



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 09:11 am GMT

PDB ID : 6ZKF
EMDB ID : EMD-11247
Title : Complex I during turnover, open3
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.80 Å (reported)
Based on initial model : 5LNK

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

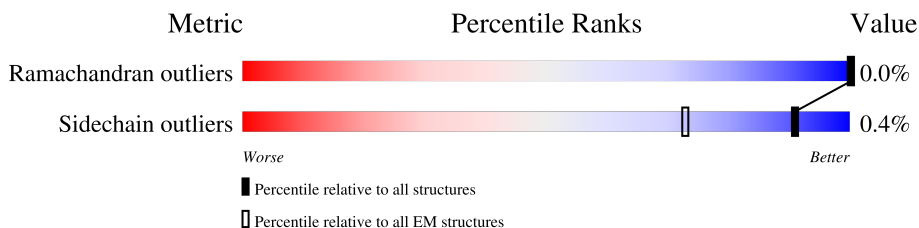
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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	1	464	
2	2	246	
3	3	727	
4	4	463	
5	5	266	
6	6	223	
7	9	217	
8	A	115	
9	H	318	

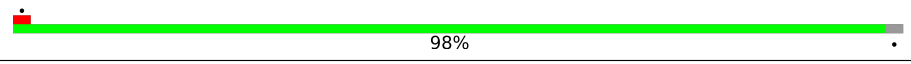
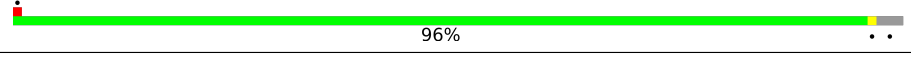
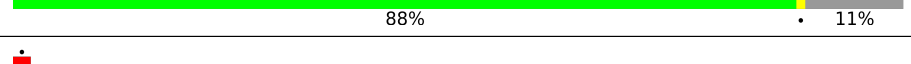
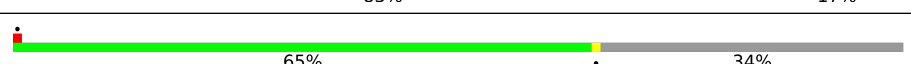
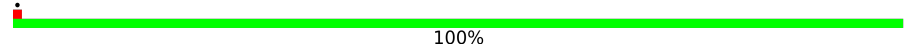

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Mol	Chain	Length	Quality of chain
10	J	175	97%
11	K	98	98%
12	L	606	99%
13	M	459	99%
14	N	347	100%
15	V	141	99%
16	W	189	74% 26%
17	X	157	55% 45%
17	j	157	52% 48%
18	Y	172	99%
19	Z	175	98%
20	a	109	40% 60%
21	b	124	77% 23%
22	c	170	74% 26%
23	d	380	78% 22%
24	e	99	87% 13%
25	f	116	97%
26	g	140	81% 19%
27	h	114	83% 16%
28	i	145	100%
29	k	355	90% 10%
30	l	106	99%
31	m	84	95% 5%
32	n	98	81% 19%
33	o	122	98%

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Mol	Chain	Length	Quality of chain
34	p	130	 98%
35	q	144	 96%
36	r	128	 77% 23%
37	s	137	 88% 11%
38	t	179	 98%
39	u	108	 60% 40%
40	v	186	 83% 17%
41	w	154	 65% 34%
42	x	76	 64% 36%
43	y	58	 86% 14%
44	z	70	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	CDL	L	1003	X	-	-	-
53	CDL	V	204	X	-	-	-
53	CDL	Y	201	X	-	-	-
53	CDL	o	201	X	-	-	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 67440 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	213	1655	1058	278	309	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	421	3390	2165	581	619	25	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	208	1726	1112	296	315	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	156	1247	795	225	213	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	312	Total	C	N	O	S	0	0
			2488	1680	378	411	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	169	Total	C	N	O	S	0	0
			1294	870	185	226	13		

- 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	Total	C	N	O	S	0	0
			749	490	112	132	15		

- 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	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- 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	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- 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	2723	1808	416	459	40	0	0

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

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

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	87	701	451	103	142	5	0	0
17	j	82	660	425	98	132	5	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

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

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

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

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

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	b	95	737	451	139	144	3	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	c	126	1024	646	182	193	3	0	0

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	d	297	2372	1516	432	419	5	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	f	113	917	595	153	167	2	0	0

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	g	114	969	619	180	166	4	0	0

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	h	96	769	480	146	140	3	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	i	145	1209	778	216	210	5	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

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

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

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

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

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

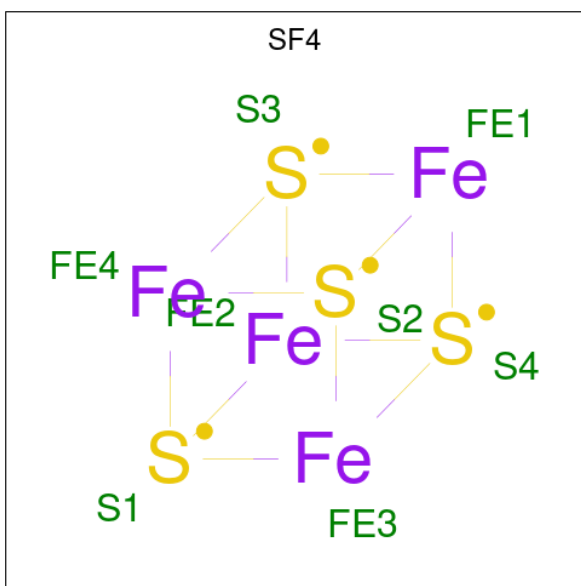
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

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

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



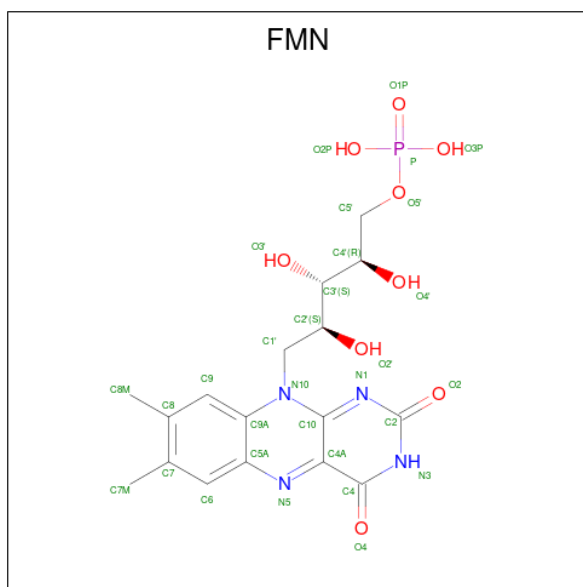
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	1	1	8	4	4	0
45	3	1	16	8	8	0
45	3	1	16	8	8	0
45	6	1	8	4	4	0

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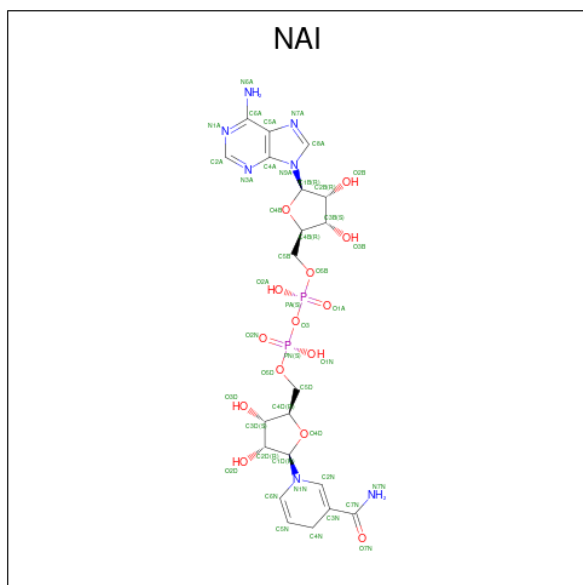
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			16	8	8	
45	9	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



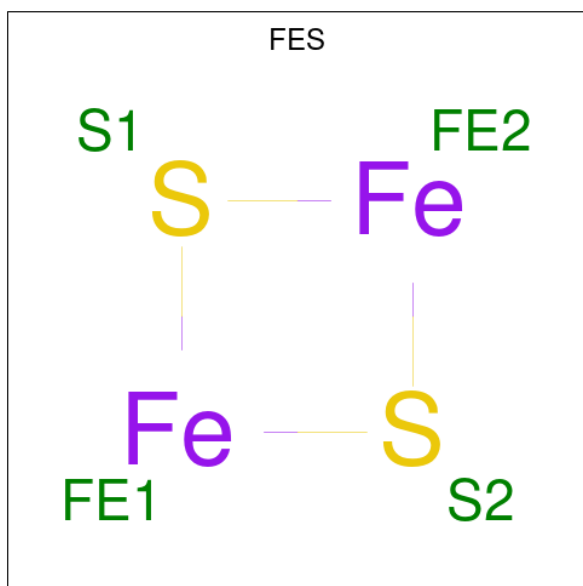
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
47	1	1	44	21	7	14	2	0

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

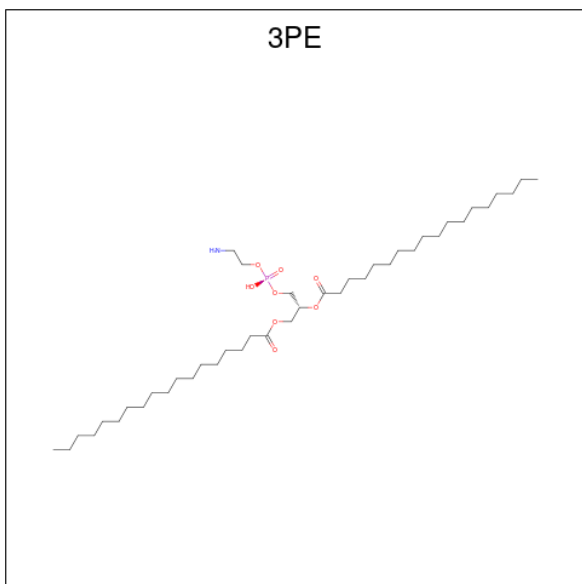


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	2	1	4	2	2	0
48	3	1	4	2	2	0

- Molecule 49 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
49	3	1	Total K 1 1	0

- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



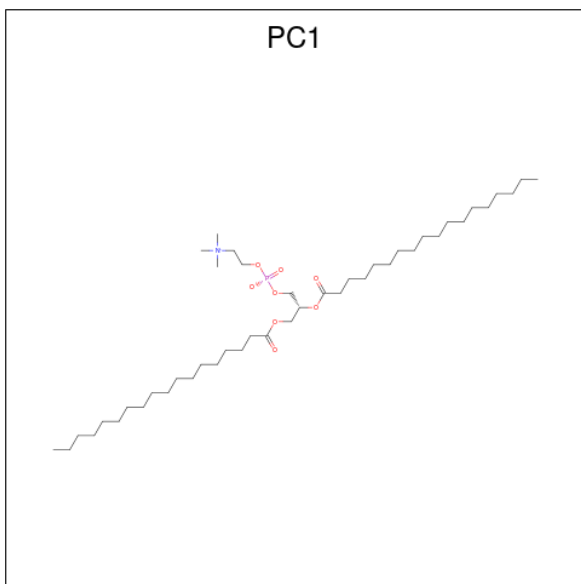
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	4	1	Total 40	C 30	N 1	O 8	P 1	0
50	A	1	Total 51	C 41	N 1	O 8	P 1	0
50	H	1	Total 51	C 41	N 1	O 8	P 1	0
50	K	1	Total 40	C 30	N 1	O 8	P 1	0
50	L	1	Total 82	C 62	N 2	O 16	P 2	0
50	L	1	Total 82	C 62	N 2	O 16	P 2	0
50	M	1	Total 44	C 34	N 1	O 8	P 1	0
50	N	1	Total 82	C 62	N 2	O 16	P 2	0
50	N	1	Total 82	C 62	N 2	O 16	P 2	0
50	V	1	Total 99	C 70	N 2	O 24	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	V	1	Total	C	N	O	P	0
			99	70	2	24	3	
50	V	1	Total	C	N	O	P	0
			99	70	2	24	3	
50	i	1	Total	C	N	O	P	0
			102	82	2	16	2	
50	i	1	Total	C	N	O	P	0
			102	82	2	16	2	

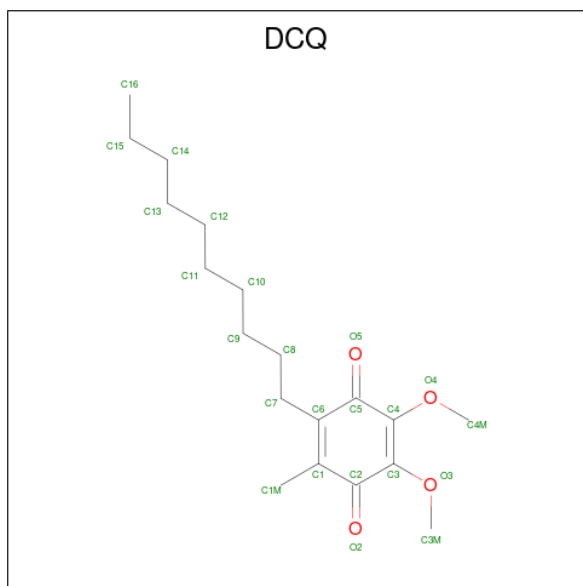
- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
51	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	M	1	Total	C	N	O	P	0
			108	88	2	16	2	
51	M	1	Total	C	N	O	P	0
			108	88	2	16	2	

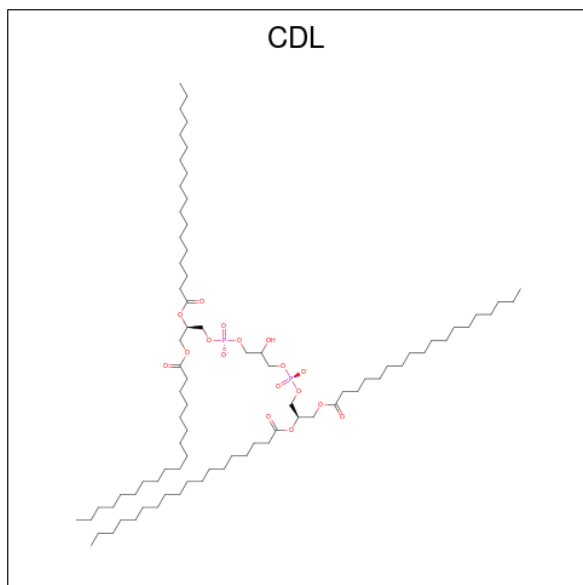
- Molecule 52 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter

code: DCQ) (formula: C₁₉H₃₀O₄).



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

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



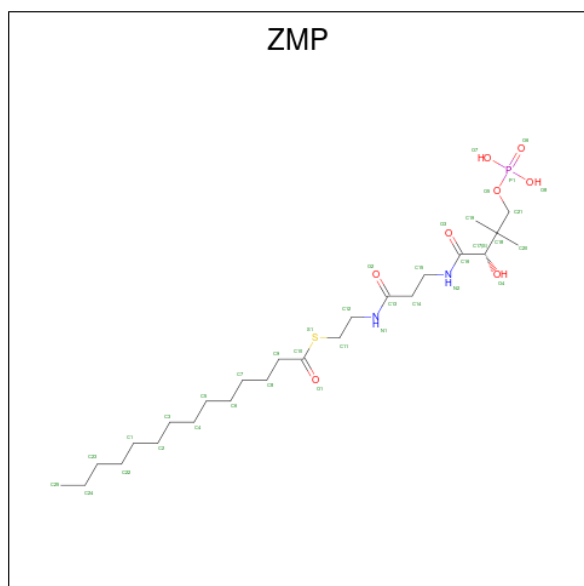
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	L	1	100	81	17	2	0
53	M	1	90	71	17	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	V	1	Total 179	C 141	O 34	P 4	0
53	V	1	Total 179	C 141	O 34	P 4	0
53	W	1	Total 100	C 81	O 17	P 2	0
53	Y	1	Total 100	C 81	O 17	P 2	0
53	o	1	Total 75	C 56	O 17	P 2	0
53	z	1	Total 58	C 39	O 17	P 2	0

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

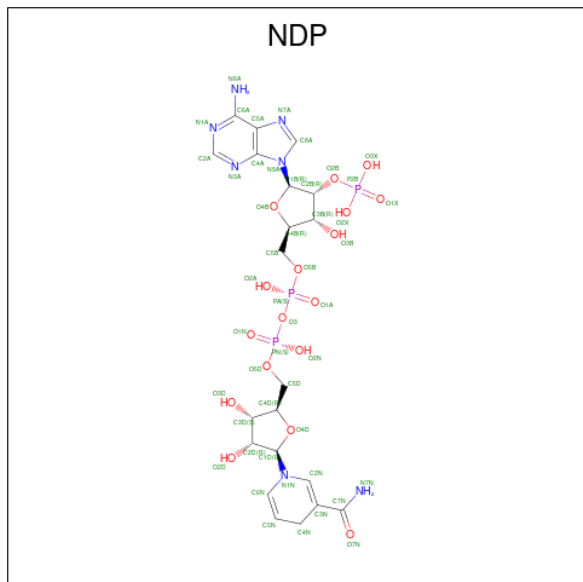


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
54	X	1	Total 31	C 20	N 2	O 7	P 1	S 1	0
54	g	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

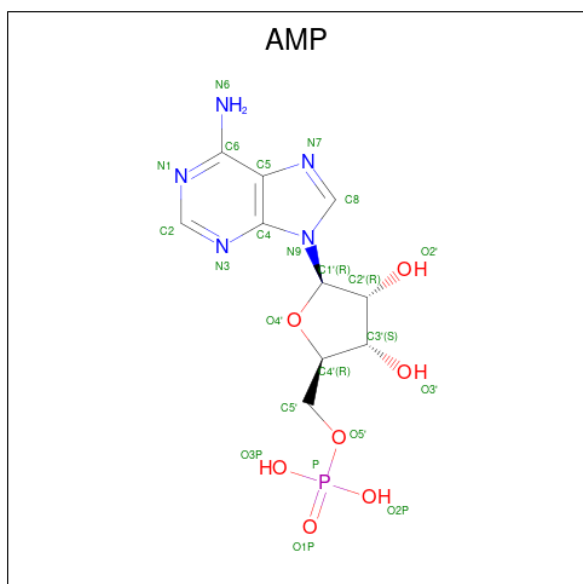
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	b	1	Total 1	Zn 1	0

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



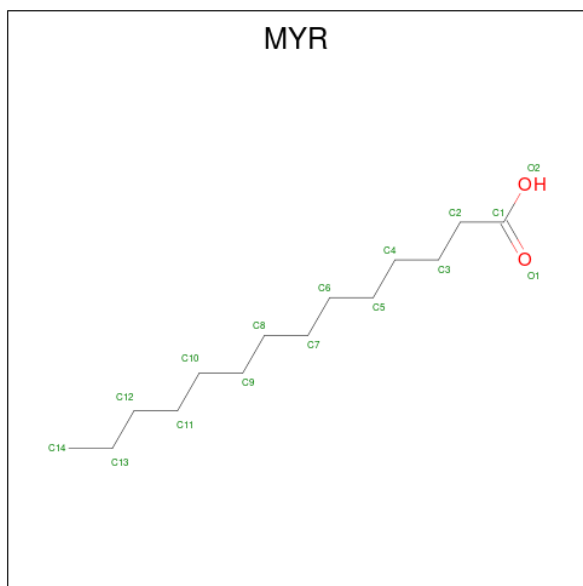
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	d	1	48	21	7	17	3	0

- Molecule 57 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 58 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



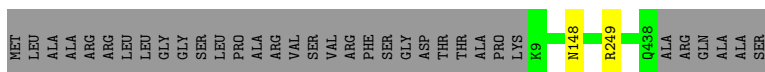
Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

3 Residue-property plots


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

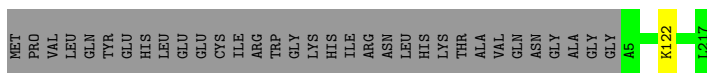
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:  92% 7%



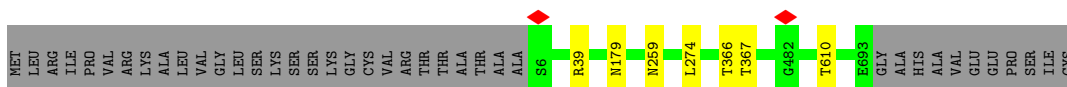
- Molecule 2: Mitochondrial complex I, 24 kDa subunit

Chain 2:  86% 13%




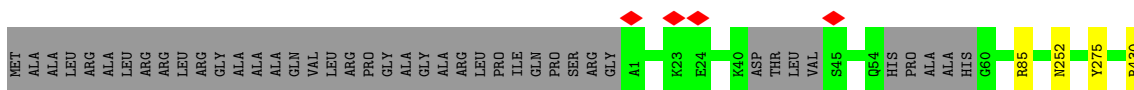
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain 3:  94% 5%




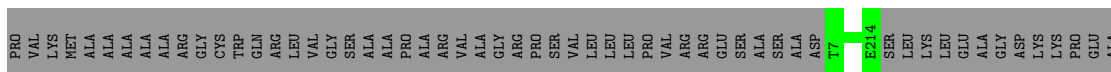
- Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4:  90% 9%



- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:  78% 22%



LYS


- Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6:  69% 30%

MET LEU PRO LEU LEU LEU PHE LYS PRO ARG GLY ARG GLY GLY ALA ALA PRO ARG LEU LEU PHE HIS HIS PRO LEU LEU VAL VAL ARG SER GLY MET GLY ALA ALA LEU GLN VAL ARG GLY VAL HIS SER SER MET MET ALA ALA ASP SER SER SER THR GLN PRO PRO ALA VAL VAL GLN ALA ARG VAL VAL PRO

LYS PRO ALA ALA LEU PRO SER S24 C54 R71 R111 R179

- Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9:  81% 19%

MET ARG LYS PRO MET MET ARG CYS LEU THR MET PRO VAL LEU ARG ALA LEU ALA GLN ALA GLN ALA ARG ALA ALA GLY HIS ALA SER GLY ARG LEU HIS SER SER ALA VAL ALA ALA T1 R176

- Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A:  5% 96%

M1 E32 S36 P36 TYR GLU CYS GLY PHE D42 G46 S46 A47 R48 E115

- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H:  97%

M1 E204 SER GLU LEU VAL SER GLY F211 F259 L285 T318

- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  97%

M1 Y79 PRO GLU VAL TRP VAL SER N86 N175

- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  98%

M1 L19 N50 C98

- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



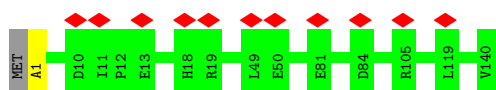
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



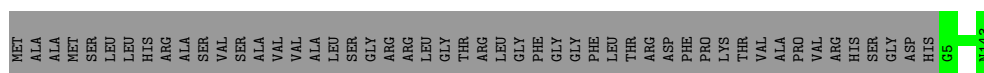
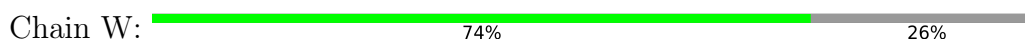
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



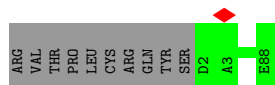
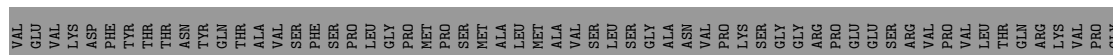
- Molecule 15: Mitochondrial complex I, B14.7 subunit



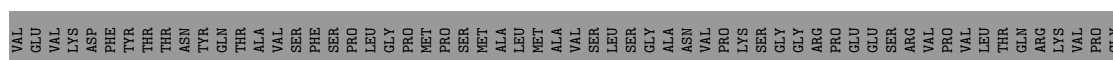
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

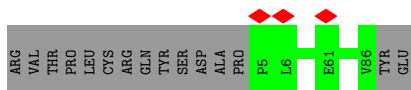


- Molecule 17: Acyl carrier protein

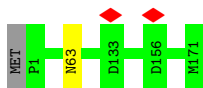


- Molecule 17: Acyl carrier protein

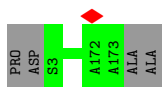




- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



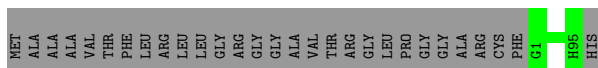
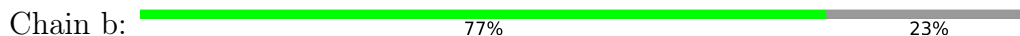
- Molecule 19: Mitochondrial complex I, PDSW subunit



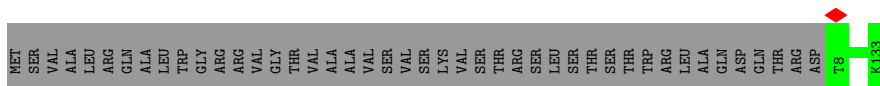
- Molecule 20: Mitochondrial complex I, 10 kDa subunit



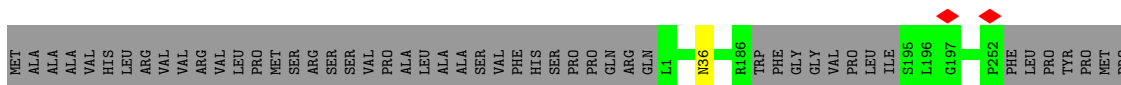
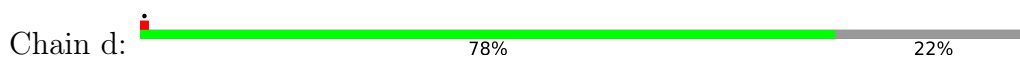
- Molecule 21: Mitochondrial complex I, 13 kDa subunit



- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

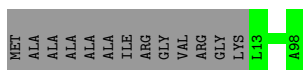
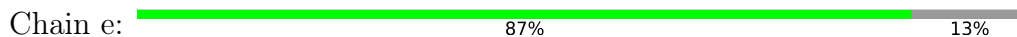


- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

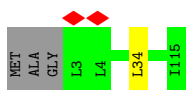




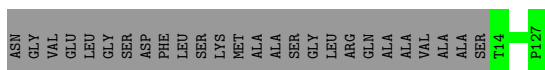
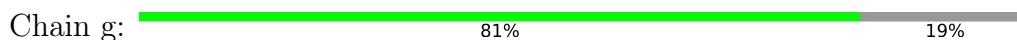
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



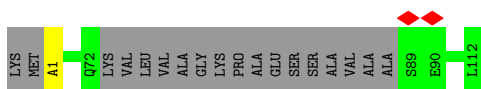
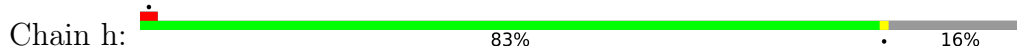
- Molecule 25: Mitochondrial complex I, B13 subunit



- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6



- Molecule 27: Mitochondrial complex I, B14.5a subunit

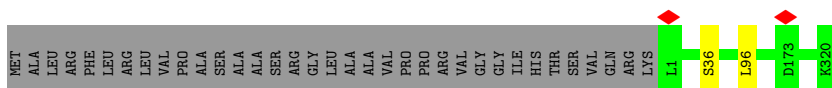
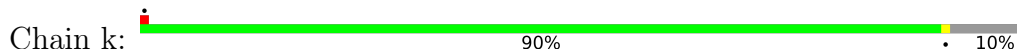


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



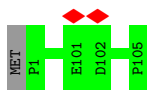
There are no outlier residues recorded for this chain.

- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



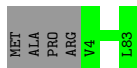
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5





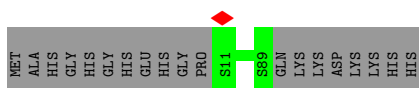
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain m: 95% 5%



- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n: 81% 19%



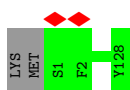
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o: 98%



- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain p: 98%



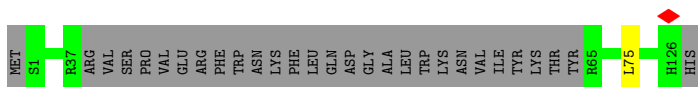
- Molecule 35: Mitochondrial complex I, B16.6 subunit

Chain q: 96%

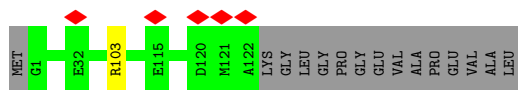
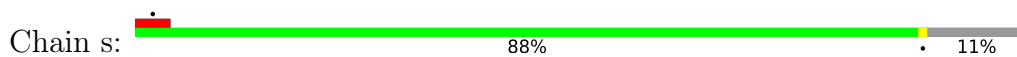


- Molecule 36: Mitochondrial complex I, B17 subunit

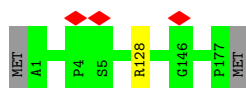
Chain r: 77% 23%



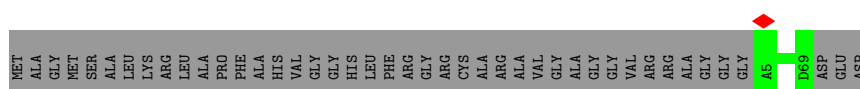
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



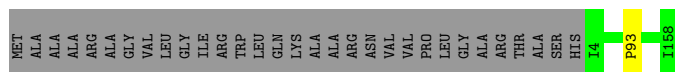
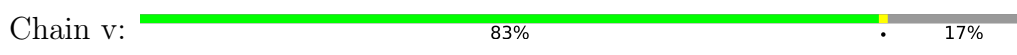
• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



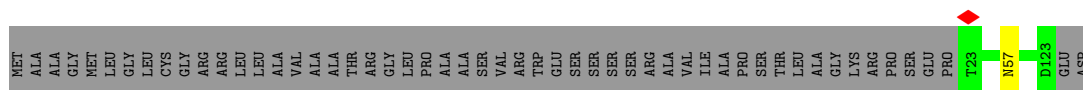
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



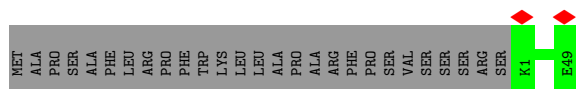
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



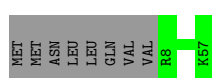
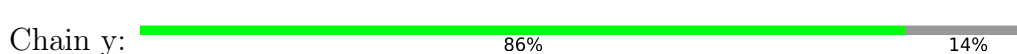
• Molecule 41: Mitochondrial complex I, ESSS subunit



• Molecule 42: Mitochondrial complex I, KFYI subunit



• Molecule 43: Mitochondrial complex I, MNLL subunit



- Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.400	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	170.821, 197.346, 287.531	wwPDB
Map dimensions	271, 186, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, DCQ, MYR, CDL, ZN, PC1, SEP, FES, 2MR, AYA, NDP, NAI, ZMP, FMN, FME, 3PE, SF4, AMP

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	1	0.39	0/3386	0.57	0/4575
2	2	0.37	0/1695	0.56	0/2306
3	3	0.40	0/5362	0.57	2/7266 (0.0%)
4	4	0.44	0/3463	0.57	0/4687
5	5	0.41	0/1776	0.56	0/2417
6	6	0.48	0/1278	0.55	0/1728
7	9	0.49	0/1445	0.59	0/1956
8	A	0.33	0/902	0.60	0/1234
9	H	0.41	0/2562	0.63	0/3504
10	J	0.41	0/1324	0.61	0/1790
11	K	0.35	0/749	0.66	1/1014 (0.1%)
12	L	0.36	0/4924	0.56	0/6698
13	M	0.37	0/3731	0.61	2/5085 (0.0%)
14	N	0.37	0/2787	0.59	1/3795 (0.0%)
15	V	0.28	0/1041	0.51	0/1412
16	W	0.33	0/1188	0.50	0/1607
17	X	0.31	0/713	0.49	0/963
17	j	0.31	0/670	0.51	0/902
18	Y	0.36	0/1440	0.53	0/1942
19	Z	0.34	0/1475	0.48	0/1989
20	a	0.31	0/383	0.49	0/518
21	b	0.37	0/749	0.50	0/1009
22	c	0.36	0/1047	0.52	0/1415
23	d	0.34	0/2424	0.52	0/3276
24	e	0.31	0/702	0.51	0/945
25	f	0.32	0/937	0.52	1/1271 (0.1%)
26	g	0.35	0/993	0.53	0/1336
27	h	0.38	0/779	0.55	0/1053
28	i	0.39	0/1250	0.51	0/1698
29	k	0.34	0/2646	0.49	1/3579 (0.0%)
30	l	0.35	0/896	0.52	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	m	0.33	0/647	0.51	0/890
32	n	0.31	0/653	0.45	0/882
33	o	0.38	0/1035	0.49	0/1398
34	p	0.30	0/1085	0.48	0/1467
35	q	0.35	0/1171	0.50	0/1579
36	r	0.31	0/874	0.51	1/1188 (0.1%)
37	s	0.28	0/1072	0.46	0/1436
38	t	0.33	0/1573	0.50	0/2130
39	u	0.30	0/590	0.45	0/810
40	v	0.32	0/1361	0.50	1/1861 (0.1%)
41	w	0.36	0/872	0.54	0/1185
42	x	0.29	0/425	0.42	0/576
43	y	0.31	0/449	0.48	0/605
44	z	0.40	0/591	0.59	0/795
All	All	0.37	0/67115	0.55	10/90972 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2
4	4	0	1
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	146	LEU	CA-CB-CG	6.18	129.51	115.30
40	v	93	PRO	C-N-CA	5.89	136.43	121.70
3	3	610	THR	C-N-CA	5.67	135.88	121.70
13	M	458	LEU	CA-CB-CG	5.54	128.04	115.30
29	k	96	LEU	CA-CB-CG	5.38	127.67	115.30
36	r	75	LEU	CA-CB-CG	5.35	127.61	115.30
11	K	19	LEU	CA-CB-CG	5.25	127.38	115.30
25	f	34	LEU	CA-CB-CG	5.24	127.36	115.30
13	M	89	LEU	CA-CB-CG	5.13	127.10	115.30
3	3	274	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide

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	1	428/464 (92%)	408 (95%)	20 (5%)	0	100	100
2	2	211/246 (86%)	198 (94%)	13 (6%)	0	100	100
3	3	686/727 (94%)	660 (96%)	25 (4%)	1 (0%)	51	81
4	4	414/463 (89%)	401 (97%)	13 (3%)	0	100	100
5	5	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
6	6	154/223 (69%)	148 (96%)	6 (4%)	0	100	100
7	9	174/217 (80%)	165 (95%)	9 (5%)	0	100	100
8	A	106/115 (92%)	96 (91%)	10 (9%)	0	100	100
9	H	308/318 (97%)	299 (97%)	9 (3%)	0	100	100
10	J	165/175 (94%)	156 (94%)	9 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	579 (96%)	25 (4%)	0	100	100
13	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
14	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
15	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	W	137/189 (72%)	137 (100%)	0	0	100	100
17	X	85/157 (54%)	84 (99%)	1 (1%)	0	100	100
17	j	80/157 (51%)	75 (94%)	5 (6%)	0	100	100
18	Y	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
21	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
22	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
23	d	289/380 (76%)	284 (98%)	5 (2%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
25	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
26	g	112/140 (80%)	108 (96%)	4 (4%)	0	100	100
27	h	92/114 (81%)	88 (96%)	4 (4%)	0	100	100
28	i	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
29	k	317/355 (89%)	307 (97%)	10 (3%)	0	100	100
30	l	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
31	m	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
33	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
34	p	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
37	s	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
38	t	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
39	u	63/108 (58%)	60 (95%)	3 (5%)	0	100	100
40	v	153/186 (82%)	145 (95%)	8 (5%)	0	100	100
41	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	48 (100%)	0	0	100	100
44	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
All	All	8046/9247 (87%)	7769 (97%)	276 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	367	THR

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	1	344/368 (94%)	342 (99%)	2 (1%)	86	96
2	2	183/210 (87%)	182 (100%)	1 (0%)	88	96
3	3	578/608 (95%)	576 (100%)	2 (0%)	92	98
4	4	363/391 (93%)	361 (99%)	2 (1%)	86	96
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	129 (98%)	3 (2%)	50	82
7	9	151/179 (84%)	151 (100%)	0	100	100
8	A	99/103 (96%)	99 (100%)	0	100	100
9	H	273/278 (98%)	271 (99%)	2 (1%)	84	95
10	J	138/144 (96%)	138 (100%)	0	100	100
11	K	86/86 (100%)	85 (99%)	1 (1%)	71	92
12	L	538/538 (100%)	534 (99%)	4 (1%)	84	95
13	M	411/411 (100%)	409 (100%)	2 (0%)	88	96
14	N	315/315 (100%)	315 (100%)	0	100	100
15	V	101/102 (99%)	101 (100%)	0	100	100
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	153 (99%)	1 (1%)	86	96
19	Z	155/157 (99%)	155 (100%)	0	100	100
20	a	43/93 (46%)	43 (100%)	0	100	100
21	b	79/97 (81%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	c	113/150 (75%)	113 (100%)	0	100	100
23	d	255/326 (78%)	254 (100%)	1 (0%)	91	97
24	e	76/82 (93%)	76 (100%)	0	100	100
25	f	101/102 (99%)	101 (100%)	0	100	100
26	g	107/124 (86%)	107 (100%)	0	100	100
27	h	84/96 (88%)	84 (100%)	0	100	100
28	i	131/131 (100%)	131 (100%)	0	100	100
29	k	283/309 (92%)	283 (100%)	0	100	100
30	l	94/95 (99%)	94 (100%)	0	100	100
31	m	69/72 (96%)	69 (100%)	0	100	100
32	n	61/76 (80%)	61 (100%)	0	100	100
33	o	107/109 (98%)	107 (100%)	0	100	100
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	118 (99%)	1 (1%)	81	94
36	r	95/122 (78%)	95 (100%)	0	100	100
37	s	110/120 (92%)	109 (99%)	1 (1%)	78	94
38	t	159/161 (99%)	158 (99%)	1 (1%)	86	96
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	91 (99%)	1 (1%)	73	92
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7128/7955 (90%)	7103 (100%)	25 (0%)	91	97

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	249	ARG
2	2	122	LYS
3	3	39	ARG
3	3	179	ASN
4	4	252	ASN

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Mol	Chain	Res	Type
4	4	430	ARG
6	6	54	CYS
6	6	71	ARG
6	6	111	ARG
9	H	259	PHE
9	H	285	LEU
11	K	50	ASN
12	L	135	ASN
12	L	270	ASN
12	L	442	ASN
12	L	541	ASN
13	M	138	ASN
13	M	144	ASN
18	Y	63	ASN
23	d	36	ASN
35	q	67	ARG
37	s	103	ARG
38	t	128	ARG
41	w	57	ASN

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

Mol	Chain	Res	Type
1	1	148	ASN
2	2	9	HIS
2	2	121	GLN
3	3	401	HIS
4	4	149	ASN
4	4	252	ASN
12	L	135	ASN
12	L	175	ASN
12	L	199	GLN
12	L	405	ASN
12	L	446	ASN
16	W	143	ASN
20	a	40	ASN
21	b	36	ASN
23	d	87	HIS
25	f	20	HIS
25	f	49	GLN
26	g	125	HIS
29	k	107	GLN

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Mol	Chain	Res	Type
33	o	61	GLN
34	p	47	GLN
40	v	87	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 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
13	FME	M	1	13	8,9,10	0.92	0	7,9,11	0.82	0
15	AYA	V	1	15	6,7,8	1.25	1 (16%)	5,8,10	2.28	2 (40%)
29	SEP	k	36	29	8,9,10	1.54	1 (12%)	8,12,14	1.56	2 (25%)
27	AYA	h	1	27	6,7,8	1.26	1 (16%)	5,8,10	1.09	1 (20%)
12	FME	L	1	12	8,9,10	0.97	0	7,9,11	0.77	0
11	FME	K	1	11	8,9,10	0.98	0	7,9,11	0.61	0
4	2MR	4	85	4	10,12,13	2.31	3 (30%)	5,13,15	2.18	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	M	1	13	-	2/7/9/11	-
15	AYA	V	1	15	-	2/4/6/8	-
29	SEP	k	36	29	-	4/5/8/10	-
27	AYA	h	1	27	-	0/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L	1	12	-	2/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
4	2MR	4	85	4	-	0/10/13/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.55	1.43	1.33
4	4	85	2MR	CZ-NE	4.31	1.43	1.34
29	k	36	SEP	P-O1P	3.38	1.61	1.50
27	h	1	AYA	CA-N	-2.52	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.41	1.41	1.46
15	V	1	AYA	CA-N	-2.28	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	85	2MR	NE-CZ-NH2	-4.32	115.52	119.48
15	V	1	AYA	CB-CA-N	3.96	114.01	109.61
29	k	36	SEP	P-OG-CB	-3.06	109.87	118.30
15	V	1	AYA	CA-N-CT	2.56	125.24	121.52
29	k	36	SEP	OG-CB-CA	2.56	110.63	108.14
27	h	1	AYA	CB-CA-N	2.13	111.98	109.61

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
29	k	36	SEP	CB-OG-P-O1P
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
15	V	1	AYA	OT-CT-N-CA
15	V	1	AYA	CM-CT-N-CA
13	M	1	FME	C-CA-CB-CG
29	k	36	SEP	CA-CB-OG-P
13	M	1	FME	CB-CA-N-CN
12	L	1	FME	N-CA-CB-CG
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 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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
53	CDL	W	201	-	99,99,99	0.29	0	105,111,111	0.31	0
50	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.45	0
50	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.33	0
56	NDP	d	401	-	45,52,52	0.58	0	53,80,80	0.57	1 (1%)
54	ZMP	X	101	17	24,30,36	0.68	0	29,37,45	1.10	1 (3%)
50	3PE	A	202	-	50,50,50	0.31	0	53,55,55	0.36	0
53	CDL	Y	201	-	99,99,99	0.26	0	105,111,111	0.34	0
48	FES	2	300	2	0,4,4	-	-	-	-	-
51	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.38	0
53	CDL	M	504	-	89,89,99	0.31	0	95,101,111	0.41	0
58	MYR	s	201	37	14,14,15	0.20	0	13,13,15	0.21	0
46	FMN	1	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.33	8 (16%)
53	CDL	V	204	-	84,84,99	0.29	0	90,96,111	0.27	0
53	CDL	z	101	-	57,57,99	0.35	0	63,69,111	0.32	0
50	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.43	1 (1%)
50	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.31	0
51	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.50	1 (1%)
50	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.79	2 (6%)
48	FES	3	803	3	0,4,4	-	-	-	-	-
45	SF4	9	403	7	0,12,12	-	-	-	-	-
45	SF4	1	501	1	0,12,12	-	-	-	-	-
45	SF4	3	801	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	3PE	i	502	-	50,50,50	0.31	0	53,55,55	0.28	0
54	ZMP	g	201	-	27,33,36	0.71	1 (3%)	32,40,45	1.34	4 (12%)
45	SF4	6	201	6	0,12,12	-	-	-	-	-
50	3PE	V	202	-	36,36,50	0.34	0	39,41,55	0.34	0
53	CDL	L	1003	-	99,99,99	0.26	0	105,111,111	0.29	0
50	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.39	0
47	NAI	1	503	-	42,48,48	0.58	0	47,73,73	1.94	4 (8%)
50	3PE	V	205	-	26,26,50	0.48	0	30,31,55	0.48	1 (3%)
51	PC1	A	201	-	36,36,53	0.36	0	42,44,61	0.59	1 (2%)
53	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.28	0
51	PC1	L	1002	-	53,53,53	0.30	0	59,61,61	0.61	2 (3%)
50	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.53	2 (3%)
50	3PE	4	501	-	39,39,50	0.33	0	42,44,55	0.35	0
50	3PE	N	402	-	30,30,50	0.38	0	33,35,55	0.43	0
53	CDL	o	201	-	74,74,99	0.31	0	80,86,111	0.44	1 (1%)
51	PC1	6	202	-	45,45,53	0.33	0	51,53,61	0.31	0
45	SF4	3	802	3	0,12,12	-	-	-	-	-
50	3PE	i	501	-	50,50,50	0.30	0	53,55,55	0.31	0
52	DCQ	H	501	-	23,23,23	0.16	0	26,29,29	0.70	0
45	SF4	9	402	7	0,12,12	-	-	-	-	-
51	PC1	M	503	-	53,53,53	0.30	0	59,61,61	0.37	0
57	AMP	k	501	-	22,25,25	0.88	1 (4%)	25,38,38	1.18	2 (8%)

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
53	CDL	W	201	-	-	23/110/110/110	-
50	3PE	M	501	-	-	18/47/47/54	-
50	3PE	L	1001	-	-	8/54/54/54	-
56	NDP	d	401	-	-	3/30/77/77	0/5/5/5
54	ZMP	X	101	17	-	14/35/37/43	-
53	CDL	Y	201	-	1/1/9/9	25/110/110/110	-
50	3PE	A	202	-	-	8/54/54/54	-
48	FES	2	300	2	-	-	0/1/1/1
51	PC1	M	502	-	-	12/57/57/57	-
53	CDL	M	504	-	-	34/100/100/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MYR	s	201	37	-	2/11/12/13	-
46	FMN	1	502	-	-	6/18/18/18	0/3/3/3
53	CDL	V	204	-	1/1/9/9	34/95/95/110	-
53	CDL	z	101	-	-	21/68/68/110	-
50	3PE	H	502	-	-	15/54/54/54	-
50	3PE	V	201	-	-	9/38/38/54	-
51	PC1	9	401	-	-	19/57/57/57	-
50	3PE	L	1004	-	-	11/34/34/54	-
48	FES	3	803	3	-	-	0/1/1/1
45	SF4	9	403	7	-	-	0/6/5/5
45	SF4	1	501	1	-	-	0/6/5/5
50	3PE	i	502	-	-	11/54/54/54	-
45	SF4	3	801	3	-	-	0/6/5/5
54	ZMP	g	201	-	-	3/38/40/43	-
45	SF4	6	201	6	-	-	0/6/5/5
50	3PE	V	202	-	-	9/40/40/54	-
53	CDL	L	1003	-	1/1/9/9	33/110/110/110	-
50	3PE	K	101	-	-	8/43/43/54	-
47	NAI	1	503	-	-	11/25/72/72	0/5/5/5
50	3PE	V	205	-	-	5/27/27/54	-
51	PC1	A	201	-	-	8/40/40/57	-
53	CDL	V	203	-	-	34/104/104/110	-
51	PC1	L	1002	-	-	16/57/57/57	-
50	3PE	N	401	-	-	16/54/54/54	-
50	3PE	4	501	-	-	10/43/43/54	-
53	CDL	o	201	-	2/2/9/9	22/85/85/110	-
50	3PE	N	402	-	-	4/34/34/54	-
51	PC1	6	202	-	-	6/49/49/57	-
45	SF4	3	802	3	-	-	0/6/5/5
50	3PE	i	501	-	-	13/54/54/54	-
52	DCQ	H	501	-	-	5/14/38/38	0/1/1/1
45	SF4	9	402	7	-	-	0/6/5/5
51	PC1	M	503	-	-	21/57/57/57	-
57	AMP	k	501	-	-	6/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	502	FMN	C4A-N5	3.23	1.37	1.30
57	k	501	AMP	C5-C4	2.47	1.47	1.40
54	g	201	ZMP	C9-C10	2.28	1.53	1.50
46	1	502	FMN	C4A-C10	-2.07	1.38	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.47	72.05	109.07
47	1	503	NAI	O2A-PA-O1A	-8.10	72.17	112.24
54	g	201	ZMP	C15-C14-C13	-3.73	106.14	112.36
46	1	502	FMN	C4-N3-C2	-3.51	119.15	125.64
57	k	501	AMP	N3-C2-N1	-3.28	123.55	128.68
46	1	502	FMN	C4A-C10-N10	3.27	121.27	116.48
54	X	101	ZMP	O1-C10-C9	-3.04	120.39	123.99
54	g	201	ZMP	O1-C10-C9	-2.89	120.58	123.99
46	1	502	FMN	C4A-C4-N3	2.68	120.00	113.19
46	1	502	FMN	C4A-C10-N1	-2.63	118.63	124.73
46	1	502	FMN	C10-C4A-N5	-2.55	119.44	124.86
51	L	1002	PC1	C2-O21-C21	2.55	124.07	117.79
54	g	201	ZMP	C14-C15-N2	-2.54	106.77	111.90
50	N	401	3PE	O21-C2-C1	2.49	117.42	108.40
47	1	503	NAI	O2A-PA-O5B	2.42	118.98	107.75
46	1	502	FMN	O4-C4-C4A	-2.40	120.24	126.60
54	g	201	ZMP	C9-C10-S1	2.36	116.20	113.46
50	L	1004	3PE	C2-O21-C21	2.35	123.59	117.79
51	L	1002	PC1	O21-C2-C1	2.31	116.78	108.40
47	1	503	NAI	C5A-C6A-N6A	2.28	123.82	120.35
46	1	502	FMN	C4-C4A-C10	2.27	120.60	116.79
56	d	401	NDP	C5A-C6A-N6A	2.26	123.79	120.35
51	A	201	PC1	C2-O21-C21	2.17	123.13	117.79
50	H	502	3PE	O31-C3-C2	2.16	114.72	108.43
50	L	1004	3PE	O21-C2-C3	2.14	116.15	108.40
50	V	205	3PE	O12-P-O14	2.13	119.03	110.68
57	k	501	AMP	C4-C5-N7	-2.10	107.21	109.40
51	9	401	PC1	O21-C2-C1	2.05	115.82	108.40
46	1	502	FMN	C10-N1-C2	2.02	120.94	116.90
53	o	201	CDL	CB4-OB6-CB5	2.01	122.75	117.79
50	N	401	3PE	C2-O21-C21	2.00	122.72	117.79

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	1003	CDL	CB4
53	V	204	CDL	CB4
53	Y	201	CDL	CB4
53	o	201	CDL	CB4
53	o	201	CDL	CA4

All (503) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
47	1	503	NAI	PN-O3-PA-O5B
47	1	503	NAI	C5D-O5D-PN-O3
50	4	501	3PE	C1-O11-P-O12
50	4	501	3PE	C1-O11-P-O14
50	4	501	3PE	C11-O13-P-O11
50	4	501	3PE	C11-O13-P-O12
50	4	501	3PE	C11-O13-P-O14
50	H	502	3PE	C11-O13-P-O11
50	H	502	3PE	C11-O13-P-O12
50	H	502	3PE	C11-O13-P-O14
50	K	101	3PE	C1-O11-P-O12
50	K	101	3PE	C1-O11-P-O14
50	K	101	3PE	O13-C11-C12-N
50	L	1001	3PE	O13-C11-C12-N
50	L	1004	3PE	C1-O11-P-O12
50	L	1004	3PE	C1-O11-P-O14
50	M	501	3PE	C1-O11-P-O14
50	M	501	3PE	C11-O13-P-O11
50	M	501	3PE	C11-O13-P-O14
50	N	401	3PE	C1-O11-P-O12
50	N	401	3PE	C11-O13-P-O14
50	V	201	3PE	C1-O11-P-O12
50	V	201	3PE	C1-O11-P-O14
50	V	201	3PE	O13-C11-C12-N
50	V	202	3PE	C1-O11-P-O12
50	V	202	3PE	C1-O11-P-O13
50	V	202	3PE	C1-O11-P-O14
50	V	205	3PE	C1-O11-P-O12
50	i	501	3PE	C1-O11-P-O12
50	i	501	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
50	i	502	3PE	C11-O13-P-O14
50	i	502	3PE	O13-C11-C12-N
51	9	401	PC1	C11-O13-P-O14
51	A	201	PC1	C1-O11-P-O14
51	L	1002	PC1	C1-O11-P-O12
51	M	502	PC1	C11-O13-P-O12
51	M	502	PC1	C1-O11-P-O14
51	M	502	PC1	O13-C11-C12-N
51	M	503	PC1	C11-O13-P-O14
53	L	1003	CDL	CA2-C1-CB2-OB2
53	L	1003	CDL	CA2-OA2-PA1-OA3
53	L	1003	CDL	CA3-OA5-PA1-OA3
53	L	1003	CDL	CA3-OA5-PA1-OA4
53	L	1003	CDL	CB3-OB5-PB2-OB3
53	M	504	CDL	O1-C1-CB2-OB2
53	M	504	CDL	CA2-C1-CB2-OB2
53	M	504	CDL	CA3-OA5-PA1-OA3
53	M	504	CDL	CB2-OB2-PB2-OB3
53	V	203	CDL	CB2-OB2-PB2-OB3
53	V	203	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CB3-OB5-PB2-OB3
53	V	204	CDL	CA2-OA2-PA1-OA3
53	V	204	CDL	CA2-OA2-PA1-OA4
53	V	204	CDL	CA3-OA5-PA1-OA4
53	V	204	CDL	CB2-OB2-PB2-OB3
53	V	204	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	CA2-OA2-PA1-OA4
53	W	201	CDL	CA3-OA5-PA1-OA3
53	W	201	CDL	CB2-OB2-PB2-OB3
53	o	201	CDL	CA2-OA2-PA1-OA3
53	o	201	CDL	CB2-OB2-PB2-OB3
53	o	201	CDL	CB2-OB2-PB2-OB4
53	o	201	CDL	CB3-OB5-PB2-OB3
53	z	101	CDL	CA3-OA5-PA1-OA4
53	z	101	CDL	CB3-OB5-PB2-OB3
54	X	101	ZMP	C17-C18-C21-O5
54	X	101	ZMP	O4-C17-C18-C21
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	C16-C17-C18-C20
54	X	101	ZMP	O3-C16-C17-O4
54	X	101	ZMP	C17-C16-N2-C15
54	g	201	ZMP	S1-C11-C12-N1

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Mol	Chain	Res	Type	Atoms
57	k	501	AMP	C5'-O5'-P-O1P
57	k	501	AMP	C5'-O5'-P-O2P
57	k	501	AMP	C5'-O5'-P-O3P
57	k	501	AMP	C3'-C4'-C5'-O5'
58	s	201	MYR	C1-C2-C3-C4
52	H	501	DCQ	C6-C7-C8-C9
53	V	204	CDL	O1-C1-CB2-OB2
53	Y	201	CDL	O1-C1-CB2-OB2
54	X	101	ZMP	O3-C16-N2-C15
53	M	504	CDL	C1-CA2-OA2-PA1
53	W	201	CDL	CB2-C1-CA2-OA2
51	6	202	PC1	C11-C12-N-C14
51	M	503	PC1	C11-C12-N-C14
50	V	201	3PE	C31-C32-C33-C34
53	L	1003	CDL	CB7-C71-C72-C73
51	6	202	PC1	C11-C12-N-C15
51	M	503	PC1	C11-C12-N-C15
50	M	501	3PE	C31-C32-C33-C34
53	L	1003	CDL	O1-C1-CB2-OB2
50	N	401	3PE	C21-C22-C23-C24
53	W	201	CDL	CA5-C11-C12-C13
50	4	501	3PE	C1-O11-P-O13
50	A	202	3PE	C11-O13-P-O11
50	K	101	3PE	C1-O11-P-O13
50	L	1004	3PE	C1-O11-P-O13
50	L	1004	3PE	C11-O13-P-O11
50	N	401	3PE	C11-O13-P-O11
50	V	201	3PE	C1-O11-P-O13
50	V	202	3PE	C11-O13-P-O11
50	i	501	3PE	C1-O11-P-O13
50	i	501	3PE	C11-O13-P-O11
51	9	401	PC1	C11-O13-P-O11
51	A	201	PC1	C1-O11-P-O13
51	M	502	PC1	C11-O13-P-O11
53	L	1003	CDL	CA3-OA5-PA1-OA2
53	L	1003	CDL	CB2-OB2-PB2-OB5
53	M	504	CDL	CA2-OA2-PA1-OA5
53	M	504	CDL	CA3-OA5-PA1-OA2
53	M	504	CDL	CB2-OB2-PB2-OB5
53	V	203	CDL	CB2-OB2-PB2-OB5
53	V	203	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	V	204	CDL	CA3-OA5-PA1-OA2
53	V	204	CDL	CB3-OB5-PB2-OB2
53	W	201	CDL	CA2-OA2-PA1-OA5
53	W	201	CDL	CA3-OA5-PA1-OA2
53	W	201	CDL	CB2-OB2-PB2-OB5
53	o	201	CDL	CA2-OA2-PA1-OA5
53	o	201	CDL	CB2-OB2-PB2-OB5
53	o	201	CDL	CB3-OB5-PB2-OB2
53	z	101	CDL	CA3-OA5-PA1-OA2
53	z	101	CDL	CB2-OB2-PB2-OB5
53	z	101	CDL	CB3-OB5-PB2-OB2
50	H	502	3PE	C33-C34-C35-C36
53	L	1003	CDL	C22-C23-C24-C25
51	L	1002	PC1	C37-C38-C39-C3A
53	L	1003	CDL	C82-C83-C84-C85
53	M	504	CDL	C78-C79-C80-C81
53	Y	201	CDL	C52-C53-C54-C55
53	L	1003	CDL	C21-C22-C23-C24
51	9	401	PC1	C3C-C3D-C3E-C3F
53	L	1003	CDL	C77-C78-C79-C80
51	L	1002	PC1	C2-C1-O11-P
50	i	501	3PE	C3C-C3D-C3E-C3F
53	W	201	CDL	O1-C1-CA2-OA2
53	o	201	CDL	O1-C1-CB2-OB2
53	V	204	CDL	C71-C72-C73-C74
50	V	205	3PE	C21-C22-C23-C24
50	L	1001	3PE	C3B-C3C-C3D-C3E
53	L	1003	CDL	C34-C35-C36-C37
53	Y	201	CDL	C13-C14-C15-C16
50	A	202	3PE	C38-C39-C3A-C3B
53	Y	201	CDL	C59-C60-C61-C62
50	K	101	3PE	C34-C35-C36-C37
53	V	203	CDL	C79-C80-C81-C82
54	X	101	ZMP	C6-C7-C8-C9
51	6	202	PC1	C3B-C3C-C3D-C3E
53	Y	201	CDL	CB5-C51-C52-C53
53	o	201	CDL	CA7-C31-C32-C33
50	N	401	3PE	C32-C33-C34-C35
51	9	401	PC1	C3B-C3C-C3D-C3E
53	V	203	CDL	C38-C39-C40-C41
53	V	203	CDL	C40-C41-C42-C43
50	A	202	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
53	M	504	CDL	CB5-C51-C52-C53
53	L	1003	CDL	C56-C57-C58-C59
50	i	502	3PE	C29-C2A-C2B-C2C
51	M	502	PC1	C27-C28-C29-C2A
52	H	501	DCQ	C10-C11-C12-C13
53	V	204	CDL	C15-C16-C17-C18
53	W	201	CDL	CB5-C51-C52-C53
51	M	503	PC1	C3A-C3B-C3C-C3D
53	W	201	CDL	C35-C36-C37-C38
53	V	204	CDL	CA2-C1-CB2-OB2
51	M	503	PC1	C11-C12-N-C13
51	9	401	PC1	C22-C23-C24-C25
51	L	1002	PC1	C38-C39-C3A-C3B
53	Y	201	CDL	C15-C16-C17-C18
51	L	1002	PC1	C23-C24-C25-C26
53	M	504	CDL	C82-C83-C84-C85
53	Y	201	CDL	CA5-C11-C12-C13
53	M	504	CDL	C81-C82-C83-C84
53	M	504	CDL	C56-C57-C58-C59
53	V	203	CDL	C31-C32-C33-C34
53	V	203	CDL	CA7-C31-C32-C33
51	9	401	PC1	C22-C21-O21-C2
50	M	501	3PE	C25-C26-C27-C28
51	L	1002	PC1	C2A-C2B-C2C-C2D
51	9	401	PC1	O22-C21-O21-C2
51	6	202	PC1	C11-C12-N-C13
53	V	203	CDL	C11-C12-C13-C14
57	k	501	AMP	O4'-C4'-C5'-O5'
50	M	501	3PE	C1-O11-P-O13
51	M	502	PC1	C1-O11-P-O13
53	L	1003	CDL	CB3-OB5-PB2-OB2
50	H	502	3PE	O11-C1-C2-C3
51	L	1002	PC1	O11-C1-C2-C3
53	Y	201	CDL	C81-C82-C83-C84
51	A	201	PC1	C22-C23-C24-C25
51	L	1002	PC1	C36-C37-C38-C39
50	V	201	3PE	C22-C23-C24-C25
51	M	503	PC1	C25-C26-C27-C28
53	V	203	CDL	CB3-CB4-CB6-OB8
53	V	204	CDL	CB3-CB4-CB6-OB8
53	Y	201	CDL	CA3-CA4-CA6-OA8
53	Y	201	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
53	M	504	CDL	CB7-C71-C72-C73
51	M	503	PC1	O31-C31-C32-C33
53	W	201	CDL	C72-C73-C74-C75
53	L	1003	CDL	C17-C18-C19-C20
53	V	204	CDL	C14-C15-C16-C17
46	1	502	FMN	C5'-O5'-P-O1P
50	L	1004	3PE	C2-C1-O11-P
50	L	1004	3PE	O11-C1-C2-O21
50	N	401	3PE	O11-C1-C2-O21
53	V	203	CDL	OA5-CA3-CA4-OA6
53	o	201	CDL	OA5-CA3-CA4-OA6
51	9	401	PC1	C2C-C2D-C2E-C2F
53	M	504	CDL	OA6-CA4-CA6-OA8
53	V	204	CDL	OB6-CB4-CB6-OB8
53	V	204	CDL	C21-C22-C23-C24
53	Y	201	CDL	C63-C64-C65-C66
50	i	501	3PE	C23-C24-C25-C26
50	V	205	3PE	C22-C23-C24-C25
50	L	1001	3PE	C24-C25-C26-C27
51	M	502	PC1	C3E-C3F-C3G-C3H
47	1	503	NAI	C2D-C1D-N1N-C2N
53	M	504	CDL	C64-C65-C66-C67
51	M	503	PC1	O11-C1-C2-C3
53	L	1003	CDL	OB5-CB3-CB4-CB6
53	V	203	CDL	OA5-CA3-CA4-CA6
50	H	502	3PE	O13-C11-C12-N
51	M	503	PC1	C31-C32-C33-C34
53	V	203	CDL	O1-C1-CB2-OB2
53	V	204	CDL	C52-C53-C54-C55
53	L	1003	CDL	CA4-CA3-OA5-PA1
53	z	101	CDL	C1-CB2-OB2-PB2
53	z	101	CDL	CB4-CB3-OB5-PB2
51	L	1002	PC1	C33-C34-C35-C36
53	M	504	CDL	C31-C32-C33-C34
53	V	204	CDL	C77-C78-C79-C80
50	N	401	3PE	C1-C2-C3-O31
53	M	504	CDL	CA3-CA4-CA6-OA8
53	z	101	CDL	CA3-CA4-CA6-OA8
53	W	201	CDL	C31-C32-C33-C34
51	M	503	PC1	O11-C1-C2-O21
53	o	201	CDL	OB5-CB3-CB4-OB6
51	9	401	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
53	L	1003	CDL	C58-C59-C60-C61
53	V	203	CDL	OB6-CB4-CB6-OB8
53	V	204	CDL	OA6-CA4-CA6-OA8
53	Y	201	CDL	CA2-C1-CB2-OB2
53	z	101	CDL	CA2-C1-CB2-OB2
51	M	503	PC1	C2B-C2C-C2D-C2E
46	1	502	FMN	C4'-C5'-O5'-P
51	M	503	PC1	C2-C1-O11-P
53	L	1003	CDL	C1-CA2-OA2-PA1
53	L	1003	CDL	CB4-CB3-OB5-PB2
53	M	504	CDL	CB4-CB3-OB5-PB2
53	V	203	CDL	C1-CA2-OA2-PA1
50	K	101	3PE	C24-C25-C26-C27
50	M	501	3PE	C38-C39-C3A-C3B
53	L	1003	CDL	C55-C56-C57-C58
53	L	1003	CDL	C81-C82-C83-C84
50	4	501	3PE	O31-C31-C32-C33
50	i	501	3PE	C2D-C2E-C2F-C2G
50	L	1001	3PE	C39-C3A-C3B-C3C
50	N	401	3PE	C2B-C2C-C2D-C2E
50	H	502	3PE	C2-C1-O11-P
50	M	501	3PE	C2-C1-O11-P
53	M	504	CDL	CA4-CA3-OA5-PA1
53	W	201	CDL	C1-CA2-OA2-PA1
53	z	101	CDL	CB3-CB4-CB6-OB8
53	L	1003	CDL	OB5-CB3-CB4-OB6
53	V	203	CDL	CA2-C1-CB2-OB2
54	X	101	ZMP	C16-C17-C18-C19
47	1	503	NAI	O4D-C1D-N1N-C2N
53	M	504	CDL	C73-C74-C75-C76
53	V	203	CDL	C78-C79-C80-C81
50	M	501	3PE	C33-C34-C35-C36
50	M	501	3PE	O21-C2-C3-O31
50	N	401	3PE	O21-C2-C3-O31
53	Y	201	CDL	OA6-CA4-CA6-OA8
53	z	101	CDL	OA6-CA4-CA6-OA8
51	M	502	PC1	C31-C32-C33-C34
53	Y	201	CDL	C14-C15-C16-C17
53	Y	201	CDL	C82-C83-C84-C85
51	M	502	PC1	C26-C27-C28-C29
50	N	401	3PE	C1-O11-P-O13
50	i	502	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
51	A	201	PC1	C11-O13-P-O11
53	Y	201	CDL	CB3-OB5-PB2-OB2
50	V	202	3PE	C2-C1-O11-P
53	V	204	CDL	C1-CA2-OA2-PA1
53	V	204	CDL	C1-CB2-OB2-PB2
57	k	501	AMP	C4'-C5'-O5'-P
47	1	503	NAI	C5B-O5B-PA-O2A
47	1	503	NAI	C5D-O5D-PN-O1N
50	A	202	3PE	C11-O13-P-O14
50	L	1004	3PE	C11-O13-P-O14
50	M	501	3PE	C1-O11-P-O12
50	N	401	3PE	C1-O11-P-O14
50	V	202	3PE	C11-O13-P-O14
50	i	501	3PE	C11-O13-P-O14
51	9	401	PC1	C11-O13-P-O12
51	A	201	PC1	C1-O11-P-O12
51	L	1002	PC1	C1-O11-P-O14
51	M	502	PC1	C11-O13-P-O14
51	M	502	PC1	C1-O11-P-O12
53	L	1003	CDL	CB2-OB2-PB2-OB3
53	L	1003	CDL	CB3-OB5-PB2-OB4
53	M	504	CDL	CA2-OA2-PA1-OA3
53	M	504	CDL	CA2-OA2-PA1-OA4
53	M	504	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CB3-OB5-PB2-OB4
53	V	204	CDL	CB3-OB5-PB2-OB4
53	W	201	CDL	CB2-OB2-PB2-OB4
53	o	201	CDL	CA2-OA2-PA1-OA4
53	o	201	CDL	CB3-OB5-PB2-OB4
53	z	101	CDL	CA3-OA5-PA1-OA3
53	z	101	CDL	CB2-OB2-PB2-OB3
53	z	101	CDL	CB3-OB5-PB2-OB4
53	V	204	CDL	OA5-CA3-CA4-CA6
53	o	201	CDL	OA5-CA3-CA4-CA6
53	M	504	CDL	C19-C20-C21-C22
52	H	501	DCQ	C5-C4-O4-C4M
50	4	501	3PE	C12-C11-O13-P
50	H	502	3PE	C12-C11-O13-P
51	9	401	PC1	C12-C11-O13-P
51	M	503	PC1	C27-C28-C29-C2A
50	i	501	3PE	C36-C37-C38-C39
53	M	504	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
50	M	501	3PE	C35-C36-C37-C38
53	V	204	CDL	C22-C23-C24-C25
51	A	201	PC1	O11-C1-C2-O21
51	L	1002	PC1	O11-C1-C2-O21
53	V	204	CDL	OA5-CA3-CA4-OA6
53	Y	201	CDL	C32-C33-C34-C35
47	1	503	NAI	C2D-C1D-N1N-C6N
50	M	501	3PE	C1-C2-C3-O31
51	9	401	PC1	O13-C11-C12-N
51	L	1002	PC1	O13-C11-C12-N
51	9	401	PC1	C2-C1-O11-P
51	A	201	PC1	O21-C21-C22-C23
53	V	203	CDL	C23-C24-C25-C26
53	L	1003	CDL	C41-C42-C43-C44
50	4	501	3PE	C24-C25-C26-C27
50	K	101	3PE	C23-C24-C25-C26
53	M	504	CDL	C83-C84-C85-C86
54	X	101	ZMP	C19-C18-C21-O5
54	X	101	ZMP	C20-C18-C21-O5
51	9	401	PC1	C3-C2-O21-C21
50	L	1004	3PE	C21-C22-C23-C24
51	L	1002	PC1	C3E-C3F-C3G-C3H
50	H	502	3PE	O11-C1-C2-O21
50	A	202	3PE	C1-O11-P-O13
50	L	1001	3PE	C11-O13-P-O11
50	N	402	3PE	C11-O13-P-O11
50	V	201	3PE	C11-O13-P-O11
51	9	401	PC1	C1-O11-P-O13
51	M	503	PC1	C11-O13-P-O11
53	o	201	CDL	CA3-OA5-PA1-OA2
53	z	101	CDL	CA2-OA2-PA1-OA5
54	X	101	ZMP	O4-C17-C18-C19
50	i	501	3PE	C3D-C3E-C3F-C3G
53	o	201	CDL	CA5-C11-C12-C13
51	M	503	PC1	C39-C3A-C3B-C3C
50	H	502	3PE	C2A-C2B-C2C-C2D
50	K	101	3PE	C2-C1-O11-P
50	H	502	3PE	C3F-C3G-C3H-C3I
51	M	503	PC1	O21-C21-C22-C23
50	i	501	3PE	C35-C36-C37-C38
53	W	201	CDL	C22-C23-C24-C25
53	V	203	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
50	N	401	3PE	O11-C1-C2-C3
56	d	401	NDP	O4D-C1D-N1N-C6N
53	z	101	CDL	C52-C53-C54-C55
53	o	201	CDL	CB7-C71-C72-C73
53	Y	201	CDL	C79-C80-C81-C82
51	M	503	PC1	C3B-C3C-C3D-C3E
50	H	502	3PE	C29-C2A-C2B-C2C
53	Y	201	CDL	C58-C59-C60-C61
58	s	201	MYR	C11-C10-C9-C8
50	L	1004	3PE	C1-C2-O21-C21
51	L	1002	PC1	C1-C2-O21-C21
53	L	1003	CDL	C37-C38-C39-C40
53	o	201	CDL	C73-C74-C75-C76
51	L	1002	PC1	C1-O11-P-O13
53	z	101	CDL	OA5-CA3-CA4-OA6
53	V	203	CDL	OB5-CB3-CB4-CB6
54	g	201	ZMP	C12-C11-S1-C10
47	1	503	NAI	O4D-C1D-N1N-C6N
51	6	202	PC1	C26-C27-C28-C29
51	M	503	PC1	O32-C31-C32-C33
50	V	205	3PE	C26-C27-C28-C29
50	i	501	3PE	C33-C34-C35-C36
53	M	504	CDL	C71-C72-C73-C74
51	9	401	PC1	C27-C28-C29-C2A
51	9	401	PC1	C2B-C2C-C2D-C2E
51	A	201	PC1	O31-C31-C32-C33
50	H	502	3PE	C31-C32-C33-C34
51	9	401	PC1	C3E-C3F-C3G-C3H
50	i	502	3PE	C36-C37-C38-C39
53	W	201	CDL	C53-C54-C55-C56
50	i	501	3PE	O11-C1-C2-O21
53	V	203	CDL	OB5-CB3-CB4-OB6
51	M	503	PC1	C2F-C2G-C2H-C2I
50	L	1001	3PE	C37-C38-C39-C3A
50	M	501	3PE	C3E-C3F-C3G-C3H
52	H	501	DCQ	C7-C8-C9-C10
53	V	203	CDL	CA5-C11-C12-C13
53	W	201	CDL	C15-C16-C17-C18
50	N	401	3PE	O13-C11-C12-N
53	o	201	CDL	CA2-C1-CB2-OB2
50	H	502	3PE	C32-C31-O31-C3
50	V	205	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
54	X	101	ZMP	N2-C16-C17-O4
53	V	204	CDL	CB2-OB2-PB2-OB5
54	g	201	ZMP	C19-C18-C21-O5
53	M	504	CDL	C12-C13-C14-C15
53	V	204	CDL	C34-C35-C36-C37
53	z	101	CDL	CB7-C71-C72-C73
50	A	202	3PE	C3C-C3D-C3E-C3F
50	V	202	3PE	O31-C31-C32-C33
51	L	1002	PC1	C2D-C2E-C2F-C2G
50	H	502	3PE	C3C-C3D-C3E-C3F
51	M	503	PC1	C2C-C2D-C2E-C2F
51	M	502	PC1	C23-C24-C25-C26
50	A	202	3PE	O21-C21-C22-C23
53	V	204	CDL	CA3-CA4-CA6-OA8
53	W	201	CDL	CA3-CA4-CA6-OA8
53	W	201	CDL	C58-C59-C60-C61
53	W	201	CDL	OB5-CB3-CB4-OB6
50	L	1004	3PE	O21-C21-C22-C23
50	N	401	3PE	O31-C31-C32-C33
53	W	201	CDL	C12-C11-CA5-OA6
53	L	1003	CDL	C35-C36-C37-C38
53	V	203	CDL	C80-C81-C82-C83
50	L	1001	3PE	C23-C24-C25-C26
50	N	402	3PE	C22-C23-C24-C25
50	i	502	3PE	O21-C21-C22-C23
53	z	101	CDL	O1-C1-CB2-OB2
51	9	401	PC1	C2D-C2E-C2F-C2G
53	V	204	CDL	C52-C51-CB5-OB6
53	Y	201	CDL	C57-C58-C59-C60
50	V	201	3PE	O11-C1-C2-C3
53	o	201	CDL	OB5-CB3-CB4-CB6
53	V	203	CDL	C72-C71-CB7-OB8
53	L	1003	CDL	OA6-CA4-CA6-OA8
53	V	203	CDL	OA6-CA4-CA6-OA8
53	V	204	CDL	C32-C31-CA7-OA8
54	X	101	ZMP	O4-C17-C18-C20
56	d	401	NDP	C2B-O2B-P2B-O2X
53	M	504	CDL	C76-C77-C78-C79
52	H	501	DCQ	C3-C4-O4-C4M
56	d	401	NDP	O4B-C4B-C5B-O5B
50	4	501	3PE	O32-C31-C32-C33
47	1	503	NAI	PA-O3-PN-O1N

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Mol	Chain	Res	Type	Atoms
53	V	203	CDL	C41-C42-C43-C44
53	V	204	CDL	C51-C52-C53-C54
53	Y	201	CDL	C72-C71-CB7-OB8
53	V	203	CDL	C34-C35-C36-C37
50	L	1004	3PE	O22-C21-C22-C23
50	N	401	3PE	O32-C31-C32-C33
53	o	201	CDL	C72-C71-CB7-OB8
53	M	504	CDL	C72-C73-C74-C75
50	A	202	3PE	O22-C21-C22-C23
50	i	502	3PE	O31-C31-C32-C33
50	V	202	3PE	O32-C31-C32-C33
50	i	502	3PE	O22-C21-C22-C23
53	W	201	CDL	C12-C11-CA5-OA7
47	1	503	NAI	C5D-O5D-PN-O2N
47	1	503	NAI	C2N-C3N-C7N-N7N
50	N	402	3PE	C11-O13-P-O14
50	i	502	3PE	C1-O11-P-O14
51	6	202	PC1	C1-O11-P-O14
53	M	504	CDL	CB3-OB5-PB2-OB3
53	Y	201	CDL	CB2-OB2-PB2-OB3
53	Y	201	CDL	CB3-OB5-PB2-OB3
53	z	101	CDL	CA2-OA2-PA1-OA3
50	V	202	3PE	C25-C26-C27-C28
53	V	204	CDL	C32-C31-CA7-OA9
53	V	204	CDL	C52-C51-CB5-OB7
53	M	504	CDL	OB5-CB3-CB4-CB6
50	M	501	3PE	O13-C11-C12-N
53	V	203	CDL	C13-C14-C15-C16
50	N	402	3PE	C25-C26-C27-C28
53	V	203	CDL	C72-C71-CB7-OB9
51	M	503	PC1	C12-C11-O13-P
53	M	504	CDL	CB3-CB4-OB6-CB5
53	o	201	CDL	CB6-CB4-OB6-CB5
53	Y	201	CDL	C52-C51-CB5-OB6
53	V	204	CDL	C75-C76-C77-C78
53	V	203	CDL	C32-C31-CA7-OA8
50	M	501	3PE	C34-C35-C36-C37
53	L	1003	CDL	C72-C71-CB7-OB8
50	i	502	3PE	C26-C27-C28-C29
50	V	201	3PE	O11-C1-C2-O21
50	i	502	3PE	O32-C31-C32-C33
50	L	1001	3PE	C35-C36-C37-C38

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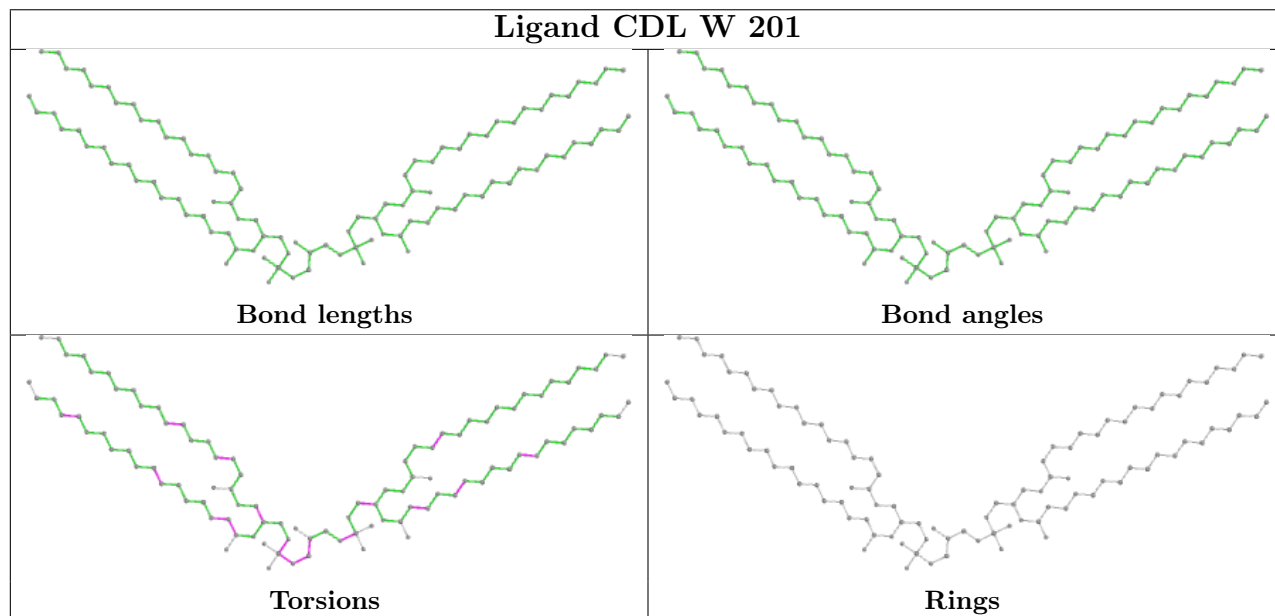
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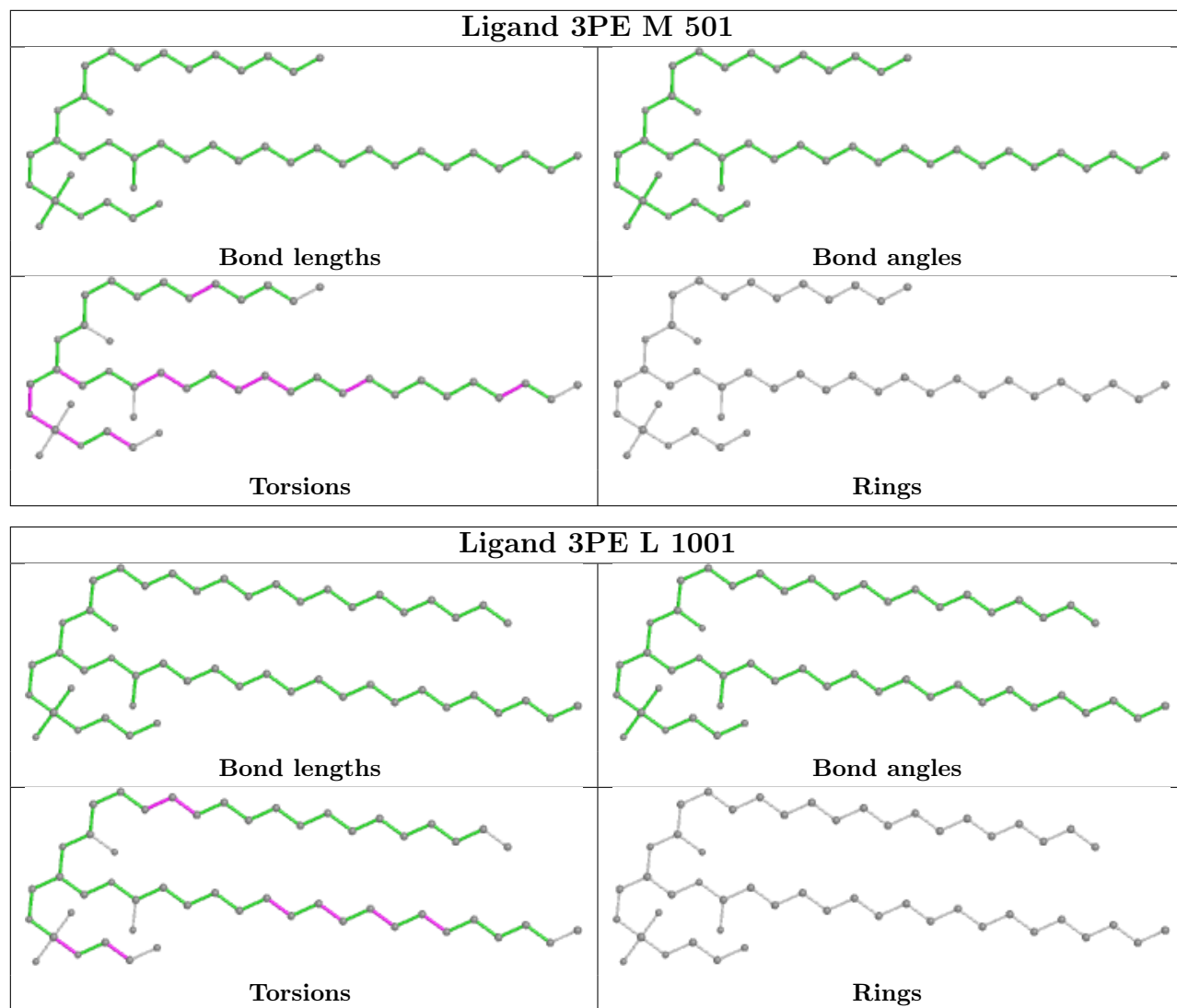
Mol	Chain	Res	Type	Atoms
50	M	501	3PE	O31-C31-C32-C33
53	z	101	CDL	C52-C51-CB5-OB6
53	L	1003	CDL	C80-C81-C82-C83
50	N	401	3PE	C38-C39-C3A-C3B
53	Y	201	CDL	C12-C11-CA5-OA6
53	V	203	CDL	C32-C31-CA7-OA9
50	M	501	3PE	O32-C31-C32-C33

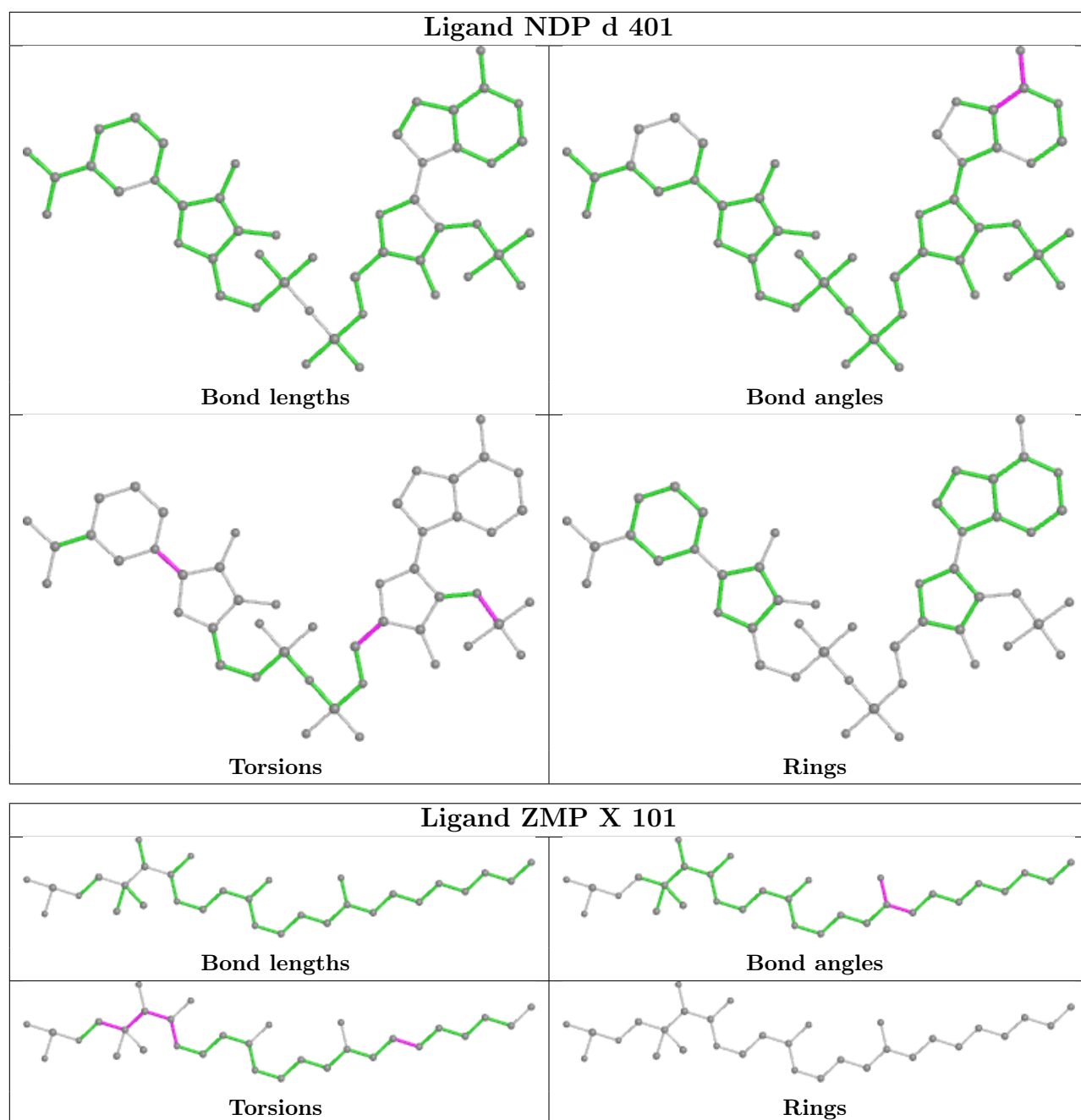
There are no ring outliers.

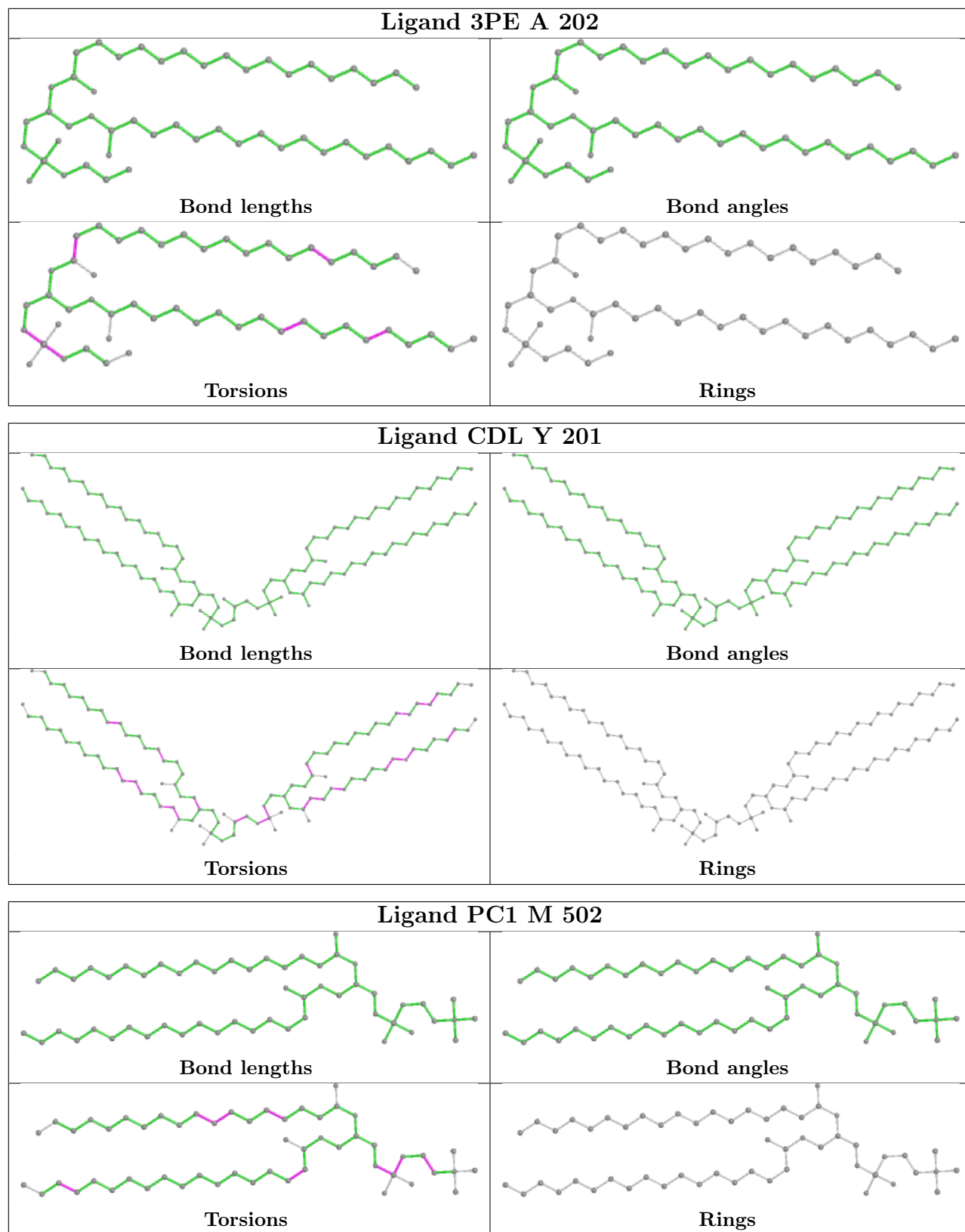
No monomer is involved in short contacts.

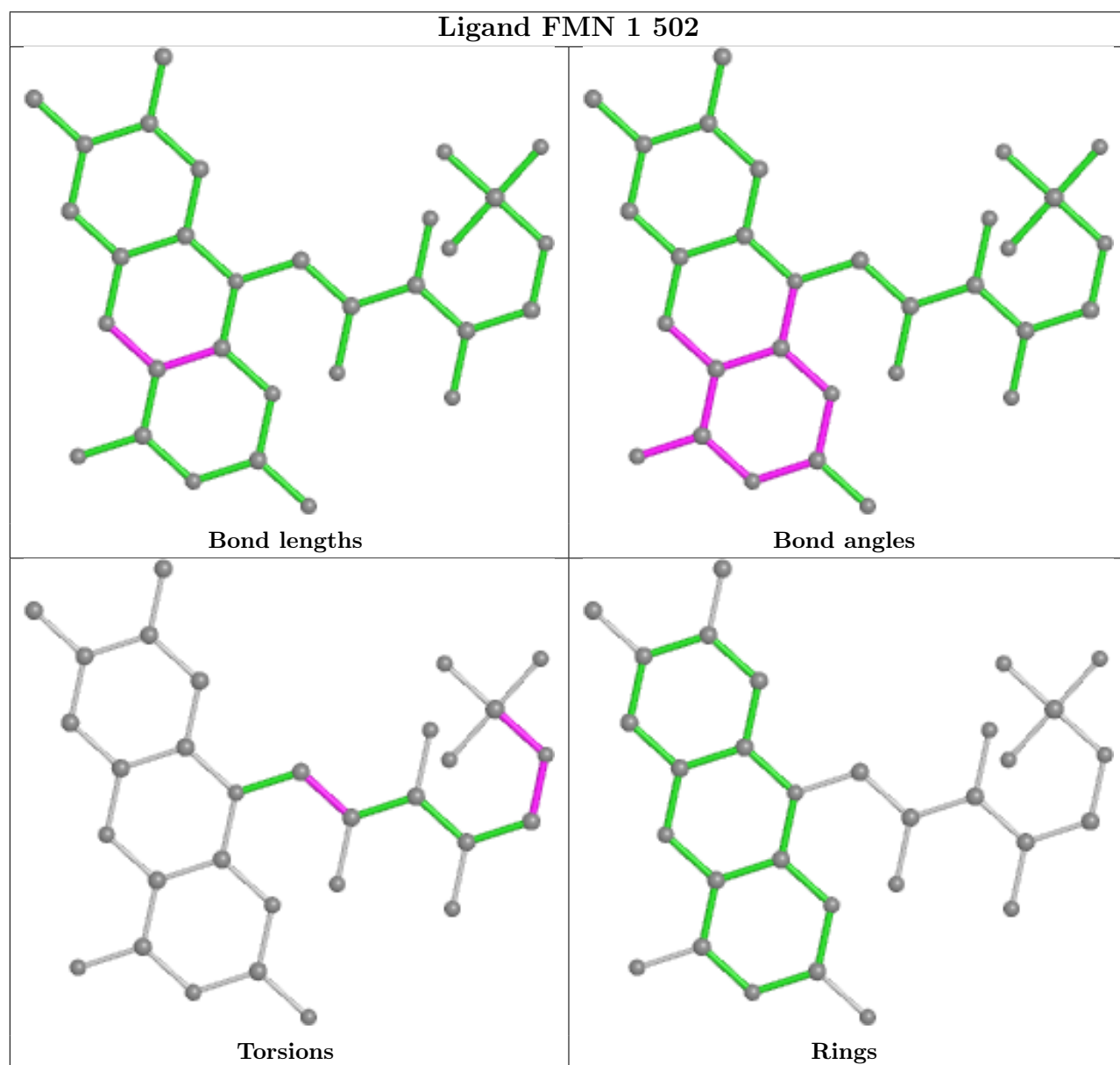
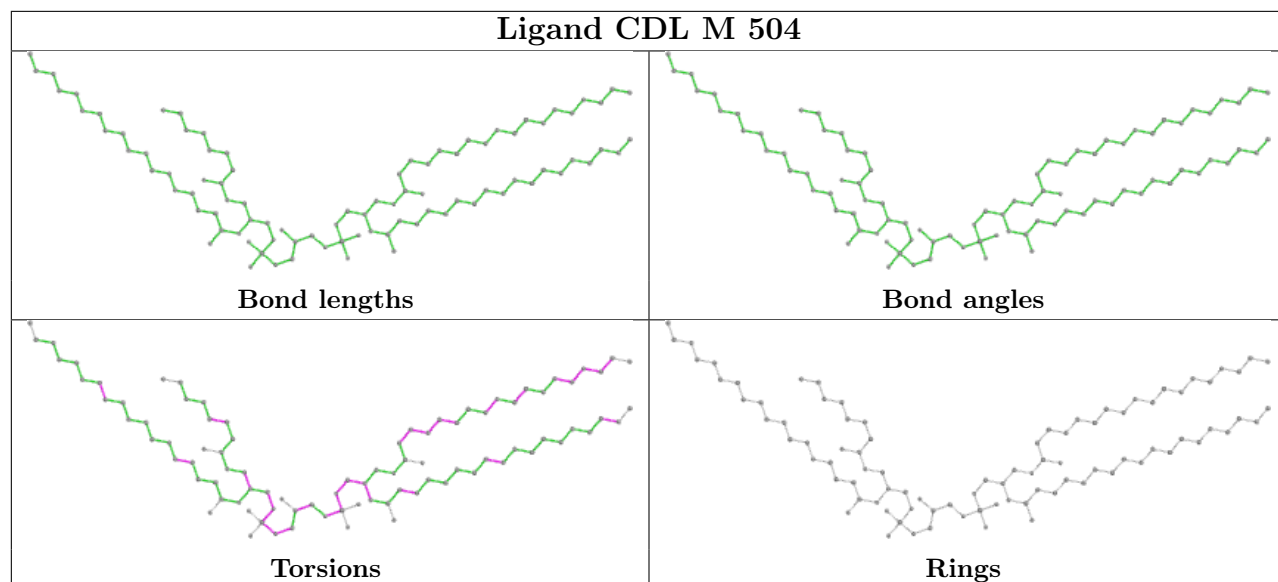
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

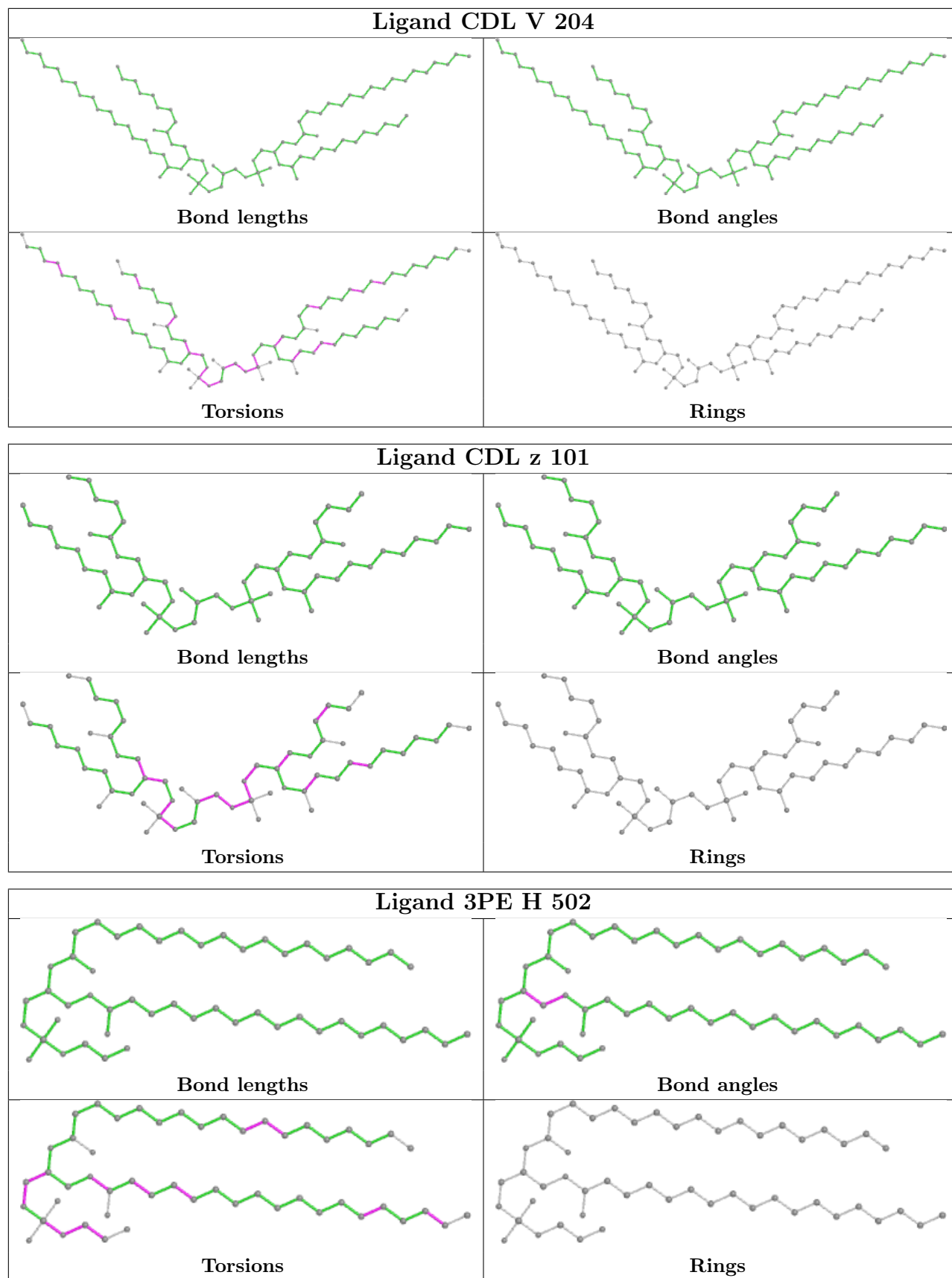


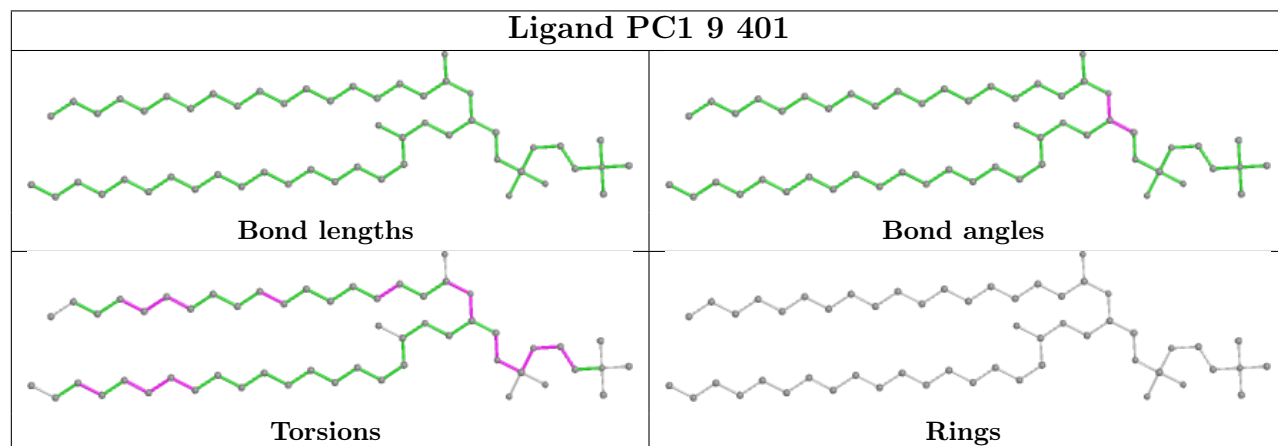
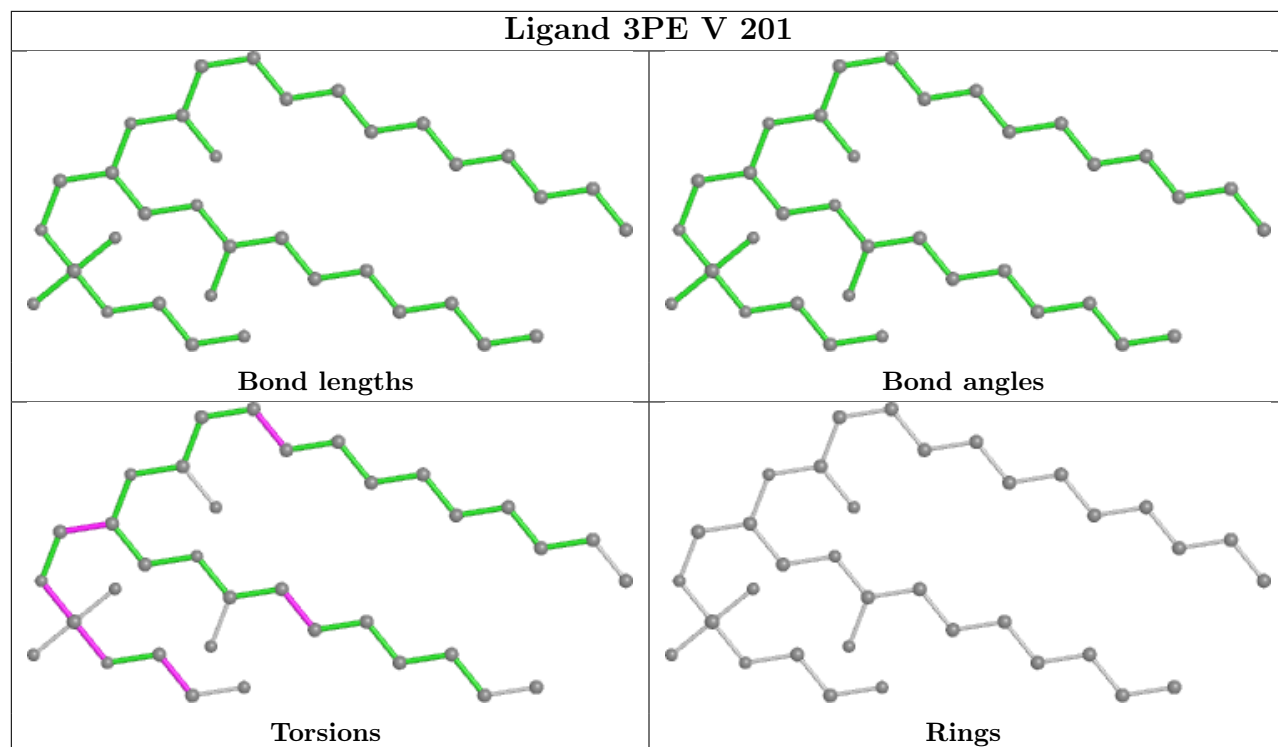


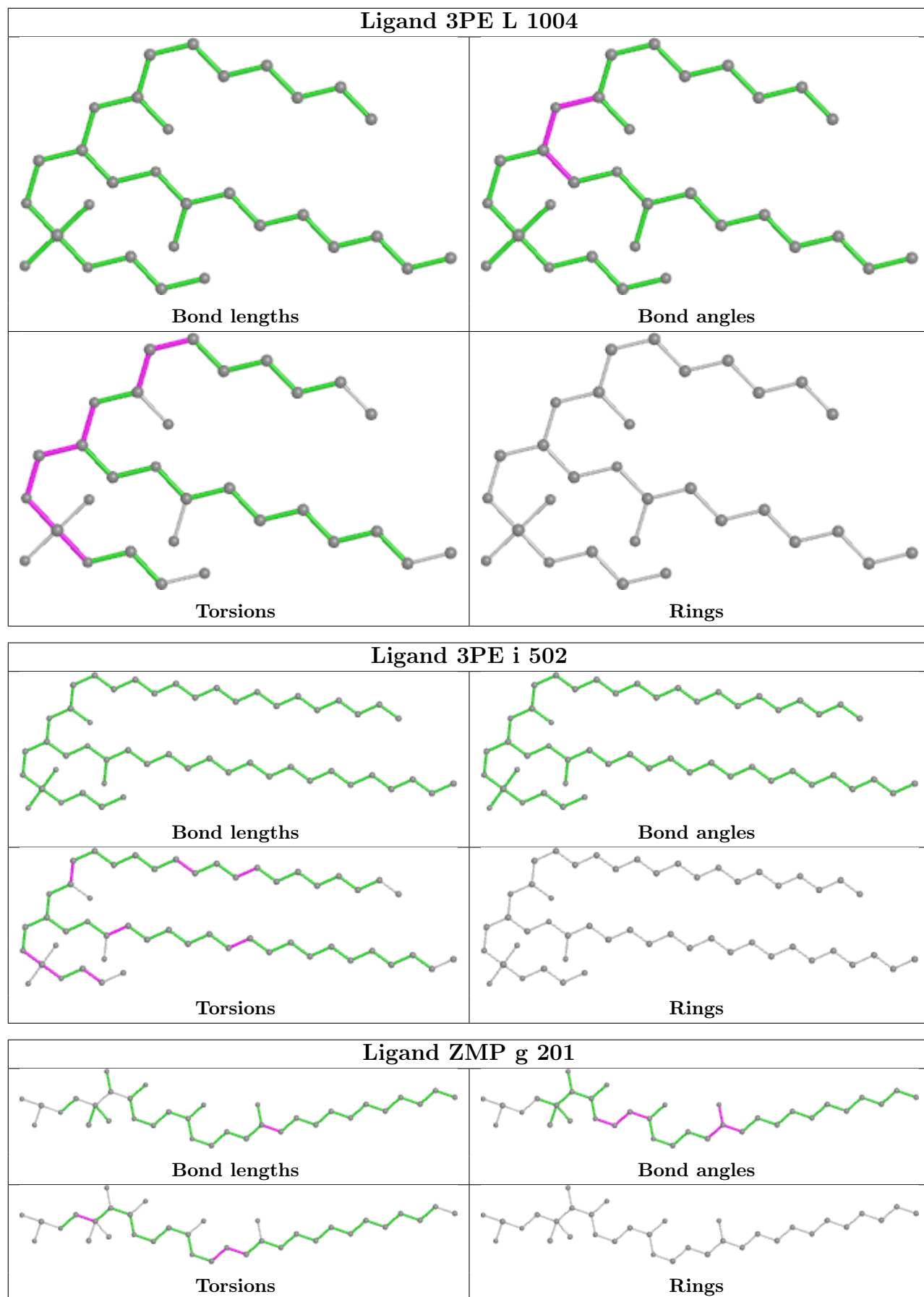


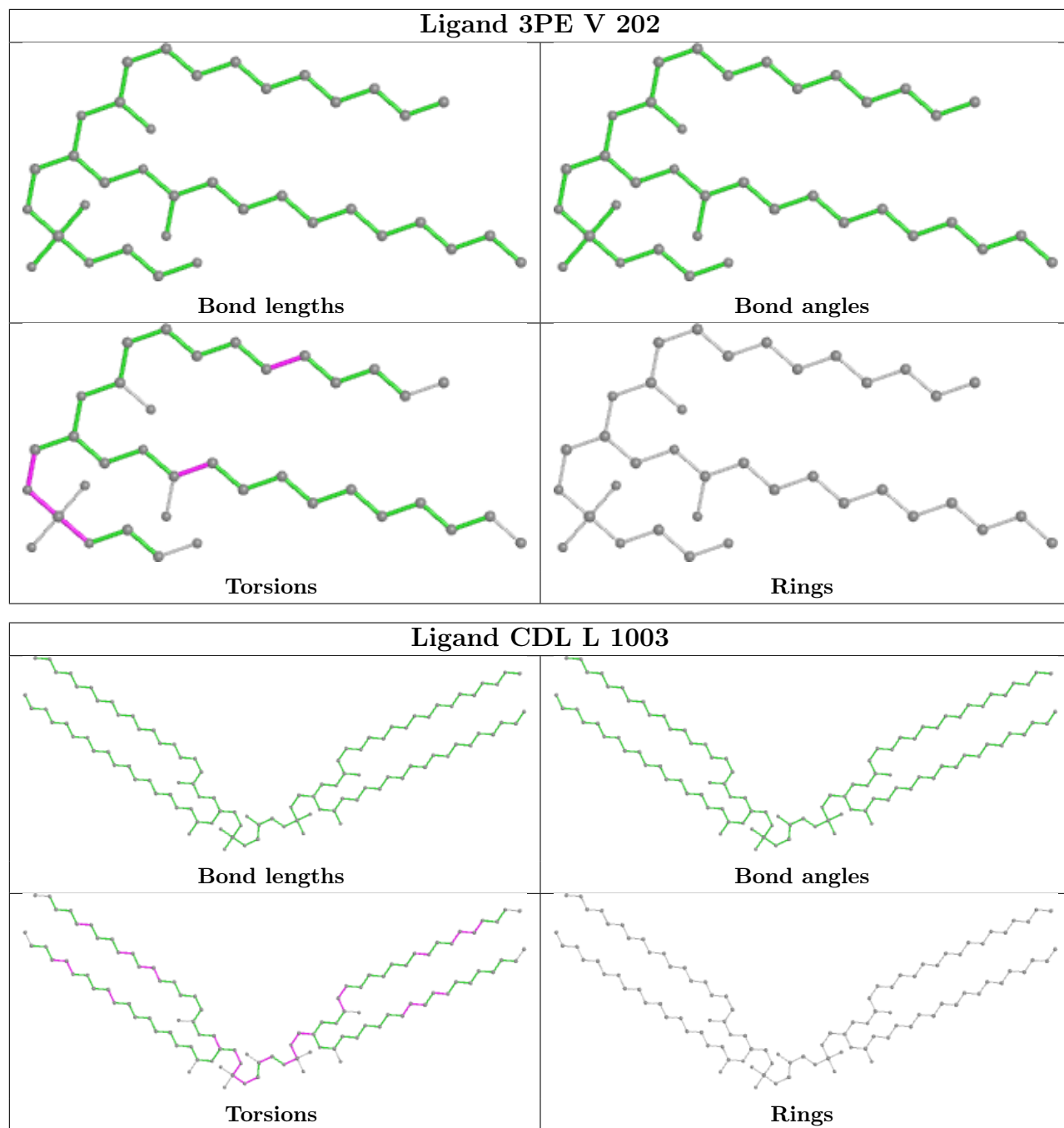


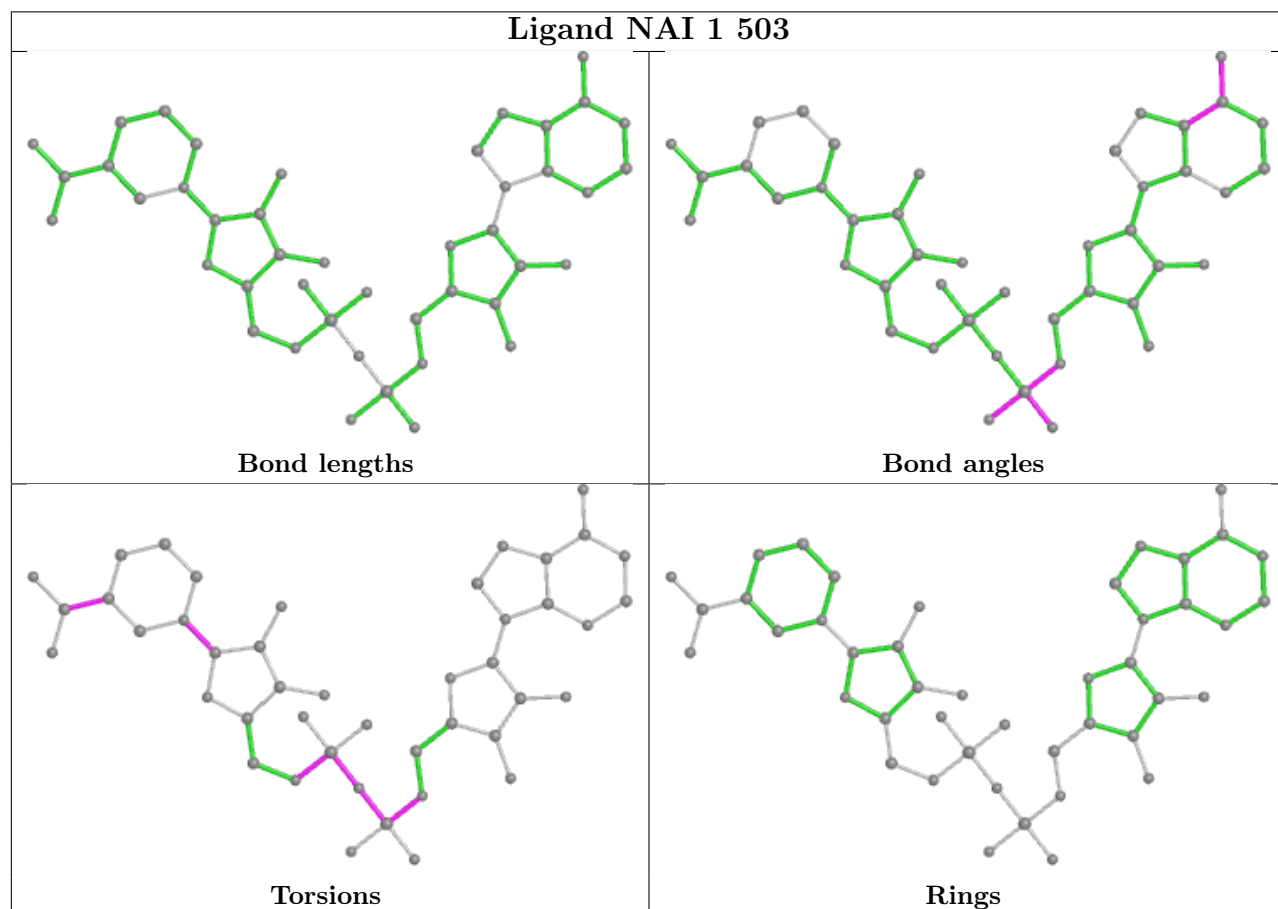
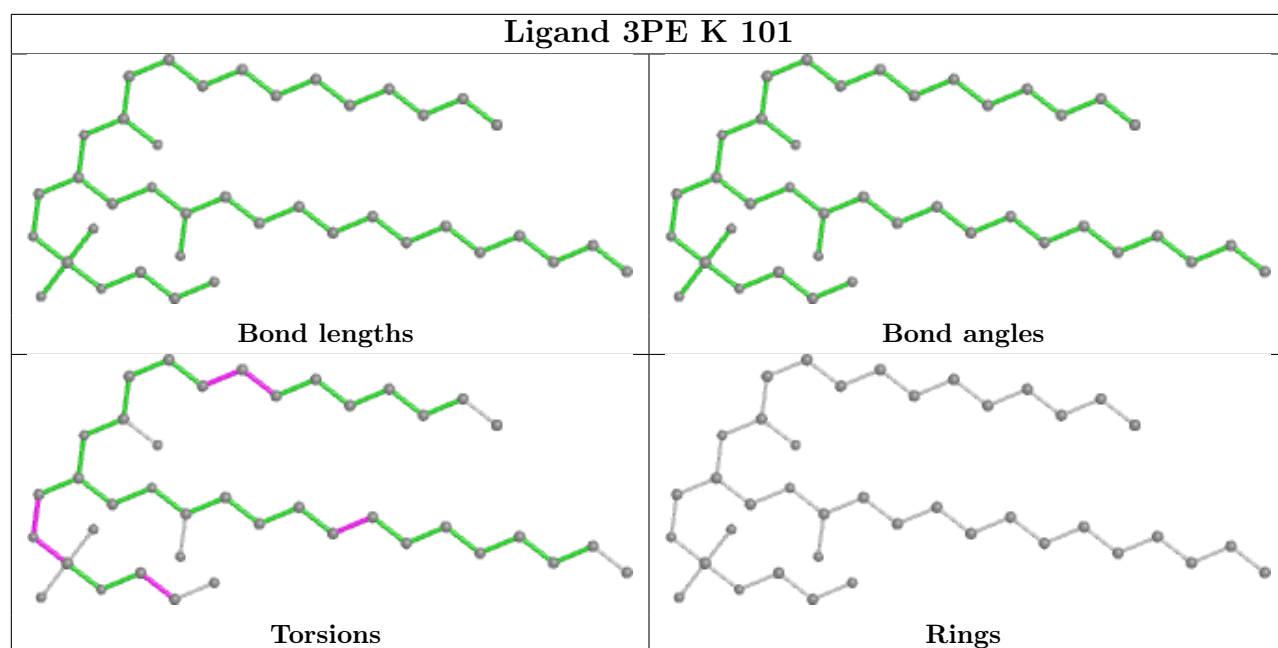


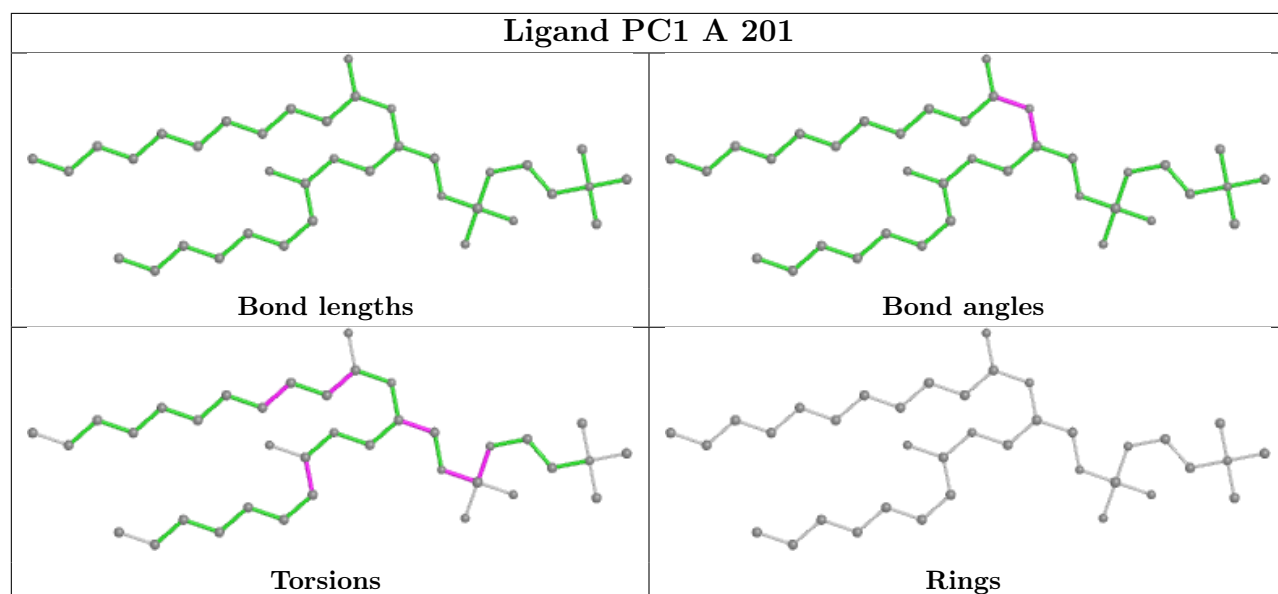
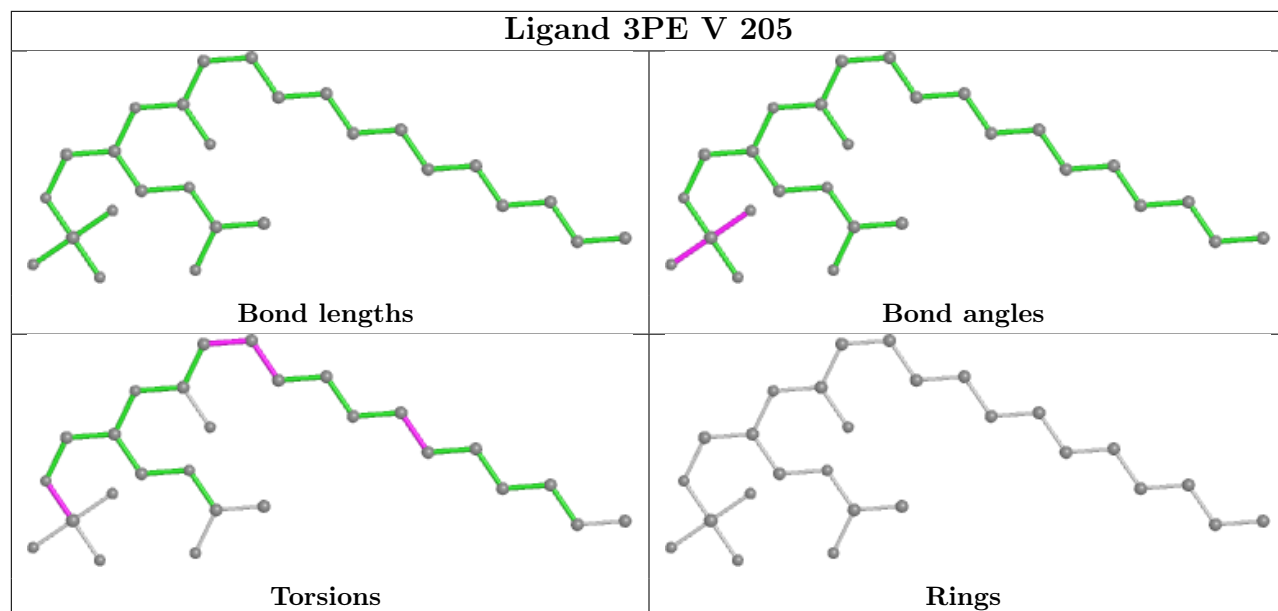


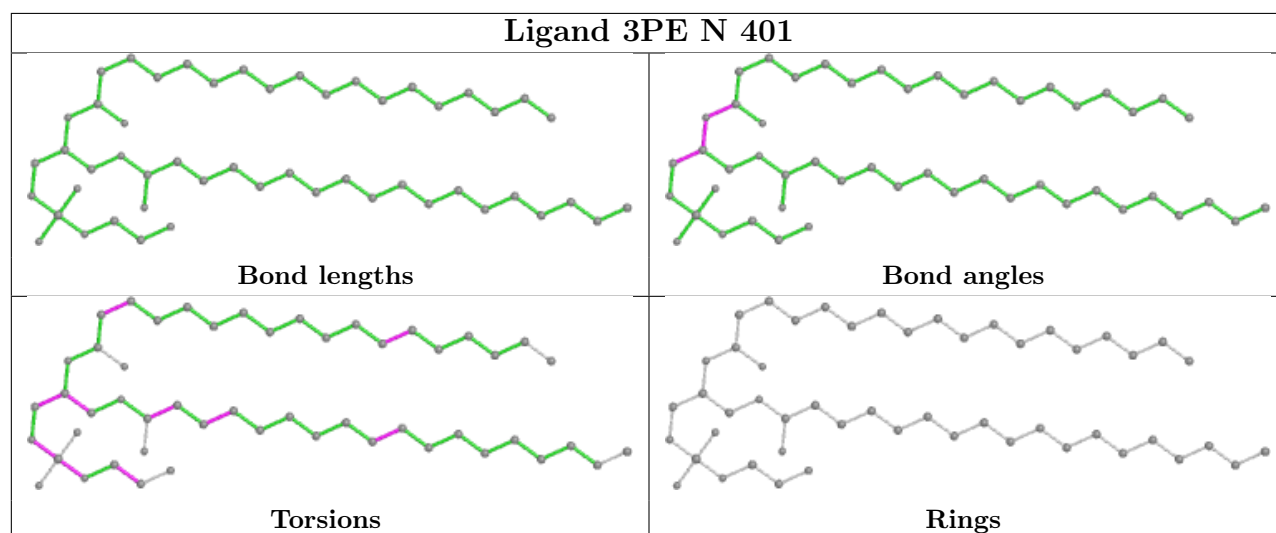
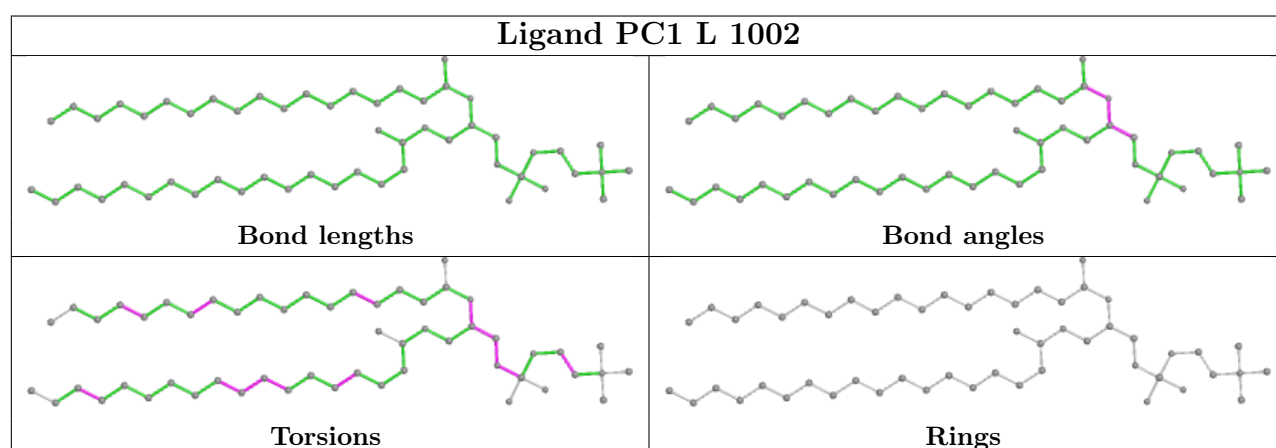
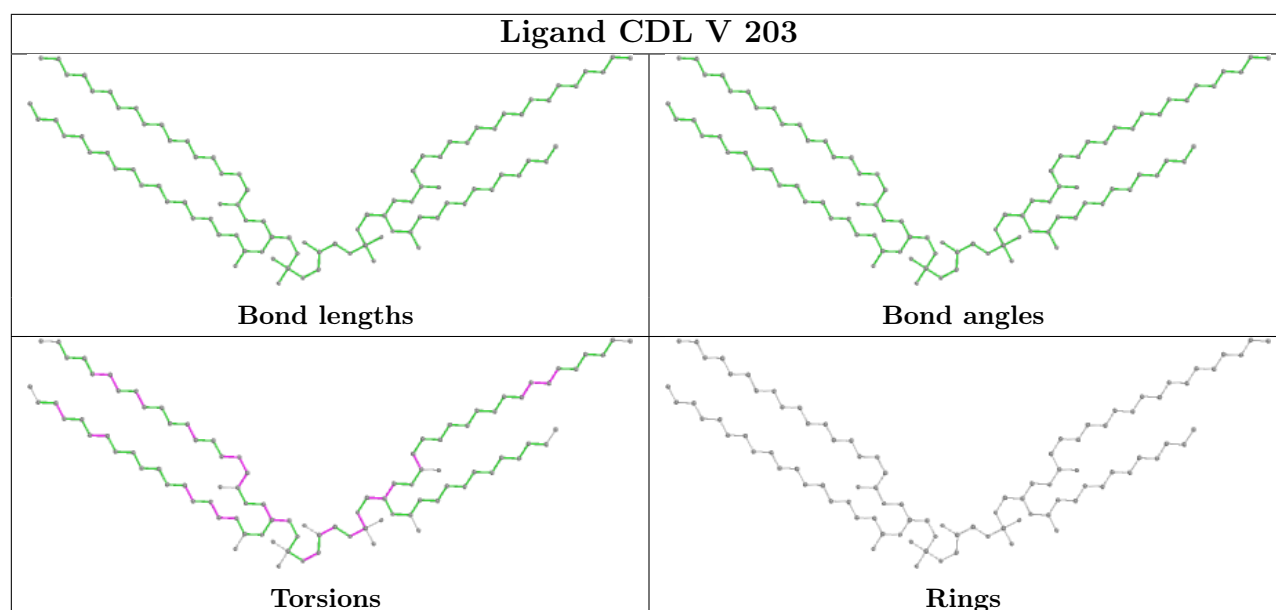


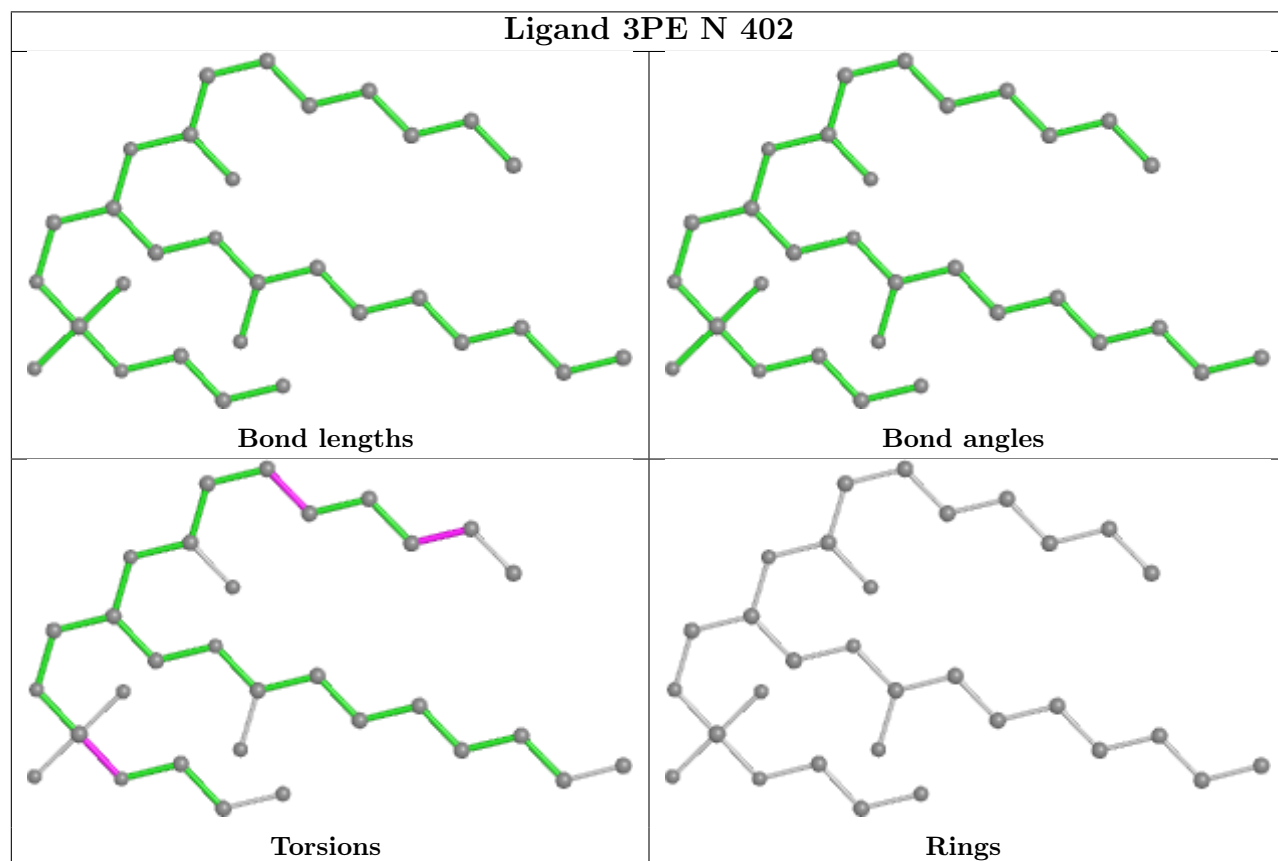
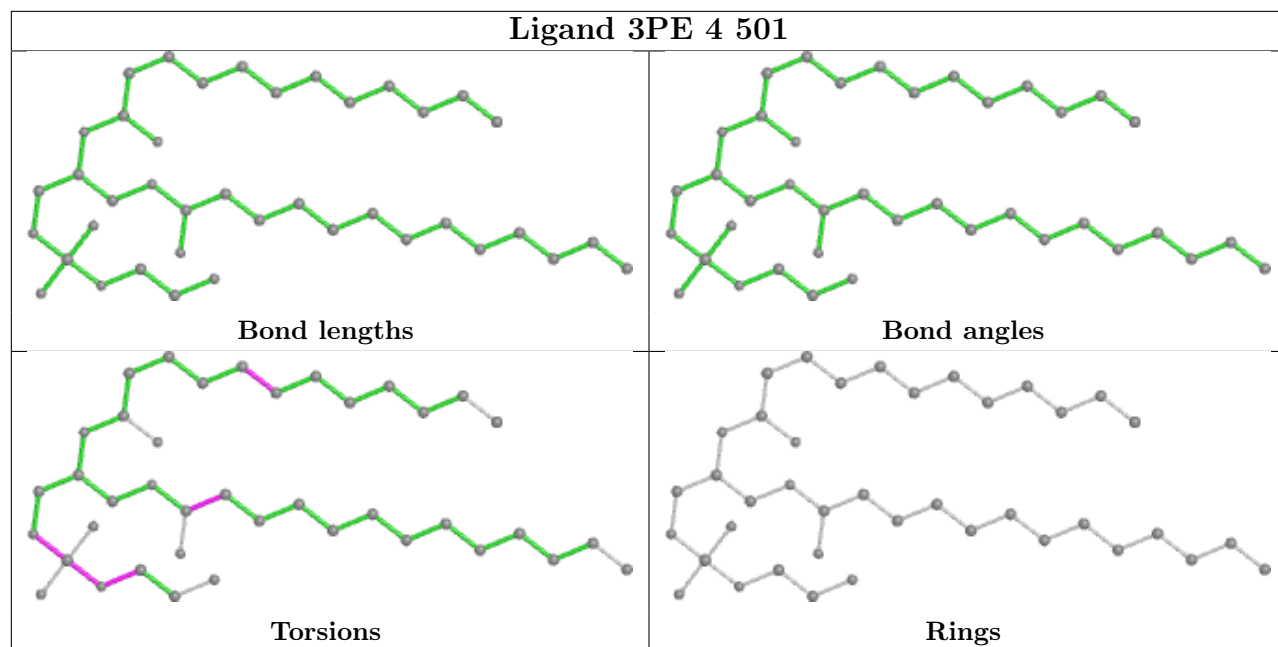


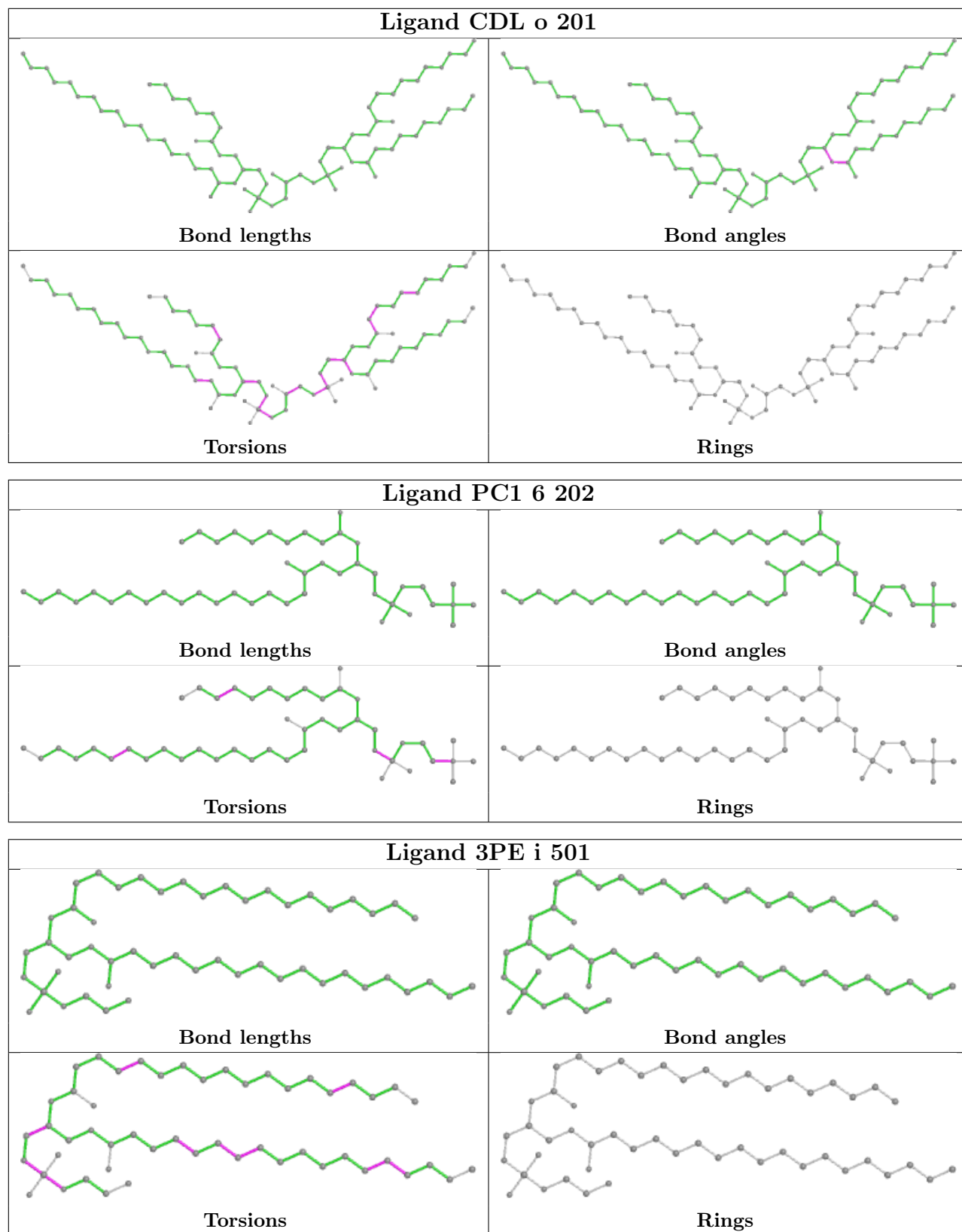


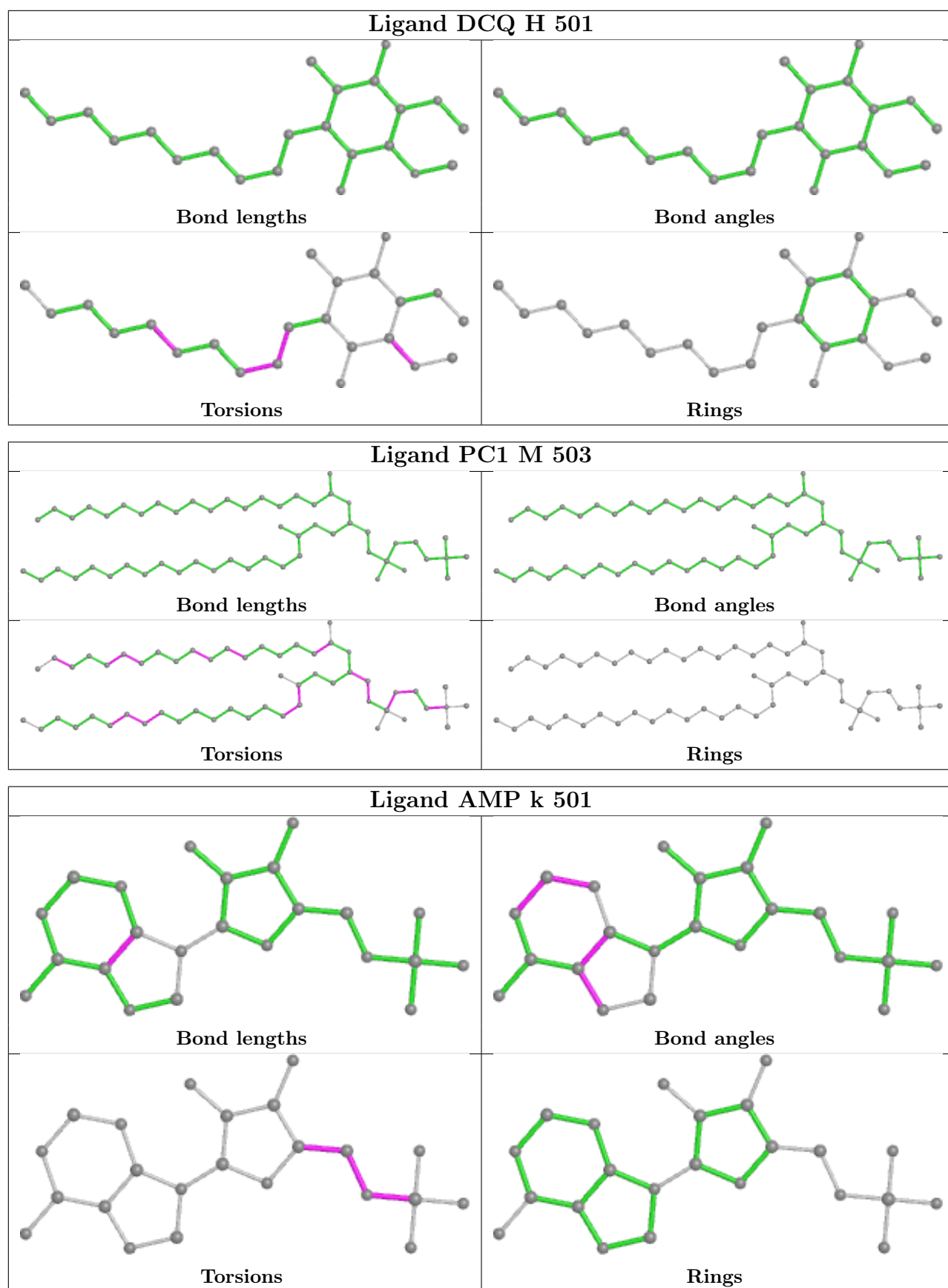












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

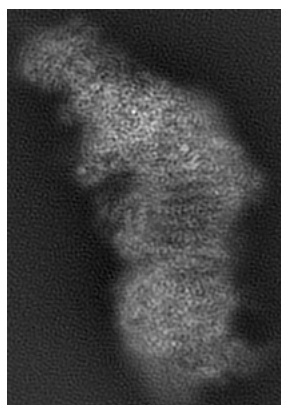
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11247. These allow visual inspection of the internal detail of the map and identification of artifacts.

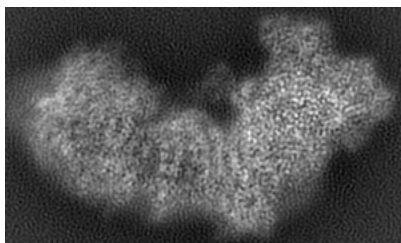
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

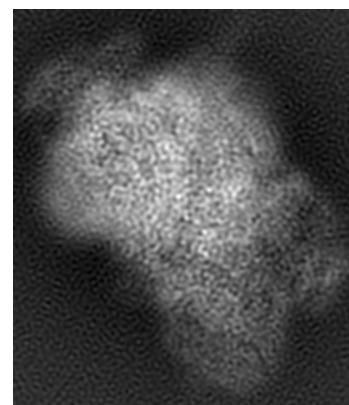
6.1.1 Primary map



X



Y

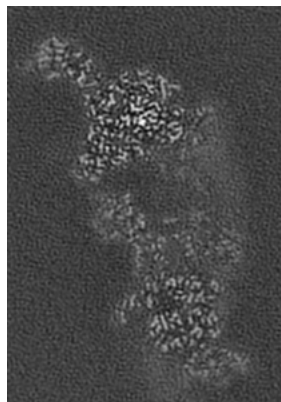


Z

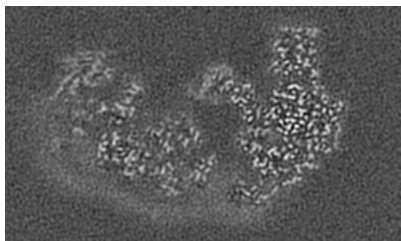
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

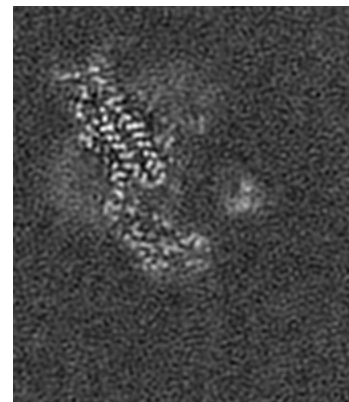
6.2.1 Primary map



X Index: 80



Y Index: 93

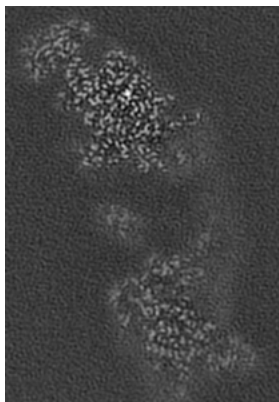


Z Index: 135

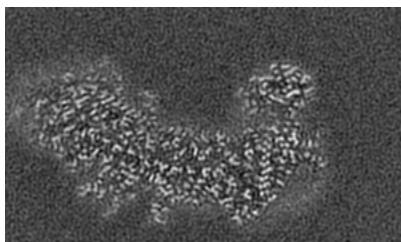
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

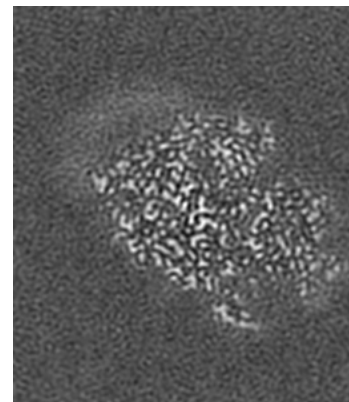
6.3.1 Primary map



X Index: 90



Y Index: 120



Z Index: 197

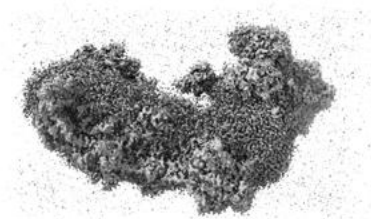
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

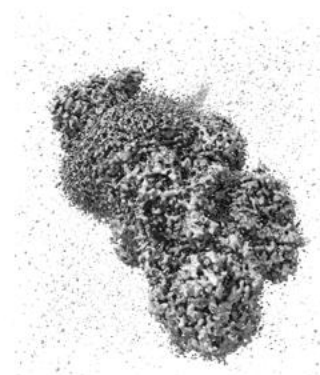
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

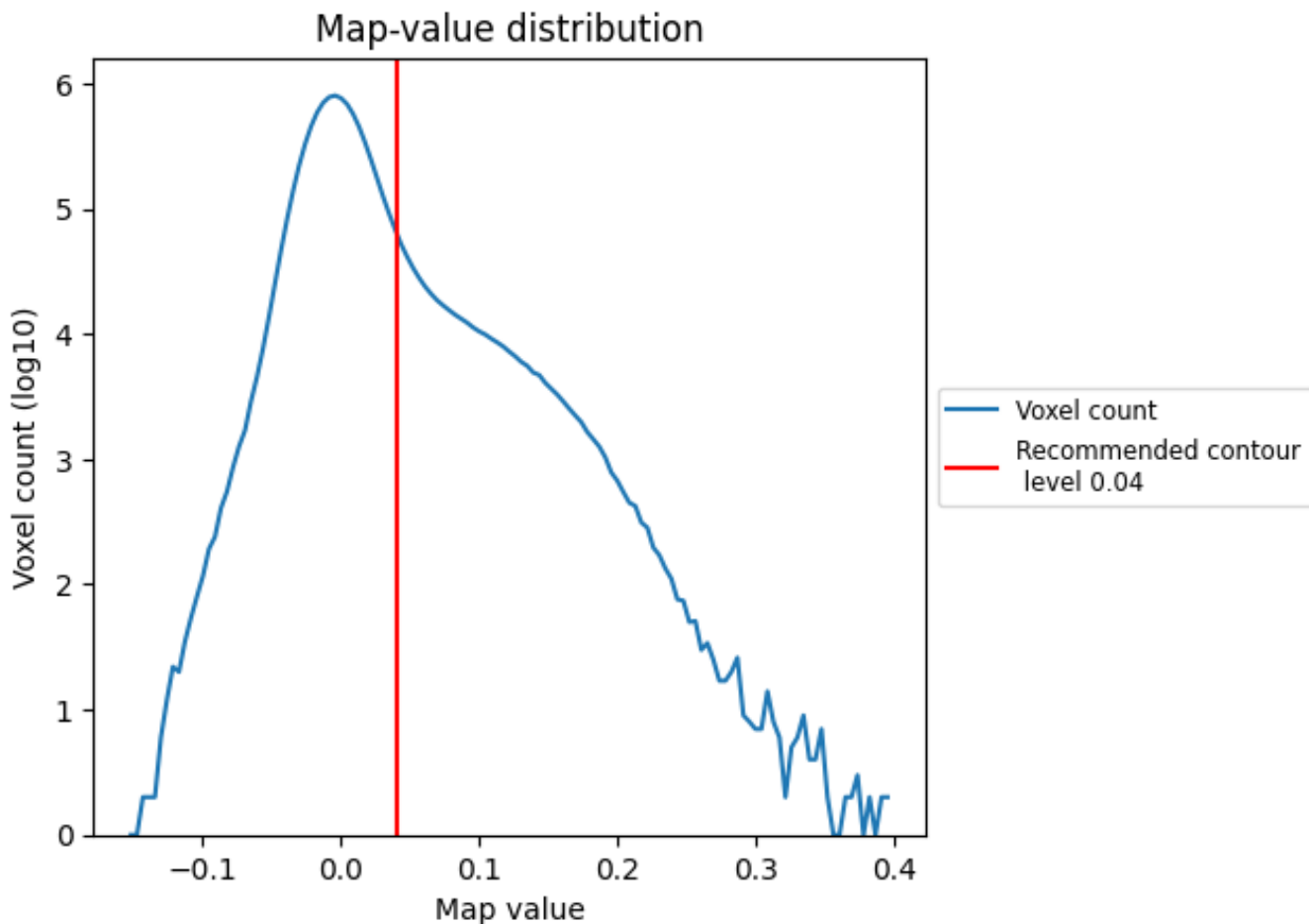
6.5 Mask visualisation

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

7 Map analysis [i](#)

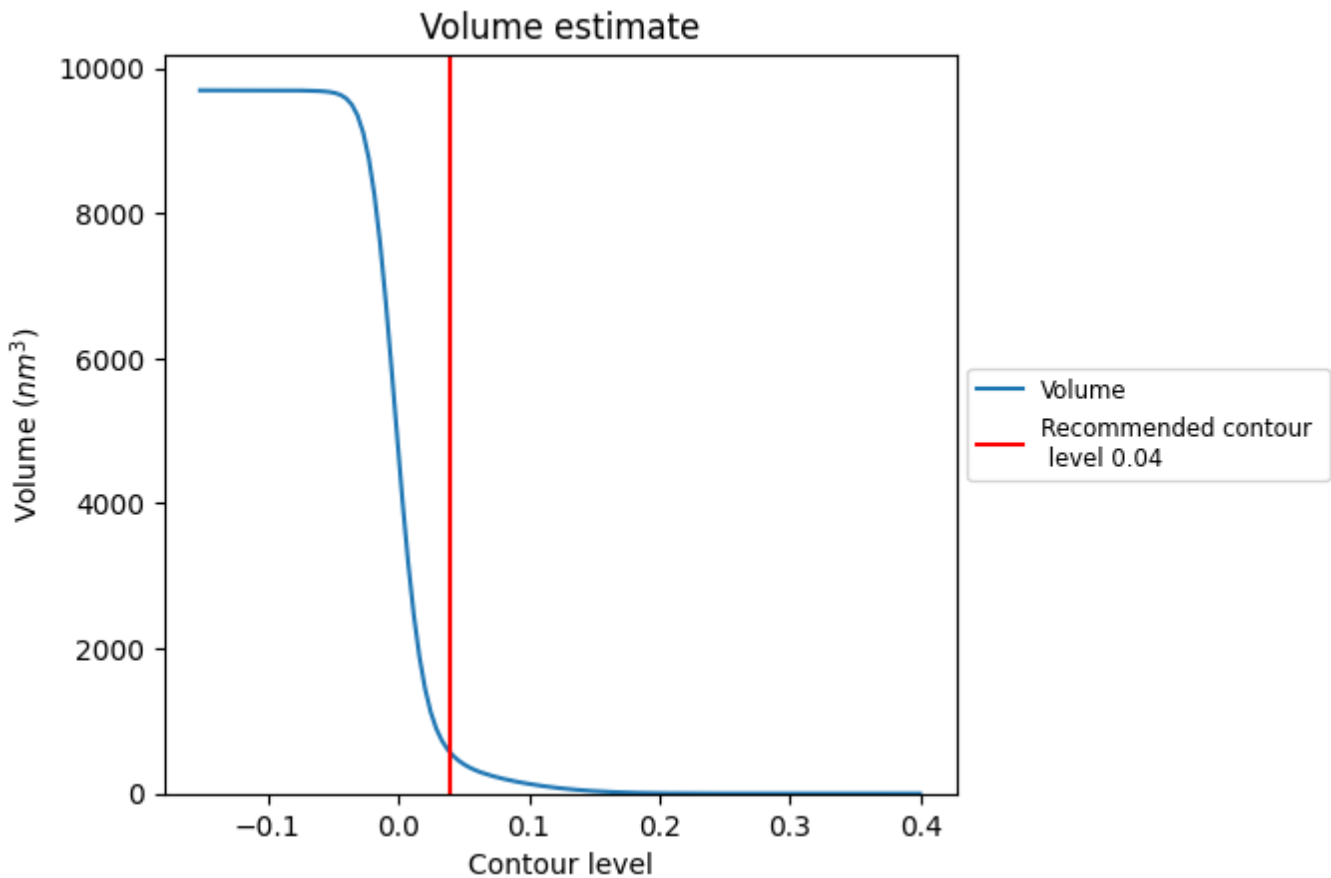
This section contains the results of statistical analysis of the map.

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 561 nm³; this corresponds to an approximate mass of 507 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.

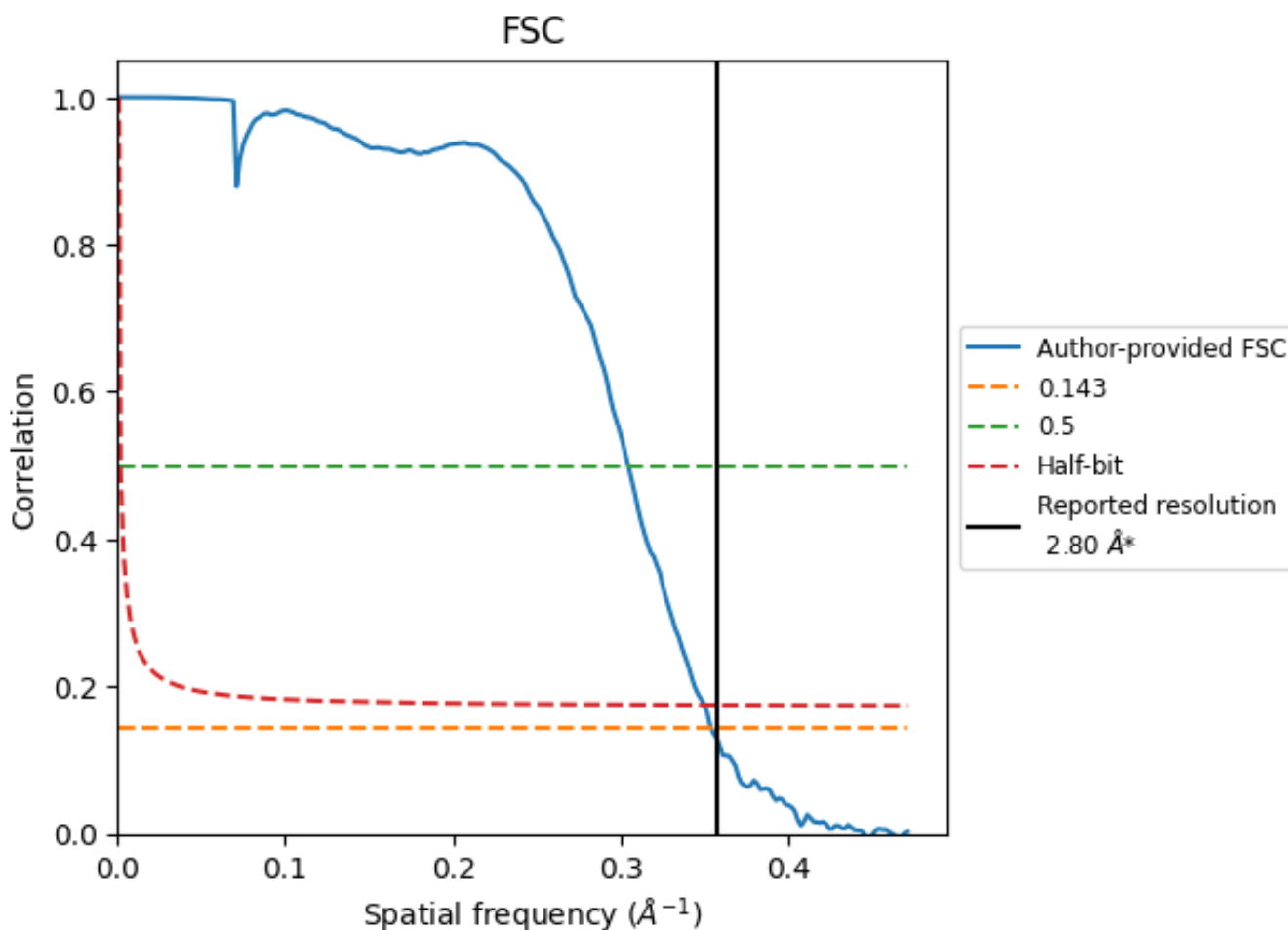
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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](#)

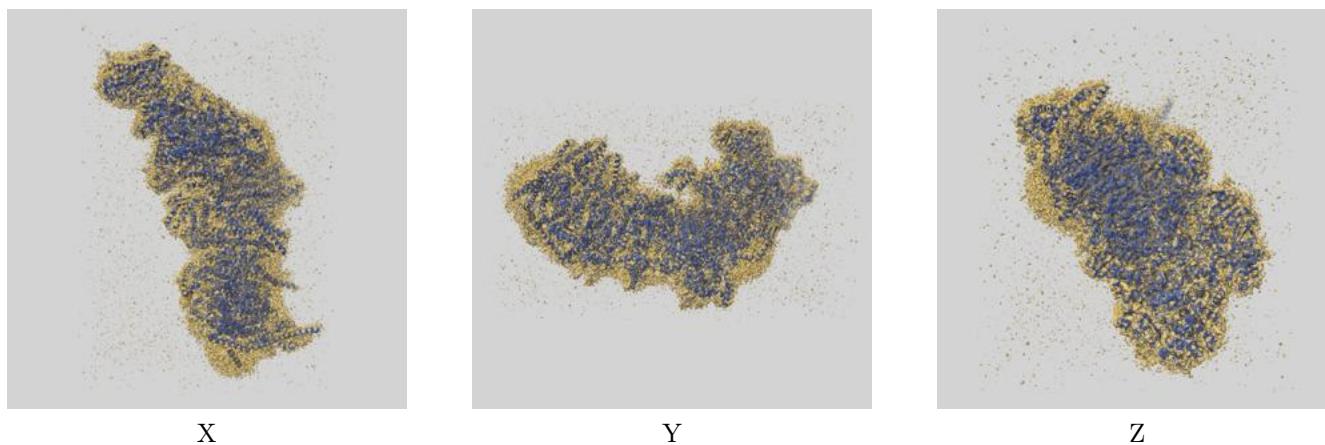
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.28	2.86
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

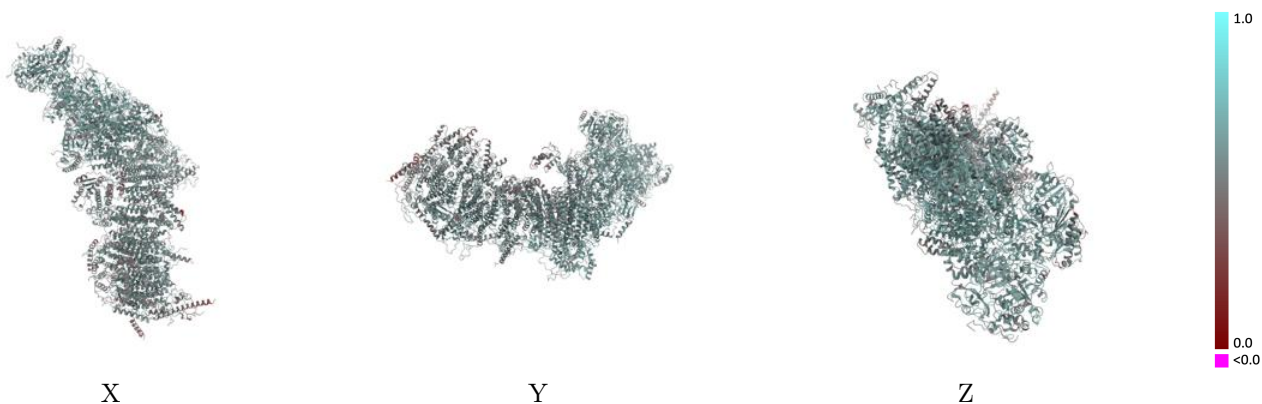
This section contains information regarding the fit between EMDB map EMD-11247 and PDB model 6ZKF. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



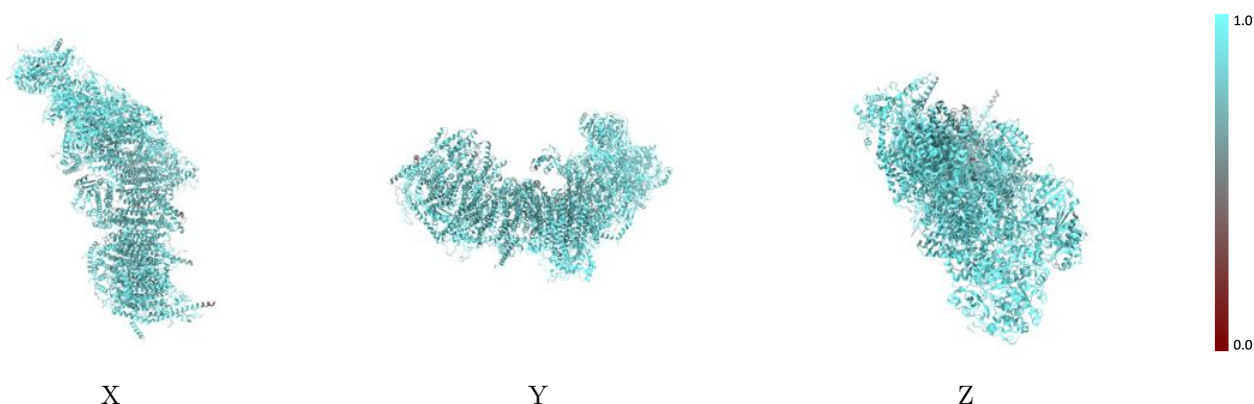
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



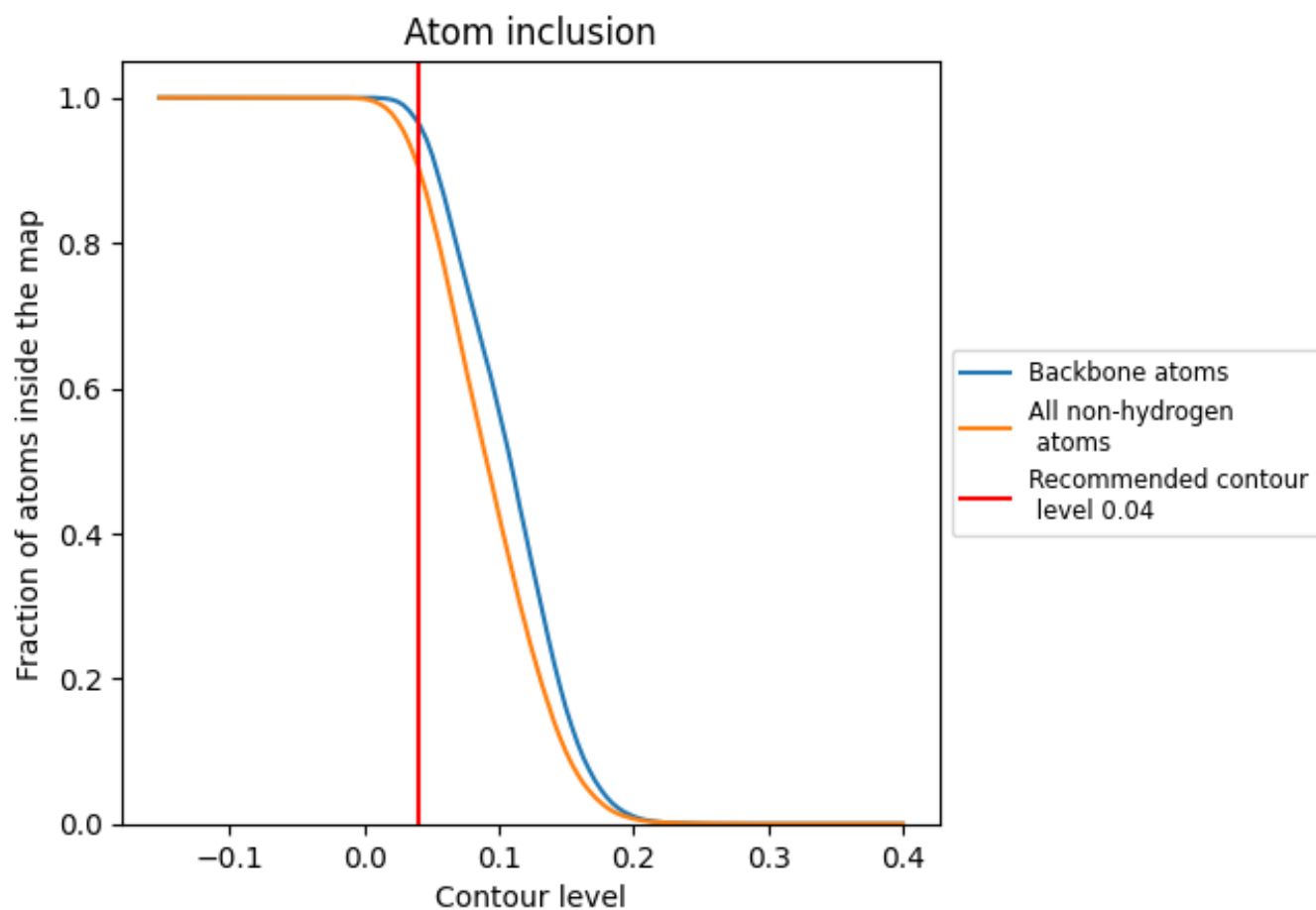
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9053	 0.5640
1	 0.9488	 0.5760
2	 0.9272	 0.5680
3	 0.9409	 0.5930
4	 0.9391	 0.6080
5	 0.9571	 0.6220
6	 0.9577	 0.6110
9	 0.9570	 0.6180
A	 0.8424	 0.5340
H	 0.9366	 0.5960
J	 0.8749	 0.5530
K	 0.9017	 0.5800
L	 0.8918	 0.5530
M	 0.9291	 0.5920
N	 0.9352	 0.5960
V	 0.7043	 0.4720
W	 0.9078	 0.5710
X	 0.8444	 0.4970
Y	 0.9121	 0.5640
Z	 0.8819	 0.5340
a	 0.9392	 0.5610
b	 0.9513	 0.6010
c	 0.9261	 0.6050
d	 0.9145	 0.5600
e	 0.9003	 0.5430
f	 0.9049	 0.5550
g	 0.9107	 0.5780
h	 0.9246	 0.5910
i	 0.9159	 0.5910
j	 0.7725	 0.4440
k	 0.8673	 0.5290
l	 0.8875	 0.5530
m	 0.9121	 0.5630
n	 0.7896	 0.4350
o	 0.8958	 0.5580



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Chain	Atom inclusion	Q-score
p	 0.8541	 0.5170
q	 0.9365	 0.5770
r	 0.8624	 0.5070
s	 0.8319	 0.4600
t	 0.8650	 0.5010
u	 0.8595	 0.4880
v	 0.8741	 0.5270
w	 0.8677	 0.5440
x	 0.8586	 0.5280
y	 0.8629	 0.5100
z	 0.9313	 0.5810