



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:44 PM UTC

PDB ID : 8RGR / pdb_00008rgr
EMDB ID : EMD-19147
Title : Closed Complex I from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-12-14
Resolution : 2.90 Å(reported)
Based on initial model : 6g2j

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

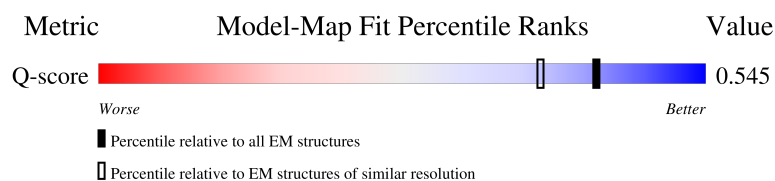
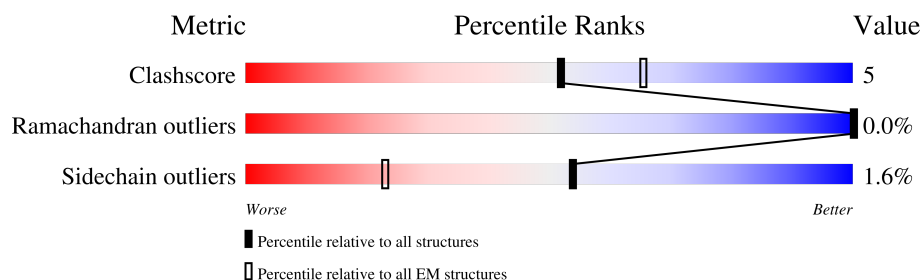
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 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.



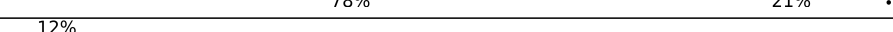
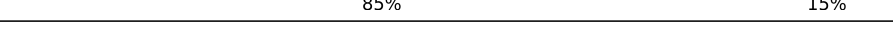
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	55% 14% 30%
2	C	263	67% 12% 21%
3	D	463	5% 76% 16% 7%
4	2	248	72% 14% 14%

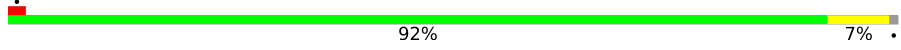
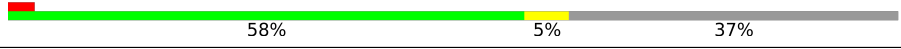
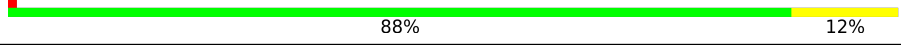
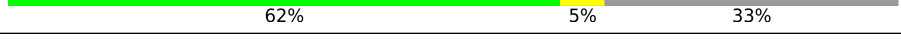
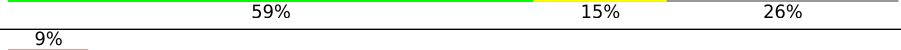
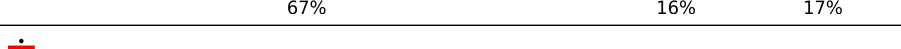
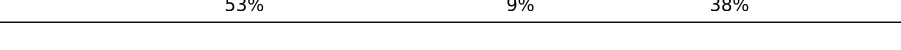
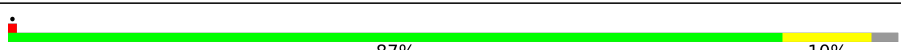
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	1	464	
6	3	727	
7	9	212	
8	P	377	
9	Q	175	
10	7	116	
11	S	99	
12	T	156	
12	U	156	
13	V	116	
14	W	131	
15	q	145	
16	r	113	
17	s	104	
18	A	115	
19	H	318	
20	J	172	
21	K	98	
22	L	607	
23	M	459	
24	N	345	
25	O	355	
26	X	172	
27	Y	141	
28	Z	144	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	a	70	
30	b	84	
31	c	76	
32	d	120	
33	e	106	
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
45	SF4	9	201	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68141 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
1	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	s	42	Total	C	N	O	0	0
			351	219	62	70		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

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

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

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

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

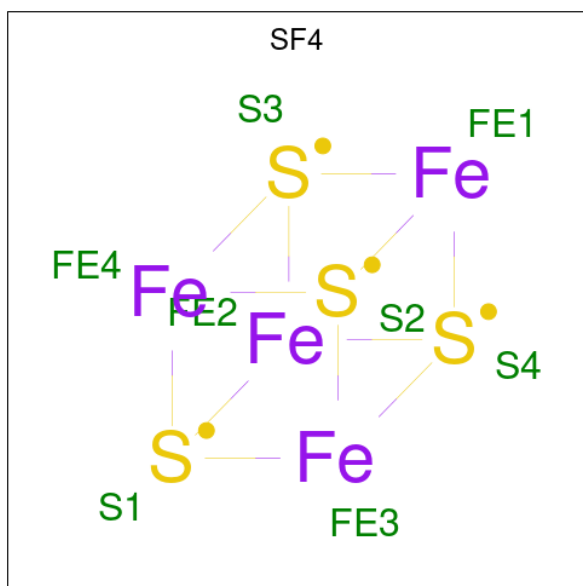
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

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

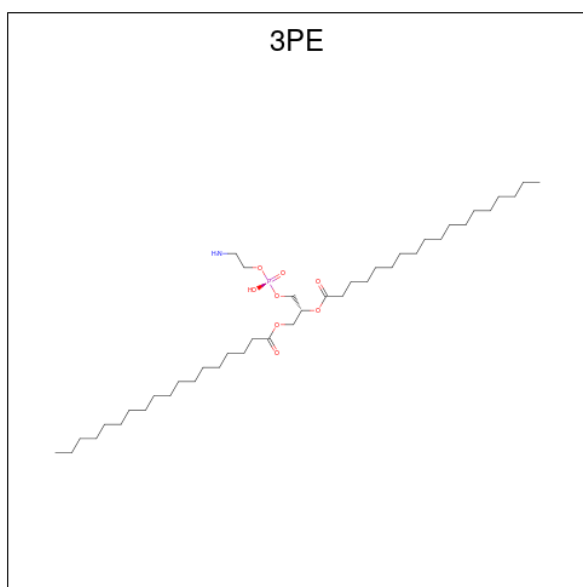
Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	170	Total	C	N	O	S	0	0
			1438	903	258	269	8		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).



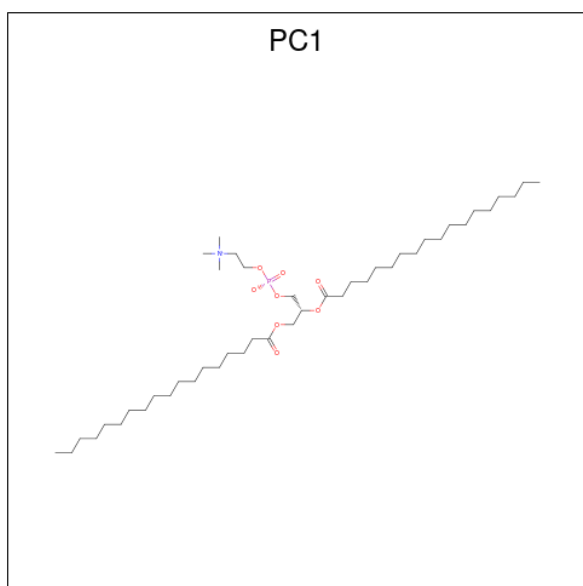
Mol	Chain	Residues	Atoms					AltConf
46	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	r	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	K	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	Y	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	d	1	Total	C	N	O	P	0
			31	21	1	8	1	

Continued on next page...

Continued from previous page...

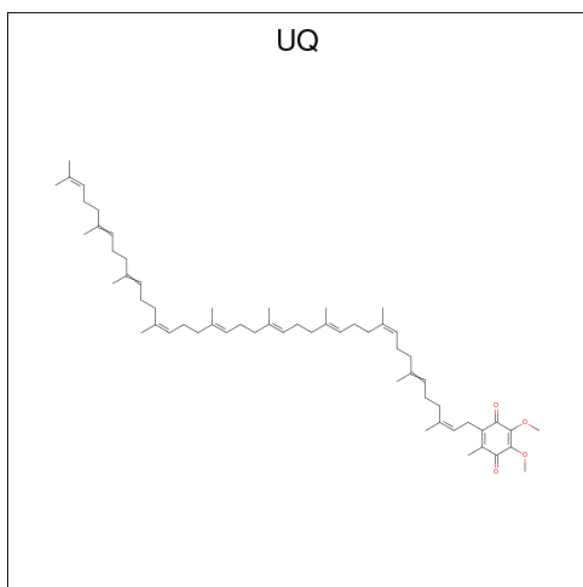
Mol	Chain	Residues	Atoms					AltConf
46	d	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	m	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



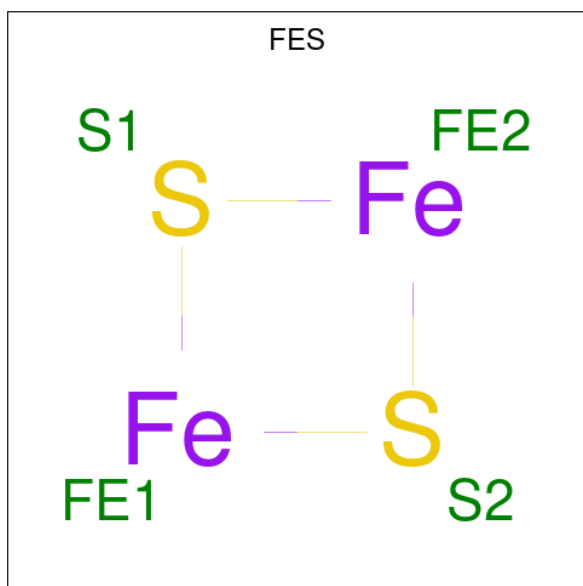
Mol	Chain	Residues	Atoms					AltConf
47	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
47	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	N	1	Total	C	N	O	P	0
			54	44	1	8	1	

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



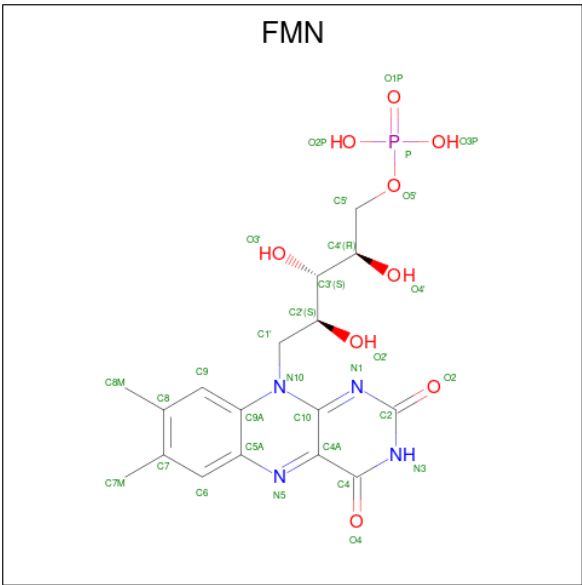
Mol	Chain	Residues	Atoms			AltConf
48	D	1	Total	C	O	0
			63	59	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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

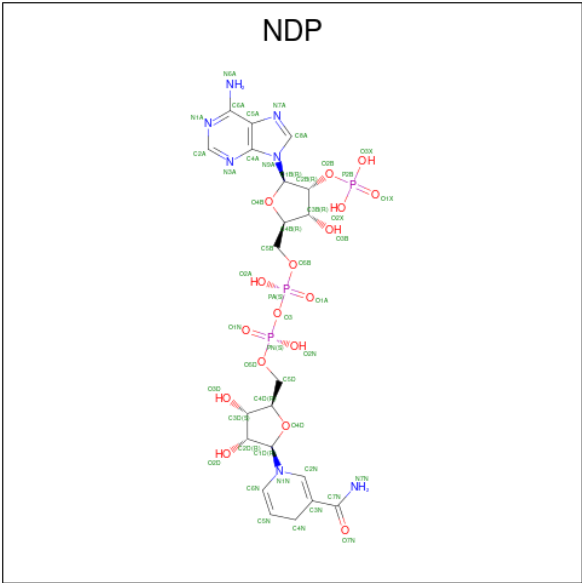


Mol	Chain	Residues	Atoms					AltConf
50	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (CCD ID: 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 (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

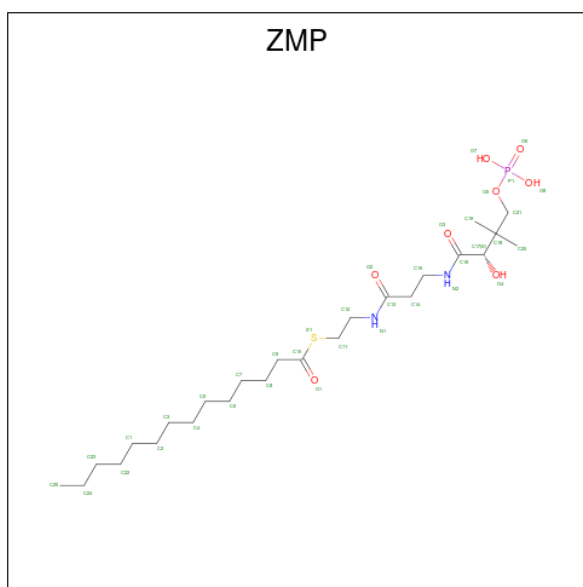


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

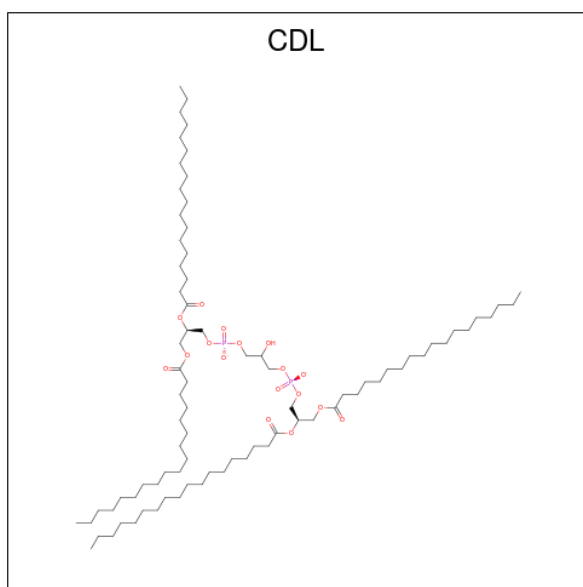
Mol	Chain	Residues	Atoms		AltConf
53	7	1	Total	Zn	0
			1	1	

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



Mol	Chain	Residues	Atoms						AltConf
54	W	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
54	n	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
55	r	1	Total	C	O	P	0
			57	38	17	2	
55	H	1	Total	C	O	P	0
			51	33	16	2	
55	L	1	Total	C	O	P	0
			78	59	17	2	
55	L	1	Total	C	O	P	0
			46	27	17	2	
55	N	1	Total	C	O	P	0
			90	71	17	2	
55	Y	1	Total	C	O	P	0
			94	75	17	2	
55	Y	1	Total	C	O	P	0
			57	38	17	2	
55	d	1	Total	C	O	P	0
			67	48	17	2	
55	h	1	Total	C	O	P	0
			70	51	17	2	
55	m	1	Total	C	O	P	0
			72	53	17	2	

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



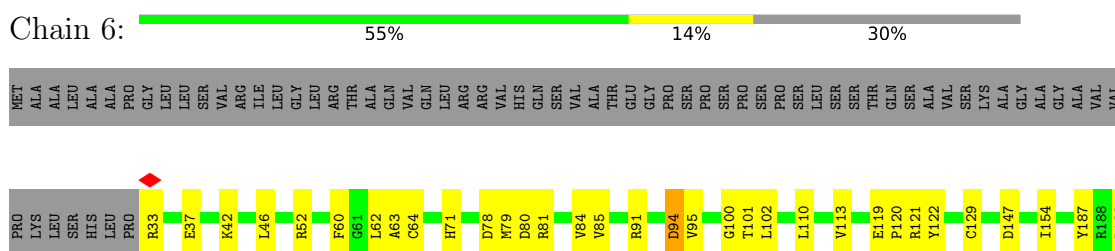
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

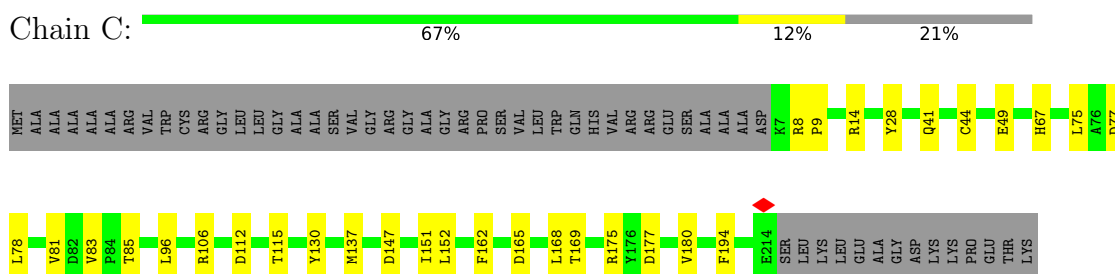
3 Residue-property plots

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.

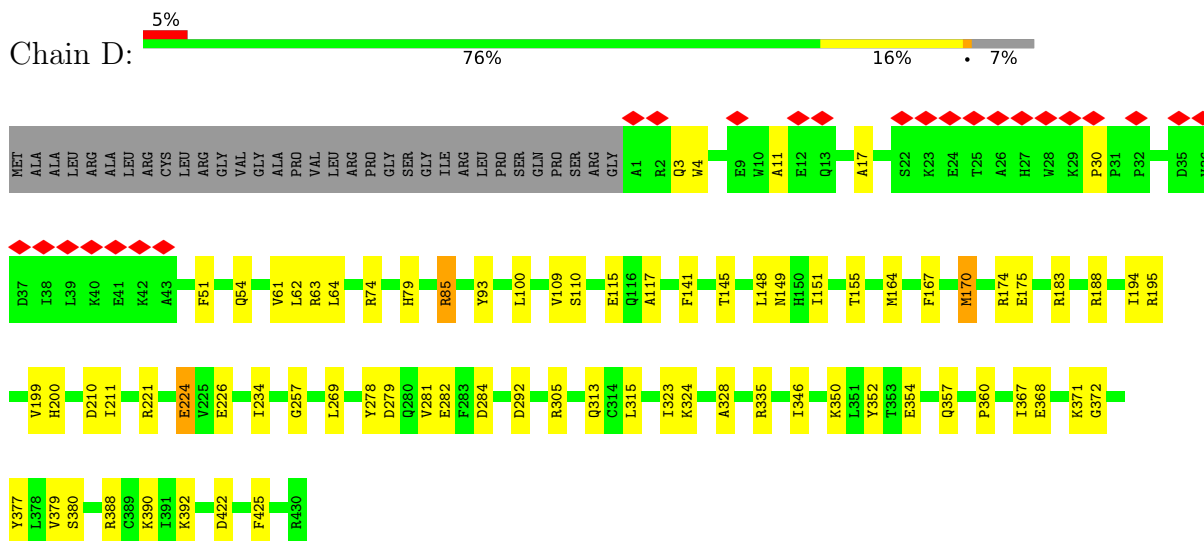
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

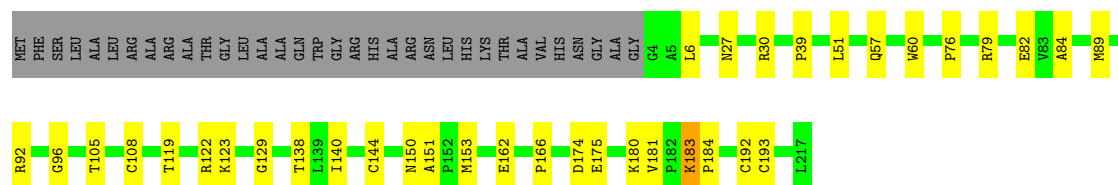


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



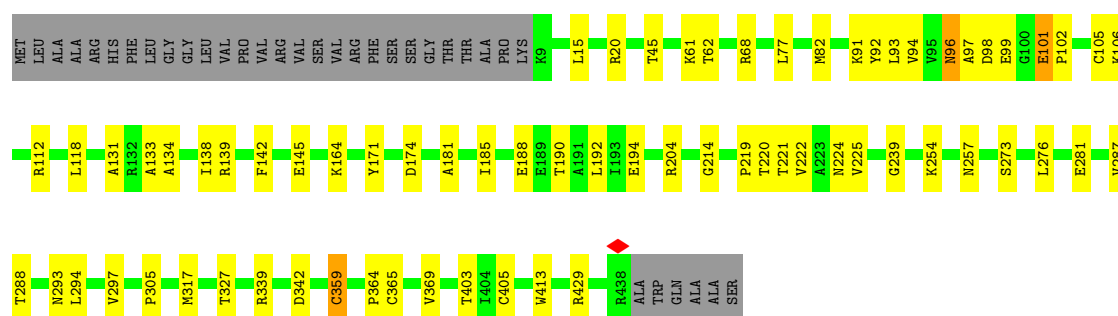
- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2: 



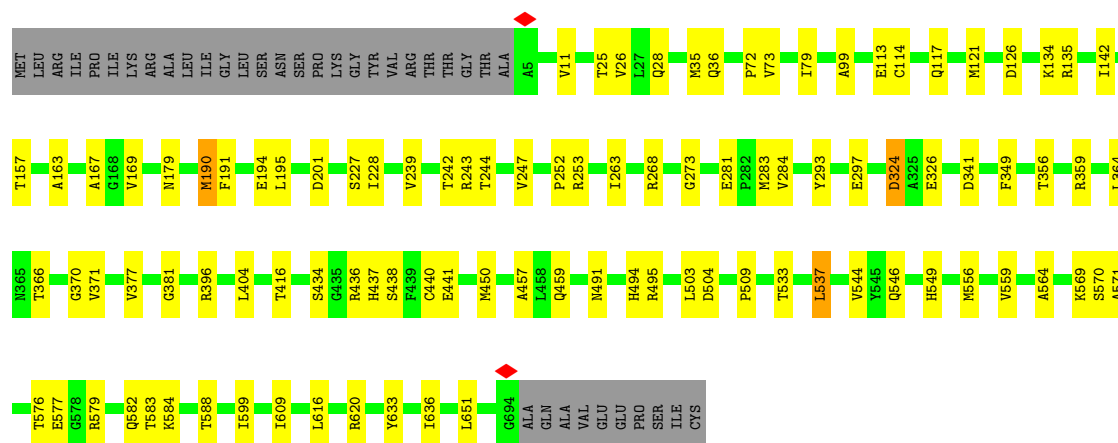
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 



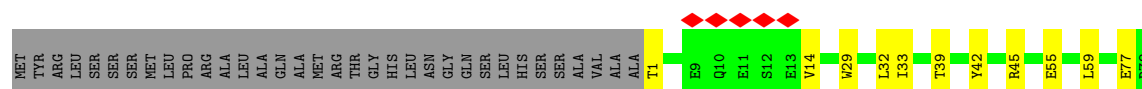
- Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

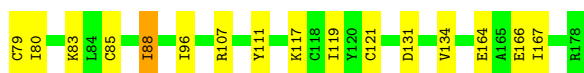
Chain 3: 



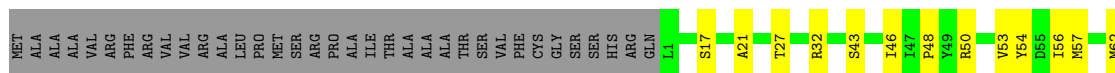
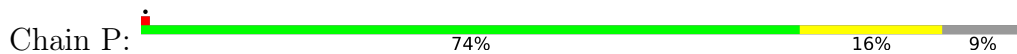
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9: 

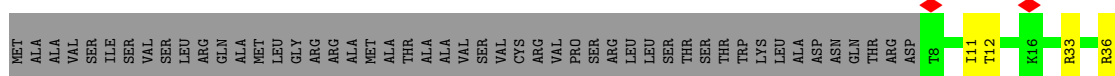




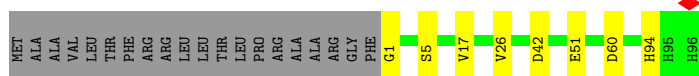
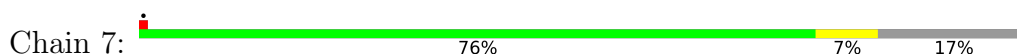
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



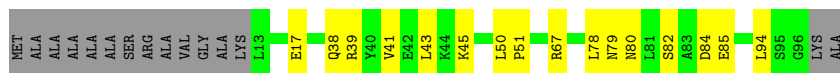
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



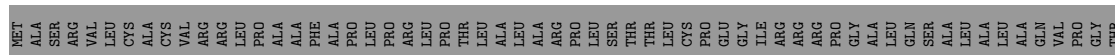
- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

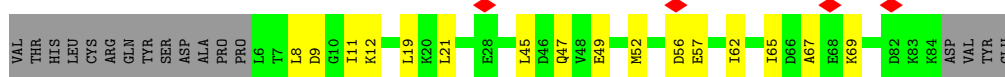


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

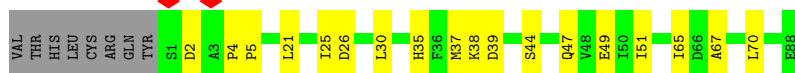


- Molecule 12: Acyl carrier protein, mitochondrial

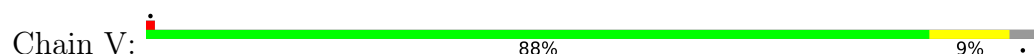




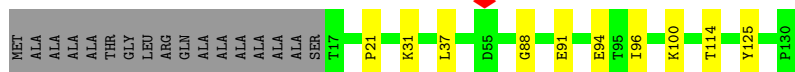
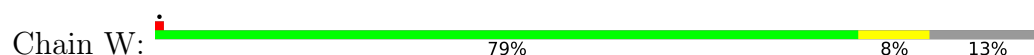
- Molecule 12: Acyl carrier protein, mitochondrial



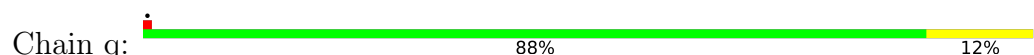
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



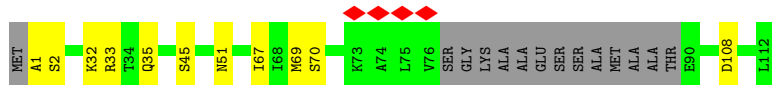
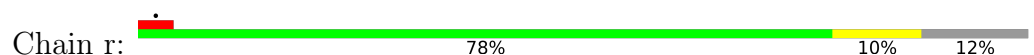
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



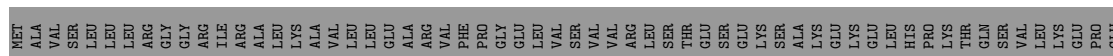
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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

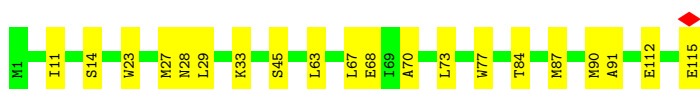
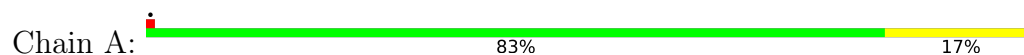


- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

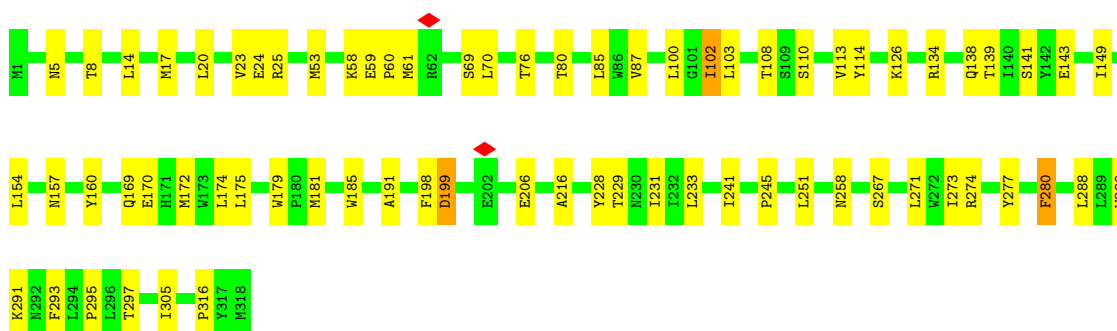
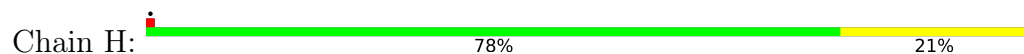




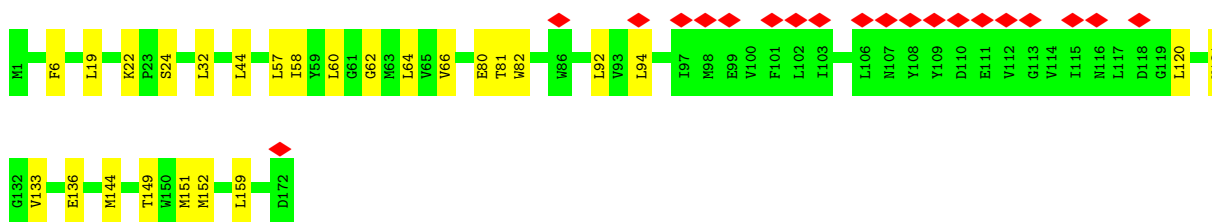
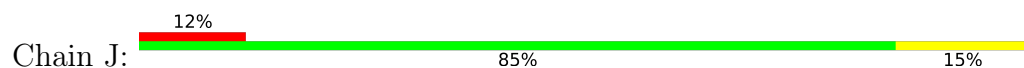
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



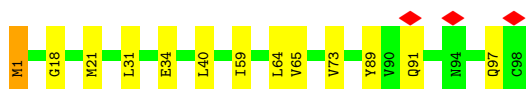
- Molecule 19: NADH-ubiquinone oxidoreductase chain 1



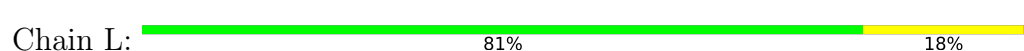
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6

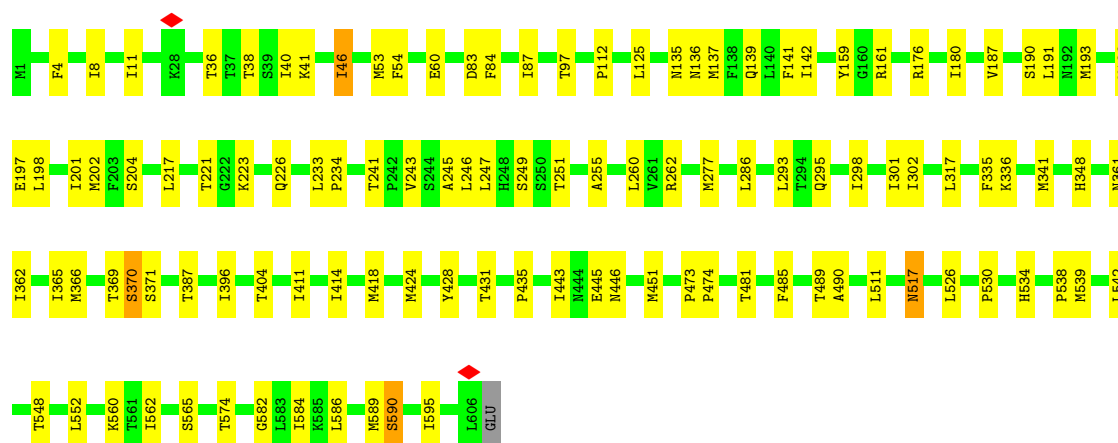


- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L



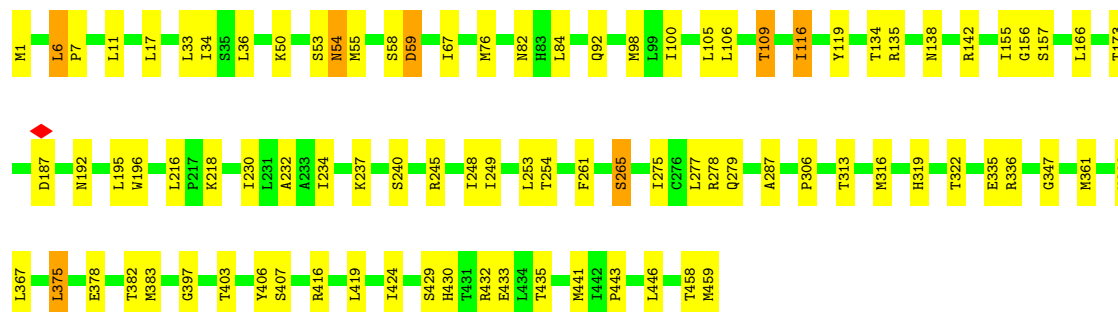
- Molecule 22: NADH-ubiquinone oxidoreductase chain 5





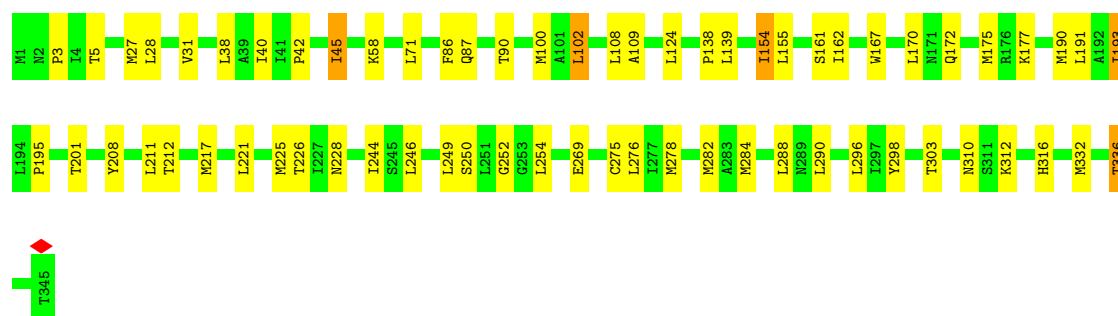
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain M: 80% 18%



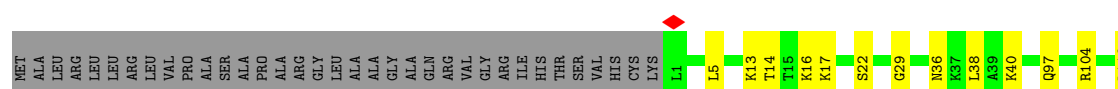
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

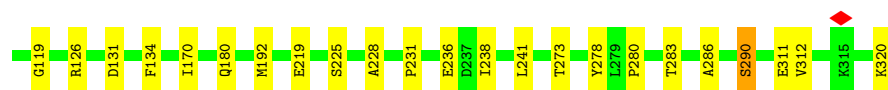
Chain N: 81% 17%



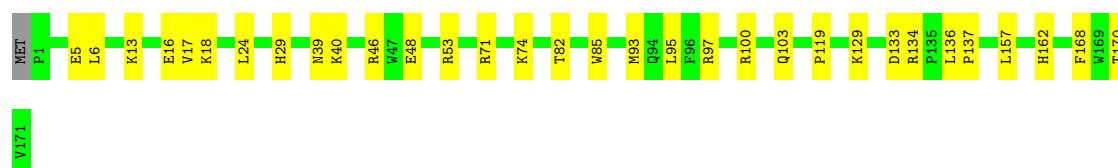
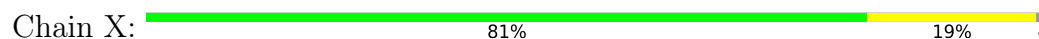
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 80% 10% 10%

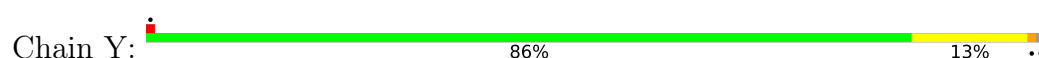




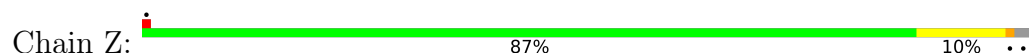
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



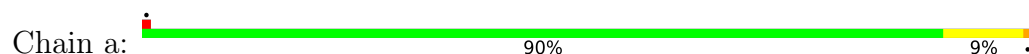
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



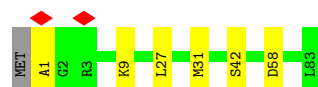
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

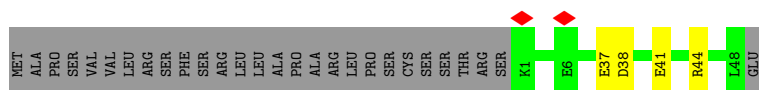


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

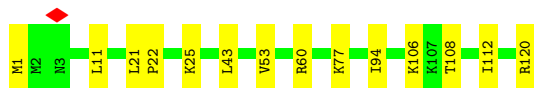
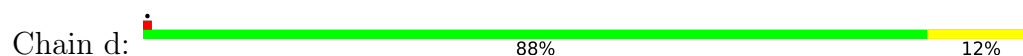


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

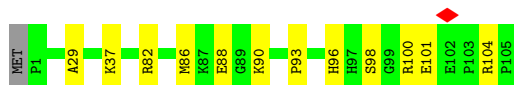
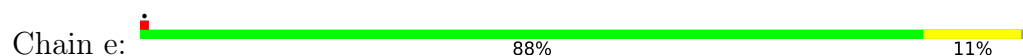




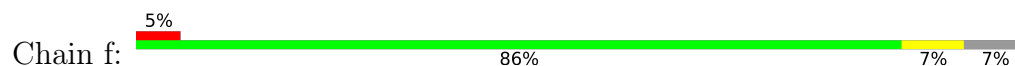
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2



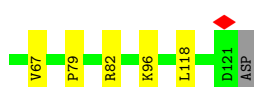
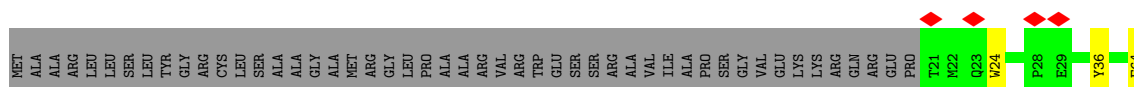
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



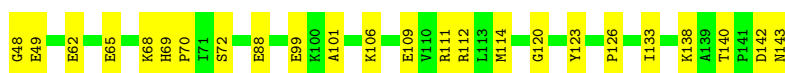
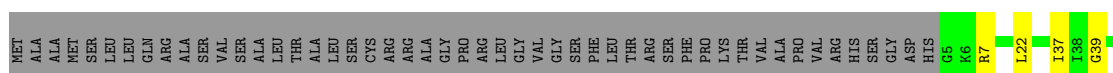
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



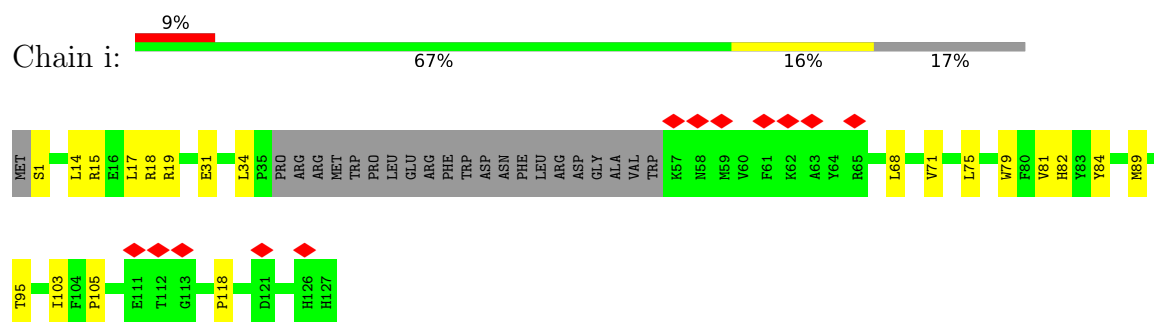
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



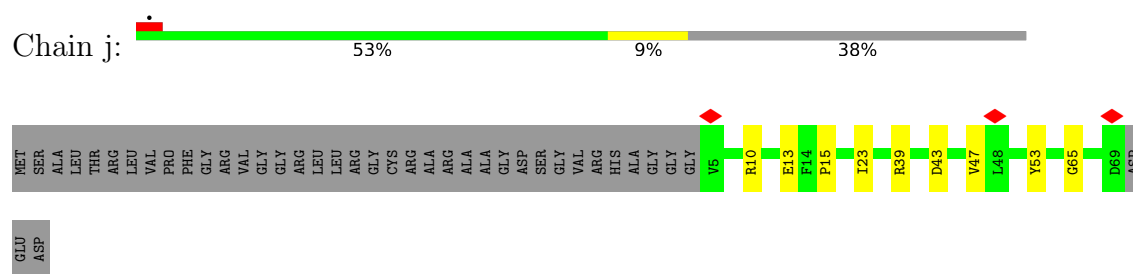
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



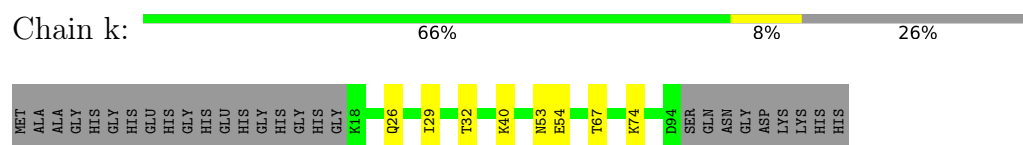
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



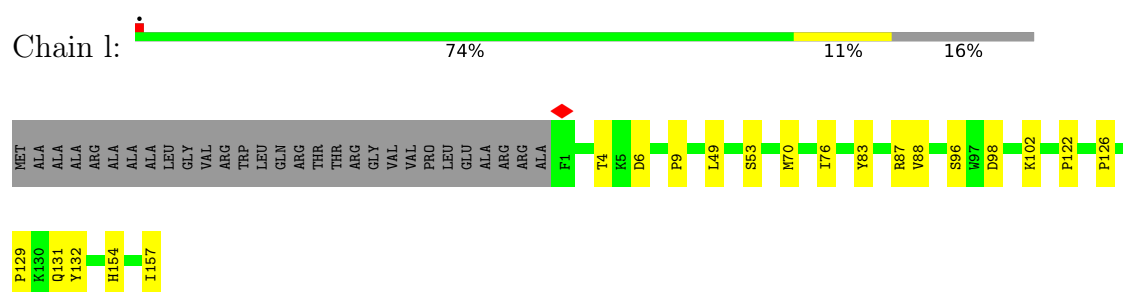
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



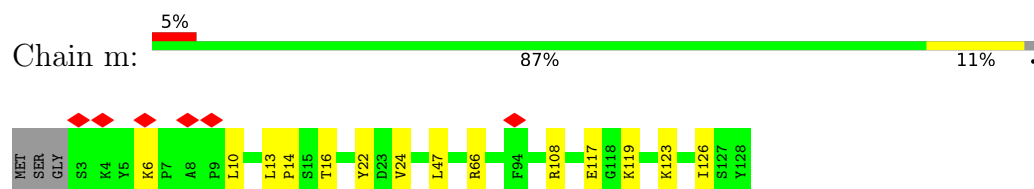
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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



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



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

Chain n:  88% 12%



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

Chain o:  76% 10% 14%



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

Chain p:  87% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	604185	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)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	226.83998, 213.05998, 203.51999	wwPDB
Map dimensions	214, 201, 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: FME, 3PE, PC1, NDP, 2MR, FES, ZN, MG, UQ, FMN, ZMP, AYA, SF4, CDL, DGT, K, SAC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	6	0.25	0/1289	0.43	1/1744 (0.1%)
2	C	0.22	0/1780	0.36	0/2424
3	D	0.24	0/3540	0.38	0/4795
4	2	0.25	0/1700	0.40	0/2316
5	1	0.27	0/3396	0.48	3/4586 (0.1%)
6	3	0.25	0/5392	0.39	0/7305
7	9	0.25	0/1461	0.37	0/1974
8	P	0.22	0/2823	0.39	0/3828
9	Q	0.24	0/1045	0.32	0/1411
10	7	0.23	0/773	0.33	0/1041
11	S	0.22	0/682	0.38	0/920
12	T	0.17	0/646	0.44	0/869
12	U	0.18	0/718	0.36	0/970
13	V	0.20	0/945	0.33	0/1281
14	W	0.20	0/993	0.34	0/1335
15	q	0.21	0/1251	0.34	0/1702
16	r	0.21	0/806	0.30	0/1090
17	s	0.20	0/360	0.37	0/489
18	A	0.23	0/948	0.41	0/1295
19	H	0.28	0/2607	0.48	0/3564
20	J	0.21	0/1330	0.38	0/1810
21	K	0.24	0/738	0.41	0/1002
22	L	0.24	0/4913	0.46	0/6686
23	M	0.25	0/3709	0.42	0/5052
24	N	0.24	0/2755	0.44	0/3751
25	O	0.20	0/2674	0.37	0/3626
26	X	0.18	0/1434	0.35	0/1937
27	Y	0.16	0/1061	0.30	0/1439
28	Z	0.19	0/1198	0.31	0/1616
29	a	0.21	0/585	0.36	0/788
30	b	0.18	0/666	0.35	0/914
31	c	0.16	0/409	0.28	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.18	0/1028	0.35	0/1387
33	e	0.17	0/900	0.35	0/1199
34	f	0.16	0/468	0.30	0/630
35	g	0.17	0/878	0.36	0/1196
36	h	0.20	0/1201	0.36	0/1626
37	i	0.19	0/917	0.36	0/1243
38	j	0.16	0/587	0.35	0/804
39	k	0.18	0/646	0.28	0/873
40	l	0.19	0/1379	0.34	0/1882
41	m	0.19	0/1079	0.34	0/1463
42	n	0.21	0/1596	0.35	0/2162
43	o	0.18	0/1039	0.33	0/1394
44	p	0.18	0/1471	0.30	0/1988
All	All	0.22	0/67816	0.39	4/91962 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	96	ASN	N-CA-C	-7.60	96.89	108.67
5	1	101	GLU	CA-C-N	5.26	125.20	119.78
5	1	101	GLU	C-N-CA	5.26	125.20	119.78
1	6	63	ALA	N-CA-C	5.11	114.78	108.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	1258	0	1268	29	0
2	C	1730	0	1686	20	0
3	D	3464	0	3416	58	0
4	2	1660	0	1653	21	0
5	1	3321	0	3278	43	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3	5305	0	5330	62	0
7	9	1431	0	1383	22	0
8	P	2748	0	2768	42	0
9	Q	1022	0	1023	14	0
10	7	758	0	731	5	0
11	S	671	0	688	9	0
12	T	637	0	640	5	0
12	U	706	0	699	12	0
13	V	923	0	965	6	0
14	W	970	0	991	5	0
15	q	1209	0	1170	11	0
16	r	796	0	831	7	0
17	s	351	0	331	4	0
18	A	932	0	967	17	0
19	H	2540	0	2626	55	0
20	J	1308	0	1319	21	0
21	K	737	0	768	15	0
22	L	4800	0	4985	72	0
23	M	3632	0	3853	61	0
24	N	2703	0	2902	44	0
25	O	2607	0	2566	22	0
26	X	1396	0	1385	24	0
27	Y	1037	0	1025	12	0
28	Z	1167	0	1166	13	0
29	a	572	0	583	7	0
30	b	651	0	653	4	0
31	c	398	0	401	2	0
32	d	996	0	1001	11	0
33	e	877	0	871	9	0
34	f	456	0	452	3	0
35	g	850	0	783	7	0
36	h	1166	0	1166	23	0
37	i	897	0	902	13	0
38	j	562	0	515	7	0
39	k	626	0	620	5	0
40	l	1323	0	1216	15	0
41	m	1050	0	1061	10	0
42	n	1541	0	1473	16	0
43	o	1014	0	1002	12	0
44	p	1438	0	1404	15	0
45	1	8	0	0	0	0
45	3	16	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	6	8	0	0	1	0
45	9	16	0	0	2	0
46	6	32	0	38	1	0
46	A	43	0	60	1	0
46	D	51	0	82	5	0
46	K	41	0	59	2	0
46	L	51	0	82	2	0
46	M	138	0	210	7	0
46	N	38	0	50	2	0
46	Y	70	0	88	2	0
46	Z	51	0	82	0	0
46	d	63	0	74	1	0
46	i	42	0	61	2	0
46	m	30	0	34	0	0
46	r	46	0	66	0	0
47	6	43	0	63	0	0
47	9	101	0	159	4	0
47	A	31	0	36	1	0
47	N	54	0	88	7	0
48	D	63	0	90	3	0
49	2	4	0	0	0	0
49	3	4	0	0	0	0
50	1	31	0	19	2	0
51	3	1	0	0	0	0
52	P	48	0	26	7	0
53	7	1	0	0	0	0
54	W	34	0	40	2	0
54	n	32	0	36	2	0
55	H	51	0	52	3	0
55	L	124	0	136	2	0
55	N	90	0	133	7	0
55	Y	151	0	199	3	0
55	d	67	0	81	5	0
55	h	70	0	87	4	0
55	m	72	0	91	1	0
55	r	57	0	58	3	0
56	O	31	0	12	1	0
57	O	1	0	0	0	0
All	All	68141	0	68908	746	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 746 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1:99:GLU:OE2	5:1:105:CYS:HA	1.68	0.91
5:1:99:GLU:OE2	5:1:105:CYS:CA	2.25	0.84
43:o:5:THR:O	43:o:9:LEU:HB2	1.86	0.74
5:1:93:LEU:O	5:1:134:ALA:HA	1.90	0.72
6:3:570:SER:HA	6:3:583:THR:O	1.91	0.71

There are no symmetry-related clashes.

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	6	155/224 (69%)	149 (96%)	6 (4%)	0	100	100
2	C	206/263 (78%)	199 (97%)	7 (3%)	0	100	100
3	D	427/463 (92%)	414 (97%)	13 (3%)	0	100	100
4	2	212/248 (86%)	201 (95%)	10 (5%)	1 (0%)	24	54
5	1	428/464 (92%)	411 (96%)	17 (4%)	0	100	100
6	3	688/727 (95%)	662 (96%)	26 (4%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	340/377 (90%)	327 (96%)	13 (4%)	0	100	100
9	Q	124/175 (71%)	120 (97%)	4 (3%)	0	100	100
10	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
11	S	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
12	T	77/156 (49%)	77 (100%)	0	0	100	100
12	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
13	V	111/116 (96%)	110 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	W	112/131 (86%)	109 (97%)	3 (3%)	0	100	100
15	q	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
16	r	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
17	s	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
18	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
19	H	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
20	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
22	L	604/607 (100%)	574 (95%)	30 (5%)	0	100	100
23	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
24	N	343/345 (99%)	333 (97%)	10 (3%)	0	100	100
25	O	318/355 (90%)	298 (94%)	20 (6%)	0	100	100
26	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
27	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
28	Z	139/144 (96%)	137 (99%)	2 (1%)	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%)	46 (100%)	0	0	100	100
32	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
33	e	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
34	f	51/57 (90%)	51 (100%)	0	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
37	i	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
38	j	63/105 (60%)	60 (95%)	3 (5%)	0	100	100
39	k	75/104 (72%)	74 (99%)	1 (1%)	0	100	100
40	l	155/186 (83%)	154 (99%)	1 (1%)	0	100	100
41	m	124/129 (96%)	123 (99%)	1 (1%)	0	100	100
42	n	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
43	o	116/137 (85%)	107 (92%)	9 (8%)	0	100	100
44	p	168/176 (96%)	167 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8141/9212 (88%)	7858 (96%)	282 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2	183	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	133/185 (72%)	130 (98%)	3 (2%)	44	76
2	C	190/227 (84%)	189 (100%)	1 (0%)	81	93
3	D	370/394 (94%)	366 (99%)	4 (1%)	65	88
4	2	184/206 (89%)	182 (99%)	2 (1%)	65	88
5	1	345/370 (93%)	340 (99%)	5 (1%)	59	85
6	3	580/610 (95%)	573 (99%)	7 (1%)	63	86
7	9	152/178 (85%)	149 (98%)	3 (2%)	48	78
8	P	299/325 (92%)	296 (99%)	3 (1%)	68	89
9	Q	113/153 (74%)	111 (98%)	2 (2%)	51	80
10	7	81/96 (84%)	81 (100%)	0	100	100
11	S	74/80 (92%)	72 (97%)	2 (3%)	39	73
12	T	73/135 (54%)	67 (92%)	6 (8%)	10	32
12	U	81/135 (60%)	80 (99%)	1 (1%)	63	86
13	V	101/102 (99%)	99 (98%)	2 (2%)	48	78
14	W	108/114 (95%)	105 (97%)	3 (3%)	38	72
15	q	131/131 (100%)	129 (98%)	2 (2%)	57	84
16	r	88/96 (92%)	88 (100%)	0	100	100
17	s	41/95 (43%)	39 (95%)	2 (5%)	22	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	A	103/103 (100%)	101 (98%)	2 (2%)	50	79
19	H	279/279 (100%)	272 (98%)	7 (2%)	42	74
20	J	137/137 (100%)	134 (98%)	3 (2%)	45	77
21	K	87/87 (100%)	87 (100%)	0	100	100
22	L	548/549 (100%)	539 (98%)	9 (2%)	55	83
23	M	414/414 (100%)	404 (98%)	10 (2%)	43	75
24	N	307/307 (100%)	295 (96%)	12 (4%)	28	63
25	O	284/309 (92%)	281 (99%)	3 (1%)	65	88
26	X	153/154 (99%)	151 (99%)	2 (1%)	61	86
27	Y	105/106 (99%)	102 (97%)	3 (3%)	37	71
28	Z	122/123 (99%)	121 (99%)	1 (1%)	73	90
29	a	60/60 (100%)	59 (98%)	1 (2%)	53	82
30	b	72/73 (99%)	72 (100%)	0	100	100
31	c	42/67 (63%)	41 (98%)	1 (2%)	43	75
32	d	107/107 (100%)	106 (99%)	1 (1%)	70	90
33	e	93/94 (99%)	93 (100%)	0	100	100
34	f	49/53 (92%)	48 (98%)	1 (2%)	48	78
35	g	92/129 (71%)	91 (99%)	1 (1%)	65	88
36	h	123/162 (76%)	123 (100%)	0	100	100
37	i	99/119 (83%)	95 (96%)	4 (4%)	28	62
38	j	61/87 (70%)	60 (98%)	1 (2%)	55	83
39	k	60/78 (77%)	57 (95%)	3 (5%)	22	53
40	l	142/161 (88%)	141 (99%)	1 (1%)	76	92
41	m	112/114 (98%)	111 (99%)	1 (1%)	70	90
42	n	163/164 (99%)	162 (99%)	1 (1%)	78	93
43	o	109/121 (90%)	109 (100%)	0	100	100
44	p	155/158 (98%)	154 (99%)	1 (1%)	78	93
All	All	7222/7947 (91%)	7105 (98%)	117 (2%)	54	83

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	J	131	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	k	29	ILE
23	M	109	THR
38	j	47	VAL
28	Z	70	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
22	L	505	ASN
43	o	43	GLN
24	N	174	GLN
40	l	54	GLN
35	g	23	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
24	FME	N	1	24	8,9,10	1.00	0	8,9,11	0.96	0
37	SAC	i	1	37	7,8,9	1.05	0	7,9,11	0.94	1 (14%)
30	AYA	b	1	30	6,7,8	1.27	1 (16%)	6,8,10	1.24	1 (16%)
3	2MR	D	85	3	10,12,13	2.61	2 (20%)	5,13,15	2.56	2 (40%)
23	FME	M	1	23	8,9,10	1.02	1 (12%)	8,9,11	0.72	0
21	FME	K	1	21	8,9,10	0.94	0	8,9,11	1.78	2 (25%)
19	FME	H	1	19	8,9,10	0.96	0	8,9,11	0.97	0
16	AYA	r	1	16	6,7,8	1.36	1 (16%)	6,8,10	1.11	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	FME	L	1	22	8,9,10	0.96	0	8,9,11	0.98	0
20	FME	J	1	20	8,9,10	0.96	0	8,9,11	0.77	0
18	FME	A	1	18	8,9,10	0.99	0	8,9,11	0.88	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
24	FME	N	1	24	-	1/7/9/11	-
37	SAC	i	1	37	-	0/7/8/10	-
30	AYA	b	1	30	-	1/5/6/8	-
3	2MR	D	85	3	-	3/10/13/15	-
23	FME	M	1	23	-	1/7/9/11	-
21	FME	K	1	21	-	3/7/9/11	-
19	FME	H	1	19	-	1/7/9/11	-
16	AYA	r	1	16	-	1/5/6/8	-
22	FME	L	1	22	-	4/7/9/11	-
20	FME	J	1	20	-	1/7/9/11	-
18	FME	A	1	18	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.84	1.46	1.34
3	D	85	2MR	CZ-NH2	5.22	1.44	1.33
16	r	1	AYA	CA-N	-2.81	1.43	1.46
30	b	1	AYA	CA-N	-2.28	1.44	1.46
23	M	1	FME	CA-N	-2.05	1.43	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	85	2MR	CD-NE-CZ	4.31	131.47	123.36
21	K	1	FME	C-CA-N	4.18	117.56	109.50
3	D	85	2MR	NE-CZ-NH2	-3.09	116.64	119.48
30	b	1	AYA	CB-CA-N	2.67	112.70	109.68
16	r	1	AYA	CB-CA-N	2.54	112.55	109.68

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	O-C-CA-CB
16	r	1	AYA	O-C-CA-CB
21	K	1	FME	O1-CN-N-CA
22	L	1	FME	N-CA-CB-CG
30	b	1	AYA	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	85	2MR	1	0
21	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 3 are monoatomic - leaving 46 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	$\# Z > 2$
55	CDL	Y	404	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
55	CDL	N	402	-	89,89,99	0.31	0	95,101,111	0.41	1 (1%)
45	SF4	1	502	5	0,12,12	-	-	-		
46	3PE	D	502	-	50,50,50	0.30	0	53,55,55	0.31	0
46	3PE	d	203	-	31,31,50	0.37	0	34,36,55	0.35	0
47	PC1	9	204	-	46,46,53	0.31	0	52,54,61	0.33	0
46	3PE	Y	403	-	41,41,50	0.32	0	44,46,55	0.34	0
48	UQ	D	501	-	63,63,63	0.32	0	78,79,79	0.72	2 (2%)
54	ZMP	n	201	-	26,31,36	0.74	1 (3%)	30,38,45	0.90	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.48	0
46	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.35	0
46	3PE	M	502	-	50,50,50	0.29	0	53,55,55	0.29	0
46	3PE	M	501	-	50,50,50	0.30	0	53,55,55	0.33	0
54	ZMP	W	201	-	28,33,36	0.61	0	32,40,45	1.11	2 (6%)
55	CDL	H	401	-	50,50,99	0.42	0	55,61,111	0.38	0
45	SF4	9	202	7	0,12,12	-	-	-		
46	3PE	Z	401	-	50,50,50	0.31	0	53,55,55	0.49	1 (1%)
46	3PE	m	202	-	29,29,50	0.38	0	32,34,55	0.34	0
46	3PE	A	602	-	42,42,50	0.33	0	45,47,55	0.33	0
46	3PE	M	503	-	35,35,50	0.35	0	38,40,55	0.31	0
52	NDP	P	501	-	51,52,52	0.38	0	71,80,80	0.44	0
55	CDL	h	201	-	69,69,99	0.36	0	75,81,111	0.45	1 (1%)
55	CDL	L	702	-	77,77,99	0.33	0	83,89,111	0.30	0
46	3PE	N	403	-	37,37,50	0.34	0	40,42,55	0.34	0
55	CDL	r	202	-	56,56,99	0.40	0	62,68,111	0.48	1 (1%)
55	CDL	m	201	-	71,71,99	0.35	0	77,83,111	0.44	1 (1%)
55	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.33	0
45	SF4	3	802	6	0,12,12	-	-	-		
46	3PE	Y	402	-	27,27,50	0.40	0	30,32,55	0.36	0
49	FES	2	301	4	0,4,4	-	-	-		
47	PC1	N	401	-	53,53,53	0.28	0	59,61,61	0.37	0
46	3PE	d	202	-	30,30,50	0.38	0	33,35,55	0.35	0
47	PC1	A	601	-	30,30,53	0.40	0	36,38,61	0.58	0
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.32	0
55	CDL	Y	401	-	93,93,99	0.30	0	99,105,111	0.29	0
56	DGT	O	401	57	32,33,33	0.31	0	48,52,52	0.31	0
45	SF4	9	201	7	0,12,12	-	-	-		
46	3PE	i	201	-	41,41,50	0.33	0	44,46,55	0.32	0
47	PC1	9	203	-	53,53,53	0.29	0	59,61,61	0.46	0
46	3PE	r	201	-	45,45,50	0.31	0	48,50,55	0.30	0
49	FES	3	803	6	0,4,4	-	-	-		
50	FMN	1	501	-	33,33,33	0.38	0	48,50,50	0.38	0
55	CDL	L	703	-	45,45,99	0.42	0	51,57,111	0.36	0
45	SF4	6	201	1	0,12,12	-	-	-		
45	SF4	3	801	6	0,12,12	-	-	-		
47	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.51	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
55	CDL	Y	404	-	-	17/67/67/110	-
55	CDL	N	402	-	-	15/100/100/110	-
45	SF4	1	502	5	-	-	0/6/5/5
46	3PE	D	502	-	-	7/54/54/54	-
46	3PE	d	203	-	-	6/35/35/54	-
47	PC1	9	204	-	-	10/50/50/57	-
46	3PE	Y	403	-	-	7/45/45/54	-
48	UQ	D	501	-	-	13/63/87/87	0/1/1/1
54	ZMP	n	201	-	-	14/36/38/43	-
46	3PE	L	701	-	-	7/54/54/54	-
46	3PE	6	202	-	-	4/35/35/54	-
46	3PE	M	502	-	-	9/54/54/54	-
46	3PE	M	501	-	-	13/54/54/54	-
54	ZMP	W	201	-	-	5/38/40/43	-
55	CDL	H	401	-	-	13/59/59/110	-
45	SF4	9	202	7	-	-	0/6/5/5
46	3PE	Z	401	-	-	11/54/54/54	-
46	3PE	m	202	-	-	7/33/33/54	-
46	3PE	A	602	-	-	10/46/46/54	-
46	3PE	M	503	-	-	10/39/39/54	-
52	NDP	P	501	-	-	7/34/77/77	0/5/5/5
55	CDL	h	201	-	-	23/80/80/110	-
55	CDL	L	702	-	-	19/88/88/110	-
46	3PE	N	403	-	-	10/41/41/54	-
55	CDL	r	202	-	-	11/67/67/110	-
55	CDL	m	201	-	-	19/82/82/110	-
55	CDL	d	201	-	-	12/77/77/110	-
45	SF4	3	802	6	-	-	0/6/5/5
46	3PE	Y	402	-	-	6/31/31/54	-
49	FES	2	301	4	-	-	0/1/1/1
47	PC1	N	401	-	-	12/57/57/57	-
46	3PE	d	202	-	-	9/34/34/54	-
47	PC1	A	601	-	-	12/34/34/57	-
46	3PE	K	201	-	-	9/44/44/54	-
55	CDL	Y	401	-	-	13/104/104/110	-
56	DGT	O	401	57	-	5/22/34/34	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	9	201	7	-	-	0/6/5/5
46	3PE	i	201	-	-	2/45/45/54	-
47	PC1	9	203	-	-	11/57/57/57	-
46	3PE	r	201	-	-	5/49/49/54	-
50	FMN	1	501	-	-	6/18/18/18	0/3/3/3
55	CDL	L	703	-	-	12/56/56/110	-
49	FES	3	803	6	-	-	0/1/1/1
45	SF4	6	201	1	-	-	0/6/5/5
45	SF4	3	801	6	-	-	0/6/5/5
47	PC1	6	203	-	-	10/46/46/57	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	n	201	ZMP	C9-C10	2.56	1.53	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	D	501	UQ	C37-C36-C34	-2.86	103.72	113.19
54	W	201	ZMP	O1-C10-C9	-2.81	120.74	123.98
48	D	501	UQ	C7-C6-C1	-2.78	115.29	118.52
54	W	201	ZMP	C15-C14-C13	-2.67	107.95	112.39
54	n	201	ZMP	O1-C10-C9	-2.42	121.19	123.98

There are no chirality outliers.

5 of 391 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	O13-C11-C12-N

There are no ring outliers.

34 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	Y	404	CDL	2	0

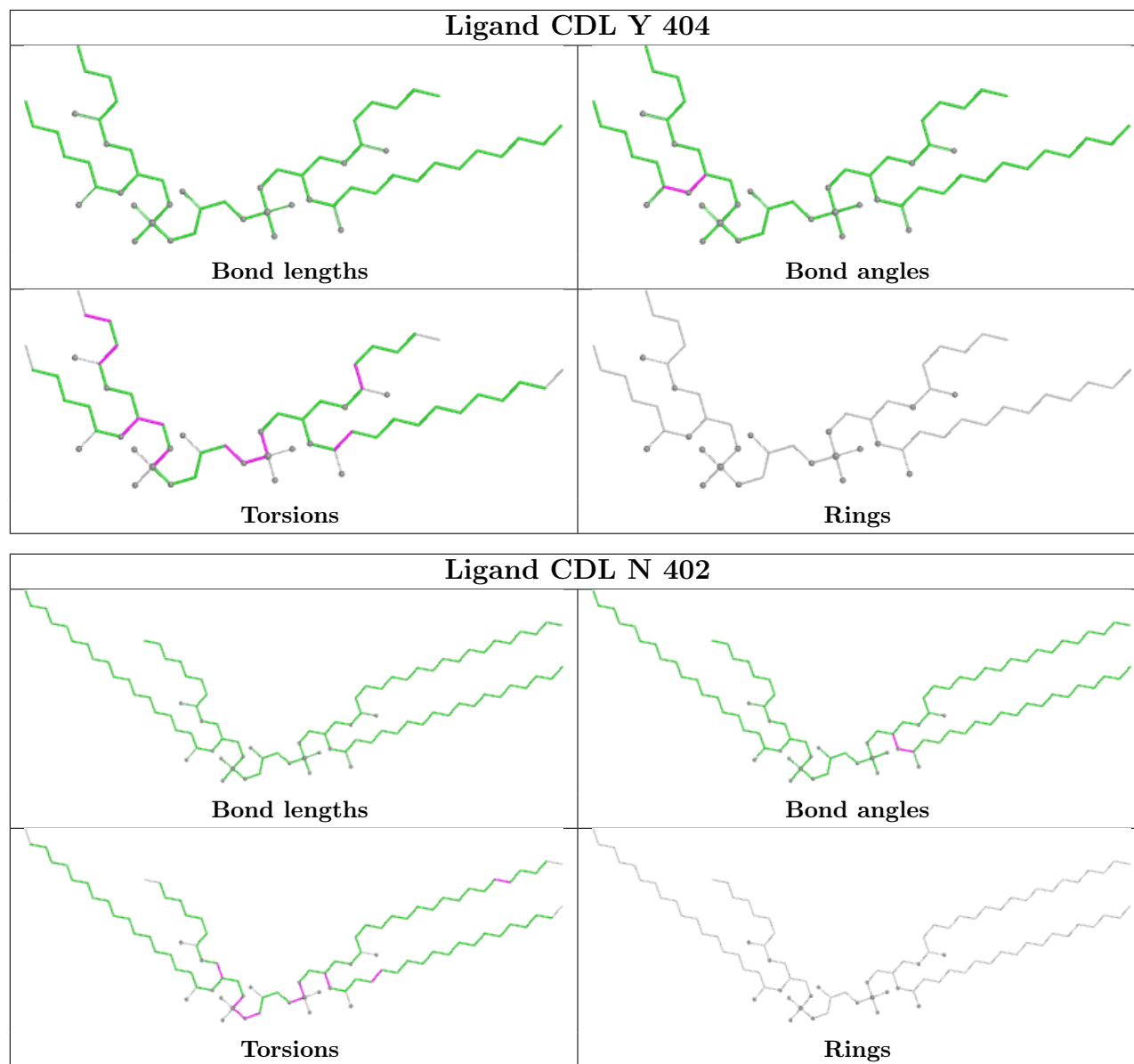
Continued on next page...

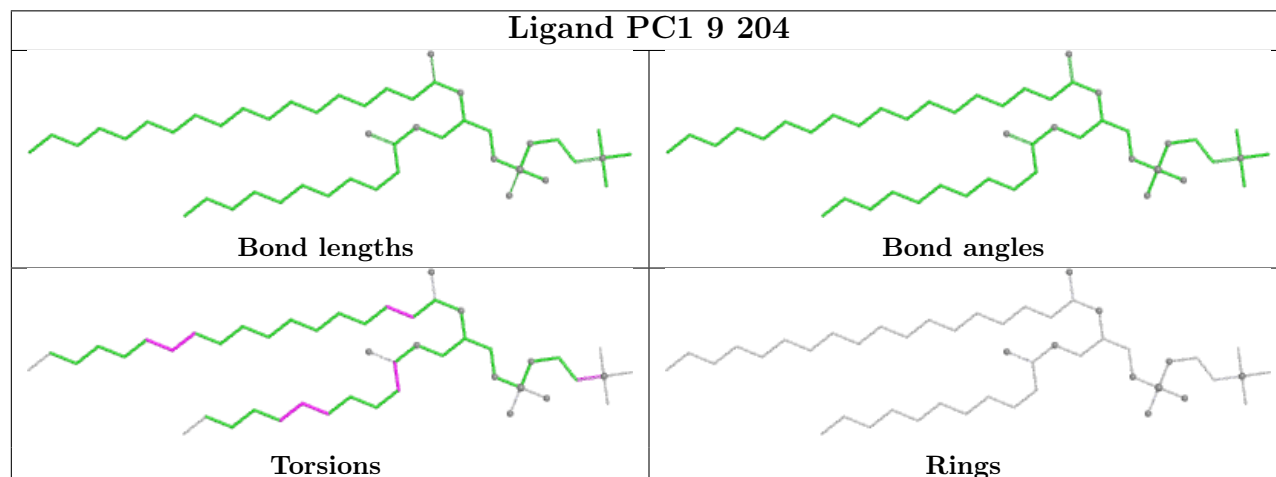
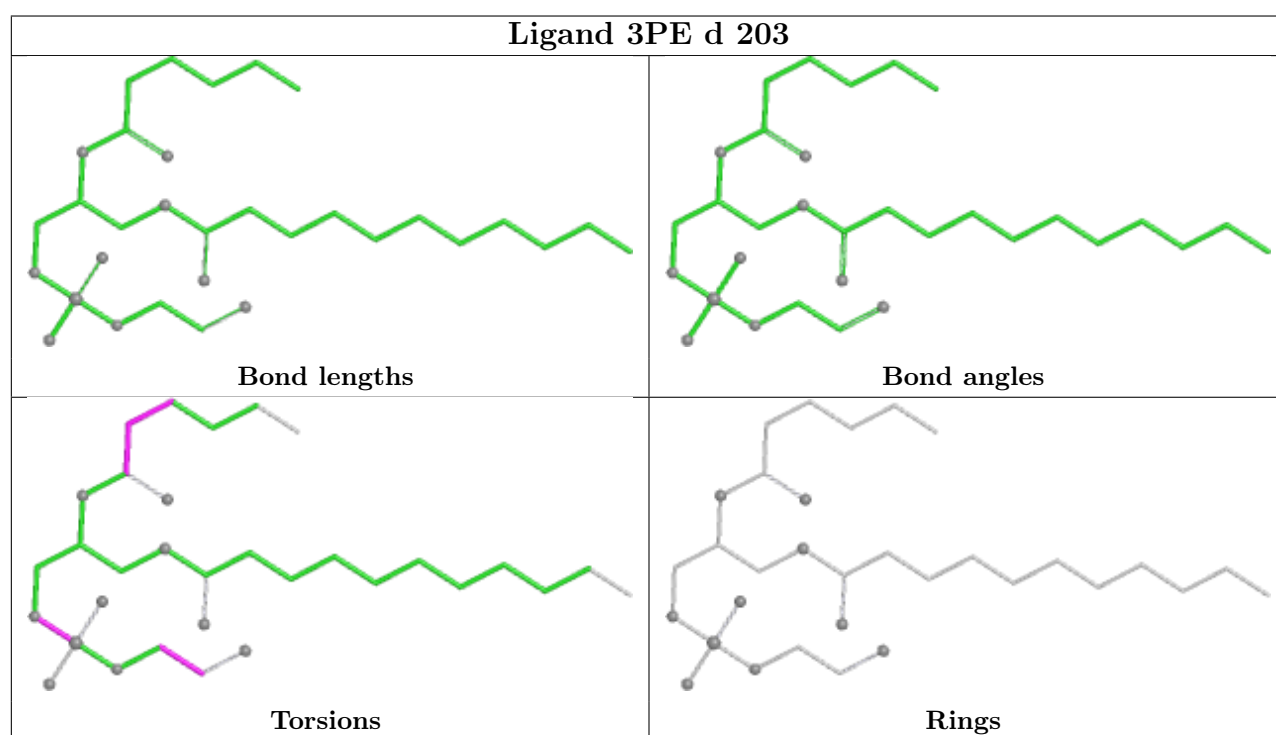
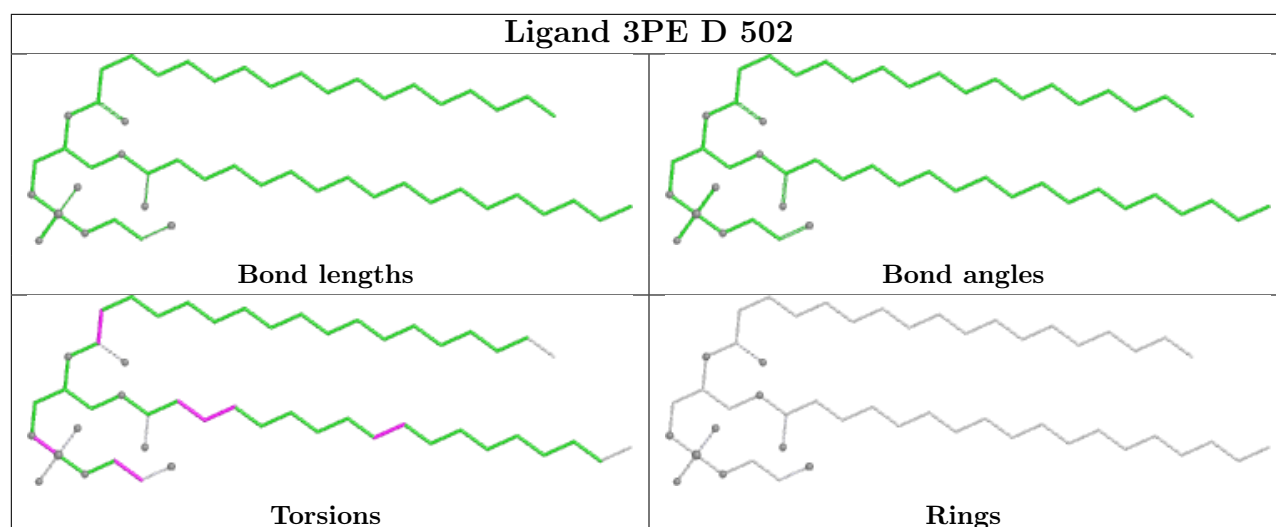
Continued from previous page...

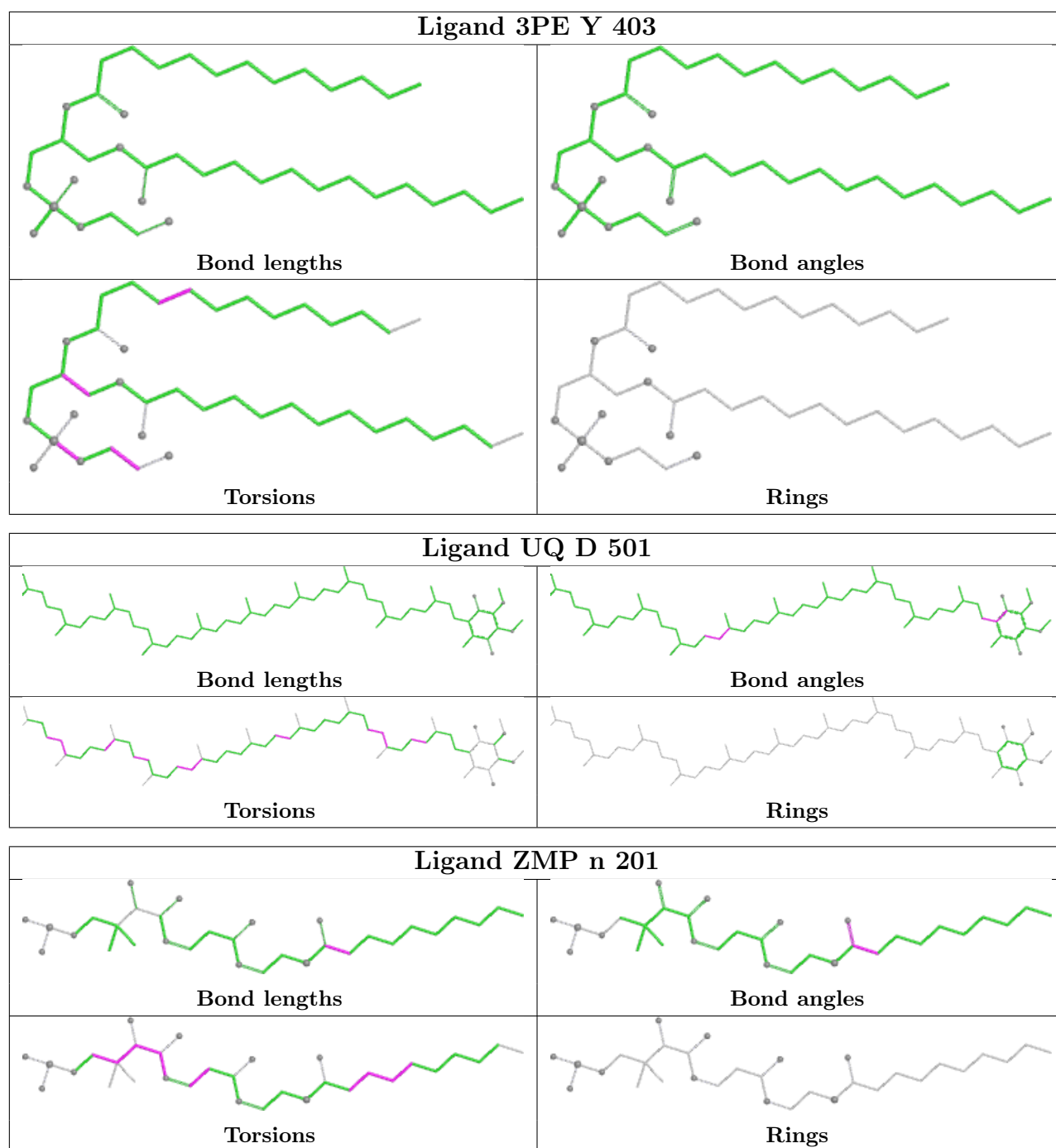
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	N	402	CDL	7	0
46	D	502	3PE	5	0
47	9	204	PC1	2	0
46	Y	403	3PE	2	0
48	D	501	UQ	3	0
54	n	201	ZMP	2	0
46	L	701	3PE	2	0
46	6	202	3PE	1	0
46	M	502	3PE	3	0
46	M	501	3PE	4	0
54	W	201	ZMP	2	0
55	H	401	CDL	3	0
46	A	602	3PE	1	0
52	P	501	NDP	7	0
55	h	201	CDL	4	0
55	L	702	CDL	1	0
46	N	403	3PE	2	0
55	r	202	CDL	3	0
55	m	201	CDL	1	0
55	d	201	CDL	5	0
45	3	802	SF4	1	0
47	N	401	PC1	7	0
46	d	202	3PE	1	0
47	A	601	PC1	1	0
46	K	201	3PE	2	0
55	Y	401	CDL	1	0
56	O	401	DGT	1	0
45	9	201	SF4	2	0
46	i	201	3PE	2	0
47	9	203	PC1	2	0
50	1	501	FMN	2	0
55	L	703	CDL	1	0
45	6	201	SF4	1	0

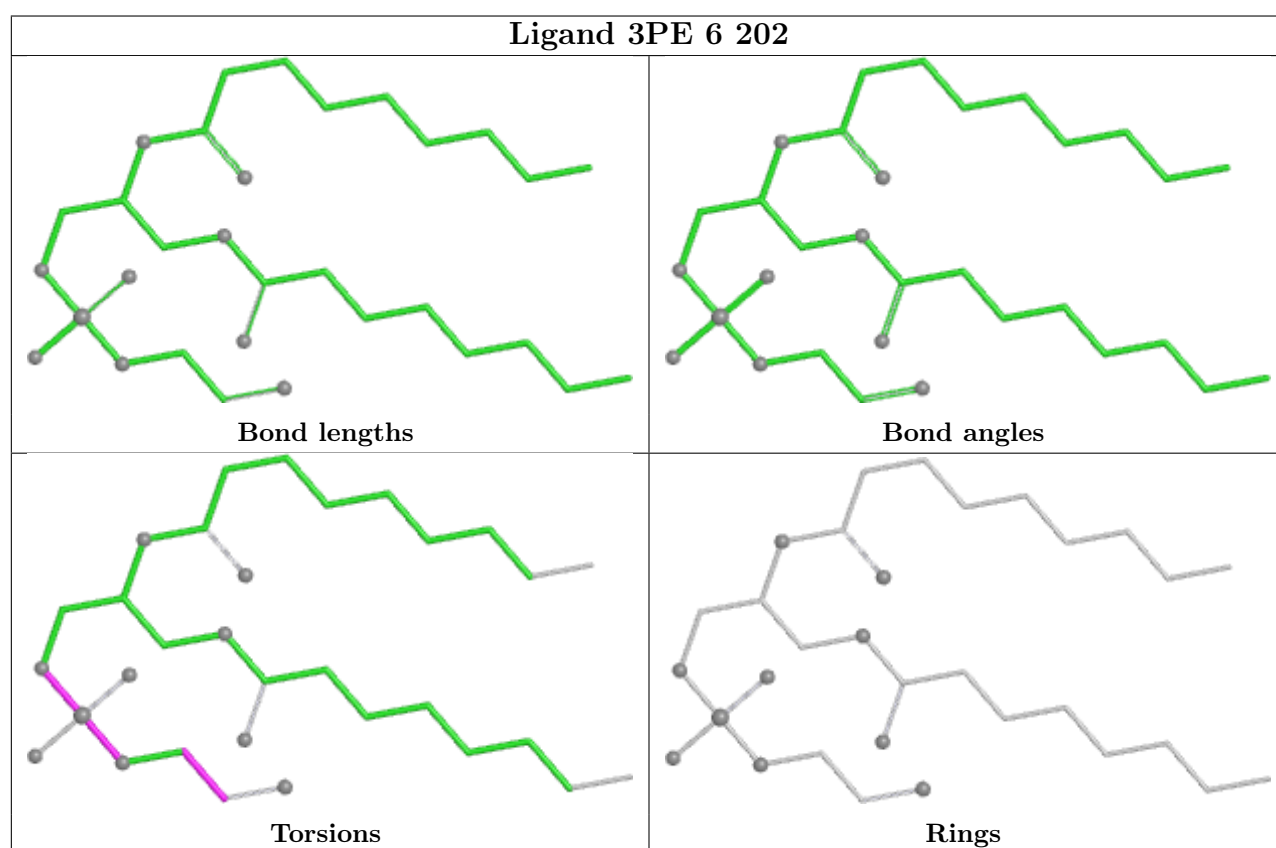
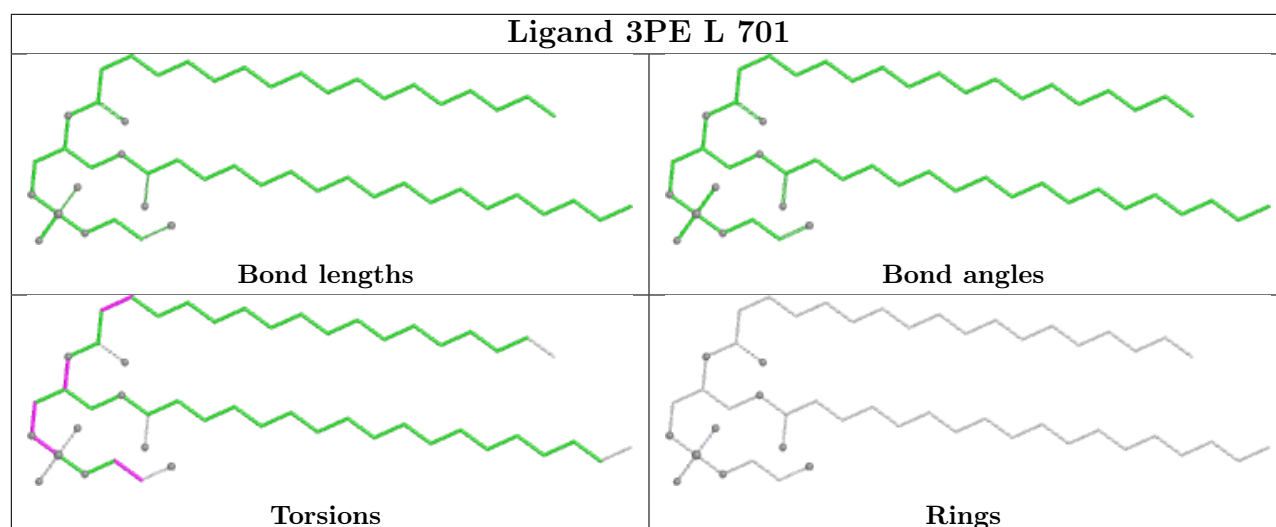
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

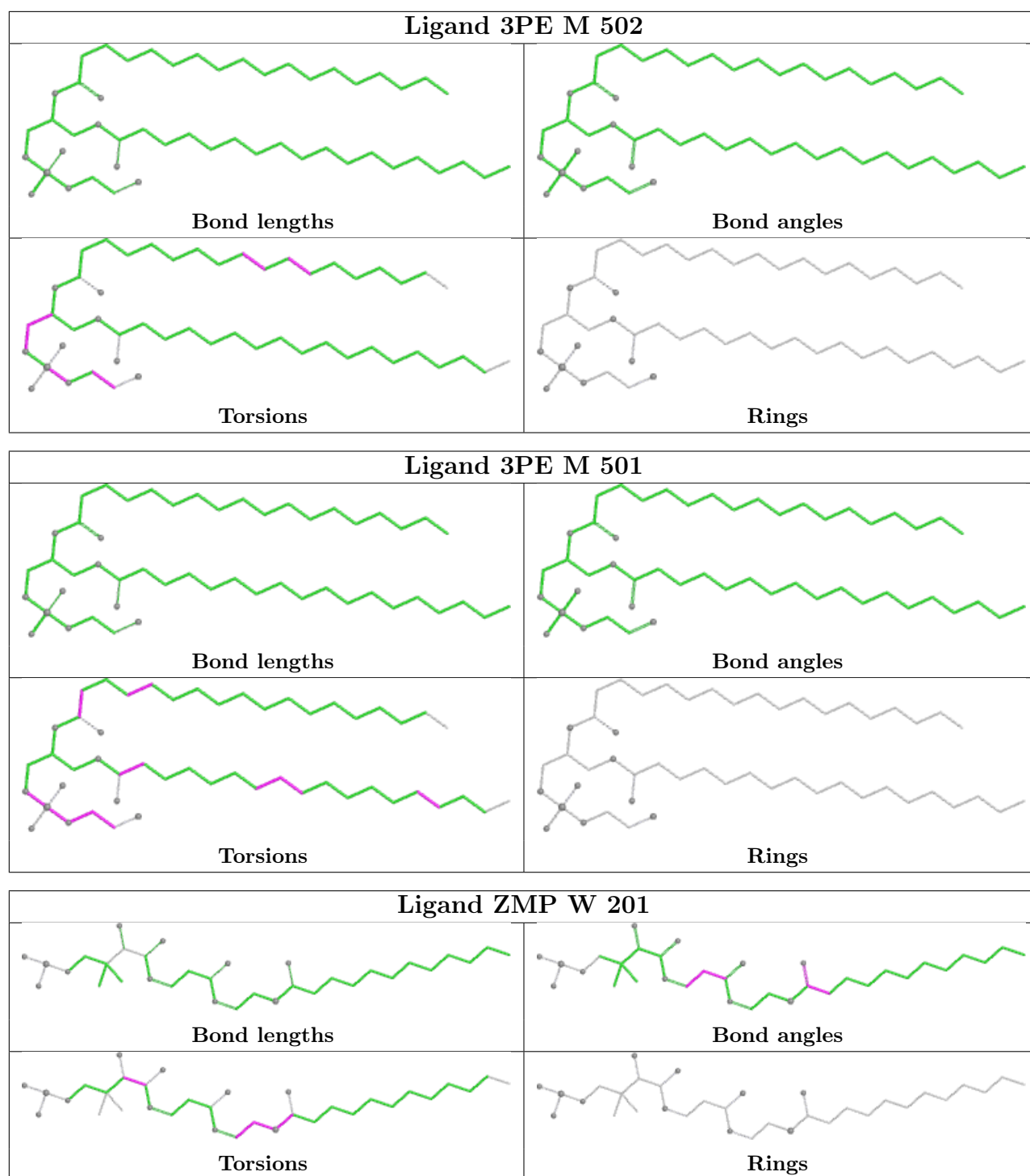
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

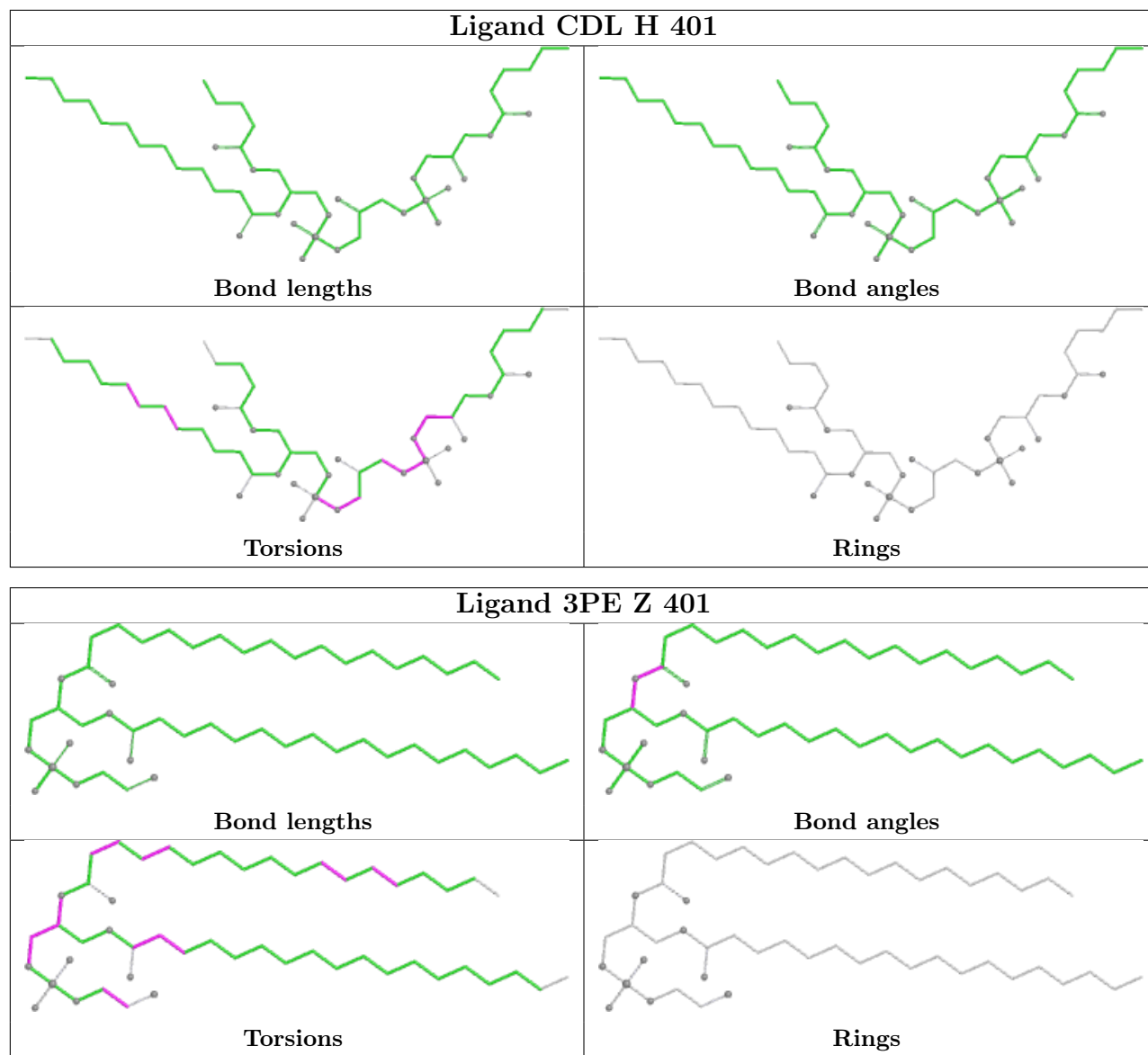


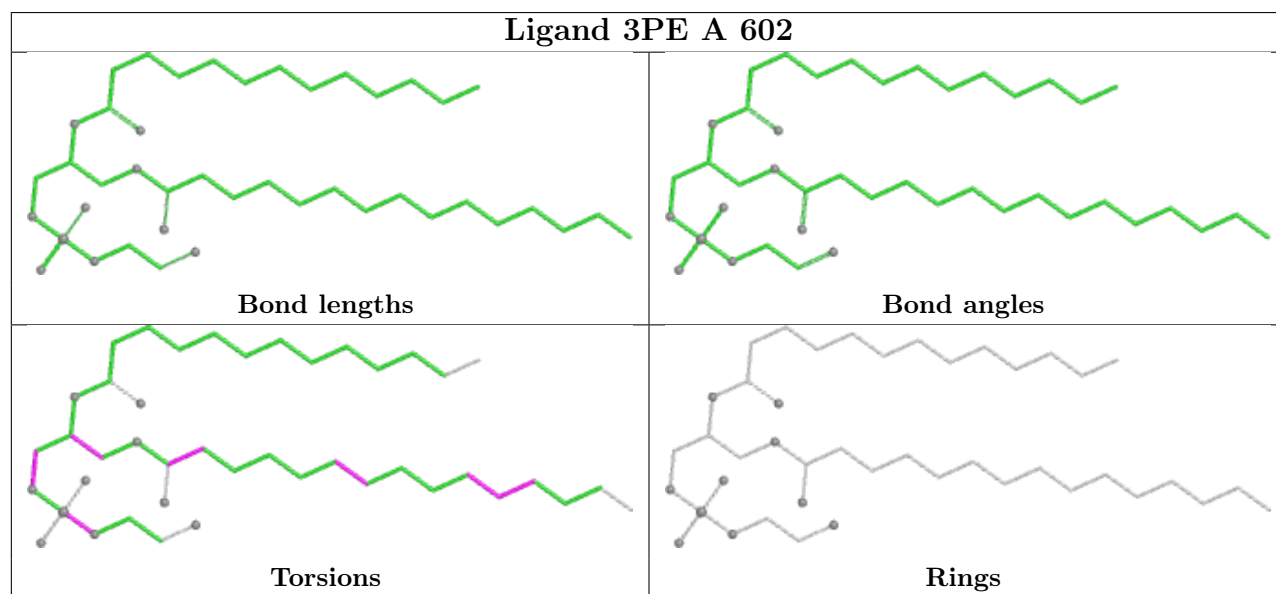
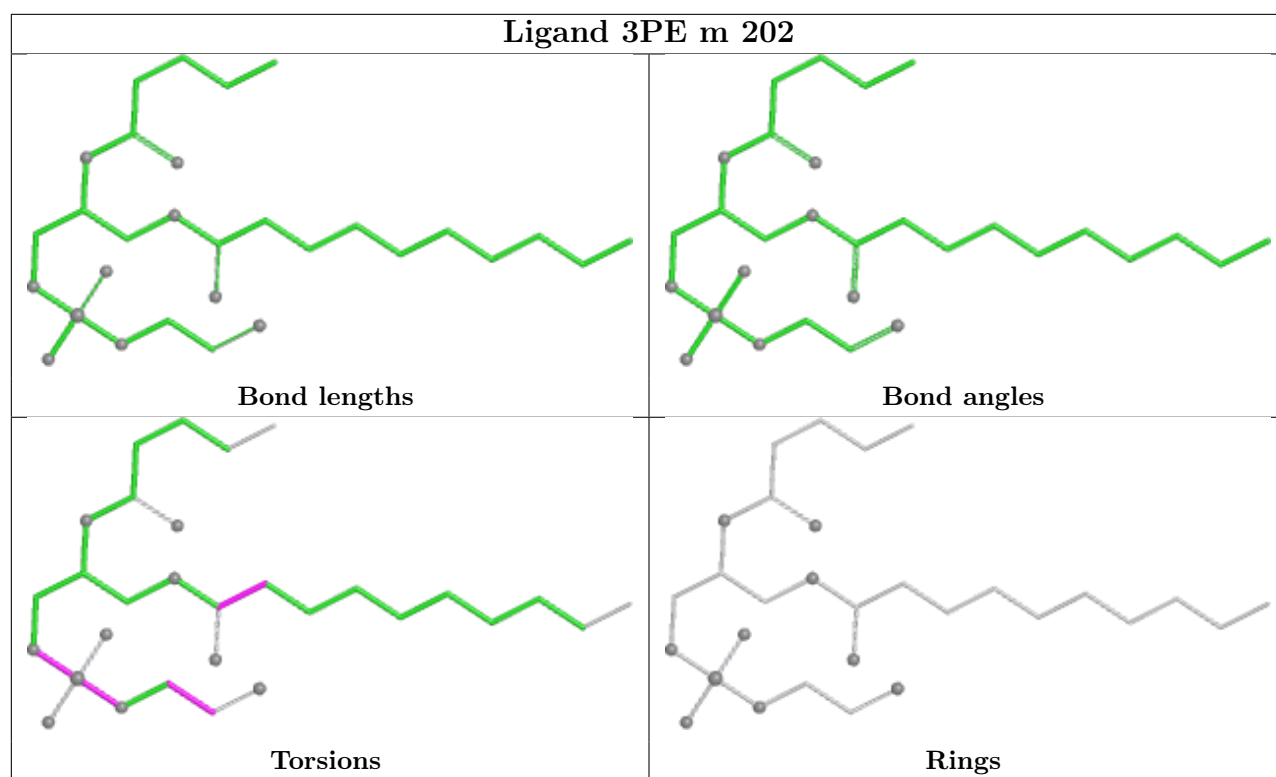


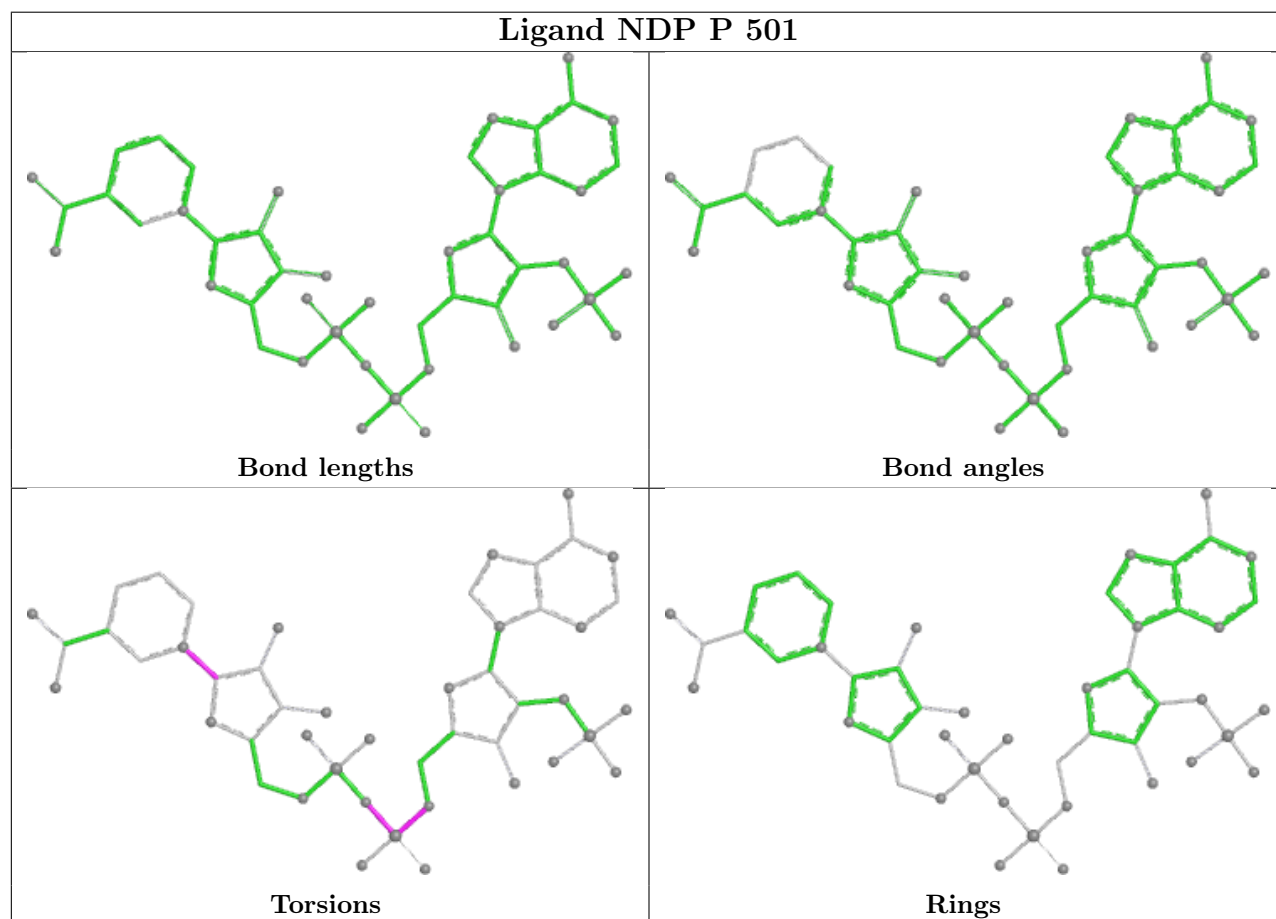
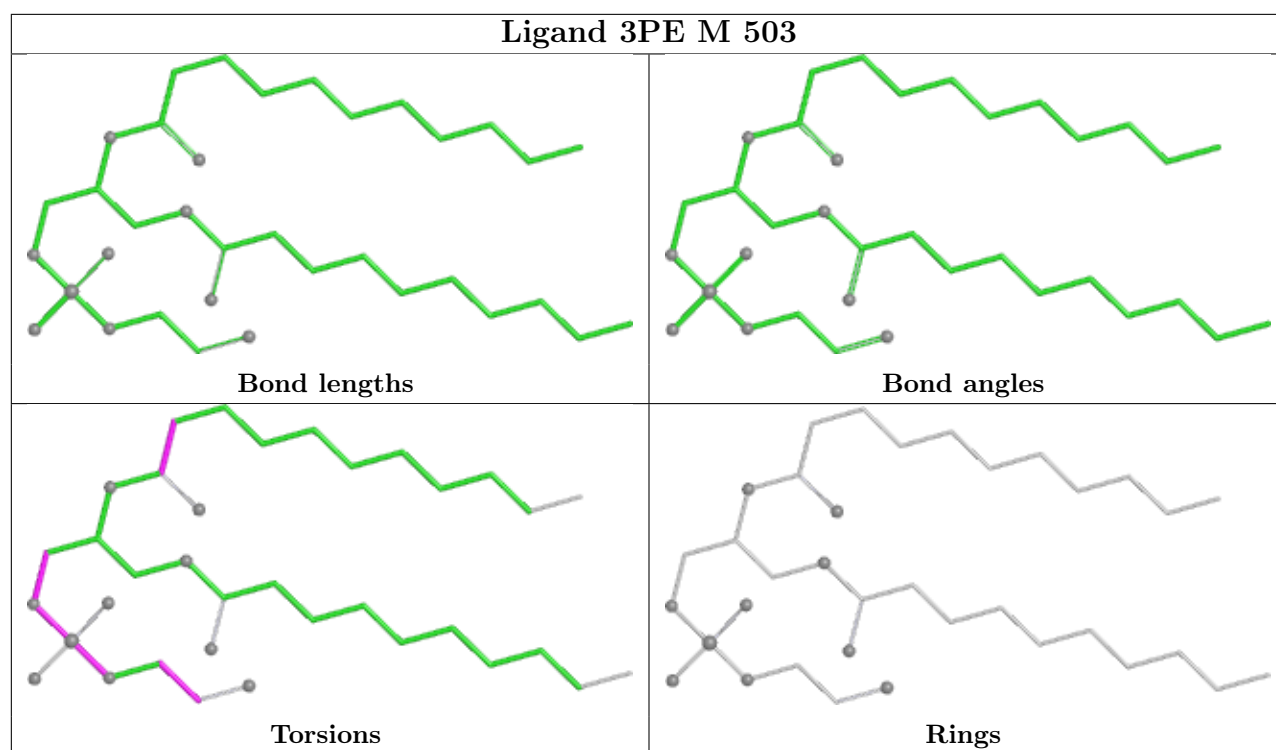


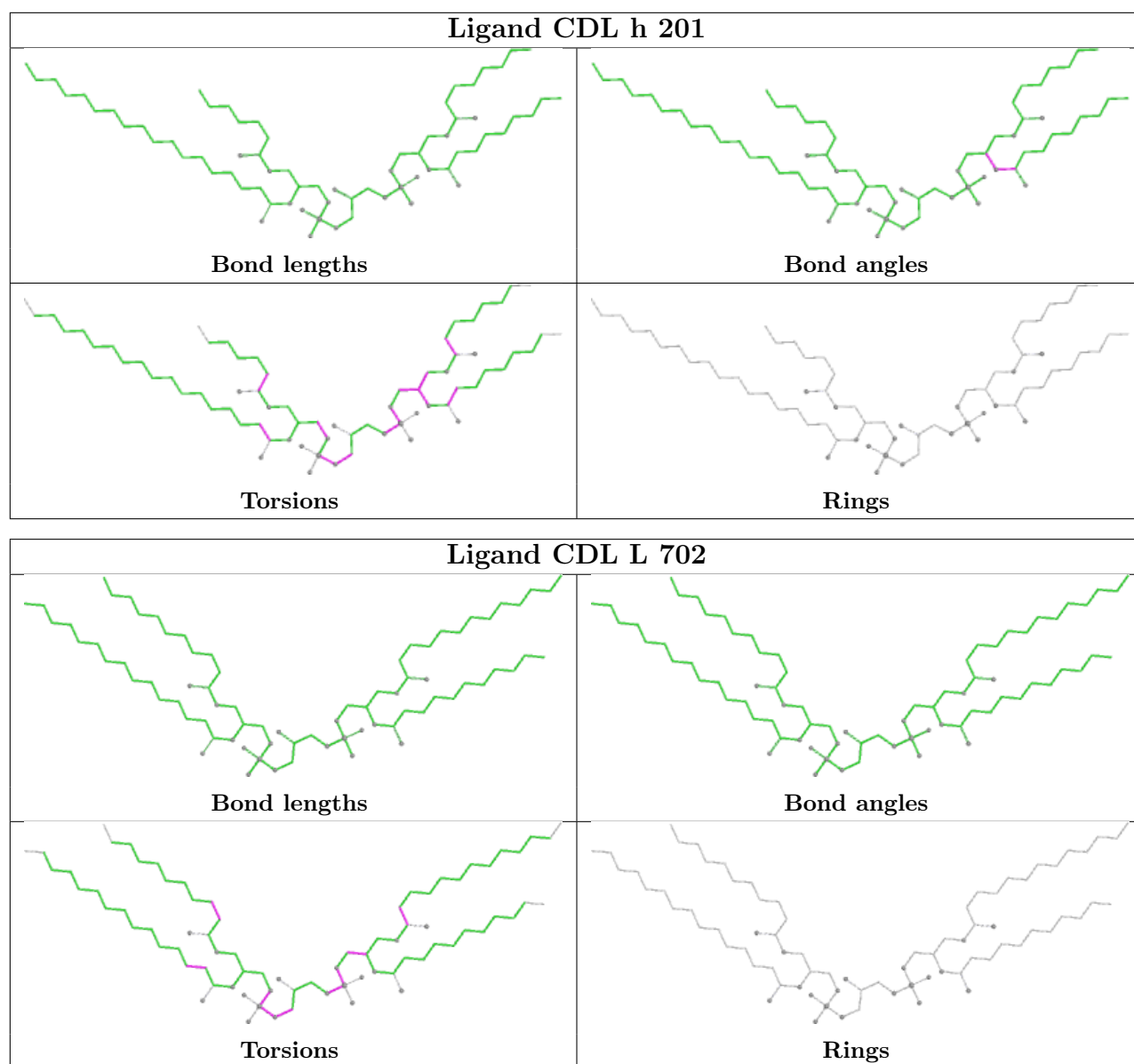


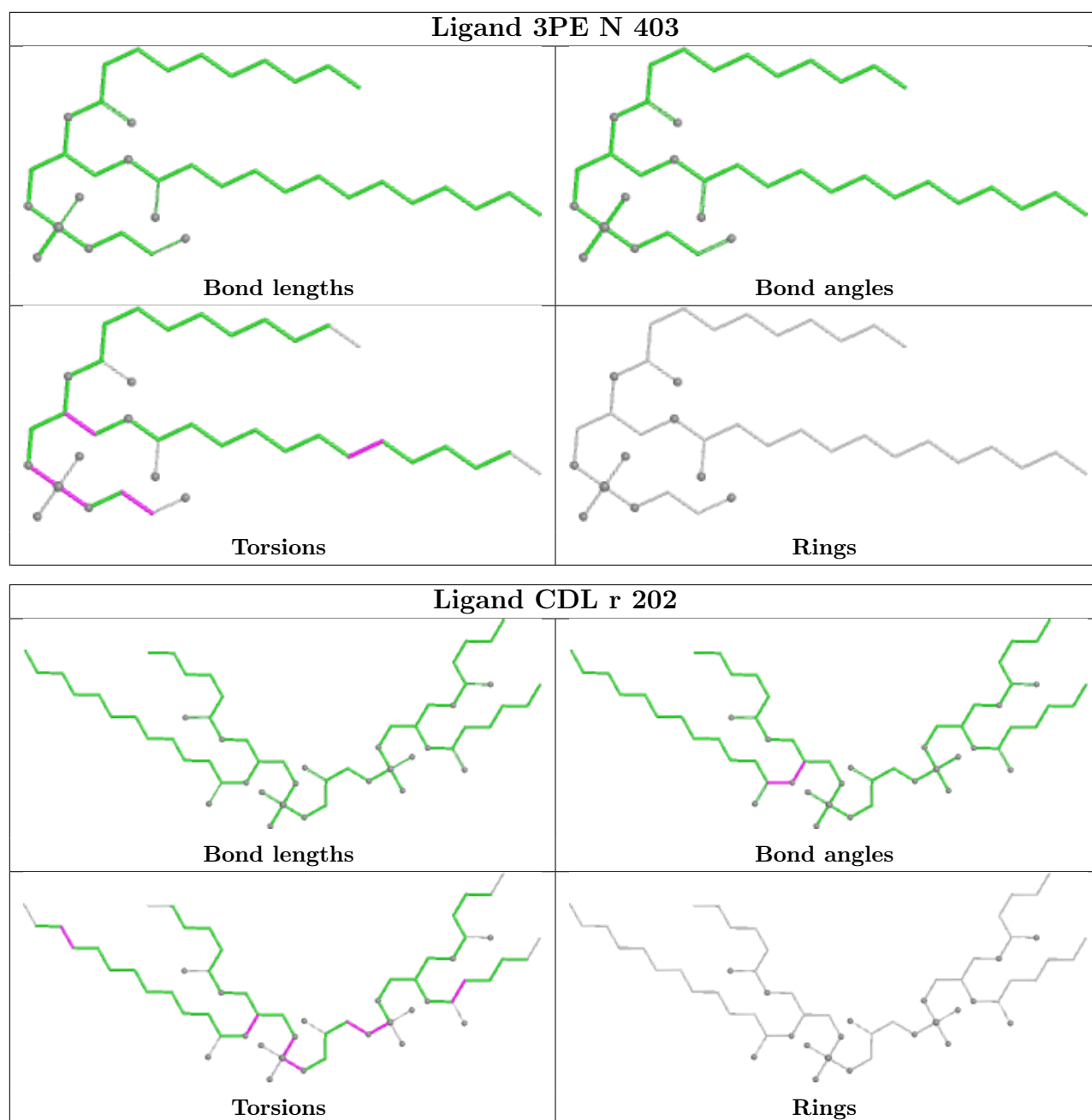


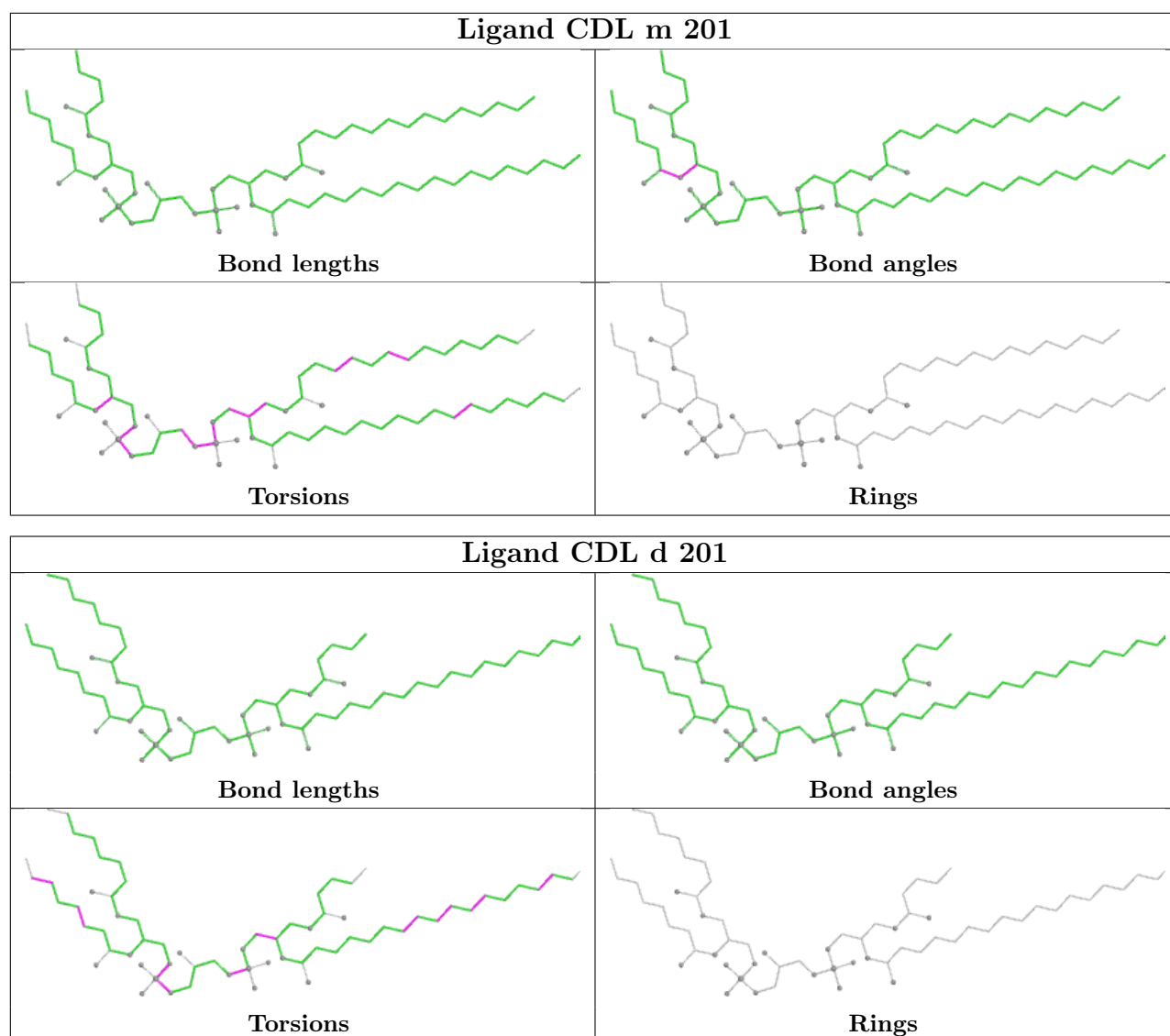


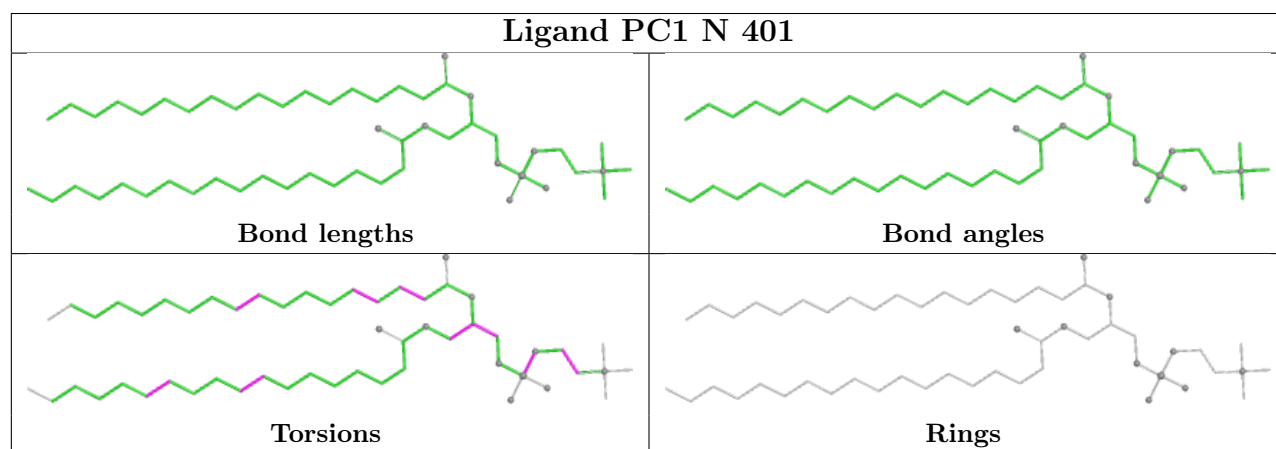
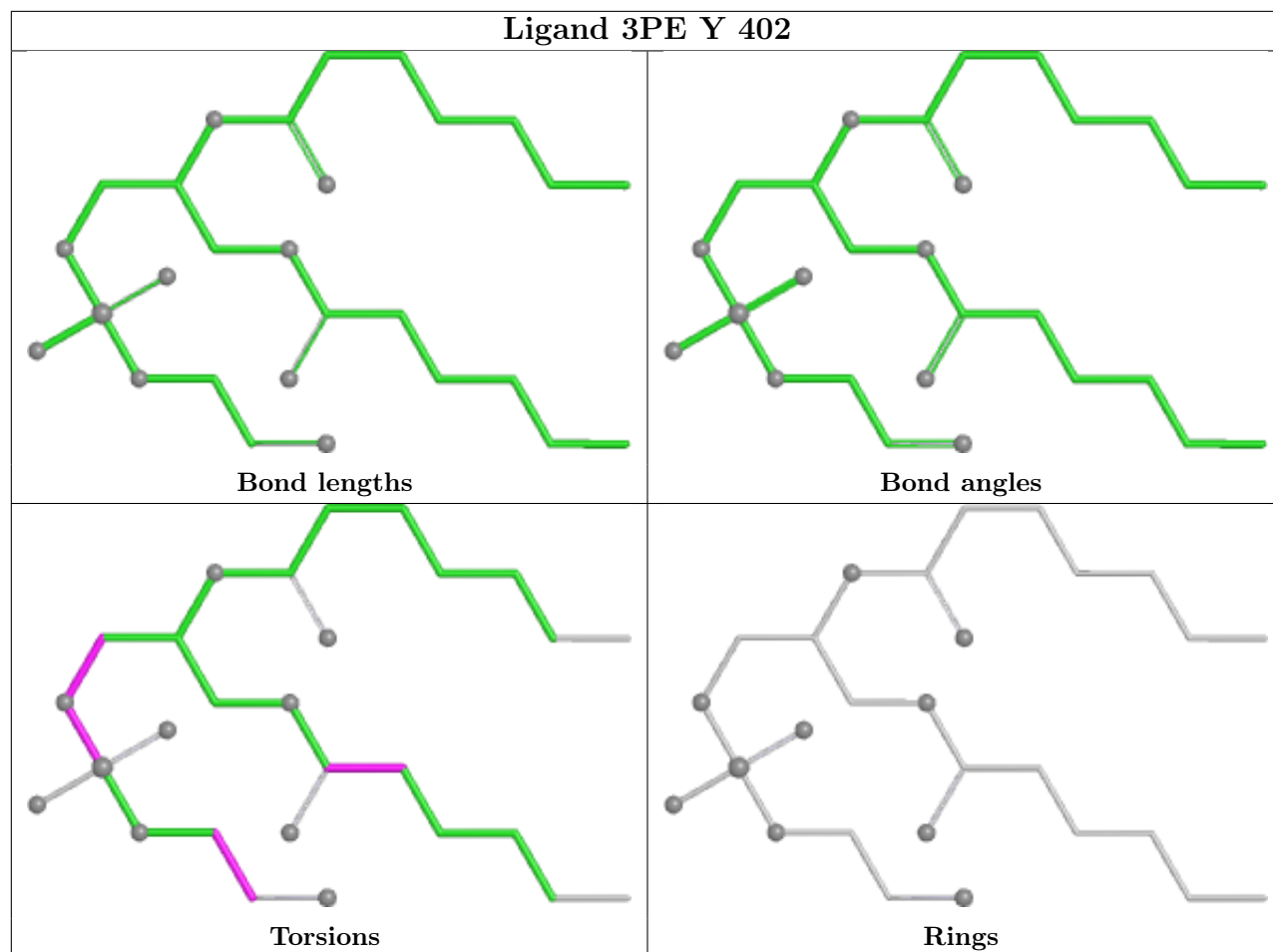


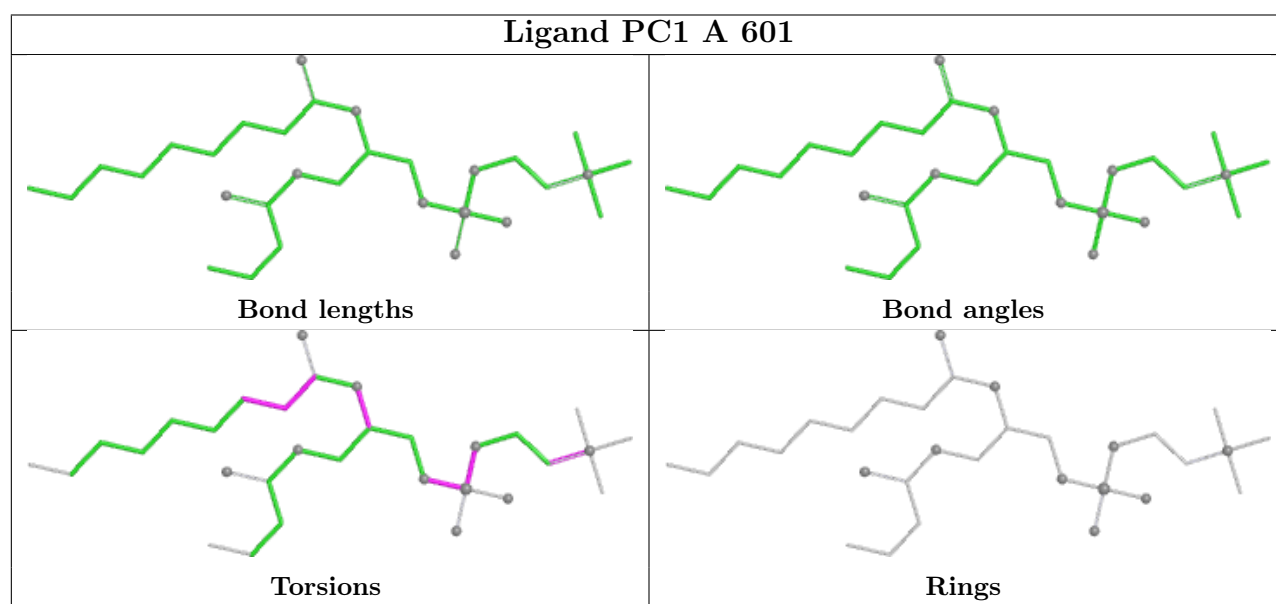
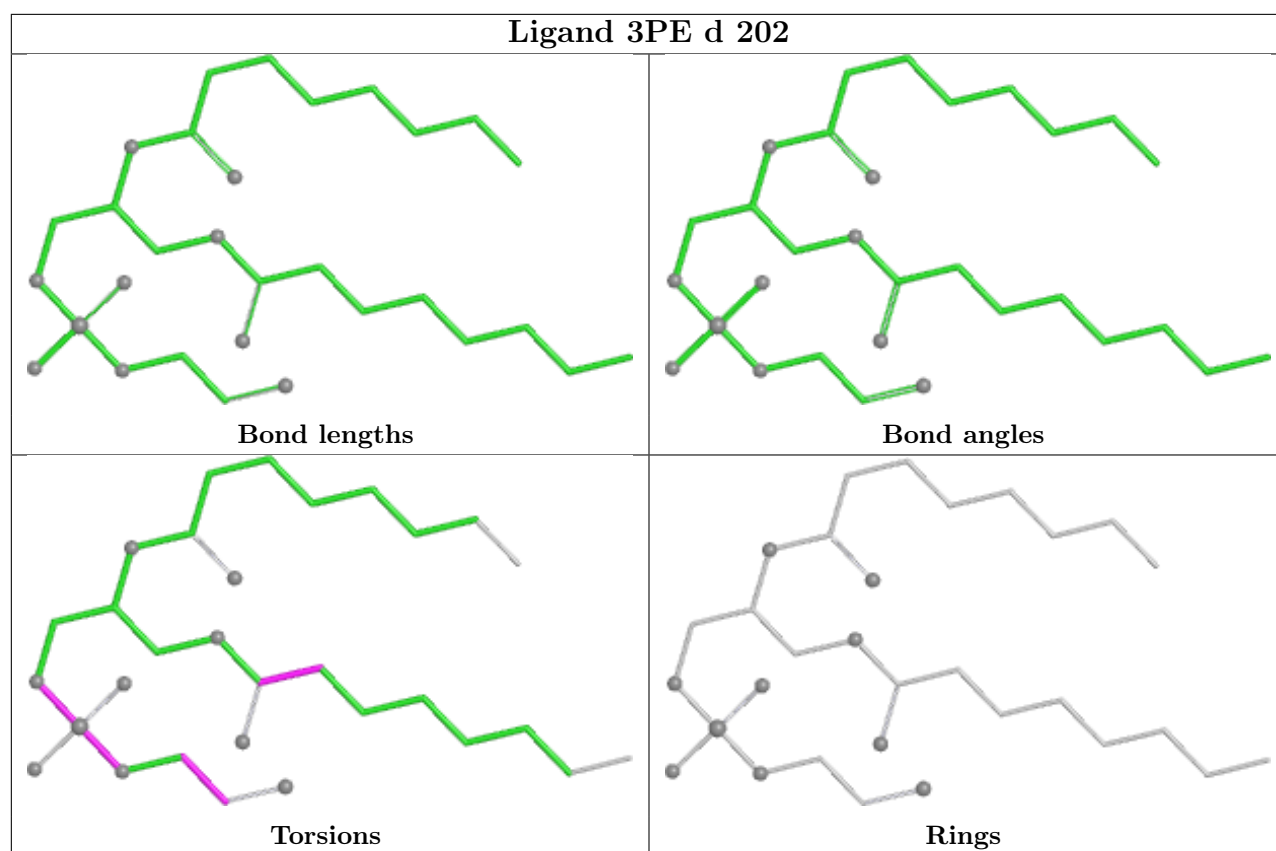


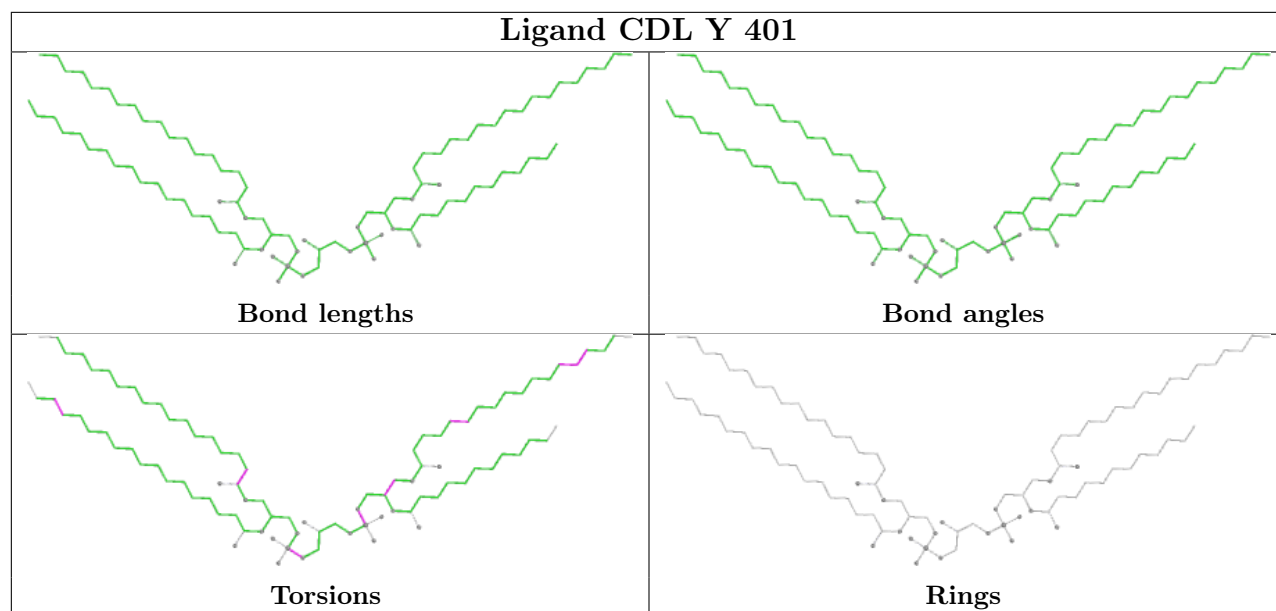
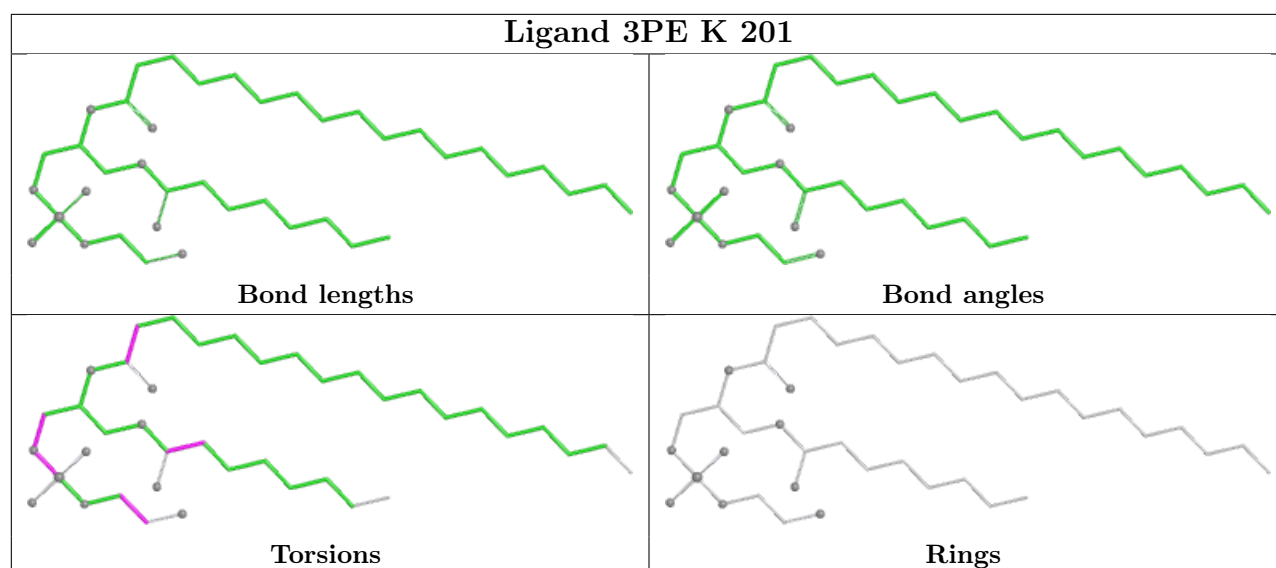


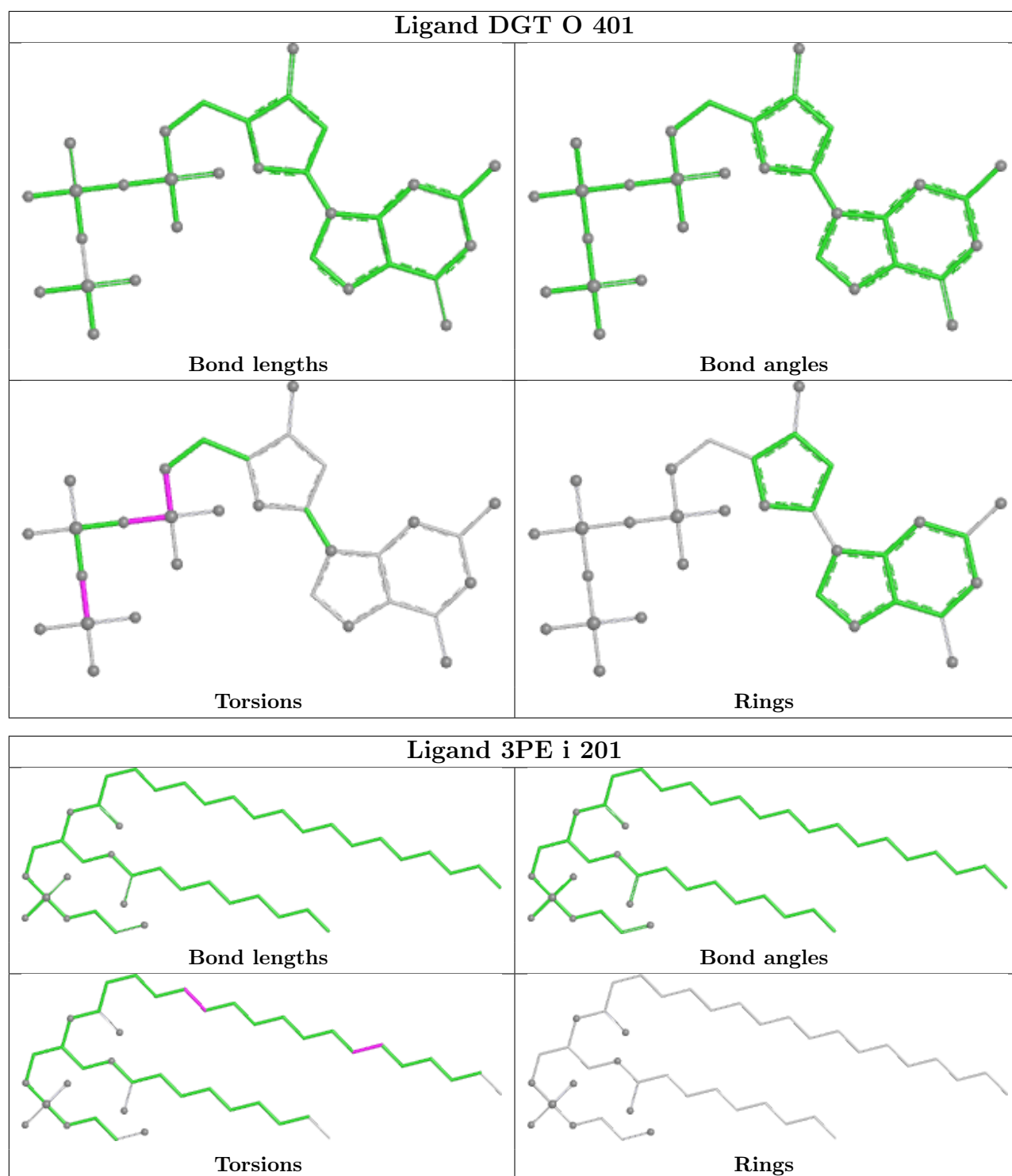


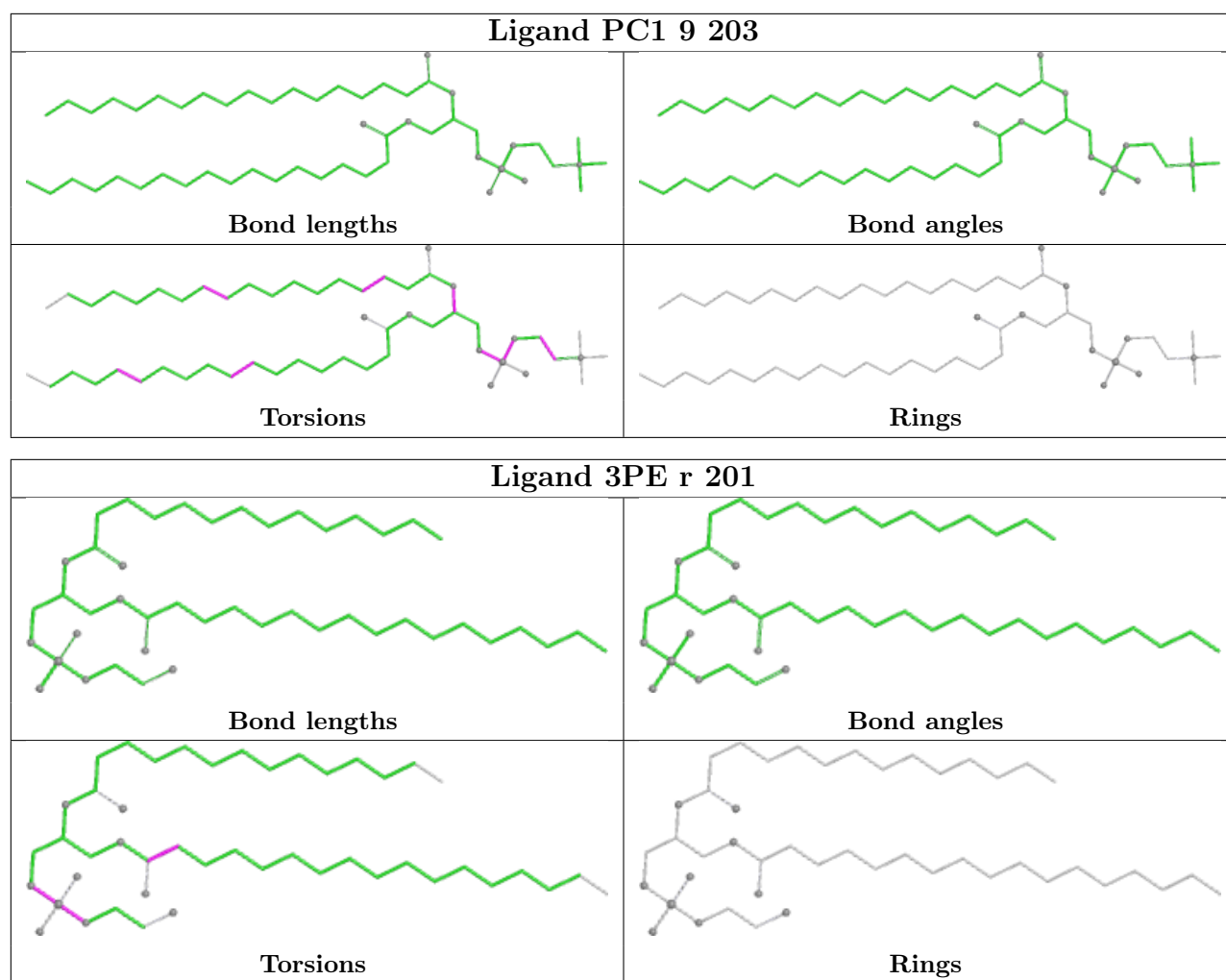


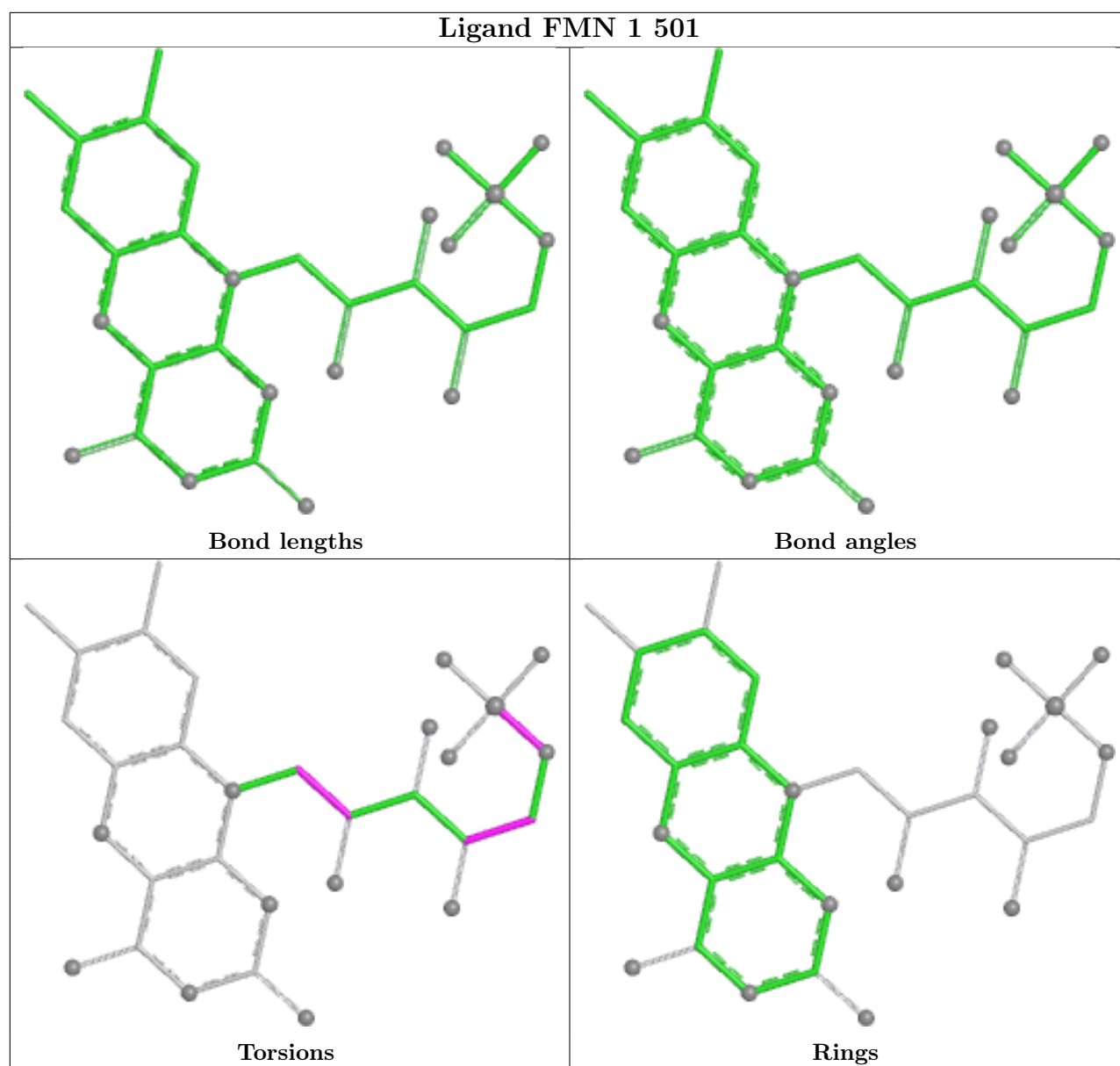


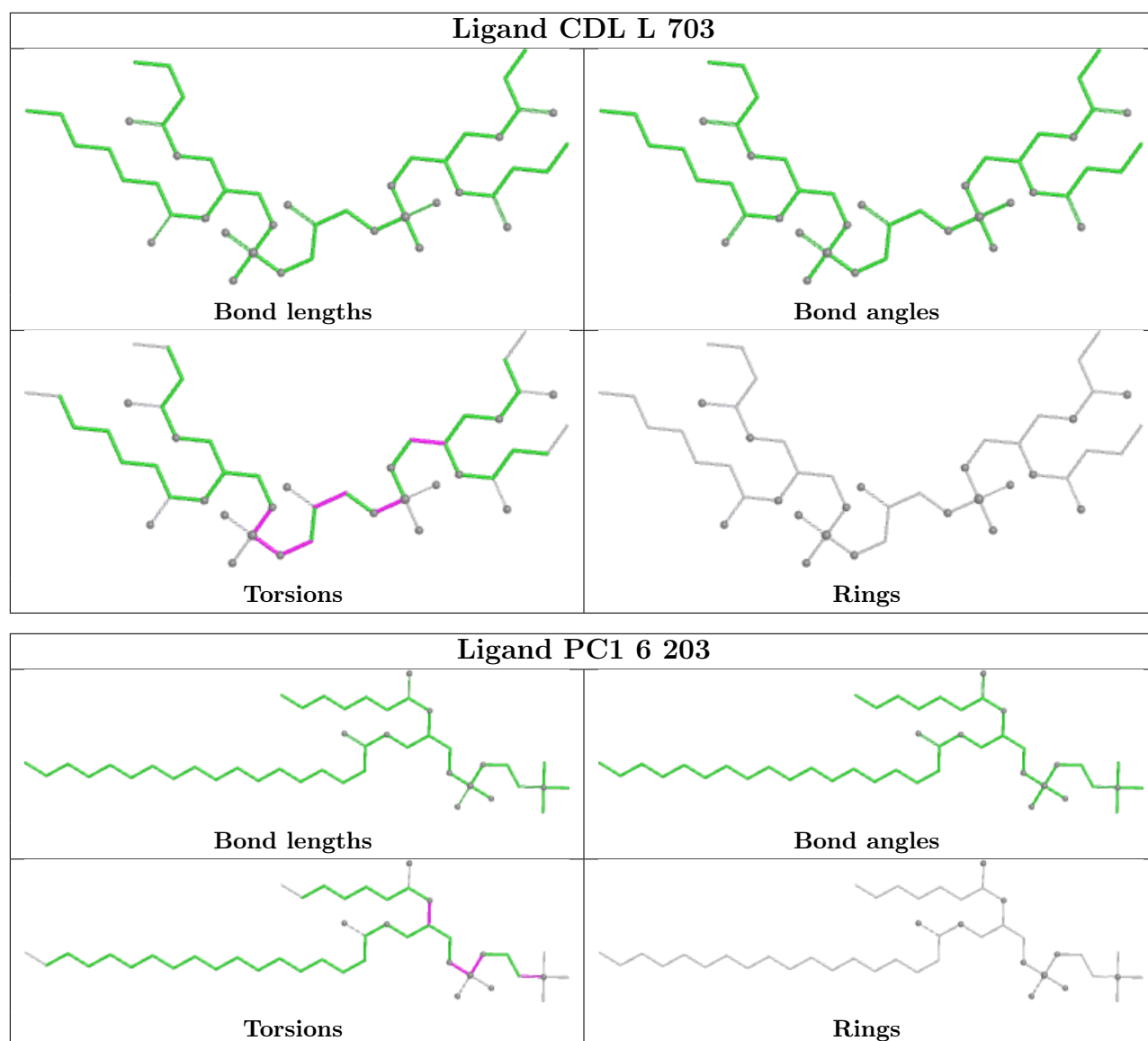












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

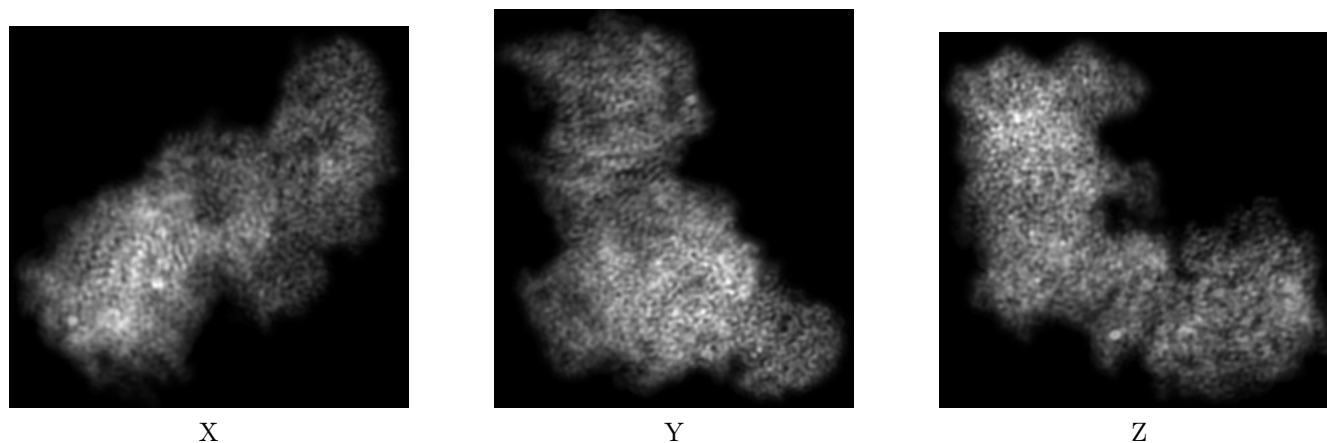
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19147. 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](#)

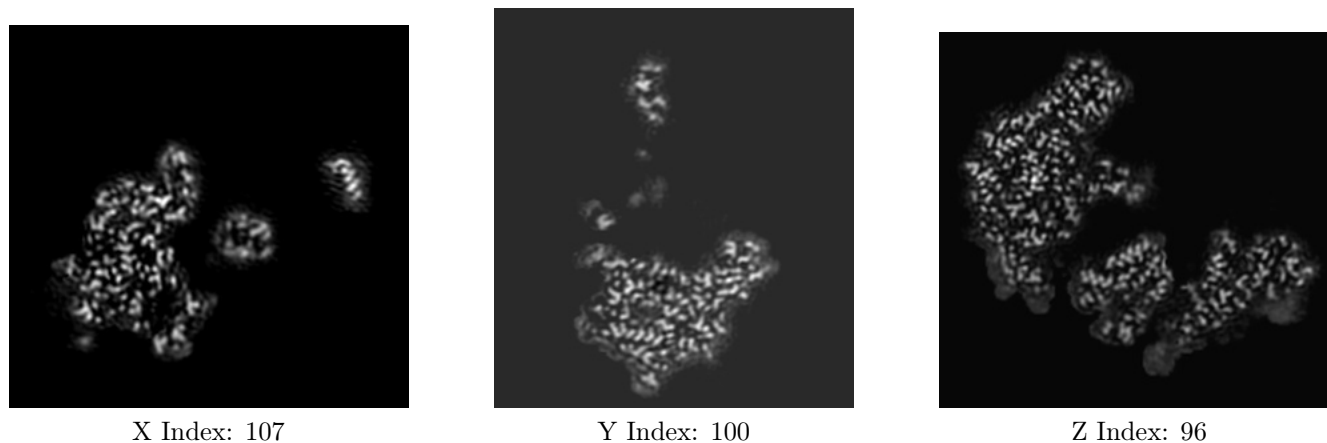
6.1.1 Primary map



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

6.2 Central slices [i](#)

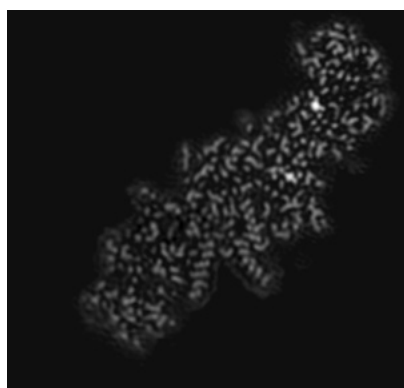
6.2.1 Primary map



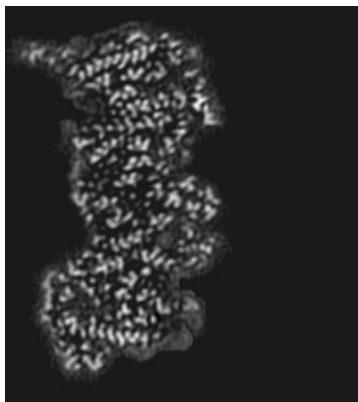
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

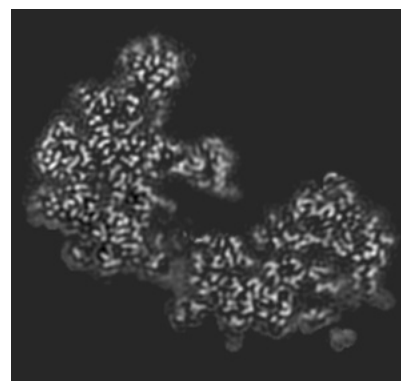
6.3.1 Primary map



X Index: 41



Y Index: 63



Z Index: 87

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

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

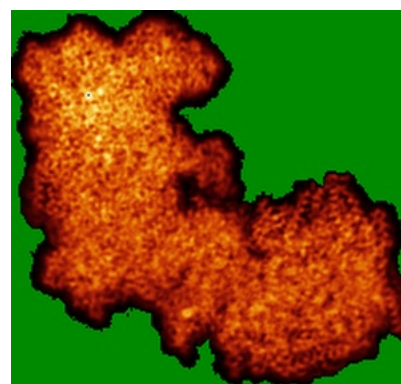
6.4.1 Primary map



X



Y

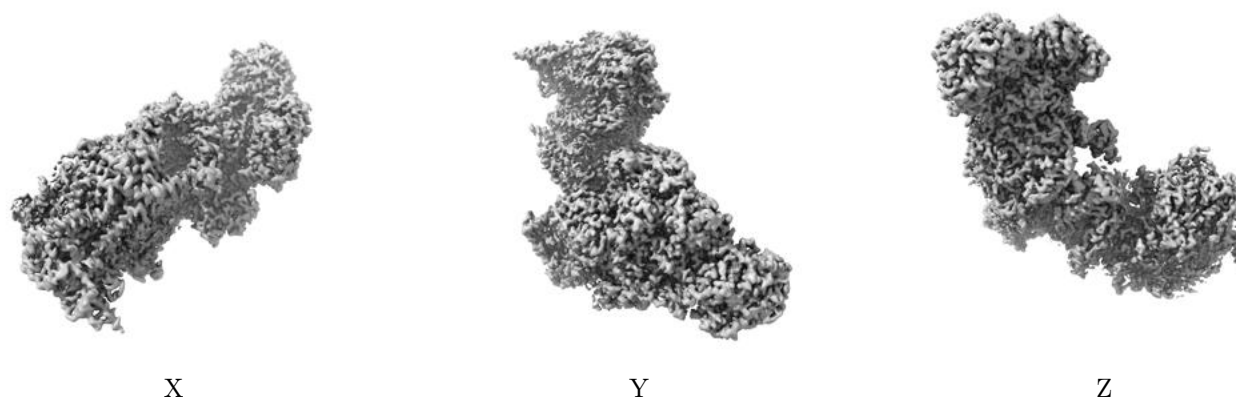


Z

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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

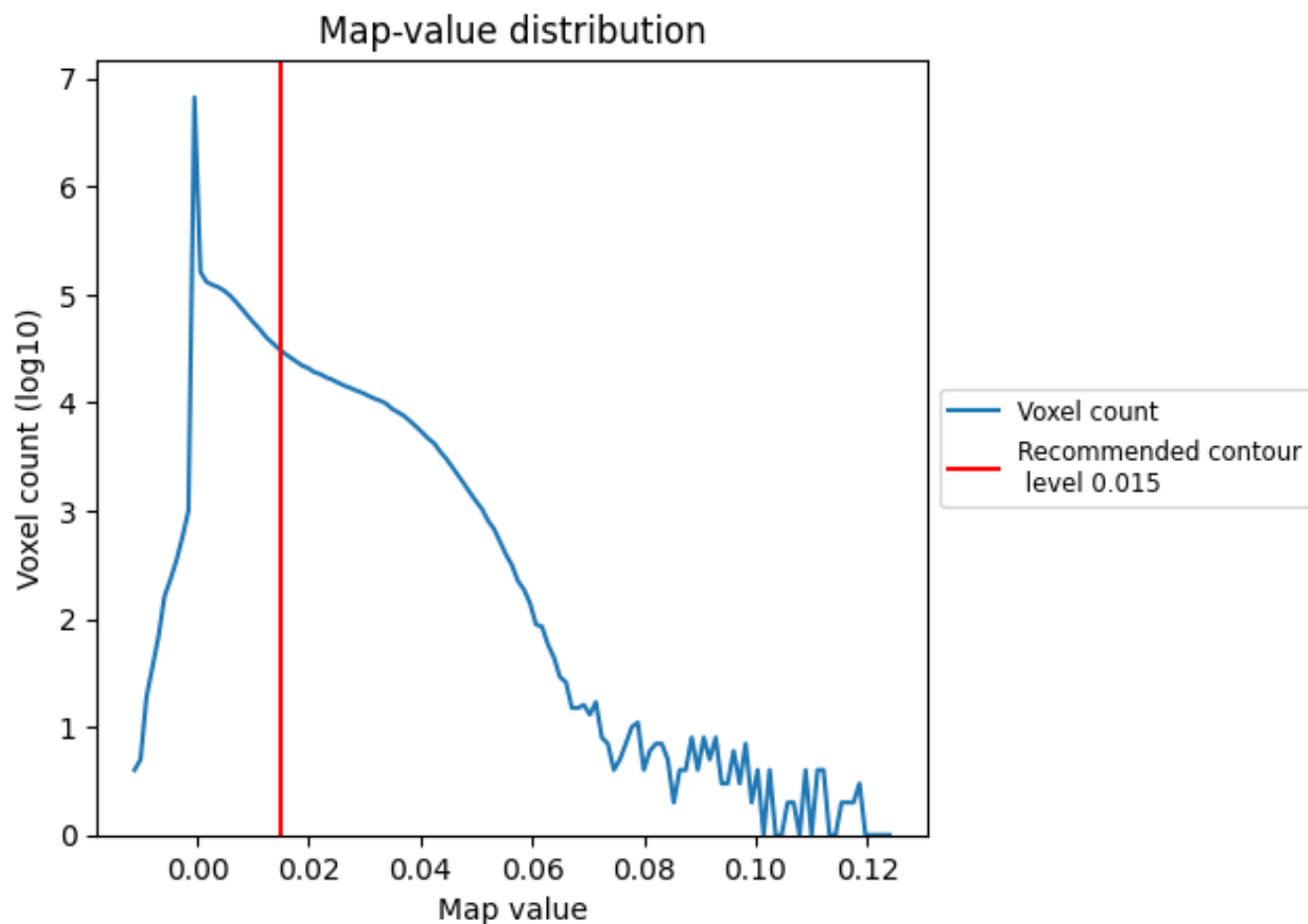
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

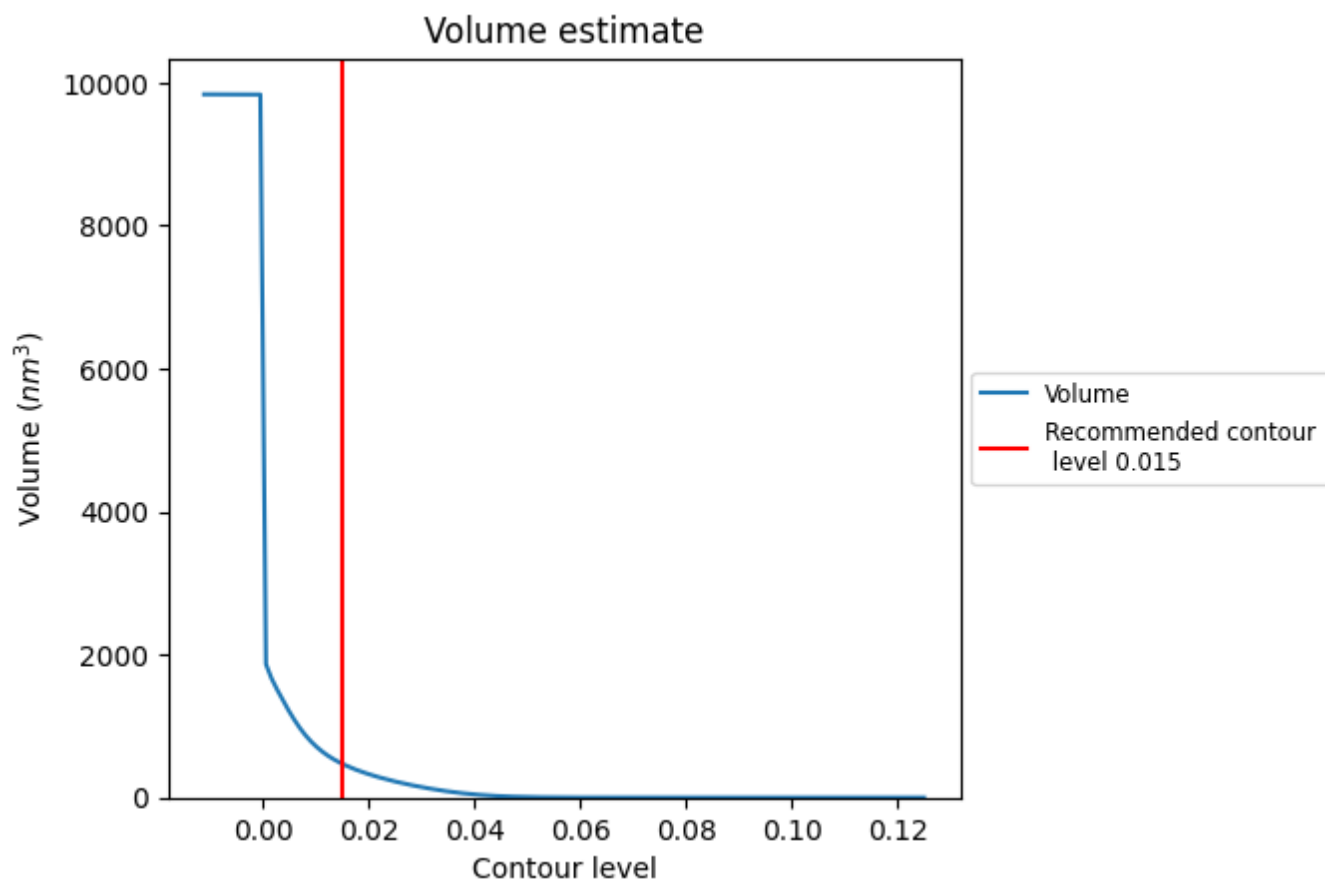
This section contains the results of statistical analysis of the map.

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 470 nm³; this corresponds to an approximate mass of 425 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.

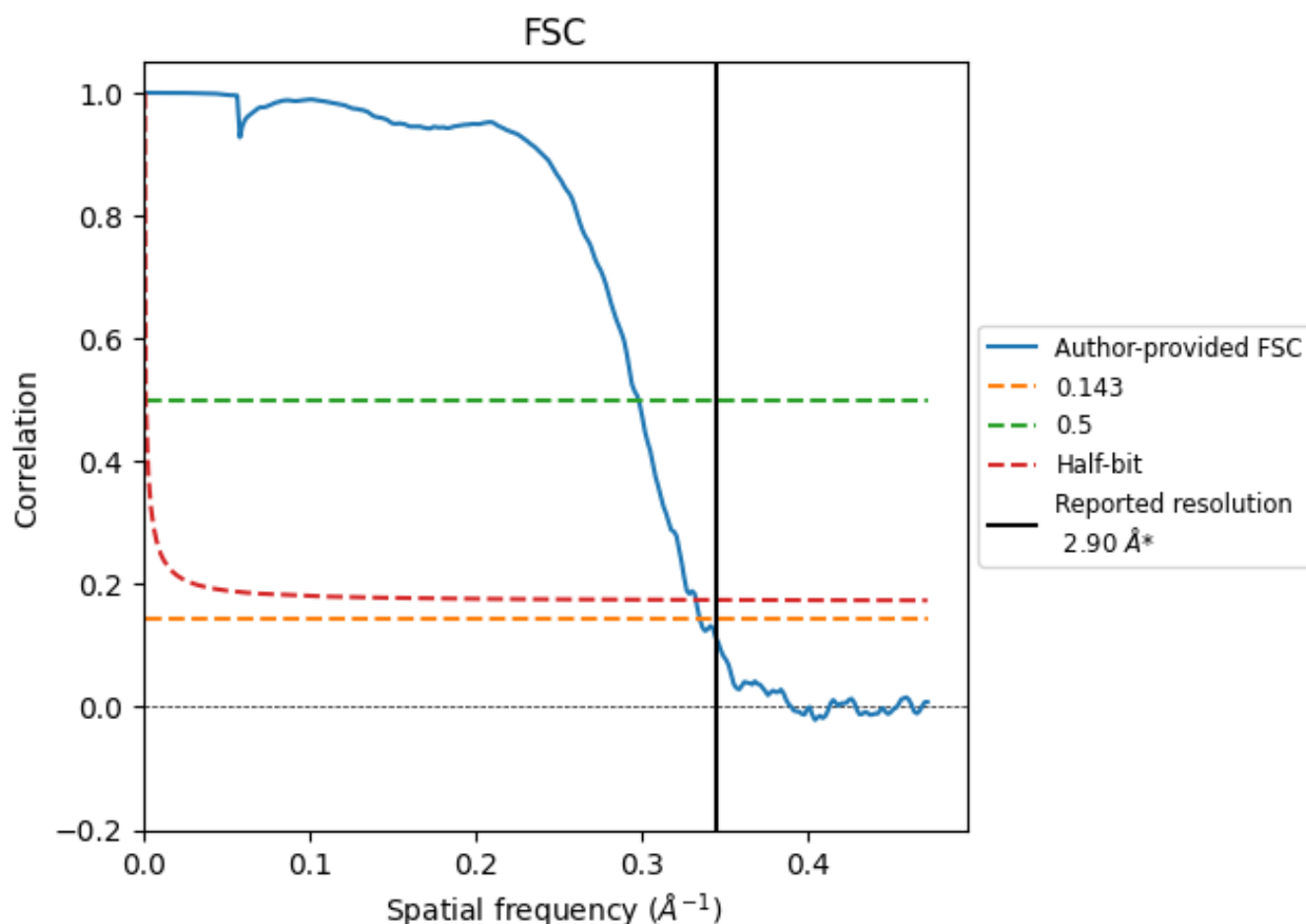
7.3 Rotationally averaged power spectrum [i](#)

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

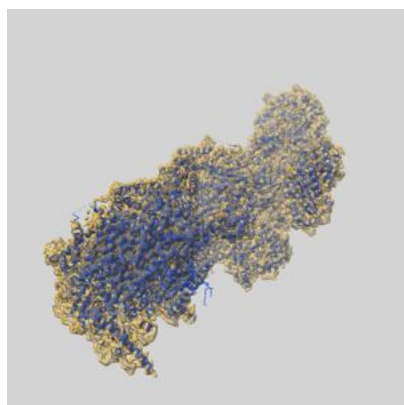
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.99	3.36	3.01
Unmasked-calculated*	-	-	-

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

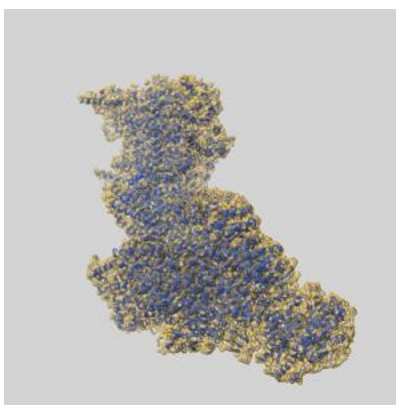
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19147 and PDB model 8RGR. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

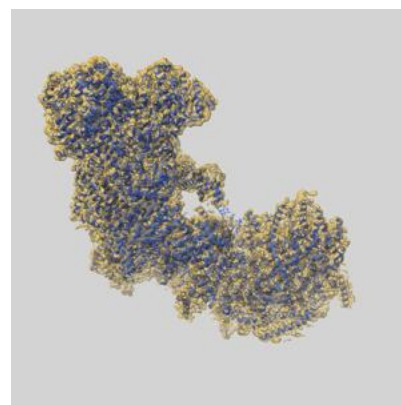
9.1 Map-model overlay [i](#)



X



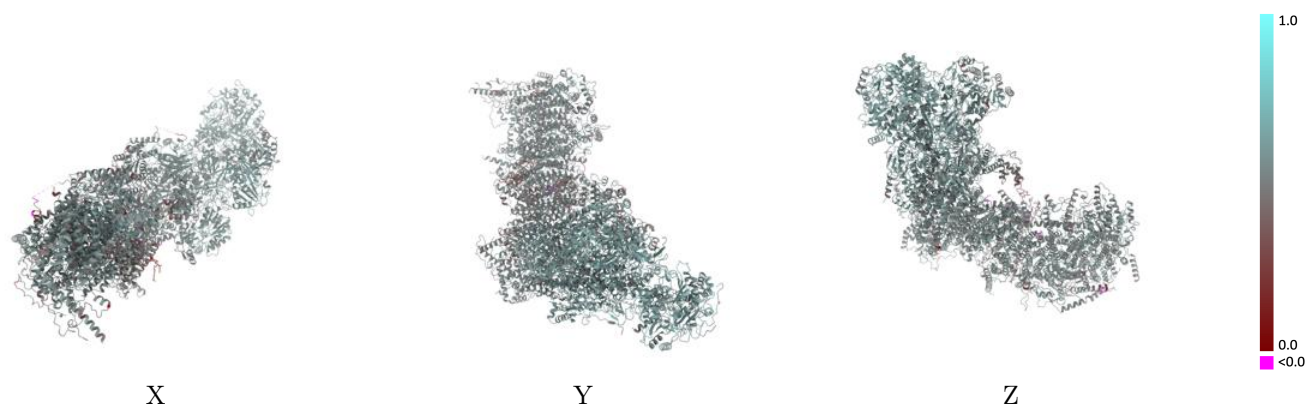
Y



Z

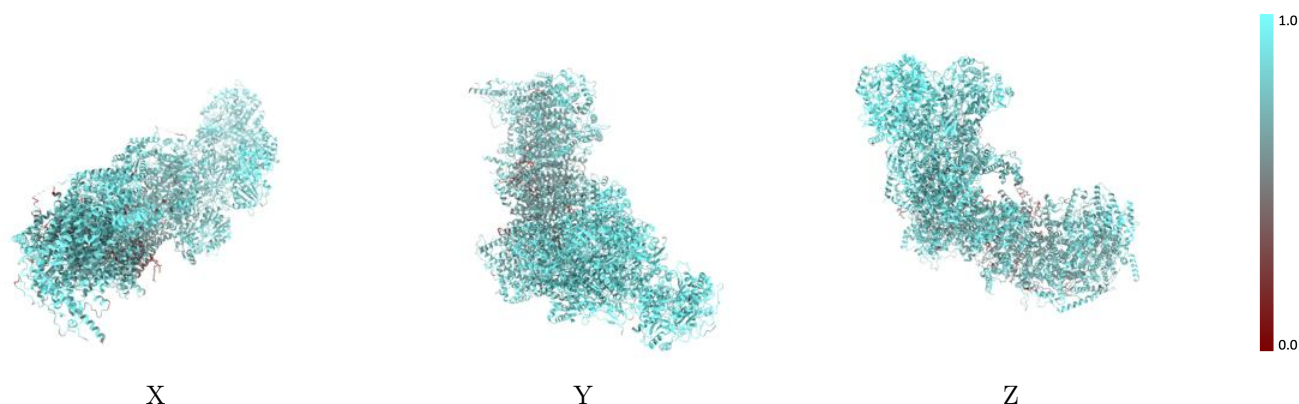
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



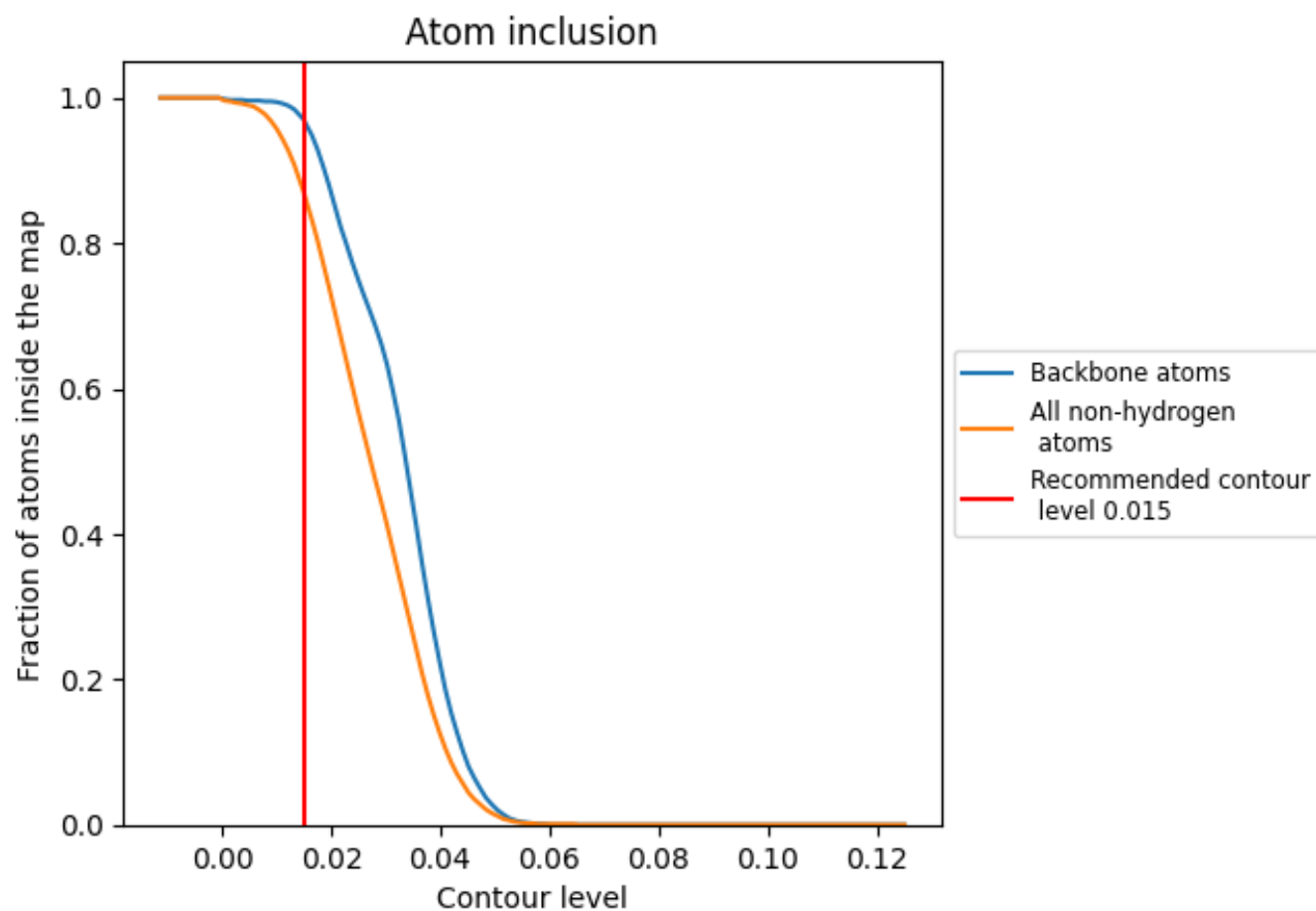
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.5450
1	 0.9570	 0.5860
2	 0.9460	 0.5790
3	 0.9350	 0.5810
6	 0.9070	 0.5730
7	 0.9370	 0.5870
9	 0.9180	 0.5830
A	 0.8040	 0.5400
C	 0.9260	 0.5820
D	 0.8600	 0.5450
H	 0.8610	 0.5450
J	 0.7320	 0.4960
K	 0.7890	 0.5290
L	 0.8390	 0.5340
M	 0.8410	 0.5460
N	 0.8060	 0.5360
O	 0.8900	 0.5340
P	 0.9030	 0.5650
Q	 0.9040	 0.5870
S	 0.9320	 0.5320
T	 0.7780	 0.4510
U	 0.8690	 0.5230
V	 0.8990	 0.5510
W	 0.8940	 0.5570
X	 0.9030	 0.5320
Y	 0.6830	 0.4630
Z	 0.8700	 0.5390
a	 0.8860	 0.5440
b	 0.8640	 0.5200
c	 0.8220	 0.5100
d	 0.8070	 0.5290
e	 0.8520	 0.5340
f	 0.7970	 0.5070
g	 0.8320	 0.5050
h	 0.8770	 0.5330



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7880	 0.4810
j	 0.8500	 0.4990
k	 0.8930	 0.5230
l	 0.8650	 0.5430
m	 0.7550	 0.4960
n	 0.8790	 0.5320
o	 0.8490	 0.5000
p	 0.8960	 0.5300
q	 0.9390	 0.5790
r	 0.8610	 0.5560
s	 0.9090	 0.5610