



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:10 PM UTC

PDB ID : 9FZL / pdb_00009fzl
EMDB ID : EMD-50491
Title : Perkinsus marinus respiratory supercomplex CII2CIII2CIV2 in an intermediate state
Authors : Wu, F.; Amunts, A.
Deposited on : 2024-07-05
Resolution : 2.20 Å(reported)

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:

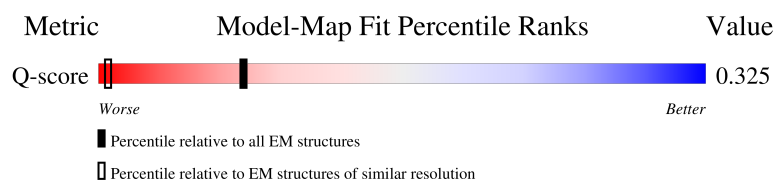
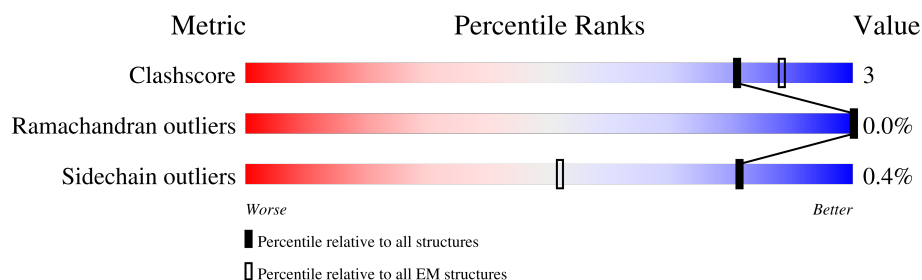
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.20 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.



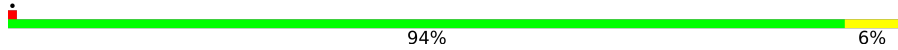
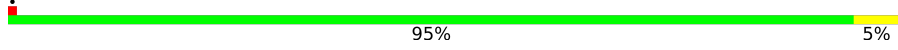
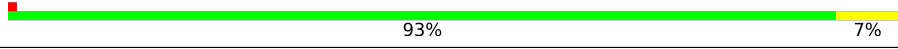
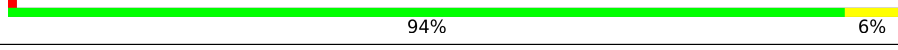
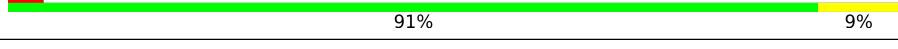
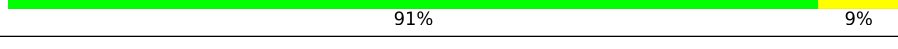
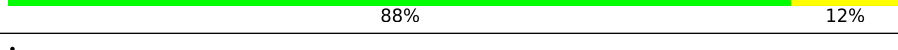
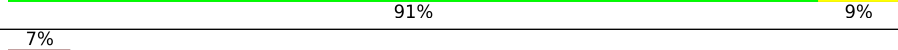
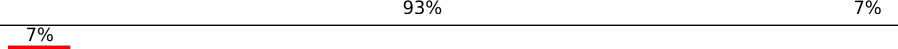
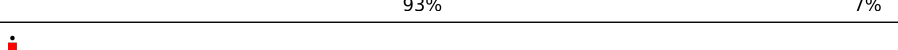
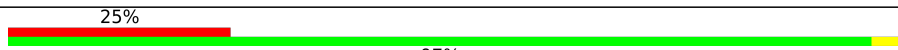
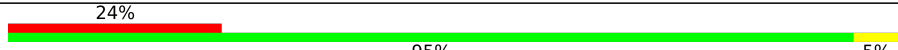
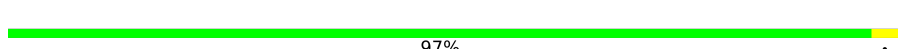
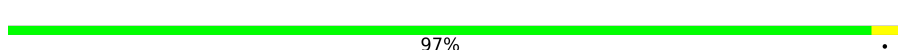
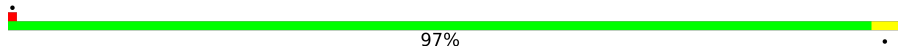
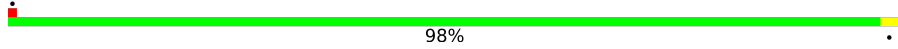
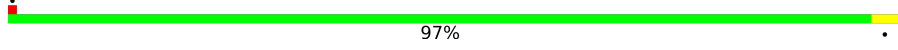
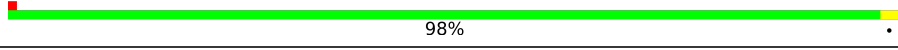
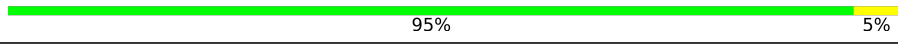
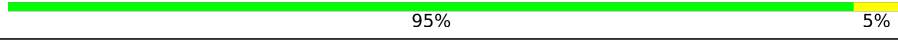
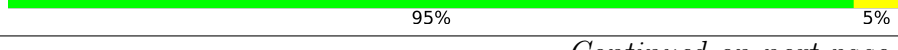
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	2M	604	77% 94% 6%
1	2m	604	77% 94% 6%
2	2N	259	24% 95% 5%
2	2n	259	23% 95% 5%

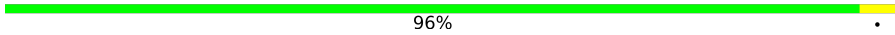
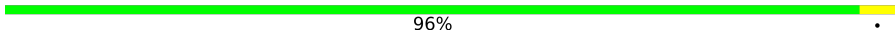
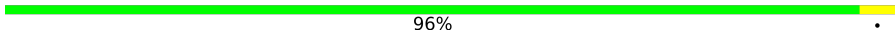
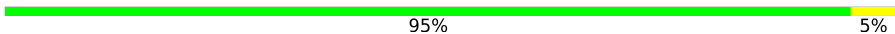
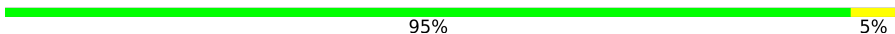
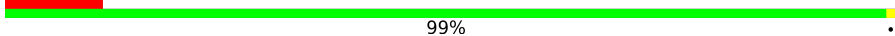
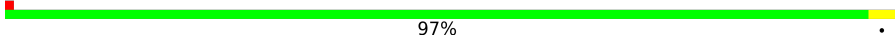
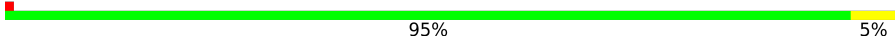
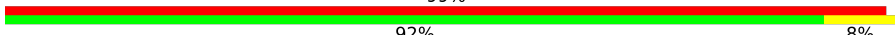
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Mol	Chain	Length	Quality of chain
3	2O	160	
3	2o	160	
4	2P	158	
4	2p	158	
5	2Q	69	
5	2q	69	
6	2R	117	
6	2r	117	
7	2S	165	
7	2s	165	
8	2T	82	
8	2t	82	
9	2U	48	
9	2u	48	
10	2V	87	
10	2v	87	
11	3A	454	
11	3a	454	
12	3B	496	
12	3b	496	
13	3C	241	
13	3c	241	
14	3D	95	
14	3d	95	
15	3E	92	

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Mol	Chain	Length	Quality of chain
15	3e	92	 96% .
16	3F	84	 96% .
16	3f	84	 96% .
17	3G	354	 90% 10%
17	3g	354	 90% 10%
18	3H	326	 30% 87% 13%
18	3h	326	 30% 87% 13%
19	3I	176	 95% 5%
19	3i	176	 95% 5%
20	3J	92	 11% 99% .
20	3j	92	 11% 99% .
21	3K	79	 97% .
21	3k	79	 95% 5%
22	3L	69	 29% 87% 13%
22	3l	69	 29% 87% 13%
23	40	230	 100% 90% 10%
23	41	230	 100% 90% 10%
24	4A	100	 100% 91% 9%
24	4a	100	 100% 91% 9%
25	4B	93	 98% 91% 8% .
25	4b	93	 98% 91% 8% .
26	4C	75	 96% 88% 11% .
26	4c	75	 96% 88% 11% .
27	4D	90	 99% 92% 8% .
27	4d	90	 100% 93% 7% .

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Mol	Chain	Length	Quality of chain
28	4E	152	100% 5%
28	4e	152	100% 5%
29	4F	73	99% 96% .
29	4f	73	99% 96% .
30	4G	100	99% 98% .
30	4g	100	99% 98% .
31	4H	141	100% 96% .
31	4h	141	100% 95% 5%
32	4I	196	100% 95% 5%
32	4i	196	100% 94% 6%
33	4J	186	100% 92% 8%
33	4j	186	100% 91% 9%
34	4K	93	100% 95% 5%
34	4k	93	100% 95% 5%
35	4L	122	100% 96% .
35	4l	122	100% 96% .
36	4M	98	100% 93% 7%
36	4m	98	100% 93% 7%
37	4N	131	100% 95% 5%
37	4n	131	100% 95% 5%
38	4O	47	100% 91% 9%
38	4o	47	100% 91% 9%
39	4P	180	100% 96% .
39	4p	180	100% 96% .
40	4Q	459	100% 88% 12%

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Mol	Chain	Length	Quality of chain
40	4q	459	100% 88% 12%
41	4R	103	100% 97%
41	4r	103	100% 96%
42	4S	65	100% 97%
42	4s	65	100% 100%
43	4T	121	100% 93% 7%
43	4t	121	100% 93% 7%
44	4U	91	100% 88% 12%
44	4u	91	100% 89% 11%
45	4V	185	100% 93% 7%
45	4v	185	100% 93% 7%
46	4W	141	100% 96%
46	4w	141	100% 96%
47	4X	226	100% 91% 9%
47	4x	226	100% 90% 10%
48	4Y	107	100% 95% 5%
48	4y	107	100% 95% 5%
49	4Z	186	100% 98%
49	4z	186	100% 98%

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
61	AJP	40	304	X	-	-	-
61	AJP	41	304	X	-	-	-

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 142424 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2M	604	Total	C	N	O	S	0	0
			4610	2880	831	873	26		
1	2m	604	Total	C	N	O	S	0	0
			4610	2880	831	873	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2N	259	Total	C	N	O	S	0	0
			2068	1309	355	378	26		
2	2n	259	Total	C	N	O	S	0	0
			2068	1309	355	378	26		

- Molecule 3 is a protein called SDHG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2O	160	Total	C	N	O	S	0	0
			1254	806	229	213	6		
3	2o	160	Total	C	N	O	S	0	0
			1254	806	229	213	6		

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2P	158	Total	C	N	O	S	0	0
			1309	846	246	211	6		
4	2p	158	Total	C	N	O	S	0	0
			1309	846	246	211	6		

- Molecule 5 is a protein called Kinesin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2Q	69	Total	C	N	O	S	0	0
			564	367	100	94	3		
5	2q	69	Total	C	N	O	S	0	0
			564	367	100	94	3		

- Molecule 6 is a protein called SDHH.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2R	117	Total	C	N	O	S	0	0
			950	621	166	157	6		
6	2r	117	Total	C	N	O	S	0	0
			950	621	166	157	6		

- Molecule 7 is a protein called DUF6827 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2S	165	Total	C	N	O	S	0	0
			1323	832	223	257	11		
7	2s	165	Total	C	N	O	S	0	0
			1323	832	223	257	11		

- Molecule 8 is a protein called Rab-GAP TBC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2T	82	Total	C	N	O	S	0	0
			695	446	117	128	4		
8	2t	82	Total	C	N	O	S	0	0
			695	446	117	128	4		

- Molecule 9 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2U	48	Total	C	N	O	S	0	0
			390	246	68	75	1		
9	2u	48	Total	C	N	O	S	0	0
			390	246	68	75	1		

- Molecule 10 is a protein called SDHI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2V	87	Total	C	N	O	S	0	0
			709	457	119	126	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2v	87	Total	C	N	O	S	0	0
			709	457	119	126	7		

- Molecule 11 is a protein called Mitochondrial processing peptidase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3A	454	Total	C	N	O	S	0	0
			3622	2285	621	698	18		
11	3a	454	Total	C	N	O	S	0	0
			3622	2285	621	698	18		

- Molecule 12 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3B	496	Total	C	N	O	S	0	0
			3884	2459	669	734	22		
12	3b	496	Total	C	N	O	S	0	0
			3884	2459	669	734	22		

- Molecule 13 is a protein called Iso-1-cytochrome c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3C	241	Total	C	N	O	S	0	0
			1921	1225	334	349	13		
13	3c	241	Total	C	N	O	S	0	0
			1921	1225	334	349	13		

- Molecule 14 is a protein called QCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3D	95	Total	C	N	O	S	0	0
			836	551	146	135	4		
14	3d	95	Total	C	N	O	S	0	0
			836	551	146	135	4		

- Molecule 15 is a protein called QCR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3E	92	Total	C	N	O	S	0	0
			813	545	138	127	3		
15	3e	92	Total	C	N	O	S	0	0
			813	545	138	127	3		

- Molecule 16 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3F	84	Total	C	N	O	S	0	0
			734	493	123	114	4		
16	3f	84	Total	C	N	O	S	0	0
			734	493	123	114	4		

- Molecule 17 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3G	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		
17	3g	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		

- Molecule 18 is a protein called Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3H	326	Total	C	N	O	S	0	0
			2628	1669	478	466	15		
18	3h	326	Total	C	N	O	S	0	0
			2628	1669	478	466	15		

- Molecule 19 is a protein called Ubiquinol-cytochrome C reductase complex 14kD subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3I	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		
19	3i	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		

- Molecule 20 is a protein called Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3J	92	Total	C	N	O	S	0	0
			755	471	134	139	11		
20	3j	92	Total	C	N	O	S	0	0
			755	471	134	139	11		

- Molecule 21 is a protein called Cu-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3K	79	Total	C	N	O	S	0	0
			608	391	110	103	4		
21	3k	79	Total	C	N	O	S	0	0
			608	391	110	103	4		

- Molecule 22 is a protein called Aurora kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3L	69	Total	C	N	O	S	0	0
			509	327	91	89	2		
22	3l	69	Total	C	N	O	S	0	0
			509	327	91	89	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	40	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		
23	41	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4A	100	Total	C	N	O	S	0	0
			841	518	157	157	9		
24	4a	100	Total	C	N	O	S	0	0
			841	518	157	157	9		

- Molecule 25 is a protein called Peptidase M14 carboxypeptidase A domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4B	93	Total	C	N	O	S	0	0
			732	479	116	129	8		
25	4b	93	Total	C	N	O	S	0	0
			732	479	116	129	8		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4C	75	Total	C	N	O	S	0	0
			626	414	95	113	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	4c	75	Total	C	N	O	S	0	0
			626	414	95	113	4		

- Molecule 27 is a protein called Cytochrome c oxidase subunit 34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4D	90	Total	C	N	O	S	0	0
			787	525	128	131	3		
27	4d	90	Total	C	N	O	S	0	0
			787	525	128	131	3		

- Molecule 28 is a protein called Merozoite surface protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4E	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		
28	4e	152	Total	C	N	O	S	0	0
			1313	840	229	229	15		

- Molecule 29 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4F	73	Total	C	N	O	S	0	0
			613	406	108	97	2		
29	4f	73	Total	C	N	O	S	0	0
			613	406	108	97	2		

- Molecule 30 is a protein called Cytochrome c oxidase subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4G	100	Total	C	N	O	S	0	0
			854	550	156	144	4		
30	4g	100	Total	C	N	O	S	0	0
			854	550	156	144	4		

- Molecule 31 is a protein called Cytochrome c oxidase subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4H	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		
31	4h	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		

- Molecule 32 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4I	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		
32	4i	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		

- Molecule 33 is a protein called Cytochrome c oxidase subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4J	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		
33	4j	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		

- Molecule 34 is a protein called Cytochrome c oxidase subunit 37.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4K	93	Total	C	N	O	S	0	0
			722	473	129	118	2		
34	4k	93	Total	C	N	O	S	0	0
			722	473	129	118	2		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4L	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		
35	4l	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4M	98	Total	C	N	O	S	0	0
			773	498	147	127	1		
36	4m	98	Total	C	N	O	S	0	0
			773	498	147	127	1		

- Molecule 37 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4N	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		
37	4n	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		

- Molecule 38 is a protein called GINS subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4O	47	Total	C	N	O	S	0	0
			383	257	60	63	3		
38	4o	47	Total	C	N	O	S	0	0
			383	257	60	63	3		

- Molecule 39 is a protein called Cytochrome c oxidase subunit 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4P	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		
39	4p	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		

- Molecule 40 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4Q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		
40	4q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

- Molecule 41 is a protein called Cytochrome c oxidase subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	4R	103	Total	C	N	O	S	0	0
			916	609	156	145	6		
41	4r	103	Total	C	N	O	S	0	0
			916	609	156	145	6		

- Molecule 42 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4S	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	4s	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4T	121	Total	C	N	O	S	0	0
			983	634	170	167	12		
43	4t	121	Total	C	N	O	S	0	0
			983	634	170	167	12		

- Molecule 44 is a protein called Amino acid transporter transmembrane domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	4U	91	Total	C	N	O	S	0	0
			758	503	125	127	3		
44	4u	91	Total	C	N	O	S	0	0
			758	503	125	127	3		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4V	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		
45	4v	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4W	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		
46	4w	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		

- Molecule 47 is a protein called Cytochrome Coxidase subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4X	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
47	4x	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

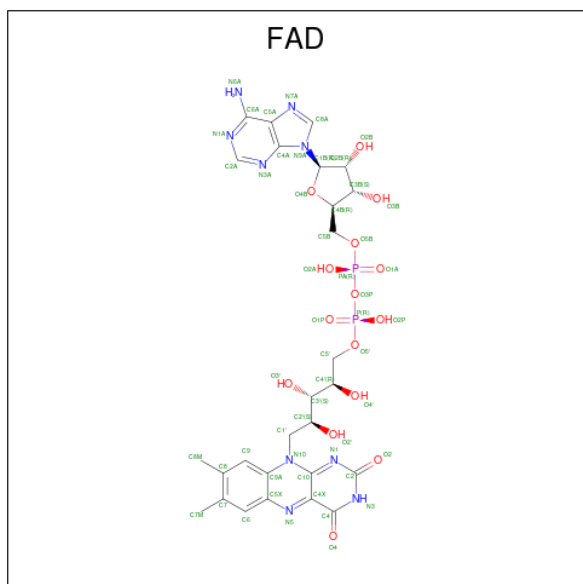
- Molecule 48 is a protein called Cytochrome c oxidase subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4Y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		
48	4y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 31.

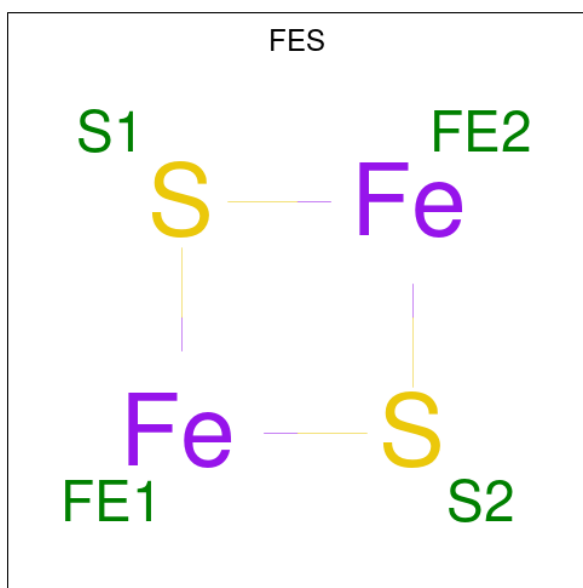
Mol	Chain	Residues	Atoms					AltConf	Trace
49	4Z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		
49	4z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		

- Molecule 50 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



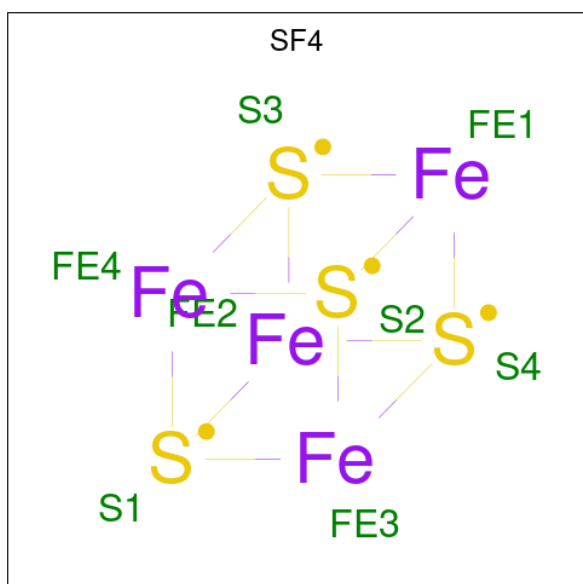
Mol	Chain	Residues	Atoms					AltConf
50	2M	1	Total	C	N	O	P	0
			53	27	9	15	2	
50	2m	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



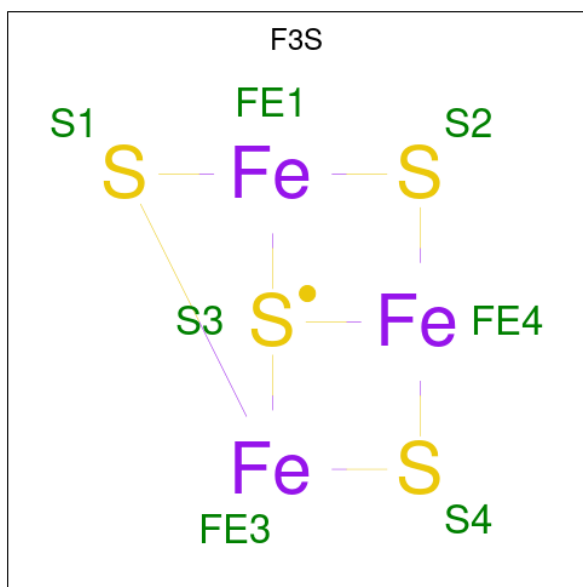
Mol	Chain	Residues	Atoms			AltConf
51	2N	1	Total	Fe	S	0
			4	2	2	
51	3H	1	Total	Fe	S	0
			4	2	2	
51	2n	1	Total	Fe	S	0
			4	2	2	
51	3h	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
52	2N	1	Total	Fe	S	0
			8	4	4	
52	2n	1	Total	Fe	S	0
			8	4	4	

- Molecule 53 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

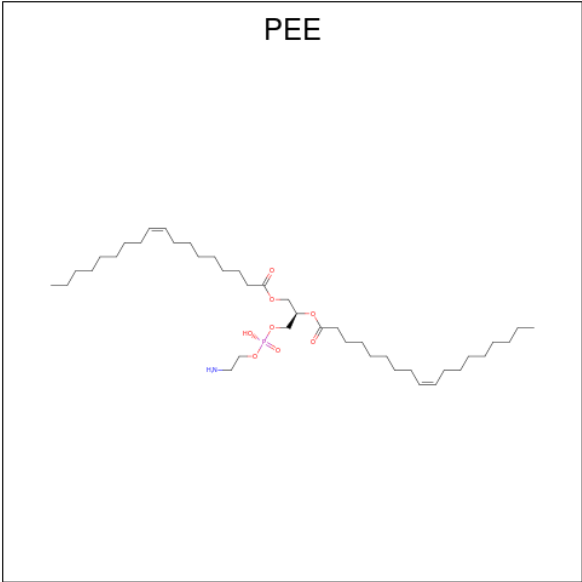


Mol	Chain	Residues	Atoms			AltConf
53	2N	1	Total	Fe	S	0
			7	3	4	
53	2n	1	Total	Fe	S	0
			7	3	4	

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
54	2N	1	Total	K	0
			1	1	
54	4Q	1	Total	K	0
			1	1	
54	2n	1	Total	K	0
			1	1	
54	4q	1	Total	K	0
			1	1	

- Molecule 55 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $\text{C}_{41}\text{H}_{78}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



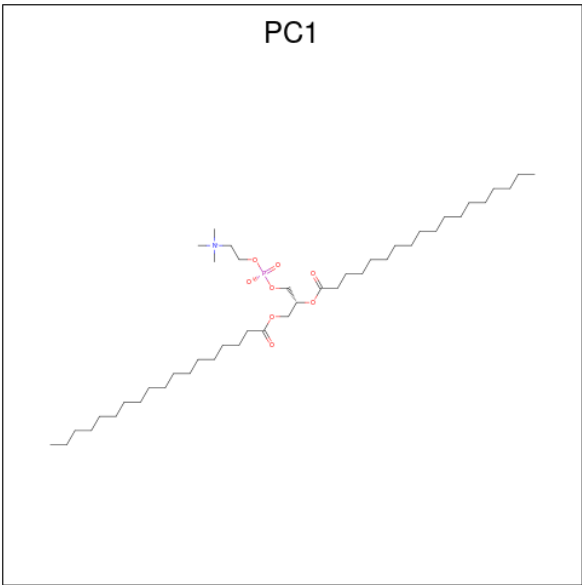
Mol	Chain	Residues	Atoms					AltConf
55	2O	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2P	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2P	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2R	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3F	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	40	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	40	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	40	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4D	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4R	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4S	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
55	4W	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2o	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2p	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2p	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	2r	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3c	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	3f	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4l	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4l	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4l	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4d	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4q	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4r	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4s	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4w	1	Total	C	N	O	P	0
			51	41	1	8	1	
55	4z	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 56 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



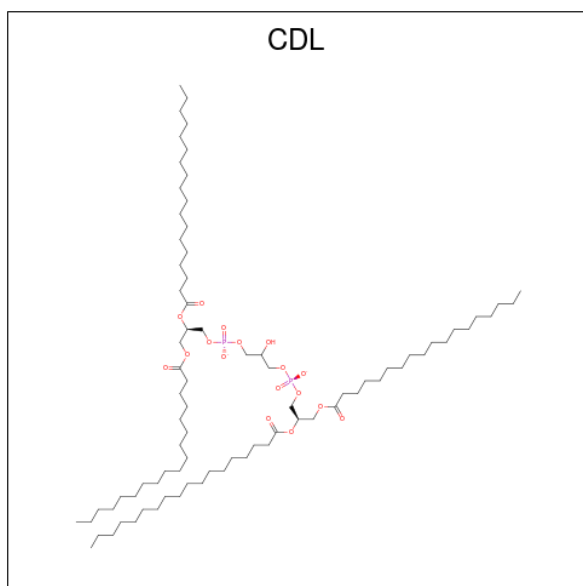
Mol	Chain	Residues	Atoms					AltConf
56	2O	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2O	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2P	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2R	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2T	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3A	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3A	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3H	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	4E	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2o	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2o	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2p	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2r	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	2t	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
56	3a	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3a	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	3h	1	Total	C	N	O	P	0
			54	44	1	8	1	
56	4e	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 57 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	2O	1	Total	C	O	P	0
			100	81	17	2	
57	2P	1	Total	C	O	P	0
			100	81	17	2	
57	2Q	1	Total	C	O	P	0
			100	81	17	2	
57	2U	1	Total	C	O	P	0
			100	81	17	2	
57	3D	1	Total	C	O	P	0
			100	81	17	2	
57	3D	1	Total	C	O	P	0
			100	81	17	2	
57	3E	1	Total	C	O	P	0
			100	81	17	2	

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Mol	Chain	Residues	Atoms				AltConf
57	3E	1	Total 100	C 81	O 17	P 2	0
57	3E	1	Total 100	C 81	O 17	P 2	0
57	3G	1	Total 100	C 81	O 17	P 2	0
57	3H	1	Total 100	C 81	O 17	P 2	0
57	3I	1	Total 100	C 81	O 17	P 2	0
57	3I	1	Total 100	C 81	O 17	P 2	0
57	3I	1	Total 100	C 81	O 17	P 2	0
57	3L	1	Total 100	C 81	O 17	P 2	0
57	3L	1	Total 100	C 81	O 17	P 2	0
57	4E	1	Total 100	C 81	O 17	P 2	0
57	4J	1	Total 100	C 81	O 17	P 2	0
57	4K	1	Total 100	C 81	O 17	P 2	0
57	4K	1	Total 100	C 81	O 17	P 2	0
57	4L	1	Total 100	C 81	O 17	P 2	0
57	4M	1	Total 100	C 81	O 17	P 2	0
57	4Q	1	Total 100	C 81	O 17	P 2	0
57	4Q	1	Total 100	C 81	O 17	P 2	0
57	4S	1	Total 100	C 81	O 17	P 2	0
57	4T	1	Total 100	C 81	O 17	P 2	0
57	4U	1	Total 100	C 81	O 17	P 2	0
57	4W	1	Total 100	C 81	O 17	P 2	0

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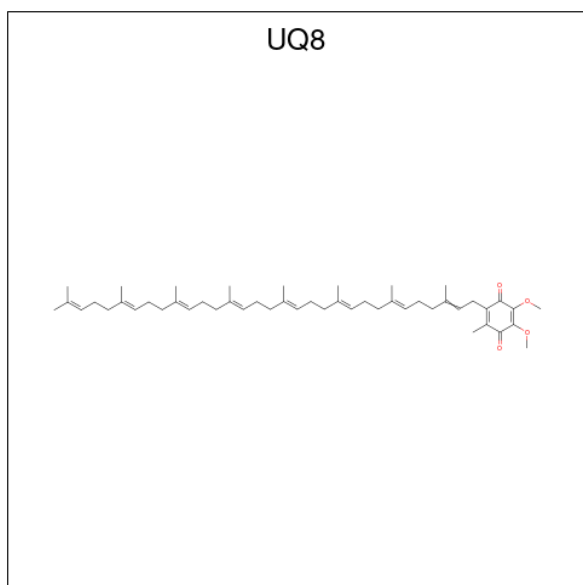
Mol	Chain	Residues	Atoms				AltConf
57	4W	1	Total 100	C 81	O 17	P 2	0
57	4Z	1	Total 100	C 81	O 17	P 2	0
57	2o	1	Total 100	C 81	O 17	P 2	0
57	2p	1	Total 100	C 81	O 17	P 2	0
57	2q	1	Total 100	C 81	O 17	P 2	0
57	2u	1	Total 100	C 81	O 17	P 2	0
57	3d	1	Total 100	C 81	O 17	P 2	0
57	3d	1	Total 100	C 81	O 17	P 2	0
57	3e	1	Total 100	C 81	O 17	P 2	0
57	3e	1	Total 100	C 81	O 17	P 2	0
57	3e	1	Total 100	C 81	O 17	P 2	0
57	3g	1	Total 100	C 81	O 17	P 2	0
57	3h	1	Total 100	C 81	O 17	P 2	0
57	3i	1	Total 100	C 81	O 17	P 2	0
57	3i	1	Total 100	C 81	O 17	P 2	0
57	3i	1	Total 100	C 81	O 17	P 2	0
57	3l	1	Total 100	C 81	O 17	P 2	0
57	3l	1	Total 100	C 81	O 17	P 2	0
57	4e	1	Total 100	C 81	O 17	P 2	0
57	4j	1	Total 100	C 81	O 17	P 2	0
57	4k	1	Total 100	C 81	O 17	P 2	0

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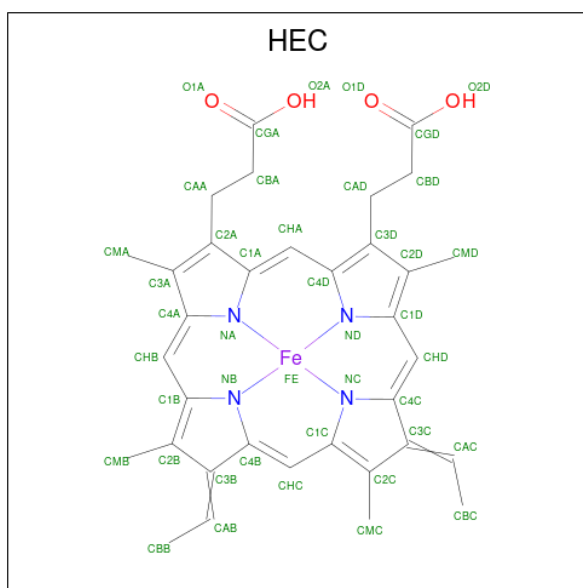
Mol	Chain	Residues	Atoms				AltConf
57	4k	1	Total 100	C 81	O 17	P 2	0
57	4l	1	Total 100	C 81	O 17	P 2	0
57	4m	1	Total 100	C 81	O 17	P 2	0
57	4q	1	Total 100	C 81	O 17	P 2	0
57	4q	1	Total 100	C 81	O 17	P 2	0
57	4s	1	Total 100	C 81	O 17	P 2	0
57	4t	1	Total 100	C 81	O 17	P 2	0
57	4u	1	Total 100	C 81	O 17	P 2	0
57	4w	1	Total 100	C 81	O 17	P 2	0
57	4w	1	Total 100	C 81	O 17	P 2	0
57	4z	1	Total 100	C 81	O 17	P 2	0

- Molecule 58 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



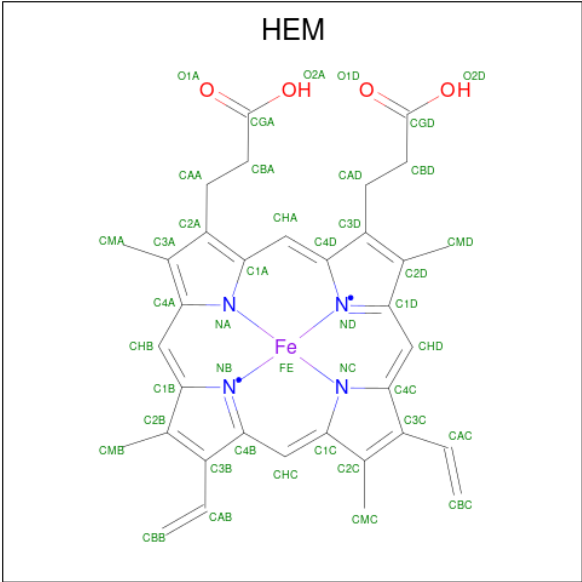
Mol	Chain	Residues	Atoms			AltConf
58	2S	1	Total	C	O	0
			53	49	4	
58	3D	1	Total	C	O	0
			53	49	4	
58	3G	1	Total	C	O	0
			53	49	4	
58	3G	1	Total	C	O	0
			53	49	4	
58	2s	1	Total	C	O	0
			53	49	4	
58	3d	1	Total	C	O	0
			53	49	4	
58	3g	1	Total	C	O	0
			53	49	4	
58	3g	1	Total	C	O	0
			53	49	4	

- Molecule 59 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



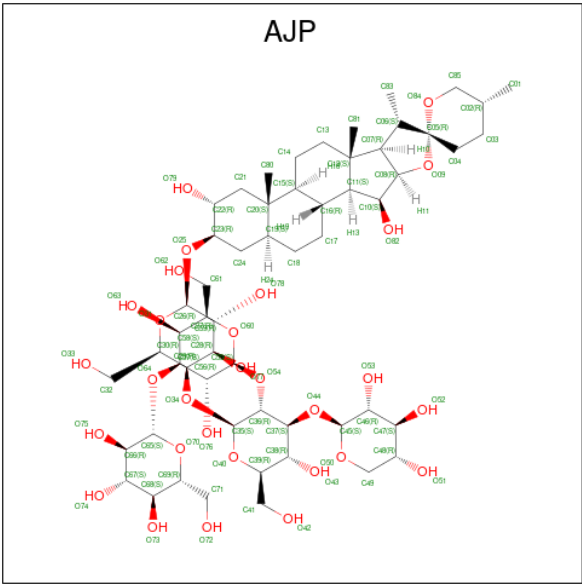
Mol	Chain	Residues	Atoms					AltConf
59	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
59	3c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 60 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



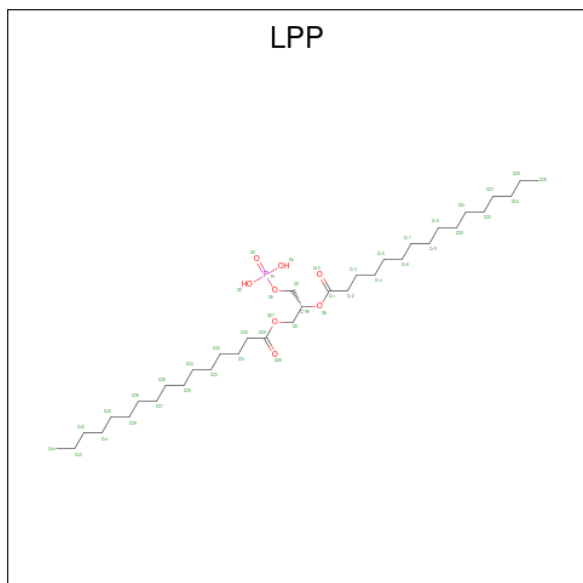
Mol	Chain	Residues	Atoms					AltConf
60	3G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
60	3G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
60	3g	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
60	3g	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 61 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



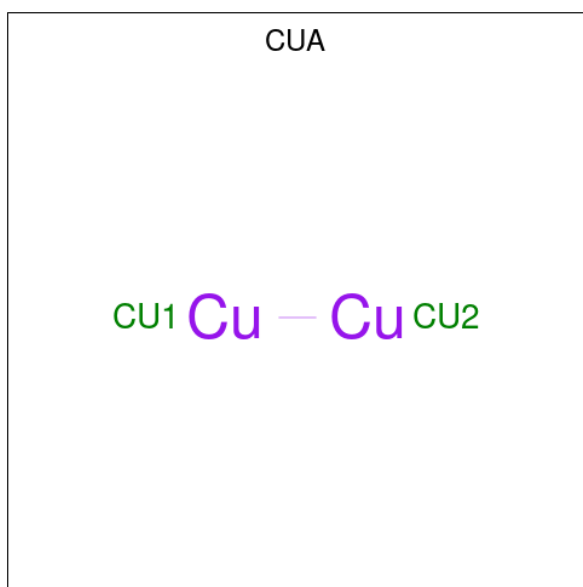
Mol	Chain	Residues	Atoms			AltConf
61	40	1	Total	C	O	0
			43	33	10	
61	41	1	Total	C	O	0
			43	33	10	

- Molecule 62 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
62	4C	1	Total	C	O	P	0
			44	35	8	1	
62	4D	1	Total	C	O	P	0
			44	35	8	1	
62	4c	1	Total	C	O	P	0
			44	35	8	1	
62	4d	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 63 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
63	4N	1	Total	Cu	0
			2	2	
63	4n	1	Total	Cu	0
			2	2	

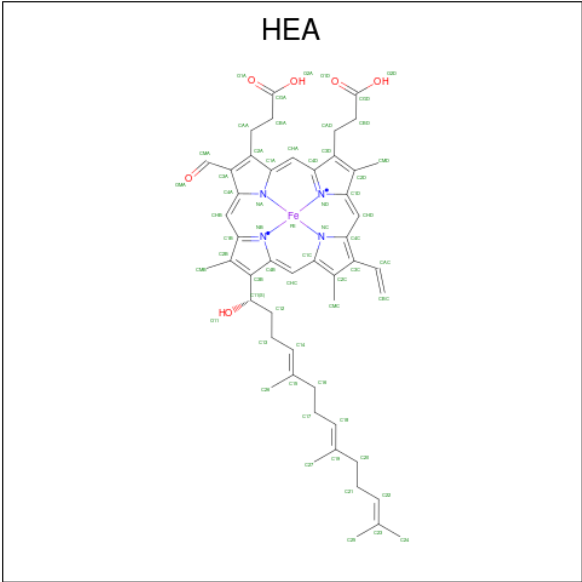
- Molecule 64 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
64	4Q	1	Total	Cu	0
			1	1	
64	4q	1	Total	Cu	0
			1	1	

- Molecule 65 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

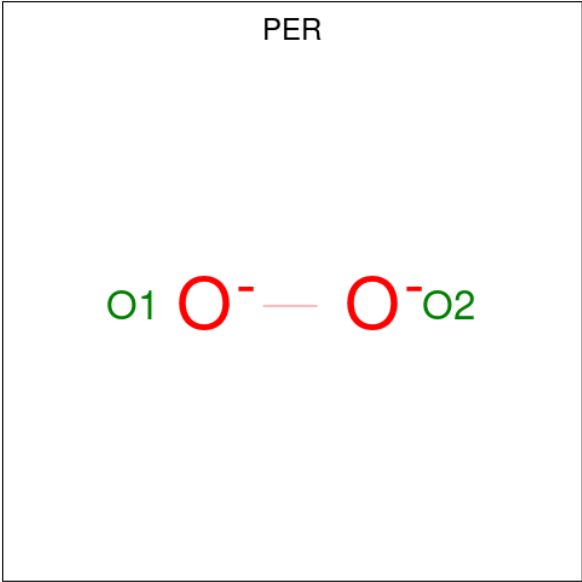
Mol	Chain	Residues	Atoms		AltConf
65	4Q	1	Total	Mg	0
			1	1	
65	4q	1	Total	Mg	0
			1	1	

- Molecule 66 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
66	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
66	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
66	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
66	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 67 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		AltConf
67	4Q	1	Total	O	0
			2	2	
67	4q	1	Total	O	0
			2	2	

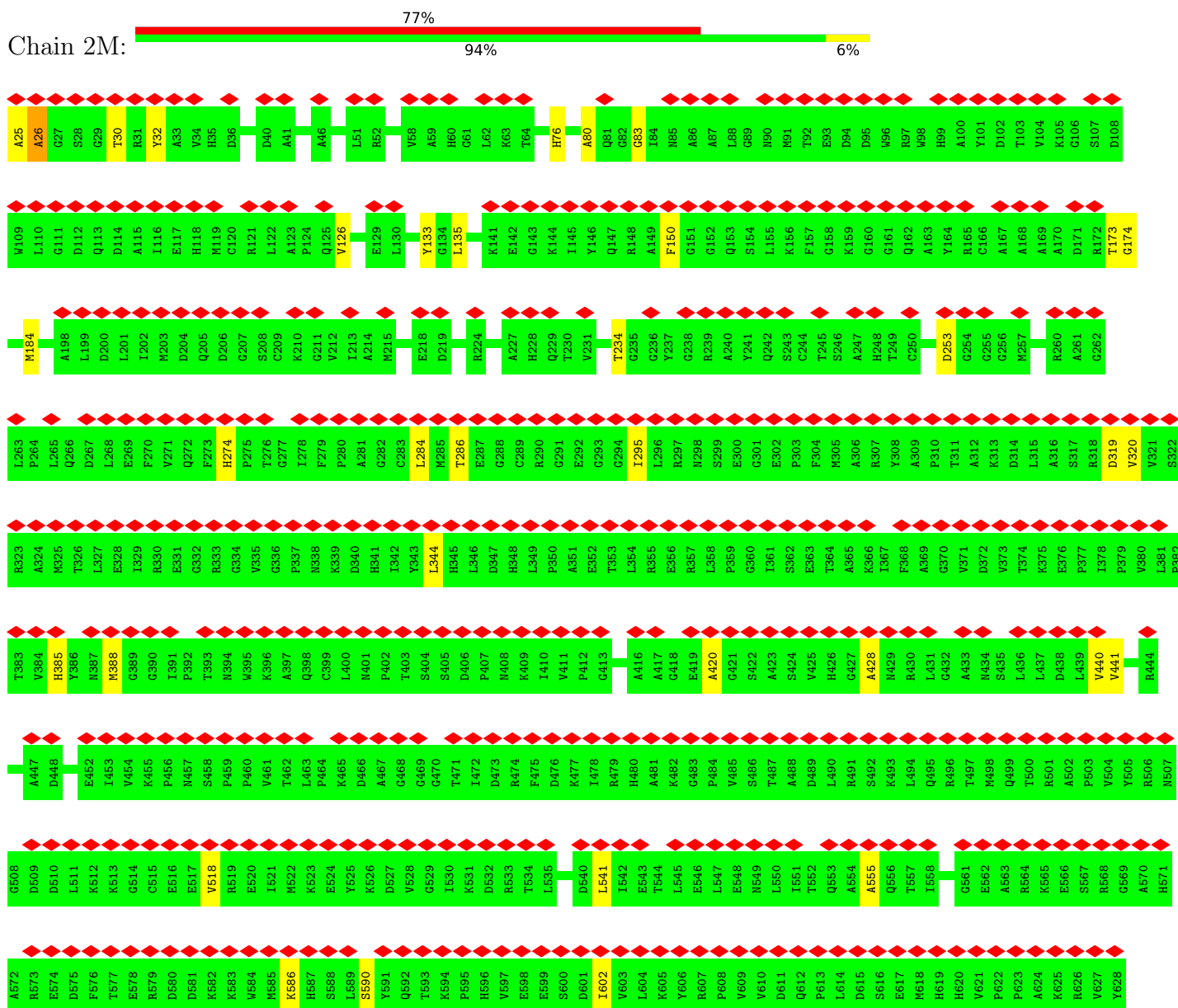
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	4T	2	Total	Zn	0
			2	2	
68	4X	1	Total	Zn	0
			1	1	
68	4t	2	Total	Zn	0
			2	2	
68	4x	1	Total	Zn	0
			1	1	

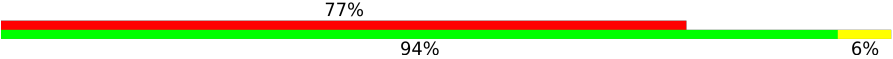
3 Residue-property plots

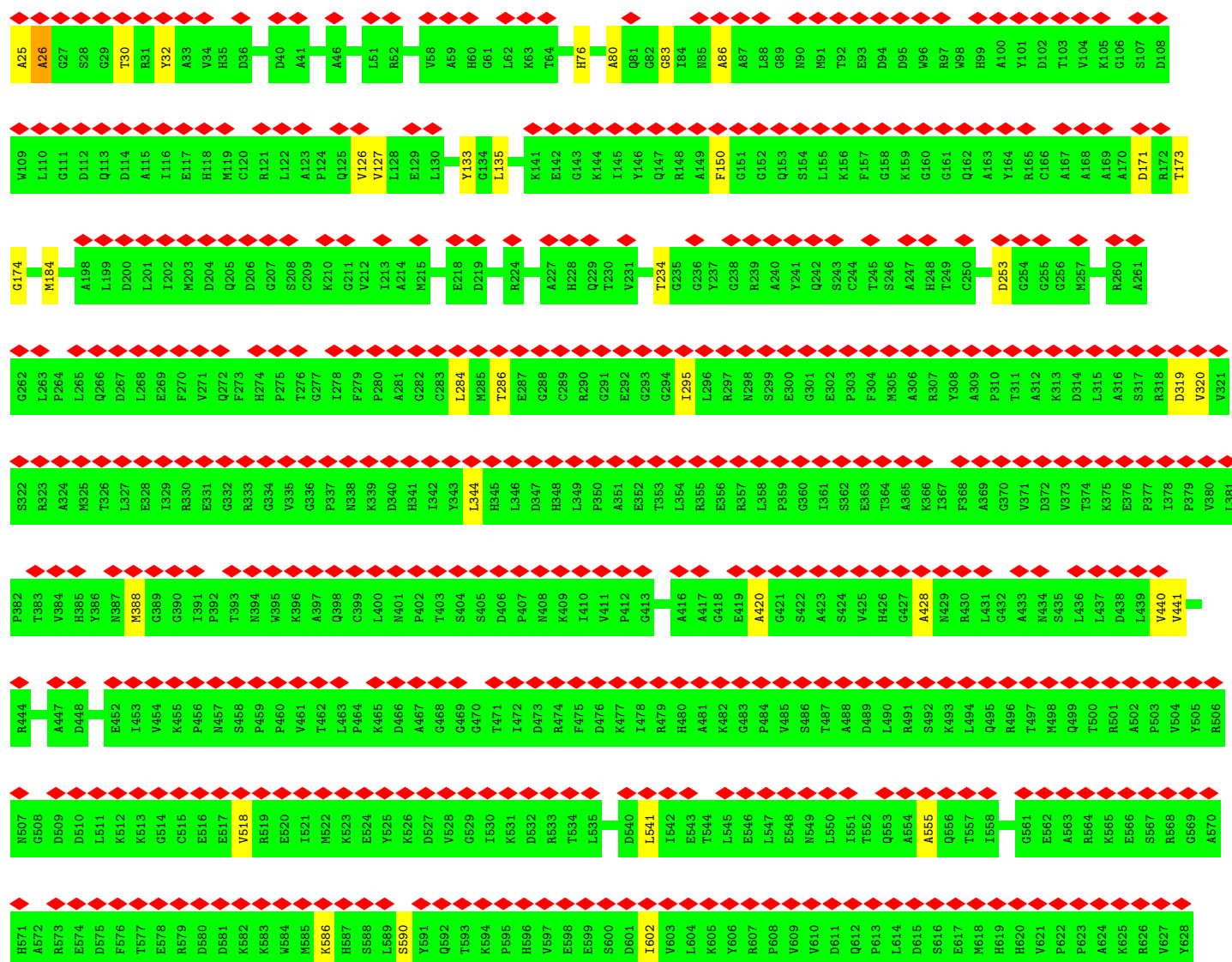
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

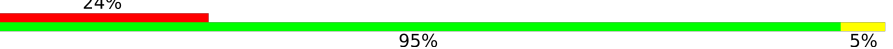


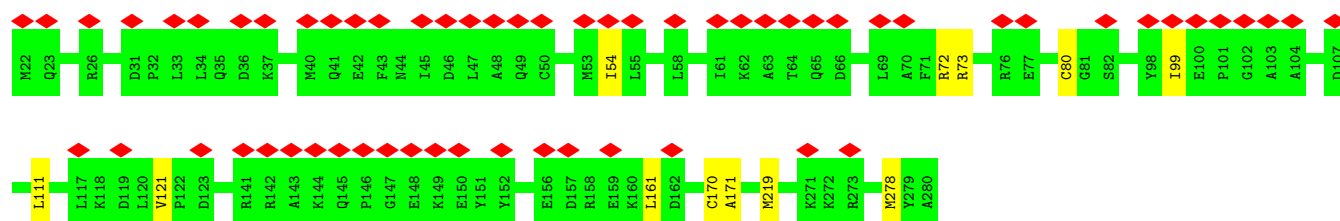
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain 2m: 

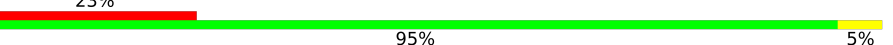


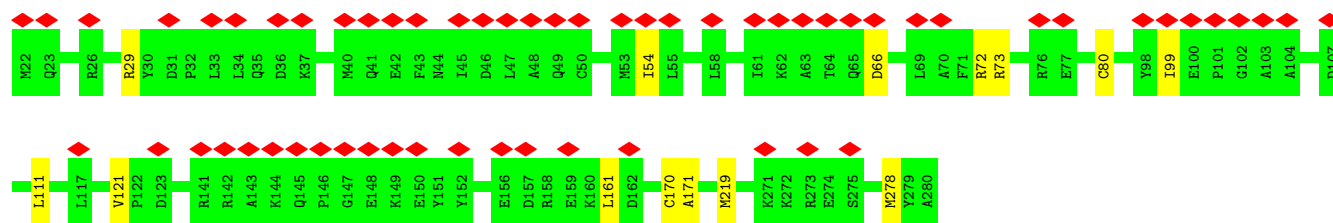
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain 2N: 



- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain 2n: 



- Molecule 3: SDHG



- Molecule 3: SDHG



- Molecule 4: Transmembrane protein



- Molecule 4: Transmembrane protein



- Molecule 5: Kinesin-like protein

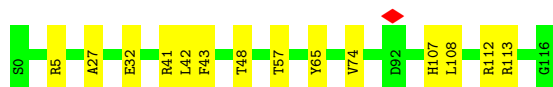
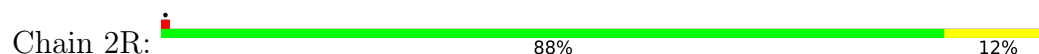


- Molecule 5: Kinesin-like protein





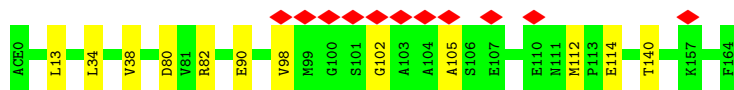
- Molecule 6: SDHH



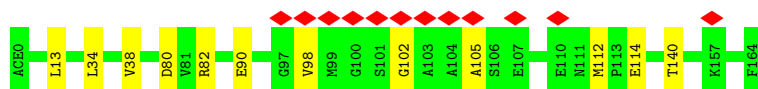
- Molecule 6: SDHH



- Molecule 7: DUF6827 domain-containing protein



- Molecule 7: DUF6827 domain-containing protein



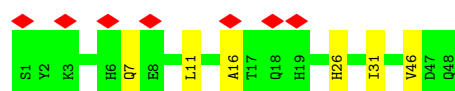
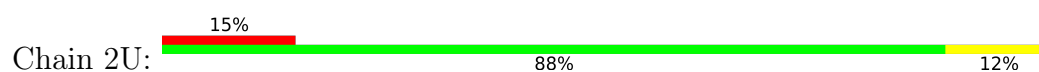
- Molecule 8: Rab-GAP TBC domain-containing protein



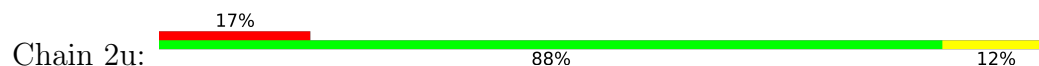
- Molecule 8: Rab-GAP TBC domain-containing protein



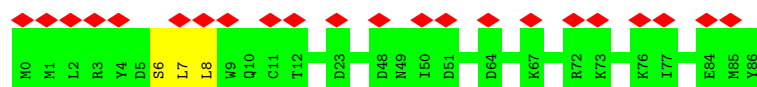
- Molecule 9: Syntaxin-1A



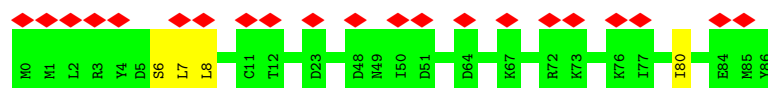
• Molecule 9: Syntaxin-1A



• Molecule 10: SDHI



• Molecule 10: SDHI



• Molecule 11: Mitochondrial processing peptidase beta subunit



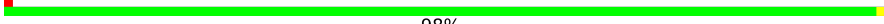
• Molecule 11: Mitochondrial processing peptidase beta subunit



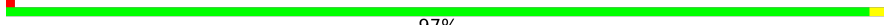
• Molecule 12: Alpha-MPP



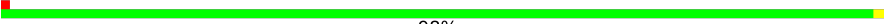
• Molecule 12: Alpha-MPP

Chain 3b:  98%

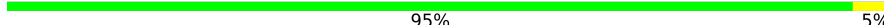
• Molecule 13: Iso-1-cytochrome c

Chain 3C:  97%

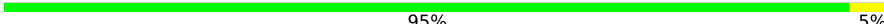
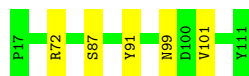
• Molecule 13: Iso-1-cytochrome c

Chain 3c:  98%

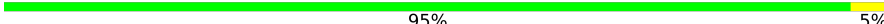
• Molecule 14: QCR8

Chain 3D:  95%

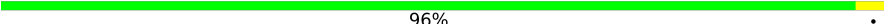
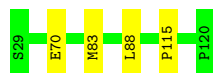
• Molecule 14: QCR8

Chain 3d:  95%

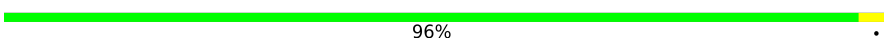
• Molecule 15: QCR9

Chain 3E:  95%

• Molecule 15: QCR9

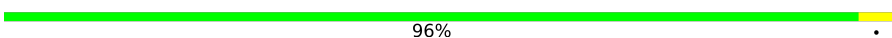
Chain 3e:  96%

- Molecule 16: QCR10

Chain 3F:  96%

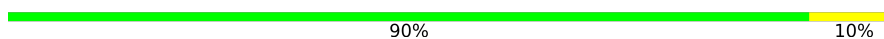


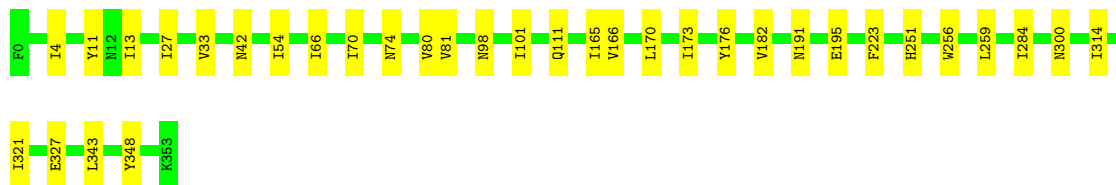
- Molecule 16: QCR10

Chain 3f:  96%



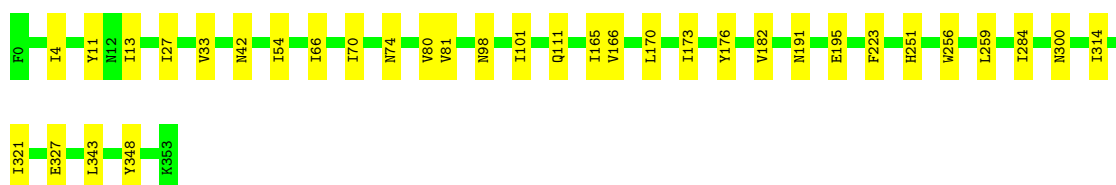
- Molecule 17: Cytochrome b

Chain 3G:  90% 10%

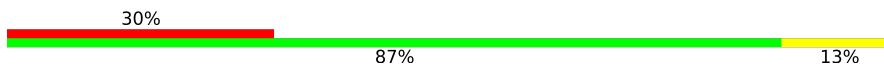


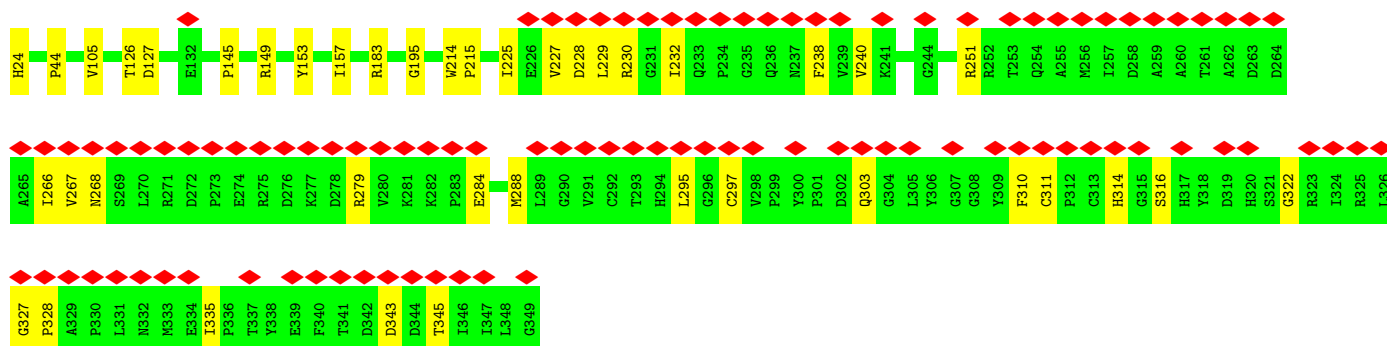
- Molecule 17: Cytochrome b

Chain 3g:  90% 10%

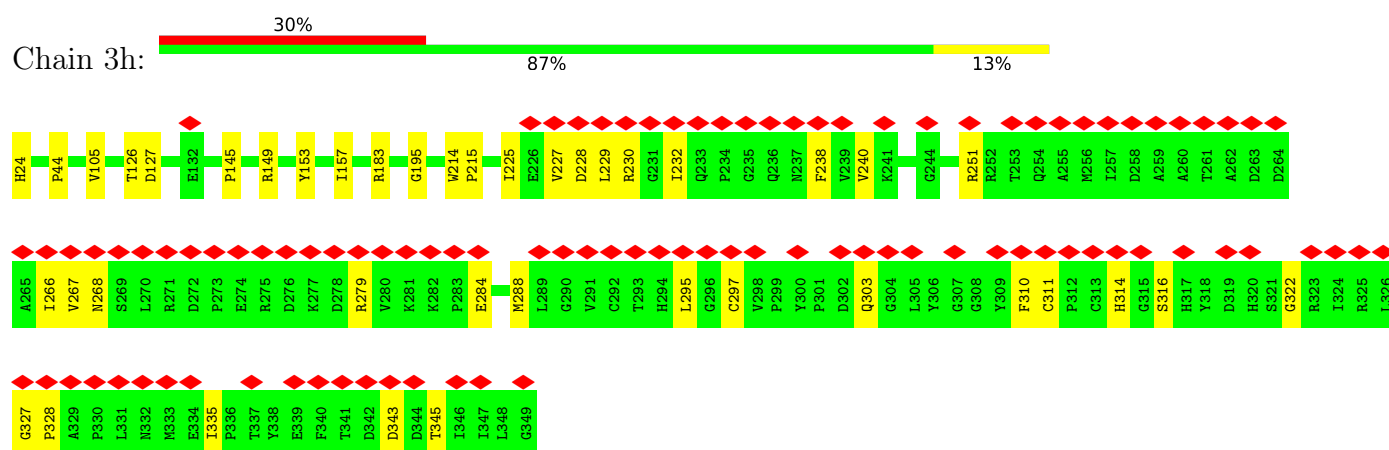


- Molecule 18: Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative

Chain 3H:  30% 87% 13%



- Molecule 18: Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative



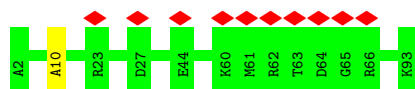
- Molecule 19: Ubiquinol-cytochrome C reductase complex 14kD subunit, putative



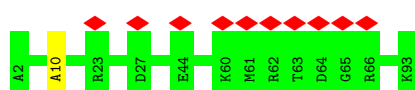
- Molecule 19: Ubiquinol-cytochrome C reductase complex 14kD subunit, putative



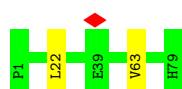
- Molecule 20: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative



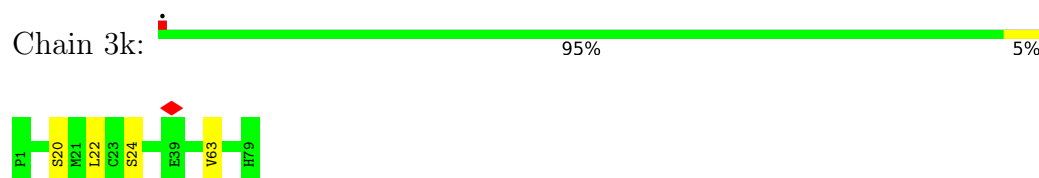
- Molecule 20: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative



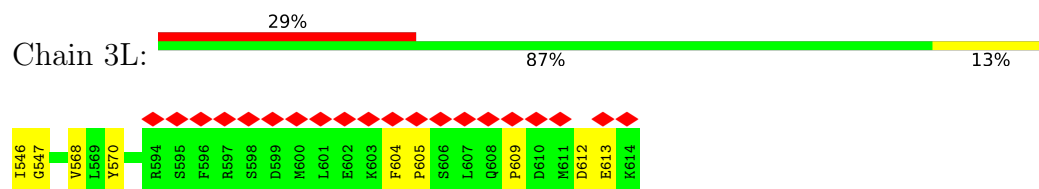
- Molecule 21: Cu-binding protein



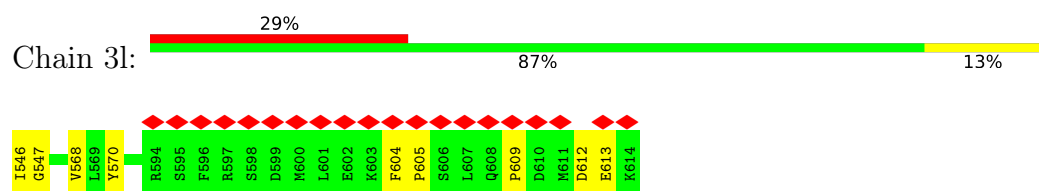
- Molecule 21: Cu-binding protein



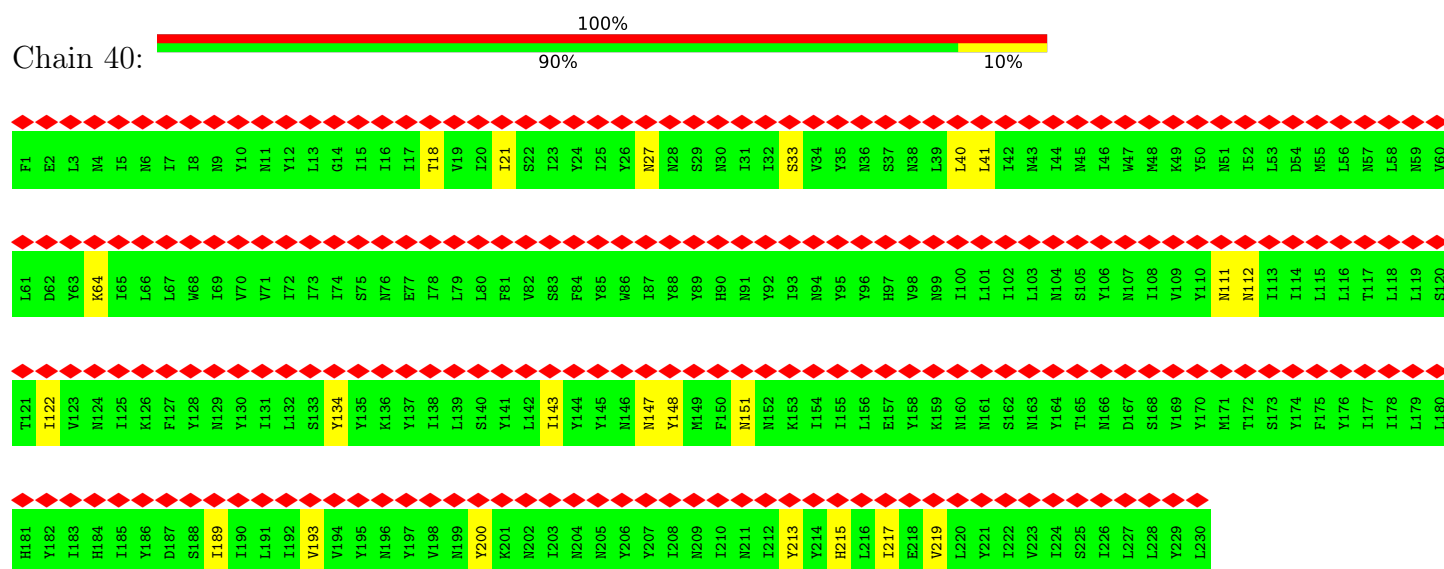
- Molecule 22: Aurora kinase



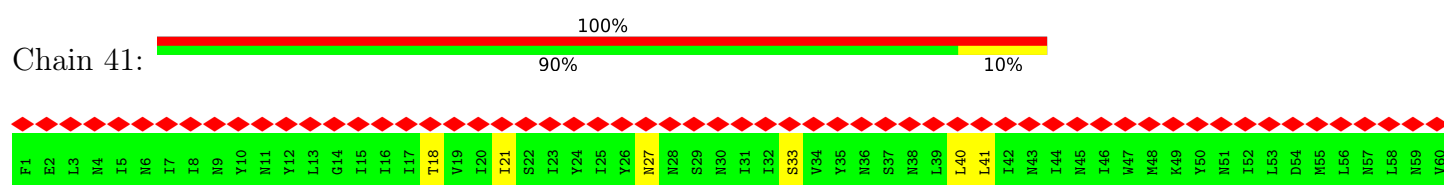
- Molecule 22: Aurora kinase

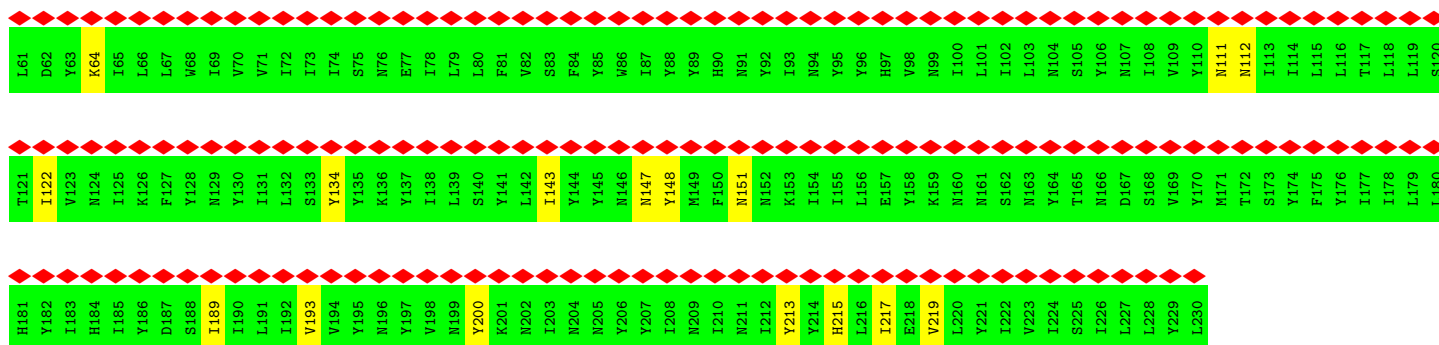


- Molecule 23: Cytochrome c oxidase subunit 3

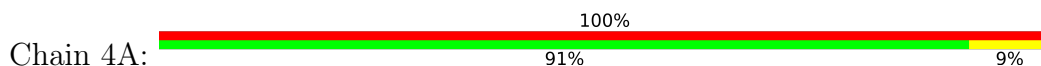


- Molecule 23: Cytochrome c oxidase subunit 3

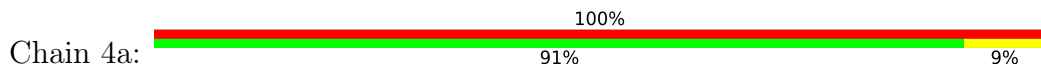




• Molecule 24: Cytochrome c oxidase subunit 6B



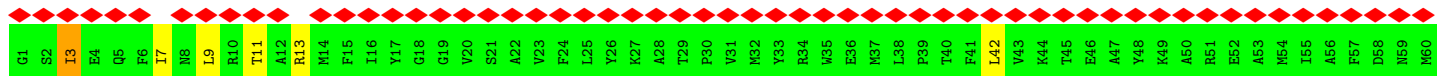
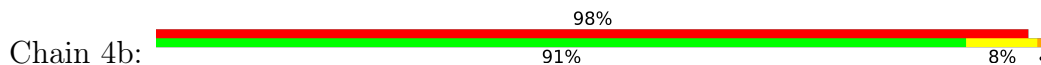
• Molecule 24: Cytochrome c oxidase subunit 6B

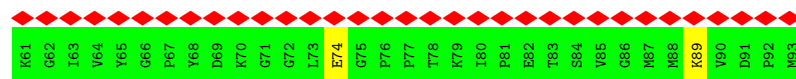


• Molecule 25: Peptidase M14 carboxypeptidase A domain-containing protein

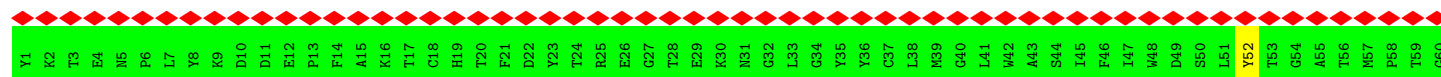


• Molecule 25: Peptidase M14 carboxypeptidase A domain-containing protein

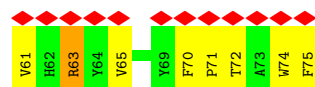
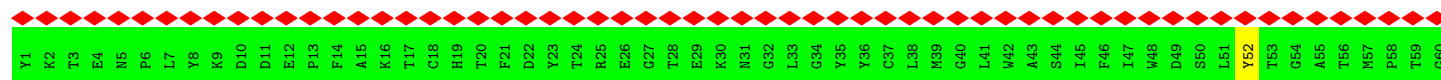
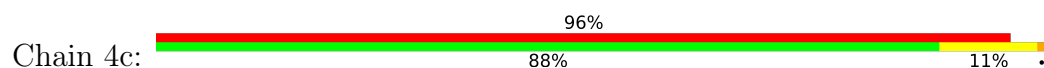




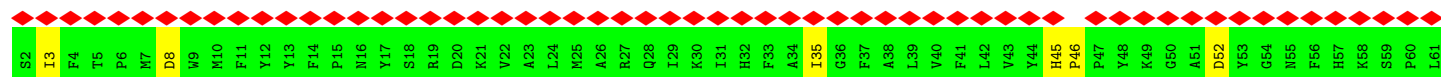
• Molecule 26: Cytochrome c oxidase subunit 40



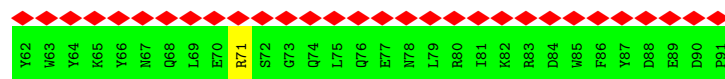
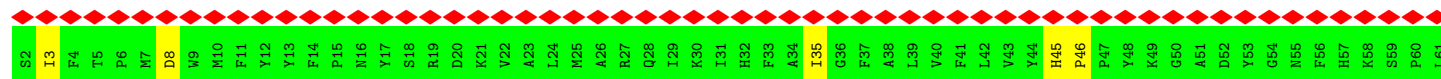
• Molecule 26: Cytochrome c oxidase subunit 40



• Molecule 27: Cytochrome c oxidase subunit 34

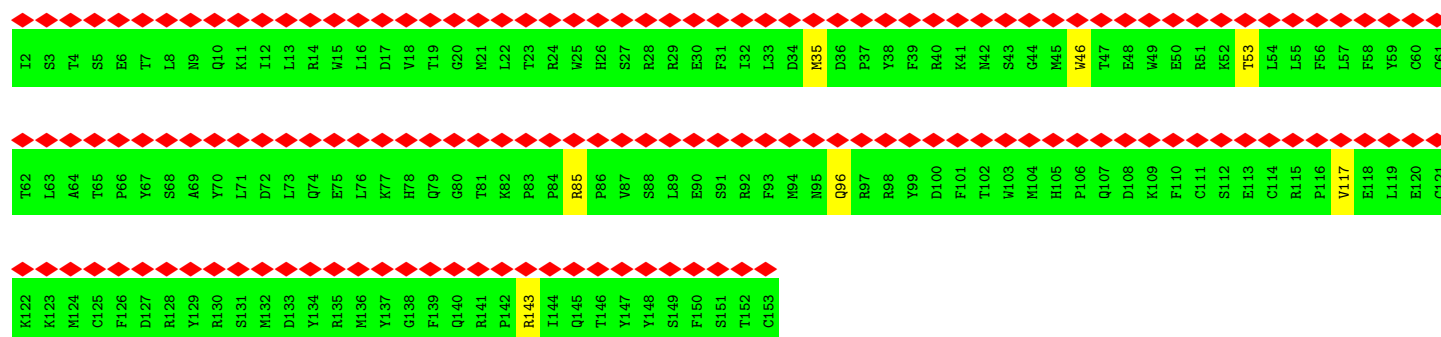


• Molecule 27: Cytochrome c oxidase subunit 34

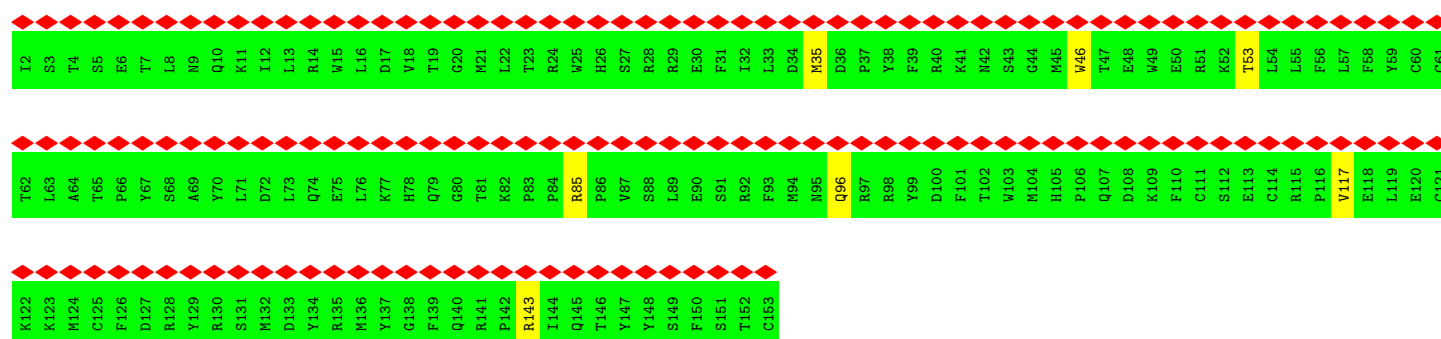


• Molecule 28: Merozoite surface protein, putative

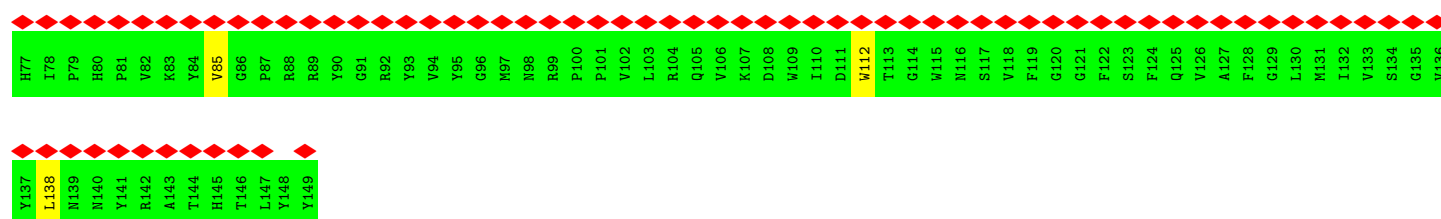




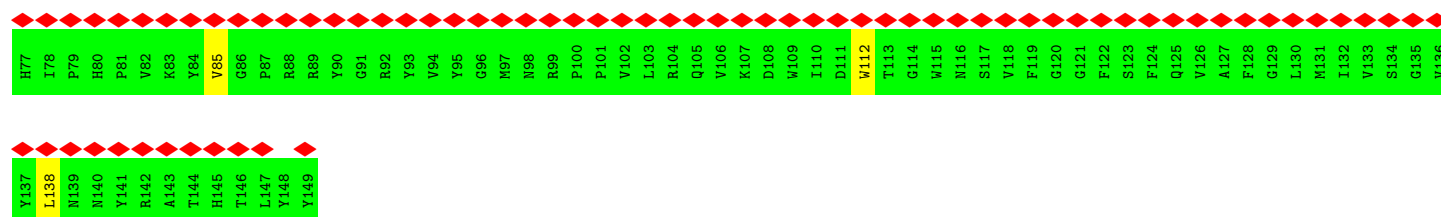
• Molecule 28: Merozoite surface protein, putative



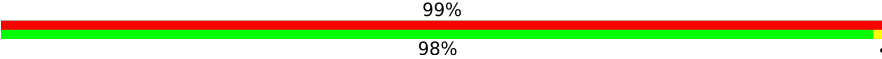
• Molecule 29: Ubiquitin, putative



• Molecule 29: Ubiquitin, putative

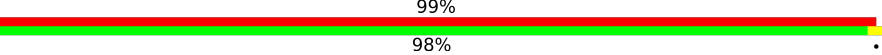


• Molecule 30: Cytochrome c oxidase subunit 33

Chain 4G: 

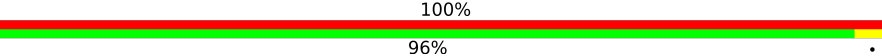


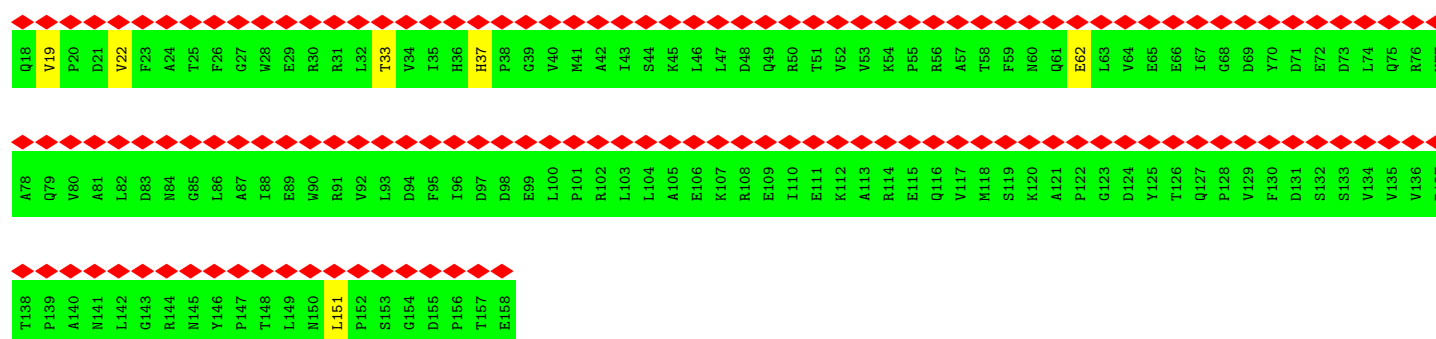
• Molecule 30: Cytochrome c oxidase subunit 33

Chain 4g: 



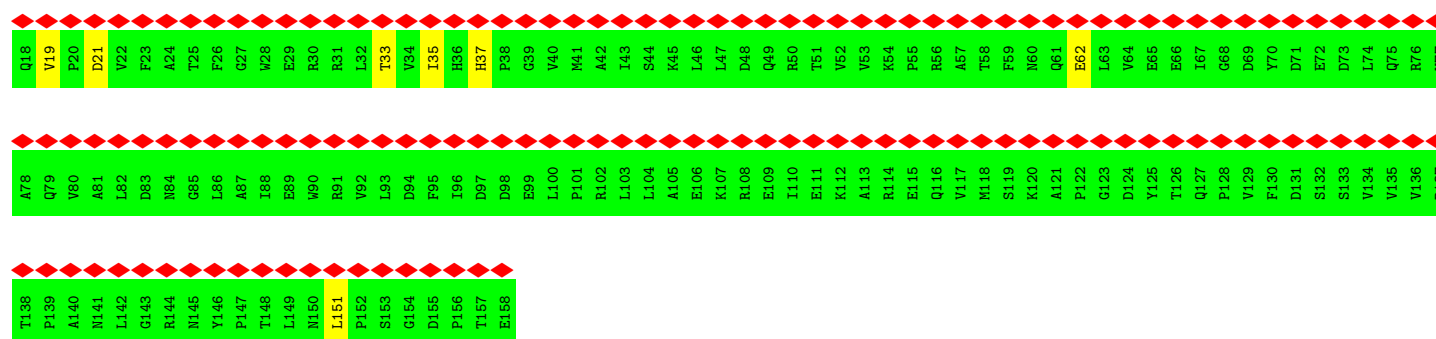
• Molecule 31: Cytochrome c oxidase subunit 30

Chain 4H: 

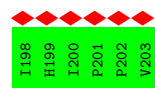


• Molecule 31: Cytochrome c oxidase subunit 30

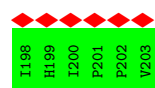
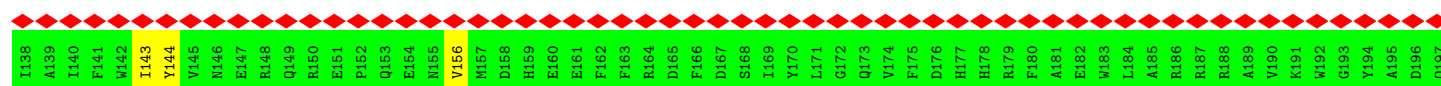
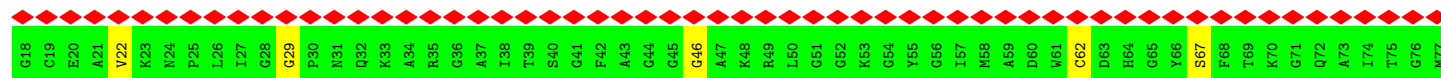
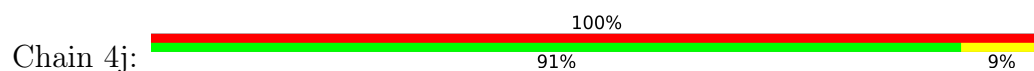
Chain 4h: 



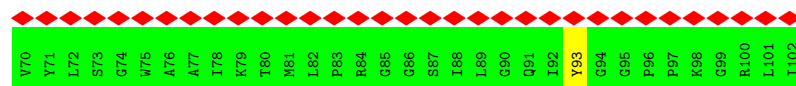
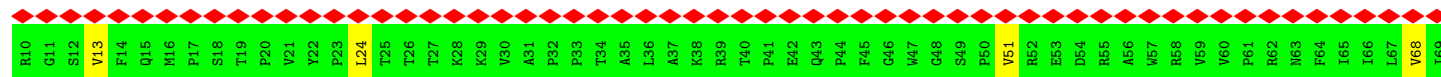
• Molecule 32: Cytochrome c oxidase subunit 6C



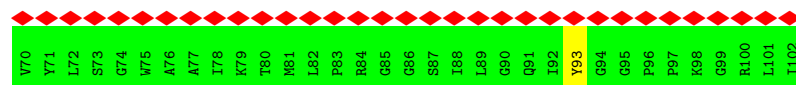
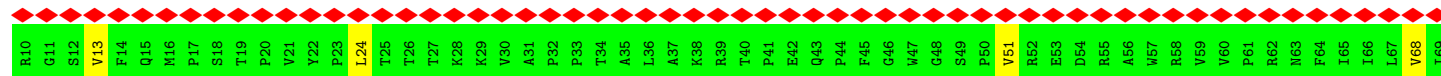
• Molecule 33: Cytochrome c oxidase subunit 24



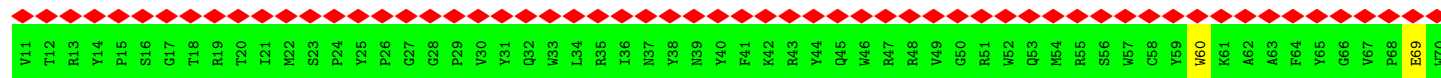
• Molecule 34: Cytochrome c oxidase subunit 37



• Molecule 34: Cytochrome c oxidase subunit 37



• Molecule 35: Cytochrome c oxidase subunit 7A





• Molecule 35: Cytochrome c oxidase subunit 7A



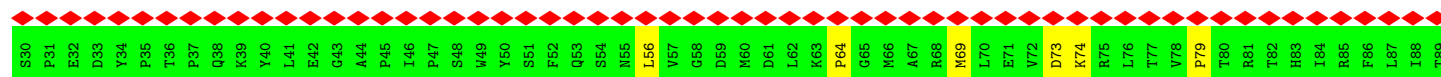
• Molecule 36: Cytochrome c oxidase subunit 35

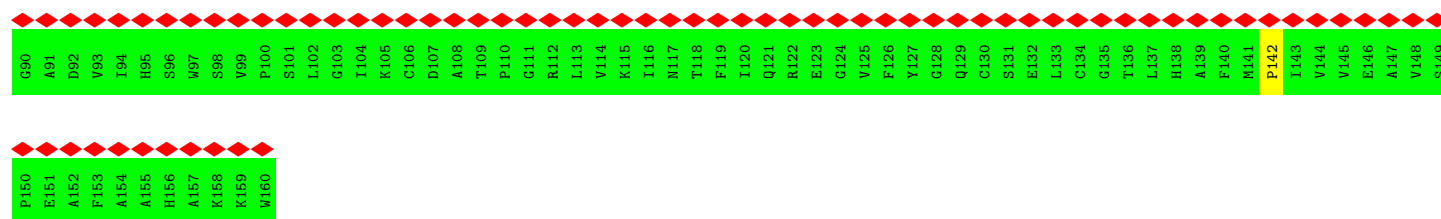


• Molecule 36: Cytochrome c oxidase subunit 35

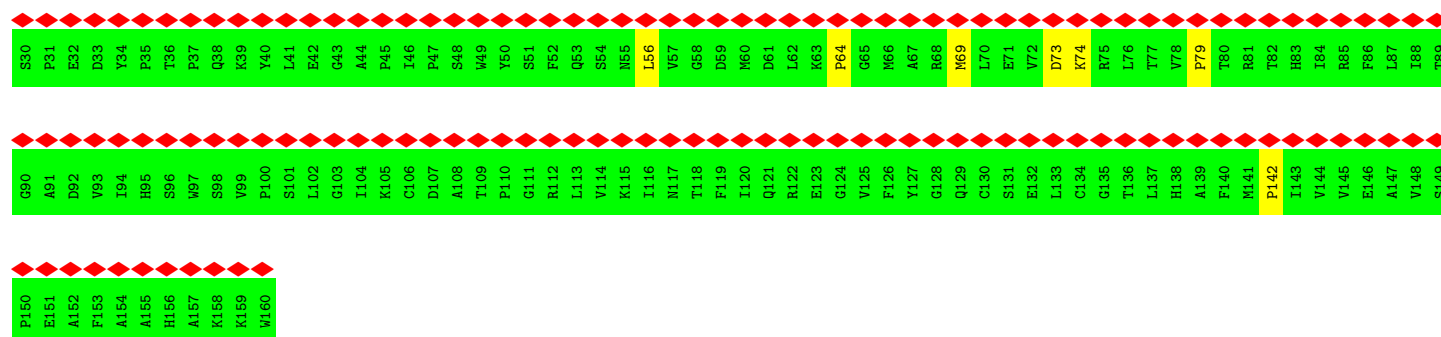


• Molecule 37: Cytochrome c oxidase polypeptide II

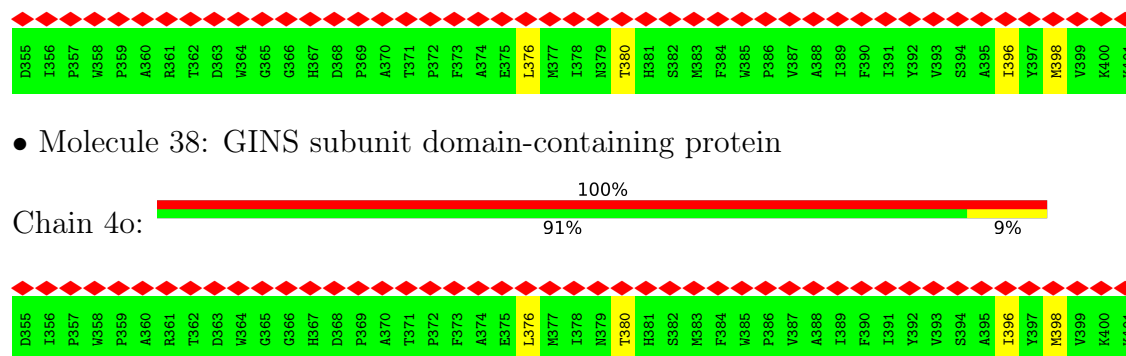




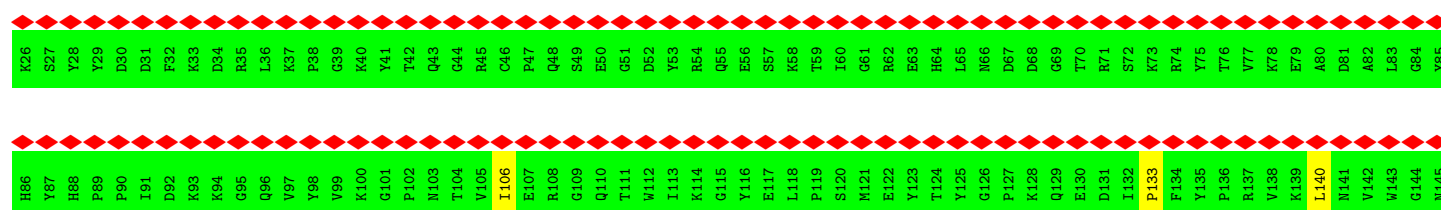
• Molecule 37: Cytochrome c oxidase polypeptide II



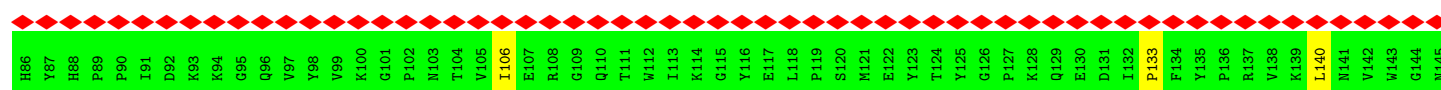
• Molecule 38: GINS subunit domain-containing protein



• Molecule 38: GINS subunit domain-containing protein

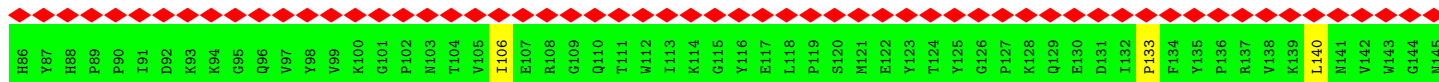


• Molecule 39: Cytochrome c oxidase subunit 2A

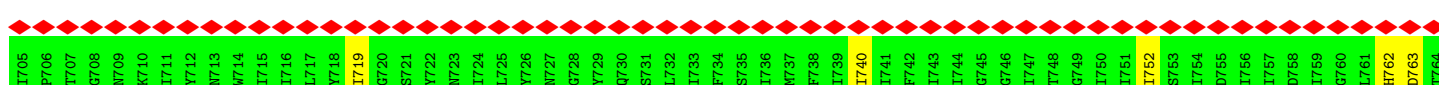
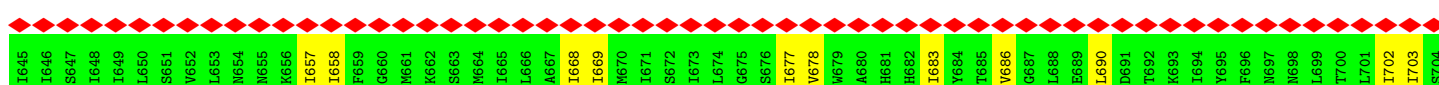
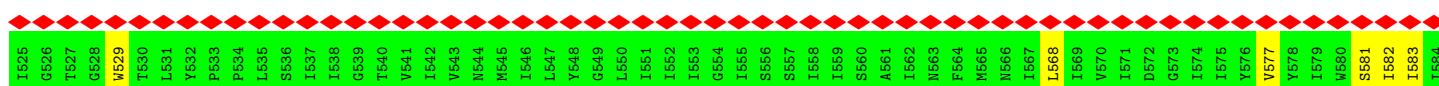
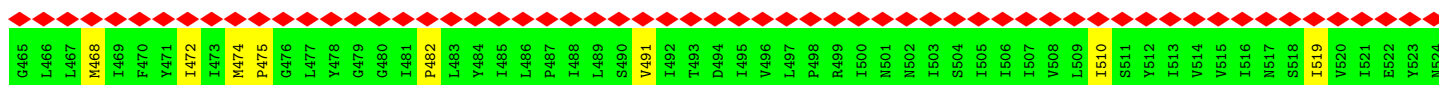
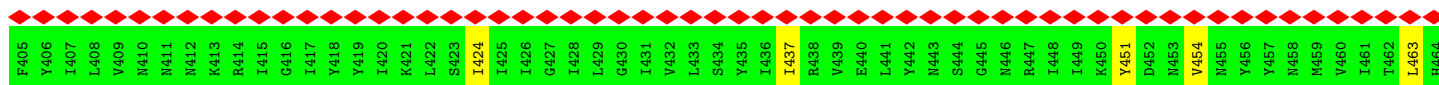
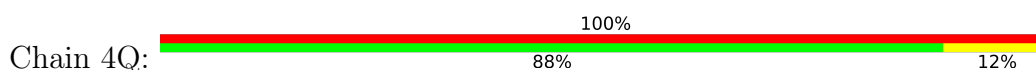


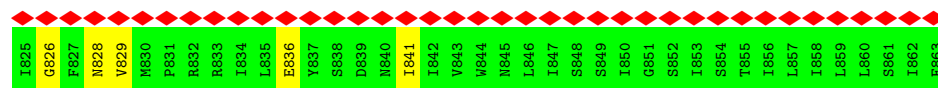


• Molecule 39: Cytochrome c oxidase subunit 2A

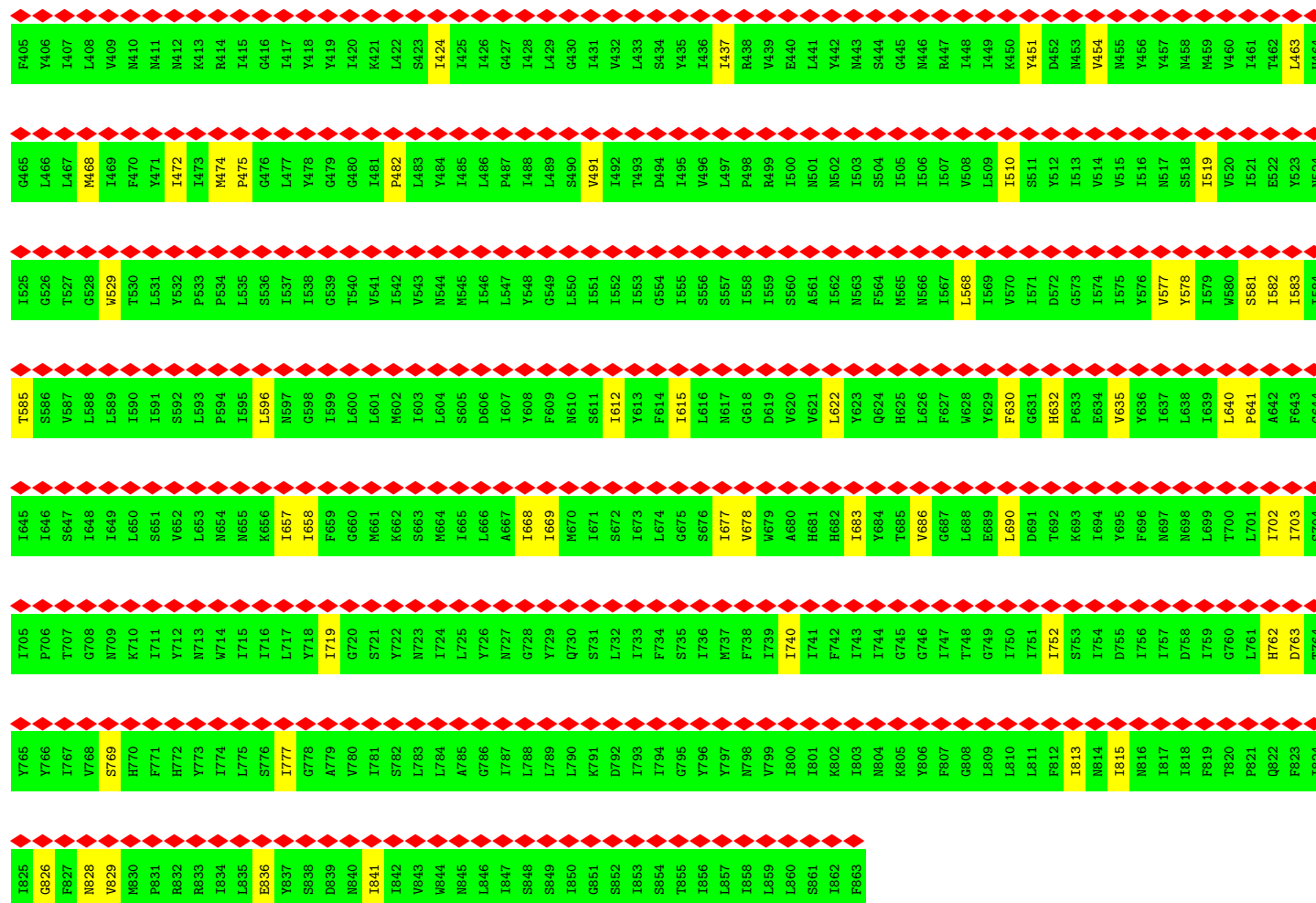
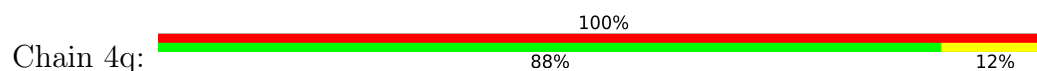


• Molecule 40: Cytochrome c oxidase subunit 1





• Molecule 40: Cytochrome c oxidase subunit 1



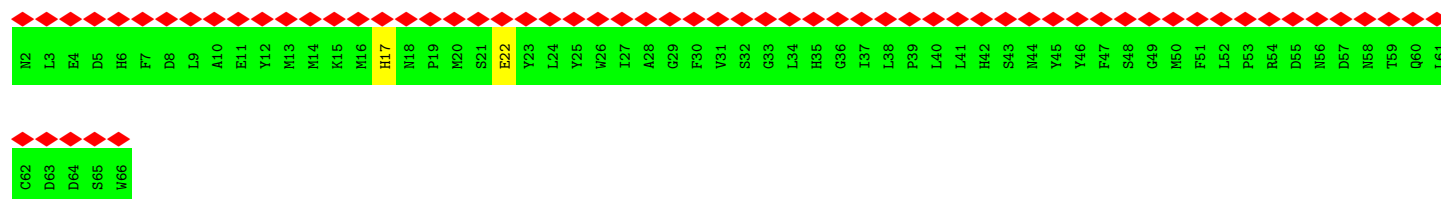
• Molecule 41: Cytochrome c oxidase subunit 32



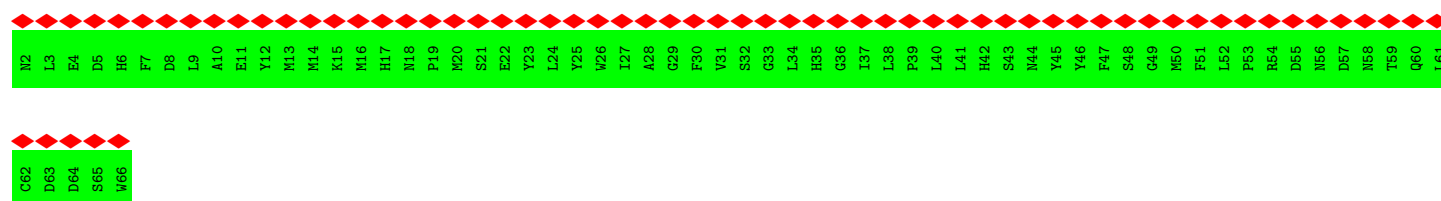
• Molecule 41: Cytochrome c oxidase subunit 32



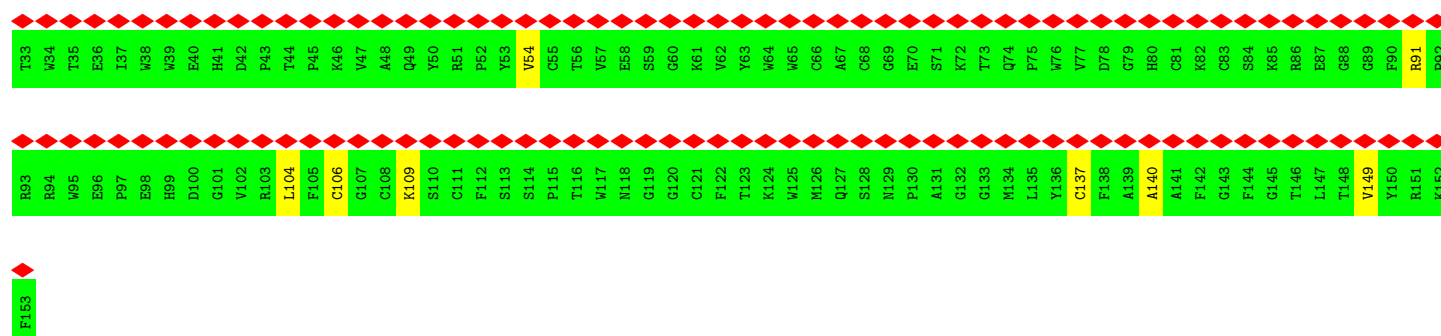
• Molecule 42: Cytochrome c oxidase subunit 7C



• Molecule 42: Cytochrome c oxidase subunit 7C

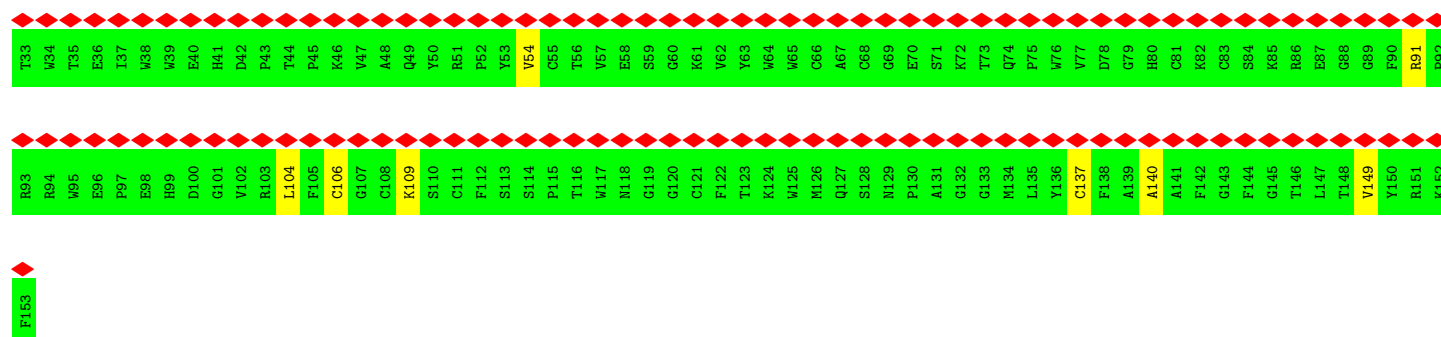


• Molecule 43: Cytochrome c oxidase subunit 13

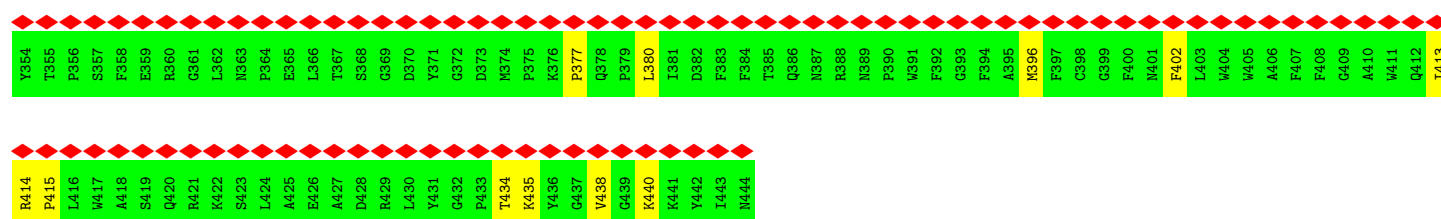
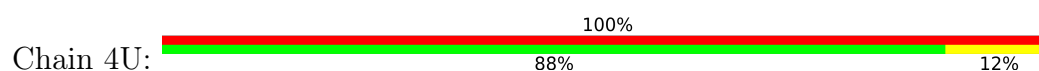


• Molecule 43: Cytochrome c oxidase subunit 13

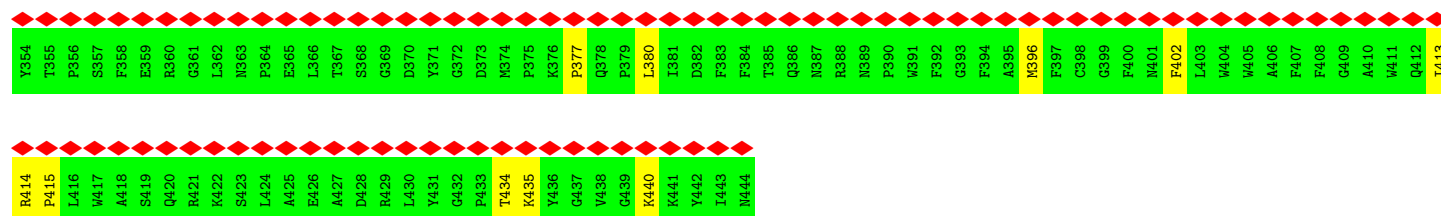
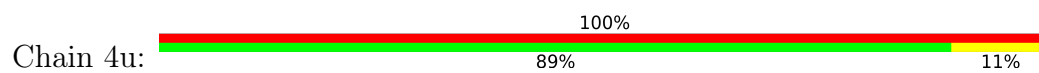




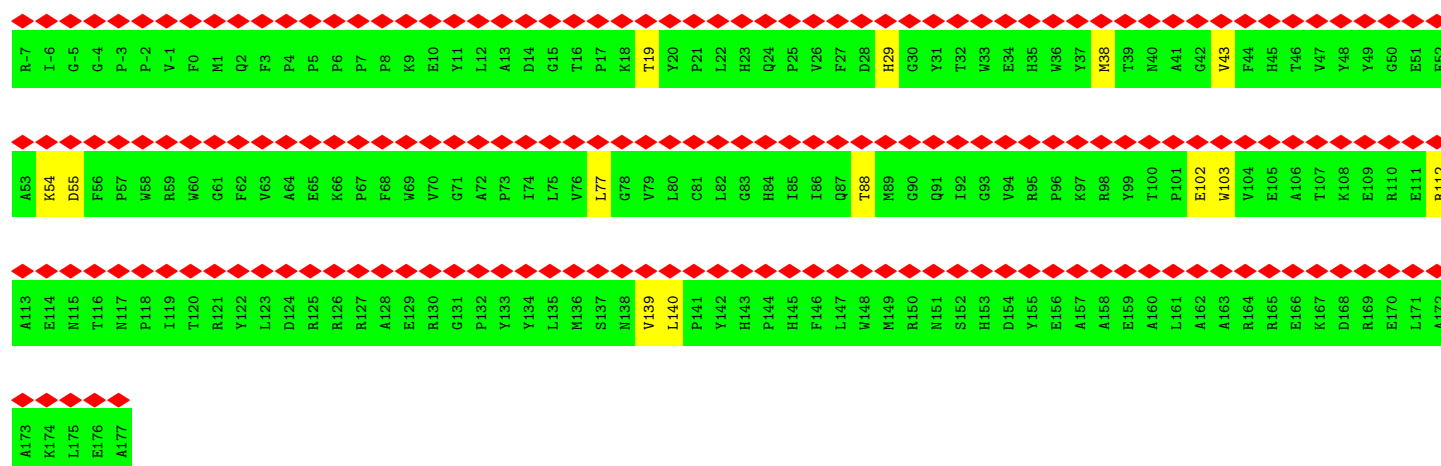
• Molecule 44: Amino acid transporter transmembrane domain-containing protein



• Molecule 44: Amino acid transporter transmembrane domain-containing protein

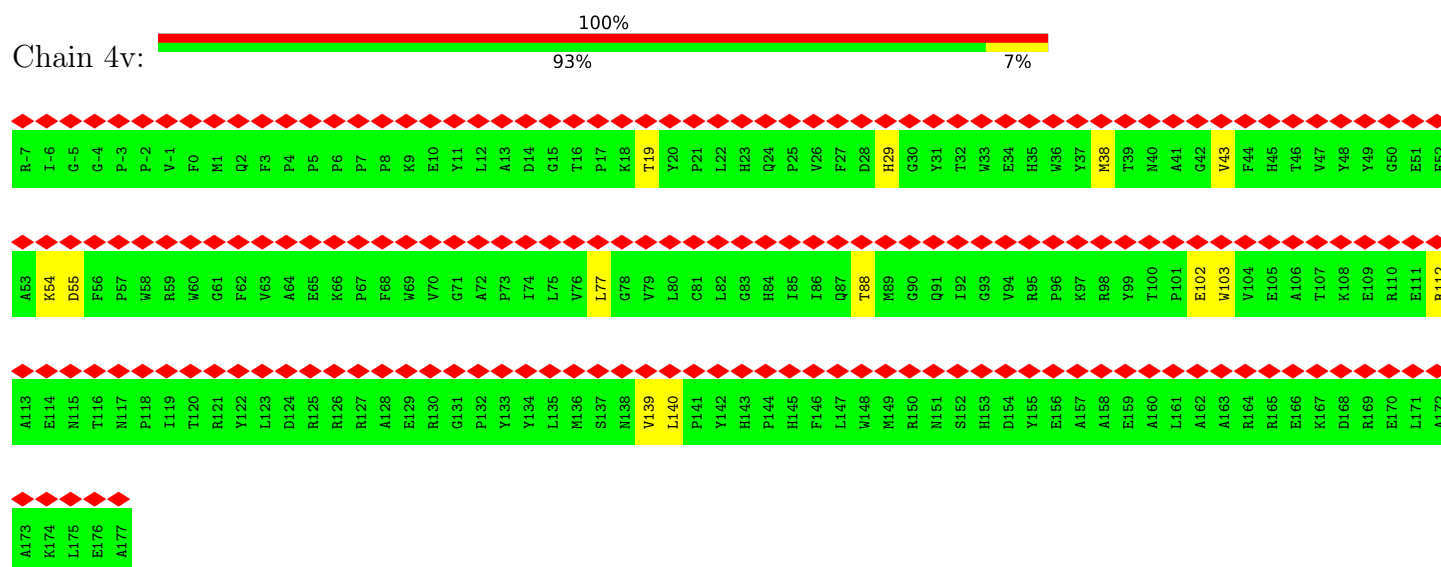


• Molecule 45: Cytochrome c oxidase subunit 4



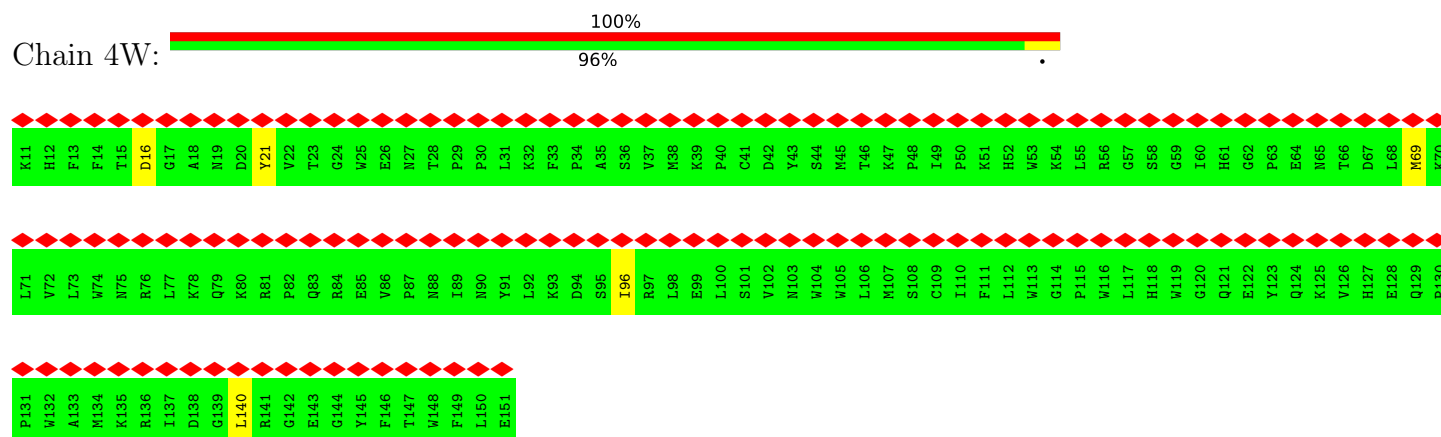
- Molecule 45: Cytochrome c oxidase subunit 4

Chain 4v:



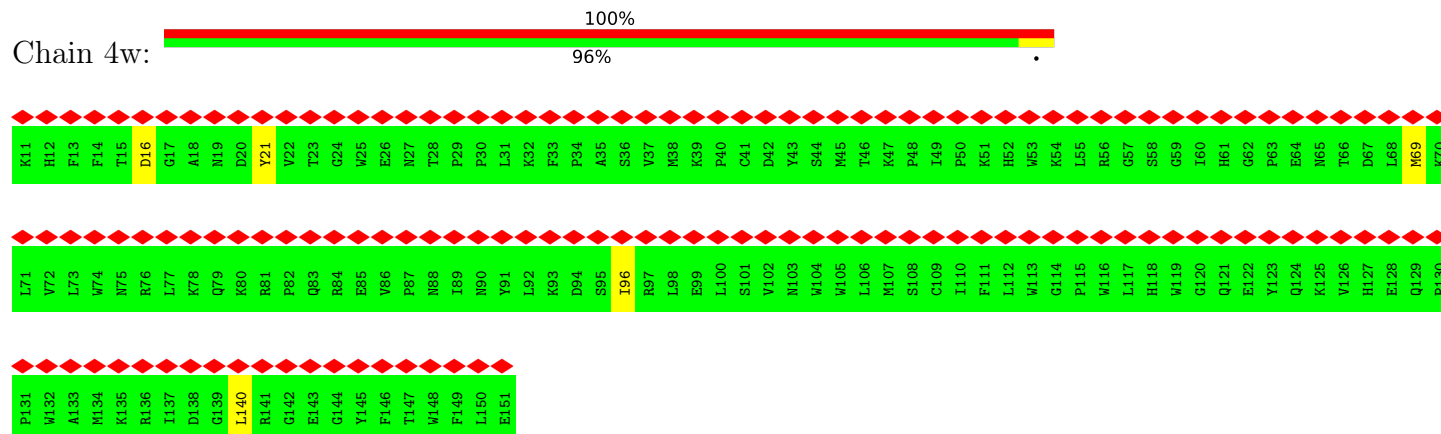
- Molecule 46: Cytochrome c oxidase subunit 19

Chain 4W:



- Molecule 46: Cytochrome c oxidase subunit 19

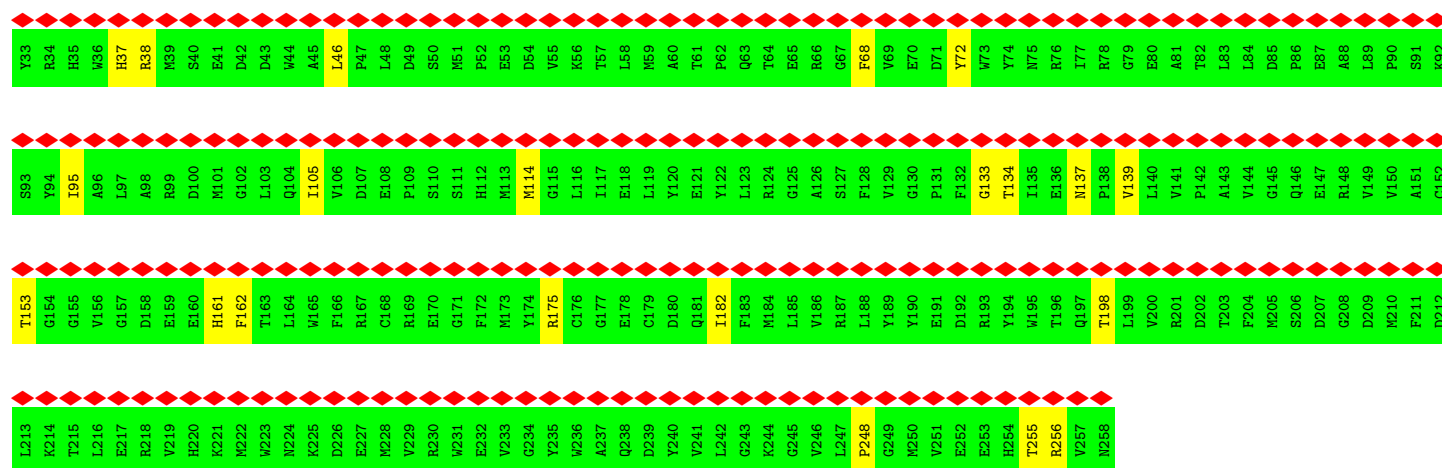
Chain 4w:



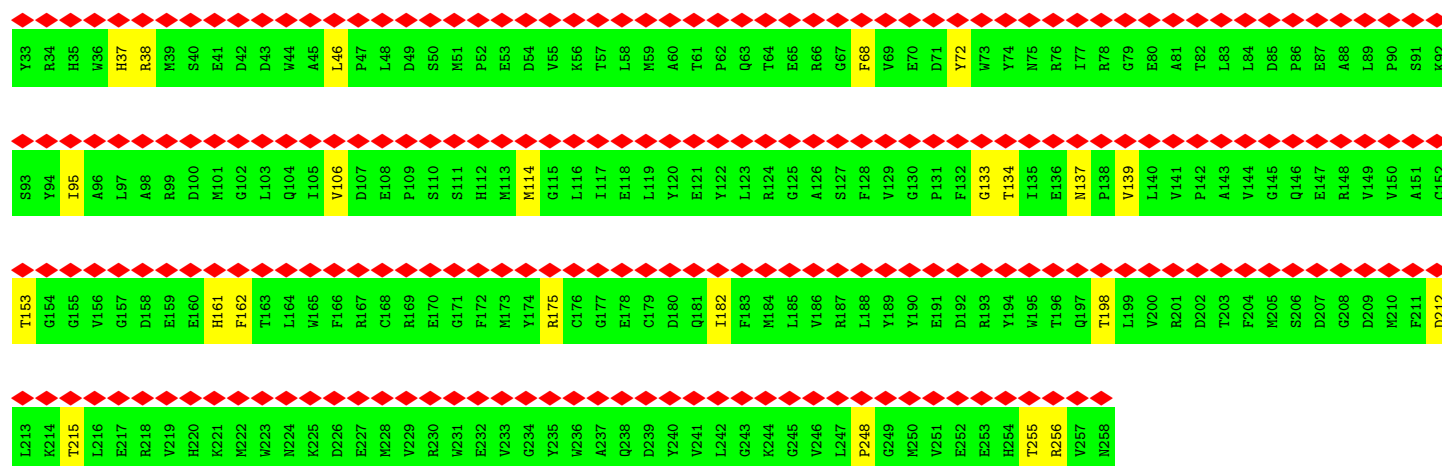
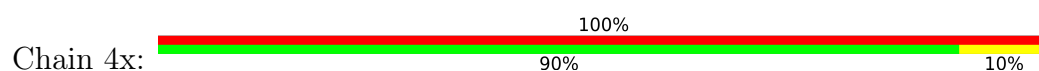
- Molecule 47: Cytochrome Coxidase subunit, putative

Chain 4X:



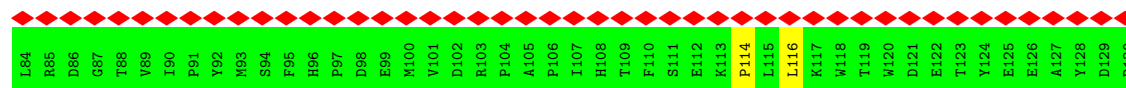


- Molecule 47: Cytochrome Coxidase subunit, putative

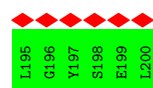
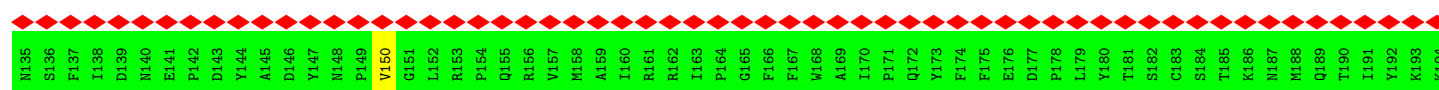
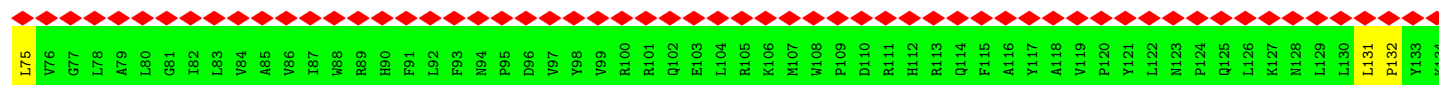
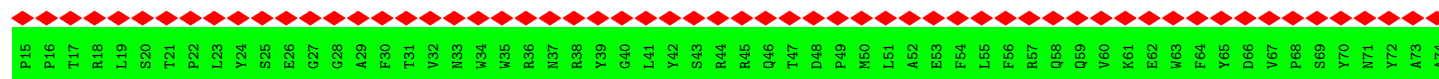


- Molecule 48: Cytochrome c oxidase subunit 18

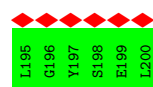
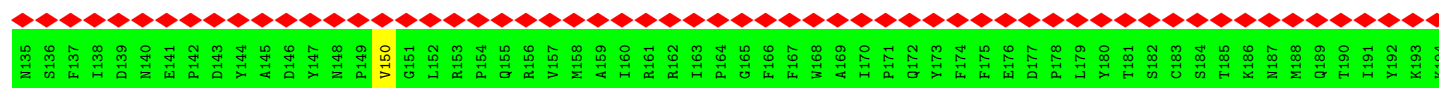




• Molecule 49: Cytochrome c oxidase subunit 31



• Molecule 49: Cytochrome c oxidase subunit 31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296890	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0203	Depositor
Map size ($\text{\AA}$)	423.2, 423.2, 423.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, UQ8, HEM, AJP, F3S, CDL, PER, HEA, K, ACE, HEC, MG, PEE, PC1, FAD, SF4, CU, ZN, CUA, FES

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	2M	0.16	0/4709	0.29	0/6372
1	2m	0.16	0/4709	0.29	0/6372
2	2N	0.20	0/2118	0.27	0/2863
2	2n	0.20	0/2118	0.27	0/2863
3	2O	0.24	0/1292	0.25	0/1759
3	2o	0.24	0/1292	0.25	0/1759
4	2P	0.23	0/1342	0.25	0/1812
4	2p	0.23	0/1342	0.25	0/1812
5	2Q	0.22	0/580	0.31	0/788
5	2q	0.22	0/580	0.31	0/788
6	2R	0.25	0/985	0.26	0/1336
6	2r	0.25	0/985	0.26	0/1336
7	2S	0.24	0/1350	0.23	0/1828
7	2s	0.24	0/1350	0.23	0/1828
8	2T	0.27	0/714	0.24	0/971
8	2t	0.27	0/714	0.24	0/971
9	2U	0.23	0/400	0.22	0/547
9	2u	0.23	0/400	0.22	0/547
10	2V	0.19	0/724	0.21	0/975
10	2v	0.19	0/724	0.21	0/975
11	3A	0.25	0/3701	0.32	0/5025
11	3a	0.25	0/3701	0.32	0/5025
12	3B	0.26	0/3967	0.26	0/5371
12	3b	0.26	0/3967	0.26	0/5371
13	3C	0.39	0/1988	0.44	0/2712
13	3c	0.39	0/1988	0.44	0/2712
14	3D	0.30	0/872	0.28	0/1182
14	3d	0.30	0/872	0.28	0/1182
15	3E	0.31	0/848	0.25	0/1148
15	3e	0.31	0/848	0.25	0/1148
16	3F	0.31	0/767	0.30	0/1042

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	3f	0.31	0/767	0.30	0/1042
17	3G	0.31	0/3098	0.30	0/4231
17	3g	0.31	0/3098	0.30	0/4231
18	3H	0.22	0/2713	0.32	0/3693
18	3h	0.22	0/2713	0.32	0/3693
19	3I	0.28	0/1514	0.33	0/2045
19	3i	0.28	0/1514	0.33	0/2045
20	3J	0.20	0/776	0.29	0/1045
20	3j	0.20	0/776	0.29	0/1045
21	3K	0.23	0/627	0.28	0/847
21	3k	0.23	0/627	0.28	0/847
22	3L	0.26	0/521	0.50	2/713 (0.3%)
22	3l	0.26	0/521	0.50	2/713 (0.3%)
23	40	0.20	0/2060	0.27	0/2822
23	41	0.20	0/2060	0.27	0/2822
24	4A	0.18	0/863	0.25	0/1166
24	4a	0.18	0/863	0.25	0/1166
25	4B	0.20	0/751	0.31	0/1013
25	4b	0.20	0/751	0.31	0/1013
26	4C	0.18	0/653	0.31	0/891
26	4c	0.18	0/653	0.31	0/891
27	4D	0.19	0/819	0.24	0/1110
27	4d	0.19	0/819	0.23	0/1110
28	4E	0.20	0/1353	0.27	0/1824
28	4e	0.20	0/1353	0.27	0/1824
29	4F	0.18	0/638	0.26	0/870
29	4f	0.18	0/638	0.26	0/870
30	4G	0.18	0/883	0.22	0/1199
30	4g	0.18	0/883	0.22	0/1199
31	4H	0.18	0/1149	0.22	0/1565
31	4h	0.18	0/1149	0.22	0/1565
32	4I	0.21	0/1757	0.24	0/2386
32	4i	0.21	0/1757	0.24	0/2386
33	4J	0.20	0/1573	0.24	0/2131
33	4j	0.20	0/1573	0.24	0/2131
34	4K	0.17	0/745	0.22	0/1017
34	4k	0.17	0/745	0.22	0/1017
35	4L	0.21	0/1131	0.26	0/1537
35	4l	0.21	0/1131	0.26	0/1537
36	4M	0.18	0/800	0.22	0/1097
36	4m	0.18	0/800	0.22	0/1097
37	4N	0.19	0/1055	0.27	0/1436
37	4n	0.19	0/1055	0.27	0/1436

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	4O	0.20	0/400	0.24	0/549
38	4o	0.20	0/400	0.24	0/549
39	4P	0.19	0/1551	0.25	0/2106
39	4p	0.19	0/1551	0.25	0/2106
40	4Q	0.19	0/3774	0.30	0/5155
40	4q	0.19	0/3774	0.30	0/5155
41	4R	0.18	0/958	0.20	0/1301
41	4r	0.18	0/958	0.20	0/1301
42	4S	0.18	0/560	0.23	0/760
42	4s	0.18	0/560	0.23	0/760
43	4T	0.20	0/1024	0.27	0/1391
43	4t	0.20	0/1024	0.27	0/1391
44	4U	0.16	0/790	0.31	0/1073
44	4u	0.16	0/790	0.31	0/1073
45	4V	0.19	0/1600	0.24	0/2183
45	4v	0.19	0/1600	0.24	0/2183
46	4W	0.19	0/1240	0.29	0/1686
46	4w	0.19	0/1240	0.29	0/1686
47	4X	0.19	0/1912	0.23	0/2592
47	4x	0.19	0/1912	0.23	0/2592
48	4Y	0.19	0/929	0.24	0/1261
48	4y	0.19	0/929	0.24	0/1261
49	4Z	0.22	0/1639	0.24	0/2233
49	4z	0.22	0/1639	0.24	0/2233
All	All	0.23	0/136426	0.28	4/185318 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2N	0	1
2	2n	0	1
4	2P	0	1
4	2p	0	1
6	2R	0	1
6	2r	0	1
11	3A	0	1
11	3a	0	1
13	3C	0	1
13	3c	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
18	3H	0	2
18	3h	0	2
26	4C	0	1
26	4c	0	1
28	4E	0	1
28	4e	0	1
All	All	0	18

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	609	PRO	N-CA-CB	7.75	110.20	103.31
22	3l	609	PRO	N-CA-CB	7.74	110.19	103.31
22	3L	605	PRO	N-CA-CB	6.97	109.94	103.46
22	3l	605	PRO	N-CA-CB	6.95	109.92	103.46

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2N	73	ARG	Sidechain
4	2P	41	ARG	Sidechain
6	2R	5	ARG	Sidechain
2	2n	73	ARG	Sidechain
4	2p	41	ARG	Sidechain
6	2r	5	ARG	Sidechain
11	3A	71	ARG	Sidechain
13	3C	180	ARG	Sidechain
18	3H	149	ARG	Sidechain
18	3H	183	ARG	Sidechain
11	3a	71	ARG	Sidechain
13	3c	180	ARG	Sidechain
18	3h	149	ARG	Sidechain
18	3h	183	ARG	Sidechain
26	4C	63	ARG	Sidechain
28	4E	143	ARG	Sidechain
26	4c	63	ARG	Sidechain
28	4e	143	ARG	Sidechain

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	2M	4610	0	4538	28	0
1	2m	4610	0	4538	29	0
2	2N	2068	0	2025	6	0
2	2n	2068	0	2025	7	0
3	2O	1254	0	1263	8	0
3	2o	1254	0	1263	7	0
4	2P	1309	0	1367	11	0
4	2p	1309	0	1367	11	0
5	2Q	564	0	567	6	0
5	2q	564	0	567	6	0
6	2R	950	0	935	12	0
6	2r	950	0	935	10	0
7	2S	1323	0	1261	9	0
7	2s	1323	0	1261	9	0
8	2T	695	0	672	9	0
8	2t	695	0	672	9	0
9	2U	390	0	369	7	0
9	2u	390	0	369	6	0
10	2V	709	0	723	3	0
10	2v	709	0	723	4	0
11	3A	3622	0	3508	8	0
11	3a	3622	0	3508	8	0
12	3B	3884	0	3842	10	0
12	3b	3884	0	3842	9	0
13	3C	1921	0	1816	8	0
13	3c	1921	0	1816	6	0
14	3D	836	0	798	5	0
14	3d	836	0	798	5	0
15	3E	813	0	776	5	0
15	3e	813	0	776	4	0
16	3F	734	0	704	2	0
16	3f	734	0	704	2	0
17	3G	3016	0	3162	28	0
17	3g	3016	0	3162	28	0
18	3H	2628	0	2541	26	0
18	3h	2628	0	2541	26	0
19	3I	1472	0	1436	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	3i	1472	0	1436	7	0
20	3J	755	0	693	1	0
20	3j	755	0	693	1	0
21	3K	608	0	617	2	0
21	3k	608	0	617	3	0
22	3L	509	0	475	5	0
22	3l	509	0	475	5	0
23	40	2004	0	2032	17	0
23	41	2004	0	2032	17	0
24	4A	841	0	766	9	0
24	4a	841	0	766	9	0
25	4B	732	0	746	6	0
25	4b	732	0	746	6	0
26	4C	626	0	575	10	0
26	4c	626	0	575	10	0
27	4D	787	0	745	6	0
27	4d	787	0	745	5	0
28	4E	1313	0	1269	7	0
28	4e	1313	0	1269	7	0
29	4F	613	0	591	3	0
29	4f	613	0	591	3	0
30	4G	854	0	811	1	0
30	4g	854	0	811	1	0
31	4H	1125	0	1112	6	0
31	4h	1125	0	1112	7	0
32	4I	1695	0	1593	7	0
32	4i	1695	0	1593	8	0
33	4J	1517	0	1435	10	0
33	4j	1517	0	1435	11	0
34	4K	722	0	760	5	0
34	4k	722	0	760	5	0
35	4L	1083	0	1027	5	0
35	4l	1083	0	1027	5	0
36	4M	773	0	797	7	0
36	4m	773	0	797	7	0
37	4N	1025	0	1018	6	0
37	4n	1025	0	1018	6	0
38	4O	383	0	368	3	0
38	4o	383	0	368	3	0
39	4P	1504	0	1461	8	0
39	4p	1504	0	1461	9	0
40	4Q	3687	0	3955	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	4q	3687	0	3955	42	0
41	4R	916	0	854	2	0
41	4r	916	0	854	3	0
42	4S	541	0	489	1	0
42	4s	541	0	489	0	0
43	4T	983	0	902	9	0
43	4t	983	0	902	9	0
44	4U	758	0	713	10	0
44	4u	758	0	713	9	0
45	4V	1539	0	1482	11	0
45	4v	1539	0	1482	11	0
46	4W	1193	0	1164	6	0
46	4w	1193	0	1164	6	0
47	4X	1860	0	1764	16	0
47	4x	1860	0	1764	17	0
48	4Y	905	0	835	5	0
48	4y	905	0	835	5	0
49	4Z	1582	0	1548	4	0
49	4z	1582	0	1548	4	0
50	2M	53	0	31	11	0
50	2m	53	0	31	11	0
51	2N	4	0	0	0	0
51	2n	4	0	0	0	0
51	3H	4	0	0	1	0
51	3h	4	0	0	1	0
52	2N	8	0	0	0	0
52	2n	8	0	0	0	0
53	2N	7	0	0	0	0
53	2n	7	0	0	0	0
54	2N	1	0	0	0	0
54	2n	1	0	0	0	0
54	4Q	1	0	0	0	0
54	4q	1	0	0	0	0
55	2O	51	0	82	0	0
55	2P	102	0	164	0	0
55	2R	51	0	82	0	0
55	2o	51	0	82	0	0
55	2p	102	0	164	0	0
55	2r	51	0	82	0	0
55	3C	51	0	82	1	0
55	3F	51	0	82	1	0
55	3c	51	0	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	3f	51	0	82	1	0
55	40	153	0	246	1	0
55	41	153	0	246	1	0
55	4D	51	0	82	0	0
55	4Q	102	0	164	2	0
55	4R	51	0	82	0	0
55	4S	51	0	82	0	0
55	4W	51	0	82	0	0
55	4Z	51	0	82	0	0
55	4d	51	0	82	0	0
55	4q	102	0	164	2	0
55	4r	51	0	82	0	0
55	4s	51	0	82	0	0
55	4w	51	0	82	0	0
55	4z	51	0	82	0	0
56	2O	108	0	176	5	0
56	2P	54	0	88	2	0
56	2R	54	0	88	1	0
56	2T	54	0	88	1	0
56	2o	108	0	176	5	0
56	2p	54	0	88	2	0
56	2r	54	0	88	1	0
56	2t	54	0	88	1	0
56	3A	108	0	176	2	0
56	3H	54	0	88	0	0
56	3a	108	0	176	2	0
56	3h	54	0	88	0	0
56	4E	54	0	88	2	0
56	4e	54	0	88	2	0
57	2O	100	0	156	1	0
57	2P	100	0	156	3	0
57	2Q	100	0	156	2	0
57	2U	100	0	156	2	0
57	2o	100	0	156	1	0
57	2p	100	0	156	3	0
57	2q	100	0	156	2	0
57	2u	100	0	156	2	0
57	3D	200	0	312	0	0
57	3E	300	0	468	0	0
57	3G	100	0	156	5	0
57	3H	100	0	156	1	0
57	3I	300	0	468	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	3L	200	0	312	1	0
57	3d	200	0	312	0	0
57	3e	300	0	468	0	0
57	3g	100	0	156	4	0
57	3h	100	0	156	1	0
57	3i	300	0	468	3	0
57	3l	200	0	312	1	0
57	4E	100	0	156	0	0
57	4J	100	0	156	1	0
57	4K	200	0	312	2	0
57	4L	100	0	156	0	0
57	4M	100	0	156	0	0
57	4Q	200	0	312	3	0
57	4S	100	0	156	0	0
57	4T	100	0	156	3	0
57	4U	100	0	156	2	0
57	4W	200	0	312	1	0
57	4Z	100	0	156	0	0
57	4e	100	0	156	0	0
57	4j	100	0	156	1	0
57	4k	200	0	312	3	0
57	4l	100	0	156	0	0
57	4m	100	0	156	0	0
57	4q	200	0	312	3	0
57	4s	100	0	156	1	0
57	4t	100	0	156	3	0
57	4u	100	0	156	2	0
57	4w	200	0	312	1	0
57	4z	100	0	156	0	0
58	2S	53	0	74	2	0
58	2s	53	0	74	2	0
58	3D	53	0	74	12	0
58	3G	106	0	148	15	0
58	3d	53	0	74	12	0
58	3g	106	0	148	15	0
59	3C	43	0	31	6	0
59	3c	43	0	31	5	0
60	3G	86	0	60	5	0
60	3g	86	0	60	5	0
61	40	43	0	0	1	0
61	41	43	0	0	1	0
62	4C	44	0	67	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	4D	44	0	67	1	0
62	4c	44	0	67	0	0
62	4d	44	0	67	1	0
63	4N	2	0	0	0	0
63	4n	2	0	0	0	0
64	4Q	1	0	0	0	0
64	4q	1	0	0	0	0
65	4Q	1	0	0	0	0
65	4q	1	0	0	0	0
66	4Q	120	0	108	6	0
66	4q	120	0	108	6	0
67	4Q	2	0	0	0	0
67	4q	2	0	0	0	0
68	4T	2	0	0	0	0
68	4X	1	0	0	0	0
68	4t	2	0	0	0	0
68	4x	1	0	0	0	0
All	All	142424	0	144688	735	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 3.

All (735) 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)
1:2M:76:HIS:CE1	50:2M:701:FAD:HM82	1.21	1.70
1:2m:76:HIS:CE1	50:2m:701:FAD:HM82	1.21	1.65
1:2m:76:HIS:NE2	50:2m:701:FAD:C8M	1.75	1.46
1:2M:76:HIS:NE2	50:2M:701:FAD:C8M	1.75	1.45
13:3C:76:CYS:SG	59:3C:301:HEC:HAC	1.67	1.34
13:3c:76:CYS:SG	59:3c:301:HEC:HAC	1.67	1.33
13:3c:76:CYS:SG	59:3c:301:HEC:CAC	2.17	1.32
1:2M:76:HIS:CE1	50:2M:701:FAD:C8M	2.07	1.31
13:3C:76:CYS:SG	59:3C:301:HEC:CAC	2.17	1.31
1:2m:76:HIS:CE1	50:2m:701:FAD:C8M	2.07	1.30
1:2M:76:HIS:NE2	50:2M:701:FAD:HM82	0.90	1.22
1:2m:76:HIS:NE2	50:2m:701:FAD:HM82	0.90	1.21
13:3c:76:CYS:HG	59:3c:301:HEC:HAC	0.94	1.02
1:2M:76:HIS:NE2	50:2M:701:FAD:C8	2.40	0.84
13:3C:76:CYS:HG	59:3C:301:HEC:HAC	0.98	0.84
1:2m:76:HIS:NE2	50:2m:701:FAD:C8	2.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2m:76:HIS:HE1	50:2m:701:FAD:C8M	1.96	0.74
17:3G:176:TYR:OH	17:3g:176:TYR:OH	2.02	0.72
40:4q:762:HIS:CD2	40:4q:763:ASP:OD2	2.42	0.72
40:4Q:762:HIS:CD2	40:4Q:763:ASP:OD2	2.43	0.71
40:4q:468:MET:HB3	66:4q:904:HEA:CAC	2.21	0.71
1:2M:76:HIS:HE1	50:2M:701:FAD:C8M	1.96	0.71
40:4Q:468:MET:HB3	66:4Q:904:HEA:CAC	2.21	0.70
17:3G:173:ILE:HG21	58:3G:404:UQ8:H35A	1.75	0.69
17:3g:173:ILE:HG21	58:3g:404:UQ8:H35A	1.75	0.69
40:4Q:678:VAL:HG21	40:4Q:703:ILE:HD11	1.74	0.68
44:4u:396:MET:HA	57:4u:501:CDL:H431	1.76	0.68
58:3d:203:UQ8:H3MB	58:3d:203:UQ8:H4MA	1.75	0.67
40:4q:678:VAL:HG21	40:4q:703:ILE:HD11	1.74	0.67
58:3D:203:UQ8:H4MA	58:3D:203:UQ8:H3MB	1.75	0.67
44:4U:396:MET:HA	57:4U:501:CDL:H431	1.76	0.67
58:3d:203:UQ8:H20A	26:4c:72:THR:HG21	1.77	0.66
1:2M:76:HIS:CE1	50:2M:701:FAD:HM83	2.27	0.66
58:3D:203:UQ8:H20A	26:4C:72:THR:HG21	1.77	0.66
1:2m:253:ASP:CB	50:2m:701:FAD:H61A	2.09	0.66
1:2M:253:ASP:CB	50:2M:701:FAD:H61A	2.09	0.65
4:2P:106:ASN:ND2	4:2P:108:GLN:OE1	2.30	0.65
4:2p:106:ASN:ND2	4:2p:108:GLN:OE1	2.30	0.64
3:2o:131:LEU:HD23	8:2t:72:ALA:HB2	1.80	0.64
31:4h:19:VAL:HG11	31:4h:37:HIS:NE2	2.12	0.64
31:4H:19:VAL:HG11	31:4H:37:HIS:NE2	2.12	0.64
1:2m:76:HIS:CE1	50:2m:701:FAD:HM83	2.27	0.63
3:2O:131:LEU:HD23	8:2T:72:ALA:HB2	1.80	0.62
40:4Q:632:HIS:O	40:4Q:635:VAL:HG22	2.00	0.62
40:4q:632:HIS:O	40:4q:635:VAL:HG22	2.00	0.62
56:2o:204:PC1:H371	6:2r:48:THR:HA	1.82	0.62
56:2O:203:PC1:H371	6:2R:48:THR:HA	1.82	0.61
17:3G:74:ASN:CG	57:3G:403:CDL:H873	2.26	0.61
13:3C:76:CYS:SG	59:3C:301:HEC:C3C	2.89	0.61
17:3g:223:PHE:CE2	57:3g:403:CDL:H872	2.36	0.60
17:3G:223:PHE:CE2	57:3G:403:CDL:H872	2.36	0.60
40:4q:468:MET:HA	40:4q:472:ILE:HD12	1.83	0.60
3:2o:13:ALA:H	3:2o:18:THR:HG22	1.66	0.60
17:3g:74:ASN:CG	57:3g:403:CDL:H873	2.26	0.60
23:41:215:HIS:O	23:41:219:VAL:HG23	2.02	0.60
60:3G:401:HEM:HBC2	60:3G:401:HEM:HMC2	1.84	0.60
1:2M:126:VAL:HG21	1:2M:441:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2O:13:ALA:H	3:2O:18:THR:HG22	1.66	0.59
23:40:215:HIS:O	23:40:219:VAL:HG23	2.02	0.59
17:3G:111:GLN:HE21	58:3G:404:UQ8:H35	1.67	0.59
40:4Q:468:MET:HA	40:4Q:472:ILE:HD12	1.83	0.59
1:2m:126:VAL:HG21	1:2m:441:VAL:HG22	1.84	0.59
13:3c:76:CYS:SG	59:3c:301:HEC:C3C	2.89	0.59
23:40:200:TYR:HH	35:4L:60:TRP:CD1	2.20	0.59
17:3g:321:ILE:HG22	26:4c:63:ARG:HD2	1.85	0.58
17:3G:321:ILE:HG22	26:4C:63:ARG:HD2	1.85	0.58
17:3g:111:GLN:HE21	58:3g:404:UQ8:H35	1.67	0.58
60:3g:401:HEM:HMC2	60:3g:401:HEM:HBC2	1.84	0.58
58:3G:404:UQ8:H3MA	58:3G:404:UQ8:H4MB	1.84	0.58
43:4T:106:CYS:SG	43:4T:109:LYS:N	2.77	0.58
58:3g:404:UQ8:H4MB	58:3g:404:UQ8:H3MA	1.84	0.58
27:4d:3:ILE:HD12	62:4d:102:LPP:H263	1.86	0.58
26:4c:70:PHE:CD1	26:4c:71:PRO:HD2	2.39	0.58
5:2Q:11:SER:OG	6:2R:57:THR:HG22	2.04	0.57
36:4M:59:VAL:HG13	43:4T:137:CYS:SG	2.45	0.57
37:4N:73:ASP:OD1	37:4N:74:LYS:N	2.37	0.57
37:4n:69:MET:HE2	40:4q:836:GLU:HB2	1.86	0.57
24:4A:20:LEU:HD12	24:4A:28:LEU:HA	1.86	0.57
5:2q:11:SER:OG	6:2r:57:THR:HG22	2.04	0.57
27:4D:3:ILE:HD12	62:4D:102:LPP:H263	1.86	0.57
11:3a:131:ILE:HD13	11:3a:228:VAL:HG12	1.86	0.57
24:4a:20:LEU:HD12	24:4a:28:LEU:HA	1.85	0.57
37:4n:73:ASP:OD1	37:4n:74:LYS:N	2.37	0.57
37:4N:69:MET:HE2	40:4Q:836:GLU:HB2	1.86	0.57
3:2o:158:MET:SD	3:2o:158:MET:N	2.78	0.57
28:4e:117:VAL:HG12	28:4e:117:VAL:O	2.05	0.57
36:4m:59:VAL:HG13	43:4t:137:CYS:SG	2.45	0.57
11:3A:131:ILE:HD13	11:3A:228:VAL:HG12	1.86	0.56
12:3B:537:ARG:NH2	12:3b:537:ARG:HH22	2.03	0.56
12:3B:369:THR:HG21	21:3K:22:LEU:HG	1.88	0.56
26:4C:70:PHE:CD1	26:4C:71:PRO:HD2	2.39	0.56
28:4E:117:VAL:HG12	28:4E:117:VAL:O	2.05	0.56
17:3g:284:ILE:HG21	17:3g:343:LEU:HD13	1.87	0.56
12:3B:537:ARG:HH22	12:3b:537:ARG:NH2	2.03	0.56
15:3e:70:GLU:OE1	15:3e:70:GLU:N	2.36	0.56
17:3G:284:ILE:HG21	17:3G:343:LEU:HD13	1.88	0.56
40:4Q:581:SER:O	40:4Q:585:THR:HG23	2.06	0.56
3:2O:158:MET:SD	3:2O:158:MET:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2o:204:PC1:H3F1	6:2r:43:PHE:HB2	1.88	0.55
43:4t:106:CYS:SG	43:4t:109:LYS:N	2.77	0.55
7:2s:112:MET:HA	7:2s:112:MET:HE3	1.88	0.55
12:3b:369:THR:HG21	21:3k:22:LEU:HG	1.88	0.55
56:2O:203:PC1:H3F1	6:2R:43:PHE:HB2	1.88	0.55
33:4J:108:GLU:OE1	33:4J:108:GLU:N	2.40	0.55
40:4Q:669:ILE:HG21	57:4Q:908:CDL:H621	1.88	0.55
33:4j:108:GLU:N	33:4j:108:GLU:OE1	2.40	0.55
17:3g:173:ILE:HD13	58:3g:404:UQ8:H37A	1.89	0.55
33:4j:22:VAL:HG21	33:4j:110:ILE:HA	1.89	0.55
47:4x:133:GLY:HA3	47:4x:139:VAL:HG23	1.89	0.55
17:3G:173:ILE:HD13	58:3G:404:UQ8:H37A	1.89	0.55
18:3H:153:TYR:CE1	18:3H:157:ILE:HG21	2.41	0.55
44:4U:402:PHE:HB2	45:4V:77:LEU:HD21	1.89	0.55
13:3c:41:PRO:HA	26:4c:61:VAL:HG12	1.89	0.55
58:3g:404:UQ8:H4MB	58:3g:404:UQ8:C3M	2.37	0.55
40:4q:581:SER:O	40:4q:585:THR:HG23	2.06	0.55
14:3d:87:SER:HB2	58:3d:203:UQ8:H35B	1.89	0.55
13:3C:41:PRO:HA	26:4C:61:VAL:HG12	1.89	0.54
40:4q:669:ILE:HG21	57:4q:908:CDL:H621	1.88	0.54
18:3h:153:TYR:CE1	18:3h:157:ILE:HG21	2.41	0.54
18:3h:343:ASP:OD1	18:3h:343:ASP:O	2.25	0.54
1:2M:234:THR:O	1:2M:420:ALA:HB2	2.08	0.54
7:2S:112:MET:HE3	7:2S:112:MET:HA	1.89	0.54
23:41:200:TYR:HH	35:4l:60:TRP:CD1	2.26	0.54
18:3h:266:ILE:HG22	18:3h:266:ILE:O	2.08	0.54
18:3H:266:ILE:HG22	18:3H:266:ILE:O	2.08	0.54
1:2m:234:THR:O	1:2m:420:ALA:HB2	2.08	0.54
14:3D:87:SER:HB2	58:3D:203:UQ8:H35B	1.89	0.54
18:3H:343:ASP:O	18:3H:343:ASP:OD1	2.25	0.54
33:4J:22:VAL:HG21	33:4J:110:ILE:HA	1.89	0.54
47:4X:133:GLY:HA3	47:4X:139:VAL:HG23	1.89	0.54
7:2S:98:VAL:HG11	58:2S:201:UQ8:H22A	1.90	0.53
58:3G:404:UQ8:H4MB	58:3G:404:UQ8:C3M	2.37	0.53
1:2m:388:MET:HE3	1:2m:428:ALA:O	2.08	0.53
23:41:111:ASN:OD1	23:41:112:ASN:N	2.42	0.53
23:40:111:ASN:OD1	23:40:112:ASN:N	2.42	0.53
40:4q:596:LEU:HD22	40:4q:630:PHE:CE2	2.44	0.53
17:3G:165:ILE:HD11	17:3g:42:ASN:HD22	1.74	0.53
18:3H:266:ILE:O	18:3H:266:ILE:CG2	2.57	0.53
40:4Q:596:LEU:HD22	40:4Q:630:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2s:98:VAL:HG11	58:2s:201:UQ8:H22A	1.90	0.53
1:2M:388:MET:HE3	1:2M:428:ALA:O	2.08	0.53
1:2M:518:VAL:HG11	1:2M:555:ALA:HA	1.91	0.53
17:3g:182:VAL:HG12	58:3g:405:UQ8:H10A	1.91	0.53
32:4i:157:GLU:OE1	32:4i:157:GLU:N	2.39	0.53
19:3I:65:ARG:NH1	17:3g:195:GLU:OE2	2.42	0.52
18:3h:266:ILE:O	18:3h:266:ILE:CG2	2.57	0.52
44:4u:402:PHE:HB2	45:4v:77:LEU:HD21	1.89	0.52
60:3G:401:HEM:HMB1	60:3G:401:HEM:HBB2	1.91	0.52
36:4M:71:GLN:HG3	43:4T:149:VAL:HG21	1.90	0.52
15:3E:70:GLU:N	15:3E:70:GLU:OE1	2.36	0.52
40:4Q:828:ASN:N	40:4Q:829:VAL:HA	2.24	0.52
60:3g:401:HEM:HBB2	60:3g:401:HEM:HMB1	1.91	0.52
32:4I:157:GLU:OE1	32:4I:157:GLU:N	2.39	0.52
32:4I:193:ILE:HG23	57:4T:203:CDL:H362	1.92	0.52
7:2s:80:ASP:OD1	8:2t:17:ARG:NH2	2.42	0.52
17:3G:195:GLU:OE2	19:3i:65:ARG:NH1	2.42	0.52
40:4Q:451:TYR:O	40:4Q:454:VAL:HG23	2.10	0.52
32:4i:193:ILE:HG23	57:4t:203:CDL:H362	1.92	0.52
40:4q:451:TYR:O	40:4q:454:VAL:HG23	2.10	0.52
17:3G:42:ASN:HD22	17:3g:165:ILE:HD11	1.74	0.51
18:3H:227:VAL:HG12	18:3H:229:LEU:HD23	1.92	0.51
21:3K:63:VAL:HG12	21:3K:63:VAL:O	2.10	0.51
6:2r:27:ALA:HB1	6:2r:32:GLU:HG3	1.92	0.51
1:2m:518:VAL:HG11	1:2m:555:ALA:HA	1.91	0.51
6:2R:27:ALA:HB1	6:2R:32:GLU:HG3	1.92	0.51
24:4A:28:LEU:HD11	49:4Z:150:VAL:HG11	1.93	0.51
40:4q:828:ASN:N	40:4q:829:VAL:HA	2.24	0.51
44:4U:396:MET:CA	57:4U:501:CDL:H431	2.40	0.51
7:2S:80:ASP:OD1	8:2T:17:ARG:NH2	2.42	0.51
24:4a:28:LEU:HD11	49:4z:150:VAL:HG11	1.93	0.51
36:4m:71:GLN:HG3	43:4t:149:VAL:HG21	1.90	0.51
21:3k:63:VAL:HG12	21:3k:63:VAL:O	2.10	0.51
23:4I:148:TYR:CE1	33:4j:143:ILE:HD11	2.45	0.51
23:40:148:TYR:CE1	33:4J:143:ILE:HD11	2.45	0.51
59:3c:301:HEC:HBB3	59:3c:301:HEC:HMB3	1.92	0.51
18:3h:279:ARG:CZ	18:3h:335:ILE:HD11	2.41	0.51
24:4a:34:HIS:O	39:4p:184:THR:OG1	2.28	0.51
17:3G:182:VAL:HG12	58:3G:405:UQ8:H10A	1.91	0.51
18:3H:279:ARG:CZ	18:3H:335:ILE:HD11	2.41	0.51
18:3H:314:HIS:HB2	51:3H:401:FES:S2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3h:227:VAL:HG12	18:3h:229:LEU:HD23	1.92	0.51
11:3a:469:ARG:O	56:3a:501:PC1:H143	2.11	0.50
40:4q:491:VAL:HG12	40:4q:491:VAL:O	2.11	0.50
24:4A:63:GLU:OE2	30:4G:46:TRP:NE1	2.44	0.50
39:4P:140:LEU:HD13	40:4Q:657:ILE:HD11	1.93	0.50
1:2m:83:GLY:HA2	1:2m:173:THR:HG21	1.94	0.50
59:3C:301:HEC:HMB3	59:3C:301:HEC:HBB3	1.92	0.50
25:4b:3:ILE:HD12	25:4b:3:ILE:H	1.77	0.50
1:2M:83:GLY:HA2	1:2M:173:THR:HG21	1.94	0.50
1:2M:126:VAL:HG13	1:2M:440:VAL:CG1	2.42	0.50
23:40:64:LYS:NZ	46:4W:16:ASP:OD2	2.44	0.50
40:4Q:468:MET:HB3	66:4Q:904:HEA:CBC	2.42	0.50
57:2p:201:CDL:H721	57:3i:202:CDL:H322	1.94	0.50
58:3D:203:UQ8:C18	26:4C:65:VAL:HG11	2.42	0.50
24:4A:34:HIS:O	39:4P:184:THR:OG1	2.28	0.50
40:4Q:424:ILE:HG13	66:4Q:904:HEA:H242	1.94	0.50
18:3h:314:HIS:HB2	51:3h:401:FES:S2	2.51	0.50
47:4x:153:THR:HG21	48:4y:116:LEU:HD21	1.94	0.50
4:2P:139:THR:HG22	8:2T:52:GLU:HG3	1.94	0.49
4:2p:139:THR:HG22	8:2t:52:GLU:HG3	1.94	0.49
57:2p:201:CDL:H722	57:3i:202:CDL:H342	1.94	0.49
58:3d:203:UQ8:C18	26:4c:65:VAL:HG11	2.42	0.49
40:4q:577:VAL:HG21	40:4q:658:ILE:HD13	1.94	0.49
40:4Q:826:GLY:O	40:4Q:829:VAL:HG13	2.12	0.49
44:4u:396:MET:CA	57:4u:501:CDL:H431	2.40	0.49
11:3A:469:ARG:O	56:3A:501:PC1:H143	2.11	0.49
18:3H:227:VAL:O	18:3H:345:THR:HA	2.12	0.49
40:4Q:491:VAL:HG12	40:4Q:491:VAL:O	2.11	0.49
40:4Q:640:LEU:HD22	40:4Q:668:ILE:HG23	1.93	0.49
7:2s:114:GLU:OE1	7:2s:114:GLU:N	2.42	0.49
39:4p:140:LEU:HD13	40:4q:657:ILE:HD11	1.93	0.49
40:4q:640:LEU:HD22	40:4q:668:ILE:HG23	1.94	0.49
17:3G:54:ILE:HD11	60:3G:401:HEM:O2D	2.13	0.49
41:4r:103:ARG:NH1	41:4r:113:PRO:O	2.45	0.49
14:3D:91:TYR:HA	58:3D:203:UQ8:H31	1.94	0.49
23:40:189:ILE:O	23:40:193:VAL:HG13	2.13	0.49
40:4Q:577:VAL:HG21	40:4Q:658:ILE:HD13	1.94	0.49
24:4a:63:GLU:OE2	30:4g:46:TRP:NE1	2.44	0.49
1:2M:80:ALA:HB3	1:2M:174:GLY:HA3	1.94	0.49
32:4I:166:ASN:OD1	47:4X:175:ARG:NH2	2.46	0.49
24:4a:105:PRO:HB3	46:4w:140:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4q:826:GLY:O	40:4q:829:VAL:HG13	2.12	0.49
41:4R:103:ARG:NH1	41:4R:113:PRO:O	2.45	0.49
47:4X:153:THR:HG21	48:4Y:116:LEU:HD21	1.94	0.49
25:4B:3:ILE:HD12	25:4B:3:ILE:H	1.76	0.49
23:41:64:LYS:NZ	46:4w:16:ASP:OD2	2.44	0.49
40:4q:468:MET:HB3	66:4q:904:HEA:CBC	2.42	0.49
57:2P:201:CDL:H722	57:3I:201:CDL:H342	1.94	0.49
8:2T:50:TRP:CG	56:2T:101:PC1:H132	2.48	0.49
35:4L:69:GLU:N	35:4L:69:GLU:OE1	2.40	0.49
1:2m:126:VAL:HG13	1:2m:440:VAL:CG1	2.42	0.49
23:41:134:TYR:CD1	28:4e:35:MET:HE3	2.48	0.49
28:4E:53:THR:HG21	46:4W:96:ILE:CD1	2.43	0.49
39:4P:176:PHE:HD1	40:4Q:690:LEU:HD21	1.78	0.49
23:41:21:ILE:HD11	55:4q:910:PEE:H31	1.95	0.49
23:41:189:ILE:O	23:41:193:VAL:HG13	2.13	0.49
4:2P:101:SER:HA	57:2P:201:CDL:OA3	2.13	0.48
11:3a:87:VAL:HG12	11:3a:87:VAL:O	2.13	0.48
28:4e:53:THR:HG21	46:4w:96:ILE:CD1	2.43	0.48
57:2P:201:CDL:H721	57:3I:201:CDL:H322	1.94	0.48
23:40:134:TYR:CD1	28:4E:35:MET:HE3	2.48	0.48
1:2m:80:ALA:HB3	1:2m:174:GLY:HA3	1.94	0.48
4:2p:101:SER:HA	57:2p:201:CDL:OA3	2.13	0.48
7:2s:102:GLY:HA2	7:2s:105:ALA:HB2	1.96	0.48
18:3h:227:VAL:O	18:3h:345:THR:HA	2.12	0.48
39:4p:176:PHE:HD1	40:4q:690:LEU:HD21	1.78	0.48
40:4q:424:ILE:HG13	66:4q:904:HEA:H242	1.94	0.48
7:2S:13:LEU:O	7:2S:13:LEU:HD23	2.14	0.48
24:4A:105:PRO:HB3	46:4W:140:LEU:HD11	1.95	0.48
1:2m:253:ASP:CG	50:2m:701:FAD:H61A	2.21	0.48
17:3g:98:ASN:HB3	17:3g:101:ILE:HD12	1.95	0.48
8:2t:50:TRP:CG	56:2t:101:PC1:H132	2.48	0.48
14:3d:91:TYR:HA	58:3d:203:UQ8:H31	1.95	0.48
2:2N:72:ARG:NE	2:2N:121:VAL:HG13	2.29	0.48
11:3A:87:VAL:HG12	11:3A:87:VAL:O	2.13	0.48
58:3d:203:UQ8:H15	17:3g:314:ILE:HA	1.96	0.48
23:40:18:THR:HG22	40:4Q:510:ILE:HG13	1.96	0.48
56:4E:202:PC1:H143	29:4F:112:TRP:CG	2.49	0.48
40:4Q:813:ILE:HG23	57:4T:203:CDL:H873	1.96	0.48
7:2s:13:LEU:HD23	7:2s:13:LEU:O	2.14	0.48
28:4e:96:GLN:CD	40:4q:615:ILE:HD12	2.39	0.48
40:4q:669:ILE:HG21	57:4q:908:CDL:C62	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3G:33:VAL:HG11	57:3G:403:CDL:H871	1.95	0.48
23:40:122:ILE:HG21	23:40:143:ILE:HG13	1.95	0.48
23:40:213:TYR:CE2	23:40:217:ILE:HD11	2.49	0.48
40:4Q:669:ILE:HG21	57:4Q:908:CDL:C62	2.44	0.48
44:4U:435:LYS:O	44:4U:440:LYS:NZ	2.47	0.48
17:3g:54:ILE:HD11	60:3g:401:HEM:O2D	2.13	0.48
9:2U:46:VAL:HG12	9:2U:46:VAL:O	2.14	0.48
25:4B:74:GLU:OE1	25:4B:74:GLU:N	2.44	0.48
28:4E:96:GLN:CD	40:4Q:615:ILE:HD12	2.39	0.48
2:2n:72:ARG:NE	2:2n:121:VAL:HG13	2.29	0.48
18:3h:232:ILE:HG12	18:3h:238:PHE:CE2	2.49	0.48
39:4p:176:PHE:CD1	40:4q:690:LEU:HD21	2.49	0.48
1:2M:253:ASP:CG	50:2M:701:FAD:H61A	2.21	0.47
18:3H:232:ILE:HG12	18:3H:238:PHE:CE2	2.49	0.47
7:2S:102:GLY:HA2	7:2S:105:ALA:HB2	1.96	0.47
58:3D:203:UQ8:H15	17:3G:314:ILE:HA	1.96	0.47
17:3G:98:ASN:HB3	17:3G:101:ILE:HD12	1.95	0.47
39:4P:176:PHE:CD1	40:4Q:690:LEU:HD21	2.49	0.47
56:2o:203:PC1:H153	56:2o:203:PC1:O13	2.14	0.47
18:3H:24:HIS:N	19:3i:168:THR:HG1	2.12	0.47
40:4q:813:ILE:HG23	57:4t:203:CDL:H873	1.96	0.47
47:4x:68:PHE:CE1	47:4x:198:THR:HG21	2.50	0.47
1:2M:126:VAL:HG13	1:2M:440:VAL:HG11	1.97	0.47
4:2P:87:LEU:HD23	4:2P:87:LEU:C	2.40	0.47
8:2T:55:GLU:OE1	8:2T:55:GLU:N	2.46	0.47
18:3H:126:THR:HG22	18:3H:127:ASP:H	1.79	0.47
23:40:21:ILE:HD11	55:4Q:910:PEE:H31	1.95	0.47
47:4X:68:PHE:CE1	47:4X:198:THR:HG21	2.50	0.47
9:2u:46:VAL:HG12	9:2u:46:VAL:O	2.14	0.47
23:41:213:TYR:CE2	23:41:217:ILE:HD11	2.49	0.47
32:4i:166:ASN:OD1	47:4x:175:ARG:NH2	2.46	0.47
32:4i:177:ARG:CG	36:4m:27:VAL:HG11	2.45	0.47
2:2N:54:ILE:HD13	2:2N:99:ILE:HG12	1.97	0.47
1:2M:133:TYR:CD2	1:2M:184:MET:HE2	2.50	0.47
22:3L:546:ILE:HD12	22:3L:547:GLY:N	2.30	0.47
33:4J:144:TYR:CZ	57:4J:301:CDL:HB61	2.49	0.47
4:2p:87:LEU:HD23	4:2p:87:LEU:C	2.39	0.47
22:3l:546:ILE:HD12	22:3l:547:GLY:N	2.30	0.47
56:4e:202:PC1:H143	29:4f:112:TRP:CG	2.49	0.47
31:4h:151:LEU:N	31:4h:151:LEU:HD23	2.30	0.47
56:2O:202:PC1:H153	56:2O:202:PC1:O13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:3d:203:UQ8:C18	58:3d:203:UQ8:C15	2.93	0.47
17:3g:170:LEU:CD1	58:3g:404:UQ8:H35B	2.45	0.47
18:3h:126:THR:HG22	18:3h:127:ASP:H	1.79	0.47
1:2M:284:LEU:HD21	1:2M:286:THR:HA	1.96	0.47
58:3D:203:UQ8:C18	58:3D:203:UQ8:C15	2.93	0.47
58:3D:203:UQ8:H15A	58:3D:203:UQ8:C19	2.45	0.47
36:4M:31:ARG:NH1	48:4Y:32:GLU:OE1	2.48	0.47
47:4X:182:ILE:HD12	47:4X:182:ILE:N	2.30	0.47
17:3g:33:VAL:HG11	57:3g:403:CDL:H871	1.96	0.47
47:4x:182:ILE:N	47:4x:182:ILE:HD12	2.30	0.47
12:3B:537:ARG:NH2	12:3b:537:ARG:NH2	2.61	0.46
17:3G:170:LEU:CD1	58:3G:404:UQ8:H35B	2.45	0.46
25:4b:74:GLU:OE1	25:4b:74:GLU:N	2.44	0.46
36:4m:31:ARG:NH1	48:4y:32:GLU:OE1	2.48	0.46
37:4n:64:PRO:HA	45:4v:103:TRP:CD2	2.50	0.46
3:2O:82:TYR:CD1	57:3I:201:CDL:HA61	2.51	0.46
2:2n:54:ILE:HD13	2:2n:99:ILE:HG12	1.97	0.46
23:4I:18:THR:HG22	40:4q:510:ILE:HG13	1.96	0.46
23:4I:122:ILE:HG21	23:4I:143:ILE:HG13	1.95	0.46
7:2S:82:ARG:NH1	7:2S:140:THR:O	2.45	0.46
32:4I:177:ARG:CG	36:4M:27:VAL:HG11	2.45	0.46
41:4R:33:TYR:O	45:4V:19:THR:OG1	2.29	0.46
18:3h:214:TRP:CD2	18:3h:215:PRO:HD2	2.51	0.46
33:4j:46:GLY:O	47:4x:256:ARG:NH1	2.42	0.46
35:4I:69:GLU:OE1	35:4I:69:GLU:N	2.41	0.46
1:2M:76:HIS:HE1	50:2M:701:FAD:HM83	1.74	0.46
3:2o:82:TYR:CD1	57:3i:202:CDL:HA61	2.51	0.46
33:4j:144:TYR:CZ	57:4j:301:CDL:HB61	2.50	0.46
56:3A:501:PC1:O13	56:3A:501:PC1:H152	2.16	0.46
31:4H:151:LEU:N	31:4H:151:LEU:HD23	2.30	0.46
45:4V:29:HIS:O	45:4V:54:LYS:NZ	2.49	0.46
1:2m:133:TYR:CD2	1:2m:184:MET:HE2	2.50	0.46
1:2m:284:LEU:HD21	1:2m:286:THR:HA	1.96	0.46
7:2s:82:ARG:NH1	7:2s:140:THR:O	2.45	0.46
8:2t:55:GLU:OE1	8:2t:55:GLU:N	2.46	0.46
18:3h:228:ASP:C	18:3h:230:ARG:H	2.24	0.46
44:4u:435:LYS:O	44:4u:440:LYS:NZ	2.47	0.46
27:4D:3:ILE:HD11	27:4D:35:ILE:HD11	1.97	0.46
57:2q:101:CDL:H792	9:2u:31:ILE:HD11	1.97	0.46
17:3g:4:ILE:HG23	58:3g:405:UQ8:H18	1.97	0.46
1:2M:319:ASP:OD1	1:2M:320:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2R:107:HIS:ND1	6:2R:113:ARG:O	2.44	0.46
58:3d:203:UQ8:C19	58:3d:203:UQ8:H15A	2.45	0.46
27:4d:3:ILE:HD11	27:4d:35:ILE:HD11	1.96	0.46
3:2O:35:PRO:HG3	18:3h:44:PRO:HD2	1.98	0.46
44:4U:434:THR:HG23	45:4V:112:ARG:HH12	1.81	0.46
4:2p:134:TRP:CE3	56:2p:204:PC1:H133	2.50	0.46
24:4a:100:ASP:OD1	24:4a:100:ASP:N	2.48	0.46
40:4q:841:ILE:HG22	40:4q:841:ILE:O	2.16	0.46
18:3H:214:TRP:CD2	18:3H:215:PRO:HD2	2.51	0.46
18:3H:228:ASP:C	18:3H:230:ARG:H	2.24	0.46
57:3H:402:CDL:HA61	22:3L:570:TYR:CE1	2.51	0.46
37:4N:64:PRO:HA	45:4V:103:TRP:CD2	2.50	0.46
57:3h:402:CDL:HA61	22:3l:570:TYR:CE1	2.51	0.46
40:4Q:841:ILE:HG22	40:4Q:841:ILE:O	2.16	0.45
28:4e:53:THR:HG21	46:4w:96:ILE:HD11	1.97	0.45
43:4t:54:VAL:HG22	43:4t:104:LEU:CD2	2.46	0.45
44:4u:434:THR:HG23	45:4v:112:ARG:HH12	1.81	0.45
47:4x:161:HIS:ND1	47:4x:162:PHE:O	2.44	0.45
18:3H:44:PRO:HD2	3:2o:35:PRO:HG3	1.98	0.45
1:2m:126:VAL:HG13	1:2m:440:VAL:HG11	1.96	0.45
49:4z:131:LEU:N	49:4z:132:PRO:HD2	2.31	0.45
4:2P:134:TRP:CE3	56:2P:204:PC1:H133	2.50	0.45
57:2Q:101:CDL:H792	9:2U:31:ILE:HD11	1.97	0.45
17:3G:4:ILE:HG23	58:3G:405:UQ8:H18	1.97	0.45
19:3I:136:GLU:HG3	18:3h:145:PRO:HG3	1.98	0.45
28:4E:53:THR:HG21	46:4W:96:ILE:HD11	1.97	0.45
31:4H:62:GLU:OE1	31:4H:62:GLU:N	2.48	0.45
38:4O:396:ILE:HD12	40:4Q:740:ILE:HG12	1.99	0.45
56:3a:501:PC1:O13	56:3a:501:PC1:H152	2.16	0.45
22:3L:568:VAL:HG21	57:3L:701:CDL:C11	2.47	0.45
27:4D:52:ASP:OD1	27:4D:52:ASP:N	2.49	0.45
39:4P:133:PRO:HB2	45:4V:38:MET:HE1	1.99	0.45
49:4Z:131:LEU:N	49:4Z:132:PRO:HD2	2.31	0.45
19:3I:33:PRO:CG	25:4b:7:ILE:HG22	2.47	0.45
22:3l:568:VAL:HG21	57:3l:701:CDL:C11	2.47	0.45
40:4Q:463:LEU:HD13	40:4Q:519:ILE:HD11	1.99	0.45
18:3h:316:SER:HA	18:3h:327:GLY:HA3	1.99	0.45
17:3G:259:LEU:HD11	17:3G:321:ILE:HD11	1.99	0.45
25:4B:7:ILE:HG22	19:3i:33:PRO:CG	2.47	0.45
43:4T:54:VAL:HG22	43:4T:104:LEU:CD2	2.47	0.45
45:4V:55:ASP:OD2	48:4Y:58:ARG:NH2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3a:261:ALA:HB2	11:3a:449:GLU:HB3	1.99	0.45
37:4n:56:LEU:HD13	37:4n:142:PRO:HG3	1.98	0.45
11:3A:261:ALA:HB2	11:3A:449:GLU:HB3	1.99	0.45
12:3B:123:MET:HE2	12:3B:298:PHE:HB2	1.99	0.45
17:3G:11:TYR:CE2	17:3G:13:ILE:HD11	2.52	0.45
58:3G:404:UQ8:H43	58:3g:405:UQ8:H38	1.99	0.45
34:4K:68:VAL:HG21	57:4K:201:CDL:H631	1.99	0.45
37:4N:56:LEU:HD13	37:4N:142:PRO:HG3	1.98	0.45
40:4Q:585:THR:HG21	40:4Q:641:PRO:HD3	1.99	0.45
17:3g:259:LEU:HD11	17:3g:321:ILE:HD11	1.99	0.45
18:3h:251:ARG:NE	18:3h:284:GLU:OE2	2.49	0.45
31:4h:151:LEU:HD23	31:4h:151:LEU:H	1.82	0.45
1:2m:319:ASP:OD1	1:2m:320:VAL:N	2.49	0.45
40:4q:777:ILE:HG23	40:4q:815:ILE:HD12	1.99	0.45
41:4r:33:TYR:O	45:4v:19:THR:OG1	2.29	0.45
18:3H:145:PRO:HG3	19:3i:136:GLU:HG3	1.98	0.45
21:3k:20:SER:O	21:3k:24:SER:OG	2.32	0.45
34:4k:68:VAL:HG21	57:4k:201:CDL:H631	1.99	0.45
38:4o:396:ILE:HD12	40:4q:740:ILE:HG12	1.99	0.45
58:3d:203:UQ8:H15	17:3g:314:ILE:HG12	1.99	0.44
24:4a:20:LEU:HD13	24:4a:27:ARG:HG2	1.99	0.44
47:4x:46:LEU:HD12	47:4x:72:TYR:CD1	2.52	0.44
58:3D:203:UQ8:H15	17:3G:314:ILE:HG12	1.99	0.44
43:4T:91:ARG:NE	48:4Y:46:GLU:OE2	2.50	0.44
27:4d:8:ASP:OD1	27:4d:8:ASP:N	2.49	0.44
12:3B:201:LEU:HD13	12:3B:209:ALA:HB2	2.00	0.44
24:4A:100:ASP:OD1	24:4A:100:ASP:N	2.48	0.44
31:4H:151:LEU:HD23	31:4H:151:LEU:H	1.82	0.44
39:4P:169:ILE:N	39:4P:169:ILE:HD12	2.33	0.44
2:2n:111:LEU:O	9:2u:7:GLN:NE2	2.49	0.44
43:4t:91:ARG:NE	48:4y:46:GLU:OE2	2.50	0.44
27:4D:8:ASP:OD1	27:4D:8:ASP:N	2.49	0.44
12:3b:201:LEU:HD13	12:3b:209:ALA:HB2	1.99	0.44
32:4i:140:LYS:C	46:4w:69:MET:HE2	2.42	0.44
45:4v:29:HIS:O	45:4v:54:LYS:NZ	2.49	0.44
9:2U:11:LEU:O	10:2V:6:SER:OG	2.36	0.44
12:3B:467:MET:O	12:3B:470:GLU:HG2	2.18	0.44
44:4U:414:ARG:N	44:4U:415:PRO:HD2	2.32	0.44
50:2m:701:FAD:H9	50:2m:701:FAD:H1'1	1.77	0.44
6:2R:65:TYR:HB2	8:2T:79:LEU:HD13	2.00	0.44
10:2V:8:LEU:C	10:2V:8:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3b:123:MET:HE2	12:3b:298:PHE:HB2	1.99	0.44
19:3I:168:THR:HG1	18:3h:24:HIS:N	2.14	0.44
24:4A:20:LEU:HD13	24:4A:27:ARG:HG2	1.99	0.44
45:4V:139:VAL:HG23	45:4V:140:LEU:HG	1.99	0.44
6:2r:65:TYR:HB2	8:2t:79:LEU:HD13	2.00	0.44
55:3f:101:PEE:O4	55:3f:101:PEE:O3	2.35	0.44
39:4p:106:ILE:HG23	39:4p:106:ILE:O	2.18	0.44
18:3H:225:ILE:HG21	18:3H:240:VAL:HG11	2.00	0.44
47:4X:46:LEU:HD12	47:4X:72:TYR:CD1	2.52	0.44
57:4k:202:CDL:H873	35:4l:99:MET:HG3	2.00	0.44
44:4u:414:ARG:N	44:4u:415:PRO:HD2	2.32	0.44
58:3D:203:UQ8:H10B	58:3D:203:UQ8:H13	2.00	0.44
18:3H:295:LEU:HD12	18:3H:314:HIS:CE1	2.53	0.44
19:3I:65:ARG:NH2	17:3g:300:ASN:OD1	2.51	0.44
29:4F:138:LEU:HD21	57:4W:202:CDL:H261	2.00	0.44
5:2q:6:VAL:HG13	27:4d:71:ARG:O	2.18	0.44
5:2q:50:ARG:HD2	8:2t:20:LEU:HD13	2.00	0.44
12:3b:467:MET:O	12:3b:470:GLU:HG2	2.18	0.44
29:4f:138:LEU:HD21	57:4w:202:CDL:H261	2.00	0.44
39:4p:133:PRO:HB2	45:4v:38:MET:HE1	1.99	0.44
39:4p:169:ILE:N	39:4p:169:ILE:HD12	2.33	0.44
40:4q:585:THR:HG21	40:4q:641:PRO:HD3	1.99	0.44
47:4x:134:THR:HG23	47:4x:137:ASN:H	1.83	0.44
2:2N:170:CYS:O	2:2N:171:ALA:HB3	2.18	0.43
18:3H:316:SER:HA	18:3H:327:GLY:HA3	1.99	0.43
34:4K:13:VAL:HG12	34:4K:13:VAL:O	2.17	0.43
17:3g:11:TYR:CE2	17:3g:13:ILE:HD11	2.52	0.43
17:3G:300:ASN:OD1	19:3i:65:ARG:NH2	2.51	0.43
32:4I:140:LYS:C	46:4W:69:MET:HE2	2.42	0.43
40:4Q:777:ILE:HG23	40:4Q:815:ILE:HD12	1.99	0.43
10:2v:8:LEU:HD23	10:2v:8:LEU:C	2.43	0.43
4:2P:123:ILE:HG23	57:2U:101:CDL:H152	2.00	0.43
8:2T:66:PRO:HG3	15:3E:115:PRO:HD3	2.01	0.43
12:3B:67:VAL:O	12:3B:71:VAL:HG23	2.18	0.43
56:4E:202:PC1:H31	56:4E:202:PC1:O22	2.17	0.43
47:4X:134:THR:HG23	47:4X:137:ASN:H	1.83	0.43
9:2u:11:LEU:O	10:2v:6:SER:OG	2.36	0.43
12:3b:67:VAL:O	12:3b:71:VAL:HG23	2.18	0.43
31:4h:62:GLU:OE1	31:4h:62:GLU:N	2.48	0.43
50:2M:701:FAD:H9	50:2M:701:FAD:H1'1	1.77	0.43
4:2P:116:PHE:HB3	57:2Q:101:CDL:H431	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:3D:203:UQ8:H18	26:4C:65:VAL:HG11	2.00	0.43
58:3G:405:UQ8:H38	58:3g:404:UQ8:H43	1.99	0.43
18:3H:251:ARG:NE	18:3H:284:GLU:OE2	2.49	0.43
40:4Q:752:ILE:HG13	66:4Q:905:HEA:CMA	2.48	0.43
4:2p:101:SER:O	8:2t:27:LYS:NZ	2.50	0.43
4:2p:134:TRP:CD2	56:2p:204:PC1:H133	2.53	0.43
18:3h:225:ILE:HG21	18:3h:240:VAL:HG11	2.00	0.43
18:3h:295:LEU:HD12	18:3h:314:HIS:CE1	2.53	0.43
7:2S:114:GLU:OE1	7:2S:114:GLU:N	2.42	0.43
27:4D:45:HIS:O	27:4D:46:PRO:C	2.62	0.43
6:2r:107:HIS:ND1	6:2r:113:ARG:O	2.44	0.43
58:3d:203:UQ8:H20	58:3d:203:UQ8:H17A	1.78	0.43
56:4e:202:PC1:O22	56:4e:202:PC1:H31	2.17	0.43
40:4q:463:LEU:HD13	40:4q:519:ILE:HD11	1.99	0.43
45:4v:139:VAL:HG23	45:4v:140:LEU:HG	1.99	0.43
5:2Q:6:VAL:HG13	27:4D:71:ARG:O	2.18	0.43
5:2Q:50:ARG:HD2	8:2T:20:LEU:HD13	2.00	0.43
6:2R:42:LEU:HD23	6:2R:42:LEU:O	2.19	0.43
55:3F:101:PEE:O4	55:3F:101:PEE:O3	2.35	0.43
58:3G:405:UQ8:H17	58:3G:405:UQ8:H20	1.88	0.43
40:4Q:612:ILE:HB	40:4Q:615:ILE:HD11	2.00	0.43
40:4Q:702:ILE:HG23	49:4Z:75:LEU:HD11	2.01	0.43
47:4X:255:THR:HG23	47:4X:255:THR:O	2.18	0.43
4:2p:123:ILE:HG23	57:2u:101:CDL:H152	2.00	0.43
60:3g:401:HEM:HBC2	60:3g:401:HEM:CMC	2.48	0.43
18:3H:297:CYS:HB2	18:3H:311:CYS:SG	2.59	0.43
61:40:304:AJP:O82	61:40:304:AJP:C81	2.67	0.43
37:4N:79:PRO:HG3	39:4P:186:MET:HE1	2.01	0.43
34:4k:13:VAL:O	34:4k:13:VAL:HG12	2.17	0.43
36:4m:71:GLN:CG	43:4t:149:VAL:HG21	2.49	0.43
37:4n:79:PRO:HG3	39:4p:186:MET:HE1	2.01	0.43
3:2o:58:PRO:O	57:2o:201:CDL:OB5	2.37	0.43
17:3g:166:VAL:HG11	58:3g:404:UQ8:H21	2.00	0.43
27:4d:45:HIS:O	27:4d:46:PRO:C	2.62	0.43
40:4q:752:ILE:HG13	66:4q:905:HEA:CMA	2.48	0.43
47:4x:95:ILE:HD12	47:4x:95:ILE:H	1.84	0.43
58:3D:203:UQ8:H20	58:3D:203:UQ8:H17A	1.78	0.43
23:40:41:LEU:HD21	33:4J:129:TYR:HE2	1.84	0.43
39:4P:106:ILE:HG23	39:4P:106:ILE:O	2.18	0.43
40:4Q:622:LEU:C	40:4Q:622:LEU:HD23	2.43	0.43
2:2n:170:CYS:O	2:2n:171:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:4j:29:GLY:HA2	34:4k:51:VAL:HG22	2.00	0.43
40:4q:474:MET:HB3	40:4q:475:PRO:HD3	2.01	0.43
40:4q:612:ILE:HB	40:4q:615:ILE:HD11	2.00	0.43
1:2M:30:THR:C	1:2M:32:TYR:H	2.27	0.43
4:2P:134:TRP:CD2	56:2P:204:PC1:H133	2.53	0.43
58:2S:201:UQ8:H37A	58:2S:201:UQ8:H40	1.81	0.43
14:3D:101:VAL:HG22	17:3G:327:GLU:HB2	2.01	0.43
57:4K:202:CDL:H873	35:4L:99:MET:HG3	2.00	0.43
6:2r:42:LEU:HD23	6:2r:42:LEU:C	2.44	0.43
9:2u:16:ALA:HB2	10:2v:7:LEU:HA	2.01	0.43
18:3h:267:VAL:O	18:3h:268:ASN:HB2	2.19	0.43
23:4i:134:TYR:HB2	28:4e:46:TRP:HZ2	1.84	0.43
25:4b:42:LEU:HD23	25:4b:42:LEU:C	2.44	0.43
36:4m:53:PRO:O	36:4m:57:VAL:HG23	2.19	0.43
11:3A:271:MET:SD	11:3A:456:GLY:HA2	2.59	0.42
14:3d:101:VAL:HG22	17:3g:327:GLU:HB2	2.01	0.42
58:3d:203:UQ8:H10B	58:3d:203:UQ8:H13	2.00	0.42
58:3g:405:UQ8:H30	58:3g:405:UQ8:H27A	1.81	0.42
61:41:304:AJP:O82	61:41:304:AJP:C81	2.67	0.42
6:2R:74:VAL:HG22	56:2R:202:PC1:H322	2.01	0.42
11:3A:82:HIS:HA	11:3A:115:THR:HG21	2.00	0.42
33:4J:29:GLY:HA2	34:4K:51:VAL:HG22	2.00	0.42
3:2o:110:ILE:HG12	56:2o:203:PC1:H351	2.01	0.42
11:3a:82:HIS:HA	11:3a:115:THR:HG21	2.00	0.42
40:4q:622:LEU:C	40:4q:622:LEU:HD23	2.43	0.42
4:2P:101:SER:O	8:2T:27:LYS:NZ	2.50	0.42
17:3G:66:ILE:HG22	17:3G:70:ILE:HD12	2.01	0.42
17:3G:166:VAL:HG11	58:3G:404:UQ8:H21	2.00	0.42
17:3G:191:ASN:ND2	60:3G:402:HEM:O2D	2.45	0.42
23:40:147:ASN:O	23:40:151:ASN:ND2	2.53	0.42
36:4M:53:PRO:O	36:4M:57:VAL:HG23	2.19	0.42
40:4Q:568:LEU:HD21	40:4Q:583:ILE:HD13	2.01	0.42
43:4T:54:VAL:HG21	44:4U:380:LEU:HA	2.01	0.42
4:2p:116:PHE:HB3	57:2q:101:CDL:H431	2.00	0.42
8:2t:66:PRO:HG3	15:3e:115:PRO:HD3	2.01	0.42
58:3d:203:UQ8:H18	26:4c:65:VAL:HG11	2.00	0.42
18:3h:297:CYS:HB2	18:3h:311:CYS:SG	2.59	0.42
40:4q:702:ILE:HG23	49:4z:75:LEU:HD11	2.01	0.42
47:4x:95:ILE:HD12	47:4x:95:ILE:N	2.34	0.42
47:4x:255:THR:HG23	47:4x:255:THR:O	2.18	0.42
26:4C:70:PHE:CD2	26:4C:72:THR:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:4V:88:THR:O	45:4V:88:THR:HG22	2.19	0.42
46:4W:21:TYR:O	47:4X:38:ARG:NH2	2.50	0.42
58:2s:201:UQ8:H7	58:2s:201:UQ8:H10	1.85	0.42
23:41:147:ASN:O	23:41:151:ASN:ND2	2.53	0.42
44:4u:402:PHE:HB2	45:4v:77:LEU:CD2	2.49	0.42
60:3G:401:HEM:HBC2	60:3G:401:HEM:CMC	2.48	0.42
58:3G:404:UQ8:H22A	58:3G:404:UQ8:H25	1.85	0.42
22:3L:546:ILE:HD12	22:3L:546:ILE:C	2.45	0.42
44:4U:402:PHE:HB2	45:4V:77:LEU:CD2	2.49	0.42
47:4X:161:HIS:ND1	47:4X:162:PHE:O	2.44	0.42
1:2m:76:HIS:HE1	50:2m:701:FAD:HM83	1.74	0.42
31:4h:33:THR:HG21	47:4x:114:MET:HE2	2.02	0.42
43:4t:54:VAL:HG21	44:4u:380:LEU:HA	2.01	0.42
43:4t:140:ALA:HB3	57:4t:203:CDL:H471	2.02	0.42
36:4M:38:ILE:HD12	36:4M:38:ILE:N	2.34	0.42
47:4X:95:ILE:HD12	47:4X:95:ILE:N	2.34	0.42
6:2r:42:LEU:HD23	6:2r:42:LEU:O	2.19	0.42
18:3h:316:SER:OG	18:3h:328:PRO:HD2	2.19	0.42
25:4B:42:LEU:HD23	25:4B:42:LEU:C	2.44	0.42
25:4B:89:LYS:NZ	34:4K:93:TYR:O	2.52	0.42
38:4O:398:MET:HB3	40:4Q:719:ILE:HD11	2.01	0.42
40:4Q:683:ILE:HG23	40:4Q:686:VAL:HG21	2.02	0.42
32:4i:193:ILE:HD13	32:4i:196:MET:CE	2.50	0.42
56:2O:203:PC1:H3F2	6:2R:43:PHE:HB3	2.01	0.42
43:4T:140:ALA:HB3	57:4T:203:CDL:H471	2.02	0.42
46:4w:21:TYR:O	47:4x:38:ARG:NH2	2.50	0.42
2:2N:111:LEU:O	9:2U:7:GLN:NE2	2.49	0.42
6:2R:42:LEU:HD23	6:2R:42:LEU:C	2.44	0.42
12:3B:537:ARG:HH22	12:3b:537:ARG:HH22	1.65	0.42
16:3F:31:LEU:N	16:3F:32:PRO:CD	2.83	0.42
66:4Q:905:HEA:OMA	66:4Q:905:HEA:HHB	2.20	0.42
11:3a:271:MET:SD	11:3a:456:GLY:HA2	2.59	0.42
22:3l:546:ILE:HD12	22:3l:546:ILE:C	2.45	0.42
32:4i:84:PRO:HA	32:4i:87:SER:HG	1.85	0.42
40:4q:683:ILE:HG23	40:4q:686:VAL:HG21	2.02	0.42
1:2M:25:ALA:O	1:2M:26:ALA:C	2.63	0.42
1:2M:135:LEU:HD23	1:2M:135:LEU:C	2.45	0.42
9:2U:16:ALA:HB2	10:2V:7:LEU:HA	2.01	0.42
18:3H:267:VAL:O	18:3H:268:ASN:HB2	2.19	0.42
29:4F:85:VAL:O	29:4F:85:VAL:HG22	2.20	0.42
32:4I:193:ILE:HD13	32:4I:196:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:4S:17:HIS:NE2	42:4S:22:GLU:OE2	2.47	0.42
17:3g:66:ILE:HG22	17:3g:70:ILE:HD12	2.01	0.42
25:4b:89:LYS:NZ	34:4k:93:TYR:O	2.52	0.42
40:4q:568:LEU:HD21	40:4q:583:ILE:HD13	2.01	0.42
47:4x:212:ASP:O	47:4x:215:THR:OG1	2.36	0.42
3:2O:58:PRO:O	57:2O:204:CDL:OB5	2.37	0.41
15:3E:88:LEU:C	15:3E:88:LEU:HD23	2.45	0.41
19:3I:176:THR:O	19:3I:177:MET:C	2.63	0.41
23:40:134:TYR:HB2	28:4E:46:TRP:HZ2	1.84	0.41
40:4Q:482:PRO:HB3	40:4Q:582:ILE:HD13	2.02	0.41
1:2m:25:ALA:O	1:2m:26:ALA:C	2.63	0.41
1:2m:30:THR:C	1:2m:32:TYR:H	2.27	0.41
1:2m:295:ILE:O	1:2m:344:LEU:HD12	2.20	0.41
1:2m:541:LEU:HD23	1:2m:541:LEU:O	2.20	0.41
6:2r:74:VAL:HG22	56:2r:202:PC1:H322	2.01	0.41
11:3a:475:ARG:O	11:3a:476:TYR:C	2.63	0.41
58:3g:404:UQ8:H22A	58:3g:404:UQ8:H25	1.85	0.41
45:4v:88:THR:O	45:4v:88:THR:HG22	2.19	0.41
18:3H:316:SER:OG	18:3H:328:PRO:HD2	2.19	0.41
23:40:200:TYR:CD2	33:4J:82:LEU:HD12	2.55	0.41
40:4Q:491:VAL:HG13	48:4Y:114:PRO:HB2	2.02	0.41
15:3e:88:LEU:HD23	15:3e:88:LEU:C	2.45	0.41
58:3g:404:UQ8:H30A	58:3g:404:UQ8:C33	2.50	0.41
23:41:41:LEU:HD21	33:4j:129:TYR:HE2	1.84	0.41
35:4l:100:TYR:HB3	57:4q:907:CDL:H322	2.02	0.41
3:2O:110:ILE:HG12	56:2O:202:PC1:H351	2.01	0.41
58:3G:404:UQ8:H30A	58:3G:404:UQ8:C33	2.50	0.41
22:3L:612:ASP:O	22:3L:613:GLU:C	2.62	0.41
23:40:27:ASN:ND2	23:40:33:SER:OG	2.54	0.41
47:4X:95:ILE:HD12	47:4X:95:ILE:H	1.84	0.41
1:2m:602:ILE:N	1:2m:602:ILE:HD12	2.35	0.41
2:2n:161:LEU:N	2:2n:161:LEU:HD12	2.36	0.41
22:3l:612:ASP:O	22:3l:613:GLU:C	2.62	0.41
36:4m:38:ILE:HD12	36:4m:38:ILE:N	2.34	0.41
38:4o:398:MET:HB3	40:4q:719:ILE:HD11	2.01	0.41
4:2P:123:ILE:HG23	57:2U:101:CDL:C15	2.50	0.41
23:40:40:LEU:HD23	55:40:302:PEE:C23	2.51	0.41
34:4K:24:LEU:HD12	47:4X:248:PRO:HB3	2.03	0.41
36:4M:71:GLN:CG	43:4T:149:VAL:HG21	2.49	0.41
40:4Q:474:MET:HB3	40:4Q:475:PRO:HD3	2.01	0.41
1:2m:86:ALA:HB2	1:2m:127:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2o:204:PC1:H3F2	6:2r:43:PHE:HB3	2.01	0.41
16:3f:31:LEU:N	16:3f:32:PRO:CD	2.83	0.41
18:3h:288:MET:HE1	18:3h:322:GLY:HA3	2.02	0.41
18:3h:303:GLN:HB2	18:3h:310:PHE:HB3	2.02	0.41
23:41:200:TYR:CD2	33:4j:82:LEU:HD12	2.56	0.41
57:3G:403:CDL:OA7	57:3G:403:CDL:HA62	2.20	0.41
33:4J:113:TYR:O	33:4J:117:THR:HG23	2.21	0.41
37:4n:64:PRO:HA	45:4v:103:TRP:CE3	2.55	0.41
40:4q:437:ILE:HG21	66:4q:904:HEA:CMA	2.51	0.41
1:2M:274:HIS:HB2	1:2M:385:HIS:HB2	2.02	0.41
1:2M:541:LEU:O	1:2M:541:LEU:HD23	2.20	0.41
14:3D:99:ASN:HB3	26:4C:52:TYR:CD1	2.56	0.41
18:3H:288:MET:HE1	18:3H:322:GLY:HA3	2.02	0.41
24:4A:28:LEU:HD21	49:4Z:150:VAL:HG13	2.02	0.41
40:4Q:437:ILE:HG21	66:4Q:904:HEA:CMA	2.51	0.41
44:4U:438:VAL:O	44:4U:438:VAL:HG12	2.21	0.41
4:2p:123:ILE:HG23	57:2u:101:CDL:C15	2.50	0.41
43:4t:54:VAL:O	44:4u:377:PRO:HA	2.21	0.41
2:2N:161:LEU:N	2:2N:161:LEU:HD12	2.36	0.41
9:2U:31:ILE:HD12	9:2U:31:ILE:N	2.36	0.41
19:3I:113:LYS:HD3	14:3d:72:ARG:HG3	2.03	0.41
38:4O:376:LEU:O	38:4O:380:THR:HG23	2.20	0.41
40:4Q:677:ILE:HG22	55:4Q:909:PEE:H63	2.02	0.41
7:2s:34:LEU:O	7:2s:38:VAL:HG23	2.21	0.41
17:3g:27:ILE:CG1	17:3g:81:VAL:HG12	2.51	0.41
19:3i:176:THR:O	19:3i:177:MET:C	2.63	0.41
24:4a:28:LEU:HD21	49:4z:150:VAL:HG13	2.02	0.41
26:4c:70:PHE:CD2	26:4c:72:THR:HG22	2.55	0.41
40:4q:482:PRO:HB3	40:4q:582:ILE:HD13	2.02	0.41
7:2S:34:LEU:O	7:2S:38:VAL:HG23	2.21	0.41
12:3B:366:VAL:HB	12:3B:367:PRO:HD3	2.03	0.41
37:4N:64:PRO:HA	45:4V:103:TRP:CE3	2.55	0.41
43:4T:54:VAL:O	44:4U:377:PRO:HA	2.21	0.41
1:2m:135:LEU:HD23	1:2m:135:LEU:C	2.45	0.41
1:2m:171:ASP:O	1:2m:171:ASP:CG	2.64	0.41
13:3c:276:THR:HG23	13:3c:276:THR:O	2.21	0.41
55:3c:302:PEE:H10	20:3j:10:ALA:HB3	2.03	0.41
57:3g:403:CDL:OA7	57:3g:403:CDL:HA62	2.20	0.41
31:4h:21:ASP:HB2	47:4x:106:VAL:HG22	2.03	0.41
33:4j:113:TYR:O	33:4j:117:THR:HG23	2.21	0.41
1:2M:602:ILE:HD12	1:2M:602:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2Q:51:THR:HG23	7:2S:90:GLU:CG	2.51	0.41
11:3A:475:ARG:O	11:3A:476:TYR:C	2.63	0.41
16:3F:13:GLU:HG2	18:3h:105:VAL:HG11	2.03	0.41
17:3G:27:ILE:CG1	17:3G:81:VAL:HG12	2.51	0.41
18:3H:303:GLN:HB2	18:3H:310:PHE:HB3	2.02	0.41
26:4C:71:PRO:HA	26:4C:74:TRP:CD2	2.56	0.41
28:4E:85:ARG:O	33:4J:156:VAL:HA	2.21	0.41
31:4H:33:THR:HG21	47:4X:114:MET:HE2	2.02	0.41
35:4L:100:TYR:HB3	57:4Q:907:CDL:H322	2.02	0.41
2:2n:29:ARG:NH1	2:2n:66:ASP:OD2	2.54	0.41
2:2n:219:MET:SD	5:2q:43:MET:HE3	2.61	0.41
4:2p:5:VAL:HG12	10:2v:80:ILE:HD12	2.03	0.41
5:2q:34:ARG:HH11	9:2u:26:HIS:CE1	2.39	0.41
23:41:27:ASN:ND2	23:41:33:SER:OG	2.54	0.41
23:41:40:LEU:HD23	55:41:302:PEE:C23	2.51	0.41
28:4e:85:ARG:O	33:4j:156:VAL:HA	2.21	0.41
29:4f:85:VAL:HG22	29:4f:85:VAL:O	2.20	0.41
34:4k:24:LEU:HD12	47:4x:248:PRO:HB3	2.03	0.41
38:4o:376:LEU:O	38:4o:380:THR:HG23	2.20	0.41
40:4q:677:ILE:HG22	55:4q:909:PEE:H63	2.02	0.41
41:4r:62:ILE:HD11	57:4s:101:CDL:H732	2.02	0.41
1:2M:295:ILE:O	1:2M:344:LEU:HD12	2.20	0.41
11:3A:63:GLY:C	11:3A:64:LEU:HD22	2.46	0.41
14:3D:72:ARG:HG3	19:3i:113:LYS:HD3	2.03	0.41
25:4B:9:LEU:O	25:4B:13:ARG:HG2	2.21	0.41
26:4C:75:PHE:OXT	26:4C:75:PHE:CG	2.74	0.41
31:4H:22:VAL:HG12	47:4X:105:ILE:HD13	2.03	0.41
35:4L:113:LEU:HD13	35:4L:113:LEU:C	2.45	0.41
24:4a:81:VAL:O	24:4a:81:VAL:HG22	2.21	0.41
33:4j:135:PRO:HB3	57:4k:202:CDL:C62	2.51	0.41
45:4v:55:ASP:OD2	48:4y:58:ARG:NH2	2.43	0.41
18:3H:105:VAL:HG11	16:3f:13:GLU:HG2	2.03	0.40
5:2q:51:THR:HG23	7:2s:90:GLU:CG	2.51	0.40
26:4c:75:PHE:OXT	26:4c:75:PHE:CG	2.74	0.40
2:2N:219:MET:SD	5:2Q:43:MET:HE3	2.61	0.40
15:3E:83:MET:HE3	18:3H:195:GLY:HA3	2.03	0.40
11:3a:63:GLY:C	11:3a:64:LEU:HD22	2.46	0.40
66:4q:905:HEA:OMA	66:4q:905:HEA:HHB	2.20	0.40
4:2P:88:LEU:HB3	4:2P:89:PRO:HD3	2.03	0.40
5:2Q:34:ARG:HH11	9:2U:26:HIS:CE1	2.39	0.40
6:2R:108:LEU:O	6:2R:112:ARG:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3C:197:PRO:HD2	59:3C:301:HEC:HBC2	2.03	0.40
55:3C:302:PEE:H10	20:3J:10:ALA:HB3	2.03	0.40
24:4A:81:VAL:O	24:4A:81:VAL:HG22	2.20	0.40
25:4b:9:LEU:O	25:4b:13:ARG:HG2	2.21	0.40
31:4h:35:ILE:HG13	32:4i:142:LEU:HD23	2.04	0.40
35:4l:113:LEU:C	35:4l:113:LEU:HD13	2.45	0.40
40:4q:578:TYR:CE2	40:4q:582:ILE:HD11	2.57	0.40
3:2O:104:VAL:O	6:2R:41:ARG:HD3	2.22	0.40
13:3C:276:THR:O	13:3C:276:THR:HG23	2.21	0.40
58:3G:405:UQ8:H38	58:3g:404:UQ8:H41A	2.04	0.40
14:3d:99:ASN:HB3	26:4c:52:TYR:CD1	2.56	0.40
15:3e:83:MET:HE3	18:3h:195:GLY:HA3	2.03	0.40
17:3g:80:VAL:HG23	17:3g:256:TRP:CZ2	2.57	0.40
17:3g:191:ASN:ND2	60:3g:402:HEM:O2D	2.45	0.40
40:4q:491:VAL:HG13	48:4y:114:PRO:HB2	2.02	0.40
13:3C:208:GLU:OE1	15:3E:116:TYR:OH	2.29	0.40
17:3G:80:VAL:HG23	17:3G:256:TRP:CZ2	2.57	0.40
57:3G:403:CDL:OA7	57:3G:403:CDL:CA6	2.69	0.40
32:4I:115:LYS:N	32:4I:116:PRO:HD2	2.37	0.40
33:4J:46:GLY:O	47:4X:256:ARG:NH1	2.42	0.40
26:4c:71:PRO:HA	26:4c:74:TRP:CD2	2.56	0.40
39:4p:169:ILE:HD12	39:4p:169:ILE:H	1.86	0.40

There are no symmetry-related clashes.

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	2M	602/604 (100%)	586 (97%)	15 (2%)	1 (0%)	43	51
1	2m	602/604 (100%)	586 (97%)	15 (2%)	1 (0%)	43	51
2	2N	257/259 (99%)	250 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2n	257/259 (99%)	250 (97%)	7 (3%)	0	100	100
3	2O	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
3	2o	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
4	2P	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	2p	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
5	2Q	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
5	2q	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
6	2R	115/117 (98%)	115 (100%)	0	0	100	100
6	2r	115/117 (98%)	115 (100%)	0	0	100	100
7	2S	163/165 (99%)	162 (99%)	1 (1%)	0	100	100
7	2s	163/165 (99%)	162 (99%)	1 (1%)	0	100	100
8	2T	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
8	2t	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
9	2U	46/48 (96%)	46 (100%)	0	0	100	100
9	2u	46/48 (96%)	46 (100%)	0	0	100	100
10	2V	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
10	2v	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
11	3A	452/454 (100%)	447 (99%)	5 (1%)	0	100	100
11	3a	452/454 (100%)	447 (99%)	5 (1%)	0	100	100
12	3B	494/496 (100%)	489 (99%)	5 (1%)	0	100	100
12	3b	494/496 (100%)	489 (99%)	5 (1%)	0	100	100
13	3C	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
13	3c	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
14	3D	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
14	3d	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
15	3E	90/92 (98%)	90 (100%)	0	0	100	100
15	3e	90/92 (98%)	90 (100%)	0	0	100	100
16	3F	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
16	3f	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
17	3G	352/354 (99%)	340 (97%)	12 (3%)	0	100	100
17	3g	352/354 (99%)	340 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	3H	324/326 (99%)	314 (97%)	10 (3%)	0	100	100
18	3h	324/326 (99%)	314 (97%)	10 (3%)	0	100	100
19	3I	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
19	3i	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
20	3J	90/92 (98%)	90 (100%)	0	0	100	100
20	3j	90/92 (98%)	90 (100%)	0	0	100	100
21	3K	77/79 (98%)	77 (100%)	0	0	100	100
21	3k	77/79 (98%)	77 (100%)	0	0	100	100
22	3L	67/69 (97%)	64 (96%)	2 (3%)	1 (2%)	8	6
22	3l	67/69 (97%)	64 (96%)	2 (3%)	1 (2%)	8	6
23	40	228/230 (99%)	226 (99%)	2 (1%)	0	100	100
23	41	228/230 (99%)	226 (99%)	2 (1%)	0	100	100
24	4A	98/100 (98%)	98 (100%)	0	0	100	100
24	4a	98/100 (98%)	98 (100%)	0	0	100	100
25	4B	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
25	4b	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
26	4C	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
26	4c	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
27	4D	88/90 (98%)	88 (100%)	0	0	100	100
27	4d	88/90 (98%)	88 (100%)	0	0	100	100
28	4E	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
28	4e	150/152 (99%)	146 (97%)	4 (3%)	0	100	100
29	4F	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
29	4f	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
30	4G	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
30	4g	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
31	4H	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
31	4h	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
32	4I	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
32	4i	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
33	4J	184/186 (99%)	178 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	4j	184/186 (99%)	178 (97%)	6 (3%)	0	100	100
34	4K	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
34	4k	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
35	4L	120/122 (98%)	120 (100%)	0	0	100	100
35	4l	120/122 (98%)	120 (100%)	0	0	100	100
36	4M	96/98 (98%)	96 (100%)	0	0	100	100
36	4m	96/98 (98%)	96 (100%)	0	0	100	100
37	4N	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
37	4n	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
38	4O	45/47 (96%)	45 (100%)	0	0	100	100
38	4o	45/47 (96%)	45 (100%)	0	0	100	100
39	4P	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
39	4p	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
40	4Q	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
40	4q	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
41	4R	101/103 (98%)	101 (100%)	0	0	100	100
41	4r	101/103 (98%)	101 (100%)	0	0	100	100
42	4S	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
42	4s	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
43	4T	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
43	4t	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
44	4U	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
44	4u	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
45	4V	183/185 (99%)	182 (100%)	1 (0%)	0	100	100
45	4v	183/185 (99%)	182 (100%)	1 (0%)	0	100	100
46	4W	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
46	4w	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
47	4X	224/226 (99%)	221 (99%)	3 (1%)	0	100	100
47	4x	224/226 (99%)	221 (99%)	3 (1%)	0	100	100
48	4Y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
48	4y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	4Z	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
49	4z	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
All	All	16000/16196 (99%)	15719 (98%)	277 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	3L	604	PHE
22	3l	604	PHE
1	2M	26	ALA
1	2m	26	ALA

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	2M	481/481 (100%)	478 (99%)	3 (1%)	78	89
1	2m	481/481 (100%)	478 (99%)	3 (1%)	78	89
2	2N	221/221 (100%)	219 (99%)	2 (1%)	70	84
2	2n	221/221 (100%)	219 (99%)	2 (1%)	70	84
3	2O	130/130 (100%)	130 (100%)	0	100	100
3	2o	130/130 (100%)	130 (100%)	0	100	100
4	2P	139/139 (100%)	139 (100%)	0	100	100
4	2p	139/139 (100%)	139 (100%)	0	100	100
5	2Q	60/60 (100%)	60 (100%)	0	100	100
5	2q	60/60 (100%)	60 (100%)	0	100	100
6	2R	100/100 (100%)	100 (100%)	0	100	100
6	2r	100/100 (100%)	100 (100%)	0	100	100
7	2S	144/144 (100%)	144 (100%)	0	100	100
7	2s	144/144 (100%)	144 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2T	73/73 (100%)	73 (100%)	0	100	100
8	2t	73/73 (100%)	73 (100%)	0	100	100
9	2U	43/43 (100%)	43 (100%)	0	100	100
9	2u	43/43 (100%)	43 (100%)	0	100	100
10	2V	76/76 (100%)	76 (100%)	0	100	100
10	2v	76/76 (100%)	76 (100%)	0	100	100
11	3A	386/386 (100%)	386 (100%)	0	100	100
11	3a	386/386 (100%)	386 (100%)	0	100	100
12	3B	423/423 (100%)	422 (100%)	1 (0%)	87	94
12	3b	423/423 (100%)	422 (100%)	1 (0%)	87	94
13	3C	204/204 (100%)	203 (100%)	1 (0%)	81	90
13	3c	204/204 (100%)	203 (100%)	1 (0%)	81	90
14	3D	88/88 (100%)	88 (100%)	0	100	100
14	3d	88/88 (100%)	88 (100%)	0	100	100
15	3E	81/81 (100%)	81 (100%)	0	100	100
15	3e	81/81 (100%)	81 (100%)	0	100	100
16	3F	72/72 (100%)	72 (100%)	0	100	100
16	3f	72/72 (100%)	72 (100%)	0	100	100
17	3G	336/336 (100%)	334 (99%)	2 (1%)	78	89
17	3g	336/336 (100%)	334 (99%)	2 (1%)	78	89
18	3H	280/280 (100%)	280 (100%)	0	100	100
18	3h	280/280 (100%)	280 (100%)	0	100	100
19	3I	154/154 (100%)	153 (99%)	1 (1%)	78	89
19	3i	154/154 (100%)	153 (99%)	1 (1%)	78	89
20	3J	79/79 (100%)	79 (100%)	0	100	100
20	3j	79/79 (100%)	79 (100%)	0	100	100
21	3K	67/67 (100%)	67 (100%)	0	100	100
21	3k	67/67 (100%)	67 (100%)	0	100	100
22	3L	48/60 (80%)	48 (100%)	0	100	100
22	3l	48/60 (80%)	48 (100%)	0	100	100
23	40	229/229 (100%)	229 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	4I	229/229 (100%)	229 (100%)	0	100	100
24	4A	91/91 (100%)	90 (99%)	1 (1%)	65	79
24	4a	91/91 (100%)	90 (99%)	1 (1%)	65	79
25	4B	77/77 (100%)	75 (97%)	2 (3%)	40	55
25	4b	77/77 (100%)	75 (97%)	2 (3%)	40	55
26	4C	64/64 (100%)	64 (100%)	0	100	100
26	4c	64/64 (100%)	64 (100%)	0	100	100
27	4D	81/81 (100%)	81 (100%)	0	100	100
27	4d	81/81 (100%)	81 (100%)	0	100	100
28	4E	146/146 (100%)	146 (100%)	0	100	100
28	4e	146/146 (100%)	146 (100%)	0	100	100
29	4F	63/63 (100%)	63 (100%)	0	100	100
29	4f	63/63 (100%)	63 (100%)	0	100	100
30	4G	83/83 (100%)	82 (99%)	1 (1%)	63	78
30	4g	83/83 (100%)	82 (99%)	1 (1%)	63	78
31	4H	124/124 (100%)	124 (100%)	0	100	100
31	4h	124/124 (100%)	124 (100%)	0	100	100
32	4I	180/180 (100%)	178 (99%)	2 (1%)	65	79
32	4i	180/180 (100%)	178 (99%)	2 (1%)	65	79
33	4J	148/148 (100%)	145 (98%)	3 (2%)	48	64
33	4j	148/148 (100%)	145 (98%)	3 (2%)	48	64
34	4K	77/77 (100%)	77 (100%)	0	100	100
34	4k	77/77 (100%)	77 (100%)	0	100	100
35	4L	108/108 (100%)	108 (100%)	0	100	100
35	4l	108/108 (100%)	108 (100%)	0	100	100
36	4M	85/85 (100%)	85 (100%)	0	100	100
36	4m	85/85 (100%)	85 (100%)	0	100	100
37	4N	112/112 (100%)	112 (100%)	0	100	100
37	4n	112/112 (100%)	112 (100%)	0	100	100
38	4O	40/40 (100%)	40 (100%)	0	100	100
38	4o	40/40 (100%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	4P	163/163 (100%)	163 (100%)	0	100	100
39	4p	163/163 (100%)	163 (100%)	0	100	100
40	4Q	419/419 (100%)	417 (100%)	2 (0%)	81	90
40	4q	419/419 (100%)	417 (100%)	2 (0%)	81	90
41	4R	92/92 (100%)	92 (100%)	0	100	100
41	4r	92/92 (100%)	92 (100%)	0	100	100
42	4S	59/59 (100%)	59 (100%)	0	100	100
42	4s	59/59 (100%)	59 (100%)	0	100	100
43	4T	102/102 (100%)	102 (100%)	0	100	100
43	4t	102/102 (100%)	102 (100%)	0	100	100
44	4U	76/76 (100%)	75 (99%)	1 (1%)	61	76
44	4u	76/76 (100%)	75 (99%)	1 (1%)	61	76
45	4V	156/156 (100%)	154 (99%)	2 (1%)	61	76
45	4v	156/156 (100%)	154 (99%)	2 (1%)	61	76
46	4W	128/128 (100%)	128 (100%)	0	100	100
46	4w	128/128 (100%)	128 (100%)	0	100	100
47	4X	198/198 (100%)	197 (100%)	1 (0%)	81	90
47	4x	198/198 (100%)	197 (100%)	1 (0%)	81	90
48	4Y	100/100 (100%)	100 (100%)	0	100	100
48	4y	100/100 (100%)	100 (100%)	0	100	100
49	4Z	167/167 (100%)	167 (100%)	0	100	100
49	4z	167/167 (100%)	167 (100%)	0	100	100
All	All	14106/14130 (100%)	14056 (100%)	50 (0%)	81	92

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2M	150	PHE
1	2M	586	LYS
1	2M	590	SER
2	2N	80	CYS
2	2N	278	MET
12	3B	219	PHE
13	3C	183	LEU

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Mol	Chain	Res	Type
17	3G	251	HIS
17	3G	348	TYR
19	3I	32	SER
24	4A	26	ASP
25	4B	3	ILE
25	4B	11	THR
30	4G	24	TRP
32	4I	67	GLU
32	4I	74	ASP
33	4J	62	CYS
33	4J	67	SER
33	4J	104	GLN
40	4Q	529	TRP
40	4Q	769	SER
44	4U	413	ILE
45	4V	43	VAL
45	4V	102	GLU
47	4X	37	HIS
1	2m	150	PHE
1	2m	586	LYS
1	2m	590	SER
2	2n	80	CYS
2	2n	278	MET
12	3b	219	PHE
13	3c	183	LEU
17	3g	251	HIS
17	3g	348	TYR
19	3i	32	SER
24	4a	26	ASP
25	4b	3	ILE
25	4b	11	THR
30	4g	24	TRP
32	4i	67	GLU
32	4i	74	ASP
33	4j	62	CYS
33	4j	67	SER
33	4j	104	GLN
40	4q	529	TRP
40	4q	769	SER
44	4u	413	ILE
45	4v	43	VAL
45	4v	102	GLU

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Mol	Chain	Res	Type
47	4x	37	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	2M	147	GLN
1	2M	228	HIS
1	2M	248	HIS
1	2M	274	HIS
1	2M	341	HIS
1	2M	434	ASN
1	2M	571	HIS
2	2N	49	GLN
2	2N	88	ASN
2	2N	97	GLN
2	2N	130	GLN
2	2N	195	GLN
3	2O	32	HIS
4	2P	142	GLN
7	2S	14	GLN
7	2S	69	HIS
7	2S	160	HIS
9	2U	26	HIS
11	3A	112	ASN
11	3A	144	ASN
11	3A	213	ASN
11	3A	214	ASN
11	3A	230	HIS
11	3A	363	HIS
11	3A	470	GLN
12	3B	76	HIS
12	3B	86	HIS
12	3B	108	GLN
13	3C	57	HIS
13	3C	224	GLN
13	3C	261	HIS
15	3E	37	HIS
16	3F	34	GLN
17	3G	137	ASN
17	3G	186	HIS
17	3G	205	ASN
17	3G	228	ASN

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Mol	Chain	Res	Type
18	3H	100	HIS
18	3H	156	ASN
18	3H	187	HIS
23	40	38	ASN
23	40	59	ASN
23	40	91	ASN
23	40	97	HIS
23	40	146	ASN
24	4A	32	HIS
28	4E	9	ASN
32	4I	89	GLN
33	4J	64	HIS
33	4J	100	HIS
33	4J	123	ASN
38	4O	381	HIS
39	4P	55	GLN
39	4P	88	HIS
39	4P	110	GLN
39	4P	147	ASN
39	4P	178	GLN
40	4Q	446	ASN
40	4Q	502	ASN
40	4Q	681	HIS
40	4Q	697	ASN
44	4U	378	GLN
45	4V	40	ASN
46	4W	12	HIS
46	4W	61	HIS
46	4W	118	HIS
47	4X	37	HIS
47	4X	104	GLN
47	4X	137	ASN
49	4Z	140	ASN
1	2m	147	GLN
1	2m	228	HIS
1	2m	248	HIS
1	2m	274	HIS
1	2m	341	HIS
1	2m	434	ASN
1	2m	571	HIS
2	2n	49	GLN
2	2n	88	ASN

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Mol	Chain	Res	Type
2	2n	97	GLN
2	2n	130	GLN
2	2n	195	GLN
3	2o	32	HIS
4	2p	142	GLN
7	2s	14	GLN
7	2s	50	HIS
7	2s	160	HIS
9	2u	26	HIS
11	3a	112	ASN
11	3a	144	ASN
11	3a	213	ASN
11	3a	214	ASN
11	3a	230	HIS
11	3a	363	HIS
11	3a	470	GLN
13	3c	224	GLN
13	3c	261	HIS
15	3e	37	HIS
16	3f	6	HIS
16	3f	34	GLN
17	3g	137	ASN
17	3g	186	HIS
17	3g	190	ASN
17	3g	205	ASN
17	3g	228	ASN
18	3h	156	ASN
18	3h	187	HIS
23	4l	38	ASN
23	4l	59	ASN
23	4l	91	ASN
23	4l	146	ASN
23	4l	151	ASN
24	4a	32	HIS
28	4e	9	ASN
32	4i	89	GLN
33	4j	64	HIS
33	4j	100	HIS
33	4j	123	ASN
33	4j	199	HIS
35	4l	96	ASN
37	4n	117	ASN

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Mol	Chain	Res	Type
38	4o	381	HIS
39	4p	88	HIS
39	4p	110	GLN
39	4p	178	GLN
40	4q	446	ASN
40	4q	502	ASN
40	4q	681	HIS
45	4v	40	ASN
46	4w	12	HIS
46	4w	61	HIS
46	4w	118	HIS
47	4x	104	GLN
47	4x	137	ASN
49	4z	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 162 ligands modelled in this entry, 14 are monoatomic - leaving 148 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
57	CDL	4S	101	-	99,99,99	0.28	0	105,111,111	0.39	0
57	CDL	4q	907	-	99,99,99	0.29	0	105,111,111	0.48	1 (0%)
57	CDL	4k	201	-	99,99,99	0.28	0	105,111,111	0.33	0
57	CDL	4K	201	-	99,99,99	0.28	0	105,111,111	0.33	0
57	CDL	2u	101	-	99,99,99	0.29	0	105,111,111	0.31	0
62	LPP	4C	101	-	43,43,43	0.26	0	46,48,48	0.34	0
56	PC1	2T	101	-	53,53,53	0.29	0	59,61,61	0.35	0
57	CDL	3e	202	-	99,99,99	0.29	0	105,111,111	0.37	0
55	PEE	4r	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.58	0
57	CDL	4l	201	-	99,99,99	0.28	0	105,111,111	0.34	0
57	CDL	3H	402	-	99,99,99	0.30	0	105,111,111	0.41	0
51	FES	2N	301	2	0,4,4	-	-	-	-	-
66	HEA	4q	904	40	67,67,67	1.37	7 (10%)	81,103,103	2.08	25 (30%)
58	UQ8	3G	405	-	53,53,53	1.86	6 (11%)	66,67,67	1.53	15 (22%)
55	PEE	4W	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
61	AJP	4l	304	-	49,49,95	1.08	3 (6%)	75,80,149	1.56	13 (17%)
55	PEE	4Z	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.54	0
57	CDL	2U	101	-	99,99,99	0.29	0	105,111,111	0.31	0
51	FES	2n	301	2	0,4,4	-	-	-	-	-
55	PEE	4l	303	-	50,50,50	0.79	2 (4%)	53,55,55	0.53	0
57	CDL	3l	702	-	99,99,99	0.30	0	105,111,111	0.32	0
55	PEE	2R	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.50	0
55	PEE	2o	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.66	0
55	PEE	4Q	910	-	50,50,50	0.79	2 (4%)	53,55,55	0.61	1 (1%)
57	CDL	4s	101	-	99,99,99	0.28	0	105,111,111	0.39	0
63	CUA	4n	201	37	0,1,1	-	-	-	-	-
57	CDL	4j	301	-	99,99,99	0.29	0	105,111,111	0.43	0
60	HEM	3g	402	17	50,50,50	1.47	7 (14%)	67,82,82	1.32	7 (10%)
57	CDL	4Q	907	-	99,99,99	0.29	0	105,111,111	0.48	1 (0%)
56	PC1	2t	101	-	53,53,53	0.29	0	59,61,61	0.35	0
57	CDL	2p	201	-	99,99,99	0.29	0	105,111,111	0.33	0
58	UQ8	3g	405	-	53,53,53	1.87	6 (11%)	66,67,67	1.53	15 (22%)
55	PEE	4o	301	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
56	PC1	3A	502	-	53,53,53	0.30	0	59,61,61	0.41	0
55	PEE	2r	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.50	0
50	FAD	2M	701	-	58,58,58	0.70	3 (5%)	85,89,89	0.97	4 (4%)
57	CDL	3D	201	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
55	PEE	4d	101	-	50,50,50	0.77	2 (4%)	53,55,55	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PEE	2P	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.57	0
58	UQ8	3G	404	-	53,53,53	1.83	6 (11%)	66,67,67	1.72	17 (25%)
57	CDL	4M	201	-	99,99,99	0.28	0	105,111,111	0.30	0
57	CDL	4q	908	-	99,99,99	0.29	0	105,111,111	0.33	0
57	CDL	4w	201	-	99,99,99	0.28	0	105,111,111	0.34	0
50	FAD	2m	701	-	58,58,58	0.70	3 (5%)	85,89,89	0.97	4 (4%)
57	CDL	2P	201	-	99,99,99	0.29	0	105,111,111	0.33	0
57	CDL	3d	201	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
57	CDL	3i	203	-	99,99,99	0.29	0	105,111,111	0.46	1 (0%)
67	PER	4Q	906	64,66	1,1,1	0.18	0	-		
55	PEE	2P	202	-	50,50,50	0.77	2 (4%)	53,55,55	0.52	0
56	PC1	2O	203	-	53,53,53	0.28	0	59,61,61	0.57	1 (1%)
55	PEE	2O	201	-	50,50,50	0.78	2 (4%)	53,55,55	0.66	0
57	CDL	3e	201	-	99,99,99	0.30	0	105,111,111	0.44	0
57	CDL	2q	101	-	99,99,99	0.29	0	105,111,111	0.37	1 (0%)
57	CDL	3h	402	-	99,99,99	0.30	0	105,111,111	0.41	0
57	CDL	4k	202	-	99,99,99	0.28	0	105,111,111	0.41	0
56	PC1	2O	202	-	53,53,53	0.28	0	59,61,61	0.42	0
55	PEE	2p	202	-	50,50,50	0.77	2 (4%)	53,55,55	0.52	0
60	HEM	3G	401	17	50,50,50	1.50	7 (14%)	67,82,82	1.26	5 (7%)
57	CDL	4J	301	-	99,99,99	0.29	0	105,111,111	0.43	0
55	PEE	40	303	-	50,50,50	0.79	2 (4%)	53,55,55	0.53	0
55	PEE	4R	201	-	50,50,50	0.77	2 (4%)	53,55,55	0.58	0
57	CDL	4L	201	-	99,99,99	0.29	0	105,111,111	0.34	0
57	CDL	4z	301	-	99,99,99	0.28	0	105,111,111	0.43	1 (0%)
57	CDL	4m	201	-	99,99,99	0.28	0	105,111,111	0.30	0
57	CDL	3E	202	-	99,99,99	0.29	0	105,111,111	0.37	0
58	UQ8	2S	201	-	53,53,53	1.84	7 (13%)	66,67,67	1.62	16 (24%)
57	CDL	3D	202	-	99,99,99	0.32	0	105,111,111	0.47	0
57	CDL	4Q	908	-	99,99,99	0.29	0	105,111,111	0.33	0
57	CDL	2o	201	-	99,99,99	0.29	0	105,111,111	0.32	0
57	CDL	2Q	101	-	99,99,99	0.29	0	105,111,111	0.37	1 (0%)
55	PEE	4q	909	-	50,50,50	0.77	2 (4%)	53,55,55	0.65	1 (1%)
57	CDL	3I	203	-	99,99,99	0.30	0	105,111,111	0.39	0
56	PC1	3a	501	-	53,53,53	0.30	0	59,61,61	0.55	1 (1%)
59	HEC	3c	301	13	46,50,50	1.96	6 (13%)	58,82,82	1.78	5 (8%)
60	HEM	3G	402	17	50,50,50	1.47	7 (14%)	67,82,82	1.32	7 (10%)
62	LPP	4d	102	-	43,43,43	0.21	0	46,48,48	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PC1	2r	202	-	53,53,53	0.29	0	59,61,61	0.46	0
58	UQ8	3D	203	-	53,53,53	1.90	5 (9%)	66,67,67	1.66	12 (18%)
57	CDL	3G	403	-	99,99,99	0.30	0	105,111,111	0.40	1 (0%)
57	CDL	4e	201	-	99,99,99	0.28	0	105,111,111	0.40	0
57	CDL	4W	201	-	99,99,99	0.28	0	105,111,111	0.34	0
58	UQ8	3d	203	-	53,53,53	1.90	5 (9%)	66,67,67	1.66	12 (18%)
56	PC1	4e	202	-	53,53,53	0.29	0	59,61,61	0.46	0
57	CDL	4T	203	-	99,99,99	0.29	0	105,111,111	0.29	0
55	PEE	4Q	909	-	50,50,50	0.76	2 (4%)	53,55,55	0.65	1 (1%)
57	CDL	3i	201	-	99,99,99	0.30	0	105,111,111	0.39	0
63	CUA	4N	201	37	0,1,1	-	-	-	-	-
55	PEE	3C	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.68	1 (1%)
56	PC1	3a	502	-	53,53,53	0.30	0	59,61,61	0.41	0
53	F3S	2N	303	2	0,9,9	-	-	-	-	-
52	SF4	2n	302	2	0,12,12	-	-	-	-	-
55	PEE	4D	101	-	50,50,50	0.77	2 (4%)	53,55,55	0.48	0
55	PEE	3c	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.68	1 (1%)
57	CDL	4U	501	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
57	CDL	3e	203	-	99,99,99	0.28	0	105,111,111	0.40	1 (0%)
62	LPP	4D	102	-	43,43,43	0.21	0	46,48,48	0.31	0
56	PC1	4E	202	-	53,53,53	0.29	0	59,61,61	0.46	0
57	CDL	2O	204	-	99,99,99	0.29	0	105,111,111	0.32	0
51	FES	3h	401	18	0,4,4	-	-	-	-	-
57	CDL	3g	403	-	99,99,99	0.31	0	105,111,111	0.40	1 (0%)
61	AJP	40	304	-	49,49,95	1.08	3 (6%)	75,80,149	1.56	13 (17%)
59	HEC	3C	301	13	46,50,50	1.95	6 (13%)	58,82,82	1.78	6 (10%)
53	F3S	2n	303	2	0,9,9	-	-	-	-	-
66	HEA	4Q	905	67,40	67,67,67	1.36	9 (13%)	81,103,103	2.05	24 (29%)
51	FES	3H	401	18	0,4,4	-	-	-	-	-
56	PC1	2p	204	-	53,53,53	0.28	0	59,61,61	0.36	0
66	HEA	4Q	904	40	67,67,67	1.37	7 (10%)	81,103,103	2.08	25 (30%)
57	CDL	3I	202	-	99,99,99	0.29	0	105,111,111	0.46	1 (0%)
57	CDL	3d	202	-	99,99,99	0.31	0	105,111,111	0.47	0
55	PEE	4I	301	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
56	PC1	2o	203	-	53,53,53	0.28	0	59,61,61	0.42	0
57	CDL	3i	202	-	99,99,99	0.29	0	105,111,111	0.47	1 (0%)
57	CDL	4t	203	-	99,99,99	0.29	0	105,111,111	0.29	0
57	CDL	4w	202	-	99,99,99	0.28	0	105,111,111	0.33	0
55	PEE	40	302	-	50,50,50	0.76	2 (4%)	53,55,55	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PEE	4S	102	-	50,50,50	0.78	2 (4%)	53,55,55	0.55	0
60	HEM	3g	401	17	50,50,50	1.50	8 (16%)	67,82,82	1.26	5 (7%)
56	PC1	3H	403	-	53,53,53	0.30	0	59,61,61	0.42	0
57	CDL	3l	701	-	99,99,99	0.30	0	105,111,111	0.37	0
52	SF4	2N	302	2	0,12,12	-	-	-		
55	PEE	3F	101	-	50,50,50	0.78	2 (4%)	53,55,55	0.58	0
55	PEE	4l	302	-	50,50,50	0.76	2 (4%)	53,55,55	0.51	0
57	CDL	4Z	301	-	99,99,99	0.28	0	105,111,111	0.43	1 (0%)
56	PC1	2o	204	-	53,53,53	0.28	0	59,61,61	0.57	1 (1%)
57	CDL	3E	203	-	99,99,99	0.29	0	105,111,111	0.40	1 (0%)
67	PER	4q	906	64,66	1,1,1	0.18	0	-		
57	CDL	3l	201	-	99,99,99	0.29	0	105,111,111	0.47	1 (0%)
57	CDL	4W	202	-	99,99,99	0.28	0	105,111,111	0.33	0
58	UQ8	2s	201	-	53,53,53	1.84	7 (13%)	66,67,67	1.62	16 (24%)
57	CDL	4E	201	-	99,99,99	0.28	0	105,111,111	0.41	0
57	CDL	4K	202	-	99,99,99	0.28	0	105,111,111	0.41	0
62	LPP	4c	101	-	43,43,43	0.26	0	46,48,48	0.34	0
57	CDL	3L	702	-	99,99,99	0.30	0	105,111,111	0.32	0
55	PEE	2p	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.57	0
55	PEE	3f	101	-	50,50,50	0.78	2 (4%)	53,55,55	0.58	0
57	CDL	4u	501	-	99,99,99	0.29	0	105,111,111	0.43	1 (0%)
55	PEE	4s	102	-	50,50,50	0.78	2 (4%)	53,55,55	0.55	0
66	HEA	4q	905	67,40	67,67,67	1.36	9 (13%)	81,103,103	2.04	24 (29%)
55	PEE	4q	910	-	50,50,50	0.79	2 (4%)	53,55,55	0.61	1 (1%)
57	CDL	3E	201	-	99,99,99	0.30	0	105,111,111	0.44	0
56	PC1	2P	204	-	53,53,53	0.28	0	59,61,61	0.36	0
55	PEE	4z	302	-	50,50,50	0.79	2 (4%)	53,55,55	0.54	0
56	PC1	2R	202	-	53,53,53	0.29	0	59,61,61	0.46	0
56	PC1	3A	501	-	53,53,53	0.29	0	59,61,61	0.55	1 (1%)
55	PEE	4w	203	-	50,50,50	0.77	2 (4%)	53,55,55	0.55	0
56	PC1	3h	403	-	53,53,53	0.29	0	59,61,61	0.42	0
58	UQ8	3g	404	-	53,53,53	1.83	7 (13%)	66,67,67	1.72	17 (25%)
57	CDL	3L	701	-	99,99,99	0.30	0	105,111,111	0.37	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
57	CDL	4S	101	-	-	20/110/110/110	-
57	CDL	4q	907	-	-	38/110/110/110	-
57	CDL	4k	201	-	-	28/110/110/110	-
57	CDL	4K	201	-	-	28/110/110/110	-
57	CDL	2u	101	-	-	18/110/110/110	-
62	LPP	4C	101	-	-	13/45/45/45	-
56	PC1	2T	101	-	-	13/57/57/57	-
57	CDL	3e	202	-	-	26/110/110/110	-
55	PEE	4r	201	-	-	16/54/54/54	-
57	CDL	4l	201	-	-	14/110/110/110	-
57	CDL	3H	402	-	-	13/110/110/110	-
51	FES	2N	301	2	-	-	0/1/1/1
66	HEA	4q	904	40	-	7/36/76/76	-
58	UQ8	3G	405	-	-	6/51/75/75	0/1/1/1
55	PEE	4W	203	-	-	11/54/54/54	-
61	AJP	4l	304	-	3/3/19/38	3/6/121/220	0/7/7/11
55	PEE	4Z	302	-	-	24/54/54/54	-
57	CDL	2U	101	-	-	18/110/110/110	-
51	FES	2n	301	2	-	-	0/1/1/1
55	PEE	4l	303	-	-	19/54/54/54	-
57	CDL	3l	702	-	-	22/110/110/110	-
55	PEE	2R	201	-	-	18/54/54/54	-
55	PEE	2o	202	-	-	16/54/54/54	-
55	PEE	4Q	910	-	-	13/54/54/54	-
57	CDL	4s	101	-	-	20/110/110/110	-
57	CDL	4j	301	-	-	32/110/110/110	-
60	HEM	3g	402	17	-	4/14/54/54	-
57	CDL	4Q	907	-	-	38/110/110/110	-
56	PC1	2t	101	-	-	13/57/57/57	-
57	CDL	2p	201	-	-	21/110/110/110	-
58	UQ8	3g	405	-	-	6/51/75/75	0/1/1/1
55	PEE	40	301	-	-	13/54/54/54	-
56	PC1	3A	502	-	-	15/57/57/57	-
55	PEE	2r	201	-	-	18/54/54/54	-
50	FAD	2M	701	-	-	4/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	3D	201	-	-	38/110/110/110	-
55	PEE	4d	101	-	-	15/54/54/54	-
55	PEE	2P	203	-	-	17/54/54/54	-
58	UQ8	3G	404	-	-	14/51/75/75	0/1/1/1
57	CDL	4M	201	-	-	16/110/110/110	-
57	CDL	4q	908	-	-	19/110/110/110	-
57	CDL	4w	201	-	-	16/110/110/110	-
50	FAD	2m	701	-	-	4/34/50/50	0/6/6/6
57	CDL	2P	201	-	-	21/110/110/110	-
57	CDL	3d	201	-	-	38/110/110/110	-
57	CDL	3i	203	-	-	37/110/110/110	-
55	PEE	2P	202	-	-	18/54/54/54	-
56	PC1	2O	203	-	-	14/57/57/57	-
55	PEE	2O	201	-	-	16/54/54/54	-
57	CDL	3e	201	-	-	28/110/110/110	-
57	CDL	2q	101	-	-	31/110/110/110	-
57	CDL	3h	402	-	-	12/110/110/110	-
57	CDL	4k	202	-	-	29/110/110/110	-
56	PC1	2O	202	-	-	9/57/57/57	-
55	PEE	2p	202	-	-	18/54/54/54	-
60	HEM	3G	401	17	-	5/14/54/54	-
57	CDL	4J	301	-	-	32/110/110/110	-
55	PEE	40	303	-	-	19/54/54/54	-
55	PEE	4R	201	-	-	16/54/54/54	-
57	CDL	4L	201	-	-	14/110/110/110	-
57	CDL	4z	301	-	-	16/110/110/110	-
57	CDL	4m	201	-	-	16/110/110/110	-
57	CDL	3E	202	-	-	26/110/110/110	-
58	UQ8	2S	201	-	-	8/51/75/75	0/1/1/1
57	CDL	3D	202	-	-	56/110/110/110	-
57	CDL	4Q	908	-	-	19/110/110/110	-
57	CDL	2o	201	-	-	21/110/110/110	-
57	CDL	2Q	101	-	-	31/110/110/110	-
55	PEE	4q	909	-	-	21/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	3I	203	-	-	22/110/110/110	-
56	PC1	3a	501	-	-	19/57/57/57	-
59	HEC	3c	301	13	-	9/14/54/54	-
60	HEM	3G	402	17	-	4/14/54/54	-
62	LPP	4d	102	-	-	5/45/45/45	-
56	PC1	2r	202	-	-	16/57/57/57	-
58	UQ8	3D	203	-	-	12/51/75/75	0/1/1/1
57	CDL	3G	403	-	-	22/110/110/110	-
57	CDL	4e	201	-	-	29/110/110/110	-
57	CDL	4W	201	-	-	16/110/110/110	-
58	UQ8	3d	203	-	-	12/51/75/75	0/1/1/1
56	PC1	4e	202	-	-	10/57/57/57	-
57	CDL	4T	203	-	-	23/110/110/110	-
55	PEE	4Q	909	-	-	21/54/54/54	-
57	CDL	3i	201	-	-	22/110/110/110	-
55	PEE	3C	302	-	-	14/54/54/54	-
56	PC1	3a	502	-	-	14/57/57/57	-
53	F3S	2N	303	2	-	-	0/3/3/3
52	SF4	2n	302	2	-	-	0/6/5/5
55	PEE	4D	101	-	-	15/54/54/54	-
55	PEE	3c	302	-	-	14/54/54/54	-
57	CDL	4U	501	-	-	33/110/110/110	-
57	CDL	3e	203	-	-	36/110/110/110	-
62	LPP	4D	102	-	-	5/45/45/45	-
56	PC1	4E	202	-	-	10/57/57/57	-
57	CDL	2O	204	-	-	21/110/110/110	-
51	FES	3h	401	18	-	-	0/1/1/1
61	AJP	40	304	-	3/3/19/38	3/6/121/220	0/7/7/11
57	CDL	3g	403	-	-	22/110/110/110	-
59	HEC	3C	301	13	-	9/14/54/54	-
53	F3S	2n	303	2	-	-	0/3/3/3
66	HEA	4Q	905	67,40	-	9/36/76/76	-
51	FES	3H	401	18	-	-	0/1/1/1
56	PC1	2p	204	-	-	4/57/57/57	-
66	HEA	4Q	904	40	-	7/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CDL	3I	202	-	-	37/110/110/110	-
57	CDL	3d	202	-	-	56/110/110/110	-
55	PEE	4I	301	-	-	13/54/54/54	-
56	PC1	2o	203	-	-	9/57/57/57	-
57	CDL	3i	202	-	-	25/110/110/110	-
57	CDL	4t	203	-	-	23/110/110/110	-
57	CDL	4w	202	-	-	28/110/110/110	-
55	PEE	40	302	-	-	5/54/54/54	-
55	PEE	4S	102	-	-	10/54/54/54	-
60	HEM	3g	401	17	-	5/14/54/54	-
56	PC1	3H	403	-	-	16/57/57/57	-
57	CDL	3I	701	-	-	31/110/110/110	-
52	SF4	2N	302	2	-	-	0/6/5/5
55	PEE	3F	101	-	-	16/54/54/54	-
55	PEE	4I	302	-	-	5/54/54/54	-
57	CDL	4Z	301	-	-	16/110/110/110	-
56	PC1	2o	204	-	-	14/57/57/57	-
57	CDL	3E	203	-	-	36/110/110/110	-
57	CDL	3I	201	-	-	25/110/110/110	-
57	CDL	4W	202	-	-	28/110/110/110	-
58	UQ8	2s	201	-	-	8/51/75/75	0/1/1/1
57	CDL	4E	201	-	-	29/110/110/110	-
57	CDL	4K	202	-	-	29/110/110/110	-
62	LPP	4c	101	-	-	12/45/45/45	-
57	CDL	3L	702	-	-	21/110/110/110	-
55	PEE	2p	203	-	-	17/54/54/54	-
55	PEE	3f	101	-	-	16/54/54/54	-
57	CDL	4u	501	-	-	35/110/110/110	-
55	PEE	4s	102	-	-	10/54/54/54	-
66	HEA	4q	905	67,40	-	9/36/76/76	-
55	PEE	4q	910	-	-	13/54/54/54	-
57	CDL	3E	201	-	-	29/110/110/110	-
56	PC1	2P	204	-	-	4/57/57/57	-
55	PEE	4z	302	-	-	24/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PC1	2R	202	-	-	16/57/57/57	-
56	PC1	3A	501	-	-	19/57/57/57	-
55	PEE	4w	203	-	-	11/54/54/54	-
56	PC1	3h	403	-	-	16/57/57/57	-
58	UQ8	3g	404	-	-	14/51/75/75	0/1/1/1
57	CDL	3L	701	-	-	30/110/110/110	-

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	3D	203	UQ8	C6-C1	10.42	1.53	1.35
58	3d	203	UQ8	C6-C1	10.40	1.53	1.35
58	3G	405	UQ8	C6-C1	9.95	1.53	1.35
58	3g	405	UQ8	C6-C1	9.94	1.53	1.35
58	2s	201	UQ8	C6-C1	9.92	1.53	1.35
58	2S	201	UQ8	C6-C1	9.85	1.52	1.35
58	3G	404	UQ8	C6-C1	9.78	1.52	1.35
58	3g	404	UQ8	C6-C1	9.78	1.52	1.35
59	3C	301	HEC	CAC-C3C	7.25	1.58	1.35
59	3c	301	HEC	CAC-C3C	7.25	1.58	1.35
59	3c	301	HEC	CAB-C3B	6.64	1.56	1.35
59	3C	301	HEC	CAB-C3B	6.62	1.56	1.35
58	3g	405	UQ8	C4-C3	4.68	1.53	1.36
58	3G	405	UQ8	C4-C3	4.67	1.53	1.36
58	3D	203	UQ8	C4-C3	4.59	1.52	1.36
58	3d	203	UQ8	C4-C3	4.59	1.52	1.36
58	2S	201	UQ8	C4-C3	4.56	1.52	1.36
58	2s	201	UQ8	C4-C3	4.53	1.52	1.36
58	3g	404	UQ8	C4-C3	4.38	1.52	1.36
58	3G	404	UQ8	C4-C3	4.36	1.52	1.36
66	4Q	904	HEA	C3B-C2B	4.23	1.44	1.34
66	4q	904	HEA	C3B-C2B	4.23	1.44	1.34
66	4q	905	HEA	C3B-C2B	4.05	1.43	1.34
66	4Q	905	HEA	C3B-C2B	4.02	1.43	1.34
60	3G	401	HEM	CBB-CAB	3.82	1.48	1.30
60	3G	402	HEM	CBB-CAB	3.81	1.48	1.30
60	3g	402	HEM	CBB-CAB	3.81	1.48	1.30
60	3g	401	HEM	CBB-CAB	3.80	1.48	1.30
60	3G	401	HEM	CBC-CAC	3.77	1.48	1.30
60	3g	401	HEM	CBC-CAC	3.77	1.48	1.30
66	4Q	905	HEA	C3D-C2D	3.75	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	3G	402	HEM	CBC-CAC	3.74	1.48	1.30
60	3g	402	HEM	CBC-CAC	3.74	1.48	1.30
66	4q	905	HEA	C3D-C2D	3.74	1.44	1.36
55	4Z	302	PEE	C39-C38	3.70	1.52	1.31
55	4z	302	PEE	C39-C38	3.70	1.52	1.31
55	4l	303	PEE	C18-C19	3.67	1.52	1.31
55	4R	201	PEE	C39-C38	3.66	1.52	1.31
55	4r	201	PEE	C39-C38	3.66	1.52	1.31
55	40	303	PEE	C18-C19	3.66	1.52	1.31
55	4W	203	PEE	C18-C19	3.65	1.52	1.31
55	4w	203	PEE	C18-C19	3.65	1.52	1.31
55	2o	202	PEE	C39-C38	3.64	1.52	1.31
55	4z	302	PEE	C18-C19	3.64	1.52	1.31
55	4S	102	PEE	C18-C19	3.64	1.52	1.31
55	3C	302	PEE	C18-C19	3.64	1.52	1.31
55	2O	201	PEE	C39-C38	3.63	1.52	1.31
55	2r	201	PEE	C18-C19	3.63	1.52	1.31
55	4Q	910	PEE	C18-C19	3.63	1.52	1.31
55	4q	910	PEE	C18-C19	3.63	1.52	1.31
55	3c	302	PEE	C18-C19	3.63	1.52	1.31
55	3f	101	PEE	C18-C19	3.63	1.52	1.31
55	4s	102	PEE	C18-C19	3.63	1.52	1.31
55	2P	203	PEE	C39-C38	3.62	1.52	1.31
55	2p	203	PEE	C39-C38	3.62	1.52	1.31
55	2R	201	PEE	C18-C19	3.62	1.52	1.31
55	4Q	909	PEE	C18-C19	3.62	1.52	1.31
55	4q	909	PEE	C18-C19	3.62	1.52	1.31
55	4Z	302	PEE	C18-C19	3.62	1.52	1.31
55	4Q	910	PEE	C39-C38	3.62	1.52	1.31
55	4q	910	PEE	C39-C38	3.62	1.52	1.31
55	3F	101	PEE	C18-C19	3.62	1.52	1.31
55	4l	301	PEE	C39-C38	3.61	1.52	1.31
55	4d	101	PEE	C18-C19	3.60	1.52	1.31
55	4D	101	PEE	C18-C19	3.60	1.52	1.31
55	40	301	PEE	C39-C38	3.60	1.52	1.31
55	40	302	PEE	C39-C38	3.60	1.52	1.31
55	2P	202	PEE	C18-C19	3.60	1.52	1.31
55	40	303	PEE	C39-C38	3.59	1.52	1.31
55	4l	302	PEE	C39-C38	3.59	1.52	1.31
55	4l	303	PEE	C39-C38	3.59	1.52	1.31
55	4s	102	PEE	C39-C38	3.59	1.52	1.31
66	4Q	904	HEA	C3D-C2D	3.59	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	4q	904	HEA	C3D-C2D	3.59	1.44	1.36
55	2p	202	PEE	C18-C19	3.59	1.52	1.31
55	4S	102	PEE	C39-C38	3.58	1.52	1.31
55	2O	201	PEE	C18-C19	3.58	1.52	1.31
55	3c	302	PEE	C39-C38	3.58	1.52	1.31
55	4D	101	PEE	C39-C38	3.58	1.52	1.31
55	40	301	PEE	C18-C19	3.57	1.52	1.31
55	3C	302	PEE	C39-C38	3.57	1.52	1.31
55	2p	202	PEE	C39-C38	3.57	1.52	1.31
55	2o	202	PEE	C18-C19	3.56	1.51	1.31
55	4d	101	PEE	C39-C38	3.56	1.51	1.31
55	4l	301	PEE	C18-C19	3.56	1.51	1.31
55	4R	201	PEE	C18-C19	3.56	1.51	1.31
55	2P	202	PEE	C39-C38	3.55	1.51	1.31
55	2R	201	PEE	C39-C38	3.55	1.51	1.31
55	4q	909	PEE	C39-C38	3.54	1.51	1.31
55	4r	201	PEE	C18-C19	3.54	1.51	1.31
55	2P	203	PEE	C18-C19	3.53	1.51	1.31
55	2r	201	PEE	C39-C38	3.53	1.51	1.31
55	4Q	909	PEE	C39-C38	3.52	1.51	1.31
55	2p	203	PEE	C18-C19	3.52	1.51	1.31
61	40	304	AJP	O09-C05	3.50	1.49	1.42
61	4l	304	AJP	O09-C05	3.50	1.49	1.42
55	3f	101	PEE	C39-C38	3.48	1.51	1.31
55	3F	101	PEE	C39-C38	3.46	1.51	1.31
55	4W	203	PEE	C39-C38	3.46	1.51	1.31
55	4w	203	PEE	C39-C38	3.46	1.51	1.31
59	3C	301	HEC	CBC-CAC	-3.45	1.36	1.49
59	3c	301	HEC	CBC-CAC	-3.45	1.36	1.49
55	40	302	PEE	C18-C19	3.45	1.51	1.31
55	4l	302	PEE	C18-C19	3.45	1.51	1.31
66	4Q	904	HEA	C3A-C2A	3.23	1.44	1.37
66	4q	904	HEA	C3A-C2A	3.23	1.44	1.37
66	4q	905	HEA	C3A-C2A	3.10	1.44	1.37
66	4Q	905	HEA	C3A-C2A	3.08	1.44	1.37
66	4q	905	HEA	C4B-C3B	3.03	1.50	1.44
61	40	304	AJP	O09-C08	3.02	1.48	1.43
61	4l	304	AJP	O09-C08	3.02	1.48	1.43
66	4Q	905	HEA	C4B-C3B	3.01	1.50	1.44
50	2M	701	FAD	C4-N3	-2.87	1.33	1.38
50	2m	701	FAD	C4-N3	-2.87	1.33	1.38
60	3g	402	HEM	FE-ND	2.82	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	3G	402	HEM	FE-ND	2.81	2.03	1.94
60	3g	402	HEM	FE-NC	2.74	2.04	1.95
60	3G	402	HEM	FE-NC	2.74	2.04	1.95
60	3G	401	HEM	FE-NC	2.70	2.04	1.95
60	3g	401	HEM	FE-NC	2.69	2.04	1.95
60	3G	401	HEM	FE-ND	2.68	2.03	1.94
60	3g	401	HEM	FE-ND	2.66	2.03	1.94
60	3G	402	HEM	FE-NB	2.53	2.02	1.94
66	4Q	904	HEA	C1D-ND	-2.52	1.35	1.40
60	3g	402	HEM	FE-NB	2.52	2.02	1.94
66	4Q	904	HEA	C1C-C2C	2.50	1.49	1.43
66	4q	904	HEA	C1C-C2C	2.49	1.49	1.43
60	3g	401	HEM	FE-NA	2.49	2.03	1.95
66	4q	904	HEA	C1D-ND	-2.49	1.35	1.40
60	3g	401	HEM	FE-NB	2.48	2.02	1.94
60	3G	401	HEM	FE-NA	2.48	2.03	1.95
60	3G	401	HEM	FE-NB	2.47	2.02	1.94
58	3G	405	UQ8	O3-C3M	-2.45	1.39	1.45
58	3g	405	UQ8	O3-C3M	-2.45	1.39	1.45
58	3G	404	UQ8	O3-C3M	-2.43	1.39	1.45
58	3g	404	UQ8	O3-C3M	-2.43	1.39	1.45
58	3g	405	UQ8	C6-C5	2.42	1.53	1.46
58	3d	203	UQ8	O4-C4M	-2.41	1.39	1.45
58	3D	203	UQ8	O4-C4M	-2.41	1.39	1.45
58	3G	405	UQ8	C6-C5	2.41	1.53	1.46
66	4Q	905	HEA	C1C-C2C	2.38	1.48	1.43
58	3D	203	UQ8	C6-C5	2.38	1.53	1.46
58	3d	203	UQ8	C6-C5	2.38	1.53	1.46
60	3g	402	HEM	C2A-C3A	-2.38	1.32	1.38
58	2S	201	UQ8	C6-C5	2.37	1.53	1.46
58	2s	201	UQ8	C6-C5	2.37	1.53	1.46
66	4q	905	HEA	C1C-C2C	2.36	1.48	1.43
58	3g	404	UQ8	O4-C4M	-2.35	1.40	1.45
60	3G	402	HEM	FE-NA	2.34	2.02	1.95
59	3c	301	HEC	C3D-C2D	-2.34	1.32	1.38
60	3g	402	HEM	FE-NA	2.34	2.02	1.95
58	3G	404	UQ8	O4-C4M	-2.34	1.40	1.45
58	3G	404	UQ8	C6-C5	2.33	1.53	1.46
60	3G	402	HEM	C2A-C3A	-2.33	1.32	1.38
59	3C	301	HEC	C3D-C2D	-2.33	1.32	1.38
66	4Q	905	HEA	C1D-ND	-2.32	1.36	1.40
66	4Q	904	HEA	C4B-C3B	2.32	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	4q	904	HEA	C4B-C3B	2.32	1.48	1.44
66	4q	905	HEA	C1D-ND	-2.31	1.36	1.40
59	3c	301	HEC	CBB-CAB	-2.31	1.40	1.49
58	3g	404	UQ8	C6-C5	2.31	1.53	1.46
59	3C	301	HEC	CBB-CAB	-2.28	1.41	1.49
59	3c	301	HEC	C4B-NB	-2.28	1.35	1.39
66	4q	905	HEA	C1D-C2D	2.23	1.49	1.44
59	3C	301	HEC	C4B-NB	-2.23	1.35	1.39
66	4Q	905	HEA	C1D-C2D	2.21	1.49	1.44
58	3D	203	UQ8	O3-C3M	-2.21	1.40	1.45
58	3d	203	UQ8	O3-C3M	-2.21	1.40	1.45
58	2S	201	UQ8	O5-C5	-2.20	1.18	1.23
60	3G	401	HEM	C2A-C3A	-2.20	1.33	1.38
60	3g	401	HEM	C2A-C3A	-2.20	1.33	1.38
58	2s	201	UQ8	O3-C3M	-2.17	1.40	1.45
66	4Q	905	HEA	C4D-C3D	2.17	1.48	1.45
58	2S	201	UQ8	O3-C3M	-2.16	1.40	1.45
50	2M	701	FAD	C4X-C10	-2.15	1.37	1.44
66	4q	905	HEA	C4D-C3D	2.15	1.48	1.45
58	2S	201	UQ8	O4-C4M	-2.15	1.40	1.45
50	2m	701	FAD	C4X-C10	-2.15	1.37	1.44
58	2s	201	UQ8	O5-C5	-2.14	1.18	1.23
58	3G	405	UQ8	O2-C2	-2.14	1.18	1.23
58	2s	201	UQ8	O4-C4M	-2.13	1.40	1.45
58	3G	404	UQ8	O5-C5	-2.13	1.18	1.23
58	3g	405	UQ8	O2-C2	-2.13	1.18	1.23
58	2S	201	UQ8	O2-C2	-2.12	1.18	1.23
58	2s	201	UQ8	O2-C2	-2.12	1.18	1.23
66	4Q	904	HEA	C11-C3B	-2.12	1.48	1.51
66	4q	904	HEA	C11-C3B	-2.12	1.48	1.51
58	3g	405	UQ8	O4-C4M	-2.11	1.40	1.45
58	3g	404	UQ8	O5-C5	-2.07	1.18	1.23
58	3G	405	UQ8	O4-C4M	-2.07	1.40	1.45
66	4q	905	HEA	C3C-C4C	2.06	1.48	1.42
66	4Q	905	HEA	C3C-C4C	2.04	1.48	1.42
58	3g	404	UQ8	O2-C2	-2.04	1.18	1.23
60	3g	401	HEM	C4D-ND	-2.02	1.36	1.40
61	40	304	AJP	C10-C08	2.01	1.57	1.53
61	41	304	AJP	C10-C08	2.01	1.57	1.53
50	2M	701	FAD	C9A-N10	-2.01	1.37	1.41
50	2m	701	FAD	C9A-N10	-2.01	1.37	1.41

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	3C	301	HEC	CBB-CAB-C3B	-8.15	111.15	127.43
59	3c	301	HEC	CBB-CAB-C3B	-8.14	111.17	127.43
66	4Q	904	HEA	C3A-C2A-C1A	-6.64	100.77	107.05
66	4q	904	HEA	C3A-C2A-C1A	-6.64	100.77	107.05
59	3C	301	HEC	CBC-CAC-C3C	-6.47	114.50	127.43
59	3c	301	HEC	CBC-CAC-C3C	-6.46	114.52	127.43
66	4Q	905	HEA	C3A-C2A-C1A	-6.29	101.09	107.05
66	4q	905	HEA	C3A-C2A-C1A	-6.29	101.09	107.05
50	2m	701	FAD	C4-N3-C2	-5.16	116.48	125.64
50	2M	701	FAD	C4-N3-C2	-5.15	116.49	125.64
61	40	304	AJP	O09-C08-C10	5.09	120.50	110.20
61	41	304	AJP	O09-C08-C10	5.09	120.50	110.20
66	4q	905	HEA	CMC-C2C-C3C	4.80	137.83	126.55
66	4Q	905	HEA	CMC-C2C-C3C	4.79	137.81	126.55
66	4Q	904	HEA	C2A-C1A-NA	4.78	114.93	110.32
66	4q	904	HEA	C2A-C1A-NA	4.77	114.92	110.32
66	4q	904	HEA	CMC-C2C-C3C	4.68	137.55	126.55
66	4Q	904	HEA	CMC-C2C-C3C	4.67	137.54	126.55
66	4Q	905	HEA	C3D-C4D-ND	4.66	114.86	110.35
61	41	304	AJP	O09-C05-C06	-4.65	98.38	104.56
61	40	304	AJP	O09-C05-C06	-4.64	98.39	104.56
66	4q	905	HEA	C3D-C4D-ND	4.62	114.81	110.35
66	4q	905	HEA	C2A-C1A-NA	4.51	114.68	110.32
66	4Q	905	HEA	C2A-C1A-NA	4.51	114.68	110.32
66	4q	905	HEA	CMC-C2C-C1C	-4.42	118.69	125.42
66	4Q	905	HEA	CMC-C2C-C1C	-4.38	118.75	125.42
58	3D	203	UQ8	C20-C19-C21	4.29	122.67	115.23
58	3d	203	UQ8	C20-C19-C21	4.27	122.63	115.23
66	4q	904	HEA	C3D-C4D-ND	4.25	114.46	110.35
66	4Q	904	HEA	C3D-C4D-ND	4.22	114.43	110.35
66	4q	904	HEA	CMC-C2C-C1C	-4.20	119.02	125.42
66	4Q	904	HEA	CMC-C2C-C1C	-4.18	119.05	125.42
58	3G	404	UQ8	C40-C39-C41	4.15	122.43	115.23
58	3g	404	UQ8	C40-C39-C41	4.15	122.43	115.23
61	41	304	AJP	C26-O25-C23	4.10	122.12	115.27
61	40	304	AJP	C26-O25-C23	4.09	122.10	115.27
58	3G	404	UQ8	C15-C14-C16	4.06	122.28	115.23
58	3g	404	UQ8	C15-C14-C16	4.06	122.28	115.23
58	3g	404	UQ8	C7-C8-C9	-3.97	119.99	126.83
58	3G	404	UQ8	C7-C8-C9	-3.96	120.00	126.83
66	4Q	904	HEA	CHA-C1A-C2A	-3.95	118.63	124.86
66	4q	904	HEA	CHA-C1A-C2A	-3.94	118.64	124.86
58	3d	203	UQ8	C15-C14-C13	-3.91	113.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	3D	203	UQ8	C15-C14-C13	-3.91	113.58	123.63
58	3D	203	UQ8	C7-C8-C9	-3.80	120.28	126.83
58	3d	203	UQ8	C7-C8-C9	-3.75	120.38	126.83
58	3G	404	UQ8	C20-C19-C21	3.69	121.63	115.23
58	3g	404	UQ8	C20-C19-C21	3.69	121.63	115.23
66	4Q	905	HEA	CHA-C4D-C3D	-3.67	119.42	124.77
58	3D	203	UQ8	C37-C38-C39	-3.66	119.25	127.62
66	4q	905	HEA	CHA-C4D-C3D	-3.65	119.45	124.77
58	3d	203	UQ8	C37-C38-C39	-3.64	119.29	127.62
59	3c	301	HEC	O1D-CGD-CBD	-3.62	111.62	123.09
60	3g	401	HEM	C1B-NB-C4B	3.61	109.48	105.21
60	3G	401	HEM	C1B-NB-C4B	3.61	109.48	105.21
59	3C	301	HEC	O1D-CGD-CBD	-3.60	111.68	123.09
58	3D	203	UQ8	C25-C24-C26	3.58	121.44	115.23
66	4Q	905	HEA	C4D-C3D-C2D	-3.57	101.69	106.89
66	4Q	904	HEA	CHA-C4D-C3D	-3.57	119.56	124.77
58	3d	203	UQ8	C25-C24-C26	3.57	121.42	115.23
66	4q	904	HEA	CHA-C4D-C3D	-3.56	119.59	124.77
66	4q	905	HEA	C4D-C3D-C2D	-3.54	101.74	106.89
66	4Q	905	HEA	CHA-C1A-C2A	-3.45	119.42	124.86
66	4q	905	HEA	CHA-C1A-C2A	-3.44	119.42	124.86
61	40	304	AJP	C05-C06-C07	-3.44	98.30	103.37
61	41	304	AJP	C05-C06-C07	-3.42	98.33	103.37
58	2s	201	UQ8	C40-C39-C41	3.40	121.13	115.23
66	4Q	905	HEA	CAD-C3D-C4D	3.40	130.62	124.70
58	2S	201	UQ8	C40-C39-C41	3.39	121.11	115.23
66	4q	905	HEA	CAD-C3D-C4D	3.38	130.58	124.70
66	4Q	905	HEA	CAA-C2A-C1A	3.31	131.57	124.85
66	4q	905	HEA	CAA-C2A-C1A	3.30	131.57	124.85
58	3D	203	UQ8	C15-C14-C16	3.27	120.90	115.23
58	3d	203	UQ8	C15-C14-C16	3.26	120.88	115.23
66	4Q	904	HEA	C3C-C2C-C1C	-3.21	103.39	107.17
58	3g	404	UQ8	C30-C29-C31	3.19	120.77	115.23
66	4q	904	HEA	C3C-C2C-C1C	-3.18	103.42	107.17
58	3G	404	UQ8	C30-C29-C31	3.18	120.76	115.23
58	2S	201	UQ8	C10-C9-C11	3.17	120.73	115.23
66	4Q	905	HEA	C3C-C2C-C1C	-3.17	103.44	107.17
58	2s	201	UQ8	C10-C9-C11	3.16	120.71	115.23
58	3g	405	UQ8	C15-C14-C16	3.15	120.70	115.23
66	4q	905	HEA	C3C-C2C-C1C	-3.14	103.47	107.17
58	3G	405	UQ8	C15-C14-C16	3.13	120.67	115.23
66	4Q	904	HEA	C4D-C3D-C2D	-3.12	102.36	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	4q	904	HEA	C4D-C3D-C2D	-3.12	102.36	106.89
60	3G	402	HEM	C1B-NB-C4B	3.11	108.89	105.21
58	3g	405	UQ8	C7-C8-C9	-3.11	121.48	126.83
58	2S	201	UQ8	C32-C33-C34	-3.10	120.52	127.62
50	2M	701	FAD	C4X-C4-N3	3.10	121.14	113.25
58	2s	201	UQ8	C32-C33-C34	-3.10	120.53	127.62
50	2m	701	FAD	C4X-C4-N3	3.10	121.14	113.25
60	3g	402	HEM	C1B-NB-C4B	3.09	108.87	105.21
58	3G	405	UQ8	C30-C29-C31	3.09	120.59	115.23
58	3g	405	UQ8	C30-C29-C31	3.09	120.59	115.23
58	3G	405	UQ8	C7-C8-C9	-3.07	121.54	126.83
60	3g	402	HEM	C2A-C1A-NA	-3.05	106.77	110.15
66	4q	905	HEA	C13-C12-C11	-3.04	109.54	114.39
60	3G	402	HEM	C2A-C1A-NA	-3.03	106.79	110.15
66	4Q	905	HEA	C13-C12-C11	-3.01	109.59	114.39
66	4Q	904	HEA	C3C-C4C-NC	2.99	112.32	109.80
56	2O	203	PC1	O31-C3-C2	-2.97	99.83	108.40
56	2o	204	PC1	O31-C3-C2	-2.97	99.83	108.40
59	3C	301	HEC	C1D-C2D-C3D	2.97	110.22	106.82
66	4q	904	HEA	C3C-C4C-NC	2.97	112.30	109.80
66	4Q	904	HEA	CAD-C3D-C4D	2.95	129.83	124.70
66	4q	904	HEA	CAD-C3D-C4D	2.95	129.83	124.70
59	3c	301	HEC	C1D-C2D-C3D	2.95	110.19	106.82
58	2S	201	UQ8	C7-C6-C1	-2.94	119.86	124.89
58	2s	201	UQ8	C7-C6-C1	-2.93	119.87	124.89
58	3G	405	UQ8	C10-C9-C11	2.92	120.29	115.23
66	4Q	904	HEA	CMB-C2B-C1B	-2.91	120.49	125.03
66	4q	904	HEA	CMB-C2B-C1B	-2.91	120.49	125.03
58	3g	405	UQ8	C10-C9-C11	2.89	120.25	115.23
58	3d	203	UQ8	C27-C28-C29	-2.89	121.02	127.62
58	2S	201	UQ8	C17-C18-C19	-2.88	121.02	127.62
58	2s	201	UQ8	C17-C18-C19	-2.87	121.04	127.62
58	3D	203	UQ8	C27-C28-C29	-2.87	121.06	127.62
61	40	304	AJP	C04-C05-C06	-2.85	110.50	115.66
58	3G	404	UQ8	C7-C6-C1	-2.85	120.01	124.89
58	3g	404	UQ8	C7-C6-C1	-2.85	120.01	124.89
66	4Q	904	HEA	CAA-C2A-C1A	2.85	130.64	124.85
66	4q	904	HEA	CAA-C2A-C1A	2.85	130.64	124.85
61	41	304	AJP	C04-C05-C06	-2.83	110.53	115.66
58	3d	203	UQ8	C10-C9-C11	2.83	120.14	115.23
58	3D	203	UQ8	C10-C9-C11	2.81	120.11	115.23
58	3G	405	UQ8	C17-C18-C19	-2.80	121.21	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	3g	405	UQ8	C17-C18-C19	-2.80	121.21	127.62
58	3G	405	UQ8	C22-C23-C24	-2.79	121.23	127.62
58	2S	201	UQ8	C30-C29-C31	2.78	120.05	115.23
58	3g	405	UQ8	C22-C23-C24	-2.77	121.28	127.62
58	2S	201	UQ8	C22-C23-C24	-2.77	121.29	127.62
58	2s	201	UQ8	C22-C23-C24	-2.76	121.30	127.62
58	2s	201	UQ8	C30-C29-C31	2.76	120.02	115.23
66	4Q	905	HEA	CAA-CBA-CGA	-2.76	106.34	113.67
58	2S	201	UQ8	C15-C14-C16	2.75	120.01	115.23
66	4q	905	HEA	CAA-CBA-CGA	-2.75	106.38	113.67
58	2s	201	UQ8	C27-C28-C29	-2.74	121.34	127.62
58	2s	201	UQ8	C15-C14-C16	2.74	119.98	115.23
58	2S	201	UQ8	C27-C28-C29	-2.73	121.39	127.62
58	3G	404	UQ8	C1M-C1-C6	-2.71	119.99	124.45
58	3g	404	UQ8	C1M-C1-C6	-2.71	119.99	124.45
58	2s	201	UQ8	C12-C13-C14	-2.70	121.44	127.62
58	2S	201	UQ8	C12-C13-C14	-2.70	121.44	127.62
58	3G	405	UQ8	C25-C24-C26	2.67	119.86	115.23
58	3G	404	UQ8	C27-C26-C24	-2.66	104.36	113.19
58	3g	404	UQ8	C27-C26-C24	-2.66	104.37	113.19
58	3g	405	UQ8	C25-C24-C26	2.66	119.84	115.23
61	40	304	AJP	C12-C11-C16	-2.63	110.23	113.90
61	41	304	AJP	C12-C11-C16	-2.62	110.25	113.90
66	4Q	905	HEA	C17-C18-C19	-2.59	121.70	127.62
57	3d	201	CDL	OB8-CB6-CB4	-2.59	100.94	108.40
58	3G	404	UQ8	C32-C33-C34	-2.59	121.70	127.62
58	3g	404	UQ8	C32-C33-C34	-2.58	121.71	127.62
60	3G	402	HEM	C3D-C4D-ND	-2.58	107.34	110.17
50	2m	701	FAD	C4X-C10-N10	2.57	120.17	116.48
66	4q	905	HEA	C17-C18-C19	-2.57	121.74	127.62
57	3D	201	CDL	OB8-CB6-CB4	-2.57	101.00	108.40
50	2M	701	FAD	C4X-C10-N10	2.56	120.14	116.48
58	2s	201	UQ8	C35-C34-C36	2.55	119.65	115.23
58	3G	405	UQ8	C1M-C1-C6	-2.54	120.27	124.45
58	3d	203	UQ8	C35-C34-C33	-2.54	117.10	123.63
58	3G	404	UQ8	C35-C34-C36	2.54	119.63	115.23
58	3g	405	UQ8	C40-C39-C41	2.54	119.63	115.23
58	2S	201	UQ8	C35-C34-C36	2.53	119.63	115.23
58	3D	203	UQ8	C35-C34-C33	-2.53	117.12	123.63
58	3g	405	UQ8	C1M-C1-C6	-2.53	120.29	124.45
58	3G	405	UQ8	C40-C39-C41	2.53	119.61	115.23
58	3d	203	UQ8	C35-C34-C36	2.52	119.61	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	3g	405	UQ8	C40-C39-C38	-2.52	117.15	123.63
58	3g	404	UQ8	C35-C34-C36	2.52	119.61	115.23
60	3g	402	HEM	C3D-C4D-ND	-2.52	107.41	110.17
58	3G	404	UQ8	C27-C28-C29	-2.52	121.86	127.62
58	3g	404	UQ8	C27-C28-C29	-2.52	121.86	127.62
58	3D	203	UQ8	C35-C34-C36	2.52	119.59	115.23
58	3G	405	UQ8	C40-C39-C38	-2.51	117.17	123.63
58	2S	201	UQ8	C7-C8-C9	-2.51	122.50	126.83
58	2s	201	UQ8	C7-C8-C9	-2.51	122.50	126.83
58	2s	201	UQ8	C1M-C1-C6	-2.51	120.33	124.45
57	4Z	301	CDL	OA8-CA6-CA4	-2.49	101.20	108.40
58	2s	201	UQ8	C37-C38-C39	-2.49	121.93	127.62
57	4z	301	CDL	OA8-CA6-CA4	-2.49	101.22	108.40
66	4Q	905	HEA	CAD-CBD-CGD	-2.49	107.07	113.67
66	4q	905	HEA	CAD-CBD-CGD	-2.49	107.07	113.67
58	2S	201	UQ8	C37-C38-C39	-2.49	121.93	127.62
58	2S	201	UQ8	C1M-C1-C6	-2.47	120.38	124.45
58	3G	405	UQ8	C12-C13-C14	-2.46	122.00	127.62
66	4Q	905	HEA	CHB-C1B-C2B	-2.45	121.16	125.03
58	3G	404	UQ8	C37-C38-C39	-2.45	122.02	127.62
58	3g	405	UQ8	C12-C13-C14	-2.45	122.02	127.62
58	3g	404	UQ8	C37-C38-C39	-2.44	122.03	127.62
57	3I	201	CDL	OA8-CA6-CA4	-2.44	101.37	108.40
57	3i	202	CDL	OA8-CA6-CA4	-2.42	101.41	108.40
61	40	304	AJP	C11-C10-C08	-2.42	97.79	103.05
61	41	304	AJP	C11-C10-C08	-2.42	97.79	103.05
66	4q	905	HEA	CHB-C1B-C2B	-2.42	121.21	125.03
61	41	304	AJP	C20-C15-C16	-2.42	109.97	112.43
59	3c	301	HEC	O1A-CGA-CBA	-2.41	115.43	123.09
58	2S	201	UQ8	C25-C24-C26	2.41	119.42	115.23
58	2s	201	UQ8	C25-C24-C26	2.41	119.42	115.23
61	40	304	AJP	C20-C15-C16	-2.40	109.99	112.43
66	4Q	904	HEA	CMD-C2D-C3D	2.40	132.63	126.15
66	4q	904	HEA	CMD-C2D-C3D	2.40	132.63	126.15
66	4Q	904	HEA	CAA-CBA-CGA	-2.40	107.31	113.67
58	3G	404	UQ8	C25-C24-C26	2.39	119.38	115.23
58	3g	404	UQ8	C25-C24-C26	2.39	119.38	115.23
59	3C	301	HEC	O1A-CGA-CBA	-2.39	115.51	123.09
66	4q	904	HEA	CAA-CBA-CGA	-2.38	107.34	113.67
66	4q	905	HEA	CMB-C2B-C1B	-2.37	121.33	125.03
57	3I	202	CDL	OB8-CB6-CB4	-2.37	101.56	108.40
57	3i	203	CDL	OB8-CB6-CB4	-2.37	101.56	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	3G	405	UQ8	C35-C34-C36	2.36	119.33	115.23
66	4Q	905	HEA	CMB-C2B-C1B	-2.36	121.34	125.03
58	3g	405	UQ8	C35-C34-C36	2.36	119.32	115.23
58	3g	405	UQ8	C32-C33-C34	-2.34	122.26	127.62
55	4Q	909	PEE	O3-C3-C2	-2.34	101.65	108.40
55	4q	909	PEE	O3-C3-C2	-2.34	101.66	108.40
58	3G	405	UQ8	C32-C33-C34	-2.32	122.32	127.62
55	3C	302	PEE	O3-C3-C2	2.31	115.05	108.40
55	3c	302	PEE	O3-C3-C2	2.31	115.04	108.40
66	4Q	905	HEA	CHC-C1C-C2C	-2.30	120.75	127.43
66	4q	905	HEA	CHC-C1C-C2C	-2.29	120.78	127.43
66	4Q	904	HEA	C26-C15-C16	2.29	119.20	115.23
66	4Q	905	HEA	C4B-C3B-C2B	-2.28	103.60	107.44
66	4Q	904	HEA	CHB-C1B-C2B	-2.28	121.43	125.03
66	4q	904	HEA	CHB-C1B-C2B	-2.28	121.43	125.03
66	4q	904	HEA	C26-C15-C16	2.28	119.18	115.23
66	4q	904	HEA	C17-C18-C19	-2.27	122.42	127.62
61	4l	304	AJP	C14-C15-C20	-2.27	111.35	113.91
66	4q	905	HEA	C4B-C3B-C2B	-2.27	103.62	107.44
58	3g	404	UQ8	C17-C18-C19	-2.26	122.45	127.62
66	4Q	904	HEA	C25-C23-C24	2.26	119.78	114.59
66	4Q	904	HEA	C17-C18-C19	-2.25	122.48	127.62
58	3G	404	UQ8	C17-C18-C19	-2.25	122.48	127.62
58	3g	405	UQ8	C7-C6-C1	-2.25	121.04	124.89
66	4q	904	HEA	C25-C23-C24	2.24	119.74	114.59
58	3G	405	UQ8	C7-C6-C1	-2.23	121.06	124.89
61	4o	304	AJP	C14-C15-C20	-2.23	111.40	113.91
66	4Q	904	HEA	C27-C19-C20	2.22	119.09	115.23
66	4q	904	HEA	C27-C19-C20	2.21	119.06	115.23
58	3D	203	UQ8	C21-C19-C18	-2.19	116.25	121.17
60	3g	401	HEM	C3A-C4A-NA	-2.18	106.65	110.14
58	3d	203	UQ8	C21-C19-C18	-2.18	116.28	121.17
60	3G	401	HEM	C3A-C4A-NA	-2.17	106.66	110.14
57	3e	203	CDL	OB8-CB6-CB4	2.17	114.64	108.40
50	2M	701	FAD	O4-C4-C4X	-2.16	120.82	126.53
57	4Q	907	CDL	OA8-CA6-CA4	-2.16	102.16	108.40
57	4q	907	CDL	OA8-CA6-CA4	-2.16	102.16	108.40
66	4q	905	HEA	C3B-C4B-NB	2.16	112.32	109.84
57	3E	203	CDL	OB8-CB6-CB4	2.16	114.62	108.40
60	3G	401	HEM	CMD-C2D-C1D	2.16	128.41	125.03
66	4Q	905	HEA	C3B-C4B-NB	2.16	112.32	109.84
61	4o	304	AJP	O09-C05-C04	2.16	112.92	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	4l	304	AJP	O09-C05-C04	2.16	112.92	108.54
50	2m	701	FAD	O4-C4-C4X	-2.15	120.84	126.53
61	40	304	AJP	C14-C13-C12	-2.15	109.11	112.74
66	4q	904	HEA	C2D-C1D-ND	2.15	112.31	109.84
66	4q	905	HEA	CMD-C2D-C3D	2.15	131.97	126.15
57	3g	403	CDL	OA8-CA6-CA4	-2.15	102.19	108.40
61	4l	304	AJP	C14-C13-C12	-2.15	109.11	112.74
60	3g	402	HEM	CMD-C2D-C1D	2.15	128.39	125.03
66	4Q	904	HEA	CMB-C2B-C3B	2.15	134.43	130.28
66	4q	904	HEA	CMB-C2B-C3B	2.15	134.43	130.28
57	3G	403	CDL	OA8-CA6-CA4	-2.15	102.20	108.40
66	4Q	905	HEA	CMD-C2D-C3D	2.14	131.94	126.15
66	4q	905	HEA	CMD-C2D-C1D	-2.14	121.69	125.03
60	3G	401	HEM	CHD-C4C-NC	2.14	126.78	124.45
60	3g	401	HEM	CHD-C4C-NC	2.14	126.78	124.45
66	4Q	904	HEA	C2D-C1D-ND	2.13	112.29	109.84
66	4Q	905	HEA	CMD-C2D-C1D	-2.13	121.71	125.03
60	3g	401	HEM	CMD-C2D-C1D	2.13	128.36	125.03
66	4Q	904	HEA	CMD-C2D-C1D	-2.13	121.71	125.03
66	4q	904	HEA	CMD-C2D-C1D	-2.13	121.71	125.03
60	3G	402	HEM	CMD-C2D-C1D	2.12	128.35	125.03
58	3d	203	UQ8	C32-C33-C34	-2.12	122.78	127.62
58	3D	203	UQ8	C32-C33-C34	-2.11	122.79	127.62
55	4Q	910	PEE	O3-C3-C2	-2.11	102.32	108.40
58	3G	404	UQ8	C46-C44-C45	2.10	119.42	114.59
58	3g	404	UQ8	C46-C44-C45	2.10	119.42	114.59
66	4q	905	HEA	C2B-C1B-NB	2.10	112.33	109.90
55	4q	910	PEE	O3-C3-C2	-2.09	102.37	108.40
56	3A	501	PC1	O31-C3-C2	-2.09	102.37	108.40
66	4Q	905	HEA	C2B-C1B-NB	2.09	112.32	109.90
66	4Q	904	HEA	CHC-C1C-C2C	-2.09	121.37	127.43
56	3a	501	PC1	O31-C3-C2	-2.08	102.39	108.40
60	3g	402	HEM	C3A-C4A-NA	-2.08	106.81	110.14
66	4q	904	HEA	CHC-C1C-C2C	-2.08	121.39	127.43
60	3G	402	HEM	C2B-C1B-NB	-2.07	107.46	109.84
58	2s	201	UQ8	C8-C7-C6	-2.07	106.99	112.08
60	3g	402	HEM	C2B-C1B-NB	-2.07	107.47	109.84
60	3g	401	HEM	C2B-C1B-NB	-2.06	107.47	109.84
66	4q	904	HEA	CHB-C1B-NB	2.06	126.64	124.42
58	3G	404	UQ8	C10-C9-C11	2.06	118.80	115.23
58	3g	404	UQ8	C12-C13-C14	-2.06	122.91	127.62
58	2S	201	UQ8	C8-C7-C6	-2.06	107.02	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	4U	501	CDL	OA8-CA6-CA4	2.06	114.32	108.40
57	4u	501	CDL	OA8-CA6-CA4	2.06	114.32	108.40
58	3g	404	UQ8	C10-C9-C11	2.05	118.80	115.23
60	3G	402	HEM	C3A-C4A-NA	-2.05	106.86	110.14
60	3G	402	HEM	C4D-ND-C1D	2.04	107.63	105.21
58	3G	405	UQ8	C20-C19-C21	2.04	118.76	115.23
61	41	304	AJP	C04-C03-C02	-2.04	107.61	111.67
66	4Q	904	HEA	CHB-C1B-NB	2.04	126.61	124.42
58	3G	404	UQ8	C12-C13-C14	-2.03	122.97	127.62
66	4Q	905	HEA	C26-C15-C16	2.03	118.76	115.23
61	40	304	AJP	C04-C03-C02	-2.03	107.62	111.67
60	3G	401	HEM	C2B-C1B-NB	-2.03	107.51	109.84
58	3g	405	UQ8	C20-C19-C21	2.02	118.73	115.23
60	3g	402	HEM	C4D-ND-C1D	2.01	107.59	105.21
57	2q	101	CDL	OA8-CA6-CA4	-2.01	102.60	108.40
57	2Q	101	CDL	OA8-CA6-CA4	-2.01	102.60	108.40
61	40	304	AJP	C20-C21-C22	-2.01	110.87	114.17
61	41	304	AJP	C20-C21-C22	-2.01	110.87	114.17
66	4q	905	HEA	C26-C15-C16	2.01	118.71	115.23
59	3C	301	HEC	CMB-C2B-C1B	2.00	128.47	125.42

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
61	40	304	AJP	C30
61	40	304	AJP	C28
61	40	304	AJP	C29
61	41	304	AJP	C30
61	41	304	AJP	C28
61	41	304	AJP	C29

All (2496) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	2M	701	FAD	C5B-O5B-PA-O3P
50	2M	701	FAD	N10-C1'-C2'-O2'
50	2m	701	FAD	C5B-O5B-PA-O3P
50	2m	701	FAD	N10-C1'-C2'-O2'
55	2O	201	PEE	C11-C10-O2-C2
55	2O	201	PEE	C1-O3P-P-O1P
55	2O	201	PEE	C1-O3P-P-O4P
55	2P	202	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
55	2P	202	PEE	C1-O3P-P-O4P
55	2P	202	PEE	C4-O4P-P-O3P
55	2P	202	PEE	C4-O4P-P-O2P
55	2P	202	PEE	C4-O4P-P-O1P
55	2P	203	PEE	C4-O4P-P-O3P
55	2R	201	PEE	C1-O3P-P-O2P
55	2R	201	PEE	C1-O3P-P-O1P
55	2R	201	PEE	C1-O3P-P-O4P
55	2R	201	PEE	C4-O4P-P-O3P
55	2R	201	PEE	C4-O4P-P-O1P
55	3C	302	PEE	C1-O3P-P-O2P
55	3C	302	PEE	C1-O3P-P-O4P
55	3C	302	PEE	C4-O4P-P-O3P
55	3C	302	PEE	C4-O4P-P-O2P
55	3C	302	PEE	C4-O4P-P-O1P
55	3F	101	PEE	C1-O3P-P-O1P
55	3F	101	PEE	C1-O3P-P-O4P
55	3F	101	PEE	C4-O4P-P-O3P
55	3F	101	PEE	C4-O4P-P-O1P
55	40	303	PEE	C1-O3P-P-O2P
55	40	303	PEE	C1-O3P-P-O1P
55	40	303	PEE	C1-O3P-P-O4P
55	40	303	PEE	O4P-C4-C5-N
55	4D	101	PEE	C1-O3P-P-O4P
55	4Q	909	PEE	C1-O3P-P-O2P
55	4Q	909	PEE	C1-O3P-P-O4P
55	4Q	909	PEE	O4P-C4-C5-N
55	4Q	910	PEE	C4-O4P-P-O3P
55	4Q	910	PEE	C4-O4P-P-O2P
55	4Q	910	PEE	C4-O4P-P-O1P
55	4R	201	PEE	C1-O3P-P-O4P
55	4S	102	PEE	C4-O4P-P-O3P
55	4S	102	PEE	C4-O4P-P-O2P
55	4S	102	PEE	C4-O4P-P-O1P
55	4Z	302	PEE	C1-O3P-P-O4P
55	4Z	302	PEE	C4-O4P-P-O3P
55	4Z	302	PEE	C4-O4P-P-O2P
55	4Z	302	PEE	C4-O4P-P-O1P
55	2o	202	PEE	C11-C10-O2-C2
55	2o	202	PEE	C1-O3P-P-O1P
55	2o	202	PEE	C1-O3P-P-O4P
55	2p	202	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
55	2p	202	PEE	C1-O3P-P-O4P
55	2p	202	PEE	C4-O4P-P-O3P
55	2p	202	PEE	C4-O4P-P-O2P
55	2p	202	PEE	C4-O4P-P-O1P
55	2p	203	PEE	C4-O4P-P-O3P
55	2r	201	PEE	C1-O3P-P-O2P
55	2r	201	PEE	C1-O3P-P-O1P
55	2r	201	PEE	C1-O3P-P-O4P
55	2r	201	PEE	C4-O4P-P-O3P
55	2r	201	PEE	C4-O4P-P-O1P
55	3c	302	PEE	C1-O3P-P-O2P
55	3c	302	PEE	C1-O3P-P-O4P
55	3c	302	PEE	C4-O4P-P-O3P
55	3c	302	PEE	C4-O4P-P-O2P
55	3c	302	PEE	C4-O4P-P-O1P
55	3f	101	PEE	C1-O3P-P-O1P
55	3f	101	PEE	C1-O3P-P-O4P
55	3f	101	PEE	C4-O4P-P-O3P
55	3f	101	PEE	C4-O4P-P-O1P
55	4l	303	PEE	C1-O3P-P-O2P
55	4l	303	PEE	C1-O3P-P-O1P
55	4l	303	PEE	C1-O3P-P-O4P
55	4l	303	PEE	O4P-C4-C5-N
55	4d	101	PEE	C1-O3P-P-O4P
55	4q	909	PEE	C1-O3P-P-O2P
55	4q	909	PEE	C1-O3P-P-O4P
55	4q	909	PEE	O4P-C4-C5-N
55	4q	910	PEE	C4-O4P-P-O3P
55	4q	910	PEE	C4-O4P-P-O2P
55	4q	910	PEE	C4-O4P-P-O1P
55	4r	201	PEE	C1-O3P-P-O4P
55	4s	102	PEE	C4-O4P-P-O3P
55	4s	102	PEE	C4-O4P-P-O2P
55	4s	102	PEE	C4-O4P-P-O1P
55	4z	302	PEE	C1-O3P-P-O4P
55	4z	302	PEE	C4-O4P-P-O3P
55	4z	302	PEE	C4-O4P-P-O2P
55	4z	302	PEE	C4-O4P-P-O1P
56	2O	202	PC1	C3-C2-O21-C21
56	2R	202	PC1	C11-O13-P-O14
56	2R	202	PC1	C1-O11-P-O14
56	2R	202	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
56	2R	202	PC1	O13-C11-C12-N
56	2T	101	PC1	C11-O13-P-O12
56	2T	101	PC1	C11-O13-P-O11
56	3A	501	PC1	C11-O13-P-O12
56	3A	501	PC1	C11-O13-P-O14
56	3A	501	PC1	C11-O13-P-O11
56	3A	501	PC1	C1-O11-P-O13
56	3A	501	PC1	O13-C11-C12-N
56	3A	502	PC1	C11-O13-P-O11
56	3A	502	PC1	C1-O11-P-O14
56	3A	502	PC1	C1-O11-P-O13
56	3A	502	PC1	O13-C11-C12-N
56	3H	403	PC1	C1-O11-P-O13
56	3H	403	PC1	O21-C2-C3-O31
56	4E	202	PC1	C3-C2-O21-C21
56	2o	203	PC1	C3-C2-O21-C21
56	2r	202	PC1	C11-O13-P-O14
56	2r	202	PC1	C1-O11-P-O14
56	2r	202	PC1	C1-O11-P-O13
56	2r	202	PC1	O13-C11-C12-N
56	2t	101	PC1	C11-O13-P-O12
56	2t	101	PC1	C11-O13-P-O11
56	3a	501	PC1	C11-O13-P-O12
56	3a	501	PC1	C11-O13-P-O14
56	3a	501	PC1	C11-O13-P-O11
56	3a	501	PC1	C1-O11-P-O13
56	3a	501	PC1	O13-C11-C12-N
56	3a	502	PC1	C11-O13-P-O11
56	3a	502	PC1	C1-O11-P-O14
56	3a	502	PC1	C1-O11-P-O13
56	3a	502	PC1	O13-C11-C12-N
56	3h	403	PC1	C1-O11-P-O13
56	3h	403	PC1	O21-C2-C3-O31
56	4e	202	PC1	C3-C2-O21-C21
57	2O	204	CDL	CA2-OA2-PA1-OA4
57	2O	204	CDL	CA2-OA2-PA1-OA5
57	2O	204	CDL	CB3-OB5-PB2-OB2
57	2O	204	CDL	CB3-OB5-PB2-OB4
57	2P	201	CDL	O1-C1-CA2-OA2
57	2P	201	CDL	O1-C1-CB2-OB2
57	2P	201	CDL	CA2-OA2-PA1-OA4
57	2P	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
57	2P	201	CDL	CB2-OB2-PB2-OB4
57	2P	201	CDL	CB2-OB2-PB2-OB5
57	2Q	101	CDL	CA2-OA2-PA1-OA3
57	2Q	101	CDL	CA2-OA2-PA1-OA5
57	2Q	101	CDL	CA3-OA5-PA1-OA2
57	2Q	101	CDL	CB2-OB2-PB2-OB3
57	2Q	101	CDL	CB2-OB2-PB2-OB4
57	2Q	101	CDL	CB2-OB2-PB2-OB5
57	2U	101	CDL	CA3-OA5-PA1-OA3
57	2U	101	CDL	CB2-OB2-PB2-OB4
57	2U	101	CDL	CB2-OB2-PB2-OB5
57	3D	201	CDL	CB2-OB2-PB2-OB3
57	3D	201	CDL	CB3-OB5-PB2-OB2
57	3D	201	CDL	CB3-OB5-PB2-OB4
57	3D	202	CDL	O1-C1-CA2-OA2
57	3D	202	CDL	CB2-C1-CA2-OA2
57	3D	202	CDL	CA3-OA5-PA1-OA2
57	3D	202	CDL	CA3-OA5-PA1-OA3
57	3D	202	CDL	CA3-OA5-PA1-OA4
57	3E	201	CDL	CB2-OB2-PB2-OB3
57	3E	202	CDL	O1-C1-CA2-OA2
57	3E	202	CDL	CA2-OA2-PA1-OA4
57	3E	202	CDL	CA2-OA2-PA1-OA5
57	3E	202	CDL	CA3-OA5-PA1-OA2
57	3E	202	CDL	CA3-OA5-PA1-OA4
57	3E	203	CDL	CA2-OA2-PA1-OA4
57	3E	203	CDL	CA2-OA2-PA1-OA5
57	3E	203	CDL	CB3-OB5-PB2-OB2
57	3E	203	CDL	CB3-OB5-PB2-OB4
57	3G	403	CDL	CA2-OA2-PA1-OA3
57	3G	403	CDL	CA2-OA2-PA1-OA5
57	3G	403	CDL	C1-CB2-OB2-PB2
57	3H	402	CDL	CA2-C1-CB2-OB2
57	3H	402	CDL	CA3-OA5-PA1-OA4
57	3H	402	CDL	CB2-OB2-PB2-OB3
57	3H	402	CDL	CB2-OB2-PB2-OB5
57	3I	201	CDL	CB2-C1-CA2-OA2
57	3I	201	CDL	C11-CA5-OA6-CA4
57	3I	201	CDL	CB2-OB2-PB2-OB4
57	3I	201	CDL	CB2-OB2-PB2-OB5
57	3I	202	CDL	CA2-OA2-PA1-OA4
57	3I	202	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
57	3I	202	CDL	CA3-OA5-PA1-OA2
57	3I	202	CDL	CA3-OA5-PA1-OA4
57	3I	202	CDL	CB2-OB2-PB2-OB3
57	3I	202	CDL	CB2-OB2-PB2-OB4
57	3I	202	CDL	CB2-OB2-PB2-OB5
57	3I	202	CDL	CB3-OB5-PB2-OB2
57	3I	202	CDL	CB3-OB5-PB2-OB4
57	3I	203	CDL	CA2-OA2-PA1-OA3
57	3I	203	CDL	CB3-OB5-PB2-OB2
57	3I	203	CDL	CB3-OB5-PB2-OB3
57	3I	203	CDL	CB3-OB5-PB2-OB4
57	3I	203	CDL	OB6-CB4-CB6-OB8
57	3L	701	CDL	CB2-C1-CA2-OA2
57	3L	702	CDL	CA3-OA5-PA1-OA2
57	3L	702	CDL	CA3-OA5-PA1-OA4
57	3L	702	CDL	CB2-OB2-PB2-OB3
57	4E	201	CDL	CA2-OA2-PA1-OA3
57	4E	201	CDL	CA2-OA2-PA1-OA4
57	4E	201	CDL	CA2-OA2-PA1-OA5
57	4E	201	CDL	CA3-OA5-PA1-OA3
57	4E	201	CDL	C11-CA5-OA6-CA4
57	4E	201	CDL	CB3-OB5-PB2-OB2
57	4E	201	CDL	CB3-OB5-PB2-OB4
57	4E	201	CDL	CB4-CB3-OB5-PB2
57	4J	301	CDL	CA2-OA2-PA1-OA3
57	4J	301	CDL	CA2-OA2-PA1-OA5
57	4J	301	CDL	CA3-OA5-PA1-OA2
57	4J	301	CDL	C11-CA5-OA6-CA4
57	4J	301	CDL	CB2-OB2-PB2-OB3
57	4K	201	CDL	O1-C1-CB2-OB2
57	4K	201	CDL	CA2-C1-CB2-OB2
57	4K	201	CDL	CA2-OA2-PA1-OA3
57	4K	201	CDL	CA2-OA2-PA1-OA5
57	4K	201	CDL	CB2-OB2-PB2-OB3
57	4K	201	CDL	CB2-OB2-PB2-OB4
57	4K	201	CDL	CB2-OB2-PB2-OB5
57	4K	201	CDL	CB3-OB5-PB2-OB2
57	4K	201	CDL	CB3-OB5-PB2-OB4
57	4K	202	CDL	O1-C1-CA2-OA2
57	4K	202	CDL	CB2-C1-CA2-OA2
57	4K	202	CDL	CA2-OA2-PA1-OA4
57	4K	202	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
57	4K	202	CDL	CA3-OA5-PA1-OA2
57	4K	202	CDL	CA3-OA5-PA1-OA3
57	4K	202	CDL	CB2-OB2-PB2-OB4
57	4K	202	CDL	CB2-OB2-PB2-OB5
57	4L	201	CDL	CA3-OA5-PA1-OA2
57	4L	201	CDL	CA3-OA5-PA1-OA4
57	4M	201	CDL	CA3-OA5-PA1-OA2
57	4M	201	CDL	CA3-OA5-PA1-OA3
57	4Q	907	CDL	O1-C1-CA2-OA2
57	4Q	907	CDL	CA2-C1-CB2-OB2
57	4Q	907	CDL	CA2-OA2-PA1-OA5
57	4Q	907	CDL	CA3-OA5-PA1-OA2
57	4Q	907	CDL	C11-CA5-OA6-CA4
57	4Q	907	CDL	CB3-OB5-PB2-OB2
57	4Q	907	CDL	CB3-OB5-PB2-OB4
57	4Q	908	CDL	CB2-OB2-PB2-OB4
57	4Q	908	CDL	CB2-OB2-PB2-OB5
57	4S	101	CDL	CA2-OA2-PA1-OA5
57	4S	101	CDL	CA3-OA5-PA1-OA2
57	4S	101	CDL	CA3-OA5-PA1-OA3
57	4S	101	CDL	CB3-OB5-PB2-OB2
57	4T	203	CDL	CA2-OA2-PA1-OA3
57	4T	203	CDL	CB2-OB2-PB2-OB3
57	4T	203	CDL	CB2-OB2-PB2-OB5
57	4T	203	CDL	CB3-OB5-PB2-OB2
57	4T	203	CDL	CB3-OB5-PB2-OB4
57	4U	501	CDL	CA2-OA2-PA1-OA3
57	4U	501	CDL	CA2-OA2-PA1-OA5
57	4U	501	CDL	CA3-OA5-PA1-OA2
57	4U	501	CDL	CA3-OA5-PA1-OA3
57	4U	501	CDL	CA3-OA5-PA1-OA4
57	4U	501	CDL	CA4-CA3-OA5-PA1
57	4W	201	CDL	CA2-OA2-PA1-OA5
57	4W	202	CDL	O1-C1-CB2-OB2
57	4W	202	CDL	CA2-OA2-PA1-OA4
57	4W	202	CDL	CA2-OA2-PA1-OA5
57	4W	202	CDL	CB3-OB5-PB2-OB2
57	4W	202	CDL	CB4-CB3-OB5-PB2
57	2o	201	CDL	CA2-OA2-PA1-OA4
57	2o	201	CDL	CA2-OA2-PA1-OA5
57	2o	201	CDL	CB3-OB5-PB2-OB2
57	2o	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
57	2p	201	CDL	O1-C1-CA2-OA2
57	2p	201	CDL	O1-C1-CB2-OB2
57	2p	201	CDL	CA2-OA2-PA1-OA4
57	2p	201	CDL	CA2-OA2-PA1-OA5
57	2p	201	CDL	CB2-OB2-PB2-OB4
57	2p	201	CDL	CB2-OB2-PB2-OB5
57	2q	101	CDL	CA2-OA2-PA1-OA3
57	2q	101	CDL	CA2-OA2-PA1-OA5
57	2q	101	CDL	CA3-OA5-PA1-OA2
57	2q	101	CDL	CB2-OB2-PB2-OB3
57	2q	101	CDL	CB2-OB2-PB2-OB4
57	2q	101	CDL	CB2-OB2-PB2-OB5
57	2u	101	CDL	CA3-OA5-PA1-OA3
57	2u	101	CDL	CB2-OB2-PB2-OB4
57	2u	101	CDL	CB2-OB2-PB2-OB5
57	3d	201	CDL	CB2-OB2-PB2-OB3
57	3d	201	CDL	CB3-OB5-PB2-OB2
57	3d	201	CDL	CB3-OB5-PB2-OB4
57	3d	202	CDL	O1-C1-CA2-OA2
57	3d	202	CDL	CB2-C1-CA2-OA2
57	3d	202	CDL	CA3-OA5-PA1-OA2
57	3d	202	CDL	CA3-OA5-PA1-OA3
57	3d	202	CDL	CA3-OA5-PA1-OA4
57	3e	201	CDL	CB2-OB2-PB2-OB3
57	3e	202	CDL	O1-C1-CA2-OA2
57	3e	202	CDL	CA2-OA2-PA1-OA4
57	3e	202	CDL	CA2-OA2-PA1-OA5
57	3e	202	CDL	CA3-OA5-PA1-OA2
57	3e	202	CDL	CA3-OA5-PA1-OA4
57	3e	203	CDL	CA2-OA2-PA1-OA4
57	3e	203	CDL	CA2-OA2-PA1-OA5
57	3e	203	CDL	CB3-OB5-PB2-OB2
57	3e	203	CDL	CB3-OB5-PB2-OB4
57	3g	403	CDL	CA2-OA2-PA1-OA3
57	3g	403	CDL	CA2-OA2-PA1-OA5
57	3g	403	CDL	C1-CB2-OB2-PB2
57	3h	402	CDL	CA2-C1-CB2-OB2
57	3h	402	CDL	CA3-OA5-PA1-OA4
57	3h	402	CDL	CB2-OB2-PB2-OB3
57	3h	402	CDL	CB2-OB2-PB2-OB5
57	3i	201	CDL	CA2-OA2-PA1-OA3
57	3i	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
57	3i	201	CDL	CB3-OB5-PB2-OB3
57	3i	201	CDL	CB3-OB5-PB2-OB4
57	3i	201	CDL	OB6-CB4-CB6-OB8
57	3i	202	CDL	CB2-C1-CA2-OA2
57	3i	202	CDL	C11-CA5-OA6-CA4
57	3i	202	CDL	CB2-OB2-PB2-OB4
57	3i	202	CDL	CB2-OB2-PB2-OB5
57	3i	203	CDL	CA2-OA2-PA1-OA4
57	3i	203	CDL	CA2-OA2-PA1-OA5
57	3i	203	CDL	CA3-OA5-PA1-OA2
57	3i	203	CDL	CA3-OA5-PA1-OA4
57	3i	203	CDL	CB2-OB2-PB2-OB3
57	3i	203	CDL	CB2-OB2-PB2-OB4
57	3i	203	CDL	CB2-OB2-PB2-OB5
57	3i	203	CDL	CB3-OB5-PB2-OB2
57	3i	203	CDL	CB3-OB5-PB2-OB4
57	3l	701	CDL	CB2-C1-CA2-OA2
57	3l	702	CDL	CA3-OA5-PA1-OA2
57	3l	702	CDL	CA3-OA5-PA1-OA4
57	3l	702	CDL	CB2-OB2-PB2-OB3
57	4e	201	CDL	CA2-OA2-PA1-OA3
57	4e	201	CDL	CA2-OA2-PA1-OA4
57	4e	201	CDL	CA2-OA2-PA1-OA5
57	4e	201	CDL	CA3-OA5-PA1-OA3
57	4e	201	CDL	C11-CA5-OA6-CA4
57	4e	201	CDL	CB3-OB5-PB2-OB2
57	4e	201	CDL	CB3-OB5-PB2-OB4
57	4e	201	CDL	CB4-CB3-OB5-PB2
57	4j	301	CDL	CA2-OA2-PA1-OA3
57	4j	301	CDL	CA2-OA2-PA1-OA5
57	4j	301	CDL	CA3-OA5-PA1-OA2
57	4j	301	CDL	C11-CA5-OA6-CA4
57	4j	301	CDL	CB2-OB2-PB2-OB3
57	4k	201	CDL	O1-C1-CB2-OB2
57	4k	201	CDL	CA2-C1-CB2-OB2
57	4k	201	CDL	CA2-OA2-PA1-OA3
57	4k	201	CDL	CA2-OA2-PA1-OA5
57	4k	201	CDL	CB2-OB2-PB2-OB3
57	4k	201	CDL	CB2-OB2-PB2-OB4
57	4k	201	CDL	CB2-OB2-PB2-OB5
57	4k	201	CDL	CB3-OB5-PB2-OB2
57	4k	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
57	4k	202	CDL	O1-C1-CA2-OA2
57	4k	202	CDL	CB2-C1-CA2-OA2
57	4k	202	CDL	CA2-OA2-PA1-OA4
57	4k	202	CDL	CA2-OA2-PA1-OA5
57	4k	202	CDL	CA3-OA5-PA1-OA2
57	4k	202	CDL	CA3-OA5-PA1-OA3
57	4k	202	CDL	CB2-OB2-PB2-OB4
57	4k	202	CDL	CB2-OB2-PB2-OB5
57	4l	201	CDL	CA3-OA5-PA1-OA2
57	4l	201	CDL	CA3-OA5-PA1-OA4
57	4l	201	CDL	OA5-CA3-CA4-OA6
57	4m	201	CDL	CA3-OA5-PA1-OA2
57	4m	201	CDL	CA3-OA5-PA1-OA3
57	4q	907	CDL	O1-C1-CA2-OA2
57	4q	907	CDL	CA2-C1-CB2-OB2
57	4q	907	CDL	CA2-OA2-PA1-OA5
57	4q	907	CDL	CA3-OA5-PA1-OA2
57	4q	907	CDL	C11-CA5-OA6-CA4
57	4q	907	CDL	CB3-OB5-PB2-OB2
57	4q	907	CDL	CB3-OB5-PB2-OB4
57	4q	908	CDL	CB2-OB2-PB2-OB4
57	4q	908	CDL	CB2-OB2-PB2-OB5
57	4s	101	CDL	CA2-OA2-PA1-OA5
57	4s	101	CDL	CA3-OA5-PA1-OA2
57	4s	101	CDL	CA3-OA5-PA1-OA3
57	4s	101	CDL	CB3-OB5-PB2-OB2
57	4t	203	CDL	CA2-OA2-PA1-OA3
57	4t	203	CDL	CB2-OB2-PB2-OB3
57	4t	203	CDL	CB2-OB2-PB2-OB5
57	4t	203	CDL	CB3-OB5-PB2-OB2
57	4t	203	CDL	CB3-OB5-PB2-OB4
57	4u	501	CDL	CA2-OA2-PA1-OA3
57	4u	501	CDL	CA2-OA2-PA1-OA5
57	4u	501	CDL	CA3-OA5-PA1-OA2
57	4u	501	CDL	CA3-OA5-PA1-OA3
57	4u	501	CDL	CA3-OA5-PA1-OA4
57	4u	501	CDL	CA4-CA3-OA5-PA1
57	4w	201	CDL	CA2-OA2-PA1-OA5
57	4w	202	CDL	O1-C1-CB2-OB2
57	4w	202	CDL	CA2-OA2-PA1-OA4
57	4w	202	CDL	CA2-OA2-PA1-OA5
57	4w	202	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
57	4w	202	CDL	CB4-CB3-OB5-PB2
58	3G	404	UQ8	C18-C19-C21-C22
58	3g	404	UQ8	C18-C19-C21-C22
59	3C	301	HEC	C2B-C3B-CAB-CBB
59	3C	301	HEC	C4B-C3B-CAB-CBB
59	3C	301	HEC	C2C-C3C-CAC-CBC
59	3C	301	HEC	C4C-C3C-CAC-CBC
59	3c	301	HEC	C2B-C3B-CAB-CBB
59	3c	301	HEC	C4B-C3B-CAB-CBB
59	3c	301	HEC	C2C-C3C-CAC-CBC
59	3c	301	HEC	C4C-C3C-CAC-CBC
62	4C	101	LPP	C6-O5-P1-O2
62	4C	101	LPP	C6-O5-P1-O3
62	4C	101	LPP	C6-O5-P1-O4
62	4c	101	LPP	C6-O5-P1-O2
62	4c	101	LPP	C6-O5-P1-O3
62	4c	101	LPP	C6-O5-P1-O4
57	4Q	907	CDL	OA7-CA5-OA6-CA4
57	4q	907	CDL	OA7-CA5-OA6-CA4
57	4K	202	CDL	C31-CA7-OA8-CA6
57	4k	202	CDL	C31-CA7-OA8-CA6
56	4E	202	PC1	C22-C21-O21-C2
56	4e	202	PC1	C22-C21-O21-C2
58	3D	203	UQ8	C20-C19-C21-C22
58	3G	404	UQ8	C40-C39-C41-C42
58	3G	404	UQ8	C20-C19-C21-C22
58	3d	203	UQ8	C20-C19-C21-C22
58	3g	404	UQ8	C40-C39-C41-C42
58	3g	404	UQ8	C20-C19-C21-C22
58	3D	203	UQ8	C18-C19-C21-C22
58	3d	203	UQ8	C18-C19-C21-C22
57	4U	501	CDL	C31-CA7-OA8-CA6
57	4u	501	CDL	C31-CA7-OA8-CA6
55	2O	201	PEE	C17-C18-C19-C20
55	2P	202	PEE	C17-C18-C19-C20
55	2P	203	PEE	C37-C38-C39-C40
55	40	303	PEE	C37-C38-C39-C40
55	4R	201	PEE	C37-C38-C39-C40
55	2o	202	PEE	C17-C18-C19-C20
55	2p	202	PEE	C17-C18-C19-C20
55	2p	203	PEE	C37-C38-C39-C40
55	41	303	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
55	4r	201	PEE	C37-C38-C39-C40
57	3I	201	CDL	OA7-CA5-OA6-CA4
57	3i	202	CDL	OA7-CA5-OA6-CA4
57	2U	101	CDL	O1-C1-CA2-OA2
57	3I	202	CDL	O1-C1-CA2-OA2
57	4M	201	CDL	O1-C1-CB2-OB2
57	4Q	908	CDL	O1-C1-CB2-OB2
57	2u	101	CDL	O1-C1-CA2-OA2
57	3i	203	CDL	O1-C1-CA2-OA2
57	4m	201	CDL	O1-C1-CB2-OB2
57	4q	908	CDL	O1-C1-CB2-OB2
55	3C	302	PEE	C31-C30-O3-C3
55	3c	302	PEE	C31-C30-O3-C3
57	3I	201	CDL	C31-CA7-OA8-CA6
57	3i	202	CDL	C31-CA7-OA8-CA6
56	3A	501	PC1	C22-C21-O21-C2
56	3a	501	PC1	C22-C21-O21-C2
57	4U	501	CDL	C11-CA5-OA6-CA4
57	4u	501	CDL	C11-CA5-OA6-CA4
58	3G	404	UQ8	C15-C14-C16-C17
58	3g	404	UQ8	C15-C14-C16-C17
58	3G	404	UQ8	C38-C39-C41-C42
58	3G	404	UQ8	C13-C14-C16-C17
58	3g	404	UQ8	C38-C39-C41-C42
58	3g	404	UQ8	C13-C14-C16-C17
56	4E	202	PC1	O22-C21-O21-C2
56	4e	202	PC1	O22-C21-O21-C2
57	4J	301	CDL	OA7-CA5-OA6-CA4
57	4j	301	CDL	OA7-CA5-OA6-CA4
58	2S	201	UQ8	C19-C21-C22-C23
58	3D	203	UQ8	C24-C26-C27-C28
58	3G	404	UQ8	C19-C21-C22-C23
58	3G	405	UQ8	C34-C36-C37-C38
58	3G	405	UQ8	C29-C31-C32-C33
58	3G	405	UQ8	C24-C26-C27-C28
58	2s	201	UQ8	C19-C21-C22-C23
58	3d	203	UQ8	C24-C26-C27-C28
58	3g	404	UQ8	C19-C21-C22-C23
58	3g	405	UQ8	C34-C36-C37-C38
58	3g	405	UQ8	C29-C31-C32-C33
58	3g	405	UQ8	C24-C26-C27-C28
57	3D	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
57	3d	201	CDL	C1-CB2-OB2-PB2
55	2R	201	PEE	C17-C18-C19-C20
55	2R	201	PEE	C37-C38-C39-C40
55	2r	201	PEE	C17-C18-C19-C20
55	2r	201	PEE	C37-C38-C39-C40
57	4K	202	CDL	OA9-CA7-OA8-CA6
57	4U	501	CDL	OA9-CA7-OA8-CA6
57	4k	202	CDL	OA9-CA7-OA8-CA6
57	4u	501	CDL	OA9-CA7-OA8-CA6
57	3D	202	CDL	C41-C42-C43-C44
57	3d	202	CDL	C41-C42-C43-C44
55	2O	201	PEE	O4-C10-O2-C2
55	2o	202	PEE	O4-C10-O2-C2
57	4E	201	CDL	OA7-CA5-OA6-CA4
57	4e	201	CDL	OA7-CA5-OA6-CA4
57	4Q	907	CDL	CB2-C1-CA2-OA2
57	4Q	908	CDL	CA2-C1-CB2-OB2
57	4U	501	CDL	CB2-C1-CA2-OA2
57	4W	202	CDL	CA2-C1-CB2-OB2
57	4q	907	CDL	CB2-C1-CA2-OA2
57	4q	908	CDL	CA2-C1-CB2-OB2
57	4u	501	CDL	CB2-C1-CA2-OA2
57	4w	202	CDL	CA2-C1-CB2-OB2
55	3F	101	PEE	C31-C30-O3-C3
55	3f	101	PEE	C31-C30-O3-C3
56	2R	202	PC1	C32-C31-O31-C3
56	2r	202	PC1	C32-C31-O31-C3
57	3D	202	CDL	C31-CA7-OA8-CA6
57	3I	202	CDL	C71-CB7-OB8-CB6
57	3d	202	CDL	C31-CA7-OA8-CA6
57	3i	203	CDL	C71-CB7-OB8-CB6
57	4W	202	CDL	O1-C1-CA2-OA2
57	4w	202	CDL	O1-C1-CA2-OA2
55	3C	302	PEE	O5-C30-O3-C3
55	3c	302	PEE	O5-C30-O3-C3
57	3I	201	CDL	OA9-CA7-OA8-CA6
57	3i	202	CDL	OA9-CA7-OA8-CA6
57	3D	202	CDL	CB7-C71-C72-C73
57	3d	202	CDL	CB7-C71-C72-C73
57	3D	202	CDL	OA9-CA7-OA8-CA6
57	3d	202	CDL	OA9-CA7-OA8-CA6
57	2O	204	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
57	4L	201	CDL	OA5-CA3-CA4-OA6
57	2o	201	CDL	OB5-CB3-CB4-OB6
57	4Q	907	CDL	C51-CB5-OB6-CB4
57	4q	907	CDL	C51-CB5-OB6-CB4
57	2U	101	CDL	OB6-CB4-CB6-OB8
57	3D	201	CDL	OB6-CB4-CB6-OB8
57	4W	201	CDL	OA6-CA4-CA6-OA8
57	2u	101	CDL	OB6-CB4-CB6-OB8
57	3d	201	CDL	OB6-CB4-CB6-OB8
57	4w	201	CDL	OA6-CA4-CA6-OA8
57	4J	301	CDL	C71-CB7-OB8-CB6
57	4j	301	CDL	C71-CB7-OB8-CB6
55	4Q	909	PEE	C17-C18-C19-C20
55	4q	909	PEE	C17-C18-C19-C20
56	3A	502	PC1	C21-C22-C23-C24
56	3a	502	PC1	C21-C22-C23-C24
58	2S	201	UQ8	C29-C31-C32-C33
58	2s	201	UQ8	C29-C31-C32-C33
57	3D	202	CDL	CB5-C51-C52-C53
57	3d	202	CDL	CB5-C51-C52-C53
56	2R	202	PC1	O32-C31-O31-C3
56	2r	202	PC1	O32-C31-O31-C3
57	3I	202	CDL	OB9-CB7-OB8-CB6
57	3i	203	CDL	OB9-CB7-OB8-CB6
57	3D	201	CDL	C71-CB7-OB8-CB6
57	3d	201	CDL	C71-CB7-OB8-CB6
55	4Z	302	PEE	C10-C11-C12-C13
55	4z	302	PEE	C10-C11-C12-C13
57	4W	202	CDL	CA5-C11-C12-C13
57	4w	202	CDL	CA5-C11-C12-C13
55	3F	101	PEE	O5-C30-O3-C3
55	3f	101	PEE	O5-C30-O3-C3
57	3D	201	CDL	O1-C1-CB2-OB2
57	3E	203	CDL	O1-C1-CA2-OA2
57	3H	402	CDL	O1-C1-CB2-OB2
57	3I	201	CDL	O1-C1-CA2-OA2
57	3L	701	CDL	O1-C1-CA2-OA2
57	4E	201	CDL	O1-C1-CB2-OB2
57	4Q	907	CDL	O1-C1-CB2-OB2
57	4U	501	CDL	O1-C1-CA2-OA2
57	3d	201	CDL	O1-C1-CB2-OB2
57	3e	203	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
57	3h	402	CDL	O1-C1-CB2-OB2
57	3i	202	CDL	O1-C1-CA2-OA2
57	3l	701	CDL	O1-C1-CA2-OA2
57	4e	201	CDL	O1-C1-CB2-OB2
57	4q	907	CDL	O1-C1-CB2-OB2
57	4u	501	CDL	O1-C1-CA2-OA2
57	4K	202	CDL	CA7-C31-C32-C33
57	4k	202	CDL	CA7-C31-C32-C33
55	4D	101	PEE	C17-C18-C19-C20
55	4Z	302	PEE	C37-C38-C39-C40
55	4d	101	PEE	C17-C18-C19-C20
55	4z	302	PEE	C37-C38-C39-C40
61	40	304	AJP	O31-C30-C32-O33
61	41	304	AJP	O31-C30-C32-O33
57	3D	202	CDL	CA5-C11-C12-C13
57	3d	202	CDL	CA5-C11-C12-C13
57	4J	301	CDL	C51-CB5-OB6-CB4
57	4j	301	CDL	C51-CB5-OB6-CB4
57	4W	201	CDL	CA5-C11-C12-C13
57	4w	201	CDL	CA5-C11-C12-C13
56	3A	501	PC1	O22-C21-O21-C2
56	3a	501	PC1	O22-C21-O21-C2
57	4U	501	CDL	OA7-CA5-OA6-CA4
57	4u	501	CDL	OA7-CA5-OA6-CA4
57	2P	201	CDL	CB2-C1-CA2-OA2
57	2P	201	CDL	CA2-C1-CB2-OB2
57	3D	201	CDL	CA2-C1-CB2-OB2
57	3E	203	CDL	CB2-C1-CA2-OA2
57	4E	201	CDL	CA2-C1-CB2-OB2
57	4W	202	CDL	CB2-C1-CA2-OA2
57	2p	201	CDL	CB2-C1-CA2-OA2
57	2p	201	CDL	CA2-C1-CB2-OB2
57	3d	201	CDL	CA2-C1-CB2-OB2
57	3e	203	CDL	CB2-C1-CA2-OA2
57	4e	201	CDL	CA2-C1-CB2-OB2
57	4w	202	CDL	CB2-C1-CA2-OA2
57	3E	201	CDL	C71-CB7-OB8-CB6
57	3e	201	CDL	C71-CB7-OB8-CB6
57	3H	402	CDL	CA5-C11-C12-C13
57	3h	402	CDL	CA5-C11-C12-C13
58	2S	201	UQ8	C40-C39-C41-C42
58	2s	201	UQ8	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
56	2O	202	PC1	C22-C21-O21-C2
56	2o	203	PC1	C22-C21-O21-C2
57	3I	202	CDL	C11-CA5-OA6-CA4
57	4Z	301	CDL	C11-CA5-OA6-CA4
57	3i	203	CDL	C11-CA5-OA6-CA4
57	4z	301	CDL	C11-CA5-OA6-CA4
62	4C	101	LPP	C36-C37-C38-C39
62	4c	101	LPP	C36-C37-C38-C39
57	4J	301	CDL	OB7-CB5-OB6-CB4
57	4Q	907	CDL	OB7-CB5-OB6-CB4
57	4j	301	CDL	OB7-CB5-OB6-CB4
57	4q	907	CDL	OB7-CB5-OB6-CB4
55	2O	201	PEE	C37-C38-C39-C40
55	4Q	910	PEE	C37-C38-C39-C40
55	2o	202	PEE	C37-C38-C39-C40
55	4q	910	PEE	C37-C38-C39-C40
58	3G	404	UQ8	C29-C31-C32-C33
58	3g	404	UQ8	C29-C31-C32-C33
57	3G	403	CDL	O1-C1-CA2-OA2
57	3g	403	CDL	O1-C1-CA2-OA2
57	4J	301	CDL	C31-CA7-OA8-CA6
57	4j	301	CDL	C31-CA7-OA8-CA6
57	4K	201	CDL	C71-C72-C73-C74
57	4k	201	CDL	C71-C72-C73-C74
57	4U	501	CDL	CA5-C11-C12-C13
57	4u	501	CDL	CA5-C11-C12-C13
57	4E	201	CDL	CA6-CA4-OA6-CA5
57	4J	301	CDL	CA6-CA4-OA6-CA5
57	4e	201	CDL	CA6-CA4-OA6-CA5
57	4j	301	CDL	CA6-CA4-OA6-CA5
57	3g	403	CDL	C62-C63-C64-C65
57	3G	403	CDL	C62-C63-C64-C65
57	4Z	301	CDL	C31-CA7-OA8-CA6
57	4z	301	CDL	C31-CA7-OA8-CA6
56	2T	101	PC1	C2B-C2C-C2D-C2E
56	2t	101	PC1	C2B-C2C-C2D-C2E
57	3D	202	CDL	C32-C33-C34-C35
57	3E	203	CDL	C79-C80-C81-C82
57	2p	201	CDL	C32-C33-C34-C35
57	3e	203	CDL	C79-C80-C81-C82
55	2P	203	PEE	C40-C41-C42-C43
55	2p	203	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
57	2P	201	CDL	C32-C33-C34-C35
57	3d	202	CDL	C32-C33-C34-C35
57	4J	301	CDL	OB9-CB7-OB8-CB6
57	4j	301	CDL	OB9-CB7-OB8-CB6
57	3D	202	CDL	C20-C21-C22-C23
57	3E	201	CDL	C77-C78-C79-C80
57	3I	203	CDL	C53-C54-C55-C56
57	4Q	908	CDL	C58-C59-C60-C61
57	3d	201	CDL	C79-C80-C81-C82
57	3d	202	CDL	C20-C21-C22-C23
57	3e	201	CDL	C77-C78-C79-C80
57	3i	201	CDL	C53-C54-C55-C56
57	3D	201	CDL	C79-C80-C81-C82
57	4q	908	CDL	C58-C59-C60-C61
57	4K	201	CDL	C11-C12-C13-C14
57	4k	201	CDL	C11-C12-C13-C14
62	4C	101	LPP	C12-C13-C14-C15
62	4c	101	LPP	C12-C13-C14-C15
55	40	301	PEE	C11-C10-O2-C2
57	3D	201	CDL	C11-CA5-OA6-CA4
57	3d	201	CDL	C11-CA5-OA6-CA4
56	2O	203	PC1	C3E-C3F-C3G-C3H
57	3D	201	CDL	O1-C1-CA2-OA2
57	3d	201	CDL	O1-C1-CA2-OA2
57	4U	501	CDL	CA7-C31-C32-C33
57	4u	501	CDL	CA7-C31-C32-C33
56	2o	204	PC1	C3E-C3F-C3G-C3H
57	3H	402	CDL	C60-C61-C62-C63
57	3L	701	CDL	C39-C40-C41-C42
57	3L	702	CDL	C40-C41-C42-C43
57	3h	402	CDL	C60-C61-C62-C63
57	3l	701	CDL	C39-C40-C41-C42
57	3l	702	CDL	C40-C41-C42-C43
57	3D	201	CDL	OB9-CB7-OB8-CB6
57	3d	201	CDL	OB9-CB7-OB8-CB6
56	2r	202	PC1	C38-C39-C3A-C3B
57	2Q	101	CDL	C36-C37-C38-C39
57	2q	101	CDL	C36-C37-C38-C39
55	4Q	909	PEE	C31-C32-C33-C34
55	4q	909	PEE	C31-C32-C33-C34
56	2R	202	PC1	C38-C39-C3A-C3B
57	4w	202	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
57	4W	202	CDL	C51-C52-C53-C54
57	3E	203	CDL	C55-C56-C57-C58
57	3e	203	CDL	C55-C56-C57-C58
57	3G	403	CDL	CB2-C1-CA2-OA2
57	3g	403	CDL	CB2-C1-CA2-OA2
57	4J	301	CDL	C51-C52-C53-C54
57	4M	201	CDL	C40-C41-C42-C43
57	4j	301	CDL	C51-C52-C53-C54
57	4u	501	CDL	C31-C32-C33-C34
55	4R	201	PEE	C22-C23-C24-C25
55	4r	201	PEE	C22-C23-C24-C25
57	2Q	101	CDL	C17-C18-C19-C20
57	3E	203	CDL	C52-C53-C54-C55
57	4U	501	CDL	C31-C32-C33-C34
57	2q	101	CDL	C17-C18-C19-C20
57	3d	201	CDL	C56-C57-C58-C59
57	3e	203	CDL	C52-C53-C54-C55
57	4m	201	CDL	C40-C41-C42-C43
61	40	304	AJP	C29-C30-C32-O33
61	41	304	AJP	C29-C30-C32-O33
57	3D	201	CDL	C56-C57-C58-C59
57	3L	701	CDL	C17-C18-C19-C20
57	3l	701	CDL	C17-C18-C19-C20
55	4Q	909	PEE	C13-C14-C15-C16
55	4q	909	PEE	C13-C14-C15-C16
57	3L	701	CDL	C76-C77-C78-C79
57	4K	201	CDL	C59-C60-C61-C62
57	3l	701	CDL	C76-C77-C78-C79
56	3H	403	PC1	C31-C32-C33-C34
56	3h	403	PC1	C31-C32-C33-C34
57	3I	202	CDL	CA7-C31-C32-C33
57	3i	203	CDL	CA7-C31-C32-C33
55	40	302	PEE	C42-C43-C44-C45
55	41	302	PEE	C42-C43-C44-C45
57	4k	201	CDL	C59-C60-C61-C62
55	3C	302	PEE	C11-C10-O2-C2
55	3c	302	PEE	C11-C10-O2-C2
55	41	301	PEE	C11-C10-O2-C2
56	2O	203	PC1	C22-C21-O21-C2
56	2o	204	PC1	C22-C21-O21-C2
57	4E	201	CDL	C51-CB5-OB6-CB4
57	4e	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
55	4Q	909	PEE	C31-C30-O3-C3
55	4q	909	PEE	C31-C30-O3-C3
56	3H	403	PC1	C32-C31-O31-C3
56	3h	403	PC1	C32-C31-O31-C3
57	3D	201	CDL	C31-CA7-OA8-CA6
57	3d	201	CDL	C31-CA7-OA8-CA6
55	3F	101	PEE	C17-C18-C19-C20
55	3f	101	PEE	C17-C18-C19-C20
57	3E	203	CDL	C15-C16-C17-C18
57	3e	203	CDL	C15-C16-C17-C18
60	3G	401	HEM	C3D-CAD-CBD-CGD
60	3g	401	HEM	C3D-CAD-CBD-CGD
55	4D	101	PEE	C10-C11-C12-C13
55	4d	101	PEE	C10-C11-C12-C13
57	3d	202	CDL	C55-C56-C57-C58
56	2O	202	PC1	O22-C21-O21-C2
56	2o	203	PC1	O22-C21-O21-C2
57	3i	203	CDL	OA7-CA5-OA6-CA4
57	3D	202	CDL	C55-C56-C57-C58
58	2S	201	UQ8	C38-C39-C41-C42
58	2s	201	UQ8	C38-C39-C41-C42
55	40	301	PEE	C32-C33-C34-C35
56	2P	204	PC1	C37-C38-C39-C3A
56	4E	202	PC1	C33-C34-C35-C36
56	2p	204	PC1	C37-C38-C39-C3A
56	4e	202	PC1	C33-C34-C35-C36
57	2U	101	CDL	C21-C22-C23-C24
57	3D	202	CDL	C62-C63-C64-C65
57	2u	101	CDL	C21-C22-C23-C24
57	3d	202	CDL	C62-C63-C64-C65
56	2O	203	PC1	C32-C31-O31-C3
56	2o	204	PC1	C32-C31-O31-C3
55	40	303	PEE	C23-C24-C25-C26
55	41	301	PEE	C32-C33-C34-C35
55	41	303	PEE	C23-C24-C25-C26
55	4Z	302	PEE	C34-C35-C36-C37
55	4z	302	PEE	C34-C35-C36-C37
57	4M	201	CDL	C81-C82-C83-C84
57	4m	201	CDL	C81-C82-C83-C84
56	2O	203	PC1	C3B-C3C-C3D-C3E
56	2o	204	PC1	C3B-C3C-C3D-C3E
55	40	303	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
55	4l	303	PEE	C14-C15-C16-C17
56	3A	502	PC1	C29-C2A-C2B-C2C
56	3a	502	PC1	C29-C2A-C2B-C2C
55	4Q	910	PEE	C31-C30-O3-C3
55	4q	910	PEE	C31-C30-O3-C3
55	2P	203	PEE	C11-C10-O2-C2
55	4Q	909	PEE	C11-C10-O2-C2
55	2p	203	PEE	C11-C10-O2-C2
55	4q	909	PEE	C11-C10-O2-C2
57	3D	202	CDL	C11-CA5-OA6-CA4
57	3E	201	CDL	C11-CA5-OA6-CA4
57	3L	701	CDL	C11-CA5-OA6-CA4
57	4L	201	CDL	C11-CA5-OA6-CA4
57	4Z	301	CDL	C51-CB5-OB6-CB4
57	3d	202	CDL	C11-CA5-OA6-CA4
57	3e	201	CDL	C11-CA5-OA6-CA4
57	3l	701	CDL	C11-CA5-OA6-CA4
57	4l	201	CDL	C11-CA5-OA6-CA4
57	4z	301	CDL	C51-CB5-OB6-CB4
57	3E	203	CDL	CB5-C51-C52-C53
57	3I	203	CDL	CB5-C51-C52-C53
57	3e	203	CDL	CB5-C51-C52-C53
57	3L	702	CDL	C61-C62-C63-C64
57	3l	702	CDL	C61-C62-C63-C64
55	40	301	PEE	O4-C10-O2-C2
55	41	301	PEE	O4-C10-O2-C2
57	3D	201	CDL	OA7-CA5-OA6-CA4
57	3I	202	CDL	OA7-CA5-OA6-CA4
57	4Z	301	CDL	OA7-CA5-OA6-CA4
57	3d	201	CDL	OA7-CA5-OA6-CA4
57	4z	301	CDL	OA7-CA5-OA6-CA4
57	4U	501	CDL	C16-C17-C18-C19
57	4u	501	CDL	C16-C17-C18-C19
57	3i	201	CDL	CB5-C51-C52-C53
57	2Q	101	CDL	C13-C14-C15-C16
57	3E	201	CDL	C16-C17-C18-C19
57	2q	101	CDL	C13-C14-C15-C16
57	3e	201	CDL	C16-C17-C18-C19
57	3d	202	CDL	C79-C80-C81-C82
55	2p	203	PEE	C32-C33-C34-C35
57	3D	202	CDL	C79-C80-C81-C82
55	2P	203	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
57	4L	201	CDL	C12-C13-C14-C15
57	4l	201	CDL	C12-C13-C14-C15
57	2O	204	CDL	C62-C63-C64-C65
57	2o	201	CDL	C62-C63-C64-C65
57	4q	907	CDL	C20-C21-C22-C23
57	3I	202	CDL	C21-C22-C23-C24
57	4Q	907	CDL	C20-C21-C22-C23
57	3i	203	CDL	C21-C22-C23-C24
56	4E	202	PC1	C21-C22-C23-C24
56	4e	202	PC1	C21-C22-C23-C24
57	3I	203	CDL	OB5-CB3-CB4-OB6
57	4J	301	CDL	OB5-CB3-CB4-OB6
57	3i	201	CDL	OB5-CB3-CB4-OB6
57	4j	301	CDL	OB5-CB3-CB4-OB6
55	40	303	PEE	C21-C22-C23-C24
55	41	303	PEE	C21-C22-C23-C24
57	3E	202	CDL	C19-C20-C21-C22
57	3e	202	CDL	C19-C20-C21-C22
57	2P	201	CDL	C52-C53-C54-C55
57	3E	201	CDL	C13-C14-C15-C16
57	3E	201	CDL	C76-C77-C78-C79
57	3I	201	CDL	C38-C39-C40-C41
57	3I	202	CDL	C57-C58-C59-C60
57	2p	201	CDL	C52-C53-C54-C55
57	3e	201	CDL	C13-C14-C15-C16
57	3e	201	CDL	C76-C77-C78-C79
57	3i	202	CDL	C38-C39-C40-C41
57	3i	203	CDL	C57-C58-C59-C60
57	4T	203	CDL	C38-C39-C40-C41
57	4t	203	CDL	C38-C39-C40-C41
55	2R	201	PEE	C15-C16-C17-C18
55	2r	201	PEE	C15-C16-C17-C18
57	4U	501	CDL	C42-C43-C44-C45
57	3D	202	CDL	C43-C44-C45-C46
57	3d	202	CDL	C43-C44-C45-C46
57	4u	501	CDL	C42-C43-C44-C45
57	3E	202	CDL	CA4-CA3-OA5-PA1
57	3e	202	CDL	CA4-CA3-OA5-PA1
57	2p	201	CDL	C56-C57-C58-C59
57	3D	202	CDL	C76-C77-C78-C79
57	3d	202	CDL	C76-C77-C78-C79
56	2O	203	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
56	2o	204	PC1	O22-C21-O21-C2
57	2U	101	CDL	CB2-C1-CA2-OA2
57	3E	202	CDL	CB2-C1-CA2-OA2
57	2u	101	CDL	CB2-C1-CA2-OA2
57	3e	202	CDL	CB2-C1-CA2-OA2
55	4Q	910	PEE	C12-C13-C14-C15
55	4q	910	PEE	C12-C13-C14-C15
57	2P	201	CDL	C56-C57-C58-C59
57	3D	201	CDL	C76-C77-C78-C79
57	3d	201	CDL	C76-C77-C78-C79
57	3i	201	CDL	C83-C84-C85-C86
55	4Q	909	PEE	C14-C15-C16-C17
55	4Z	302	PEE	C20-C21-C22-C23
55	4q	909	PEE	C14-C15-C16-C17
55	4z	302	PEE	C20-C21-C22-C23
56	2T	101	PC1	C23-C24-C25-C26
56	2t	101	PC1	C23-C24-C25-C26
57	3I	203	CDL	C83-C84-C85-C86
55	4Z	302	PEE	C11-C10-O2-C2
55	4z	302	PEE	C11-C10-O2-C2
57	3E	203	CDL	C51-CB5-OB6-CB4
57	4W	201	CDL	C11-CA5-OA6-CA4
57	3e	203	CDL	C51-CB5-OB6-CB4
57	4w	201	CDL	C11-CA5-OA6-CA4
57	2P	201	CDL	C22-C23-C24-C25
57	2p	201	CDL	C22-C23-C24-C25
57	3i	201	CDL	C79-C80-C81-C82
57	3E	201	CDL	OB9-CB7-OB8-CB6
57	4J	301	CDL	OA9-CA7-OA8-CA6
57	3e	201	CDL	OB9-CB7-OB8-CB6
57	4j	301	CDL	OA9-CA7-OA8-CA6
57	3I	203	CDL	C79-C80-C81-C82
57	2U	101	CDL	C31-C32-C33-C34
57	3D	202	CDL	C18-C19-C20-C21
57	4L	201	CDL	C52-C53-C54-C55
57	2u	101	CDL	C31-C32-C33-C34
57	4l	201	CDL	C52-C53-C54-C55
57	3I	202	CDL	C34-C35-C36-C37
57	3d	202	CDL	C18-C19-C20-C21
57	3i	203	CDL	C34-C35-C36-C37
55	4Z	302	PEE	C35-C36-C37-C38
57	4Z	301	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	4z	301	CDL	OA9-CA7-OA8-CA6
56	3A	502	PC1	O11-C1-C2-C3
56	3a	502	PC1	O11-C1-C2-C3
57	3I	201	CDL	OB5-CB3-CB4-CB6
57	3I	203	CDL	OB5-CB3-CB4-CB6
57	3L	701	CDL	OB5-CB3-CB4-CB6
57	3L	702	CDL	OB5-CB3-CB4-CB6
57	4K	202	CDL	OA5-CA3-CA4-CA6
57	4L	201	CDL	OA5-CA3-CA4-CA6
57	4M	201	CDL	OB5-CB3-CB4-CB6
57	4Q	907	CDL	OB5-CB3-CB4-CB6
57	4S	101	CDL	OB5-CB3-CB4-CB6
57	4U	501	CDL	OA5-CA3-CA4-CA6
57	4U	501	CDL	OB5-CB3-CB4-CB6
57	3i	201	CDL	OB5-CB3-CB4-CB6
57	3i	202	CDL	OB5-CB3-CB4-CB6
57	3l	701	CDL	OB5-CB3-CB4-CB6
57	3l	702	CDL	OB5-CB3-CB4-CB6
57	4k	202	CDL	OA5-CA3-CA4-CA6
57	4l	201	CDL	OA5-CA3-CA4-CA6
57	4m	201	CDL	OB5-CB3-CB4-CB6
57	4q	907	CDL	OB5-CB3-CB4-CB6
57	4s	101	CDL	OB5-CB3-CB4-CB6
57	4u	501	CDL	OA5-CA3-CA4-CA6
57	4u	501	CDL	OB5-CB3-CB4-CB6
57	3L	701	CDL	OA7-CA5-OA6-CA4
57	3l	701	CDL	OA7-CA5-OA6-CA4
57	4K	201	CDL	C75-C76-C77-C78
57	4l	201	CDL	C72-C73-C74-C75
57	3E	203	CDL	CA5-C11-C12-C13
57	3e	203	CDL	CA5-C11-C12-C13
57	3E	203	CDL	C19-C20-C21-C22
57	3I	202	CDL	C40-C41-C42-C43
57	3I	202	CDL	C83-C84-C85-C86
57	4L	201	CDL	C72-C73-C74-C75
57	3e	203	CDL	C19-C20-C21-C22
57	3i	203	CDL	C40-C41-C42-C43
57	3i	203	CDL	C83-C84-C85-C86
57	4k	201	CDL	C75-C76-C77-C78
56	3a	501	PC1	C28-C29-C2A-C2B
56	3a	501	PC1	C29-C2A-C2B-C2C
57	4E	201	CDL	CB4-CB6-OB8-CB7

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Mol	Chain	Res	Type	Atoms
57	4e	201	CDL	CB4-CB6-OB8-CB7
56	3A	501	PC1	C28-C29-C2A-C2B
56	3A	501	PC1	C29-C2A-C2B-C2C
57	3E	202	CDL	C14-C15-C16-C17
57	3e	202	CDL	C14-C15-C16-C17
57	3E	203	CDL	C71-CB7-OB8-CB6
57	3L	701	CDL	C71-CB7-OB8-CB6
57	3e	203	CDL	C71-CB7-OB8-CB6
57	3l	701	CDL	C71-CB7-OB8-CB6
55	40	302	PEE	C43-C44-C45-C46
55	41	302	PEE	C43-C44-C45-C46
55	2P	203	PEE	O4-C10-O2-C2
55	2p	203	PEE	O4-C10-O2-C2
57	4L	201	CDL	OA7-CA5-OA6-CA4
57	4l	201	CDL	OA7-CA5-OA6-CA4
55	3F	101	PEE	C37-C38-C39-C40
55	3f	101	PEE	C37-C38-C39-C40
55	4Q	910	PEE	C1-C2-C3-O3
55	4q	910	PEE	C1-C2-C3-O3
56	2O	203	PC1	C1-C2-C3-O31
56	3H	403	PC1	C1-C2-C3-O31
56	2o	204	PC1	C1-C2-C3-O31
56	3h	403	PC1	C1-C2-C3-O31
57	2O	204	CDL	CB3-CB4-CB6-OB8
57	3D	201	CDL	CB3-CB4-CB6-OB8
57	4K	201	CDL	CA3-CA4-CA6-OA8
57	4K	201	CDL	CB3-CB4-CB6-OB8
57	4S	101	CDL	CB3-CB4-CB6-OB8
57	2o	201	CDL	CB3-CB4-CB6-OB8
57	3d	201	CDL	CB3-CB4-CB6-OB8
57	4k	201	CDL	CA3-CA4-CA6-OA8
57	4k	201	CDL	CB3-CB4-CB6-OB8
57	4s	101	CDL	CB3-CB4-CB6-OB8
58	3D	203	UQ8	C19-C21-C22-C23
58	3d	203	UQ8	C19-C21-C22-C23
55	2P	202	PEE	C15-C16-C17-C18
55	2p	202	PEE	C15-C16-C17-C18
55	4z	302	PEE	C35-C36-C37-C38
62	4D	102	LPP	C32-C33-C34-C35
62	4d	102	LPP	C32-C33-C34-C35
55	2O	201	PEE	C31-C30-O3-C3
55	2o	202	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
57	3I	201	CDL	CB5-C51-C52-C53
57	3i	202	CDL	CB5-C51-C52-C53
55	3C	302	PEE	C41-C42-C43-C44
55	3c	302	PEE	C41-C42-C43-C44
57	4W	202	CDL	C20-C21-C22-C23
57	4w	202	CDL	C20-C21-C22-C23
55	4Q	909	PEE	O4-C10-O2-C2
55	4q	909	PEE	O4-C10-O2-C2
57	4J	301	CDL	C15-C16-C17-C18
57	4j	301	CDL	C15-C16-C17-C18
57	2P	201	CDL	C35-C36-C37-C38
57	3E	202	CDL	C71-CB7-OB8-CB6
57	3e	202	CDL	C71-CB7-OB8-CB6
55	40	303	PEE	C3-C2-O2-C10
55	41	303	PEE	C3-C2-O2-C10
57	4U	501	CDL	CA6-CA4-OA6-CA5
57	4u	501	CDL	CA6-CA4-OA6-CA5
57	2p	201	CDL	C35-C36-C37-C38
55	4Q	909	PEE	C43-C44-C45-C46
56	3h	403	PC1	C3A-C3B-C3C-C3D
57	3D	202	CDL	C74-C75-C76-C77
57	3d	202	CDL	C74-C75-C76-C77
56	3H	403	PC1	C3A-C3B-C3C-C3D
55	4q	909	PEE	C43-C44-C45-C46
57	2O	204	CDL	C33-C34-C35-C36
57	2o	201	CDL	C33-C34-C35-C36
56	2R	202	PC1	O11-C1-C2-O21
56	2r	202	PC1	O11-C1-C2-O21
57	4W	201	CDL	OB5-CB3-CB4-OB6
57	4w	201	CDL	OB5-CB3-CB4-OB6
55	40	303	PEE	C11-C10-O2-C2
55	41	303	PEE	C11-C10-O2-C2
57	3E	201	CDL	C39-C40-C41-C42
57	4W	202	CDL	C78-C79-C80-C81
57	3e	201	CDL	C39-C40-C41-C42
57	4w	202	CDL	C78-C79-C80-C81
56	3h	403	PC1	C2A-C2B-C2C-C2D
56	3H	403	PC1	C2A-C2B-C2C-C2D
57	3E	203	CDL	C56-C57-C58-C59
57	3L	702	CDL	C17-C18-C19-C20
57	3e	203	CDL	C56-C57-C58-C59
57	3l	702	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
57	3I	203	CDL	C71-CB7-OB8-CB6
57	4E	201	CDL	C71-CB7-OB8-CB6
57	4e	201	CDL	C71-CB7-OB8-CB6
57	3I	203	CDL	C75-C76-C77-C78
57	3i	201	CDL	C75-C76-C77-C78
57	3e	201	CDL	C14-C15-C16-C17
57	3E	201	CDL	C14-C15-C16-C17
57	4W	202	CDL	C75-C76-C77-C78
57	4w	202	CDL	C75-C76-C77-C78
55	2O	201	PEE	C35-C36-C37-C38
66	4Q	905	HEA	C3B-C11-C12-C13
66	4q	905	HEA	C3B-C11-C12-C13
58	3G	404	UQ8	C34-C36-C37-C38
58	3g	404	UQ8	C34-C36-C37-C38
56	2O	203	PC1	O32-C31-O31-C3
56	2o	204	PC1	O32-C31-O31-C3
57	4T	203	CDL	C78-C79-C80-C81
57	4q	908	CDL	C56-C57-C58-C59
57	4t	203	CDL	C78-C79-C80-C81
57	2Q	101	CDL	C31-CA7-OA8-CA6
57	2Q	101	CDL	C71-CB7-OB8-CB6
57	2q	101	CDL	C31-CA7-OA8-CA6
57	2q	101	CDL	C71-CB7-OB8-CB6
57	4j	301	CDL	C12-C11-CA5-OA6
57	4Q	908	CDL	C56-C57-C58-C59
57	4T	203	CDL	C11-C12-C13-C14
57	4t	203	CDL	C11-C12-C13-C14
55	4R	201	PEE	C33-C34-C35-C36
55	4r	201	PEE	C33-C34-C35-C36
57	3D	202	CDL	C12-C13-C14-C15
57	3d	202	CDL	C12-C13-C14-C15
57	4M	201	CDL	CA5-C11-C12-C13
57	4m	201	CDL	CA5-C11-C12-C13
66	4Q	905	HEA	C27-C19-C20-C21
66	4q	905	HEA	C27-C19-C20-C21
57	4J	301	CDL	C12-C11-CA5-OA6
55	4Q	909	PEE	O5-C30-O3-C3
55	4Q	910	PEE	C11-C12-C13-C14
55	4q	910	PEE	C11-C12-C13-C14
57	3I	202	CDL	C53-C54-C55-C56
55	4q	909	PEE	O5-C30-O3-C3
57	4M	201	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
57	3i	203	CDL	C53-C54-C55-C56
57	4q	907	CDL	C76-C77-C78-C79
57	4Q	907	CDL	C76-C77-C78-C79
57	4m	201	CDL	C75-C76-C77-C78
57	3i	201	CDL	C71-CB7-OB8-CB6
55	2o	202	PEE	C35-C36-C37-C38
56	2T	101	PC1	C37-C38-C39-C3A
56	3H	403	PC1	C2D-C2E-C2F-C2G
56	2t	101	PC1	C37-C38-C39-C3A
56	3h	403	PC1	C2D-C2E-C2F-C2G
57	3D	202	CDL	C22-C23-C24-C25
57	3d	202	CDL	C22-C23-C24-C25
57	3D	202	CDL	C14-C15-C16-C17
57	3d	202	CDL	C14-C15-C16-C17
57	2Q	101	CDL	CB7-C71-C72-C73
57	2q	101	CDL	CB7-C71-C72-C73
55	4Q	909	PEE	O3P-C1-C2-C3
55	4q	909	PEE	O3P-C1-C2-C3
56	2R	202	PC1	O11-C1-C2-C3
56	2r	202	PC1	O11-C1-C2-C3
57	2O	204	CDL	OB5-CB3-CB4-CB6
57	3D	202	CDL	OB5-CB3-CB4-CB6
57	3E	202	CDL	OA5-CA3-CA4-CA6
57	3E	203	CDL	OA5-CA3-CA4-CA6
57	3E	203	CDL	OB5-CB3-CB4-CB6
57	3L	702	CDL	OA5-CA3-CA4-CA6
57	4J	301	CDL	OB5-CB3-CB4-CB6
57	4W	202	CDL	OB5-CB3-CB4-CB6
57	2o	201	CDL	OB5-CB3-CB4-CB6
57	3d	202	CDL	OB5-CB3-CB4-CB6
57	3e	202	CDL	OA5-CA3-CA4-CA6
57	3e	203	CDL	OA5-CA3-CA4-CA6
57	3e	203	CDL	OB5-CB3-CB4-CB6
57	3l	702	CDL	OA5-CA3-CA4-CA6
57	4j	301	CDL	OB5-CB3-CB4-CB6
57	4w	202	CDL	OB5-CB3-CB4-CB6
57	4J	301	CDL	C77-C78-C79-C80
57	4j	301	CDL	C77-C78-C79-C80
56	3H	403	PC1	O32-C31-O31-C3
56	3h	403	PC1	O32-C31-O31-C3
57	3D	201	CDL	OA9-CA7-OA8-CA6
57	3d	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
57	4Q	907	CDL	C61-C62-C63-C64
57	3D	202	CDL	C54-C55-C56-C57
57	3D	202	CDL	C75-C76-C77-C78
57	3d	202	CDL	C54-C55-C56-C57
57	3d	202	CDL	C75-C76-C77-C78
57	3e	202	CDL	C20-C21-C22-C23
57	4q	907	CDL	C61-C62-C63-C64
56	3A	501	PC1	C26-C27-C28-C29
56	3a	501	PC1	C26-C27-C28-C29
57	3E	202	CDL	C20-C21-C22-C23
57	3G	403	CDL	C31-CA7-OA8-CA6
57	3g	403	CDL	C31-CA7-OA8-CA6
55	4Q	910	PEE	O5-C30-O3-C3
55	4q	910	PEE	O5-C30-O3-C3
57	4Q	907	CDL	C71-C72-C73-C74
57	4q	907	CDL	C71-C72-C73-C74
57	4K	202	CDL	C11-CA5-OA6-CA4
57	4k	202	CDL	C11-CA5-OA6-CA4
57	3I	202	CDL	CB2-C1-CA2-OA2
57	3i	203	CDL	CB2-C1-CA2-OA2
57	4L	201	CDL	C32-C33-C34-C35
57	4l	201	CDL	C32-C33-C34-C35
57	2U	101	CDL	CB3-CB4-CB6-OB8
57	3I	203	CDL	CB3-CB4-CB6-OB8
57	4Q	908	CDL	CA3-CA4-CA6-OA8
57	4W	201	CDL	CA3-CA4-CA6-OA8
57	2u	101	CDL	CB3-CB4-CB6-OB8
57	3i	201	CDL	CB3-CB4-CB6-OB8
57	4q	908	CDL	CA3-CA4-CA6-OA8
57	4w	201	CDL	CA3-CA4-CA6-OA8
58	3D	203	UQ8	C29-C31-C32-C33
58	3d	203	UQ8	C29-C31-C32-C33
57	3E	203	CDL	C77-C78-C79-C80
57	3e	203	CDL	C77-C78-C79-C80
56	2r	202	PC1	C39-C3A-C3B-C3C
56	2R	202	PC1	C39-C3A-C3B-C3C
58	3G	404	UQ8	C12-C11-C9-C10
58	3g	404	UQ8	C12-C11-C9-C10
55	3C	302	PEE	C11-C12-C13-C14
55	3c	302	PEE	C11-C12-C13-C14
57	3I	202	CDL	C39-C40-C41-C42
57	3i	203	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
55	4W	203	PEE	C10-C11-C12-C13
55	4w	203	PEE	C10-C11-C12-C13
55	4Q	909	PEE	O3P-C1-C2-O2
55	4q	909	PEE	O3P-C1-C2-O2
56	3A	501	PC1	O11-C1-C2-O21
56	3A	502	PC1	O11-C1-C2-O21
56	3a	501	PC1	O11-C1-C2-O21
56	3a	502	PC1	O11-C1-C2-O21
57	2Q	101	CDL	OB5-CB3-CB4-OB6
57	3L	701	CDL	OA5-CA3-CA4-OA6
57	3L	701	CDL	OB5-CB3-CB4-OB6
57	3L	702	CDL	OA5-CA3-CA4-OA6
57	4Q	907	CDL	OB5-CB3-CB4-OB6
57	4S	101	CDL	OB5-CB3-CB4-OB6
57	4U	501	CDL	OA5-CA3-CA4-OA6
57	2q	101	CDL	OB5-CB3-CB4-OB6
57	3l	701	CDL	OA5-CA3-CA4-OA6
57	3l	701	CDL	OB5-CB3-CB4-OB6
57	3l	702	CDL	OA5-CA3-CA4-OA6
57	4q	907	CDL	OB5-CB3-CB4-OB6
57	4s	101	CDL	OB5-CB3-CB4-OB6
57	4u	501	CDL	OA5-CA3-CA4-OA6
55	4s	102	PEE	C10-C11-C12-C13
57	2P	201	CDL	C72-C73-C74-C75
57	2p	201	CDL	C72-C73-C74-C75
57	3l	702	CDL	C42-C43-C44-C45
57	2Q	101	CDL	C52-C53-C54-C55
57	2Q	101	CDL	C79-C80-C81-C82
57	3L	702	CDL	C42-C43-C44-C45
57	2q	101	CDL	C52-C53-C54-C55
57	2q	101	CDL	C79-C80-C81-C82
57	3e	202	CDL	C37-C38-C39-C40
55	4Q	910	PEE	O2-C2-C3-O3
55	4q	910	PEE	O2-C2-C3-O3
55	4w	203	PEE	O2-C2-C3-O3
56	2O	203	PC1	O21-C2-C3-O31
56	2o	204	PC1	O21-C2-C3-O31
57	2O	204	CDL	OB6-CB4-CB6-OB8
57	3D	201	CDL	OA6-CA4-CA6-OA8
57	4K	201	CDL	OA6-CA4-CA6-OA8
57	4M	201	CDL	OB6-CB4-CB6-OB8
57	4Z	301	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
57	2o	201	CDL	OB6-CB4-CB6-OB8
57	3d	201	CDL	OA6-CA4-CA6-OA8
57	4k	201	CDL	OA6-CA4-CA6-OA8
57	4m	201	CDL	OB6-CB4-CB6-OB8
57	4z	301	CDL	OB6-CB4-CB6-OB8
57	3E	202	CDL	C37-C38-C39-C40
55	3C	302	PEE	O4-C10-O2-C2
55	3c	302	PEE	O4-C10-O2-C2
57	4E	201	CDL	OB7-CB5-OB6-CB4
57	4e	201	CDL	OB7-CB5-OB6-CB4
56	3A	501	PC1	C21-C22-C23-C24
56	3a	501	PC1	C21-C22-C23-C24
57	3D	201	CDL	CB7-C71-C72-C73
57	3d	201	CDL	CB7-C71-C72-C73
57	3D	202	CDL	C38-C39-C40-C41
57	3d	202	CDL	C38-C39-C40-C41
58	3G	404	UQ8	C12-C11-C9-C8
66	4Q	905	HEA	C18-C19-C20-C21
66	4q	905	HEA	C18-C19-C20-C21
57	4K	202	CDL	C57-C58-C59-C60
57	4L	201	CDL	C14-C15-C16-C17
57	4k	202	CDL	C57-C58-C59-C60
57	4l	201	CDL	C14-C15-C16-C17
56	2T	101	PC1	C22-C23-C24-C25
56	2t	101	PC1	C22-C23-C24-C25
57	4W	201	CDL	C51-C52-C53-C54
57	4w	201	CDL	C51-C52-C53-C54
55	2R	201	PEE	C10-C11-C12-C13
55	2r	201	PEE	C10-C11-C12-C13
55	4Z	302	PEE	C39-C40-C41-C42
55	4z	302	PEE	C39-C40-C41-C42
55	2P	203	PEE	C43-C44-C45-C46
50	2M	701	FAD	PA-O3P-P-O5'
50	2m	701	FAD	PA-O3P-P-O5'
55	4S	102	PEE	C10-C11-C12-C13
55	2p	203	PEE	C43-C44-C45-C46
57	3E	201	CDL	C55-C56-C57-C58
57	3e	201	CDL	C55-C56-C57-C58
62	4C	101	LPP	C15-C16-C17-C18
62	4c	101	LPP	C15-C16-C17-C18
57	4E	201	CDL	CA7-C31-C32-C33
57	4e	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
56	3H	403	PC1	C3C-C3D-C3E-C3F
56	3h	403	PC1	C3C-C3D-C3E-C3F
56	3A	502	PC1	C32-C31-O31-C3
56	3a	502	PC1	C32-C31-O31-C3
58	3g	404	UQ8	C12-C11-C9-C8
57	2Q	101	CDL	C11-CA5-OA6-CA4
57	4W	202	CDL	C51-CB5-OB6-CB4
57	2q	101	CDL	C11-CA5-OA6-CA4
57	4w	202	CDL	C51-CB5-OB6-CB4
57	4T	203	CDL	C44-C45-C46-C47
57	4t	203	CDL	C44-C45-C46-C47
57	3G	403	CDL	C64-C65-C66-C67
57	4T	203	CDL	C32-C31-CA7-OA8
57	4t	203	CDL	C32-C31-CA7-OA8
57	3g	403	CDL	C64-C65-C66-C67
55	2R	201	PEE	O3P-C1-C2-C3
55	4Z	302	PEE	O3P-C1-C2-C3
55	2r	201	PEE	O3P-C1-C2-C3
55	4z	302	PEE	O3P-C1-C2-C3
57	2Q	101	CDL	OB5-CB3-CB4-CB6
57	3L	701	CDL	OA5-CA3-CA4-CA6
57	4E	201	CDL	OA5-CA3-CA4-CA6
57	2q	101	CDL	OB5-CB3-CB4-CB6
57	3l	701	CDL	OA5-CA3-CA4-CA6
57	4e	201	CDL	OA5-CA3-CA4-CA6
57	3G	403	CDL	C13-C14-C15-C16
57	3g	403	CDL	C13-C14-C15-C16
56	3A	501	PC1	C2F-C2G-C2H-C2I
56	3a	501	PC1	C2F-C2G-C2H-C2I
57	4L	201	CDL	C36-C37-C38-C39
57	4l	201	CDL	C36-C37-C38-C39
57	3E	203	CDL	OB9-CB7-OB8-CB6
57	3L	701	CDL	OB9-CB7-OB8-CB6
57	3l	701	CDL	OB9-CB7-OB8-CB6
57	2P	201	CDL	C71-C72-C73-C74
57	2p	201	CDL	C71-C72-C73-C74
57	3e	202	CDL	C35-C36-C37-C38
55	4Z	302	PEE	C40-C41-C42-C43
55	4z	302	PEE	C40-C41-C42-C43
57	3E	202	CDL	C35-C36-C37-C38
62	4C	101	LPP	O9-C11-C12-C13
62	4c	101	LPP	O9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
57	3e	203	CDL	OB9-CB7-OB8-CB6
60	3G	402	HEM	C2B-C3B-CAB-CBB
60	3g	402	HEM	C2B-C3B-CAB-CBB
57	3L	701	CDL	CB6-CB4-OB6-CB5
57	3l	701	CDL	CB6-CB4-OB6-CB5
55	2O	201	PEE	O5-C30-O3-C3
55	2o	202	PEE	O5-C30-O3-C3
57	3E	202	CDL	OB9-CB7-OB8-CB6
57	3e	202	CDL	OB9-CB7-OB8-CB6
57	2O	204	CDL	C75-C76-C77-C78
57	4S	101	CDL	C51-C52-C53-C54
57	3l	701	CDL	C60-C61-C62-C63
57	3D	202	CDL	OA7-CA5-OA6-CA4
57	3d	202	CDL	OA7-CA5-OA6-CA4
55	2R	201	PEE	O3P-C1-C2-O2
55	2r	201	PEE	O3P-C1-C2-O2
57	3D	202	CDL	OB5-CB3-CB4-OB6
57	3E	202	CDL	OA5-CA3-CA4-OA6
57	3E	202	CDL	OB5-CB3-CB4-OB6
57	3E	203	CDL	OB5-CB3-CB4-OB6
57	4E	201	CDL	OA5-CA3-CA4-OA6
57	4W	202	CDL	OB5-CB3-CB4-OB6
57	3d	202	CDL	OB5-CB3-CB4-OB6
57	3e	202	CDL	OA5-CA3-CA4-OA6
57	3e	202	CDL	OB5-CB3-CB4-OB6
57	3e	203	CDL	OB5-CB3-CB4-OB6
57	4e	201	CDL	OA5-CA3-CA4-OA6
57	4w	202	CDL	OB5-CB3-CB4-OB6
57	4s	101	CDL	C51-C52-C53-C54
55	2P	202	PEE	C1-C2-C3-O3
55	4W	203	PEE	C1-C2-C3-O3
55	2p	202	PEE	C1-C2-C3-O3
55	4w	203	PEE	C1-C2-C3-O3
57	4J	301	CDL	CB3-CB4-CB6-OB8
57	4M	201	CDL	CB3-CB4-CB6-OB8
57	4j	301	CDL	CB3-CB4-CB6-OB8
57	4m	201	CDL	CB3-CB4-CB6-OB8
57	3L	701	CDL	C60-C61-C62-C63
57	2o	201	CDL	C75-C76-C77-C78
58	3D	203	UQ8	C40-C39-C41-C42
58	3d	203	UQ8	C40-C39-C41-C42
57	4z	301	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
55	4W	203	PEE	C5-C4-O4P-P
55	4w	203	PEE	C5-C4-O4P-P
58	3D	203	UQ8	C5-C6-C7-C8
58	3d	203	UQ8	C5-C6-C7-C8
57	3D	202	CDL	C13-C14-C15-C16
57	4Z	301	CDL	C31-C32-C33-C34
57	3d	202	CDL	C13-C14-C15-C16
55	4W	203	PEE	O2-C2-C3-O3
55	4z	302	PEE	C15-C16-C17-C18
57	3E	203	CDL	OB6-CB4-CB6-OB8
57	4J	301	CDL	OB6-CB4-CB6-OB8
57	4Q	907	CDL	OB6-CB4-CB6-OB8
57	4Q	908	CDL	OA6-CA4-CA6-OA8
57	4S	101	CDL	OB6-CB4-CB6-OB8
57	4U	501	CDL	OA6-CA4-CA6-OA8
57	3e	203	CDL	OB6-CB4-CB6-OB8
57	4j	301	CDL	OB6-CB4-CB6-OB8
57	4q	907	CDL	OB6-CB4-CB6-OB8
57	4q	908	CDL	OA6-CA4-CA6-OA8
57	4s	101	CDL	OB6-CB4-CB6-OB8
57	4u	501	CDL	OA6-CA4-CA6-OA8
57	3I	201	CDL	C53-C54-C55-C56
57	3L	702	CDL	C51-C52-C53-C54
57	3l	702	CDL	C51-C52-C53-C54
57	4E	201	CDL	OB9-CB7-OB8-CB6
57	4e	201	CDL	OB9-CB7-OB8-CB6
57	4W	202	CDL	C77-C78-C79-C80
57	4w	202	CDL	C77-C78-C79-C80
55	40	301	PEE	C10-C11-C12-C13
55	41	301	PEE	C10-C11-C12-C13
57	3i	202	CDL	C53-C54-C55-C56
56	2P	204	PC1	C3C-C3D-C3E-C3F
56	2p	204	PC1	C3C-C3D-C3E-C3F
57	4U	501	CDL	C51-C52-C53-C54
55	2P	202	PEE	C11-C10-O2-C2
55	2p	202	PEE	C11-C10-O2-C2
57	4K	201	CDL	C36-C37-C38-C39
57	4Q	907	CDL	C38-C39-C40-C41
57	3d	202	CDL	C37-C38-C39-C40
57	4q	907	CDL	C38-C39-C40-C41
57	4u	501	CDL	C51-C52-C53-C54
57	3I	201	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
57	3i	202	CDL	CB4-CB3-OB5-PB2
57	3D	202	CDL	C37-C38-C39-C40
57	4k	201	CDL	C36-C37-C38-C39
56	2T	101	PC1	O13-C11-C12-N
56	3H	403	PC1	O13-C11-C12-N
56	2t	101	PC1	O13-C11-C12-N
56	3h	403	PC1	O13-C11-C12-N
57	4M	201	CDL	CA7-C31-C32-C33
57	4m	201	CDL	CA7-C31-C32-C33
55	4Z	302	PEE	C15-C16-C17-C18
57	3L	701	CDL	C42-C43-C44-C45
57	3l	701	CDL	C42-C43-C44-C45
57	2P	201	CDL	C34-C35-C36-C37
57	3e	203	CDL	C78-C79-C80-C81
57	2p	201	CDL	C34-C35-C36-C37
57	4K	201	CDL	C84-C85-C86-C87
57	4k	201	CDL	C84-C85-C86-C87
57	3E	203	CDL	C78-C79-C80-C81
57	3E	201	CDL	C31-CA7-OA8-CA6
56	4E	202	PC1	C22-C23-C24-C25
56	4e	202	PC1	C22-C23-C24-C25
57	2Q	101	CDL	C16-C17-C18-C19
57	4L	201	CDL	C51-C52-C53-C54
57	4W	202	CDL	C16-C17-C18-C19
57	2q	101	CDL	C16-C17-C18-C19
57	3d	201	CDL	C54-C55-C56-C57
57	4w	202	CDL	C16-C17-C18-C19
57	4J	301	CDL	C58-C59-C60-C61
57	4Q	907	CDL	C60-C61-C62-C63
57	4j	301	CDL	C58-C59-C60-C61
57	4l	201	CDL	C51-C52-C53-C54
57	4q	907	CDL	C60-C61-C62-C63
57	2Q	101	CDL	OA9-CA7-OA8-CA6
57	2q	101	CDL	OA9-CA7-OA8-CA6
57	3l	702	CDL	C62-C63-C64-C65
57	3L	702	CDL	C62-C63-C64-C65
55	2P	203	PEE	O3P-C1-C2-C3
55	2p	203	PEE	O3P-C1-C2-C3
57	4Z	301	CDL	OB7-CB5-OB6-CB4
57	3e	201	CDL	OA7-CA5-OA6-CA4
57	4z	301	CDL	OB7-CB5-OB6-CB4
57	3D	201	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
57	4q	907	CDL	C41-C42-C43-C44
57	4Q	907	CDL	C41-C42-C43-C44
56	2R	202	PC1	C27-C28-C29-C2A
56	2r	202	PC1	C27-C28-C29-C2A
56	2t	101	PC1	C3C-C3D-C3E-C3F
57	3I	202	CDL	O1-C1-CB2-OB2
57	3i	203	CDL	O1-C1-CB2-OB2
56	2T	101	PC1	C3C-C3D-C3E-C3F
57	4z	301	CDL	C51-C52-C53-C54
57	3e	201	CDL	C31-CA7-OA8-CA6
57	4Z	301	CDL	C51-C52-C53-C54
62	4D	102	LPP	C34-C35-C36-C37
62	4d	102	LPP	C34-C35-C36-C37
57	4S	101	CDL	C22-C23-C24-C25
57	4s	101	CDL	C22-C23-C24-C25
55	4z	302	PEE	C13-C14-C15-C16
57	2Q	101	CDL	C32-C33-C34-C35
57	3G	403	CDL	CA4-CA3-OA5-PA1
57	3I	203	CDL	C1-CA2-OA2-PA1
57	3g	403	CDL	CA4-CA3-OA5-PA1
57	3i	201	CDL	C1-CA2-OA2-PA1
55	4I	301	PEE	C12-C13-C14-C15
57	4K	202	CDL	C72-C73-C74-C75
57	2q	101	CDL	C32-C33-C34-C35
55	40	301	PEE	C12-C13-C14-C15
55	4Z	302	PEE	C13-C14-C15-C16
57	3D	202	CDL	C56-C57-C58-C59
57	4Q	907	CDL	C12-C13-C14-C15
57	4k	202	CDL	C72-C73-C74-C75
57	4q	907	CDL	C12-C13-C14-C15
57	3d	202	CDL	C56-C57-C58-C59
55	40	303	PEE	O4-C10-O2-C2
55	4Z	302	PEE	O4-C10-O2-C2
55	4I	303	PEE	O4-C10-O2-C2
55	4z	302	PEE	O4-C10-O2-C2
57	3E	201	CDL	OA7-CA5-OA6-CA4
55	2P	203	PEE	O3P-C1-C2-O2
55	40	303	PEE	O3P-C1-C2-O2
55	4W	203	PEE	O3P-C1-C2-O2
55	4Z	302	PEE	O3P-C1-C2-O2
55	2p	203	PEE	O3P-C1-C2-O2
55	4I	303	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
55	4w	203	PEE	O3P-C1-C2-O2
55	4z	302	PEE	O3P-C1-C2-O2
56	3H	403	PC1	O11-C1-C2-O21
56	3h	403	PC1	O11-C1-C2-O21
57	3L	702	CDL	OB5-CB3-CB4-OB6
57	4M	201	CDL	OB5-CB3-CB4-OB6
57	3l	702	CDL	OB5-CB3-CB4-OB6
57	4m	201	CDL	OB5-CB3-CB4-OB6
56	2T	101	PC1	C39-C3A-C3B-C3C
57	3E	201	CDL	C20-C21-C22-C23
57	3e	201	CDL	C20-C21-C22-C23
56	2t	101	PC1	C39-C3A-C3B-C3C
57	3G	403	CDL	OA9-CA7-OA8-CA6
57	3D	202	CDL	OA6-CA4-CA6-OA8
57	4K	201	CDL	OB6-CB4-CB6-OB8
57	3d	202	CDL	OA6-CA4-CA6-OA8
57	4k	201	CDL	OB6-CB4-CB6-OB8
57	3g	403	CDL	C61-C62-C63-C64
57	3G	403	CDL	C61-C62-C63-C64
56	4E	202	PC1	C1-C2-C3-O31
56	4e	202	PC1	C1-C2-C3-O31
62	4C	101	LPP	C6-C7-C8-O27
62	4c	101	LPP	C6-C7-C8-O27
57	3g	403	CDL	OA9-CA7-OA8-CA6
57	4W	201	CDL	C73-C74-C75-C76
57	4w	201	CDL	C73-C74-C75-C76
57	3I	203	CDL	OB9-CB7-OB8-CB6
57	3i	201	CDL	OB9-CB7-OB8-CB6
55	2O	201	PEE	C38-C39-C40-C41
55	3F	101	PEE	C18-C19-C20-C21
55	4Q	910	PEE	C18-C19-C20-C21
55	4W	203	PEE	C36-C37-C38-C39
55	4W	203	PEE	C38-C39-C40-C41
55	2o	202	PEE	C38-C39-C40-C41
55	3f	101	PEE	C18-C19-C20-C21
55	4q	910	PEE	C18-C19-C20-C21
55	4w	203	PEE	C36-C37-C38-C39
55	4w	203	PEE	C38-C39-C40-C41
57	3d	202	CDL	C21-C22-C23-C24
57	3D	202	CDL	C21-C22-C23-C24
57	3E	201	CDL	C82-C83-C84-C85
57	3e	201	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
57	4W	201	CDL	OA7-CA5-OA6-CA4
57	4w	201	CDL	OA7-CA5-OA6-CA4
57	3D	202	CDL	C19-C20-C21-C22
57	3d	202	CDL	C19-C20-C21-C22
55	2O	201	PEE	C1-O3P-P-O2P
55	2R	201	PEE	C4-O4P-P-O2P
55	3F	101	PEE	C1-O3P-P-O2P
55	3F	101	PEE	C4-O4P-P-O2P
55	4O	301	PEE	C1-O3P-P-O2P
55	4D	101	PEE	C1-O3P-P-O1P
55	4D	101	PEE	O4P-C4-C5-N
55	4Q	909	PEE	C1-O3P-P-O1P
55	4R	201	PEE	C1-O3P-P-O1P
55	4R	201	PEE	C4-O4P-P-O1P
55	2o	202	PEE	C1-O3P-P-O2P
55	2r	201	PEE	C4-O4P-P-O2P
55	3f	101	PEE	C1-O3P-P-O2P
55	3f	101	PEE	C4-O4P-P-O2P
55	4l	301	PEE	C1-O3P-P-O2P
55	4d	101	PEE	C1-O3P-P-O1P
55	4d	101	PEE	O4P-C4-C5-N
55	4q	909	PEE	C1-O3P-P-O1P
55	4r	201	PEE	C1-O3P-P-O1P
55	4r	201	PEE	C4-O4P-P-O1P
56	2P	204	PC1	C11-O13-P-O11
56	2R	202	PC1	C1-O11-P-O12
56	2T	101	PC1	C11-O13-P-O14
56	2T	101	PC1	C1-O11-P-O14
56	3A	501	PC1	C1-O11-P-O14
56	3A	502	PC1	C11-O13-P-O14
56	3A	502	PC1	C1-O11-P-O12
56	3H	403	PC1	C1-O11-P-O14
56	2p	204	PC1	C11-O13-P-O11
56	2r	202	PC1	C1-O11-P-O12
56	2t	101	PC1	C11-O13-P-O14
56	2t	101	PC1	C1-O11-P-O14
56	3a	501	PC1	C1-O11-P-O14
56	3a	502	PC1	C11-O13-P-O14
56	3a	502	PC1	C1-O11-P-O12
56	3h	403	PC1	C1-O11-P-O14
57	2O	204	CDL	CB3-OB5-PB2-OB3
57	2P	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
57	2P	201	CDL	CB3-OB5-PB2-OB2
57	2Q	101	CDL	CA2-OA2-PA1-OA4
57	2U	101	CDL	CB3-OB5-PB2-OB3
57	3E	201	CDL	CA2-OA2-PA1-OA3
57	3E	201	CDL	CB2-OB2-PB2-OB4
57	3E	201	CDL	CB2-OB2-PB2-OB5
57	3G	403	CDL	CA2-OA2-PA1-OA4
57	3H	402	CDL	CB2-OB2-PB2-OB4
57	3I	201	CDL	CA3-OA5-PA1-OA3
57	3I	202	CDL	CA2-OA2-PA1-OA3
57	3I	202	CDL	CA3-OA5-PA1-OA3
57	3L	702	CDL	CB2-OB2-PB2-OB5
57	4E	201	CDL	CA3-OA5-PA1-OA2
57	4E	201	CDL	CA3-OA5-PA1-OA4
57	4J	301	CDL	CA3-OA5-PA1-OA3
57	4J	301	CDL	CB2-OB2-PB2-OB4
57	4J	301	CDL	CB2-OB2-PB2-OB5
57	4K	201	CDL	CA2-OA2-PA1-OA4
57	4K	202	CDL	CB3-OB5-PB2-OB3
57	4L	201	CDL	CA2-OA2-PA1-OA3
57	4M	201	CDL	CA2-OA2-PA1-OA3
57	4M	201	CDL	CA3-OA5-PA1-OA4
57	4M	201	CDL	CB3-OB5-PB2-OB3
57	4Q	907	CDL	CA2-OA2-PA1-OA3
57	4Q	907	CDL	CA3-OA5-PA1-OA3
57	4Q	907	CDL	CB2-OB2-PB2-OB5
57	4Q	908	CDL	CA3-OA5-PA1-OA2
57	4Q	908	CDL	CA3-OA5-PA1-OA3
57	4Q	908	CDL	CA3-OA5-PA1-OA4
57	4S	101	CDL	CA2-OA2-PA1-OA3
57	4S	101	CDL	CA3-OA5-PA1-OA4
57	4S	101	CDL	CB3-OB5-PB2-OB3
57	4T	203	CDL	CA2-OA2-PA1-OA5
57	4T	203	CDL	CB2-OB2-PB2-OB4
57	4T	203	CDL	CB3-OB5-PB2-OB3
57	4U	501	CDL	CA2-OA2-PA1-OA4
57	4W	201	CDL	CA2-OA2-PA1-OA3
57	4W	202	CDL	CB3-OB5-PB2-OB3
57	4Z	301	CDL	CB2-OB2-PB2-OB3
57	2o	201	CDL	CB3-OB5-PB2-OB3
57	2p	201	CDL	CB2-OB2-PB2-OB3
57	2p	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
57	2q	101	CDL	CA2-OA2-PA1-OA4
57	2u	101	CDL	CB3-OB5-PB2-OB3
57	3e	201	CDL	CA2-OA2-PA1-OA3
57	3e	201	CDL	CB2-OB2-PB2-OB5
57	3g	403	CDL	CA2-OA2-PA1-OA4
57	3h	402	CDL	CB2-OB2-PB2-OB4
57	3i	202	CDL	CA3-OA5-PA1-OA3
57	3i	203	CDL	CA2-OA2-PA1-OA3
57	3i	203	CDL	CA3-OA5-PA1-OA3
57	3l	702	CDL	CB2-OB2-PB2-OB5
57	4e	201	CDL	CA3-OA5-PA1-OA2
57	4e	201	CDL	CA3-OA5-PA1-OA4
57	4j	301	CDL	CA3-OA5-PA1-OA3
57	4j	301	CDL	CB2-OB2-PB2-OB4
57	4j	301	CDL	CB2-OB2-PB2-OB5
57	4k	201	CDL	CA2-OA2-PA1-OA4
57	4k	202	CDL	CB3-OB5-PB2-OB3
57	4l	201	CDL	CA2-OA2-PA1-OA3
57	4m	201	CDL	CA2-OA2-PA1-OA3
57	4m	201	CDL	CA3-OA5-PA1-OA4
57	4m	201	CDL	CB3-OB5-PB2-OB3
57	4q	907	CDL	CA2-OA2-PA1-OA3
57	4q	907	CDL	CA3-OA5-PA1-OA3
57	4q	907	CDL	CB2-OB2-PB2-OB5
57	4q	908	CDL	CA3-OA5-PA1-OA2
57	4q	908	CDL	CA3-OA5-PA1-OA3
57	4q	908	CDL	CA3-OA5-PA1-OA4
57	4s	101	CDL	CA2-OA2-PA1-OA3
57	4s	101	CDL	CA3-OA5-PA1-OA4
57	4s	101	CDL	CB3-OB5-PB2-OB3
57	4t	203	CDL	CA2-OA2-PA1-OA5
57	4t	203	CDL	CB2-OB2-PB2-OB4
57	4t	203	CDL	CB3-OB5-PB2-OB3
57	4u	501	CDL	CA2-OA2-PA1-OA4
57	4w	201	CDL	CA2-OA2-PA1-OA3
57	4w	202	CDL	CB3-OB5-PB2-OB3
57	4z	301	CDL	CB2-OB2-PB2-OB3
55	4d	101	PEE	C31-C32-C33-C34
55	4D	101	PEE	C31-C32-C33-C34
57	3E	201	CDL	C17-C18-C19-C20
57	4j	301	CDL	C76-C77-C78-C79
57	4u	501	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
58	3D	203	UQ8	C38-C39-C41-C42
58	3d	203	UQ8	C38-C39-C41-C42
55	2P	202	PEE	C12-C13-C14-C15
55	2p	202	PEE	C12-C13-C14-C15
57	4J	301	CDL	C76-C77-C78-C79
57	4U	501	CDL	C39-C40-C41-C42
57	3e	201	CDL	C17-C18-C19-C20
57	2O	204	CDL	C1-CB2-OB2-PB2
57	2Q	101	CDL	CB4-CB3-OB5-PB2
57	3D	201	CDL	CB4-CB3-OB5-PB2
57	3D	202	CDL	CB4-CB3-OB5-PB2
57	3E	203	CDL	CB4-CB3-OB5-PB2
57	4K	202	CDL	C1-CB2-OB2-PB2
57	2o	201	CDL	C1-CB2-OB2-PB2
57	2q	101	CDL	CB4-CB3-OB5-PB2
57	3d	201	CDL	CB4-CB3-OB5-PB2
57	3d	202	CDL	CB4-CB3-OB5-PB2
57	3e	203	CDL	CB4-CB3-OB5-PB2
57	4k	202	CDL	C1-CB2-OB2-PB2
57	4K	202	CDL	C76-C77-C78-C79
57	4k	202	CDL	C76-C77-C78-C79
57	4u	501	CDL	C33-C34-C35-C36
57	3I	201	CDL	C31-C32-C33-C34
57	4U	501	CDL	C33-C34-C35-C36
57	3i	202	CDL	C31-C32-C33-C34
56	2O	202	PC1	C2C-C2D-C2E-C2F
55	2P	202	PEE	C13-C14-C15-C16
55	2p	202	PEE	C13-C14-C15-C16
56	2o	203	PC1	C2C-C2D-C2E-C2F
57	4Q	907	CDL	C22-C23-C24-C25
57	3E	203	CDL	CB3-CB4-OB6-CB5
57	3G	403	CDL	CA6-CA4-OA6-CA5
57	4E	201	CDL	CB6-CB4-OB6-CB5
57	4Q	907	CDL	CA3-CA4-OA6-CA5
57	4Q	907	CDL	CA6-CA4-OA6-CA5
57	4Z	301	CDL	CA3-CA4-OA6-CA5
57	3e	203	CDL	CB3-CB4-OB6-CB5
57	3g	403	CDL	CA6-CA4-OA6-CA5
57	4e	201	CDL	CB6-CB4-OB6-CB5
57	4q	907	CDL	CA3-CA4-OA6-CA5
57	4q	907	CDL	CA6-CA4-OA6-CA5
57	4z	301	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
58	3D	203	UQ8	C39-C41-C42-C43
56	4E	202	PC1	C3F-C3G-C3H-C3I
56	4e	202	PC1	C3F-C3G-C3H-C3I
57	2U	101	CDL	C35-C36-C37-C38
57	2u	101	CDL	C35-C36-C37-C38
57	4q	907	CDL	C22-C23-C24-C25
57	4k	202	CDL	C15-C16-C17-C18
57	3I	202	CDL	OB5-CB3-CB4-CB6
57	4Q	907	CDL	OA5-CA3-CA4-CA6
57	4W	201	CDL	OB5-CB3-CB4-CB6
57	3i	203	CDL	OB5-CB3-CB4-CB6
57	4q	907	CDL	OA5-CA3-CA4-CA6
57	4w	201	CDL	OB5-CB3-CB4-CB6
55	2P	202	PEE	C34-C35-C36-C37
55	40	301	PEE	C11-C12-C13-C14
55	2p	202	PEE	C34-C35-C36-C37
55	41	301	PEE	C11-C12-C13-C14
56	2O	202	PC1	C33-C34-C35-C36
56	2o	203	PC1	C33-C34-C35-C36
57	4K	202	CDL	C15-C16-C17-C18
57	3i	202	CDL	C71-CB7-OB8-CB6
55	4S	102	PEE	C12-C13-C14-C15
55	4s	102	PEE	C12-C13-C14-C15
55	2R	201	PEE	C36-C37-C38-C39
55	3C	302	PEE	C18-C19-C20-C21
55	4R	201	PEE	C36-C37-C38-C39
55	4W	203	PEE	C18-C19-C20-C21
55	2r	201	PEE	C36-C37-C38-C39
55	3c	302	PEE	C18-C19-C20-C21
55	4r	201	PEE	C36-C37-C38-C39
55	4w	203	PEE	C18-C19-C20-C21
55	4Q	909	PEE	C30-C31-C32-C33
55	4q	909	PEE	C30-C31-C32-C33
57	4M	201	CDL	CA2-C1-CB2-OB2
57	4m	201	CDL	CA2-C1-CB2-OB2
57	3E	203	CDL	OA5-CA3-CA4-OA6
57	3I	201	CDL	OB5-CB3-CB4-OB6
57	3I	202	CDL	OB5-CB3-CB4-OB6
57	4K	202	CDL	OA5-CA3-CA4-OA6
57	4U	501	CDL	OB5-CB3-CB4-OB6
57	3e	203	CDL	OA5-CA3-CA4-OA6
57	3i	202	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
57	3i	203	CDL	OB5-CB3-CB4-OB6
57	4k	202	CDL	OA5-CA3-CA4-OA6
57	4u	501	CDL	OB5-CB3-CB4-OB6
57	3D	202	CDL	C61-C62-C63-C64
57	3d	202	CDL	C61-C62-C63-C64
57	3I	201	CDL	C71-CB7-OB8-CB6
55	2O	201	PEE	C21-C22-C23-C24
55	2o	202	PEE	C21-C22-C23-C24
57	3i	201	CDL	C77-C78-C79-C80
58	3G	404	UQ8	C5-C4-O4-C4M
58	3g	404	UQ8	C5-C4-O4-C4M
57	3I	203	CDL	C77-C78-C79-C80
56	2O	203	PC1	C2-C1-O11-P
56	2o	204	PC1	C2-C1-O11-P
57	2U	101	CDL	CA4-CA3-OA5-PA1
57	3E	202	CDL	C1-CB2-OB2-PB2
57	2u	101	CDL	CA4-CA3-OA5-PA1
57	3e	202	CDL	C1-CB2-OB2-PB2
55	4w	203	PEE	C11-C12-C13-C14
57	3L	701	CDL	OB6-CB4-CB6-OB8
57	3l	701	CDL	OB6-CB4-CB6-OB8
55	4W	203	PEE	C11-C12-C13-C14
57	2Q	101	CDL	OB9-CB7-OB8-CB6
57	2q	101	CDL	OB9-CB7-OB8-CB6
57	4K	201	CDL	C58-C59-C60-C61
57	4K	202	CDL	C71-C72-C73-C74
57	4k	202	CDL	C71-C72-C73-C74
55	4r	201	PEE	C11-C10-O2-C2
57	3D	202	CDL	C11-C12-C13-C14
57	4k	201	CDL	C58-C59-C60-C61
57	3d	202	CDL	C11-C12-C13-C14
57	3E	203	CDL	OB7-CB5-OB6-CB4
57	3e	203	CDL	OB7-CB5-OB6-CB4
57	3D	201	CDL	CA3-CA4-CA6-OA8
57	4Z	301	CDL	CB3-CB4-CB6-OB8
57	3d	201	CDL	CA3-CA4-CA6-OA8
57	4z	301	CDL	CB3-CB4-CB6-OB8
58	3d	203	UQ8	C39-C41-C42-C43
57	3E	202	CDL	CB7-C71-C72-C73
57	3e	202	CDL	CB7-C71-C72-C73
55	4R	201	PEE	C11-C10-O2-C2
55	40	302	PEE	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
55	4l	302	PEE	C44-C45-C46-C47
57	4W	202	CDL	C76-C77-C78-C79
57	4w	202	CDL	C76-C77-C78-C79
55	4l	302	PEE	C16-C17-C18-C19
58	3D	203	UQ8	C1-C6-C7-C8
58	3d	203	UQ8	C1-C6-C7-C8
57	4Z	301	CDL	C13-C14-C15-C16
57	4z	301	CDL	C13-C14-C15-C16
57	3D	202	CDL	C32-C31-CA7-OA8
57	3d	202	CDL	C32-C31-CA7-OA8
57	3E	203	CDL	C12-C13-C14-C15
57	3e	203	CDL	C12-C13-C14-C15
61	4l	304	AJP	C27-C26-O25-C23
57	3I	201	CDL	C54-C55-C56-C57
57	3i	202	CDL	C54-C55-C56-C57
55	40	302	PEE	C16-C17-C18-C19
56	4E	202	PC1	C2-C1-O11-P
56	4e	202	PC1	C2-C1-O11-P
61	40	304	AJP	C27-C26-O25-C23
57	2q	101	CDL	C35-C36-C37-C38
57	2Q	101	CDL	C35-C36-C37-C38
57	2O	204	CDL	C23-C24-C25-C26
57	2o	201	CDL	C23-C24-C25-C26
56	3A	502	PC1	O32-C31-O31-C3
57	2P	201	CDL	OA5-CA3-CA4-OA6
57	2p	201	CDL	OA5-CA3-CA4-OA6
55	2O	201	PEE	C16-C17-C18-C19
55	40	302	PEE	C36-C37-C38-C39
55	2o	202	PEE	C16-C17-C18-C19
55	4l	302	PEE	C36-C37-C38-C39
57	4Q	908	CDL	C57-C58-C59-C60
56	3a	502	PC1	O32-C31-O31-C3
57	4q	908	CDL	C57-C58-C59-C60
57	2U	101	CDL	C56-C57-C58-C59
57	3L	701	CDL	C58-C59-C60-C61
57	3I	202	CDL	C11-C12-C13-C14
57	3L	702	CDL	C35-C36-C37-C38
57	3l	701	CDL	C58-C59-C60-C61
57	3l	702	CDL	C35-C36-C37-C38
57	2Q	101	CDL	OA7-CA5-OA6-CA4
57	4K	202	CDL	OA7-CA5-OA6-CA4
57	2q	101	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
57	4k	202	CDL	OA7-CA5-OA6-CA4
57	2P	201	CDL	C74-C75-C76-C77
57	3E	202	CDL	C38-C39-C40-C41
57	2p	201	CDL	C74-C75-C76-C77
57	2u	101	CDL	C56-C57-C58-C59
57	3e	202	CDL	C38-C39-C40-C41
55	2P	203	PEE	C18-C19-C20-C21
55	2R	201	PEE	C38-C39-C40-C41
55	40	301	PEE	C36-C37-C38-C39
55	4Q	910	PEE	C38-C39-C40-C41
55	4W	203	PEE	C16-C17-C18-C19
55	4Z	302	PEE	C16-C17-C18-C19
55	4Z	302	PEE	C36-C37-C38-C39
55	2p	203	PEE	C18-C19-C20-C21
55	2r	201	PEE	C38-C39-C40-C41
55	4l	301	PEE	C36-C37-C38-C39
55	4q	910	PEE	C38-C39-C40-C41
55	4w	203	PEE	C16-C17-C18-C19
55	4z	302	PEE	C16-C17-C18-C19
55	4z	302	PEE	C36-C37-C38-C39
57	3i	203	CDL	C11-C12-C13-C14
55	2P	202	PEE	O2-C2-C3-O3
55	2p	202	PEE	O2-C2-C3-O3
57	4s	101	CDL	C71-C72-C73-C74
57	3H	402	CDL	C64-C65-C66-C67
57	3h	402	CDL	C64-C65-C66-C67
57	3I	202	CDL	C76-C77-C78-C79
57	4S	101	CDL	C71-C72-C73-C74
57	3i	203	CDL	C76-C77-C78-C79
56	2O	202	PC1	C2-C3-O31-C31
56	2o	203	PC1	C2-C3-O31-C31
55	4R	201	PEE	C20-C21-C22-C23
57	2P	201	CDL	C15-C16-C17-C18
57	3D	202	CDL	C59-C60-C61-C62
57	2p	201	CDL	C15-C16-C17-C18
57	3d	202	CDL	C59-C60-C61-C62
57	3l	701	CDL	C77-C78-C79-C80
57	4u	501	CDL	C41-C42-C43-C44
57	3L	701	CDL	C77-C78-C79-C80
55	4r	201	PEE	C20-C21-C22-C23
57	4U	501	CDL	C41-C42-C43-C44
55	2P	202	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
55	2p	202	PEE	C16-C17-C18-C19
57	3D	201	CDL	C1-CA2-OA2-PA1
57	4Z	301	CDL	CB4-CB3-OB5-PB2
57	3d	201	CDL	C1-CA2-OA2-PA1
57	4z	301	CDL	CB4-CB3-OB5-PB2
57	3i	203	CDL	C77-C78-C79-C80
57	3E	203	CDL	C80-C81-C82-C83
57	4Q	907	CDL	CB7-C71-C72-C73
57	4q	907	CDL	CB7-C71-C72-C73
57	3D	201	CDL	C20-C21-C22-C23
57	3E	202	CDL	C60-C61-C62-C63
57	3I	202	CDL	C77-C78-C79-C80
57	3d	201	CDL	C20-C21-C22-C23
57	3e	202	CDL	C60-C61-C62-C63
57	3e	203	CDL	C80-C81-C82-C83
57	3g	403	CDL	C59-C60-C61-C62
58	2S	201	UQ8	C34-C36-C37-C38
58	2s	201	UQ8	C34-C36-C37-C38
57	3d	201	CDL	C62-C63-C64-C65
57	3D	201	CDL	C62-C63-C64-C65
57	2q	101	CDL	C39-C40-C41-C42
60	3G	401	HEM	CAD-CBD-CGD-O1D
57	3I	202	CDL	C15-C16-C17-C18
56	2R	202	PC1	C31-C32-C33-C34
56	2r	202	PC1	C31-C32-C33-C34
57	2Q	101	CDL	C39-C40-C41-C42
57	3G	403	CDL	C59-C60-C61-C62
57	3i	203	CDL	C15-C16-C17-C18
60	3g	401	HEM	CAD-CBD-CGD-O1D
55	3F	101	PEE	C3-C2-O2-C10
55	3f	101	PEE	C3-C2-O2-C10
57	3D	201	CDL	CA3-CA4-OA6-CA5
57	3D	202	CDL	CA6-CA4-OA6-CA5
57	3E	203	CDL	CA3-CA4-OA6-CA5
57	3d	201	CDL	CA3-CA4-OA6-CA5
57	3d	202	CDL	CA3-CA4-OA6-CA5
57	3d	202	CDL	CA6-CA4-OA6-CA5
57	3e	203	CDL	CA3-CA4-OA6-CA5
57	4E	201	CDL	C11-C12-C13-C14
57	4e	201	CDL	C11-C12-C13-C14
58	2S	201	UQ8	C15-C14-C16-C17
58	2s	201	UQ8	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
55	3C	302	PEE	C36-C37-C38-C39
55	4S	102	PEE	C18-C19-C20-C21
55	3c	302	PEE	C36-C37-C38-C39
55	40	301	PEE	C14-C15-C16-C17
55	41	301	PEE	C14-C15-C16-C17
57	2O	204	CDL	C31-C32-C33-C34
57	2o	201	CDL	C31-C32-C33-C34
57	2u	101	CDL	C60-C61-C62-C63
57	2O	204	CDL	C73-C74-C75-C76
57	2o	201	CDL	C73-C74-C75-C76
58	3G	404	UQ8	C3-C4-O4-C4M
58	3g	404	UQ8	C3-C4-O4-C4M
57	2U	101	CDL	C60-C61-C62-C63
57	3G	403	CDL	C36-C37-C38-C39
57	2q	101	CDL	C72-C73-C74-C75
55	4Q	910	PEE	O3P-C1-C2-O2
55	4q	910	PEE	O3P-C1-C2-O2
57	3D	201	CDL	OB5-CB3-CB4-OB6
57	3d	201	CDL	OB5-CB3-CB4-OB6
57	2Q	101	CDL	C72-C73-C74-C75
57	3g	403	CDL	C36-C37-C38-C39
57	4k	202	CDL	C31-C32-C33-C34
57	3L	702	CDL	C14-C15-C16-C17
57	3e	201	CDL	C83-C84-C85-C86
66	4Q	905	HEA	CAD-CBD-CGD-O2D
66	4q	905	HEA	CAD-CBD-CGD-O2D
55	2P	203	PEE	C16-C17-C18-C19
55	4D	101	PEE	C38-C39-C40-C41
55	4Z	302	PEE	C38-C39-C40-C41
55	2p	203	PEE	C16-C17-C18-C19
55	4d	101	PEE	C38-C39-C40-C41
55	4s	102	PEE	C18-C19-C20-C21
55	4z	302	PEE	C38-C39-C40-C41
57	3E	201	CDL	C83-C84-C85-C86
57	4K	202	CDL	C31-C32-C33-C34
57	3E	201	CDL	CA4-CA3-OA5-PA1
57	3I	201	CDL	C1-CB2-OB2-PB2
57	3I	203	CDL	CA4-CA3-OA5-PA1
57	3L	702	CDL	CA4-CA3-OA5-PA1
57	4K	201	CDL	CB4-CB3-OB5-PB2
57	4Q	907	CDL	C1-CB2-OB2-PB2
57	4Q	908	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
57	4S	101	CDL	CB4-CB3-OB5-PB2
57	3e	201	CDL	CA4-CA3-OA5-PA1
57	3i	201	CDL	CA4-CA3-OA5-PA1
57	3i	202	CDL	C1-CB2-OB2-PB2
57	4k	201	CDL	CB4-CB3-OB5-PB2
57	4q	907	CDL	C1-CB2-OB2-PB2
57	4q	908	CDL	CA4-CA3-OA5-PA1
57	4s	101	CDL	CB4-CB3-OB5-PB2
57	3l	702	CDL	C14-C15-C16-C17
57	4k	202	CDL	C62-C63-C64-C65
66	4Q	904	HEA	C26-C15-C16-C17
66	4Q	904	HEA	C27-C19-C20-C21
66	4q	904	HEA	C26-C15-C16-C17
66	4q	904	HEA	C27-C19-C20-C21
57	4K	202	CDL	C62-C63-C64-C65
55	4R	201	PEE	O3P-C1-C2-C3
55	4r	201	PEE	O3P-C1-C2-C3
57	4T	203	CDL	OA5-CA3-CA4-CA6
57	4t	203	CDL	OA5-CA3-CA4-CA6
58	2S	201	UQ8	C13-C14-C16-C17
58	2s	201	UQ8	C13-C14-C16-C17
55	2P	203	PEE	C44-C45-C46-C47
57	4T	203	CDL	C53-C54-C55-C56
57	4t	203	CDL	C53-C54-C55-C56
59	3C	301	HEC	C3D-CAD-CBD-CGD
59	3c	301	HEC	C3D-CAD-CBD-CGD
55	2p	203	PEE	C44-C45-C46-C47
55	40	301	PEE	C18-C19-C20-C21
55	40	303	PEE	C18-C19-C20-C21
55	4Q	909	PEE	C36-C37-C38-C39
55	4l	301	PEE	C18-C19-C20-C21
55	4l	303	PEE	C18-C19-C20-C21
55	4q	909	PEE	C36-C37-C38-C39
57	4E	201	CDL	OB6-CB4-CB6-OB8
57	4U	501	CDL	OB6-CB4-CB6-OB8
57	4e	201	CDL	OB6-CB4-CB6-OB8
57	4u	501	CDL	OB6-CB4-CB6-OB8
62	4C	101	LPP	O9-C7-C8-O27
62	4c	101	LPP	O9-C7-C8-O27
60	3g	402	HEM	CAA-CBA-CGA-O2A
66	4Q	905	HEA	CAD-CBD-CGD-O1D
66	4q	905	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
57	3E	203	CDL	C31-C32-C33-C34
57	3e	203	CDL	C31-C32-C33-C34
57	3D	202	CDL	C63-C64-C65-C66
57	3d	202	CDL	C63-C64-C65-C66
57	2O	204	CDL	CA7-C31-C32-C33
57	4W	201	CDL	C74-C75-C76-C77
60	3G	402	HEM	CAA-CBA-CGA-O1A
60	3G	402	HEM	CAA-CBA-CGA-O2A
60	3g	402	HEM	CAA-CBA-CGA-O1A
66	4Q	904	HEA	CAA-CBA-CGA-O1A
66	4Q	905	HEA	CAA-CBA-CGA-O2A
66	4q	904	HEA	CAA-CBA-CGA-O1A
66	4q	905	HEA	CAA-CBA-CGA-O2A
57	4w	201	CDL	C74-C75-C76-C77
57	4W	202	CDL	OB7-CB5-OB6-CB4
57	4w	202	CDL	OB7-CB5-OB6-CB4
57	4K	201	CDL	C54-C55-C56-C57
57	2o	201	CDL	CA7-C31-C32-C33
60	3g	401	HEM	CAA-CBA-CGA-O1A
57	3D	202	CDL	C36-C37-C38-C39
57	4k	201	CDL	C54-C55-C56-C57
60	3G	401	HEM	CAA-CBA-CGA-O1A
66	4Q	905	HEA	CAA-CBA-CGA-O1A
57	4K	201	CDL	C73-C74-C75-C76
57	3i	202	CDL	C41-C42-C43-C44
57	4k	201	CDL	C73-C74-C75-C76
57	3I	201	CDL	C41-C42-C43-C44
57	3d	202	CDL	C36-C37-C38-C39
57	3D	201	CDL	C17-C18-C19-C20
57	3l	701	CDL	C16-C17-C18-C19
57	3L	701	CDL	C16-C17-C18-C19
57	3d	201	CDL	C17-C18-C19-C20
59	3C	301	HEC	CAA-CBA-CGA-O1A
59	3c	301	HEC	CAA-CBA-CGA-O1A
59	3c	301	HEC	CAD-CBD-CGD-O2D
57	3E	203	CDL	C18-C19-C20-C21
57	4U	501	CDL	C54-C55-C56-C57
57	4u	501	CDL	C54-C55-C56-C57
57	3e	203	CDL	C18-C19-C20-C21
57	3i	201	CDL	C74-C75-C76-C77
59	3C	301	HEC	CAD-CBD-CGD-O2D
60	3G	401	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
66	4q	905	HEA	CAA-CBA-CGA-O1A
57	4w	202	CDL	C71-CB7-OB8-CB6
57	3I	203	CDL	C74-C75-C76-C77
57	4U	501	CDL	C32-C33-C34-C35
57	4u	501	CDL	C32-C33-C34-C35
58	3d	203	UQ8	C12-C11-C9-C10
66	4Q	904	HEA	CAA-CBA-CGA-O2A
66	4q	904	HEA	CAA-CBA-CGA-O2A
55	2P	203	PEE	C2-C1-O3P-P
55	2R	201	PEE	C2-C1-O3P-P
55	4R	201	PEE	C2-C1-O3P-P
55	2p	203	PEE	C2-C1-O3P-P
55	2r	201	PEE	C2-C1-O3P-P
55	4r	201	PEE	C2-C1-O3P-P
57	3E	203	CDL	C1-CA2-OA2-PA1
57	4W	202	CDL	C1-CB2-OB2-PB2
57	3e	203	CDL	C1-CA2-OA2-PA1
57	3I	702	CDL	CA4-CA3-OA5-PA1
57	4q	907	CDL	CB4-CB3-OB5-PB2
57	4w	202	CDL	C1-CB2-OB2-PB2
57	4Q	908	CDL	C31-CA7-OA8-CA6
57	4W	202	CDL	C71-CB7-OB8-CB6
57	4q	908	CDL	C31-CA7-OA8-CA6
60	3G	401	HEM	CAD-CBD-CGD-O2D
60	3g	401	HEM	CAA-CBA-CGA-O2A
60	3g	401	HEM	CAD-CBD-CGD-O2D
56	2t	101	PC1	C3A-C3B-C3C-C3D
57	3i	202	CDL	C39-C40-C41-C42
55	2O	201	PEE	C1-C2-C3-O3
55	2o	202	PEE	C1-C2-C3-O3
58	3G	404	UQ8	C24-C26-C27-C28
58	3g	404	UQ8	C24-C26-C27-C28
57	3I	201	CDL	C39-C40-C41-C42
56	2T	101	PC1	C3A-C3B-C3C-C3D
57	3D	202	CDL	C34-C35-C36-C37
57	3G	403	CDL	C37-C38-C39-C40
57	3d	202	CDL	C34-C35-C36-C37
57	3E	201	CDL	C22-C23-C24-C25
55	4D	101	PEE	O3P-C1-C2-O2
55	4d	101	PEE	O3P-C1-C2-O2
57	4T	203	CDL	OA5-CA3-CA4-OA6
57	4t	203	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
58	3D	203	UQ8	C12-C11-C9-C10
66	4Q	905	HEA	C26-C15-C16-C17
66	4q	905	HEA	C26-C15-C16-C17
57	3e	201	CDL	C22-C23-C24-C25
57	3g	403	CDL	C37-C38-C39-C40
57	3e	201	CDL	OA9-CA7-OA8-CA6
55	2R	201	PEE	C18-C19-C20-C21
55	4D	101	PEE	C16-C17-C18-C19
55	4D	101	PEE	C36-C37-C38-C39
55	4R	201	PEE	C16-C17-C18-C19
55	2r	201	PEE	C18-C19-C20-C21
55	4d	101	PEE	C16-C17-C18-C19
55	4d	101	PEE	C36-C37-C38-C39
55	4r	201	PEE	C16-C17-C18-C19
57	3I	203	CDL	CA2-C1-CB2-OB2
57	3d	201	CDL	CB2-C1-CA2-OA2
57	3i	201	CDL	CA2-C1-CB2-OB2
57	3E	201	CDL	OA9-CA7-OA8-CA6
57	4Q	907	CDL	C36-C37-C38-C39
57	4T	203	CDL	C22-C23-C24-C25
57	4q	907	CDL	C36-C37-C38-C39
57	4q	908	CDL	C59-C60-C61-C62
57	4Q	908	CDL	C59-C60-C61-C62
57	4t	203	CDL	C22-C23-C24-C25
56	3A	501	PC1	O11-C1-C2-C3
56	3H	403	PC1	O11-C1-C2-C3
56	3a	501	PC1	O11-C1-C2-C3
56	3h	403	PC1	O11-C1-C2-C3
57	3D	202	CDL	C57-C58-C59-C60
55	2O	201	PEE	C36-C37-C38-C39
55	40	301	PEE	C38-C39-C40-C41
55	40	303	PEE	C16-C17-C18-C19
55	40	303	PEE	C36-C37-C38-C39
55	2o	202	PEE	C36-C37-C38-C39
55	41	301	PEE	C38-C39-C40-C41
55	41	303	PEE	C16-C17-C18-C19
55	41	303	PEE	C36-C37-C38-C39
57	3L	701	CDL	C1-CA2-OA2-PA1
57	3L	701	CDL	C1-CB2-OB2-PB2
57	4J	301	CDL	CA4-CA3-OA5-PA1
57	4Q	907	CDL	CB4-CB3-OB5-PB2
57	3l	701	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
57	3l	701	CDL	C1-CB2-OB2-PB2
57	4j	301	CDL	CA4-CA3-OA5-PA1
57	3d	202	CDL	C57-C58-C59-C60
57	4T	203	CDL	C34-C35-C36-C37
59	3C	301	HEC	CAA-CBA-CGA-O2A
66	4Q	904	HEA	CAD-CBD-CGD-O2D
57	4t	203	CDL	C34-C35-C36-C37
57	3E	201	CDL	C43-C44-C45-C46
57	3e	201	CDL	C43-C44-C45-C46
57	3I	203	CDL	O1-C1-CB2-OB2
57	3i	201	CDL	O1-C1-CB2-OB2
57	3G	403	CDL	C38-C39-C40-C41
57	3g	403	CDL	C38-C39-C40-C41
50	2M	701	FAD	O4B-C4B-C5B-O5B
50	2m	701	FAD	O4B-C4B-C5B-O5B
62	4C	101	LPP	O10-C11-C12-C13
62	4c	101	LPP	O10-C11-C12-C13
57	4j	301	CDL	C57-C58-C59-C60
59	3c	301	HEC	CAA-CBA-CGA-O2A
66	4q	904	HEA	CAD-CBD-CGD-O2D
55	3F	101	PEE	C36-C37-C38-C39
55	4S	102	PEE	C38-C39-C40-C41
55	4Z	302	PEE	C18-C19-C20-C21
55	3f	101	PEE	C36-C37-C38-C39
55	4s	102	PEE	C38-C39-C40-C41
55	4z	302	PEE	C18-C19-C20-C21
57	4J	301	CDL	C57-C58-C59-C60
66	4Q	904	HEA	C14-C15-C16-C17
66	4q	904	HEA	C14-C15-C16-C17
57	4T	203	CDL	C32-C31-CA7-OA9
57	4t	203	CDL	C32-C31-CA7-OA9
57	3D	202	CDL	C71-CB7-OB8-CB6
57	3d	202	CDL	C71-CB7-OB8-CB6
57	3D	202	CDL	CA3-CA4-OA6-CA5
57	3E	203	CDL	CA6-CA4-OA6-CA5
57	4S	101	CDL	CB6-CB4-OB6-CB5
57	3e	203	CDL	CA6-CA4-OA6-CA5
57	4s	101	CDL	CB6-CB4-OB6-CB5
57	3I	201	CDL	OB9-CB7-OB8-CB6
57	3i	202	CDL	OB9-CB7-OB8-CB6
55	2P	202	PEE	C38-C39-C40-C41
55	2p	202	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
57	3L	701	CDL	C78-C79-C80-C81
57	3l	701	CDL	C78-C79-C80-C81
62	4c	101	LPP	C39-C40-C41-C42
62	4C	101	LPP	C39-C40-C41-C42
55	40	303	PEE	C30-C31-C32-C33
57	3D	201	CDL	C21-C22-C23-C24
66	4Q	904	HEA	CAD-CBD-CGD-O1D
66	4q	904	HEA	CAD-CBD-CGD-O1D
56	2R	202	PC1	C32-C33-C34-C35
56	2r	202	PC1	C32-C33-C34-C35
56	2O	203	PC1	C3F-C3G-C3H-C3I
56	2o	204	PC1	C3F-C3G-C3H-C3I
57	3d	201	CDL	C21-C22-C23-C24
55	2P	202	PEE	C2-C1-O3P-P
55	4D	101	PEE	C2-C1-O3P-P
55	2p	202	PEE	C2-C1-O3P-P
55	4d	101	PEE	C2-C1-O3P-P
57	3I	202	CDL	CA4-CA3-OA5-PA1
57	4K	202	CDL	CA4-CA3-OA5-PA1
57	3i	203	CDL	CA4-CA3-OA5-PA1
57	4k	202	CDL	CA4-CA3-OA5-PA1
57	3D	201	CDL	CB2-C1-CA2-OA2
55	4R	201	PEE	C31-C32-C33-C34
57	4E	201	CDL	C73-C74-C75-C76
57	4e	201	CDL	C73-C74-C75-C76
57	3H	402	CDL	C71-CB7-OB8-CB6
57	3h	402	CDL	C71-CB7-OB8-CB6
57	3D	202	CDL	CA3-CA4-CA6-OA8
57	3d	202	CDL	CA3-CA4-CA6-OA8
55	2P	203	PEE	C41-C42-C43-C44
55	2p	203	PEE	C41-C42-C43-C44
55	4r	201	PEE	C31-C32-C33-C34
55	4l	303	PEE	C30-C31-C32-C33
57	2q	101	CDL	C76-C77-C78-C79
55	40	303	PEE	C38-C39-C40-C41
55	4Q	909	PEE	C18-C19-C20-C21
55	4S	102	PEE	C16-C17-C18-C19
55	4l	303	PEE	C38-C39-C40-C41
55	4q	909	PEE	C18-C19-C20-C21
55	4s	102	PEE	C16-C17-C18-C19
57	2Q	101	CDL	C76-C77-C78-C79
56	2o	203	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
56	2O	202	PC1	C2B-C2C-C2D-C2E
57	4Q	908	CDL	C35-C36-C37-C38
57	4q	908	CDL	C35-C36-C37-C38
55	4S	102	PEE	C13-C14-C15-C16
56	3A	502	PC1	C32-C33-C34-C35
57	3G	403	CDL	C71-C72-C73-C74
57	3g	403	CDL	C71-C72-C73-C74
55	3F	101	PEE	C41-C42-C43-C44
55	3f	101	PEE	C41-C42-C43-C44
55	4s	102	PEE	C13-C14-C15-C16
59	3C	301	HEC	C2D-C3D-CAD-CBD
59	3c	301	HEC	C2D-C3D-CAD-CBD
56	3a	502	PC1	C32-C33-C34-C35
55	4D	101	PEE	C18-C19-C20-C21
55	4R	201	PEE	C18-C19-C20-C21
55	4d	101	PEE	C18-C19-C20-C21
55	4r	201	PEE	C18-C19-C20-C21
57	3I	202	CDL	C22-C23-C24-C25
55	4W	203	PEE	O3P-C1-C2-C3
55	4w	203	PEE	O3P-C1-C2-C3
60	3G	402	HEM	CAD-CBD-CGD-O2D
60	3g	402	HEM	CAD-CBD-CGD-O2D
55	3F	101	PEE	C31-C32-C33-C34
55	4D	101	PEE	C33-C34-C35-C36
57	4W	202	CDL	C52-C53-C54-C55
55	3f	101	PEE	C31-C32-C33-C34
55	4d	101	PEE	C33-C34-C35-C36
57	4Q	908	CDL	C15-C16-C17-C18
57	3i	203	CDL	C22-C23-C24-C25
57	4w	202	CDL	C52-C53-C54-C55
57	3D	201	CDL	C12-C11-CA5-OA6
57	3d	201	CDL	C12-C11-CA5-OA6
57	4q	908	CDL	C15-C16-C17-C18
57	3L	701	CDL	C64-C65-C66-C67
66	4Q	905	HEA	C2C-C3C-CAC-CBC
66	4q	905	HEA	C2C-C3C-CAC-CBC
57	3l	701	CDL	C64-C65-C66-C67
55	2R	201	PEE	C16-C17-C18-C19
55	3F	101	PEE	C38-C39-C40-C41
55	2r	201	PEE	C16-C17-C18-C19
55	3f	101	PEE	C38-C39-C40-C41
57	2Q	101	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
56	2o	204	PC1	C2A-C2B-C2C-C2D
57	2q	101	CDL	C40-C41-C42-C43
57	4K	201	CDL	C1-CB2-OB2-PB2
57	4k	201	CDL	C1-CB2-OB2-PB2
56	2O	203	PC1	C2A-C2B-C2C-C2D
57	4j	301	CDL	C72-C71-CB7-OB8
56	2O	203	PC1	O13-C11-C12-N
56	2o	204	PC1	O13-C11-C12-N
57	2u	101	CDL	CA5-C11-C12-C13
57	4J	301	CDL	C72-C71-CB7-OB8
57	4S	101	CDL	C52-C51-CB5-OB6
57	4s	101	CDL	C52-C51-CB5-OB6
55	2P	202	PEE	O4-C10-O2-C2
55	2p	202	PEE	O4-C10-O2-C2
55	2O	201	PEE	C18-C19-C20-C21
55	2P	203	PEE	C36-C37-C38-C39
55	4Q	909	PEE	C38-C39-C40-C41
55	2o	202	PEE	C18-C19-C20-C21
55	2p	203	PEE	C36-C37-C38-C39
55	4q	909	PEE	C38-C39-C40-C41
57	2O	204	CDL	C52-C53-C54-C55
57	2o	201	CDL	C52-C53-C54-C55
57	3L	702	CDL	C51-CB5-OB6-CB4
57	3l	702	CDL	C51-CB5-OB6-CB4
57	2O	204	CDL	C43-C44-C45-C46
57	3D	201	CDL	C52-C53-C54-C55
57	2o	201	CDL	C43-C44-C45-C46
57	3d	201	CDL	C52-C53-C54-C55
57	2U	101	CDL	CA5-C11-C12-C13
57	4W	201	CDL	C36-C37-C38-C39
57	3g	403	CDL	C33-C34-C35-C36
57	4w	201	CDL	C36-C37-C38-C39
55	4z	302	PEE	C21-C22-C23-C24
57	3L	701	CDL	C73-C74-C75-C76
57	3e	202	CDL	C41-C42-C43-C44
57	3l	701	CDL	C73-C74-C75-C76
57	3I	202	CDL	C72-C71-CB7-OB8
57	3i	203	CDL	C72-C71-CB7-OB8
57	4K	202	CDL	CB5-C51-C52-C53
57	4k	202	CDL	CB5-C51-C52-C53
57	4Z	301	CDL	OA5-CA3-CA4-OA6
57	4z	301	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
62	4D	102	LPP	O5-C6-C7-O9
62	4d	102	LPP	O5-C6-C7-O9
57	3G	403	CDL	C33-C34-C35-C36
55	4Z	302	PEE	C21-C22-C23-C24
57	3E	202	CDL	C41-C42-C43-C44
58	3G	405	UQ8	C15-C14-C16-C17
58	3g	405	UQ8	C15-C14-C16-C17
56	2T	101	PC1	C36-C37-C38-C39
56	2t	101	PC1	C36-C37-C38-C39
57	3L	702	CDL	C38-C39-C40-C41
57	3l	702	CDL	C38-C39-C40-C41
55	2p	203	PEE	O2-C10-C11-C12
57	3G	403	CDL	C12-C11-CA5-OA6
57	3g	403	CDL	C12-C11-CA5-OA6
57	3L	702	CDL	C64-C65-C66-C67
57	3l	702	CDL	C64-C65-C66-C67
57	4Q	907	CDL	C18-C19-C20-C21
57	4q	907	CDL	C18-C19-C20-C21
55	4l	303	PEE	C42-C43-C44-C45
57	4w	201	CDL	C37-C38-C39-C40
55	2P	203	PEE	O2-C10-C11-C12
56	3A	501	PC1	O21-C21-C22-C23
56	3a	501	PC1	O21-C21-C22-C23
57	4W	201	CDL	C37-C38-C39-C40
57	3d	202	CDL	C77-C78-C79-C80
57	3E	203	CDL	CB3-CB4-CB6-OB8
57	3e	203	CDL	CB3-CB4-CB6-OB8
57	2U	101	CDL	C59-C60-C61-C62
57	2u	101	CDL	C59-C60-C61-C62
55	40	303	PEE	C42-C43-C44-C45
57	2U	101	CDL	C61-C62-C63-C64
57	3H	402	CDL	C33-C34-C35-C36
58	3D	203	UQ8	C5-C4-O4-C4M
58	3d	203	UQ8	C5-C4-O4-C4M
58	3G	405	UQ8	C12-C11-C9-C10
58	3g	405	UQ8	C12-C11-C9-C10
57	3d	201	CDL	C75-C76-C77-C78
55	40	303	PEE	O2-C10-C11-C12
55	4l	303	PEE	O2-C10-C11-C12
55	4q	909	PEE	O3-C30-C31-C32
56	2R	202	PC1	O21-C21-C22-C23
56	2r	202	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
57	2O	204	CDL	C52-C51-CB5-OB6
57	3D	202	CDL	C52-C51-CB5-OB6
57	4U	501	CDL	C72-C71-CB7-OB8
57	2o	201	CDL	C52-C51-CB5-OB6
57	3d	202	CDL	C52-C51-CB5-OB6
57	4u	501	CDL	C72-C71-CB7-OB8
57	3D	201	CDL	C75-C76-C77-C78
57	2u	101	CDL	C61-C62-C63-C64
57	3D	202	CDL	C77-C78-C79-C80
56	2O	202	PC1	C23-C24-C25-C26
56	2o	203	PC1	C23-C24-C25-C26
57	3h	402	CDL	C33-C34-C35-C36
57	2o	201	CDL	C76-C77-C78-C79
55	4Q	909	PEE	O3-C30-C31-C32
56	3A	501	PC1	O31-C31-C32-C33
57	4J	301	CDL	C32-C31-CA7-OA8
57	4K	202	CDL	C32-C31-CA7-OA8
57	4T	203	CDL	C52-C51-CB5-OB6
57	4W	202	CDL	C12-C11-CA5-OA6
57	4j	301	CDL	C32-C31-CA7-OA8
57	4k	202	CDL	C32-C31-CA7-OA8
57	4t	203	CDL	C52-C51-CB5-OB6
57	4w	202	CDL	C12-C11-CA5-OA6
62	4d	102	LPP	O9-C11-C12-C13
57	3h	402	CDL	C54-C55-C56-C57
57	3D	202	CDL	OA5-CA3-CA4-CA6
57	4K	202	CDL	OB5-CB3-CB4-CB6
57	3d	202	CDL	OA5-CA3-CA4-CA6
57	4k	202	CDL	OB5-CB3-CB4-CB6
56	3a	501	PC1	O31-C31-C32-C33
62	4D	102	LPP	O9-C11-C12-C13
57	2O	204	CDL	C76-C77-C78-C79
57	3H	402	CDL	C54-C55-C56-C57
57	4k	201	CDL	C11-CA5-OA6-CA4
57	3E	202	CDL	CA2-C1-CB2-OB2
57	3e	202	CDL	CA2-C1-CB2-OB2
55	4S	102	PEE	C36-C37-C38-C39
55	2p	202	PEE	C36-C37-C38-C39
57	3E	201	CDL	C72-C71-CB7-OB8
57	3e	201	CDL	C72-C71-CB7-OB8
56	3a	502	PC1	C26-C27-C28-C29
56	3A	502	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
56	3H	403	PC1	C23-C24-C25-C26
56	3h	403	PC1	C23-C24-C25-C26
57	4Q	907	CDL	CB3-CB4-OB6-CB5
57	4S	101	CDL	CB3-CB4-OB6-CB5
57	4q	907	CDL	CB3-CB4-OB6-CB5
57	4s	101	CDL	CB3-CB4-OB6-CB5
55	4d	101	PEE	C21-C22-C23-C24
57	4t	203	CDL	C61-C62-C63-C64
57	4T	203	CDL	C61-C62-C63-C64
55	4D	101	PEE	C21-C22-C23-C24
57	4Z	301	CDL	C52-C53-C54-C55
55	4R	201	PEE	O4-C10-O2-C2
55	4r	201	PEE	O4-C10-O2-C2
57	3e	202	CDL	C34-C35-C36-C37
55	2R	201	PEE	C11-C12-C13-C14
55	2r	201	PEE	C11-C12-C13-C14
57	4z	301	CDL	C52-C53-C54-C55
55	2P	202	PEE	C36-C37-C38-C39
55	4s	102	PEE	C36-C37-C38-C39
57	3E	202	CDL	C71-C72-C73-C74
57	2U	101	CDL	C1-CA2-OA2-PA1
57	4K	201	CDL	CA4-CA3-OA5-PA1
57	4W	201	CDL	CB4-CB3-OB5-PB2
57	2u	101	CDL	C1-CA2-OA2-PA1
57	4k	201	CDL	CA4-CA3-OA5-PA1
57	4w	201	CDL	CB4-CB3-OB5-PB2
57	4Q	907	CDL	C40-C41-C42-C43
55	4Q	909	PEE	O5-C30-C31-C32
55	4q	909	PEE	O5-C30-C31-C32
57	3I	202	CDL	C72-C71-CB7-OB9
57	3i	203	CDL	C72-C71-CB7-OB9
57	3e	202	CDL	C71-C72-C73-C74
57	4q	907	CDL	C40-C41-C42-C43
57	3E	202	CDL	C34-C35-C36-C37
55	4Z	302	PEE	O3-C30-C31-C32
55	4z	302	PEE	O3-C30-C31-C32
57	3L	701	CDL	C32-C31-CA7-OA8
57	3l	701	CDL	C32-C31-CA7-OA8
56	2O	202	PC1	C21-C22-C23-C24
56	2o	203	PC1	C21-C22-C23-C24
57	2Q	101	CDL	C82-C83-C84-C85
57	2q	101	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
57	4k	201	CDL	C74-C75-C76-C77
57	4K	201	CDL	C74-C75-C76-C77
57	4w	202	CDL	C72-C73-C74-C75
57	3D	202	CDL	C39-C40-C41-C42
57	3d	202	CDL	C39-C40-C41-C42
57	3l	701	CDL	C72-C73-C74-C75
55	4D	101	PEE	O2-C10-C11-C12
55	4d	101	PEE	O2-C10-C11-C12
57	4E	201	CDL	C32-C31-CA7-OA8
57	4e	201	CDL	C32-C31-CA7-OA8
55	2P	203	PEE	O4-C10-C11-C12
55	2p	203	PEE	O4-C10-C11-C12
56	3A	501	PC1	O22-C21-C22-C23
58	3G	405	UQ8	C5-C4-O4-C4M
58	3g	405	UQ8	C5-C4-O4-C4M
57	4K	201	CDL	C11-CA5-OA6-CA4
57	2Q	101	CDL	CB5-C51-C52-C53
57	2q	101	CDL	CB5-C51-C52-C53
57	3L	701	CDL	C72-C73-C74-C75
56	3a	501	PC1	O22-C21-C22-C23
57	4J	301	CDL	C12-C11-CA5-OA7
57	4j	301	CDL	C12-C11-CA5-OA7
57	4K	202	CDL	C39-C40-C41-C42
57	4W	202	CDL	C72-C73-C74-C75
56	4E	202	PC1	C2E-C2F-C2G-C2H
57	4Q	908	CDL	OA9-CA7-OA8-CA6
57	4q	908	CDL	OA9-CA7-OA8-CA6
57	3d	202	CDL	C52-C51-CB5-OB7
56	4e	202	PC1	C2E-C2F-C2G-C2H
56	2o	204	PC1	C32-C33-C34-C35
56	2O	203	PC1	C32-C33-C34-C35
57	4k	202	CDL	C39-C40-C41-C42
57	3D	202	CDL	C52-C51-CB5-OB7
57	4t	203	CDL	C52-C51-CB5-OB7
57	4E	201	CDL	C35-C36-C37-C38
57	4W	201	CDL	C24-C25-C26-C27
57	4w	201	CDL	C24-C25-C26-C27
57	3E	201	CDL	CA2-C1-CB2-OB2
57	3e	201	CDL	CA2-C1-CB2-OB2
57	3D	201	CDL	C12-C11-CA5-OA7
57	4T	203	CDL	C52-C51-CB5-OB7
57	3d	201	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
62	4D	102	LPP	O10-C11-C12-C13
62	4d	102	LPP	O10-C11-C12-C13
57	3D	201	CDL	C52-C51-CB5-OB6
57	4W	202	CDL	C72-C71-CB7-OB8
57	3d	201	CDL	C52-C51-CB5-OB6
57	4w	202	CDL	C72-C71-CB7-OB8
57	4s	101	CDL	C16-C17-C18-C19
57	3L	701	CDL	C57-C58-C59-C60
57	4S	101	CDL	C16-C17-C18-C19
57	4s	101	CDL	C19-C20-C21-C22
57	3l	701	CDL	C57-C58-C59-C60
62	4c	101	LPP	C13-C14-C15-C16
57	3L	701	CDL	CB3-CB4-CB6-OB8
57	3l	701	CDL	CB3-CB4-CB6-OB8
57	3E	201	CDL	C72-C71-CB7-OB9
57	3G	403	CDL	C12-C11-CA5-OA7
57	4J	301	CDL	C32-C31-CA7-OA9
57	3e	201	CDL	C72-C71-CB7-OB9
57	4j	301	CDL	C32-C31-CA7-OA9
58	2S	201	UQ8	C21-C22-C23-C24
58	2s	201	UQ8	C21-C22-C23-C24
57	4S	101	CDL	C19-C20-C21-C22
57	4e	201	CDL	C35-C36-C37-C38
55	3C	302	PEE	O3-C30-C31-C32
55	3c	302	PEE	O3-C30-C31-C32
56	3H	403	PC1	O21-C21-C22-C23
56	3h	403	PC1	O21-C21-C22-C23
57	3E	203	CDL	C20-C21-C22-C23
57	3e	203	CDL	C20-C21-C22-C23
62	4C	101	LPP	C13-C14-C15-C16
57	3L	701	CDL	C32-C31-CA7-OA9
57	3l	701	CDL	C32-C31-CA7-OA9
57	3D	201	CDL	C60-C61-C62-C63
57	3d	201	CDL	C60-C61-C62-C63
57	4t	203	CDL	C31-C32-C33-C34
55	40	301	PEE	O2-C10-C11-C12
57	3D	202	CDL	CB4-CB6-OB8-CB7
57	3d	202	CDL	CB4-CB6-OB8-CB7
56	3A	501	PC1	O32-C31-C32-C33
57	3g	403	CDL	C12-C11-CA5-OA7
57	3E	202	CDL	OB5-CB3-CB4-CB6
57	3e	202	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
57	3D	202	CDL	C64-C65-C66-C67
57	3i	201	CDL	C71-C72-C73-C74
57	3d	202	CDL	C64-C65-C66-C67
56	3a	501	PC1	O32-C31-C32-C33
55	4l	301	PEE	O2-C10-C11-C12
56	2o	204	PC1	C36-C37-C38-C39
57	3I	203	CDL	C71-C72-C73-C74
57	4T	203	CDL	C31-C32-C33-C34
57	4Q	908	CDL	C73-C74-C75-C76
57	4q	908	CDL	C73-C74-C75-C76
55	40	301	PEE	O4-C10-C11-C12
55	4l	301	PEE	O4-C10-C11-C12
57	4U	501	CDL	C72-C71-CB7-OB9
55	4R	201	PEE	O3-C30-C31-C32
55	4r	201	PEE	O3-C30-C31-C32
57	3I	202	CDL	C32-C31-CA7-OA8
57	3L	702	CDL	C72-C71-CB7-OB8
57	4Q	907	CDL	C32-C31-CA7-OA8
57	3i	203	CDL	C32-C31-CA7-OA8
57	3l	702	CDL	C72-C71-CB7-OB8
57	4q	907	CDL	C32-C31-CA7-OA8
56	2P	204	PC1	C38-C39-C3A-C3B
57	3l	701	CDL	C61-C62-C63-C64
55	4Z	302	PEE	O5-C30-C31-C32
55	4z	302	PEE	O5-C30-C31-C32
57	4W	202	CDL	C12-C11-CA5-OA7
57	4u	501	CDL	C72-C71-CB7-OB9
57	4w	202	CDL	C12-C11-CA5-OA7
57	3D	201	CDL	CB5-C51-C52-C53
57	3d	201	CDL	CB5-C51-C52-C53
56	2O	203	PC1	C36-C37-C38-C39
56	2p	204	PC1	C38-C39-C3A-C3B
56	3A	502	PC1	O31-C31-C32-C33
57	3E	201	CDL	C52-C51-CB5-OB6
57	3I	201	CDL	C32-C31-CA7-OA8
57	3I	201	CDL	C52-C51-CB5-OB6
57	3e	201	CDL	C52-C51-CB5-OB6
57	3i	202	CDL	C32-C31-CA7-OA8
57	3i	202	CDL	C52-C51-CB5-OB6
57	4u	501	CDL	C52-C51-CB5-OB6
56	2R	202	PC1	O22-C21-C22-C23
56	2r	202	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
57	3H	402	CDL	C72-C71-CB7-OB9
57	4E	201	CDL	C32-C31-CA7-OA9
57	3I	702	CDL	C72-C71-CB7-OB9
57	4e	201	CDL	C32-C31-CA7-OA9
62	4C	101	LPP	O28-C29-C30-C31
57	3E	201	CDL	C11-C12-C13-C14
57	3I	201	CDL	C43-C44-C45-C46
57	3e	201	CDL	C11-C12-C13-C14
57	3i	202	CDL	C43-C44-C45-C46
57	4u	501	CDL	C20-C21-C22-C23

There are no ring outliers.

83 monomers are involved in 209 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	4q	907	CDL	1	0
57	4k	201	CDL	1	0
57	4K	201	CDL	1	0
57	2u	101	CDL	2	0
56	2T	101	PC1	1	0
57	3H	402	CDL	1	0
66	4q	904	HEA	4	0
58	3G	405	UQ8	5	0
61	4I	304	AJP	1	0
57	2U	101	CDL	2	0
55	4Q	910	PEE	1	0
57	4s	101	CDL	1	0
57	4j	301	CDL	1	0
60	3g	402	HEM	1	0
57	4Q	907	CDL	1	0
56	2t	101	PC1	1	0
57	2p	201	CDL	3	0
58	3g	405	UQ8	4	0
50	2M	701	FAD	11	0
58	3G	404	UQ8	10	0
57	4q	908	CDL	2	0
50	2m	701	FAD	11	0
57	2P	201	CDL	3	0
56	2O	203	PC1	3	0
57	2q	101	CDL	2	0
57	3h	402	CDL	1	0
57	4k	202	CDL	2	0

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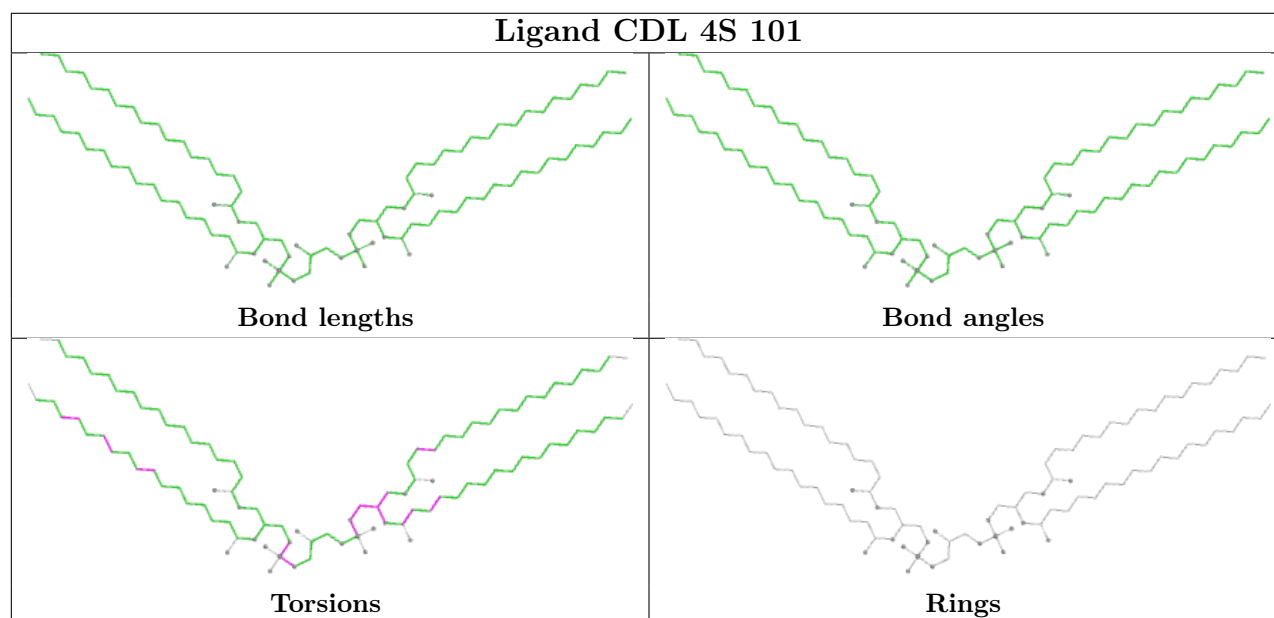
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2O	202	PC1	2	0
60	3G	401	HEM	4	0
57	4J	301	CDL	1	0
58	2S	201	UQ8	2	0
57	4Q	908	CDL	2	0
57	2o	201	CDL	1	0
57	2Q	101	CDL	2	0
55	4q	909	PEE	1	0
56	3a	501	PC1	2	0
59	3c	301	HEC	5	0
60	3G	402	HEM	1	0
62	4d	102	LPP	1	0
56	2r	202	PC1	1	0
58	3D	203	UQ8	12	0
57	3G	403	CDL	5	0
58	3d	203	UQ8	12	0
56	4e	202	PC1	2	0
57	4T	203	CDL	3	0
55	4Q	909	PEE	1	0
55	3C	302	PEE	1	0
55	3c	302	PEE	1	0
57	4U	501	CDL	2	0
62	4D	102	LPP	1	0
56	4E	202	PC1	2	0
57	2O	204	CDL	1	0
51	3h	401	FES	1	0
57	3g	403	CDL	4	0
61	40	304	AJP	1	0
59	3C	301	HEC	6	0
66	4Q	905	HEA	2	0
51	3H	401	FES	1	0
56	2p	204	PC1	2	0
66	4Q	904	HEA	4	0
56	2o	203	PC1	2	0
57	3i	202	CDL	3	0
57	4t	203	CDL	3	0
57	4w	202	CDL	1	0
55	40	302	PEE	1	0
60	3g	401	HEM	4	0
57	3l	701	CDL	1	0
55	3F	101	PEE	1	0
55	4l	302	PEE	1	0

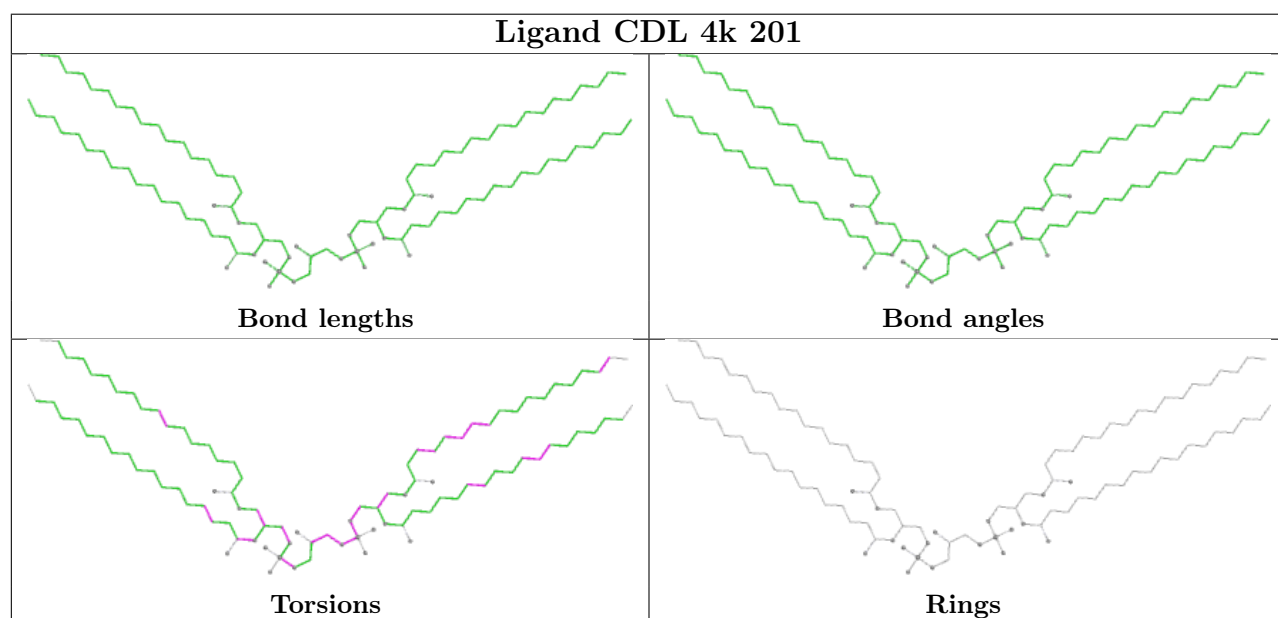
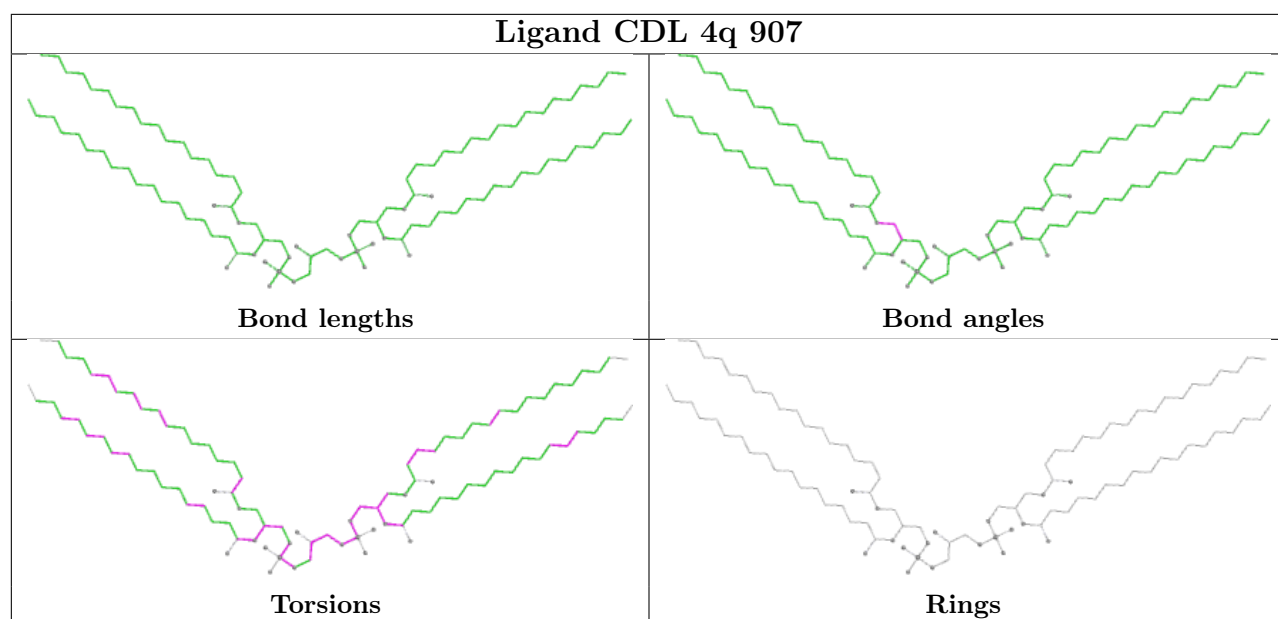
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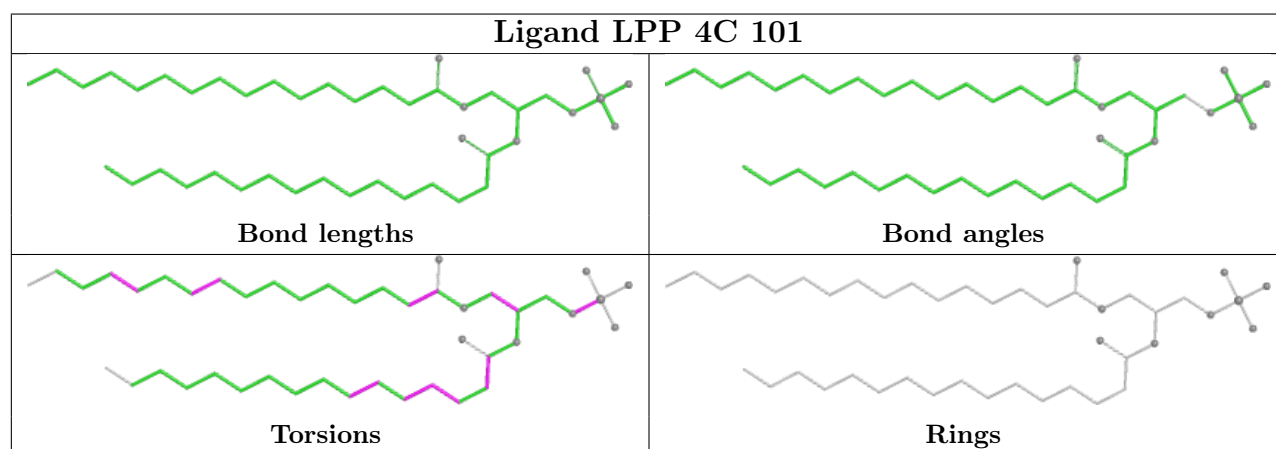
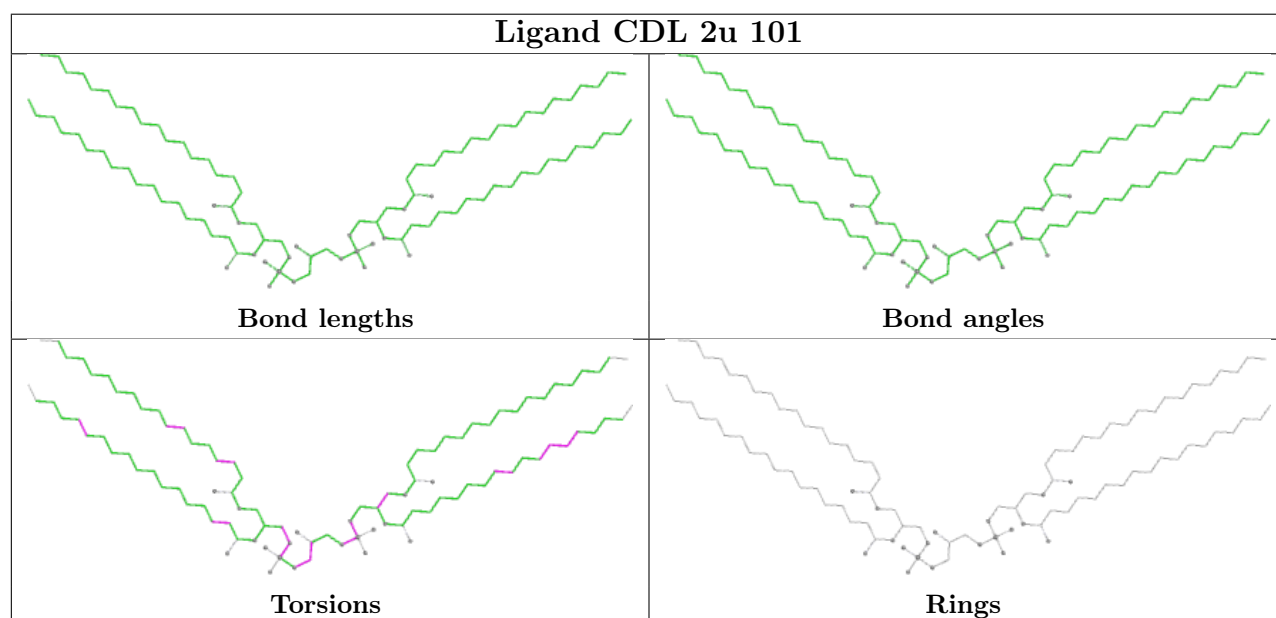
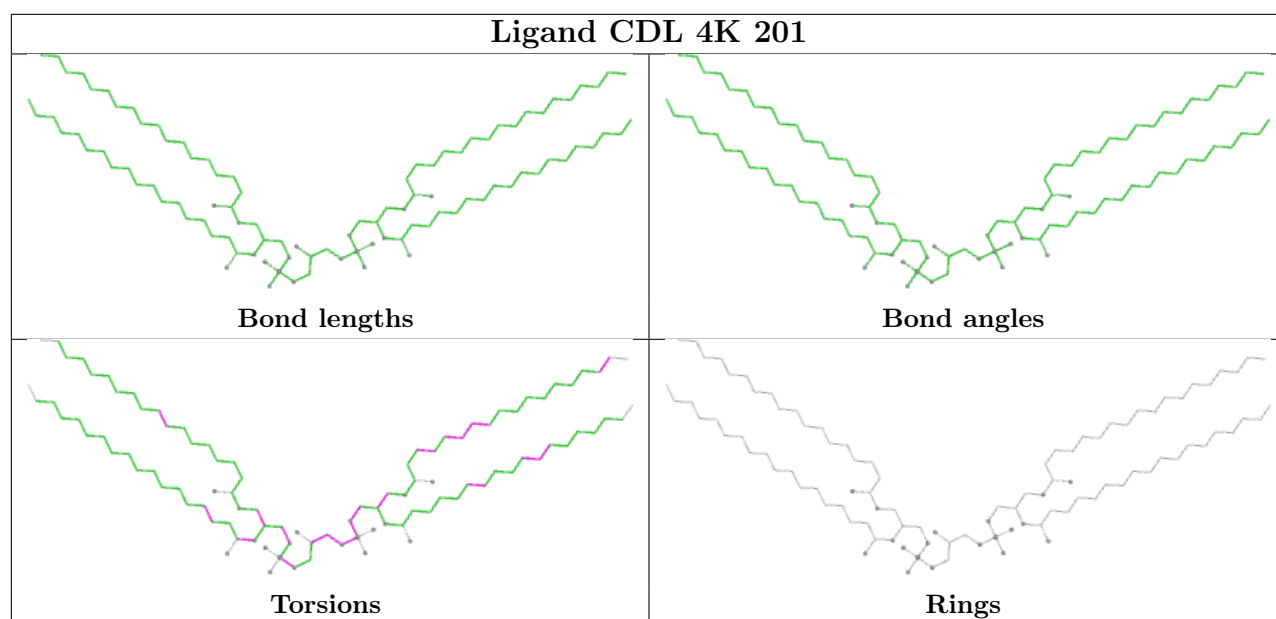
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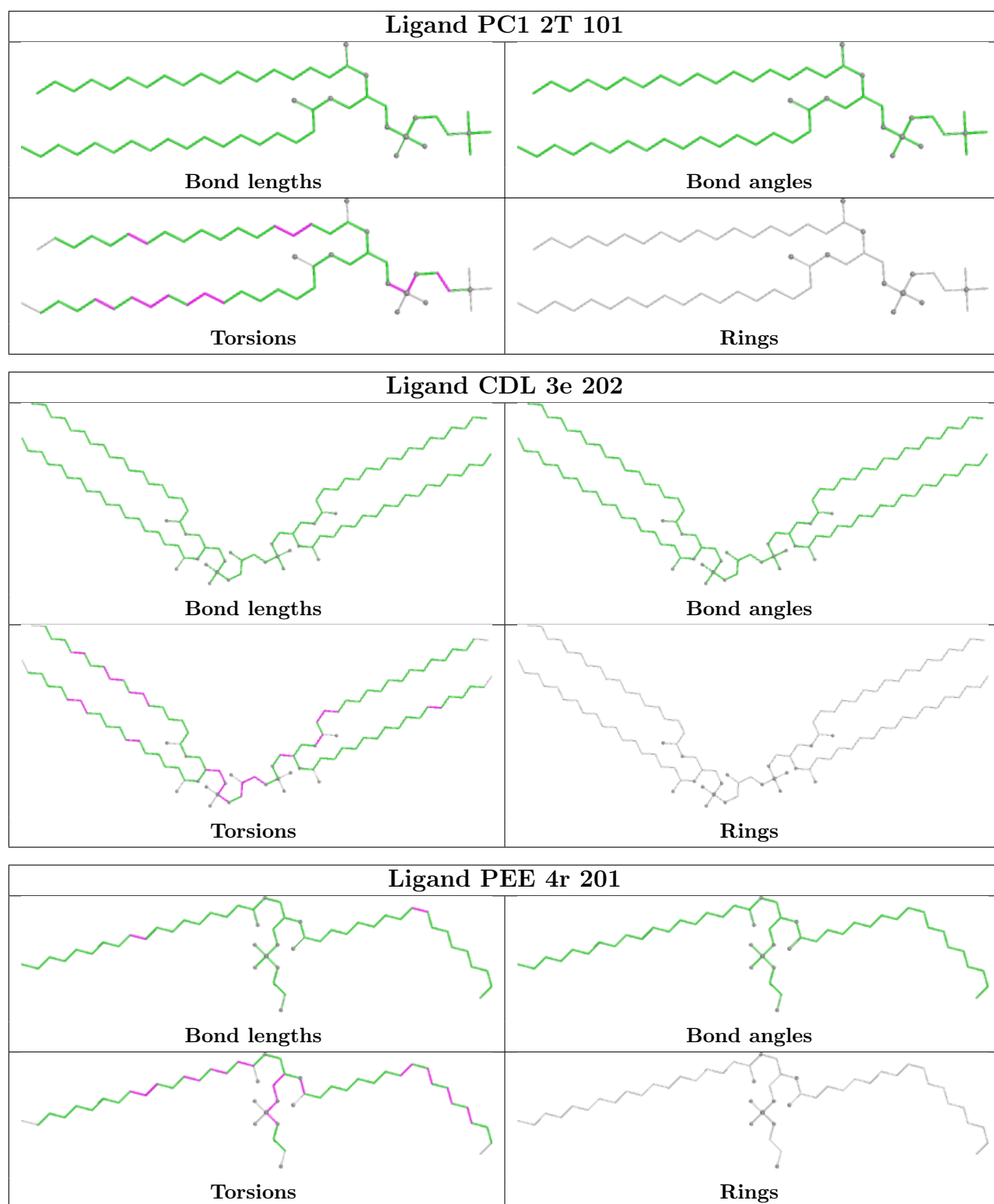
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2o	204	PC1	3	0
57	3I	201	CDL	3	0
57	4W	202	CDL	1	0
58	2s	201	UQ8	2	0
57	4K	202	CDL	1	0
55	3f	101	PEE	1	0
57	4u	501	CDL	2	0
66	4q	905	HEA	2	0
55	4q	910	PEE	1	0
56	2P	204	PC1	2	0
56	2R	202	PC1	1	0
56	3A	501	PC1	2	0
58	3g	404	UQ8	11	0
57	3L	701	CDL	1	0

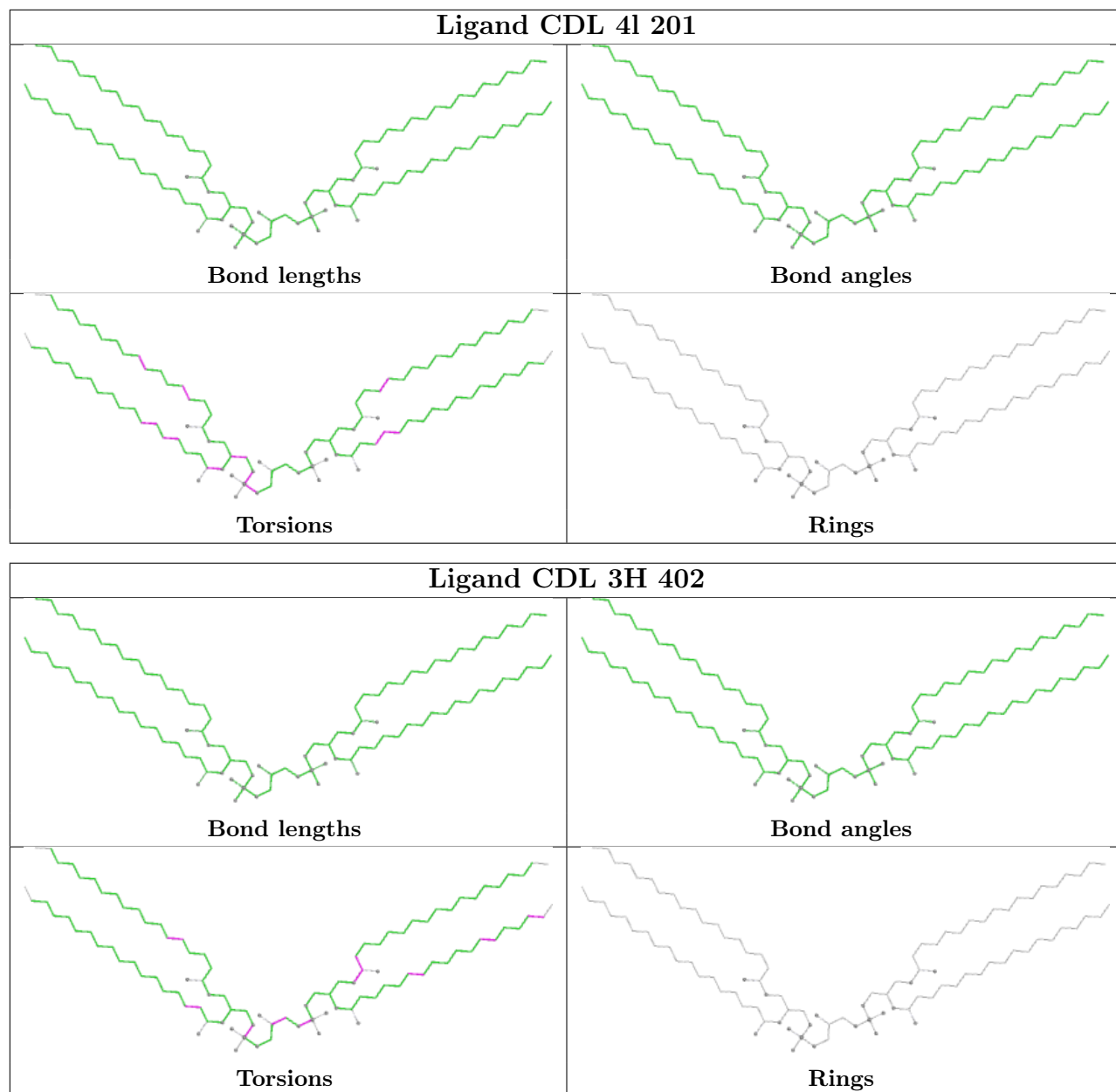
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

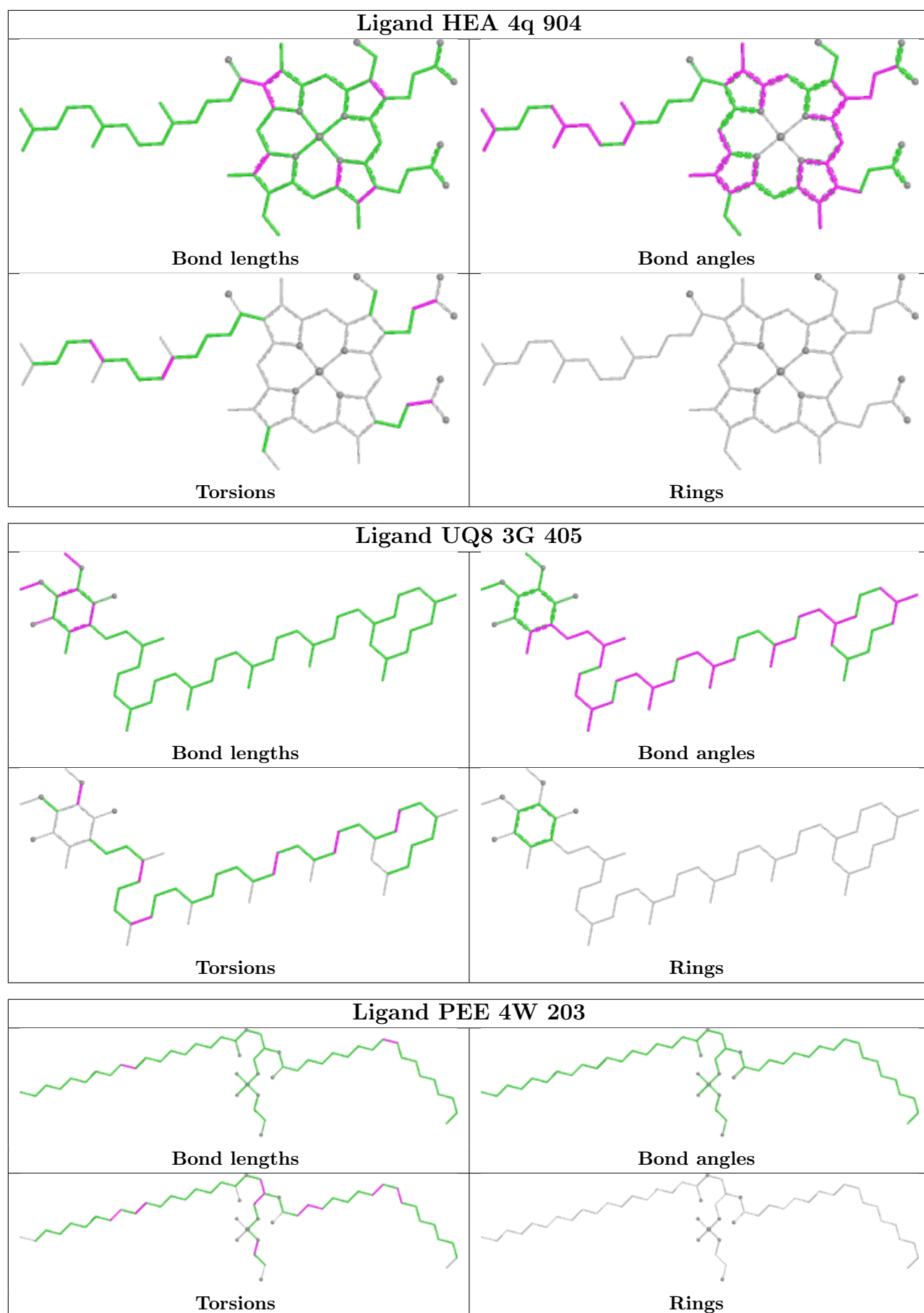


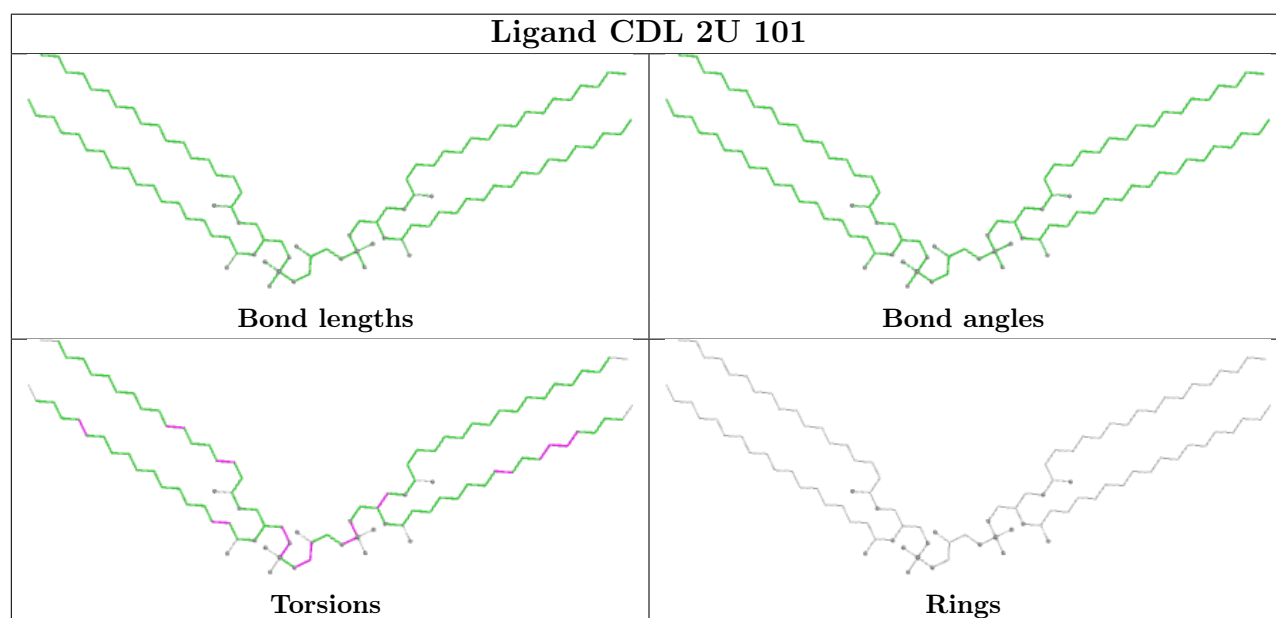
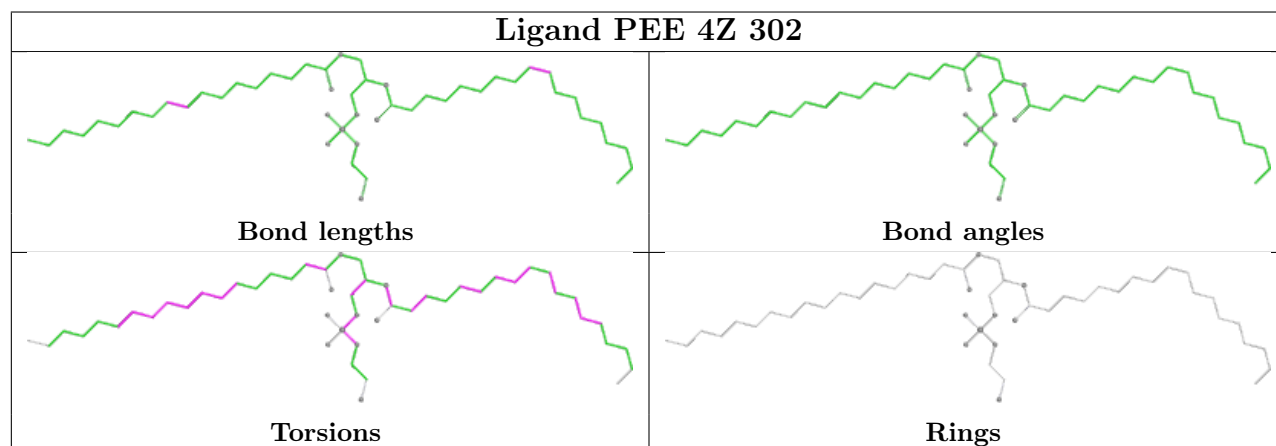
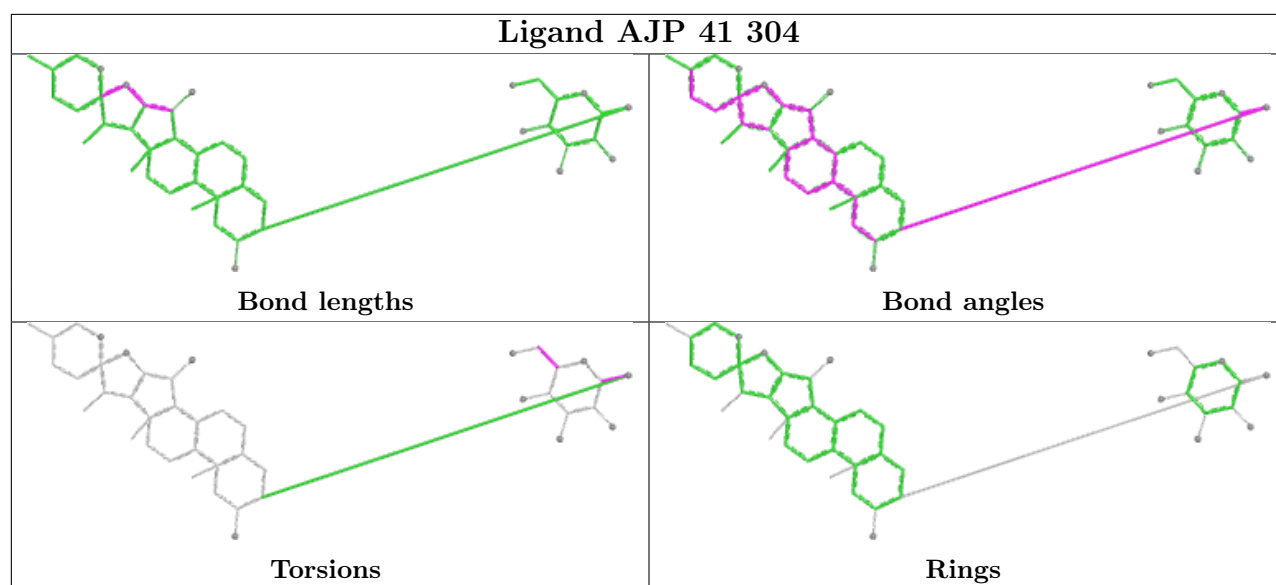


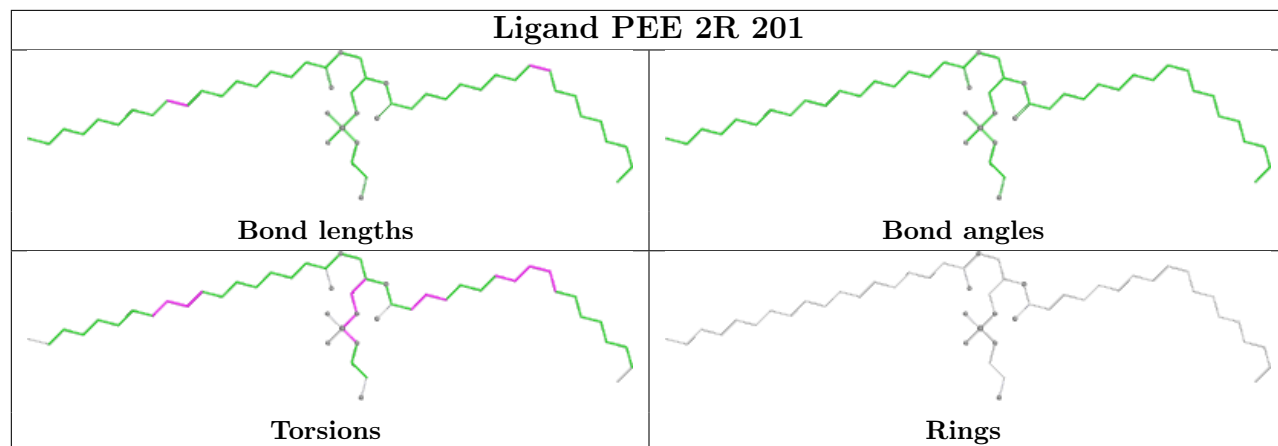
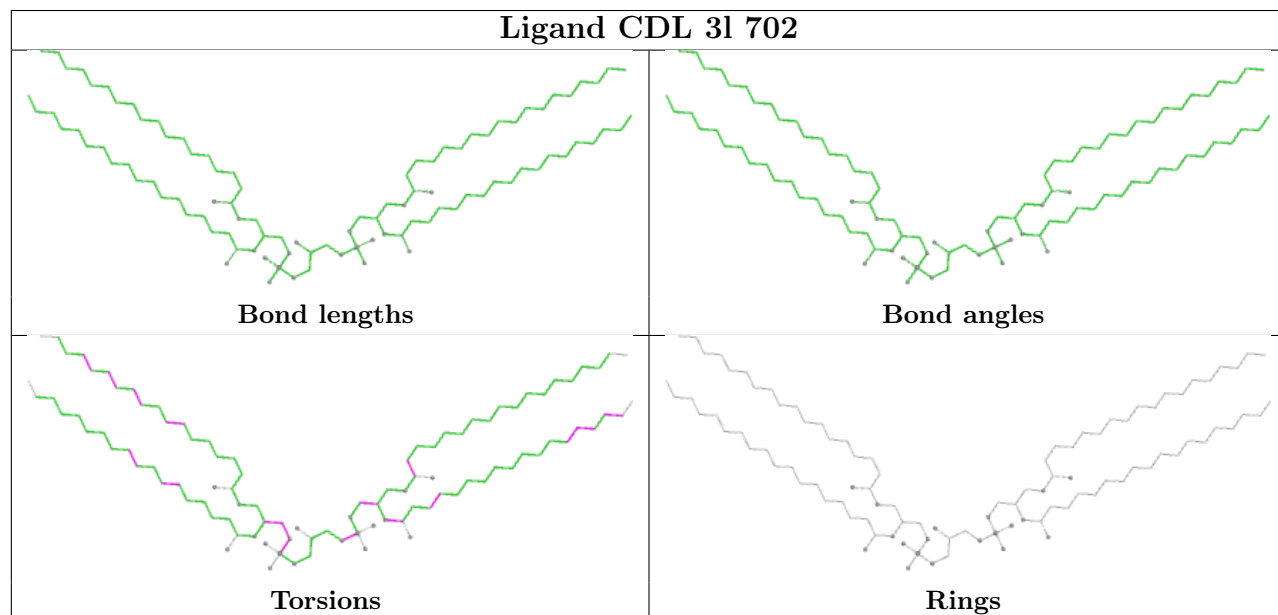
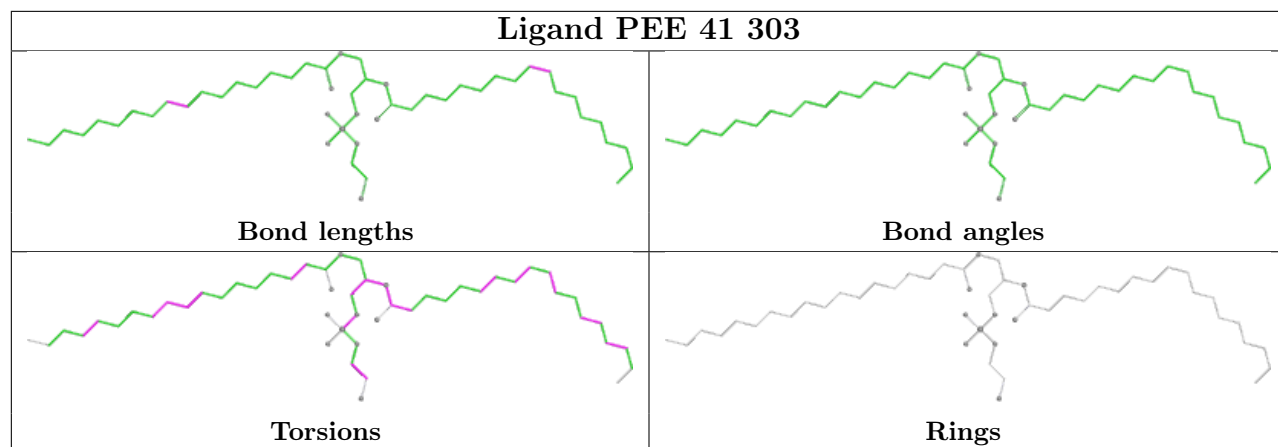


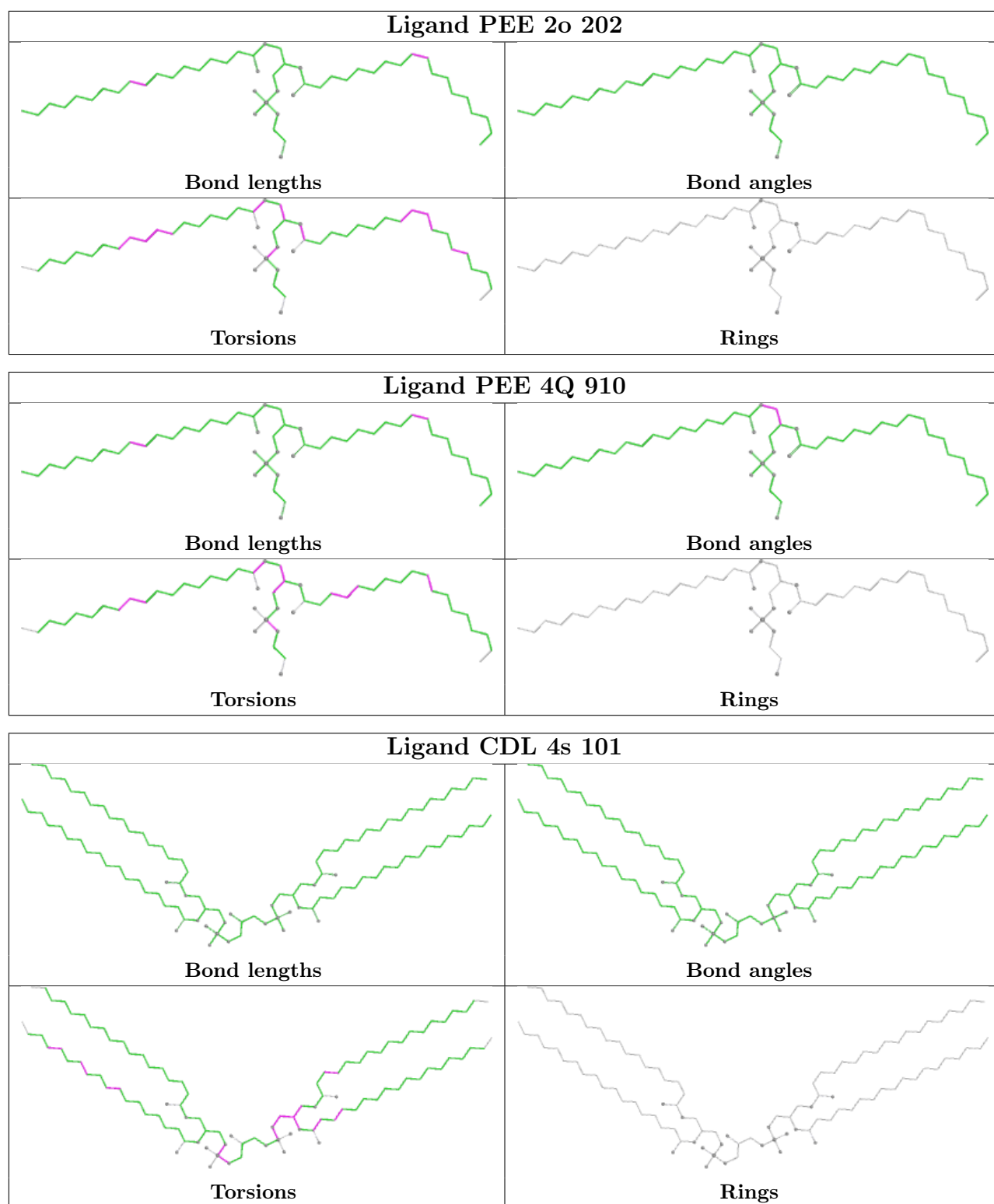


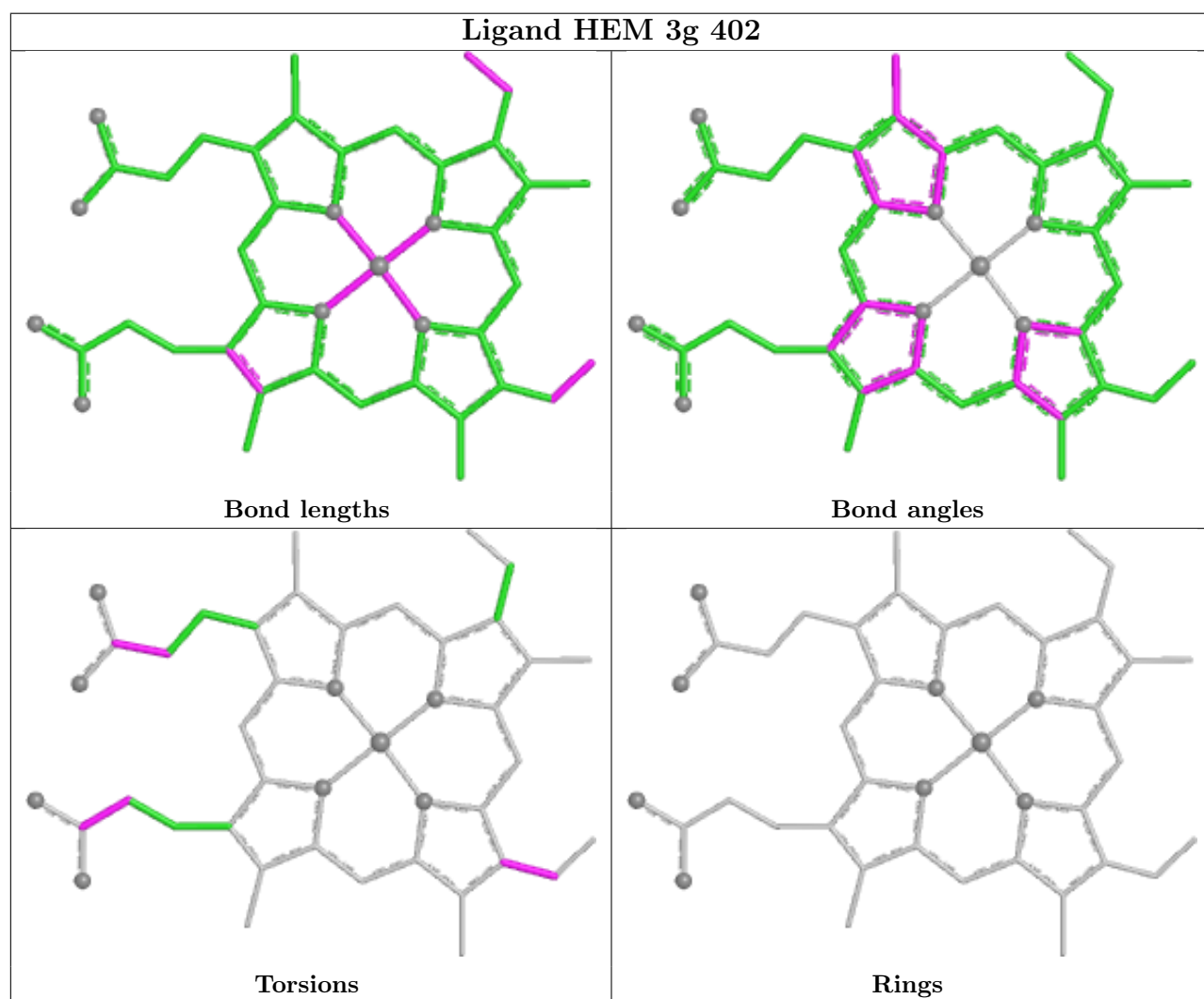
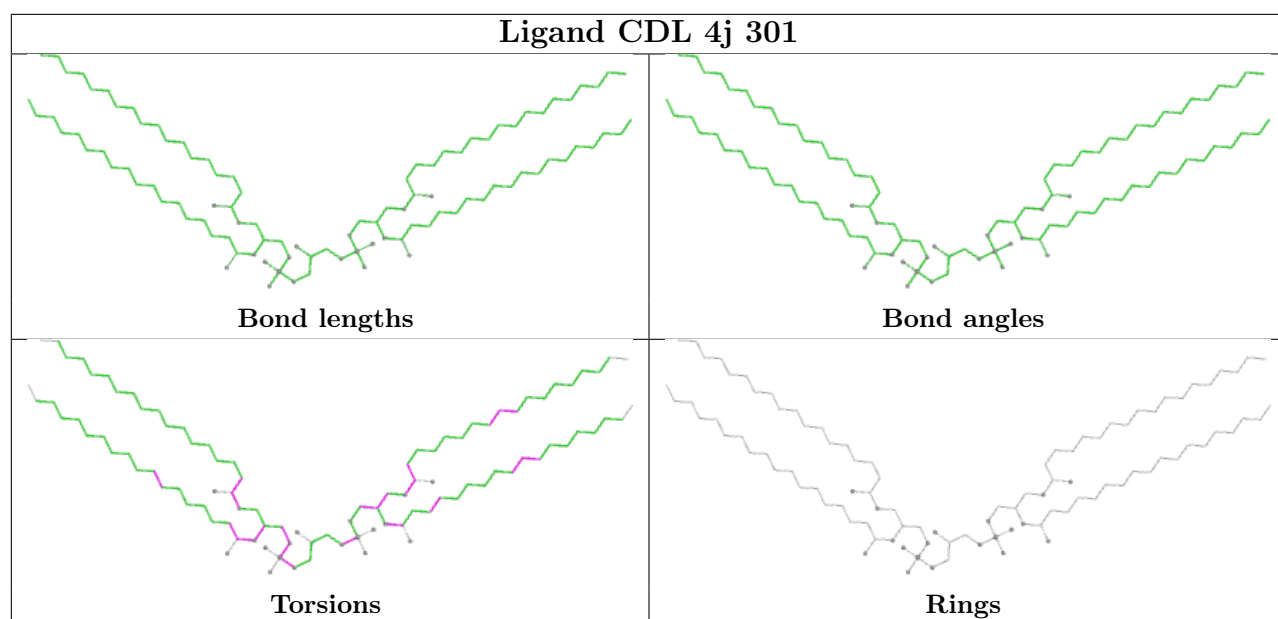


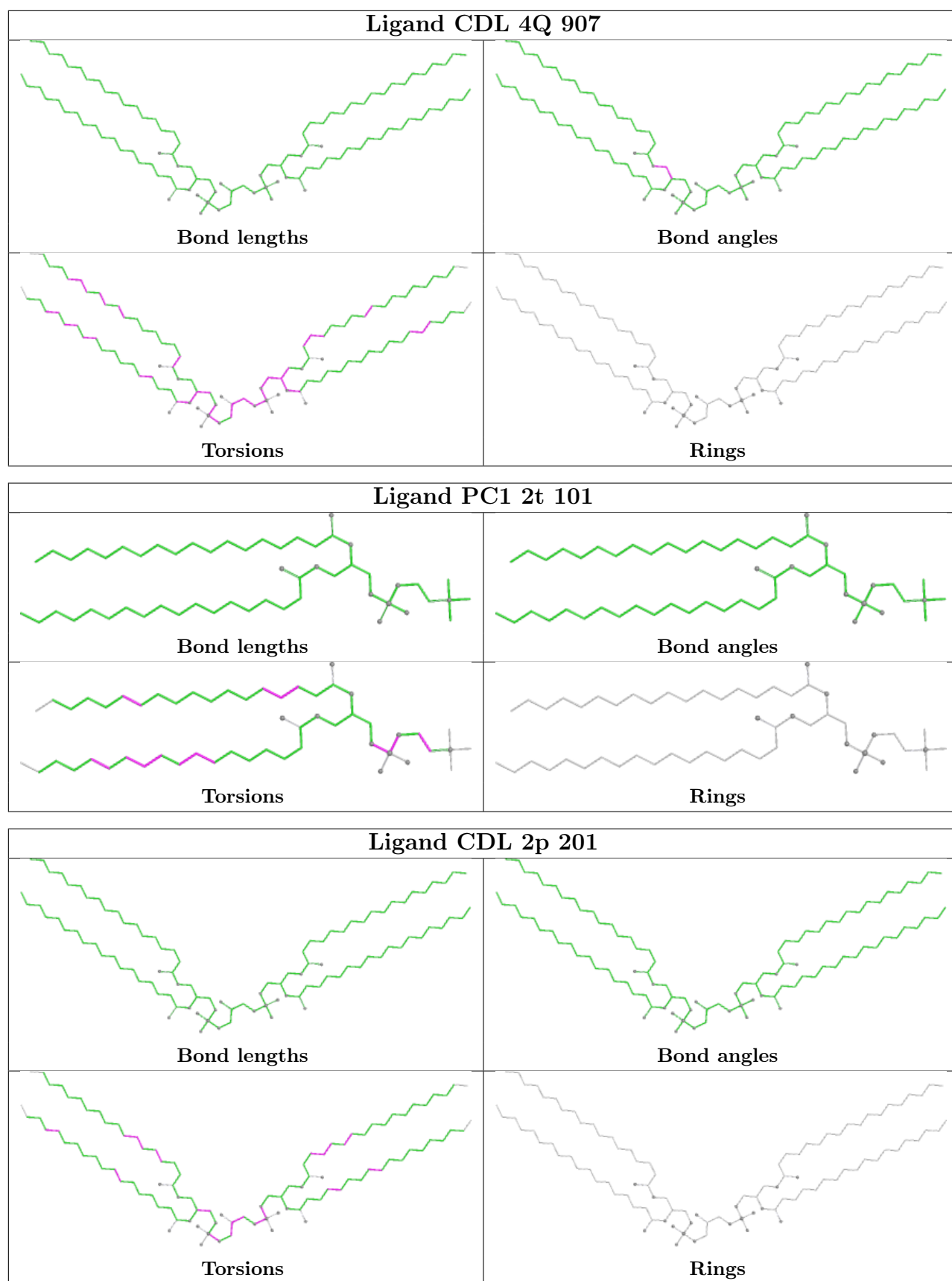


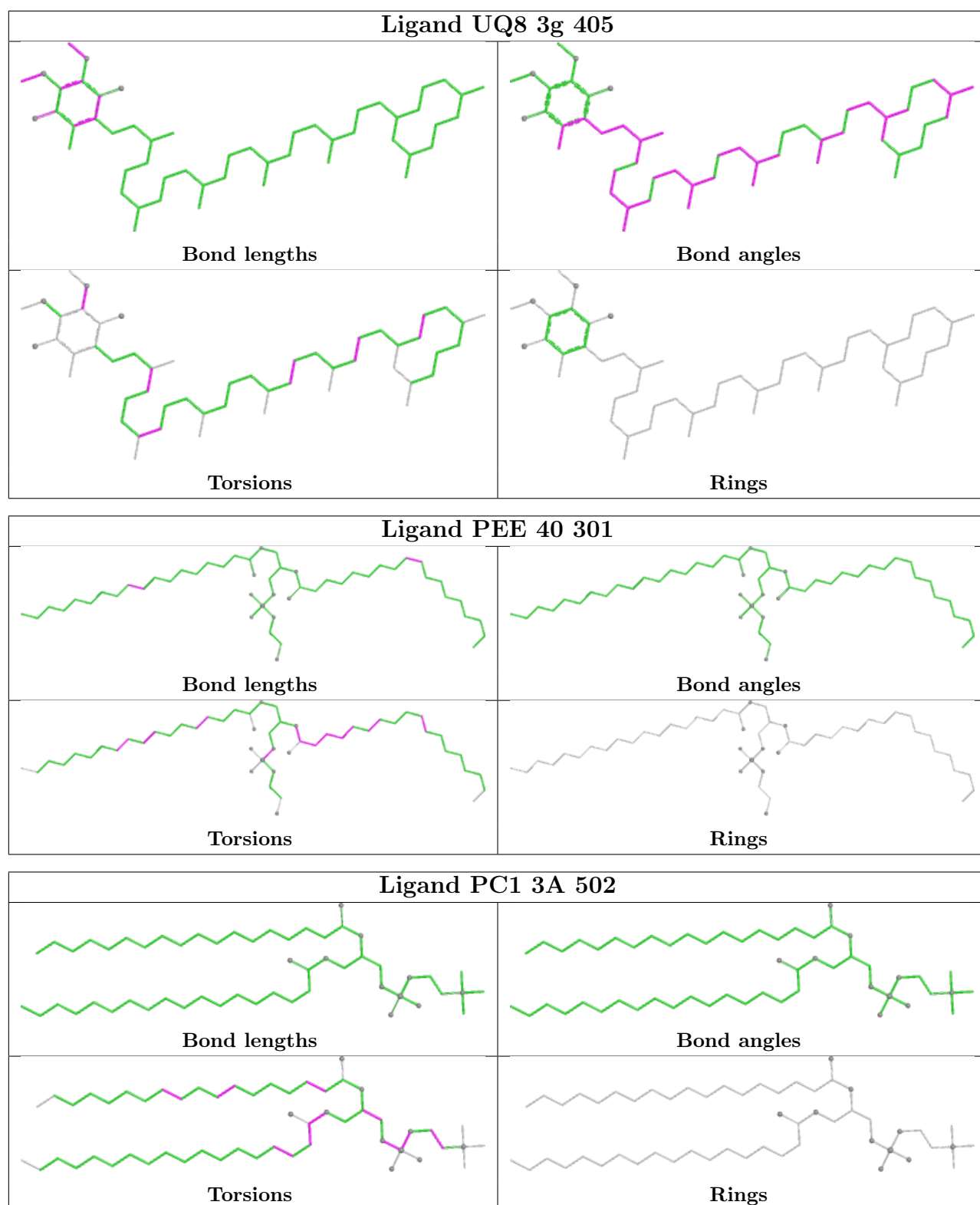


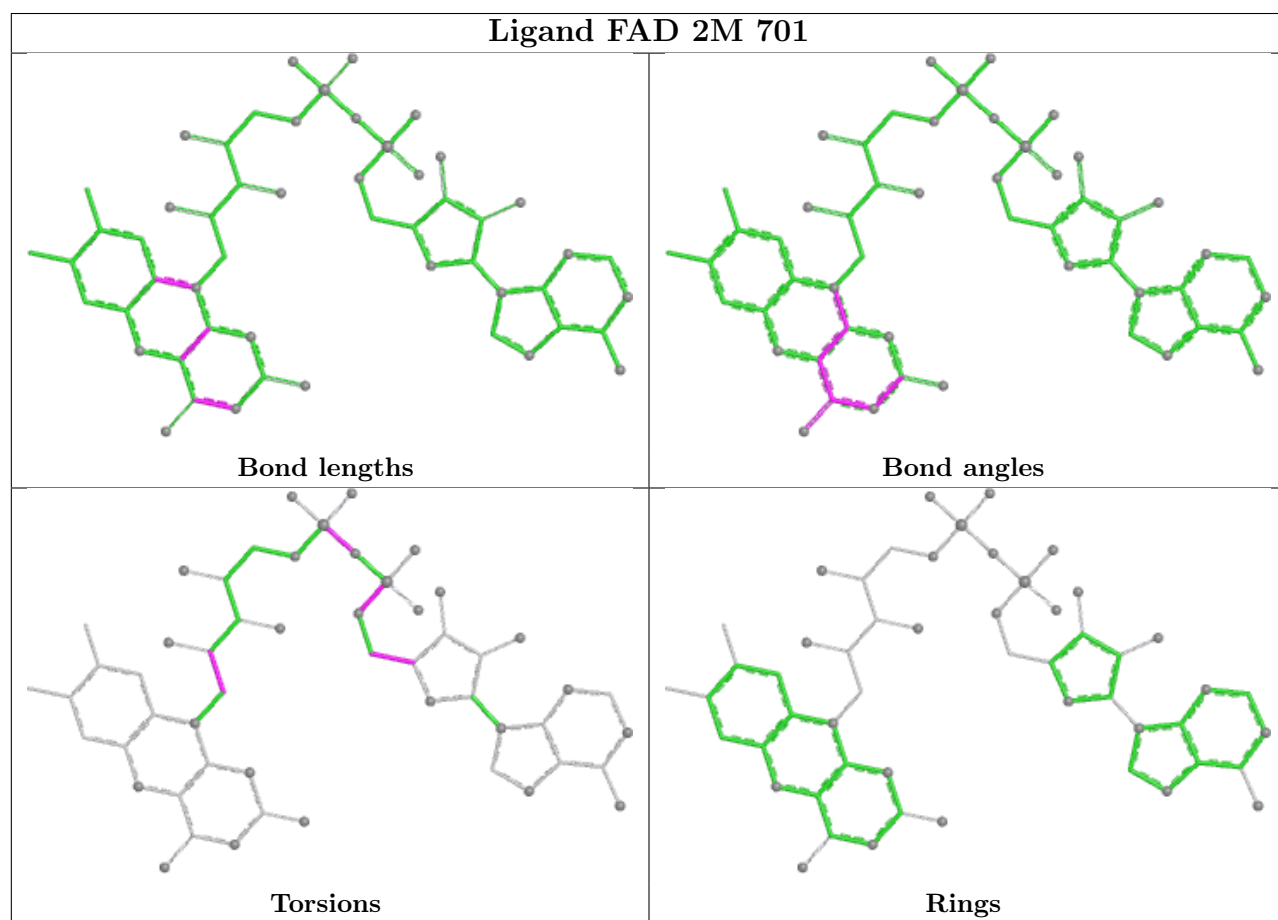
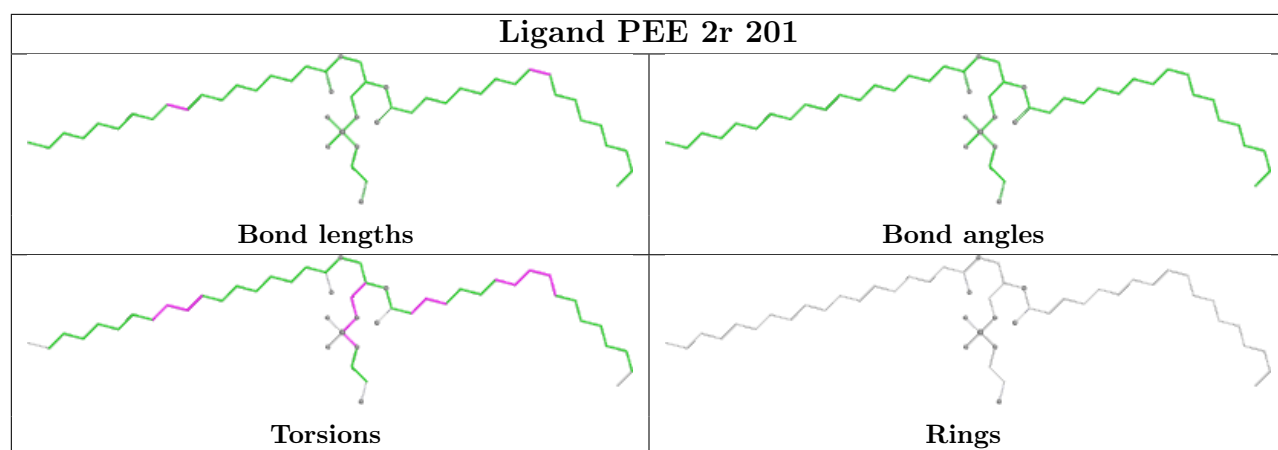


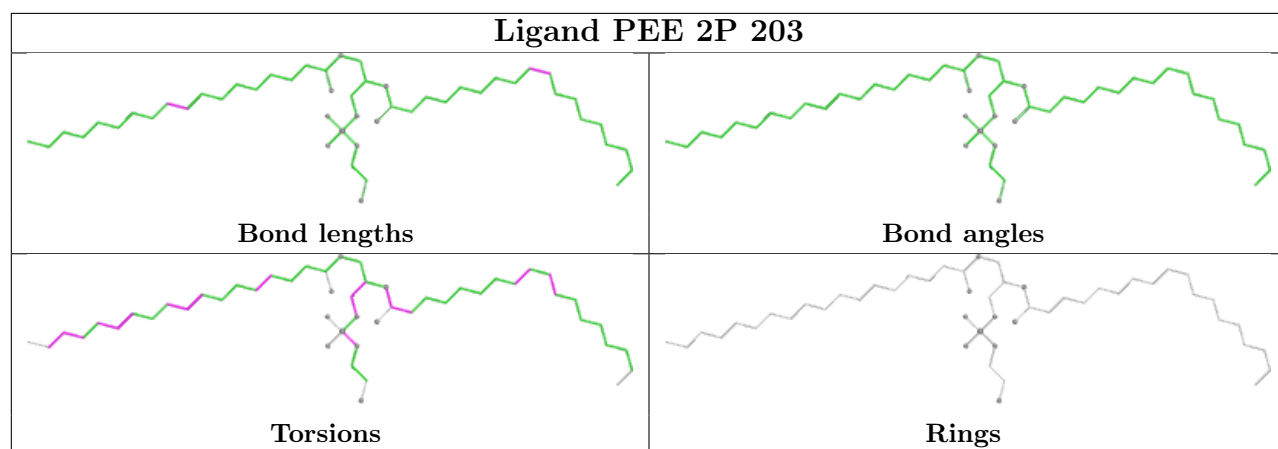
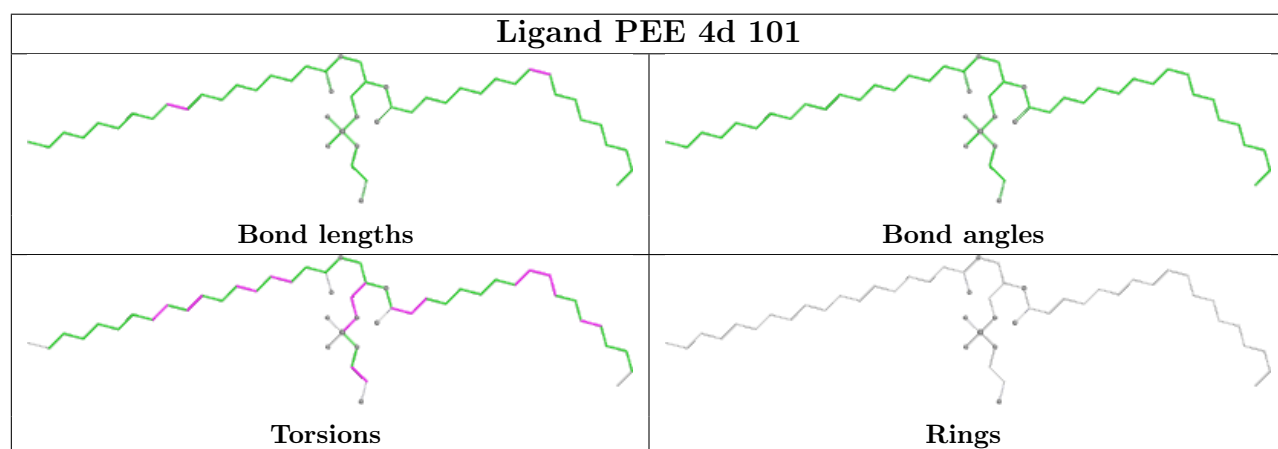
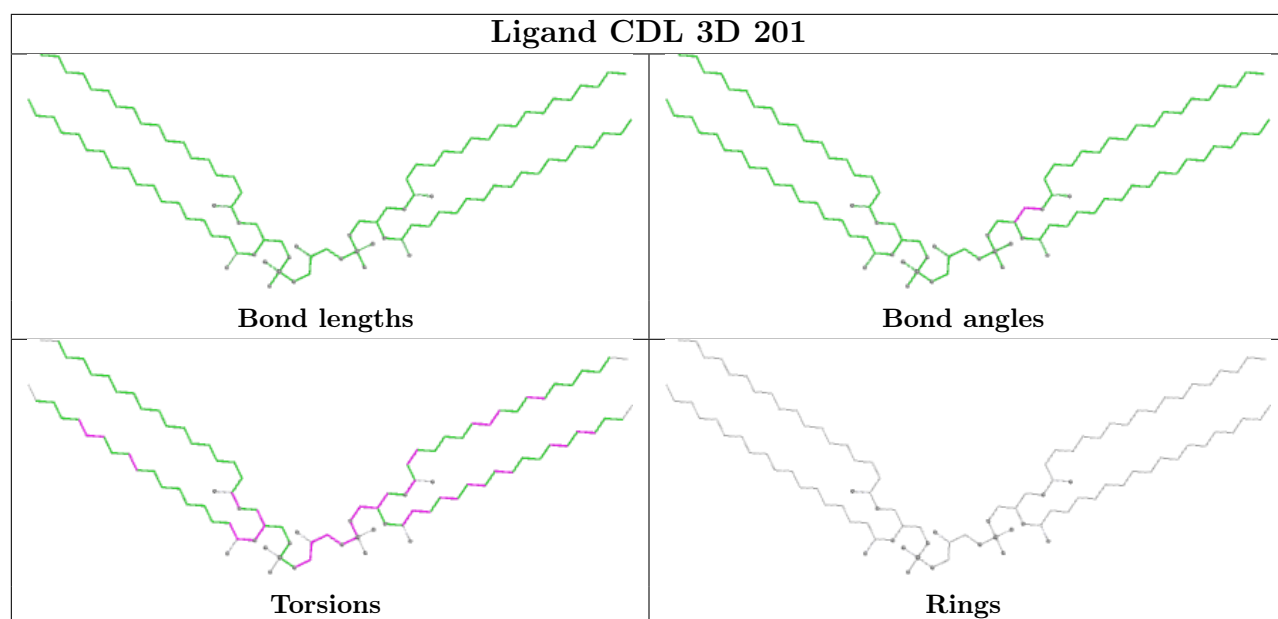


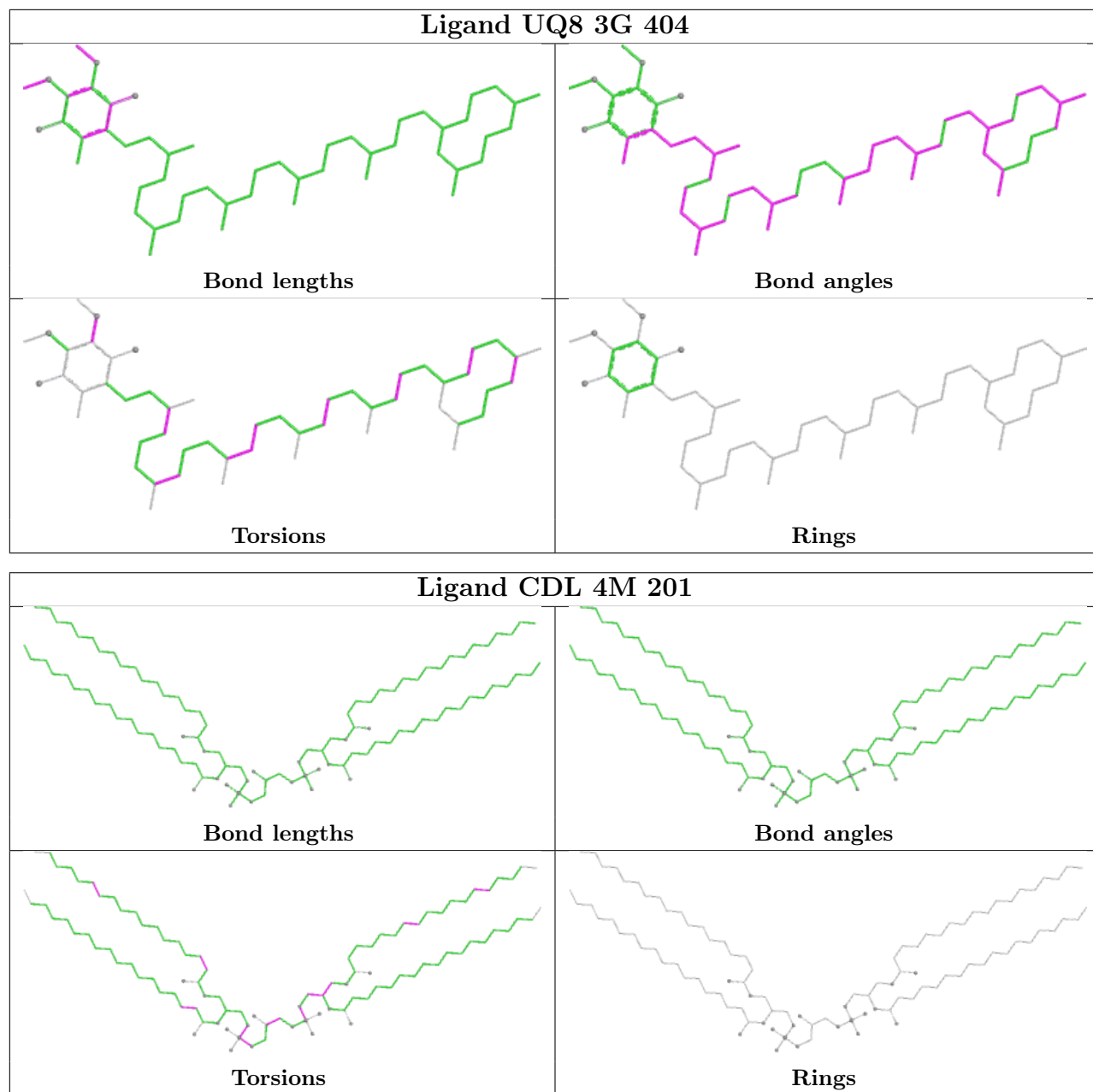


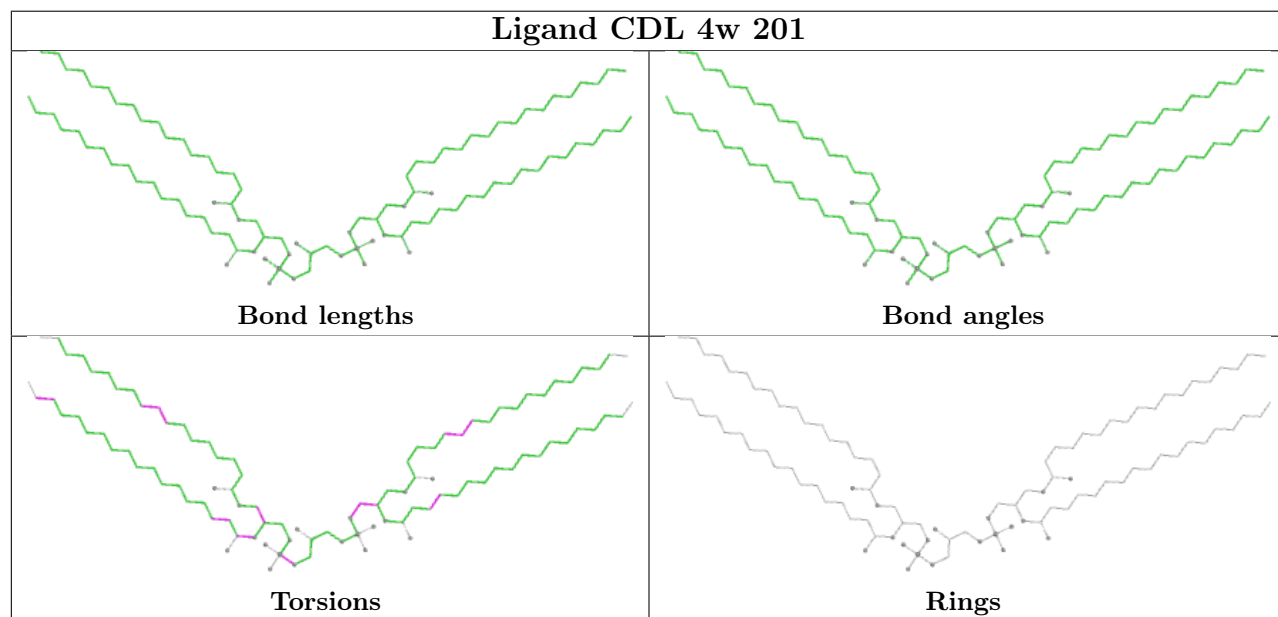
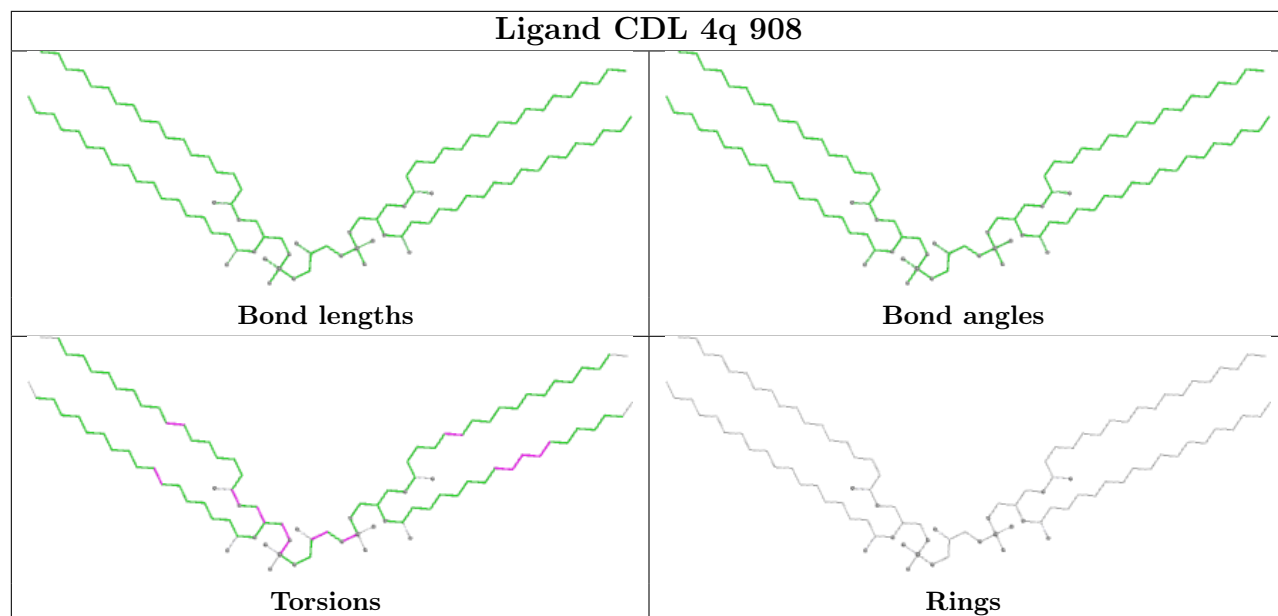


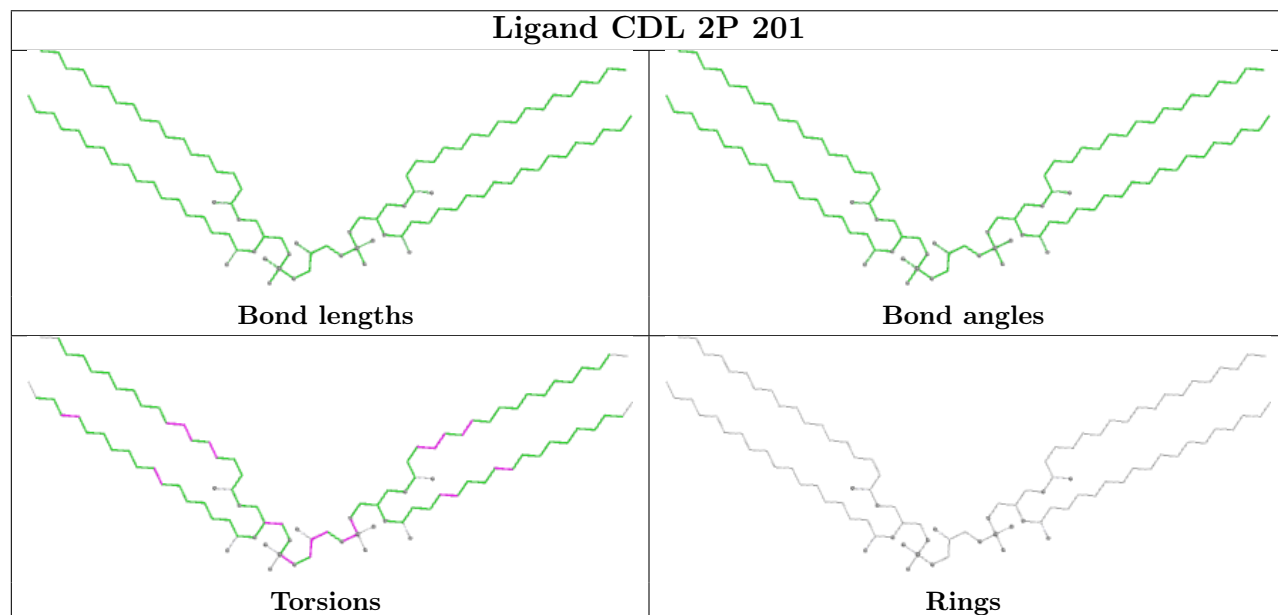
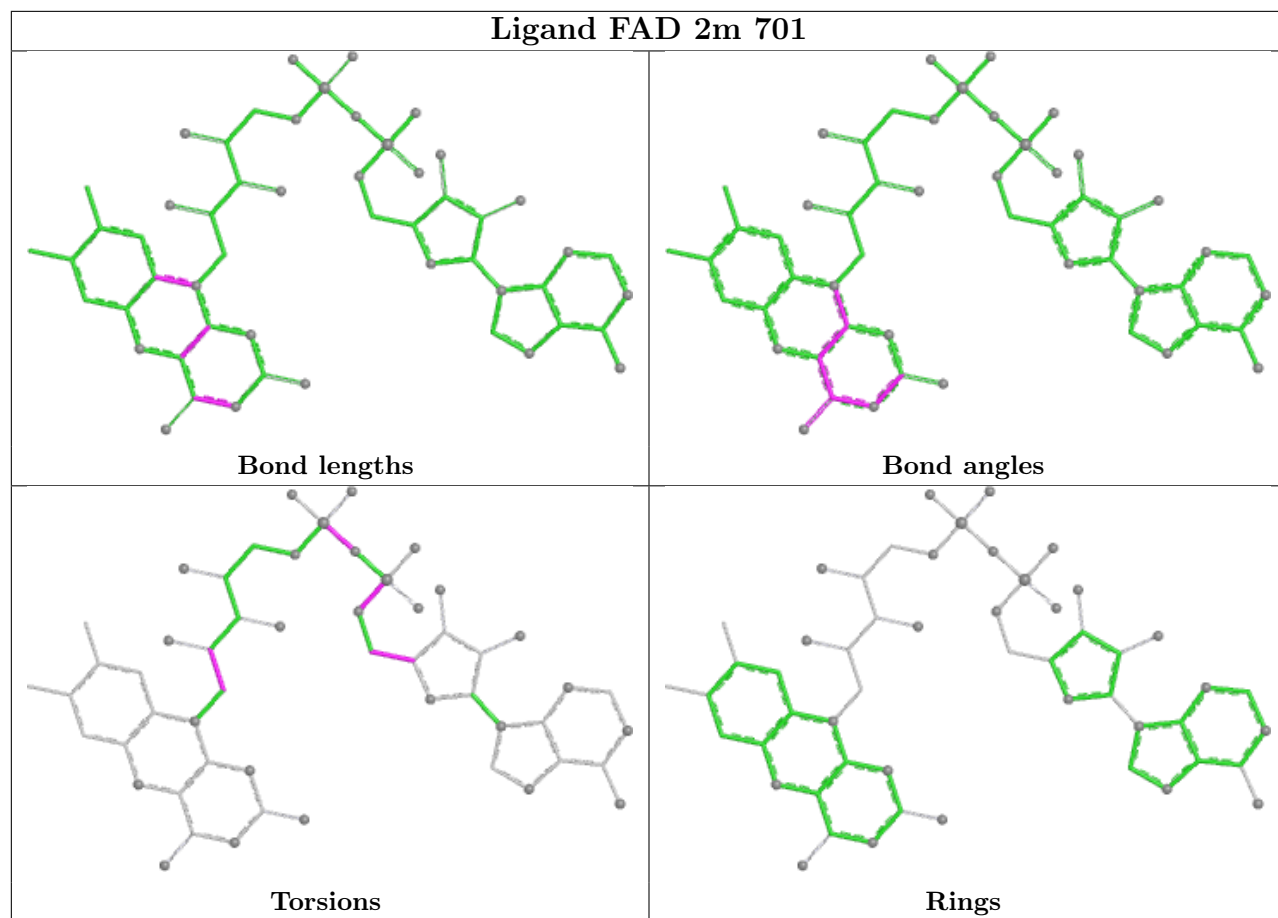


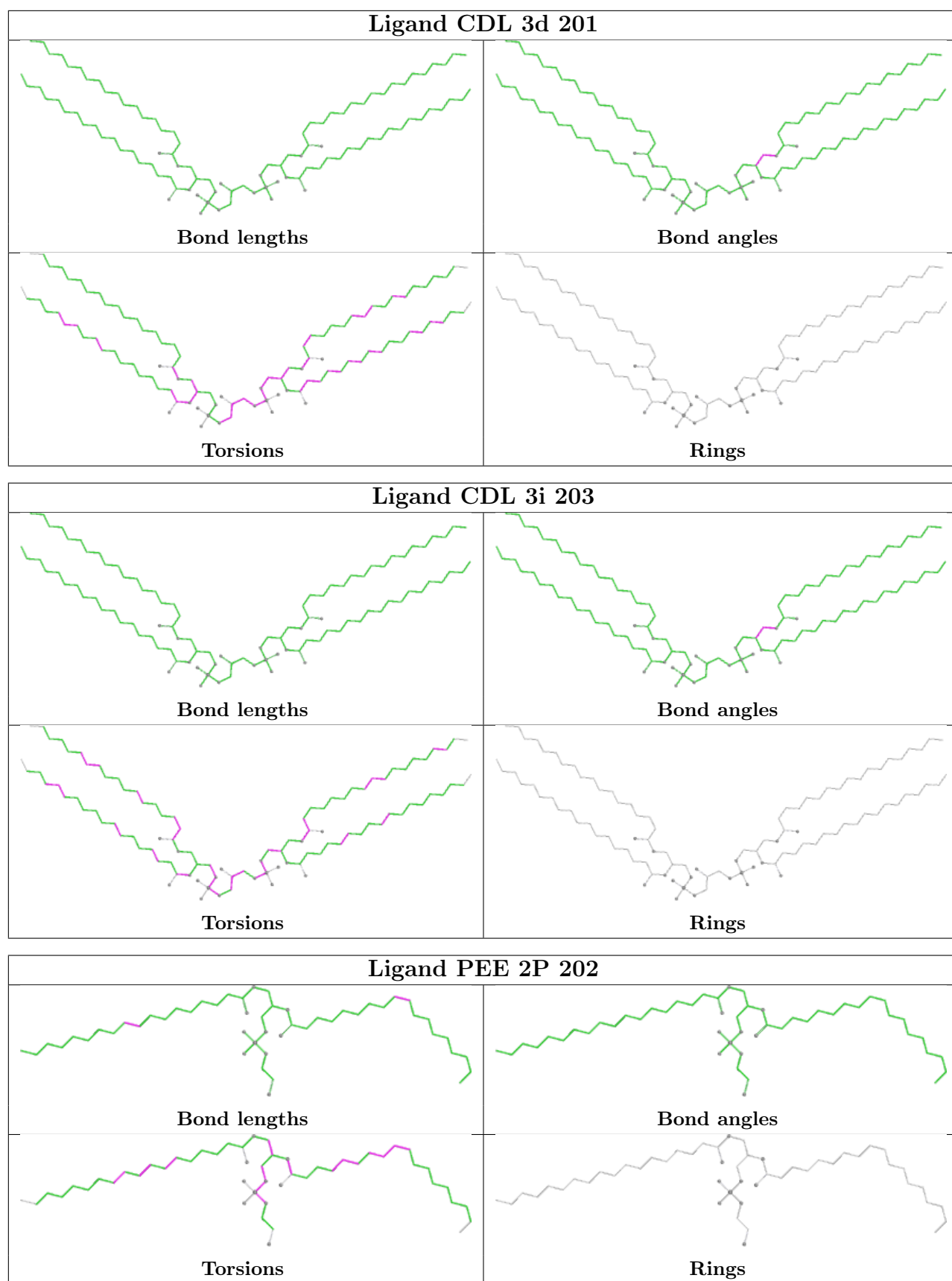


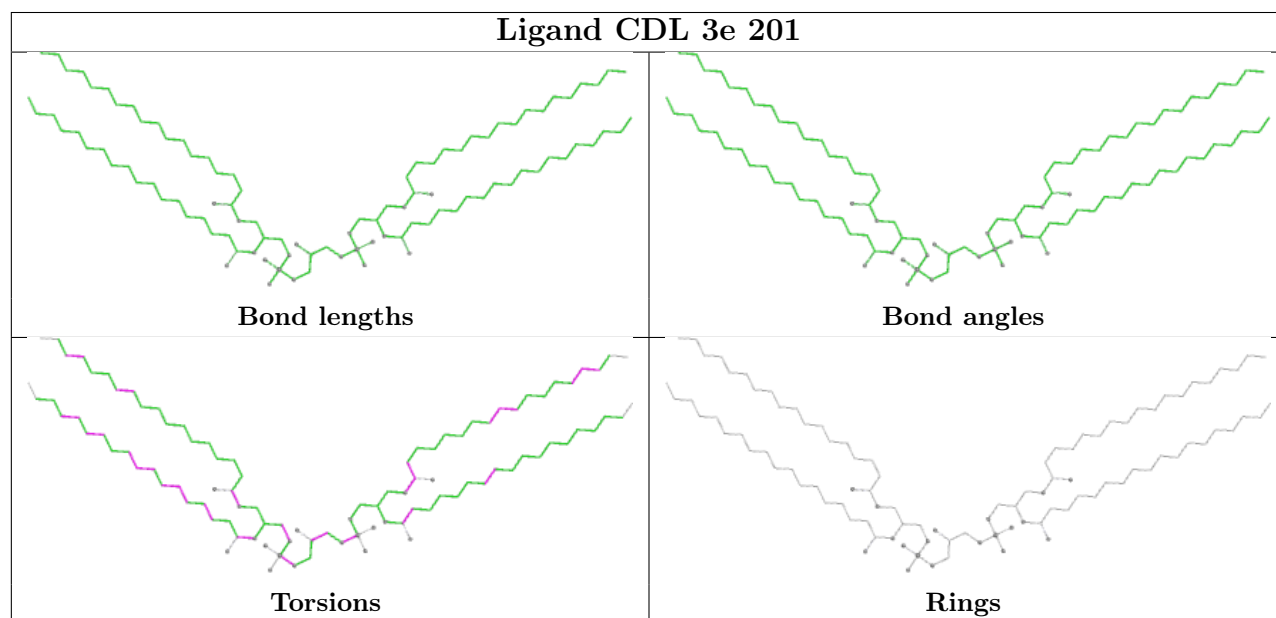
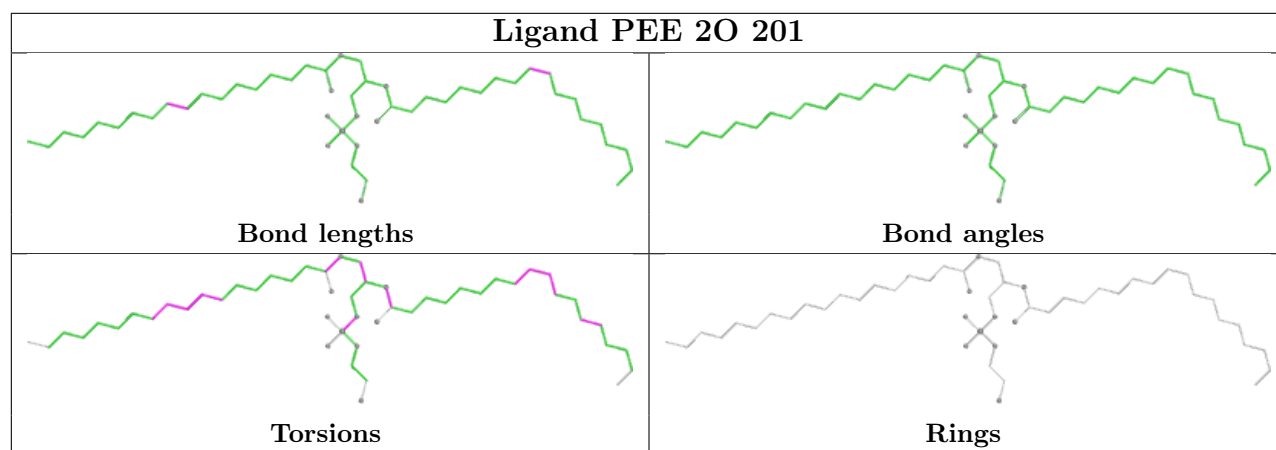
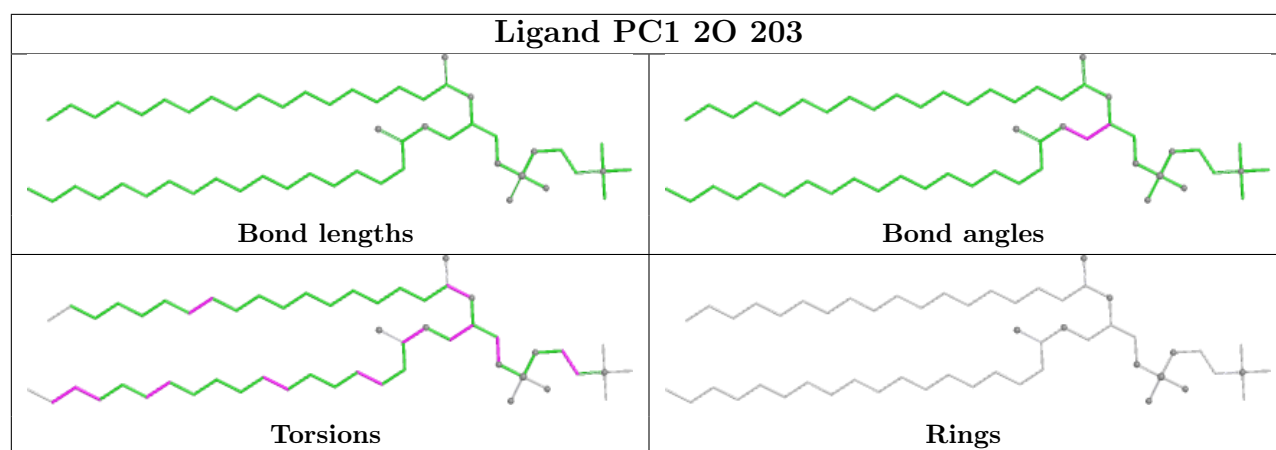


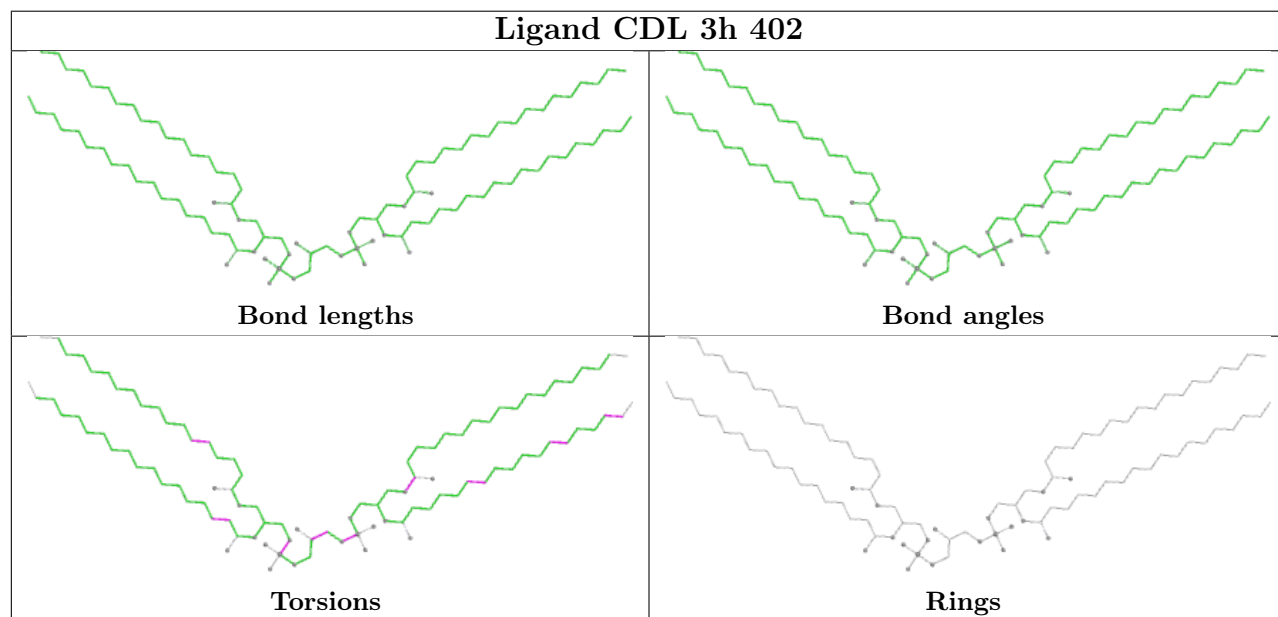
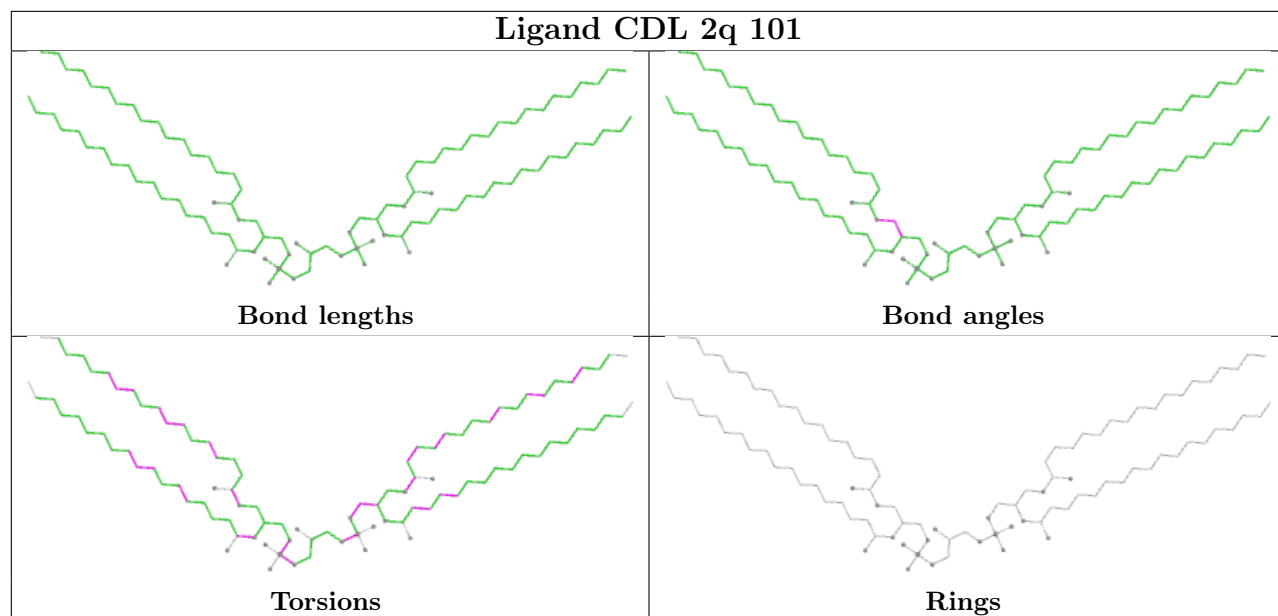


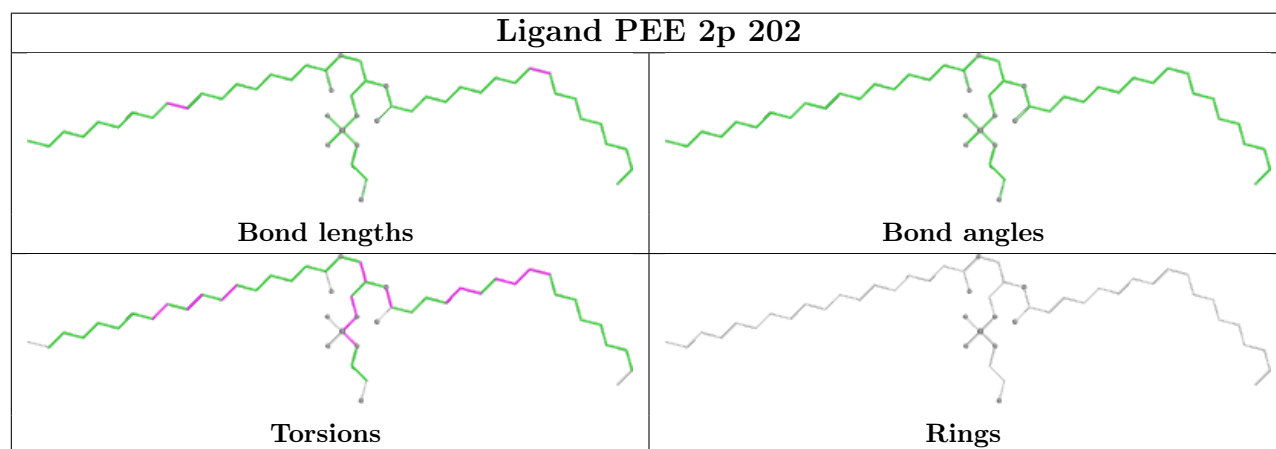
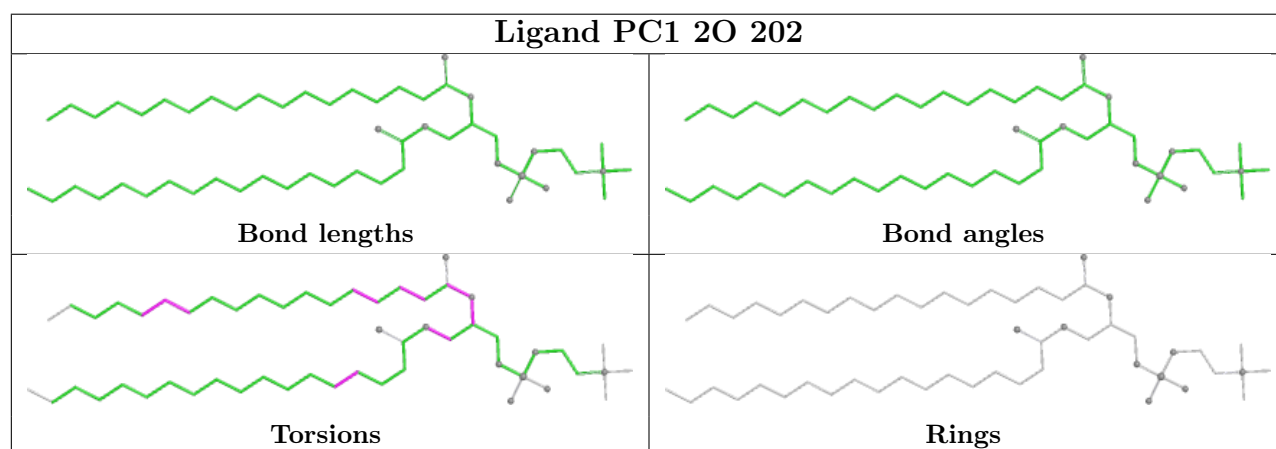
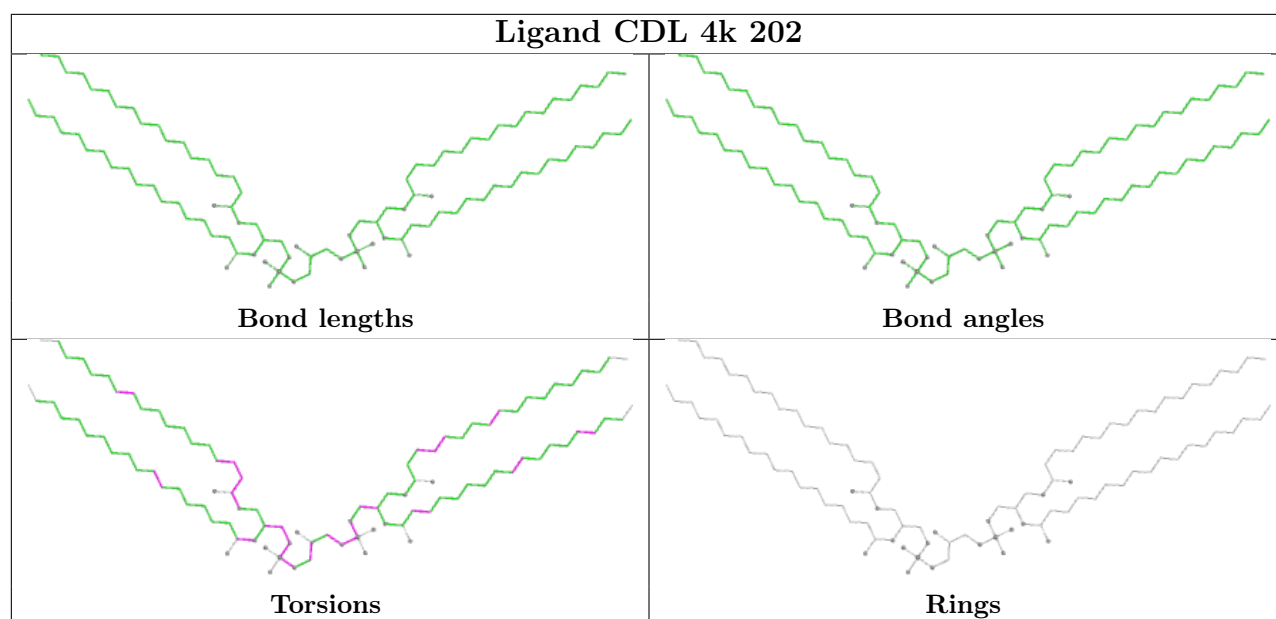




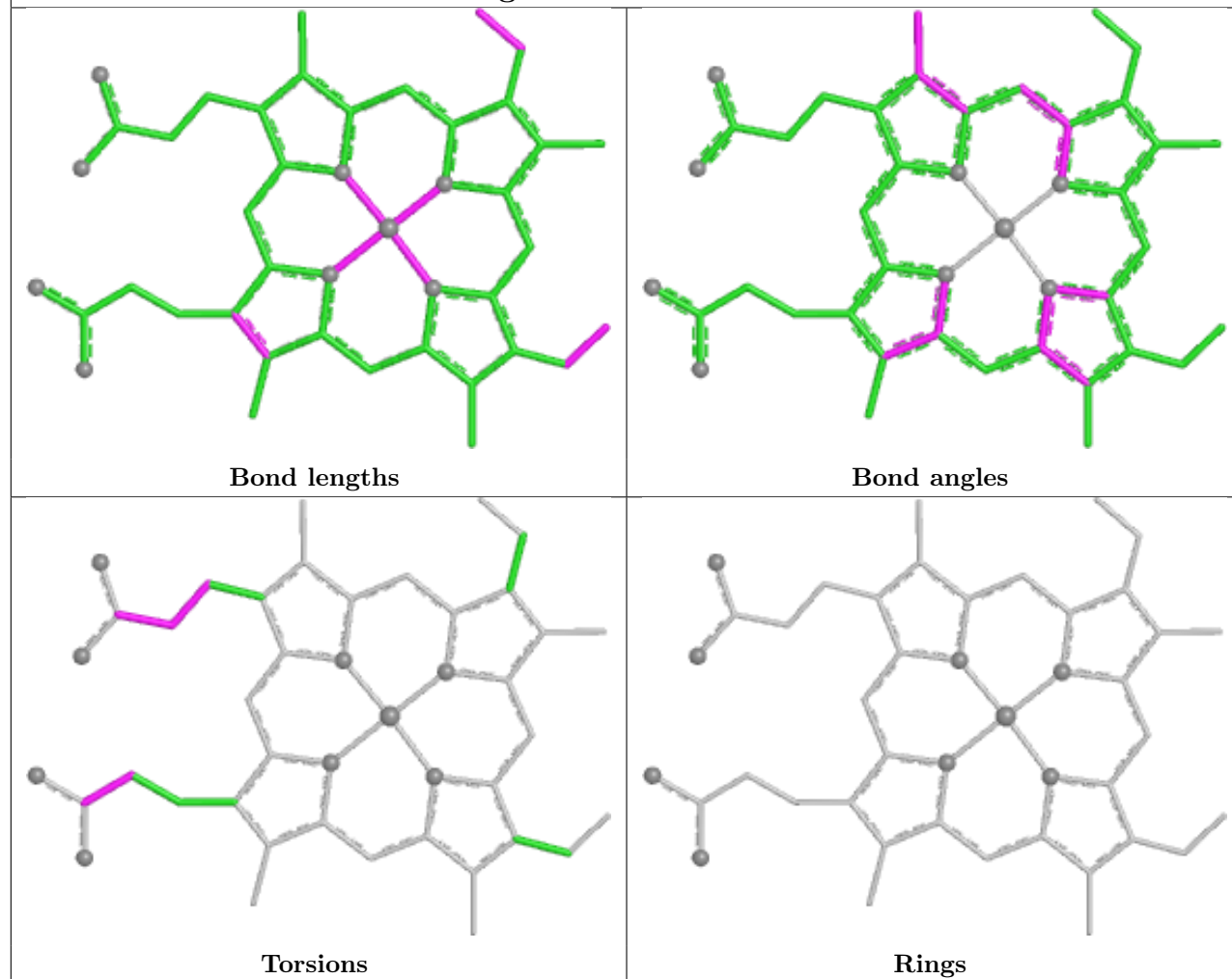




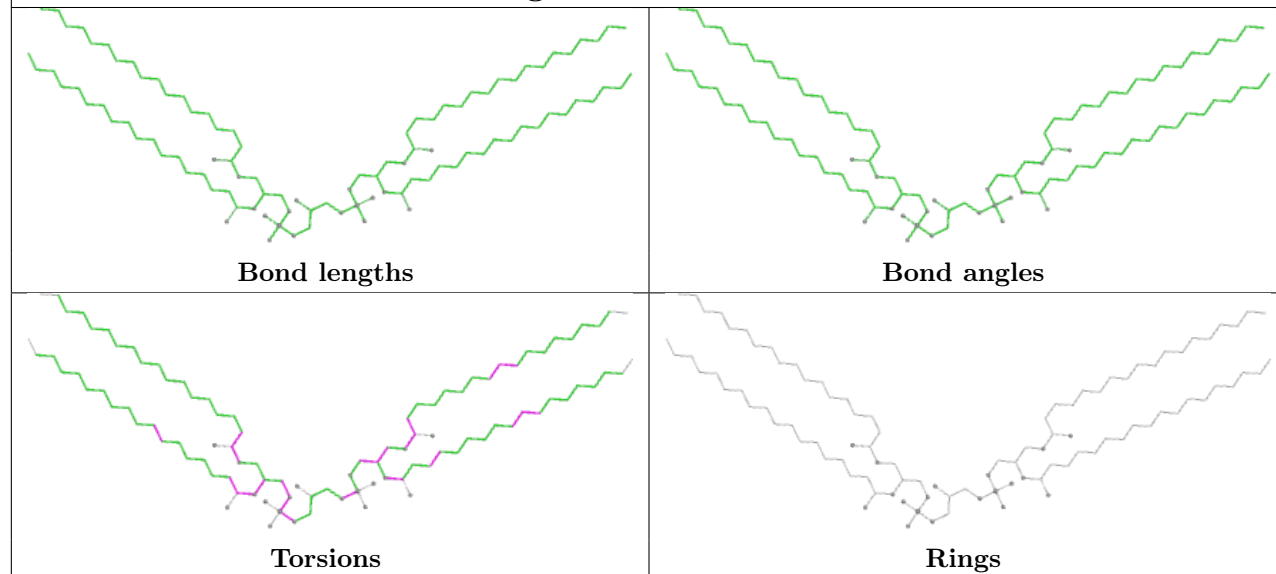


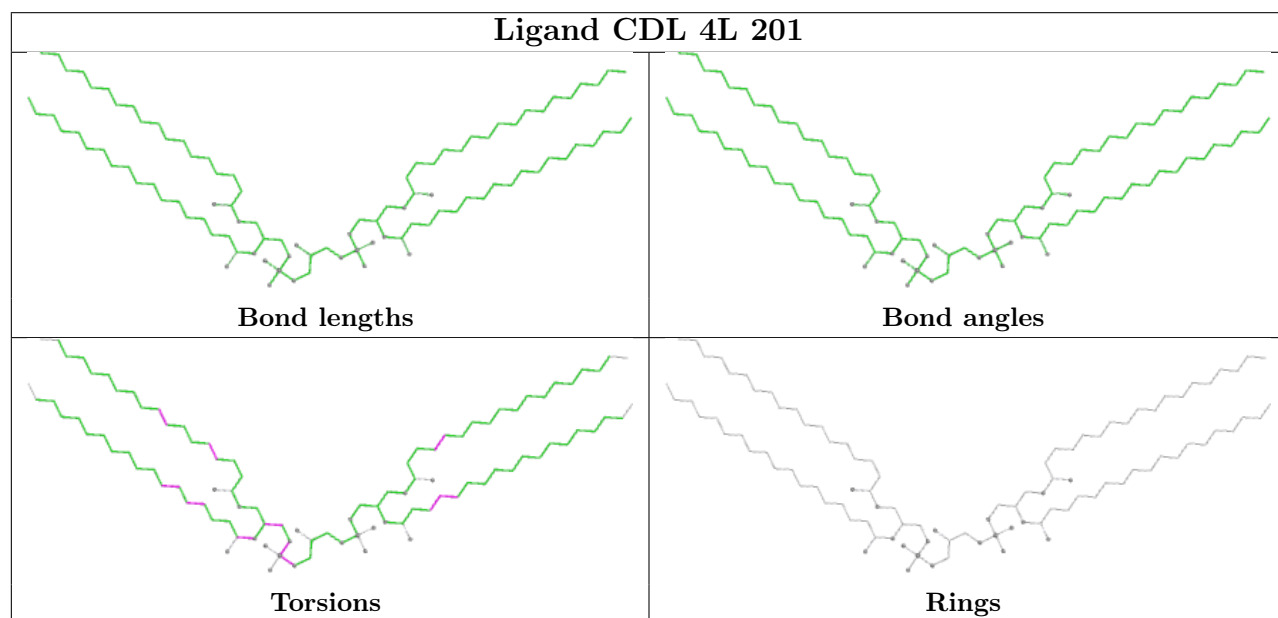
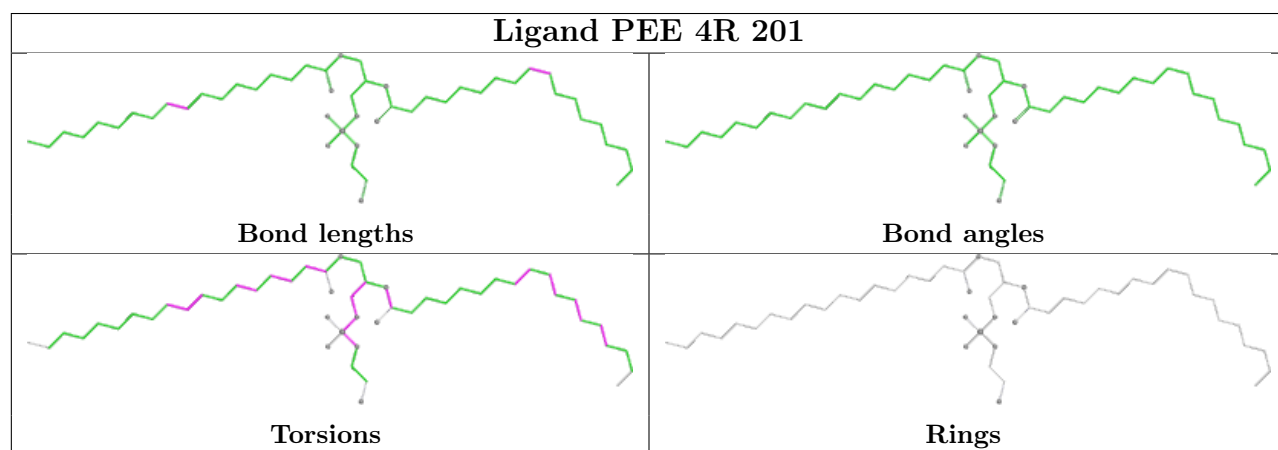
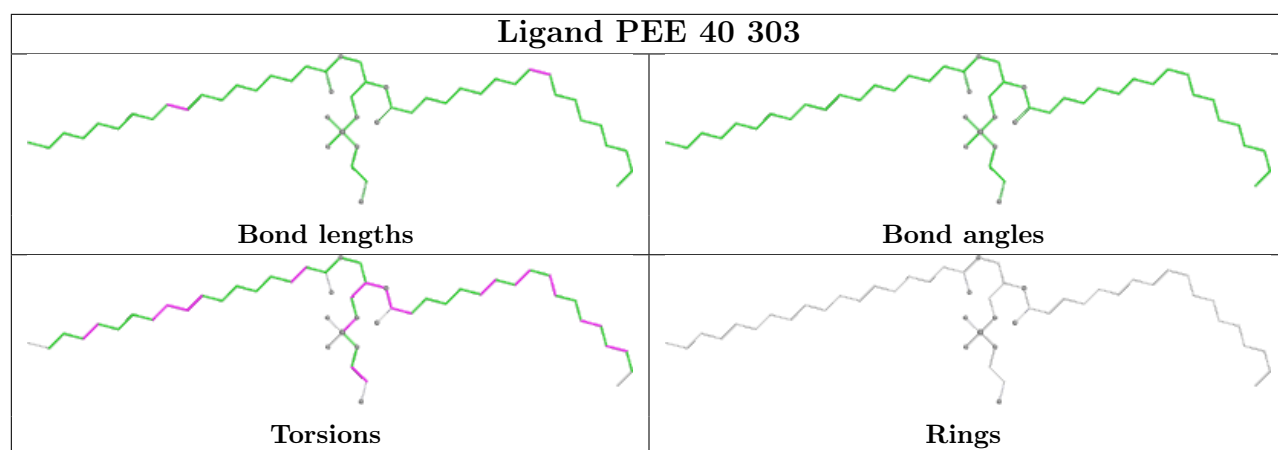


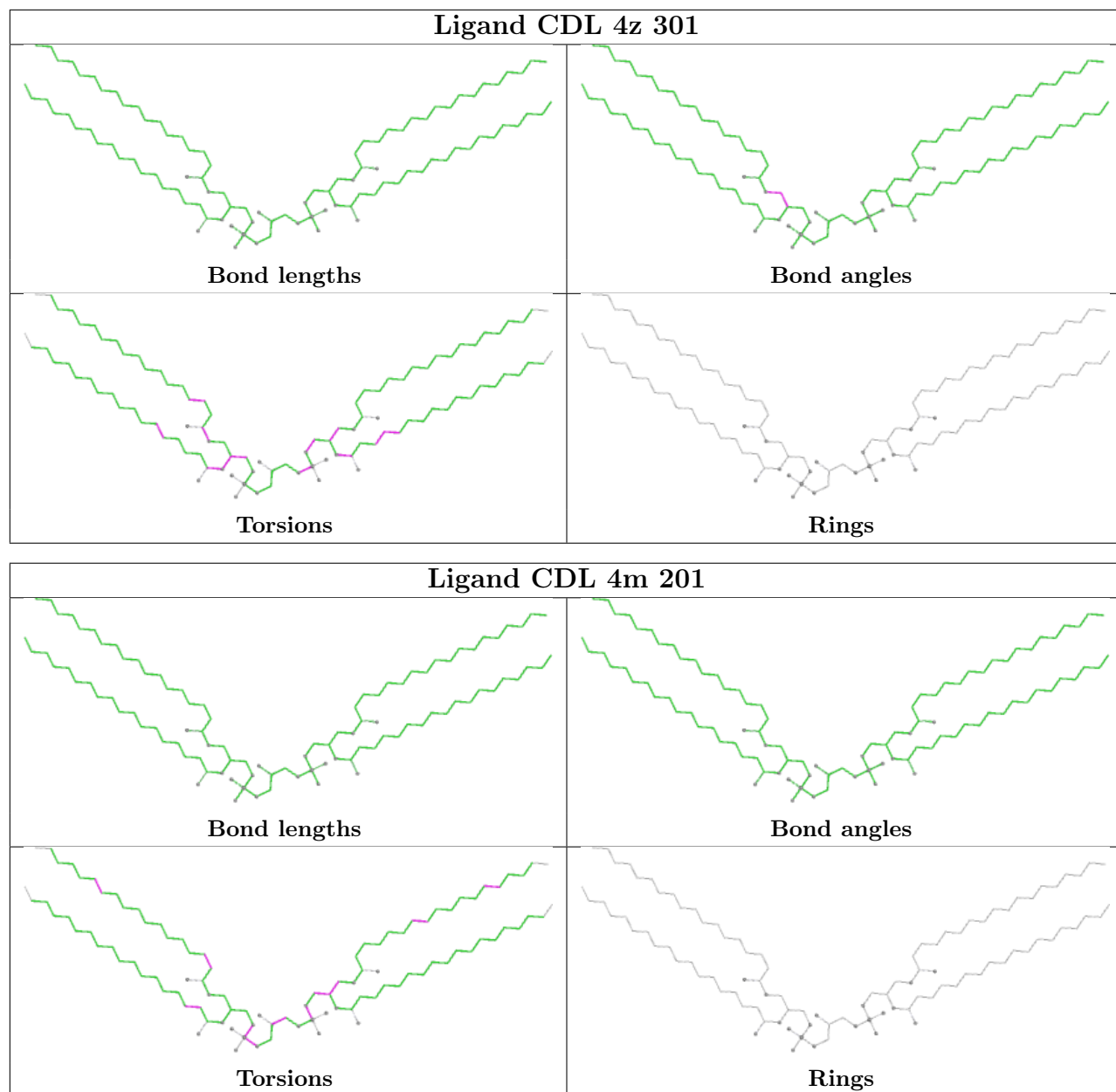
Ligand HEM 3G 401

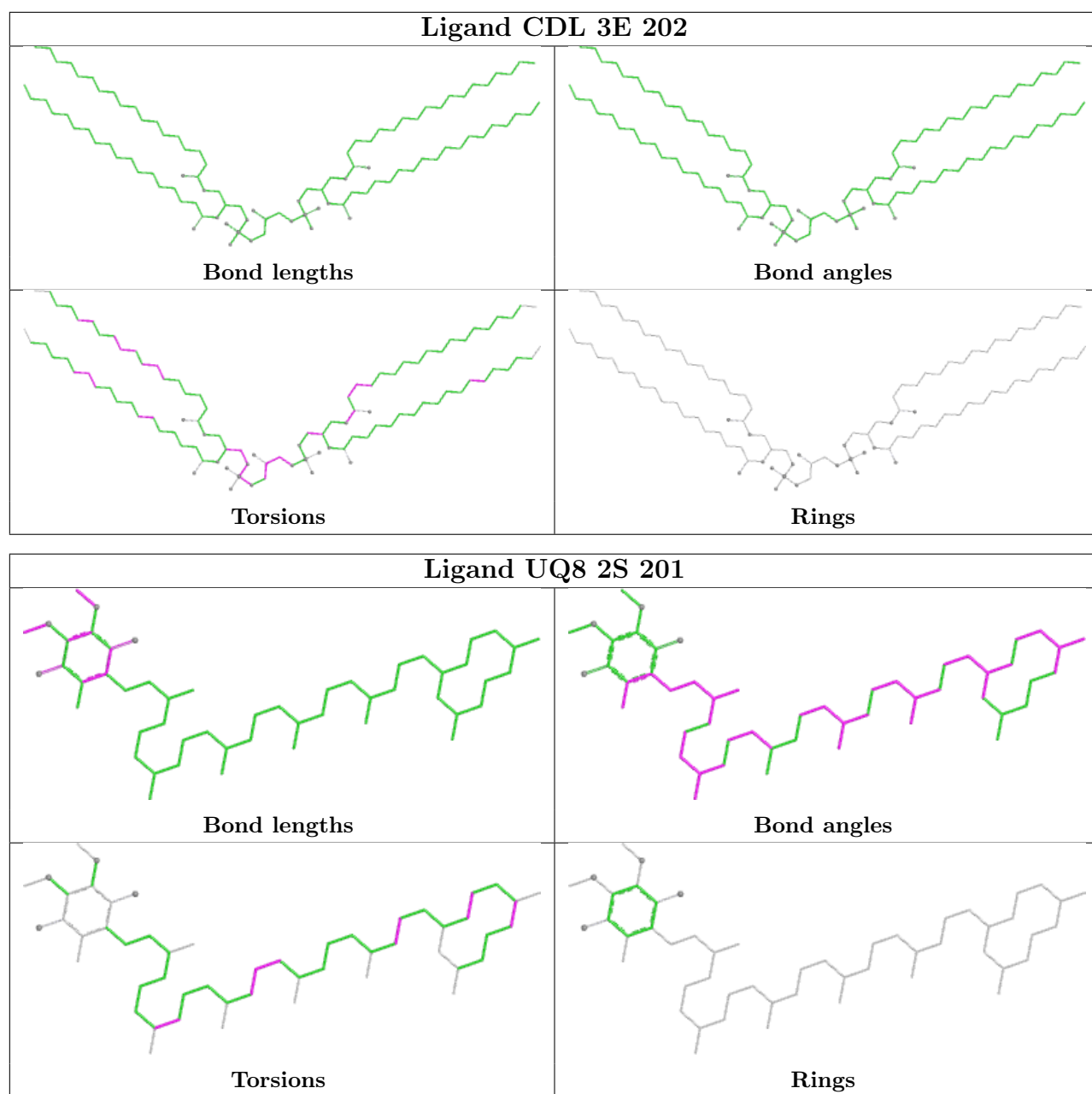


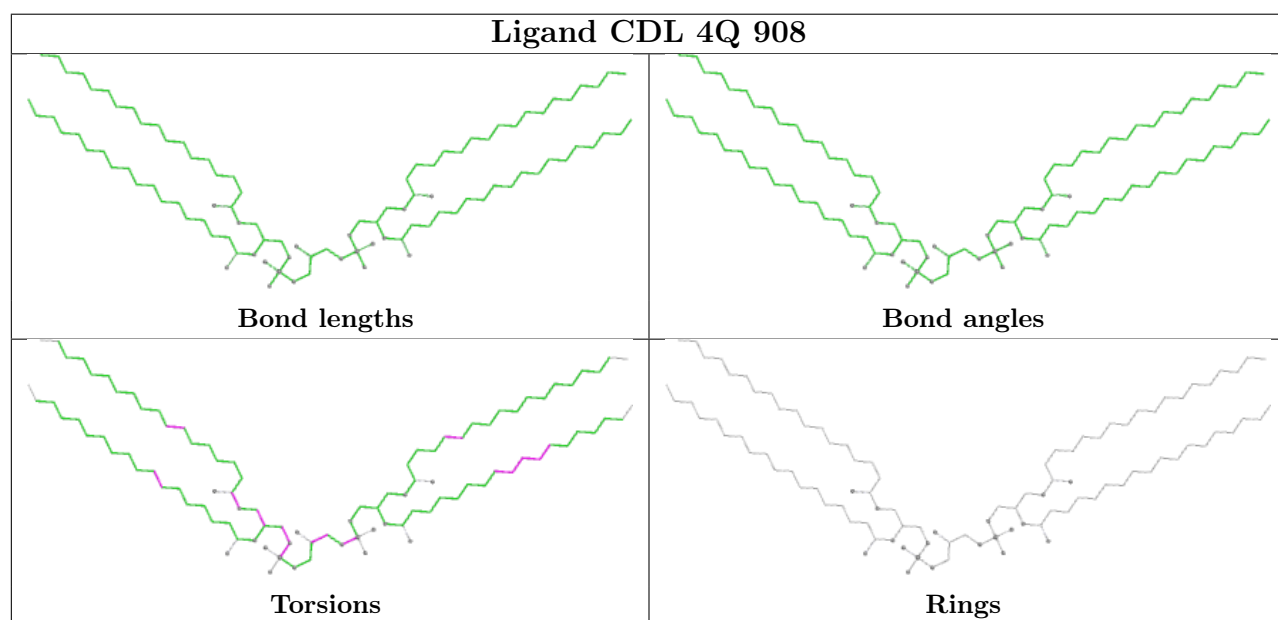
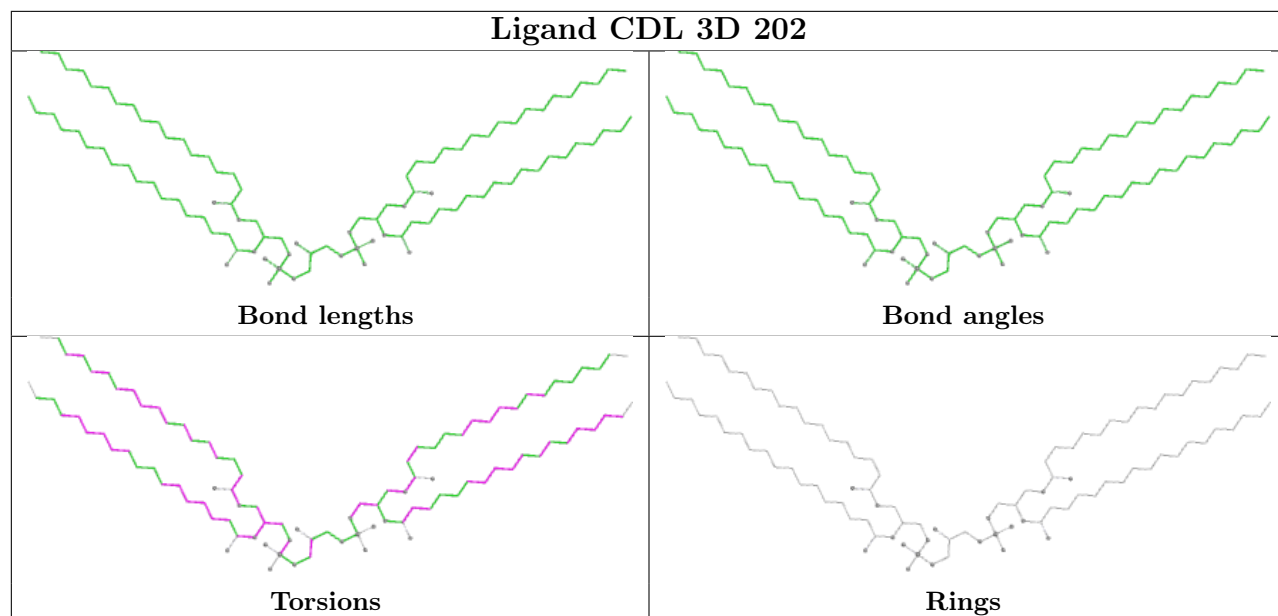
Ligand CDL 4J 301

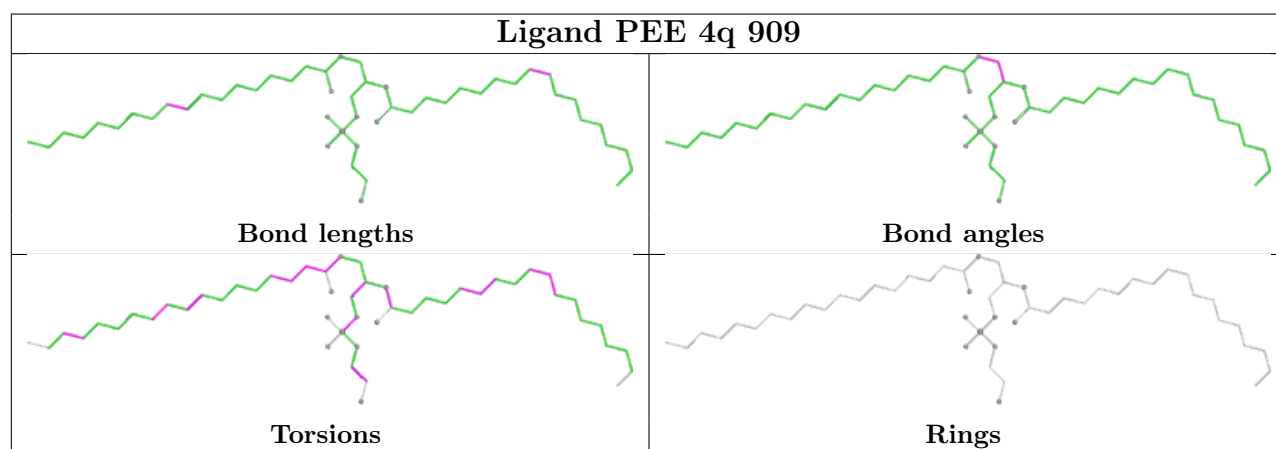
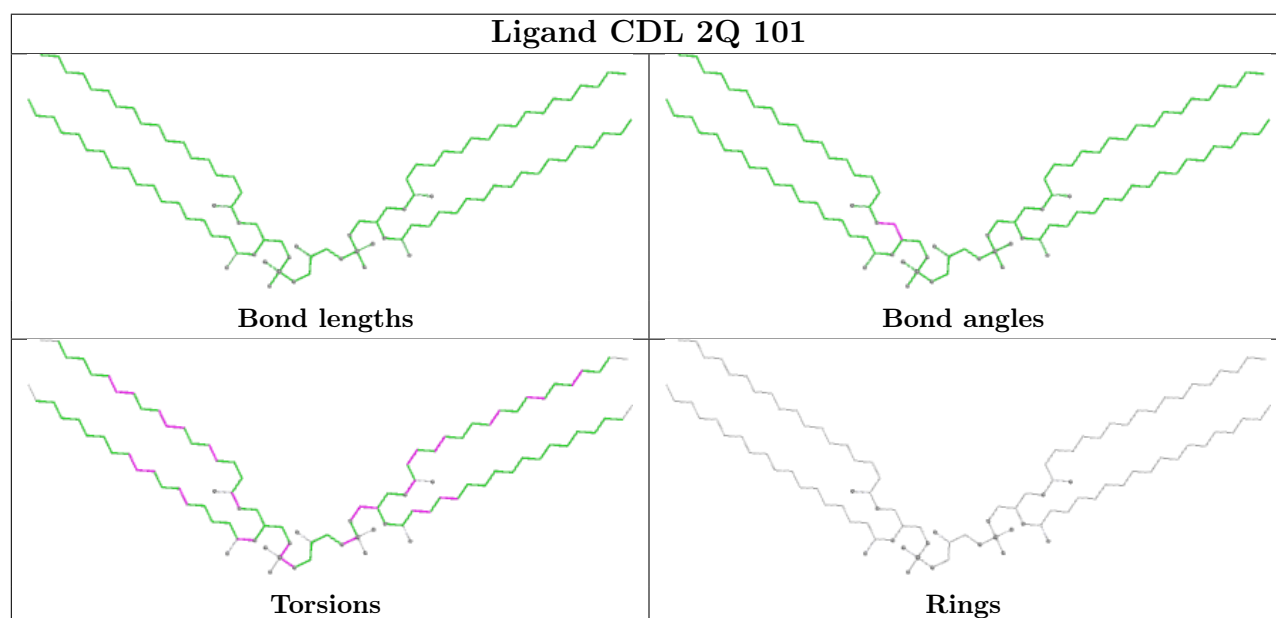
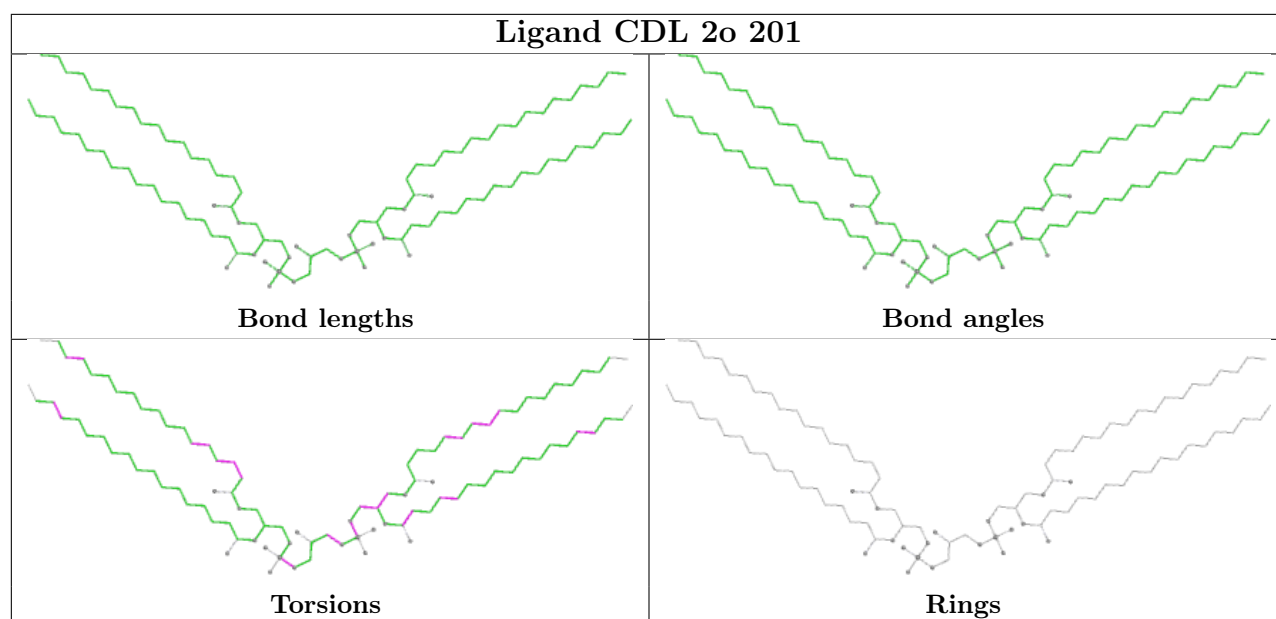


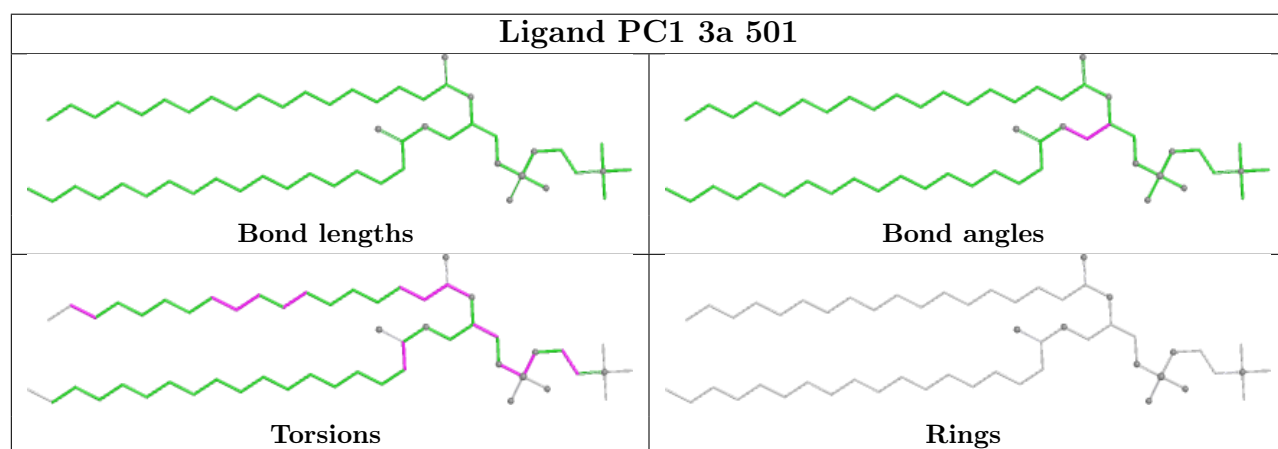
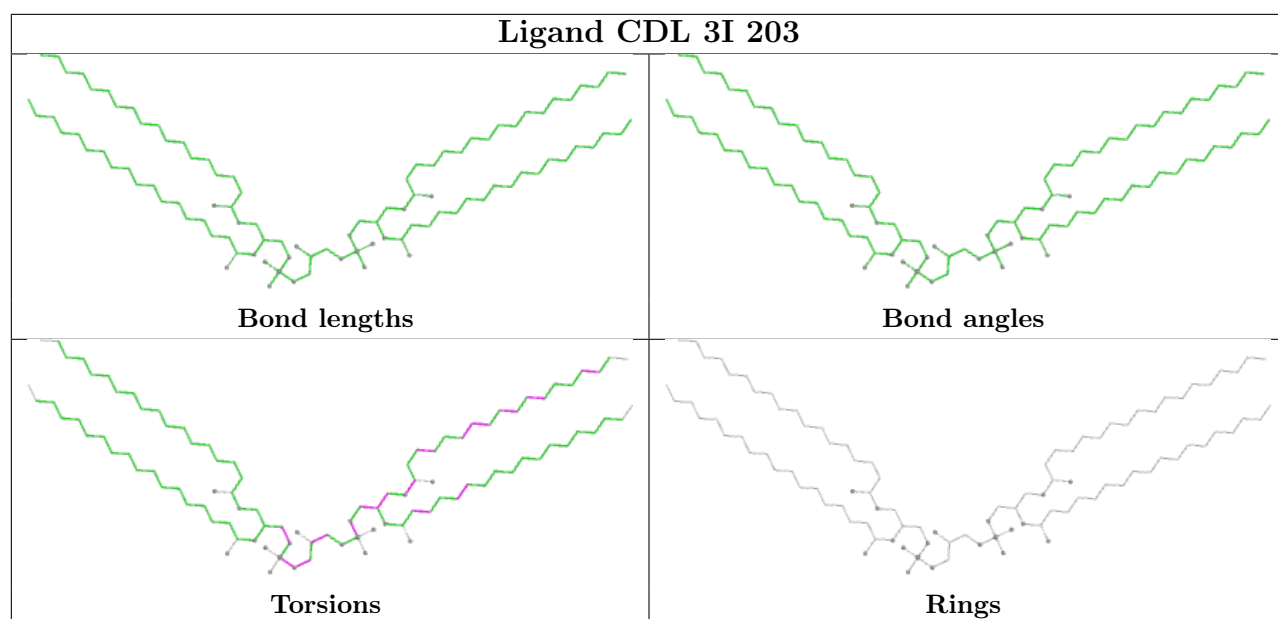


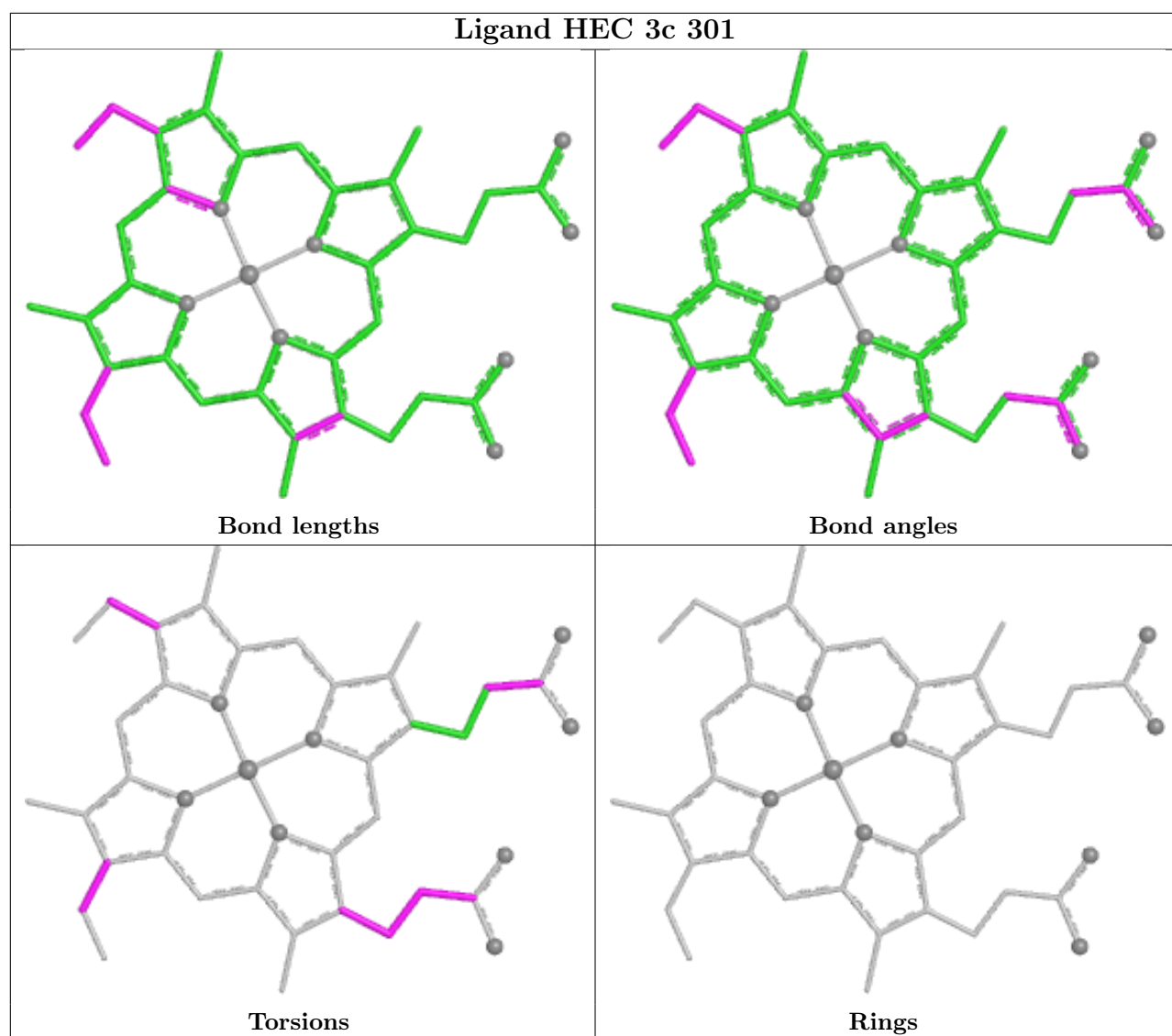




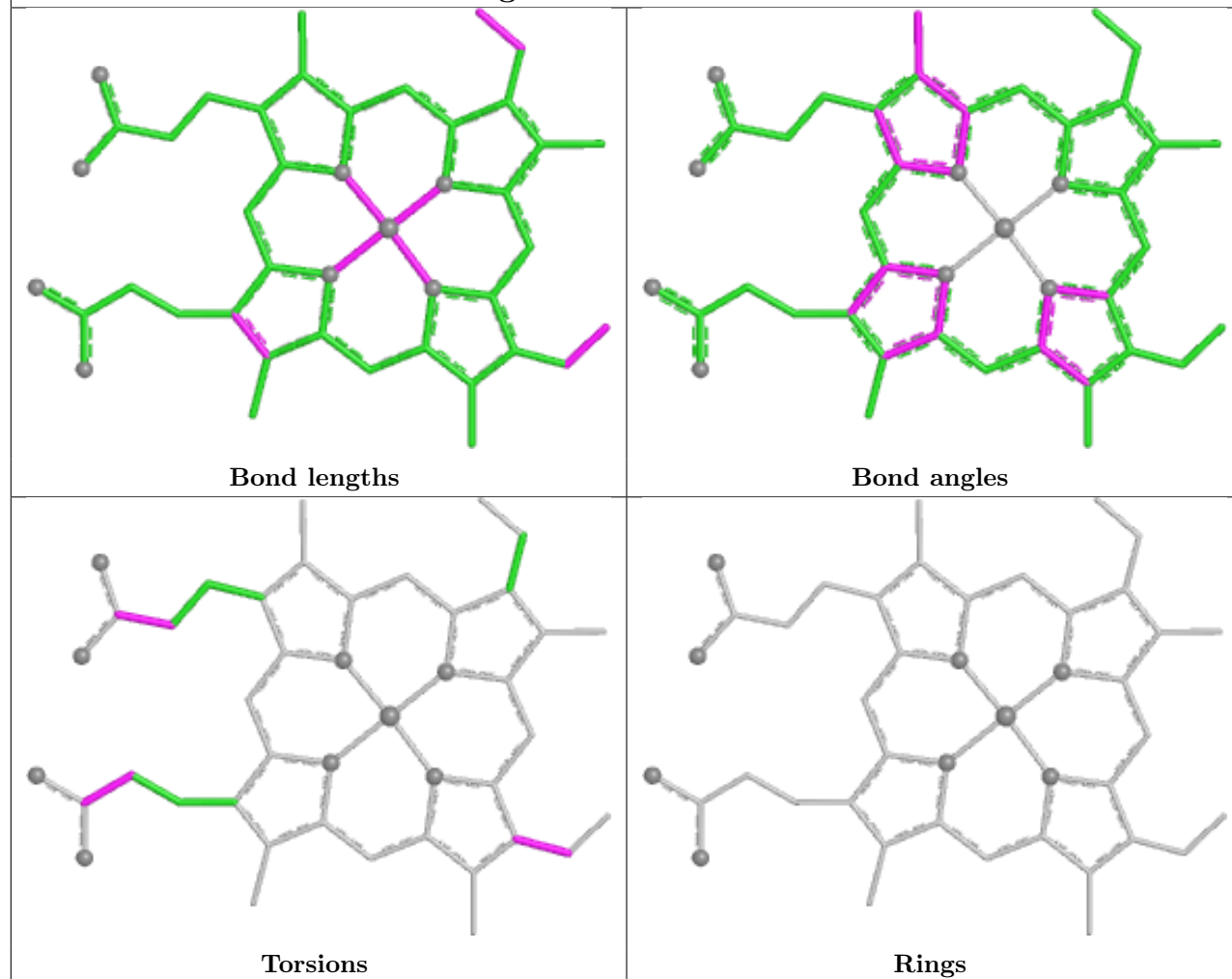




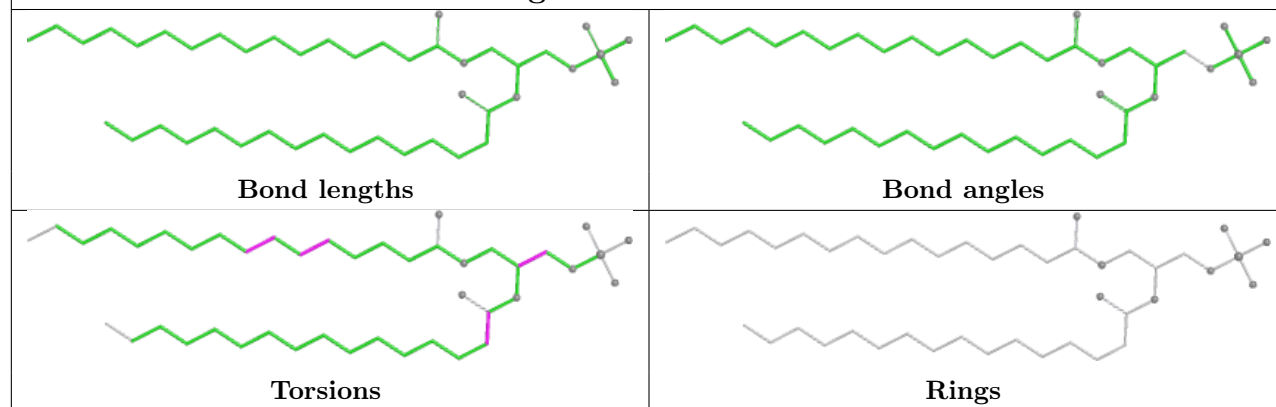


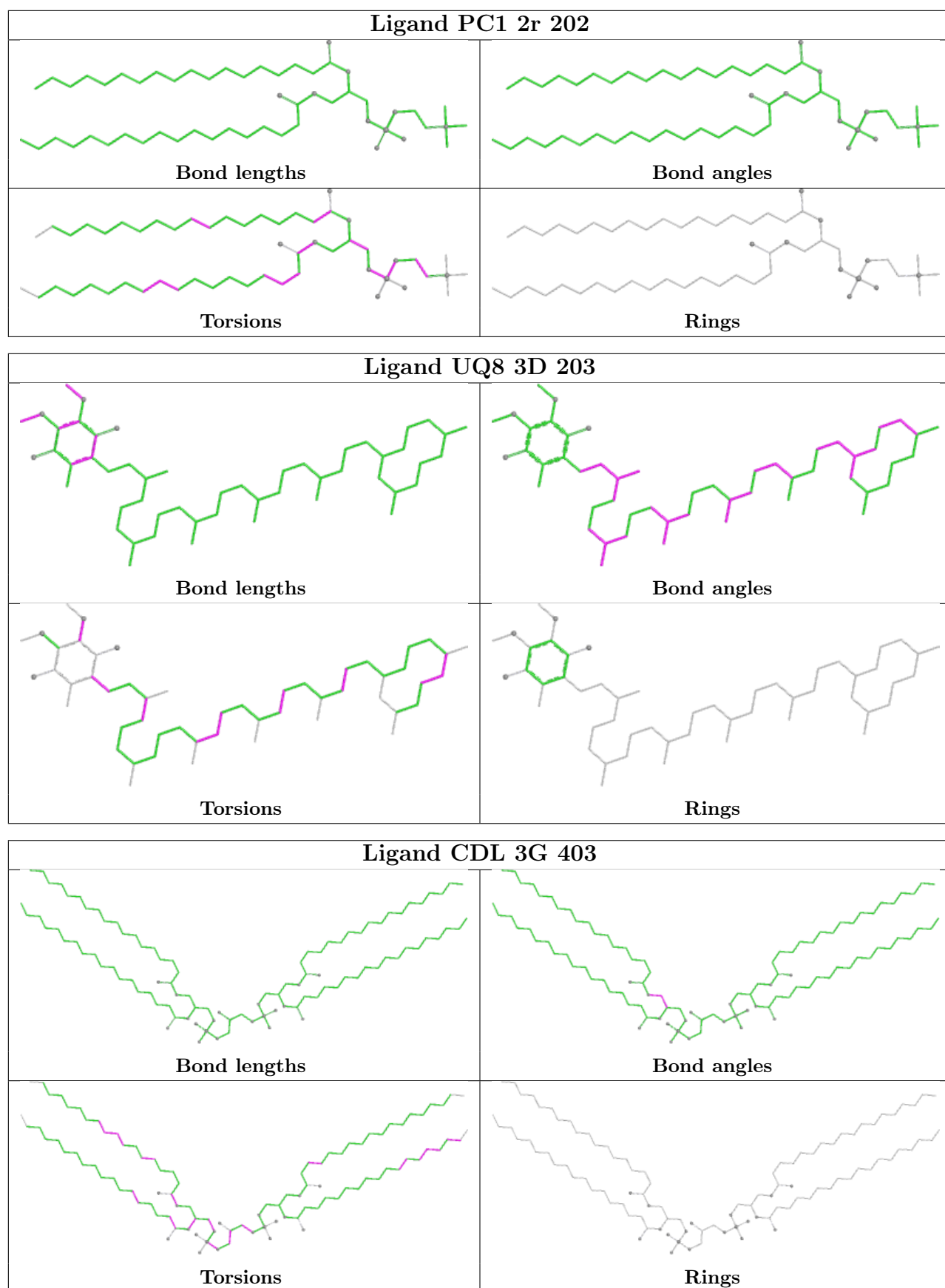


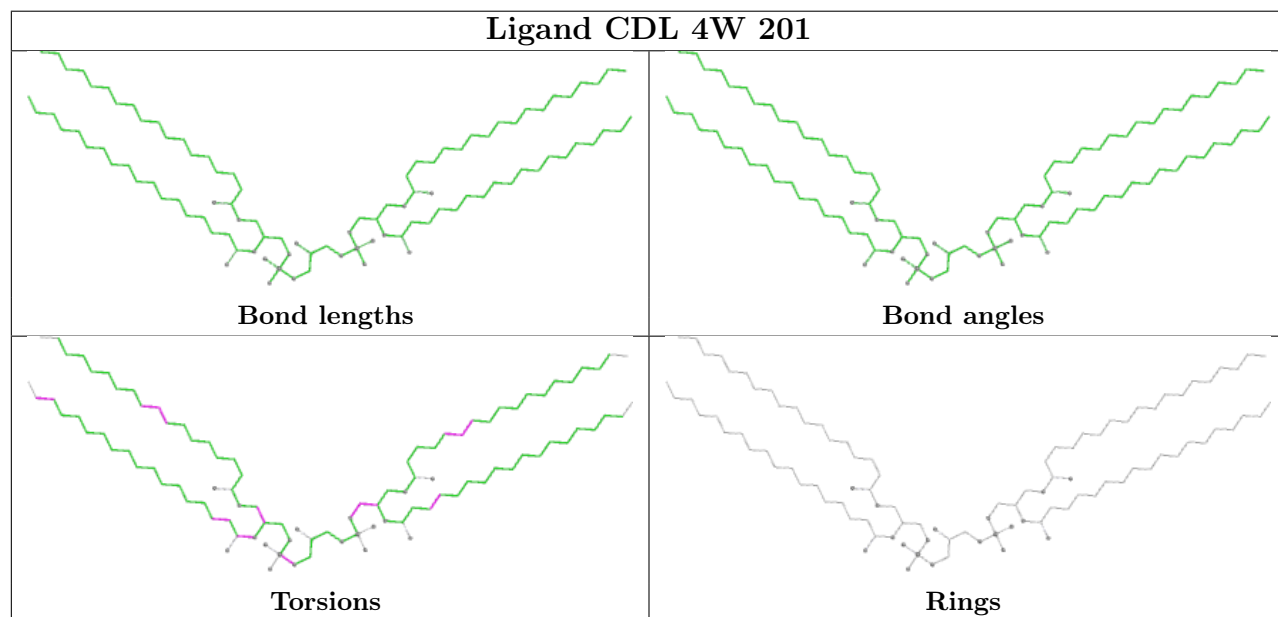
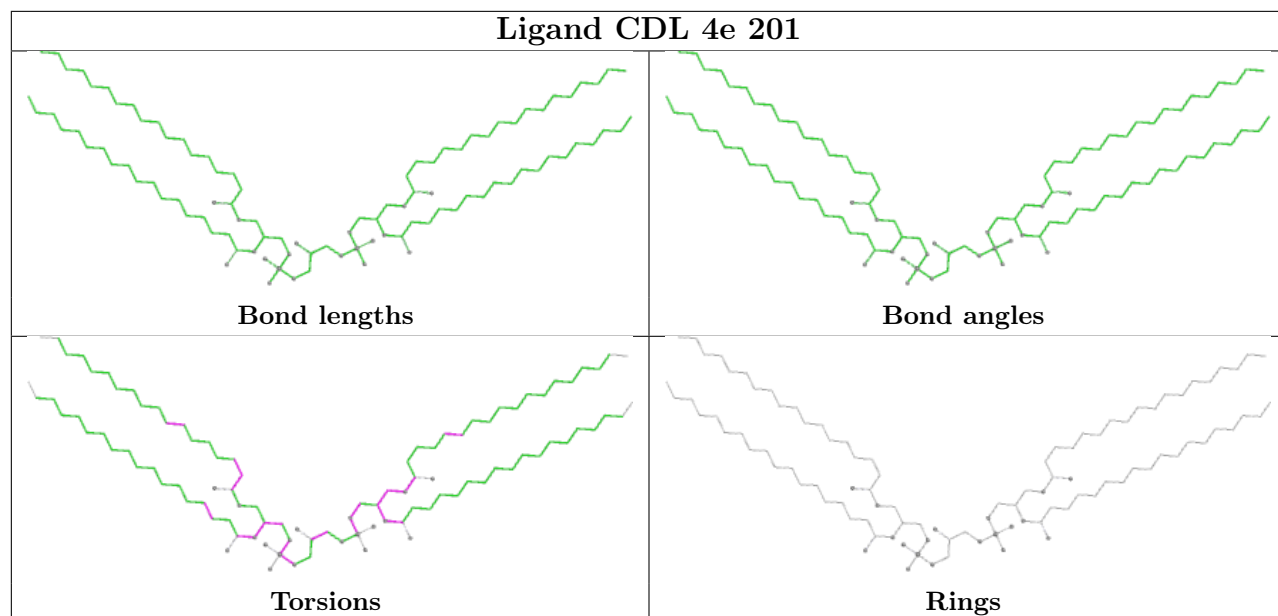
Ligand HEM 3G 402

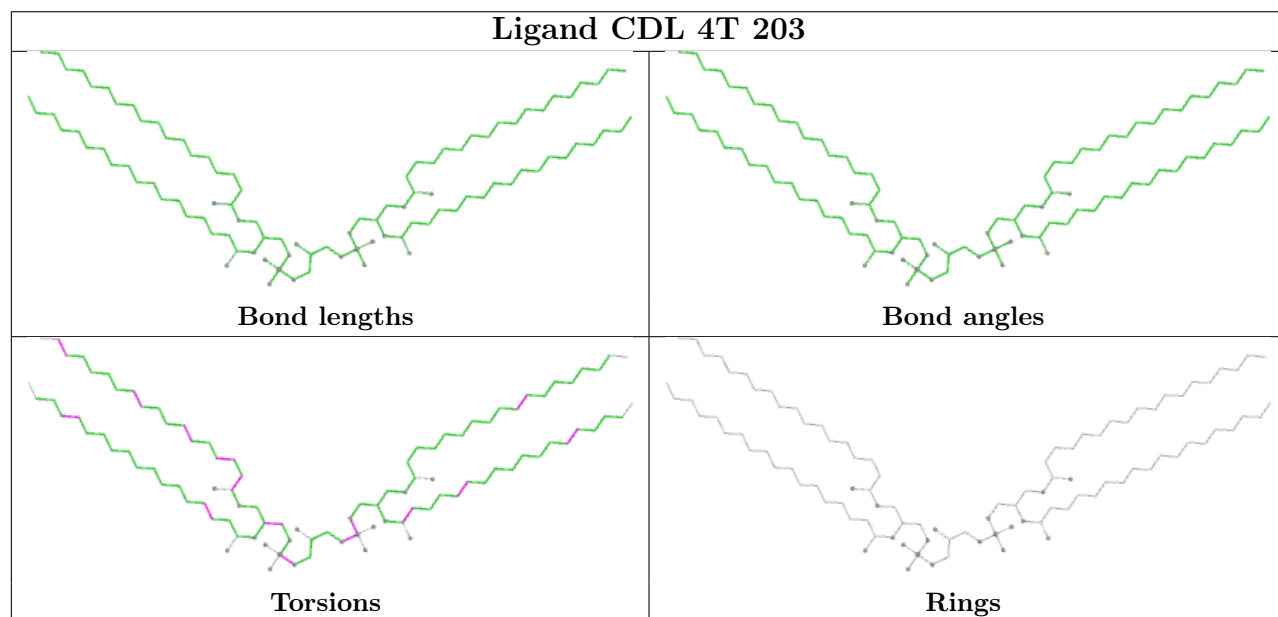
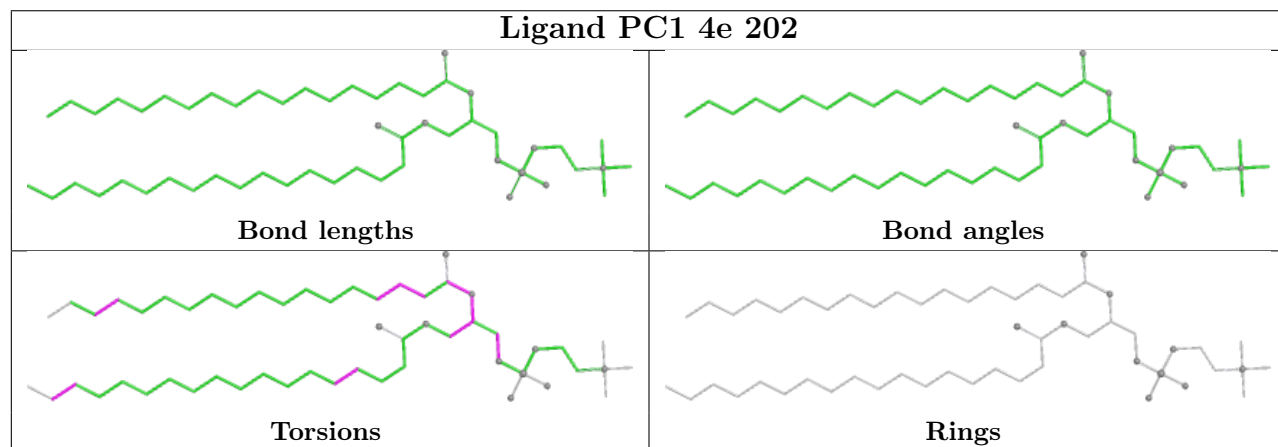
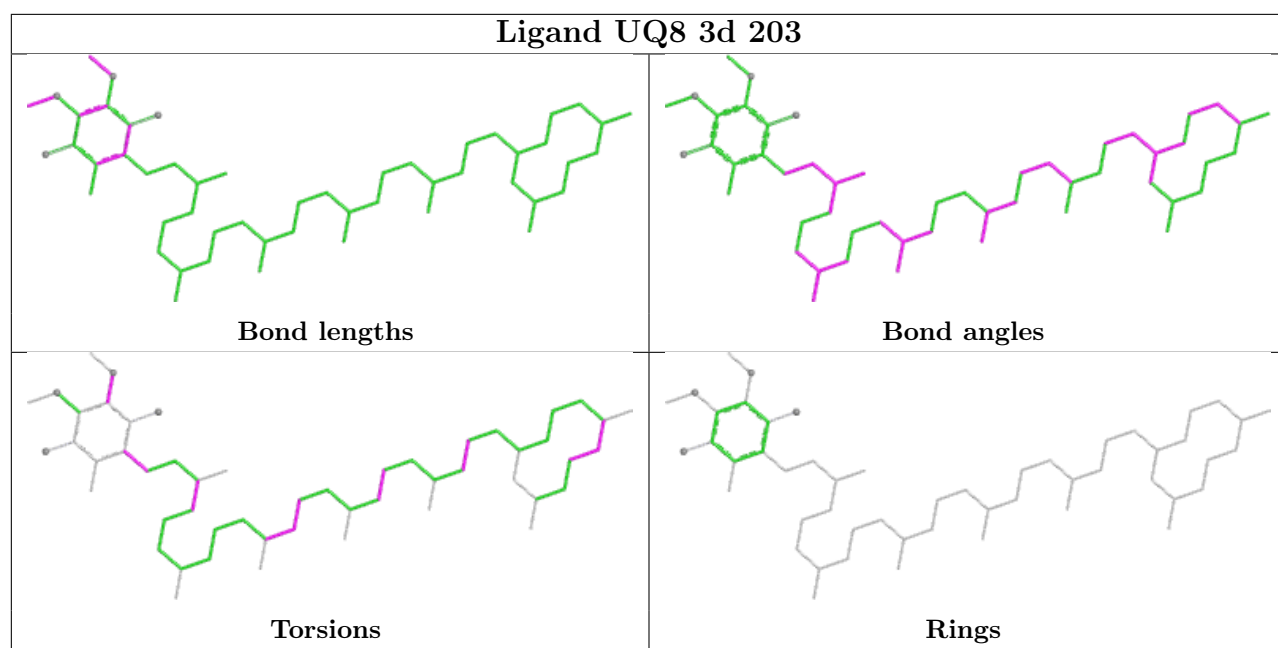


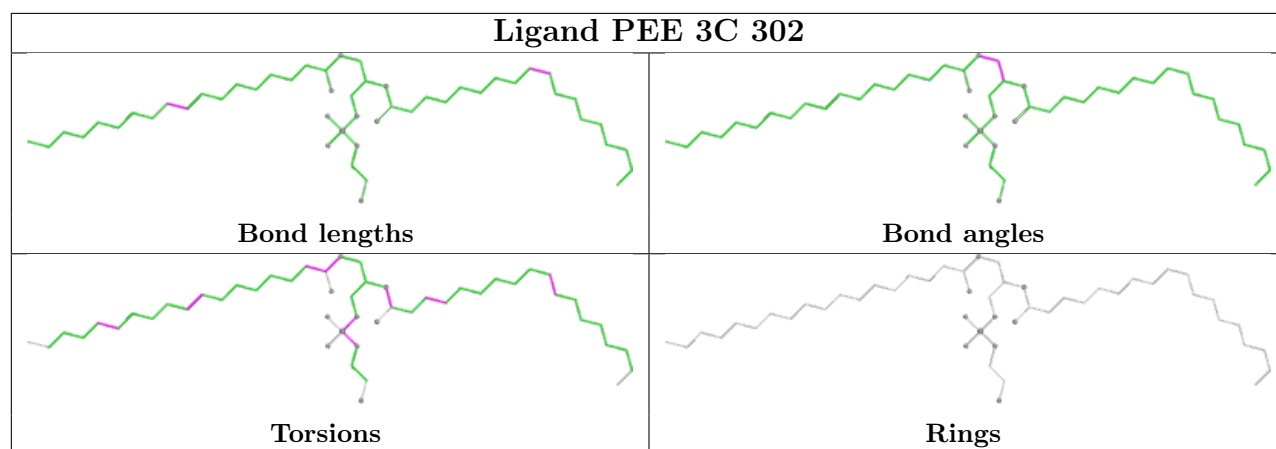
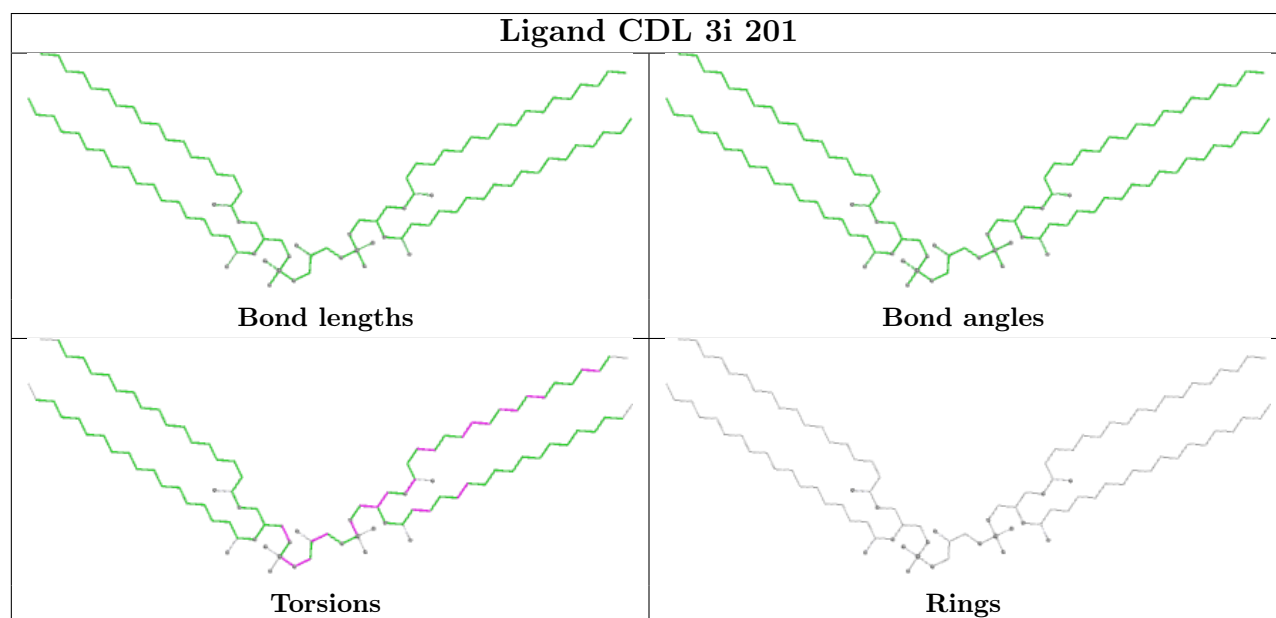
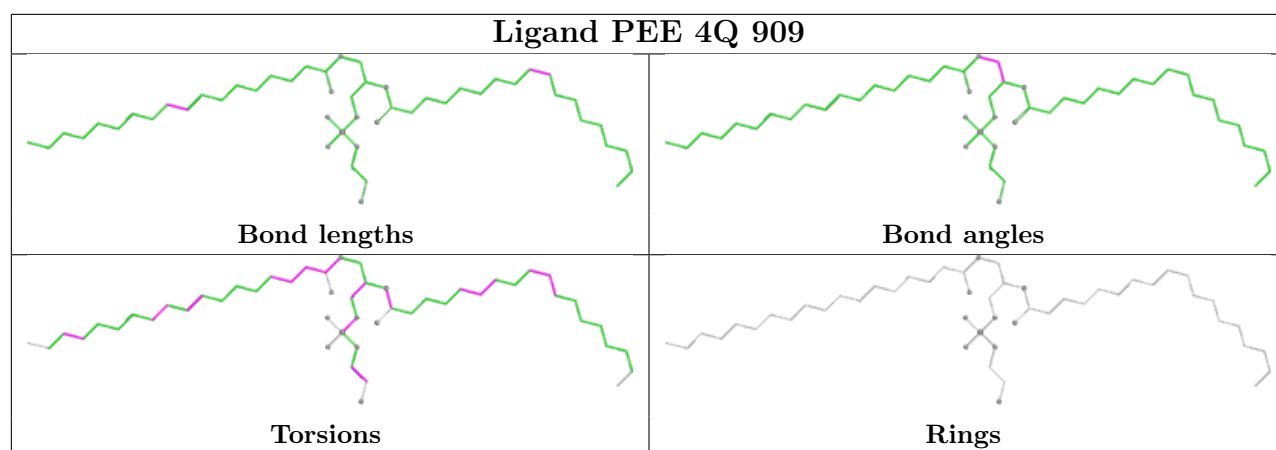
Ligand LPP 4d 102

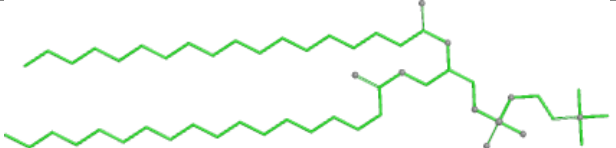
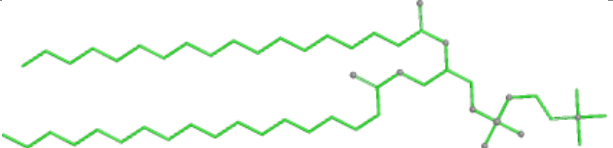
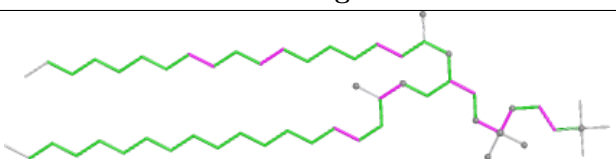
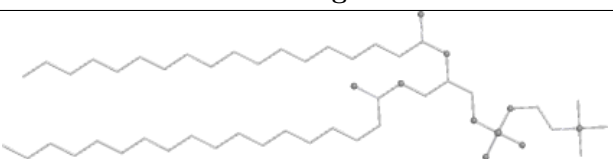
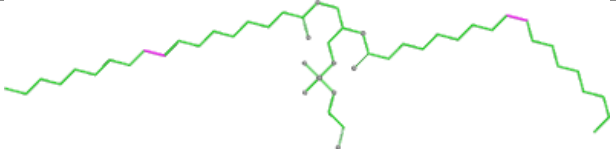
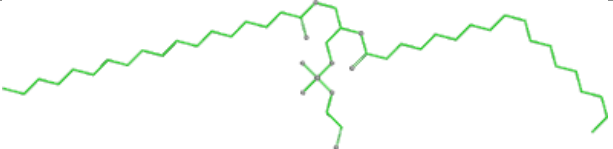
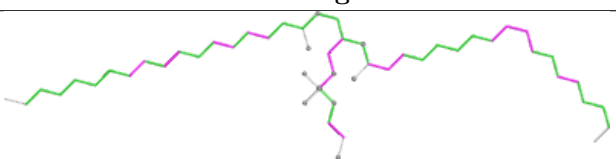
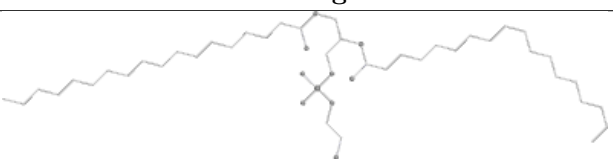
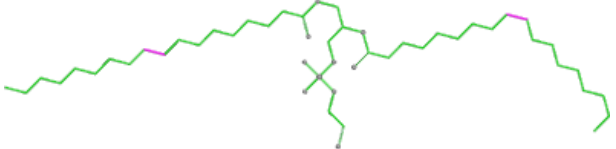
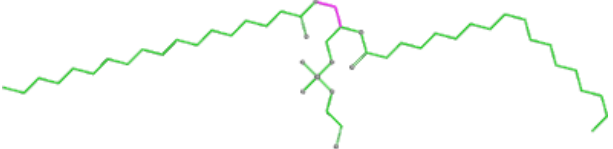
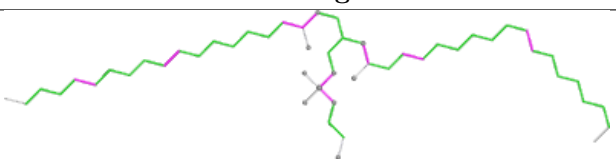
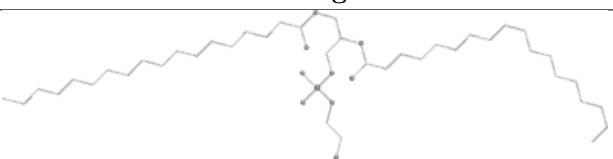


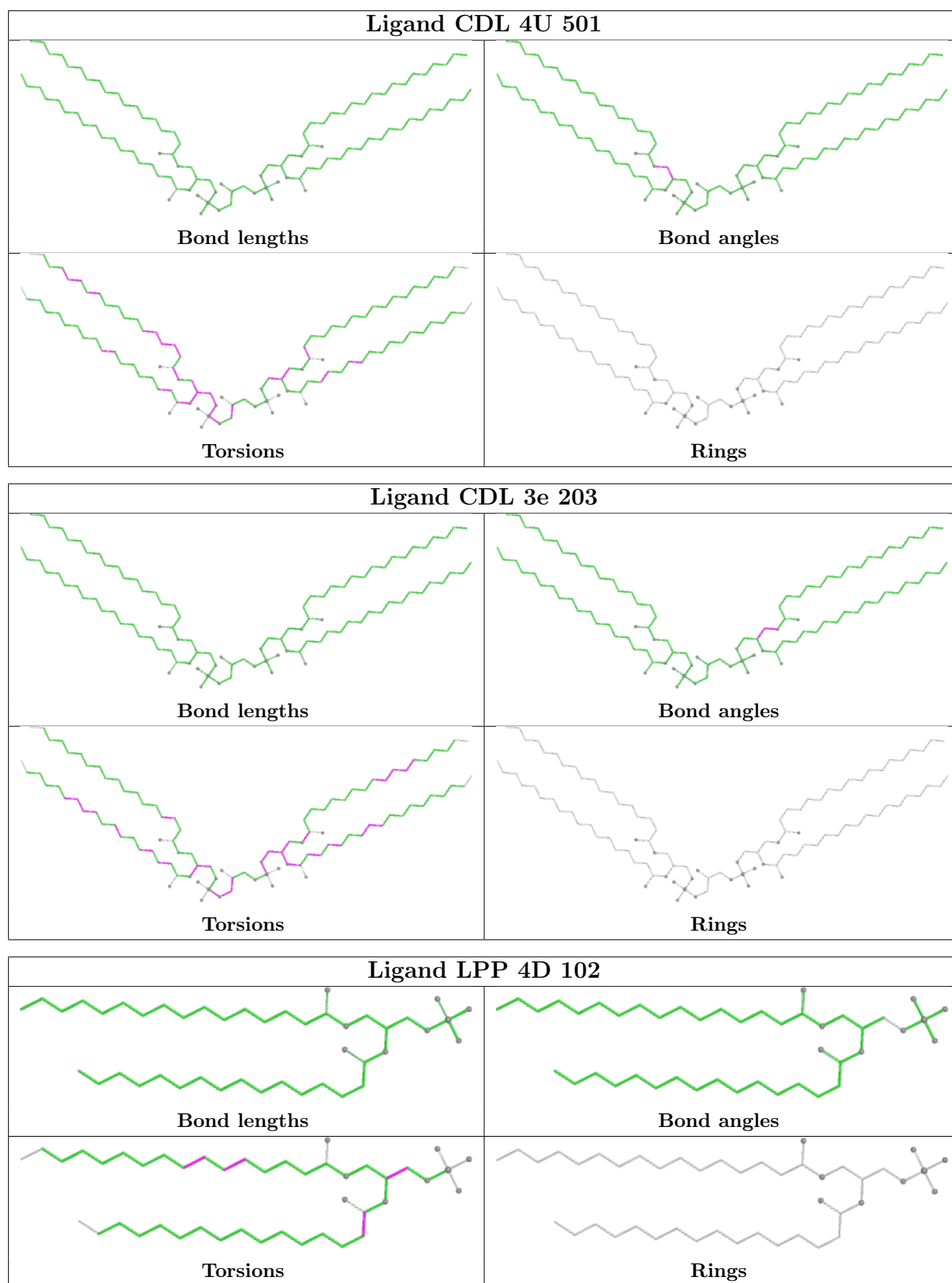


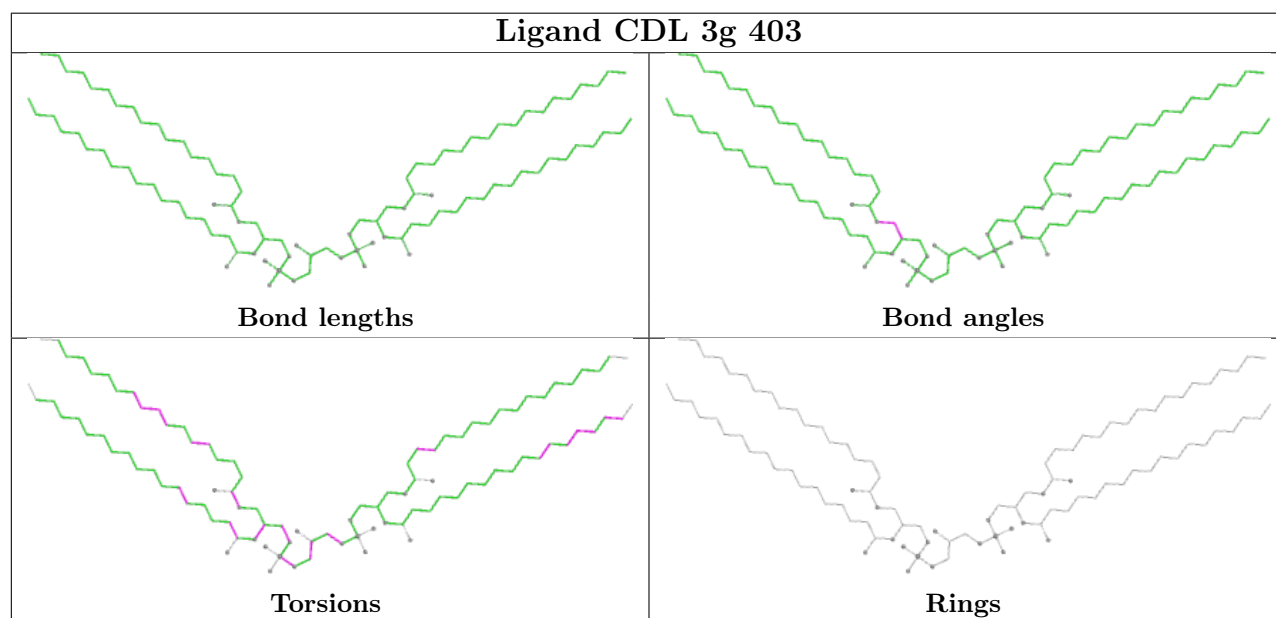
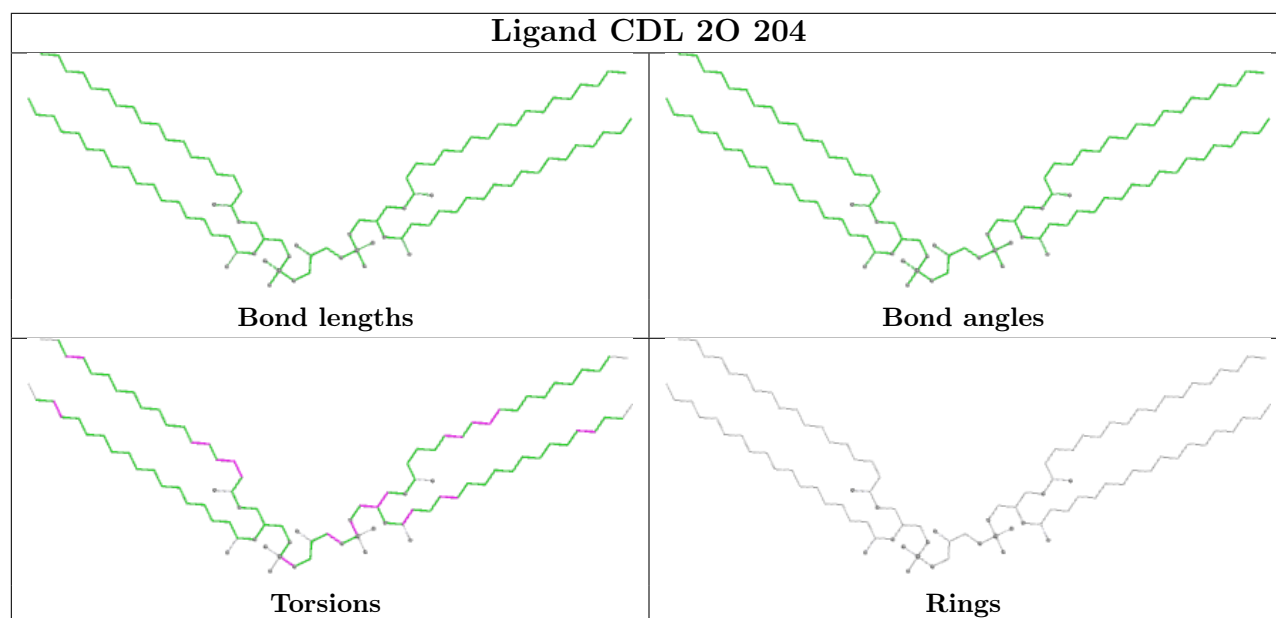
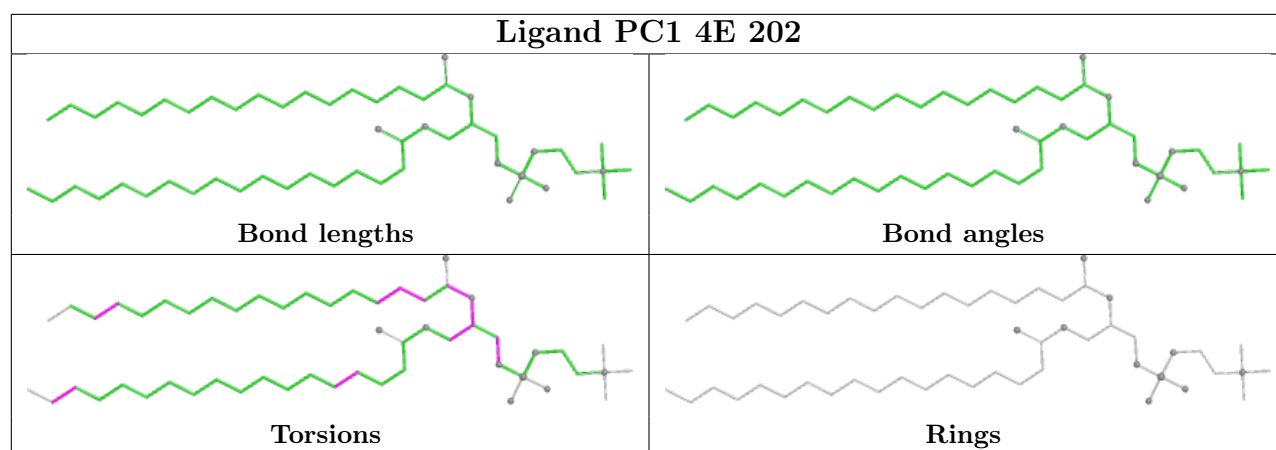


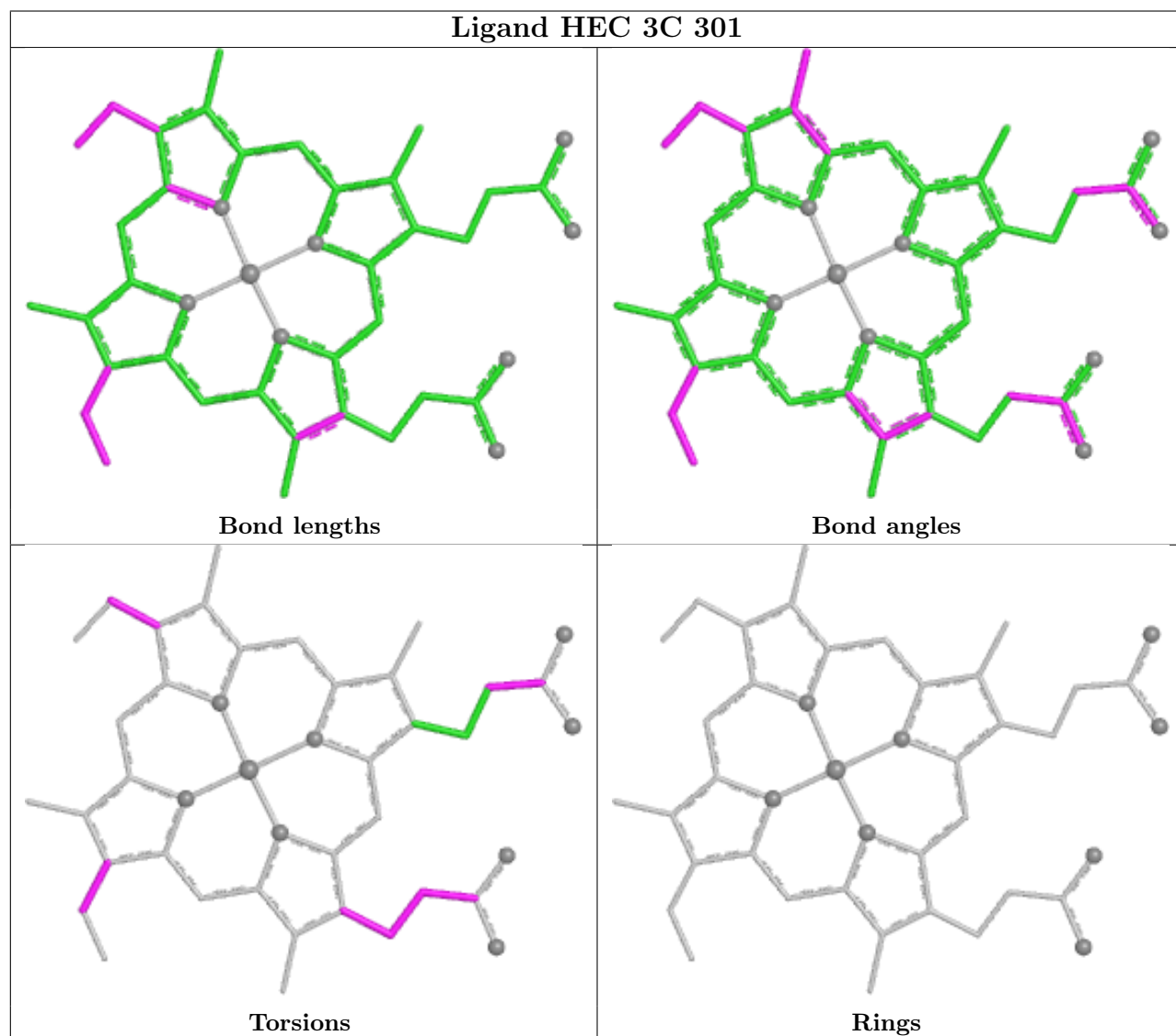
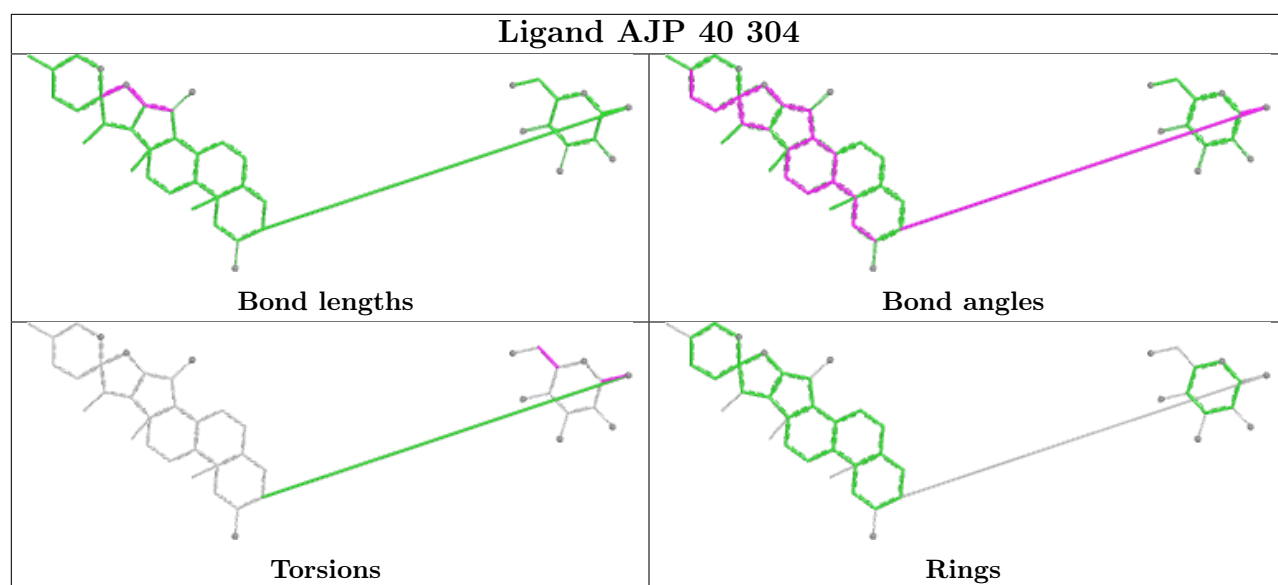


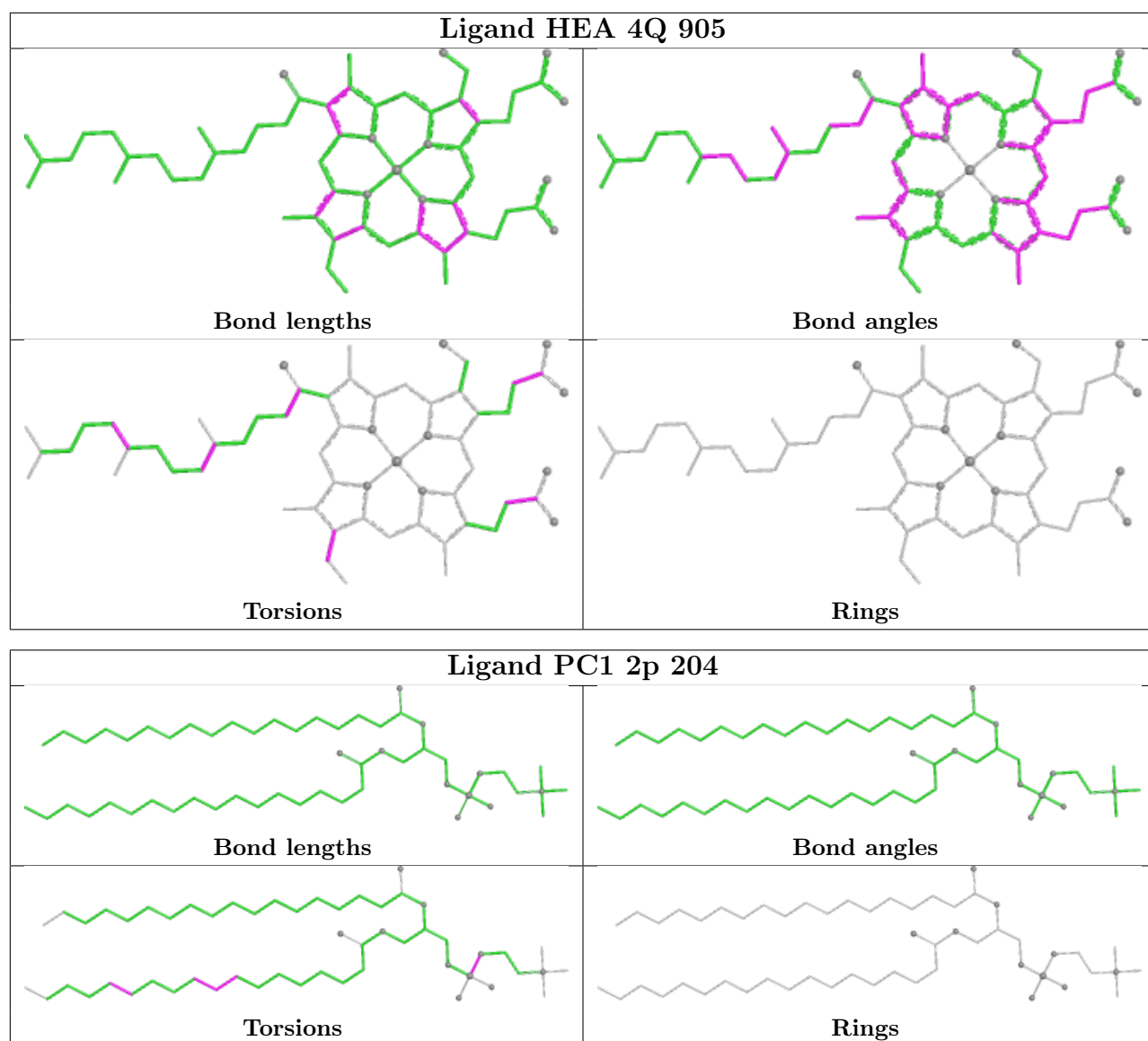


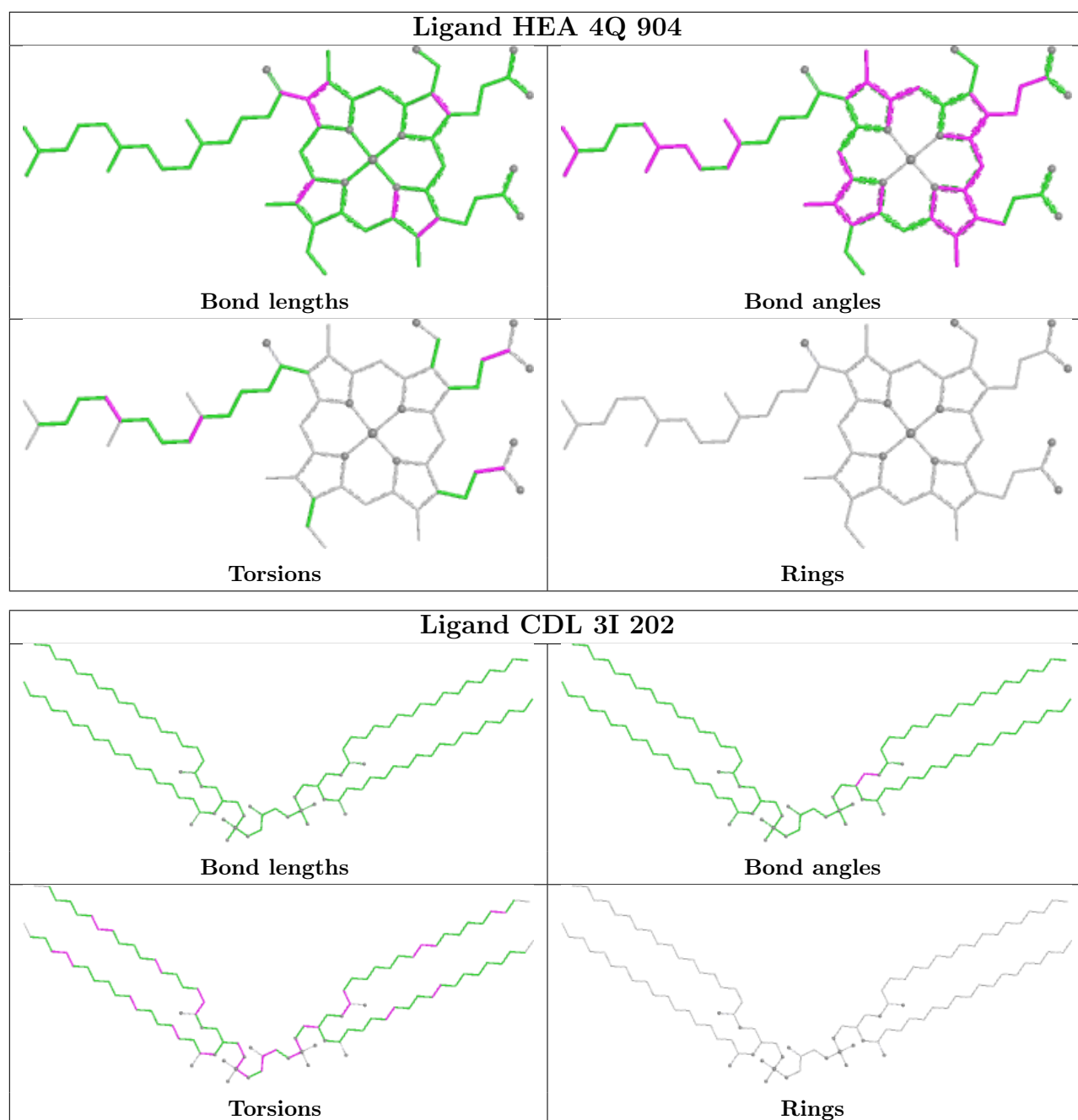
Ligand PC1 3a 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE 4D 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE 3c 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

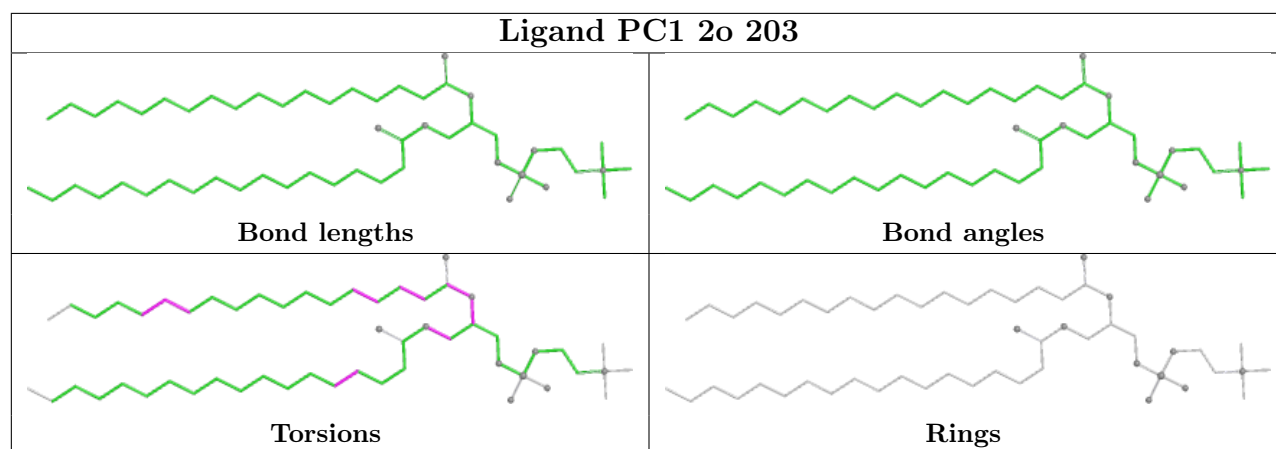
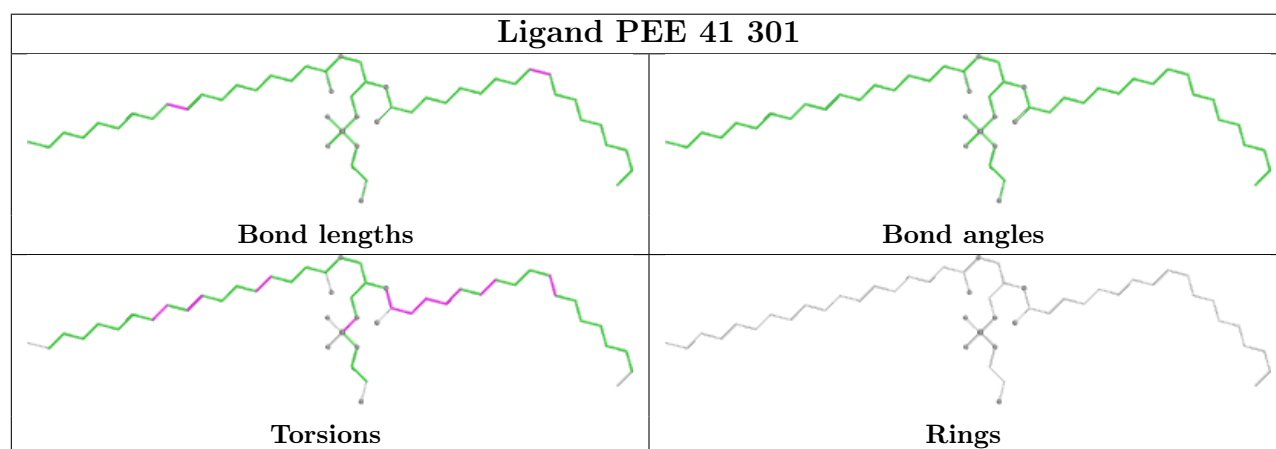
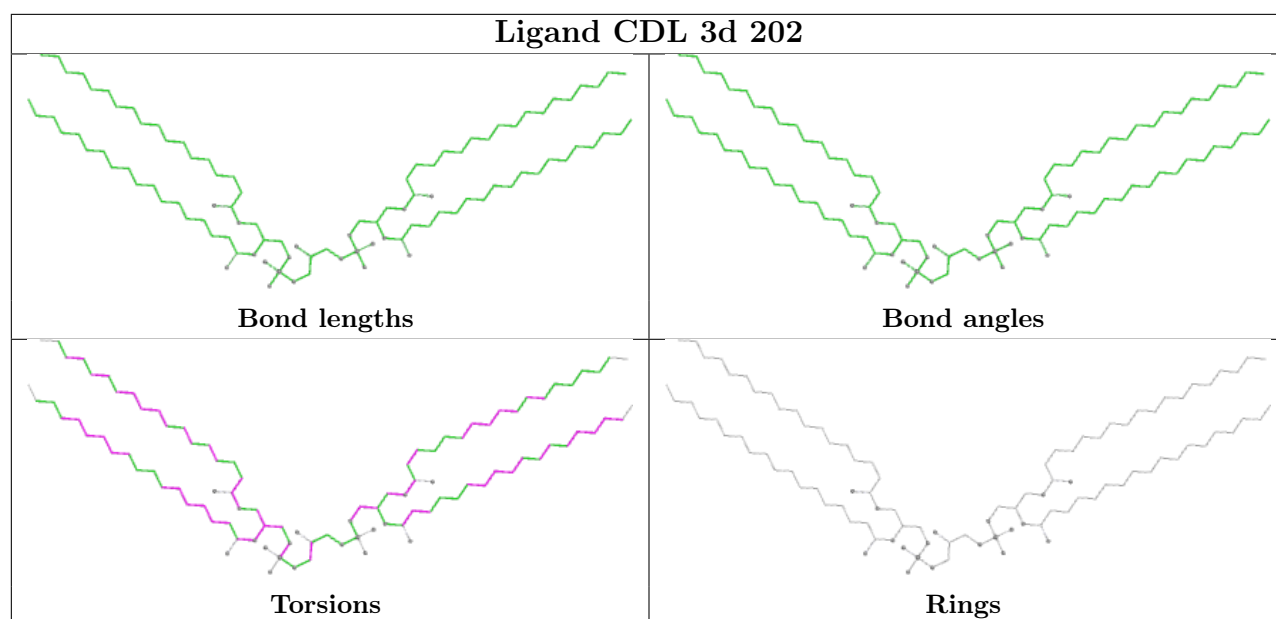


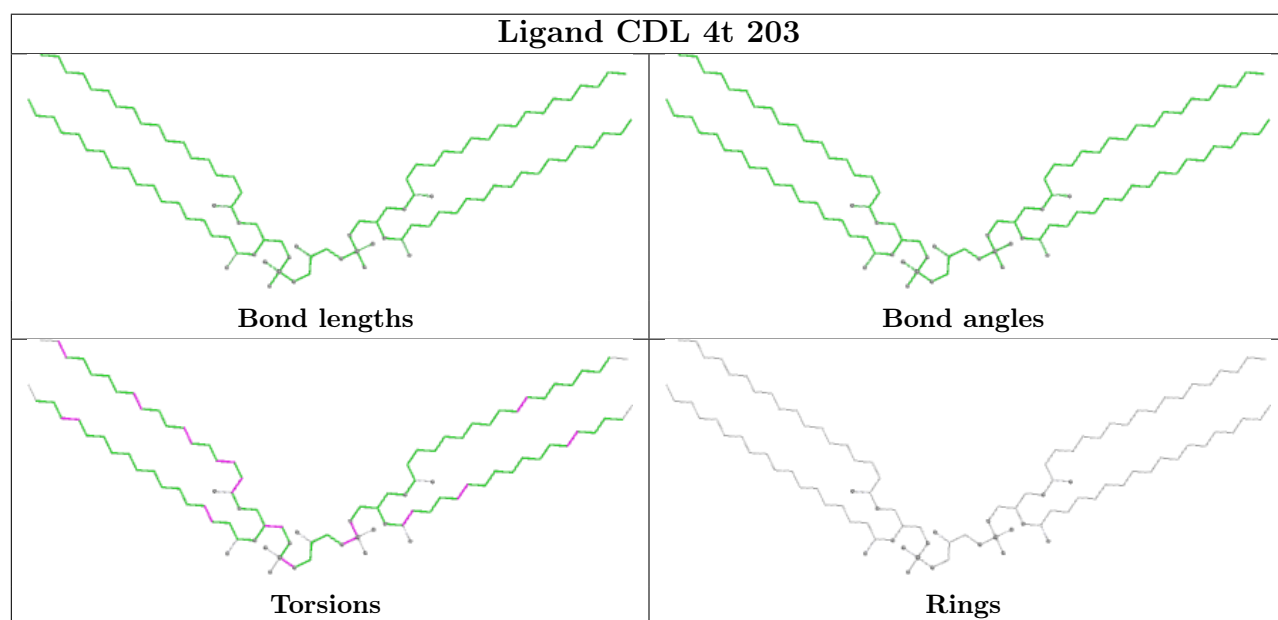
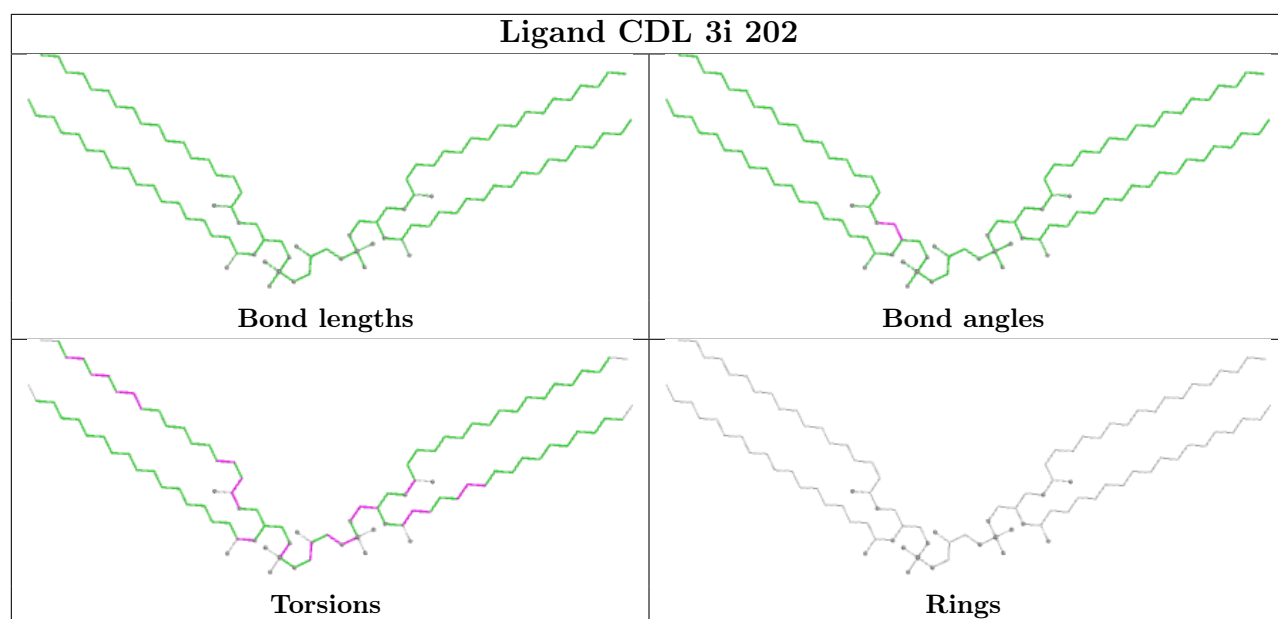


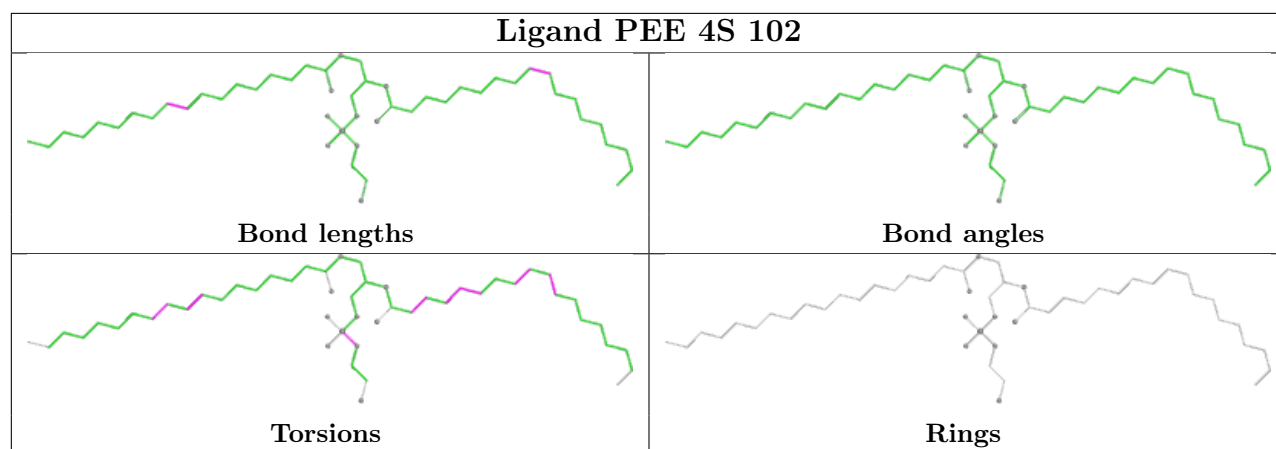
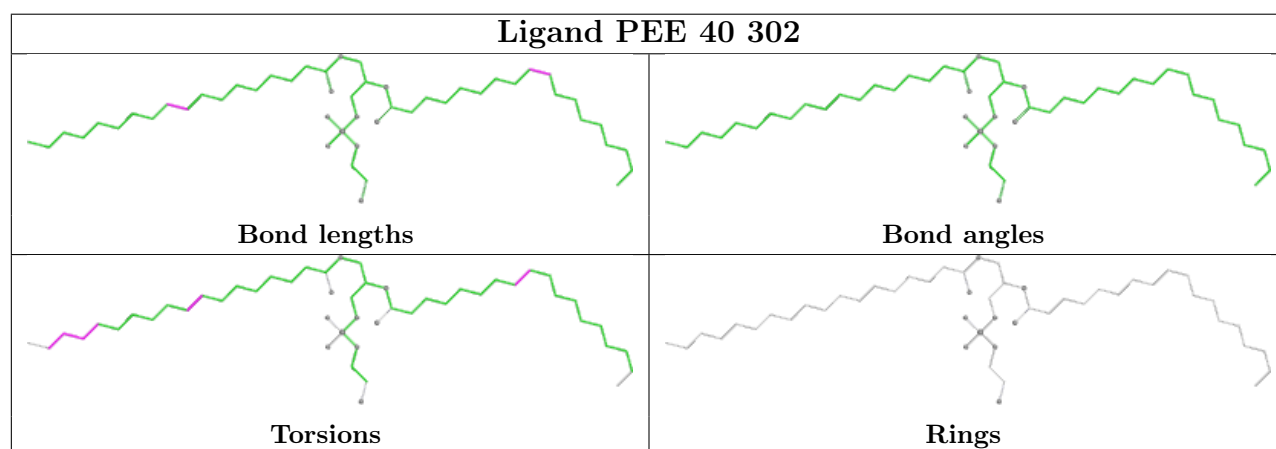
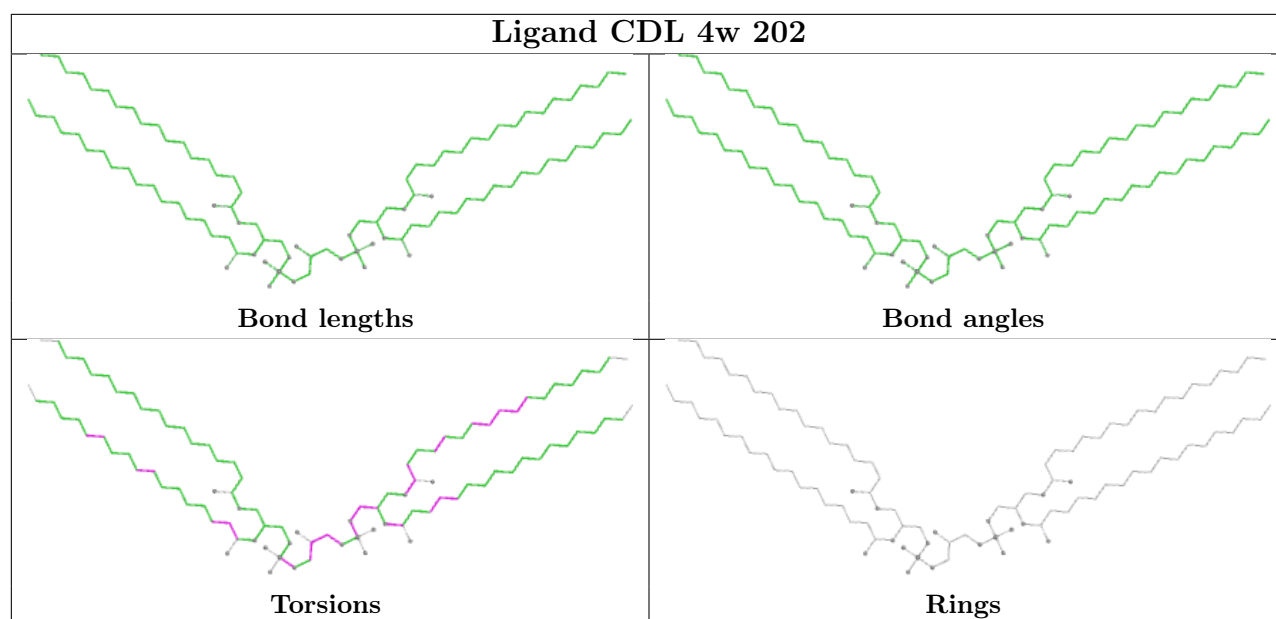




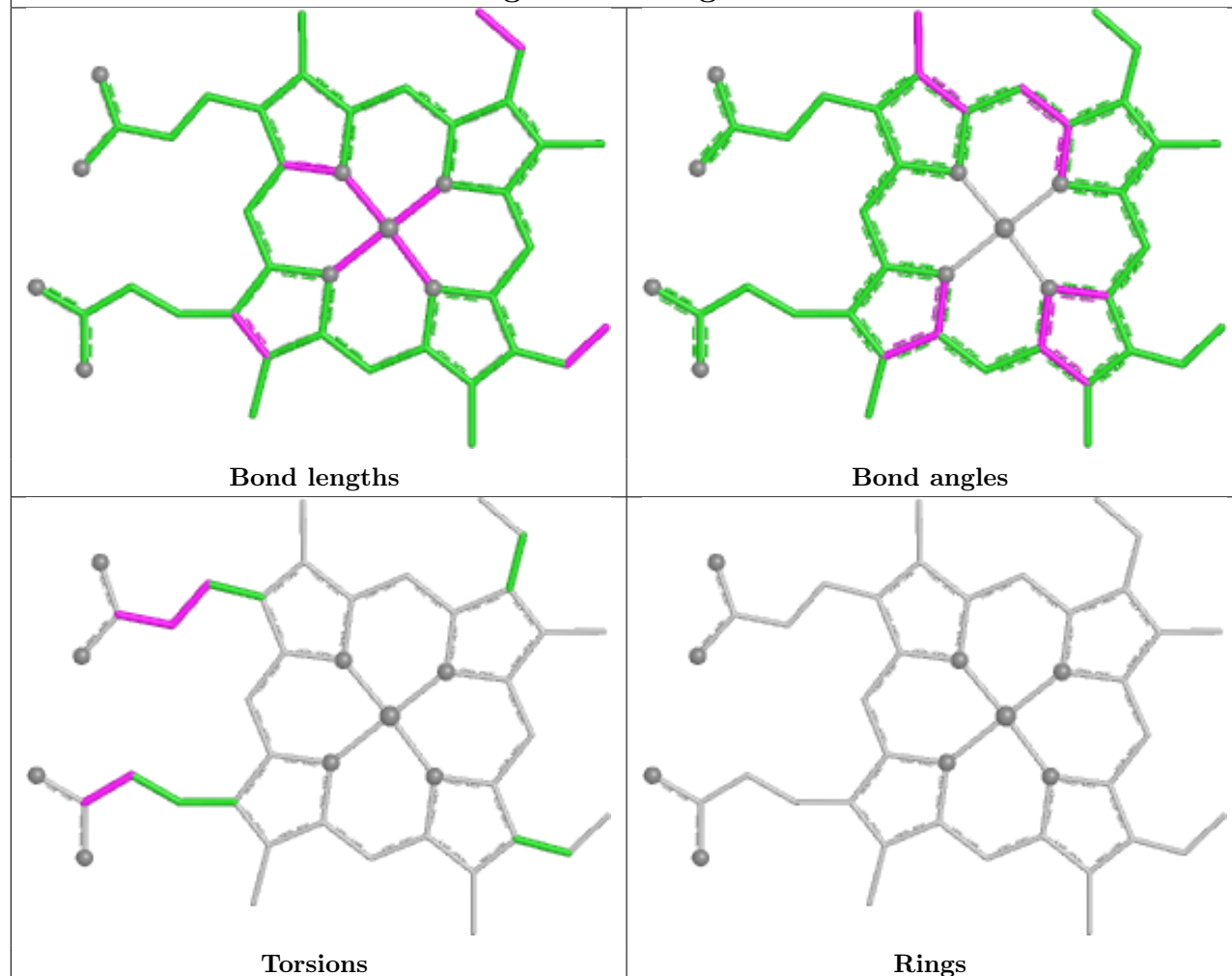




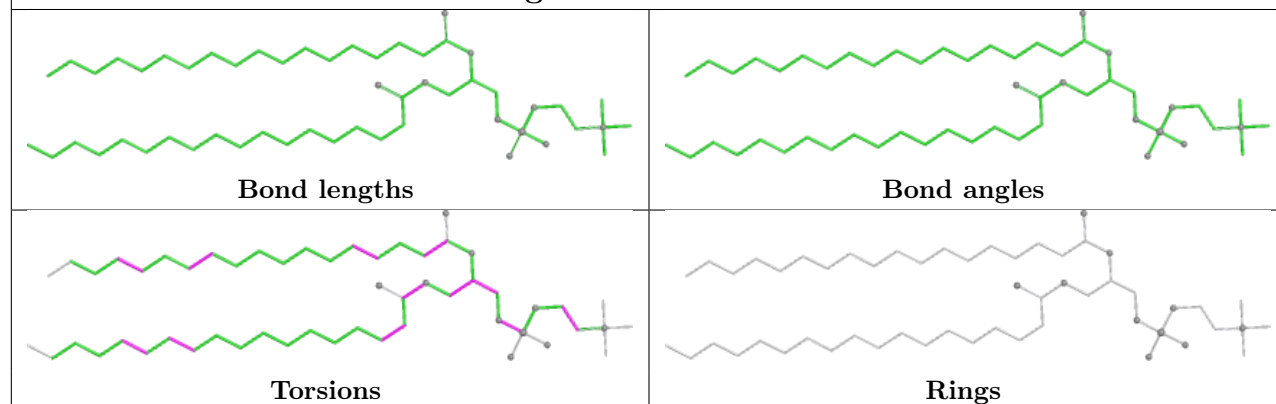


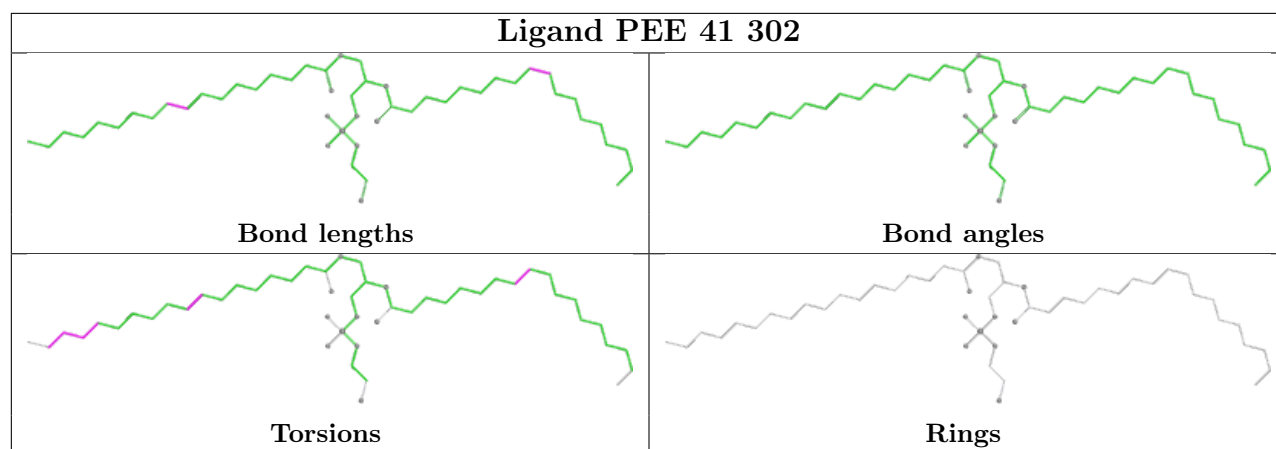
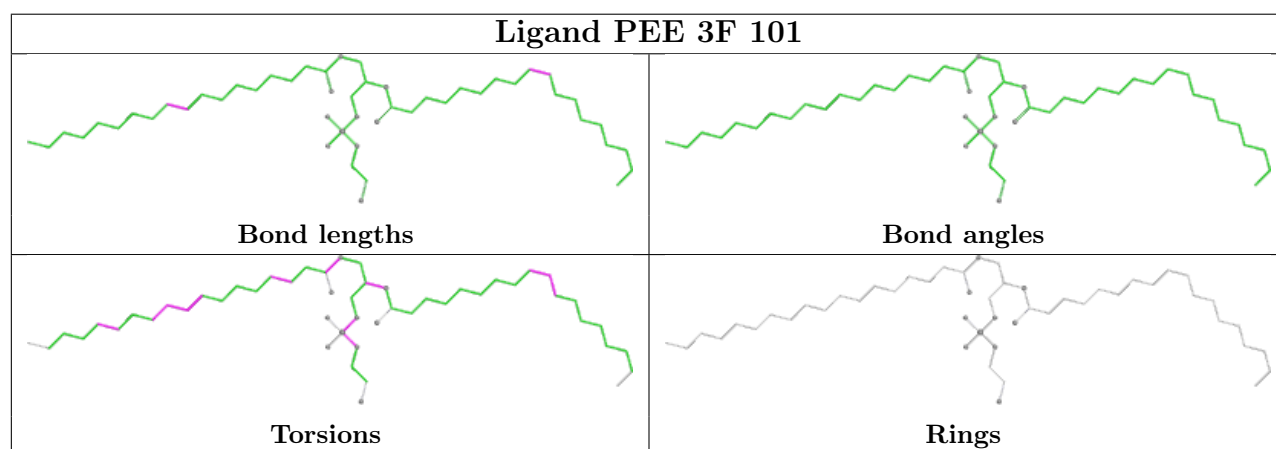
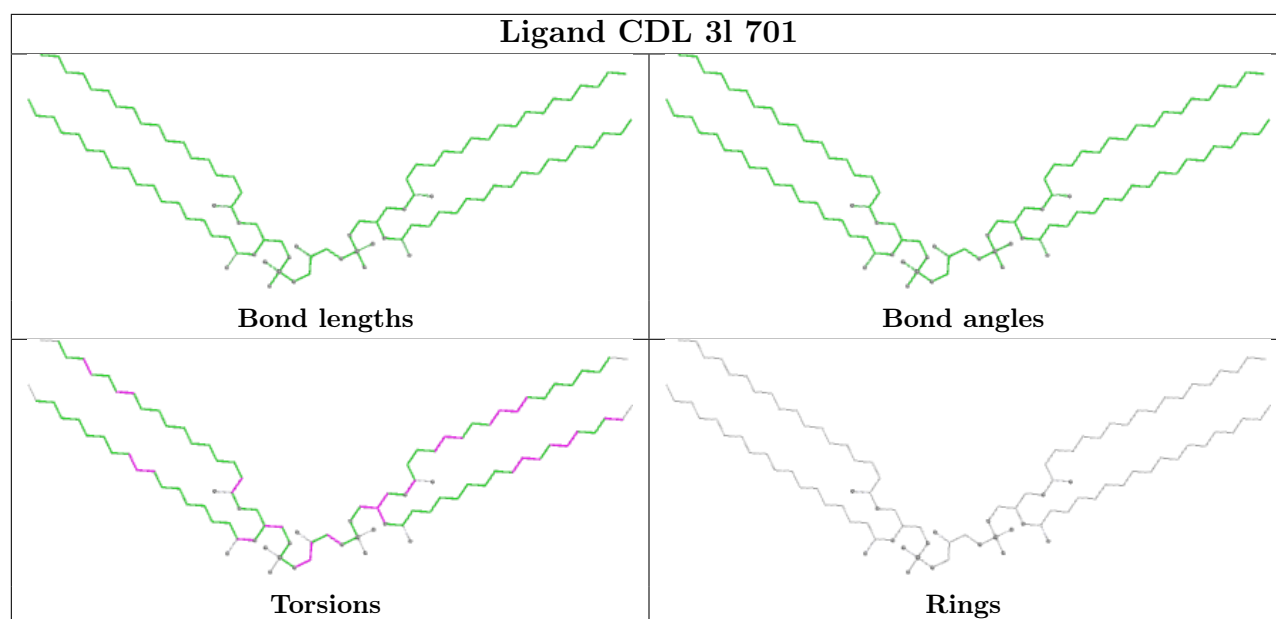


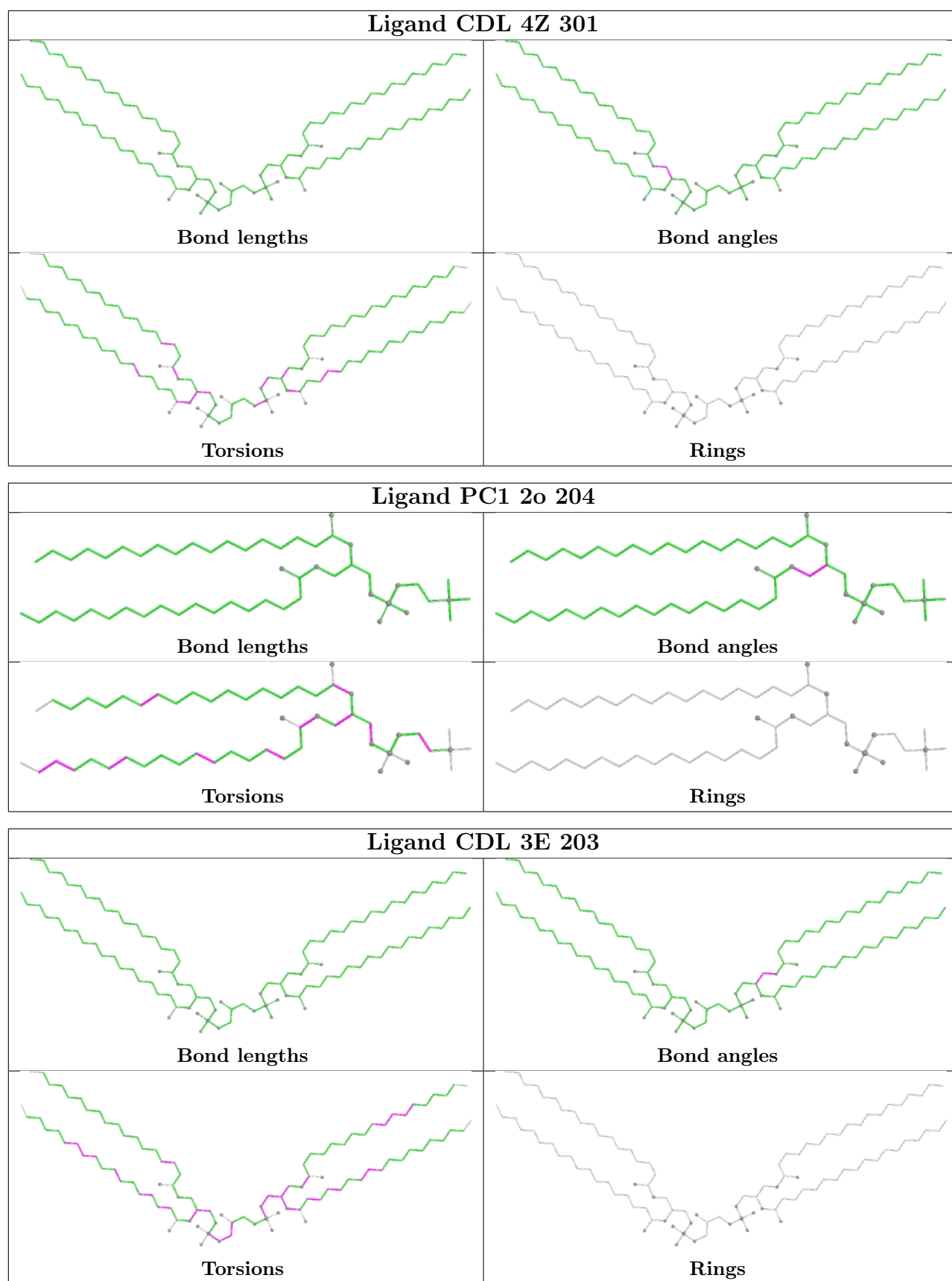
Ligand HEM 3g 401

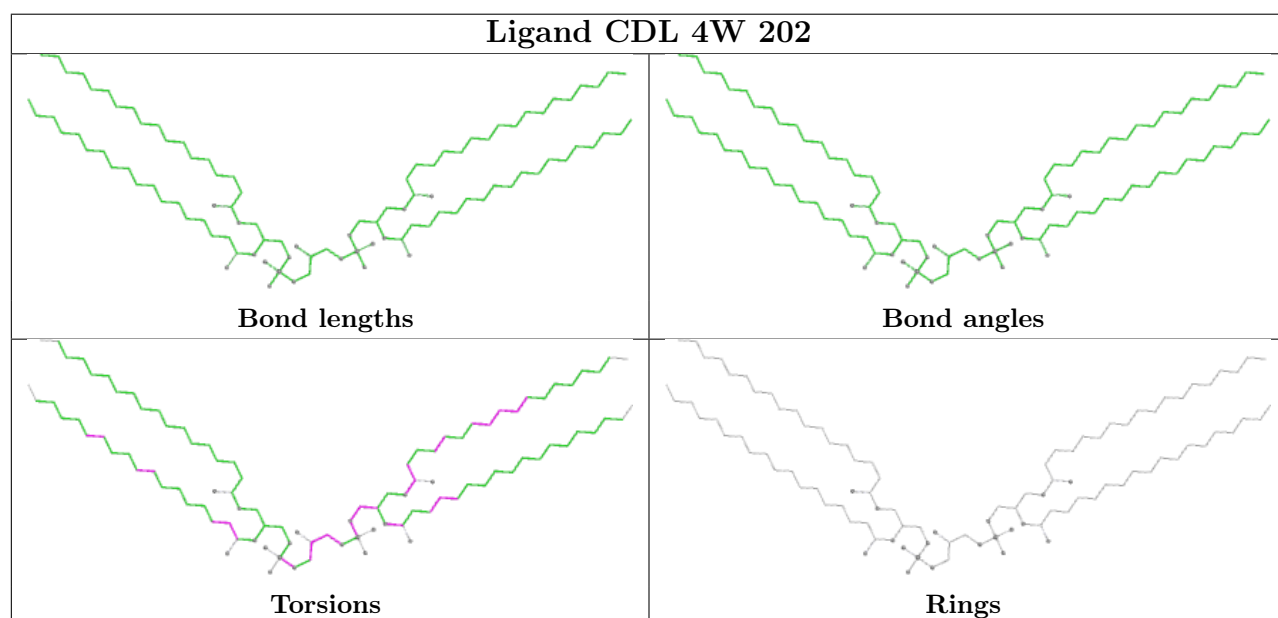
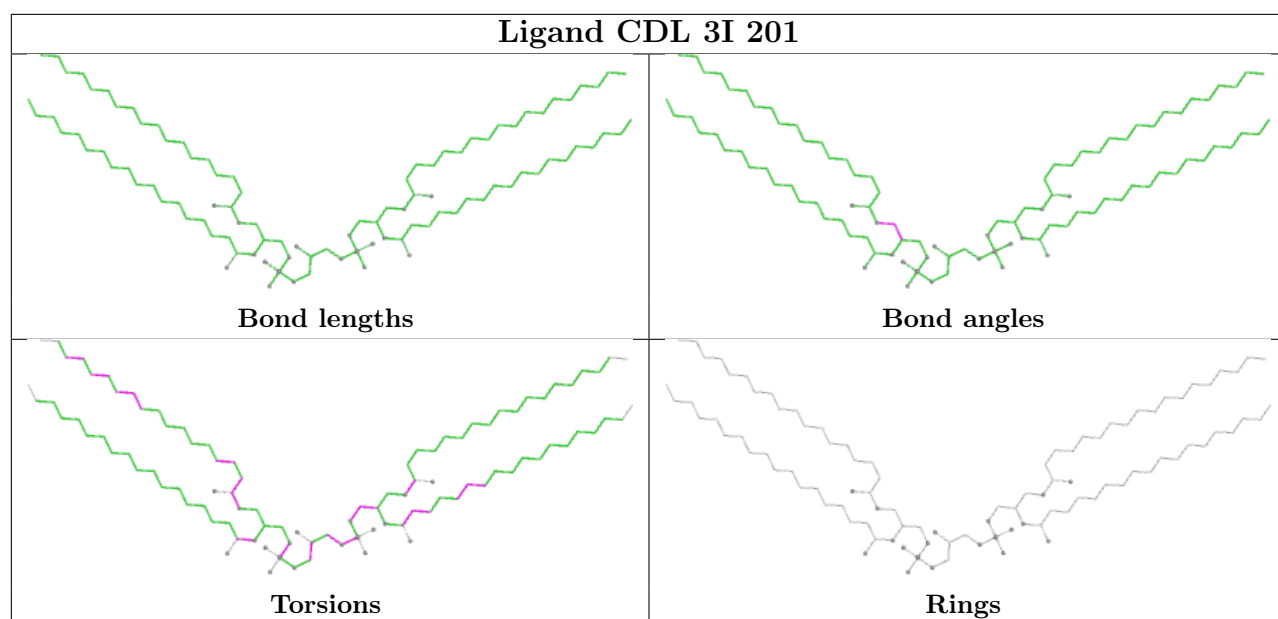


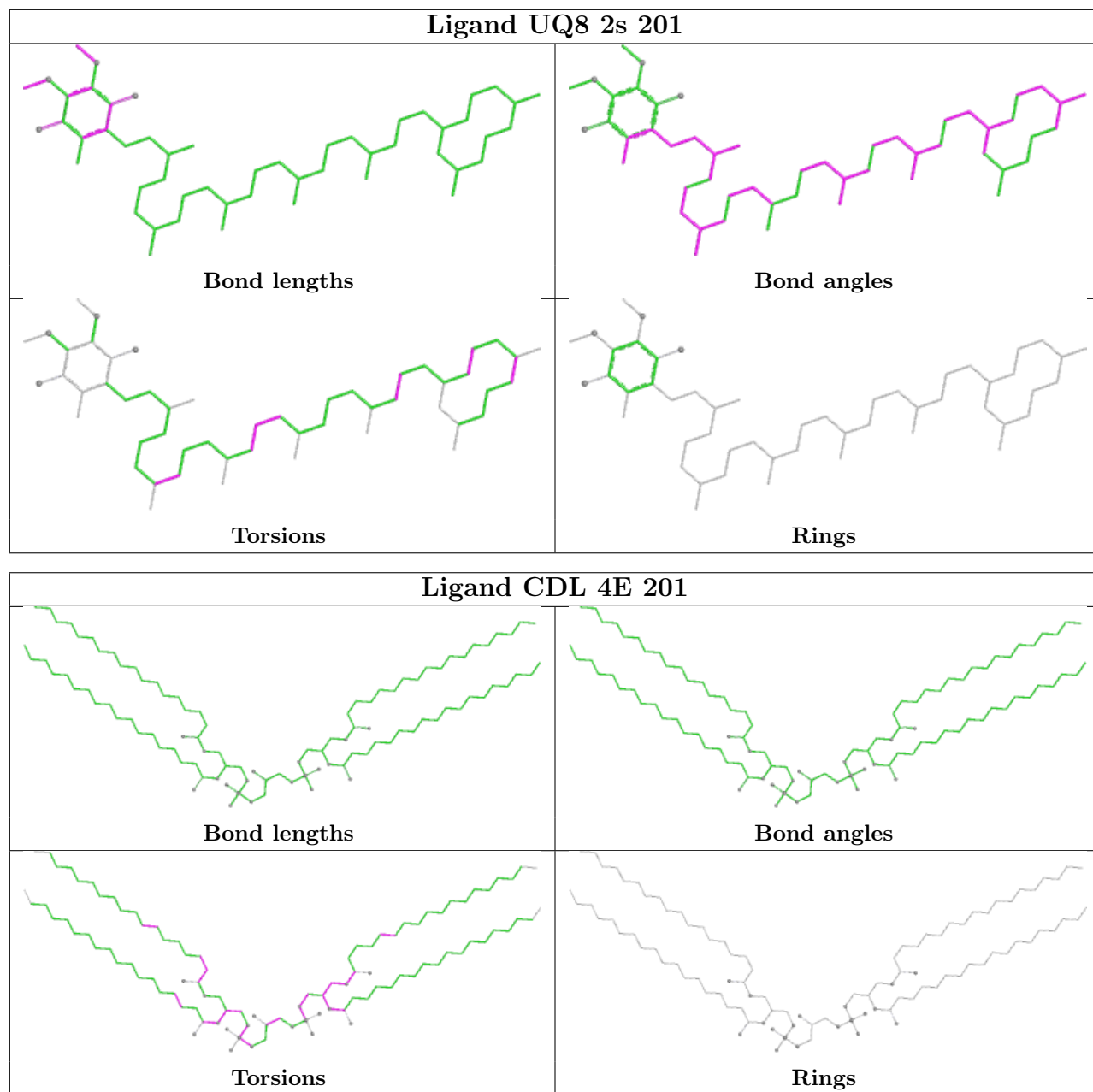
Ligand PC1 3H 403

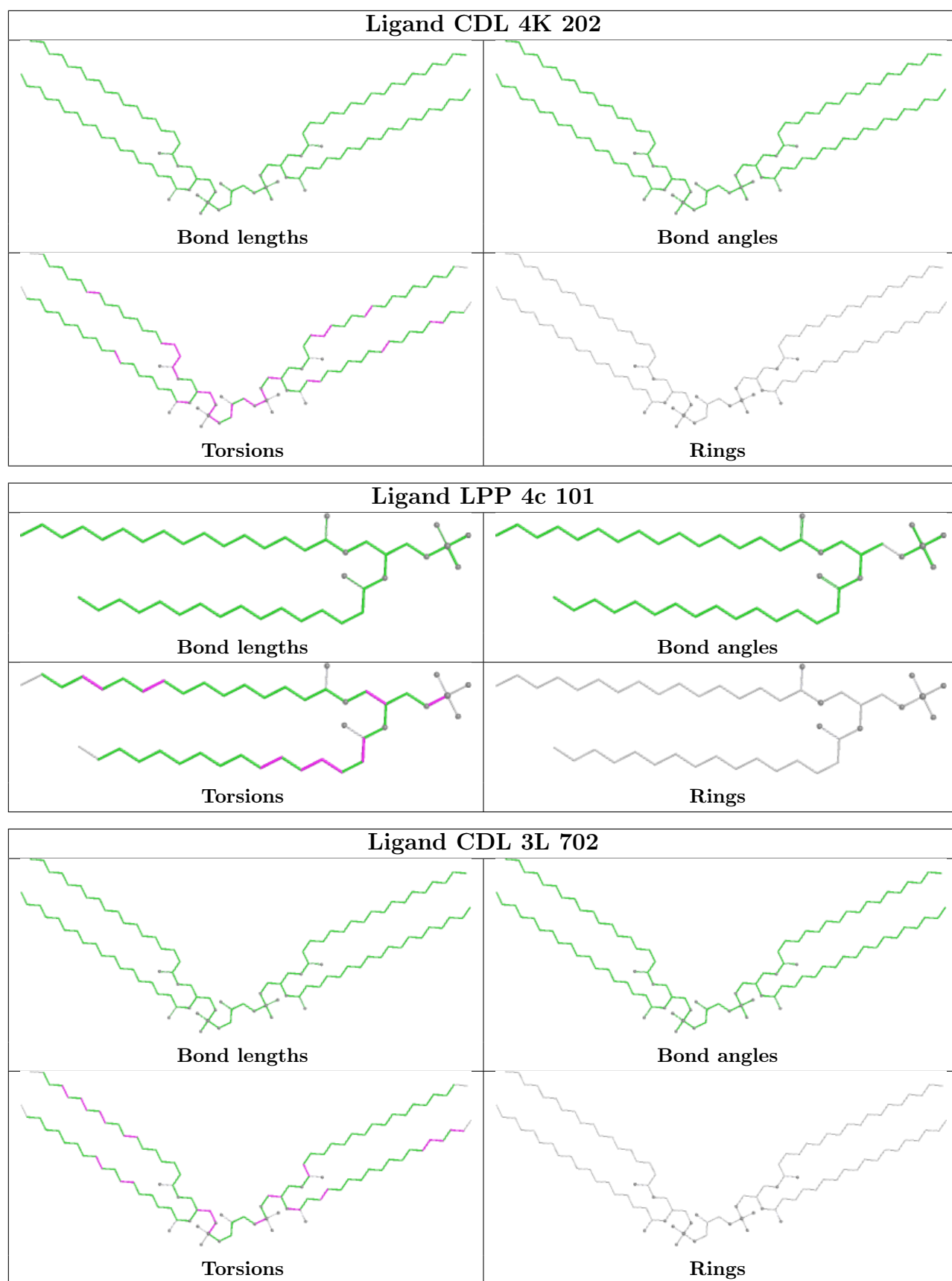


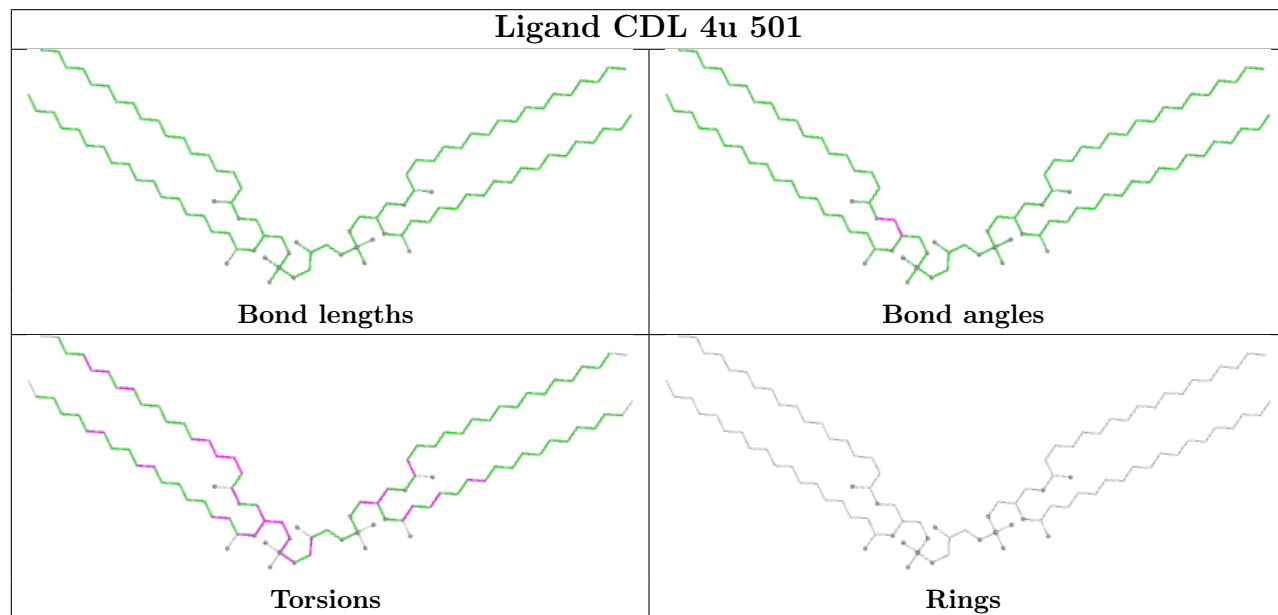
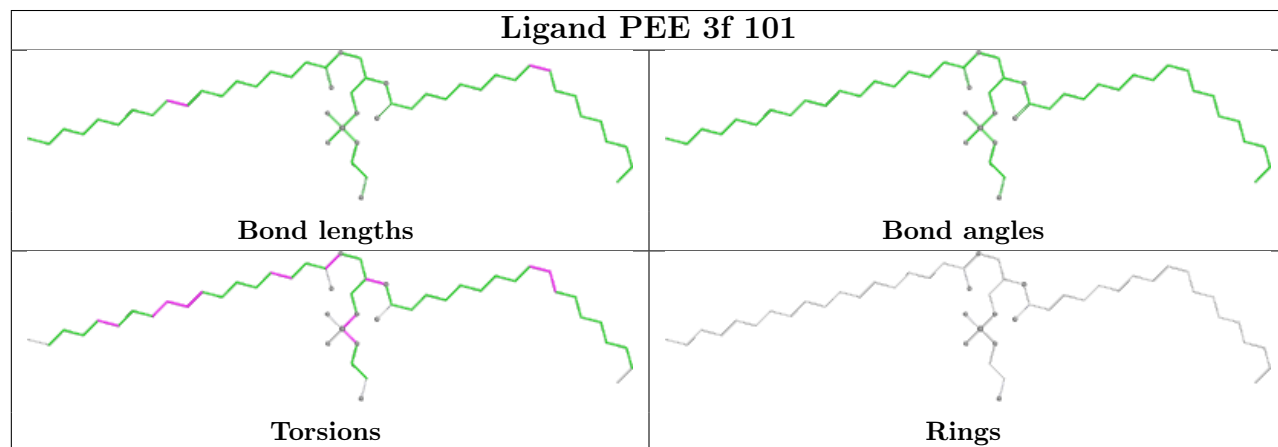
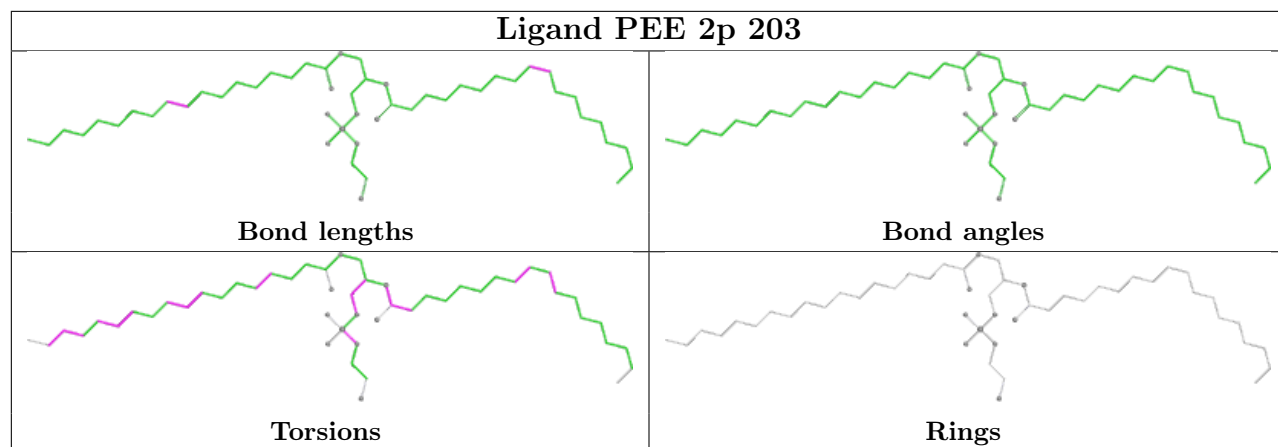


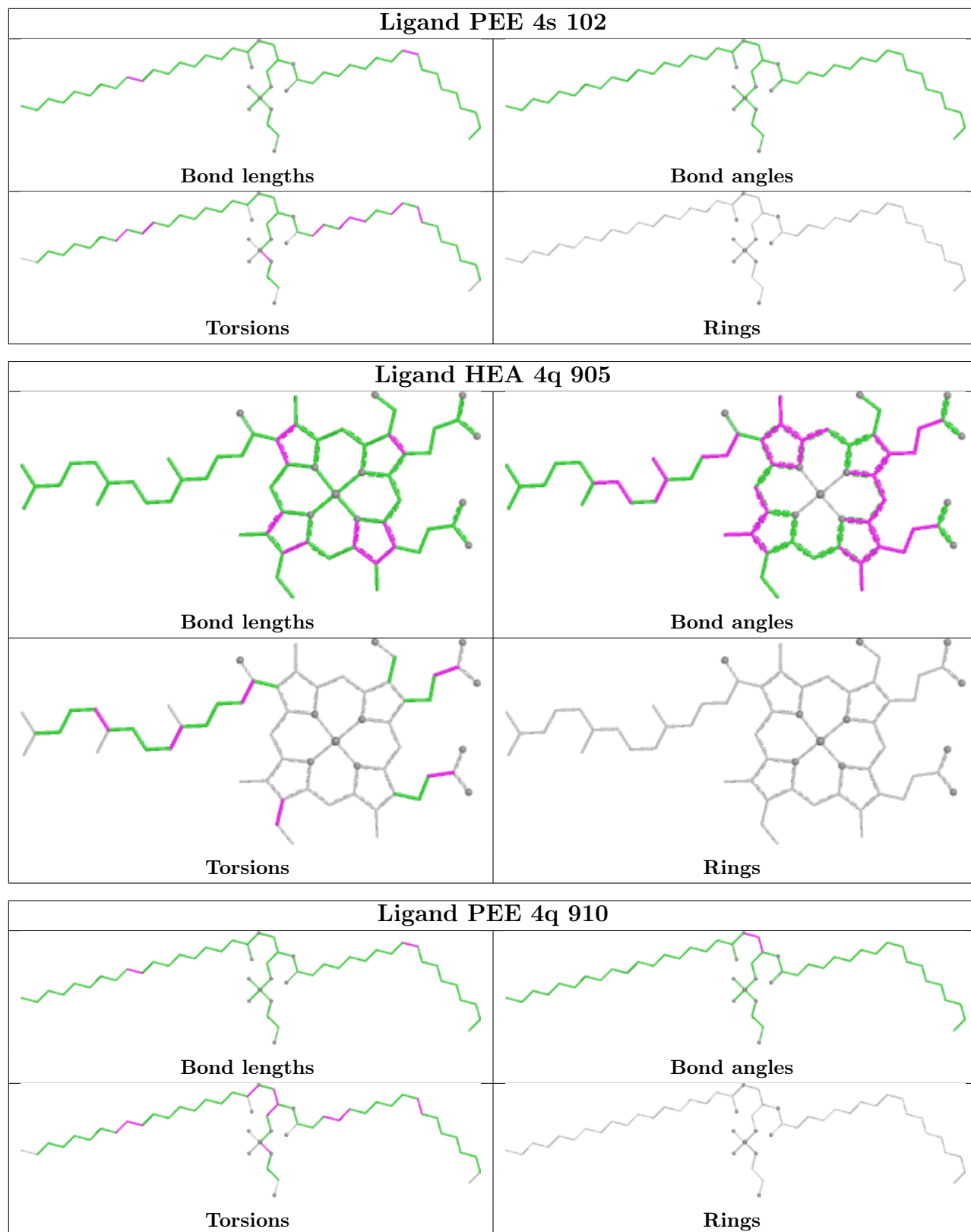


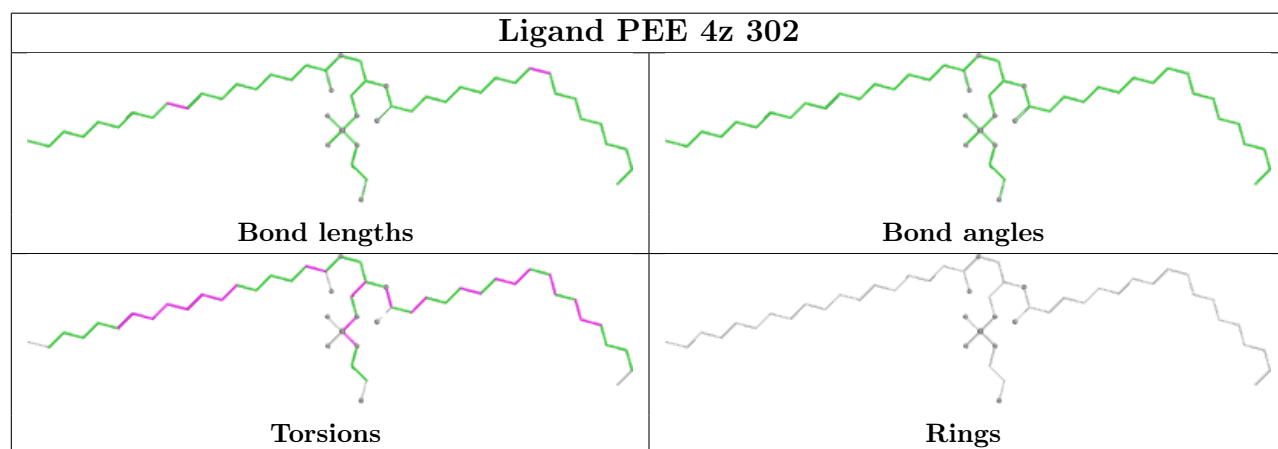
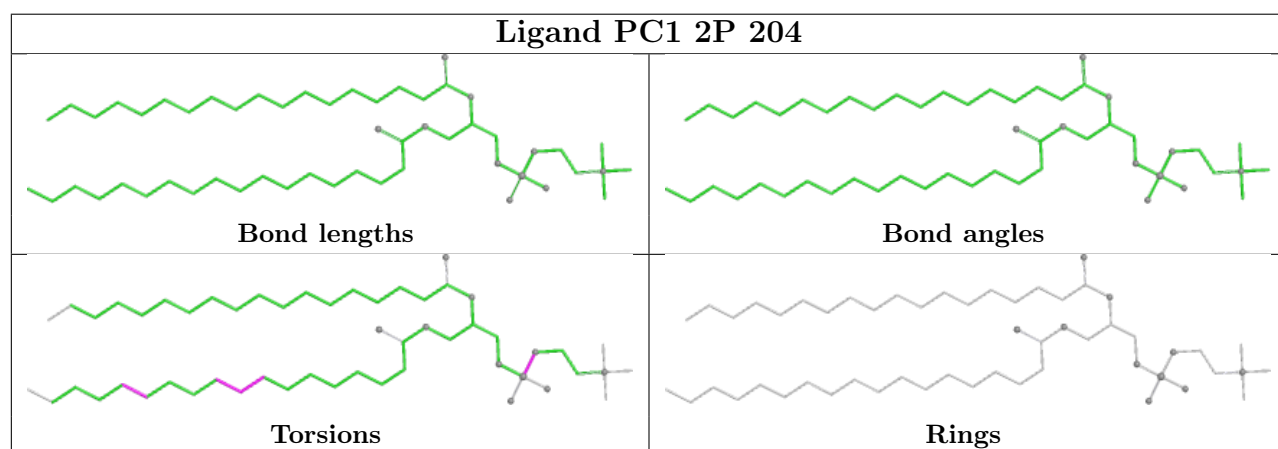
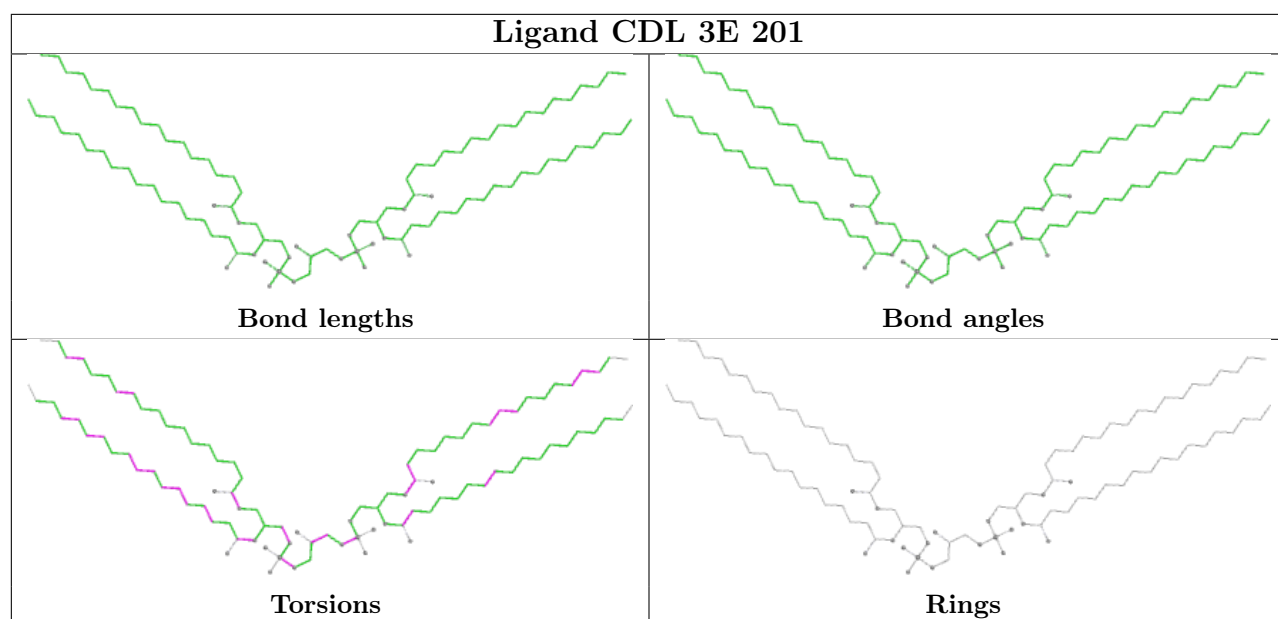


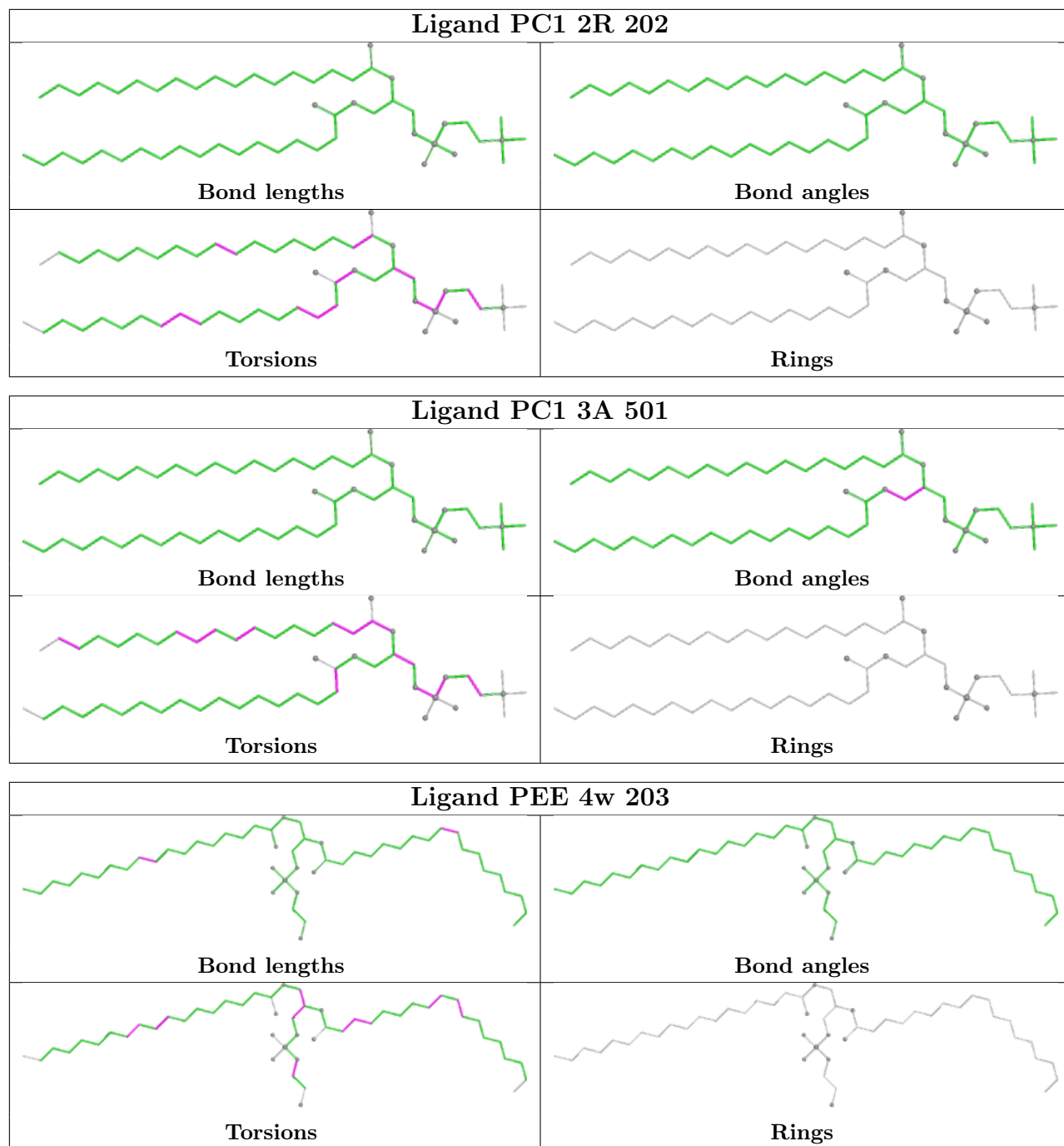


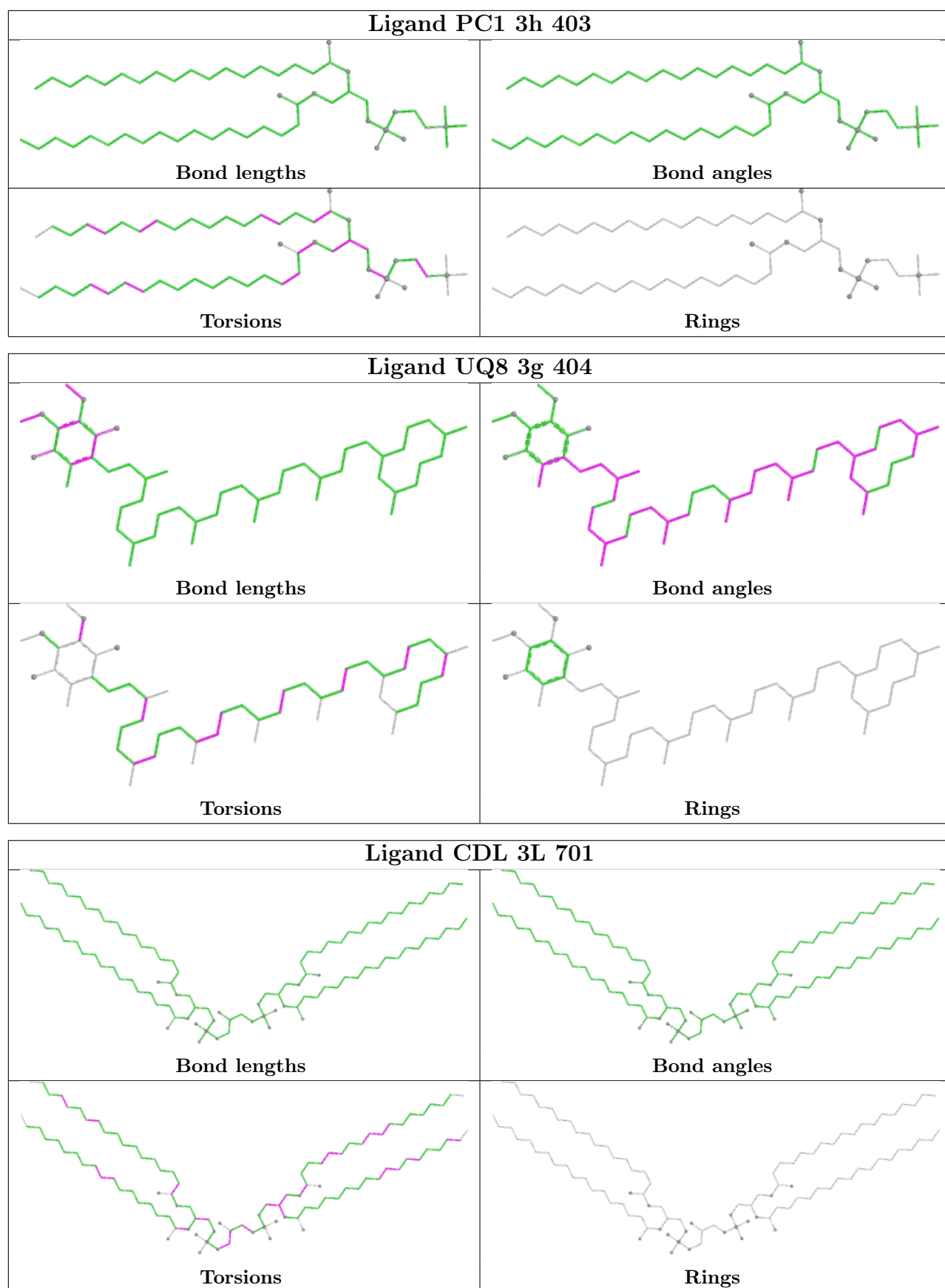












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

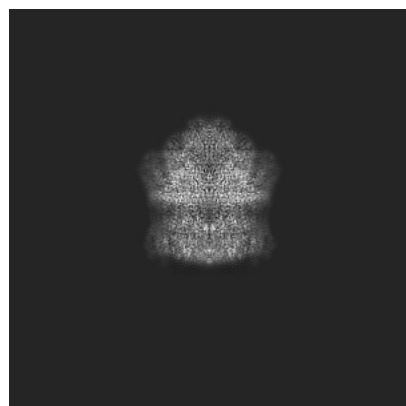
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50491. These allow visual inspection of the internal detail of the map and identification of artifacts.

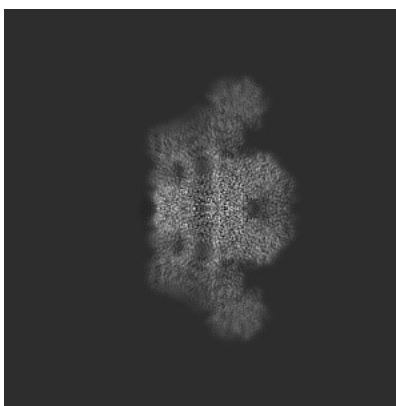
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

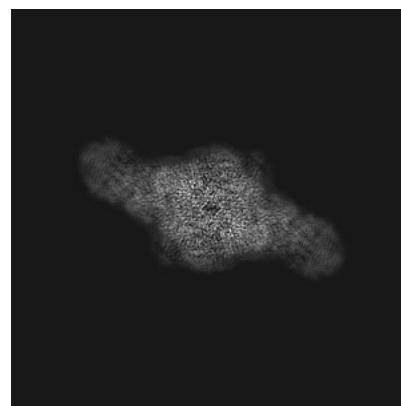
6.1.1 Primary map



X

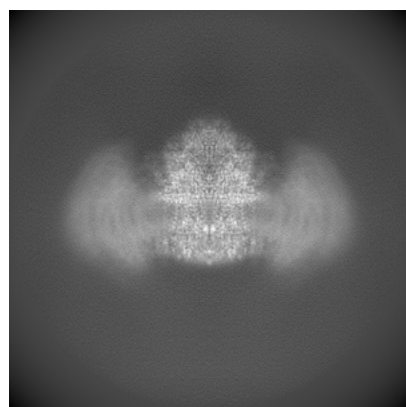


Y

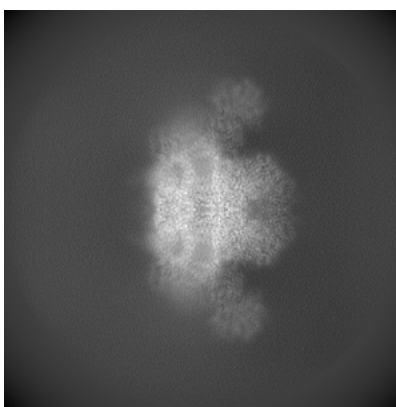


Z

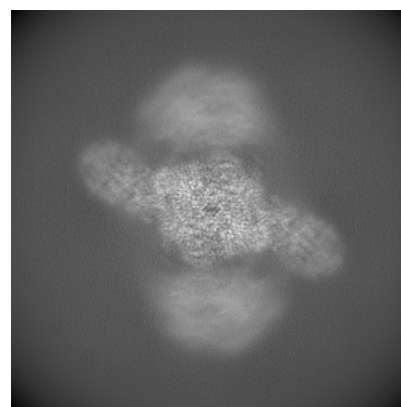
6.1.2 Raw map



X



Y



Z

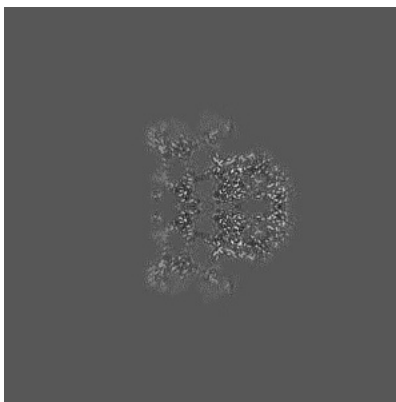
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

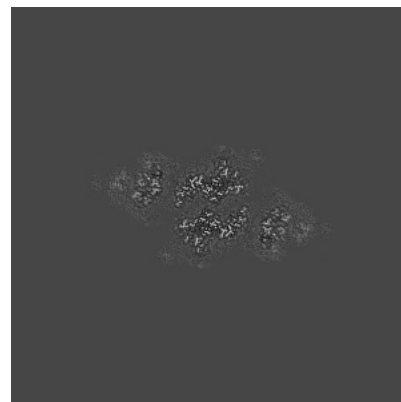
6.2.1 Primary map



X Index: 250

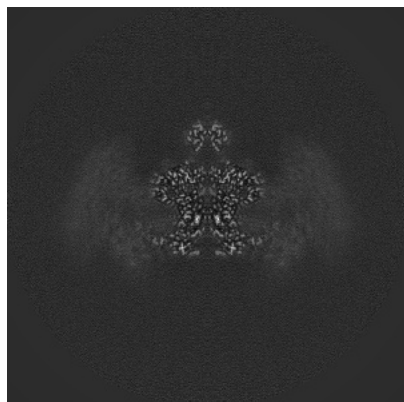


Y Index: 250

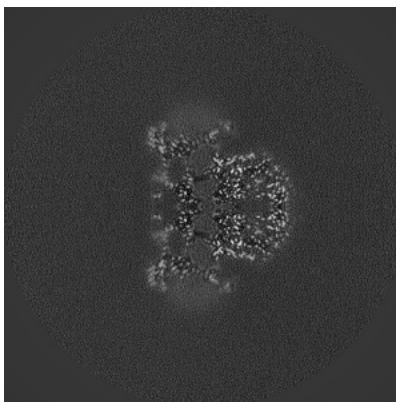


Z Index: 250

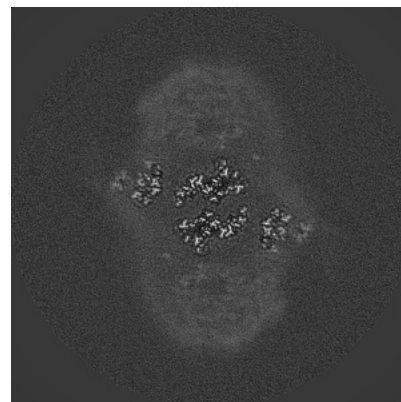
6.2.2 Raw map



X Index: 250



Y Index: 250

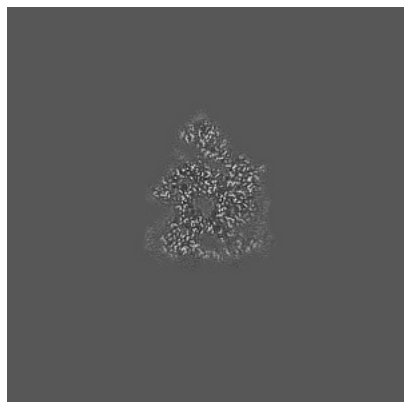


Z Index: 250

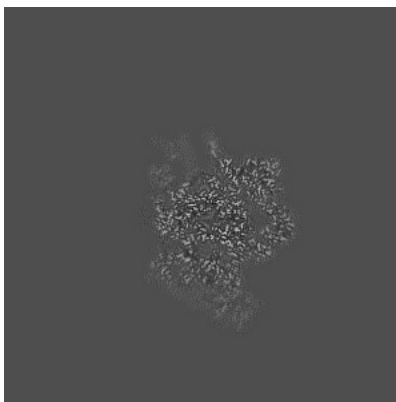
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

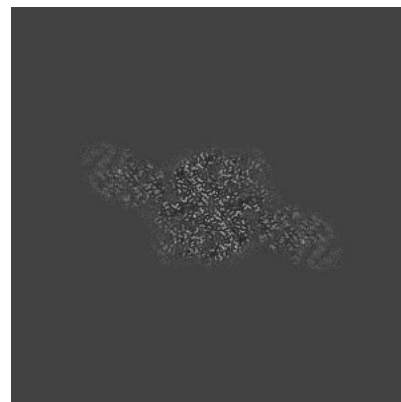
6.3.1 Primary map



X Index: 263

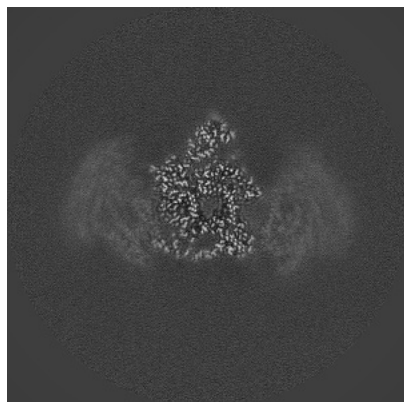


Y Index: 267

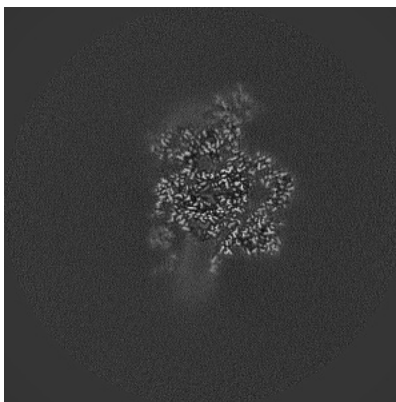


Z Index: 268

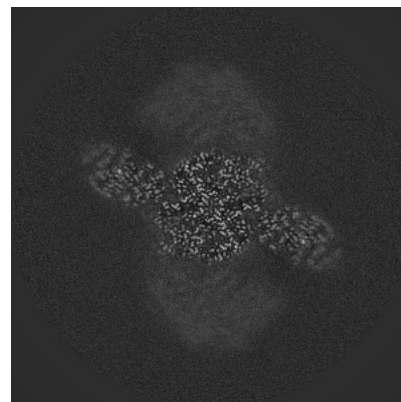
6.3.2 Raw map



X Index: 237



Y Index: 233

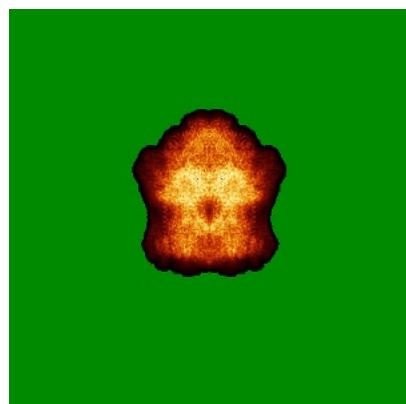


Z Index: 268

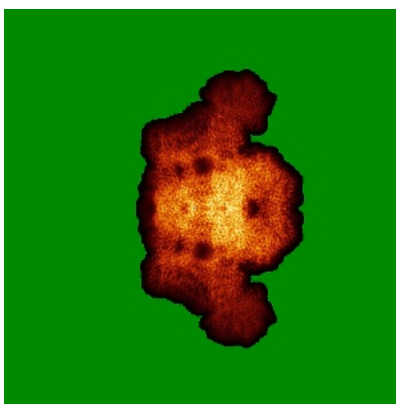
The images above show the largest variance slices of the map in three orthogonal directions.

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

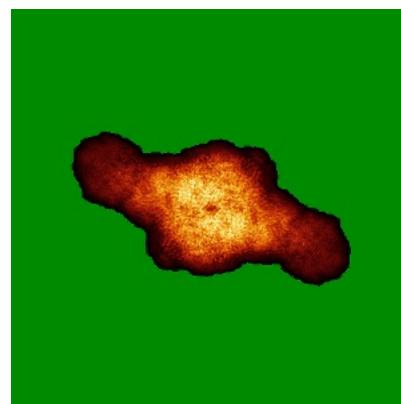
6.4.1 Primary map



X

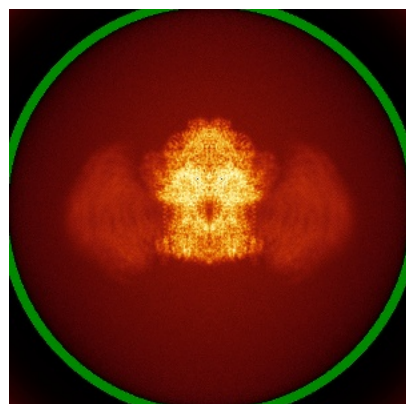


Y

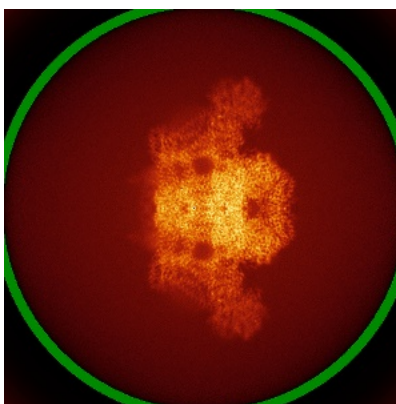


Z

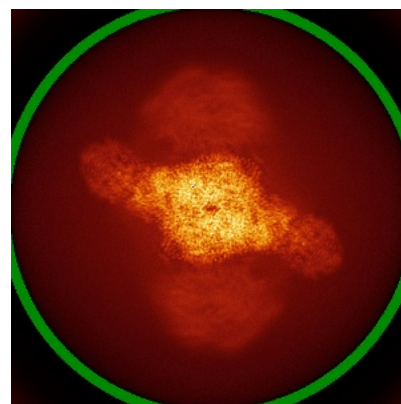
6.4.2 Raw map



X



Y

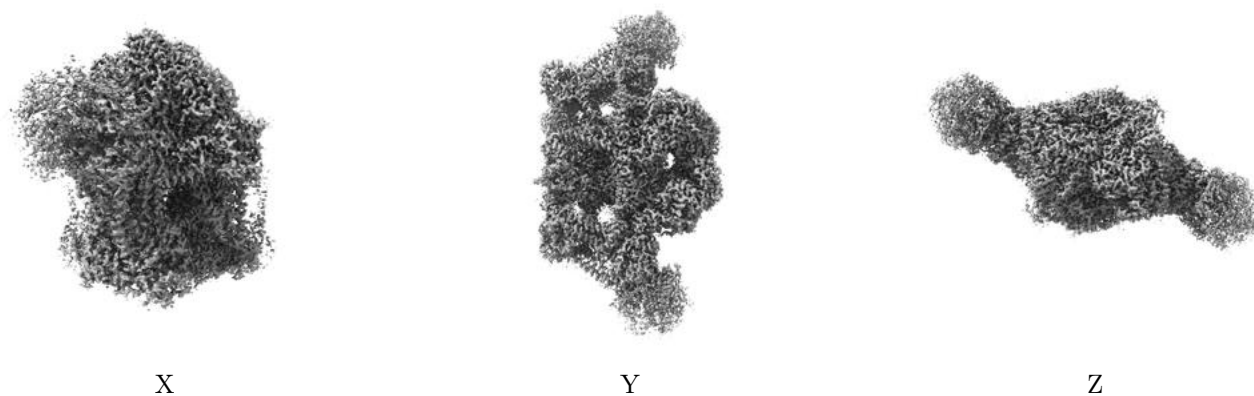


Z

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.

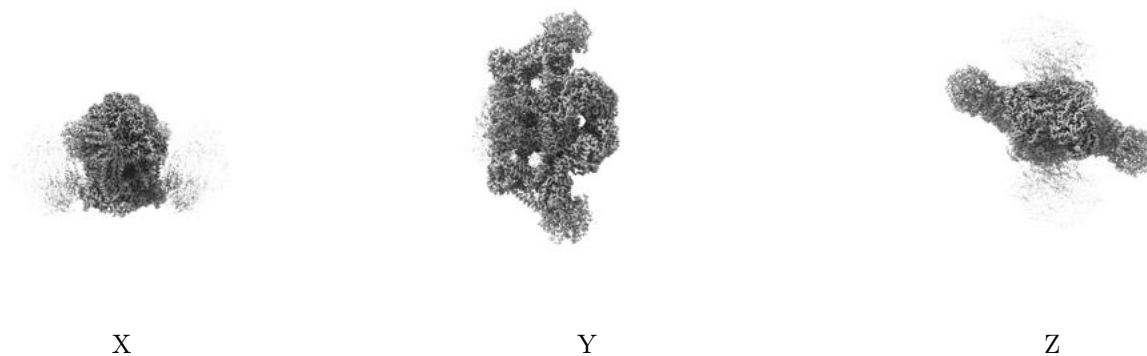
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

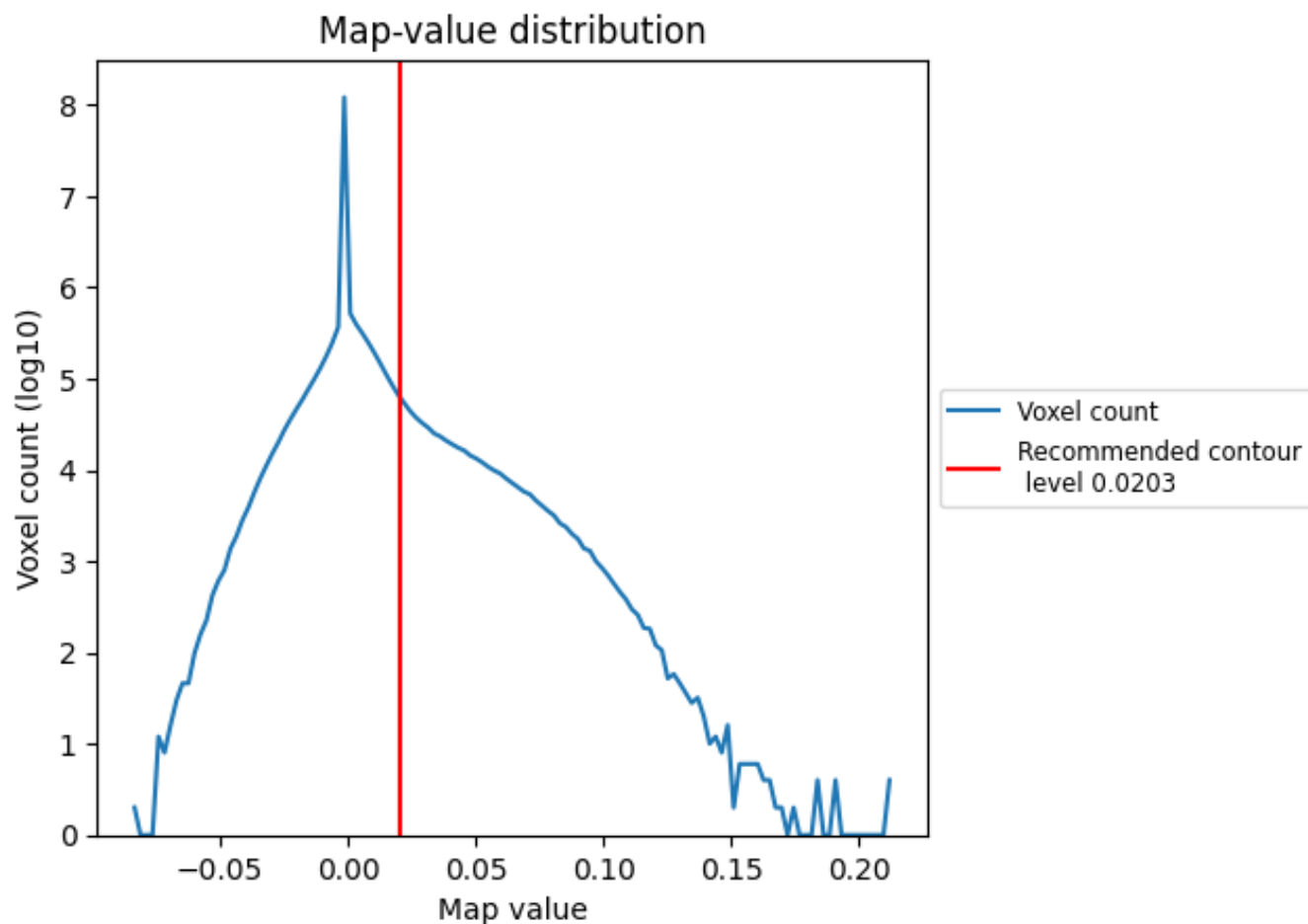
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

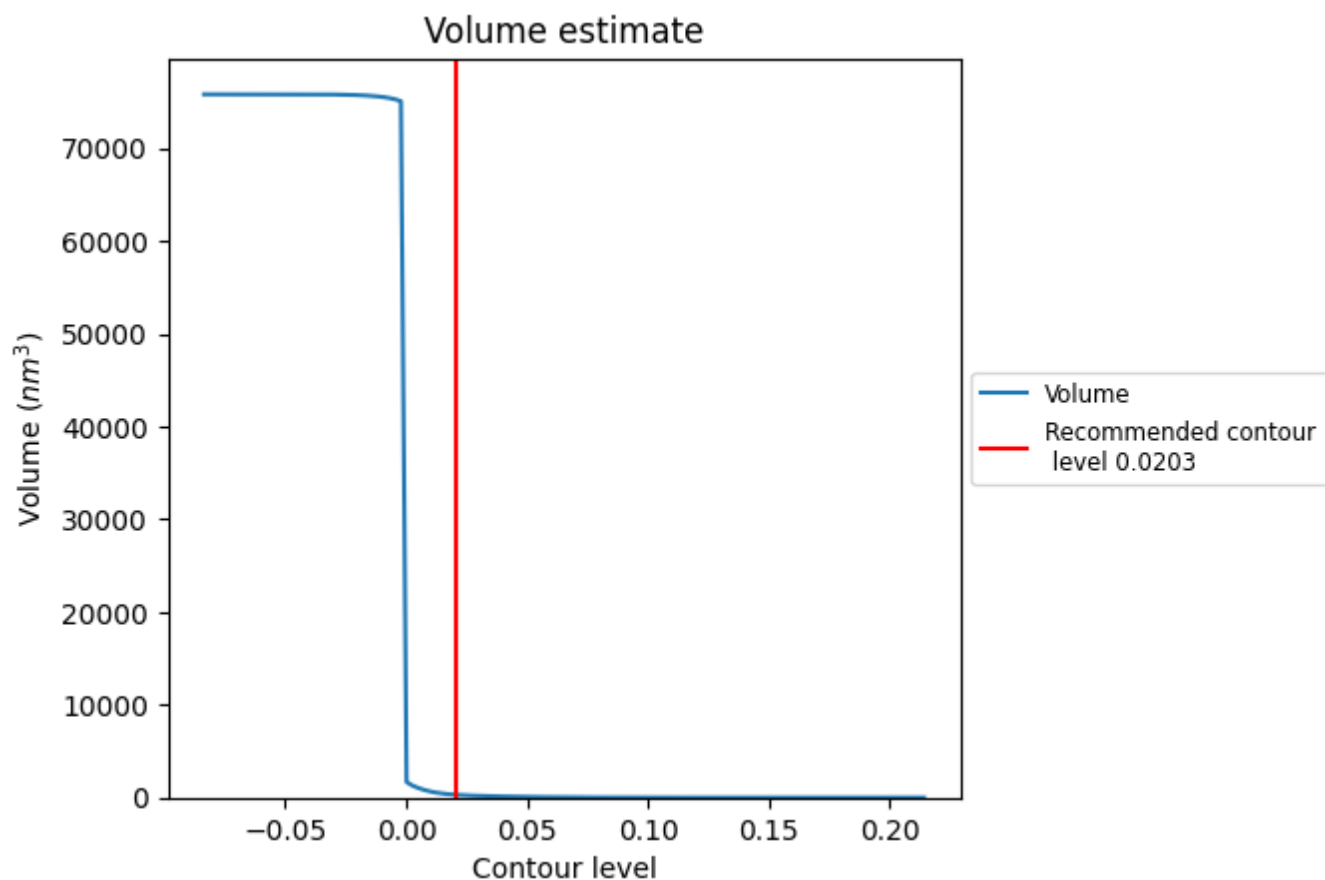
This section contains the results of statistical analysis of the map.

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.

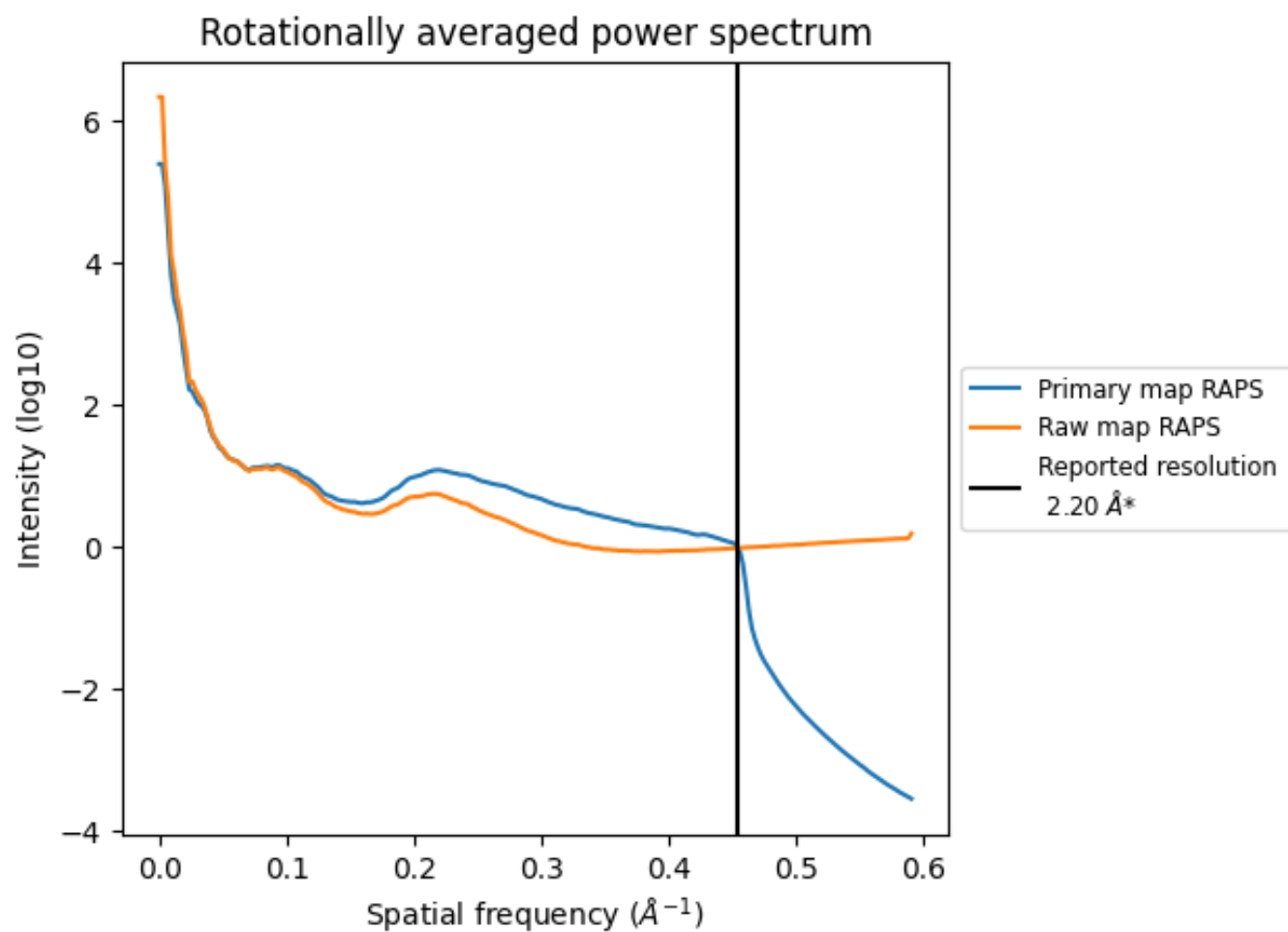
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm³; this corresponds to an approximate mass of 276 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 ⓘ

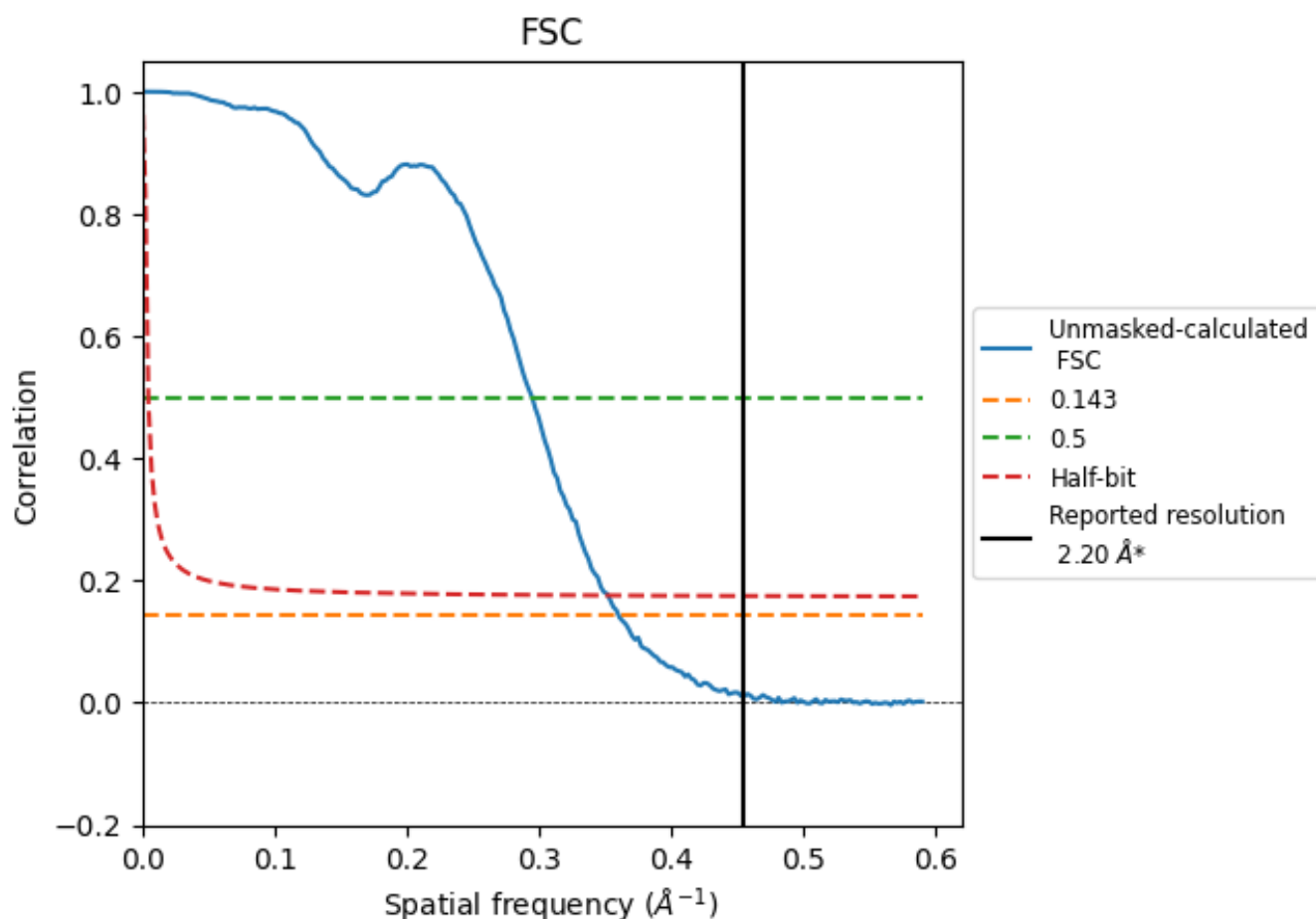


*Reported resolution corresponds to spatial frequency of 0.455 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.455 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

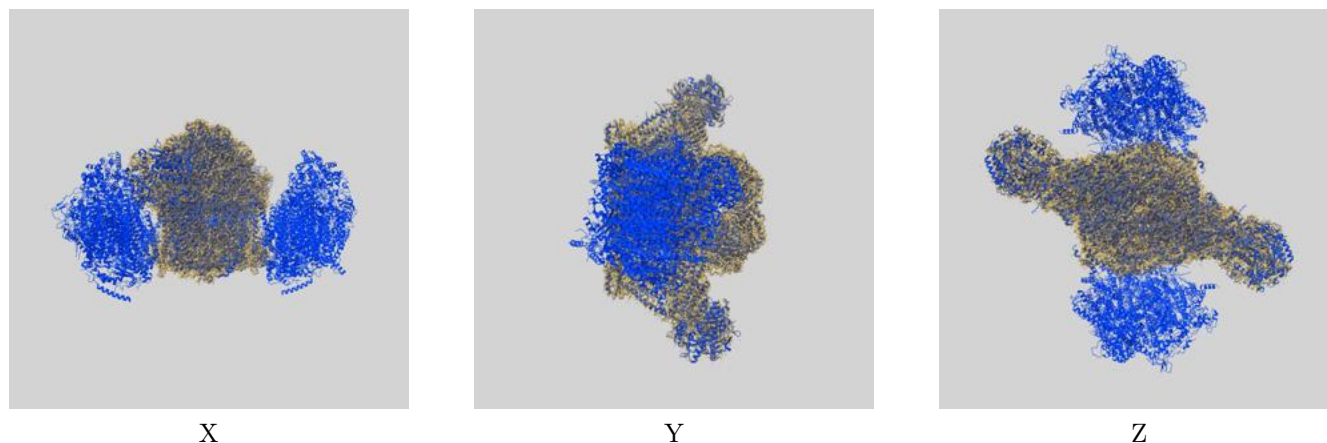
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.77	3.39	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.77 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

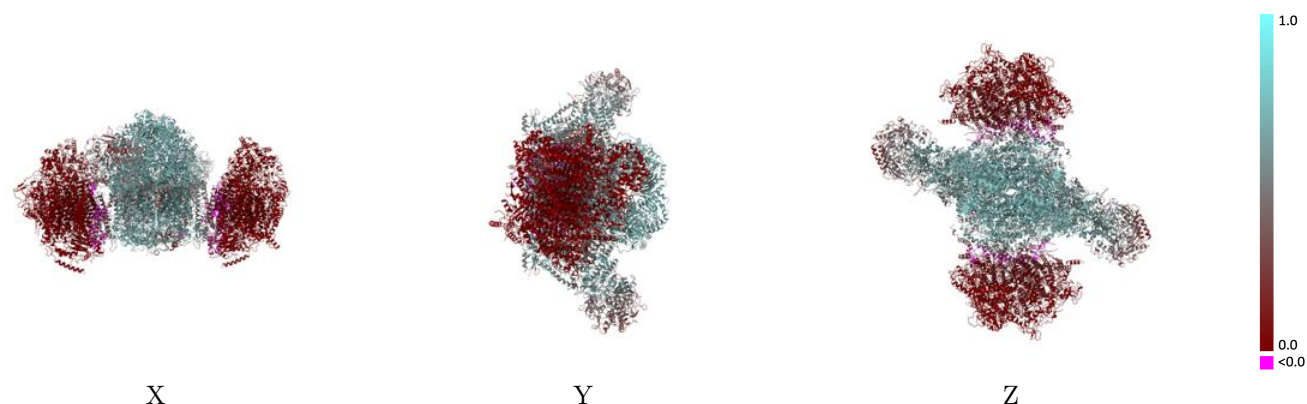
This section contains information regarding the fit between EMDB map EMD-50491 and PDB model 9FZL. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



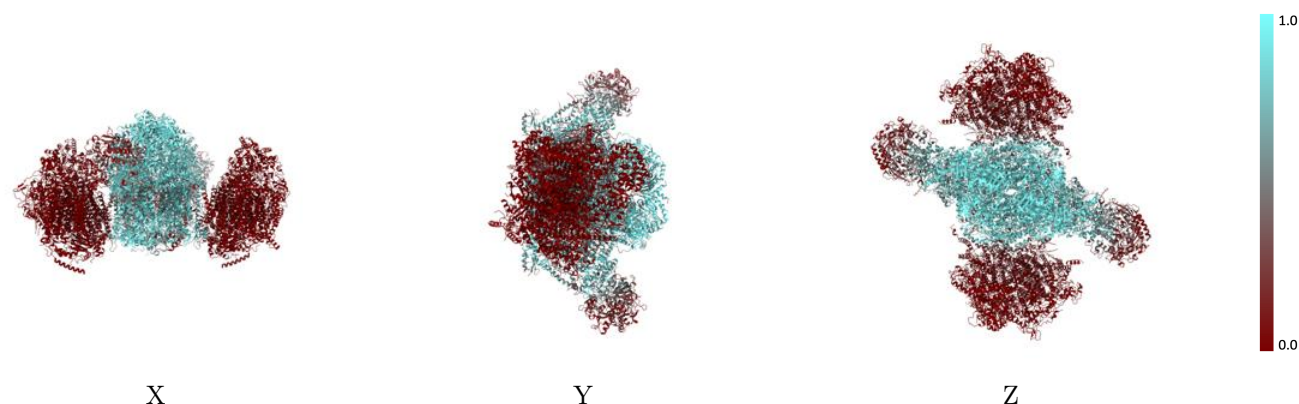
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



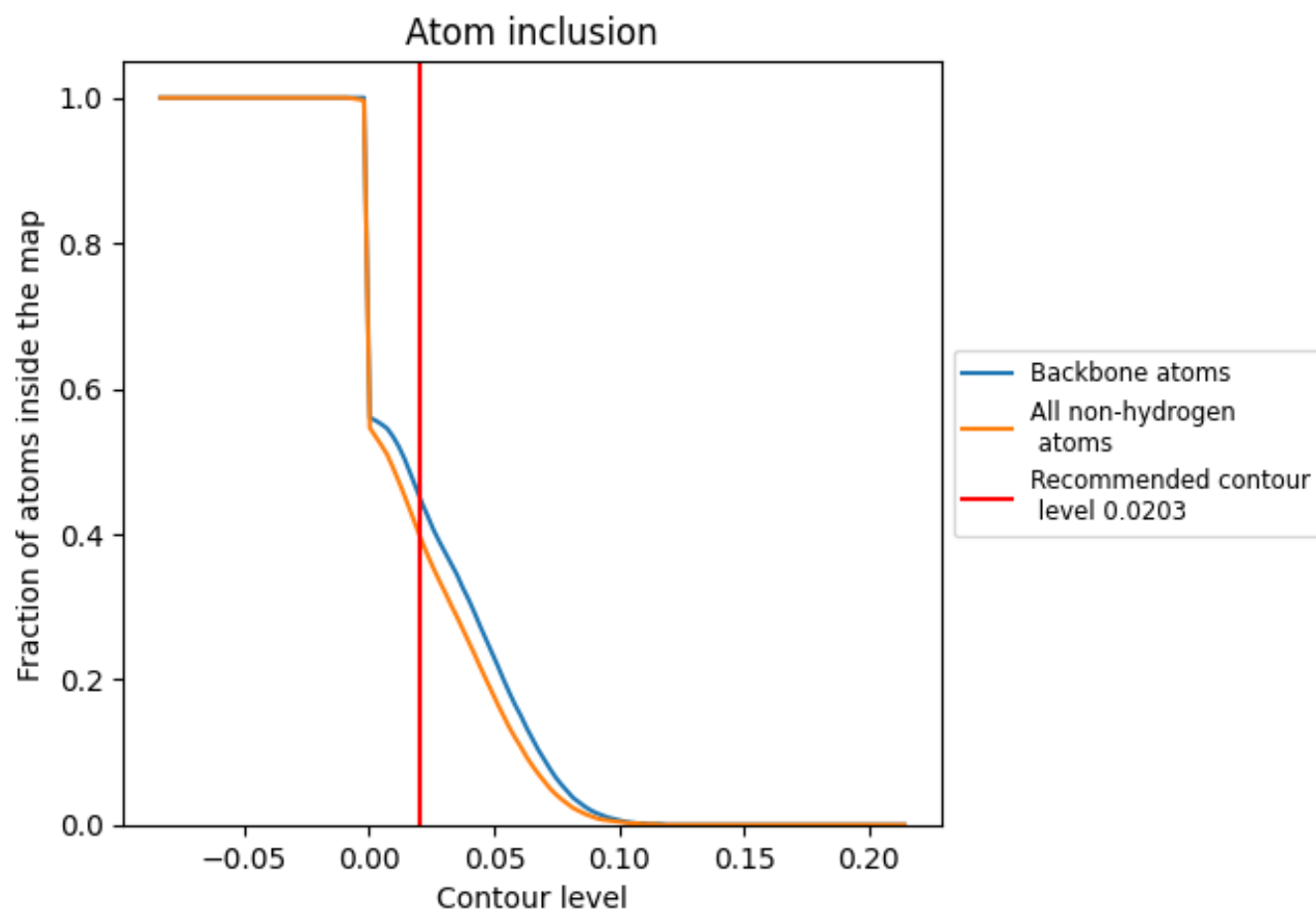
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 40% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3970	 0.3250
2M	 0.2660	 0.4070
2N	 0.6330	 0.5480
2O	 0.7970	 0.6040
2P	 0.7940	 0.5970
2Q	 0.7560	 0.5850
2R	 0.7950	 0.6090
2S	 0.8110	 0.6220
2T	 0.8780	 0.6560
2U	 0.5740	 0.5030
2V	 0.5780	 0.4910
2m	 0.2670	 0.4070
2n	 0.6360	 0.5480
2o	 0.7970	 0.6040
2p	 0.7940	 0.5950
2q	 0.7540	 0.5860
2r	 0.7950	 0.6140
2s	 0.8090	 0.6250
2t	 0.8780	 0.6580
2u	 0.5700	 0.5020
2v	 0.5730	 0.4930
3A	 0.9080	 0.6830
3B	 0.9090	 0.6720
3C	 0.9180	 0.6900
3D	 0.7940	 0.6250
3E	 0.8240	 0.6350
3F	 0.9370	 0.6950
3G	 0.9190	 0.6920
3H	 0.6570	 0.5320
3I	 0.8470	 0.6510
3J	 0.7730	 0.5920
3K	 0.9210	 0.6950
3L	 0.6370	 0.5310
3a	 0.9070	 0.6850
3b	 0.9100	 0.6730



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Chain	Atom inclusion	Q-score
3c	 0.9180	 0.6880
3d	 0.7950	 0.6260
3e	 0.8250	 0.6350
3f	 0.9370	 0.6940
3g	 0.9190	 0.6920
3h	 0.6570	 0.5330
3i	 0.8480	 0.6520
3j	 0.7750	 0.5900
3k	 0.9210	 0.6930
3l	 0.6370	 0.5320
40	 0.0000	 0.0000
41	 0.0000	 -0.0000
4A	 0.0050	 0.0700
4B	 0.0530	 0.1050
4C	 0.0720	 0.2140
4D	 0.0270	 0.1230
4E	 0.0000	 0.0000
4F	 0.0140	 0.0510
4G	 0.0220	 0.0640
4H	 0.0000	 0.0000
4I	 0.0000	 0.0000
4J	 0.0000	 0.0000
4K	 0.0000	 0.0000
4L	 0.0000	 0.0000
4M	 0.0000	 0.0000
4N	 0.0000	 0.0140
4O	 0.0000	 0.0000
4P	 0.0000	 0.0050
4Q	 0.0000	 0.0000
4R	 0.0000	 0.0000
4S	 0.0000	 0.0000
4T	 0.0000	 0.0000
4U	 0.0000	 0.0000
4V	 0.0000	 0.0000
4W	 0.0000	 -0.0030
4X	 0.0000	 0.0000
4Y	 0.0000	 0.0000
4Z	 0.0110	 0.0760
4a	 0.0050	 0.0750
4b	 0.0520	 0.1020
4c	 0.0690	 0.2070
4d	 0.0280	 0.1150

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Chain	Atom inclusion	Q-score
4e	 0.0000	 0.0000
4f	 0.0140	 0.0520
4g	 0.0230	 0.0700
4h	 0.0000	 0.0000
4i	 0.0000	 0.0000
4j	 0.0000	 0.0000
4k	 0.0000	 0.0000
4l	 0.0000	 0.0000
4m	 0.0000	 0.0000
4n	 0.0000	 0.0130
4o	 0.0000	 0.0000
4p	 0.0000	 0.0030
4q	 0.0000	 -0.0000
4r	 0.0000	 0.0000
4s	 0.0000	 0.0000
4t	 0.0000	 0.0000
4u	 0.0000	 0.0000
4v	 0.0000	 0.0000
4w	 0.0000	 -0.0040
4x	 0.0000	 0.0000
4y	 0.0000	 0.0000
4z	 0.0100	 0.0760