



Full wwPDB EM Validation Report ⓘ

Jul 20, 2024 – 08:32 am BST

PDB ID : 8RGP
EMDB ID : EMD-19145
Title : Closed Complex I from murine brain
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-12-14
Resolution : 3.00 Å (reported)
Based on initial model : 6g2j

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:

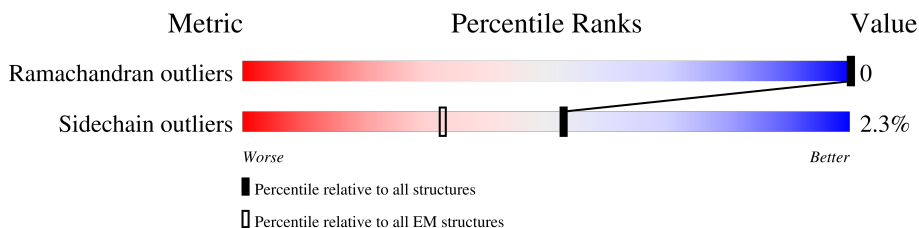
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.00 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	6	224	67% (green), 31% (grey)
2	C	263	78% (green), 21% (grey)
3	D	463	5% (red), 92% (green), 7% (grey)
4	2	248	83% (green), 14% (grey)
5	1	464	91% (green), 7% (grey)
6	3	727	93% (green), 5% (grey)
7	9	212	83% (green), 16% (grey)
8	P	377	89% (green), 9% (grey)
9	Q	175	71% (green), 28% (grey)

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Mol	Chain	Length	Quality of chain
10	7	116	82% 17%
11	S	99	82% 15%
12	T	156	50% 49%
12	U	156	56% 44%
13	V	116	93%
14	W	131	85% 13%
15	q	145	98%
16	r	113	86% 12%
17	s	104	38% 61%
18	A	115	97%
19	H	318	97%
20	J	172	12% 97%
21	K	98	98%
22	L	607	97%
23	M	459	98%
24	N	345	97%
25	O	355	88% 10%
26	X	172	95% 5%
27	Y	141	95%
28	Z	144	97%
29	a	70	100%
30	b	84	5% 96%
31	c	76	62% 37%
32	d	120	98%
33	e	106	99%

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Mol	Chain	Length	Quality of chain
34	f	57	
35	g	151	
36	h	189	
37	i	128	
38	j	105	
39	k	104	
40	l	186	
41	m	129	
42	n	179	
43	o	137	
44	p	176	

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
37	SAC	i	1	-	X	-	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 67868 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] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	155	1241	793	222	212	14	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	207	1721	1110	295	313	3	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	430	3464	2215	595	630	24	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	214	1660	1056	279	314	11	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1	430	3321	2092	596	611	22	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	3	690	5305	3326	921	1017	41	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	9	178	1431	898	245	276	12	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	342	2748	1777	483	481	7	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	126	1022	646	180	192	4	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	7	96	758	470	141	144	3	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	84	671	421	127	120	3	0	0

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	79	637	410	95	127	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	88	706	453	104	144	5	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	112	915	596	152	164	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	114	970	619	180	165	6	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	q	145	1209	777	215	212	5	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	r	99	796	504	148	141	3	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	s	41	344	215	61	68	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	A	115	932	633	132	160	7	0	0

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	318	2540	1706	384	428	22	0	0

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	172	1308	878	186	229	15	0	0

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	K	98	737	477	112	137	11	0	0

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	L	606	4800	3182	746	827	45	0	0

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	M	459	3632	2408	567	617	40	0	0

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	N	345	2703	1795	417	454	37	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	O	320	2607	1674	431	492	10	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	171	1396	889	250	247	10	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	140	1037	662	175	192	8	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	141	1167	750	207	202	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	70	572	370	101	97	4	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	83	651	427	105	115	4	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	48	398	261	69	67	1	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	120	996	651	171	165	9	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	105	877	555	162	152	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	53	456	295	82	77	2	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	101	850	549	136	161	4	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	139	1166	764	195	204	3	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	98	828	537	146	142	3	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	64	555	365	92	97	1	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	77	626	414	106	104	2	0	0

- 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	l	157	1323	855	220	237	11	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	m	126	1050	676	189	185	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	178	1541	985	276	269	11	0	0

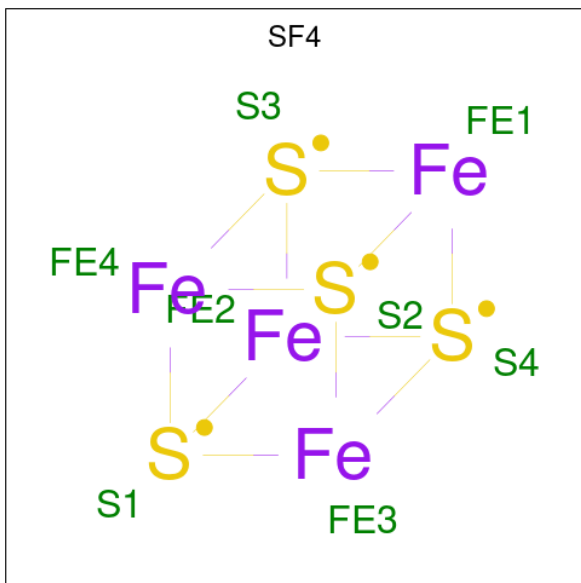
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	118	1014	639	190	177	8	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

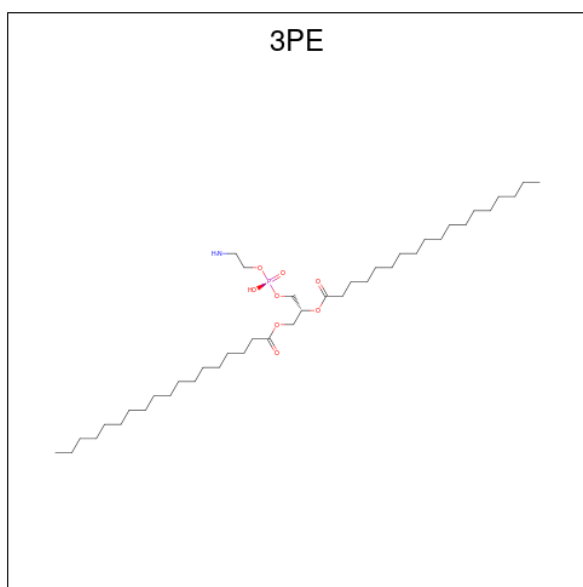
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	170	1438	903	258	269	8	0	0

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



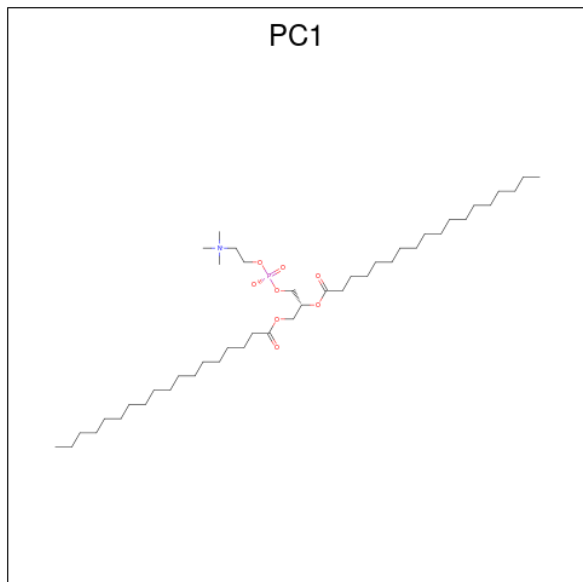
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	6	1	8	4	4	0
45	1	1	8	4	4	0
45	3	1	8	4	4	0
45	3	1	8	4	4	0
45	9	1	8	4	4	0
45	9	1	8	4	4	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



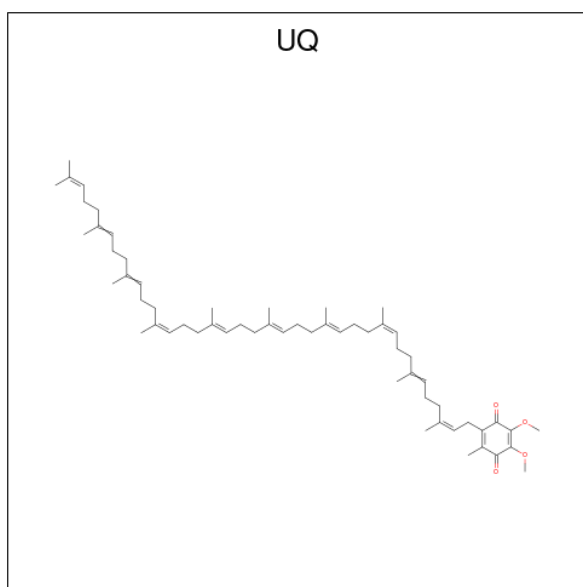
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	6	1	Total 32	22	1	8	1	0
46	D	1	Total 51	41	1	8	1	0
46	A	1	Total 43	33	1	8	1	0
46	K	1	Total 41	31	1	8	1	0
46	L	1	Total 51	41	1	8	1	0
46	L	1	Total 42	32	1	8	1	0
46	M	1	Total 51	41	1	8	1	0
46	M	1	Total 36	26	1	8	1	0
46	Y	1	Total 28	18	1	8	1	0
46	Z	1	Total 51	41	1	8	1	0
46	d	1	Total 31	21	1	8	1	0
46	h	1	Total 51	41	1	8	1	0
46	i	1	Total 42	32	1	8	1	0
46	m	1	Total 30	20	1	8	1	0

- Molecule 47 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	
47	6	1	Total 43	33	1	8	1	0
47	9	1	Total 54	44	1	8	1	0
47	H	1	Total 42	32	1	8	1	0
47	M	1	Total 54	44	1	8	1	0
47	Z	1	Total 47	37	1	8	1	0

- Molecule 48 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



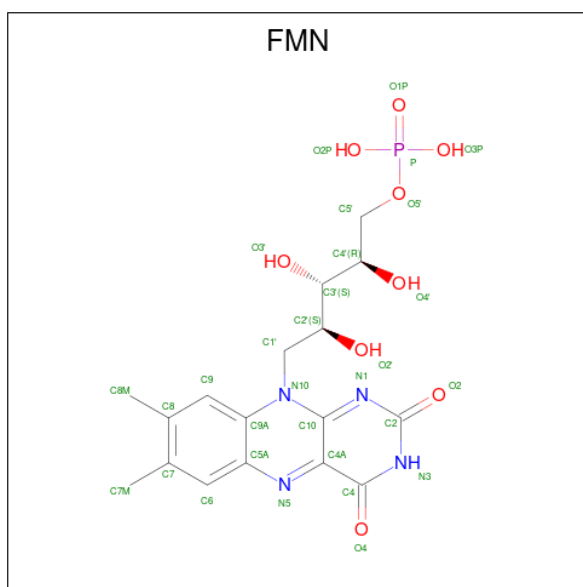
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	D	1	63	59	4	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	2	1	4	2	2	0
49	3	1	4	2	2	0

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

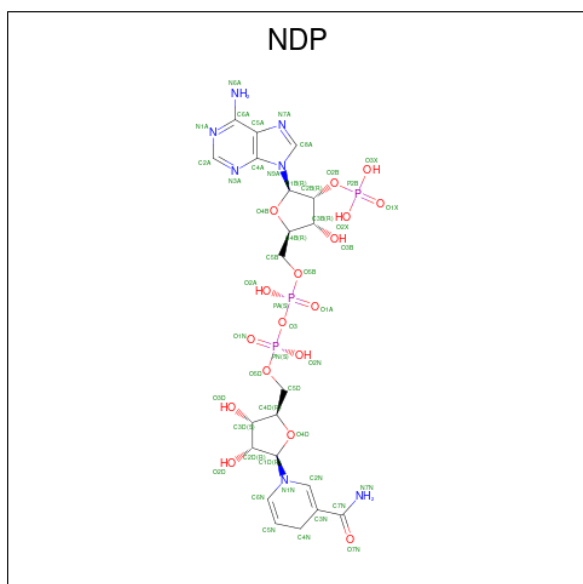


Mol	Chain	Residues	Atoms					AltConf
50	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
51	3	1	Total	K	0
			1	1	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

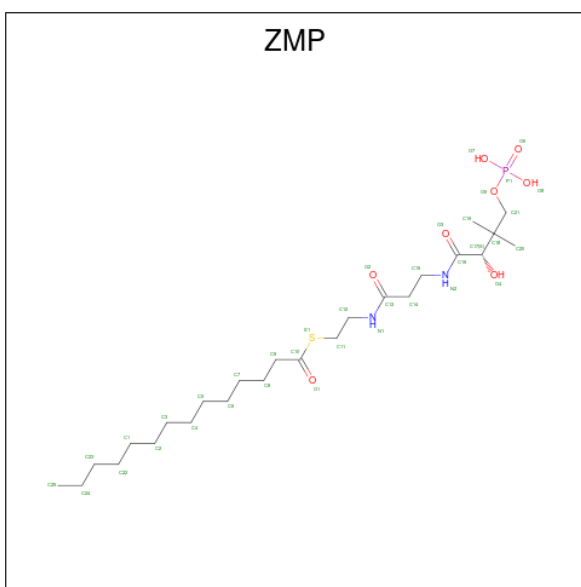


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	P	1	48	21	7	17	3	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
53	7	1	1	1	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	W	1	34	23	2	7	1	1	0
54	n	1	32	21	2	7	1	1	0

- Molecule 55 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
55	r	1	57	38	17	2	0
55	L	1	78	59	17	2	0
55	L	1	46	27	17	2	0
55	N	1	90	71	17	2	0
55	Y	1	94	75	17	2	0
55	Y	1	57	38	17	2	0
55	d	1	67	48	17	2	0
55	h	1	70	51	17	2	0
55	m	1	72	53	17	2	0

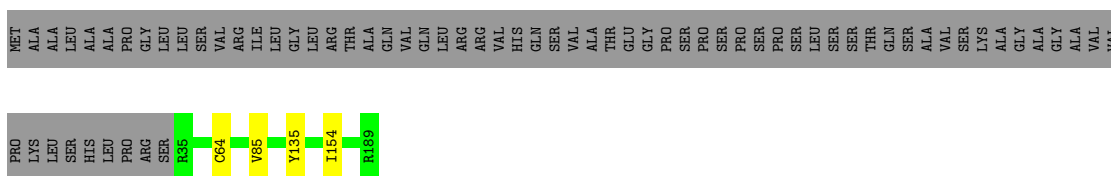
- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).

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.

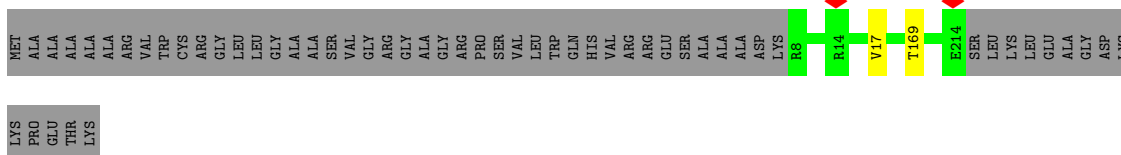
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:  67% 31%



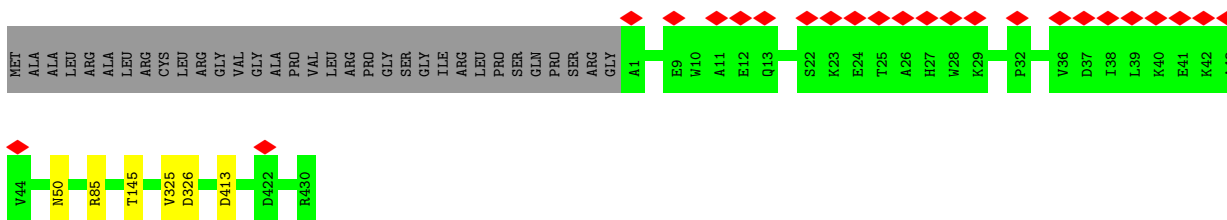
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  78% 21%




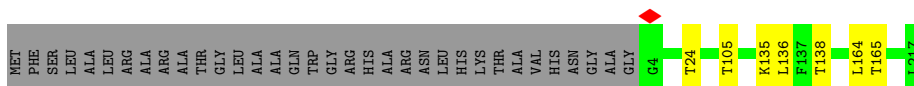
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  5% 92% 7%




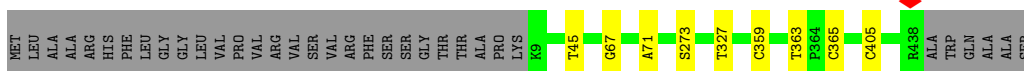
- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2:  83% 14%



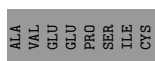
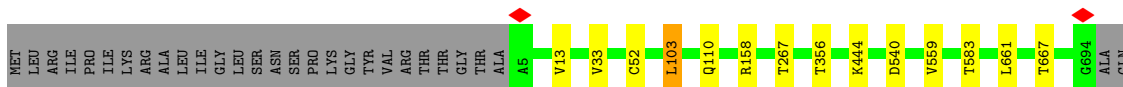
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:  91% 7%




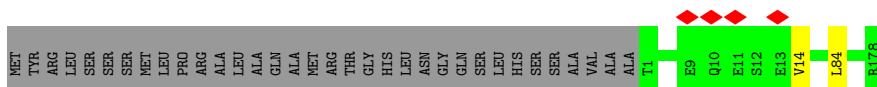
- Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:  93% 5%




- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:  83% 16%



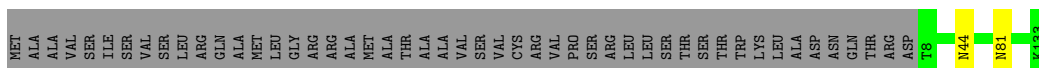
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  89% 9%




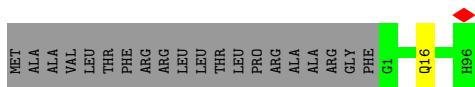
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  71% 28%

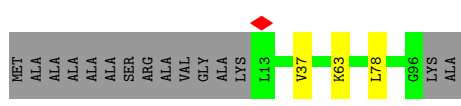
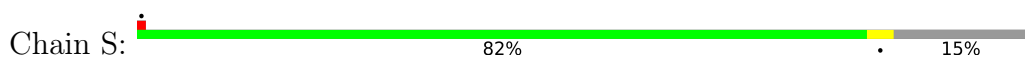


- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

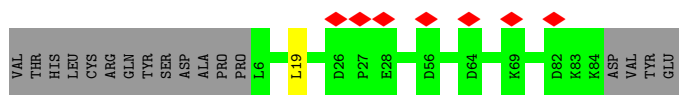
Chain 7:  82% 17%



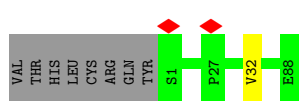
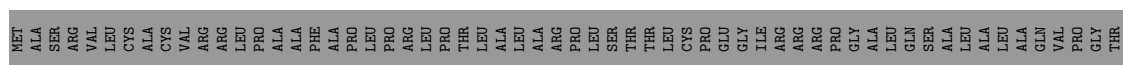
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



• Molecule 12: Acyl carrier protein, mitochondrial



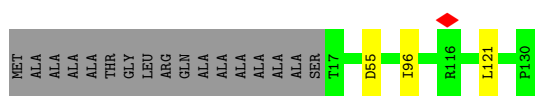
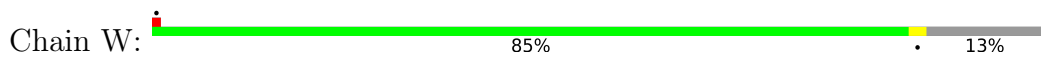
• Molecule 12: Acyl carrier protein, mitochondrial



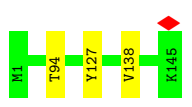
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

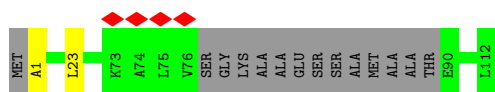


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  86% 12%



- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:  38% 61%



- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain A:  97%



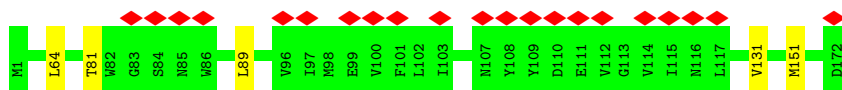
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

Chain H:  97%



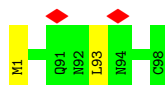
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain J:  12% 97%



- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  98%



- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain L:  97%



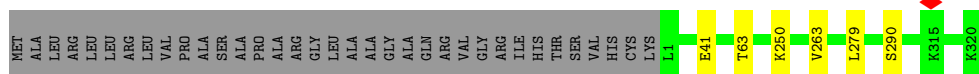
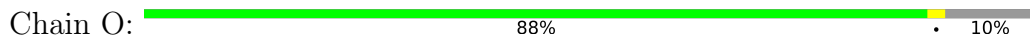
- Molecule 23: NADH-ubiquinone oxidoreductase chain 4



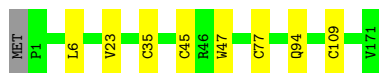
- Molecule 24: NADH-ubiquinone oxidoreductase chain 2



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



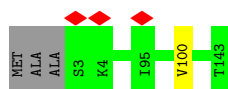
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



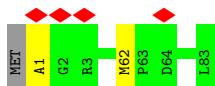
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  100%



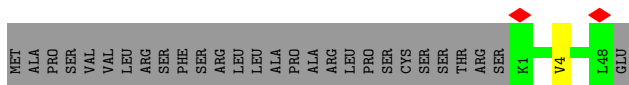
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  96% 5%



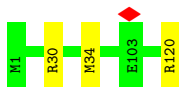
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  62% 37%



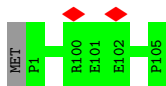
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  98%




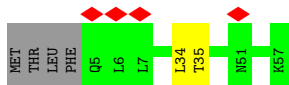
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  99%



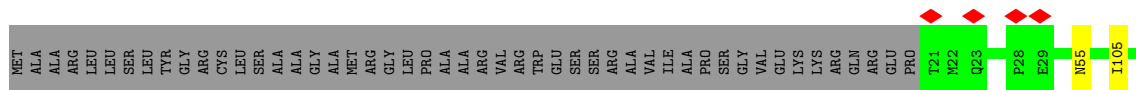
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  89% 7%

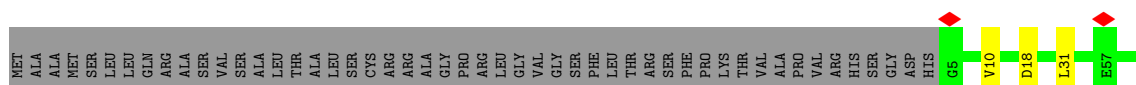


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

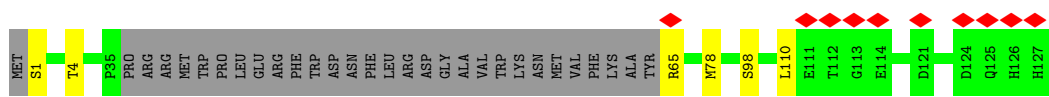
Chain g:  66% 33%



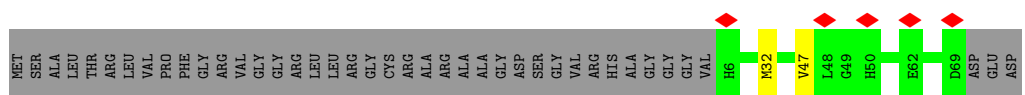
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



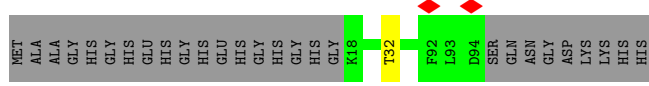
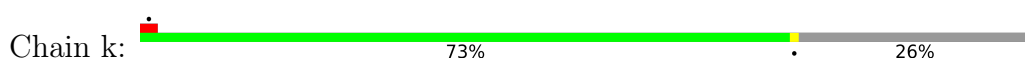
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



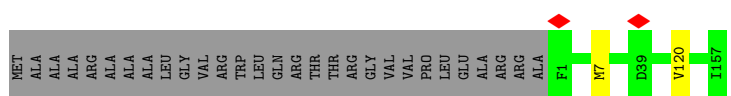
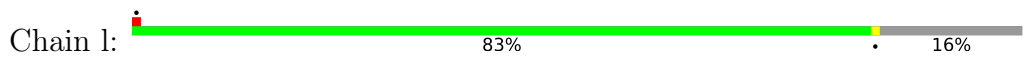
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

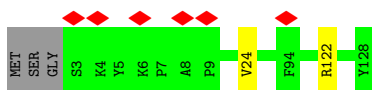


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



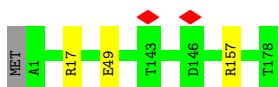
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:  5% 96% ..




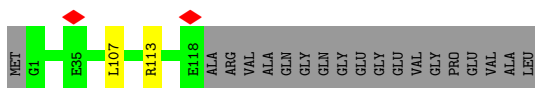
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:  98% ..



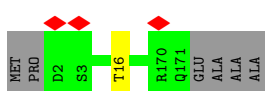
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  85% 14%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  96% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95155	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.149	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	226.83998, 214.12, 203.51999	wwPDB
Map dimensions	214, 202, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: SAC, AYA, SF4, UQ, K, ZMP, PC1, DGT, FMN, 2MR, ZN, MG, 3PE, NDP, FES, CDL, FME

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	6	0.40	0/1272	0.55	0/1722
2	C	0.35	0/1771	0.55	0/2413
3	D	0.36	0/3540	0.54	0/4795
4	2	0.33	0/1700	0.54	0/2316
5	1	0.53	2/3396 (0.1%)	0.59	3/4586 (0.1%)
6	3	0.34	0/5392	0.54	2/7305 (0.0%)
7	9	0.36	0/1461	0.55	1/1974 (0.1%)
8	P	0.33	0/2823	0.55	0/3828
9	Q	0.31	0/1045	0.51	0/1411
10	7	0.34	0/773	0.52	0/1041
11	S	0.33	0/682	0.58	1/920 (0.1%)
12	T	0.27	0/646	0.54	0/869
12	U	0.32	0/718	0.52	0/970
13	V	0.30	0/937	0.46	0/1270
14	W	0.31	0/993	0.52	0/1335
15	q	0.34	0/1251	0.55	0/1702
16	r	0.32	0/806	0.53	0/1090
17	s	0.34	0/353	0.55	0/479
18	A	0.32	0/948	0.52	1/1295 (0.1%)
19	H	0.37	0/2607	0.54	1/3564 (0.0%)
20	J	0.35	0/1330	0.48	0/1810
21	K	0.32	0/738	0.50	0/1002
22	L	0.34	0/4913	0.52	0/6686
23	M	0.34	0/3709	0.53	0/5052
24	N	0.33	0/2755	0.52	1/3751 (0.0%)
25	O	0.34	0/2674	0.49	0/3626
26	X	0.31	0/1434	0.54	0/1937
27	Y	0.31	0/1061	0.47	0/1439
28	Z	0.32	0/1198	0.51	0/1616
29	a	0.33	0/585	0.54	0/788
30	b	0.30	0/666	0.45	0/914
31	c	0.29	0/409	0.45	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.33	0/1028	0.50	0/1387
33	e	0.30	0/900	0.49	0/1199
34	f	0.29	0/468	0.56	0/630
35	g	0.34	0/878	0.48	0/1196
36	h	0.33	0/1201	0.51	0/1626
37	i	0.30	0/846	0.53	0/1149
38	j	0.31	0/580	0.48	0/794
39	k	0.30	0/646	0.47	0/873
40	l	0.34	0/1379	0.48	0/1882
41	m	0.32	0/1079	0.53	0/1463
42	n	0.33	0/1596	0.51	0/2162
43	o	0.29	0/1039	0.50	0/1394
44	p	0.31	0/1471	0.51	0/1988
All	All	0.35	2/67697 (0.0%)	0.53	10/91804 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	67	GLY	C-N	-17.12	0.94	1.34
5	1	71	ALA	C-N	15.12	1.60	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	71	ALA	O-C-N	7.01	135.13	123.20
24	N	148	LEU	CA-CB-CG	6.43	130.08	115.30
5	1	71	ALA	CA-C-N	-6.17	103.87	116.20
5	1	71	ALA	C-N-CA	-5.93	109.85	122.30
19	H	233	LEU	CB-CG-CD1	-5.71	101.28	111.00
18	A	98	LEU	CA-CB-CG	5.45	127.83	115.30
6	3	103	LEU	CA-CB-CG	5.40	127.72	115.30
11	S	78	LEU	CA-CB-CG	5.20	127.27	115.30
7	9	84	LEU	CA-CB-CG	5.09	127.02	115.30
6	3	661	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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	6	153/224 (68%)	146 (95%)	7 (5%)	0	100	100
2	C	205/263 (78%)	193 (94%)	12 (6%)	0	100	100
3	D	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
4	2	212/248 (86%)	189 (89%)	23 (11%)	0	100	100
5	1	428/464 (92%)	399 (93%)	29 (7%)	0	100	100
6	3	688/727 (95%)	643 (94%)	45 (6%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	340/377 (90%)	310 (91%)	30 (9%)	0	100	100
9	Q	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
10	7	94/116 (81%)	88 (94%)	6 (6%)	0	100	100
11	S	82/99 (83%)	73 (89%)	9 (11%)	0	100	100
12	T	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
12	U	86/156 (55%)	80 (93%)	6 (7%)	0	100	100
13	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
14	W	112/131 (86%)	105 (94%)	7 (6%)	0	100	100
15	q	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
16	r	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
17	s	39/104 (38%)	38 (97%)	1 (3%)	0	100	100
18	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
19	H	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
20	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
22	L	604/607 (100%)	558 (92%)	46 (8%)	0	100	100
23	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
24	N	343/345 (99%)	330 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	O	318/355 (90%)	295 (93%)	23 (7%)	0	100	100
26	X	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
27	Y	138/141 (98%)	138 (100%)	0	0	100	100
28	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
29	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
31	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
32	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
33	e	103/106 (97%)	91 (88%)	12 (12%)	0	100	100
34	f	51/57 (90%)	42 (82%)	9 (18%)	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	129 (94%)	8 (6%)	0	100	100
37	i	94/128 (73%)	83 (88%)	11 (12%)	0	100	100
38	j	62/105 (59%)	58 (94%)	4 (6%)	0	100	100
39	k	75/104 (72%)	72 (96%)	3 (4%)	0	100	100
40	l	155/186 (83%)	147 (95%)	8 (5%)	0	100	100
41	m	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
42	n	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
43	o	116/137 (85%)	107 (92%)	9 (8%)	0	100	100
44	p	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
All	All	8127/9212 (88%)	7635 (94%)	492 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	6	131/185 (71%)	127 (97%)	4 (3%)	40	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	189/227 (83%)	187 (99%)	2 (1%)	73	90
3	D	370/394 (94%)	365 (99%)	5 (1%)	67	88
4	2	184/206 (89%)	177 (96%)	7 (4%)	33	69
5	1	345/370 (93%)	338 (98%)	7 (2%)	55	83
6	3	580/610 (95%)	567 (98%)	13 (2%)	52	81
7	9	152/178 (85%)	151 (99%)	1 (1%)	84	94
8	P	299/325 (92%)	292 (98%)	7 (2%)	50	80
9	Q	113/153 (74%)	111 (98%)	2 (2%)	59	85
10	7	81/96 (84%)	80 (99%)	1 (1%)	71	90
11	S	74/80 (92%)	72 (97%)	2 (3%)	44	77
12	T	73/135 (54%)	72 (99%)	1 (1%)	67	88
12	U	81/135 (60%)	80 (99%)	1 (1%)	71	90
13	V	100/102 (98%)	96 (96%)	4 (4%)	31	68
14	W	108/114 (95%)	105 (97%)	3 (3%)	43	77
15	q	131/131 (100%)	128 (98%)	3 (2%)	50	80
16	r	88/96 (92%)	87 (99%)	1 (1%)	73	90
17	s	40/95 (42%)	39 (98%)	1 (2%)	47	79
18	A	103/103 (100%)	100 (97%)	3 (3%)	42	76
19	H	279/279 (100%)	270 (97%)	9 (3%)	39	74
20	J	137/137 (100%)	132 (96%)	5 (4%)	35	70
21	K	87/87 (100%)	86 (99%)	1 (1%)	73	90
22	L	548/549 (100%)	534 (97%)	14 (3%)	46	78
23	M	414/414 (100%)	407 (98%)	7 (2%)	60	85
24	N	307/307 (100%)	297 (97%)	10 (3%)	38	73
25	O	284/309 (92%)	278 (98%)	6 (2%)	53	82
26	X	153/154 (99%)	145 (95%)	8 (5%)	23	59
27	Y	105/106 (99%)	99 (94%)	6 (6%)	20	56
28	Z	122/123 (99%)	121 (99%)	1 (1%)	81	93
29	a	60/60 (100%)	60 (100%)	0	100	100
30	b	72/73 (99%)	71 (99%)	1 (1%)	67	88
31	c	42/67 (63%)	41 (98%)	1 (2%)	49	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	d	107/107 (100%)	104 (97%)	3 (3%)	43	77
33	e	93/94 (99%)	93 (100%)	0	100	100
34	f	49/53 (92%)	47 (96%)	2 (4%)	30	67
35	g	92/129 (71%)	90 (98%)	2 (2%)	52	81
36	h	123/162 (76%)	119 (97%)	4 (3%)	38	73
37	i	92/119 (77%)	87 (95%)	5 (5%)	22	57
38	j	60/87 (69%)	58 (97%)	2 (3%)	38	73
39	k	60/78 (77%)	59 (98%)	1 (2%)	60	85
40	l	142/161 (88%)	140 (99%)	2 (1%)	67	88
41	m	112/114 (98%)	110 (98%)	2 (2%)	59	85
42	n	163/164 (99%)	160 (98%)	3 (2%)	59	85
43	o	109/121 (90%)	107 (98%)	2 (2%)	59	85
44	p	155/158 (98%)	154 (99%)	1 (1%)	86	95
All	All	7209/7947 (91%)	7043 (98%)	166 (2%)	53	80

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6	64	CYS
1	6	85	VAL
1	6	135	TYR
1	6	154	ILE
2	C	17	VAL
2	C	169	THR
3	D	50	ASN
3	D	145	THR
3	D	325	VAL
3	D	326	ASP
3	D	413	ASP
4	2	24	THR
4	2	105	THR
4	2	135	LYS
4	2	136	LEU
4	2	138	THR
4	2	164	LEU
4	2	165	THR
5	1	45	THR

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Mol	Chain	Res	Type
5	1	273	SER
5	1	327	THR
5	1	359	CYS
5	1	363	THR
5	1	365	CYS
5	1	405	CYS
6	3	13	VAL
6	3	33	VAL
6	3	52	CYS
6	3	103	LEU
6	3	110	GLN
6	3	158	ARG
6	3	267	THR
6	3	356	THR
6	3	444	LYS
6	3	540	ASP
6	3	559	VAL
6	3	583	THR
6	3	667	THR
7	9	14	VAL
8	P	5	VAL
8	P	76	ARG
8	P	185	TYR
8	P	207	VAL
8	P	224	VAL
8	P	254	ILE
8	P	263	TYR
9	Q	44	ASN
9	Q	81	ASN
10	7	16	GLN
11	S	37	VAL
11	S	63	LYS
12	T	19	LEU
13	V	18	THR
13	V	58	VAL
13	V	93	MET
13	V	103	VAL
14	W	55	ASP
14	W	96	ILE
14	W	121	LEU
15	q	94	THR
15	q	127	TYR

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Mol	Chain	Res	Type
15	q	138	VAL
16	r	23	LEU
17	s	42	THR
18	A	68	GLU
18	A	86	THR
18	A	111	LEU
19	H	17	MET
19	H	54	LYS
19	H	62	ARG
19	H	172	MET
19	H	198	PHE
19	H	202	GLU
19	H	254	LEU
19	H	297	THR
19	H	318	MET
20	J	64	LEU
20	J	81	THR
20	J	89	LEU
20	J	131	VAL
20	J	151	MET
21	K	93	LEU
22	L	10	LEU
22	L	69	VAL
22	L	190	SER
22	L	194	ASN
22	L	249	SER
22	L	293	LEU
22	L	363	THR
22	L	370	SER
22	L	472	ILE
22	L	489	THR
22	L	511	LEU
22	L	517	ASN
22	L	551	THR
22	L	562	ILE
23	M	72	LEU
23	M	138	ASN
23	M	166	LEU
23	M	173	THR
23	M	205	ILE
23	M	229	MET
23	M	414	THR

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Mol	Chain	Res	Type
24	N	35	PHE
24	N	95	LEU
24	N	108	LEU
24	N	155	LEU
24	N	173	THR
24	N	201	THR
24	N	232	LEU
24	N	235	ASN
24	N	275	CYS
24	N	287	LEU
25	O	41	GLU
25	O	63	THR
25	O	250	LYS
25	O	263	VAL
25	O	279	LEU
25	O	290	SER
12	U	32	VAL
26	X	6	LEU
26	X	23	VAL
26	X	35	CYS
26	X	45	CYS
26	X	47	TRP
26	X	77	CYS
26	X	94	GLN
26	X	109	CYS
27	Y	3	ARG
27	Y	42	LEU
27	Y	82	LYS
27	Y	104	THR
27	Y	106	SER
27	Y	114	CYS
28	Z	100	VAL
30	b	62	MET
31	c	4	VAL
32	d	30	ARG
32	d	34	MET
32	d	120	ARG
34	f	34	LEU
34	f	35	THR
35	g	55	ASN
35	g	105	ILE
36	h	10	VAL

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Mol	Chain	Res	Type
36	h	18	ASP
36	h	31	LEU
36	h	117	ARG
37	i	4	THR
37	i	65	ARG
37	i	78	MET
37	i	98	SER
37	i	110	LEU
38	j	32	MET
38	j	47	VAL
39	k	32	THR
40	l	7	MET
40	l	120	VAL
41	m	24	VAL
41	m	122	ARG
42	n	17	ARG
42	n	49	GLU
42	n	157	ARG
43	o	107	LEU
43	o	113	ARG
44	p	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
6	3	237	ASN
18	A	10	ASN
19	H	258	ASN
22	L	361	ASN
25	O	45	GLN
43	o	54	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 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
16	AYA	r	1	16	6,7,8	1.34	1 (16%)	5,8,10	1.36	1 (20%)
3	2MR	D	85	3	10,12,13	1.99	1 (10%)	5,13,15	7.17	3 (60%)
19	FME	H	1	19	8,9,10	0.95	0	7,9,11	0.96	0
20	FME	J	1	20	8,9,10	0.94	0	7,9,11	0.83	0
21	FME	K	1	21	8,9,10	0.95	0	7,9,11	1.86	2 (28%)
22	FME	L	1	22	8,9,10	0.91	0	7,9,11	1.07	1 (14%)
37	SAC	i	1	37	7,8,9	1.02	0	8,9,11	3.01	4 (50%)
24	FME	N	1	24	8,9,10	0.95	0	7,9,11	0.88	0
23	FME	M	1	23	8,9,10	0.98	0	7,9,11	0.69	0
18	FME	A	1	18	8,9,10	0.98	0	7,9,11	0.87	0
30	AYA	b	1	30	6,7,8	1.25	1 (16%)	5,8,10	1.45	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
16	AYA	r	1	16	-	0/4/6/8	-
3	2MR	D	85	3	-	4/10/13/15	-
19	FME	H	1	19	-	1/7/9/11	-
20	FME	J	1	20	-	0/7/9/11	-
21	FME	K	1	21	-	4/7/9/11	-
22	FME	L	1	22	-	4/7/9/11	-
37	SAC	i	1	37	-	7/7/8/10	-
24	FME	N	1	24	-	3/7/9/11	-
23	FME	M	1	23	-	2/7/9/11	-
18	FME	A	1	18	-	1/7/9/11	-
30	AYA	b	1	30	-	1/4/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.66	1.46	1.34
16	r	1	AYA	CA-N	-2.74	1.43	1.46
30	b	1	AYA	CA-N	-2.32	1.44	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	85	2MR	NE-CZ-NH2	14.60	132.86	119.48
37	i	1	SAC	CA-N-C1A	6.04	134.29	123.15
3	D	85	2MR	CD-NE-CZ	4.51	131.85	123.41
3	D	85	2MR	CQ2-NH2-CZ	4.49	133.79	123.86
37	i	1	SAC	C2A-C1A-N	4.30	123.38	116.10
21	K	1	FME	C-CA-N	3.99	116.93	109.73
30	b	1	AYA	CB-CA-N	2.97	112.91	109.61
16	r	1	AYA	CB-CA-N	2.92	112.86	109.61
37	i	1	SAC	C-CA-N	2.35	113.98	109.73
37	i	1	SAC	OAC-C1A-N	-2.23	117.86	121.95
21	K	1	FME	O-C-CA	-2.20	119.00	124.78
22	L	1	FME	C-CA-N	2.17	113.64	109.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	O-C-CA-CB
18	A	1	FME	N-CA-CB-CG
19	H	1	FME	N-CA-CB-CG
21	K	1	FME	O1-CN-N-CA
22	L	1	FME	CB-CA-N-CN
22	L	1	FME	C-CA-CB-CG
23	M	1	FME	O-C-CA-CB
24	N	1	FME	C-CA-CB-CG
24	N	1	FME	O-C-CA-CB
37	i	1	SAC	O-C-CA-CB
37	i	1	SAC	N-CA-CB-OG
37	i	1	SAC	C-CA-CB-OG
3	D	85	2MR	NE-CD-CG-CB
37	i	1	SAC	C2A-C1A-N-CA
37	i	1	SAC	OAC-C1A-N-CA
21	K	1	FME	CA-CB-CG-SD
21	K	1	FME	CB-CG-SD-CE
21	K	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
22	L	1	FME	N-CA-CB-CG
24	N	1	FME	N-CA-CB-CG
3	D	85	2MR	CA-CB-CG-CD
22	L	1	FME	CB-CG-SD-CE
23	M	1	FME	N-CA-CB-CG
30	b	1	AYA	C-CA-N-CT
3	D	85	2MR	N-CA-CB-CG
37	i	1	SAC	C-CA-N-C1A
37	i	1	SAC	CB-CA-N-C1A

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 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 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	PC1	H	401	-	41,41,53	0.33	0	47,49,61	0.32	0
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.46	0
46	3PE	A	201	-	42,42,50	0.33	0	45,47,55	0.32	0
45	SF4	1	502	5	0,12,12	-	-	-		
45	SF4	3	802	6	0,12,12	-	-	-		
49	FES	3	803	6	0,4,4	-	-	-		
46	3PE	d	202	-	30,30,50	0.38	0	33,35,55	0.36	0
55	CDL	m	201	-	71,71,99	0.36	0	77,83,111	0.43	0
45	SF4	9	202	7	0,12,12	-	-	-		
46	3PE	Z	401	-	50,50,50	0.31	0	53,55,55	0.47	0
45	SF4	3	801	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.48	0
46	3PE	6	202	-	31,31,50	0.38	0	34,36,55	0.35	0
55	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.33	0
46	3PE	Y	402	-	27,27,50	0.40	0	30,32,55	0.38	0
45	SF4	9	201	7	0,12,12	-	-	-	-	-
46	3PE	i	201	-	41,41,50	0.32	0	44,46,55	0.31	0
49	FES	2	301	4	0,4,4	-	-	-	-	-
55	CDL	N	401	-	89,89,99	0.31	0	95,101,111	0.41	0
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.32	0
54	ZMP	W	201	-	27,33,36	0.59	0	32,40,45	1.19	3 (9%)
55	CDL	r	201	-	56,56,99	0.40	0	62,68,111	0.58	1 (1%)
55	CDL	L	703	-	45,45,99	0.43	0	51,57,111	0.34	0
46	3PE	M	502	-	50,50,50	0.30	0	53,55,55	0.32	0
55	CDL	h	201	-	69,69,99	0.35	0	75,81,111	0.43	0
46	3PE	h	202	-	50,50,50	0.31	0	53,55,55	0.27	0
46	3PE	M	503	-	35,35,50	0.35	0	38,40,55	0.30	0
47	PC1	M	501	-	53,53,53	0.29	0	59,61,61	0.37	0
50	FMN	1	501	-	33,33,33	0.38	0	48,50,50	0.57	2 (4%)
55	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.36	0
48	UQ	D	501	-	63,63,63	0.26	0	76,79,79	0.53	1 (1%)
45	SF4	6	201	1	0,12,12	-	-	-	-	-
46	3PE	m	202	-	29,29,50	0.39	0	32,34,55	0.33	0
47	PC1	Z	402	-	46,46,53	0.32	0	52,54,61	0.32	0
46	3PE	L	704	-	41,41,50	0.32	0	44,46,55	0.37	0
52	NDP	P	501	-	45,52,52	0.57	0	53,80,80	0.63	1 (1%)
54	ZMP	n	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.92	1 (3%)
55	CDL	Y	401	-	93,93,99	0.31	0	99,105,111	0.28	0
55	CDL	Y	403	-	56,56,99	0.39	0	62,68,111	0.46	1 (1%)
47	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.43	0
46	3PE	D	502	-	50,50,50	0.30	0	53,55,55	0.37	0
56	DGT	O	401	57	26,33,33	0.80	2 (7%)	32,52,52	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PC1	H	401	-	-	9/45/45/57	-
46	3PE	L	701	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	A	201	-	-	11/46/46/54	-
45	SF4	1	502	5	-	-	0/6/5/5
45	SF4	3	802	6	-	-	0/6/5/5
49	FES	3	803	6	-	-	0/1/1/1
46	3PE	d	202	-	-	7/34/34/54	-
55	CDL	m	201	-	-	18/82/82/110	-
45	SF4	9	202	7	-	-	0/6/5/5
46	3PE	Z	401	-	-	13/54/54/54	-
45	SF4	3	801	6	-	-	0/6/5/5
47	PC1	6	203	-	-	9/46/46/57	-
46	3PE	6	202	-	-	6/35/35/54	-
55	CDL	L	702	-	-	19/88/88/110	-
46	3PE	Y	402	-	-	6/31/31/54	-
45	SF4	9	201	7	-	-	0/6/5/5
46	3PE	i	201	-	-	5/45/45/54	-
55	CDL	N	401	-	-	21/100/100/110	-
49	FES	2	301	4	-	-	0/1/1/1
46	3PE	K	201	-	-	9/44/44/54	-
54	ZMP	W	201	-	-	10/38/40/43	-
55	CDL	r	201	-	-	15/67/67/110	-
55	CDL	L	703	-	-	10/56/56/110	-
46	3PE	M	502	-	-	12/54/54/54	-
55	CDL	h	201	-	-	20/80/80/110	-
46	3PE	h	202	-	-	10/54/54/54	-
46	3PE	M	503	-	-	6/39/39/54	-
47	PC1	M	501	-	-	11/57/57/57	-
50	FMN	1	501	-	-	6/18/18/18	0/3/3/3
55	CDL	d	201	-	-	26/77/77/110	-
48	UQ	D	501	-	-	20/63/87/87	0/1/1/1
45	SF4	6	201	1	-	-	0/6/5/5
46	3PE	m	202	-	-	1/33/33/54	-
47	PC1	Z	402	-	-	9/50/50/57	-
46	3PE	L	704	-	-	8/45/45/54	-
52	NDP	P	501	-	-	4/30/77/77	0/5/5/5
54	ZMP	n	201	-	-	20/36/38/43	-
55	CDL	Y	401	-	-	16/104/104/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CDL	Y	403	-	-	21/67/67/110	-
47	PC1	9	203	-	-	14/57/57/57	-
46	3PE	D	502	-	-	14/54/54/54	-
56	DGT	O	401	57	-	8/18/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	n	201	ZMP	C9-C10	2.36	1.53	1.50
56	O	401	DGT	C5-C6	-2.03	1.43	1.47
56	O	401	DGT	C5-C4	-2.01	1.38	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	W	201	ZMP	O1-C10-C9	-3.06	120.37	123.99
54	n	201	ZMP	O1-C10-C9	-2.52	121.01	123.99
54	W	201	ZMP	C15-C14-C13	-2.51	108.18	112.36
48	D	501	UQ	C7-C6-C1	-2.50	115.47	118.48
50	1	501	FMN	P-O5'-C5'	2.49	125.16	118.30
54	W	201	ZMP	C9-C10-S1	2.30	116.14	113.46
52	P	501	NDP	C5A-C6A-N6A	2.23	123.74	120.35
55	r	201	CDL	CA4-OA6-CA5	2.18	123.16	117.79
50	1	501	FMN	C1'-N10-C9A	-2.14	116.94	120.51
55	Y	403	CDL	CA4-OA6-CA5	2.02	122.77	117.79

There are no chirality outliers.

All (404) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O14
46	6	202	3PE	O13-C11-C12-N
46	D	502	3PE	C1-O11-P-O12
46	D	502	3PE	C1-O11-P-O13
46	D	502	3PE	C1-O11-P-O14
46	D	502	3PE	C11-O13-P-O11
46	D	502	3PE	C11-O13-P-O12
46	D	502	3PE	C11-O13-P-O14
46	D	502	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	A	201	3PE	C11-O13-P-O12
46	A	201	3PE	C11-O13-P-O14
46	A	201	3PE	O13-C11-C12-N
46	K	201	3PE	O13-C11-C12-N
46	L	701	3PE	C1-O11-P-O14
46	L	701	3PE	C11-O13-P-O11
46	L	701	3PE	C11-O13-P-O12
46	L	701	3PE	C11-O13-P-O14
46	L	701	3PE	O13-C11-C12-N
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C11-O13-P-O12
46	L	704	3PE	O13-C11-C12-N
46	M	502	3PE	C11-O13-P-O12
46	M	503	3PE	C1-O11-P-O14
46	M	503	3PE	O13-C11-C12-N
46	Y	402	3PE	C1-O11-P-O12
46	Y	402	3PE	O13-C11-C12-N
46	Z	401	3PE	C11-O13-P-O12
46	Z	401	3PE	O13-C11-C12-N
46	d	202	3PE	C11-O13-P-O11
46	d	202	3PE	C11-O13-P-O12
46	d	202	3PE	C11-O13-P-O14
46	d	202	3PE	O13-C11-C12-N
46	h	202	3PE	C1-O11-P-O14
46	h	202	3PE	C11-O13-P-O14
46	h	202	3PE	O13-C11-C12-N
46	i	201	3PE	O13-C11-C12-N
47	6	203	PC1	C1-O11-P-O12
47	6	203	PC1	C1-O11-P-O14
47	9	203	PC1	C11-O13-P-O14
47	9	203	PC1	C1-O11-P-O14
47	9	203	PC1	O13-C11-C12-N
47	M	501	PC1	C11-O13-P-O12
47	Z	402	PC1	C11-O13-P-O12
48	D	501	UQ	C14-C16-C17-C18
48	D	501	UQ	C24-C26-C27-C28
48	D	501	UQ	C43-C44-C46-C47
48	D	501	UQ	C45-C44-C46-C47
50	1	501	FMN	N10-C1'-C2'-O2'
50	1	501	FMN	N10-C1'-C2'-C3'
54	W	201	ZMP	C19-C18-C21-O5
54	W	201	ZMP	C20-C18-C21-O5

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Mol	Chain	Res	Type	Atoms
54	W	201	ZMP	C17-C18-C21-O5
54	W	201	ZMP	S1-C11-C12-N1
54	W	201	ZMP	C7-C8-C9-C10
54	n	201	ZMP	C17-C18-C21-O5
54	n	201	ZMP	O4-C17-C18-C21
54	n	201	ZMP	C16-C17-C18-C21
54	n	201	ZMP	O4-C17-C18-C19
54	n	201	ZMP	C16-C17-C18-C20
54	n	201	ZMP	O3-C16-C17-O4
54	n	201	ZMP	C17-C16-N2-C15
54	n	201	ZMP	O1-C10-S1-C11
54	n	201	ZMP	C9-C10-S1-C11
54	n	201	ZMP	C7-C8-C9-C10
55	r	201	CDL	CA2-OA2-PA1-OA3
55	r	201	CDL	CA2-OA2-PA1-OA4
55	r	201	CDL	CA2-OA2-PA1-OA5
55	r	201	CDL	CA3-OA5-PA1-OA3
55	r	201	CDL	CA3-OA5-PA1-OA4
55	r	201	CDL	CB2-OB2-PB2-OB3
55	r	201	CDL	CB2-OB2-PB2-OB4
55	r	201	CDL	CB2-OB2-PB2-OB5
55	r	201	CDL	CB3-OB5-PB2-OB3
55	r	201	CDL	CB3-OB5-PB2-OB4
55	L	702	CDL	CA2-OA2-PA1-OA3
55	L	702	CDL	CA2-OA2-PA1-OA4
55	L	702	CDL	CA2-OA2-PA1-OA5
55	L	702	CDL	CA3-OA5-PA1-OA3
55	L	702	CDL	CB2-OB2-PB2-OB3
55	L	702	CDL	CB2-OB2-PB2-OB4
55	L	702	CDL	CB2-OB2-PB2-OB5
55	L	702	CDL	CB3-OB5-PB2-OB2
55	L	702	CDL	CB3-OB5-PB2-OB4
55	L	703	CDL	CA2-OA2-PA1-OA3
55	L	703	CDL	CA2-OA2-PA1-OA4
55	L	703	CDL	CA2-OA2-PA1-OA5
55	L	703	CDL	CA3-OA5-PA1-OA3
55	N	401	CDL	CA2-OA2-PA1-OA4
55	N	401	CDL	CB2-OB2-PB2-OB3
55	N	401	CDL	CB2-OB2-PB2-OB4
55	N	401	CDL	CB2-OB2-PB2-OB5
55	Y	401	CDL	CA3-OA5-PA1-OA3
55	Y	403	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
55	Y	403	CDL	CA3-OA5-PA1-OA4
55	d	201	CDL	CA3-OA5-PA1-OA2
55	d	201	CDL	CA3-OA5-PA1-OA3
55	d	201	CDL	CA3-OA5-PA1-OA4
55	d	201	CDL	CB3-OB5-PB2-OB3
55	d	201	CDL	CB3-OB5-PB2-OB4
55	h	201	CDL	CA2-OA2-PA1-OA3
55	h	201	CDL	CB3-OB5-PB2-OB2
55	h	201	CDL	CB3-OB5-PB2-OB3
55	h	201	CDL	CB3-OB5-PB2-OB4
55	m	201	CDL	CB2-OB2-PB2-OB4
55	m	201	CDL	CB3-OB5-PB2-OB2
55	m	201	CDL	CB3-OB5-PB2-OB3
55	m	201	CDL	CB3-OB5-PB2-OB4
56	O	401	DGT	PB-O3B-PG-O1G
56	O	401	DGT	C5'-O5'-PA-O3A
54	n	201	ZMP	O3-C16-N2-C15
48	D	501	UQ	C12-C11-C9-C10
48	D	501	UQ	C9-C11-C12-C13
48	D	501	UQ	C39-C41-C42-C43
48	D	501	UQ	C49-C51-C52-C53
55	m	201	CDL	OB5-CB3-CB4-OB6
55	d	201	CDL	O1-C1-CB2-OB2
46	Z	401	3PE	C31-C32-C33-C34
46	M	503	3PE	C2-C1-O11-P
47	6	203	PC1	C11-C12-N-C14
46	A	201	3PE	C11-O13-P-O11
46	K	201	3PE	C1-O11-P-O13
46	K	201	3PE	C11-O13-P-O11
46	M	502	3PE	C11-O13-P-O11
46	M	503	3PE	C1-O11-P-O13
46	Y	402	3PE	C1-O11-P-O13
46	d	202	3PE	C1-O11-P-O13
47	6	203	PC1	C1-O11-P-O13
47	9	203	PC1	C1-O11-P-O13
47	M	501	PC1	C11-O13-P-O11
47	Z	402	PC1	C11-O13-P-O11
55	r	201	CDL	CA3-OA5-PA1-OA2
55	r	201	CDL	CB3-OB5-PB2-OB2
55	L	702	CDL	CA3-OA5-PA1-OA2
55	L	703	CDL	CA3-OA5-PA1-OA2
55	N	401	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
55	Y	401	CDL	CA2-OA2-PA1-OA5
55	Y	401	CDL	CA3-OA5-PA1-OA2
55	Y	401	CDL	CB3-OB5-PB2-OB2
55	Y	403	CDL	CA3-OA5-PA1-OA2
55	Y	403	CDL	CB2-OB2-PB2-OB5
55	d	201	CDL	CB3-OB5-PB2-OB2
55	h	201	CDL	CA2-OA2-PA1-OA5
55	h	201	CDL	CB2-OB2-PB2-OB5
55	m	201	CDL	CA3-OA5-PA1-OA2
47	H	401	PC1	C21-C22-C23-C24
47	M	501	PC1	C28-C29-C2A-C2B
47	H	401	PC1	C38-C39-C3A-C3B
55	N	401	CDL	C81-C82-C83-C84
46	L	701	3PE	C21-C22-C23-C24
47	Z	402	PC1	C33-C34-C35-C36
54	n	201	ZMP	C6-C7-C8-C9
46	h	202	3PE	C35-C36-C37-C38
46	M	502	3PE	O13-C11-C12-N
46	M	502	3PE	C23-C24-C25-C26
46	A	201	3PE	C39-C3A-C3B-C3C
47	6	203	PC1	C3C-C3D-C3E-C3F
47	6	203	PC1	C11-C12-N-C13
47	6	203	PC1	C11-C12-N-C15
46	M	502	3PE	C36-C37-C38-C39
46	D	502	3PE	C31-C32-C33-C34
47	H	401	PC1	O21-C2-C3-O31
48	D	501	UQ	C12-C11-C9-C8
46	L	701	3PE	C1-O11-P-O13
46	h	202	3PE	C11-O13-P-O11
55	m	201	CDL	CB2-OB2-PB2-OB5
55	N	401	CDL	OB5-CB3-CB4-CB6
47	M	501	PC1	C37-C38-C39-C3A
48	D	501	UQ	C33-C34-C36-C37
46	D	502	3PE	C1-C2-C3-O31
55	N	401	CDL	CA3-CA4-CA6-OA8
55	Y	401	CDL	C73-C74-C75-C76
55	Y	401	CDL	C82-C83-C84-C85
48	D	501	UQ	C35-C34-C36-C37
54	n	201	ZMP	C19-C18-C21-O5
54	n	201	ZMP	C20-C18-C21-O5
47	H	401	PC1	C3A-C3B-C3C-C3D
47	9	203	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
50	1	501	FMN	C5'-O5'-P-O1P
46	D	502	3PE	C37-C38-C39-C3A
55	N	401	CDL	OA6-CA4-CA6-OA8
54	n	201	ZMP	O4-C17-C18-C20
55	L	702	CDL	CA5-C11-C12-C13
55	Y	403	CDL	OB5-CB3-CB4-CB6
55	d	201	CDL	OB5-CB3-CB4-CB6
55	m	201	CDL	OB5-CB3-CB4-CB6
47	Z	402	PC1	C21-C22-C23-C24
47	9	203	PC1	C2C-C2D-C2E-C2F
46	K	201	3PE	C2-C1-O11-P
47	H	401	PC1	C1-C2-C3-O31
55	d	201	CDL	CA3-CA4-CA6-OA8
55	m	201	CDL	CB3-CB4-CB6-OB8
46	Y	402	3PE	C11-O13-P-O11
47	Z	402	PC1	C2A-C2B-C2C-C2D
55	r	201	CDL	OB5-CB3-CB4-OB6
55	d	201	CDL	OB5-CB3-CB4-OB6
55	Y	403	CDL	O1-C1-CB2-OB2
46	D	502	3PE	O21-C2-C3-O31
48	D	501	UQ	C44-C46-C47-C48
46	h	202	3PE	C2-C1-O11-P
55	h	201	CDL	C1-CA2-OA2-PA1
54	W	201	ZMP	O1-C10-S1-C11
55	r	201	CDL	OB5-CB3-CB4-CB6
55	Y	403	CDL	C31-C32-C33-C34
54	W	201	ZMP	C9-C10-S1-C11
54	n	201	ZMP	C13-C14-C15-N2
55	Y	401	CDL	CB3-CB4-CB6-OB8
55	N	401	CDL	OB5-CB3-CB4-OB6
55	Y	403	CDL	OB5-CB3-CB4-OB6
54	n	201	ZMP	C16-C17-C18-C19
56	O	401	DGT	PB-O3B-PG-O2G
47	M	501	PC1	O21-C2-C3-O31
55	Y	401	CDL	OB6-CB4-CB6-OB8
55	d	201	CDL	OA6-CA4-CA6-OA8
55	m	201	CDL	OB6-CB4-CB6-OB8
55	d	201	CDL	C55-C56-C57-C58
52	P	501	NDP	C5B-O5B-PA-O3
56	O	401	DGT	PB-O3A-PA-O1A
46	M	503	3PE	C26-C27-C28-C29
46	Z	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
55	N	401	CDL	CB4-CB3-OB5-PB2
55	h	201	CDL	CA4-CA3-OA5-PA1
46	K	201	3PE	C11-O13-P-O14
46	L	701	3PE	C1-O11-P-O12
46	M	503	3PE	C1-O11-P-O12
46	Z	401	3PE	C11-O13-P-O14
46	d	202	3PE	C1-O11-P-O12
46	d	202	3PE	C1-O11-P-O14
47	9	203	PC1	C1-O11-P-O12
55	L	702	CDL	CA3-OA5-PA1-OA4
55	L	702	CDL	CB3-OB5-PB2-OB3
55	L	703	CDL	CA3-OA5-PA1-OA4
55	N	401	CDL	CA2-OA2-PA1-OA3
55	Y	401	CDL	CA2-OA2-PA1-OA3
55	Y	401	CDL	CA3-OA5-PA1-OA4
55	Y	401	CDL	CB3-OB5-PB2-OB3
55	Y	401	CDL	CB3-OB5-PB2-OB4
55	Y	403	CDL	CB2-OB2-PB2-OB3
55	h	201	CDL	CA2-OA2-PA1-OA4
55	h	201	CDL	CB2-OB2-PB2-OB4
55	m	201	CDL	CA3-OA5-PA1-OA3
55	m	201	CDL	CB2-OB2-PB2-OB3
56	O	401	DGT	C5'-O5'-PA-O1A
56	O	401	DGT	C5'-O5'-PA-O2A
47	9	203	PC1	O11-C1-C2-C3
55	L	702	CDL	OB5-CB3-CB4-CB6
48	D	501	UQ	C19-C21-C22-C23
46	K	201	3PE	C2A-C2B-C2C-C2D
46	D	502	3PE	C12-C11-O13-P
46	M	502	3PE	C12-C11-O13-P
55	L	702	CDL	OB5-CB3-CB4-OB6
55	h	201	CDL	OB5-CB3-CB4-OB6
47	9	203	PC1	C2D-C2E-C2F-C2G
46	Z	401	3PE	C23-C24-C25-C26
47	H	401	PC1	O13-C11-C12-N
47	M	501	PC1	O13-C11-C12-N
47	Z	402	PC1	O13-C11-C12-N
55	m	201	CDL	C12-C11-CA5-OA6
46	M	502	3PE	C37-C38-C39-C3A
46	h	202	3PE	C23-C24-C25-C26
47	9	203	PC1	C3-C2-O21-C21
55	h	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
55	d	201	CDL	C63-C64-C65-C66
46	A	201	3PE	C2-C1-O11-P
46	L	701	3PE	C2-C1-O11-P
46	Z	401	3PE	O31-C31-C32-C33
46	h	202	3PE	C1-O11-P-O13
46	i	201	3PE	C11-O13-P-O11
47	6	203	PC1	C11-O13-P-O11
47	9	203	PC1	C11-O13-P-O11
47	H	401	PC1	C1-O11-P-O13
55	L	703	CDL	CB2-OB2-PB2-OB5
55	N	401	CDL	CA3-OA5-PA1-OA2
55	Y	403	CDL	CB3-OB5-PB2-OB2
55	d	201	CDL	CA2-OA2-PA1-OA5
55	m	201	CDL	CA2-OA2-PA1-OA5
48	D	501	UQ	C15-C14-C16-C17
52	P	501	NDP	O4D-C1D-N1N-C6N
55	d	201	CDL	C57-C58-C59-C60
55	Y	403	CDL	CA2-C1-CB2-OB2
47	Z	402	PC1	O21-C21-C22-C23
47	M	501	PC1	C21-C22-C23-C24
48	D	501	UQ	C34-C36-C37-C38
55	Y	403	CDL	OA5-CA3-CA4-OA6
47	9	203	PC1	C29-C2A-C2B-C2C
55	h	201	CDL	OB6-CB4-CB6-OB8
55	L	702	CDL	C12-C13-C14-C15
52	P	501	NDP	C2D-C1D-N1N-C6N
54	W	201	ZMP	C6-C7-C8-C9
55	m	201	CDL	C72-C73-C74-C75
46	M	502	3PE	C3D-C3E-C3F-C3G
55	d	201	CDL	C59-C60-C61-C62
46	Z	401	3PE	C3-C2-O21-C21
55	r	201	CDL	CA3-CA4-OA6-CA5
55	Y	401	CDL	C13-C14-C15-C16
54	W	201	ZMP	C12-C11-S1-C10
54	n	201	ZMP	C12-C11-S1-C10
55	N	401	CDL	OB6-CB4-CB6-OB8
48	D	501	UQ	C13-C14-C16-C17
46	D	502	3PE	O21-C21-C22-C23
55	L	702	CDL	C12-C11-CA5-OA6
47	9	203	PC1	C3C-C3D-C3E-C3F
54	n	201	ZMP	C5-C6-C7-C8
55	d	201	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
46	L	704	3PE	O11-C1-C2-O21
55	N	401	CDL	CA5-C11-C12-C13
46	L	704	3PE	C23-C24-C25-C26
47	M	501	PC1	C3C-C3D-C3E-C3F
55	Y	403	CDL	C72-C71-CB7-OB8
55	h	201	CDL	C72-C71-CB7-OB8
46	A	201	3PE	C35-C36-C37-C38
50	1	501	FMN	C5'-O5'-P-O2P
54	n	201	ZMP	N2-C16-C17-O4
46	Y	402	3PE	O31-C31-C32-C33
48	D	501	UQ	C50-C49-C51-C52
46	D	502	3PE	C3D-C3E-C3F-C3G
55	Y	403	CDL	C52-C51-CB5-OB6
55	Y	403	CDL	C32-C31-CA7-OA8
46	L	701	3PE	C3-C2-O21-C21
47	6	203	PC1	C3-C2-O21-C21
55	h	201	CDL	CB6-CB4-OB6-CB5
50	1	501	FMN	O4'-C4'-C5'-O5'
47	M	501	PC1	C39-C3A-C3B-C3C
55	N	401	CDL	C52-C51-CB5-OB6
55	d	201	CDL	C62-C63-C64-C65
46	Z	401	3PE	C21-C22-C23-C24
54	W	201	ZMP	C3-C4-C5-C6
46	6	202	3PE	O21-C21-C22-C23
46	A	201	3PE	C38-C39-C3A-C3B
46	i	201	3PE	C2B-C2C-C2D-C2E
46	Z	401	3PE	C2E-C2F-C2G-C2H
55	L	703	CDL	C12-C11-CA5-OA6
46	Z	401	3PE	O11-C1-C2-C3
46	A	201	3PE	O21-C2-C3-O31
46	M	502	3PE	O31-C31-C32-C33
46	M	502	3PE	O21-C21-C22-C23
55	h	201	CDL	C32-C31-CA7-OA8
55	Y	401	CDL	C32-C31-CA7-OA8
47	Z	402	PC1	O31-C31-C32-C33
55	d	201	CDL	C72-C71-CB7-OB8
55	Y	403	CDL	C52-C51-CB5-OB7
52	P	501	NDP	PN-O3-PA-O2A
56	O	401	DGT	PB-O3A-PA-O2A
46	Z	401	3PE	C2A-C2B-C2C-C2D
55	N	401	CDL	C52-C51-CB5-OB7
48	D	501	UQ	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
55	N	401	CDL	C80-C81-C82-C83
55	Y	403	CDL	C32-C31-CA7-OA9
46	M	502	3PE	O22-C21-C22-C23
47	Z	402	PC1	O32-C31-C32-C33
55	L	703	CDL	C12-C11-CA5-OA7
55	h	201	CDL	C72-C71-CB7-OB9
46	6	202	3PE	O22-C21-C22-C23
46	Y	402	3PE	O32-C31-C32-C33
55	Y	403	CDL	C72-C71-CB7-OB9
47	M	501	PC1	C1-C2-C3-O31
46	K	201	3PE	O21-C21-C22-C23
46	A	201	3PE	O31-C31-C32-C33
55	L	702	CDL	C1-CA2-OA2-PA1
46	6	202	3PE	C1-O11-P-O14
46	K	201	3PE	C1-O11-P-O14
46	L	704	3PE	C1-O11-P-O14
46	L	704	3PE	C11-O13-P-O14
46	Z	401	3PE	C1-O11-P-O14
46	i	201	3PE	C1-O11-P-O14
46	i	201	3PE	C11-O13-P-O14
47	H	401	PC1	C1-O11-P-O14
48	D	501	UQ	C6-C7-C8-C9
55	L	703	CDL	CB2-OB2-PB2-OB3
55	N	401	CDL	CA3-OA5-PA1-OA3
55	Y	403	CDL	CA2-OA2-PA1-OA3
55	Y	403	CDL	CA2-OA2-PA1-OA4
55	d	201	CDL	CB2-OB2-PB2-OB3
55	m	201	CDL	CA2-OA2-PA1-OA3
50	1	501	FMN	O3'-C3'-C4'-C5'
55	h	201	CDL	C32-C31-CA7-OA9
46	A	201	3PE	O21-C21-C22-C23
47	M	501	PC1	O11-C1-C2-C3
46	h	202	3PE	C36-C37-C38-C39
55	d	201	CDL	C61-C62-C63-C64
56	O	401	DGT	PB-O3B-PG-O3G
48	D	501	UQ	C30-C29-C31-C32
55	Y	401	CDL	C23-C24-C25-C26
46	h	202	3PE	C12-C11-O13-P
47	9	203	PC1	C12-C11-O13-P
55	N	401	CDL	CB6-CB4-OB6-CB5
55	Y	403	CDL	CA6-CA4-OA6-CA5
55	m	201	CDL	CA3-CA4-OA6-CA5

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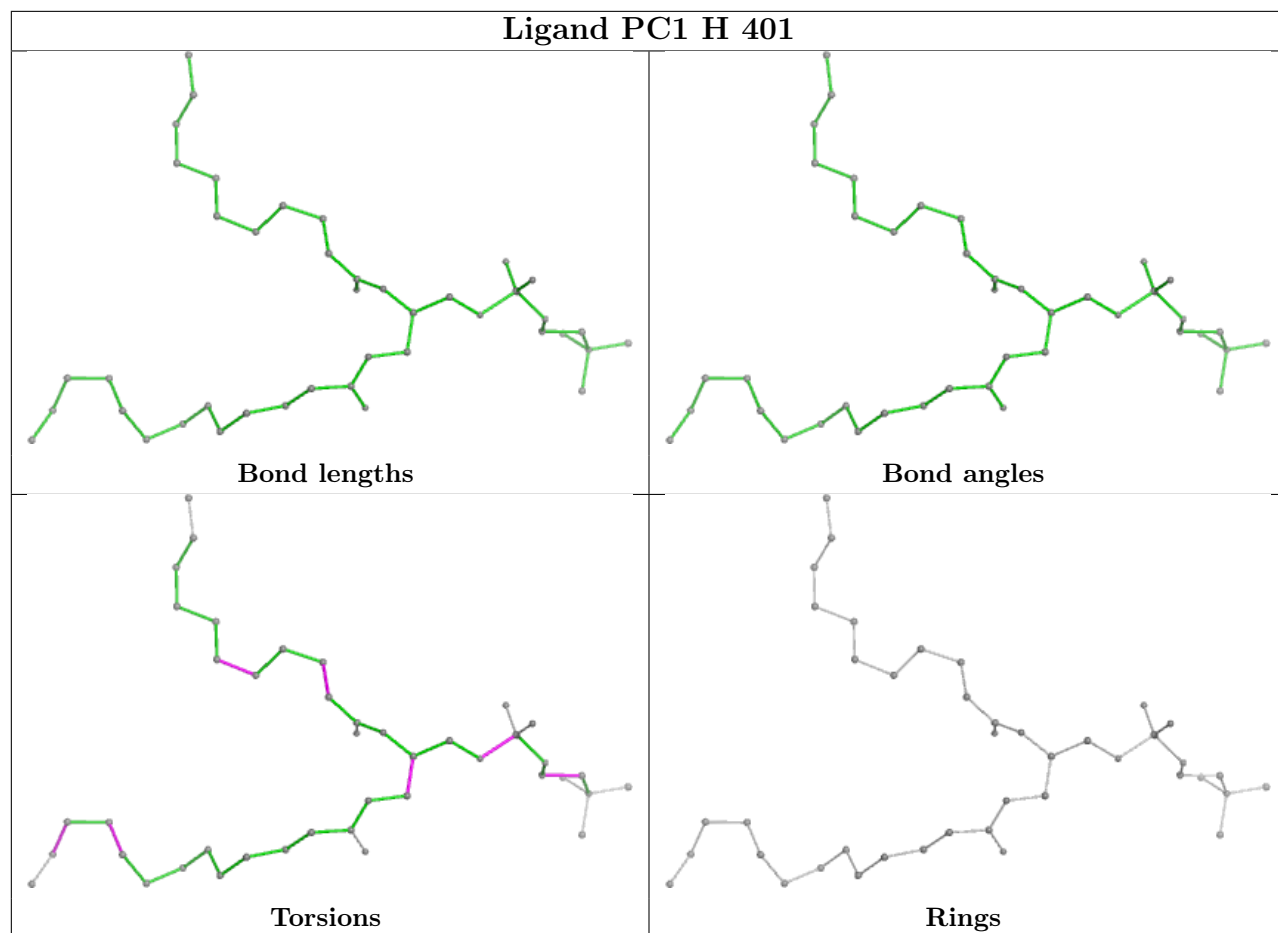
Continued from previous page...

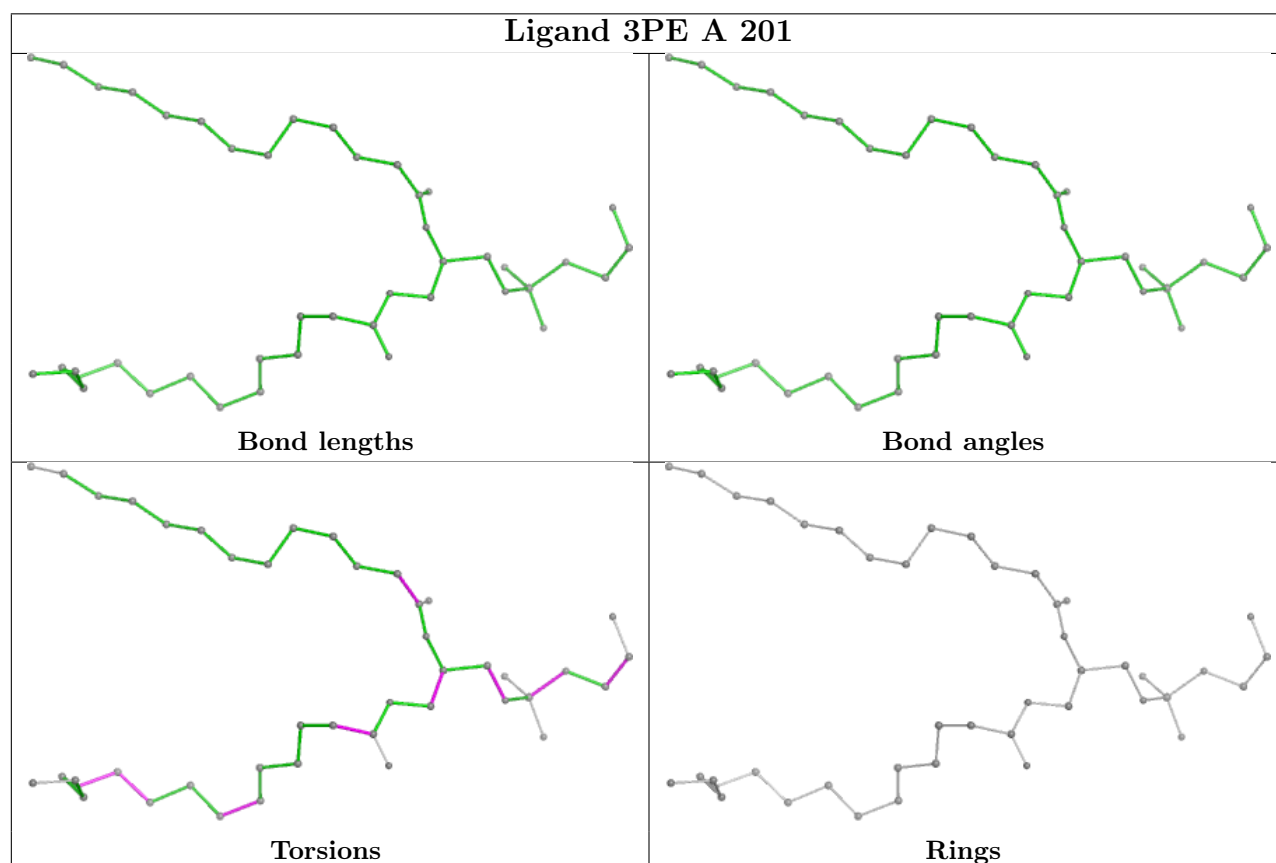
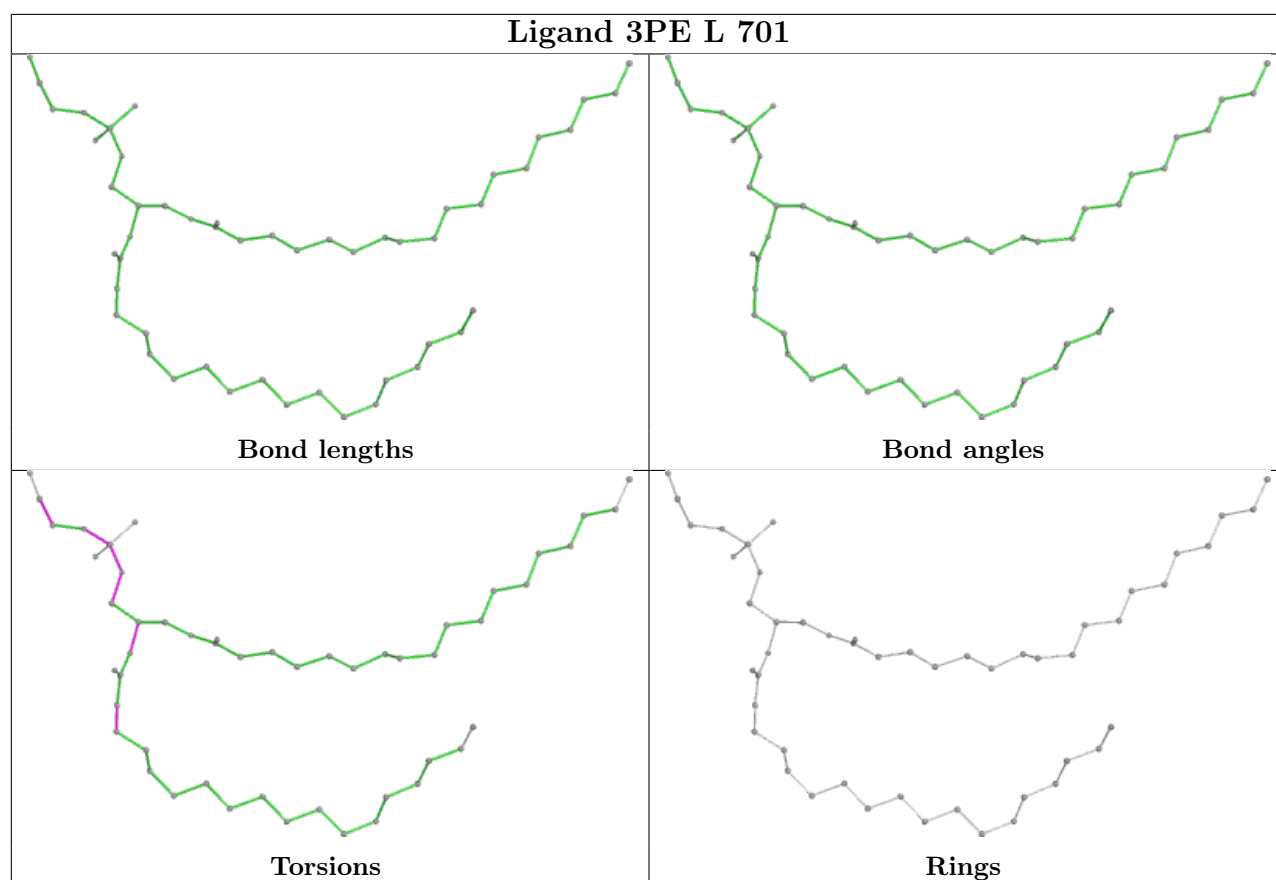
Mol	Chain	Res	Type	Atoms
55	d	201	CDL	C72-C71-CB7-OB9
46	m	202	3PE	O31-C31-C32-C33
47	H	401	PC1	C24-C25-C26-C27
55	Y	401	CDL	C32-C31-CA7-OA9
55	d	201	CDL	C32-C31-CA7-OA8
46	M	502	3PE	O32-C31-C32-C33
55	L	702	CDL	C72-C71-CB7-OB8
55	d	201	CDL	CA2-C1-CB2-OB2
55	m	201	CDL	C1-CB2-OB2-PB2
55	d	201	CDL	C14-C15-C16-C17
46	L	704	3PE	O31-C31-C32-C33
55	h	201	CDL	C52-C51-CB5-OB6
46	K	201	3PE	O22-C21-C22-C23
55	h	201	CDL	C52-C51-CB5-OB7
55	d	201	CDL	C32-C31-CA7-OA9
55	N	401	CDL	C32-C31-CA7-OA8

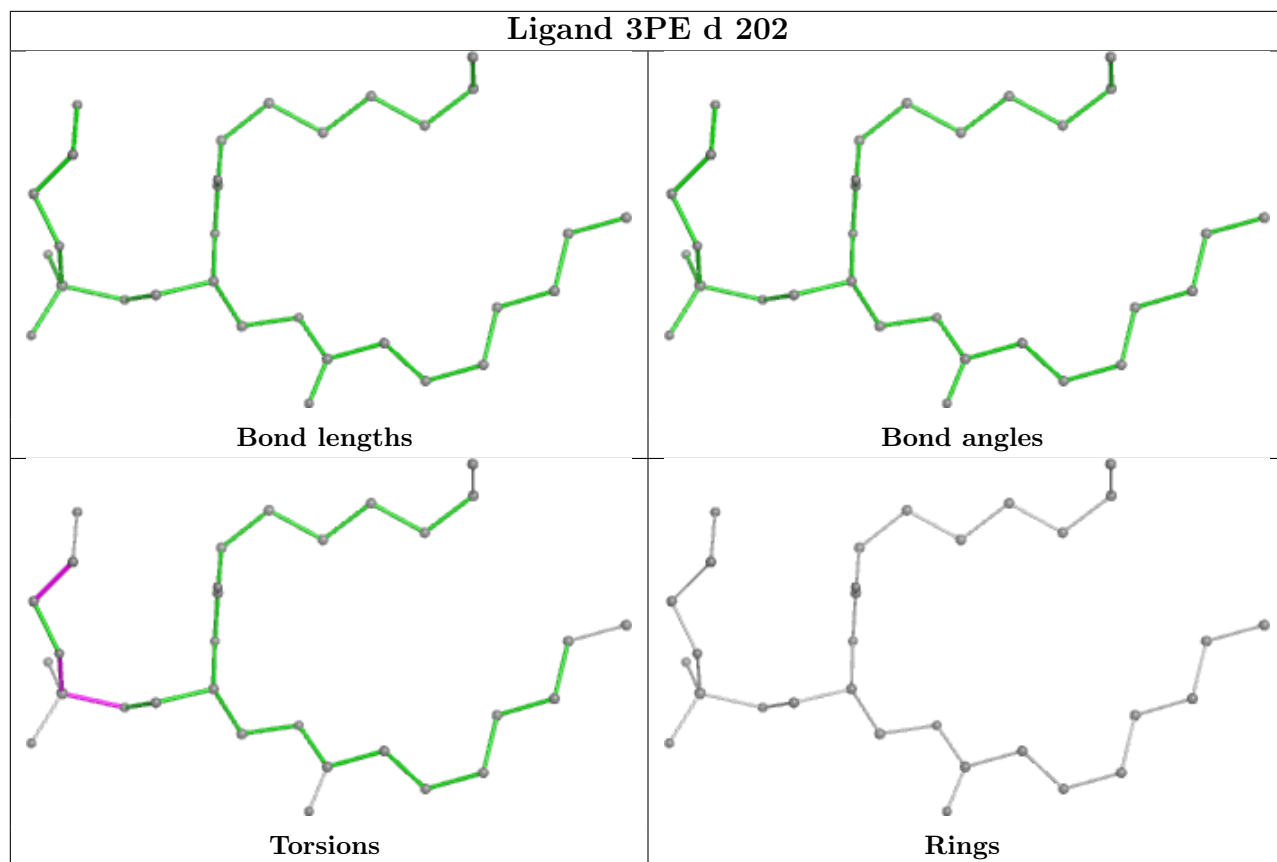
There are no ring outliers.

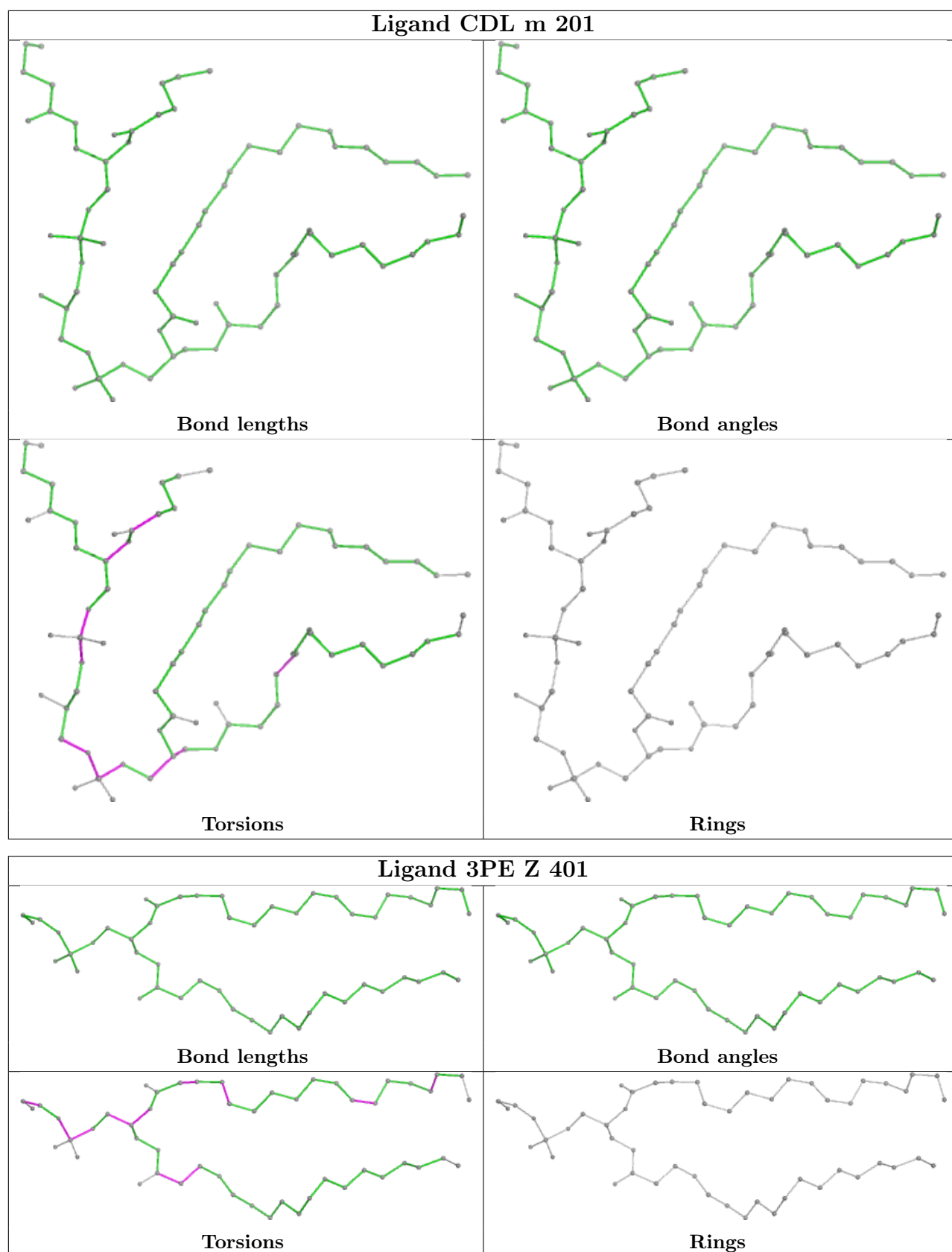
No monomer is involved in short contacts.

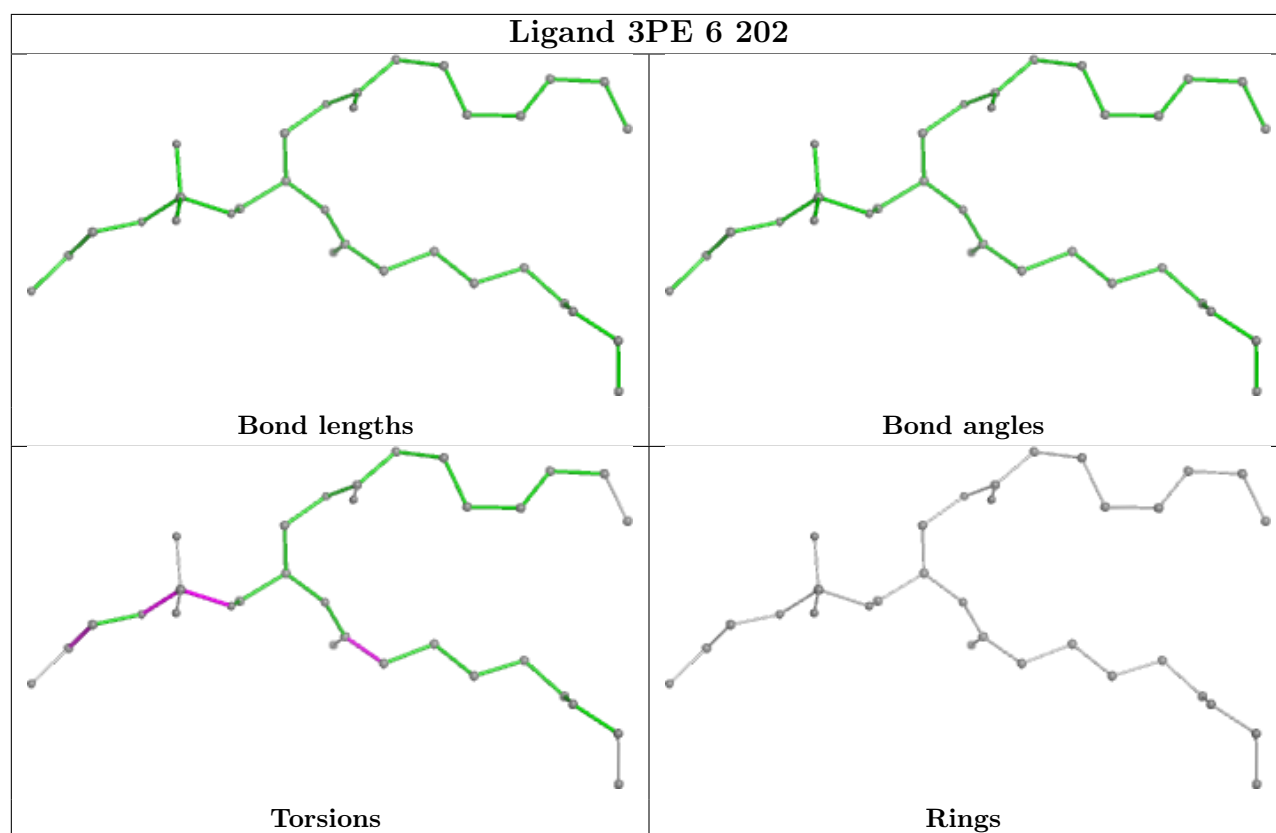
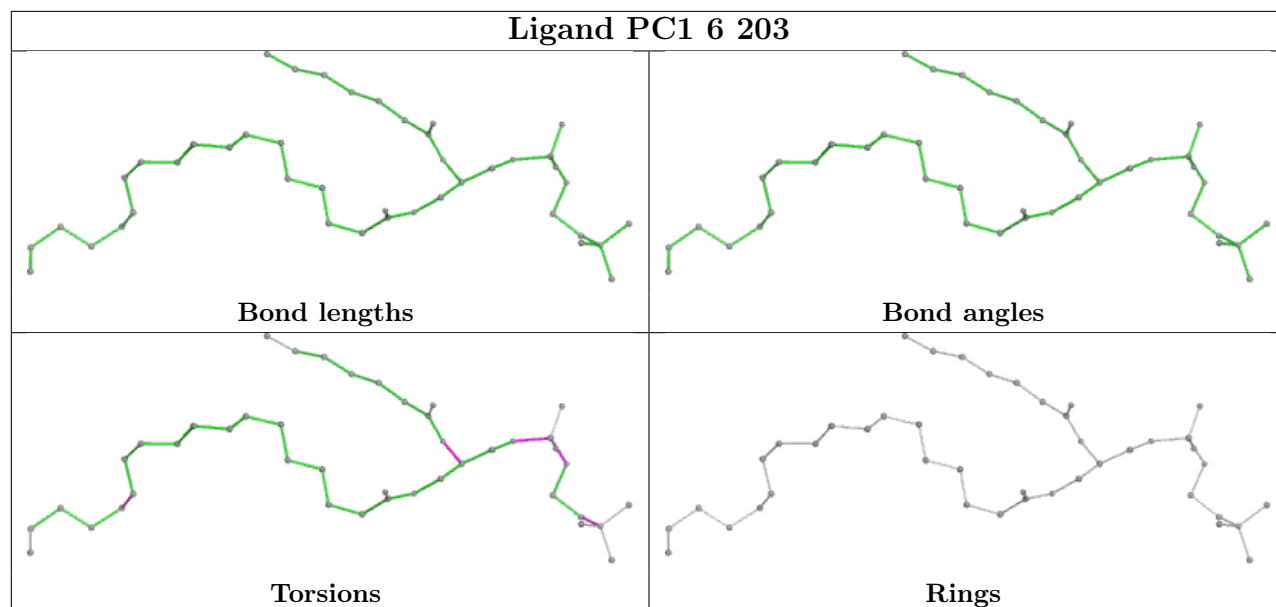
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

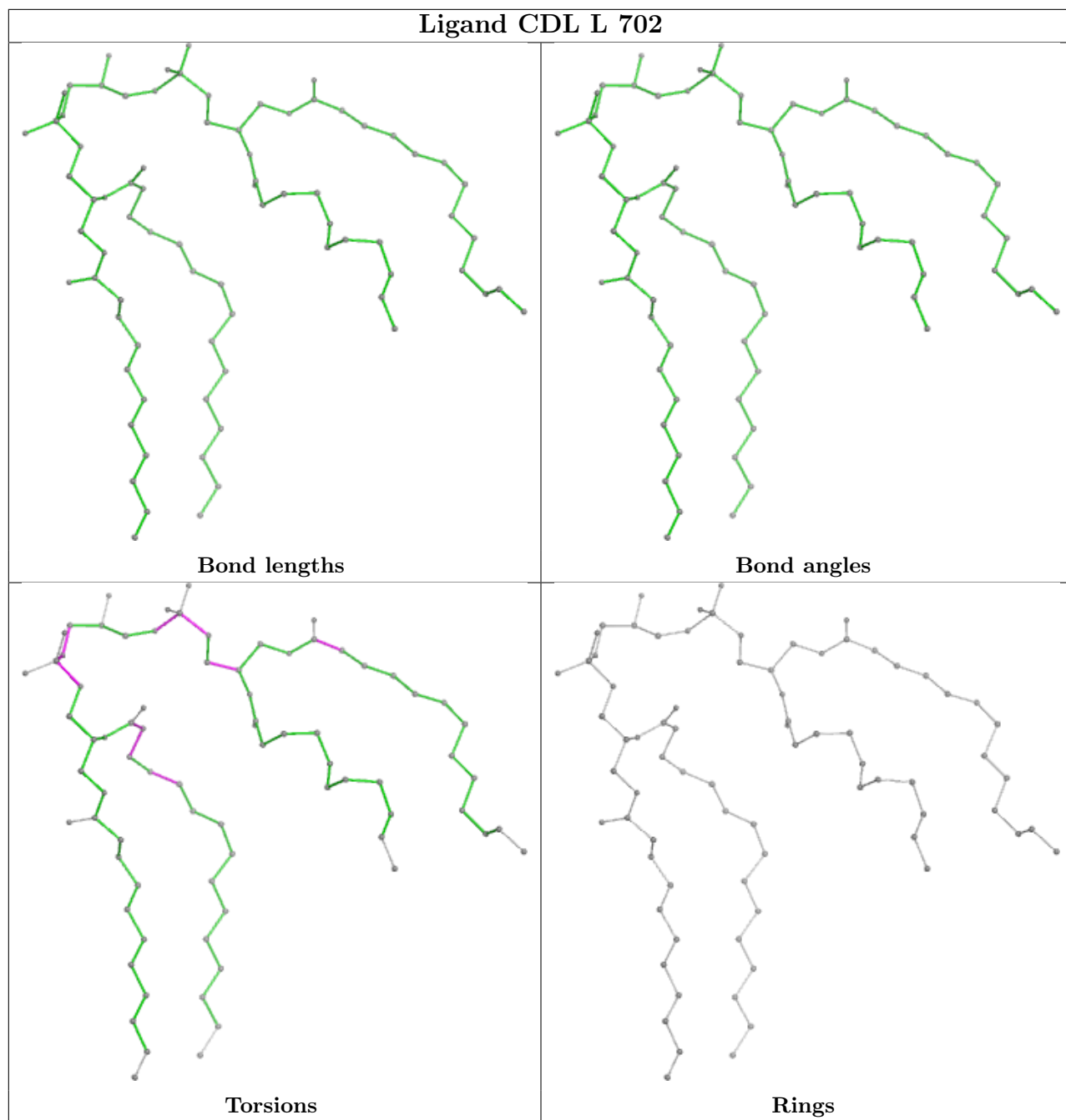


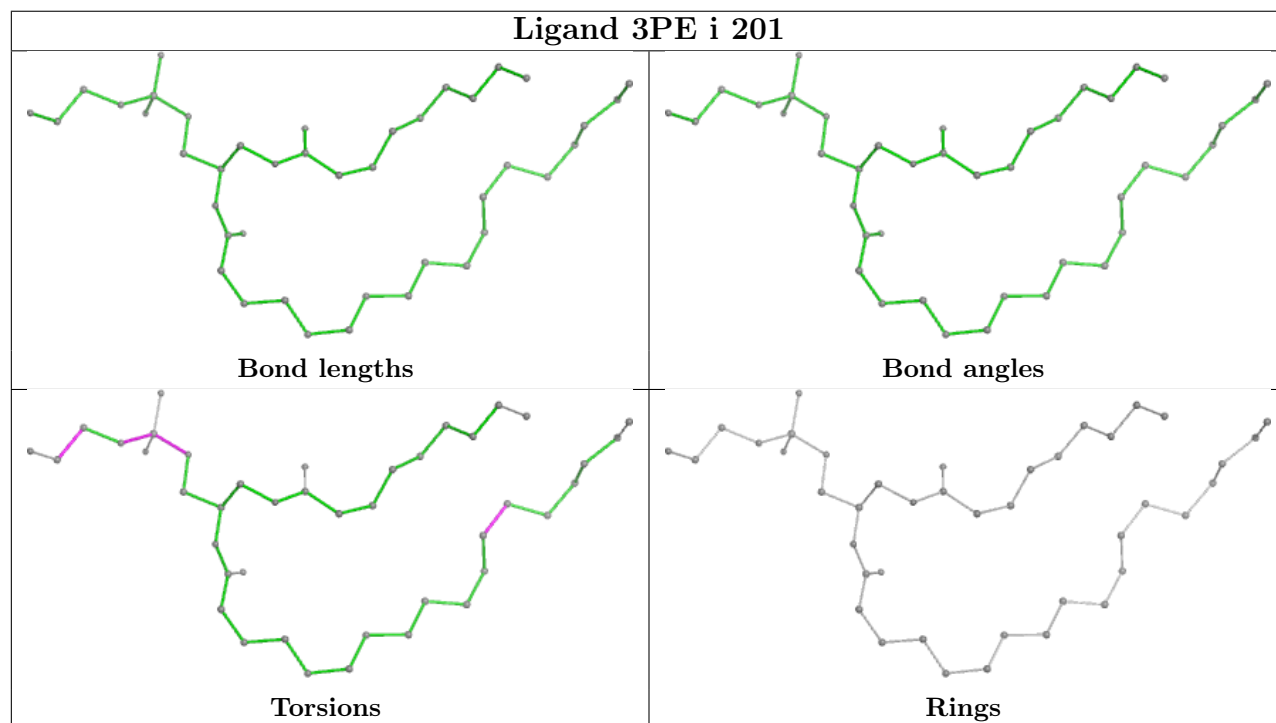
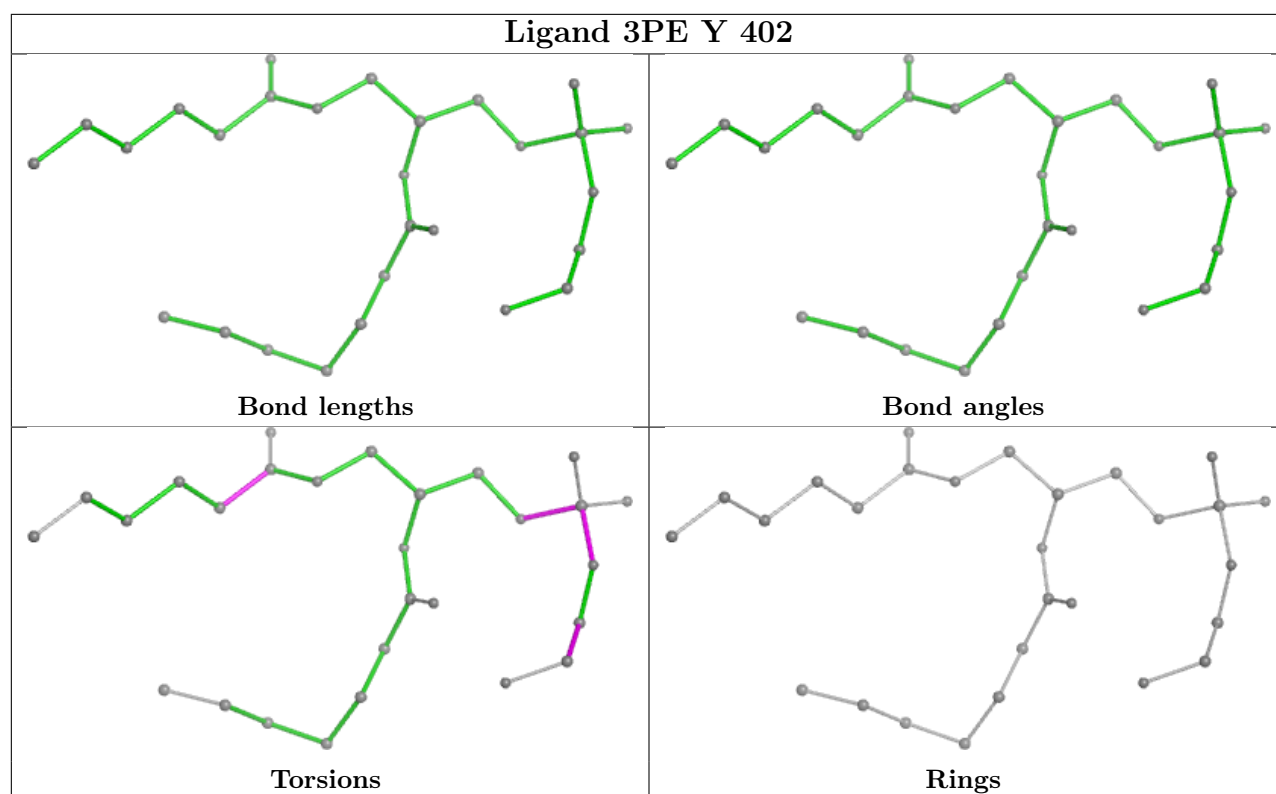


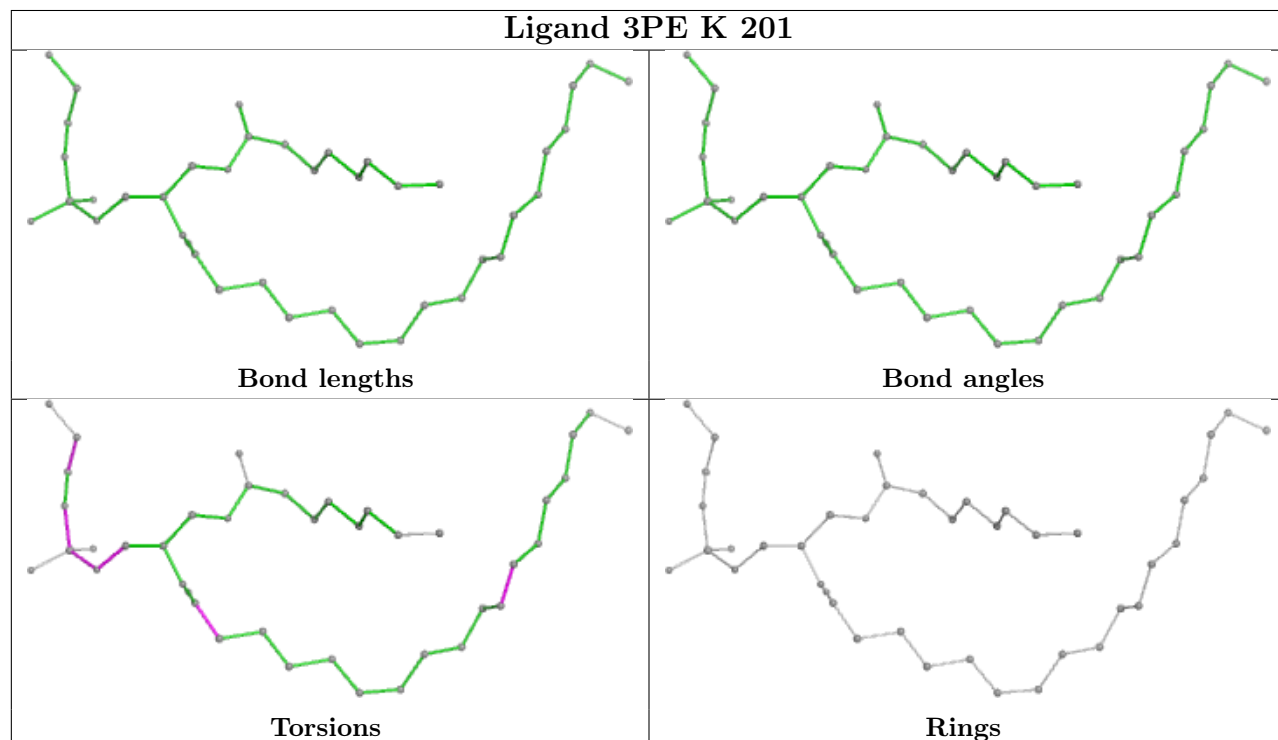
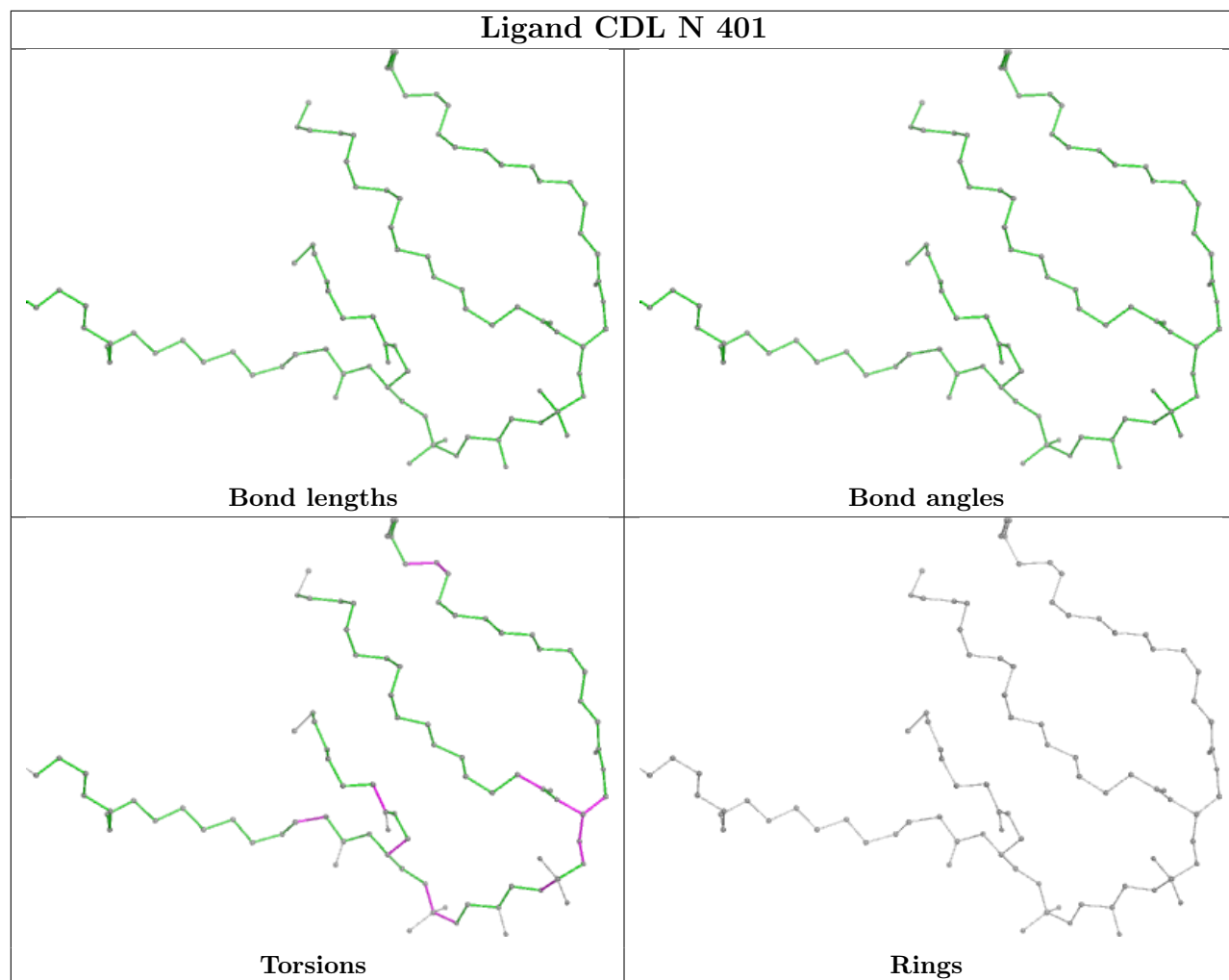


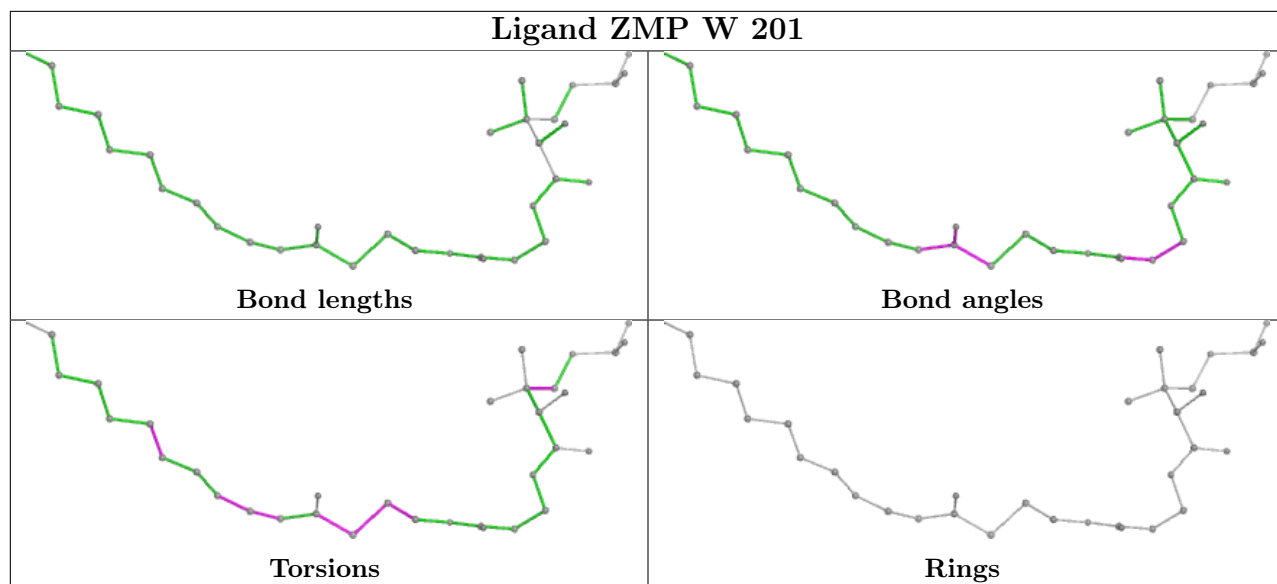


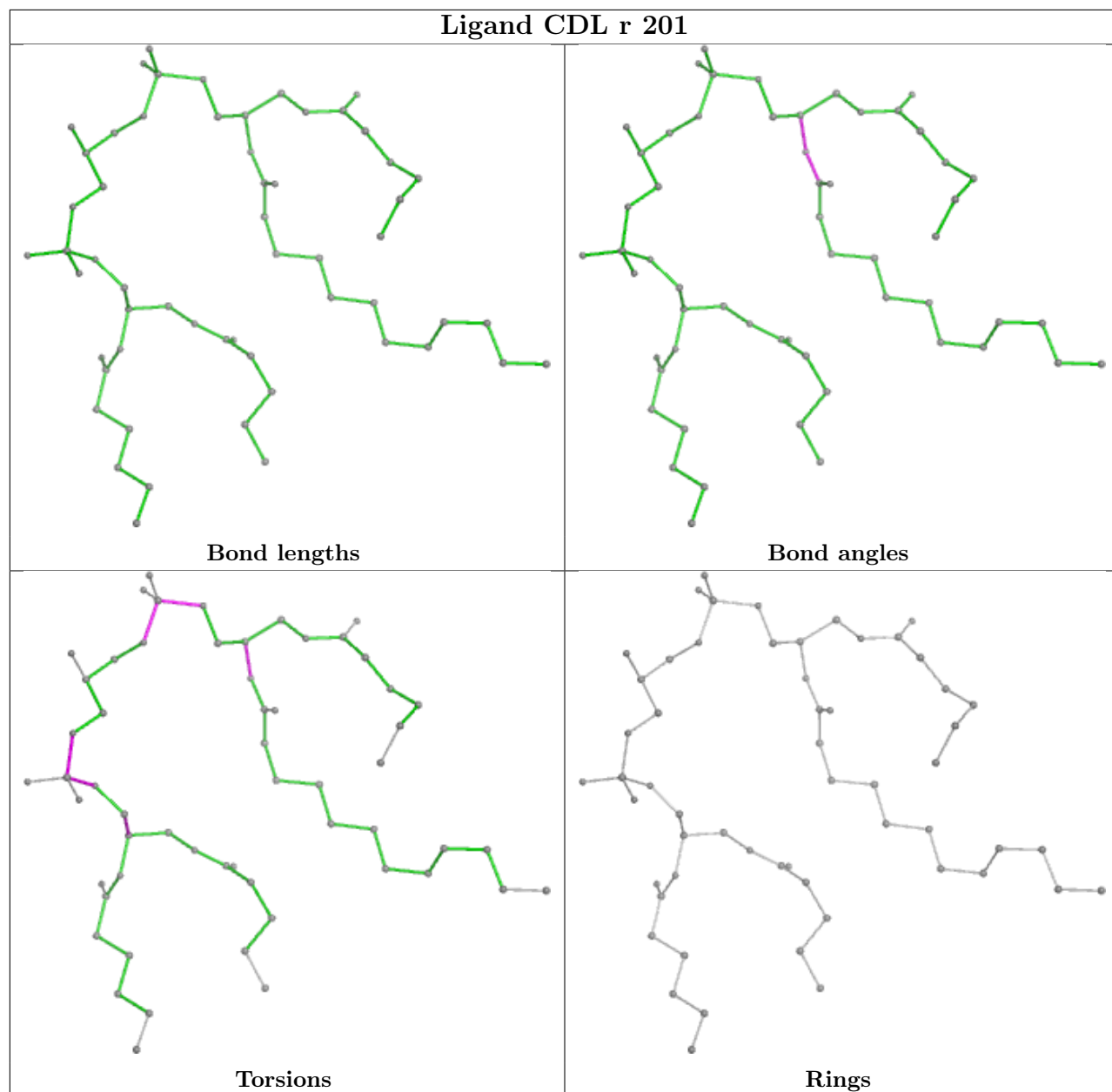


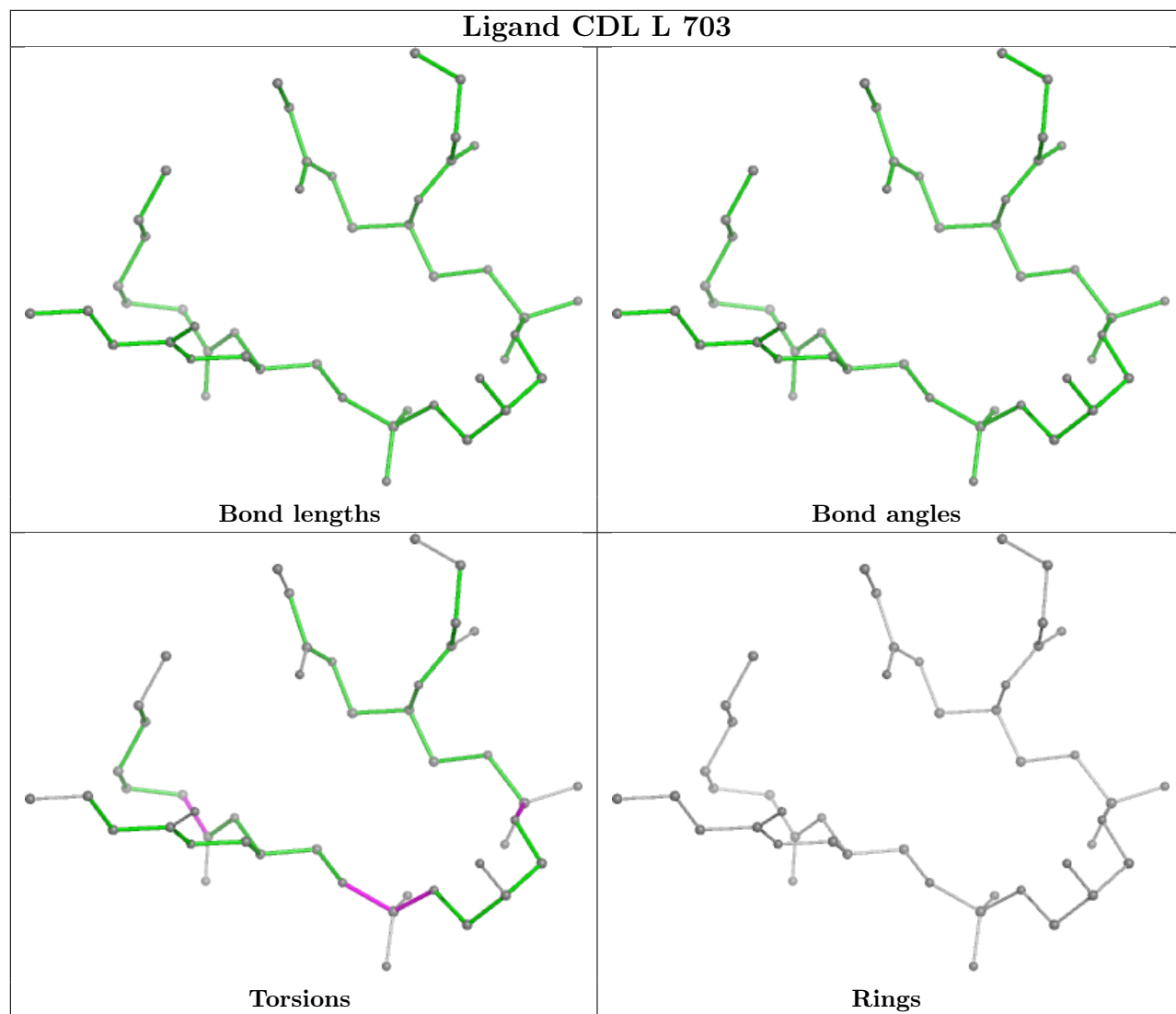


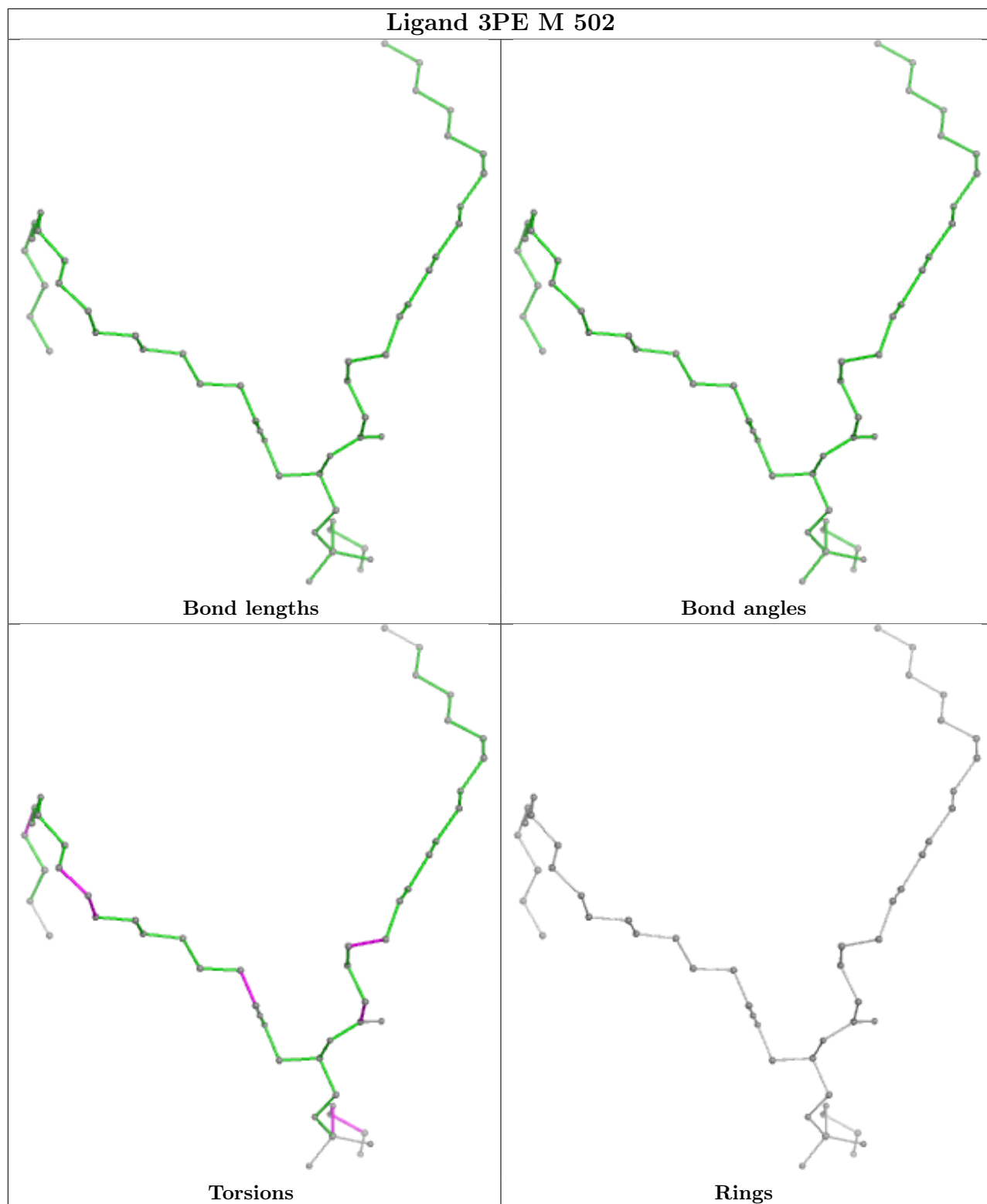


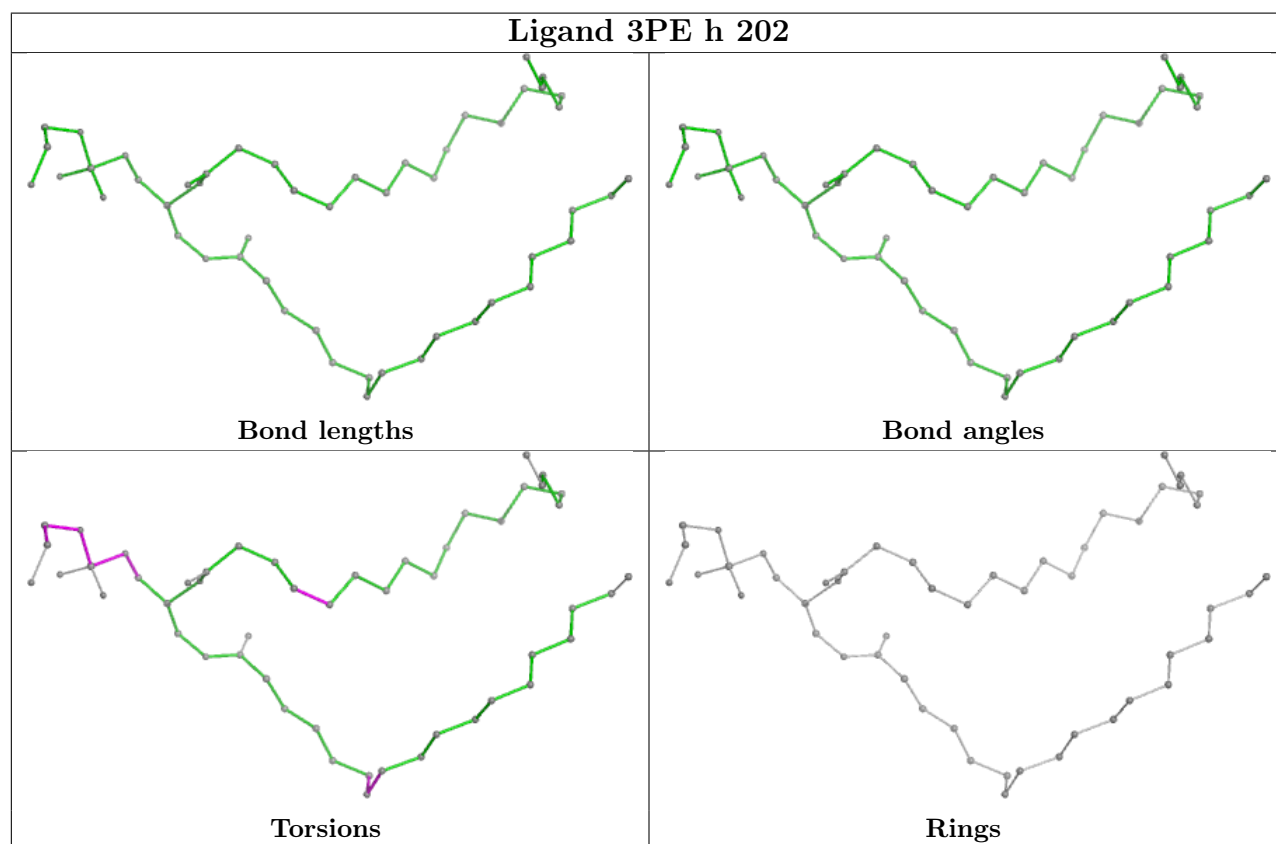
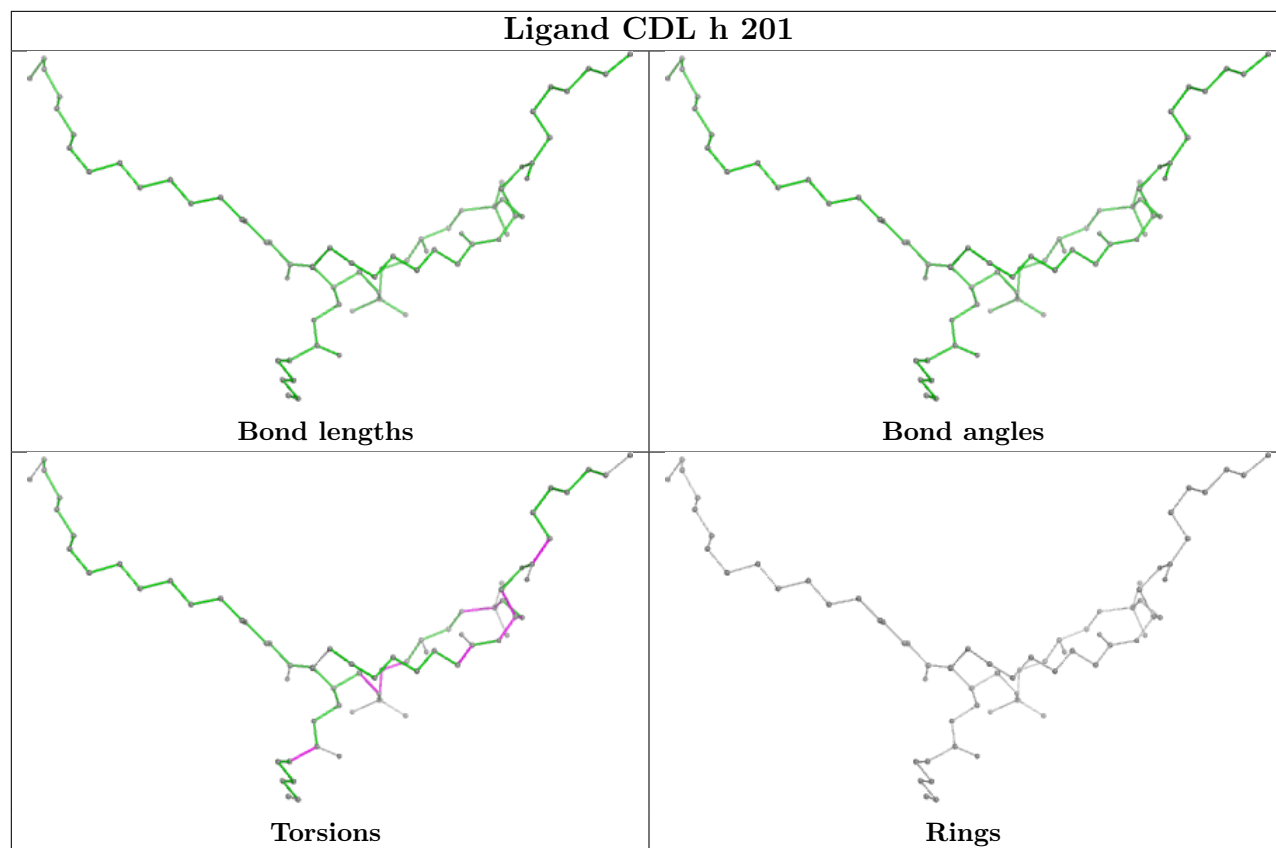


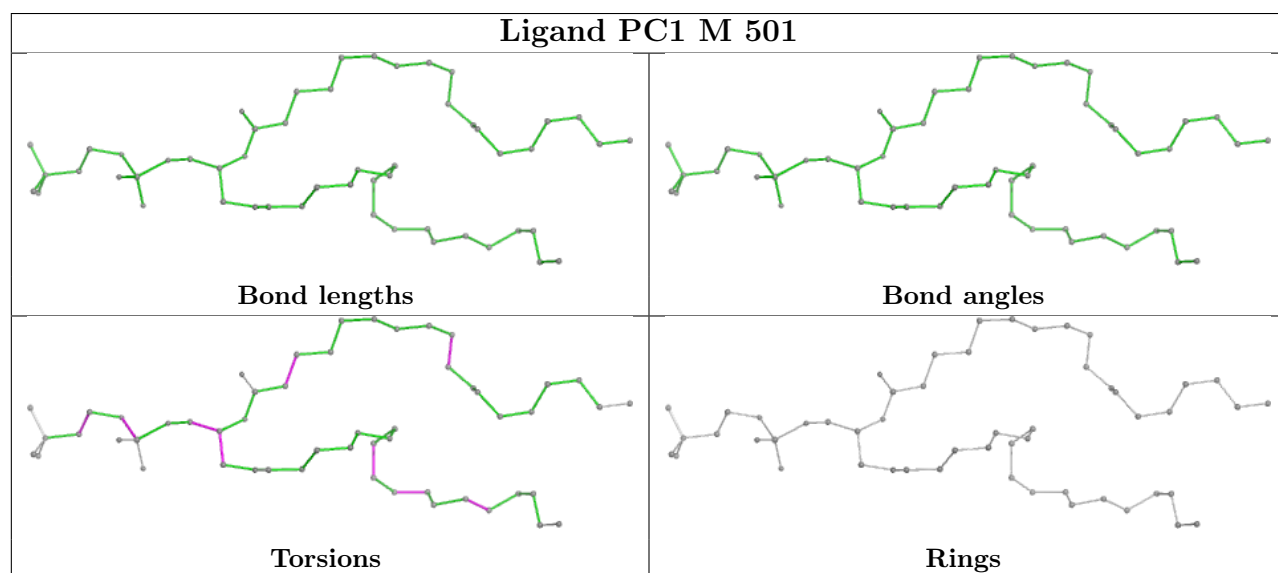
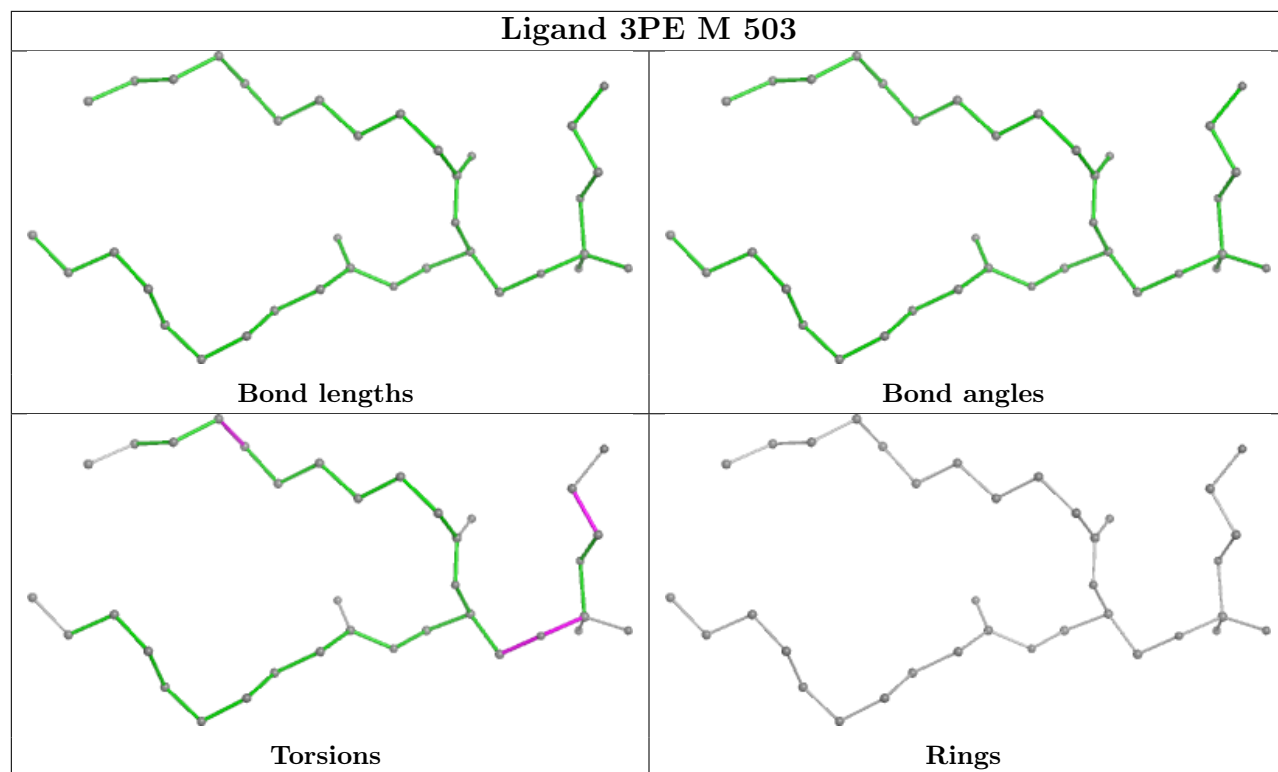


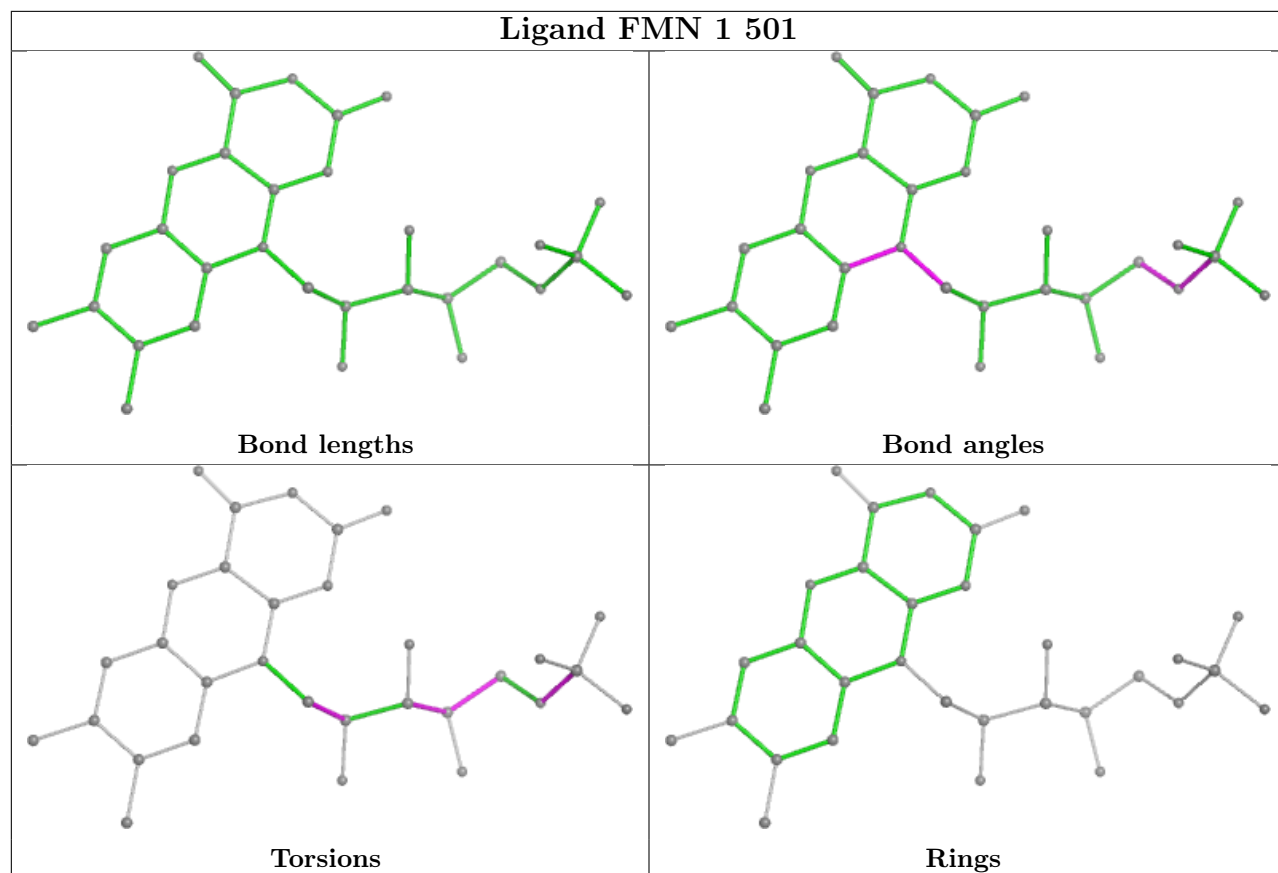


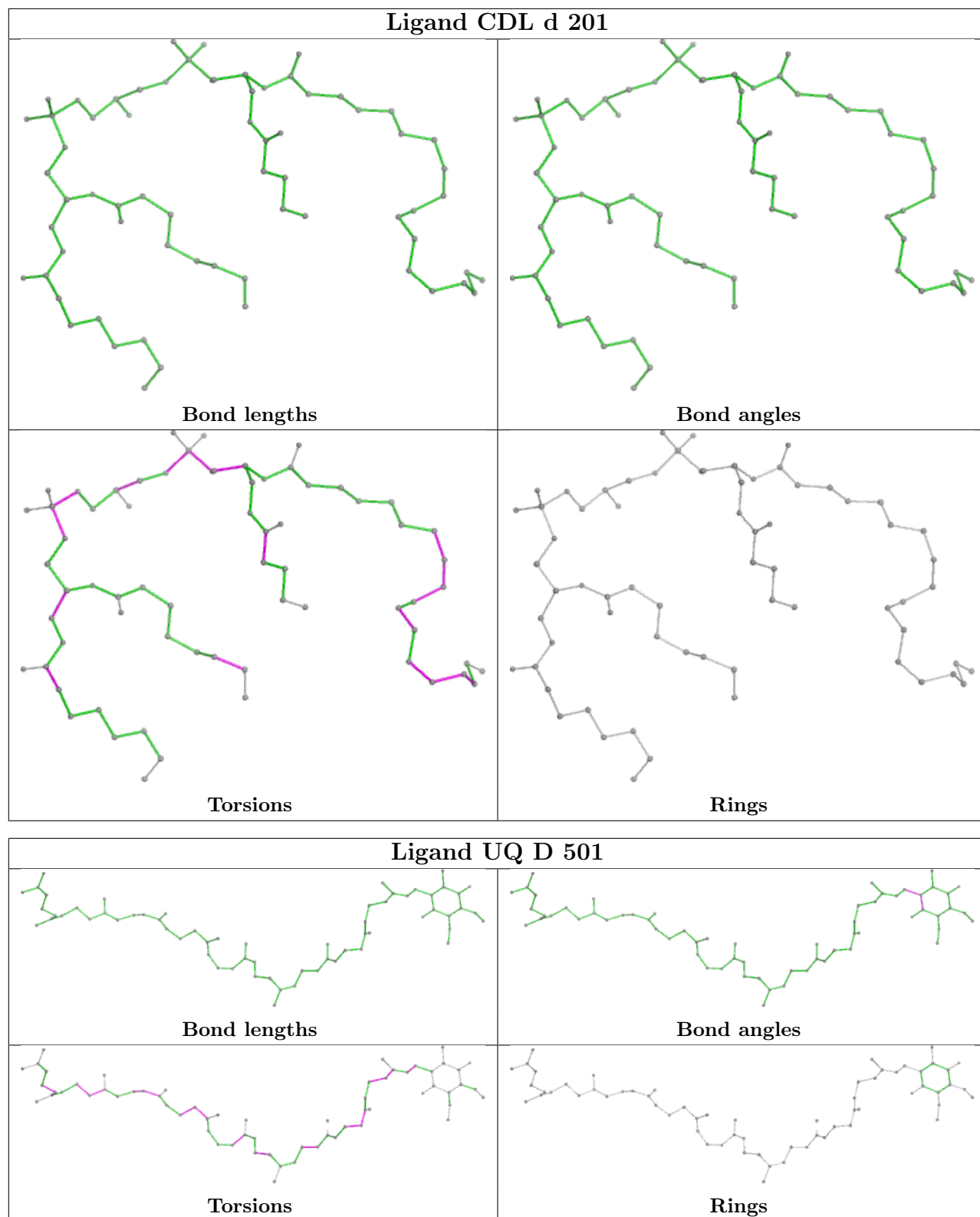


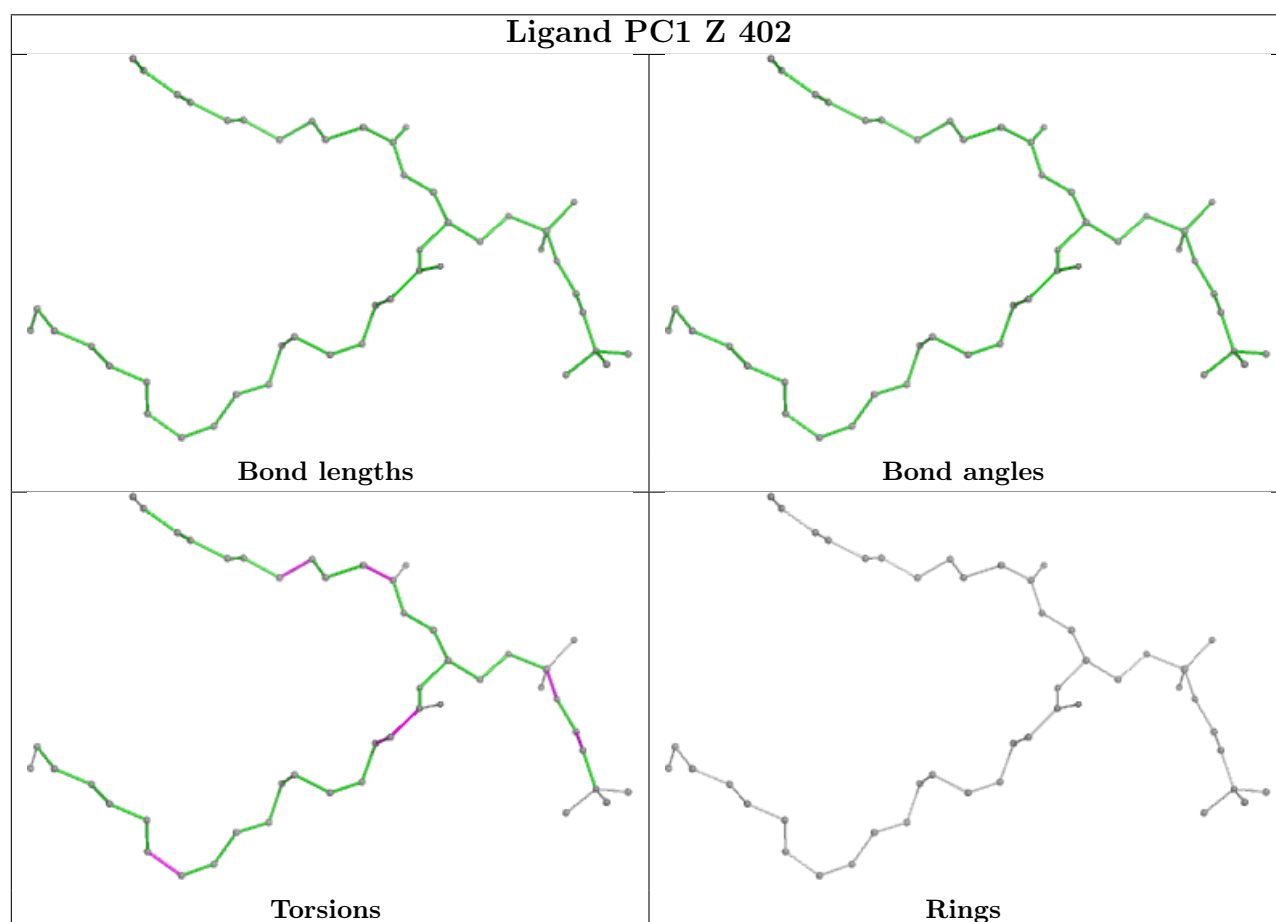
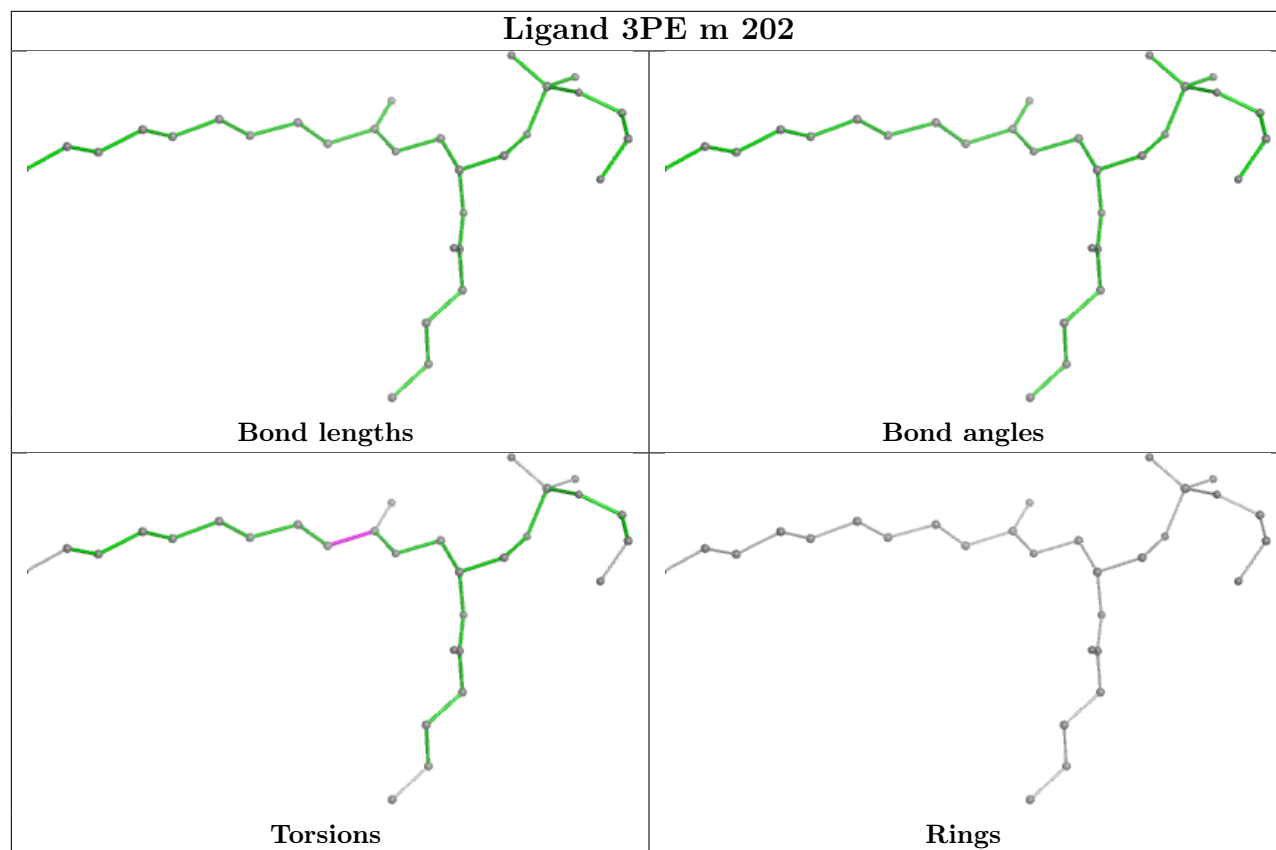


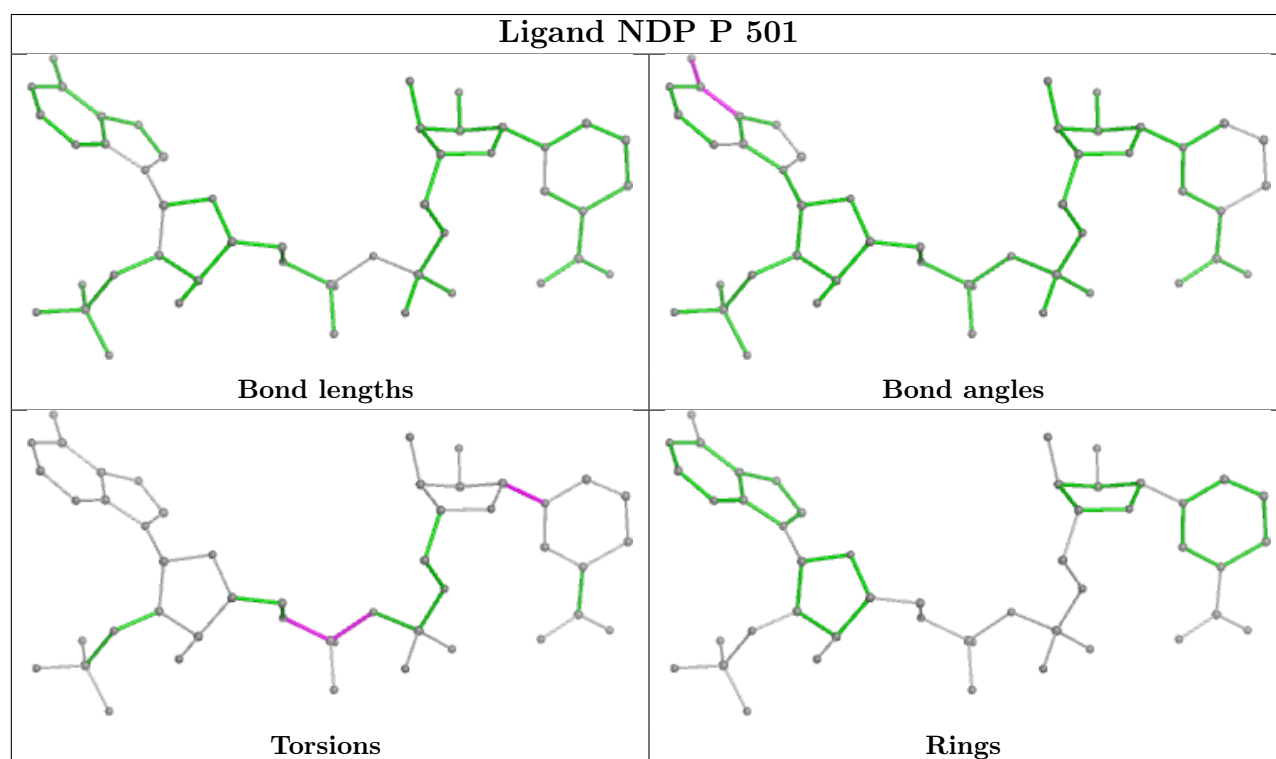
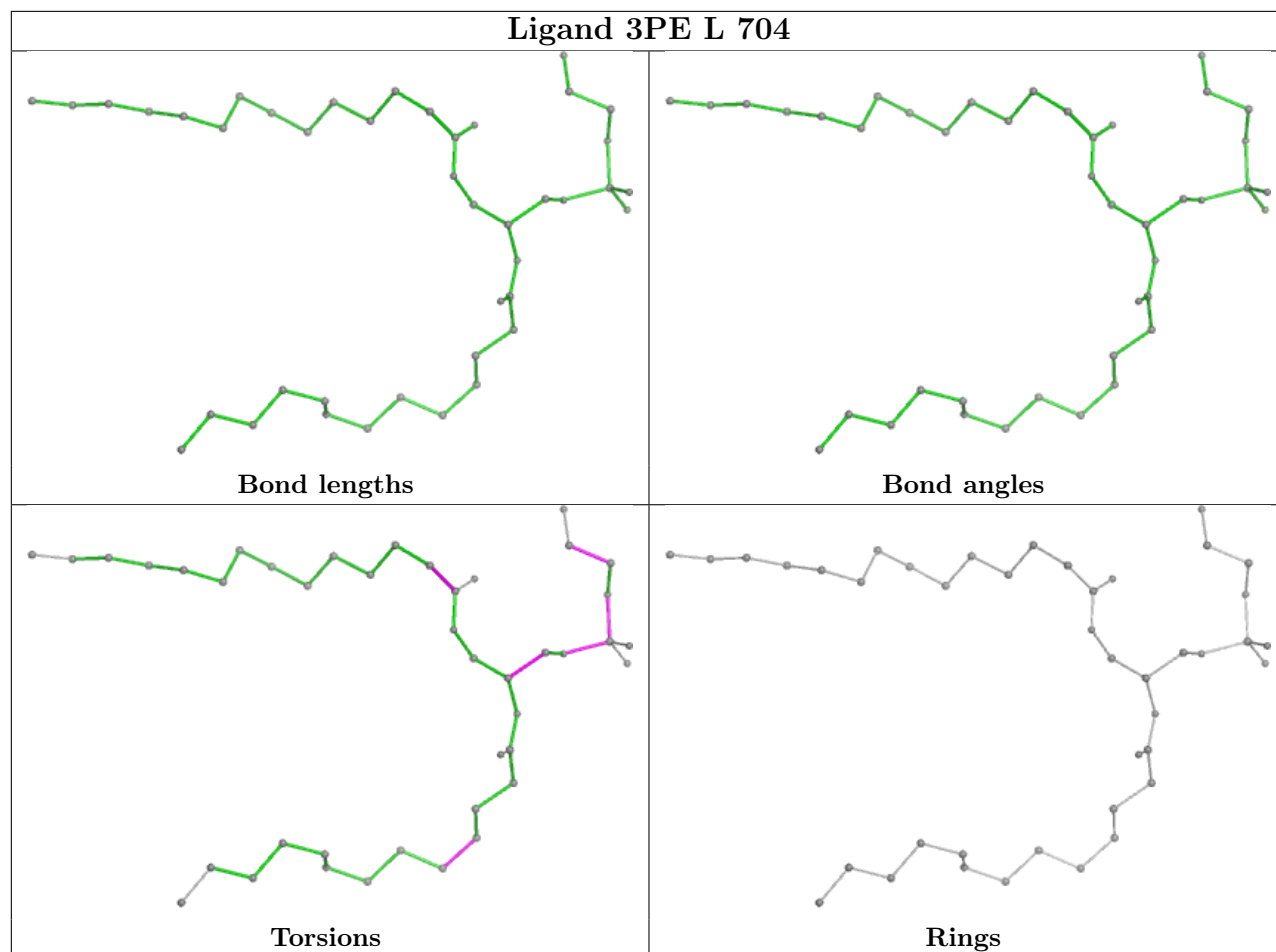


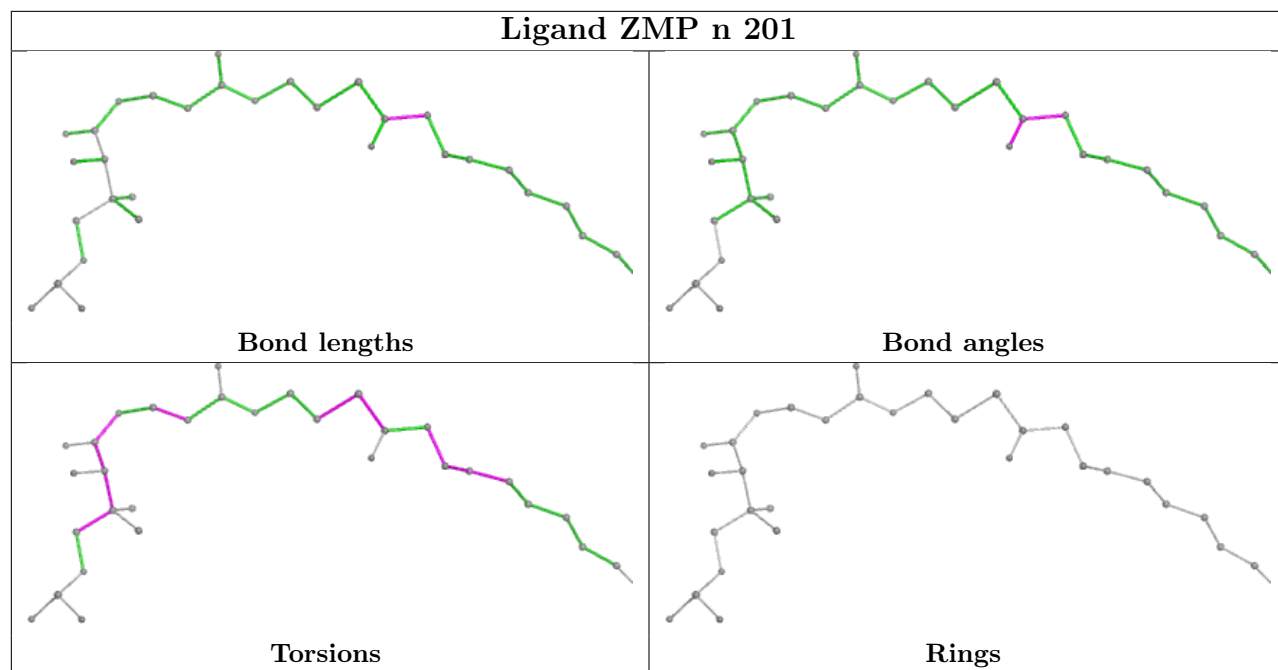


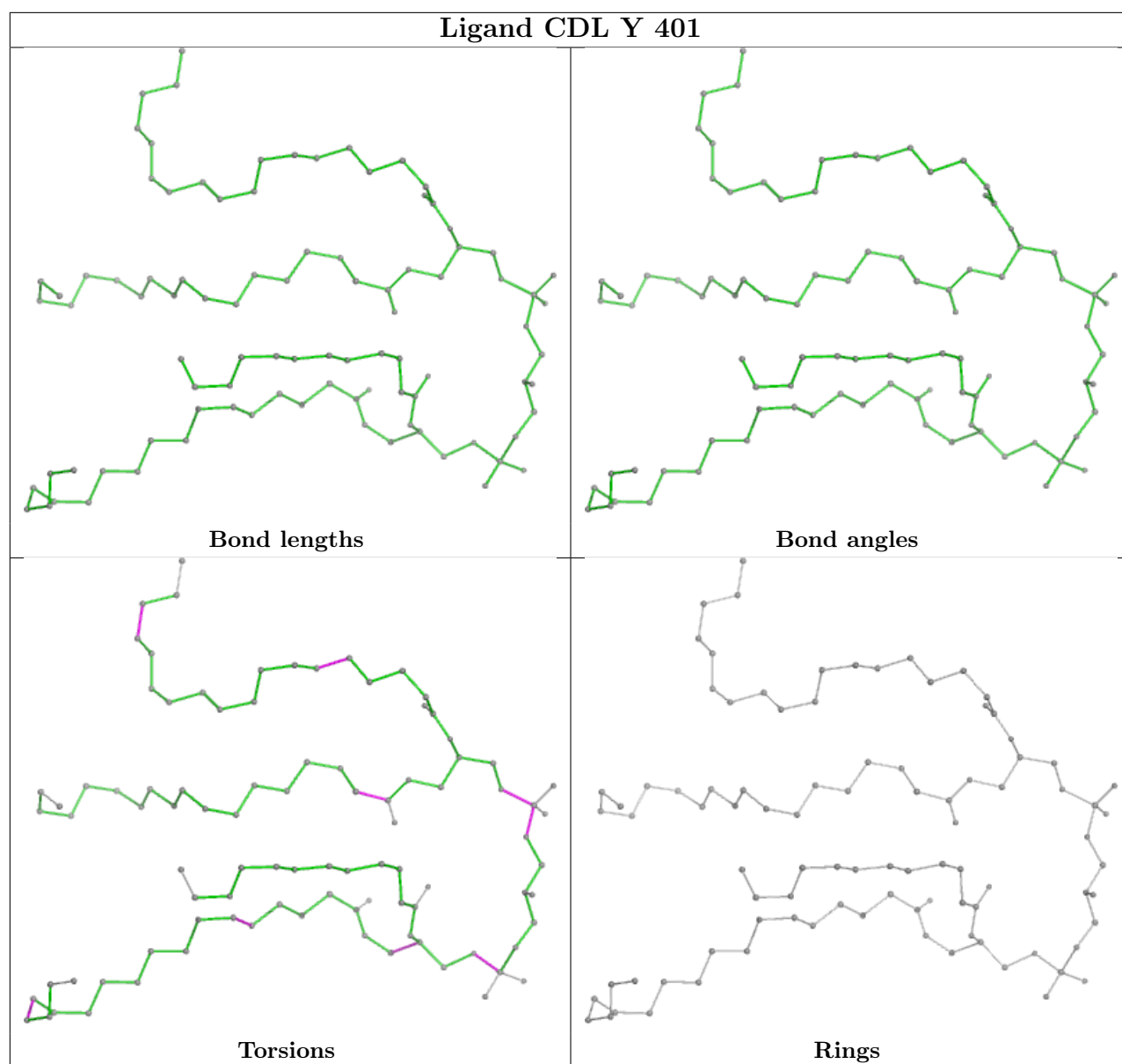


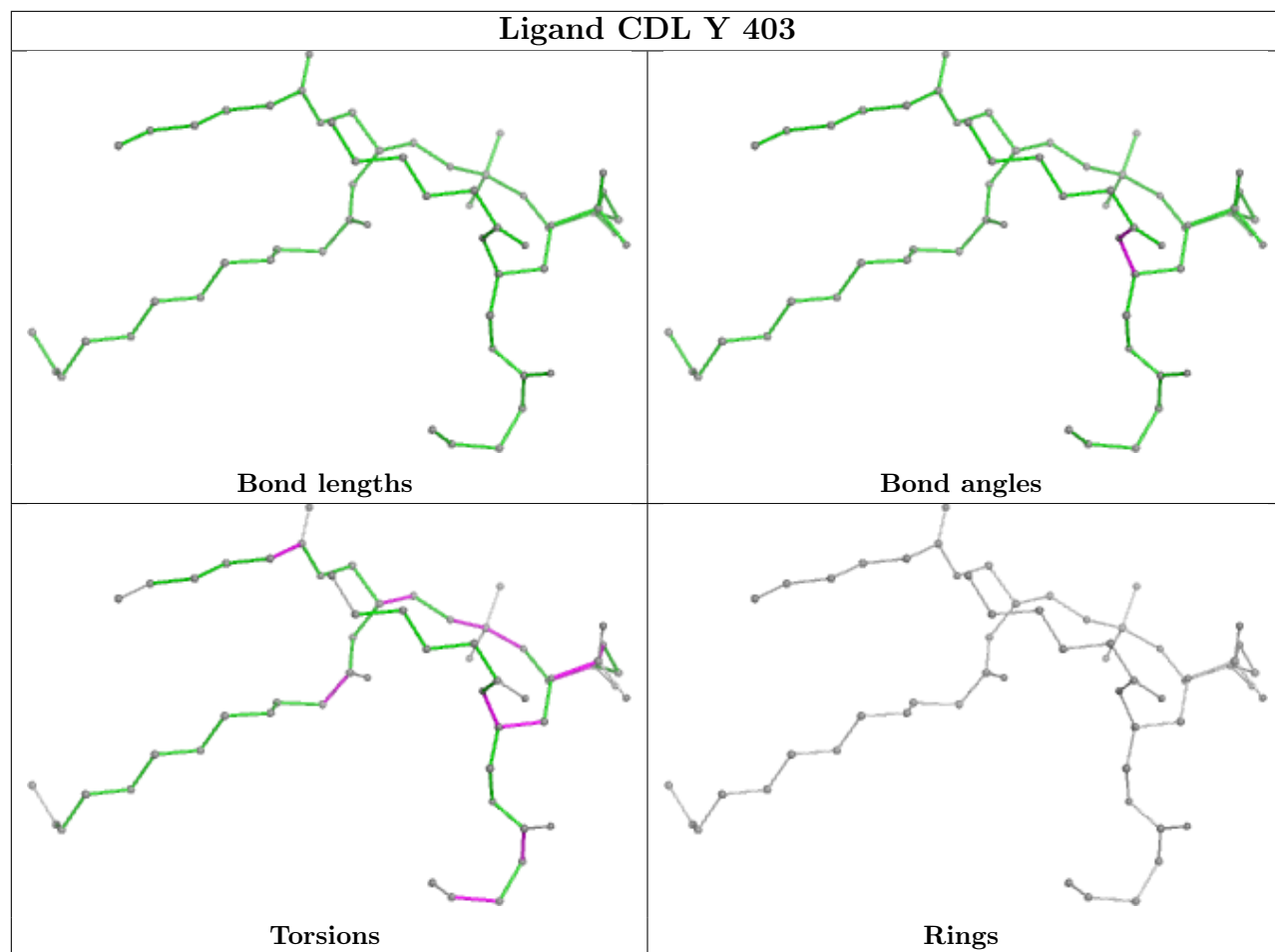


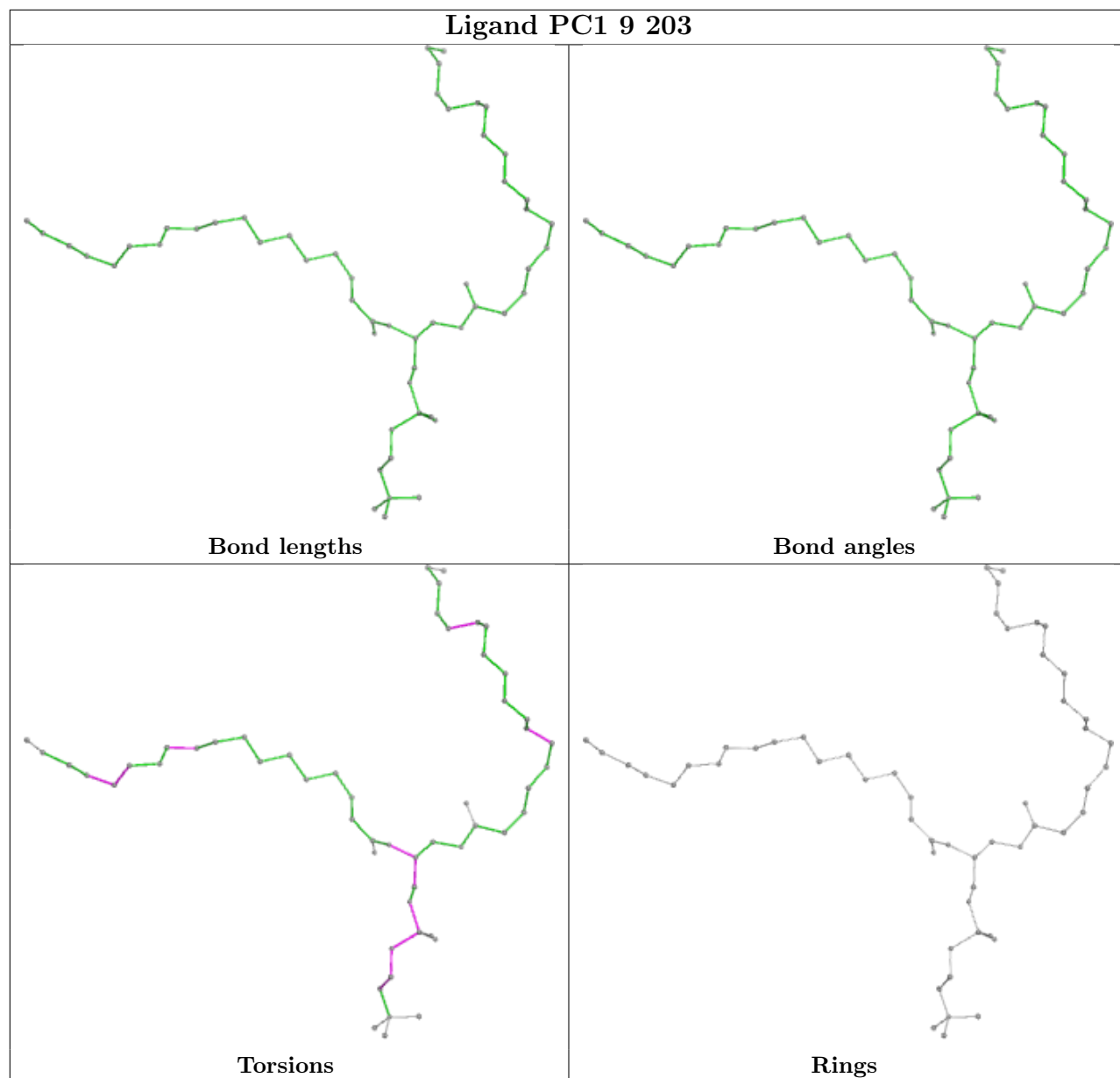


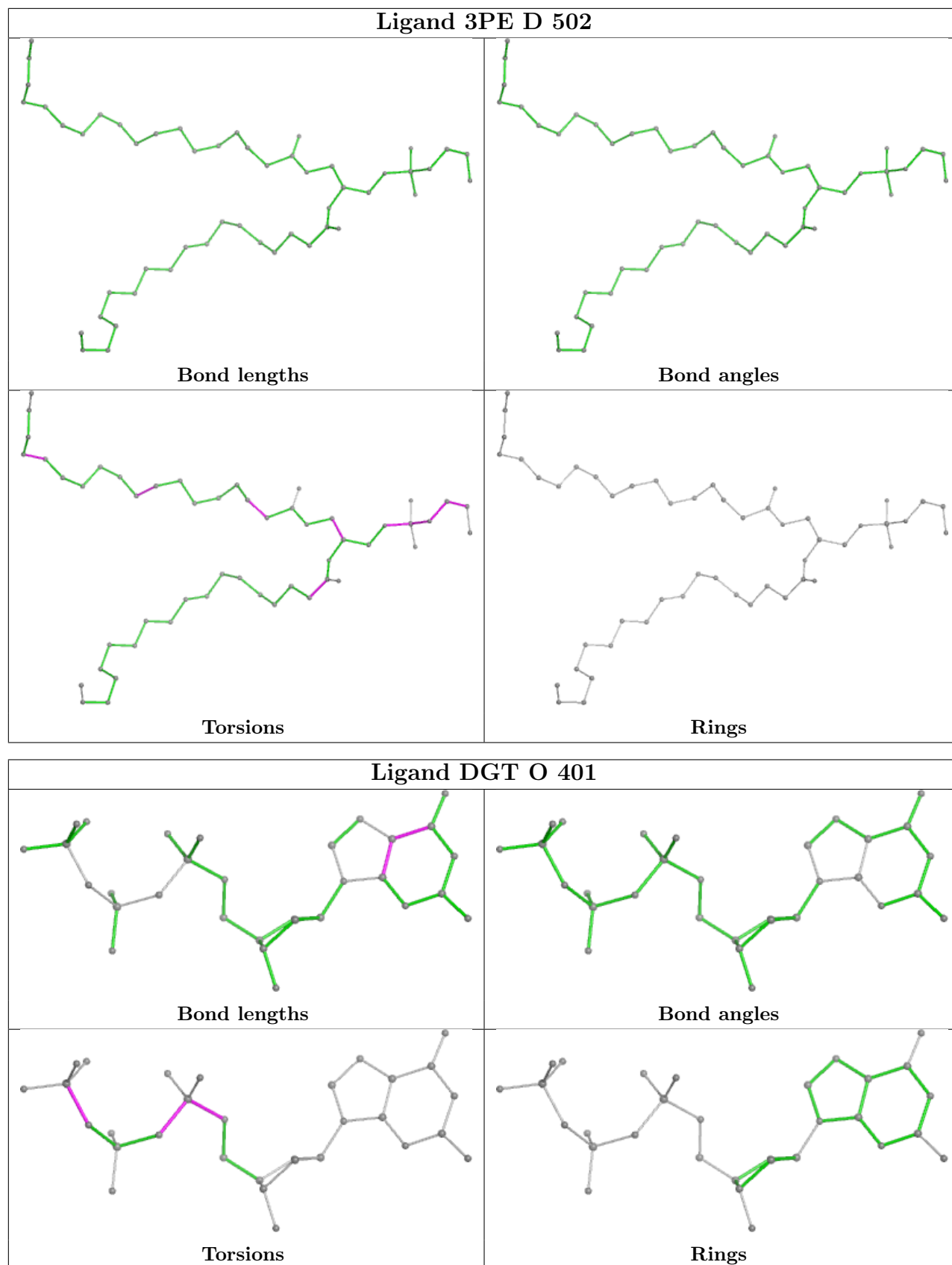












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	67:GLY	C	68:ARG	N	0.94

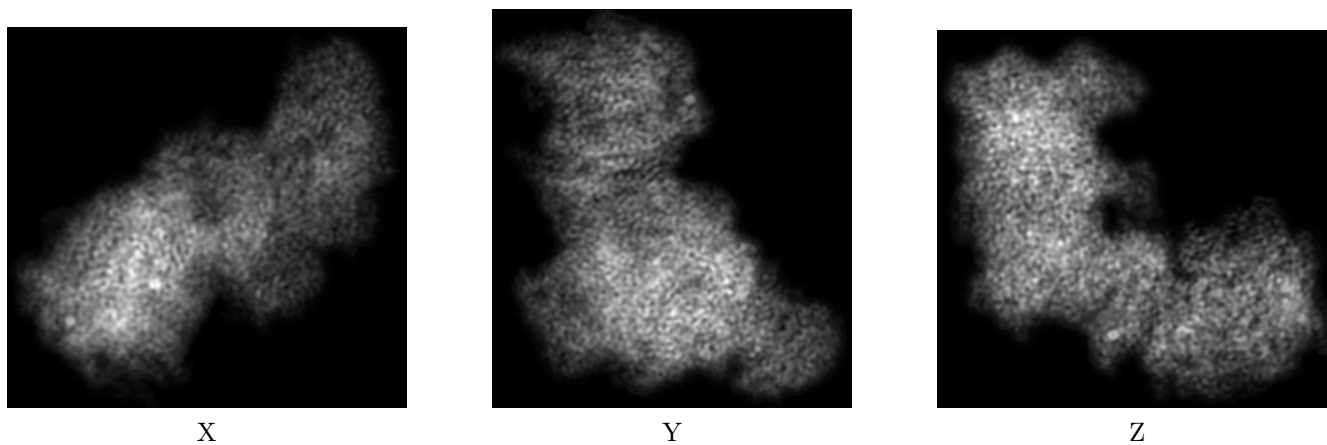
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19145. 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](#)

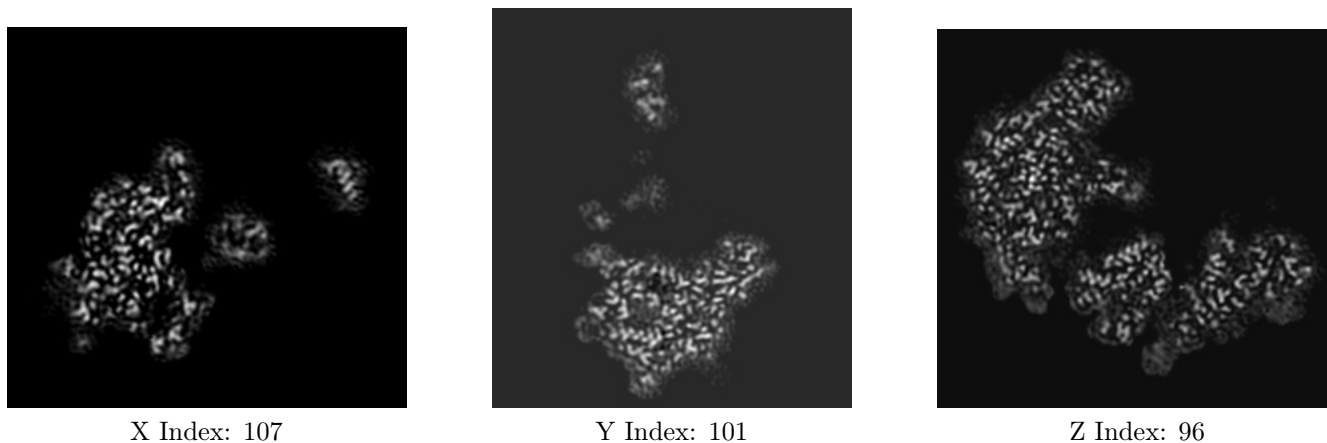
6.1.1 Primary map



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

6.2 Central slices [i](#)

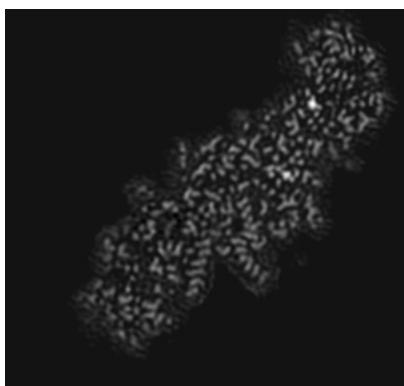
6.2.1 Primary map



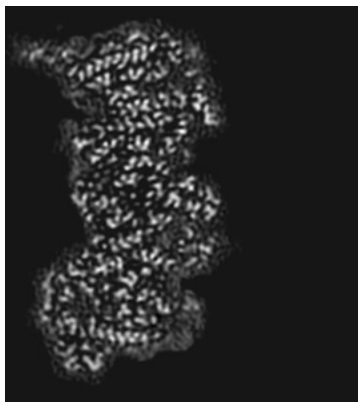
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

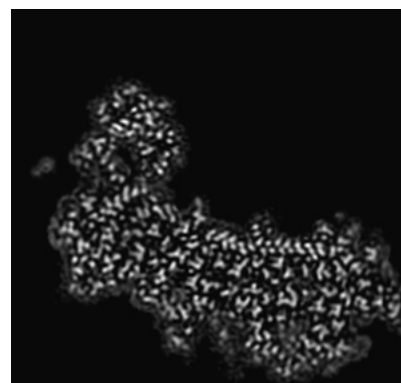
6.3.1 Primary map



X Index: 41



Y Index: 63

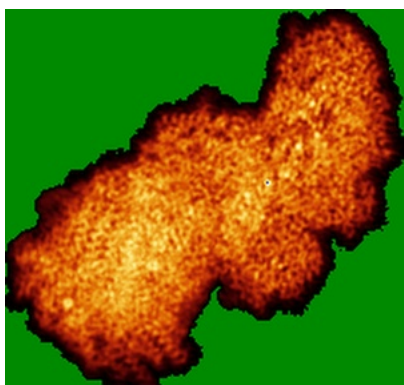


Z Index: 63

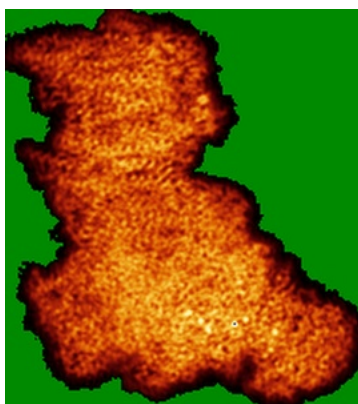
The images above show the largest variance slices of the map in three orthogonal directions.

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

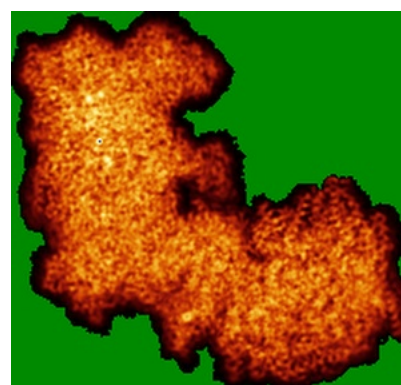
6.4.1 Primary map



X



Y

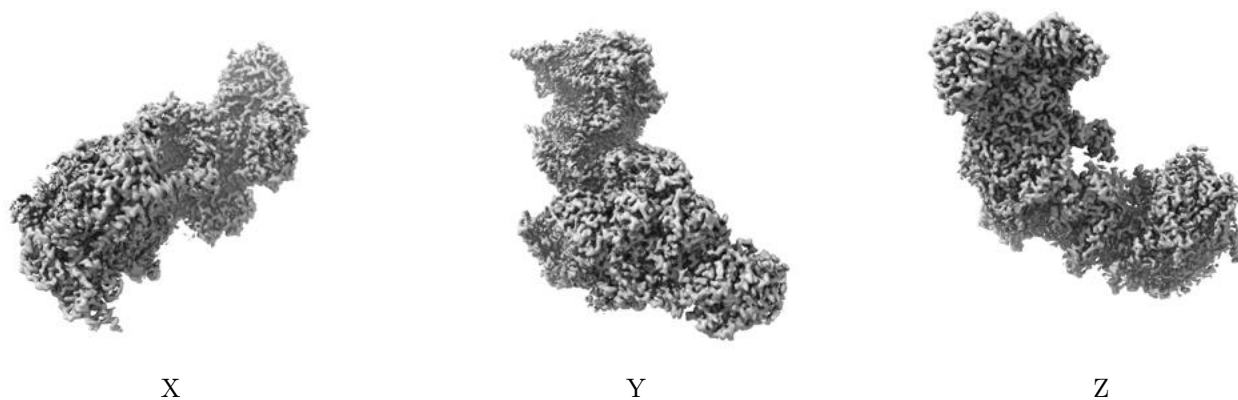


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

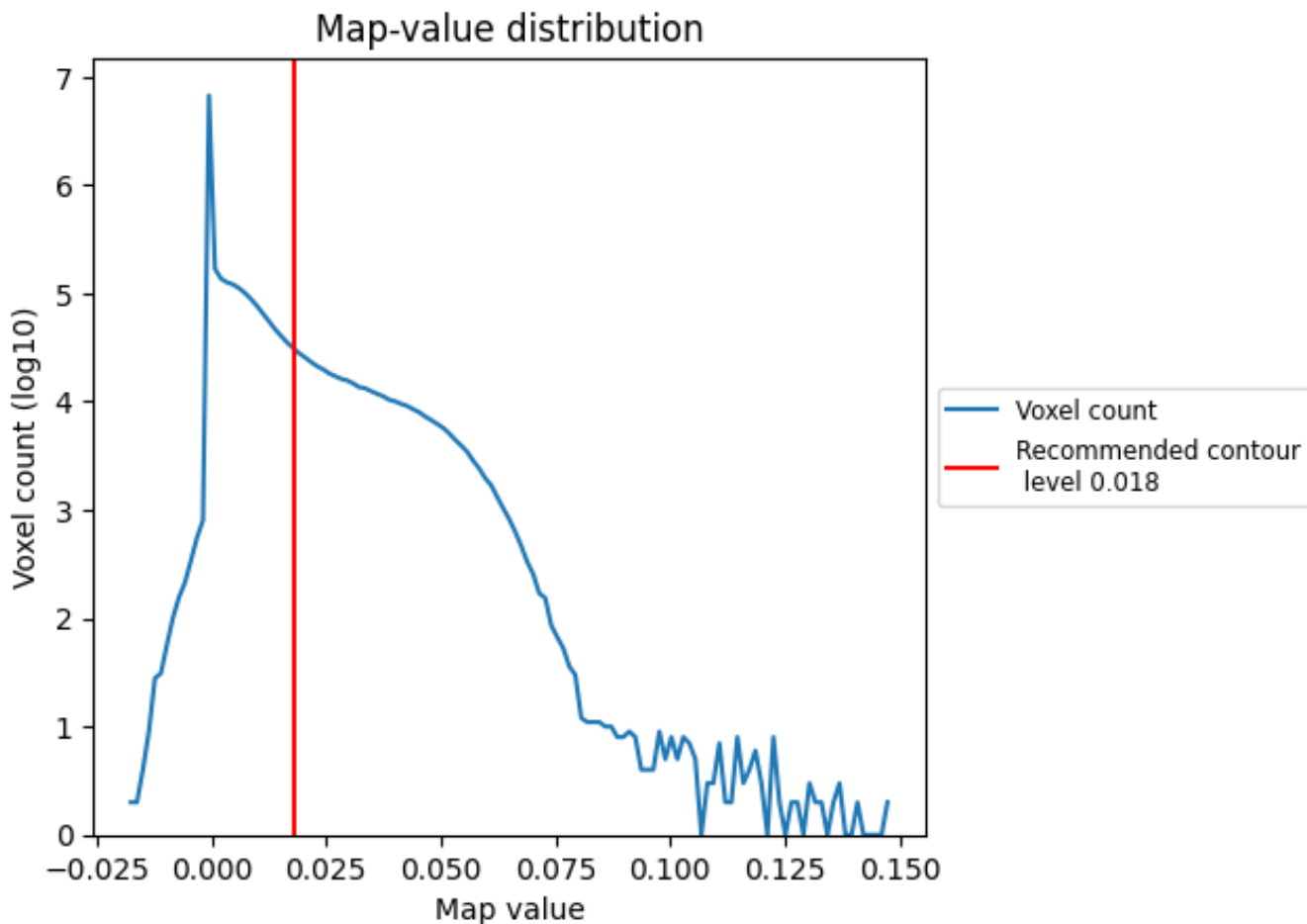
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

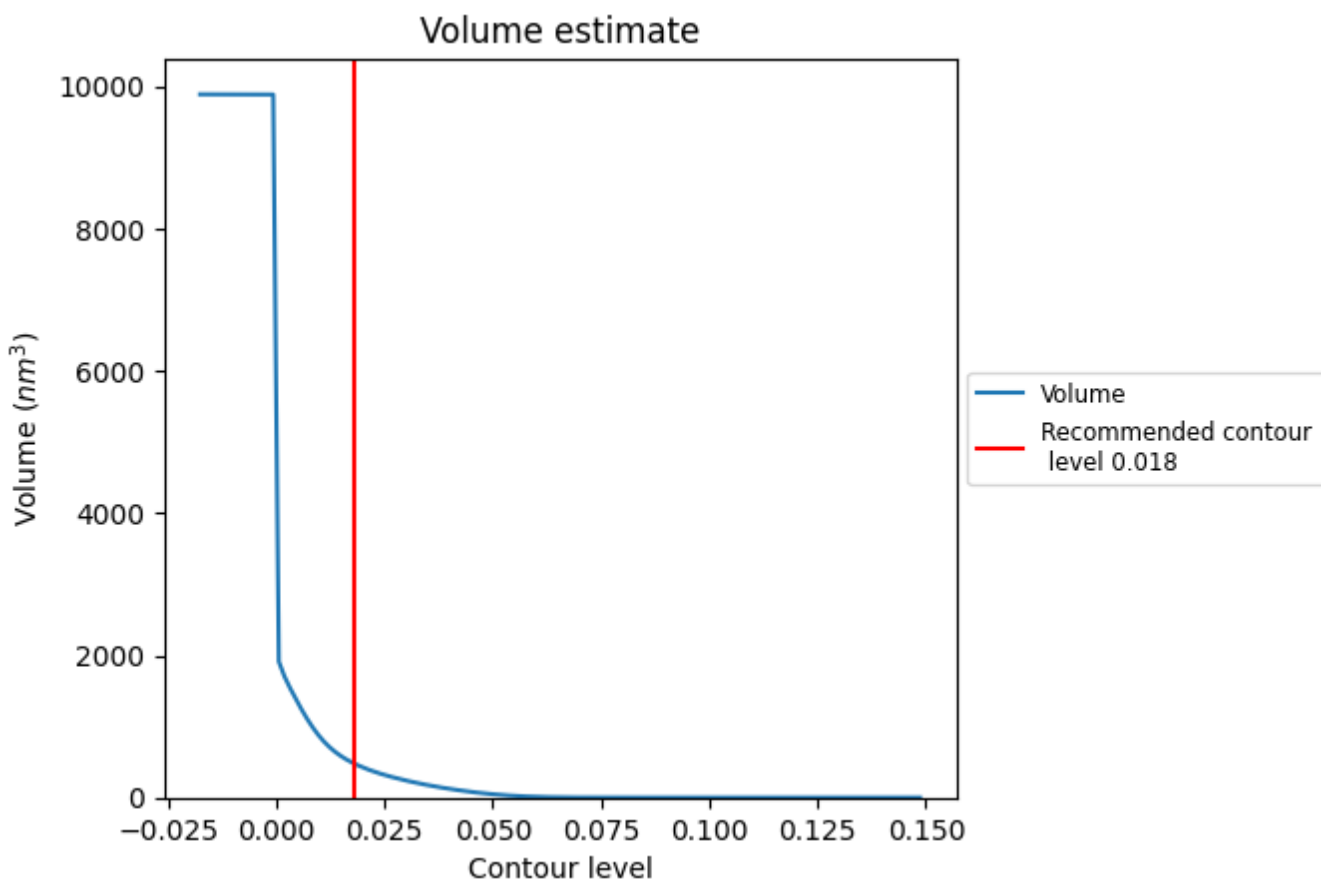
This section contains the results of statistical analysis of the map.

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 479 nm³; this corresponds to an approximate mass of 433 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.

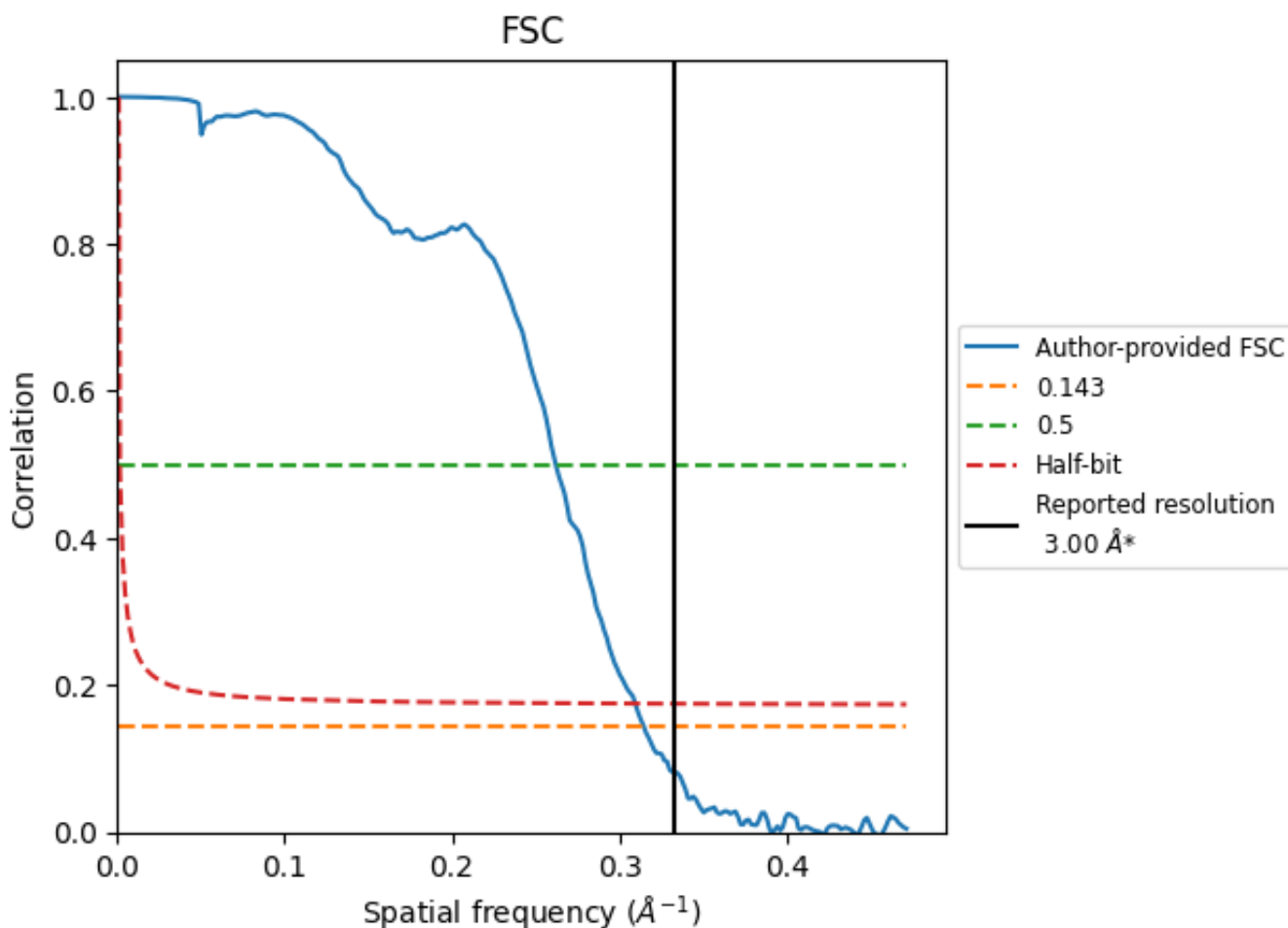
7.3 Rotationally averaged power spectrum [i](#)

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

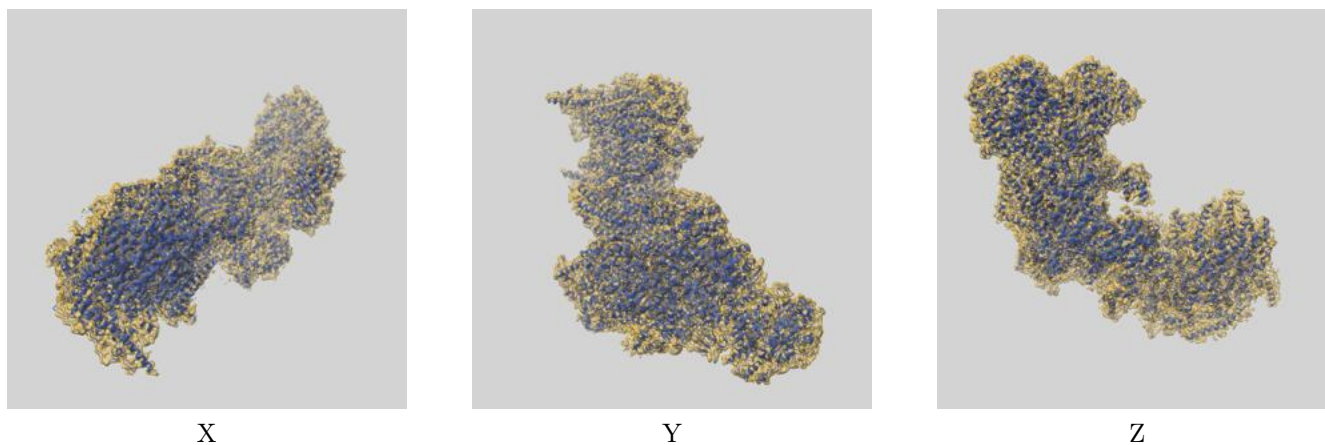
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.18	3.82	3.23
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

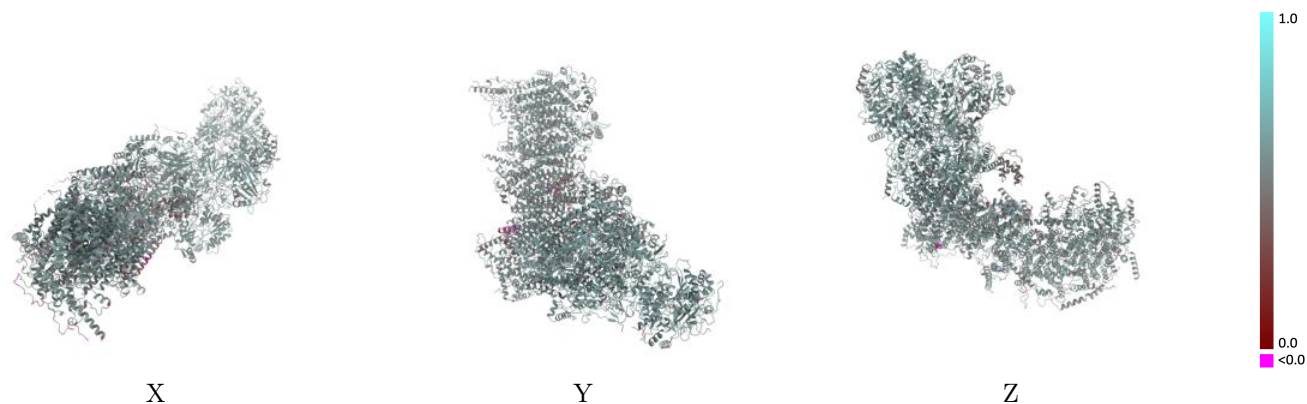
This section contains information regarding the fit between EMDB map EMD-19145 and PDB model 8RGP. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



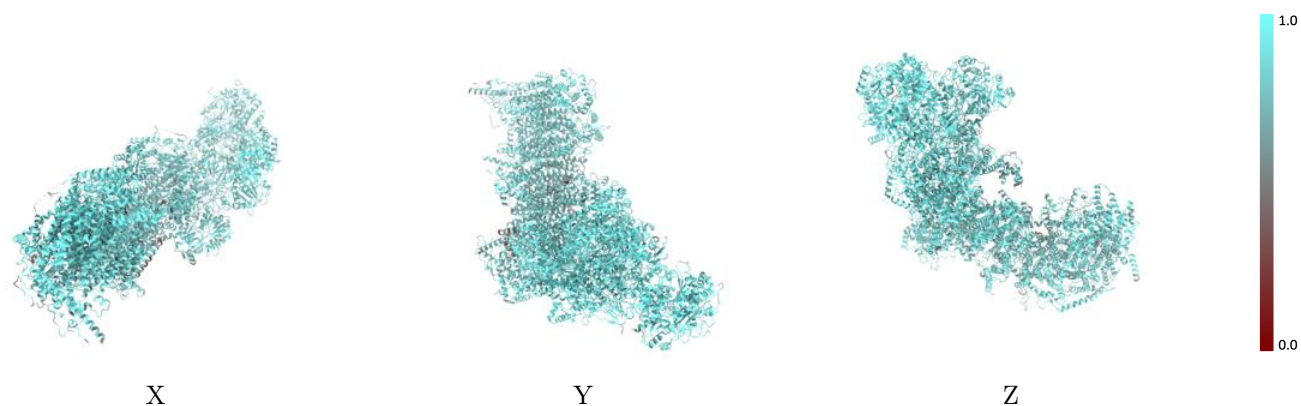
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



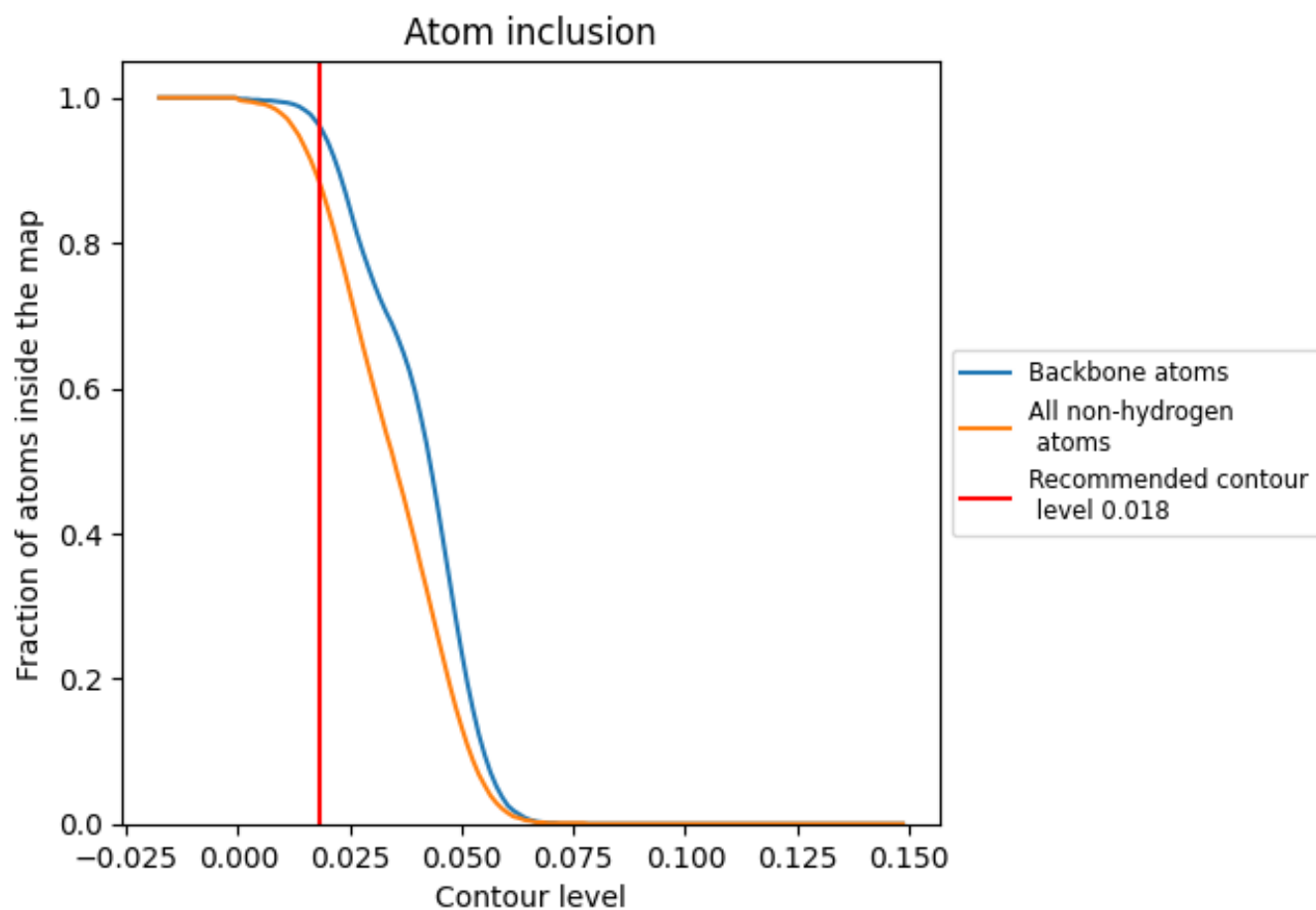
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.5450
1	 0.9190	 0.5650
2	 0.9040	 0.5490
3	 0.9090	 0.5620
6	 0.9440	 0.5730
7	 0.9140	 0.5630
9	 0.9340	 0.5780
A	 0.8790	 0.5470
C	 0.9390	 0.5860
D	 0.8860	 0.5460
H	 0.9090	 0.5490
J	 0.7760	 0.4630
K	 0.8710	 0.5380
L	 0.8910	 0.5450
M	 0.9020	 0.5640
N	 0.9020	 0.5550
O	 0.8970	 0.5430
P	 0.8910	 0.5610
Q	 0.8940	 0.5730
S	 0.8880	 0.5410
T	 0.7260	 0.4370
U	 0.8540	 0.5220
V	 0.9020	 0.5580
W	 0.8960	 0.5610
X	 0.8850	 0.5310
Y	 0.7650	 0.4720
Z	 0.8700	 0.5390
a	 0.9200	 0.5490
b	 0.8840	 0.5260
c	 0.8420	 0.5180
d	 0.8610	 0.5440
e	 0.8700	 0.5280
f	 0.8130	 0.4970
g	 0.8480	 0.5230
h	 0.8830	 0.5480



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Chain	Atom inclusion	Q-score
i	 0.8180	 0.5000
j	 0.8520	 0.4990
k	 0.8830	 0.5320
l	 0.8810	 0.5450
m	 0.7870	 0.5130
n	 0.9030	 0.5420
o	 0.8570	 0.5160
p	 0.8830	 0.5310
q	 0.9230	 0.5600
r	 0.8890	 0.5540
s	 0.9370	 0.5740