L	704	3PE	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	P	502	3PE	C35-C36-C37-C38
45	Y	201	3PE	C28-C29-C2A-C2B
45	a	101	3PE	C36-C37-C38-C39
45	f	101	3PE	C32-C33-C34-C35
46	H	403	PC1	C22-C23-C24-C25
46	h	201	PC1	C22-C23-C24-C25
52	H	402	CDL	C57-C58-C59-C60
52	H	402	CDL	C60-C61-C62-C63
52	d	202	CDL	C76-C77-C78-C79
45	q	201	3PE	O32-C31-O31-C3
52	M	602	CDL	C83-C84-C85-C86
45	Y	201	3PE	C25-C26-C27-C28
45	Y	206	3PE	C33-C34-C35-C36
46	B	203	PC1	C39-C3A-C3B-C3C
46	H	403	PC1	C37-C38-C39-C3A
52	N	401	CDL	C35-C36-C37-C38
53	M	607	PLC	C6B-C7B-C8B-C9B
45	M	603	3PE	C34-C35-C36-C37
46	I	204	PC1	C23-C24-C25-C26
52	L	701	CDL	C17-C18-C19-C20
53	M	607	PLC	C7B-C8B-C9B-CAA
45	J	202	3PE	C32-C33-C34-C35
45	M	604	3PE	C38-C39-C3A-C3B
45	N	402	3PE	C35-C36-C37-C38
46	B	203	PC1	C36-C37-C38-C39
46	H	405	PC1	C26-C27-C28-C29
46	I	204	PC1	C32-C33-C34-C35
52	L	701	CDL	C74-C75-C76-C77
52	M	602	CDL	C18-C19-C20-C21
52	i	202	CDL	C37-C38-C39-C40
52	r	201	CDL	C13-C14-C15-C16
53	b	103	PLC	C2'-C3'-C4'-C5'
45	d	203	3PE	C31-C32-C33-C34
45	N	402	3PE	C2C-C2D-C2E-C2F
45	Y	203	3PE	C33-C34-C35-C36
46	l	701	PC1	C39-C3A-C3B-C3C
52	d	201	CDL	C72-C73-C74-C75
53	Y	208	PLC	C2B-C3B-C4B-C5B
60	o	201	MYR	C3-C4-C5-C6
53	M	607	PLC	O3P-C1-C2-C3
45	A	201	3PE	C35-C36-C37-C38
45	Y	205	3PE	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	C2A-C2B-C2C-C2D
45	Y	207	3PE	C29-C2A-C2B-C2C
45	g	201	3PE	C33-C34-C35-C36
52	d	202	CDL	C58-C59-C60-C61
53	J	204	PLC	C4B-C5B-C6B-C7B
45	L	703	3PE	O13-C11-C12-N
45	M	604	3PE	C28-C29-C2A-C2B
45	N	402	3PE	C37-C38-C39-C3A
45	f	101	3PE	C33-C34-C35-C36
52	N	401	CDL	C38-C39-C40-C41
52	i	202	CDL	C74-C75-C76-C77
52	r	201	CDL	C16-C17-C18-C19
45	d	203	3PE	C21-C22-C23-C24
52	L	701	CDL	C20-C21-C22-C23
52	M	602	CDL	C40-C41-C42-C43
52	N	401	CDL	C19-C20-C21-C22
52	d	202	CDL	C52-C53-C54-C55
45	L	703	3PE	C33-C34-C35-C36
58	U	101	EHZ	S1-C10-C11-N1
45	J	202	3PE	C3C-C3D-C3E-C3F
45	L	702	3PE	C28-C29-C2A-C2B
45	Z	201	3PE	C39-C3A-C3B-C3C
45	Z	201	3PE	C23-C24-C25-C26
53	L	705	PLC	C1B-C2B-C3B-C4B
53	O	404	PLC	C1B-C2B-C3B-C4B
45	A	202	3PE	C21-C22-C23-C24
53	g	202	PLC	OB-CB-O3-C3
45	A	201	3PE	C23-C24-C25-C26
46	l	701	PC1	C32-C33-C34-C35
58	T	101	EHZ	C2-C3-C4-C5
45	N	402	3PE	C28-C29-C2A-C2B
46	H	404	PC1	C22-C23-C24-C25
45	M	604	3PE	C34-C35-C36-C37
45	N	402	3PE	C33-C34-C35-C36
46	I	204	PC1	C36-C37-C38-C39
46	H	404	PC1	C22-C21-O21-C2
52	i	202	CDL	C11-CA5-OA6-CA4
46	M	606	PC1	C23-C24-C25-C26
45	q	201	3PE	C37-C38-C39-C3A
52	L	701	CDL	O1-C1-CA2-OA2
45	Y	203	3PE	C27-C28-C29-C2A
58	U	101	EHZ	C5-C6-C7-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	M	605	PC1	C32-C31-O31-C3
52	d	201	CDL	C34-C35-C36-C37
46	Z	202	PC1	O32-C31-O31-C3
45	a	101	3PE	C33-C34-C35-C36
46	A	203	PC1	C25-C26-C27-C28
52	N	401	CDL	C22-C23-C24-C25
46	H	404	PC1	O22-C21-O21-C2
45	J	202	3PE	C37-C38-C39-C3A
46	l	701	PC1	C23-C24-C25-C26
52	d	202	CDL	C81-C82-C83-C84
46	Z	202	PC1	C35-C36-C37-C38
46	d	204	PC1	C33-C34-C35-C36
46	m	202	PC1	C24-C25-C26-C27
52	d	202	CDL	C71-C72-C73-C74
52	r	201	CDL	C11-C12-C13-C14
45	q	201	3PE	C3C-C3D-C3E-C3F
45	L	702	3PE	C21-C22-C23-C24
45	Y	206	3PE	C36-C37-C38-C39
45	b	102	3PE	C28-C29-C2A-C2B
46	I	204	PC1	C2B-C2C-C2D-C2E
46	m	202	PC1	C38-C39-C3A-C3B
46	M	606	PC1	C33-C34-C35-C36
45	Y	201	3PE	O22-C21-O21-C2
52	i	202	CDL	OA7-CA5-OA6-CA4
52	H	402	CDL	CA5-C11-C12-C13
45	Y	201	3PE	C33-C34-C35-C36
52	M	602	CDL	C74-C75-C76-C77
45	A	202	3PE	C34-C35-C36-C37
46	M	605	PC1	C2C-C2D-C2E-C2F
46	q	202	PC1	C25-C26-C27-C28
52	M	602	CDL	C73-C74-C75-C76
45	A	201	3PE	C21-C22-C23-C24
45	Y	206	3PE	C21-C22-C23-C24
45	q	201	3PE	C3A-C3B-C3C-C3D
46	H	403	PC1	C33-C34-C35-C36
46	H	403	PC1	C34-C35-C36-C37
51	H	401	U10	C9-C11-C12-C13
45	g	201	3PE	C36-C37-C38-C39
45	r	202	3PE	C35-C36-C37-C38
46	I	204	PC1	C3E-C3F-C3G-C3H
46	Z	202	PC1	C31-C32-C33-C34
52	M	602	CDL	CA5-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	603	3PE	C22-C21-O21-C2
45	Y	201	3PE	C22-C21-O21-C2
45	Y	202	3PE	C22-C21-O21-C2
45	L	704	3PE	O11-C1-C2-O21
46	A	203	PC1	O11-C1-C2-O21
52	L	701	CDL	OA5-CA3-CA4-OA6
45	M	603	3PE	C38-C39-C3A-C3B
45	a	101	3PE	C32-C33-C34-C35
46	d	204	PC1	C3B-C3C-C3D-C3E
52	i	202	CDL	C13-C14-C15-C16
45	Y	201	3PE	C22-C23-C24-C25
52	i	202	CDL	C54-C55-C56-C57
45	M	603	3PE	O22-C21-O21-C2
45	g	201	3PE	O21-C2-C3-O31
46	l	701	PC1	O21-C2-C3-O31
45	J	202	3PE	C35-C36-C37-C38
46	M	605	PC1	O32-C31-O31-C3
46	q	202	PC1	C26-C27-C28-C29
52	L	701	CDL	C12-C13-C14-C15
52	L	701	CDL	C15-C16-C17-C18
52	d	202	CDL	C54-C55-C56-C57
52	N	401	CDL	CA5-C11-C12-C13
46	q	202	PC1	C29-C2A-C2B-C2C
52	i	202	CDL	C51-C52-C53-C54
45	Y	206	3PE	C38-C39-C3A-C3B
52	L	701	CDL	C53-C54-C55-C56
52	M	602	CDL	C43-C44-C45-C46
46	H	405	PC1	C24-C25-C26-C27
52	d	202	CDL	C61-C62-C63-C64
46	A	203	PC1	C22-C21-O21-C2
46	H	403	PC1	C22-C21-O21-C2
45	L	704	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O11
45	q	201	3PE	C1-O11-P-O13
46	A	203	PC1	C11-O13-P-O11
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O13
46	Z	202	PC1	C1-O11-P-O13
52	H	402	CDL	CB3-OB5-PB2-OB2
52	d	202	CDL	CA3-OA5-PA1-OA2
52	i	202	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	h	201	PC1	C2-C1-O11-P
45	L	702	3PE	C34-C35-C36-C37
45	g	201	3PE	C35-C36-C37-C38
45	d	203	3PE	C32-C31-O31-C3
45	A	202	3PE	O11-C1-C2-C3
45	I	203	3PE	O11-C1-C2-C3
46	A	203	PC1	O11-C1-C2-C3
46	l	701	PC1	O11-C1-C2-C3
46	m	202	PC1	O11-C1-C2-C3
52	M	602	CDL	OA5-CA3-CA4-CA6
52	N	401	CDL	OB5-CB3-CB4-CB6
52	d	201	CDL	OA5-CA3-CA4-CA6
53	Y	208	PLC	O3P-C1-C2-C3
53	Z	203	PLC	O3P-C1-C2-C3
45	Y	203	3PE	C2E-C2F-C2G-C2H
45	Y	204	3PE	C35-C36-C37-C38
45	Y	205	3PE	C3A-C3B-C3C-C3D
52	d	201	CDL	C41-C42-C43-C44
46	H	403	PC1	C21-C22-C23-C24
46	Z	202	PC1	C25-C26-C27-C28
45	d	203	3PE	C34-C35-C36-C37
45	r	202	3PE	C33-C34-C35-C36
46	Z	202	PC1	C22-C23-C24-C25
45	J	201	3PE	C22-C23-C24-C25
45	a	101	3PE	C3E-C3F-C3G-C3H
52	L	701	CDL	C40-C41-C42-C43
52	M	602	CDL	C16-C17-C18-C19
45	M	604	3PE	C26-C27-C28-C29
45	Y	205	3PE	C33-C34-C35-C36
46	d	204	PC1	C38-C39-C3A-C3B
52	M	602	CDL	C36-C37-C38-C39
52	d	202	CDL	C37-C38-C39-C40
45	I	203	3PE	C25-C26-C27-C28
45	L	704	3PE	C2F-C2G-C2H-C2I
46	H	403	PC1	C2B-C2C-C2D-C2E
52	N	401	CDL	C21-C22-C23-C24
45	J	202	3PE	C1-C2-C3-O31
45	M	604	3PE	C37-C38-C39-C3A
45	Y	202	3PE	C1-C2-C3-O31
45	Y	204	3PE	C1-C2-C3-O31
45	d	203	3PE	C1-C2-C3-O31
46	A	203	PC1	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	H	404	PC1	C1-C2-C3-O31
46	J	203	PC1	C1-C2-C3-O31
46	d	204	PC1	C1-C2-C3-O31
52	i	202	CDL	CB3-CB4-CB6-OB8
45	Y	204	3PE	C2C-C2D-C2E-C2F
53	g	202	PLC	C'-C1'-C2'-C3'
45	Y	203	3PE	C38-C39-C3A-C3B
52	i	202	CDL	C15-C16-C17-C18
52	i	202	CDL	C33-C34-C35-C36
45	M	603	3PE	C2E-C2F-C2G-C2H
46	B	203	PC1	C25-C26-C27-C28
45	M	604	3PE	O21-C21-C22-C23
53	J	204	PLC	C2B-C1B-CB-O3
52	M	602	CDL	CB7-C71-C72-C73
45	Y	203	3PE	C32-C33-C34-C35
46	Z	202	PC1	C23-C24-C25-C26
45	A	202	3PE	C33-C34-C35-C36
45	P	502	3PE	C26-C27-C28-C29
53	L	705	PLC	C2'-C3'-C4'-C5'
52	H	402	CDL	C13-C14-C15-C16
46	A	203	PC1	C31-C32-C33-C34
52	d	201	CDL	C77-C78-C79-C80
46	H	405	PC1	C3E-C3F-C3G-C3H
52	L	701	CDL	C71-C72-C73-C74
52	M	602	CDL	C38-C39-C40-C41
45	b	101	3PE	C3-C2-O21-C21
45	q	201	3PE	C3-C2-O21-C21
52	d	201	CDL	C31-C32-C33-C34
45	q	201	3PE	C2-C1-O11-P
52	M	602	CDL	C58-C59-C60-C61
52	N	401	CDL	C56-C57-C58-C59
45	A	201	3PE	O11-C1-C2-O21
45	M	604	3PE	O11-C1-C2-O21
45	b	102	3PE	C25-C26-C27-C28
45	d	203	3PE	O32-C31-O31-C3
53	O	403	PLC	C2'-C3'-C4'-C5'
46	H	405	PC1	C37-C38-C39-C3A
45	N	402	3PE	O21-C2-C3-O31
45	Y	204	3PE	O21-C2-C3-O31
45	Y	206	3PE	O21-C2-C3-O31
46	H	403	PC1	C25-C26-C27-C28
46	H	403	PC1	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	J	201	3PE	C27-C28-C29-C2A
52	d	202	CDL	C80-C81-C82-C83
53	b	103	PLC	C8'-C9'-CA'-CB'
45	b	102	3PE	C27-C28-C29-C2A
46	A	203	PC1	C22-C23-C24-C25
46	q	202	PC1	C28-C29-C2A-C2B
52	L	701	CDL	C36-C37-C38-C39
56	O	402	DGT	PA-O3A-PB-O2B
57	P	501	NDP	PN-O3-PA-O1A
53	L	705	PLC	C1'-C2'-C3'-C4'
46	B	203	PC1	C22-C23-C24-C25
52	d	202	CDL	C44-C45-C46-C47
45	J	201	3PE	C2E-C2F-C2G-C2H
52	L	701	CDL	C64-C65-C66-C67
53	g	202	PLC	C7'-C8'-C9'-CA'
45	d	203	3PE	C2F-C2G-C2H-C2I
52	N	401	CDL	C76-C77-C78-C79
52	L	701	CDL	C63-C64-C65-C66
52	N	401	CDL	C24-C25-C26-C27
45	L	704	3PE	O11-C1-C2-C3
45	Y	201	3PE	O11-C1-C2-C3
45	Y	204	3PE	O11-C1-C2-C3
46	M	606	PC1	O11-C1-C2-C3
52	L	701	CDL	OA5-CA3-CA4-CA6
52	d	201	CDL	OB5-CB3-CB4-CB6
45	M	603	3PE	O13-C11-C12-N
45	q	201	3PE	C36-C37-C38-C39
45	b	102	3PE	O21-C21-C22-C23
53	b	103	PLC	C1'-C2'-C3'-C4'
45	Y	202	3PE	O22-C21-O21-C2
46	A	203	PC1	O22-C21-O21-C2
52	d	202	CDL	C35-C36-C37-C38
52	d	202	CDL	C32-C33-C34-C35
53	b	103	PLC	C4B-C5B-C6B-C7B
53	L	705	PLC	C2-C1-O3P-P
46	B	202	PC1	C26-C27-C28-C29
45	Y	201	3PE	C2B-C2C-C2D-C2E
46	B	202	PC1	C39-C3A-C3B-C3C
52	d	202	CDL	C34-C35-C36-C37
45	Y	204	3PE	C32-C31-O31-C3
52	i	202	CDL	C31-CA7-OA8-CA6
45	Y	207	3PE	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	702	3PE	C1-C2-C3-O31
45	L	704	3PE	C1-C2-C3-O31
45	Y	207	3PE	C1-C2-C3-O31
45	g	201	3PE	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31
46	h	201	PC1	C1-C2-C3-O31
52	d	202	CDL	CB3-CB4-CB6-OB8
52	r	201	CDL	CA3-CA4-CA6-OA8
53	J	204	PLC	C1-C2-C3-O3
53	O	403	PLC	C1-C2-C3-O3
45	q	201	3PE	C23-C24-C25-C26
46	H	405	PC1	C33-C34-C35-C36
52	M	602	CDL	C11-C12-C13-C14
53	b	103	PLC	C2B-C3B-C4B-C5B
46	H	405	PC1	C34-C35-C36-C37
52	M	602	CDL	C34-C35-C36-C37
46	B	202	PC1	C22-C21-O21-C2
46	A	204	PC1	C25-C26-C27-C28
45	g	201	3PE	C11-O13-P-O11
46	I	204	PC1	C11-O13-P-O11
46	m	202	PC1	C11-O13-P-O11
45	L	704	3PE	C33-C34-C35-C36
52	d	201	CDL	C11-C12-C13-C14
52	d	202	CDL	C77-C78-C79-C80
52	r	201	CDL	C18-C19-C20-C21
45	A	202	3PE	O11-C1-C2-O21
45	N	402	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
45	Y	204	3PE	O11-C1-C2-O21
45	b	101	3PE	O11-C1-C2-O21
46	B	202	PC1	O11-C1-C2-O21
46	d	204	PC1	O11-C1-C2-O21
46	l	701	PC1	O11-C1-C2-O21
52	N	401	CDL	OB5-CB3-CB4-OB6
53	L	705	PLC	O3P-C1-C2-O2
45	b	102	3PE	C39-C3A-C3B-C3C
52	r	201	CDL	C31-C32-C33-C34
52	d	201	CDL	C44-C45-C46-C47
52	d	202	CDL	C42-C43-C44-C45
45	L	702	3PE	O21-C2-C3-O31
45	L	704	3PE	O21-C2-C3-O31
45	Y	202	3PE	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	A	203	PC1	O21-C2-C3-O31
53	J	204	PLC	O2-C2-C3-O3
53	O	404	PLC	O2-C2-C3-O3
52	d	201	CDL	C31-CA7-OA8-CA6
46	A	204	PC1	C23-C24-C25-C26
46	M	605	PC1	C2A-C2B-C2C-C2D
46	B	202	PC1	O22-C21-O21-C2
52	d	202	CDL	CB7-C71-C72-C73
46	M	606	PC1	C34-C35-C36-C37
52	L	701	CDL	C59-C60-C61-C62
45	L	703	3PE	C2-C1-O11-P
45	J	202	3PE	C26-C27-C28-C29
45	d	203	3PE	C39-C3A-C3B-C3C
58	T	101	EHZ	N1-C12-C13-C14
45	g	201	3PE	C34-C35-C36-C37
52	d	201	CDL	C36-C37-C38-C39
53	M	607	PLC	C2B-C3B-C4B-C5B
46	M	605	PC1	C29-C2A-C2B-C2C
52	r	201	CDL	CA5-C11-C12-C13
45	a	101	3PE	C38-C39-C3A-C3B
46	l	701	PC1	C3C-C3D-C3E-C3F
46	B	202	PC1	C34-C35-C36-C37
57	P	501	NDP	PN-O3-PA-O5B
45	P	502	3PE	C25-C26-C27-C28
45	M	604	3PE	O11-C1-C2-C3
45	N	402	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
52	d	202	CDL	OA5-CA3-CA4-CA6
45	b	101	3PE	C34-C35-C36-C37
46	H	405	PC1	C28-C29-C2A-C2B
45	P	502	3PE	C32-C33-C34-C35
45	q	201	3PE	C2A-C2B-C2C-C2D
45	I	203	3PE	C28-C29-C2A-C2B
45	q	201	3PE	C24-C25-C26-C27
52	i	202	CDL	C39-C40-C41-C42
46	B	203	PC1	C21-C22-C23-C24
52	i	202	CDL	C72-C73-C74-C75
46	m	202	PC1	C32-C31-O31-C3
45	a	101	3PE	C3C-C3D-C3E-C3F
45	d	203	3PE	C3A-C3B-C3C-C3D
52	d	202	CDL	CA6-CA4-OA6-CA5
45	d	203	3PE	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	m	201	3PE	C25-C26-C27-C28
53	g	202	PLC	C6B-C7B-C8B-C9B
53	g	202	PLC	C7B-C8B-C9B-CAA
45	L	703	3PE	C1-C2-C3-O31
45	N	402	3PE	C2-C1-O11-P
45	P	502	3PE	C1-C2-C3-O31
45	b	101	3PE	C1-C2-C3-O31
45	b	102	3PE	C1-C2-C3-O31
46	M	605	PC1	C2-C1-O11-P
49	F	502	FMN	C4'-C5'-O5'-P
52	r	201	CDL	CB3-CB4-CB6-OB8
52	i	202	CDL	OA9-CA7-OA8-CA6
45	A	202	3PE	C24-C25-C26-C27
45	Y	201	3PE	O11-C1-C2-O21
52	d	201	CDL	OA5-CA3-CA4-OA6
53	M	607	PLC	O3P-C1-C2-O2
53	Z	203	PLC	O3P-C1-C2-O2
46	d	204	PC1	C3C-C3D-C3E-C3F
53	Y	208	PLC	C3B-C4B-C5B-C6B
58	T	101	EHZ	O1-C7-C8-C9
58	T	101	EHZ	O3-C12-C13-C14
46	H	405	PC1	C38-C39-C3A-C3B
46	d	204	PC1	C35-C36-C37-C38
46	d	204	PC1	C31-C32-C33-C34
52	d	202	CDL	C63-C64-C65-C66
45	J	202	3PE	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
46	J	203	PC1	O21-C2-C3-O31
46	h	201	PC1	O21-C2-C3-O31
52	r	201	CDL	OA6-CA4-CA6-OA8
45	b	101	3PE	C24-C25-C26-C27
56	O	402	DGT	C5'-O5'-PA-O3A
45	Y	204	3PE	O32-C31-O31-C3
52	d	201	CDL	OA9-CA7-OA8-CA6
46	B	202	PC1	C3C-C3D-C3E-C3F
52	M	602	CDL	C33-C34-C35-C36
45	Y	207	3PE	C21-C22-C23-C24
45	L	702	3PE	C3A-C3B-C3C-C3D
45	L	704	3PE	C35-C36-C37-C38
46	m	202	PC1	O32-C31-O31-C3
46	B	203	PC1	C3C-C3D-C3E-C3F
46	l	701	PC1	C37-C38-C39-C3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C11-O13-P-O11
45	Y	202	3PE	C11-O13-P-O11
45	f	101	3PE	C1-O11-P-O13
46	h	201	PC1	C11-O13-P-O11
52	d	202	CDL	CB3-OB5-PB2-OB2
53	O	404	PLC	C1-O3P-P-O4P
53	Y	208	PLC	C4-O4P-P-O3P
46	Z	202	PC1	C21-C22-C23-C24
52	L	701	CDL	C81-C82-C83-C84
52	M	602	CDL	C1-CA2-OA2-PA1
46	H	403	PC1	C28-C29-C2A-C2B
45	A	201	3PE	C11-O13-P-O14
45	I	203	3PE	C11-O13-P-O12
45	L	704	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	Y	201	3PE	C11-O13-P-O12
45	Y	202	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O12
45	Y	205	3PE	C1-O11-P-O14
45	Y	205	3PE	C11-O13-P-O14
45	Z	201	3PE	C1-O11-P-O14
45	d	203	3PE	C11-O13-P-O12
45	m	201	3PE	C11-O13-P-O12
45	q	201	3PE	C1-O11-P-O12
45	q	201	3PE	C1-O11-P-O14
45	r	202	3PE	C11-O13-P-O12
45	r	202	3PE	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O14
46	A	204	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O12
46	B	203	PC1	C1-O11-P-O14
46	H	405	PC1	C11-O13-P-O12
46	M	605	PC1	C1-O11-P-O14
46	M	606	PC1	C1-O11-P-O14
46	Z	202	PC1	C1-O11-P-O12
46	q	202	PC1	C11-O13-P-O12
52	H	402	CDL	CA2-OA2-PA1-OA4
52	H	402	CDL	CB3-OB5-PB2-OB4
52	d	202	CDL	CA2-OA2-PA1-OA4
52	d	202	CDL	CA3-OA5-PA1-OA3
52	d	202	CDL	CB3-OB5-PB2-OB4
52	r	201	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	L	705	PLC	C4-O4P-P-O2P
53	M	607	PLC	C4-O4P-P-O1P
53	O	404	PLC	C4-O4P-P-O1P
53	g	202	PLC	C1-O3P-P-O2P
56	O	402	DGT	C5'-O5'-PA-O1A
45	m	201	3PE	C37-C38-C39-C3A
45	A	201	3PE	O11-C1-C2-C3
46	q	202	PC1	O11-C1-C2-C3
53	L	705	PLC	O3P-C1-C2-C3
53	b	103	PLC	O3P-C1-C2-C3
46	B	203	PC1	C29-C2A-C2B-C2C
45	L	704	3PE	C32-C33-C34-C35
45	d	203	3PE	C25-C26-C27-C28
46	M	605	PC1	C25-C26-C27-C28
45	A	202	3PE	C12-C11-O13-P
45	L	702	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	M	604	3PE	C12-C11-O13-P
45	Y	201	3PE	C12-C11-O13-P
45	Y	204	3PE	C12-C11-O13-P
45	Y	206	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P
45	a	101	3PE	C12-C11-O13-P
45	b	102	3PE	C12-C11-O13-P
45	g	201	3PE	C12-C11-O13-P
53	L	705	PLC	C5-C4-O4P-P
53	M	607	PLC	C5-C4-O4P-P
53	Y	208	PLC	C5-C4-O4P-P
53	g	202	PLC	C5-C4-O4P-P
45	J	202	3PE	O21-C21-C22-C23
45	m	201	3PE	C3F-C3G-C3H-C3I
45	g	201	3PE	O11-C1-C2-O21
46	A	204	PC1	O11-C1-C2-O21
46	M	606	PC1	O11-C1-C2-O21
46	m	202	PC1	O11-C1-C2-O21
52	M	602	CDL	OA5-CA3-CA4-OA6
52	d	202	CDL	OA5-CA3-CA4-OA6
53	Y	208	PLC	O3P-C1-C2-O2
52	H	402	CDL	C64-C65-C66-C67
46	Z	202	PC1	C22-C21-O21-C2
45	M	604	3PE	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	H	403	PC1	C11-C12-N-C13
45	J	201	3PE	C1-C2-C3-O31
45	N	402	3PE	C1-C2-C3-O31
45	q	201	3PE	C39-C3A-C3B-C3C
46	l	701	PC1	C1-C2-C3-O31
53	M	607	PLC	O4P-C4-C5-N
53	O	404	PLC	C1-C2-C3-O3
53	b	103	PLC	O4P-C4-C5-N
45	J	201	3PE	O21-C2-C3-O31
45	P	502	3PE	O21-C2-C3-O31
45	Y	207	3PE	O21-C2-C3-O31
46	A	204	PC1	O21-C2-C3-O31
46	d	204	PC1	O21-C2-C3-O31
52	d	202	CDL	OB6-CB4-CB6-OB8
45	J	202	3PE	C36-C37-C38-C39
45	N	402	3PE	C39-C3A-C3B-C3C
45	Y	206	3PE	C2C-C2D-C2E-C2F
46	I	204	PC1	C28-C29-C2A-C2B
53	g	202	PLC	C8'-C9'-CA'-CB'
52	N	401	CDL	C72-C73-C74-C75
52	L	701	CDL	C32-C33-C34-C35
45	q	201	3PE	C32-C33-C34-C35
46	H	405	PC1	C3B-C3C-C3D-C3E
45	M	604	3PE	C23-C24-C25-C26
45	Y	204	3PE	C23-C24-C25-C26
52	M	602	CDL	C13-C14-C15-C16
45	Y	207	3PE	C2B-C2C-C2D-C2E
46	B	202	PC1	C3B-C3C-C3D-C3E
52	L	701	CDL	C84-C85-C86-C87
45	r	202	3PE	C23-C24-C25-C26
46	H	404	PC1	C31-C32-C33-C34
52	L	701	CDL	CA5-C11-C12-C13
53	O	403	PLC	C4-C5-N-C8
45	Y	202	3PE	C25-C26-C27-C28
52	H	402	CDL	C55-C56-C57-C58
53	b	103	PLC	C3B-C4B-C5B-C6B
45	Y	207	3PE	C24-C25-C26-C27
46	H	403	PC1	C35-C36-C37-C38
52	N	401	CDL	C62-C63-C64-C65
45	N	402	3PE	C2F-C2G-C2H-C2I
45	N	402	3PE	C24-C25-C26-C27
45	Y	205	3PE	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	J	201	3PE	C2D-C2E-C2F-C2G
45	P	502	3PE	C22-C23-C24-C25
45	r	202	3PE	C22-C23-C24-C25
52	d	201	CDL	C39-C40-C41-C42
52	N	401	CDL	C33-C34-C35-C36
52	L	701	CDL	C32-C31-CA7-OA8
52	N	401	CDL	C44-C45-C46-C47
52	H	402	CDL	CA6-CA4-OA6-CA5
53	Y	208	PLC	C1-C2-O2-C'
45	Y	205	3PE	C35-C36-C37-C38
46	Z	202	PC1	O22-C21-O21-C2
52	L	701	CDL	OB7-CB5-OB6-CB4
45	Y	203	3PE	C32-C31-O31-C3
46	H	405	PC1	C3C-C3D-C3E-C3F
46	A	203	PC1	C21-C22-C23-C24
52	d	202	CDL	C78-C79-C80-C81
45	M	604	3PE	C2-C1-O11-P
52	d	201	CDL	C1-CB2-OB2-PB2
45	J	201	3PE	C23-C24-C25-C26
46	H	405	PC1	C22-C23-C24-C25
52	r	201	CDL	C52-C53-C54-C55
52	L	701	CDL	C38-C39-C40-C41
46	H	403	PC1	C11-C12-N-C14
46	A	203	PC1	C32-C33-C34-C35
45	Y	203	3PE	O32-C31-O31-C3
45	Y	206	3PE	C26-C27-C28-C29
46	m	202	PC1	C32-C33-C34-C35
52	N	401	CDL	C58-C59-C60-C61
52	L	701	CDL	C51-CB5-OB6-CB4
46	q	202	PC1	O21-C2-C3-O31
52	N	401	CDL	OB6-CB4-CB6-OB8
52	H	402	CDL	C61-C62-C63-C64
52	M	602	CDL	C22-C23-C24-C25
45	M	603	3PE	C1-O11-P-O13
45	Y	204	3PE	C11-O13-P-O11
46	J	203	PC1	C11-O13-P-O11
46	Z	202	PC1	C11-O13-P-O11
52	L	701	CDL	CA2-OA2-PA1-OA5
52	M	602	CDL	CB2-OB2-PB2-OB5
52	N	401	CDL	CA2-OA2-PA1-OA5
52	i	202	CDL	CB3-OB5-PB2-OB2
53	J	204	PLC	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	M	603	3PE	C3A-C3B-C3C-C3D
52	L	701	CDL	C58-C59-C60-C61
45	A	202	3PE	C3C-C3D-C3E-C3F
45	N	402	3PE	C25-C26-C27-C28
53	Z	203	PLC	C'-C1'-C2'-C3'
45	Y	206	3PE	C1-C2-C3-O31
46	A	204	PC1	C1-C2-C3-O31
45	N	402	3PE	C22-C23-C24-C25
46	d	204	PC1	C34-C35-C36-C37
58	U	101	EHZ	C21-C22-C23-C24
45	d	203	3PE	C28-C29-C2A-C2B
46	H	405	PC1	C36-C37-C38-C39
45	Y	203	3PE	C3A-C3B-C3C-C3D
52	d	202	CDL	CA5-C11-C12-C13
45	b	102	3PE	C35-C36-C37-C38
45	L	702	3PE	C35-C36-C37-C38
45	M	603	3PE	C24-C25-C26-C27
45	Z	201	3PE	C2-C1-O11-P
53	O	404	PLC	C2-C1-O3P-P
45	Y	204	3PE	C32-C33-C34-C35
46	l	701	PC1	C38-C39-C3A-C3B
46	H	405	PC1	C25-C26-C27-C28
45	Y	207	3PE	C22-C23-C24-C25
46	M	605	PC1	C22-C23-C24-C25
45	g	201	3PE	C31-C32-C33-C34
46	M	606	PC1	C31-C32-C33-C34
52	i	202	CDL	CA5-C11-C12-C13
52	M	602	CDL	C51-C52-C53-C54
52	L	701	CDL	C41-C42-C43-C44
45	J	202	3PE	C24-C25-C26-C27
46	M	606	PC1	O21-C21-C22-C23
53	Y	208	PLC	C1B-CB-O3-C3
52	N	401	CDL	C55-C56-C57-C58
53	O	403	PLC	C4-C5-N-C7
53	J	204	PLC	C2B-C1B-CB-OB
57	P	501	NDP	O4D-C1D-N1N-C6N
45	L	703	3PE	C23-C24-C25-C26
45	M	604	3PE	O13-C11-C12-N
45	b	101	3PE	O13-C11-C12-N
45	Y	205	3PE	C3C-C3D-C3E-C3F
45	b	101	3PE	C33-C34-C35-C36
52	H	402	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C29-C2A-C2B-C2C
53	Y	208	PLC	C6'-C7'-C8'-C9'
58	T	101	EHZ	C1-C21-C22-C23
52	M	602	CDL	C31-C32-C33-C34
45	q	201	3PE	C28-C29-C2A-C2B
52	L	701	CDL	C82-C83-C84-C85
52	M	602	CDL	C72-C73-C74-C75
52	N	401	CDL	C23-C24-C25-C26
52	i	202	CDL	C11-C12-C13-C14
52	M	602	CDL	C41-C42-C43-C44
46	Z	202	PC1	O21-C2-C3-O31
53	b	103	PLC	C2-C1-O3P-P
45	M	604	3PE	O22-C21-C22-C23
46	Z	202	PC1	C26-C27-C28-C29
46	H	403	PC1	C11-C12-N-C15
51	H	401	U10	C2-C3-O3-C3M
52	L	701	CDL	C42-C43-C44-C45
45	b	102	3PE	C32-C31-O31-C3
45	L	703	3PE	C26-C27-C28-C29
45	Y	204	3PE	C3D-C3E-C3F-C3G
45	L	702	3PE	C33-C34-C35-C36
45	M	603	3PE	C29-C2A-C2B-C2C
46	H	404	PC1	C24-C25-C26-C27
45	A	201	3PE	C27-C28-C29-C2A
46	d	204	PC1	C39-C3A-C3B-C3C
52	H	402	CDL	CB2-C1-CA2-OA2
52	N	401	CDL	CB3-CB4-CB6-OB8
52	i	202	CDL	CA3-CA4-CA6-OA8
53	g	202	PLC	CB-C1B-C2B-C3B
58	U	101	EHZ	C19-C17-C20-O6
52	H	402	CDL	C52-C53-C54-C55
52	M	602	CDL	C52-C53-C54-C55
45	d	203	3PE	C3B-C3C-C3D-C3E
59	i	201	CHD	C22-C23-C24-O25
45	L	702	3PE	C1-C2-O21-C21
45	Y	203	3PE	C1-C2-O21-C21
45	Y	203	3PE	C3-C2-O21-C21
45	N	402	3PE	C26-C27-C28-C29
45	Y	205	3PE	C38-C39-C3A-C3B
53	O	403	PLC	C4-C5-N-C6
46	H	403	PC1	O21-C21-C22-C23
52	i	202	CDL	C52-C53-C54-C55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	L	705	PLC	C1-O3P-P-O4P
53	Y	208	PLC	OB-CB-O3-C3
57	P	501	NDP	C2D-C1D-N1N-C6N
52	L	701	CDL	C16-C17-C18-C19
53	Z	203	PLC	C1'-C2'-C3'-C4'
45	L	703	3PE	O11-C1-C2-O21
52	H	402	CDL	OB5-CB3-CB4-OB6
53	J	204	PLC	O3P-C1-C2-O2
53	M	607	PLC	O'-C'-O2-C2
46	A	204	PC1	O11-C1-C2-C3
59	i	201	CHD	C17-C20-C22-C23
52	L	701	CDL	C35-C36-C37-C38
52	r	201	CDL	C71-C72-C73-C74
46	H	403	PC1	C39-C3A-C3B-C3C
45	M	603	3PE	C28-C29-C2A-C2B
52	L	701	CDL	C31-C32-C33-C34
45	b	101	3PE	O21-C2-C3-O31
52	M	602	CDL	OA6-CA4-CA6-OA8
52	d	202	CDL	OA6-CA4-CA6-OA8
52	d	201	CDL	C42-C43-C44-C45
45	b	102	3PE	O32-C31-O31-C3
45	Z	201	3PE	C29-C2A-C2B-C2C
53	Z	203	PLC	C7B-C8B-C9B-CAA
45	Y	206	3PE	C29-C2A-C2B-C2C
52	L	701	CDL	C56-C57-C58-C59
46	d	204	PC1	C32-C33-C34-C35
59	i	201	CHD	C22-C23-C24-O26
52	M	602	CDL	CA7-C31-C32-C33
45	A	201	3PE	O31-C31-C32-C33
45	d	203	3PE	C27-C28-C29-C2A
52	r	201	CDL	O1-C1-CB2-OB2
45	a	101	3PE	C34-C35-C36-C37
45	N	402	3PE	C23-C24-C25-C26
46	l	701	PC1	C3B-C3C-C3D-C3E
45	M	603	3PE	C39-C3A-C3B-C3C
45	d	203	3PE	C2B-C2C-C2D-C2E
52	i	202	CDL	C38-C39-C40-C41
45	L	704	3PE	C31-C32-C33-C34
53	Y	208	PLC	O2-C'-C1'-C2'
46	q	202	PC1	O11-C1-C2-O21
45	A	201	3PE	C22-C23-C24-C25
46	H	403	PC1	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	d	203	3PE	C29-C2A-C2B-C2C
45	Y	202	3PE	O11-C1-C2-C3
45	g	201	3PE	O11-C1-C2-C3
46	B	202	PC1	O11-C1-C2-C3
46	d	204	PC1	O11-C1-C2-C3
46	I	204	PC1	C26-C27-C28-C29
46	B	202	PC1	C23-C24-C25-C26
52	N	401	CDL	C11-C12-C13-C14
45	b	102	3PE	O22-C21-C22-C23
46	A	204	PC1	C26-C27-C28-C29
45	g	201	3PE	C2-C1-O11-P
46	H	404	PC1	C2F-C2G-C2H-C2I
45	A	201	3PE	C38-C39-C3A-C3B
46	J	203	PC1	C22-C23-C24-C25
45	N	402	3PE	O31-C31-C32-C33
52	M	602	CDL	C59-C60-C61-C62
46	Z	202	PC1	C3A-C3B-C3C-C3D
52	L	701	CDL	C61-C62-C63-C64
45	q	201	3PE	C33-C34-C35-C36
52	d	201	CDL	CB7-C71-C72-C73
45	Y	202	3PE	C24-C25-C26-C27
45	Y	201	3PE	C1-O11-P-O13
52	d	202	CDL	CB2-OB2-PB2-OB5
58	U	101	EHZ	C18-C17-C20-O6
45	Y	207	3PE	C2E-C2F-C2G-C2H
52	L	701	CDL	C78-C79-C80-C81
45	L	703	3PE	O21-C21-C22-C23
52	N	401	CDL	C63-C64-C65-C66
60	o	201	MYR	C11-C10-C9-C8
45	L	703	3PE	C22-C23-C24-C25
46	l	701	PC1	C3F-C3G-C3H-C3I
46	I	204	PC1	O31-C31-C32-C33
45	Y	204	3PE	C3F-C3G-C3H-C3I
46	Z	202	PC1	C27-C28-C29-C2A
45	A	201	3PE	C1-C2-O21-C21
45	A	201	3PE	C3-C2-O21-C21
45	g	201	3PE	C32-C33-C34-C35
52	i	202	CDL	C71-C72-C73-C74
52	i	202	CDL	C36-C37-C38-C39
53	M	607	PLC	CB-C1B-C2B-C3B
45	M	603	3PE	O21-C21-C22-C23
45	Y	204	3PE	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	d	201	CDL	C72-C71-CB7-OB8
45	b	102	3PE	C2B-C2C-C2D-C2E
52	d	202	CDL	C64-C65-C66-C67
46	H	404	PC1	O31-C31-C32-C33
52	N	401	CDL	C14-C15-C16-C17
46	H	403	PC1	O32-C31-O31-C3
45	q	201	3PE	C3B-C3C-C3D-C3E
46	q	202	PC1	C1-C2-C3-O31
52	r	201	CDL	CA4-CA3-OA5-PA1
45	L	702	3PE	C3F-C3G-C3H-C3I
46	I	204	PC1	C38-C39-C3A-C3B
53	Y	208	PLC	C8'-C9'-CA'-CB'
45	f	101	3PE	O11-C1-C2-O21
52	L	701	CDL	OB5-CB3-CB4-OB6
52	N	401	CDL	OA5-CA3-CA4-OA6
45	Y	204	3PE	O31-C31-C32-C33
45	b	102	3PE	O31-C31-C32-C33
52	M	602	CDL	C52-C51-CB5-OB6
53	J	204	PLC	O2-C'-C1'-C2'
52	N	401	CDL	C73-C74-C75-C76
45	b	101	3PE	C32-C31-O31-C3
46	J	203	PC1	O21-C21-C22-C23
45	Y	205	3PE	C28-C29-C2A-C2B
52	d	202	CDL	C31-C32-C33-C34
52	M	602	CDL	C12-C11-CA5-OA6
45	A	201	3PE	C33-C34-C35-C36
52	H	402	CDL	OA5-CA3-CA4-CA6
52	H	402	CDL	OB5-CB3-CB4-CB6
45	I	203	3PE	O21-C21-C22-C23
45	r	202	3PE	C34-C35-C36-C37
52	M	602	CDL	C78-C79-C80-C81
45	A	202	3PE	O21-C2-C3-O31
45	Y	203	3PE	O21-C2-C3-O31
53	b	103	PLC	C'-C1'-C2'-C3'
53	O	404	PLC	C2'-C3'-C4'-C5'
45	A	202	3PE	O31-C31-C32-C33
45	L	702	3PE	O21-C21-C22-C23
45	r	202	3PE	O31-C31-C32-C33
52	d	202	CDL	C36-C37-C38-C39
58	U	101	EHZ	C3-C4-C5-C6
53	M	607	PLC	C1'-C'-O2-C2
52	M	602	CDL	OA7-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	d	201	CDL	C52-C51-CB5-OB6
46	B	203	PC1	C23-C24-C25-C26
46	H	404	PC1	C27-C28-C29-C2A
52	N	401	CDL	C17-C18-C19-C20
46	H	405	PC1	O31-C31-C32-C33
52	i	202	CDL	C12-C11-CA5-OA6
53	b	103	PLC	O2-C'-C1'-C2'
56	O	402	DGT	PB-O3A-PA-O1A
45	b	101	3PE	O32-C31-O31-C3
45	N	402	3PE	C3A-C3B-C3C-C3D
46	Z	202	PC1	C38-C39-C3A-C3B
45	M	603	3PE	O31-C31-C32-C33
45	J	201	3PE	C2C-C2D-C2E-C2F
45	L	702	3PE	C37-C38-C39-C3A
45	L	703	3PE	O22-C21-C22-C23
45	Y	204	3PE	O22-C21-C22-C23
45	M	603	3PE	C32-C33-C34-C35
45	Y	204	3PE	C24-C25-C26-C27
45	L	704	3PE	O21-C21-C22-C23
45	b	102	3PE	C2C-C2D-C2E-C2F
45	N	402	3PE	O32-C31-C32-C33
45	Y	207	3PE	C25-C26-C27-C28
45	f	101	3PE	C1-C2-C3-O31
45	b	102	3PE	O32-C31-C32-C33
45	A	202	3PE	C2-C1-O11-P
45	a	101	3PE	C2-C1-O11-P
53	Z	203	PLC	C2-C1-O3P-P
45	L	702	3PE	C27-C28-C29-C2A
45	Y	204	3PE	O32-C31-C32-C33
45	L	703	3PE	C1-O11-P-O14
45	M	603	3PE	C1-O11-P-O14
45	Y	204	3PE	C1-O11-P-O14
45	m	201	3PE	C1-O11-P-O12
45	q	201	3PE	C11-O13-P-O12
46	A	203	PC1	C11-O13-P-O12
46	M	605	PC1	C11-C12-N-C14
46	d	204	PC1	C11-O13-P-O14
46	d	204	PC1	C1-O11-P-O14
46	h	201	PC1	C11-O13-P-O14
46	l	701	PC1	C1-O11-P-O14
52	H	402	CDL	CA2-OA2-PA1-OA3
52	L	701	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	d	202	CDL	CA2-OA2-PA1-OA3
52	d	202	CDL	CB3-OB5-PB2-OB3
53	O	404	PLC	C1-O3P-P-O2P
57	P	501	NDP	C5D-O5D-PN-O1N
46	H	404	PC1	O32-C31-C32-C33
46	I	204	PC1	O32-C31-C32-C33
46	J	203	PC1	O22-C21-C22-C23
52	M	602	CDL	C52-C51-CB5-OB7
52	d	201	CDL	C72-C71-CB7-OB9
45	m	201	3PE	O11-C1-C2-C3
45	J	202	3PE	C23-C24-C25-C26
52	r	201	CDL	C53-C54-C55-C56
45	P	502	3PE	O13-C11-C12-N
45	I	203	3PE	O22-C21-C22-C23
45	L	702	3PE	O22-C21-C22-C23
45	M	603	3PE	O22-C21-C22-C23
45	Y	204	3PE	C22-C23-C24-C25
45	Y	205	3PE	C39-C3A-C3B-C3C
53	O	403	PLC	C3'-C4'-C5'-C6'
45	Y	203	3PE	O31-C31-C32-C33
45	A	202	3PE	C36-C37-C38-C39
45	N	402	3PE	C34-C35-C36-C37
52	i	202	CDL	C32-C31-CA7-OA8
53	J	204	PLC	O'-C'-C1'-C2'
46	I	204	PC1	C27-C28-C29-C2A
46	q	202	PC1	C36-C37-C38-C39
52	i	202	CDL	C76-C77-C78-C79
45	A	201	3PE	C12-C11-O13-P
45	I	203	3PE	C12-C11-O13-P
45	L	704	3PE	C3-C2-O21-C21
45	Y	203	3PE	C12-C11-O13-P
45	Y	207	3PE	C12-C11-O13-P
53	O	403	PLC	C1-C2-O2-C'
46	H	405	PC1	O32-C31-C32-C33
52	i	202	CDL	C12-C11-CA5-OA7
52	N	401	CDL	C77-C78-C79-C80
52	d	201	CDL	C33-C34-C35-C36
52	r	201	CDL	C12-C13-C14-C15
52	d	202	CDL	C41-C42-C43-C44
46	M	605	PC1	C11-C12-N-C13
45	Z	201	3PE	O21-C21-C22-C23
46	J	203	PC1	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

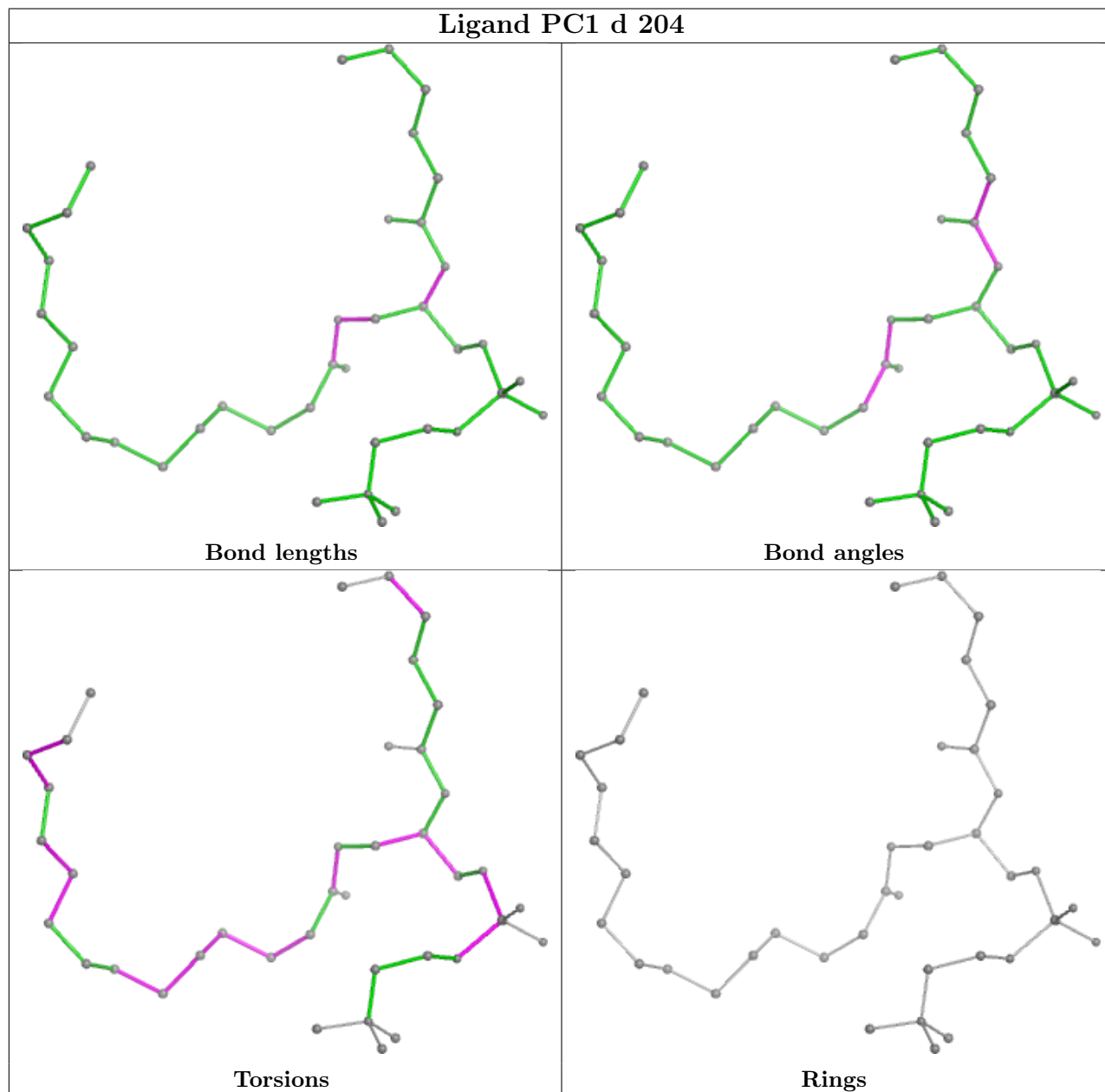
Mol	Chain	Res	Type	Atoms
52	H	402	CDL	C52-C51-CB5-OB6
45	d	203	3PE	C2D-C2E-C2F-C2G
45	A	202	3PE	C3E-C3F-C3G-C3H
45	b	101	3PE	C21-C22-C23-C24
45	A	202	3PE	O32-C31-C32-C33
52	L	701	CDL	CA4-CA6-OA8-CA7
45	d	203	3PE	C36-C37-C38-C39
52	H	402	CDL	C51-C52-C53-C54
51	H	401	U10	C15-C14-C16-C17
49	F	502	FMN	N10-C1'-C2'-O2'
52	H	402	CDL	OA5-CA3-CA4-OA6
52	r	201	CDL	OB5-CB3-CB4-OB6
52	M	602	CDL	C56-C57-C58-C59
45	L	702	3PE	O31-C31-C32-C33
45	Y	206	3PE	O31-C31-C32-C33
45	a	101	3PE	O31-C31-C32-C33
46	H	403	PC1	O31-C31-C32-C33
52	M	602	CDL	C32-C31-CA7-OA8
52	d	202	CDL	C72-C71-CB7-OB8
52	M	602	CDL	C37-C38-C39-C40
45	L	704	3PE	O22-C21-C22-C23
52	M	602	CDL	C32-C31-CA7-OA9
45	Y	201	3PE	O21-C21-C22-C23
53	L	705	PLC	C2B-C1B-CB-O3
46	d	204	PC1	C23-C24-C25-C26
46	M	605	PC1	C27-C28-C29-C2A
45	r	202	3PE	O32-C31-C32-C33
53	b	103	PLC	O'-C'-C1'-C2'
52	L	701	CDL	C52-C51-CB5-OB6
52	N	401	CDL	C72-C71-CB7-OB8
45	L	702	3PE	O32-C31-C32-C33
45	Y	206	3PE	O32-C31-C32-C33
45	Z	201	3PE	O22-C21-C22-C23
45	Y	203	3PE	C39-C3A-C3B-C3C
46	J	203	PC1	O32-C31-C32-C33

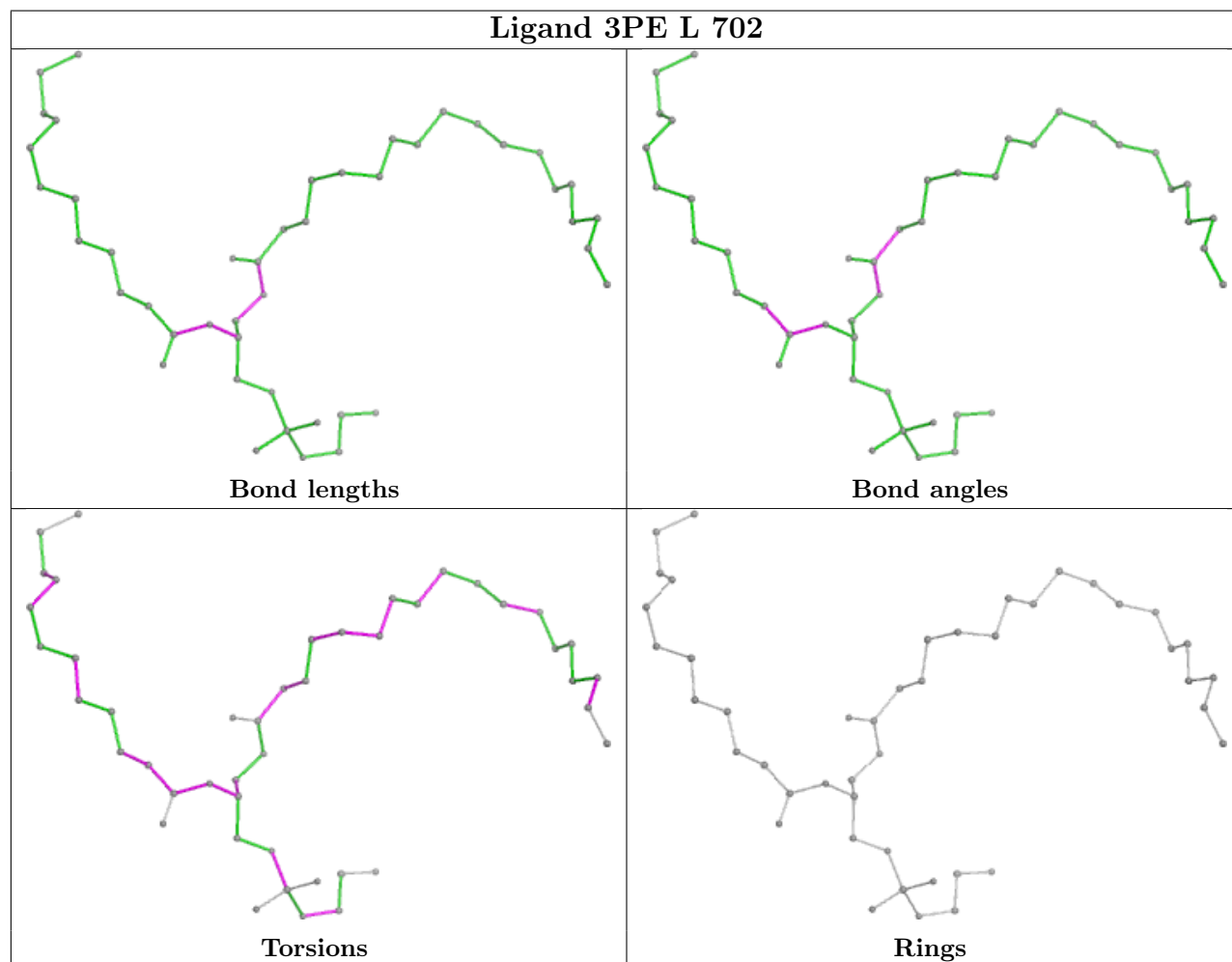
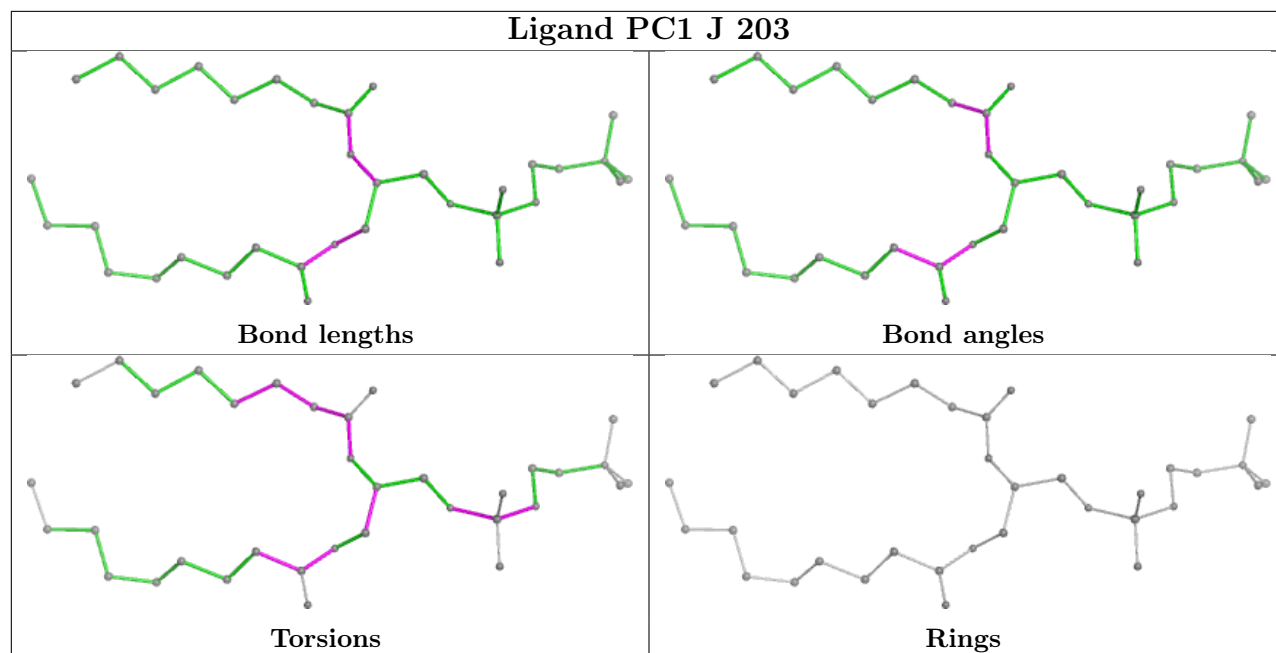
There are no ring outliers.

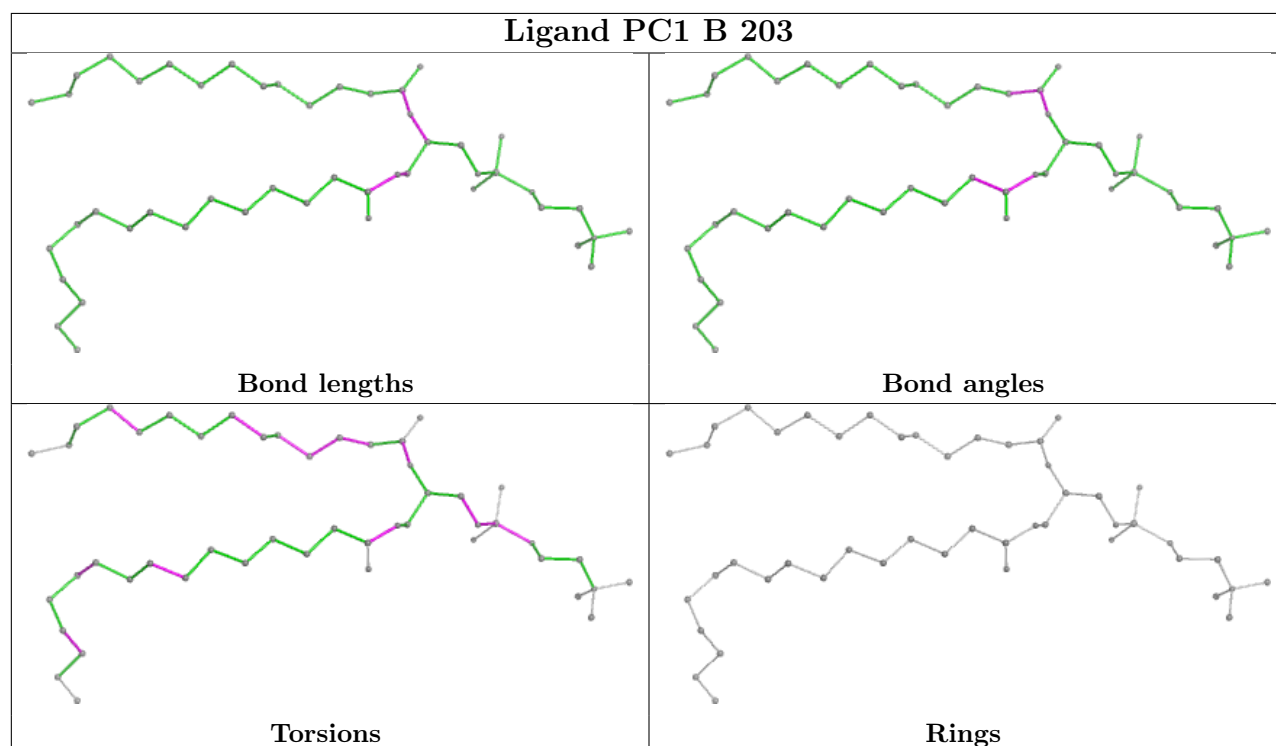
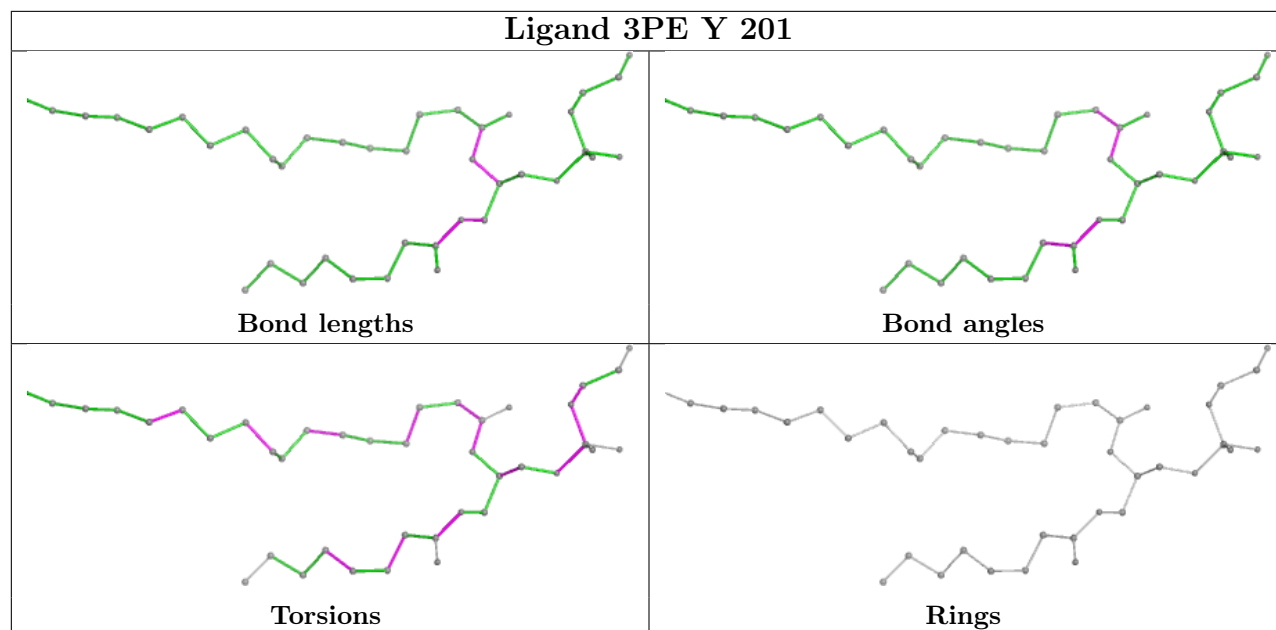
No monomer is involved in short contacts.

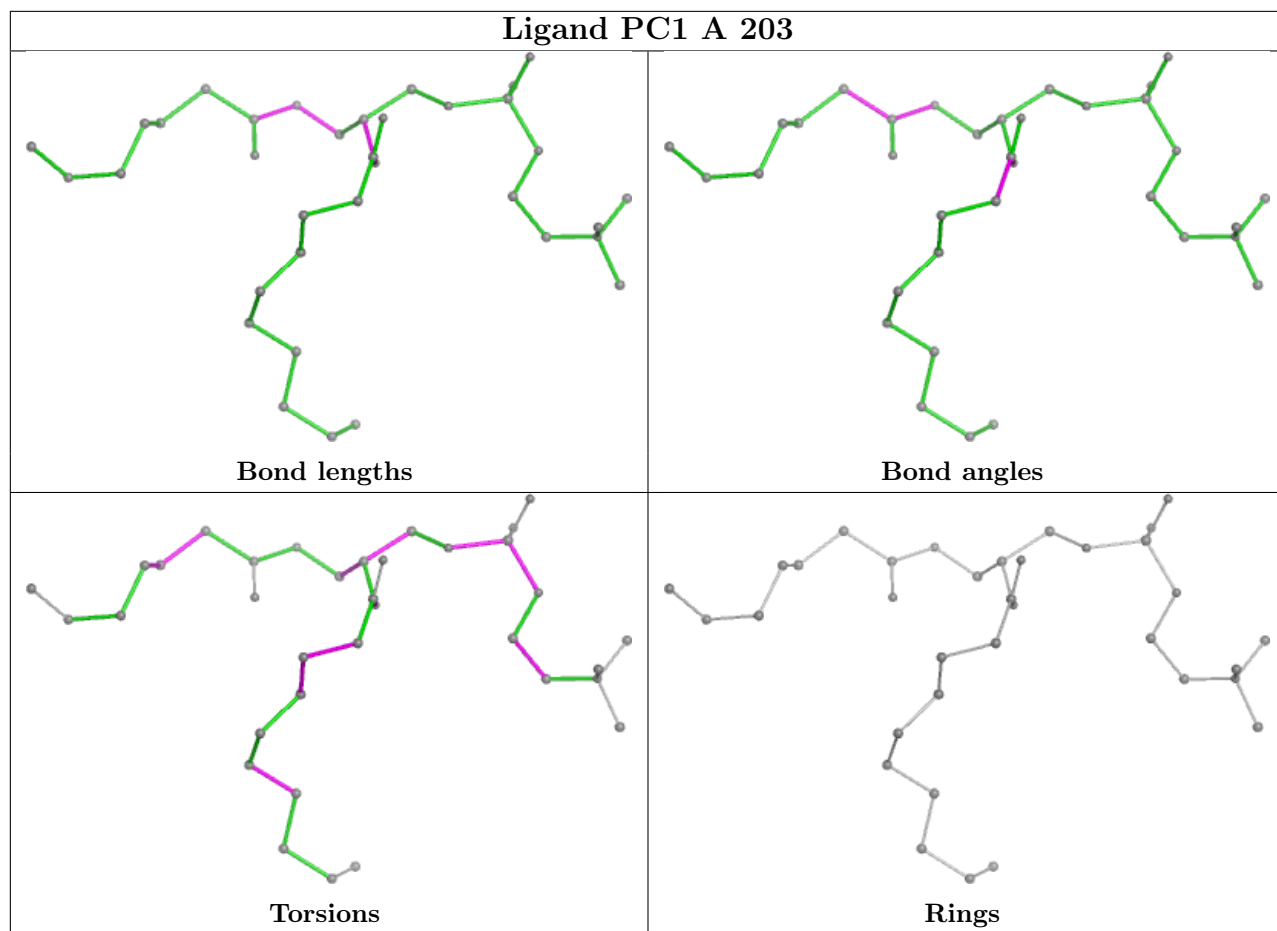
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

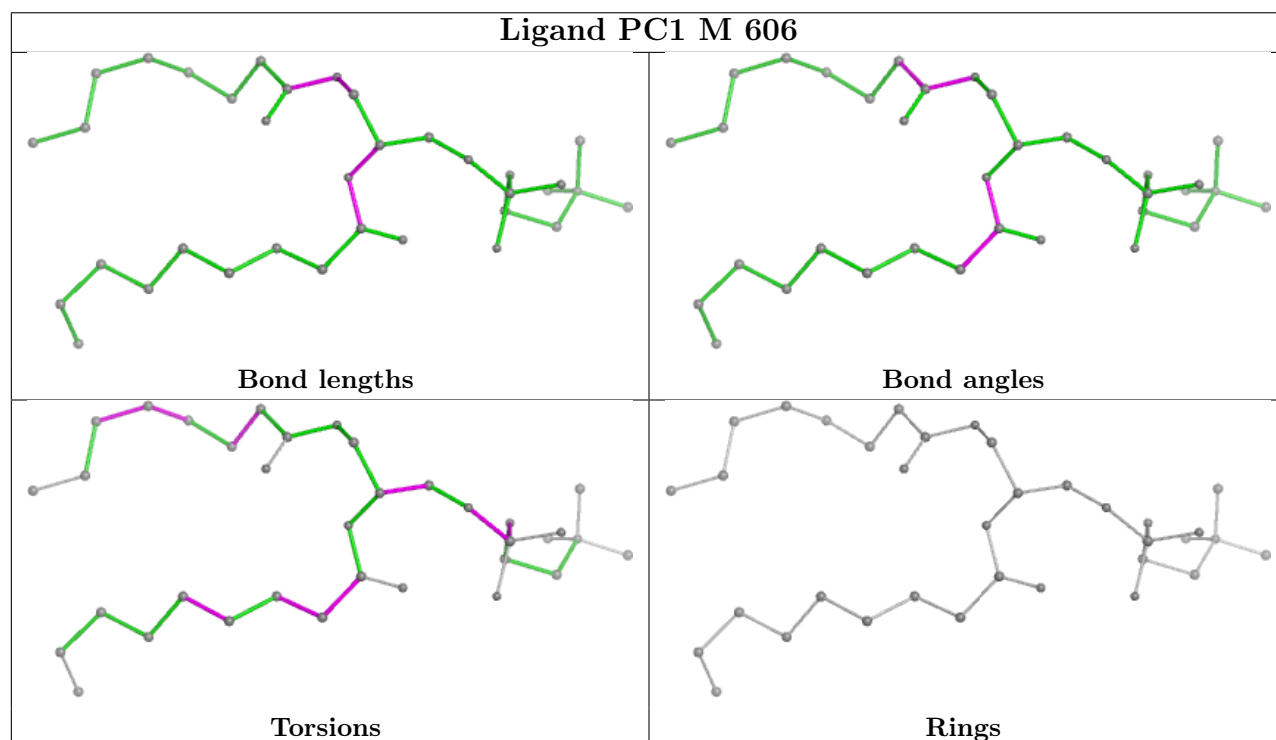
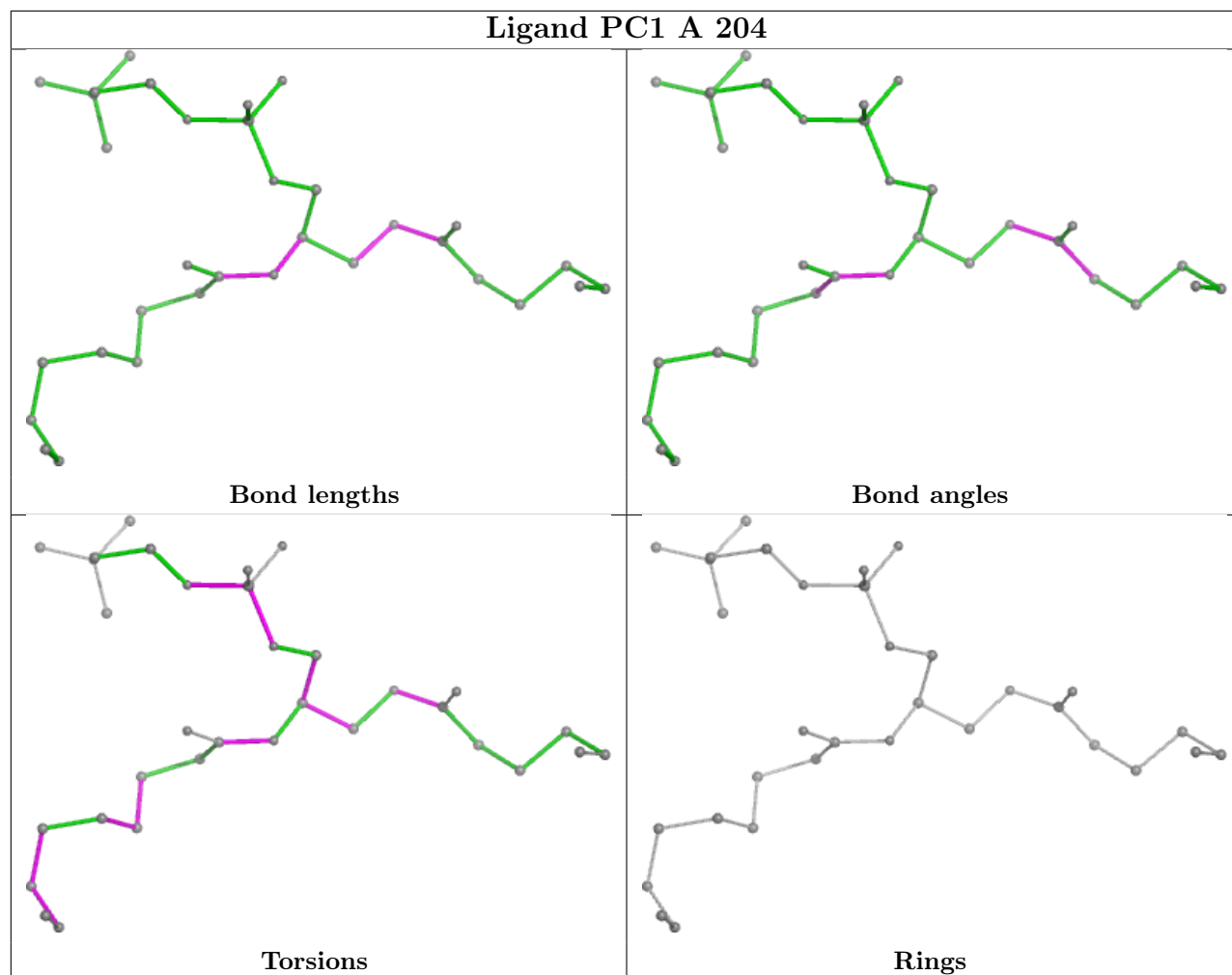
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

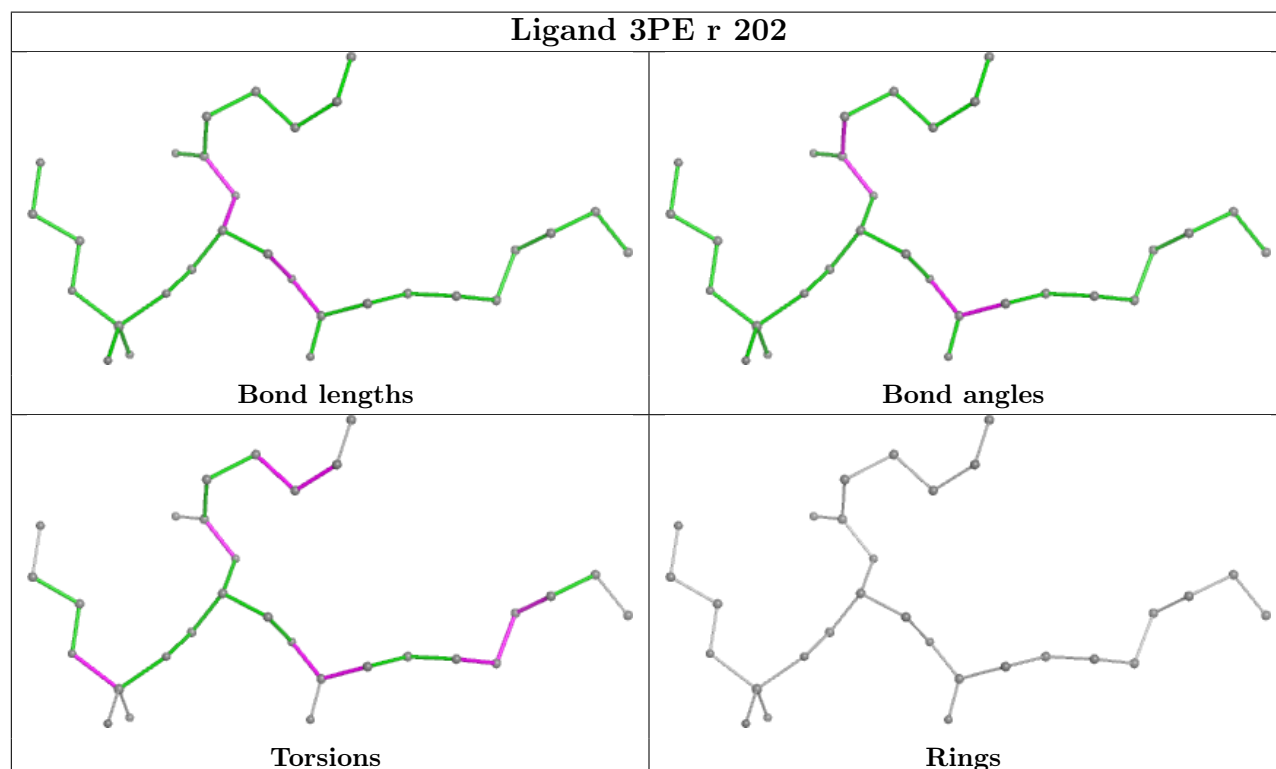
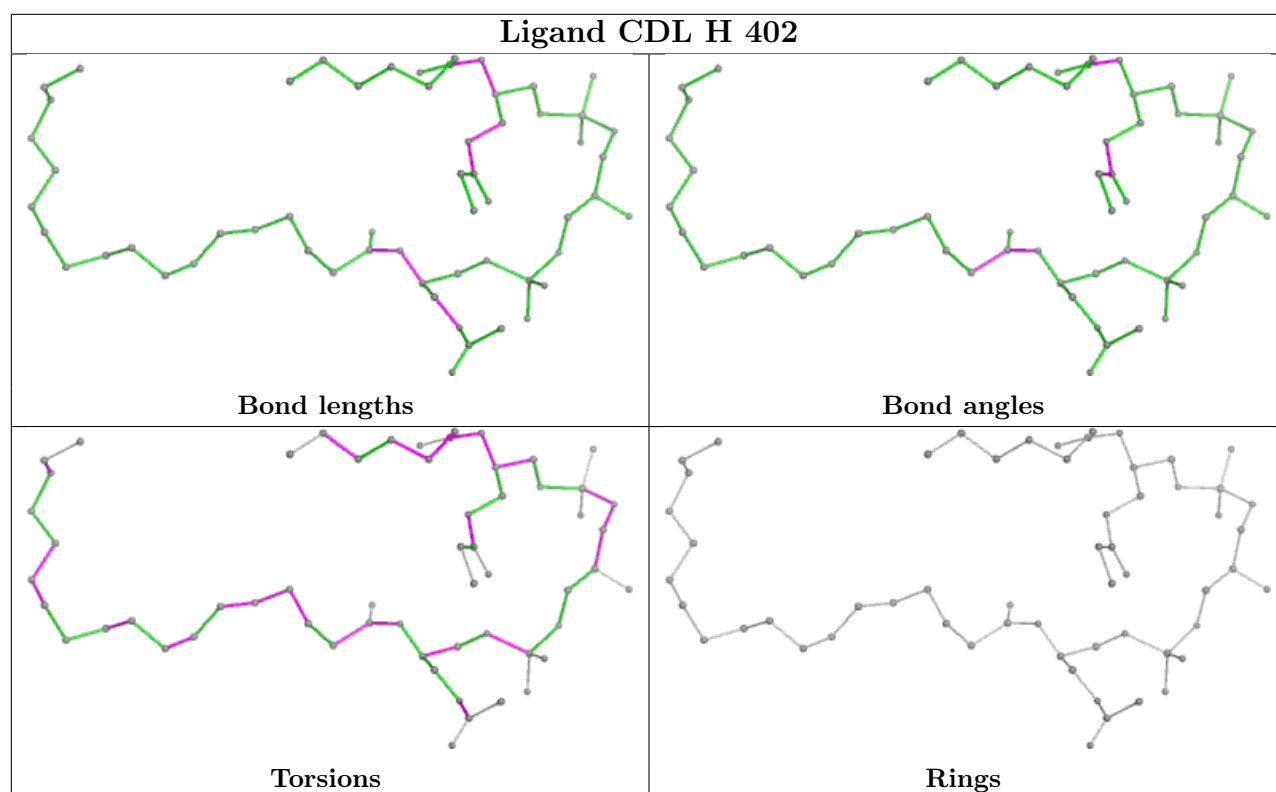


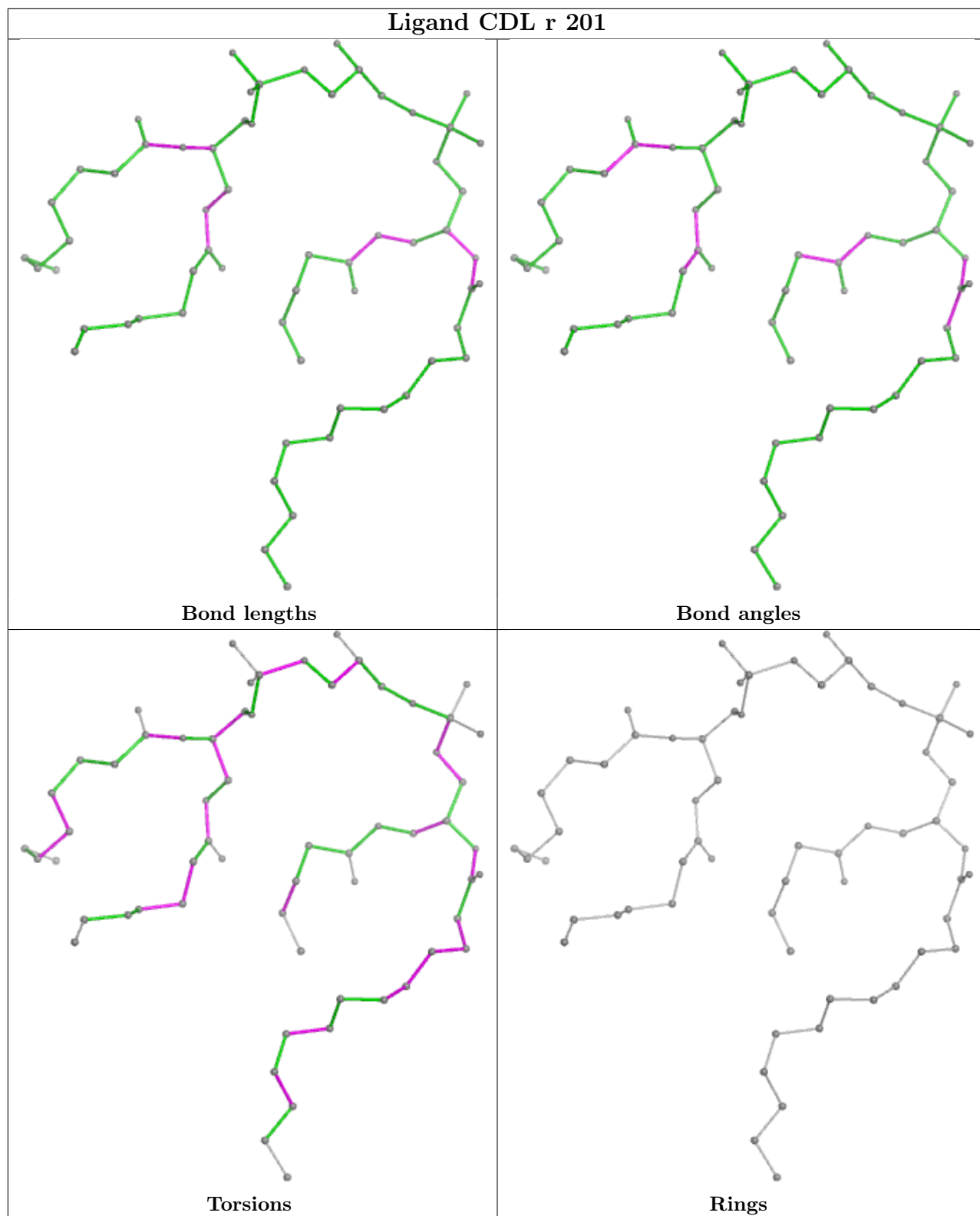


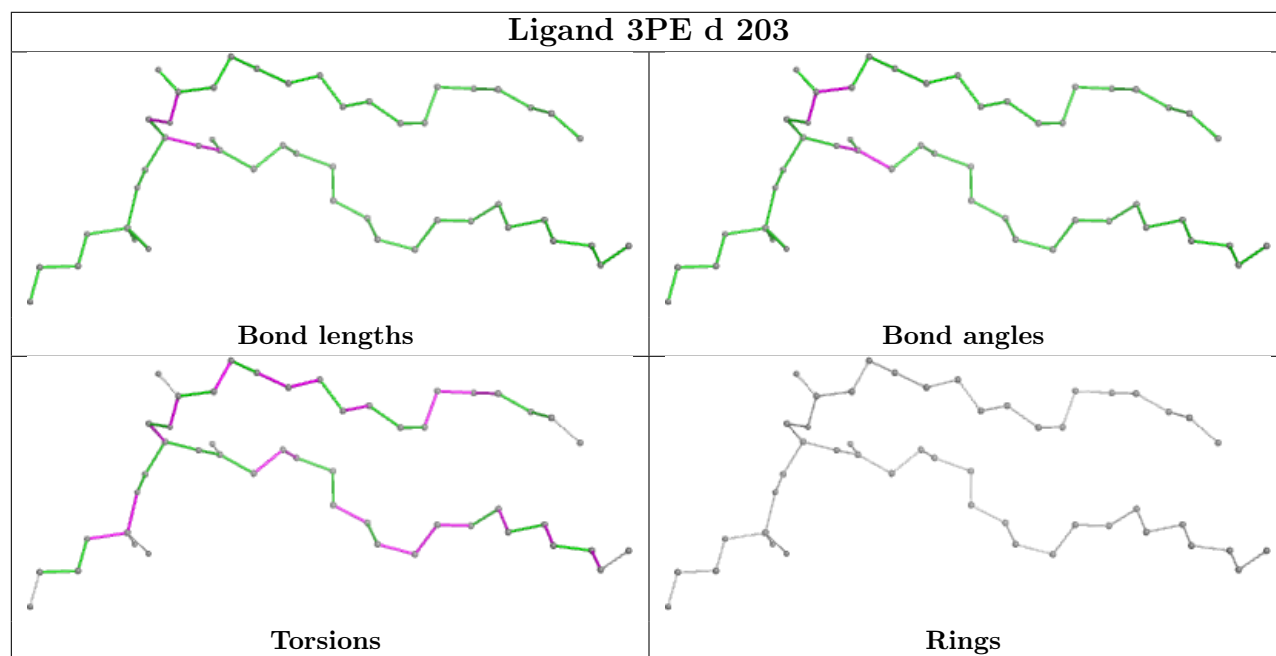
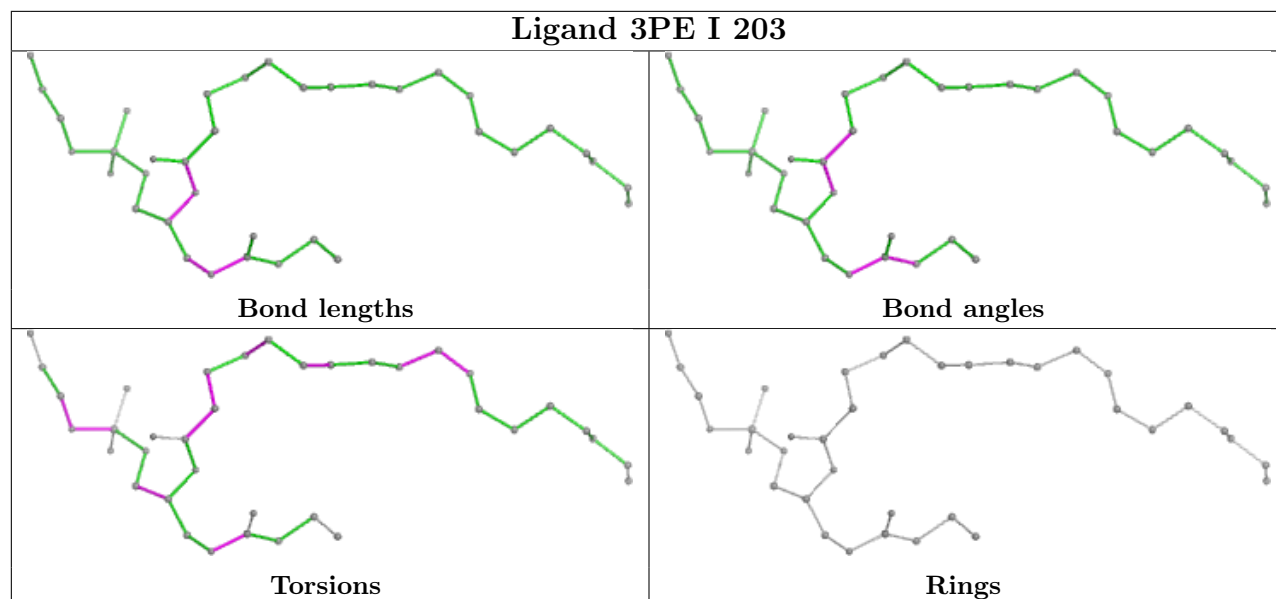


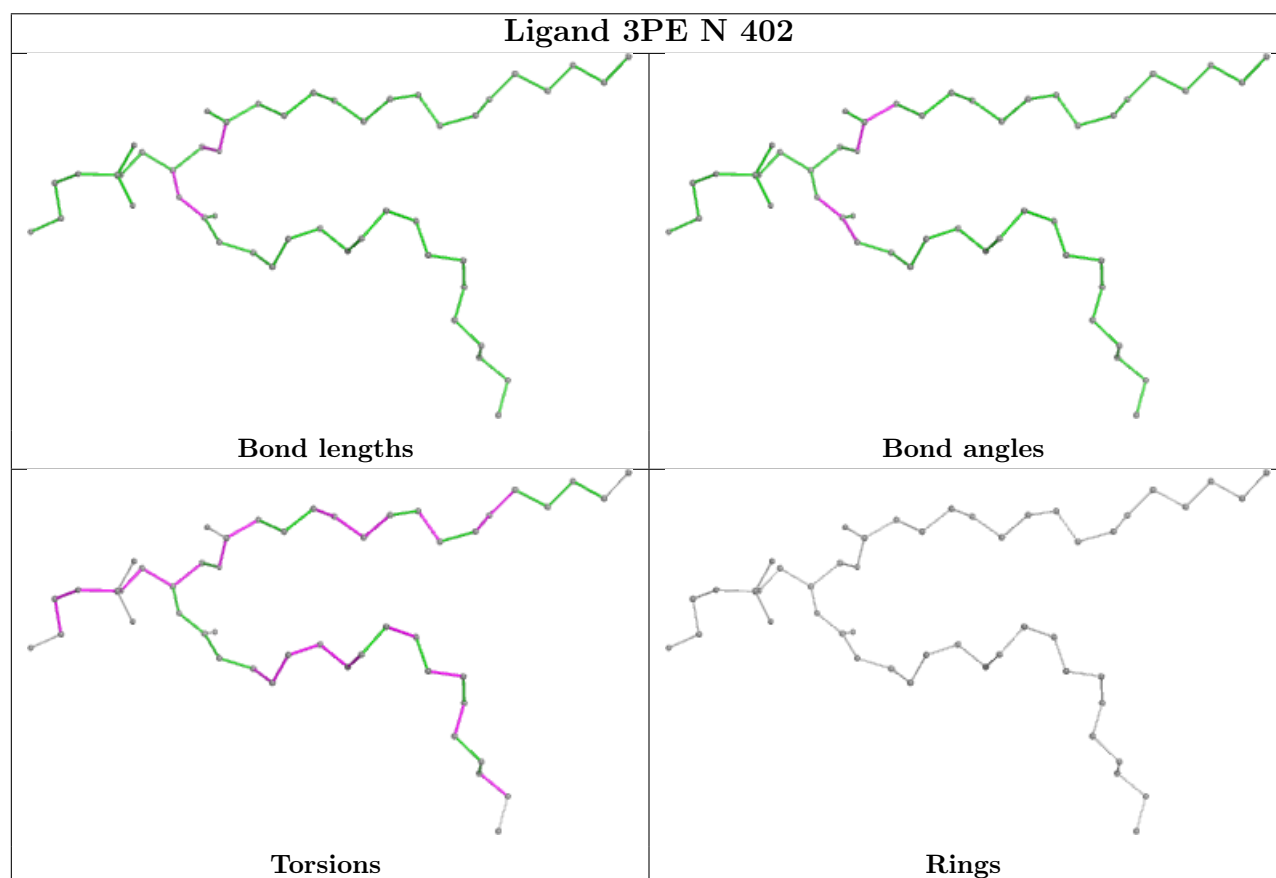
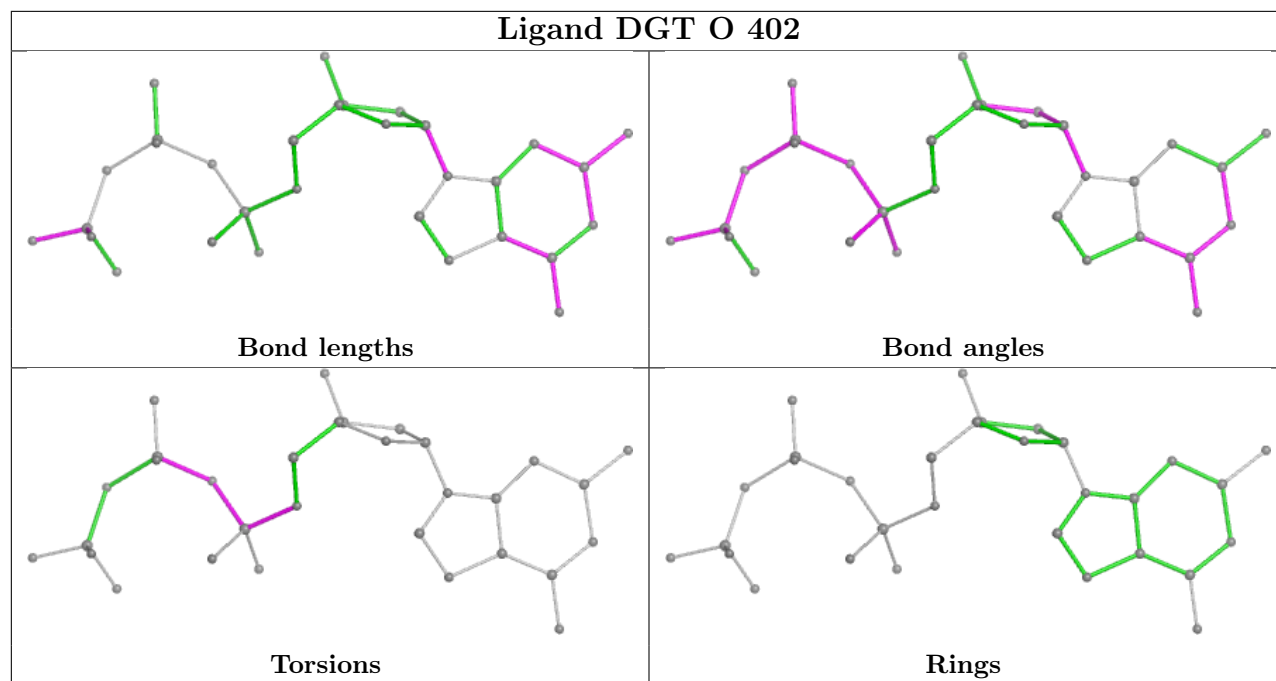


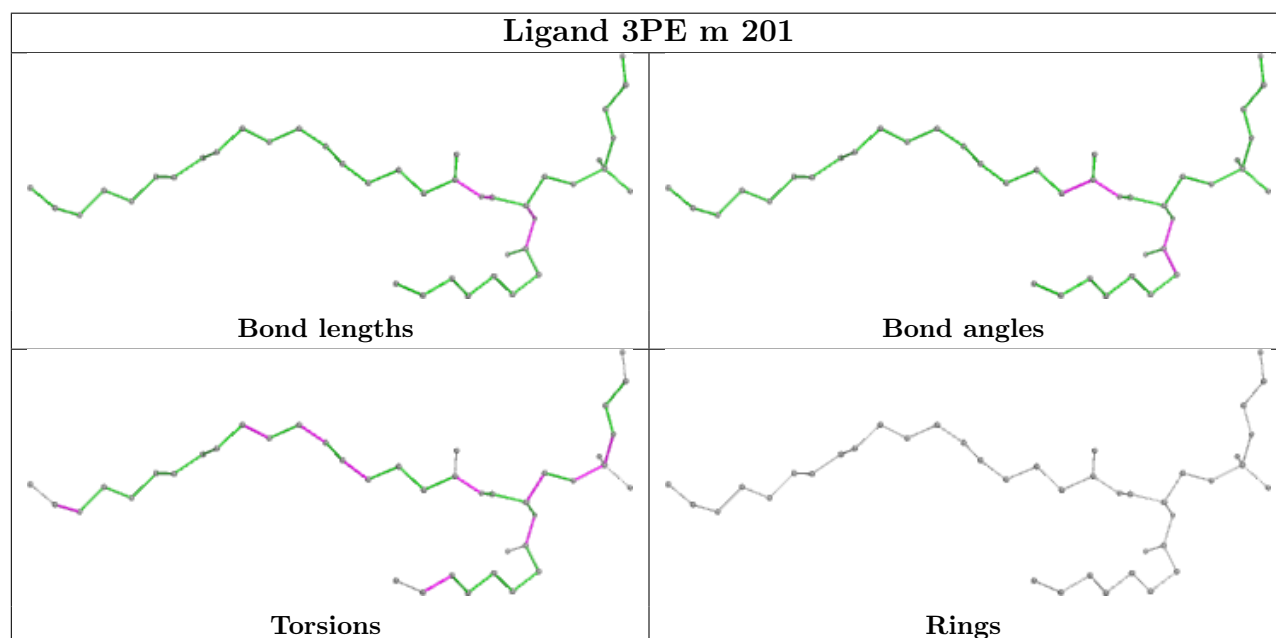
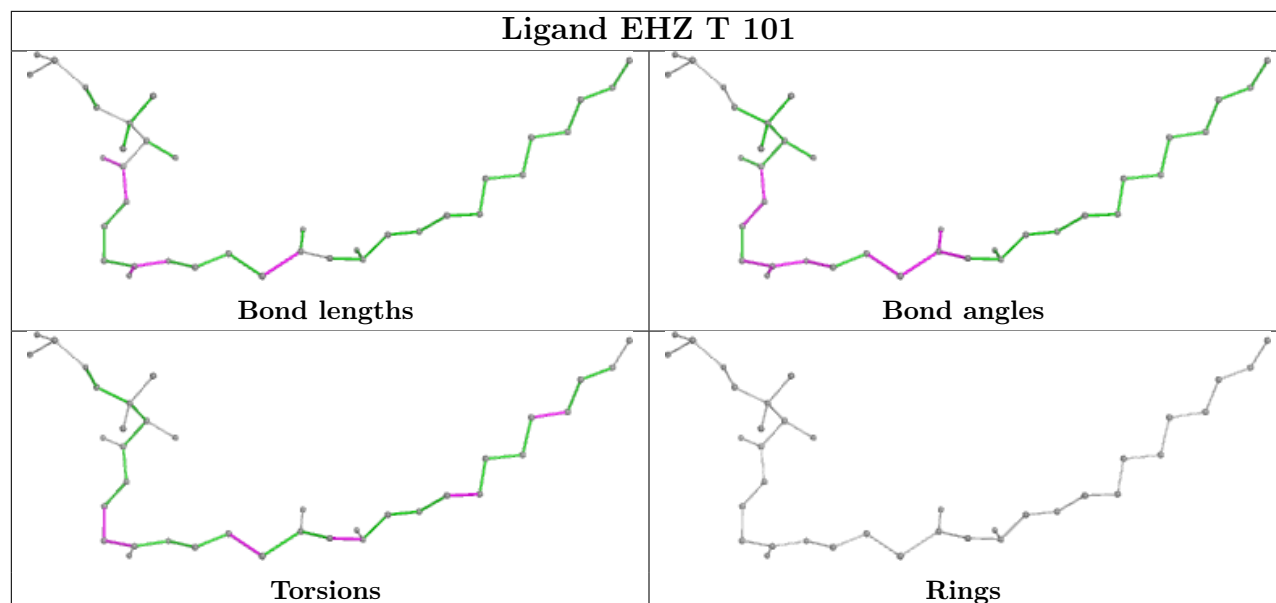


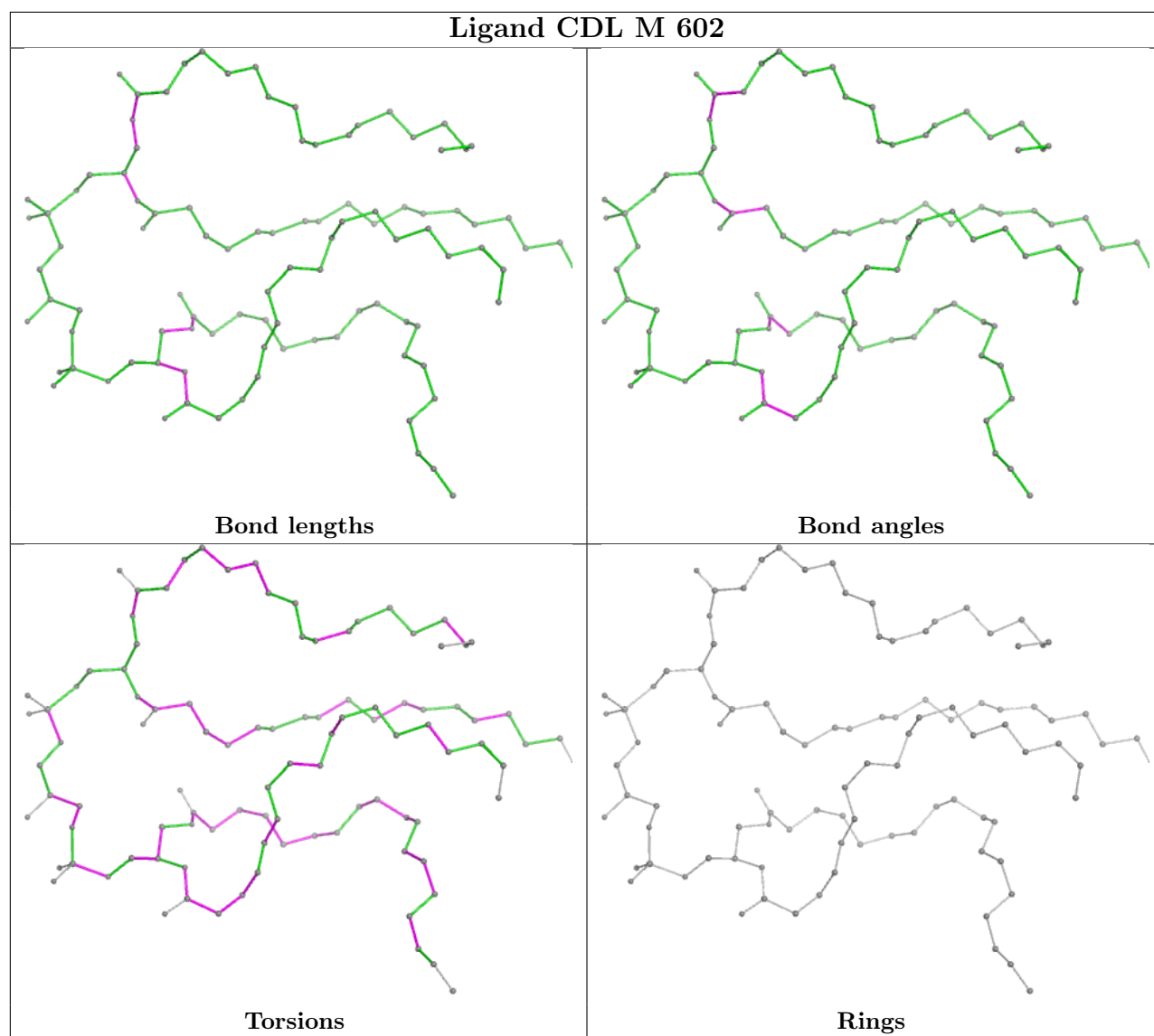
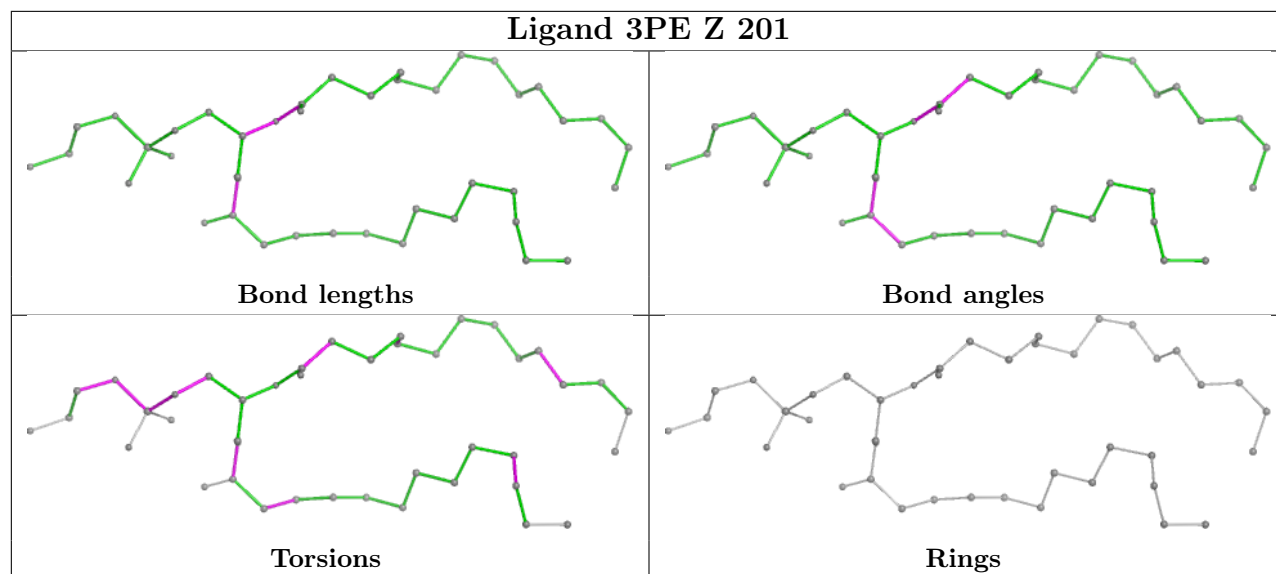


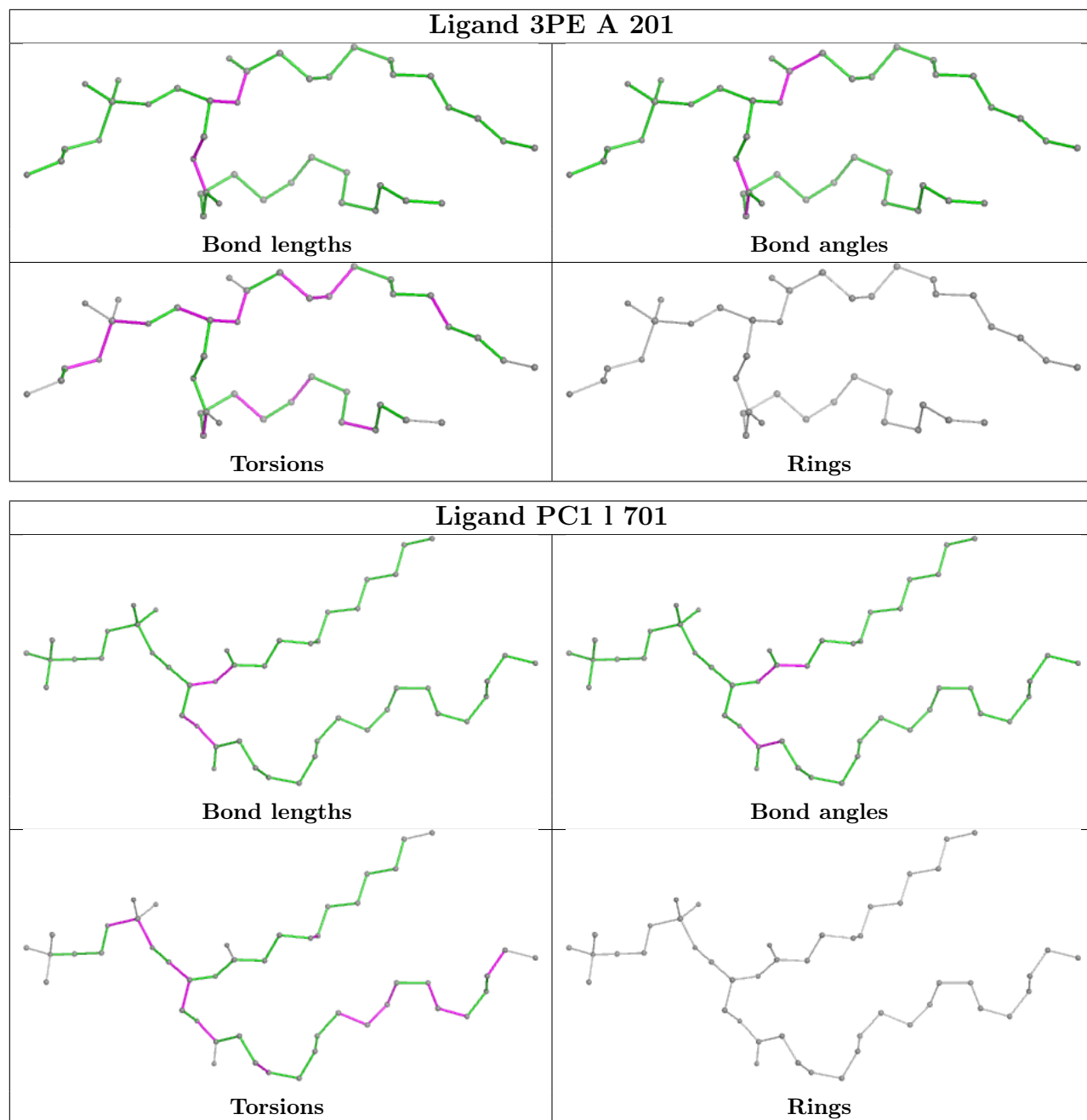


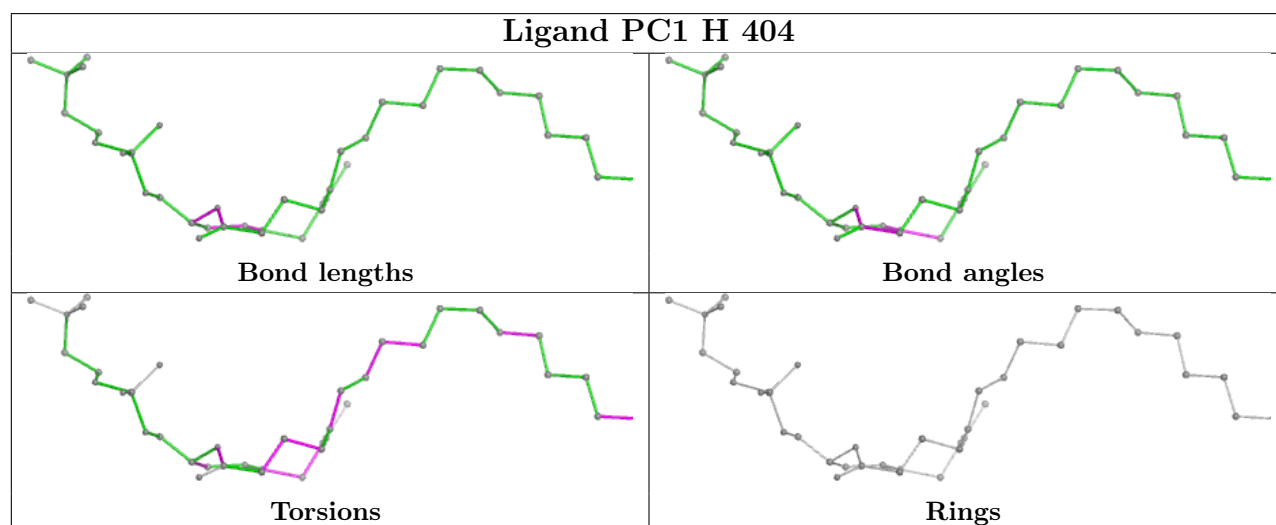
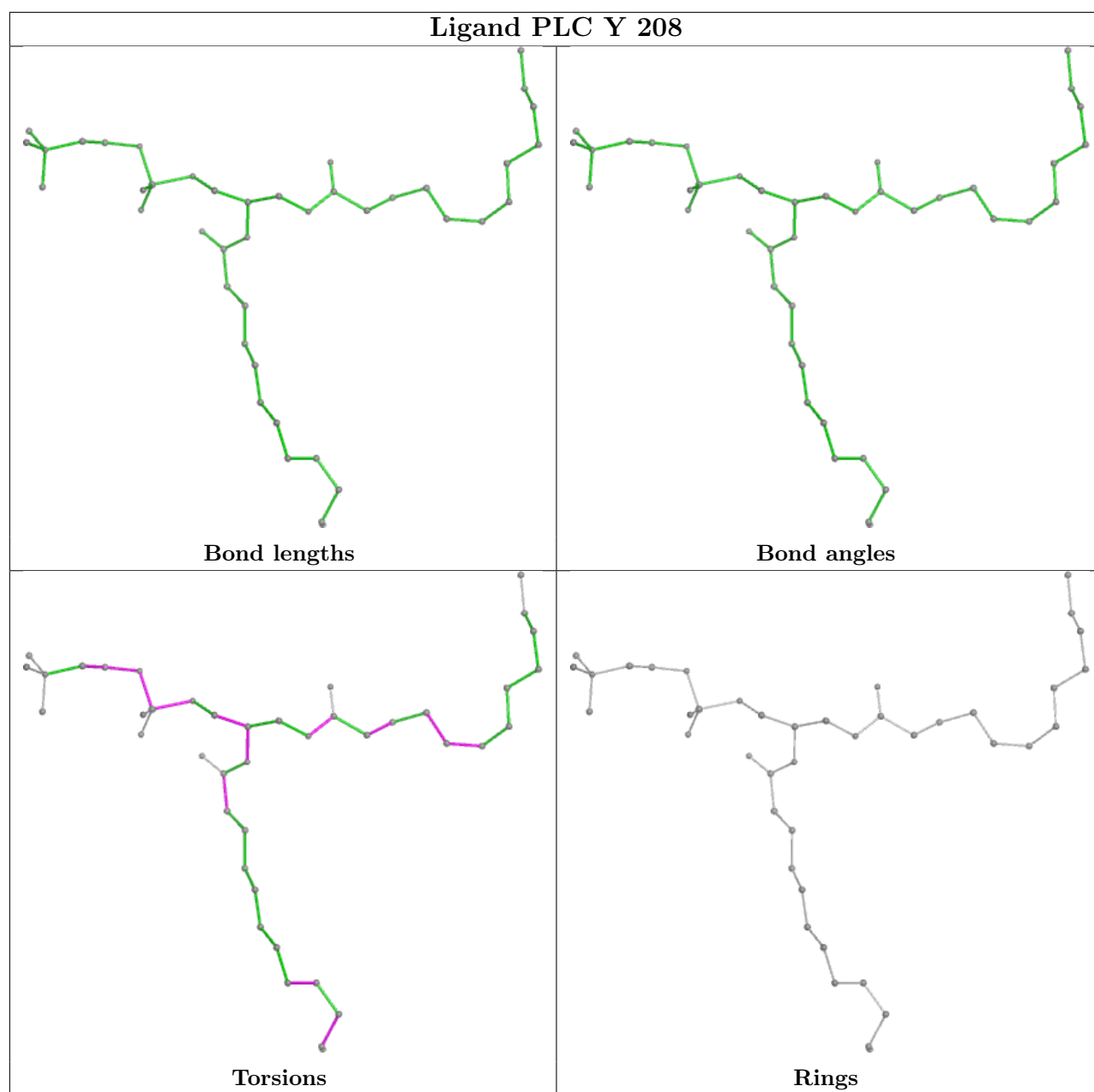


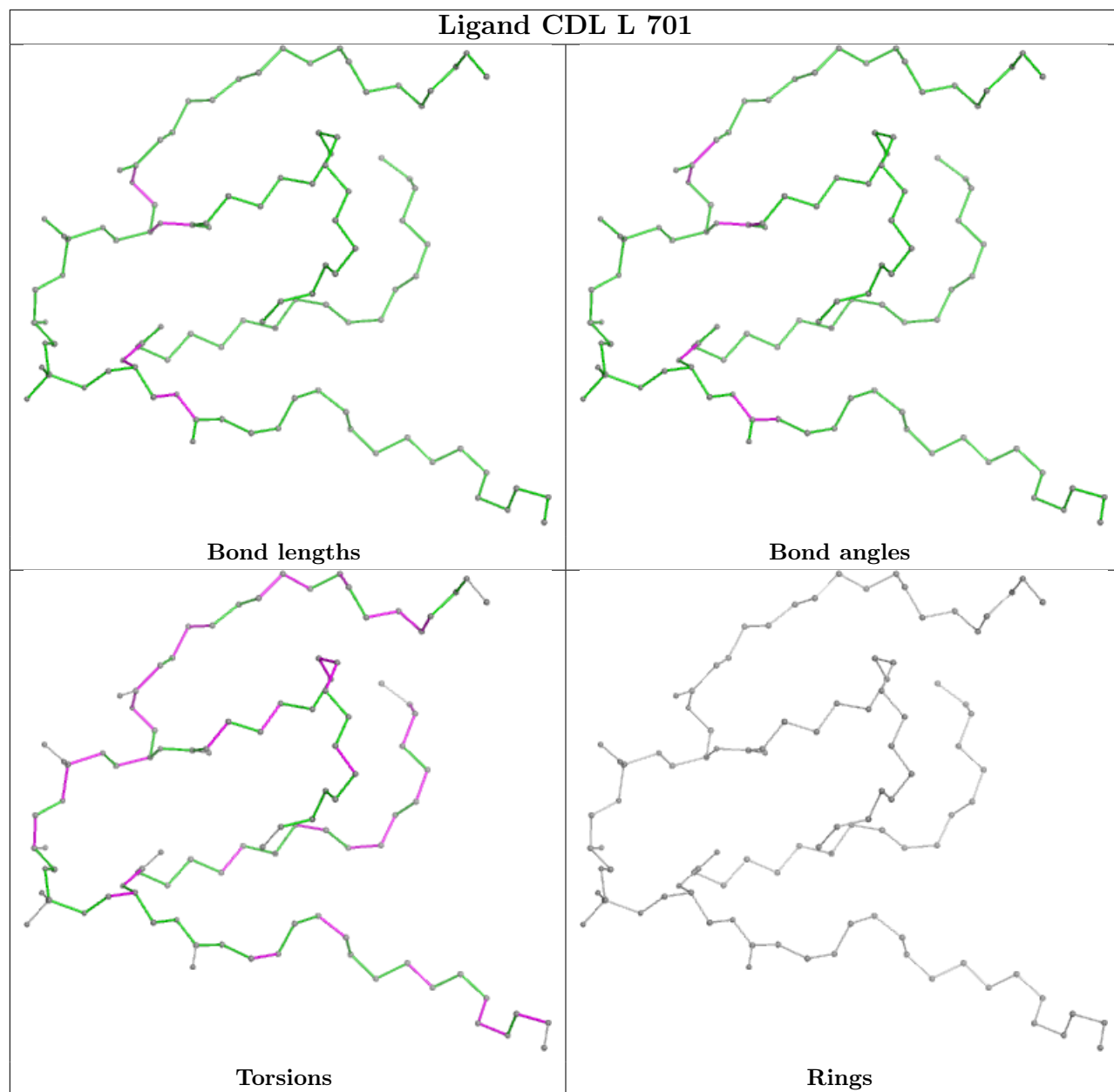


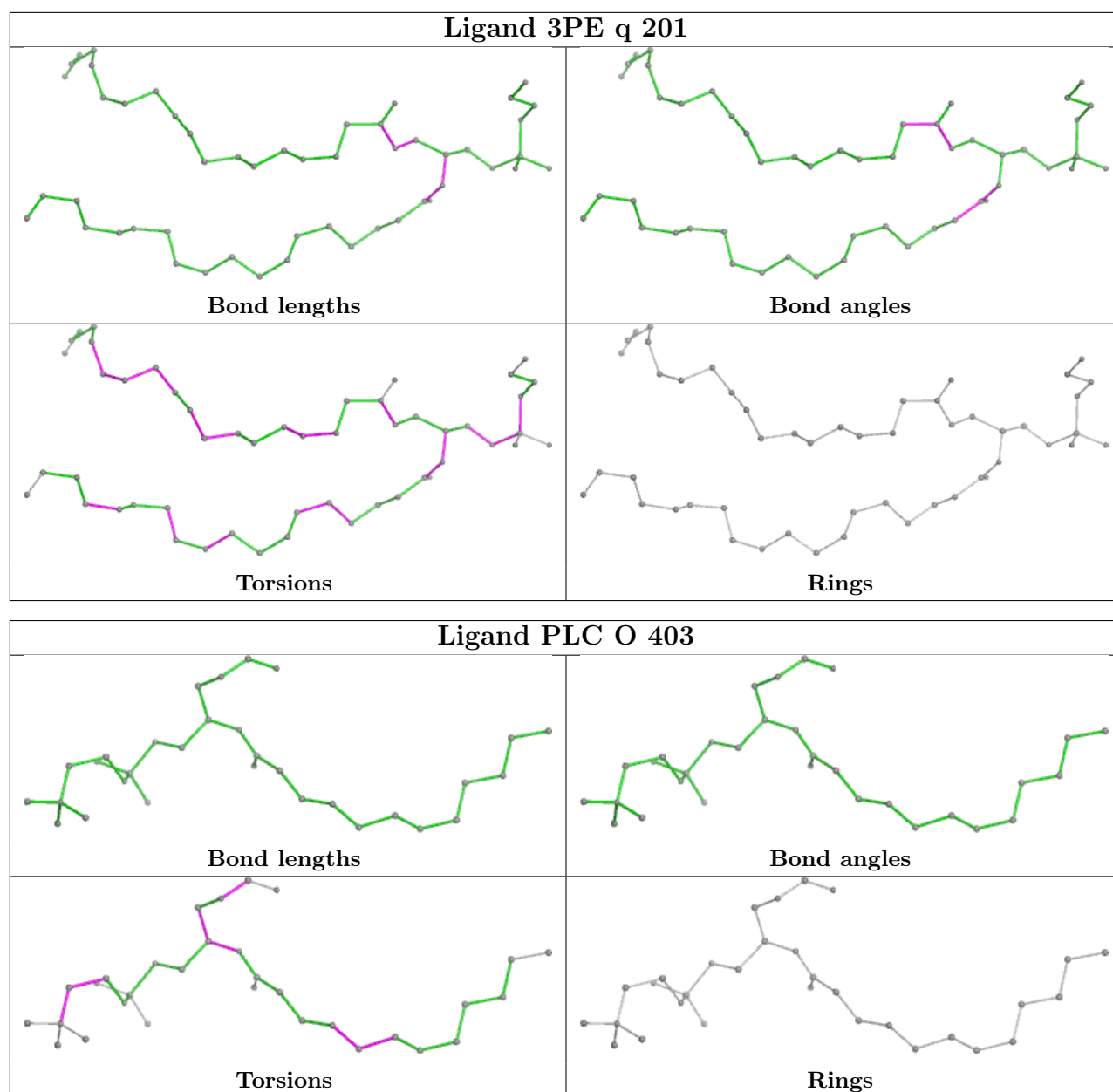


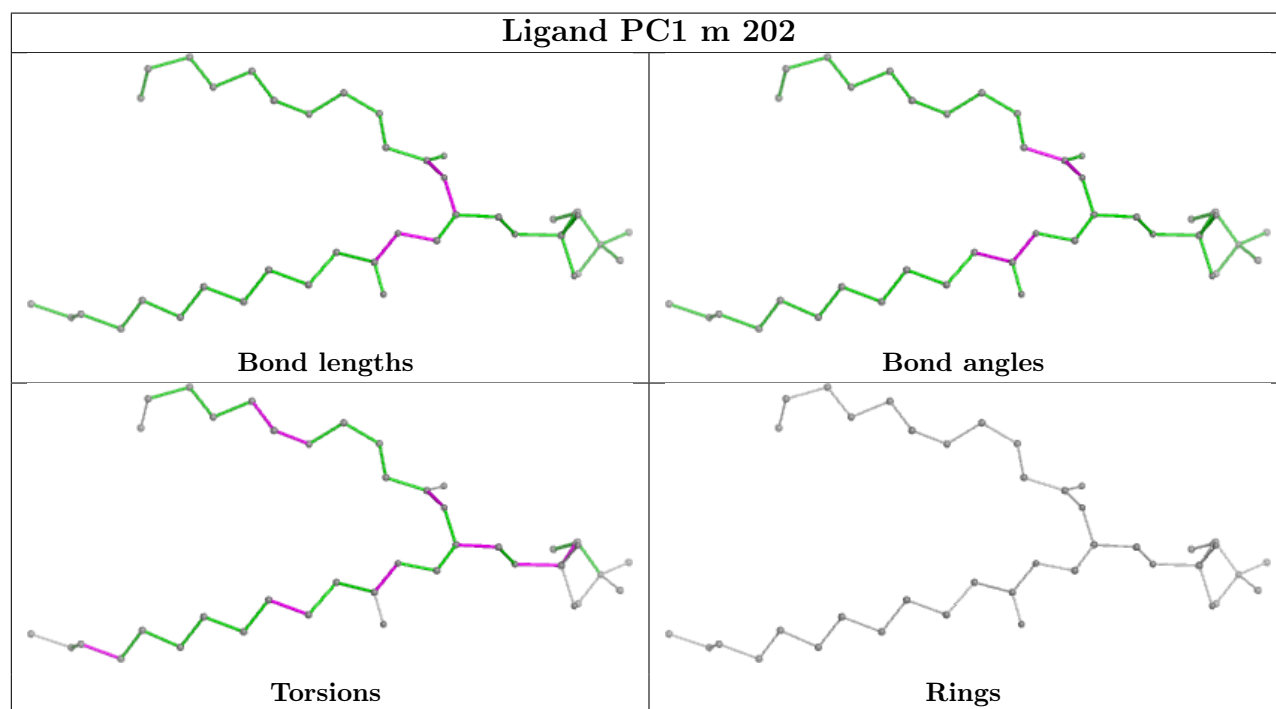
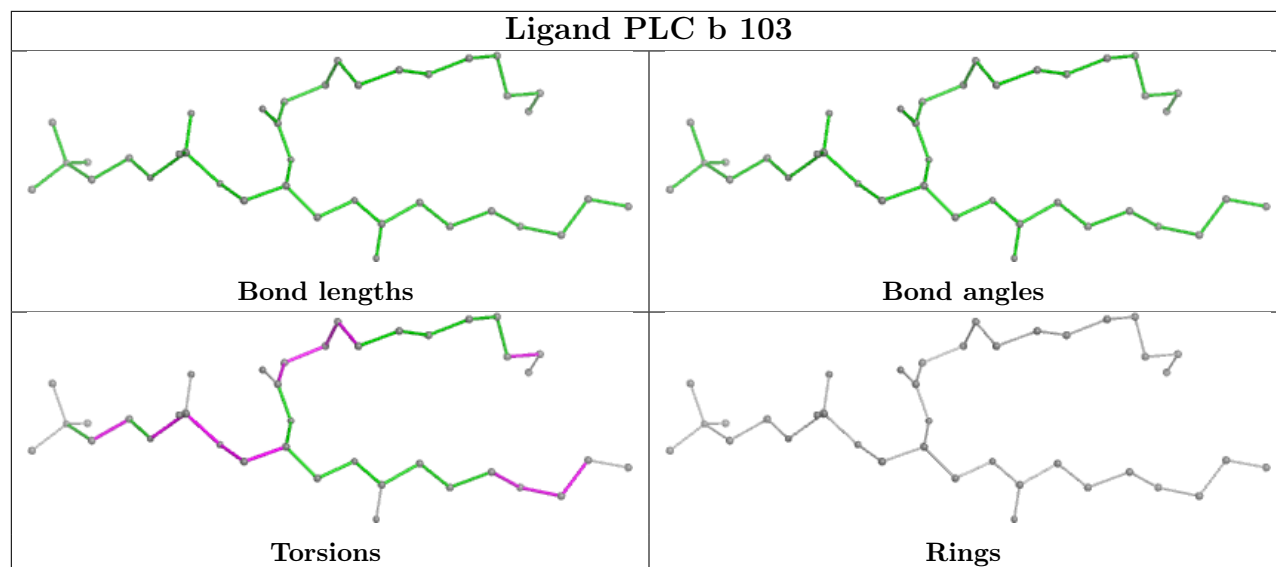


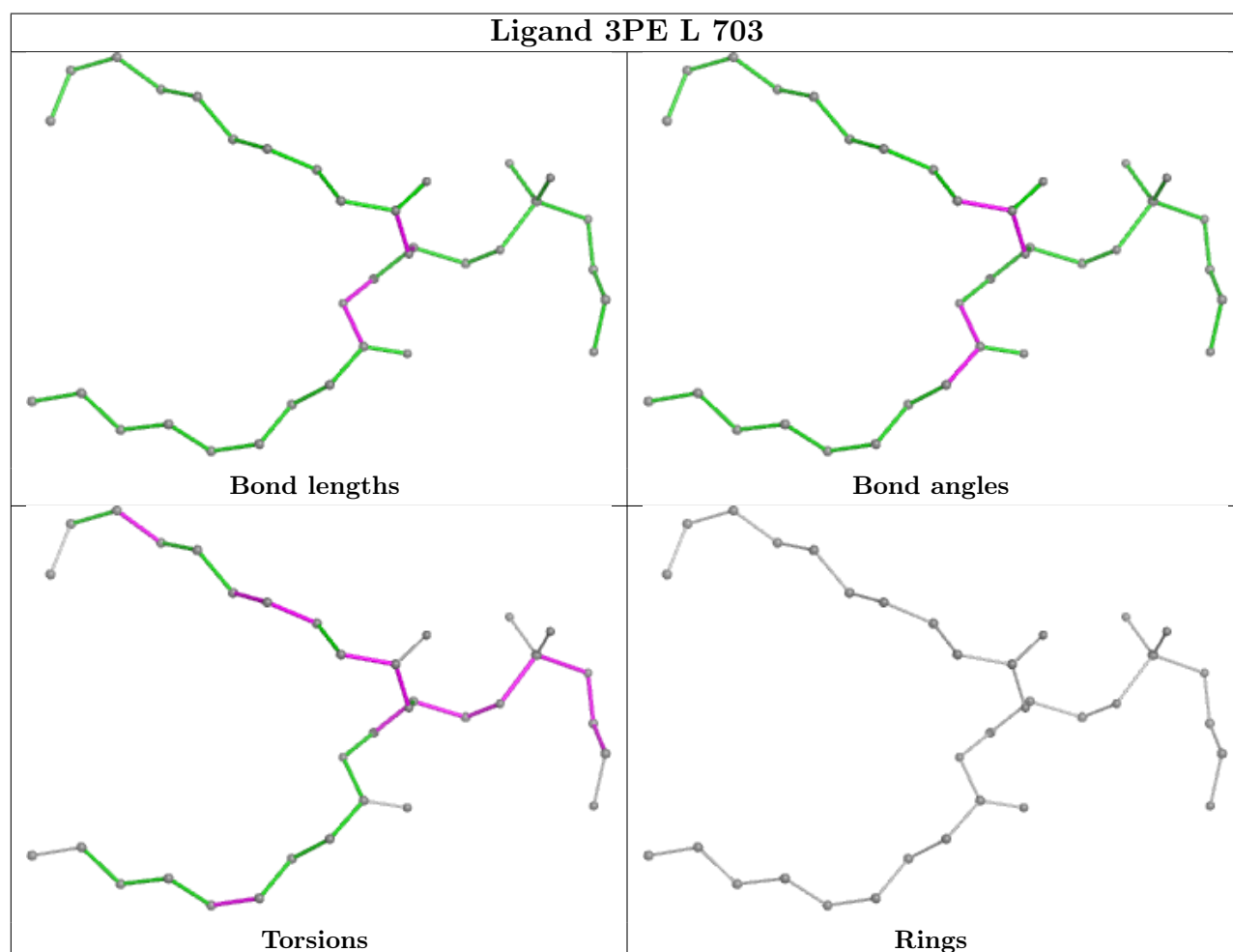
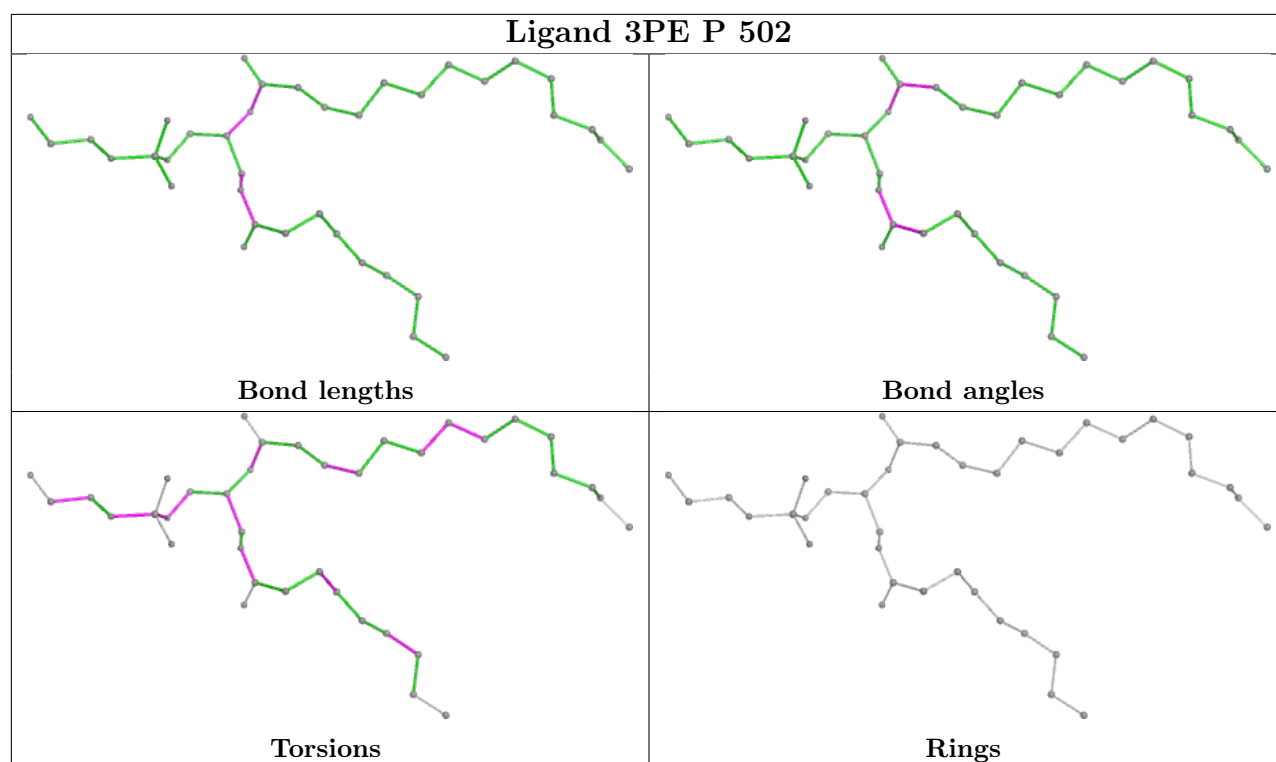


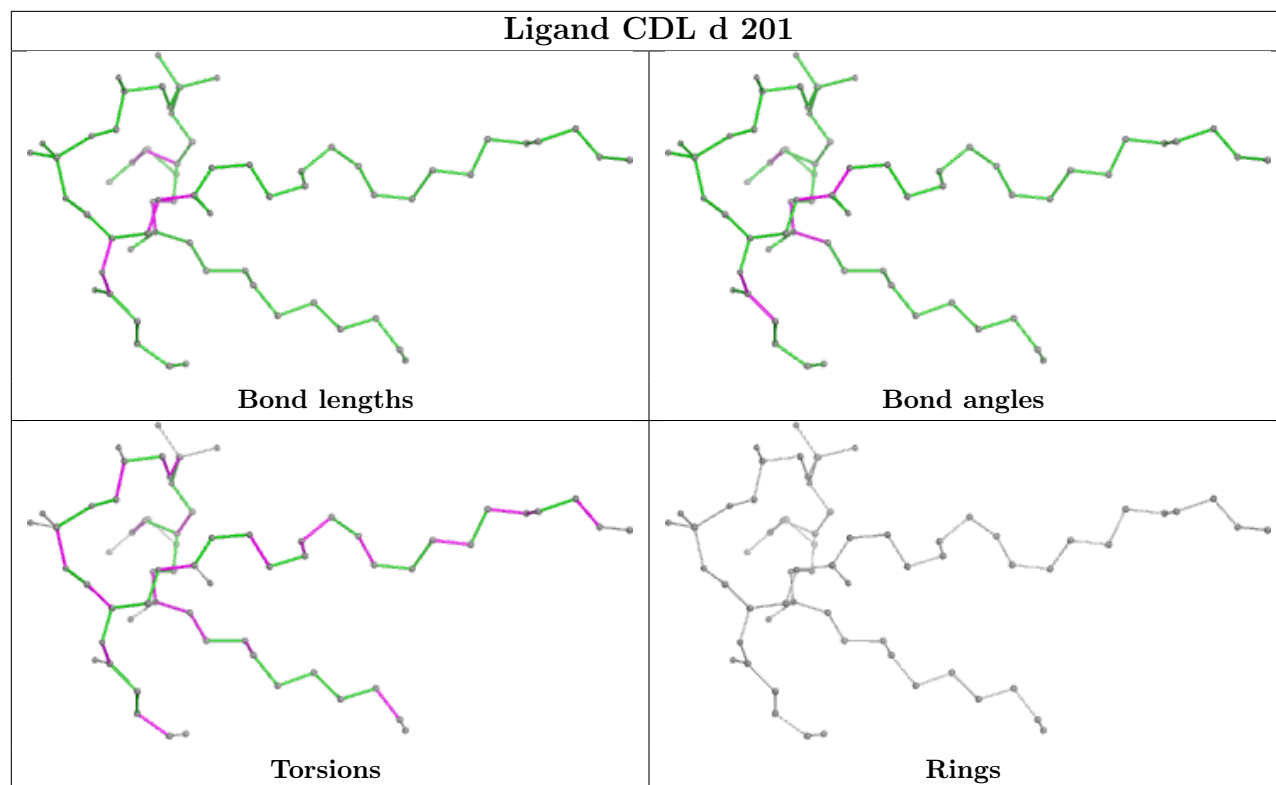


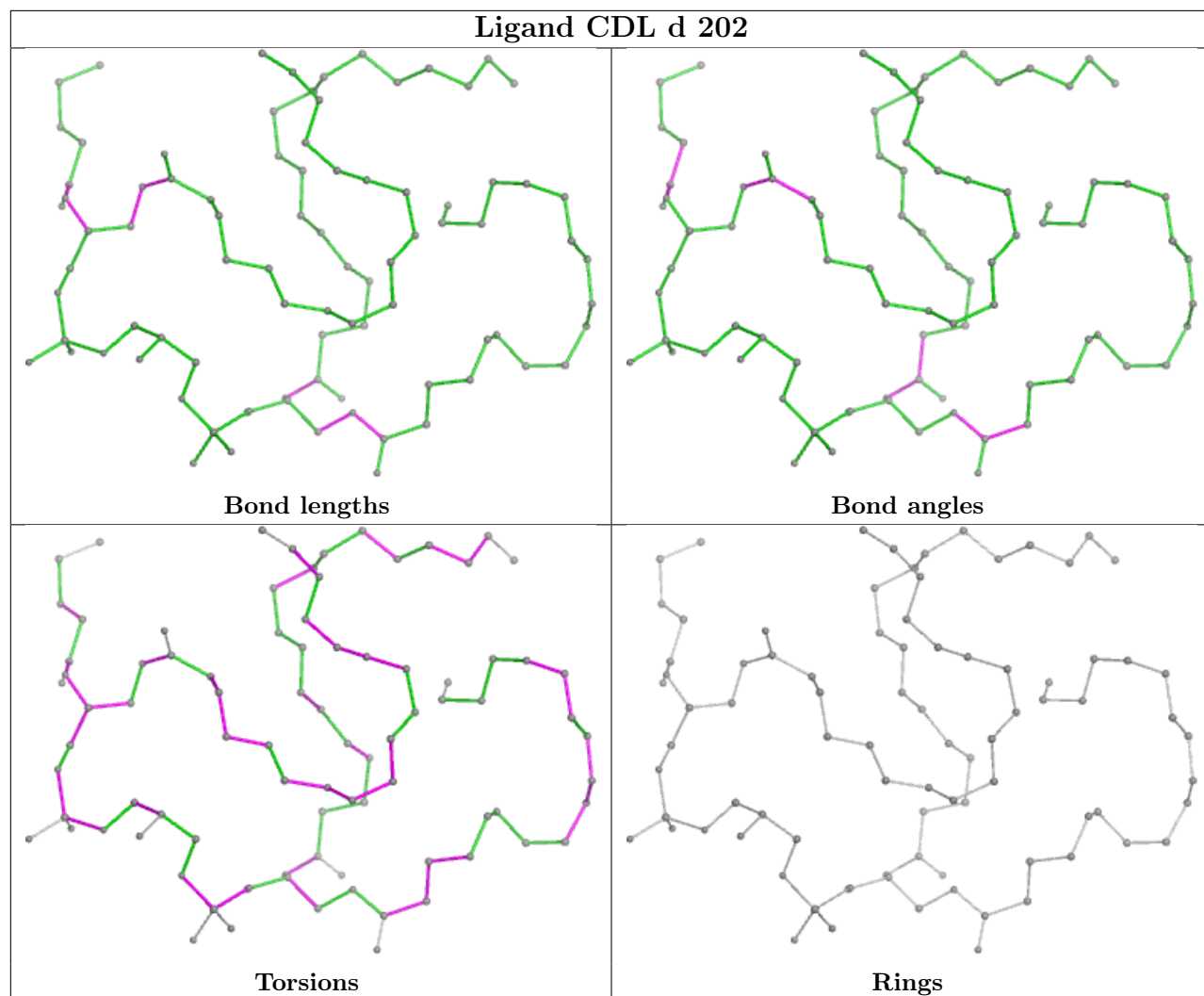


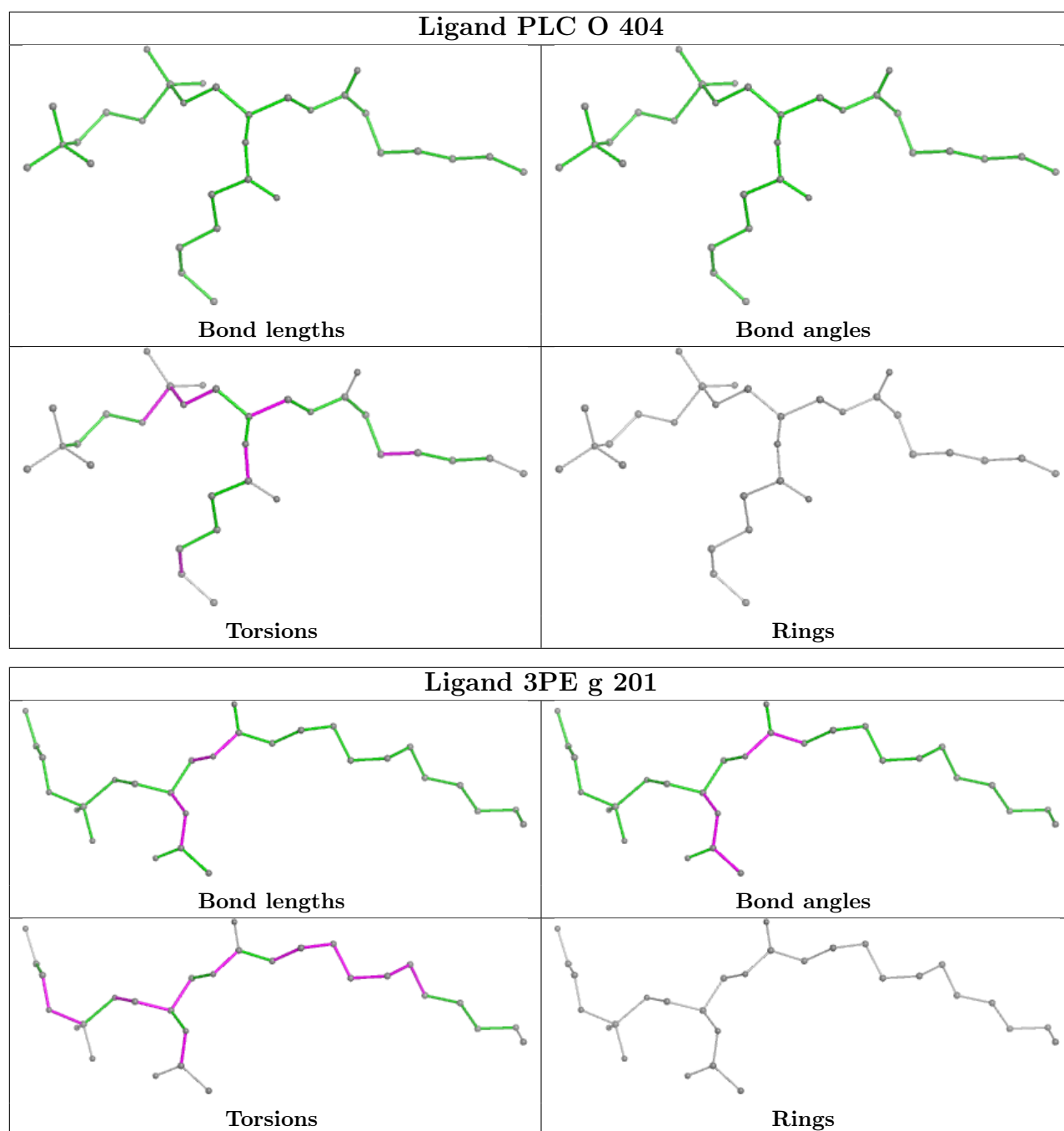


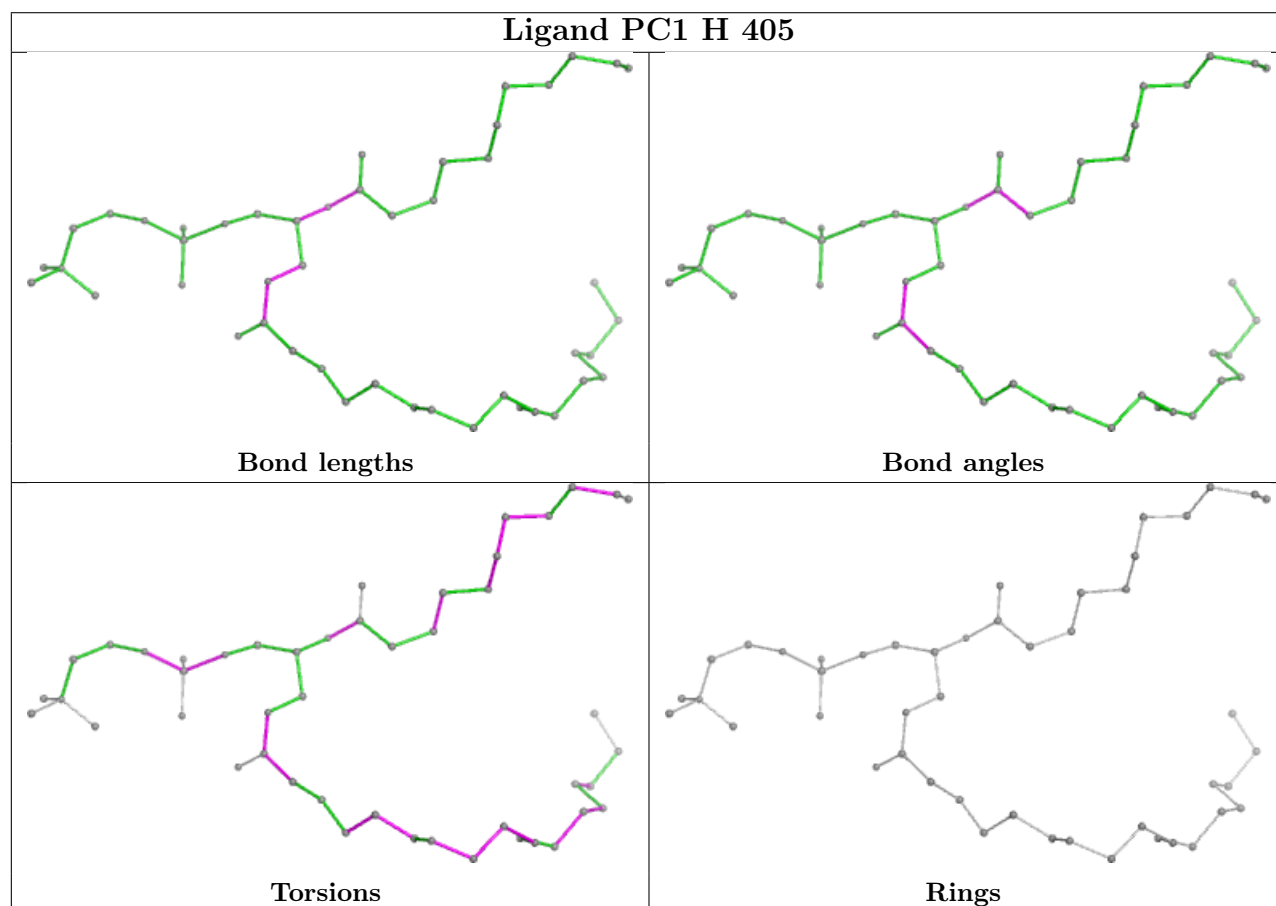
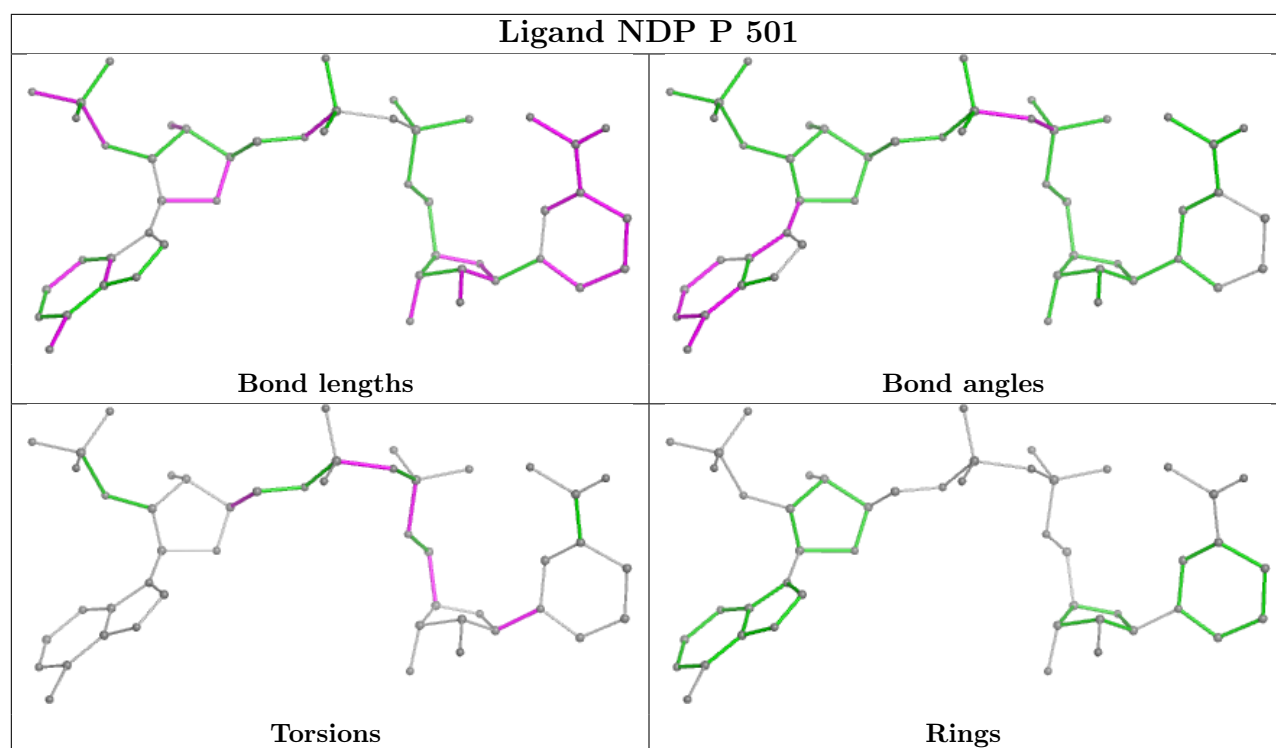


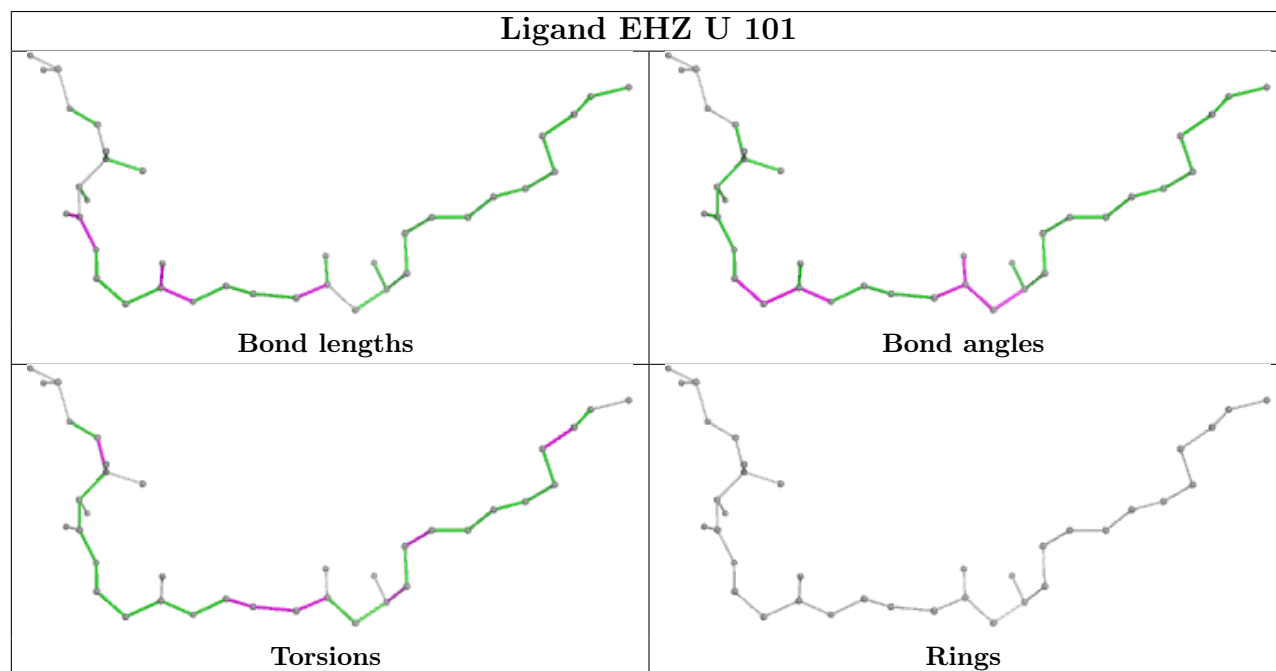
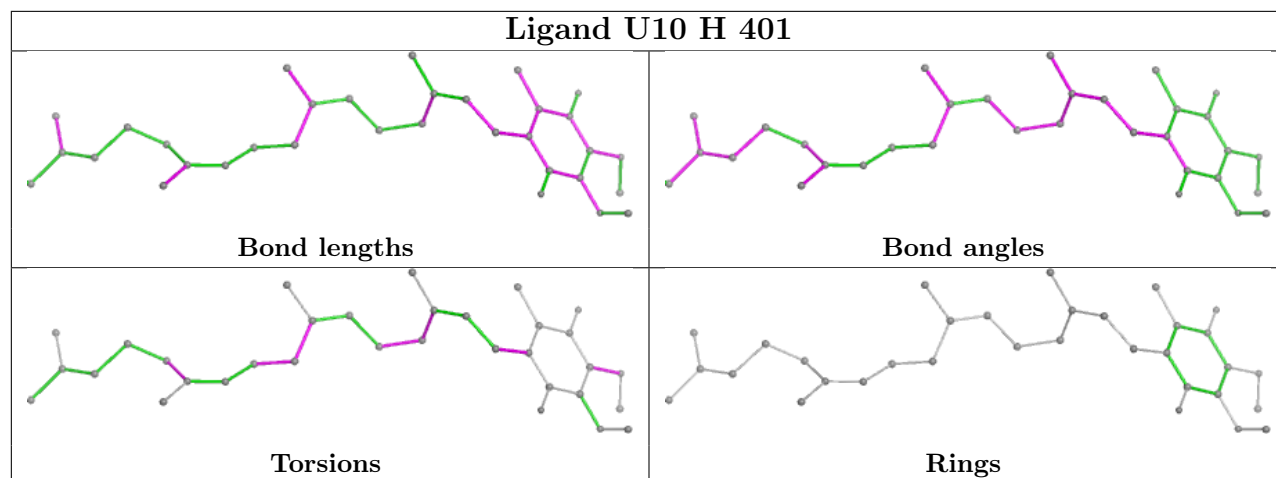


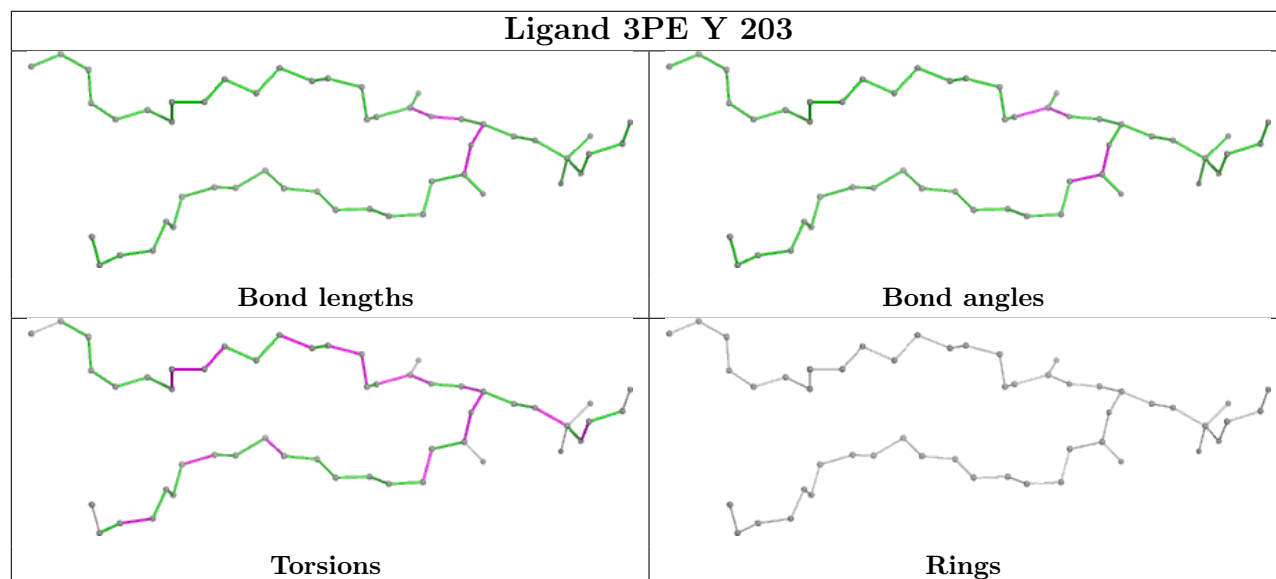
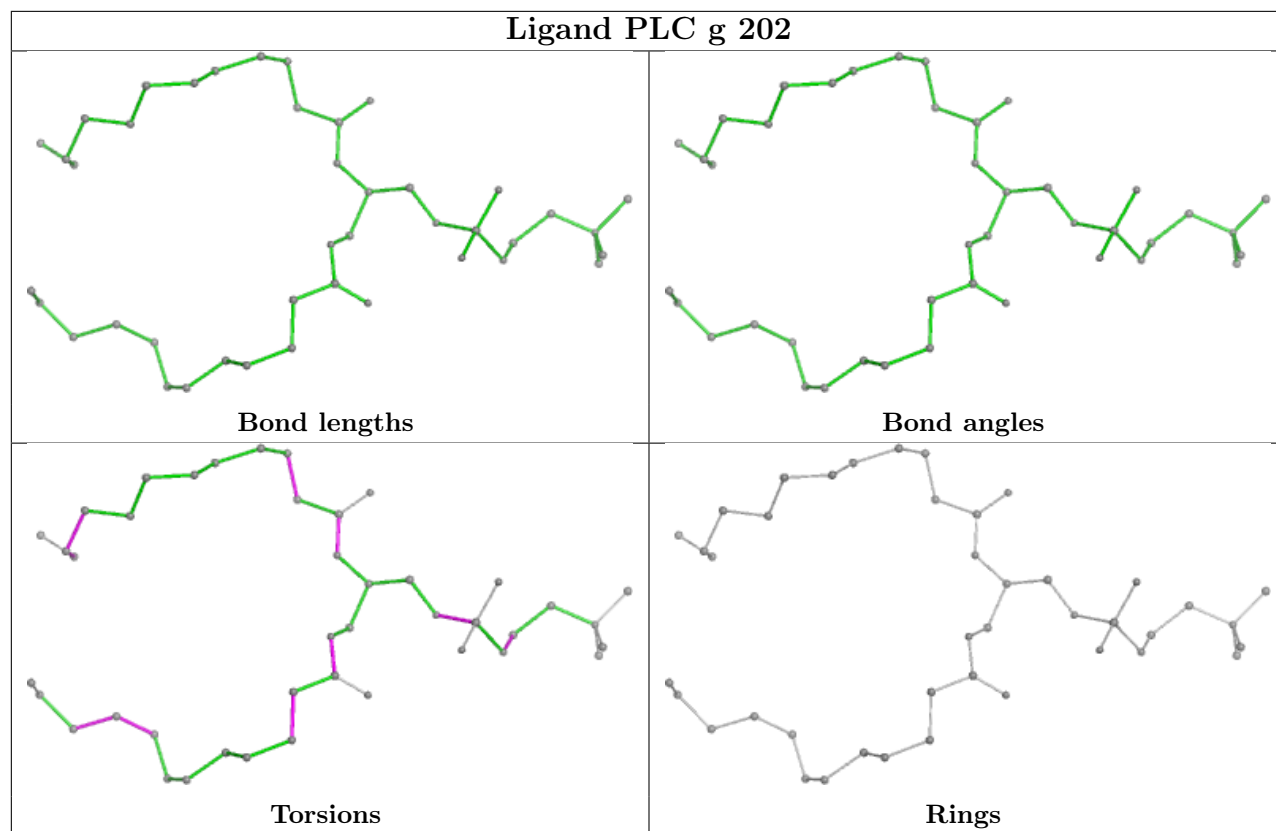


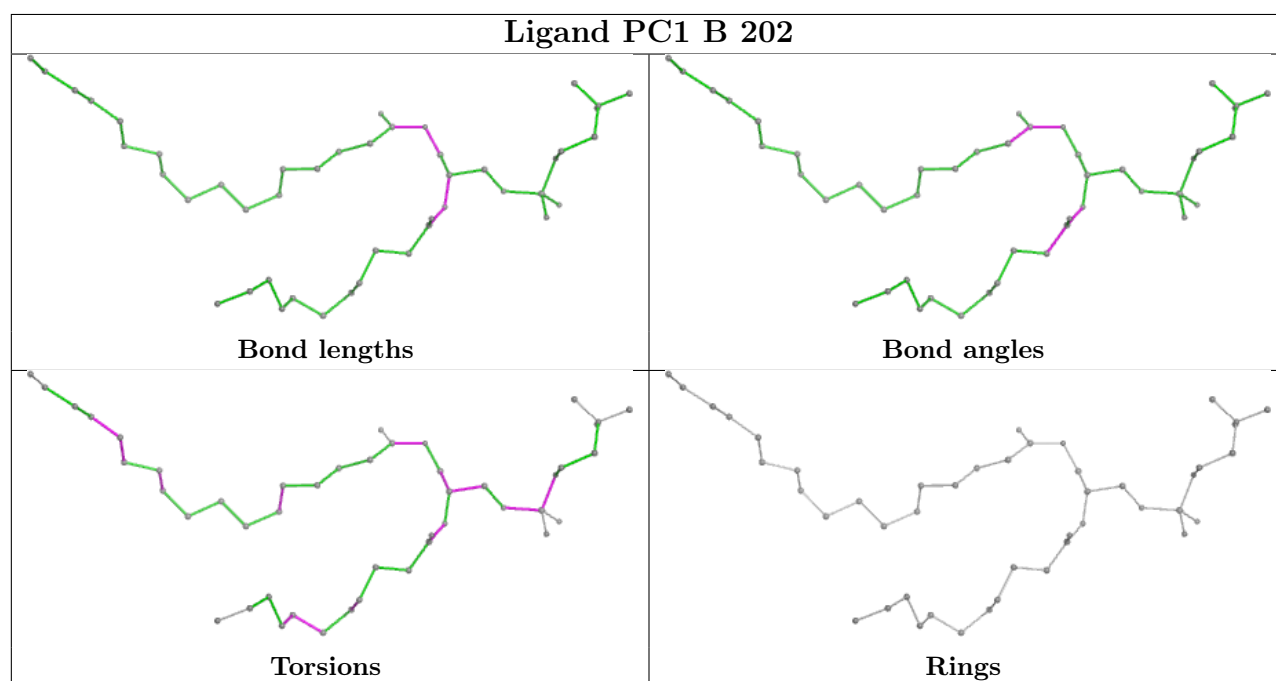
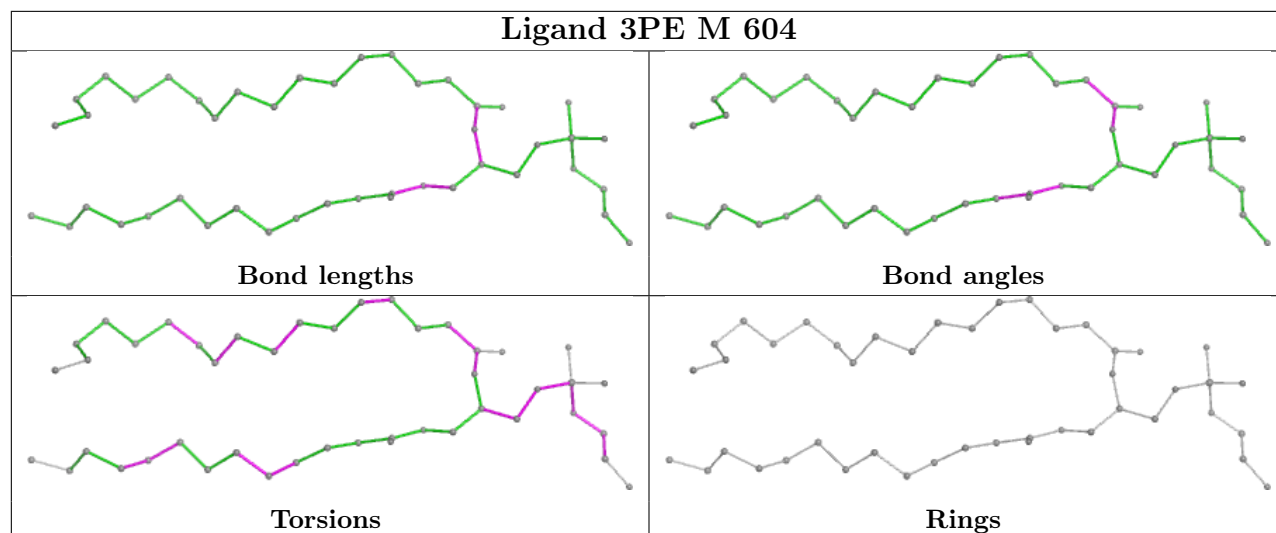


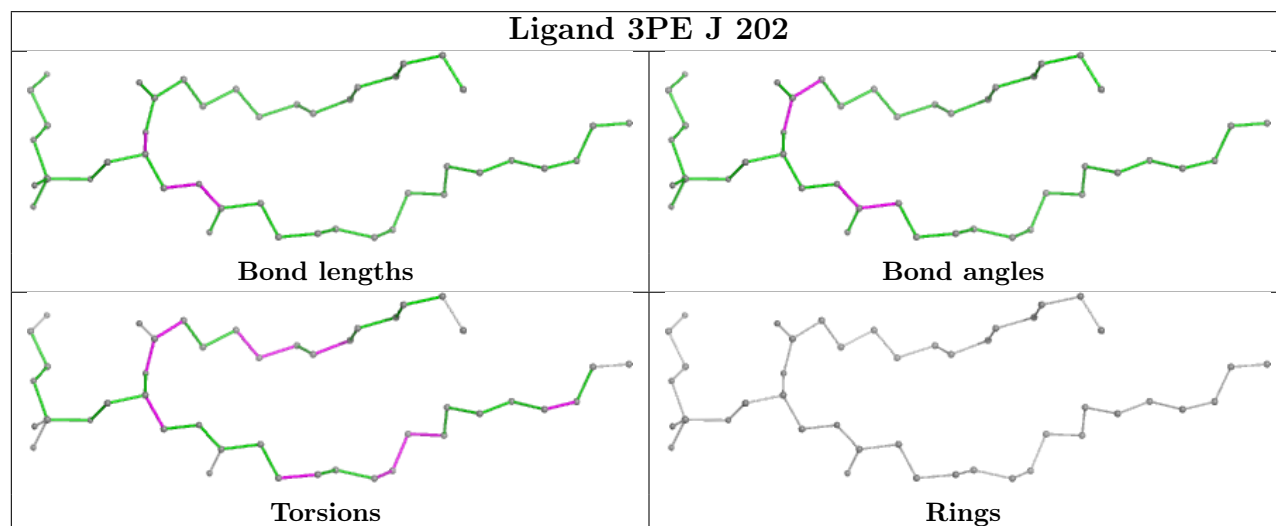
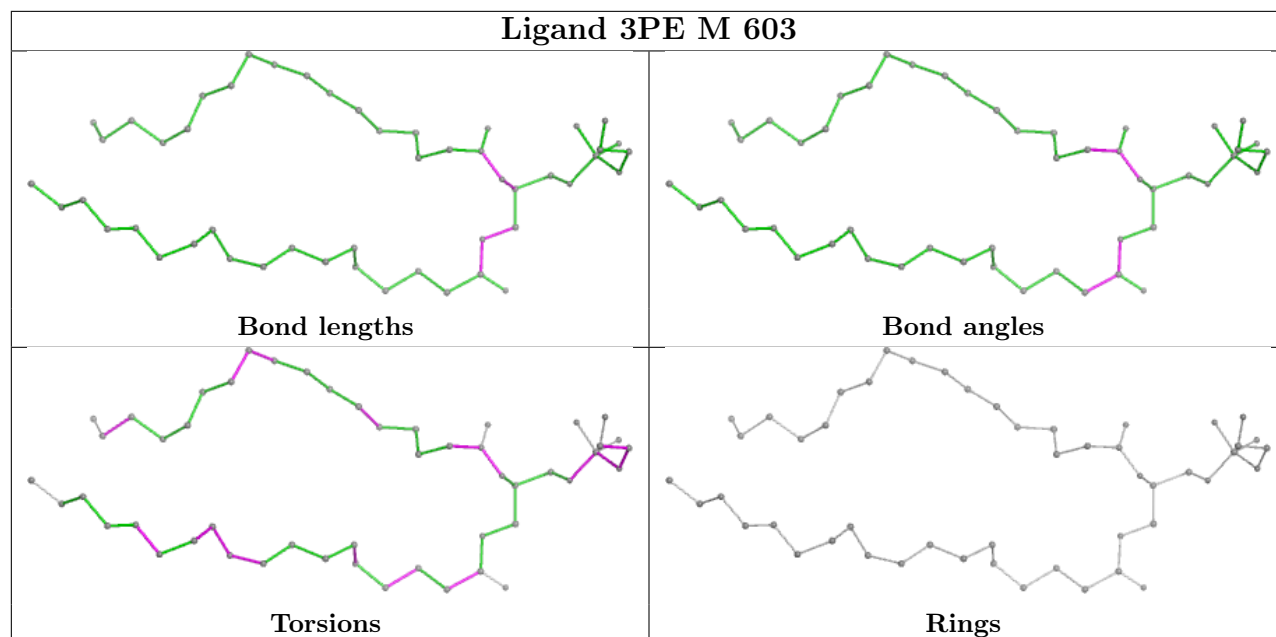


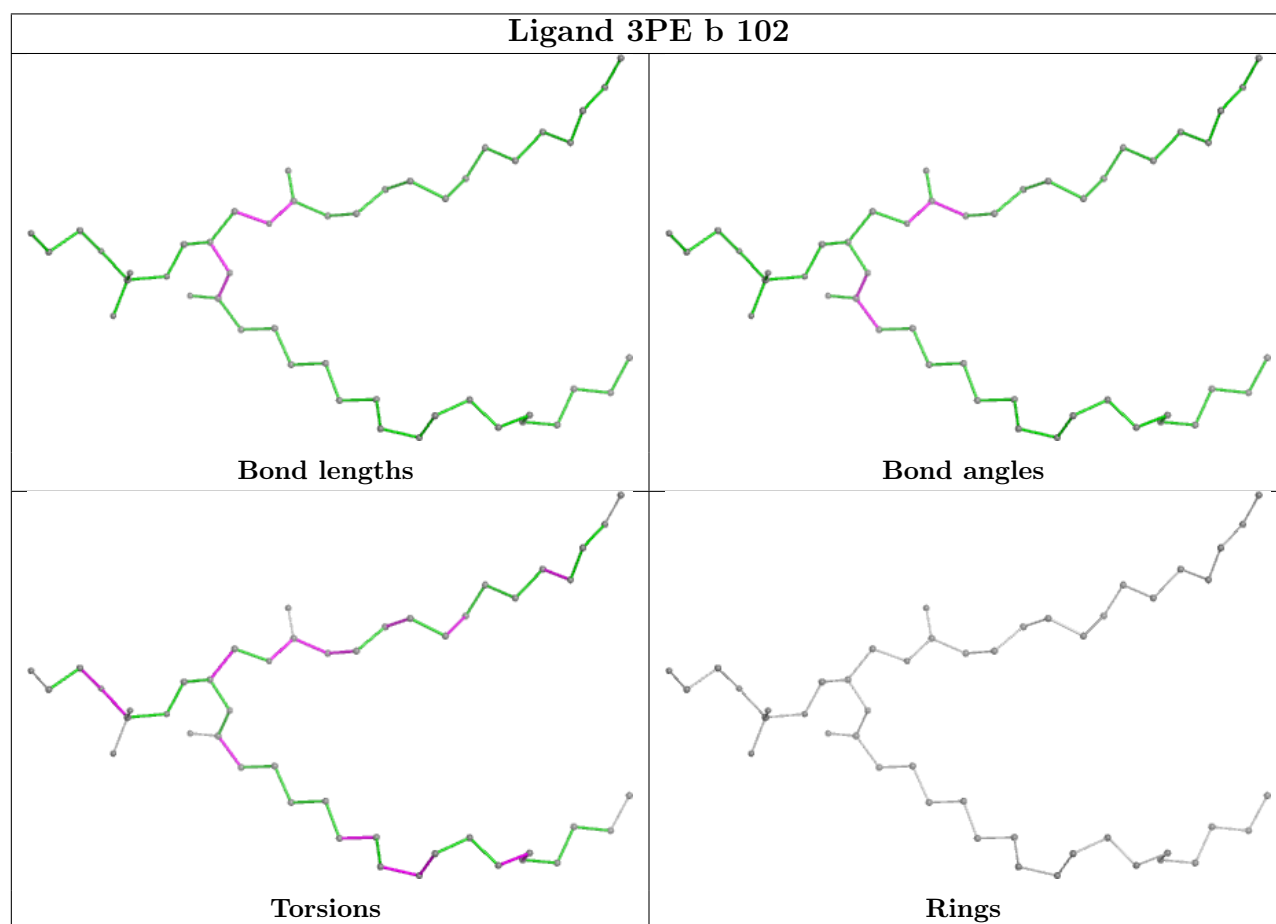
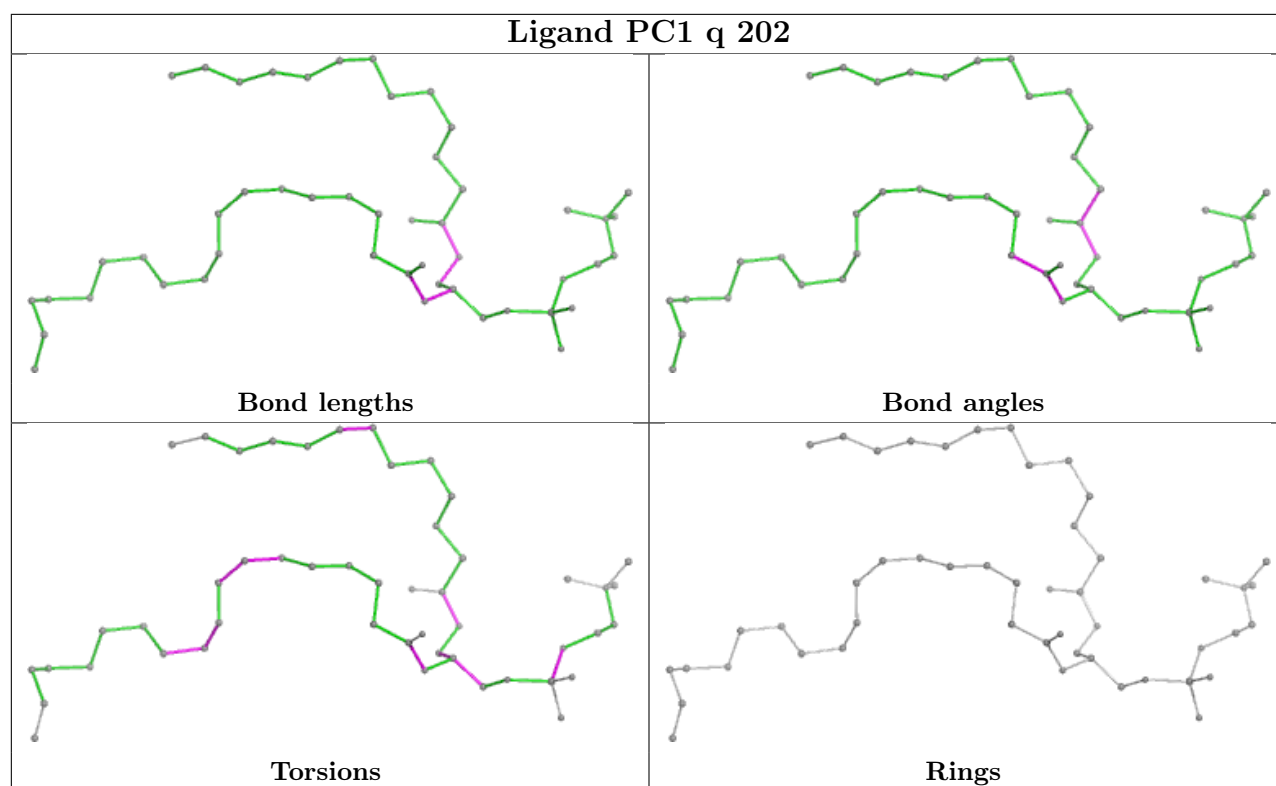


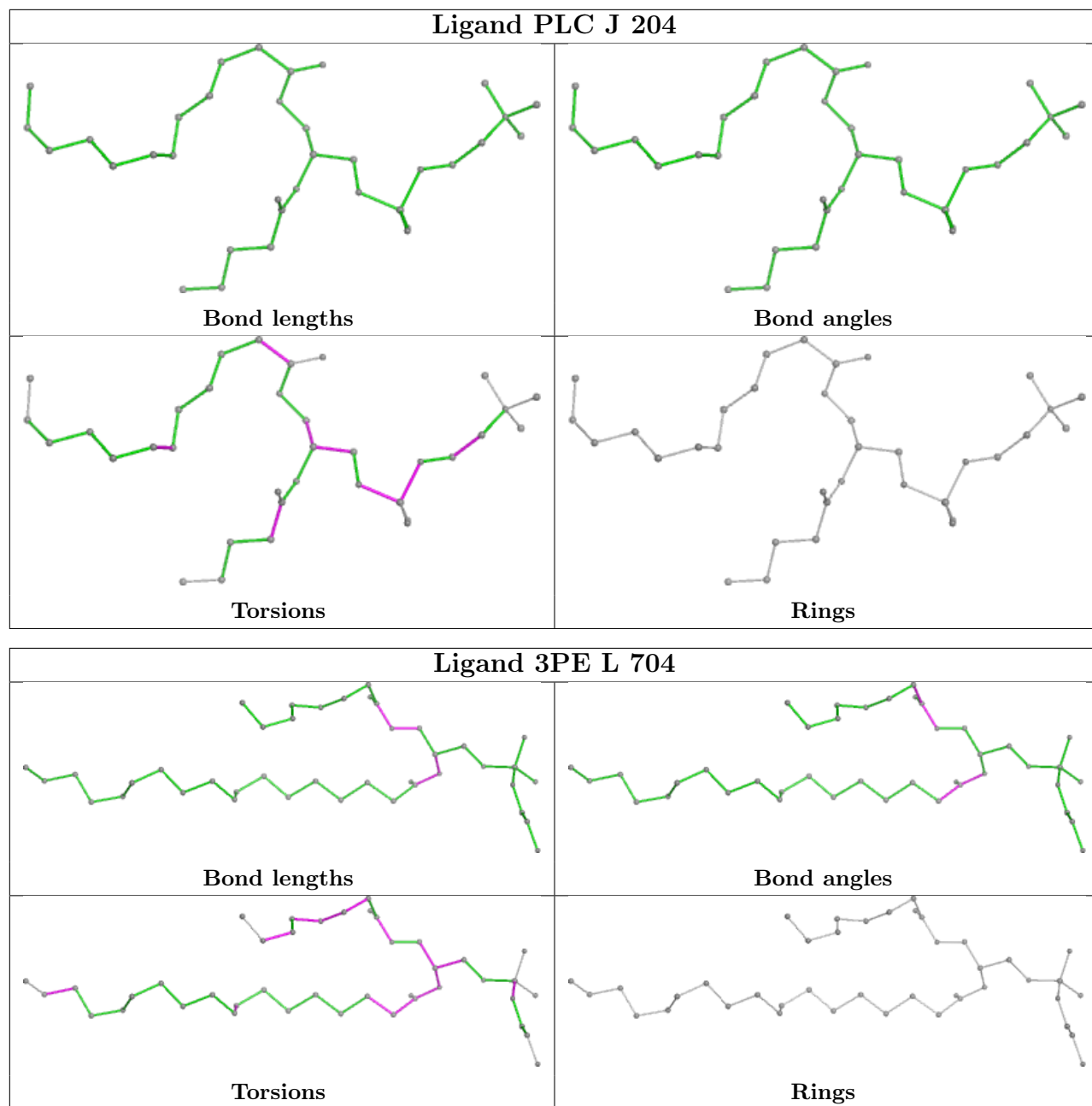


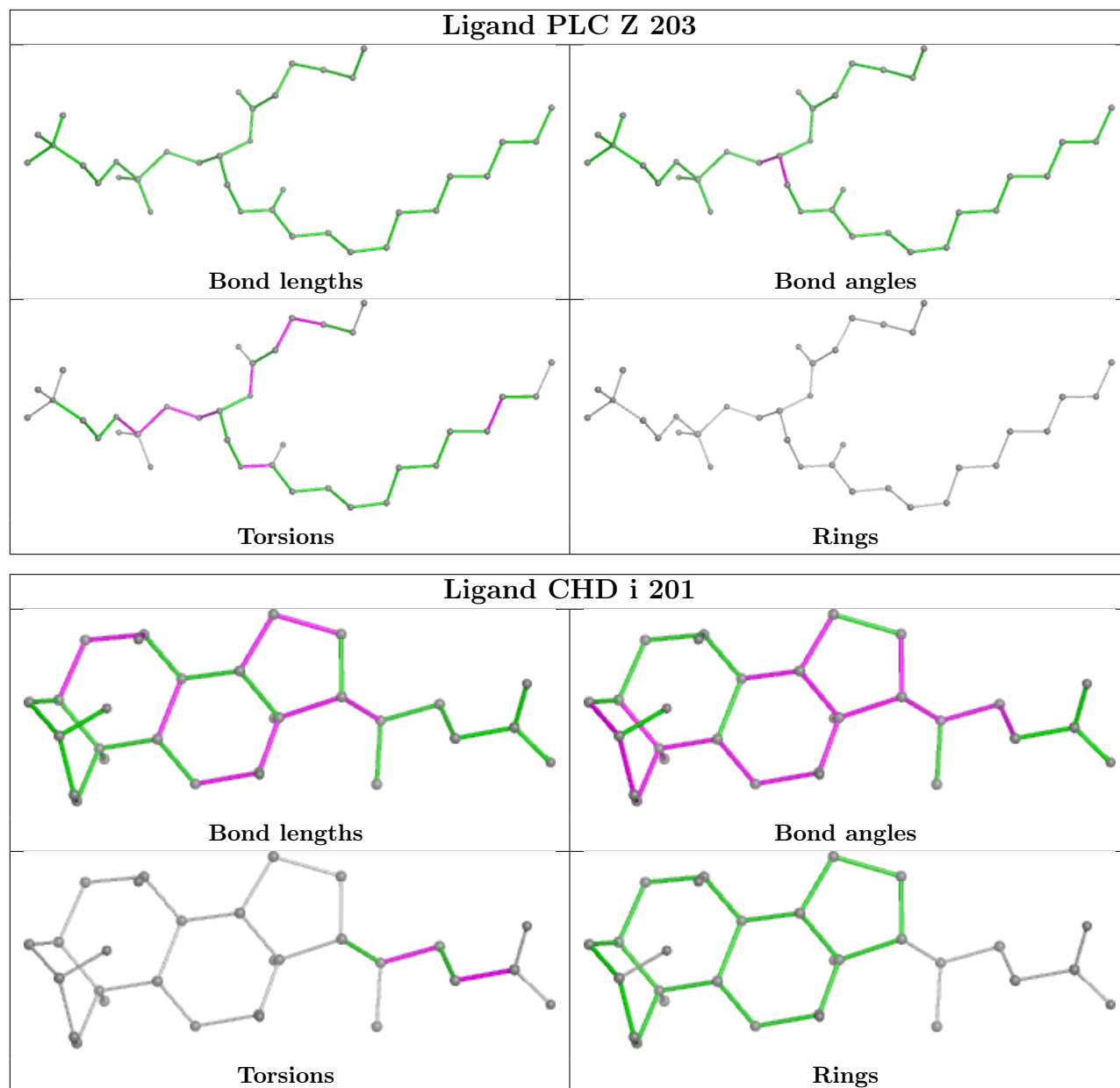


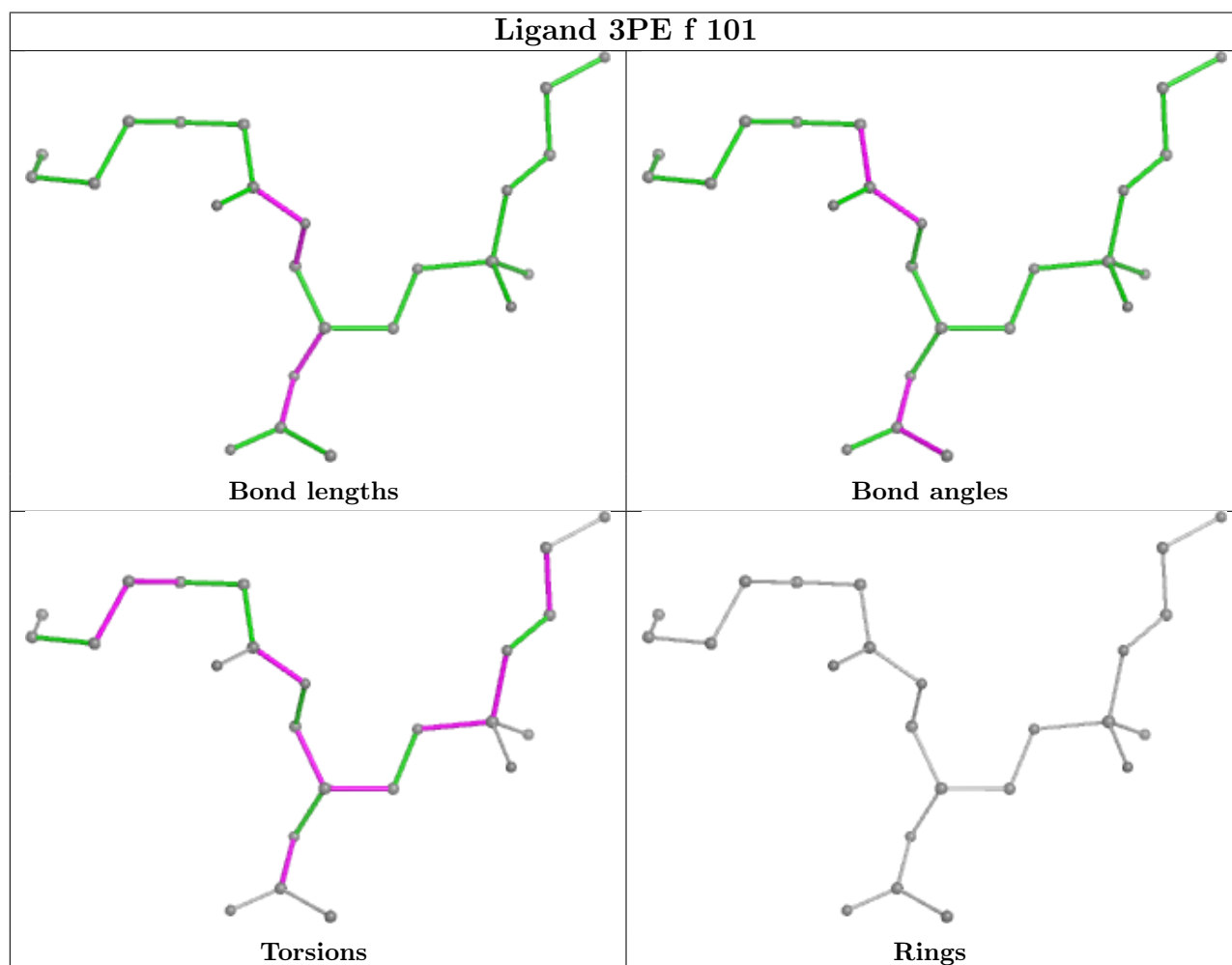
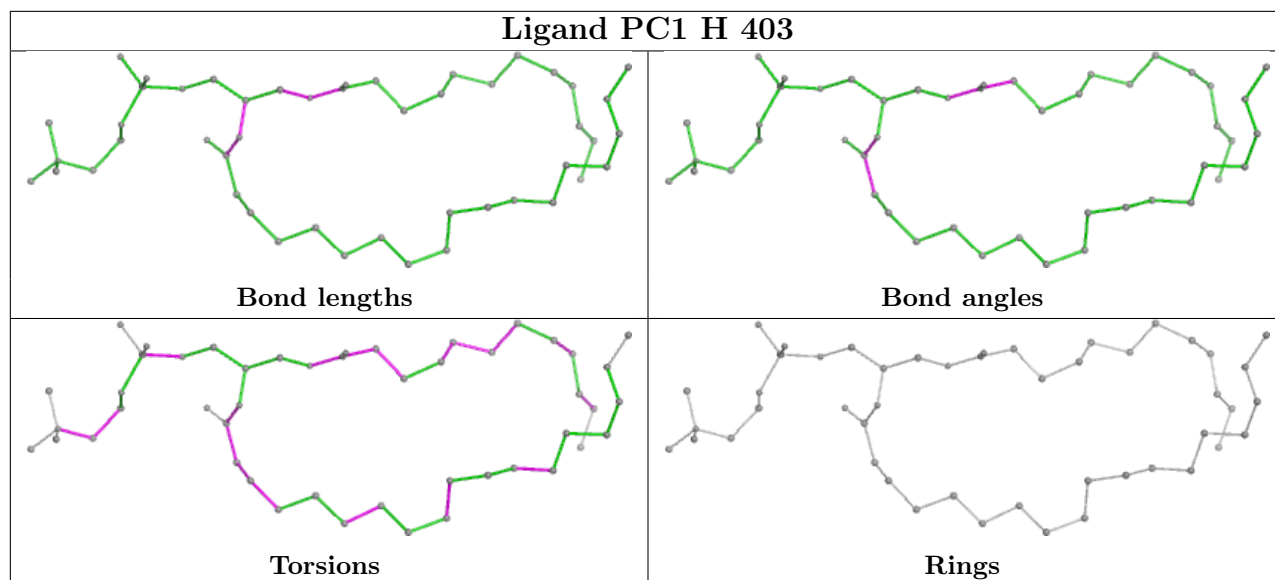


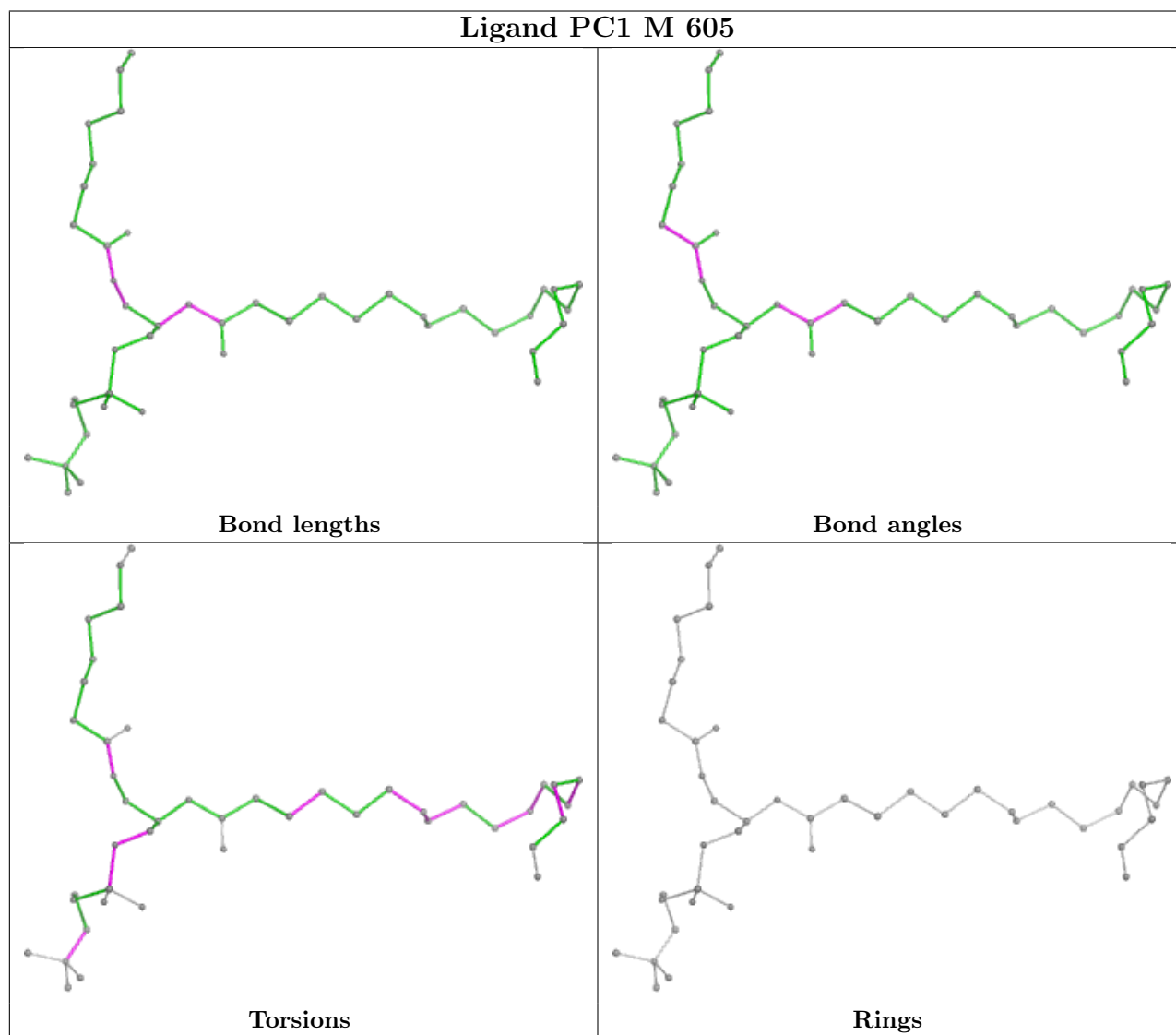
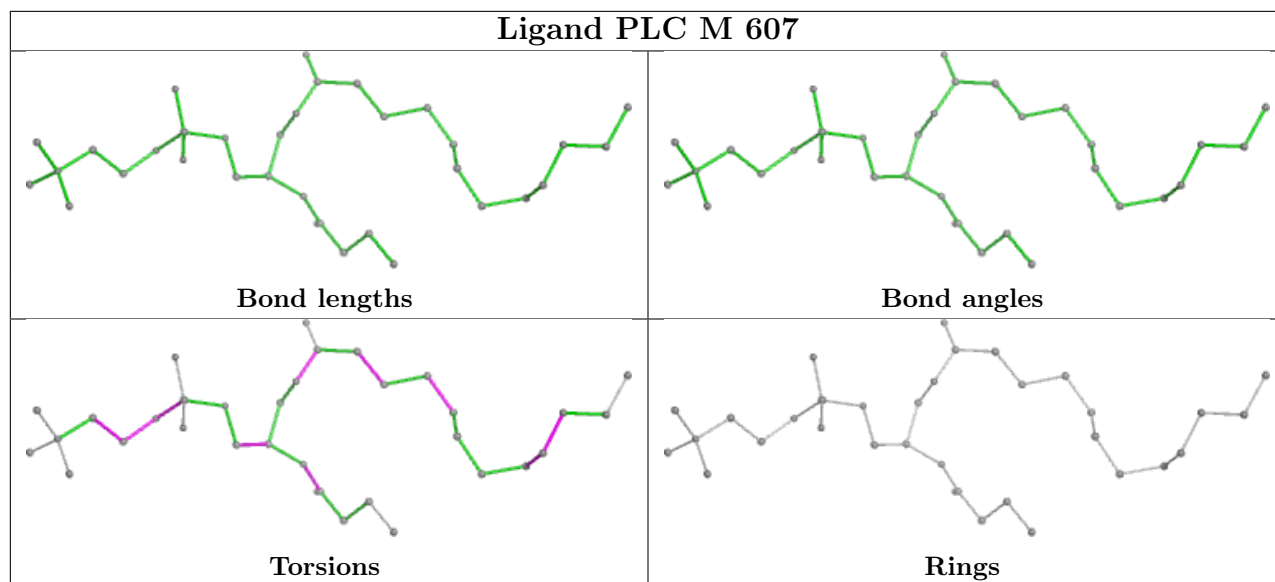


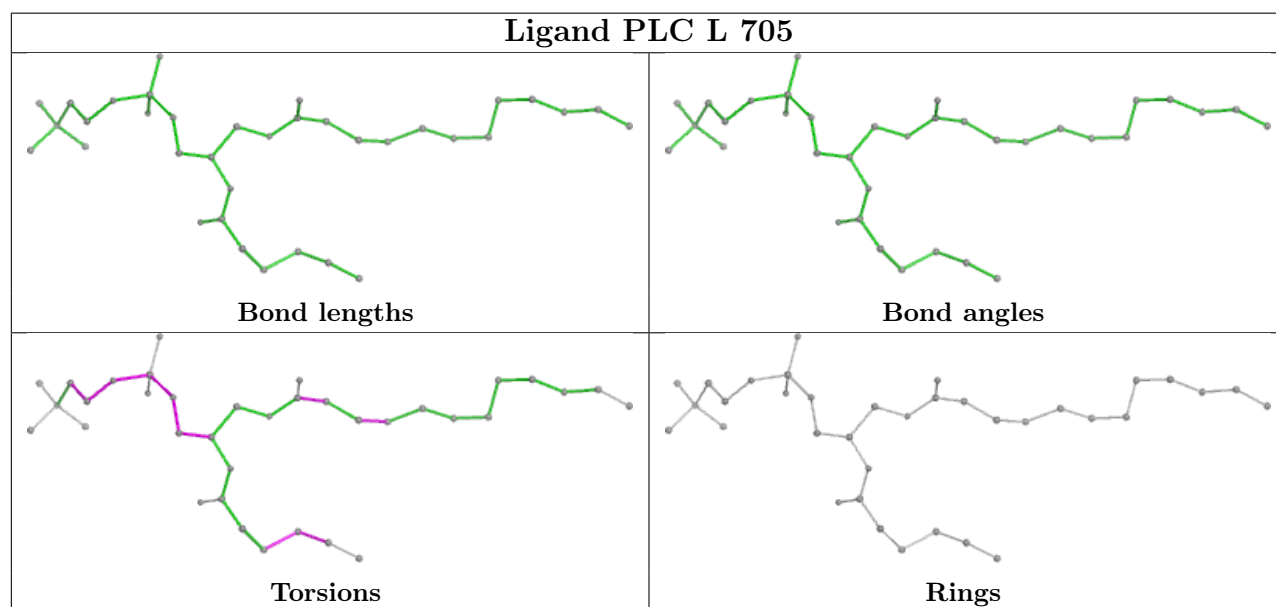
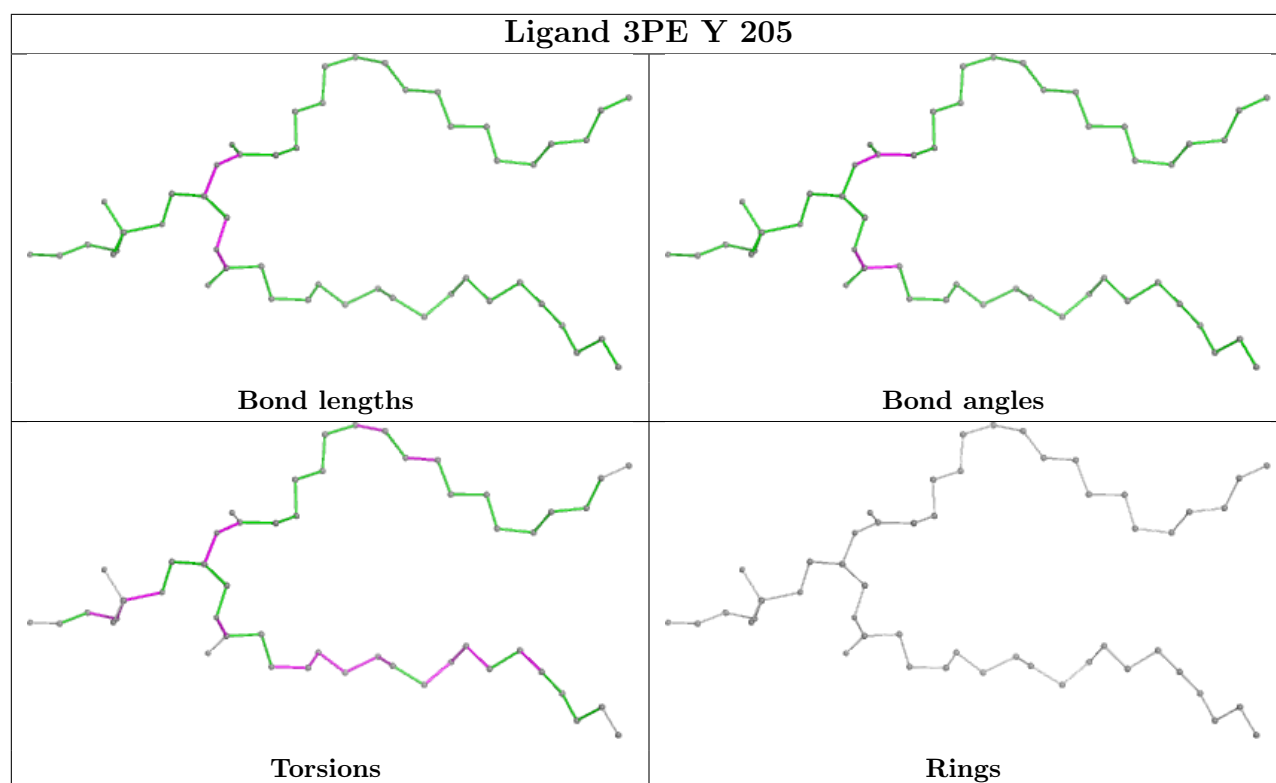


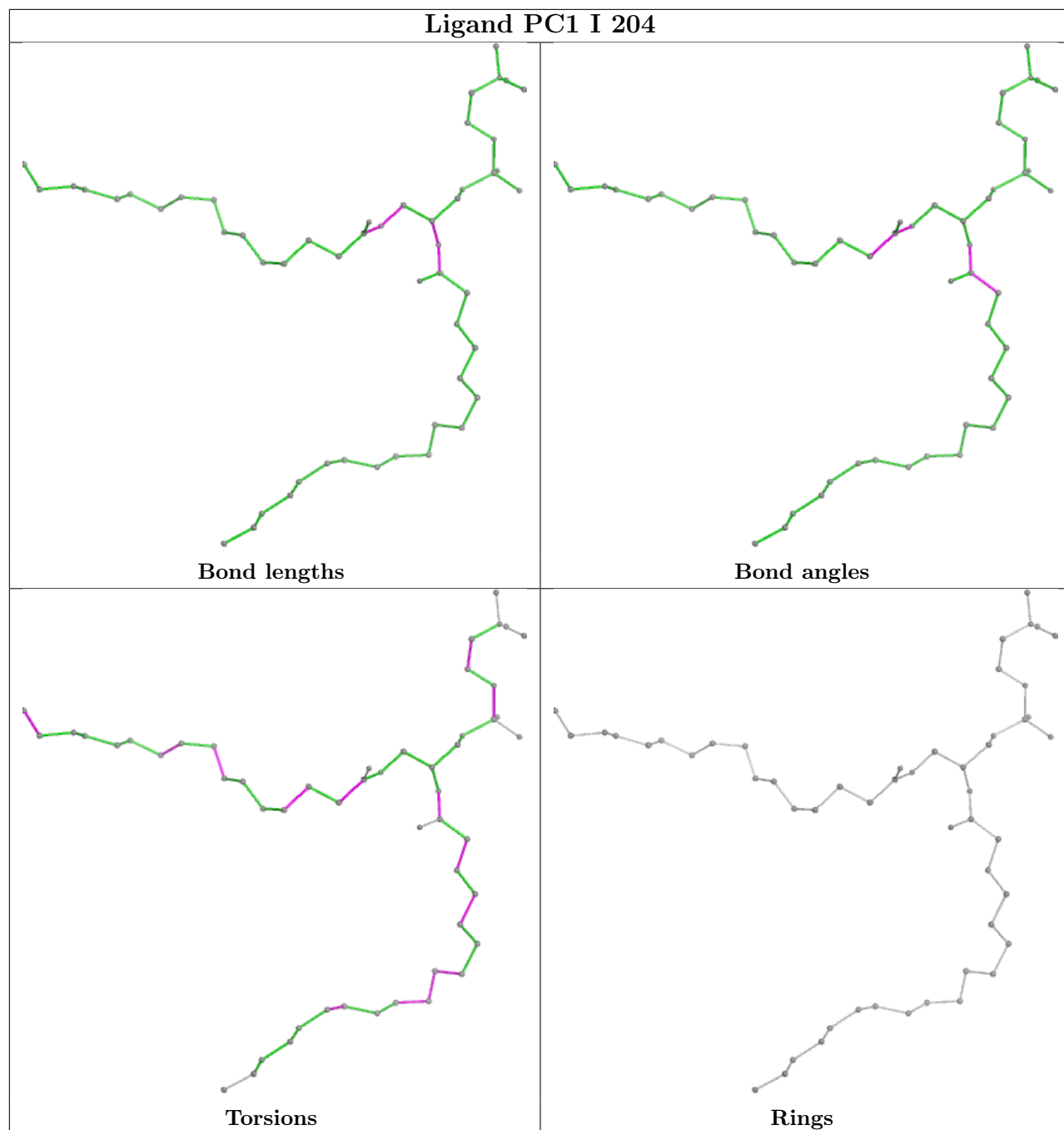


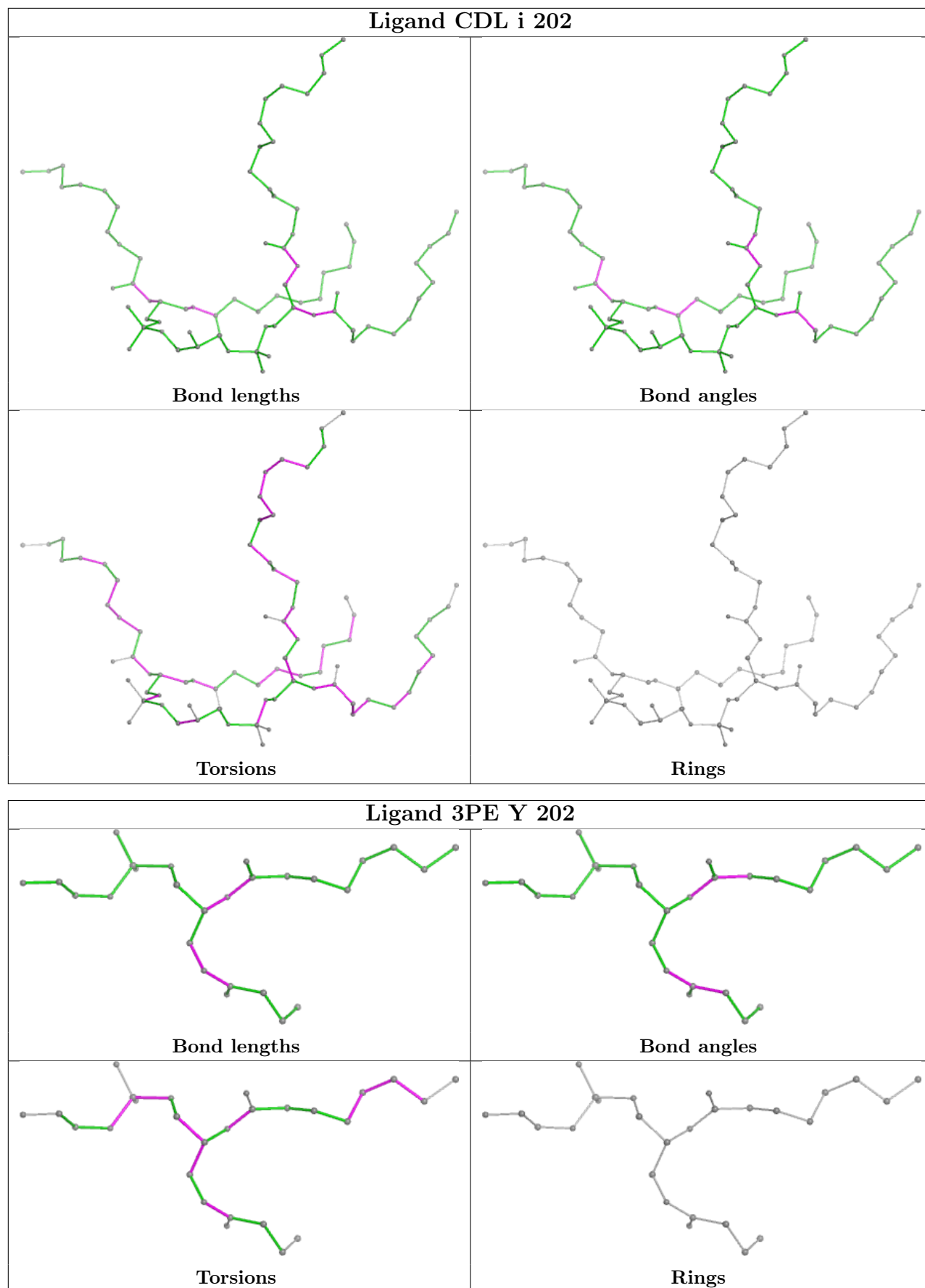


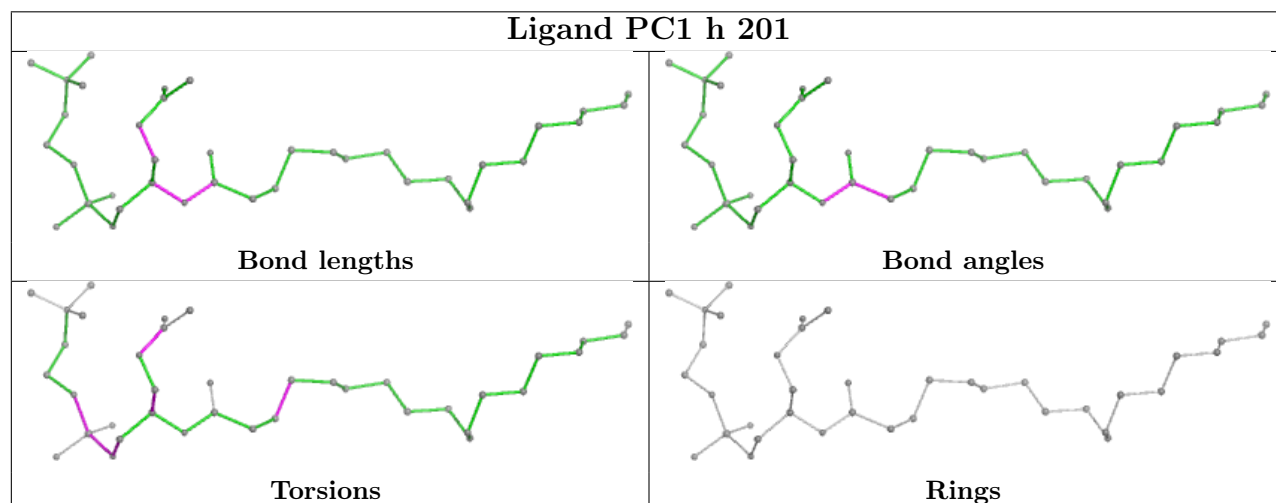
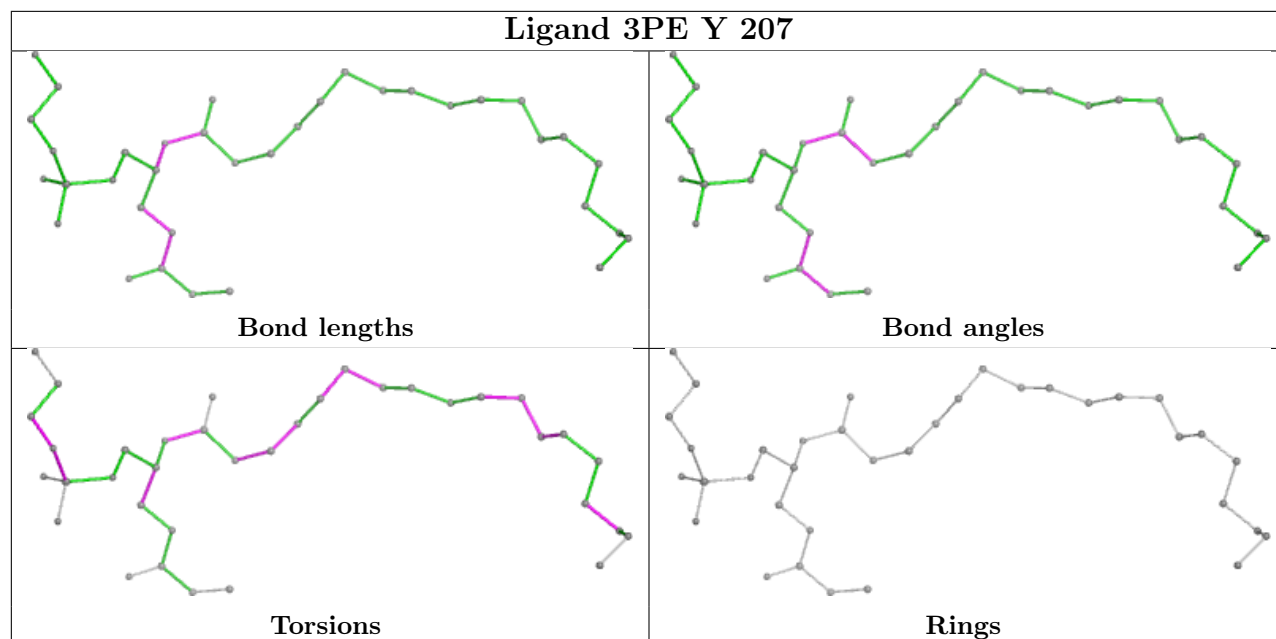


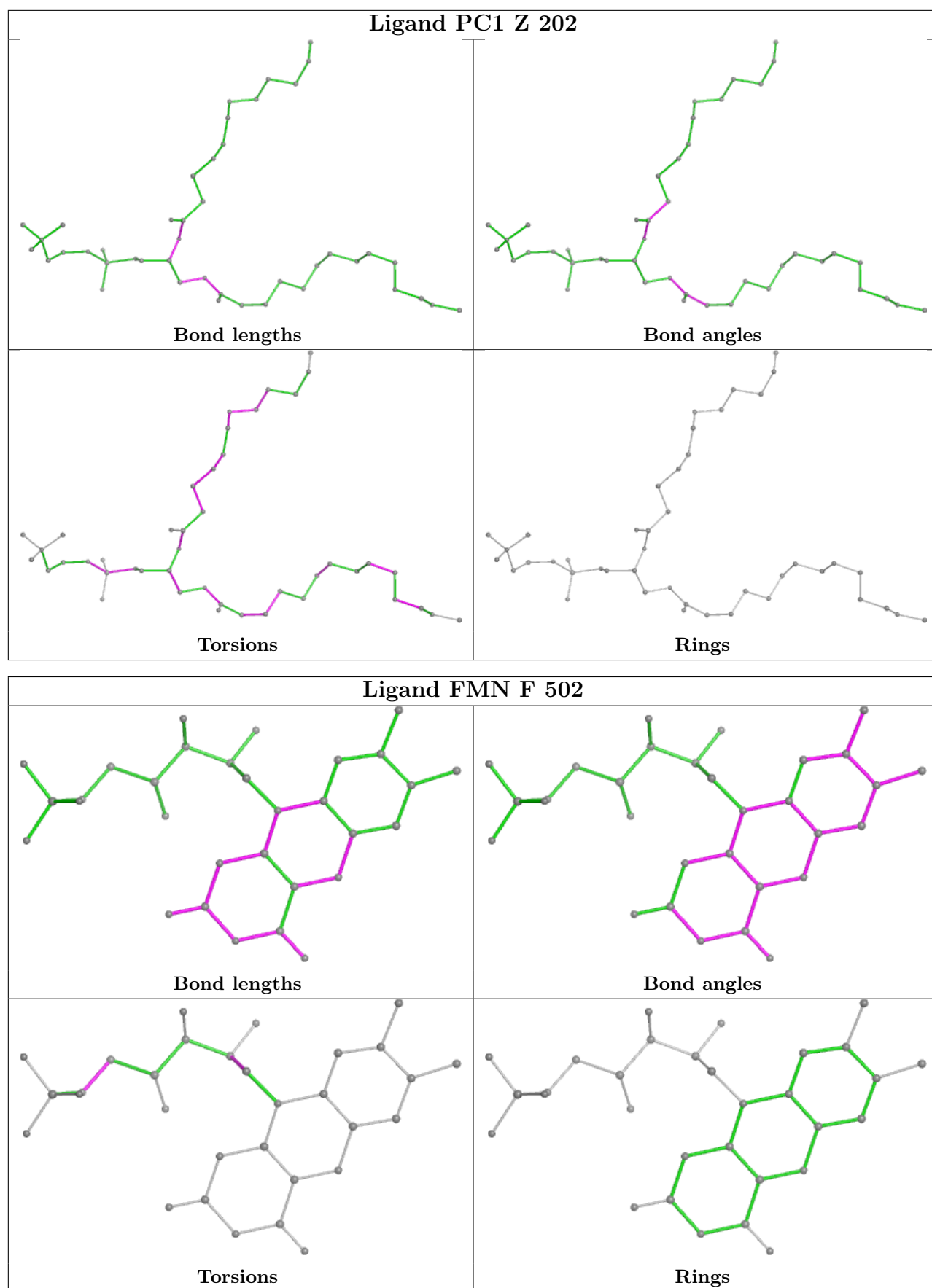


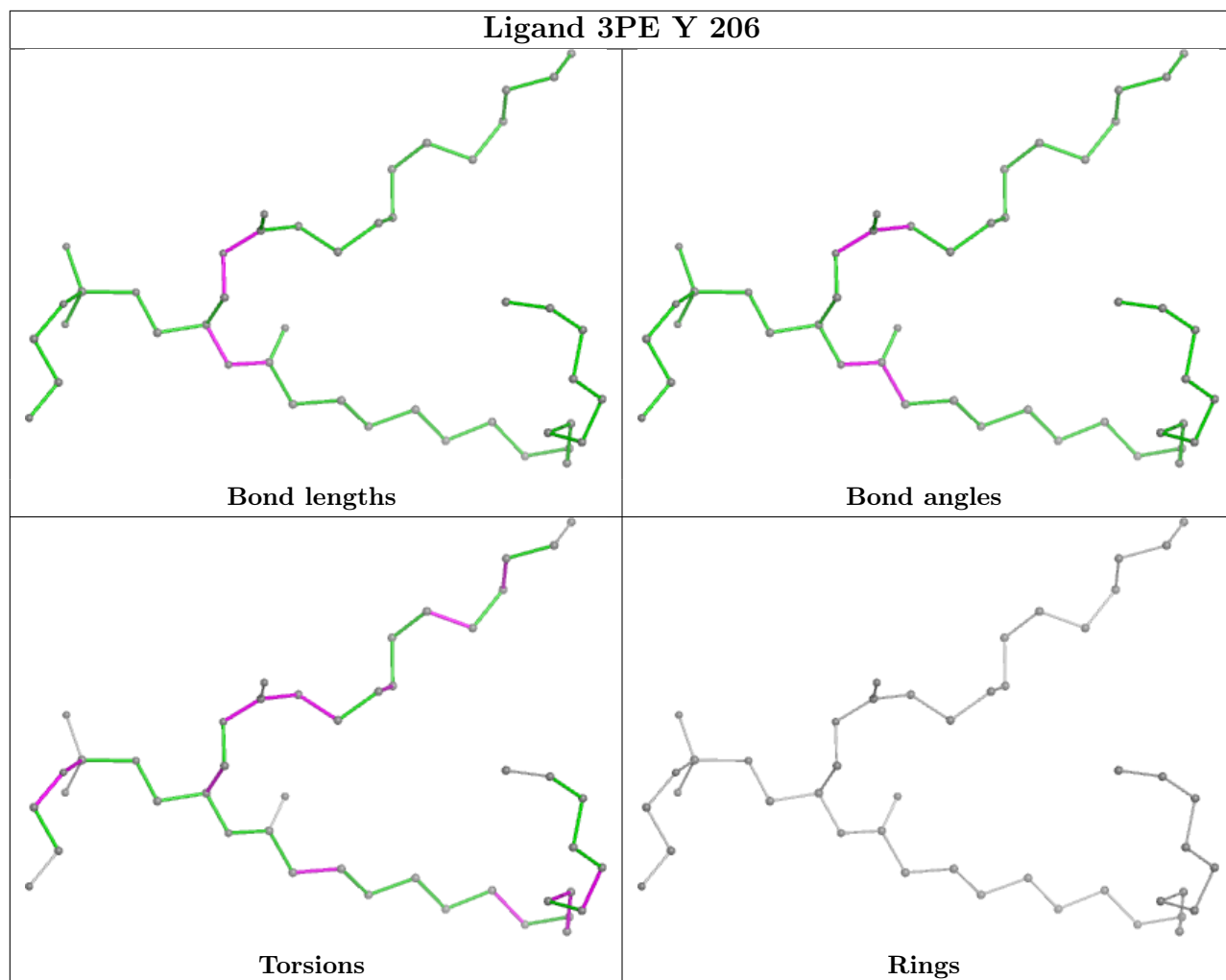


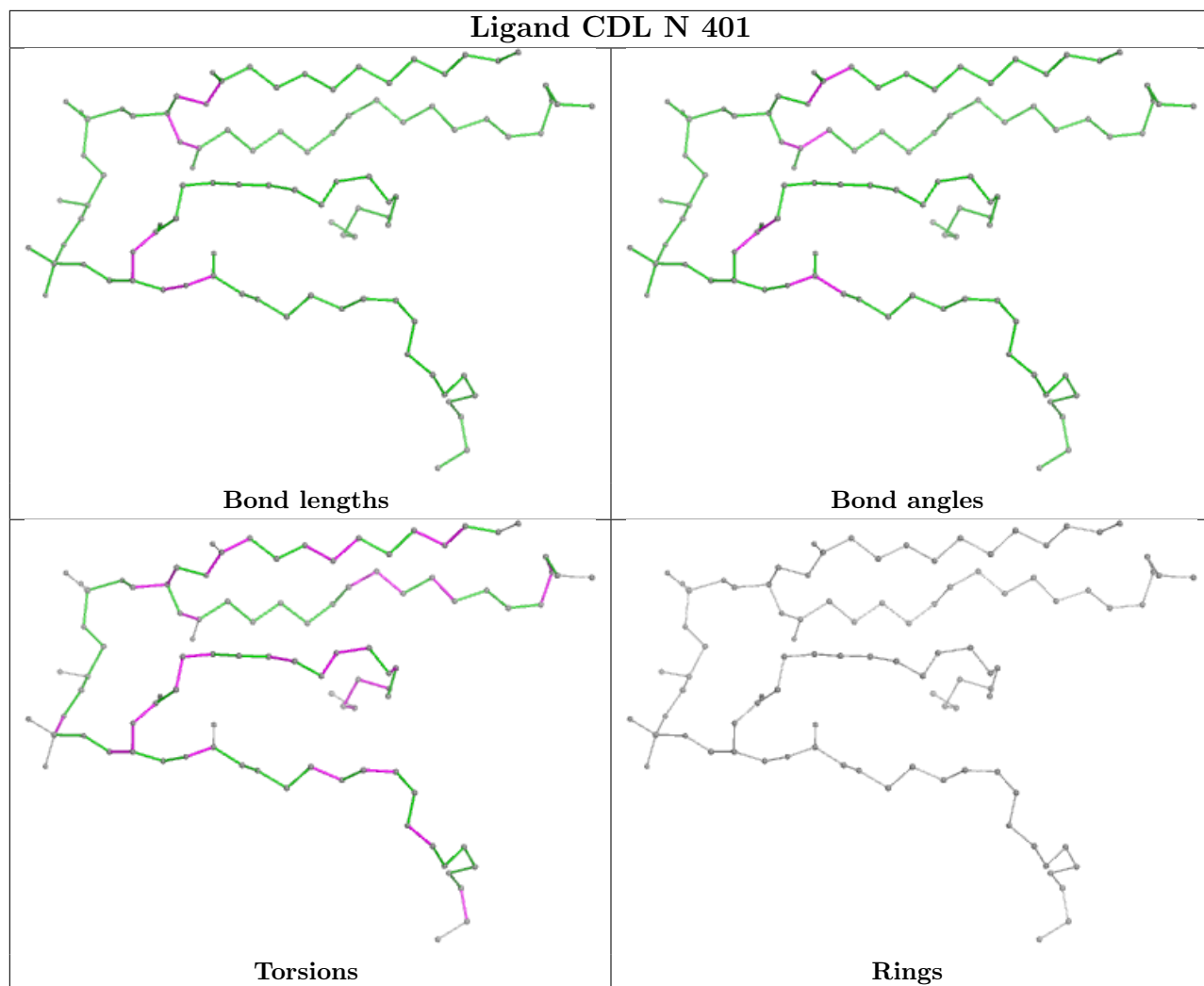


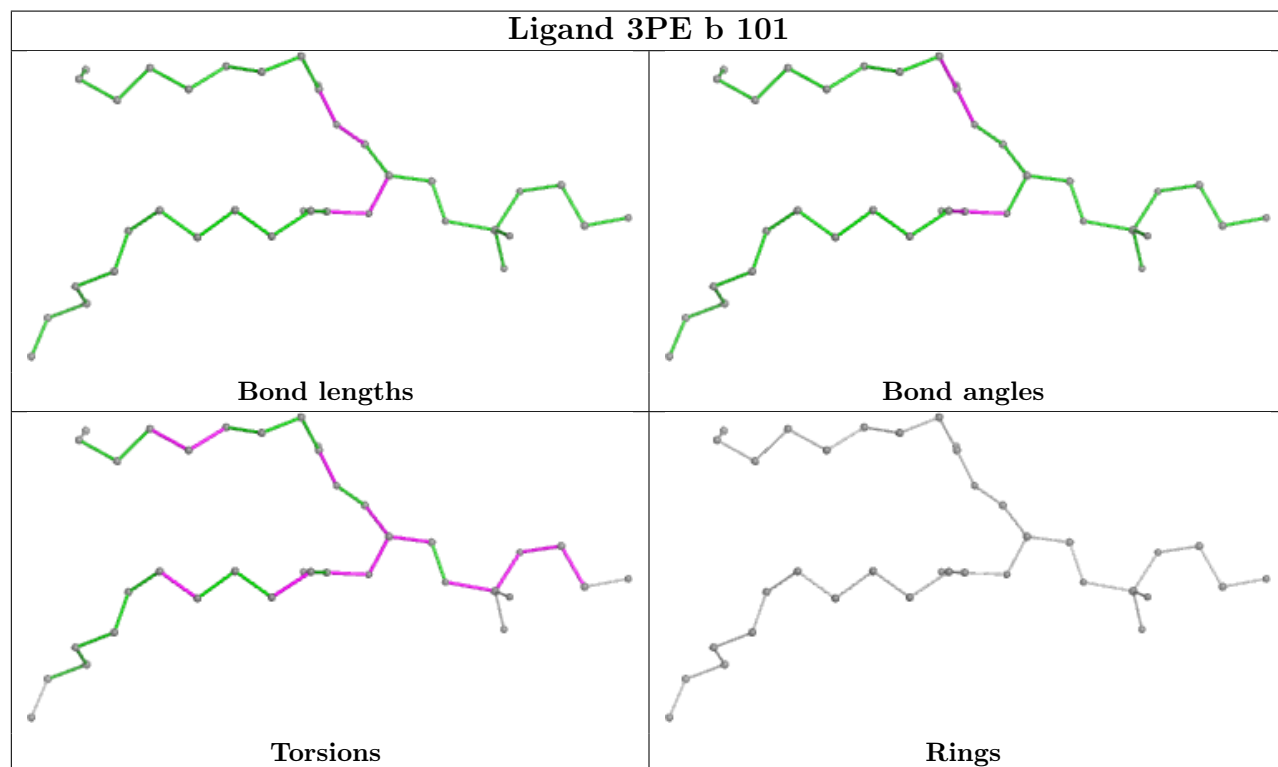
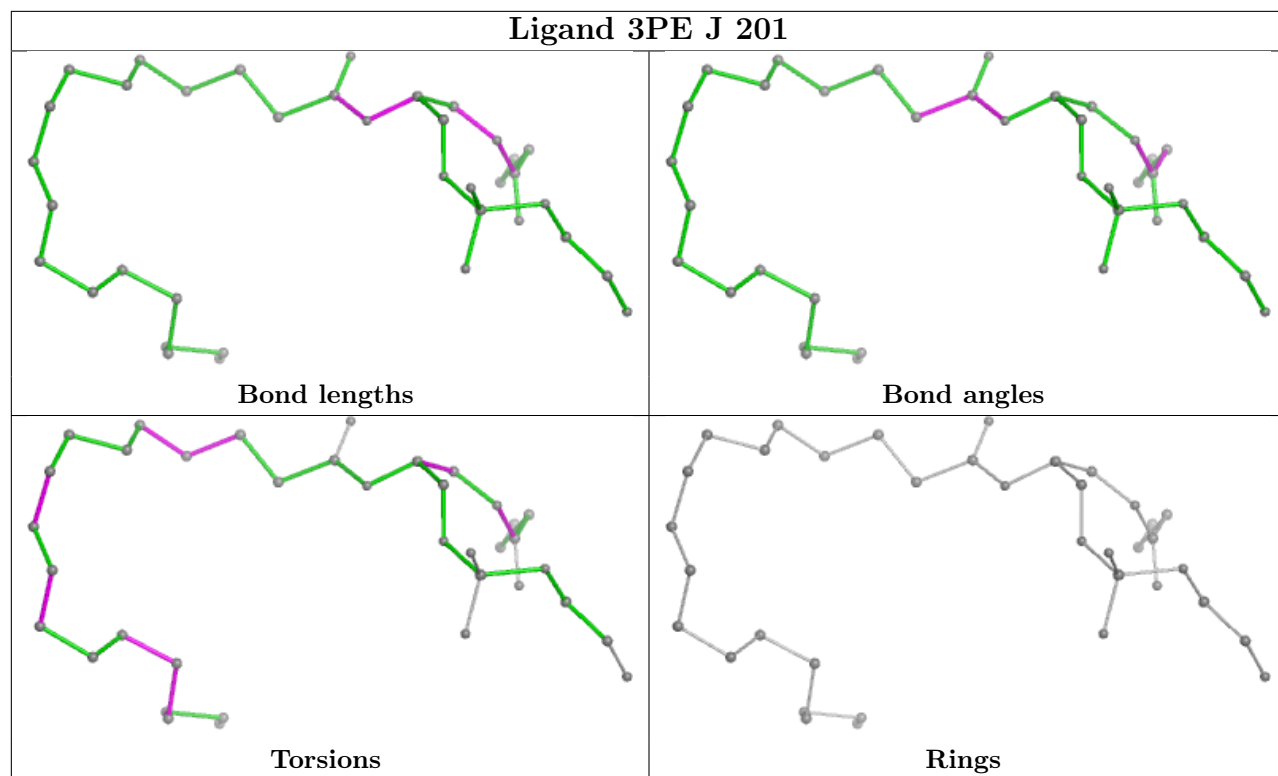


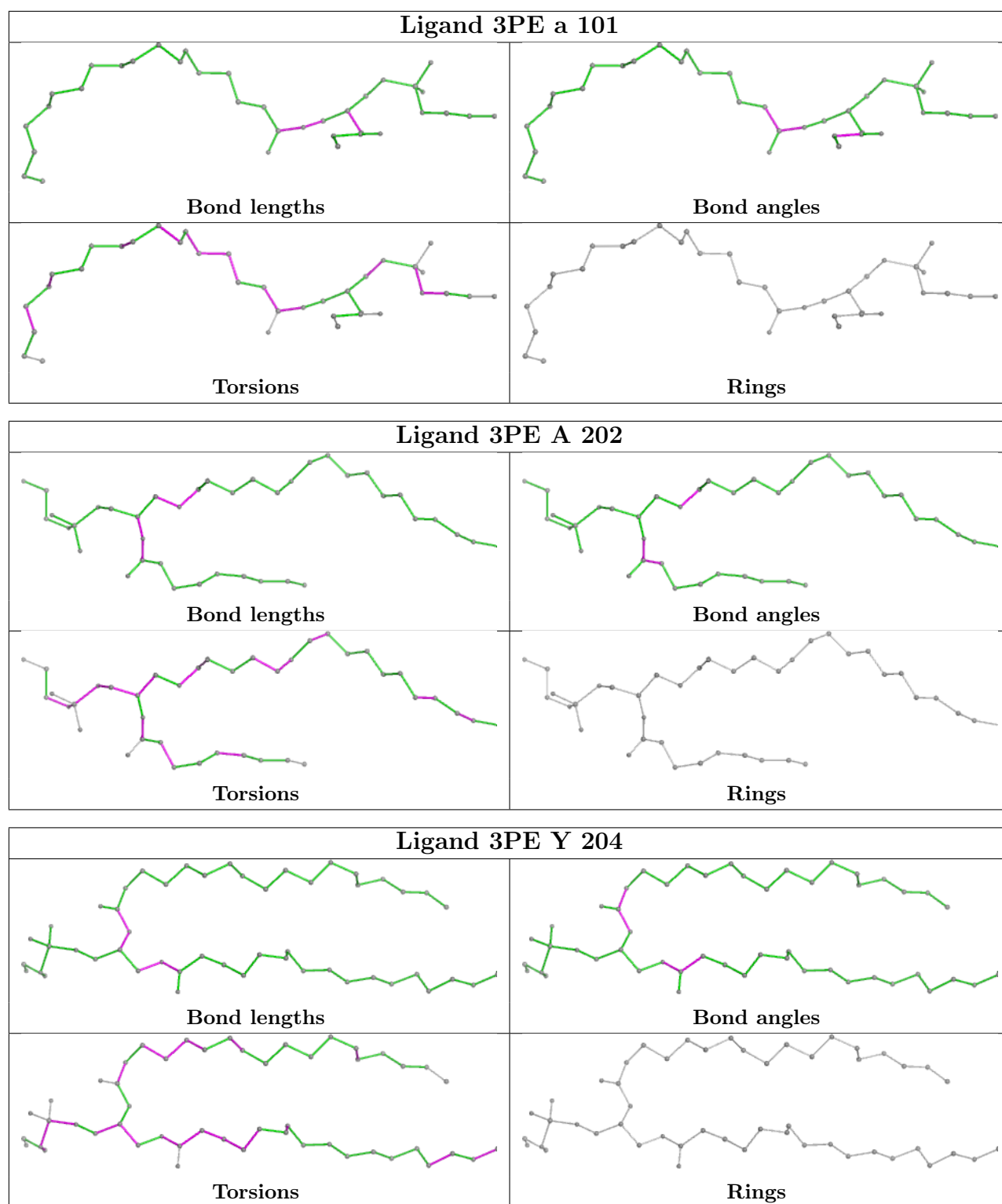












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

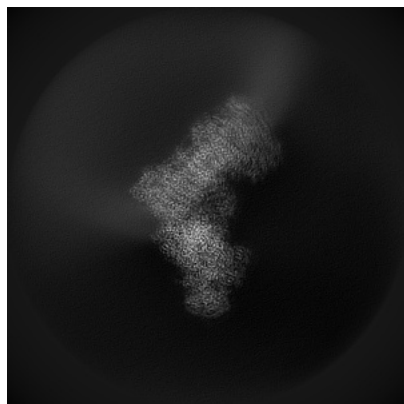
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18069. These allow visual inspection of the internal detail of the map and identification of artifacts.

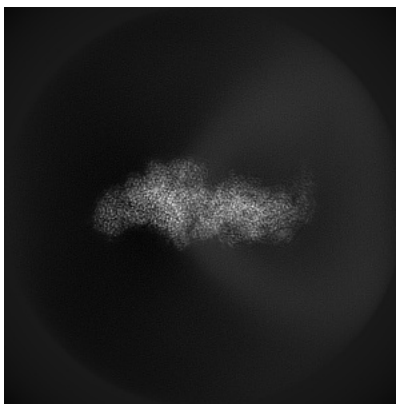
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

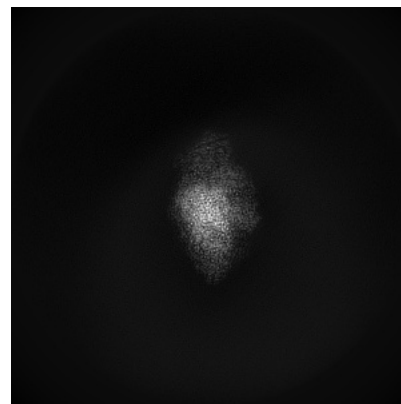
6.1.1 Primary map



X

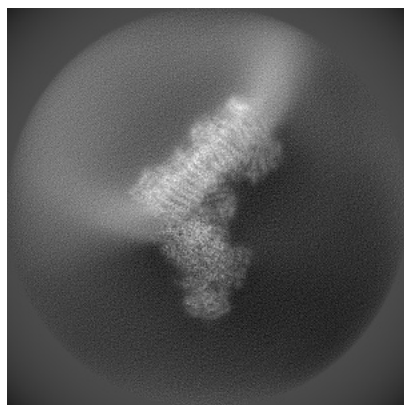


Y

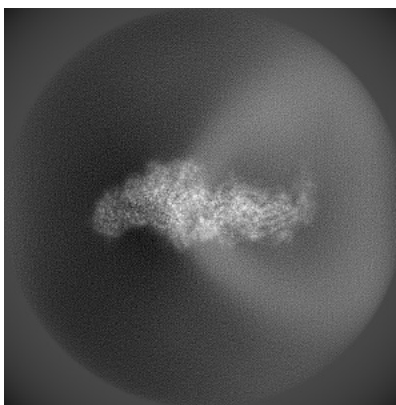


Z

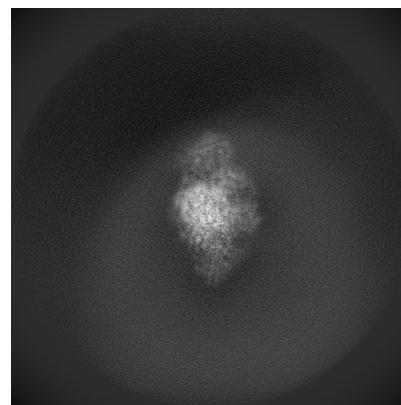
6.1.2 Raw map



X



Y



Z

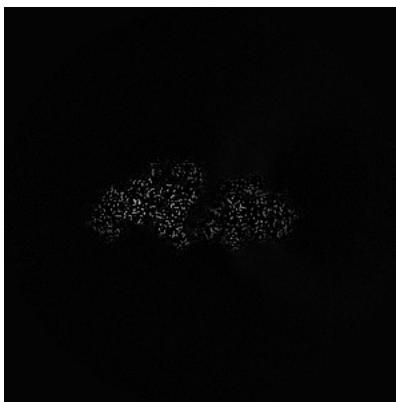
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

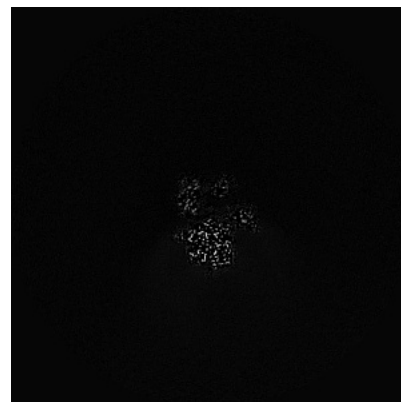
6.2.1 Primary map



X Index: 240

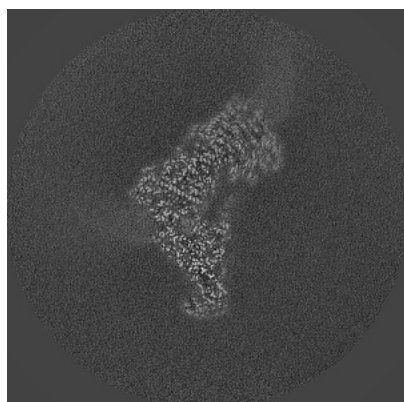


Y Index: 240

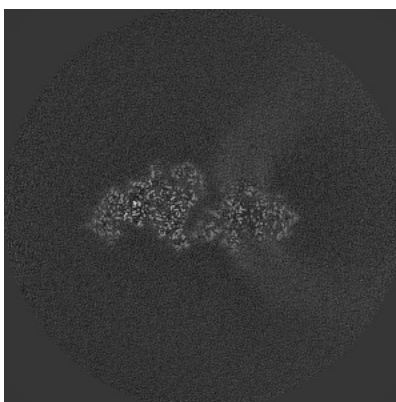


Z Index: 240

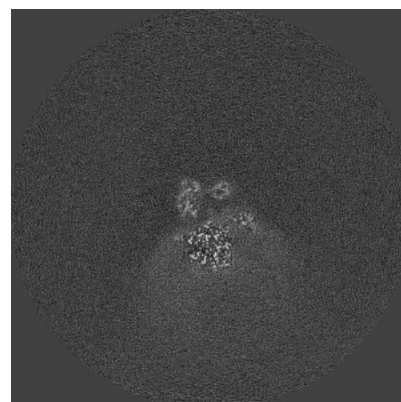
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

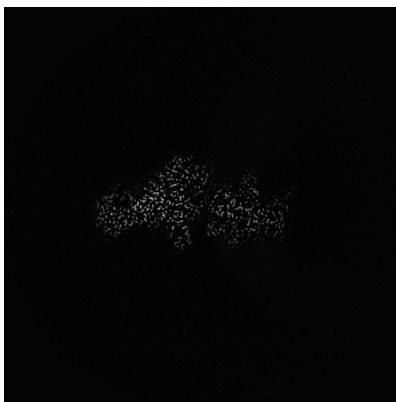
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 247

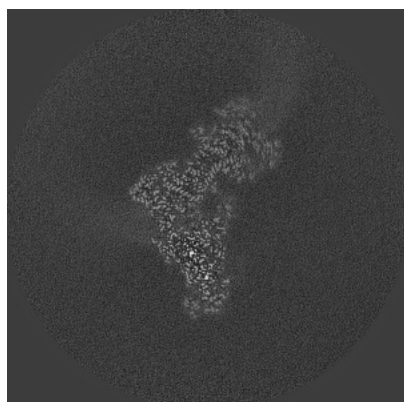


Y Index: 227

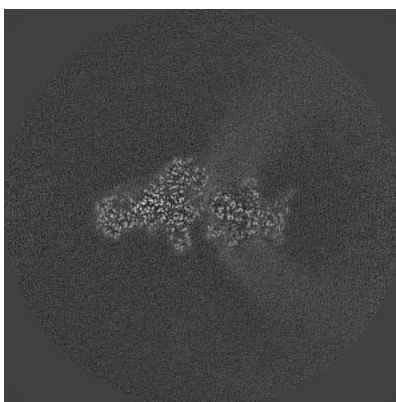


Z Index: 198

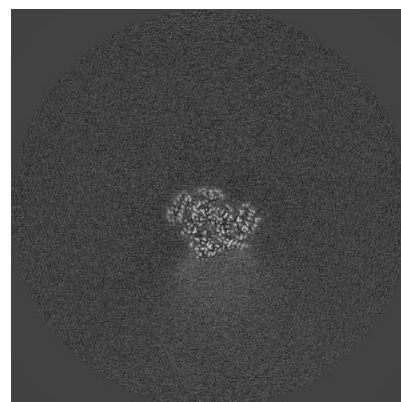
6.3.2 Raw map



X Index: 247



Y Index: 227

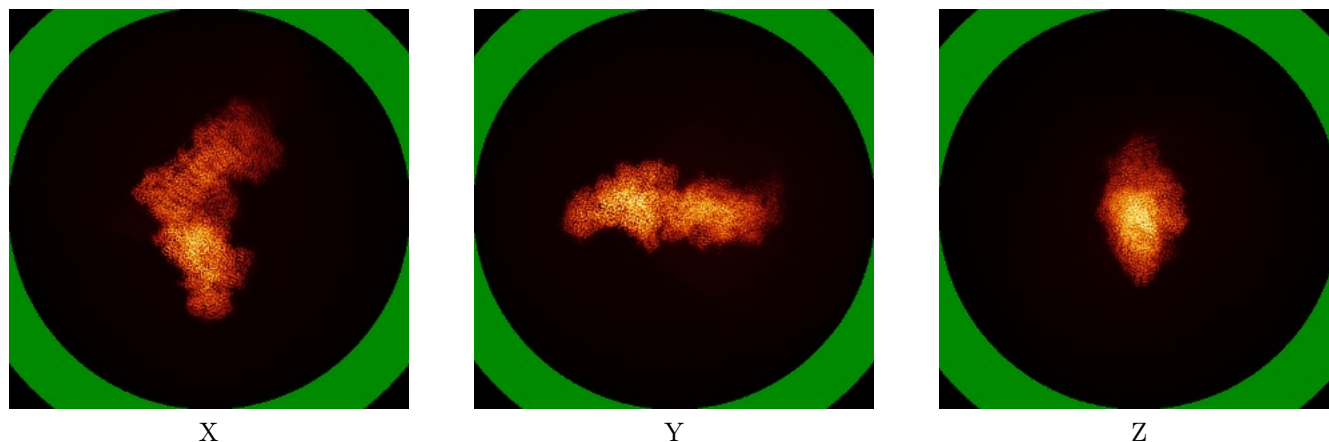


Z Index: 212

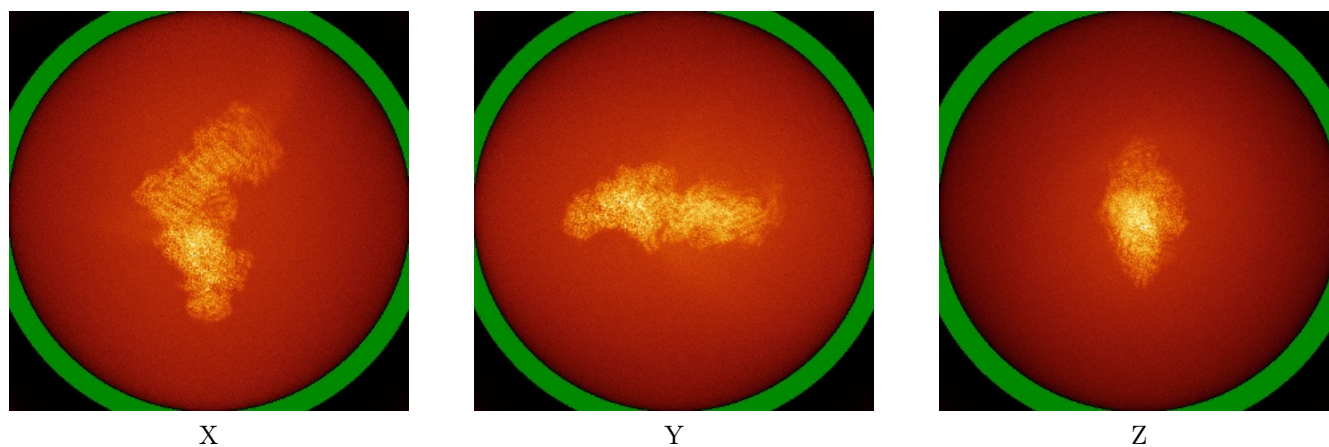
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



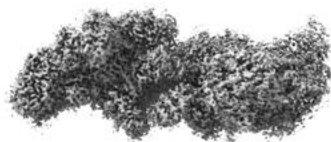
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



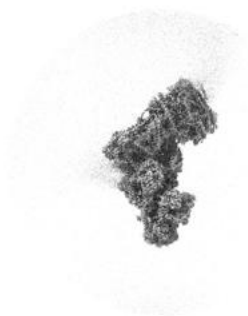
Y



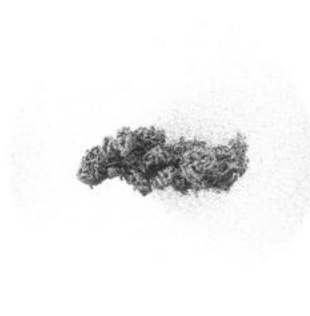
Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

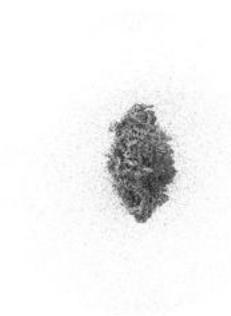
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

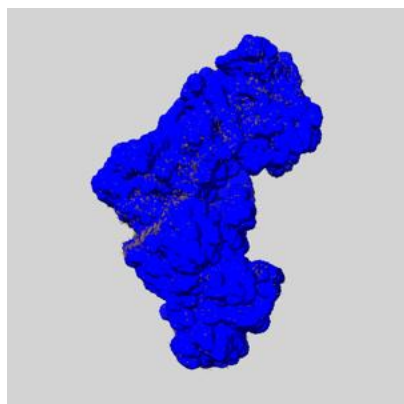
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

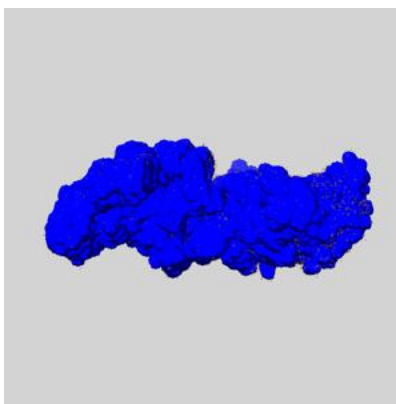
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

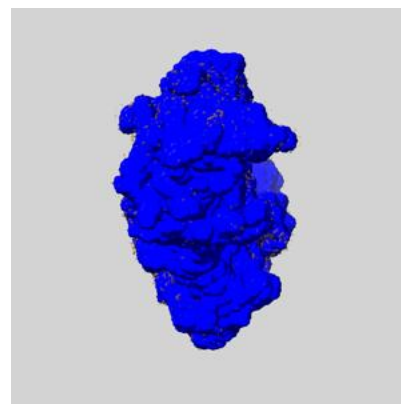
6.6.1 emd_18069_msk_1.map [i](#)



X



Y

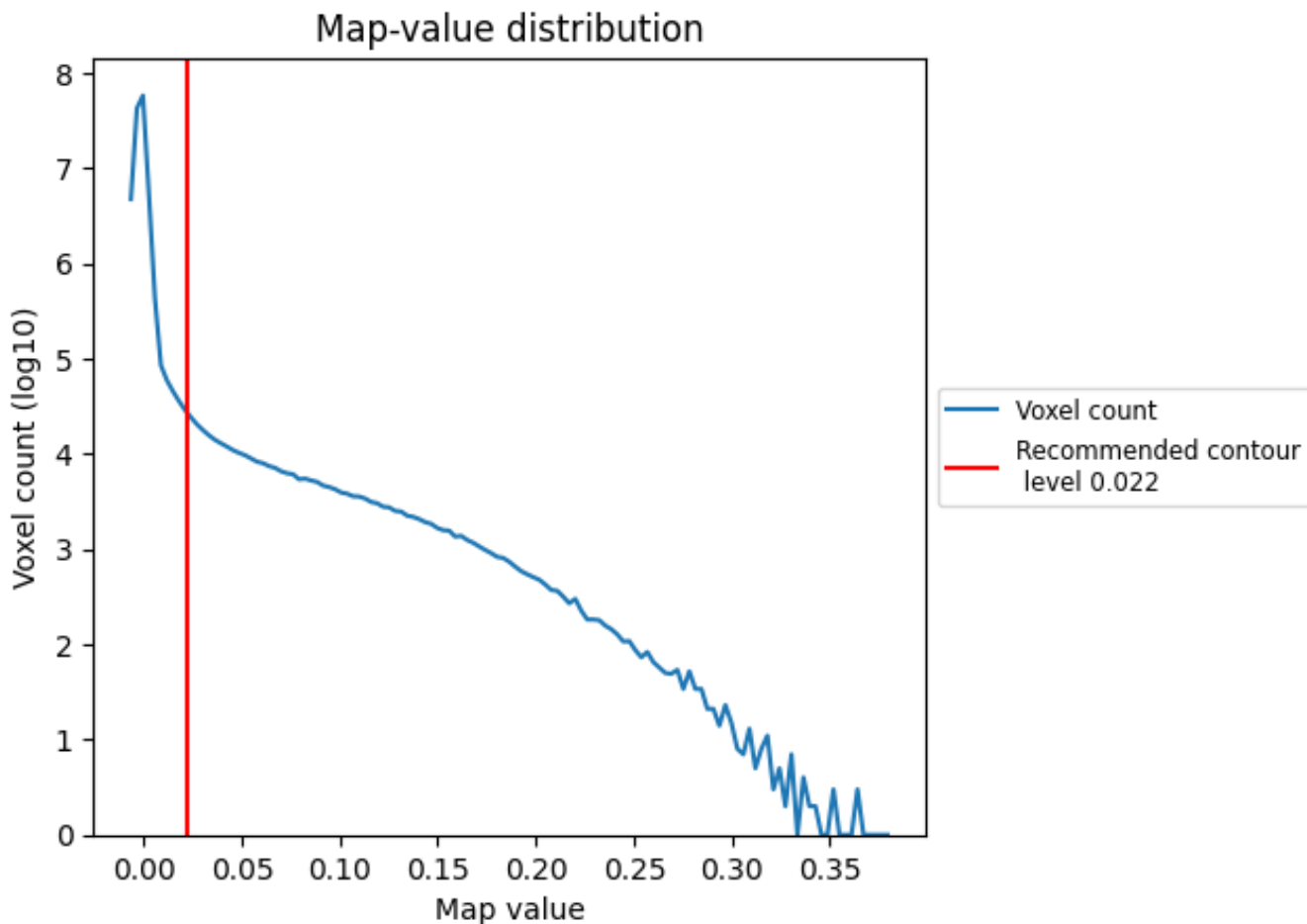


Z

7 Map analysis [i](#)

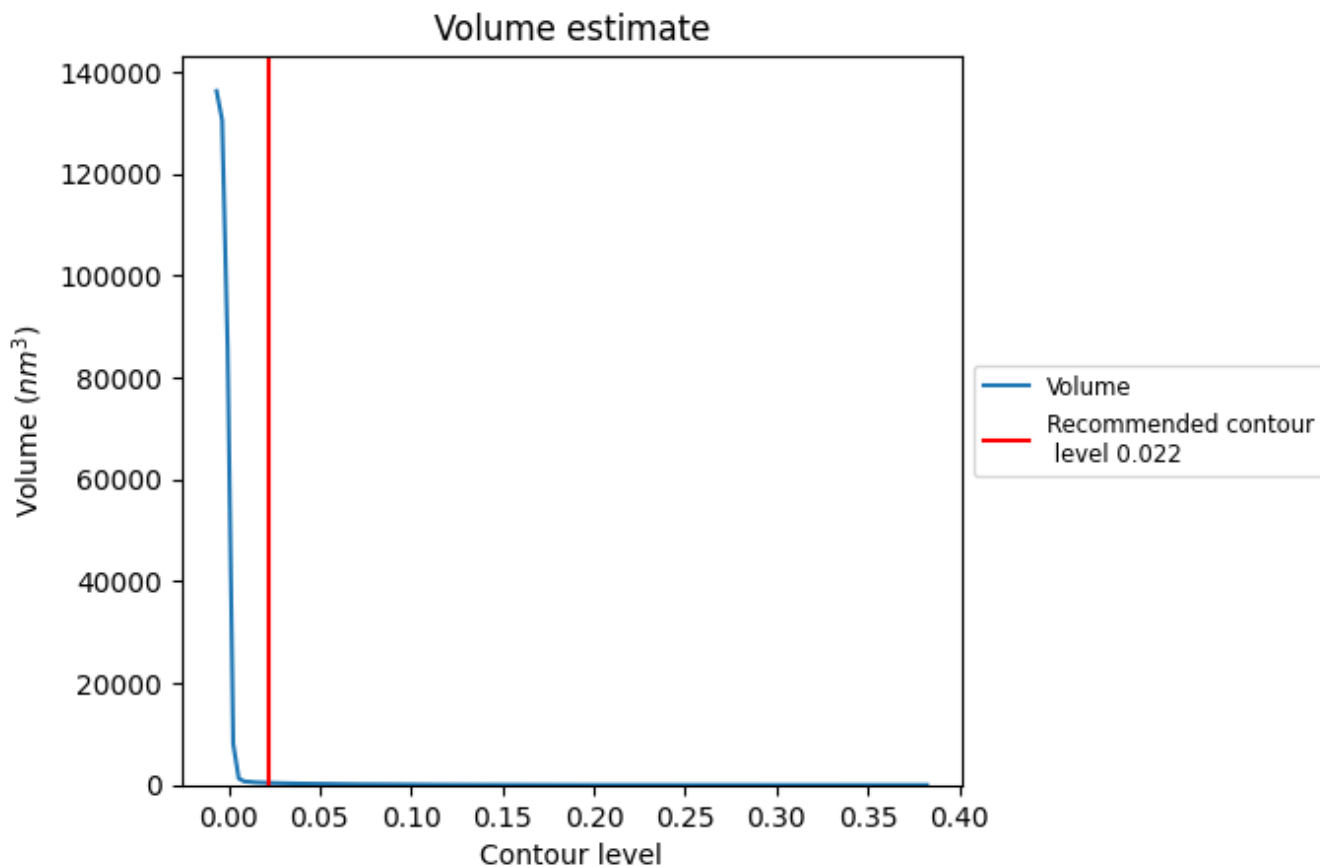
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

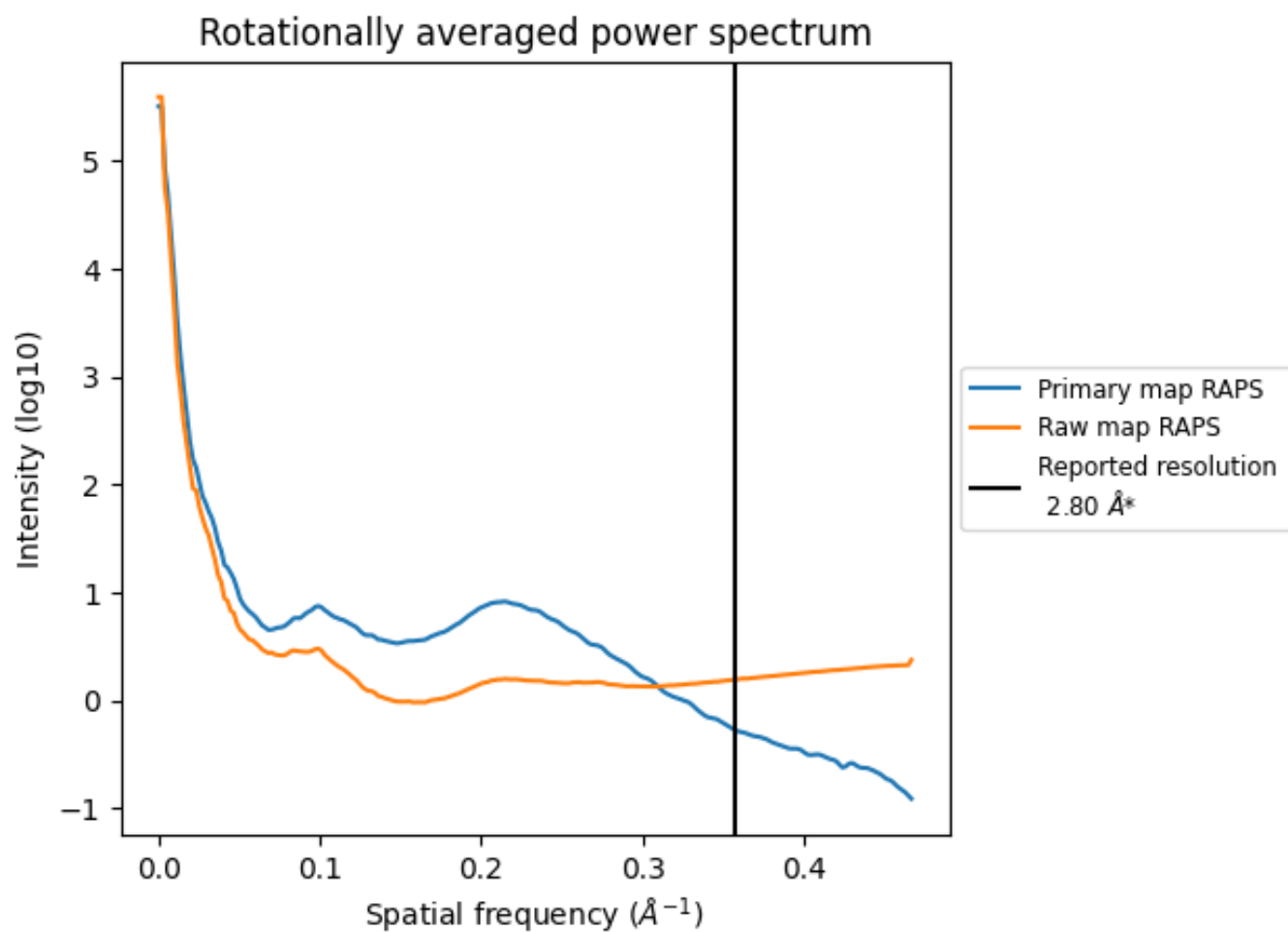
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm^3 ; this corresponds to an approximate mass of 365 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

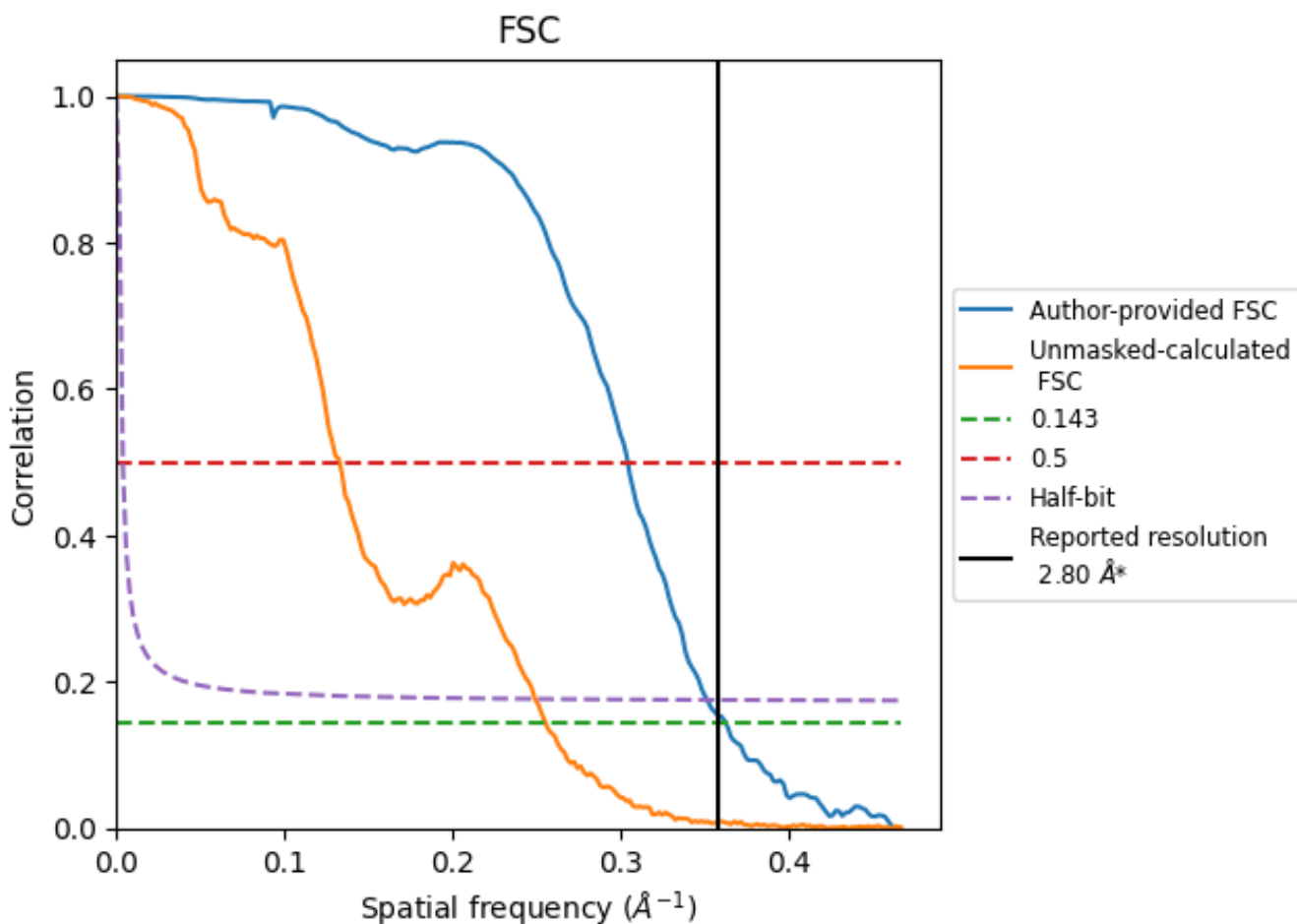


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

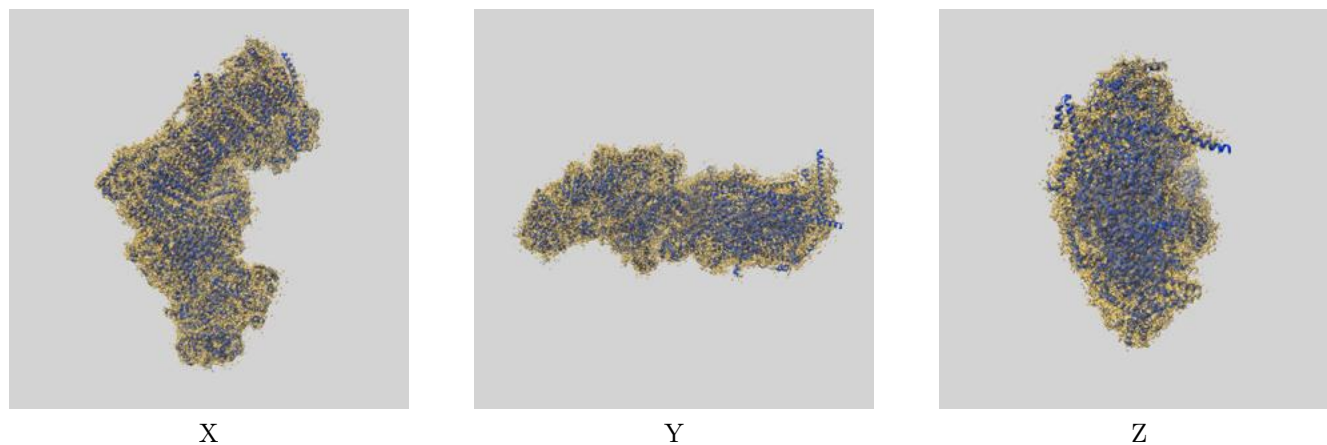
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.29	2.85
Unmasked-calculated*	3.92	7.55	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

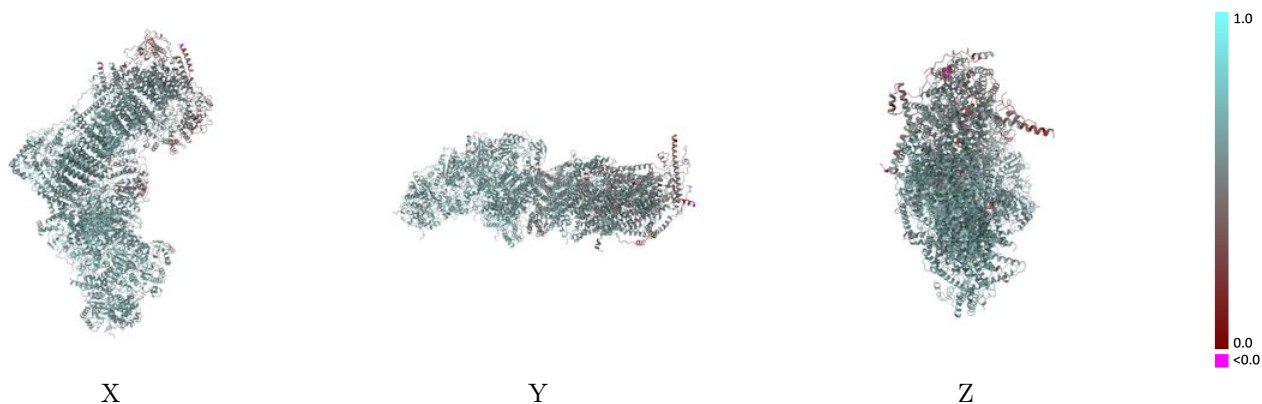
This section contains information regarding the fit between EMDB map EMD-18069 and PDB model 8Q25. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



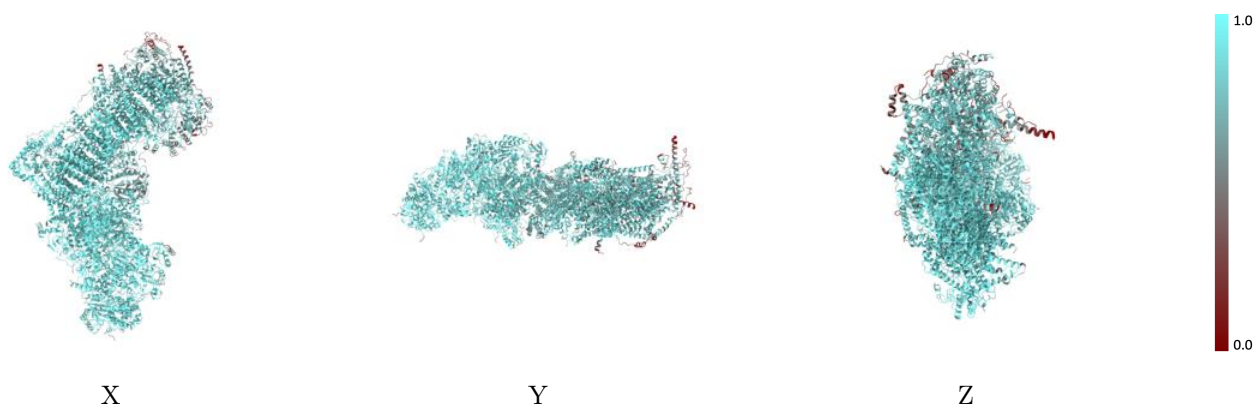
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



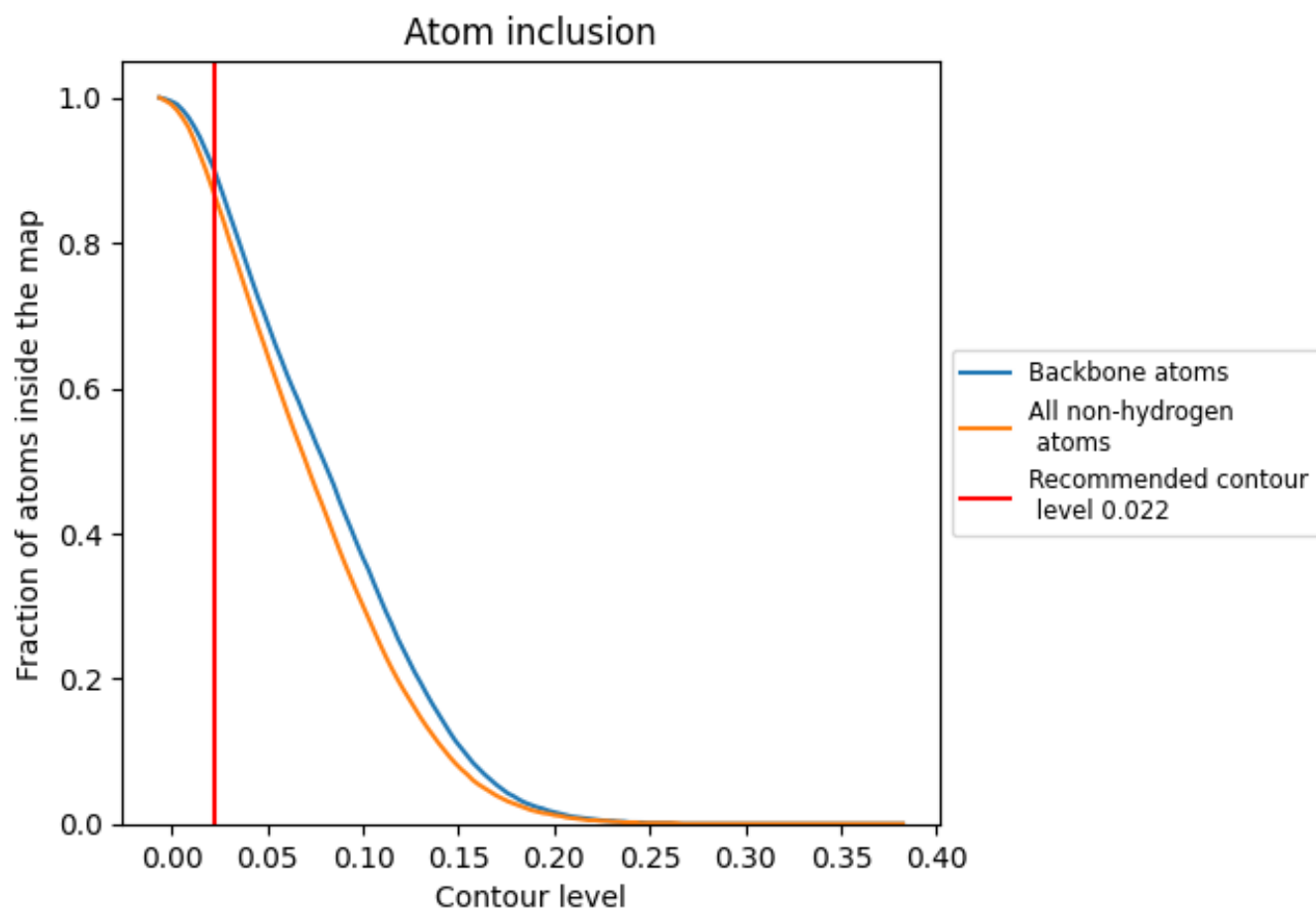
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.5970
A	 0.8980	 0.6190
B	 0.9580	 0.6580
C	 0.9680	 0.6650
D	 0.9580	 0.6630
E	 0.8860	 0.5980
F	 0.9120	 0.6170
G	 0.9280	 0.6370
H	 0.9400	 0.6390
I	 0.9590	 0.6690
J	 0.8900	 0.6010
K	 0.9590	 0.6480
L	 0.8370	 0.5630
M	 0.9350	 0.6330
N	 0.9570	 0.6540
O	 0.8160	 0.5560
P	 0.9020	 0.6180
Q	 0.9270	 0.6500
R	 0.9110	 0.6340
S	 0.7930	 0.5560
T	 0.6820	 0.4770
U	 0.6190	 0.4390
V	 0.8890	 0.6050
W	 0.9140	 0.6360
X	 0.9020	 0.6190
Y	 0.8460	 0.5860
Z	 0.8900	 0.6140
a	 0.9330	 0.6310
b	 0.8680	 0.5980
c	 0.8350	 0.5750
d	 0.9000	 0.6120
e	 0.8730	 0.6090
f	 0.7060	 0.5350
g	 0.8010	 0.5550
h	 0.8840	 0.6010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.5930	 0.4400
j	 0.5620	 0.4110
k	 0.4960	 0.3830
l	 0.7760	 0.5140
m	 0.7880	 0.5470
n	 0.7330	 0.4970
o	 0.5330	 0.3980
p	 0.7700	 0.5260
q	 0.8980	 0.6300
r	 0.9160	 0.6420
s	 0.8090	 0.5600