Full wwPDB EM Validation Report

Aug 25, 2026 – 07:34 am BST

PDB ID	:	9FQ7 / pdb_00009fq7
EMDB ID	:	EMD-50403
Title	:	Perkinsus marinus Respiratory supercomplex CII2CIII2CIV2 in c1 state
Authors	:	Wu, F.; Amunts, A.
Deposited on	:	2024-06-14
Resolution	:	2.50 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:

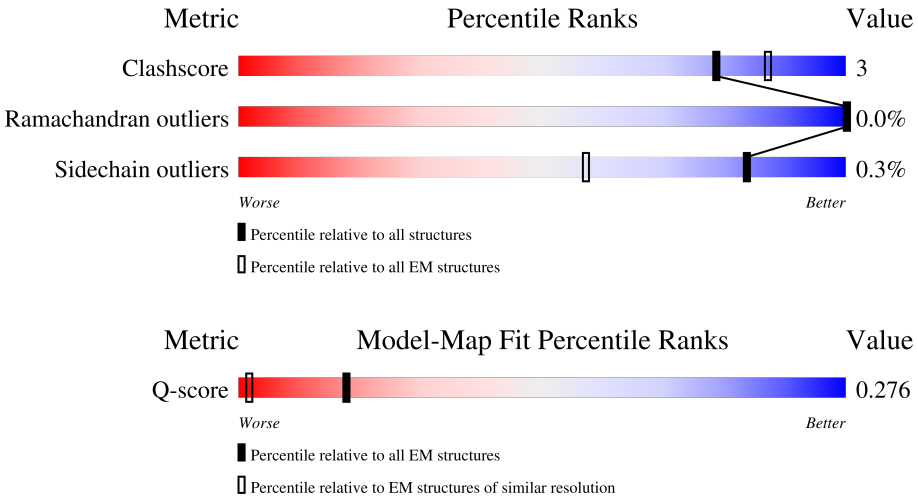
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

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 2.50 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	7115 (2.00 - 3.00)

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 <=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	94% 90% 9%
1	2m	604	93% 89% 10%
2	2N	259	62% 92% 8%
2	2n	259	61% 92% 8%

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Mol	Chain	Length	Quality of chain
3	2O	160	6% 96%
3	2o	160	8% 95% 5%
4	2P	158	11% 92% 7%
4	2p	158	9% 91% 9%
5	2Q	69	17% 96%
5	2q	69	19% 94% 6%
6	2R	117	13% 91% 9%
6	2r	117	15% 91% 9%
7	2S	164	23% 98%
7	2s	164	21% 98%
8	2T	82	10% 88% 9%
8	2t	82	6% 89% 7%
9	2U	48	46% 90% 10%
9	2u	48	46% 88% 12%
10	2V	86	58% 92% 8%
10	2v	86	53% 93% 7%
11	30	173	79% 91% 9%
12	31	159	81% 82% 15%
13	3A	454	96%
13	3a	454	5% 97%
14	3B	496	96%
14	3b	496	96%
15	3C	242	95% 5%
15	3c	242	90% 9%
16	3D	95	91% 9%

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Mol	Chain	Length	Quality of chain
16	3d	95	91% 8%
17	3E	92	93% 7%
17	3e	92	93% 7%
18	3F	84	89% 11%
18	3f	84	89% 11%
19	3G	354	91% 9%
19	3g	354	87% 13%
20	3H	326	13% 91% 9%
20	3h	326	8% 91% 9%
21	3I	176	90% 10%
21	3i	176	91% 9%
22	3J	92	20% 89% 10%
22	3j	92	20% 88% 11%
23	3K	79	95% 5%
23	3k	79	95% 5%
24	3L	68	31% 84% 16%
24	3l	68	29% 87% 13%
25	40	230	100% 94% 6%
25	41	230	100% 94% 6%
26	4A	100	99% 93% 6%
26	4a	100	100% 93% 6%
27	4B	93	99% 96%
27	4b	93	99% 96%
28	4C	75	93% 91% 9%
28	4c	75	97% 92% 8%

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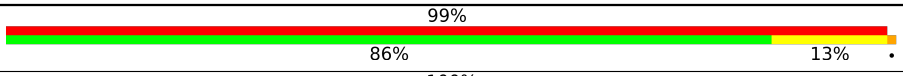
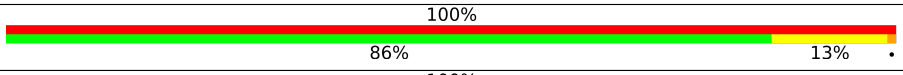
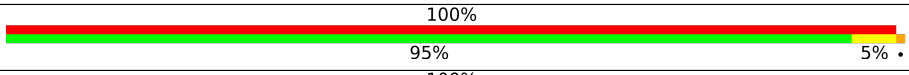
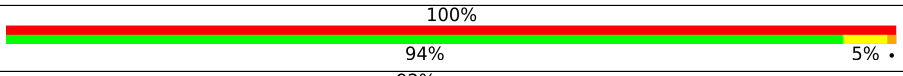
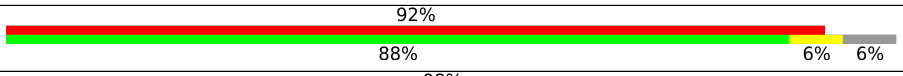
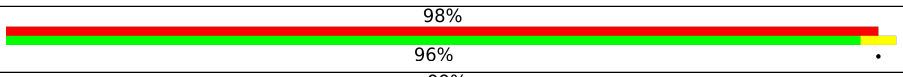
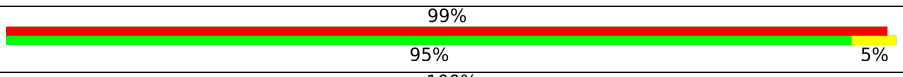
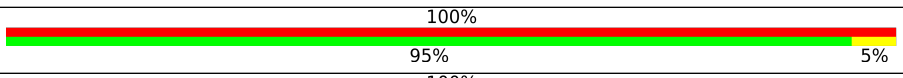
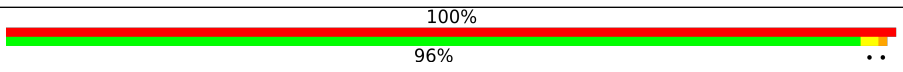
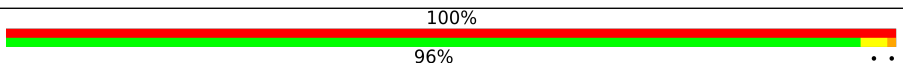
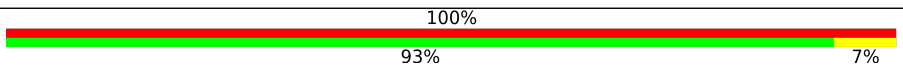
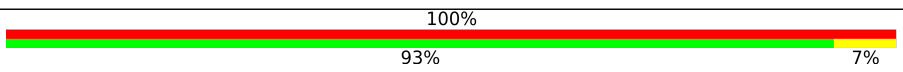
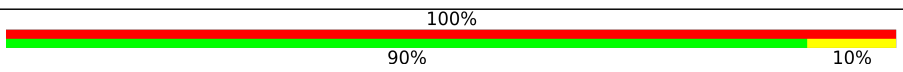
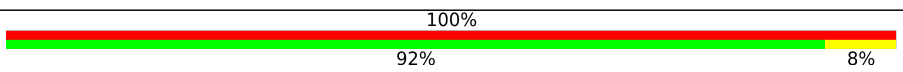
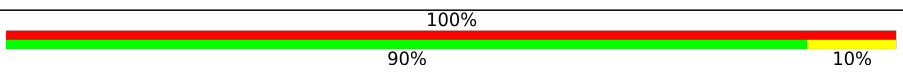
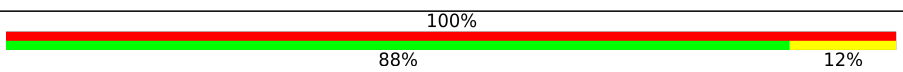
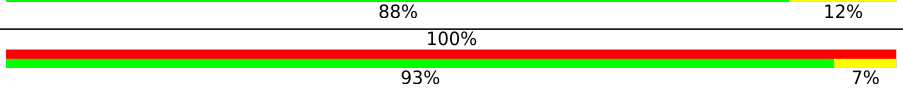
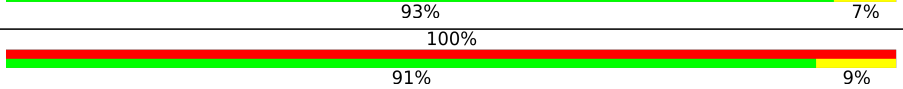
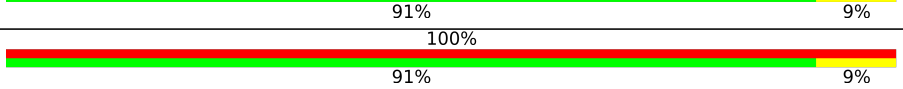
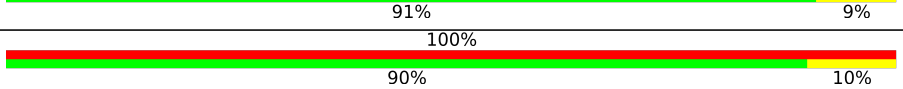
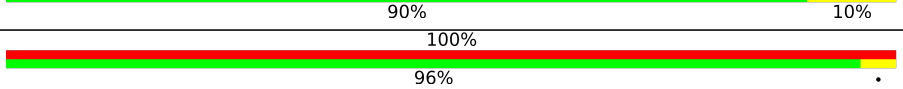
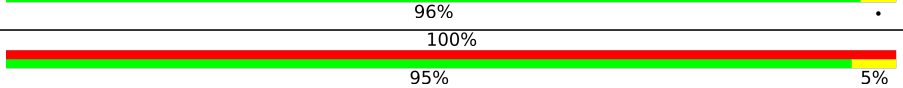
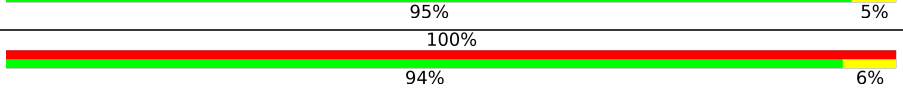
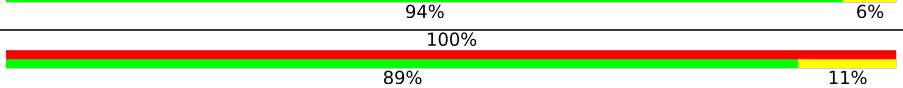
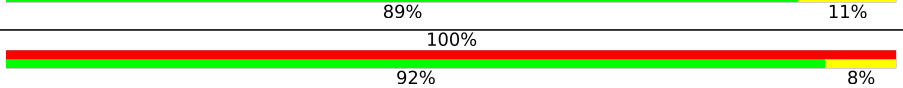
Mol	Chain	Length	Quality of chain
29	4D	90	
29	4d	90	
30	4E	152	
30	4e	152	
31	4F	85	
31	4f	85	
32	4G	100	
32	4g	100	
33	4H	141	
33	4h	141	
34	4I	196	
34	4i	196	
35	4J	186	
35	4j	186	
36	4K	93	
36	4k	93	
37	4L	122	
37	4l	122	
38	4M	99	
38	4m	99	
39	4N	131	
39	4n	131	
40	4O	47	
40	4o	47	
41	4P	180	

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Mol	Chain	Length	Quality of chain
41	4p	180	100% 92% 8%
42	4Q	459	100% 89% 11%
42	4q	459	100% 90% 10%
43	4R	103	100% 98%
43	4r	103	100% 94% 6%
44	4S	65	100% 95% 5%
44	4s	65	100% 95% 5%
45	4T	121	100% 97%
45	4t	121	100% 95% 5%
46	4U	91	100% 89% 11%
46	4u	91	100% 89% 11%
47	4V	185	100% 94% 6%
47	4v	185	100% 94% 6%
48	4W	141	100% 90% 10%
48	4w	141	100% 90% 10%
49	4X	226	100% 95% 5%
49	4x	226	100% 93% 7%
50	4Y	107	100% 95% 5%
50	4y	107	100% 94% 6%
51	4Z	186	99% 94% 6%
51	4z	186	99% 94% 6%

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	HEC	3C	302	X	-	-	-
61	HEC	3c	302	X	-	-	-

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 142971 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
			4602	2877	828	871	26		
1	2m	604	Total	C	N	O	S	0	0
			4602	2877	828	871	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	164	Total	C	N	O	S	0	0
			1323	832	223	257	11		
7	2s	164	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 SDHC.

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	86	Total	C	N	O	S	0	0
			701	452	118	125	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2v	86	Total 701	C 452	N 118	O 125	S 6	0	0

- Molecule 11 is a protein called ISPR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	30	173	Total 1181	C 723	N 209	O 242	S 7	0	0

- Molecule 12 is a protein called ISPR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	31	159	Total 1219	C 748	N 222	O 235	S 14	0	0

- Molecule 13 is a protein called Mitochondrial processing peptidase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3A	454	Total 3622	C 2285	N 621	O 698	S 18	0	0
13	3a	454	Total 3622	C 2285	N 621	O 698	S 18	0	0

- Molecule 14 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3B	496	Total 3884	C 2459	N 669	O 734	S 22	0	0
14	3b	496	Total 3884	C 2459	N 669	O 734	S 22	0	0

- Molecule 15 is a protein called CytC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3C	241	Total 1921	C 1225	N 334	O 349	S 13	0	0
15	3c	242	Total 1930	C 1230	N 335	O 352	S 13	0	0

- Molecule 16 is a protein called QCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3D	95	Total	C	N	O	S	0	0
			836	551	146	135	4		
16	3d	95	Total	C	N	O	S	0	0
			836	551	146	135	4		

- Molecule 17 is a protein called QCR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3E	92	Total	C	N	O	S	0	0
			813	545	138	127	3		
17	3e	92	Total	C	N	O	S	0	0
			813	545	138	127	3		

- Molecule 18 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3F	84	Total	C	N	O	S	0	0
			734	493	123	114	4		
18	3f	84	Total	C	N	O	S	0	0
			734	493	123	114	4		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3G	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		
19	3g	354	Total	C	N	O	S	0	0
			3016	2063	448	498	7		

- Molecule 20 is a protein called Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3H	326	Total	C	N	O	S	0	0
			2628	1669	478	466	15		
20	3h	326	Total	C	N	O	S	0	0
			2621	1663	478	465	15		

- Molecule 21 is a protein called Ubiquinol-cytochrome C reductase complex 14kD subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3I	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		
21	3i	176	Total	C	N	O	S	0	0
			1472	946	255	259	12		

- Molecule 22 is a protein called Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3J	92	Total	C	N	O	S	0	0
			755	471	134	139	11		
22	3j	92	Total	C	N	O	S	0	0
			755	471	134	139	11		

- Molecule 23 is a protein called QCR11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3K	79	Total	C	N	O	S	0	0
			608	391	110	103	4		
23	3k	79	Total	C	N	O	S	0	0
			608	391	110	103	4		

- Molecule 24 is a protein called Aurora kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3L	68	Total	C	N	O	S	0	0
			539	348	92	96	3		
24	3l	68	Total	C	N	O	S	0	0
			539	348	92	96	3		

- Molecule 25 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	40	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		
25	41	230	Total	C	N	O	S	0	0
			2004	1365	289	346	4		

- Molecule 26 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4A	100	Total	C	N	O	S	0	0
			841	518	157	157	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	4a	100	Total 841	C 518	N 157	O 157	S 9	0	0

- Molecule 27 is a protein called Peptidase M14 carboxypeptidase A domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4B	93	Total 732	C 479	N 116	O 129	S 8	0	0
27	4b	93	Total 732	C 479	N 116	O 129	S 8	0	0

- Molecule 28 is a protein called Cytochrome c oxidase subunit 40.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4C	75	Total 626	C 414	N 95	O 113	S 4	0	0
28	4c	75	Total 626	C 414	N 95	O 113	S 4	0	0

- Molecule 29 is a protein called Cytochrome c oxidase subunit 34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4D	90	Total 787	C 525	N 128	O 131	S 3	0	0
29	4d	90	Total 787	C 525	N 128	O 131	S 3	0	0

- Molecule 30 is a protein called Merozoite surface protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4E	152	Total 1313	C 840	N 229	O 229	S 15	0	0
30	4e	152	Total 1313	C 840	N 229	O 229	S 15	0	0

- Molecule 31 is a protein called Ubiquitin, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4F	80	Total 669	C 438	N 119	O 110	S 2	0	0
31	4f	85	Total 708	C 462	N 126	O 118	S 2	0	0

- Molecule 32 is a protein called Cytochrome c oxidase subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4G	100	Total	C	N	O	S	0	0
			854	550	156	144	4		
32	4g	100	Total	C	N	O	S	0	0
			854	550	156	144	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4H	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		
33	4h	141	Total	C	N	O	S	0	0
			1125	711	195	217	2		

- Molecule 34 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4I	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		
34	4i	196	Total	C	N	O	S	0	0
			1695	1105	276	305	9		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4J	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		
35	4j	186	Total	C	N	O	S	0	0
			1517	990	268	253	6		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4K	93	Total	C	N	O	S	0	0
			722	473	129	118	2		
36	4k	93	Total	C	N	O	S	0	0
			722	473	129	118	2		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4L	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		
37	4l	122	Total	C	N	O	S	0	0
			1083	715	192	168	8		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4M	99	Total	C	N	O	S	0	0
			778	501	148	128	1		
38	4m	99	Total	C	N	O	S	0	0
			778	501	148	128	1		

- Molecule 39 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4N	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		
39	4n	131	Total	C	N	O	S	0	0
			1025	661	173	184	7		

- Molecule 40 is a protein called GINS subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4O	47	Total	C	N	O	S	0	0
			383	257	60	63	3		
40	4o	47	Total	C	N	O	S	0	0
			383	257	60	63	3		

- Molecule 41 is a protein called Cytochrome oxidase subunit II copper A binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	4P	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		
41	4p	180	Total	C	N	O	S	0	0
			1504	977	246	276	5		

- Molecule 42 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4Q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	4q	459	Total	C	N	O	S	0	0
			3687	2519	545	612	11		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	4R	103	Total	C	N	O	S	0	0
			916	609	156	145	6		
43	4r	103	Total	C	N	O	S	0	0
			916	609	156	145	6		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	4S	65	Total	C	N	O	S	0	0
			541	350	85	100	6		
44	4s	65	Total	C	N	O	S	0	0
			541	350	85	100	6		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	4T	121	Total	C	N	O	S	0	0
			983	634	170	167	12		
45	4t	121	Total	C	N	O	S	0	0
			983	634	170	167	12		

- Molecule 46 is a protein called Amino acid transporter transmembrane domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	4U	91	Total	C	N	O	S	0	0
			758	503	125	127	3		
46	4u	91	Total	C	N	O	S	0	0
			758	503	125	127	3		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4V	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
47	4v	185	Total	C	N	O	S	0	0
			1539	1003	270	260	6		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4W	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		
48	4w	141	Total	C	N	O	S	0	0
			1193	782	206	198	7		

- Molecule 49 is a protein called Cytochrome Coxidase subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	4X	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		
49	4x	226	Total	C	N	O	S	0	0
			1860	1186	313	344	17		

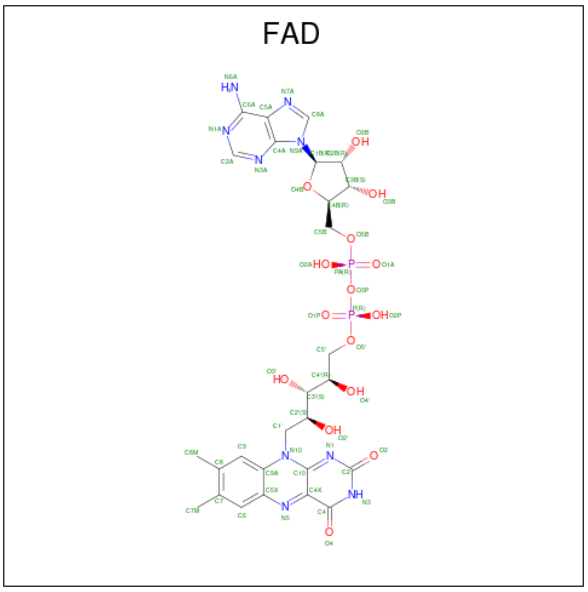
- Molecule 50 is a protein called Cytochrome c oxidase subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4Y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		
50	4y	107	Total	C	N	O	S	0	0
			905	567	153	179	6		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 31.

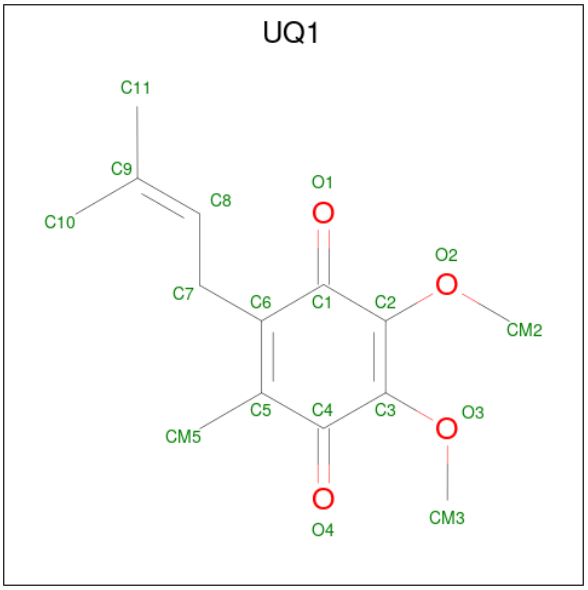
Mol	Chain	Residues	Atoms					AltConf	Trace
51	4Z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		
51	4z	186	Total	C	N	O	S	0	0
			1582	1041	270	266	5		

- Molecule 52 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
52	2M	1	Total	C	N	O	P	0
			53	27	9	15	2	
52	2m	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 53 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			AltConf
53	2N	1	Total	C	O	0
			18	14	4	
53	2p	1	Total	C	O	0
			18	14	4	

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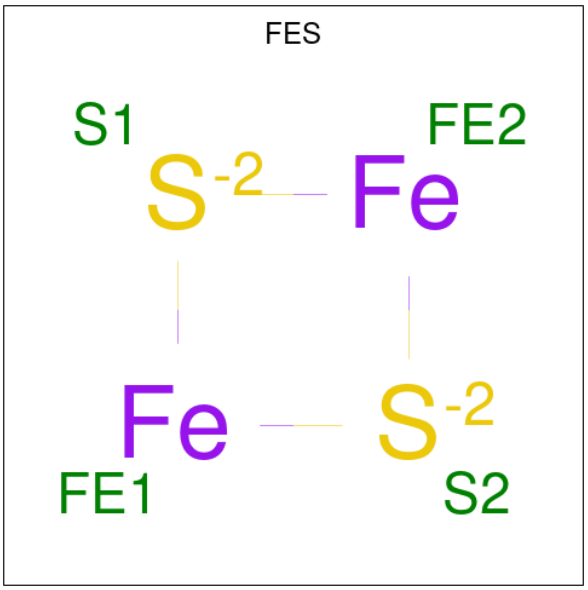
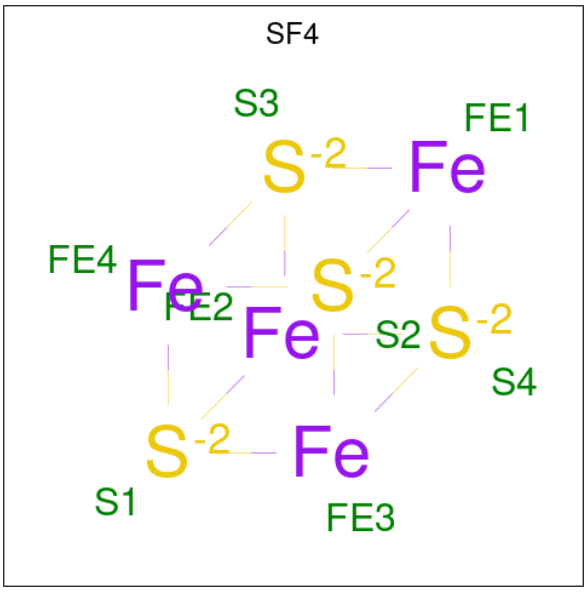
Mol	Chain	Residues	Atoms	AltConf
53	3G	1	Total C O 18 14 4	0
53	3G	1	Total C O 18 14 4	0
53	3g	1	Total C O 18 14 4	0
53	3g	1	Total C O 18 14 4	0

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



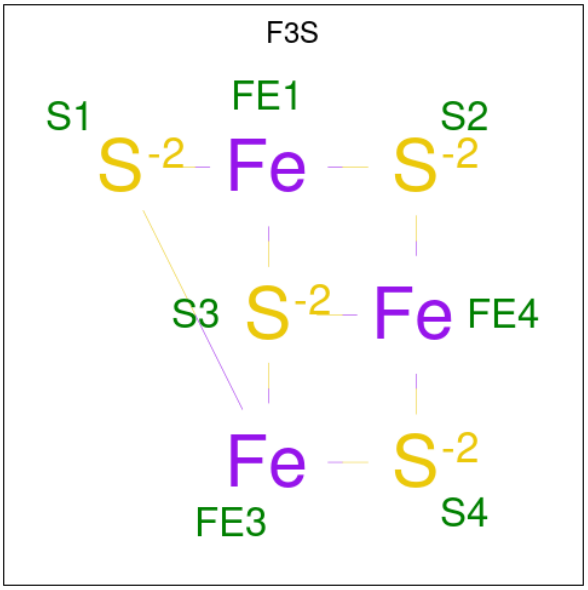
Mol	Chain	Residues	Atoms	AltConf
54	2N	1	Total Fe S 4 2 2	0
54	2n	1	Total Fe S 4 2 2	0
54	3H	1	Total Fe S 4 2 2	0
54	3h	1	Total Fe S 4 2 2	0

- Molecule 55 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
55	2N	1	Total Fe S 8 4 4	0
55	2n	1	Total Fe S 8 4 4	0

- Molecule 56 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

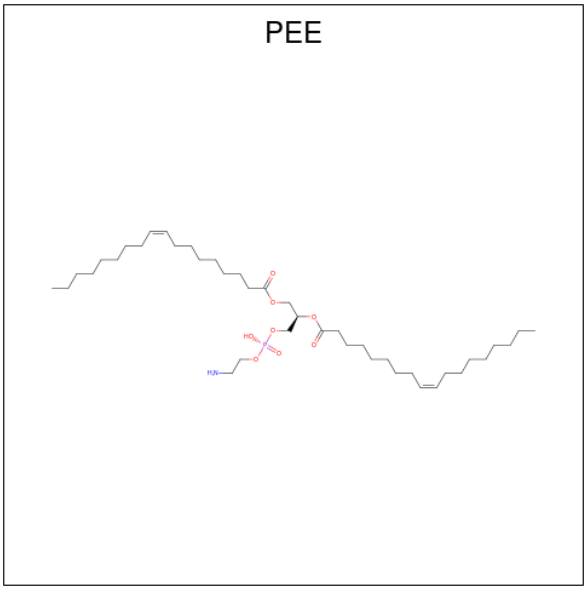


Mol	Chain	Residues	Atoms	AltConf
56	2N	1	Total Fe S 7 3 4	0
56	2n	1	Total Fe S 7 3 4	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
57	2N	1	Total K 1 1	0
57	2n	1	Total K 1 1	0
57	4Q	1	Total K 1 1	0
57	4q	1	Total K 1 1	0

- Molecule 58 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
58	2O	1	Total C N O P 39 29 1 8 1	0
58	2O	1	Total C N O P 41 31 1 8 1	0
58	2P	1	Total C N O P 46 36 1 8 1	0
58	2T	1	Total C N O P 45 35 1 8 1	0
58	2o	1	Total C N O P 24 14 1 8 1	0
58	2p	1	Total C N O P 24 14 1 8 1	0

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Mol	Chain	Residues	Atoms					AltConf
58	2r	1	Total	C	N	O	P	0
			39	29	1	8	1	
58	2t	1	Total	C	N	O	P	0
			42	32	1	8	1	
58	3C	1	Total	C	N	O	P	0
			30	20	1	8	1	
58	3H	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	3c	1	Total	C	N	O	P	0
			33	23	1	8	1	
58	3f	1	Total	C	N	O	P	0
			38	28	1	8	1	
58	40	1	Total	C	N	O	P	0
			45	35	1	8	1	
58	40	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	40	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	40	1	Total	C	N	O	P	0
			31	21	1	8	1	
58	41	1	Total	C	N	O	P	0
			45	35	1	8	1	
58	41	1	Total	C	N	O	P	0
			44	34	1	8	1	
58	41	1	Total	C	N	O	P	0
			36	26	1	8	1	
58	4D	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	4Q	1	Total	C	N	O	P	0
			36	26	1	8	1	
58	4R	1	Total	C	N	O	P	0
			43	33	1	8	1	
58	4S	1	Total	C	N	O	P	0
			27	17	1	8	1	
58	4W	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4d	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4l	1	Total	C	N	O	P	0
			38	28	1	8	1	

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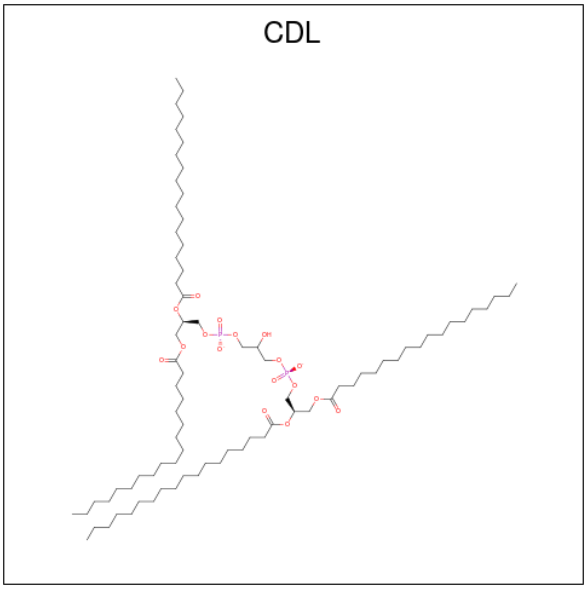
Mol	Chain	Residues	Atoms					AltConf
58	4q	1	Total	C	N	O	P	0
			37	27	1	8	1	
58	4q	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	4s	1	Total	C	N	O	P	0
			47	37	1	8	1	
58	4w	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	4z	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 59 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
59	2O	1	Total	C	O	P	0
			67	48	17	2	
59	2P	1	Total	C	O	P	0
			81	62	17	2	
59	2Q	1	Total	C	O	P	0
			100	81	17	2	
59	2T	1	Total	C	O	P	0
			71	52	17	2	
59	2o	1	Total	C	O	P	0
			86	67	17	2	
59	2p	1	Total	C	O	P	0
			74	55	17	2	

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Mol	Chain	Residues	Atoms				AltConf
59	2q	1	Total	C	O	P	0
			100	81	17	2	
59	2t	1	Total	C	O	P	0
			66	47	17	2	
59	3D	1	Total	C	O	P	0
			84	65	17	2	
59	3D	1	Total	C	O	P	0
			100	81	17	2	
59	3E	1	Total	C	O	P	0
			93	74	17	2	
59	3G	1	Total	C	O	P	0
			100	81	17	2	
59	3G	1	Total	C	O	P	0
			75	56	17	2	
59	3H	1	Total	C	O	P	0
			89	70	17	2	
59	3H	1	Total	C	O	P	0
			84	65	17	2	
59	3I	1	Total	C	O	P	0
			68	49	17	2	
59	3I	1	Total	C	O	P	0
			81	62	17	2	
59	3I	1	Total	C	O	P	0
			63	44	17	2	
59	3L	1	Total	C	O	P	0
			85	66	17	2	
59	3L	1	Total	C	O	P	0
			81	62	17	2	
59	3L	1	Total	C	O	P	0
			93	74	17	2	
59	3e	1	Total	C	O	P	0
			71	52	17	2	
59	3e	1	Total	C	O	P	0
			77	58	17	2	
59	3g	1	Total	C	O	P	0
			70	51	17	2	
59	3g	1	Total	C	O	P	0
			89	70	17	2	
59	3g	1	Total	C	O	P	0
			90	71	17	2	
59	3g	1	Total	C	O	P	0
			58	39	17	2	

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Mol	Chain	Residues	Atoms				AltConf
59	3h	1	Total	C	O	P	0
			85	66	17	2	
59	3i	1	Total	C	O	P	0
			51	32	17	2	
59	3i	1	Total	C	O	P	0
			76	57	17	2	
59	3l	1	Total	C	O	P	0
			100	81	17	2	
59	3l	1	Total	C	O	P	0
			81	62	17	2	
59	41	1	Total	C	O	P	0
			92	73	17	2	
59	4E	1	Total	C	O	P	0
			89	70	17	2	
59	4E	1	Total	C	O	P	0
			46	27	17	2	
59	4F	1	Total	C	O	P	0
			100	81	17	2	
59	4J	1	Total	C	O	P	0
			59	40	17	2	
59	4K	1	Total	C	O	P	0
			90	71	17	2	
59	4L	1	Total	C	O	P	0
			94	75	17	2	
59	4M	1	Total	C	O	P	0
			75	56	17	2	
59	4O	1	Total	C	O	P	0
			97	78	17	2	
59	4Q	1	Total	C	O	P	0
			95	76	17	2	
59	4Q	1	Total	C	O	P	0
			75	56	17	2	
59	4S	1	Total	C	O	P	0
			100	81	17	2	
59	4U	1	Total	C	O	P	0
			72	53	17	2	
59	4W	1	Total	C	O	P	0
			73	54	17	2	
59	4Z	1	Total	C	O	P	0
			48	29	17	2	
59	4e	1	Total	C	O	P	0
			50	31	17	2	

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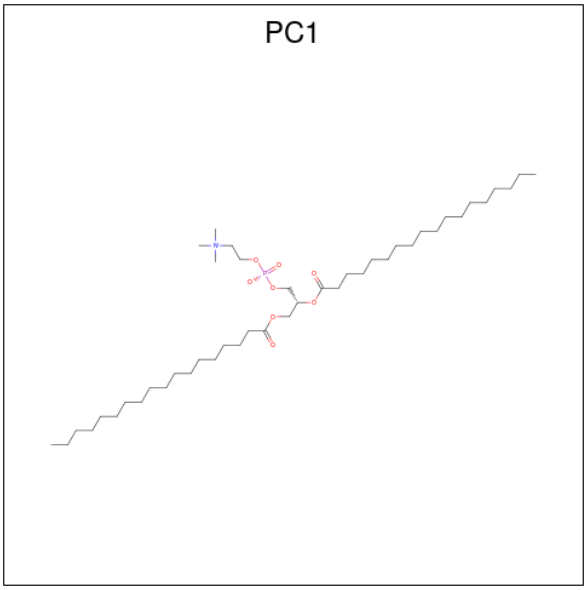
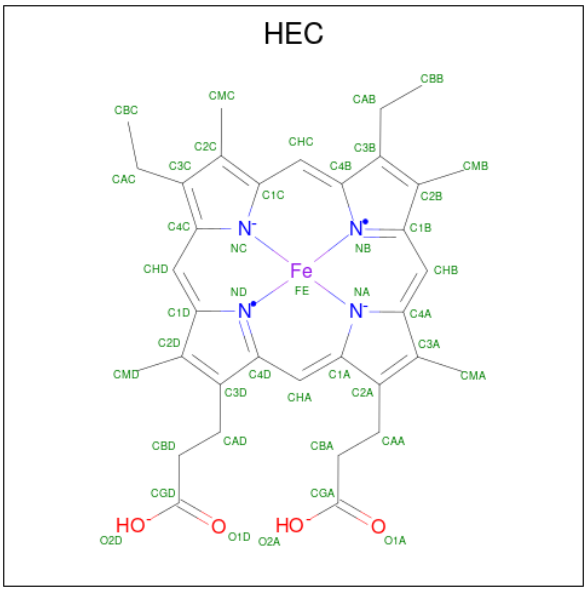
Mol	Chain	Residues	Atoms				AltConf
59	4e	1	Total	C	O	P	0
			96	77	17	2	
59	4f	1	Total	C	O	P	0
			92	73	17	2	
59	4g	1	Total	C	O	P	0
			66	47	17	2	
59	4j	1	Total	C	O	P	0
			51	32	17	2	
59	4j	1	Total	C	O	P	0
			88	69	17	2	
59	4m	1	Total	C	O	P	0
			100	81	17	2	
59	4o	1	Total	C	O	P	0
			93	74	17	2	
59	4q	1	Total	C	O	P	0
			93	74	17	2	
59	4s	1	Total	C	O	P	0
			100	81	17	2	
59	4t	1	Total	C	O	P	0
			61	42	17	2	
59	4z	1	Total	C	O	P	0
			93	74	17	2	
59	4z	1	Total	C	O	P	0
			86	67	17	2	

- Molecule 60 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



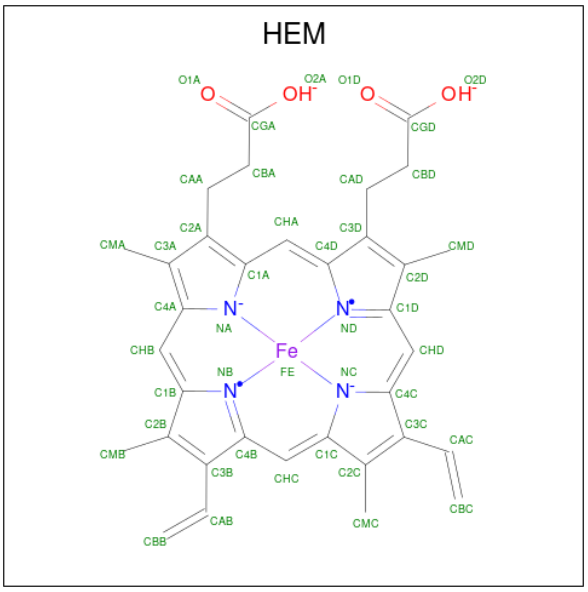
Mol	Chain	Residues	Atoms					AltConf
60	2P	1	Total	C	N	O	P	0
			35	25	1	8	1	
60	2R	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2R	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2T	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2T	1	Total	C	N	O	P	0
			45	35	1	8	1	
60	2o	1	Total	C	N	O	P	0
			39	29	1	8	1	
60	2p	1	Total	C	N	O	P	0
			41	31	1	8	1	
60	2r	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	2r	1	Total	C	N	O	P	0
			52	42	1	8	1	
60	3A	1	Total	C	N	O	P	0
			38	28	1	8	1	
60	3H	1	Total	C	N	O	P	0
			34	24	1	8	1	
60	3H	1	Total	C	N	O	P	0
			33	23	1	8	1	
60	3a	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	3f	1	Total	C	N	O	P	0
			46	36	1	8	1	
60	3h	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	3h	1	Total	C	N	O	P	0
			41	31	1	8	1	
60	4F	1	Total	C	N	O	P	0
			54	44	1	8	1	
60	4e	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 61 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
61	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
61	3c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 62 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



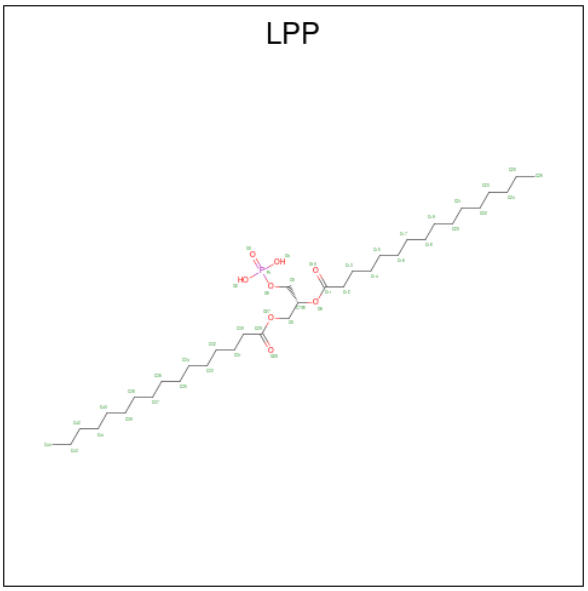
Mol	Chain	Residues	Atoms					AltConf
62	3G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

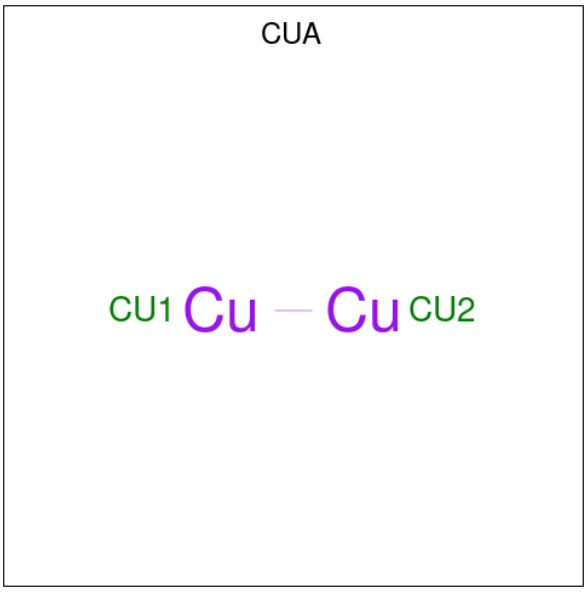
Mol	Chain	Residues	Atoms					AltConf
62	3G	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	3g	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
62	3g	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 63 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
63	4C	1	Total	C	O	P	0
			44	35	8	1	
63	4Z	1	Total	C	O	P	0
			44	35	8	1	
63	4g	1	Total	C	O	P	0
			39	30	8	1	
63	4z	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 64 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	AltConf
64	4N	1	Total Cu 2 2	0
64	4n	1	Total Cu 2 2	0

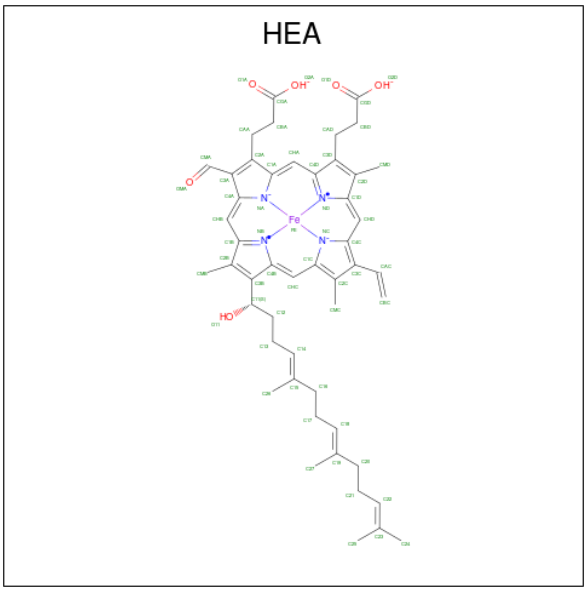
- Molecule 65 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

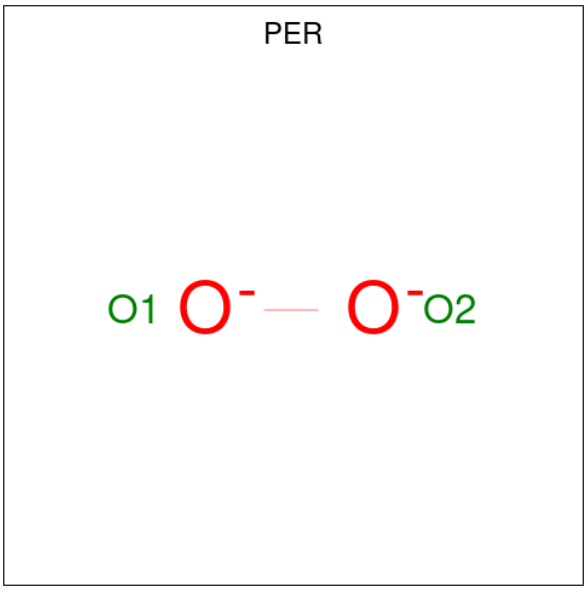
Mol	Chain	Residues	Atoms	AltConf
66	4Q	1	Total Mg 1 1	0
66	4q	1	Total Mg 1 1	0

- Molecule 67 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
67	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
67	4Q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
67	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
67	4q	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 68 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	AltConf
68	4Q	1	Total O 2 2	0
68	4q	1	Total O 2 2	0

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
69	4T	2	Total Zn 2 2	0
69	4X	1	Total Zn 1 1	0
69	4t	2	Total Zn 2 2	0
69	4x	1	Total Zn 1 1	0

- Molecule 70 is water.

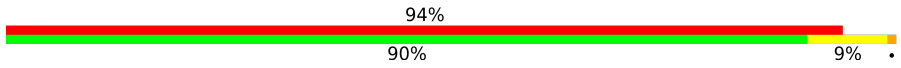
Mol	Chain	Residues	Atoms	AltConf
70	4Q	1	Total O 1 1	0
70	4n	1	Total O 1 1	0

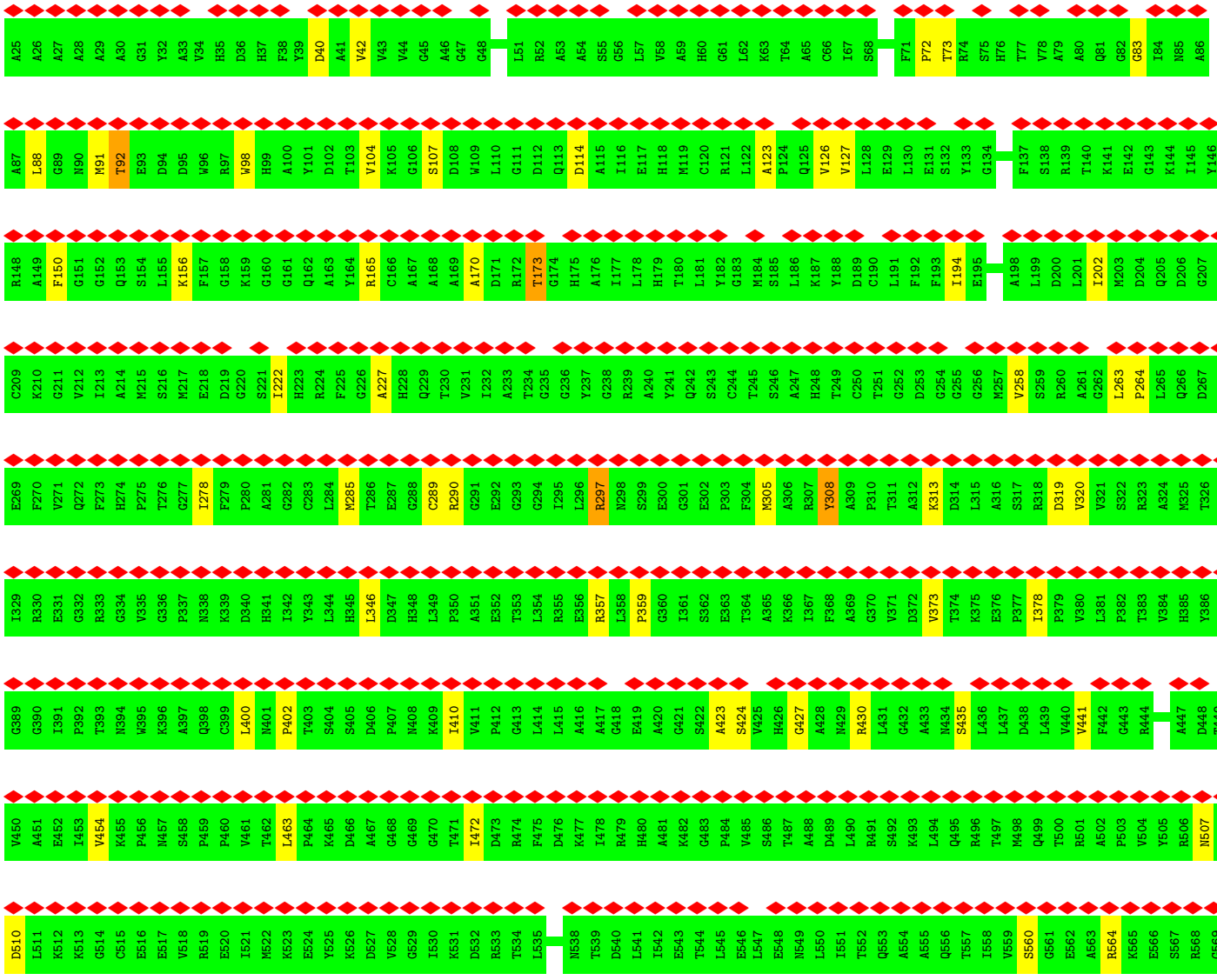
3 Residue-property plots (i)

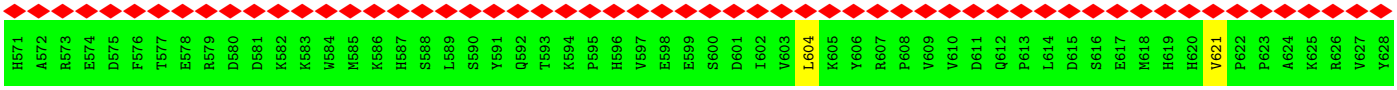
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain 2M:

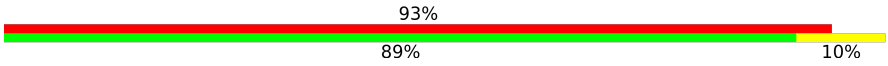


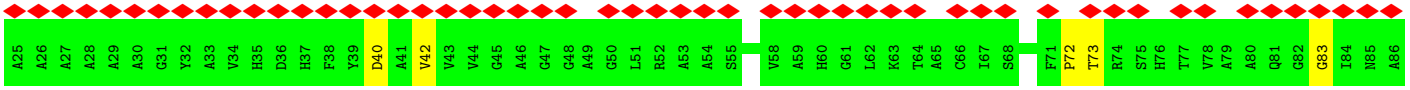


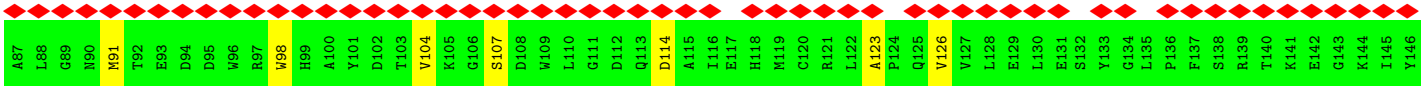


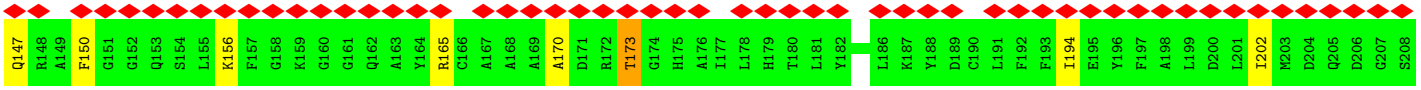
• Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

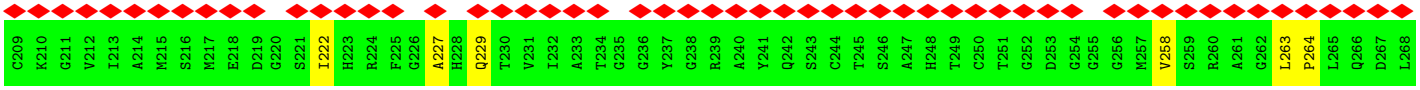
Chain 2m:

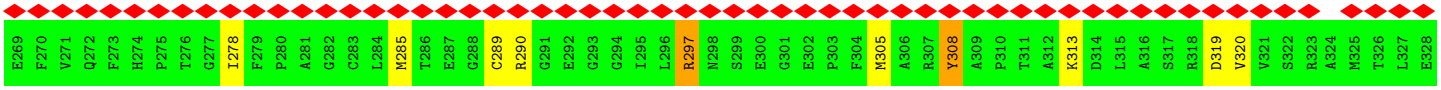


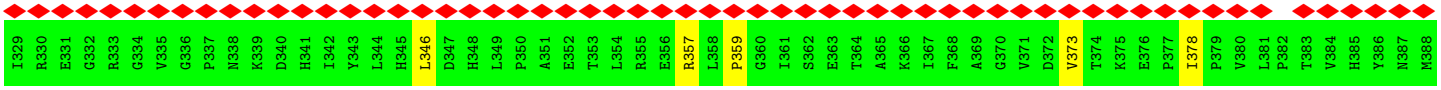


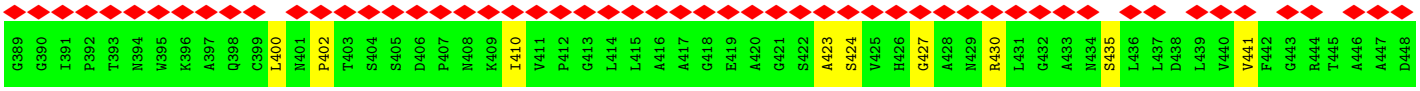


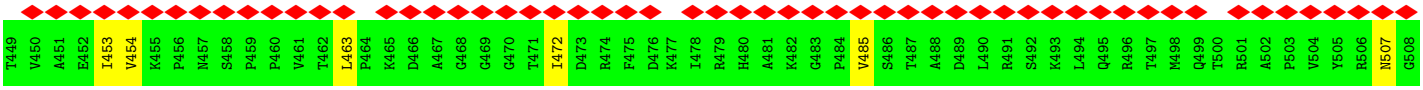


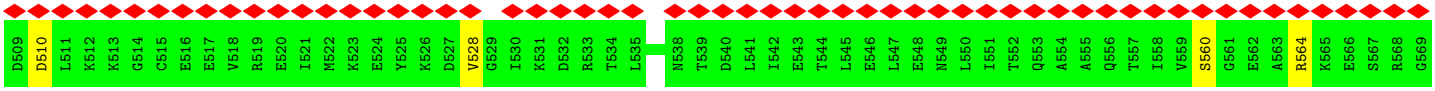


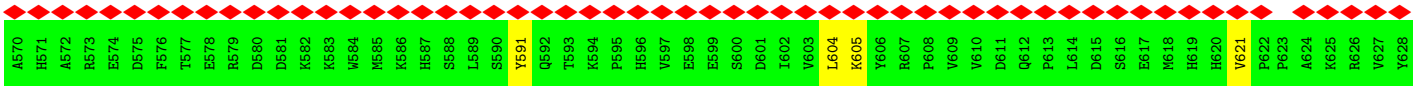






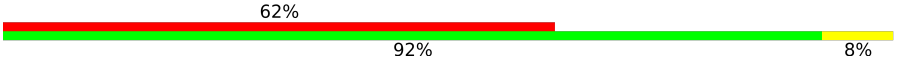


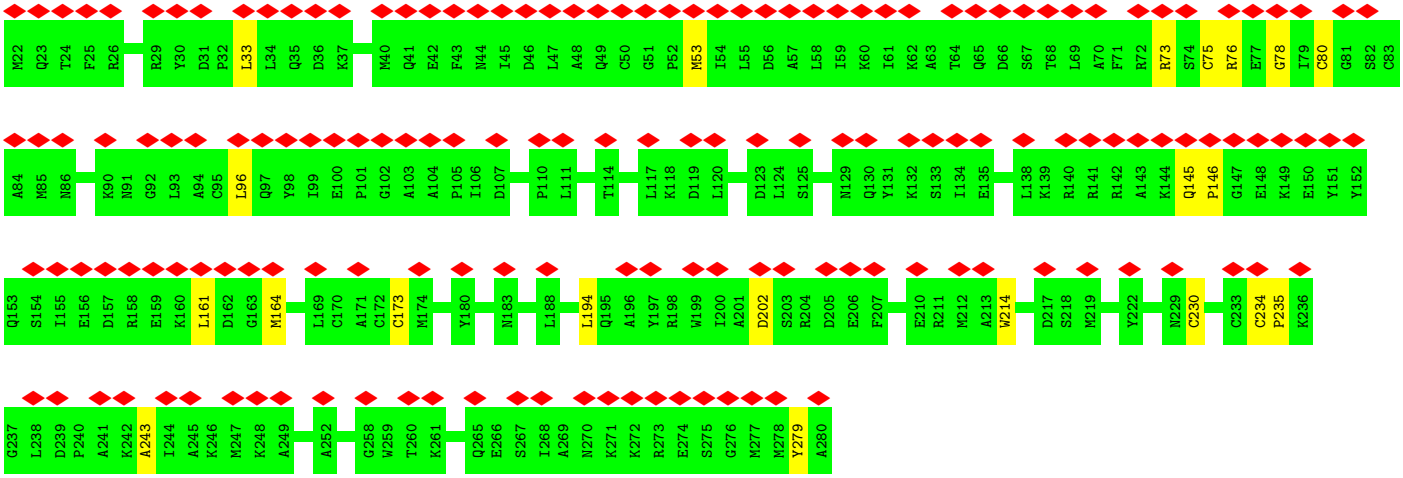




• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

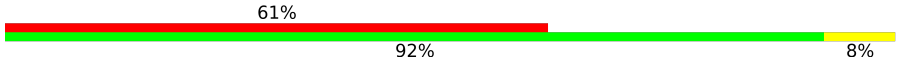
Chain 2N:

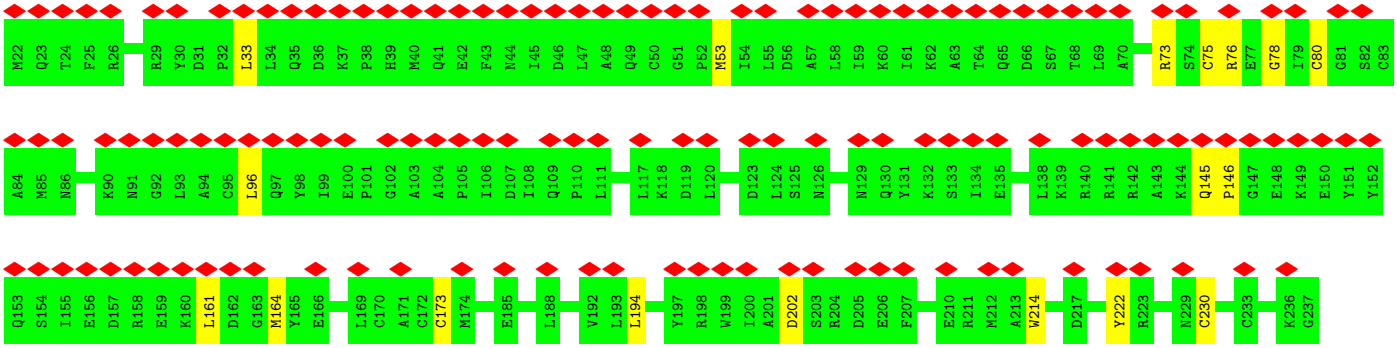




• Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

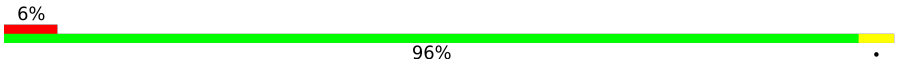
Chain 2n:

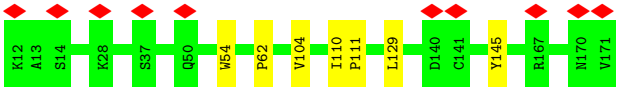




• Molecule 3: SDHG

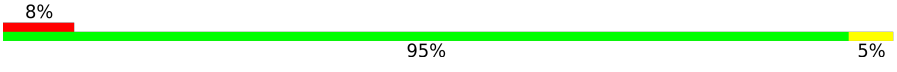
Chain 2O:

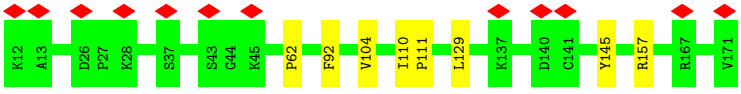




• Molecule 3: SDHG

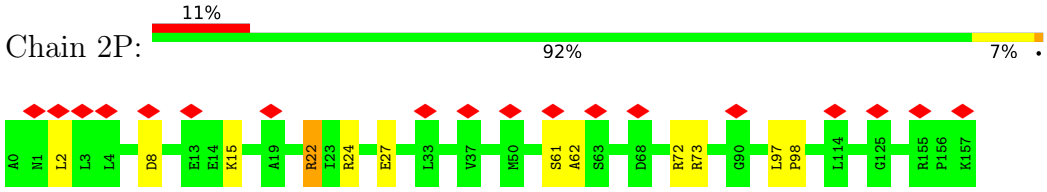
Chain 2o:





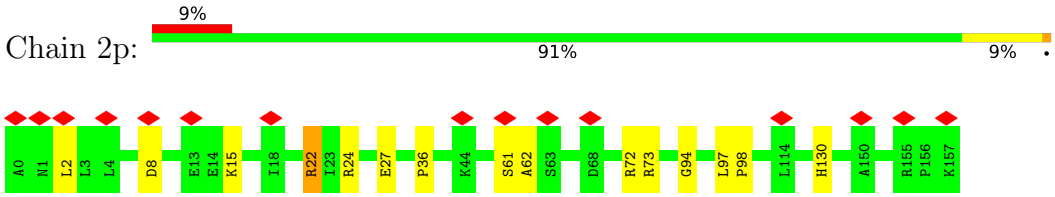
• Molecule 4: Transmembrane protein

Chain 2P:



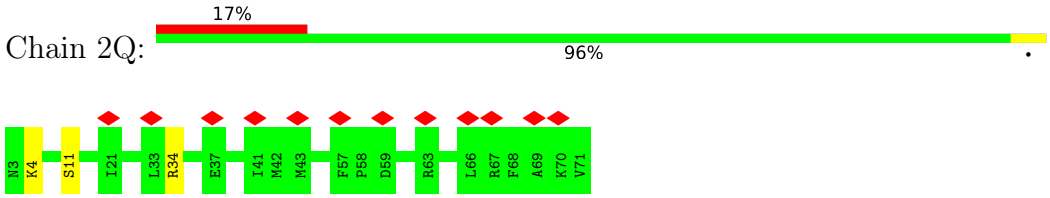
• Molecule 4: Transmembrane protein

Chain 2p:



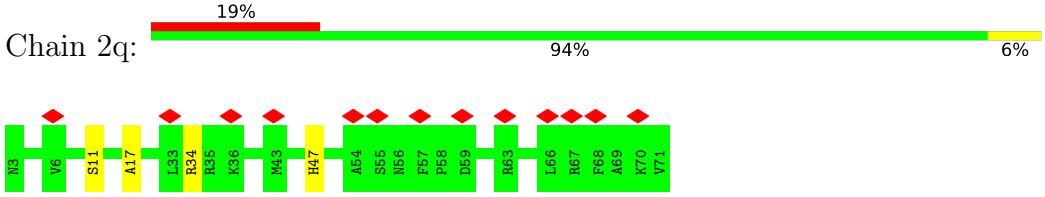
• Molecule 5: Kinesin-like protein

Chain 2Q:



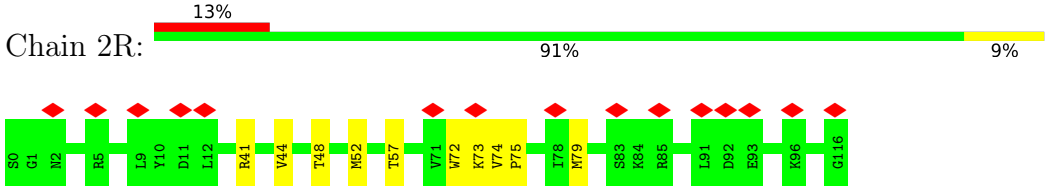
• Molecule 5: Kinesin-like protein

Chain 2q:



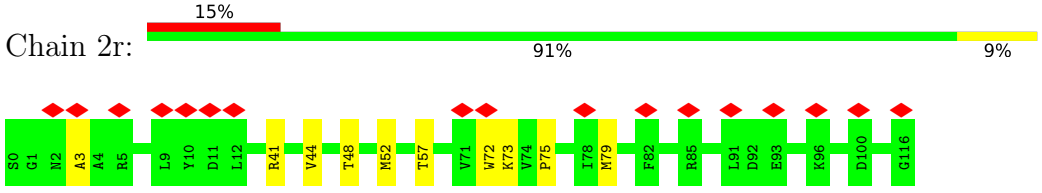
• Molecule 6: SDHH

Chain 2R:



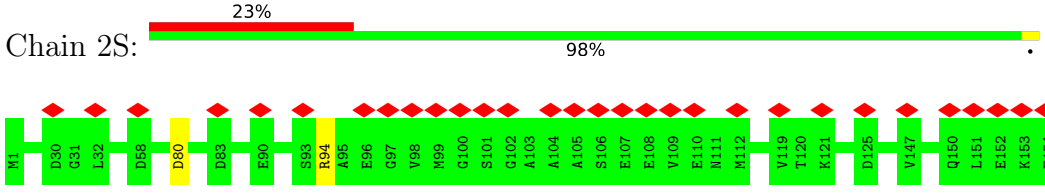
• Molecule 6: SDHH

Chain 2r:



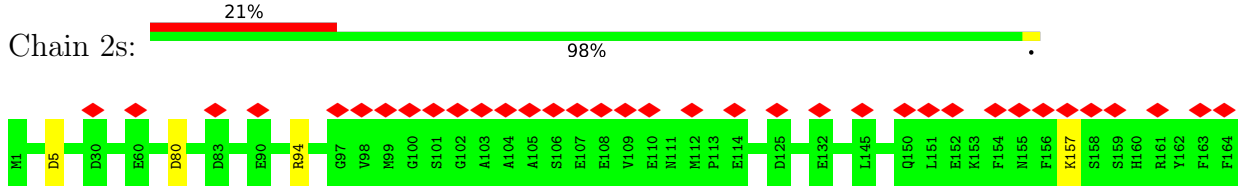
• Molecule 7: DUF6827 domain-containing protein

Chain 2S:



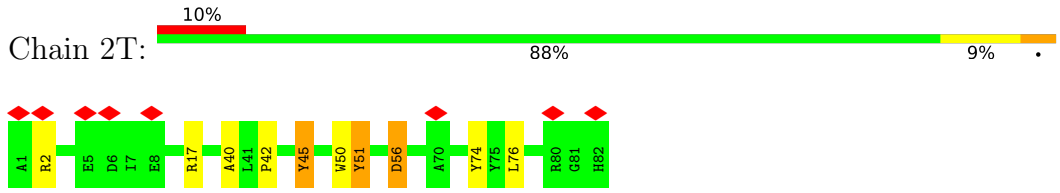
• Molecule 7: DUF6827 domain-containing protein

Chain 2s:



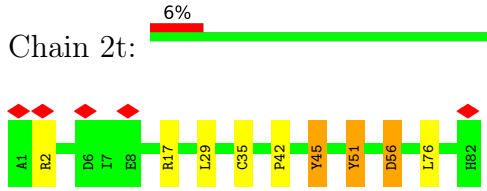
• Molecule 8: Rab-GAP TBC domain-containing protein

Chain 2T:



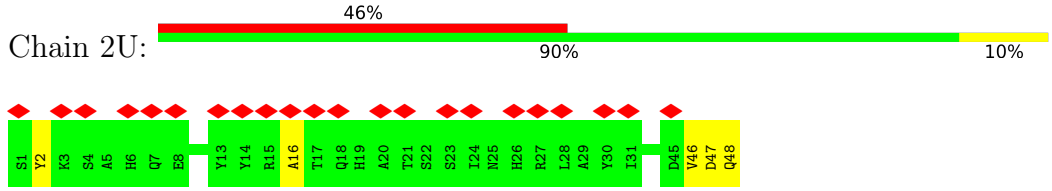
• Molecule 8: Rab-GAP TBC domain-containing protein

Chain 2t:



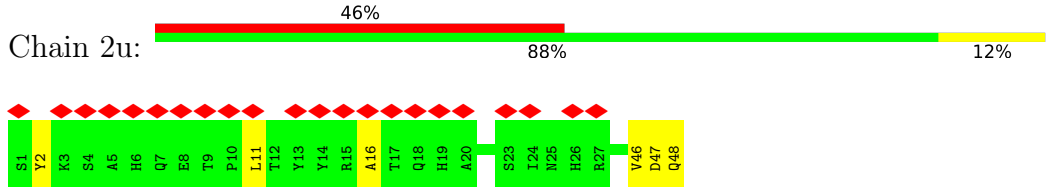
• Molecule 9: SDHC

Chain 2U:



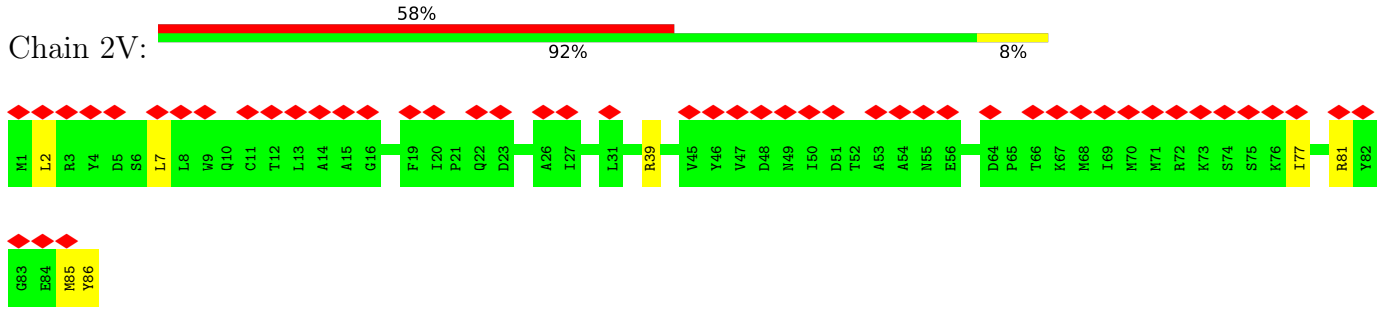
• Molecule 9: SDHC

Chain 2u:



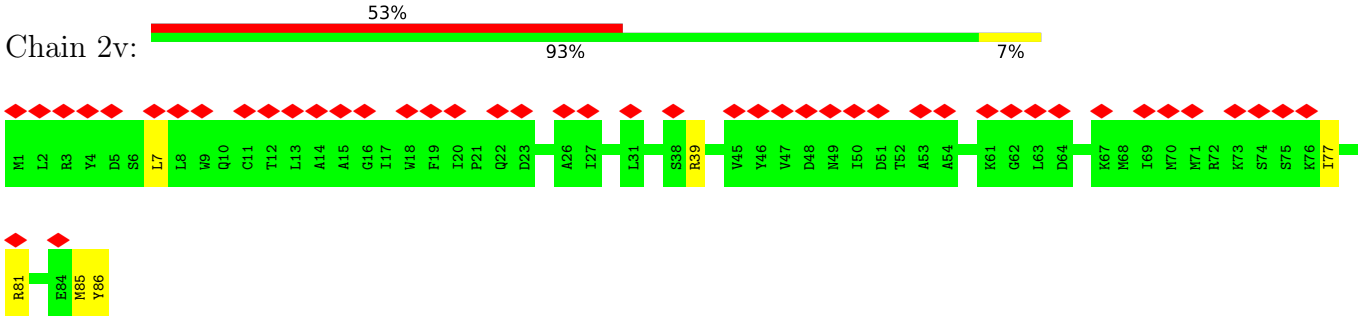
• Molecule 10: SDHI

Chain 2V:



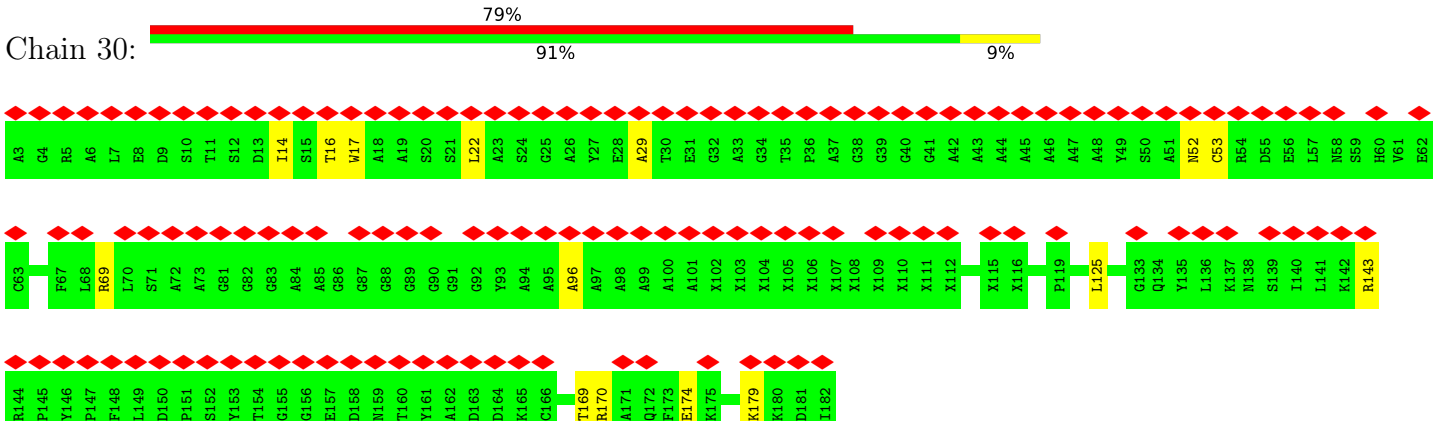
• Molecule 10: SDHI

Chain 2v:



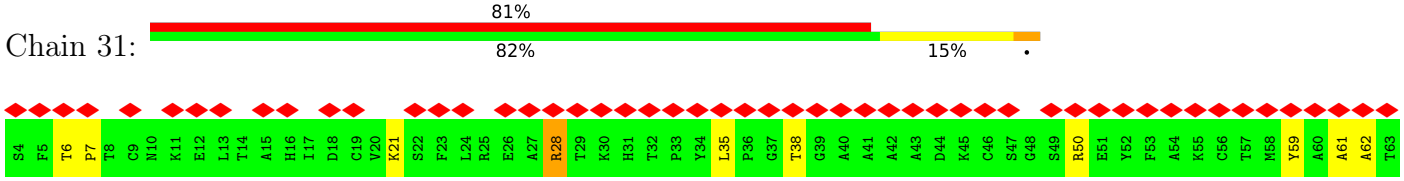
• Molecule 11: ISPR2

Chain 30:



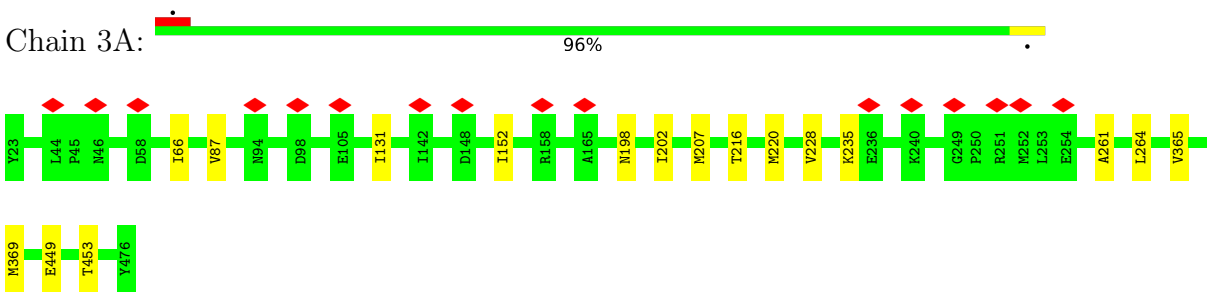
• Molecule 12: ISPR1

Chain 31:



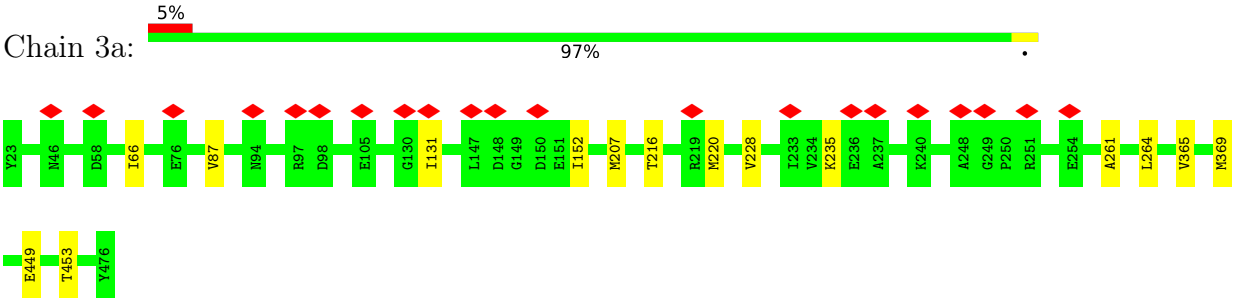
• Molecule 13: Mitochondrial processing peptidase beta subunit

Chain 3A:



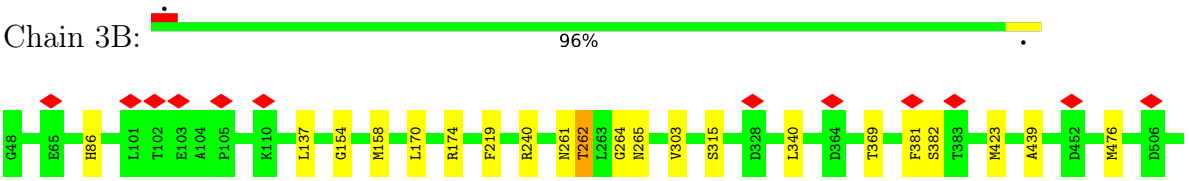
• Molecule 13: Mitochondrial processing peptidase beta subunit

Chain 3a:



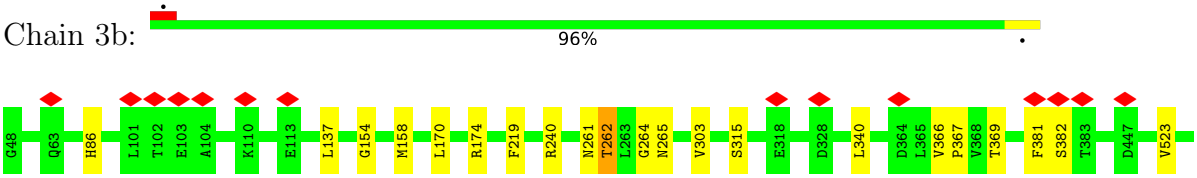
• Molecule 14: Alpha-MPP

Chain 3B:



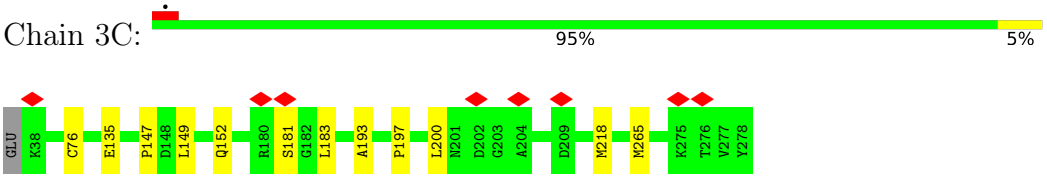
• Molecule 14: Alpha-MPP

Chain 3b:



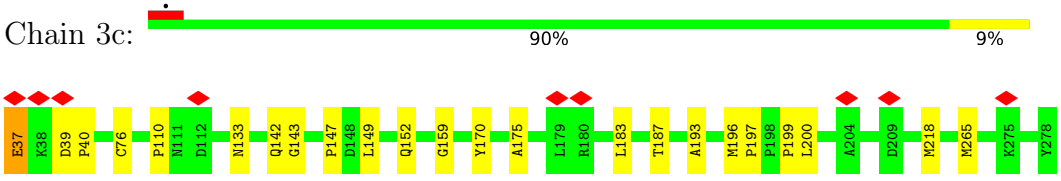
• Molecule 15: CytC1

Chain 3C:



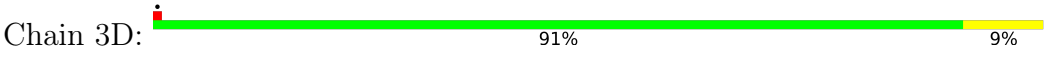
• Molecule 15: CytC1

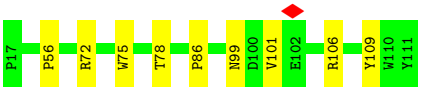
Chain 3c:



• Molecule 16: QCR8

Chain 3D:

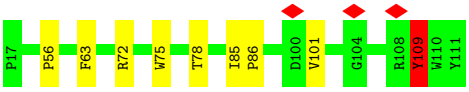




• Molecule 16: QCR8

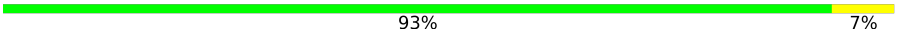
Chain 3d:

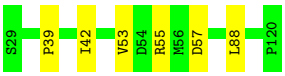




• Molecule 17: QCR9

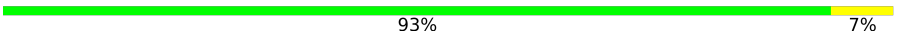
Chain 3E:





• Molecule 17: QCR9

Chain 3e:

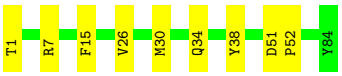




• Molecule 18: QCR10

Chain 3F:

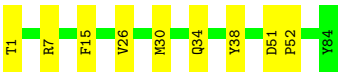




• Molecule 18: QCR10

Chain 3f:

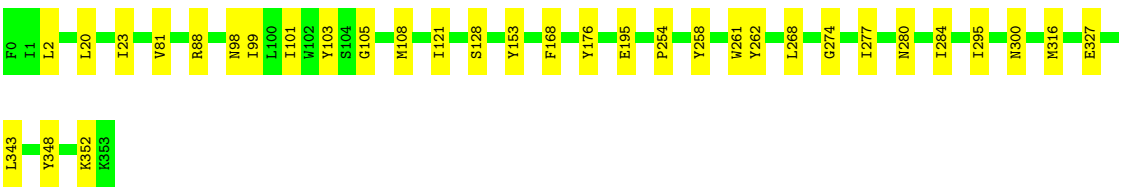




• Molecule 19: Cytochrome b

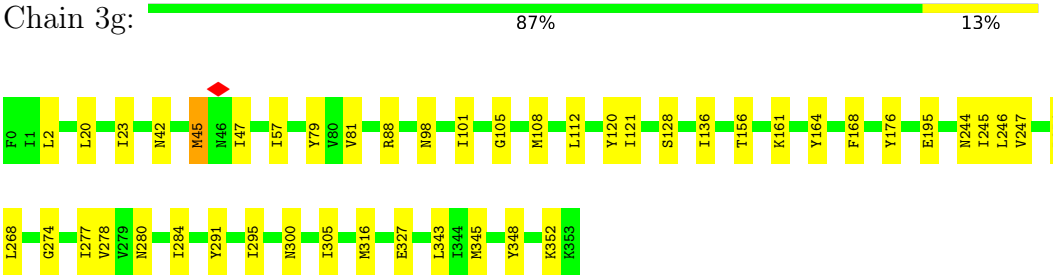
Chain 3G:





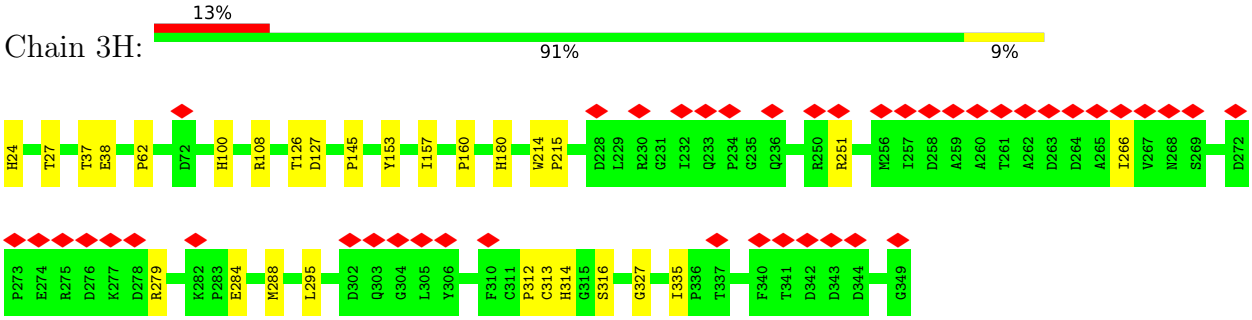
• Molecule 19: Cytochrome b

Chain 3g:



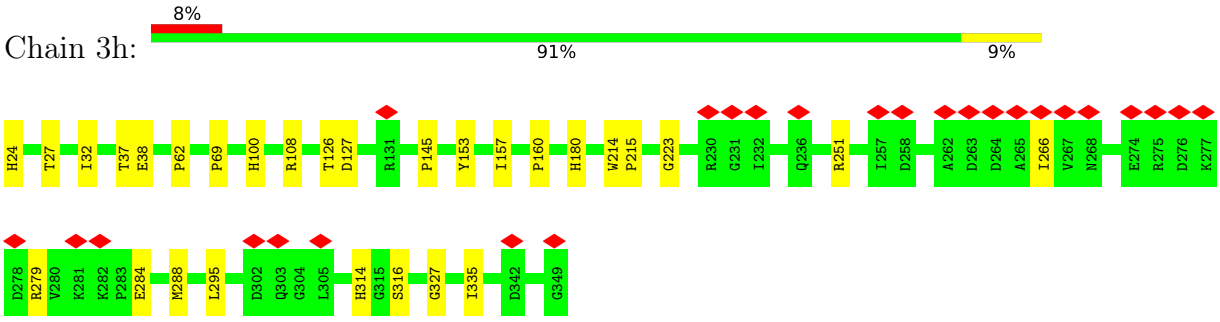
• Molecule 20: Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative

Chain 3H:



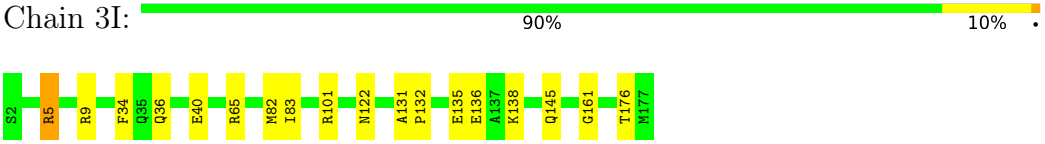
• Molecule 20: Ubiquinol-cytochrome c reductase, iron-sulfur subunit, putative

Chain 3h:



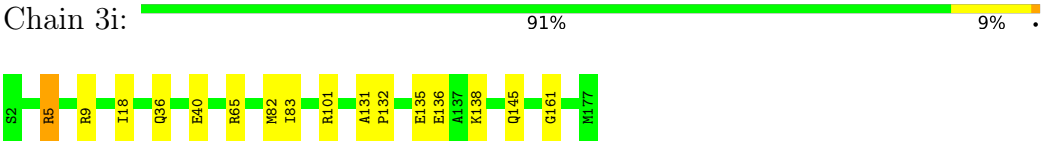
• Molecule 21: Ubiquinol-cytochrome C reductase complex 14kD subunit, putative

Chain 3I:



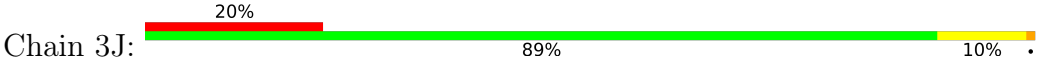
• Molecule 21: Ubiquinol-cytochrome C reductase complex 14kD subunit, putative

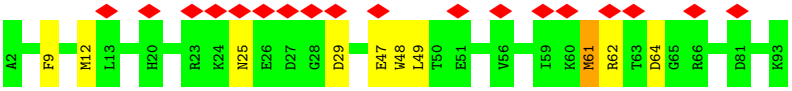
Chain 3i:



• Molecule 22: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative

Chain 3J:

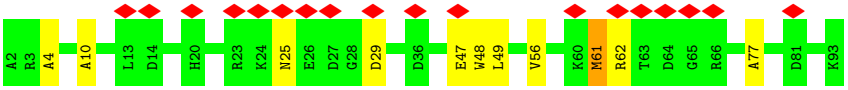




• Molecule 22: Ubiquinol-cytochrome c reductase complex 7.8 kDa protein, putative

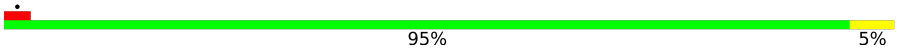
Chain 3j:





• Molecule 23: QCR11

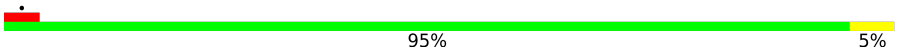
Chain 3K:

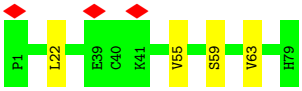




• Molecule 23: QCR11

Chain 3k:

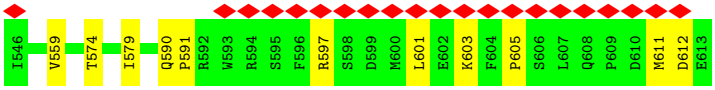




• Molecule 24: Aurora kinase

Chain 3L:

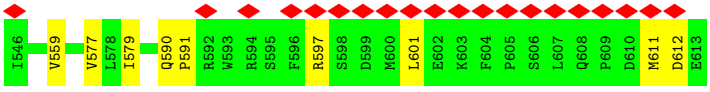




• Molecule 24: Aurora kinase

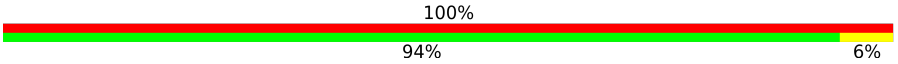
Chain 3l:

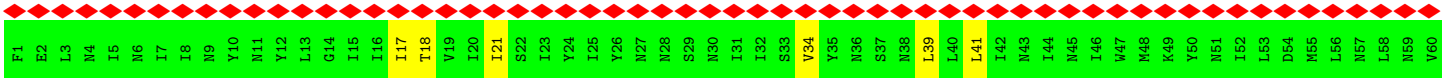


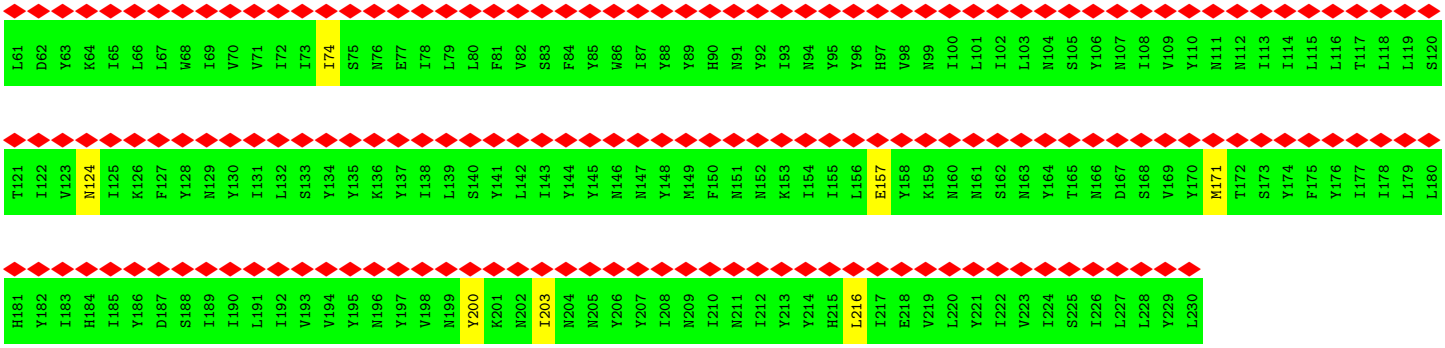


• Molecule 25: Cytochrome c oxidase subunit 3

Chain 40:

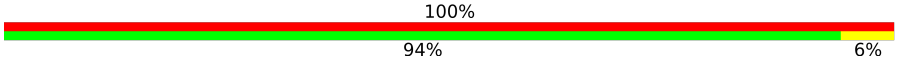


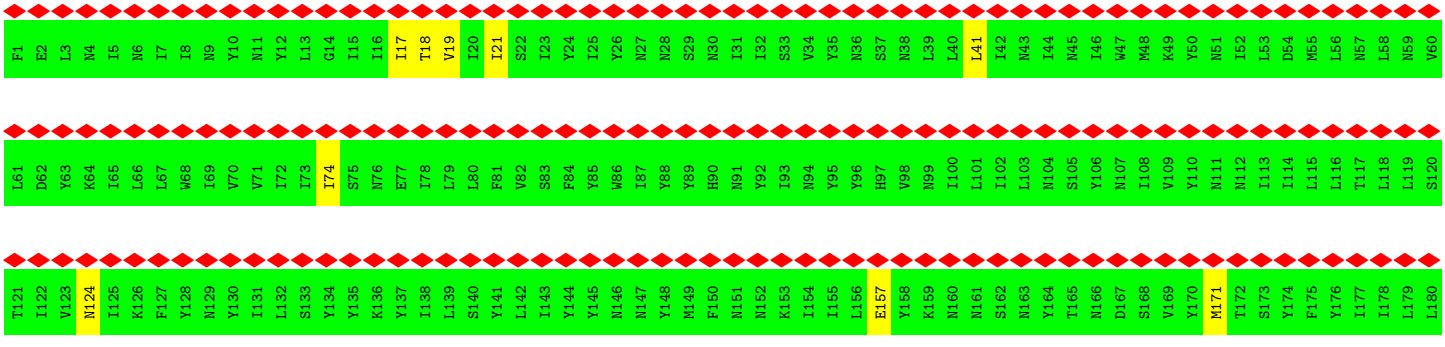




• Molecule 25: Cytochrome c oxidase subunit 3

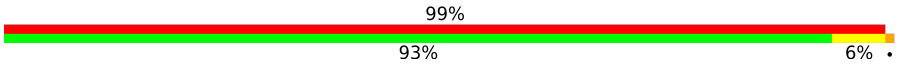
Chain 41:





• Molecule 26: Cytochrome c oxidase subunit 6B

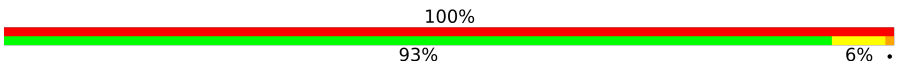
Chain 4A:





• Molecule 26: Cytochrome c oxidase subunit 6B

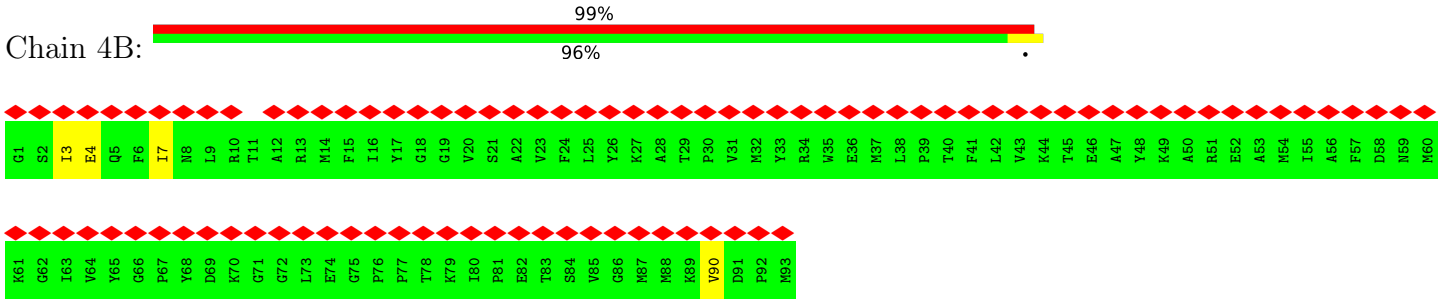
Chain 4a:





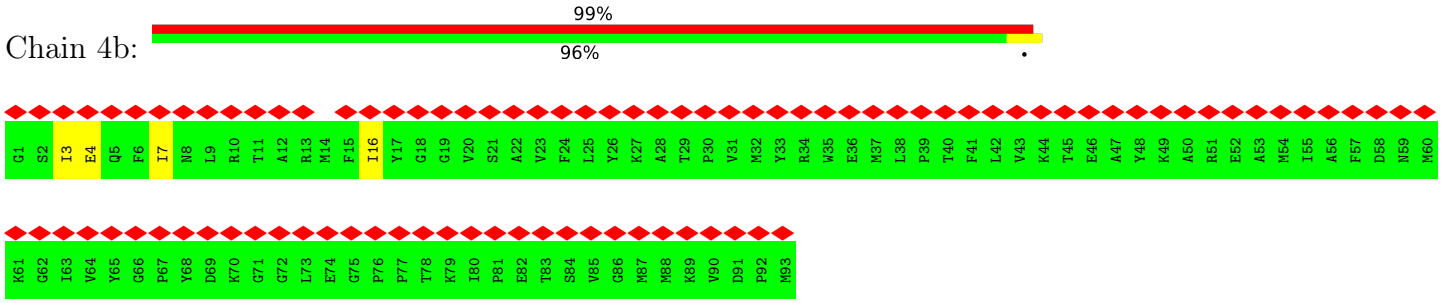
• Molecule 27: Peptidase M14 carboxypeptidase A domain-containing protein

Chain 4B:



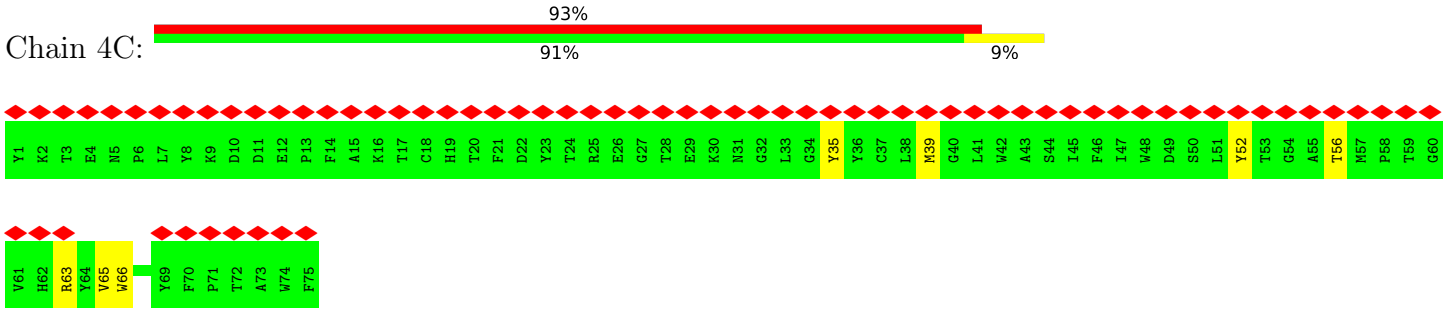
• Molecule 27: Peptidase M14 carboxypeptidase A domain-containing protein

Chain 4b:



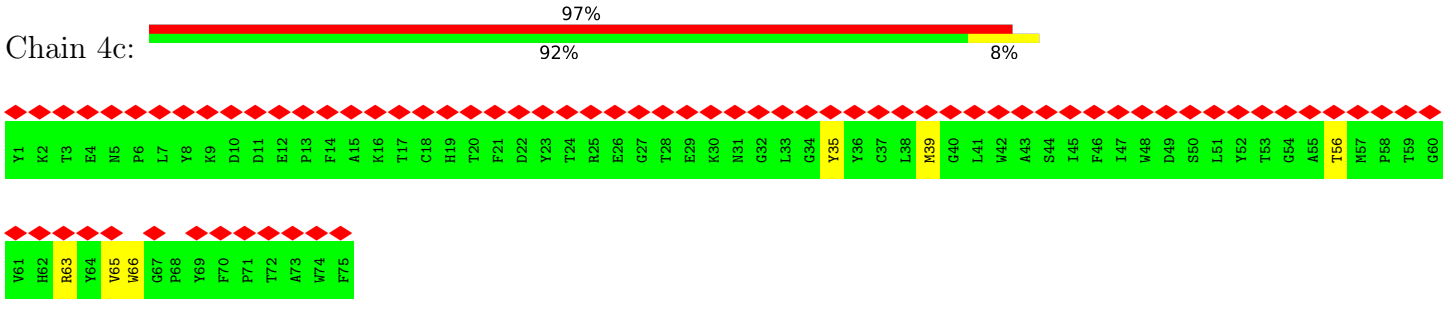
• Molecule 28: Cytochrome c oxidase subunit 40

Chain 4C:



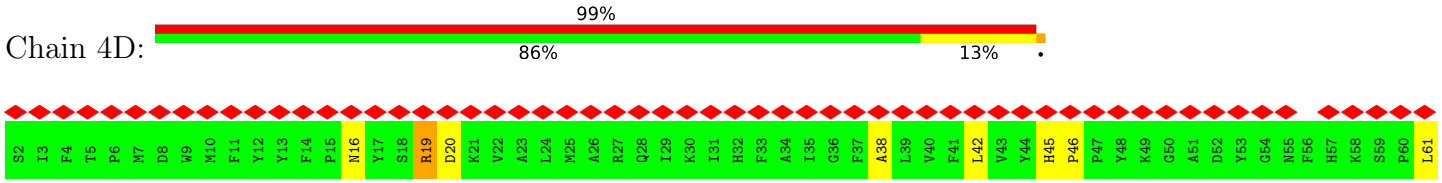
• Molecule 28: Cytochrome c oxidase subunit 40

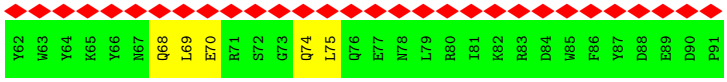
Chain 4c:



• Molecule 29: Cytochrome c oxidase subunit 34

Chain 4D:

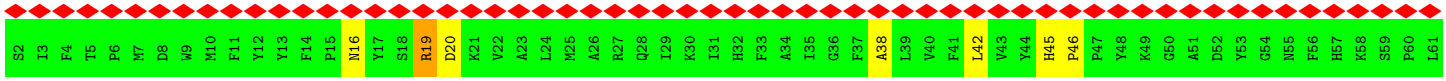


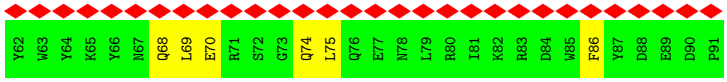


• Molecule 29: Cytochrome c oxidase subunit 34

Chain 4d:



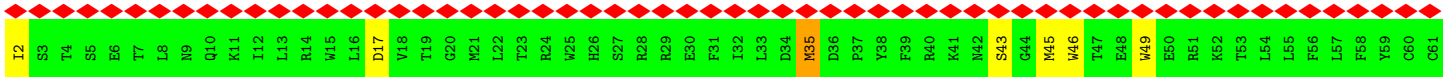


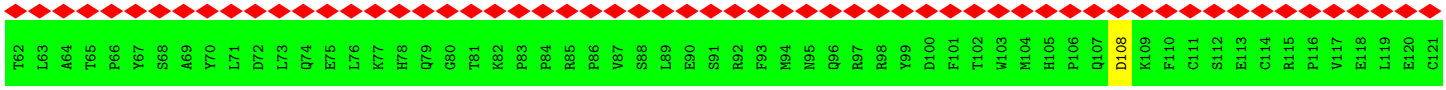


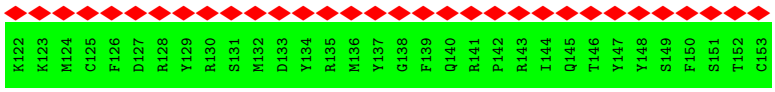
• Molecule 30: Merozoite surface protein, putative

Chain 4E:



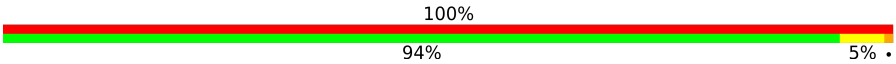


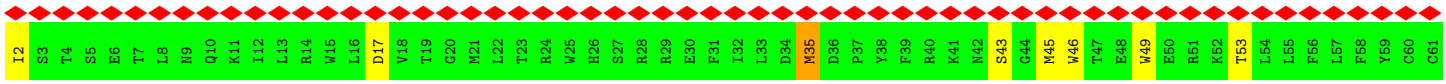


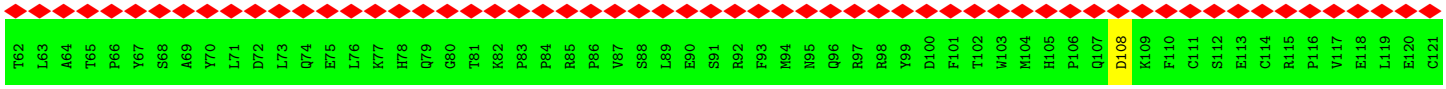


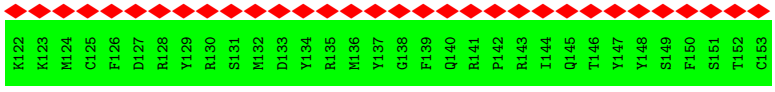
• Molecule 30: Merozoite surface protein, putative

Chain 4e:



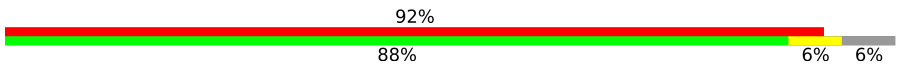


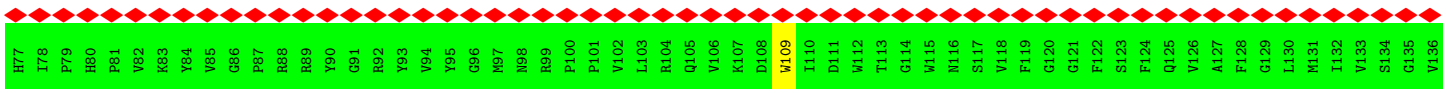


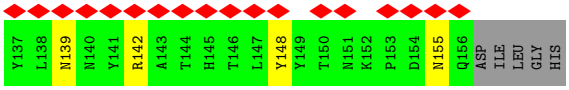


• Molecule 31: Ubiquitin, putative

Chain 4F:

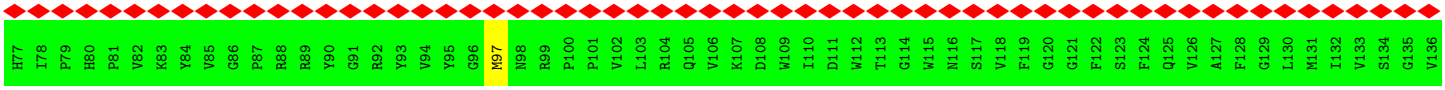


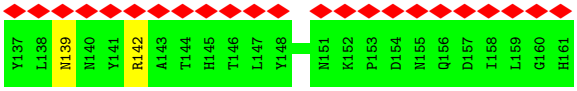




• Molecule 31: Ubiquitin, putative

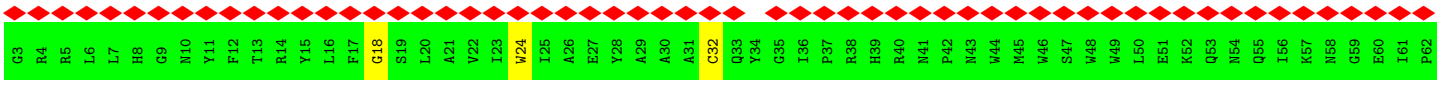


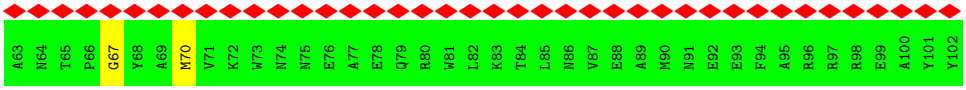




• Molecule 32: Cytochrome c oxidase subunit 33

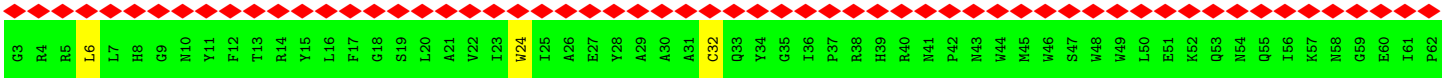


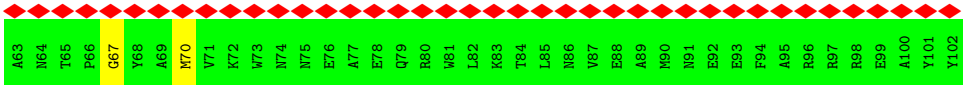




• Molecule 32: Cytochrome c oxidase subunit 33

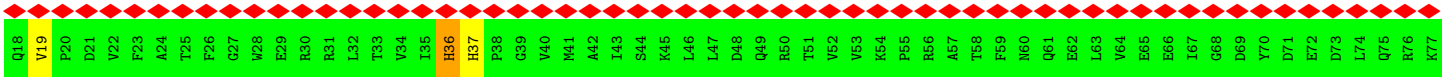


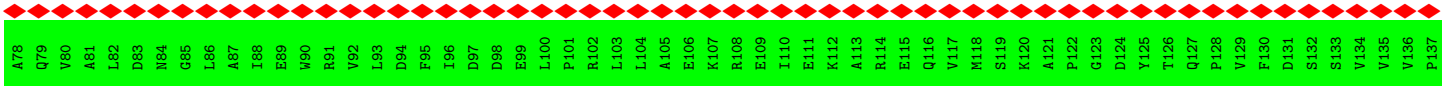


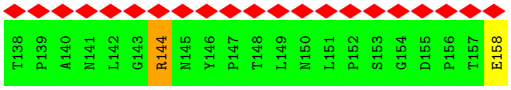


• Molecule 33: Cytochrome c oxidase subunit 30



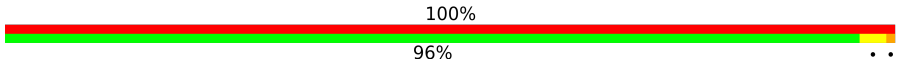


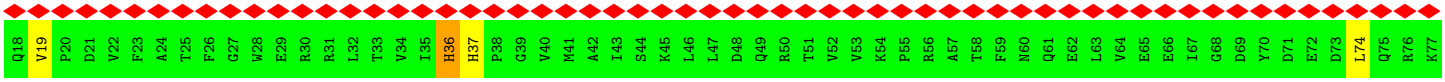


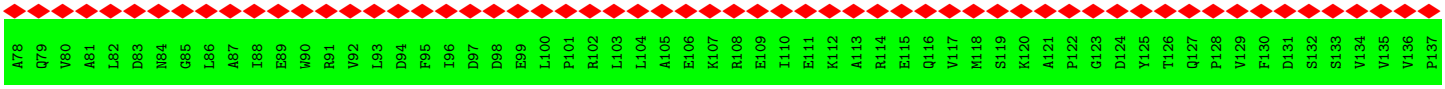


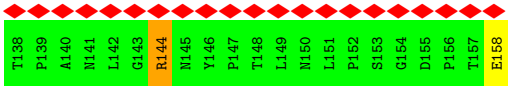
• Molecule 33: Cytochrome c oxidase subunit 30

Chain 4h:



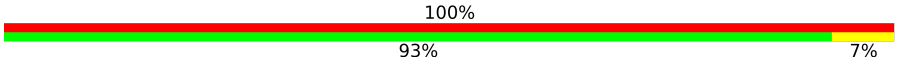


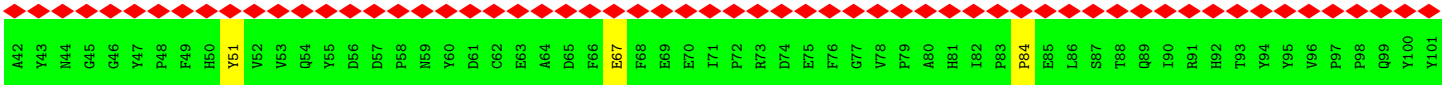


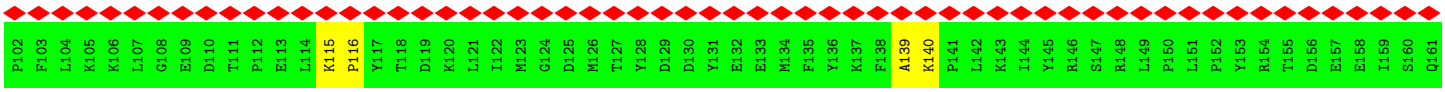


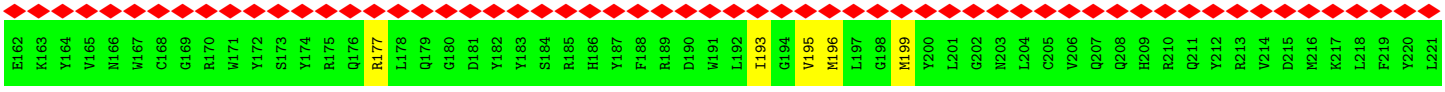
• Molecule 34: Cytochrome c oxidase subunit 6C

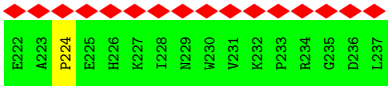
Chain 4I:





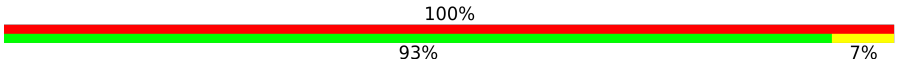


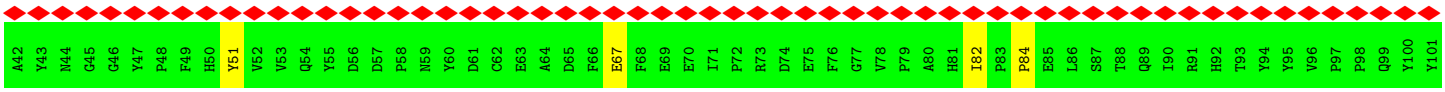


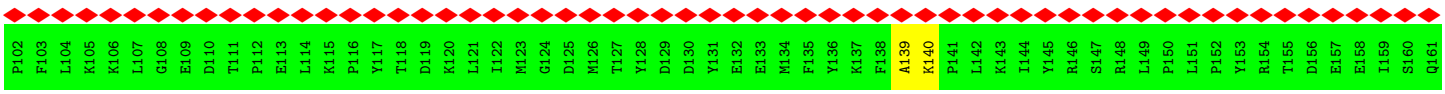


• Molecule 34: Cytochrome c oxidase subunit 6C

Chain 4i:







E162 K163 Y164 V165 N166 W167 C168 G169 R170 W171 Y172 S173 Y174 R175 Q176 R177 L178 Q179 G180 D181 Y182 Y183 S184 R185 H186 Y187 F188 R189 D190 W191 L192 I193 G194 V195 M196 L197 G198 M199 Y200 L201 G202 N203 L204 C205 V206 Q207 Q208 H209 R210 Q211 Y212 R213 V214 D215 M216 K217 L218 F219 Y220 L221

E222 A223 P224 E225 H226 K227 I228 N229 W230 V231 K232 P233 R234 G235 D236 L237

• Molecule 35: Cytochrome c oxidase subunit 24

Chain 4J:



G18 C19 E20 A21 V22 K23 N24 P25 L26 I27 G28 G29 P30 N31 Q32 K33 A34 R35 G36 A37 I38 T39 S40 G41 F42 A43 G44 G45 G46 A47 K48 R49 L50 G51 G52 K53 G54 Y55 G56 I57 M58 A59 D60 W61 C62 D63 H64 G65 Y66 S67 F68 T69 K70 G71 Q72 A73 I74 T75 G76 M77

P78 H79 W80 P81 L82 W83 C84 G85 G86 G87 V88 P89 D90 K91 F92 I93 K94 I95 D96 P97 D98 V99 H100 F101 N102 L103 Q104 G105 Y106 R107 E108 R109 I110 G111 W112 Y113 G114 F115 F116 T117 A118 F119 L120 Q121 A122 N123 Y124 H125 A126 F127 V128 Y129 F130 V131 R132 F133 I134 P135 I136 N137

I138 A139 I140 F141 W142 I143 Y144 V145 N146 E147 R148 Q149 R150 E151 P152 Q153 E154 N155 V156 M157 D158 H159 E160 E161 F162 F163 R164 D165 F166 D167 S168 I169 Y170 L171 G172 Q173 V174 F175 D176 H177 H178 R179 F180 A181 E182 W183 L184 A185 R186 R187 R188 A189 V190 K191 W192 G193 Y194 A195 D196 Q197

I198 H199 I200 P201 P202 V203

• Molecule 35: Cytochrome c oxidase subunit 24

Chain 4j:



G18 C19 E20 A21 V22 K23 N24 P25 L26 I27 G28 G29 P30 N31 Q32 K33 A34 R35 G36 A37 I38 T39 S40 G41 F42 A43 G44 G45 G46 A47 K48 R49 L50 G51 G52 K53 G54 Y55 G56 I57 M58 A59 D60 W61 C62 D63 H64 G65 Y66 S67 F68 T69 K70 G71 Q72 A73 I74 T75 G76 M77

P78 H79 W80 P81 L82 W83 C84 G85 G86 G87 V88 P89 D90 K91 F92 I93 K94 I95 D96 P97 D98 V99 H100 F101 N102 L103 Q104 G105 Y106 R107 E108 R109 I110 G111 W112 Y113 G114 F115 F116 T117 A118 F119 L120 Q121 A122 N123 Y124 H125 A126 F127 V128 Y129 F130 V131 R132 F133 I134 P135 I136 N137

I138 A139 I140 F141 W142 I143 Y144 V145 N146 E147 R148 Q149 R150 E151 P152 Q153 E154 N155 V156 M157 D158 H159 E160 E161 F162 F163 R164 D165 F166 D167 S168 I169 Y170 L171 G172 Q173 V174 F175 D176 H177 H178 R179 F180 A181 E182 W183 L184 A185 R186 R187 R188 A189 V190 K191 W192 G193 Y194 A195 D196 Q197

I198 H199 I200 P201 P202 V203

• Molecule 36: Cytochrome c oxidase subunit 37

Chain 4K:



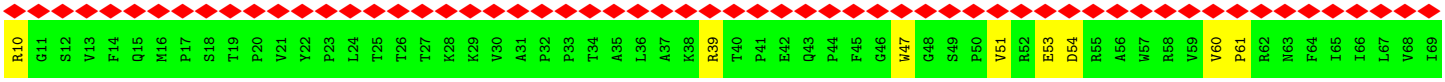
R10 G11 S12 V13 F14 Q15 M16 P17 S18 T19 P20 V21 Y22 P23 L24 T25 T26 T27 K28 K29 V30 A31 P32 P33 T34 A35 L36 A37 K38 R39 T40 P41 E42 Q43 P44 F45 G46 W47 G48 S49 P50 V51 R52 E53 D54 R55 A56 W57 R58 V59 V60 P61 R62 N63 F64 I65 I66 L67 V68 I69

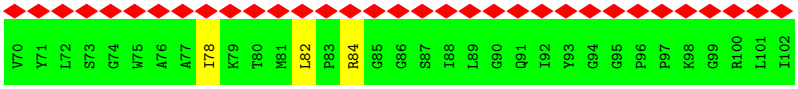


• Molecule 36: Cytochrome c oxidase subunit 37

Chain 4k:



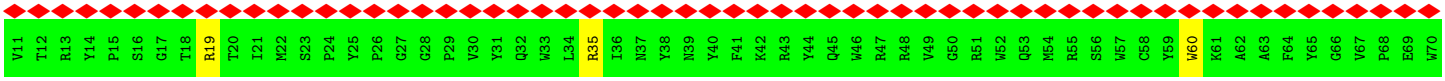


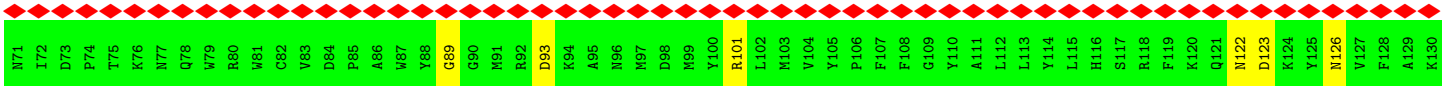


• Molecule 37: Cytochrome c oxidase subunit 7A

Chain 4L:





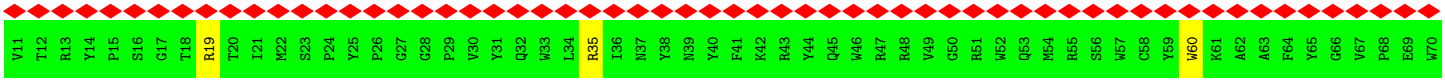


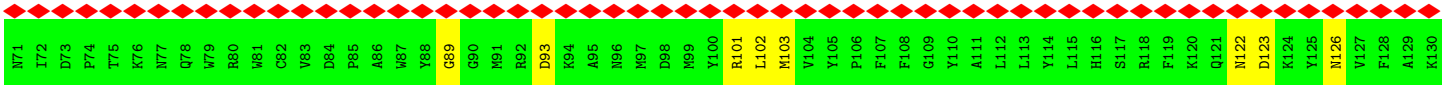


• Molecule 37: Cytochrome c oxidase subunit 7A

Chain 4l:





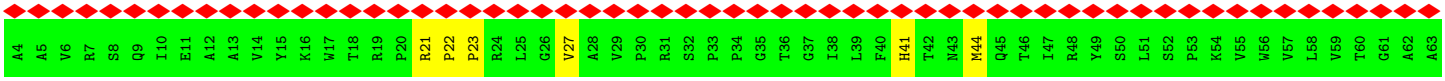


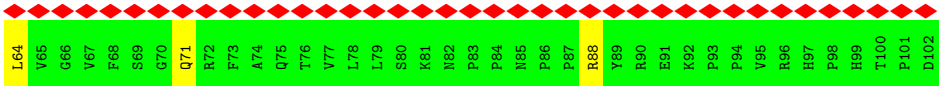


• Molecule 38: Cytochrome c oxidase subunit 35

Chain 4M:

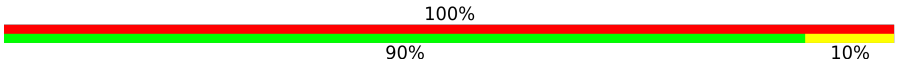


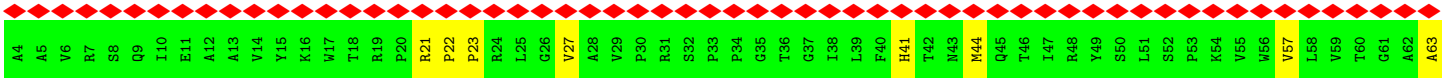


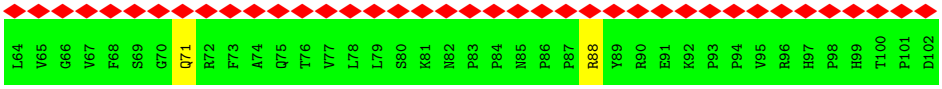


• Molecule 38: Cytochrome c oxidase subunit 35

Chain 4m:

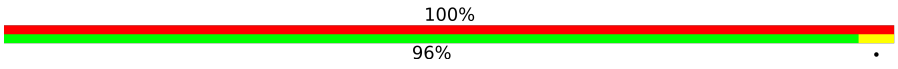


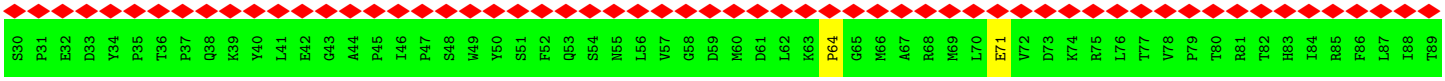


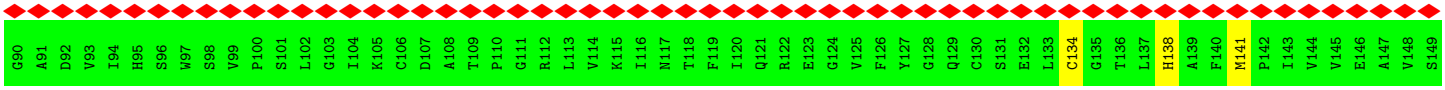


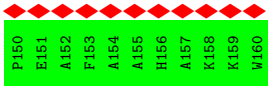
• Molecule 39: Cytochrome c oxidase polypeptide II

Chain 4N:



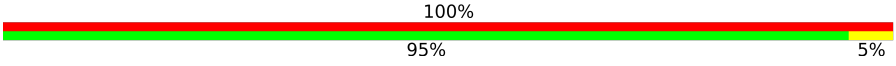


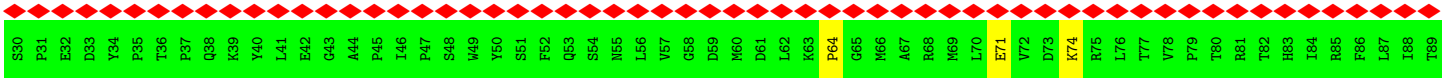


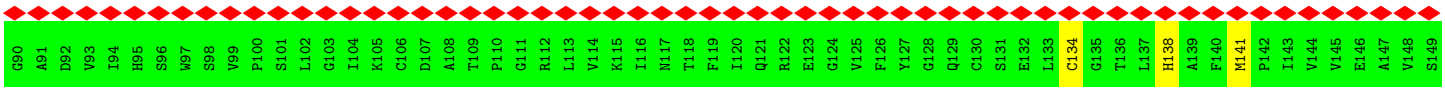


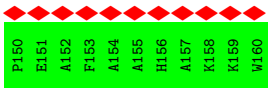
• Molecule 39: Cytochrome c oxidase polypeptide II

Chain 4n:



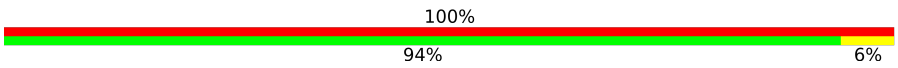


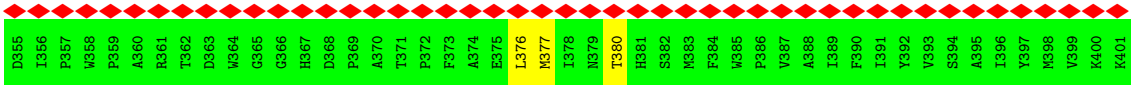




• Molecule 40: GINS subunit domain-containing protein

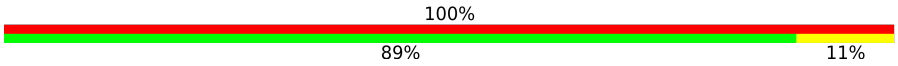
Chain 4O:





• Molecule 40: GINS subunit domain-containing protein

Chain 4o:



D355 I356 P357 W358 P359 A360 R361 T362 D363 W364 G365 G366 H367 D368 P369 A370 T371 P372 P373 A374 E375 L376 M377 I378 N379 T380 H381 S382 M383 F384 W385 P386 V387 A388 I389 F390 I391 Y392 V393 S394 A395 I396 Y397 M398 V399 K400 K401

• Molecule 41: Cytochrome oxidase subunit II copper A binding domain-containing protein

Chain 4P:



K26 S27 Y28 Y29 D30 D31 F32 K33 D34 R35 L36 K37 P38 G39 K40 Y41 T42 Q43 G44 R45 C46 P47 Q48 S49 E50 G51 D52 Y53 R54 Q55 E56 S57 K58 T59 I60 G61 R62 E63 H64 L65 N66 D67 D68 G69 T70 R71 S72 K73 R74 Y75 T76 V77 K78 E79 A80 D81 A82 L83 G84 Y85

H86 Y87 H88 P89 P90 I91 D92 K93 K94 G95 Q96 V97 Y98 V99 K100 G101 P102 N103 T104 V105 I106 E107 R108 G109 Q110 T111 W112 I113 K114 G115 Y116 E117 L118 P119 S120 M121 E122 Y123 T124 Y125 G126 P127 K128 Q129 E130 D131 I132 P133 F134 Y135 P136 R137 V138 K139 L140 N141 V142 W143 G144 N145

Y146 N147 L148 V149 M150 K151 V152 E153 F154 L155 F156 F157 Y158 L159 P160 T161 I162 I163 V164 F165 G166 I167 C168 I169 P170 V171 Y172 T173 I174 N175 F176 A177 Q178 E179 E180 V181 I182 Y183 T184 T185 M186 T187 V188 K189 V190 T191 G192 R193 Q194 W195 Y196 W197 V198 Y199 E200 V201 E202 S203 P204 T205

• Molecule 41: Cytochrome oxidase subunit II copper A binding domain-containing protein

Chain 4p:



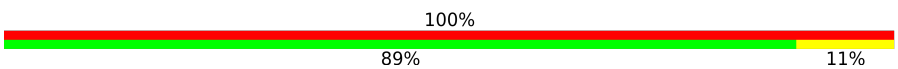
K26 S27 Y28 Y29 D30 D31 F32 K33 D34 R35 L36 K37 P38 G39 K40 Y41 T42 Q43 G44 R45 C46 P47 Q48 S49 E50 G51 D52 Y53 R54 Q55 E56 S57 K58 T59 I60 G61 R62 E63 H64 L65 N66 D67 D68 G69 T70 R71 S72 K73 R74 Y75 T76 V77 K78 E79 A80 D81 A82 L83 G84 Y85

H86 Y87 H88 P89 P90 I91 D92 K93 K94 G95 Q96 V97 Y98 V99 K100 G101 P102 N103 T104 V105 I106 E107 R108 G109 Q110 T111 W112 I113 K114 G115 Y116 E117 L118 P119 S120 M121 E122 Y123 T124 Y125 G126 P127 K128 Q129 E130 D131 I132 P133 F134 Y135 P136 R137 V138 K139 L140 N141 V142 W143 G144 N145

Y146 N147 L148 V149 M150 K151 V152 E153 F154 L155 F156 F157 Y158 L159 P160 T161 I162 I163 V164 F165 G166 I167 C168 I169 P170 V171 Y172 T173 I174 N175 F176 A177 Q178 E179 E180 V181 I182 Y183 T184 T185 M186 T187 V188 K189 V190 T191 G192 R193 Q194 W195 Y196 W197 V198 Y199 E200 V201 E202 S203 P204 T205

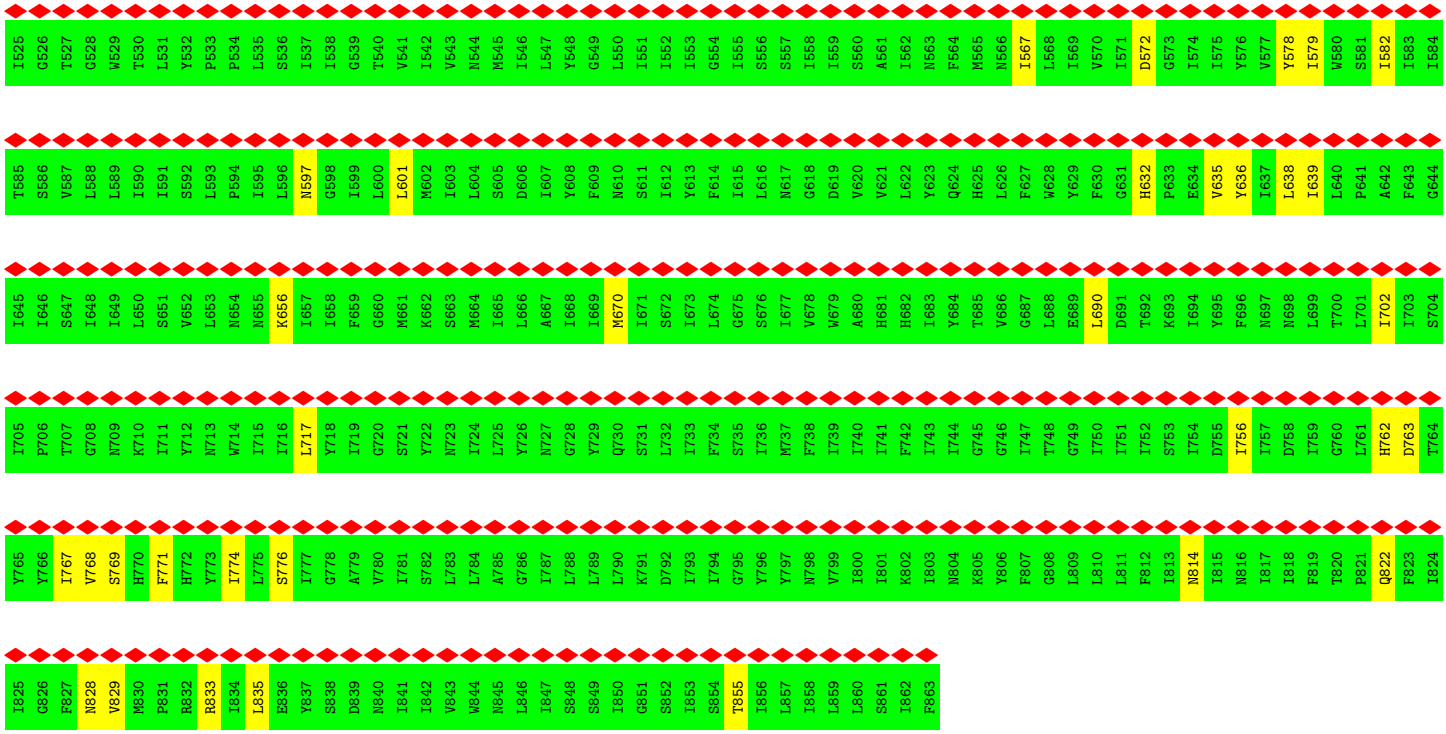
• Molecule 42: Cytochrome c oxidase subunit 1

Chain 4Q:



F405 Y406 I407 L408 V409 M410 N411 N412 K413 R414 I415 G416 I417 Y418 Y419 I420 K421 L422 S423 I424 I425 I426 G427 I428 L429 G430 I431 V432 L433 S434 Y435 I436 I437 R438 V439 E440 L441 Y442 N443 S444 G445 N446 R447 I448 I449 K450 Y451 D452 N453 V454 N455 Y456 Y457 N458 M459 V460 I461 T462 L463 H464

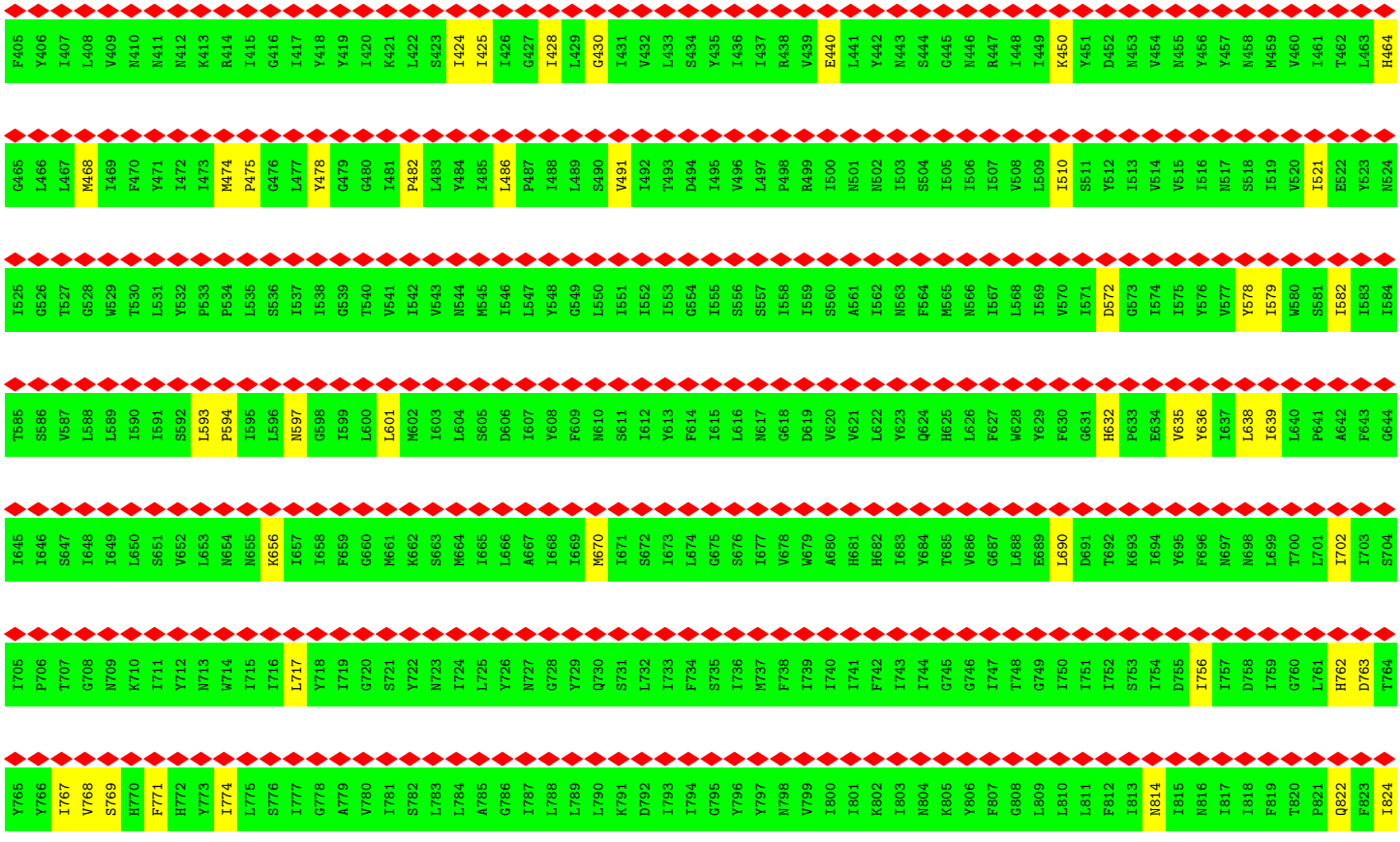
G465 L466 L467 M468 I469 F470 Y471 I472 I473 M474 P475 G476 L477 Y478 G479 G480 I481 P482 L483 Y484 I485 L486 P487 I488 L489 S490 V491 I492 T493 D494 I495 V496 L497 P498 R499 I500 N501 N502 I503 S504 I505 I506 I507 V508 L509 I510 S511 Y512 I513 V514 V515 I516 N517 S518 I519 V520 I521 E522 Y523 N524

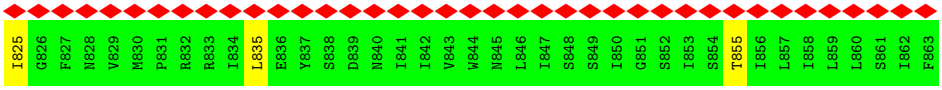


• Molecule 42: Cytochrome c oxidase subunit 1

Chain 4q:

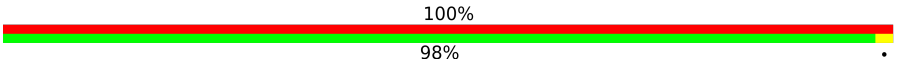


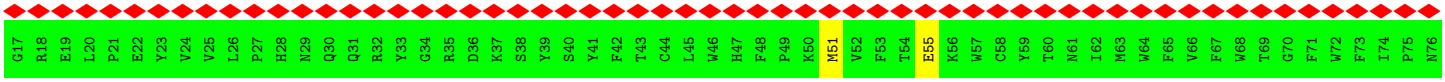


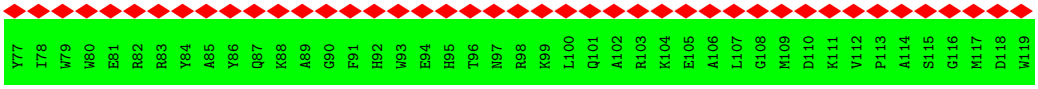


• Molecule 43: Cytochrome c oxidase subunit 32

Chain 4R:



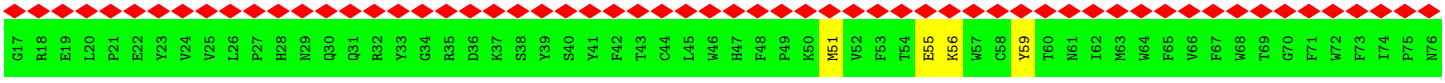


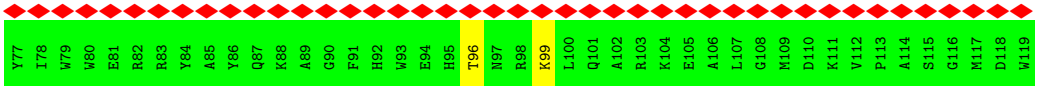


• Molecule 43: Cytochrome c oxidase subunit 32

Chain 4r:



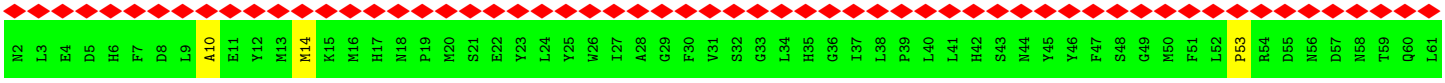


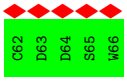


• Molecule 44: Cytochrome c oxidase subunit 7C

Chain 4S:

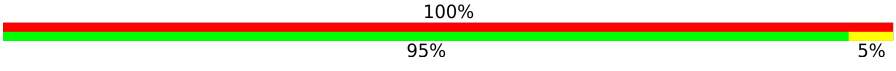


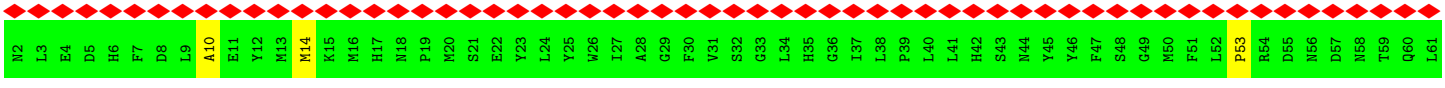


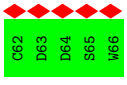


• Molecule 44: Cytochrome c oxidase subunit 7C

Chain 4s:



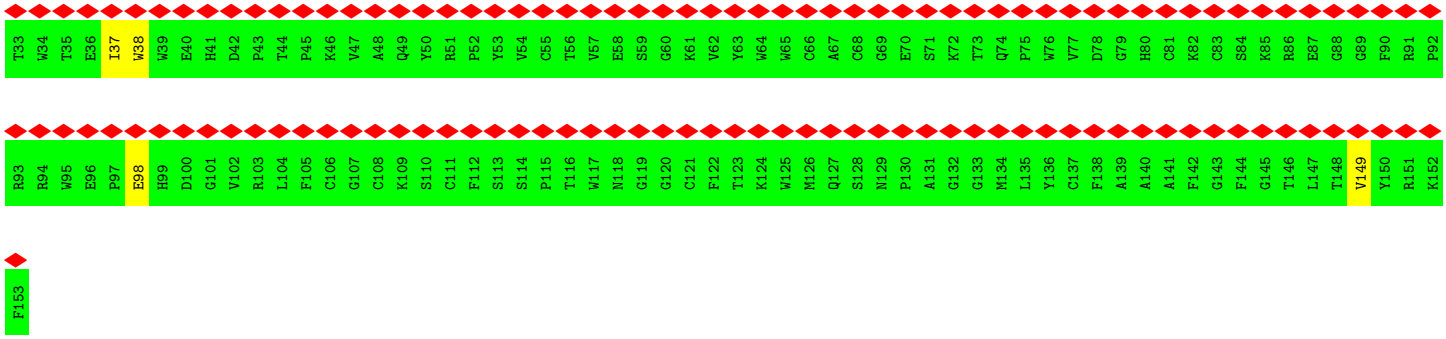




• Molecule 45: Cytochrome c oxidase subunit 13

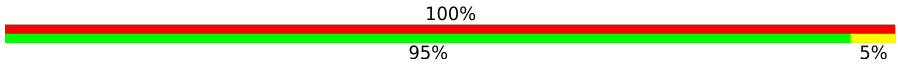
Chain 4T:

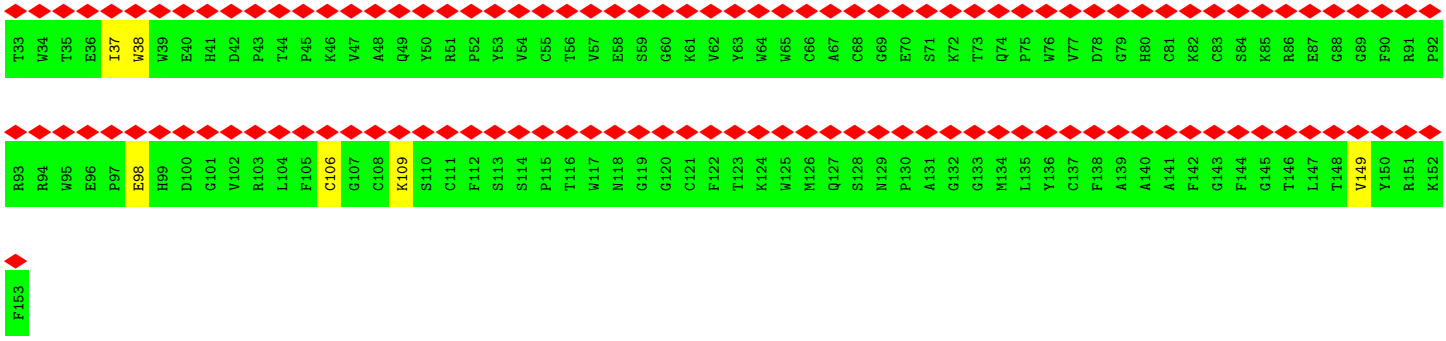




• Molecule 45: Cytochrome c oxidase subunit 13

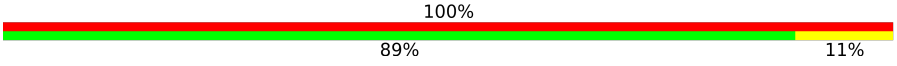
Chain 4t:

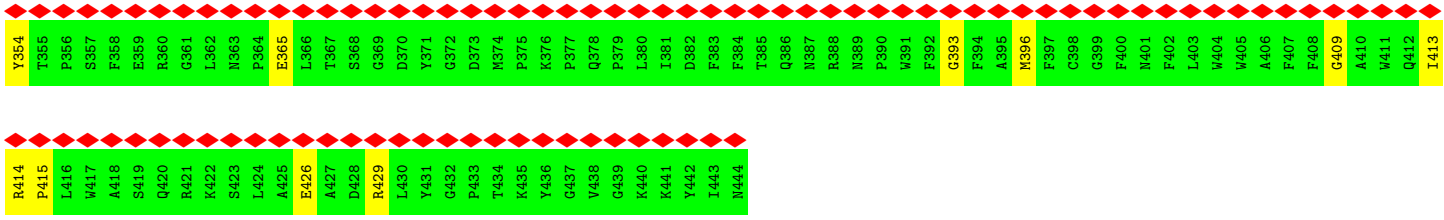




• Molecule 46: Amino acid transporter transmembrane domain-containing protein

Chain 4U:





• Molecule 46: Amino acid transporter transmembrane domain-containing protein

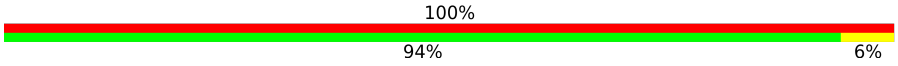
Chain 4u:





• Molecule 47: Cytochrome c oxidase subunit 4

Chain 4V:



R-7 I-6 G-5 G-4 P-3 P-2 V-1 F0 M1 Q2 F3 P4 P5 P6 P7 P8 K9 E10 Y11 L12 A13 D14 G15 T16 P17 K18 T19 Y20 P21 L22 H23 Q24 P25 V26 F27 D28 H29 G30 Y31 T32 W33 E34 H35 W36 Y37 M38 T39 N40 A41 G42 V43 F44 H45 T46 V47 Y48 Y49 G50 E51 F52

A53 K54 D55 F56 P57 W58 R59 W60 G61 F62 V63 A64 E65 K66 P67 F68 W69 V70 G71 A72 P73 I74 L75 V76 L77 G78 V79 L80 C81 L82 G83 H84 I85 I86 Q87 T88 M89 G90 Q91 I92 G93 V94 R95 P96 K97 R98 Y99 T100 P101 E102 W103 V104 E105 A106 T107 K108 E109 R110 E111 R112

A113 E114 N115 T116 N117 P118 I119 T120 R121 Y122 L123 D124 R125 R126 R127 A128 E129 R130 G131 P132 Y133 Y134 L135 M136 S137 N138 V139 L140 P141 Y142 H143 P144 H145 F146 L147 W148 M149 R150 N151 S152 H153 D154 Y155 E156 A157 A158 E159 A160 L161 A162 A163 R164 R165 E166 K167 D168 R169 E170 L171 A172

A173 K174 L175 E176 A177

• Molecule 47: Cytochrome c oxidase subunit 4

Chain 4v:



R-7 I-6 G-5 G-4 P-3 P-2 V-1 F0 M1 Q2 F3 P4 P5 P6 P7 P8 K9 E10 Y11 L12 A13 D14 G15 T16 P17 K18 T19 Y20 P21 L22 H23 Q24 P25 V26 F27 D28 H29 G30 Y31 T32 W33 E34 H35 W36 Y37 M38 T39 N40 A41 G42 V43 F44 H45 T46 V47 Y48 Y49 G50 E51 F52

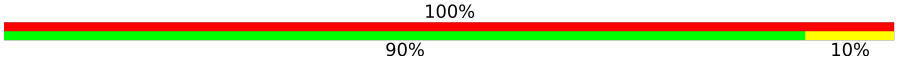
A53 K54 D55 F56 P57 W58 R59 W60 G61 F62 V63 A64 E65 K66 P67 F68 W69 V70 G71 A72 P73 I74 L75 V76 L77 G78 V79 L80 C81 L82 G83 H84 I85 I86 Q87 T88 M89 G90 Q91 I92 G93 V94 R95 P96 K97 R98 Y99 T100 P101 E102 W103 V104 E105 A106 T107 K108 E109 R110 E111 R112

A113 E114 N115 T116 N117 P118 I119 T120 R121 Y122 L123 D124 R125 R126 R127 A128 E129 R130 G131 P132 Y133 Y134 L135 M136 S137 N138 V139 L140 P141 Y142 H143 P144 H145 F146 L147 W148 M149 R150 N151 S152 H153 D154 Y155 E156 A157 A158 E159 A160 L161 A162 A163 R164 R165 E166 K167 D168 R169 E170 L171 A172

A173 K174 L175 E176 A177

• Molecule 48: Cytochrome c oxidase subunit 19

Chain 4W:



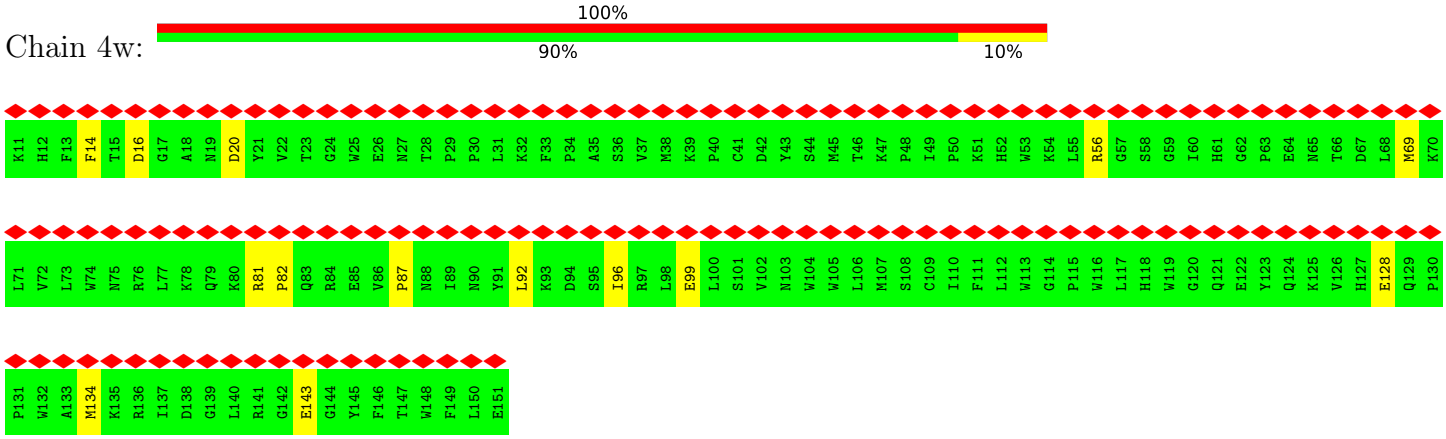
K11 H12 F13 F14 T15 D16 G17 A18 N19 D20 Y21 V22 T23 G24 W25 E26 N27 T28 P29 P30 L31 K32 F33 P34 A35 S36 V37 M38 K39 P40 C41 D42 Y43 S44 M45 T46 K47 P48 I49 P50 K51 H52 W53 K54 L55 R56 G57 S58 G59 I60 H61 G62 P63 E64 W65 T66 D67 L68 M69 K70

L71 V72 L73 W74 N75 R76 L77 K78 Q79 K80 R81 P82 Q83 R84 E85 V86 P87 N88 I89 N90 Y91 L92 K93 D94 S95 I96 R97 L98 E99 L100 S101 V102 N103 W104 W105 L106 M107 S108 C109 I110 F111 L112 W113 G114 P115 W116 L117 H118 W119 G120 Q121 E122 Y123 Q124 K125 V126 H127 E128 Q129 P130

P131 W132 A133 M134 K135 R136 I137 D138 G139 L140 R141 G142 E143 G144 Y145 F146 T147 W148 F149 L150 E151

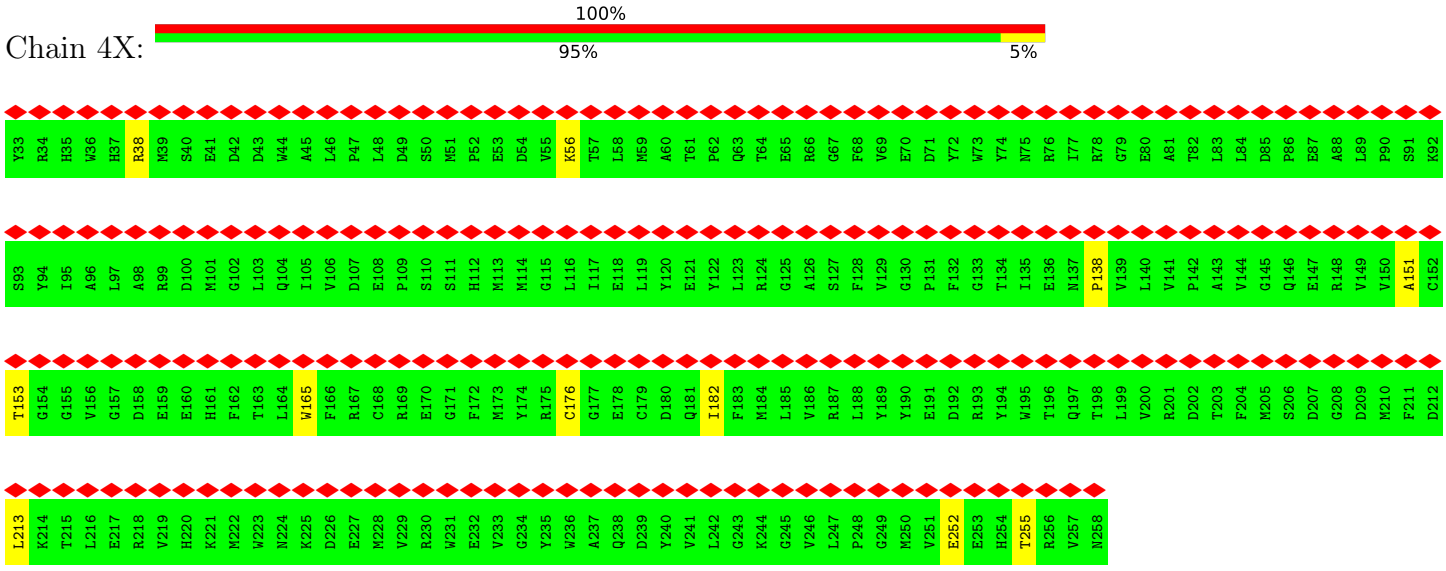
• Molecule 48: Cytochrome c oxidase subunit 19

Chain 4w:



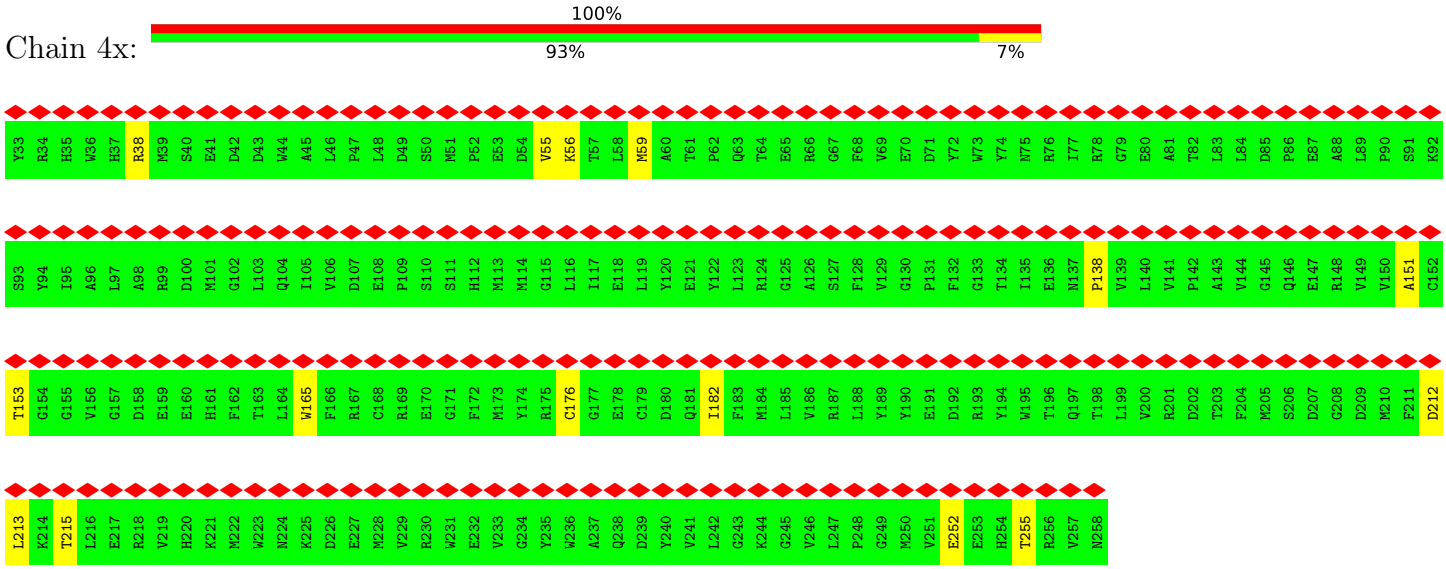
• Molecule 49: Cytochrome Coxidase subunit, putative

Chain 4X:



• Molecule 49: Cytochrome Coxidase subunit, putative

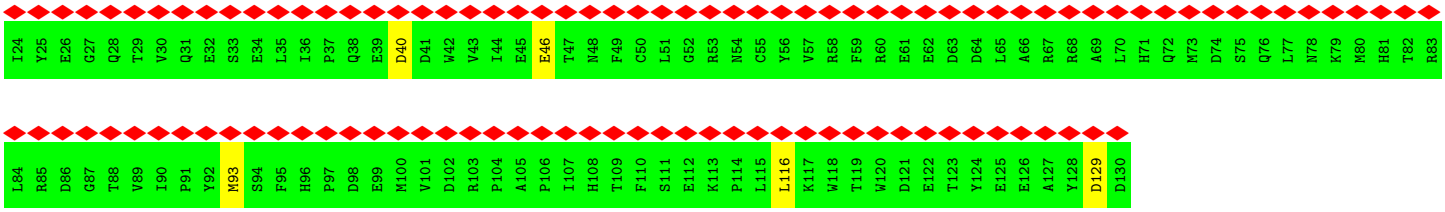
Chain 4x:



• Molecule 50: Cytochrome c oxidase subunit 18

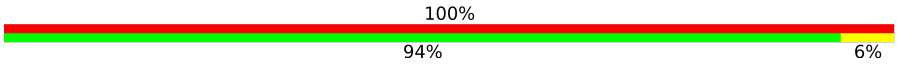
Chain 4Y:

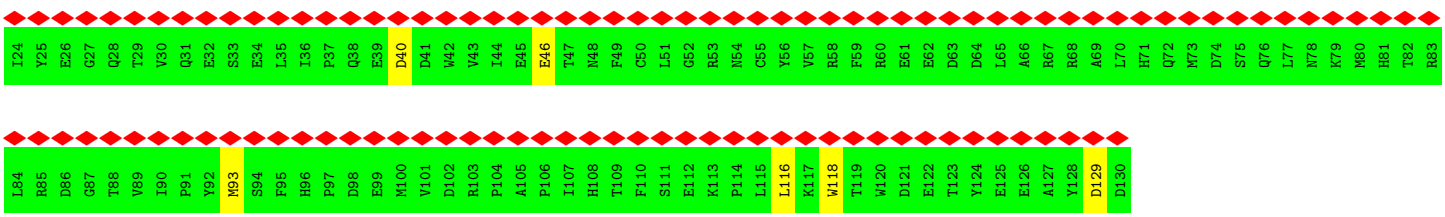




• Molecule 50: Cytochrome c oxidase subunit 18

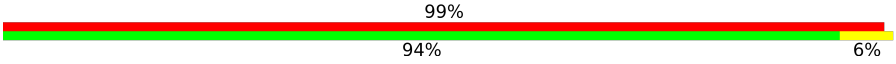
Chain 4y:

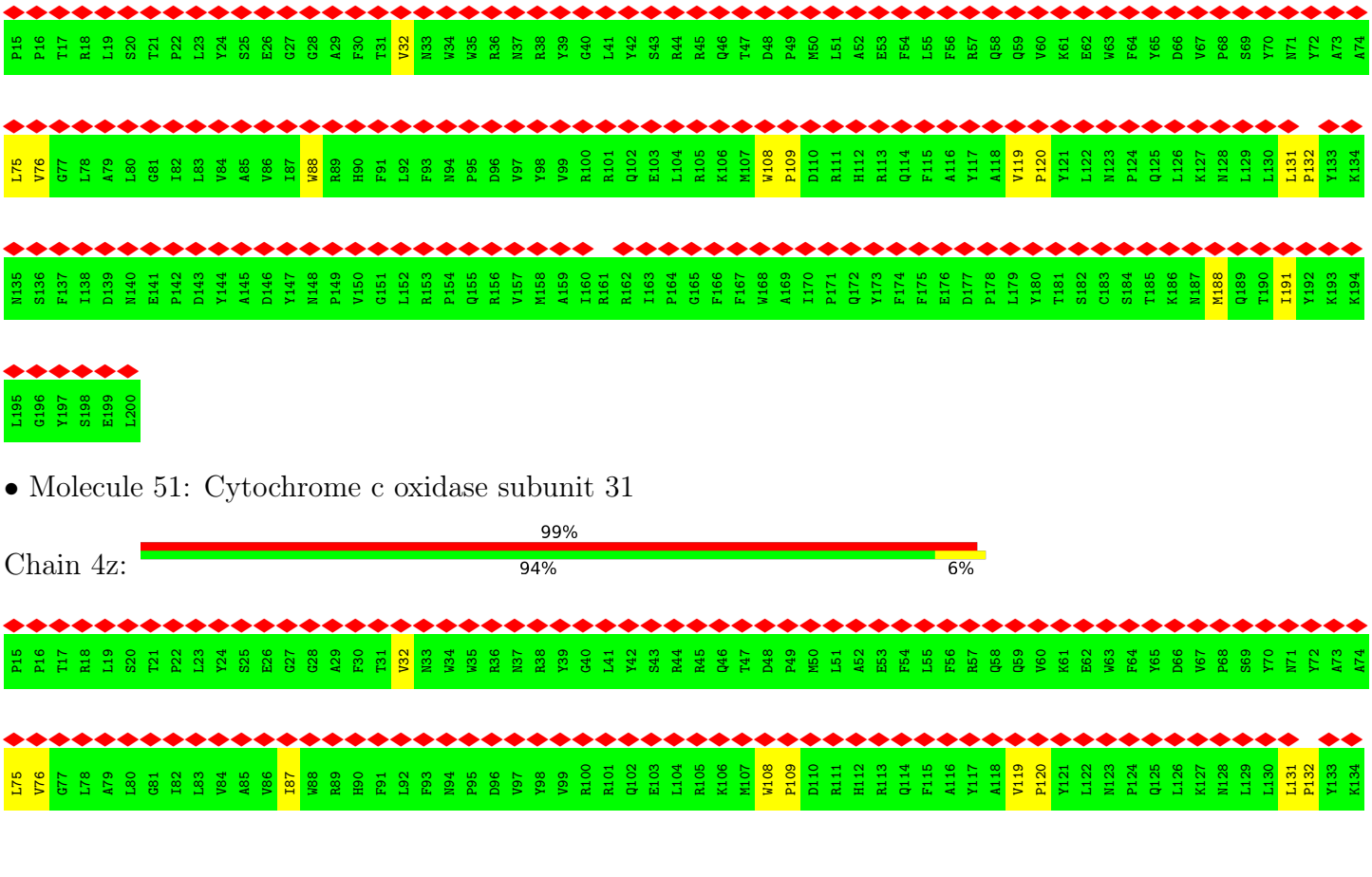




• Molecule 51: Cytochrome c oxidase subunit 31

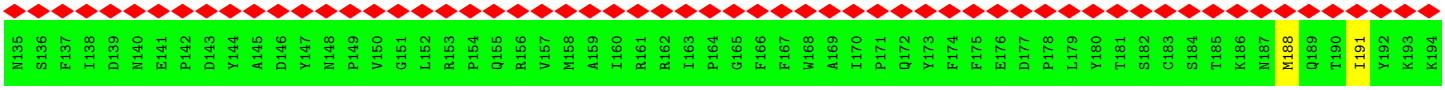
Chain 4Z:

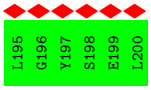




• Molecule 51: Cytochrome c oxidase subunit 31

Chain 4z:


N135
S136
F137
I138
D139
N140
E141
P142
D143
Y144
A145
D146
Y147
N148
P149
V150
G151
L152
R153
P154
Q155
R156
V157
M158
A159
I160
R161
R162
I163
P164
G165
F166
F167
W168
A169
I170
P171
Q172
Y173
F174
F175
E176
D177
P178
L179
Y180
T181
S182
C183
S184
T185
K186
N187
M188
Q189
T190
I191
Y192
K193
K194


L195
G196
Y197
S198
E199
L200

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111717	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 ($e^-/Å^2$)	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	0.173	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	423.2, 423.2, 423.2	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, HEM, PEE, AME, FES, PC1, SF4, F3S, MG, CDL, FAD, K, PER, UQ1, HEA, CUA, LPP, CU, HEC

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	0.44	6/4701 (0.1%)	0.54	5/6363 (0.1%)
1	2m	0.44	5/4701 (0.1%)	0.53	4/6363 (0.1%)
2	2N	0.23	0/2118	0.38	0/2863
2	2n	0.23	0/2118	0.38	0/2863
3	2O	0.24	0/1292	0.38	0/1759
3	2o	0.24	0/1292	0.38	0/1759
4	2P	0.17	0/1342	0.32	0/1812
4	2p	0.17	0/1342	0.32	0/1812
5	2Q	0.17	0/580	0.36	0/788
5	2q	0.17	0/580	0.36	0/788
6	2R	0.23	0/985	0.31	0/1336
6	2r	0.23	0/985	0.31	0/1336
7	2S	0.19	0/1341	0.31	0/1816
7	2s	0.18	0/1341	0.32	0/1816
8	2T	1.31	10/714 (1.4%)	1.29	11/971 (1.1%)
8	2t	1.31	10/714 (1.4%)	1.29	11/971 (1.1%)
9	2U	0.18	0/400	0.33	0/547
9	2u	0.18	0/400	0.33	0/547
10	2V	0.21	0/716	0.40	0/965
10	2v	0.21	0/716	0.39	0/965
11	30	0.35	0/1124	0.56	0/1518
12	31	0.30	0/1240	0.57	0/1667
13	3A	0.19	0/3701	0.28	0/5025
13	3a	0.19	0/3701	0.28	0/5025
14	3B	0.21	0/3967	0.31	0/5371
14	3b	0.21	0/3967	0.31	0/5371
15	3C	0.22	0/1988	0.34	0/2712
15	3c	0.21	0/1997	0.35	0/2724
16	3D	0.32	0/872	0.44	1/1182 (0.1%)
16	3d	0.88	5/872 (0.6%)	0.66	3/1182 (0.3%)
17	3E	0.24	0/848	0.33	0/1148

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	3e	0.25	0/848	0.33	0/1148
18	3F	0.21	0/767	0.33	0/1042
18	3f	0.21	0/767	0.33	0/1042
19	3G	0.20	0/3098	0.35	0/4231
19	3g	0.21	0/3098	0.40	0/4231
20	3H	0.18	0/2713	0.36	0/3693
20	3h	0.18	0/2705	0.36	0/3682
21	3I	0.20	0/1514	0.34	0/2045
21	3i	0.20	0/1514	0.34	0/2045
22	3J	0.29	0/776	0.42	1/1045 (0.1%)
22	3j	0.29	0/776	0.42	1/1045 (0.1%)
23	3K	0.15	0/627	0.32	0/847
23	3k	0.15	0/627	0.32	0/847
24	3L	0.19	0/554	0.40	0/755
24	3l	0.19	0/554	0.41	0/755
25	40	0.20	0/2060	0.36	0/2822
25	41	0.20	0/2060	0.36	0/2822
26	4A	0.16	0/863	0.32	0/1166
26	4a	0.16	0/863	0.32	0/1166
27	4B	0.17	0/751	0.30	0/1013
27	4b	0.17	0/751	0.30	0/1013
28	4C	0.16	0/653	0.30	0/891
28	4c	0.16	0/653	0.30	0/891
29	4D	0.16	0/819	0.31	0/1110
29	4d	0.16	0/819	0.31	0/1110
30	4E	0.17	0/1353	0.34	0/1824
30	4e	0.17	0/1353	0.34	0/1824
31	4F	0.22	0/695	0.34	0/948
31	4f	0.22	0/735	0.35	0/1001
32	4G	0.16	0/883	0.26	0/1199
32	4g	0.16	0/883	0.26	0/1199
33	4H	0.14	0/1149	0.26	0/1565
33	4h	0.14	0/1149	0.26	0/1565
34	4I	0.22	0/1757	0.28	0/2386
34	4i	0.22	0/1757	0.29	0/2386
35	4J	0.22	0/1573	0.33	0/2131
35	4j	0.22	0/1573	0.33	0/2131
36	4K	0.21	0/745	0.34	0/1017
36	4k	0.21	0/745	0.34	0/1017
37	4L	0.17	0/1131	0.27	0/1537
37	4l	0.17	0/1131	0.27	0/1537
38	4M	0.17	0/805	0.30	0/1104
38	4m	0.16	0/805	0.30	0/1104

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	4N	0.18	0/1055	0.32	0/1436
39	4n	0.18	0/1055	0.32	0/1436
40	4O	0.29	0/400	0.36	0/549
40	4o	0.29	0/400	0.36	0/549
41	4P	0.17	0/1551	0.30	0/2106
41	4p	0.16	0/1551	0.30	0/2106
42	4Q	0.24	0/3774	0.36	0/5155
42	4q	0.24	0/3774	0.37	0/5155
43	4R	0.14	0/958	0.25	0/1301
43	4r	0.14	0/958	0.25	0/1301
44	4S	0.15	0/560	0.24	0/760
44	4s	0.15	0/560	0.24	0/760
45	4T	0.18	0/1024	0.27	0/1391
45	4t	0.18	0/1024	0.27	0/1391
46	4U	0.14	0/790	0.35	0/1073
46	4u	0.14	0/790	0.35	0/1073
47	4V	0.23	0/1600	0.32	0/2183
47	4v	0.23	0/1600	0.32	0/2183
48	4W	0.17	0/1240	0.32	0/1686
48	4w	0.17	0/1240	0.33	0/1686
49	4X	0.18	0/1912	0.32	0/2592
49	4x	0.18	0/1912	0.32	0/2592
50	4Y	0.17	0/929	0.27	0/1261
50	4y	0.16	0/929	0.27	0/1261
51	4Z	0.18	0/1639	0.32	0/2233
51	4z	0.18	0/1639	0.32	0/2233
All	All	0.27	36/138971 (0.0%)	0.38	37/188749 (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
1	2M	0	3
1	2m	0	3
4	2P	0	3
4	2p	0	3
5	2Q	0	1
5	2q	0	1
7	2S	0	1
7	2s	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	2T	0	3
8	2t	0	3
10	2V	0	2
10	2v	0	2
11	30	0	3
12	31	0	6
16	3D	0	1
16	3d	0	2
18	3F	0	1
18	3f	0	1
20	3H	0	1
20	3h	0	1
21	3I	0	2
21	3i	0	2
26	4A	0	1
26	4a	0	1
28	4C	0	1
28	4c	0	1
29	4D	0	1
29	4d	0	1
31	4F	0	1
31	4f	0	1
33	4H	0	1
33	4h	0	1
35	4J	0	1
35	4j	0	1
36	4K	0	2
36	4k	0	2
47	4V	0	1
47	4v	0	1
49	4X	0	1
49	4x	0	1
All	All	0	66

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3d	109	TYR	CG-CD2	-16.85	1.03	1.39
8	2t	45	TYR	CG-CD2	-13.32	1.11	1.39
8	2T	45	TYR	CG-CD2	-13.25	1.11	1.39
8	2t	45	TYR	CG-CD1	-12.97	1.12	1.39
8	2T	45	TYR	CG-CD1	-12.96	1.12	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2t	51	TYR	CG-CD1	-11.88	1.14	1.39
8	2T	51	TYR	CG-CD1	-11.84	1.14	1.39
8	2t	76	LEU	CG-CD1	-11.82	1.13	1.52
8	2T	76	LEU	CG-CD1	-11.78	1.13	1.52
8	2t	51	TYR	CG-CD2	-11.35	1.15	1.39
8	2T	51	TYR	CG-CD2	-11.34	1.15	1.39
8	2t	51	TYR	CE2-CZ	-11.30	1.11	1.38
8	2T	51	TYR	CE2-CZ	-11.30	1.11	1.38
1	2m	297	ARG	NE-CZ	-11.25	1.20	1.33
1	2M	297	ARG	NE-CZ	-11.23	1.20	1.33
16	3d	109	TYR	CG-CD1	-10.22	1.17	1.39
16	3d	109	TYR	CE1-CZ	-9.94	1.14	1.38
8	2t	76	LEU	CG-CD2	-9.91	1.19	1.52
8	2T	76	LEU	CG-CD2	-9.88	1.20	1.52
8	2T	45	TYR	CE1-CZ	-8.77	1.17	1.38
8	2t	45	TYR	CE1-CZ	-8.75	1.17	1.38
8	2T	45	TYR	CE2-CZ	-8.54	1.17	1.38
8	2t	45	TYR	CE2-CZ	-8.53	1.17	1.38
1	2M	98	TRP	N-CA	-8.00	1.36	1.46
1	2m	98	TRP	N-CA	-8.00	1.36	1.46
16	3d	109	TYR	CE2-CZ	-7.97	1.19	1.38
8	2T	51	TYR	CE1-CZ	-6.57	1.22	1.38
8	2t	51	TYR	CE1-CZ	-6.56	1.22	1.38
1	2m	297	ARG	CG-CD	-6.50	1.32	1.52
1	2M	297	ARG	CG-CD	-6.50	1.32	1.52
1	2M	297	ARG	CZ-NH1	-6.17	1.24	1.32
1	2m	297	ARG	CZ-NH1	-6.15	1.24	1.32
16	3d	109	TYR	CD1-CE1	6.02	1.56	1.38
1	2M	92	THR	CB-CG2	-5.66	1.33	1.52
1	2M	156	LYS	CE-NZ	-5.17	1.33	1.49
1	2m	156	LYS	CE-NZ	-5.16	1.33	1.49

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2T	76	LEU	CD1-CG-CD2	-20.95	64.71	110.80
8	2t	76	LEU	CD1-CG-CD2	-20.94	64.74	110.80
8	2T	51	TYR	CE1-CZ-CE2	-14.89	90.51	120.30
8	2t	51	TYR	CE1-CZ-CE2	-14.85	90.59	120.30
8	2t	45	TYR	CE1-CZ-CE2	-13.43	93.43	120.30
8	2T	45	TYR	CE1-CZ-CE2	-13.41	93.47	120.30
8	2T	51	TYR	CD1-CG-CD2	-12.04	100.05	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2t	51	TYR	CD1-CG-CD2	-12.02	100.08	118.10
8	2T	45	TYR	CD1-CG-CD2	-11.40	101.00	118.10
8	2t	45	TYR	CD1-CG-CD2	-11.34	101.08	118.10
16	3d	109	TYR	CE1-CZ-CE2	-9.86	100.59	120.30
1	2M	92	THR	OG1-CB-CG2	-9.78	89.74	109.30
16	3d	109	TYR	CD1-CG-CD2	-9.75	103.48	118.10
1	2m	98	TRP	N-CA-C	8.59	121.59	111.71
1	2M	98	TRP	N-CA-C	8.56	121.56	111.71
1	2m	297	ARG	NE-CZ-NH1	-8.08	113.42	121.50
1	2M	297	ARG	NE-CZ-NH1	-8.04	113.46	121.50
16	3d	109	TYR	CZ-CE2-CD2	7.34	132.82	119.60
1	2m	297	ARG	NE-CZ-NH2	7.22	125.69	119.20
1	2M	297	ARG	NE-CZ-NH2	7.13	125.61	119.20
8	2T	45	TYR	CB-CG-CD2	7.12	131.49	120.80
8	2t	45	TYR	CB-CG-CD2	7.12	131.48	120.80
8	2T	51	TYR	CB-CG-CD2	7.03	131.34	120.80
8	2t	51	TYR	CB-CG-CD2	6.97	131.25	120.80
8	2t	76	LEU	CB-CG-CD1	6.14	129.11	110.70
8	2T	76	LEU	CB-CG-CD1	6.12	129.06	110.70
8	2T	51	TYR	CD1-CE1-CZ	6.10	130.59	119.60
8	2t	51	TYR	CD1-CE1-CZ	6.07	130.53	119.60
8	2t	45	TYR	CD1-CE1-CZ	5.95	130.31	119.60
8	2T	45	TYR	CD1-CE1-CZ	5.92	130.26	119.60
8	2T	45	TYR	CZ-CE2-CD2	5.75	129.94	119.60
8	2t	45	TYR	CZ-CE2-CD2	5.72	129.91	119.60
1	2M	297	ARG	CD-NE-CZ	-5.32	116.96	124.40
1	2m	297	ARG	CD-NE-CZ	-5.28	117.01	124.40
16	3D	109	TYR	CA-C-O	-5.08	115.39	120.77
22	3J	61	MET	CB-CG-SD	5.03	127.79	112.70
22	3j	61	MET	CB-CG-SD	5.03	127.78	112.70

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2M	165	ARG	Sidechain
1	2M	290	ARG	Sidechain
1	2M	564	ARG	Sidechain
4	2P	22	ARG	Sidechain
4	2P	72	ARG	Sidechain
4	2P	73	ARG	Sidechain
5	2Q	34	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	2S	94	ARG	Sidechain
8	2T	2	ARG	Sidechain
8	2T	45	TYR	Sidechain
8	2T	51	TYR	Sidechain
10	2V	39	ARG	Sidechain
10	2V	81	ARG	Sidechain
1	2m	165	ARG	Sidechain
1	2m	290	ARG	Sidechain
1	2m	564	ARG	Sidechain
4	2p	22	ARG	Sidechain
4	2p	72	ARG	Sidechain
4	2p	73	ARG	Sidechain
5	2q	34	ARG	Sidechain
7	2s	94	ARG	Sidechain
8	2t	2	ARG	Sidechain
8	2t	45	TYR	Sidechain
8	2t	51	TYR	Sidechain
10	2v	39	ARG	Sidechain
10	2v	81	ARG	Sidechain
11	30	143	ARG	Sidechain
11	30	170	ARG	Sidechain
11	30	69	ARG	Sidechain
12	31	121	ARG	Sidechain
12	31	154	ARG	Sidechain
12	31	28	ARG	Sidechain
12	31	50	ARG	Sidechain
12	31	67	ARG	Sidechain
12	31	68	ARG	Sidechain
16	3D	72	ARG	Sidechain
18	3F	7	ARG	Sidechain
20	3H	108	ARG	Sidechain
21	3I	5	ARG	Sidechain
21	3I	9	ARG	Sidechain
16	3d	109	TYR	Sidechain
16	3d	72	ARG	Sidechain
18	3f	7	ARG	Sidechain
20	3h	108	ARG	Sidechain
21	3i	5	ARG	Sidechain
21	3i	9	ARG	Sidechain
26	4A	27	ARG	Sidechain
28	4C	63	ARG	Sidechain
29	4D	19	ARG	Sidechain

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Mol	Chain	Res	Type	Group
31	4F	142	ARG	Sidechain
33	4H	144	ARG	Sidechain
35	4J	49	ARG	Sidechain
36	4K	10	ARG	Sidechain
36	4K	84	ARG	Sidechain
47	4V	127	ARG	Sidechain
49	4X	38	ARG	Sidechain
26	4a	27	ARG	Sidechain
28	4c	63	ARG	Sidechain
29	4d	19	ARG	Sidechain
31	4f	142	ARG	Sidechain
33	4h	144	ARG	Sidechain
35	4j	49	ARG	Sidechain
36	4k	10	ARG	Sidechain
36	4k	84	ARG	Sidechain
47	4v	127	ARG	Sidechain
49	4x	38	ARG	Sidechain

5.2 Too-close contacts (i)

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	4602	0	4530	32	0
1	2m	4602	0	4530	35	0
2	2N	2068	0	2025	14	0
2	2n	2068	0	2025	14	0
3	2O	1254	0	1263	6	0
3	2o	1254	0	1263	7	0
4	2P	1309	0	1367	7	0
4	2p	1309	0	1367	10	0
5	2Q	564	0	567	2	0
5	2q	564	0	567	3	0
6	2R	950	0	935	7	0
6	2r	950	0	935	7	0
7	2S	1323	0	1261	2	0
7	2s	1323	0	1261	3	0
8	2T	695	0	672	6	0
8	2t	695	0	672	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2U	390	0	369	4	0
9	2u	390	0	369	6	0
10	2V	701	0	714	4	0
10	2v	701	0	714	3	0
11	30	1181	0	1061	10	0
12	31	1219	0	1185	14	0
13	3A	3622	0	3508	11	0
13	3a	3622	0	3508	10	0
14	3B	3884	0	3842	13	0
14	3b	3884	0	3842	12	0
15	3C	1921	0	1816	10	0
15	3c	1930	0	1822	22	0
16	3D	836	0	798	7	0
16	3d	836	0	798	6	0
17	3E	813	0	776	5	0
17	3e	813	0	776	6	0
18	3F	734	0	704	5	0
18	3f	734	0	704	5	0
19	3G	3016	0	3162	30	0
19	3g	3016	0	3162	42	0
20	3H	2628	0	2541	23	0
20	3h	2621	0	2534	24	0
21	3I	1472	0	1436	14	0
21	3i	1472	0	1436	12	0
22	3J	755	0	693	7	0
22	3j	755	0	693	10	0
23	3K	608	0	617	3	0
23	3k	608	0	617	3	0
24	3L	539	0	536	8	0
24	3l	539	0	536	7	0
25	40	2004	0	2032	11	0
25	41	2004	0	2032	13	0
26	4A	841	0	766	7	0
26	4a	841	0	766	7	0
27	4B	732	0	746	3	0
27	4b	732	0	746	4	0
28	4C	626	0	575	4	0
28	4c	626	0	575	3	0
29	4D	787	0	745	8	0
29	4d	787	0	745	8	0
30	4E	1313	0	1269	8	0
30	4e	1313	0	1269	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4F	669	0	642	5	0
31	4f	708	0	678	2	0
32	4G	854	0	811	3	0
32	4g	854	0	811	3	0
33	4H	1125	0	1112	4	0
33	4h	1125	0	1112	5	0
34	4I	1695	0	1593	11	0
34	4i	1695	0	1593	13	0
35	4J	1517	0	1435	11	0
35	4j	1517	0	1435	10	0
36	4K	722	0	760	4	0
36	4k	722	0	760	5	0
37	4L	1083	0	1027	9	0
37	4l	1083	0	1027	12	0
38	4M	778	0	802	8	0
38	4m	778	0	802	11	0
39	4N	1025	0	1018	6	0
39	4n	1025	0	1018	6	0
40	4O	383	0	368	3	0
40	4o	383	0	368	5	0
41	4P	1504	0	1461	12	0
41	4p	1504	0	1461	13	0
42	4Q	3687	0	3956	45	0
42	4q	3687	0	3956	45	0
43	4R	916	0	854	1	0
43	4r	916	0	854	3	0
44	4S	541	0	489	2	0
44	4s	541	0	489	2	0
45	4T	983	0	902	3	0
45	4t	983	0	902	4	0
46	4U	758	0	713	8	0
46	4u	758	0	713	8	0
47	4V	1539	0	1482	10	0
47	4v	1539	0	1482	10	0
48	4W	1193	0	1164	10	0
48	4w	1193	0	1164	11	0
49	4X	1860	0	1764	7	0
49	4x	1860	0	1764	9	0
50	4Y	905	0	835	5	0
50	4y	905	0	835	6	0
51	4Z	1582	0	1548	8	0
51	4z	1582	0	1548	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	2M	53	0	30	0	0
52	2m	53	0	29	0	0
53	2N	18	0	18	0	0
53	2p	18	0	18	1	0
53	3G	36	0	36	5	0
53	3g	36	0	36	4	0
54	2N	4	0	0	0	0
54	2n	4	0	0	0	0
54	3H	4	0	0	1	0
54	3h	4	0	0	1	0
55	2N	8	0	0	0	0
55	2n	8	0	0	0	0
56	2N	7	0	0	0	0
56	2n	7	0	0	0	0
57	2N	1	0	0	0	0
57	2n	1	0	0	0	0
57	4Q	1	0	0	0	0
57	4q	1	0	0	0	0
58	2O	80	0	114	1	0
58	2P	46	0	69	0	0
58	2T	45	0	67	1	0
58	2o	24	0	24	0	0
58	2p	24	0	22	0	0
58	2r	39	0	55	0	0
58	2t	42	0	61	0	0
58	3C	30	0	34	0	0
58	3H	46	0	69	0	0
58	3c	33	0	40	1	0
58	3f	38	0	50	0	0
58	40	158	0	218	1	0
58	41	125	0	175	2	0
58	4D	40	0	57	0	0
58	4Q	36	0	46	0	0
58	4R	43	0	63	0	0
58	4S	27	0	28	0	0
58	4W	51	0	82	0	0
58	4Z	51	0	82	2	0
58	4d	51	0	82	0	0
58	4l	38	0	50	2	0
58	4q	77	0	102	0	0
58	4s	47	0	71	0	0
58	4w	51	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	4z	44	0	62	1	0
59	2O	67	0	78	2	0
59	2P	81	0	112	0	0
59	2Q	100	0	156	0	0
59	2T	71	0	89	0	0
59	2o	86	0	122	0	0
59	2p	74	0	95	1	0
59	2q	100	0	156	7	0
59	2t	66	0	76	2	0
59	3D	184	0	274	0	0
59	3E	93	0	136	0	0
59	3G	175	0	253	0	0
59	3H	173	0	246	2	0
59	3I	212	0	261	1	0
59	3L	259	0	371	5	0
59	3e	148	0	193	5	0
59	3g	307	0	405	3	0
59	3h	85	0	120	2	0
59	3i	127	0	148	3	0
59	3l	181	0	265	7	0
59	41	92	0	137	0	0
59	4E	135	0	167	2	0
59	4F	100	0	156	0	0
59	4J	59	0	64	0	0
59	4K	90	0	133	1	0
59	4L	94	0	141	1	0
59	4M	75	0	100	1	0
59	4O	97	0	147	0	0
59	4Q	170	0	243	2	0
59	4S	100	0	156	0	0
59	4U	72	0	88	0	0
59	4W	73	0	93	0	0
59	4Z	48	0	40	1	0
59	4e	146	0	189	5	0
59	4f	92	0	137	4	0
59	4g	66	0	78	1	0
59	4j	139	0	179	2	0
59	4m	100	0	156	3	0
59	4o	93	0	139	4	0
59	4q	93	0	139	3	0
59	4s	100	0	156	0	0
59	4t	61	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	4z	179	0	264	1	0
60	2P	35	0	44	0	0
60	2R	108	0	176	1	0
60	2T	99	0	155	3	0
60	2o	39	0	52	0	0
60	2p	41	0	56	0	0
60	2r	106	0	169	2	0
60	3A	38	0	53	0	0
60	3H	67	0	82	0	0
60	3a	54	0	88	0	0
60	3f	46	0	69	1	0
60	3h	81	0	116	1	0
60	4F	54	0	88	2	0
60	4e	54	0	88	0	0
61	3C	43	0	31	4	0
61	3c	43	0	31	6	0
62	3G	86	0	60	4	0
62	3g	86	0	60	7	0
63	4C	44	0	67	1	0
63	4Z	44	0	67	0	0
63	4g	39	0	54	0	0
63	4z	38	0	49	0	0
64	4N	2	0	0	0	0
64	4n	2	0	0	0	0
65	4Q	1	0	0	0	0
65	4q	1	0	0	0	0
66	4Q	1	0	0	0	0
66	4q	1	0	0	0	0
67	4Q	120	0	108	9	0
67	4q	120	0	108	11	0
68	4Q	2	0	0	0	0
68	4q	2	0	0	0	0
69	4T	2	0	0	0	0
69	4X	1	0	0	0	0
69	4t	2	0	0	0	0
69	4x	1	0	0	0	0
70	4Q	1	0	0	0	0
70	4n	1	0	0	0	0
All	All	142971	0	142850	813	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 (813) 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)
42:4q:632:HIS:NE2	42:4q:636:TYR:HE2	1.60	0.98
42:4Q:632:HIS:NE2	42:4Q:636:TYR:HE2	1.60	0.97
15:3c:76:CYS:SG	61:3c:302:HEC:CAC	2.69	0.80
19:3G:268:LEU:HD21	19:3G:277:ILE:HG13	1.63	0.80
19:3g:268:LEU:HD21	19:3g:277:ILE:HG13	1.64	0.79
42:4Q:762:HIS:CD2	42:4Q:763:ASP:OD2	2.38	0.77
25:41:124:ASN:HB3	48:4w:99:GLU:HG3	1.69	0.75
42:4q:762:HIS:CD2	42:4q:763:ASP:OD2	2.38	0.75
19:3g:120:TYR:CD1	62:3g:407:HEM:HAA2	2.23	0.74
16:3D:101:VAL:HG22	19:3G:327:GLU:HB2	1.70	0.74
2:2N:164:MET:HG2	2:2N:194:LEU:HD11	1.69	0.74
2:2n:164:MET:HG2	2:2n:194:LEU:HD11	1.69	0.73
42:4q:468:MET:HE3	67:4q:907:HEA:HMC2	1.71	0.73
42:4Q:632:HIS:HE2	42:4Q:636:TYR:HE2	1.36	0.73
17:3E:53:VAL:HG13	17:3E:55:ARG:HE	1.54	0.73
17:3e:53:VAL:HG13	17:3e:55:ARG:HE	1.54	0.72
15:3C:76:CYS:SG	61:3C:302:HEC:CAC	2.77	0.72
25:40:124:ASN:HB3	48:4W:99:GLU:HG3	1.70	0.72
42:4q:632:HIS:HE2	42:4q:636:TYR:HE2	1.36	0.71
42:4Q:632:HIS:NE2	42:4Q:636:TYR:CE2	2.52	0.70
22:3j:49:LEU:HD11	26:4a:22:VAL:HG22	1.75	0.69
15:3c:196:MET:HE3	15:3c:199:PRO:HG3	1.74	0.68
42:4q:632:HIS:NE2	42:4q:636:TYR:CE2	2.52	0.67
26:4a:20:LEU:HD11	26:4a:31:GLU:HG3	1.77	0.67
26:4A:20:LEU:HD11	26:4A:31:GLU:HG3	1.77	0.67
19:3g:278:VAL:HG11	53:3g:401:UQ1:H101	1.76	0.66
47:4V:89:MET:HE2	47:4V:89:MET:HA	1.79	0.65
19:3g:120:TYR:CE1	62:3g:407:HEM:HMA2	2.32	0.65
47:4v:89:MET:HA	47:4v:89:MET:HE2	1.79	0.65
19:3g:42:ASN:HD21	19:3g:164:TYR:HE1	1.44	0.65
39:4n:134:CYS:SG	39:4n:138:HIS:HA	2.37	0.64
39:4N:134:CYS:SG	39:4N:138:HIS:HA	2.37	0.64
19:3G:176:TYR:OH	19:3g:176:TYR:OH	1.96	0.64
26:4A:20:LEU:HD11	26:4A:31:GLU:CG	2.28	0.64
26:4A:20:LEU:HD12	26:4A:28:LEU:HA	1.79	0.64
26:4a:20:LEU:HD11	26:4a:31:GLU:CG	2.28	0.63
1:2M:83:GLY:HA2	1:2M:173:THR:HG21	1.81	0.62
16:3d:101:VAL:HG22	19:3g:327:GLU:HB2	1.82	0.62
19:3g:120:TYR:HE1	62:3g:407:HEM:HMA2	1.64	0.62
26:4a:20:LEU:HD12	26:4a:28:LEU:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4a:34:HIS:O	41:4p:184:THR:OG1	2.18	0.62
6:2R:74:VAL:HG22	60:2R:201:PC1:H322	1.81	0.61
25:40:171:MET:HE3	25:40:171:MET:HA	1.82	0.61
42:4q:767:ILE:HD12	67:4q:908:HEA:HBA1	1.83	0.61
1:2m:83:GLY:HA2	1:2m:173:THR:HG21	1.82	0.61
20:3h:38:GLU:OE1	20:3h:38:GLU:N	2.31	0.61
42:4Q:632:HIS:O	42:4Q:635:VAL:HG22	2.01	0.61
25:41:171:MET:HE3	25:41:171:MET:HA	1.82	0.60
26:4A:34:HIS:O	41:4P:184:THR:OG1	2.19	0.60
42:4Q:636:TYR:HA	42:4Q:639:ILE:HG22	1.82	0.60
42:4q:632:HIS:O	42:4q:635:VAL:HG22	2.01	0.60
25:40:74:ILE:HG23	25:40:216:LEU:HD22	1.83	0.60
17:3e:53:VAL:CG1	17:3e:55:ARG:HE	2.15	0.60
20:3H:38:GLU:OE1	20:3H:38:GLU:N	2.31	0.60
1:2m:560:SER:HA	1:2m:604:LEU:HD21	1.84	0.59
25:41:74:ILE:HG23	25:41:216:LEU:HD22	1.83	0.59
42:4q:636:TYR:HA	42:4q:639:ILE:HG22	1.82	0.59
1:2M:560:SER:HA	1:2M:604:LEU:HD21	1.84	0.59
19:3G:121:ILE:HA	19:3G:128:SER:HB3	1.85	0.59
17:3E:53:VAL:CG1	17:3E:55:ARG:HE	2.15	0.58
42:4Q:767:ILE:HD12	67:4Q:908:HEA:HBA1	1.85	0.58
25:40:200:TYR:HH	37:4L:60:TRP:CD1	2.21	0.58
19:3G:284:ILE:HG21	19:3G:343:LEU:HD13	1.86	0.58
15:3c:170:TYR:OH	15:3c:196:MET:HE2	2.02	0.58
1:2m:278:ILE:HD11	1:2m:285:MET:HE3	1.86	0.58
28:4C:65:VAL:HG22	28:4C:66:TRP:HD1	1.69	0.58
12:31:96:SER:OG	12:31:103:ALA:HB3	2.04	0.58
28:4c:65:VAL:HG22	28:4c:66:TRP:HD1	1.69	0.58
19:3g:280:ASN:ND2	59:3l:701:CDL:H672	2.18	0.57
19:3g:45:MET:HB3	19:3g:57:ILE:HD11	1.87	0.57
33:4h:144:ARG:HG2	33:4h:144:ARG:HH11	1.69	0.57
41:4P:133:PRO:HB2	47:4V:38:MET:HE2	1.87	0.57
42:4q:468:MET:HB3	67:4q:907:HEA:CAC	2.35	0.57
42:4q:468:MET:CE	67:4q:907:HEA:HMC2	2.35	0.56
17:3e:66:LEU:O	59:3e:202:CDL:H531	2.05	0.56
22:3J:49:LEU:HD11	26:4A:22:VAL:HG22	1.87	0.56
15:3c:147:PRO:HG3	61:3c:302:HEC:HAA1	1.86	0.56
19:3g:284:ILE:HG21	19:3g:343:LEU:HD13	1.87	0.56
30:4E:46:TRP:O	34:4I:84:PRO:CD	2.54	0.56
1:2M:278:ILE:HD11	1:2M:285:MET:HE3	1.86	0.56
41:4p:133:PRO:HB2	47:4v:38:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:4H:144:ARG:HH11	33:4H:144:ARG:HG2	1.69	0.56
35:4J:116:PHE:CZ	35:4J:120:LEU:HD11	2.41	0.56
20:3H:214:TRP:CD2	20:3H:215:PRO:HD2	2.40	0.56
20:3h:214:TRP:CD2	20:3h:215:PRO:HD2	2.41	0.56
59:2O:203:CDL:H372	27:4b:16:ILE:HD13	1.88	0.56
58:3c:301:PEE:H10	22:3j:10:ALA:HB3	1.88	0.56
19:3g:168:PHE:CD2	62:3g:407:HEM:HBC1	2.41	0.56
25:41:200:TYR:HH	37:4l:60:TRP:CD1	2.24	0.55
35:4j:116:PHE:CZ	35:4j:120:LEU:HD11	2.41	0.55
15:3c:159:GLY:HA3	22:3j:4:ALA:O	2.07	0.55
40:4o:377:MET:HG2	42:4q:756:ILE:HG22	1.89	0.55
8:2T:40:ALA:HB1	60:2T:102:PC1:H2D2	1.89	0.55
31:4F:109:TRP:HB2	60:4F:201:PC1:H222	1.88	0.55
46:4u:393:GLY:O	46:4u:396:MET:HE2	2.07	0.55
46:4U:393:GLY:O	46:4U:396:MET:HE2	2.07	0.55
30:4e:46:TRP:O	34:4i:84:PRO:CD	2.55	0.55
11:30:16:THR:HG22	19:3g:245:ILE:HD13	1.89	0.54
20:3H:314:HIS:HD2	15:3c:183:LEU:HD11	1.72	0.54
19:3g:47:ILE:HD13	19:3g:161:LYS:HG2	1.89	0.54
19:3G:280:ASN:CG	59:3L:703:CDL:H672	2.32	0.54
1:2m:285:MET:HA	1:2m:285:MET:HE2	1.89	0.54
42:4Q:468:MET:HB3	67:4Q:907:HEA:CAC	2.37	0.54
15:3C:183:LEU:HD11	20:3h:314:HIS:HD2	1.73	0.54
38:4m:23:PRO:HA	59:4m:201:CDL:HB22	1.89	0.54
20:3H:24:HIS:CD2	21:3i:82:MET:HE1	2.43	0.54
2:2N:75:CYS:SG	2:2N:78:GLY:N	2.81	0.54
59:3g:403:CDL:H352	59:3g:403:CDL:H312	1.88	0.54
25:41:219:VAL:HG21	59:4f:201:CDL:H772	1.89	0.53
2:2n:173:CYS:HB2	2:2n:230:CYS:HB2	1.91	0.53
30:4e:17:ASP:O	37:4l:35:ARG:NH1	2.41	0.53
2:2N:173:CYS:HB2	2:2N:230:CYS:HB2	1.91	0.53
5:2q:11:SER:OG	6:2r:57:THR:HG22	2.08	0.53
59:3e:202:CDL:H191	59:3e:202:CDL:H152	1.90	0.53
2:2N:75:CYS:HB3	2:2N:80:CYS:HB3	1.90	0.53
2:2n:75:CYS:SG	2:2n:78:GLY:N	2.81	0.53
1:2M:285:MET:HA	1:2M:285:MET:HE2	1.89	0.53
15:3C:265:MET:HE2	16:3D:56:PRO:HD3	1.91	0.53
19:3g:168:PHE:HA	62:3g:407:HEM:HBC2	1.90	0.53
30:4E:17:ASP:O	37:4L:35:ARG:NH1	2.42	0.53
22:3J:64:ASP:HB3	31:4F:155:ASN:HA	1.91	0.53
42:4Q:776:SER:HA	67:4Q:907:HEA:HMC2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:4Z:302:PEE:H54	58:4Z:302:PEE:H63	1.91	0.53
53:3g:401:UQ1:CM2	53:3g:401:UQ1:O1	2.56	0.53
2:2n:75:CYS:HB3	2:2n:80:CYS:HB3	1.90	0.52
38:4m:21:ARG:NH2	59:4m:201:CDL:OA7	2.42	0.52
20:3H:160:PRO:HG2	21:3i:101:ARG:HB3	1.91	0.52
24:3l:579:ILE:CG2	59:3l:701:CDL:H673	2.39	0.52
42:4Q:670:MET:HE2	42:4Q:670:MET:HA	1.90	0.52
38:4m:71:GLN:HG3	45:4t:149:VAL:HG21	1.91	0.52
42:4q:670:MET:HE2	42:4q:670:MET:HA	1.90	0.52
1:2M:91:MET:HG2	1:2M:147:GLN:HB2	1.92	0.52
20:3H:314:HIS:HB2	54:3H:406:FES:S2	2.49	0.52
1:2M:107:SER:HB2	1:2M:427:GLY:HA3	1.92	0.52
15:3C:200:LEU:HD22	15:3C:218:MET:HE2	1.92	0.52
29:4D:70:GLU:HG2	29:4D:75:LEU:HD23	1.92	0.52
4:2p:130:HIS:CE1	59:2p:204:CDL:H111	2.45	0.52
8:2T:56:ASP:OD1	8:2T:56:ASP:N	2.43	0.51
1:2m:91:MET:HG2	1:2m:147:GLN:HB2	1.92	0.51
8:2t:56:ASP:OD1	8:2t:56:ASP:N	2.43	0.51
5:2Q:11:SER:OG	6:2R:57:THR:HG22	2.11	0.51
19:3G:195:GLU:CD	21:3i:65:ARG:HH22	2.18	0.51
42:4Q:835:LEU:HD23	42:4Q:835:LEU:H	1.76	0.51
42:4q:835:LEU:HD23	42:4q:835:LEU:H	1.76	0.51
4:2p:97:LEU:HB2	4:2p:98:PRO:HD3	1.93	0.51
20:3h:314:HIS:HB2	54:3h:404:FES:S2	2.51	0.51
24:3l:579:ILE:HG22	59:3l:701:CDL:H673	1.92	0.51
46:4U:409:GLY:HA3	47:4V:140:LEU:HD11	1.92	0.51
49:4X:252:GLU:HA	49:4X:255:THR:HG22	1.93	0.51
38:4M:71:GLN:HG3	45:4T:149:VAL:HG21	1.92	0.51
49:4x:252:GLU:HA	49:4x:255:THR:HG22	1.93	0.51
20:3H:145:PRO:HG3	21:3i:136:GLU:HG3	1.93	0.51
21:3I:65:ARG:HH22	19:3g:195:GLU:CD	2.18	0.51
38:4M:23:PRO:HA	59:4M:201:CDL:HB22	1.92	0.51
29:4d:70:GLU:HG2	29:4d:75:LEU:HD23	1.92	0.51
14:3B:154:GLY:O	14:3B:158:MET:HG3	2.11	0.50
29:4d:20:ASP:OD1	51:4z:32:VAL:HG23	2.10	0.50
15:3c:200:LEU:HD22	15:3c:218:MET:HE2	1.92	0.50
1:2m:107:SER:HB2	1:2m:427:GLY:HA3	1.92	0.50
4:2p:94:GLY:HA2	59:2t:102:CDL:H361	1.93	0.50
4:2P:97:LEU:HB2	4:2P:98:PRO:HD3	1.93	0.50
42:4q:450:LYS:HD2	44:4s:53:PRO:HB3	1.93	0.50
1:2m:258:VAL:HG13	1:2m:263:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3I:82:MET:HE1	20:3h:24:HIS:CD2	2.46	0.50
1:2m:423:ALA:O	1:2m:424:SER:OG	2.29	0.50
11:30:17:TRP:HB2	19:3g:246:LEU:HD11	1.93	0.50
16:3D:101:VAL:HA	19:3G:327:GLU:HG3	1.94	0.50
14:3b:154:GLY:O	14:3b:158:MET:HG3	2.11	0.50
40:4O:377:MET:HG2	42:4Q:756:ILE:HG22	1.94	0.49
6:2r:48:THR:O	6:2r:52:MET:HG3	2.12	0.49
34:4i:193:ILE:HG23	59:4o:501:CDL:H362	1.94	0.49
35:4j:160:GLU:OE1	35:4j:160:GLU:HA	2.12	0.49
1:2m:373:VAL:HG22	1:2m:378:ILE:HD11	1.95	0.49
19:3g:2:LEU:HD11	21:3i:161:GLY:HA2	1.94	0.49
35:4J:22:VAL:HG21	35:4J:110:ILE:HA	1.93	0.49
42:4Q:670:MET:HE1	51:4Z:76:VAL:HB	1.94	0.49
42:4q:771:PHE:HB2	67:4q:908:HEA:HMD3	1.93	0.49
1:2M:40:ASP:HB3	1:2M:454:VAL:HG11	1.95	0.49
19:3G:262:TYR:HA	53:3G:401:UQ1:HM23	1.94	0.49
21:3I:136:GLU:HG3	20:3h:145:PRO:HG3	1.95	0.49
61:3c:302:HEC:HBC3	61:3c:302:HEC:HMC3	1.93	0.49
59:4e:203:CDL:H781	59:4e:203:CDL:H741	1.93	0.49
48:4w:56:ARG:HB2	50:4y:129:ASP:OD2	2.13	0.49
1:2M:258:VAL:HG13	1:2M:263:LEU:HB2	1.94	0.49
35:4j:22:VAL:HG21	35:4j:110:ILE:HA	1.93	0.49
46:4u:409:GLY:HA3	47:4v:140:LEU:HD11	1.94	0.49
15:3C:197:PRO:HD2	61:3C:302:HEC:HBC2	1.95	0.49
19:3G:168:PHE:CD2	62:3G:405:HEM:HBC1	2.48	0.49
15:3c:265:MET:HE2	16:3d:56:PRO:HD3	1.93	0.49
59:4Q:902:CDL:OB7	59:4Q:902:CDL:HB31	2.11	0.49
1:2M:373:VAL:HG22	1:2M:378:ILE:HD11	1.95	0.49
29:4D:20:ASP:OD1	51:4Z:32:VAL:HG23	2.13	0.49
3:2O:110:ILE:HG21	8:2T:42:PRO:HB2	1.94	0.49
22:3J:29:ASP:OD1	22:3J:29:ASP:N	2.42	0.49
67:4Q:908:HEA:O11	67:4Q:908:HEA:HHC	2.13	0.49
42:4q:670:MET:HE1	51:4z:76:VAL:HB	1.94	0.49
1:2M:222:ILE:HG21	1:2M:472:ILE:HD11	1.95	0.49
1:2M:507:ASN:OD1	1:2M:510:ASP:HB2	2.13	0.49
1:2m:222:ILE:HG21	1:2m:472:ILE:HD11	1.95	0.49
60:2r:201:PC1:H2D2	60:2r:201:PC1:H2H1	1.94	0.49
21:3I:101:ARG:HB3	20:3h:160:PRO:HG2	1.94	0.49
25:41:219:VAL:HG21	59:4f:201:CDL:C77	2.43	0.49
1:2M:42:VAL:HG23	1:2M:227:ALA:HB2	1.95	0.48
6:2R:48:THR:O	6:2R:52:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2o:110:ILE:HB	3:2o:111:PRO:HD3	1.95	0.48
59:3i:201:CDL:H512	59:3i:201:CDL:H561	1.95	0.48
46:4U:365:GLU:HA	46:4U:365:GLU:OE1	2.13	0.48
14:3B:86:HIS:CG	21:3I:5:ARG:HD3	2.48	0.48
23:3K:63:VAL:HG12	23:3K:63:VAL:O	2.14	0.48
20:3h:279:ARG:CZ	20:3h:335:ILE:HD11	2.43	0.48
59:4e:203:CDL:H781	59:4e:203:CDL:H821	1.94	0.48
42:4q:430:GLY:HA3	42:4q:468:MET:SD	2.54	0.48
67:4q:908:HEA:O11	67:4q:908:HEA:HHC	2.13	0.48
14:3B:137:LEU:HD21	14:3B:303:VAL:HG11	1.96	0.48
19:3g:20:LEU:HD23	59:3g:403:CDL:H592	1.96	0.48
42:4Q:450:LYS:HD2	44:4S:53:PRO:HB3	1.95	0.48
47:4V:150:ARG:NH2	47:4V:151:ASN:HD21	2.12	0.48
46:4u:365:GLU:HA	46:4u:365:GLU:OE1	2.13	0.48
47:4v:150:ARG:NH2	47:4v:151:ASN:HD21	2.12	0.48
17:3E:88:LEU:HD11	59:3H:404:CDL:H711	1.96	0.48
42:4Q:430:GLY:HA3	42:4Q:468:MET:SD	2.54	0.48
1:2M:278:ILE:HD11	1:2M:285:MET:CE	2.44	0.48
11:30:53:CYS:SG	11:30:96:ALA:HB3	2.54	0.48
13:3A:235:LYS:HB2	13:3A:235:LYS:NZ	2.28	0.48
34:4I:195:VAL:O	34:4I:199:MET:HG2	2.14	0.48
41:4P:42:THR:HG22	41:4P:43:GLN:HG2	1.95	0.48
14:3b:137:LEU:HD21	14:3b:303:VAL:HG11	1.96	0.48
23:3k:63:VAL:HG12	23:3k:63:VAL:O	2.14	0.48
51:4Z:131:LEU:N	51:4Z:132:PRO:HD2	2.28	0.48
29:4d:68:GLN:CD	29:4d:68:GLN:C	2.81	0.48
59:2q:101:CDL:H801	59:2q:101:CDL:H842	1.96	0.48
15:3C:135:GLU:CD	15:3c:110:PRO:HG2	2.38	0.48
15:3c:197:PRO:HD2	61:3c:302:HEC:HBC2	1.94	0.48
33:4H:158:GLU:HB2	37:4L:19:ARG:HH22	1.79	0.48
4:2p:15:LYS:HB2	4:2p:15:LYS:NZ	2.29	0.48
59:2q:101:CDL:H671	59:2q:101:CDL:H631	1.95	0.48
24:3L:611:MET:O	24:3L:612:ASP:C	2.57	0.48
3:2O:110:ILE:HB	3:2O:111:PRO:HD3	1.95	0.48
41:4P:81:ASP:OD1	41:4P:81:ASP:N	2.44	0.48
48:4W:56:ARG:HB2	50:4Y:129:ASP:OD2	2.13	0.48
36:4k:78:ILE:HG23	36:4k:82:LEU:HD12	1.96	0.48
3:2O:62:PRO:HG2	59:3I:202:CDL:HB31	1.95	0.47
4:2P:15:LYS:NZ	4:2P:15:LYS:HB2	2.28	0.47
1:2m:42:VAL:HG23	1:2m:227:ALA:HB2	1.95	0.47
20:3h:266:ILE:HG22	20:3h:266:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4D:68:GLN:C	29:4D:68:GLN:CD	2.81	0.47
36:4K:78:ILE:HG23	36:4K:82:LEU:HD12	1.96	0.47
41:4p:81:ASP:OD1	41:4p:81:ASP:N	2.44	0.47
7:2S:157:LYS:HB3	7:2S:157:LYS:NZ	2.29	0.47
2:2n:73:ARG:HD2	2:2n:73:ARG:O	2.14	0.47
53:2p:201:UQ1:HM52	9:2u:11:LEU:HD12	1.96	0.47
13:3a:235:LYS:HB2	13:3a:235:LYS:NZ	2.28	0.47
34:4i:195:VAL:O	34:4i:199:MET:HG2	2.14	0.47
51:4z:131:LEU:N	51:4z:132:PRO:HD2	2.28	0.47
19:3g:280:ASN:CG	59:3l:701:CDL:H672	2.40	0.47
33:4h:158:GLU:HB2	37:4l:19:ARG:HH22	1.80	0.47
1:2m:40:ASP:HB3	1:2m:454:VAL:HG11	1.97	0.47
1:2m:507:ASN:OD1	1:2m:510:ASP:HB2	2.13	0.47
3:2o:110:ILE:HG21	8:2t:42:PRO:HB2	1.97	0.47
29:4D:16:ASN:HA	29:4D:19:ARG:HG3	1.96	0.47
35:4J:160:GLU:OE1	35:4J:160:GLU:HA	2.12	0.47
42:4Q:464:HIS:O	42:4Q:468:MET:HG2	2.15	0.47
29:4d:16:ASN:HA	29:4d:19:ARG:HG3	1.96	0.47
1:2M:423:ALA:O	1:2M:424:SER:OG	2.29	0.47
4:2P:22:ARG:O	4:2P:24:ARG:NH1	2.47	0.47
4:2p:22:ARG:O	4:2p:24:ARG:NH1	2.47	0.47
12:31:112:GLN:HG2	12:31:118:PHE:HB3	1.96	0.47
20:3H:279:ARG:CZ	20:3H:335:ILE:HD11	2.44	0.47
19:3g:23:ILE:HG23	19:3g:81:VAL:HG13	1.96	0.47
42:4Q:474:MET:HB3	42:4Q:475:PRO:HD3	1.97	0.47
37:4l:102:LEU:CD2	58:4l:201:PEE:H11	2.45	0.47
42:4q:474:MET:HB3	42:4q:475:PRO:HD3	1.97	0.47
1:2M:123:ALA:HA	1:2M:126:VAL:HG22	1.97	0.47
1:2m:170:ALA:HB1	1:2m:359:PRO:HG3	1.96	0.47
1:2m:278:ILE:HD11	1:2m:285:MET:CE	2.44	0.47
15:3C:147:PRO:HG3	61:3C:302:HEC:HAA1	1.96	0.47
37:4L:123:ASP:OD1	37:4L:126:ASN:HB2	2.15	0.47
42:4Q:771:PHE:HB2	67:4Q:908:HEA:HMD3	1.97	0.47
59:4e:203:CDL:H821	59:4e:203:CDL:C78	2.45	0.47
37:4l:123:ASP:OD1	37:4l:126:ASN:HB2	2.15	0.47
40:4o:377:MET:HE3	42:4q:756:ILE:O	2.15	0.47
41:4p:42:THR:HG22	41:4p:43:GLN:HG2	1.95	0.47
42:4q:486:LEU:HD11	42:4q:579:ILE:HG23	1.97	0.47
11:30:179:LYS:HG3	15:3C:181:SER:HB3	1.97	0.47
19:3G:23:ILE:HG23	19:3G:81:VAL:HG13	1.96	0.47
21:3i:36:GLN:O	21:3i:40:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:3j:29:ASP:OD1	22:3j:29:ASP:N	2.42	0.47
42:4Q:702:ILE:HG23	51:4Z:75:LEU:HD11	1.97	0.47
6:2r:44:VAL:O	6:2r:48:THR:HG23	2.15	0.47
37:4L:122:ASN:ND2	42:4Q:521:ILE:O	2.45	0.47
59:2t:102:CDL:H372	59:2t:102:CDL:H332	1.96	0.47
12:31:66:PHE:CD1	12:31:66:PHE:C	2.93	0.47
19:3G:280:ASN:ND2	59:3L:703:CDL:H672	2.30	0.47
24:3L:579:ILE:HG22	59:3L:703:CDL:H673	1.96	0.47
27:4B:3:ILE:HD12	27:4B:3:ILE:N	2.30	0.47
6:2R:44:VAL:O	6:2R:48:THR:HG23	2.15	0.46
8:2T:50:TRP:CG	60:2T:102:PC1:H132	2.50	0.46
9:2U:16:ALA:HB2	10:2V:7:LEU:HA	1.95	0.46
20:3H:266:ILE:HG22	20:3H:266:ILE:O	2.14	0.46
14:3b:86:HIS:CG	21:3i:5:ARG:HD3	2.50	0.46
14:3b:264:GLY:O	14:3b:265:ASN:C	2.58	0.46
36:4k:39:ARG:HG3	36:4k:47:TRP:CZ3	2.50	0.46
1:2M:72:PRO:HD3	1:2M:194:ILE:HD12	1.96	0.46
1:2m:123:ALA:HA	1:2m:126:VAL:HG22	1.97	0.46
58:41:301:PEE:H59	51:4z:87:ILE:HG23	1.96	0.46
29:4D:61:LEU:HD22	59:4Z:303:CDL:C54	2.45	0.46
36:4K:39:ARG:HG3	36:4K:47:TRP:CZ3	2.50	0.46
37:4l:122:ASN:ND2	42:4q:521:ILE:O	2.44	0.46
42:4q:464:HIS:O	42:4q:468:MET:HG2	2.15	0.46
42:4q:597:ASN:O	42:4q:601:LEU:HG	2.15	0.46
49:4x:153:THR:HG21	50:4y:116:LEU:HD21	1.97	0.46
1:2M:170:ALA:HB1	1:2M:359:PRO:HG3	1.96	0.46
7:2s:157:LYS:NZ	7:2s:157:LYS:HB3	2.29	0.46
12:31:61:ALA:O	12:31:62:ALA:C	2.57	0.46
13:3A:131:ILE:HD13	13:3A:228:VAL:HG12	1.96	0.46
24:3L:579:ILE:CG2	59:3L:703:CDL:H673	2.45	0.46
25:41:18:THR:HG22	42:4q:510:ILE:HG13	1.98	0.46
26:4A:28:LEU:HD23	26:4A:38:PRO:HD3	1.97	0.46
49:4X:153:THR:HG21	50:4Y:116:LEU:HD21	1.98	0.46
2:2N:73:ARG:HD2	2:2N:73:ARG:O	2.15	0.46
19:3G:168:PHE:CD2	62:3G:405:HEM:CBC	2.98	0.46
29:4D:45:HIS:O	29:4D:46:PRO:C	2.59	0.46
16:3D:99:ASN:HB3	28:4C:52:TYR:CD1	2.51	0.46
19:3G:153:TYR:CE2	20:3h:223:GLY:HA3	2.51	0.46
19:3g:244:ASN:HB3	19:3g:247:VAL:HG12	1.96	0.46
24:3l:577:VAL:HG11	59:3l:701:CDL:H372	1.97	0.46
24:3l:611:MET:O	24:3l:612:ASP:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:2T:103:PEE:H68	58:2T:103:PEE:H61	1.98	0.46
14:3B:170:LEU:HD22	14:3B:174:ARG:HB3	1.98	0.46
61:3C:302:HEC:HBC3	61:3C:302:HEC:HMC1	1.98	0.46
53:3G:401:UQ1:O4	53:3G:401:UQ1:CM3	2.63	0.46
20:3H:313:CYS:SG	15:3c:143:GLY:C	2.99	0.46
21:3I:36:GLN:O	21:3I:40:GLU:HG2	2.15	0.46
13:3a:131:ILE:HD13	13:3a:228:VAL:HG12	1.96	0.46
13:3a:261:ALA:HB2	13:3a:449:GLU:HB3	1.97	0.46
59:3l:701:CDL:H561	59:3l:701:CDL:H601	1.97	0.46
29:4d:45:HIS:O	29:4d:46:PRO:C	2.59	0.46
13:3A:261:ALA:HB2	13:3A:449:GLU:HB3	1.97	0.46
14:3B:264:GLY:O	14:3B:265:ASN:C	2.59	0.46
19:3g:254:PRO:HB3	53:3g:401:UQ1:C2	2.45	0.46
22:3j:61:MET:O	22:3j:62:ARG:C	2.58	0.46
42:4Q:597:ASN:O	42:4Q:601:LEU:HG	2.15	0.46
19:3g:120:TYR:CE1	62:3g:407:HEM:HAA2	2.50	0.46
31:4F:139:ASN:O	48:4W:134:MET:HG3	2.16	0.46
37:4L:101:ARG:HD3	59:4Q:902:CDL:HA4	1.98	0.46
49:4X:151:ALA:HB2	49:4X:165:TRP:CD2	2.51	0.46
27:4b:3:ILE:HD12	27:4b:3:ILE:N	2.30	0.46
42:4q:774:ILE:HG21	67:4q:908:HEA:HMC1	1.98	0.46
47:4v:170:GLU:HA	47:4v:170:GLU:OE1	2.16	0.46
7:2s:80:ASP:OD1	8:2t:17:ARG:NH2	2.48	0.46
12:31:35:LEU:HB3	12:31:38:THR:HG21	1.98	0.46
42:4Q:486:LEU:HD11	42:4Q:579:ILE:HG23	1.97	0.46
32:4g:67:GLY:HA2	32:4g:70:MET:HE2	1.98	0.46
49:4x:151:ALA:HB2	49:4x:165:TRP:CD2	2.51	0.46
22:3J:61:MET:O	22:3J:62:ARG:C	2.58	0.45
24:3L:574:THR:HG23	59:3L:703:CDL:H361	1.98	0.45
19:3g:168:PHE:CD2	62:3g:407:HEM:CBC	2.99	0.45
19:3g:295:ILE:HG12	20:3h:100:HIS:NE2	2.31	0.45
42:4Q:491:VAL:HG23	42:4Q:572:ASP:HB2	1.99	0.45
67:4Q:907:HEA:HHC	67:4Q:907:HEA:H11	1.79	0.45
2:2N:161:LEU:HD21	2:2N:202:ASP:HB2	1.98	0.45
1:2m:72:PRO:HD3	1:2m:194:ILE:HD12	1.96	0.45
2:2n:161:LEU:HD21	2:2n:202:ASP:HB2	1.98	0.45
20:3H:266:ILE:O	20:3H:266:ILE:CG2	2.64	0.45
14:3b:170:LEU:HD22	14:3b:174:ARG:HB3	1.98	0.45
29:4D:38:ALA:HB1	29:4D:42:LEU:HD12	1.99	0.45
47:4V:170:GLU:HA	47:4V:170:GLU:OE1	2.16	0.45
50:4Y:40:ASP:OD1	50:4Y:40:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:4q:440:GLU:OE2	42:4q:835:LEU:HD12	2.16	0.45
42:4q:491:VAL:HG23	42:4q:572:ASP:HB2	1.98	0.45
11:30:52:ASN:OD1	11:30:52:ASN:C	2.58	0.45
14:3b:315:SER:HA	18:3f:1:THR:HB	1.98	0.45
15:3c:39:ASP:HB2	15:3c:40:PRO:HD2	1.97	0.45
15:3c:76:CYS:SG	61:3c:302:HEC:HAC	2.52	0.45
20:3h:126:THR:HG22	20:3h:127:ASP:N	2.31	0.45
19:3G:254:PRO:HB2	19:3G:258:TYR:HB2	1.97	0.45
19:3g:20:LEU:HB3	19:3g:88:ARG:HG3	1.98	0.45
42:4Q:440:GLU:OE2	42:4Q:835:LEU:HD12	2.16	0.45
42:4q:814:ASN:HB3	42:4q:855:THR:HG23	1.99	0.45
9:2u:16:ALA:HB2	10:2v:7:LEU:HA	1.98	0.45
13:3A:152:ILE:HG12	13:3A:207:MET:HE1	1.98	0.45
35:4J:18:GLY:O	35:4J:23:LYS:NZ	2.50	0.45
42:4Q:814:ASN:HB3	42:4Q:855:THR:HG23	1.99	0.45
51:4Z:188:MET:HE2	51:4Z:191:ILE:HD12	1.99	0.45
38:4m:44:MET:HA	41:4p:136:PRO:HG3	1.99	0.45
49:4x:176:CYS:HA	50:4y:93:MET:HE1	1.98	0.45
2:2N:161:LEU:HD11	2:2N:202:ASP:HA	1.98	0.45
3:2O:104:VAL:O	6:2R:41:ARG:HD3	2.16	0.45
19:3G:168:PHE:CE2	62:3G:405:HEM:HBC1	2.51	0.45
22:3j:25:ASN:HB3	22:3j:29:ASP:OD1	2.17	0.45
26:4a:28:LEU:HD23	26:4a:38:PRO:HD3	1.97	0.45
30:4e:49:TRP:CH2	48:4w:96:ILE:HD11	2.51	0.45
1:2M:400:LEU:HA	1:2M:410:ILE:HA	1.98	0.45
1:2m:400:LEU:HA	1:2m:410:ILE:HA	1.98	0.45
35:4j:18:GLY:O	35:4j:23:LYS:NZ	2.50	0.45
37:4l:101:ARG:HD3	59:4q:903:CDL:HA4	1.98	0.45
46:4u:413:ILE:HG23	47:4v:146:PHE:CZ	2.52	0.45
48:4w:14:PHE:CE2	48:4w:16:ASP:OD1	2.70	0.45
2:2n:194:LEU:HD13	2:2n:243:ALA:CB	2.47	0.45
19:3G:2:LEU:HD11	21:3I:161:GLY:HA2	1.98	0.45
20:3H:316:SER:HA	20:3H:327:GLY:HA3	1.99	0.45
17:3e:57:ASP:OD2	20:3h:180:HIS:HA	2.16	0.45
25:40:18:THR:HG22	42:4Q:510:ILE:HG13	1.98	0.45
37:4L:89:GLY:N	37:4L:93:ASP:OD2	2.45	0.45
41:4P:174:ILE:HD12	42:4Q:756:ILE:HB	1.99	0.45
31:4f:139:ASN:O	48:4w:134:MET:HG3	2.17	0.45
19:3g:305:ILE:HD11	19:3g:345:MET:HE3	1.99	0.45
27:4B:4:GLU:HA	27:4B:7:ILE:HD12	1.99	0.45
42:4q:702:ILE:HG23	51:4z:75:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2M:297:ARG:HH11	1:2M:297:ARG:HD3	1.38	0.45
53:3G:401:UQ1:HM23	53:3G:401:UQ1:O1	2.17	0.45
20:3h:266:ILE:O	20:3h:266:ILE:CG2	2.64	0.45
30:4E:49:TRP:CH2	48:4W:96:ILE:HD11	2.52	0.45
32:4G:67:GLY:HA2	32:4G:70:MET:HE2	1.99	0.45
2:2n:161:LEU:HD11	2:2n:202:ASP:HA	1.98	0.44
22:3J:25:ASN:HB3	22:3J:29:ASP:OD1	2.17	0.44
15:3c:187:THR:HG21	22:3j:77:ALA:HB1	1.99	0.44
48:4W:14:PHE:CE2	48:4W:16:ASP:OD1	2.70	0.44
29:4d:38:ALA:HB1	29:4d:42:LEU:HD12	1.99	0.44
10:2V:85:MET:O	10:2V:86:TYR:C	2.60	0.44
1:2m:297:ARG:HH11	1:2m:297:ARG:HD3	1.38	0.44
4:2p:36:PRO:O	9:2u:46:VAL:HG13	2.17	0.44
9:2u:46:VAL:HG12	9:2u:46:VAL:O	2.18	0.44
20:3h:27:THR:HG23	24:3l:559:VAL:HA	1.98	0.44
31:4F:109:TRP:CD1	60:4F:201:PC1:H252	2.52	0.44
3:2o:62:PRO:HG2	59:3i:202:CDL:HB31	1.98	0.44
2:2N:194:LEU:HD13	2:2N:243:ALA:CB	2.47	0.44
12:31:6:THR:HG23	12:31:7:PRO:HD2	1.99	0.44
19:3G:20:LEU:HB3	19:3G:88:ARG:HG3	1.98	0.44
19:3G:352:LYS:HG3	20:3H:37:THR:HG23	1.98	0.44
20:3H:126:THR:HG22	20:3H:127:ASP:N	2.32	0.44
15:3c:196:MET:HB2	61:3c:302:HEC:C1D	2.47	0.44
48:4w:81:ARG:HG2	48:4w:82:PRO:HD2	2.00	0.44
6:2R:75:PRO:O	6:2R:79:MET:HG3	2.18	0.44
10:2V:2:LEU:HA	10:2V:2:LEU:HD23	1.84	0.44
19:3G:268:LEU:HD22	19:3G:274:GLY:HA2	1.99	0.44
13:3a:152:ILE:HG12	13:3a:207:MET:HE1	1.98	0.44
16:3d:85:ILE:HB	16:3d:86:PRO:HD3	1.98	0.44
25:41:157:GLU:OE1	25:41:157:GLU:C	2.61	0.44
49:4X:56:LYS:HG3	49:4X:213:LEU:HD11	1.99	0.44
41:4p:174:ILE:HD12	42:4q:756:ILE:HB	1.99	0.44
19:3G:105:GLY:HA2	19:3G:108:MET:HE3	1.99	0.44
24:3l:597:ARG:O	24:3l:601:LEU:HG	2.18	0.44
25:40:157:GLU:C	25:40:157:GLU:OE1	2.61	0.44
42:4Q:762:HIS:HA	67:4Q:908:HEA:O2A	2.17	0.44
35:4j:29:GLY:HA2	36:4k:51:VAL:HG22	2.00	0.44
42:4q:424:ILE:HG13	67:4q:907:HEA:H242	1.98	0.44
2:2N:145:GLN:HG3	2:2N:146:PRO:HD2	2.00	0.44
6:2r:75:PRO:O	6:2r:79:MET:HG3	2.18	0.44
35:4J:147:GLU:HG2	35:4J:150:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4M:44:MET:HA	41:4P:136:PRO:HG3	1.98	0.44
39:4n:134:CYS:H	39:4n:138:HIS:HB2	1.83	0.44
19:3G:316:MET:HE2	19:3G:316:MET:HA	2.00	0.44
20:3H:157:ILE:HG13	20:3H:157:ILE:O	2.17	0.44
20:3h:157:ILE:O	20:3h:157:ILE:HG13	2.17	0.44
39:4N:134:CYS:H	39:4N:138:HIS:HB2	1.83	0.44
36:4k:53:GLU:HG3	36:4k:54:ASP:N	2.33	0.44
42:4q:762:HIS:HA	67:4q:908:HEA:O2A	2.17	0.44
46:4u:426:GLU:OE1	46:4u:429:ARG:NH2	2.51	0.44
47:4v:89:MET:CE	47:4v:92:ILE:HD11	2.48	0.44
51:4z:188:MET:HE2	51:4z:191:ILE:HD12	1.99	0.44
1:2M:104:VAL:HG11	1:2M:621:VAL:HB	2.00	0.44
16:3D:106:ARG:O	31:4F:148:TYR:HB2	2.18	0.44
24:3L:597:ARG:O	24:3L:601:LEU:HG	2.18	0.44
19:3g:316:MET:HE2	19:3g:316:MET:HA	2.00	0.44
20:3h:316:SER:HA	20:3h:327:GLY:HA3	1.99	0.44
46:4U:413:ILE:HG23	47:4V:146:PHE:CZ	2.53	0.44
51:4Z:88:TRP:CD1	58:4Z:302:PEE:H25	2.52	0.44
27:4b:4:GLU:HA	27:4b:7:ILE:HD12	1.99	0.44
37:4l:89:GLY:N	37:4l:93:ASP:OD2	2.45	0.44
1:2m:305:MET:O	1:2m:308:TYR:O	2.36	0.43
2:2n:145:GLN:HG3	2:2n:146:PRO:HD2	2.00	0.43
3:2o:104:VAL:O	6:2r:41:ARG:HD3	2.18	0.43
10:2v:85:MET:O	10:2v:86:TYR:C	2.60	0.43
25:40:203:ILE:HD13	35:4J:83:TRP:CD1	2.53	0.43
39:4N:71:GLU:HA	39:4N:71:GLU:OE1	2.18	0.43
49:4X:176:CYS:HA	50:4Y:93:MET:HE1	1.99	0.43
35:4j:147:GLU:HG2	35:4j:150:ARG:HH12	1.82	0.43
40:4o:362:THR:HA	42:4q:824:ILE:HG23	1.99	0.43
15:3c:175:ALA:HB3	22:3j:56:VAL:HG22	2.00	0.43
19:3g:79:TYR:CE1	19:3g:112:LEU:HG	2.53	0.43
30:4e:108:ASP:OD1	30:4e:108:ASP:N	2.51	0.43
4:2P:8:ASP:OD1	4:2P:8:ASP:N	2.51	0.43
9:2U:46:VAL:HG12	9:2U:46:VAL:O	2.18	0.43
59:3e:201:CDL:H172	59:3e:201:CDL:C21	2.49	0.43
21:3i:18:ILE:CD1	59:3i:202:CDL:HB22	2.48	0.43
49:4X:138:PRO:HB3	49:4X:182:ILE:HG22	2.00	0.43
26:4a:20:LEU:HD13	26:4a:27:ARG:HG2	1.99	0.43
28:4c:35:TYR:CE1	28:4c:39:MET:HE3	2.54	0.43
34:4i:140:LYS:C	48:4w:69:MET:HE2	2.43	0.43
14:3b:240:ARG:HA	23:3k:55:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:4f:201:CDL:H742	59:4g:202:CDL:HA62	2.00	0.43
33:4h:36:HIS:CE1	34:4i:139:ALA:HB2	2.53	0.43
35:4j:144:TYR:HB2	59:4j:301:CDL:H731	2.00	0.43
38:4m:57:VAL:HG21	59:4m:201:CDL:H311	1.99	0.43
5:2q:17:ALA:HA	60:2r:201:PC1:H371	2.00	0.43
34:4I:193:ILE:HD13	34:4I:196:MET:CE	2.48	0.43
38:4m:63:ALA:CB	59:4o:501:CDL:H352	2.47	0.43
45:4t:106:CYS:SG	45:4t:109:LYS:N	2.89	0.43
15:3c:183:LEU:HG	15:3c:193:ALA:HB1	2.00	0.43
15:3c:196:MET:HE3	15:3c:199:PRO:CG	2.46	0.43
25:40:34:VAL:HG11	59:4K:201:CDL:H112	2.00	0.43
26:4A:20:LEU:HD13	26:4A:27:ARG:HG2	2.00	0.43
46:4U:426:GLU:OE1	46:4U:429:ARG:NH2	2.51	0.43
19:3G:168:PHE:HA	62:3G:405:HEM:HBC2	2.00	0.43
13:3a:216:THR:O	13:3a:220:MET:HG3	2.19	0.43
42:4Q:478:TYR:HA	42:4Q:482:PRO:HG2	2.01	0.43
47:4V:89:MET:CE	47:4V:92:ILE:HD11	2.48	0.43
48:4W:87:PRO:HG2	48:4W:92:LEU:HD21	2.00	0.43
42:4q:656:LYS:HD3	42:4q:717:LEU:O	2.19	0.43
11:30:174:GLU:HG2	12:31:28:ARG:HD2	2.00	0.43
13:3A:216:THR:O	13:3A:220:MET:HG3	2.19	0.43
14:3B:369:THR:HG21	23:3K:22:LEU:HG	2.00	0.43
21:3I:122:ASN:ND2	20:3h:69:PRO:O	2.44	0.43
30:4e:35:MET:HE1	30:4e:43:SER:HB3	2.00	0.43
34:4i:193:ILE:HD13	34:4i:196:MET:CE	2.48	0.43
1:2M:305:MET:O	1:2M:308:TYR:O	2.36	0.43
7:2S:80:ASP:OD1	8:2T:17:ARG:NH2	2.49	0.43
1:2m:126:VAL:HG11	1:2m:441:VAL:HG22	2.01	0.43
19:3g:105:GLY:HA2	19:3g:108:MET:HE3	1.99	0.43
49:4x:138:PRO:HB3	49:4x:182:ILE:HG22	2.00	0.43
1:2M:114:ASP:OD1	1:2M:114:ASP:C	2.62	0.43
1:2M:126:VAL:HG11	1:2M:441:VAL:HG22	2.01	0.43
18:3F:51:ASP:N	18:3F:52:PRO:HD2	2.34	0.43
13:3a:87:VAL:HG12	13:3a:87:VAL:O	2.19	0.43
20:3h:153:TYR:CE2	20:3h:157:ILE:HG21	2.54	0.43
58:40:304:PEE:O4	58:40:304:PEE:H7	2.18	0.43
28:4C:35:TYR:CE1	28:4C:39:MET:HE3	2.54	0.43
34:4I:140:LYS:C	48:4W:69:MET:HE2	2.43	0.43
48:4W:81:ARG:HG2	48:4W:82:PRO:HD2	2.00	0.43
67:4q:907:HEA:HHC	67:4q:907:HEA:H11	1.79	0.43
49:4x:56:LYS:HG3	49:4x:213:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:4z:302:PEE:H52	58:4z:302:PEE:H13	2.01	0.43
4:2P:2:LEU:HB2	10:2V:77:ILE:HD13	2.00	0.42
24:3l:590:GLN:HB3	24:3l:591:PRO:HD3	2.01	0.42
25:41:19:VAL:HG11	59:4q:903:CDL:H351	2.01	0.42
34:4i:193:ILE:HD12	59:4o:501:CDL:H362	2.01	0.42
42:4q:822:GLN:HA	42:4q:825:ILE:HG12	2.00	0.42
15:3C:183:LEU:HG	15:3C:193:ALA:HB1	2.00	0.42
21:3I:132:PRO:O	21:3I:136:GLU:HG2	2.19	0.42
19:3g:352:LYS:HG3	20:3h:37:THR:HG23	2.01	0.42
34:4I:224:PRO:HA	38:4M:88:ARG:HG3	2.01	0.42
39:4n:141:MET:HE2	41:4p:197:TRP:NE1	2.34	0.42
1:2m:104:VAL:HG11	1:2m:621:VAL:HB	2.00	0.42
11:30:14:ILE:HD12	19:3g:156:THR:HA	2.01	0.42
19:3G:295:ILE:HG12	20:3H:100:HIS:NE2	2.33	0.42
20:3H:153:TYR:CE2	20:3H:157:ILE:HG21	2.54	0.42
39:4N:141:MET:HE2	41:4P:197:TRP:NE1	2.34	0.42
41:4P:149:VAL:HG12	41:4P:150:MET:HE2	2.01	0.42
37:4l:102:LEU:HD23	58:4l:201:PEE:H11	2.01	0.42
39:4n:71:GLU:OE1	39:4n:71:GLU:HA	2.18	0.42
59:4t:201:CDL:CA7	59:4t:201:CDL:H341	2.49	0.42
48:4w:87:PRO:HG2	48:4w:92:LEU:HD21	2.00	0.42
3:2O:129:LEU:HD21	3:2O:145:TYR:HB2	2.02	0.42
59:2q:101:CDL:H762	59:2q:101:CDL:C80	2.49	0.42
19:3G:98:ASN:HB3	19:3G:101:ILE:HD12	2.02	0.42
24:3L:590:GLN:HB3	24:3L:591:PRO:HD3	2.01	0.42
21:3i:83:ILE:HD13	21:3i:138:LYS:HG2	2.02	0.42
30:4E:108:ASP:OD1	30:4E:108:ASP:N	2.51	0.42
45:4T:37:ILE:HG13	45:4T:38:TRP:CD1	2.55	0.42
41:4p:174:ILE:HB	42:4q:756:ILE:HG13	2.01	0.42
1:2m:114:ASP:OD1	1:2m:114:ASP:C	2.62	0.42
5:2q:47:HIS:HB2	59:2q:101:CDL:H141	2.02	0.42
18:3F:34:GLN:HB3	18:3F:38:TYR:CE2	2.54	0.42
16:3d:63:PHE:HB2	59:3e:201:CDL:HB31	2.00	0.42
18:3f:34:GLN:HB3	18:3f:38:TYR:CE2	2.54	0.42
36:4K:53:GLU:HG3	36:4K:54:ASP:N	2.33	0.42
45:4t:98:GLU:OE1	47:4v:37:TYR:HE1	2.03	0.42
4:2p:8:ASP:OD1	4:2p:8:ASP:N	2.51	0.42
14:3B:261:ASN:O	14:3B:262:THR:C	2.62	0.42
14:3B:476:MET:HE2	14:3B:476:MET:HB3	1.99	0.42
19:3g:98:ASN:HB3	19:3g:101:ILE:HD12	2.02	0.42
59:3g:404:CDL:C63	59:3h:403:CDL:C42	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3h:62:PRO:CB	20:3h:157:ILE:HD11	2.50	0.42
40:4o:376:LEU:O	40:4o:380:THR:HG23	2.19	0.42
42:4q:768:VAL:HA	42:4q:771:PHE:CE2	2.55	0.42
12:31:160:LEU:HD11	19:3g:136:ILE:HG21	2.01	0.42
13:3A:87:VAL:HG12	13:3A:87:VAL:O	2.19	0.42
13:3a:365:VAL:O	13:3a:369:MET:HG3	2.20	0.42
18:3f:51:ASP:N	18:3f:52:PRO:HD2	2.34	0.42
19:3g:195:GLU:OE2	19:3g:300:ASN:ND2	2.45	0.42
20:3h:251:ARG:NE	20:3h:284:GLU:OE2	2.52	0.42
37:4L:123:ASP:O	37:4L:123:ASP:CG	2.62	0.42
42:4Q:656:LYS:HD3	42:4Q:717:LEU:O	2.19	0.42
39:4n:64:PRO:HA	47:4v:103:TRP:CD2	2.55	0.42
51:4z:119:VAL:N	51:4z:120:PRO:HD2	2.35	0.42
13:3A:66:ILE:HG12	13:3A:220:MET:HE3	2.02	0.42
13:3a:369:MET:HE2	13:3a:369:MET:HB3	1.96	0.42
14:3b:261:ASN:O	14:3b:262:THR:C	2.63	0.42
17:3e:92:TYR:CD2	59:3h:403:CDL:H512	2.55	0.42
25:41:17:ILE:O	25:41:21:ILE:HG12	2.20	0.42
58:41:303:PEE:O4	58:41:303:PEE:H7	2.20	0.42
30:4E:35:MET:HE1	30:4E:43:SER:HB3	2.00	0.42
34:4I:196:MET:SD	38:4M:64:LEU:HD11	2.59	0.42
42:4Q:828:ASN:N	42:4Q:829:VAL:HA	2.35	0.42
48:4w:14:PHE:CE1	48:4w:20:ASP:HA	2.55	0.42
3:2o:129:LEU:HD21	3:2o:145:TYR:HB2	2.02	0.42
7:2s:5:ASP:OD2	17:3e:67:ARG:NH2	2.42	0.42
34:4I:177:ARG:CG	38:4M:27:VAL:HG11	2.49	0.42
42:4Q:424:ILE:HG13	67:4Q:907:HEA:H242	2.01	0.42
28:4c:56:THR:HG23	32:4g:32:CYS:HA	2.00	0.42
31:4f:97:MET:HE2	31:4f:97:MET:HB2	1.91	0.42
37:4l:123:ASP:CG	37:4l:123:ASP:O	2.62	0.42
50:4y:116:LEU:HD22	50:4y:118:TRP:CE2	2.55	0.42
2:2N:214:TRP:HB2	2:2N:279:TYR:CE2	2.55	0.42
60:2T:102:PC1:H133	60:2T:102:PC1:H112	1.87	0.42
1:2m:289:CYS:HB3	1:2m:346:LEU:HD21	2.01	0.42
11:30:22:LEU:HB3	11:30:29:ALA:HA	2.01	0.42
14:3B:240:ARG:HA	23:3K:55:VAL:HG22	2.02	0.42
19:3G:261:TRP:HB2	53:3G:401:UQ1:H72	2.02	0.42
20:3h:32:ILE:HD13	60:3h:402:PC1:C14	2.50	0.42
21:3i:132:PRO:O	21:3i:136:GLU:HG2	2.19	0.42
33:4H:19:VAL:HG11	33:4H:37:HIS:NE2	2.35	0.42
42:4Q:768:VAL:HA	42:4Q:771:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:4U:414:ARG:N	46:4U:415:PRO:HD2	2.35	0.42
48:4W:14:PHE:CE1	48:4W:20:ASP:HA	2.55	0.42
29:4d:69:LEU:HD22	29:4d:74:GLN:HB3	2.02	0.42
42:4q:578:TYR:CE2	42:4q:582:ILE:HD11	2.54	0.42
1:2m:305:MET:HB3	1:2m:313:LYS:O	2.21	0.41
59:2q:101:CDL:C36	8:2t:35:CYS:SG	3.08	0.41
14:3B:340:LEU:HG	14:3B:523:VAL:HB	2.02	0.41
53:3g:401:UQ1:O2	53:3g:401:UQ1:CM3	2.67	0.41
25:41:41:LEU:HD21	35:4j:129:TYR:HE2	1.85	0.41
29:4D:69:LEU:HD22	29:4D:74:GLN:HB3	2.02	0.41
30:4e:2:ILE:HA	59:4e:202:CDL:OB3	2.20	0.41
42:4q:425:ILE:HA	42:4q:428:ILE:HD12	2.02	0.41
58:2O:201:PEE:H3	58:2O:202:PEE:H13	2.02	0.41
20:3H:251:ARG:NE	20:3H:284:GLU:OE2	2.52	0.41
21:3I:83:ILE:HD13	21:3I:138:LYS:HG2	2.02	0.41
16:3d:109:TYR:CD1	16:3d:109:TYR:N	2.88	0.41
19:3g:121:ILE:HD13	19:3g:128:SER:HB3	2.00	0.41
63:4C:101:LPP:H311	32:4G:18:GLY:HA3	2.02	0.41
46:4U:354:TYR:O	46:4U:354:TYR:CG	2.72	0.41
49:4X:151:ALA:HB2	49:4X:165:TRP:CE3	2.55	0.41
38:4m:41:HIS:CD2	50:4y:46:GLU:HG2	2.55	0.41
45:4t:37:ILE:HG13	45:4t:38:TRP:CD1	2.55	0.41
1:2M:123:ALA:O	1:2M:126:VAL:HG22	2.20	0.41
1:2M:289:CYS:HB3	1:2M:346:LEU:HD21	2.02	0.41
2:2N:33:LEU:HD13	9:2U:2:TYR:CE1	2.56	0.41
3:2o:157:ARG:HD2	8:2t:56:ASP:OD2	2.19	0.41
12:31:74:MET:HE3	20:3H:312:PRO:HB3	2.02	0.41
12:31:109:GLY:HA3	12:31:114:GLU:HG2	2.03	0.41
14:3B:381:PHE:CD1	14:3B:382:SER:N	2.89	0.41
16:3D:75:TRP:HA	16:3D:78:THR:HG22	2.03	0.41
20:3H:62:PRO:CB	20:3H:157:ILE:HD11	2.50	0.41
59:3e:201:CDL:H351	59:3e:201:CDL:H311	2.02	0.41
37:4L:123:ASP:OD1	37:4L:126:ASN:ND2	2.53	0.41
38:4M:21:ARG:HB3	38:4M:22:PRO:HD2	2.02	0.41
42:4Q:769:SER:HB3	42:4Q:822:GLN:HB2	2.02	0.41
59:4e:202:CDL:HB4	59:4e:202:CDL:OB9	2.21	0.41
32:4g:6:LEU:HD11	59:4z:303:CDL:H371	2.03	0.41
33:4h:74:LEU:HD13	34:4i:82:ILE:HD11	2.02	0.41
41:4p:149:VAL:HG12	41:4p:150:MET:HE2	2.01	0.41
42:4q:478:TYR:HA	42:4q:482:PRO:HG2	2.01	0.41
9:2U:47:ASP:OD1	9:2U:48:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:3H:27:THR:HG23	24:3L:559:VAL:HA	2.02	0.41
13:3a:66:ILE:HG12	13:3a:220:MET:HE3	2.02	0.41
15:3c:149:LEU:HD23	15:3c:152:GLN:HG3	2.02	0.41
19:3g:195:GLU:CD	19:3g:195:GLU:H	2.29	0.41
49:4x:151:ALA:HB2	49:4x:165:TRP:CE3	2.55	0.41
49:4x:212:ASP:O	49:4x:215:THR:OG1	2.37	0.41
50:4y:40:ASP:OD1	50:4y:40:ASP:N	2.49	0.41
1:2M:430:ARG:HD2	1:2M:435:SER:HB2	2.02	0.41
1:2m:123:ALA:O	1:2m:126:VAL:HG22	2.20	0.41
1:2m:264:PRO:HG3	1:2m:402:PRO:HD2	2.03	0.41
9:2u:47:ASP:OD1	9:2u:48:GLN:N	2.53	0.41
13:3A:365:VAL:O	13:3A:369:MET:HG3	2.20	0.41
14:3b:369:THR:HG21	23:3k:22:LEU:HG	2.01	0.41
25:40:41:LEU:HD21	35:4J:129:TYR:HE2	1.86	0.41
41:4P:174:ILE:HB	42:4Q:756:ILE:HG13	2.02	0.41
34:4i:177:ARG:CG	38:4m:27:VAL:HG11	2.50	0.41
37:4l:123:ASP:OD1	37:4l:126:ASN:ND2	2.53	0.41
41:4p:194:GLN:HA	41:4p:195:TRP:HA	1.85	0.41
1:2M:202:ILE:HG21	1:2M:463:LEU:HD22	2.03	0.41
1:2m:202:ILE:HG21	1:2m:463:LEU:HD22	2.03	0.41
2:2n:214:TRP:HB2	2:2n:279:TYR:CE2	2.55	0.41
12:31:75:PRO:HB2	15:3c:142:GLN:HA	2.02	0.41
39:4N:64:PRO:HA	47:4V:103:TRP:CD2	2.55	0.41
42:4Q:578:TYR:CE2	42:4Q:582:ILE:HD11	2.54	0.41
51:4Z:119:VAL:N	51:4Z:120:PRO:HD2	2.35	0.41
37:4l:103:MET:HE2	59:4q:903:CDL:H411	2.02	0.41
43:4r:51:MET:HA	43:4r:55:GLU:HG2	2.03	0.41
1:2M:88:LEU:HD11	1:2M:127:VAL:HG11	2.03	0.41
13:3A:264:LEU:O	13:3A:453:THR:HG23	2.21	0.41
19:3G:195:GLU:OE2	19:3G:300:ASN:ND2	2.45	0.41
15:3c:175:ALA:CB	22:3j:56:VAL:HG22	2.51	0.41
30:4E:46:TRP:O	34:4I:84:PRO:HD2	2.21	0.41
33:4H:36:HIS:CE1	34:4I:139:ALA:HB2	2.55	0.41
42:4Q:474:MET:HB2	42:4Q:638:LEU:HD21	2.02	0.41
33:4h:19:VAL:HG11	33:4h:37:HIS:NE2	2.35	0.41
4:2p:2:LEU:HB2	10:2v:77:ILE:HD13	2.02	0.41
17:3E:57:ASP:OD2	20:3H:180:HIS:HA	2.21	0.41
21:3I:176:THR:O	21:3I:176:THR:HG22	2.21	0.41
16:3d:75:TRP:HA	16:3d:78:THR:HG22	2.03	0.41
20:3h:295:LEU:HD12	20:3h:314:HIS:CE1	2.56	0.41
25:40:17:ILE:O	25:40:21:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4B:90:VAL:HG21	35:4J:194:TYR:HB2	2.02	0.41
40:4O:376:LEU:O	40:4O:380:THR:HG23	2.20	0.41
29:4d:86:PHE:CE1	38:4m:88:ARG:HD3	2.55	0.41
34:4i:224:PRO:HA	38:4m:88:ARG:HG3	2.02	0.41
1:2M:305:MET:HB3	1:2M:313:LYS:O	2.21	0.41
2:2N:53:MET:HE3	2:2N:96:LEU:C	2.46	0.41
2:2N:75:CYS:O	2:2N:76:ARG:HB3	2.20	0.41
59:2O:203:CDL:H342	21:3I:34:PHE:HB3	2.03	0.41
4:2P:24:ARG:HB2	4:2P:27:GLU:HG3	2.03	0.41
1:2m:73:THR:O	1:2m:73:THR:HG22	2.20	0.41
2:2n:53:MET:HE3	2:2n:96:LEU:C	2.46	0.41
4:2p:24:ARG:HB2	4:2p:27:GLU:HG3	2.03	0.41
14:3b:340:LEU:HG	14:3b:523:VAL:HB	2.02	0.41
18:3f:15:PHE:CZ	21:3i:145:GLN:HG2	2.56	0.41
19:3g:268:LEU:HD22	19:3g:274:GLY:HA2	2.03	0.41
19:3g:291:TYR:CE2	59:3l:701:CDL:H571	2.56	0.41
35:4J:146:ASN:O	35:4J:149:GLN:HG2	2.21	0.41
38:4M:41:HIS:CD2	50:4Y:46:GLU:HG2	2.56	0.41
42:4Q:774:ILE:HG21	67:4Q:908:HEA:HMC1	2.02	0.41
45:4T:98:GLU:OE1	47:4V:37:TYR:HE1	2.04	0.41
35:4j:131:VAL:HG13	59:4j:302:CDL:H581	2.03	0.41
42:4q:474:MET:HB2	42:4q:638:LEU:HD21	2.02	0.41
42:4q:593:LEU:N	42:4q:594:PRO:HD2	2.36	0.41
43:4r:96:THR:HA	43:4r:99:LYS:HE2	2.03	0.41
6:2r:72:TRP:CD1	6:2r:73:LYS:HG3	2.56	0.41
15:3C:149:LEU:HD23	15:3C:152:GLN:HG3	2.02	0.41
16:3D:86:PRO:HG3	59:3H:405:CDL:H832	2.03	0.41
19:3G:195:GLU:CD	19:3G:195:GLU:H	2.29	0.41
21:3I:131:ALA:O	21:3I:135:GLU:HG2	2.21	0.41
22:3J:9:PHE:HB2	22:3J:12:MET:HG3	2.03	0.41
13:3a:264:LEU:O	13:3a:453:THR:HG23	2.21	0.41
19:3g:254:PRO:HG2	19:3g:259:LEU:HD23	2.03	0.41
22:3j:47:GLU:HG2	22:3j:48:TRP:N	2.36	0.41
41:4P:194:GLN:HA	41:4P:195:TRP:HA	1.85	0.41
46:4U:413:ILE:HG23	47:4V:146:PHE:CE2	2.56	0.41
51:4Z:108:TRP:N	51:4Z:109:PRO:HD2	2.36	0.41
48:4w:128:GLU:O	48:4w:143:GLU:HA	2.21	0.41
6:2R:72:TRP:CD1	6:2R:73:LYS:HG3	2.56	0.40
11:30:16:THR:HG22	19:3g:245:ILE:CD1	2.50	0.40
12:31:144:GLU:HG2	15:3c:37:GLU:HG3	2.03	0.40
18:3F:15:PHE:CZ	21:3I:145:GLN:HG2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3F:26:VAL:O	18:3F:30:MET:HG2	2.21	0.40
30:4E:2:ILE:HA	59:4E:202:CDL:OB3	2.20	0.40
35:4J:29:GLY:HA2	36:4K:51:VAL:HG22	2.03	0.40
41:4P:175:ASN:HB3	42:4Q:690:LEU:HD11	2.03	0.40
42:4Q:486:LEU:HG	42:4Q:567:ILE:HD13	2.03	0.40
44:4S:10:ALA:O	44:4S:14:MET:HG2	2.21	0.40
34:4i:236:ASP:OD1	39:4n:74:LYS:HG2	2.21	0.40
41:4p:176:PHE:CD1	42:4q:690:LEU:HD21	2.56	0.40
44:4s:10:ALA:O	44:4s:14:MET:HG2	2.21	0.40
46:4u:414:ARG:N	46:4u:415:PRO:HD2	2.35	0.40
49:4x:55:VAL:O	49:4x:59:MET:HG2	2.22	0.40
4:2P:61:SER:O	4:2P:62:ALA:C	2.64	0.40
5:2Q:4:LYS:HA	8:2T:74:TYR:O	2.21	0.40
2:2n:75:CYS:O	2:2n:76:ARG:HB3	2.20	0.40
11:30:125:LEU:HG	12:31:21:LYS:HD2	2.03	0.40
14:3B:315:SER:HA	18:3F:1:THR:HB	2.02	0.40
19:3G:254:PRO:HB3	53:3G:401:UQ1:HM32	2.04	0.40
14:3b:381:PHE:CD1	14:3b:382:SER:N	2.89	0.40
60:3f:101:PC1:H133	60:3f:101:PC1:H112	1.86	0.40
28:4C:56:THR:HG23	32:4G:32:CYS:HA	2.02	0.40
30:4E:45:MET:HE3	34:4I:51:TYR:CD2	2.56	0.40
34:4I:115:LYS:N	34:4I:116:PRO:HD2	2.37	0.40
35:4J:80:TRP:HB2	35:4J:84:CYS:SG	2.61	0.40
42:4Q:425:ILE:HA	42:4Q:428:ILE:HD12	2.02	0.40
30:4e:53:THR:HG21	48:4w:96:ILE:CD1	2.51	0.40
59:4o:501:CDL:H621	59:4o:501:CDL:H662	2.02	0.40
46:4u:354:TYR:O	46:4u:354:TYR:CG	2.72	0.40
1:2M:73:THR:O	1:2M:73:THR:HG22	2.21	0.40
1:2M:264:PRO:HG3	1:2M:402:PRO:HD2	2.03	0.40
3:2O:54:TRP:CH2	27:4b:7:ILE:HD11	2.56	0.40
1:2m:430:ARG:HD2	1:2m:435:SER:HB2	2.02	0.40
2:2n:33:LEU:HD13	9:2u:2:TYR:CE1	2.56	0.40
2:2n:222:TYR:CE1	6:2r:3:ALA:HA	2.57	0.40
3:2o:92:PHE:CD2	8:2t:29:LEU:HD13	2.57	0.40
19:3G:99:ILE:HG13	19:3G:103:TYR:CE2	2.56	0.40
20:3H:295:LEU:HD12	20:3H:314:HIS:CE1	2.56	0.40
25:41:219:VAL:CG2	59:4f:201:CDL:H772	2.52	0.40
40:4O:377:MET:HE3	42:4Q:756:ILE:O	2.21	0.40
41:4P:176:PHE:HD1	42:4Q:690:LEU:HD21	1.87	0.40
30:4e:45:MET:HE3	34:4i:51:TYR:CD2	2.57	0.40
36:4k:60:VAL:N	36:4k:61:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4m:21:ARG:HB3	38:4m:22:PRO:HD2	2.02	0.40
42:4q:769:SER:HB3	42:4q:822:GLN:HB2	2.02	0.40
43:4r:56:LYS:HA	43:4r:59:TYR:CZ	2.57	0.40
46:4u:413:ILE:HG23	47:4v:146:PHE:CE2	2.56	0.40
1:2m:485:VAL:HG13	1:2m:528:VAL:HA	2.04	0.40
1:2m:591:TYR:CE1	1:2m:605:LYS:HE2	2.56	0.40
4:2p:61:SER:O	4:2p:62:ALA:C	2.64	0.40
59:2q:101:CDL:H361	8:2t:35:CYS:SG	2.61	0.40
13:3A:198:ASN:O	13:3A:202:ILE:HG12	2.22	0.40
13:3A:369:MET:HE2	13:3A:369:MET:HB3	1.96	0.40
17:3E:39:PRO:HD2	17:3E:42:ILE:HD12	2.04	0.40
22:3J:47:GLU:HG2	22:3J:48:TRP:N	2.36	0.40
14:3b:366:VAL:HB	14:3b:367:PRO:HD3	2.03	0.40
25:40:39:LEU:HD21	59:4L:201:CDL:H841	2.02	0.40
25:41:203:ILE:HD13	35:4j:83:TRP:CD1	2.55	0.40
59:4E:202:CDL:HB61	59:4E:202:CDL:OB7	2.22	0.40
43:4R:51:MET:HA	43:4R:55:GLU:HG2	2.03	0.40
48:4W:128:GLU:O	48:4W:143:GLU:HA	2.21	0.40
34:4i:201:LEU:HD12	40:4o:393:VAL:HG21	2.04	0.40
41:4p:160:PRO:HB3	67:4q:908:HEA:H253	2.03	0.40
41:4p:176:PHE:HD1	42:4q:690:LEU:HD21	1.85	0.40
1:2M:319:ASP:OD1	1:2M:320:VAL:N	2.55	0.40
2:2N:234:CYS:HA	2:2N:235:PRO:HD3	1.97	0.40
1:2m:229:GLN:NE2	1:2m:453:ILE:HG21	2.37	0.40
1:2m:319:ASP:OD1	1:2m:320:VAL:N	2.55	0.40
1:2m:400:LEU:CD1	1:2m:410:ILE:HG22	2.51	0.40
59:2q:101:CDL:H552	59:2q:101:CDL:H352	2.02	0.40
12:31:161:GLY:O	12:31:162:ALA:C	2.65	0.40
14:3B:423:MET:HE1	14:3B:439:ALA:HA	2.04	0.40
24:3L:603:LYS:C	24:3L:605:PRO:HD3	2.47	0.40
18:3f:26:VAL:O	18:3f:30:MET:HG2	2.21	0.40
21:3i:131:ALA:O	21:3i:135:GLU:HG2	2.21	0.40
39:4N:138:HIS:HD2	42:4Q:833:ARG:O	2.05	0.40
42:4Q:632:HIS:CD2	42:4Q:636:TYR:HE2	2.34	0.40
51:4z:108:TRP:N	51:4z:109:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2M	602/604 (100%)	579 (96%)	23 (4%)	0	100	100
1	2m	602/604 (100%)	579 (96%)	23 (4%)	0	100	100
2	2N	257/259 (99%)	244 (95%)	13 (5%)	0	100	100
2	2n	257/259 (99%)	244 (95%)	13 (5%)	0	100	100
3	2O	158/160 (99%)	158 (100%)	0	0	100	100
3	2o	158/160 (99%)	158 (100%)	0	0	100	100
4	2P	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	2p	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
5	2Q	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
5	2q	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
6	2R	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
6	2r	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
7	2S	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
7	2s	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
8	2T	80/82 (98%)	80 (100%)	0	0	100	100
8	2t	80/82 (98%)	80 (100%)	0	0	100	100
9	2U	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
9	2u	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
10	2V	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
10	2v	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
11	30	154/173 (89%)	149 (97%)	5 (3%)	0	100	100
12	31	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
13	3A	452/454 (100%)	445 (98%)	7 (2%)	0	100	100
13	3a	452/454 (100%)	445 (98%)	7 (2%)	0	100	100
14	3B	494/496 (100%)	489 (99%)	4 (1%)	1 (0%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	3b	494/496 (100%)	489 (99%)	4 (1%)	1 (0%)	43	63
15	3C	239/242 (99%)	232 (97%)	7 (3%)	0	100	100
15	3c	240/242 (99%)	234 (98%)	6 (2%)	0	100	100
16	3D	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
16	3d	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
17	3E	90/92 (98%)	90 (100%)	0	0	100	100
17	3e	90/92 (98%)	90 (100%)	0	0	100	100
18	3F	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
18	3f	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
19	3G	352/354 (99%)	342 (97%)	10 (3%)	0	100	100
19	3g	352/354 (99%)	336 (96%)	16 (4%)	0	100	100
20	3H	324/326 (99%)	313 (97%)	11 (3%)	0	100	100
20	3h	324/326 (99%)	313 (97%)	11 (3%)	0	100	100
21	3I	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
21	3i	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
22	3J	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
22	3j	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
23	3K	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
23	3k	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
24	3L	66/68 (97%)	58 (88%)	8 (12%)	0	100	100
24	3l	66/68 (97%)	58 (88%)	8 (12%)	0	100	100
25	40	228/230 (99%)	225 (99%)	3 (1%)	0	100	100
25	41	228/230 (99%)	225 (99%)	3 (1%)	0	100	100
26	4A	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
26	4a	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
27	4B	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
27	4b	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
28	4C	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
28	4c	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
29	4D	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
29	4d	88/90 (98%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	4E	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
30	4e	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
31	4F	78/85 (92%)	74 (95%)	4 (5%)	0	100	100
31	4f	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
32	4G	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
32	4g	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
33	4H	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
33	4h	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
34	4I	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
34	4i	194/196 (99%)	193 (100%)	1 (0%)	0	100	100
35	4J	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
35	4j	184/186 (99%)	179 (97%)	5 (3%)	0	100	100
36	4K	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
36	4k	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
37	4L	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
37	4l	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
38	4M	97/99 (98%)	97 (100%)	0	0	100	100
38	4m	97/99 (98%)	97 (100%)	0	0	100	100
39	4N	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
39	4n	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
40	4O	45/47 (96%)	45 (100%)	0	0	100	100
40	4o	45/47 (96%)	45 (100%)	0	0	100	100
41	4P	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
41	4p	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
42	4Q	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
42	4q	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
43	4R	101/103 (98%)	101 (100%)	0	0	100	100
43	4r	101/103 (98%)	101 (100%)	0	0	100	100
44	4S	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
44	4s	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
45	4T	119/121 (98%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	4t	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
46	4U	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
46	4u	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
47	4V	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
47	4v	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
48	4W	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
48	4w	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
49	4X	224/226 (99%)	220 (98%)	4 (2%)	0	100	100
49	4x	224/226 (99%)	220 (98%)	4 (2%)	0	100	100
50	4Y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
50	4y	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
51	4Z	184/186 (99%)	181 (98%)	3 (2%)	0	100	100
51	4z	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
All	All	16327/16550 (99%)	15930 (98%)	395 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	3B	262	THR
14	3b	262	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2M	478/478 (100%)	473 (99%)	5 (1%)	68	86
1	2m	478/478 (100%)	474 (99%)	4 (1%)	73	88
2	2N	221/221 (100%)	221 (100%)	0	100	100
2	2n	221/221 (100%)	221 (100%)	0	100	100
3	2O	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	143/143 (100%)	143 (100%)	0	100	100
7	2s	143/143 (100%)	143 (100%)	0	100	100
8	2T	73/73 (100%)	72 (99%)	1 (1%)	59	81
8	2t	73/73 (100%)	72 (99%)	1 (1%)	59	81
9	2U	43/43 (100%)	43 (100%)	0	100	100
9	2u	43/43 (100%)	43 (100%)	0	100	100
10	2V	75/75 (100%)	75 (100%)	0	100	100
10	2v	75/75 (100%)	75 (100%)	0	100	100
11	30	102/102 (100%)	101 (99%)	1 (1%)	68	86
12	31	126/126 (100%)	121 (96%)	5 (4%)	28	54
13	3A	386/386 (100%)	386 (100%)	0	100	100
13	3a	386/386 (100%)	386 (100%)	0	100	100
14	3B	423/423 (100%)	422 (100%)	1 (0%)	87	95
14	3b	423/423 (100%)	422 (100%)	1 (0%)	87	95
15	3C	204/205 (100%)	204 (100%)	0	100	100
15	3c	205/205 (100%)	203 (99%)	2 (1%)	68	86
16	3D	88/88 (100%)	88 (100%)	0	100	100
16	3d	88/88 (100%)	88 (100%)	0	100	100
17	3E	81/81 (100%)	81 (100%)	0	100	100
17	3e	81/81 (100%)	81 (100%)	0	100	100
18	3F	72/72 (100%)	72 (100%)	0	100	100
18	3f	72/72 (100%)	72 (100%)	0	100	100
19	3G	336/336 (100%)	335 (100%)	1 (0%)	86	94
19	3g	336/336 (100%)	334 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	3H	280/280 (100%)	279 (100%)	1 (0%)	84 93
20	3h	279/280 (100%)	278 (100%)	1 (0%)	84 93
21	3I	154/154 (100%)	154 (100%)	0	100 100
21	3i	154/154 (100%)	154 (100%)	0	100 100
22	3J	79/79 (100%)	79 (100%)	0	100 100
22	3j	79/79 (100%)	79 (100%)	0	100 100
23	3K	67/67 (100%)	66 (98%)	1 (2%)	57 80
23	3k	67/67 (100%)	66 (98%)	1 (2%)	57 80
24	3L	59/59 (100%)	59 (100%)	0	100 100
24	3l	59/59 (100%)	59 (100%)	0	100 100
25	40	229/229 (100%)	229 (100%)	0	100 100
25	41	229/229 (100%)	229 (100%)	0	100 100
26	4A	91/91 (100%)	91 (100%)	0	100 100
26	4a	91/91 (100%)	91 (100%)	0	100 100
27	4B	77/77 (100%)	77 (100%)	0	100 100
27	4b	77/77 (100%)	77 (100%)	0	100 100
28	4C	64/64 (100%)	64 (100%)	0	100 100
28	4c	64/64 (100%)	64 (100%)	0	100 100
29	4D	81/81 (100%)	81 (100%)	0	100 100
29	4d	81/81 (100%)	81 (100%)	0	100 100
30	4E	146/146 (100%)	145 (99%)	1 (1%)	76 89
30	4e	146/146 (100%)	145 (99%)	1 (1%)	76 89
31	4F	70/74 (95%)	70 (100%)	0	100 100
31	4f	74/74 (100%)	74 (100%)	0	100 100
32	4G	83/83 (100%)	82 (99%)	1 (1%)	63 83
32	4g	83/83 (100%)	82 (99%)	1 (1%)	63 83
33	4H	124/124 (100%)	123 (99%)	1 (1%)	73 88
33	4h	124/124 (100%)	123 (99%)	1 (1%)	73 88
34	4I	180/180 (100%)	179 (99%)	1 (1%)	78 91
34	4i	180/180 (100%)	179 (99%)	1 (1%)	78 91
35	4J	148/148 (100%)	148 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	4j	148/148 (100%)	148 (100%)	0	100	100
36	4K	77/77 (100%)	77 (100%)	0	100	100
36	4k	77/77 (100%)	77 (100%)	0	100	100
37	4L	108/108 (100%)	108 (100%)	0	100	100
37	4l	108/108 (100%)	108 (100%)	0	100	100
38	4M	85/85 (100%)	85 (100%)	0	100	100
38	4m	85/85 (100%)	85 (100%)	0	100	100
39	4N	112/112 (100%)	112 (100%)	0	100	100
39	4n	112/112 (100%)	112 (100%)	0	100	100
40	4O	40/40 (100%)	40 (100%)	0	100	100
40	4o	40/40 (100%)	40 (100%)	0	100	100
41	4P	163/163 (100%)	162 (99%)	1 (1%)	78	91
41	4p	163/163 (100%)	162 (99%)	1 (1%)	78	91
42	4Q	419/419 (100%)	419 (100%)	0	100	100
42	4q	419/419 (100%)	419 (100%)	0	100	100
43	4R	92/92 (100%)	92 (100%)	0	100	100
43	4r	92/92 (100%)	92 (100%)	0	100	100
44	4S	59/59 (100%)	59 (100%)	0	100	100
44	4s	59/59 (100%)	59 (100%)	0	100	100
45	4T	102/102 (100%)	102 (100%)	0	100	100
45	4t	102/102 (100%)	102 (100%)	0	100	100
46	4U	76/76 (100%)	76 (100%)	0	100	100
46	4u	76/76 (100%)	76 (100%)	0	100	100
47	4V	156/156 (100%)	156 (100%)	0	100	100
47	4v	156/156 (100%)	156 (100%)	0	100	100
48	4W	128/128 (100%)	128 (100%)	0	100	100
48	4w	128/128 (100%)	128 (100%)	0	100	100
49	4X	198/198 (100%)	198 (100%)	0	100	100
49	4x	198/198 (100%)	198 (100%)	0	100	100
50	4Y	100/100 (100%)	100 (100%)	0	100	100
50	4y	100/100 (100%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	4Z	167/167 (100%)	167 (100%)	0	100 100
51	4z	167/167 (100%)	167 (100%)	0	100 100
All	All	14364/14370 (100%)	14326 (100%)	38 (0%)	84 94

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2M	92	THR
1	2M	150	PHE
1	2M	173	THR
1	2M	308	TYR
1	2M	357	ARG
8	2T	56	ASP
1	2m	150	PHE
1	2m	173	THR
1	2m	308	TYR
1	2m	357	ARG
8	2t	56	ASP
11	30	169	THR
12	31	59	TYR
12	31	66	PHE
12	31	74	MET
12	31	158	THR
12	31	160	LEU
14	3B	219	PHE
19	3G	348	TYR
20	3H	288	MET
23	3K	59	SER
14	3b	219	PHE
15	3c	37	GLU
15	3c	133	ASN
19	3g	45	MET
19	3g	348	TYR
20	3h	288	MET
23	3k	59	SER
30	4E	35	MET
32	4G	24	TRP
33	4H	36	HIS
34	4I	67	GLU
41	4P	186	MET
30	4e	35	MET

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Mol	Chain	Res	Type
32	4g	24	TRP
33	4h	36	HIS
34	4i	67	GLU
41	4p	186	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	2M	35	HIS
1	2M	85	ASN
1	2M	118	HIS
1	2M	153	GLN
1	2M	228	HIS
1	2M	429	ASN
1	2M	571	HIS
2	2N	39	HIS
2	2N	113	HIS
2	2N	195	GLN
5	2Q	48	HIS
6	2R	81	HIS
7	2S	69	HIS
7	2S	84	HIS
7	2S	139	GLN
7	2S	160	HIS
1	2m	35	HIS
1	2m	85	ASN
1	2m	118	HIS
1	2m	153	GLN
1	2m	228	HIS
1	2m	429	ASN
1	2m	571	HIS
2	2n	39	HIS
2	2n	113	HIS
2	2n	195	GLN
5	2q	48	HIS
7	2s	84	HIS
7	2s	139	GLN
8	2t	32	ASN
11	30	128	HIS
12	31	157	GLN
13	3A	144	ASN
13	3A	214	ASN

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Mol	Chain	Res	Type
14	3B	58	ASN
14	3B	64	GLN
14	3B	76	HIS
14	3B	108	GLN
15	3C	261	HIS
18	3F	6	HIS
18	3F	25	GLN
19	3G	22	ASN
19	3G	191	ASN
20	3H	24	HIS
21	3I	171	HIS
23	3K	79	HIS
24	3L	554	GLN
24	3L	576	ASN
24	3L	590	GLN
13	3a	99	GLN
13	3a	144	ASN
13	3a	214	ASN
13	3a	232	GLN
14	3b	58	ASN
14	3b	64	GLN
14	3b	76	HIS
14	3b	108	GLN
15	3c	261	HIS
16	3d	52	GLN
16	3d	99	ASN
18	3f	6	HIS
18	3f	25	GLN
19	3g	22	ASN
19	3g	42	ASN
19	3g	46	ASN
19	3g	49	ASN
19	3g	191	ASN
19	3g	330	ASN
20	3h	24	HIS
20	3h	187	HIS
21	3i	4	HIS
21	3i	171	HIS
23	3k	79	HIS
24	3l	554	GLN
24	3l	576	ASN
24	3l	590	GLN

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Mol	Chain	Res	Type
25	40	43	ASN
25	40	59	ASN
25	40	181	HIS
25	40	199	ASN
25	40	215	HIS
25	41	43	ASN
25	41	59	ASN
25	41	147	ASN
25	41	181	HIS
25	41	199	ASN
25	41	215	HIS
26	4A	56	GLN
29	4D	57	HIS
29	4D	74	GLN
30	4E	26	HIS
30	4E	42	ASN
31	4F	77	HIS
31	4F	125	GLN
33	4H	36	HIS
34	4I	50	HIS
34	4I	89	GLN
35	4J	64	HIS
35	4J	79	HIS
35	4J	123	ASN
38	4M	99	HIS
40	4O	381	HIS
41	4P	88	HIS
41	4P	110	GLN
41	4P	178	GLN
42	4Q	443	ASN
42	4Q	502	ASN
42	4Q	654	ASN
43	4R	30	GLN
43	4R	97	ASN
44	4S	35	HIS
47	4V	143	HIS
48	4W	61	HIS
48	4W	83	GLN
49	4X	35	HIS
49	4X	104	GLN
50	4Y	108	HIS
51	4Z	125	GLN

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Mol	Chain	Res	Type
51	4Z	187	ASN
29	4d	74	GLN
30	4e	26	HIS
30	4e	42	ASN
31	4f	77	HIS
31	4f	125	GLN
31	4f	156	GLN
33	4h	36	HIS
34	4i	50	HIS
34	4i	89	GLN
35	4j	64	HIS
35	4j	79	HIS
35	4j	123	ASN
38	4m	99	HIS
40	4o	381	HIS
41	4p	88	HIS
41	4p	110	GLN
41	4p	178	GLN
42	4q	443	ASN
42	4q	502	ASN
42	4q	654	ASN
42	4q	709	ASN
43	4r	30	GLN
43	4r	97	ASN
44	4s	35	HIS
48	4w	61	HIS
48	4w	83	GLN
49	4x	35	HIS
49	4x	104	GLN
50	4y	108	HIS
51	4z	125	GLN
51	4z	187	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	AME	2S	1	7	9,10,11	0.27	0	9,11,13	0.48	0
7	AME	2s	1	7	9,10,11	0.30	0	9,11,13	0.49	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
7	AME	2S	1	7	-	2/9/10/12	-
7	AME	2s	1	7	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2S	1	AME	O-C-CA-CB
7	2S	1	AME	C-CA-N-CT1
7	2s	1	AME	O-C-CA-CB
7	2s	1	AME	C-CA-N-CT1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 158 ligands modelled in this entry, 14 are monoatomic - leaving 144 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	$\#\|Z\| > 2$
59	CDL	3l	702	-	80,80,99	0.33	0	86,92,111	0.48	0
67	HEA	4q	907	42	66,67,67	1.35	7 (10%)	78,103,103	2.42	28 (35%)
55	SF4	2n	302	2	0,12,12	-	-	-		
59	CDL	4f	201	-	91,91,99	0.32	0	97,103,111	0.45	0
59	CDL	3I	201	-	66,66,99	0.35	0	71,77,111	0.43	0
56	F3S	2N	304	2	0,9,9	-	-	-		
68	PER	4Q	909	67,65	1,1,1	0.26	0	-		
54	FES	3h	404	20	0,4,4	-	-	-		
59	CDL	4M	201	-	74,74,99	0.32	0	80,86,111	0.43	0
59	CDL	4L	201	-	93,93,99	0.29	0	99,105,111	0.35	0
53	UQ1	2p	201	-	18,18,18	1.13	2 (11%)	22,25,25	0.63	0
58	PEE	4z	302	-	43,43,50	0.81	2 (4%)	46,48,55	0.56	0
60	PC1	3a	501	-	53,53,53	0.28	0	59,61,61	0.37	0
59	CDL	4m	201	-	99,99,99	0.28	0	105,111,111	0.50	0
60	PC1	4F	201	-	53,53,53	0.29	0	59,61,61	0.41	0
58	PEE	2P	202	-	45,45,50	0.77	2 (4%)	48,50,55	0.59	0
59	CDL	3i	202	-	75,75,99	0.33	0	81,87,111	0.49	0
68	PER	4q	909	67,65	1,1,1	0.25	0	-		
58	PEE	4Z	302	-	50,50,50	0.76	2 (4%)	53,55,55	0.55	0
59	CDL	3D	201	-	83,83,99	0.31	0	89,95,111	0.41	0
60	PC1	2R	201	-	53,53,53	0.29	0	59,61,61	0.48	1 (1%)
59	CDL	3D	202	-	99,99,99	0.29	0	105,111,111	0.39	0
61	HEC	3C	302	15	50,50,50	1.48	9 (18%)	68,82,82	1.99	12 (17%)
64	CUA	4n	201	39	0,1,1	-	-	-		
59	CDL	2q	101	-	99,99,99	0.30	0	105,111,111	0.47	0
59	CDL	4Q	902	-	94,94,99	0.30	0	100,106,111	0.47	0
63	LPP	4z	301	-	37,37,43	0.24	0	41,42,48	0.47	0
58	PEE	4S	101	-	26,26,50	0.37	0	29,31,55	0.34	0
58	PEE	40	304	-	30,30,50	0.32	0	33,35,55	0.52	0
62	HEM	3g	407	19	50,50,50	1.43	7 (14%)	66,82,82	1.42	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	CDL	3H	405	-	83,83,99	0.32	0	89,95,111	0.39	0
53	UQ1	2N	301	-	18,18,18	1.07	2 (11%)	22,25,25	0.75	0
58	PEE	2r	203	-	38,38,50	0.61	1 (2%)	41,43,55	0.46	0
59	CDL	4t	201	-	60,60,99	0.37	0	66,72,111	0.45	0
59	CDL	4U	501	-	71,71,99	0.34	0	77,83,111	0.44	0
60	PC1	3H	401	-	33,33,53	0.35	0	39,41,61	0.77	1 (2%)
59	CDL	3I	202	-	80,80,99	0.32	0	86,92,111	0.44	0
54	FES	2n	301	2	0,4,4	-	-	-		
58	PEE	4O	301	-	44,44,50	0.78	2 (4%)	46,49,55	0.55	0
60	PC1	2o	202	-	38,38,53	0.33	0	44,46,61	0.48	0
59	CDL	3e	202	-	76,76,99	0.33	0	82,88,111	0.43	0
60	PC1	3h	402	-	40,40,53	0.34	0	46,48,61	0.44	0
63	LPP	4Z	301	-	43,43,43	0.23	0	47,48,48	0.44	0
58	PEE	4q	902	-	39,39,50	0.85	2 (5%)	41,44,55	0.64	0
63	LPP	4C	101	-	43,43,43	0.24	0	47,48,48	0.38	0
60	PC1	2r	201	-	53,53,53	0.30	0	59,61,61	0.57	1 (1%)
59	CDL	3g	406	-	57,57,99	0.38	0	63,69,111	0.55	0
60	PC1	2r	202	-	51,51,53	0.29	0	57,59,61	0.40	0
58	PEE	4q	901	-	36,36,50	0.89	2 (5%)	38,41,55	0.64	0
60	PC1	3h	401	-	39,39,53	0.33	0	45,47,61	0.46	0
58	PEE	4D	101	-	39,39,50	0.66	1 (2%)	42,44,55	0.45	0
52	FAD	2M	701	1	56,58,58	0.73	2 (3%)	81,89,89	1.01	4 (4%)
59	CDL	4J	301	-	58,58,99	0.36	0	62,69,111	0.49	0
59	CDL	2p	204	-	73,73,99	0.33	0	79,85,111	0.50	0
67	HEA	4q	908	42,68	66,67,67	1.38	7 (10%)	78,103,103	2.38	29 (37%)
59	CDL	4z	303	-	92,92,99	0.30	0	98,104,111	0.51	1 (1%)
59	CDL	4E	201	-	88,88,99	0.30	0	94,100,111	0.37	0
58	PEE	4s	101	-	46,46,50	0.80	2 (4%)	49,51,55	0.52	0
58	PEE	3H	403	-	45,45,50	0.79	2 (4%)	48,50,55	0.75	1 (2%)
59	CDL	4Z	303	-	47,47,99	0.40	0	53,59,111	0.49	0
59	CDL	4O	501	-	96,96,99	0.30	0	102,108,111	0.41	0
62	HEM	3G	406	19	50,50,50	1.51	8 (16%)	66,82,82	1.54	9 (13%)
54	FES	3H	406	20	0,4,4	-	-	-		
60	PC1	4e	201	-	53,53,53	0.28	0	59,61,61	0.35	0
59	CDL	41	304	-	91,91,99	0.29	0	97,103,111	0.41	0
58	PEE	3c	301	-	32,32,50	0.70	1 (3%)	34,37,55	0.43	0
59	CDL	3E	201	-	92,92,99	0.30	0	98,104,111	0.37	0
58	PEE	41	301	-	44,44,50	0.80	2 (4%)	46,49,55	0.43	0
59	CDL	2T	104	-	70,70,99	0.34	0	76,82,111	0.56	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	PEE	3f	102	-	37,37,50	0.66	1 (2%)	40,42,55	0.51	0
58	PEE	4w	201	-	50,50,50	0.75	2 (4%)	53,55,55	0.52	0
53	UQ1	3g	402	-	18,18,18	1.07	2 (11%)	22,25,25	0.64	0
59	CDL	2O	203	-	66,66,99	0.35	0	72,78,111	0.56	0
60	PC1	2T	102	-	44,44,53	0.31	0	50,52,61	0.37	0
58	PEE	41	303	-	35,35,50	0.67	1 (2%)	38,40,55	0.56	0
58	PEE	2t	101	-	41,41,50	0.62	1 (2%)	44,46,55	0.46	0
53	UQ1	3G	402	-	18,18,18	1.06	2 (11%)	22,25,25	0.65	0
59	CDL	4q	903	-	92,92,99	0.29	0	98,104,111	0.51	0
60	PC1	2p	202	-	40,40,53	0.31	0	46,48,61	0.35	0
58	PEE	2O	202	-	40,40,50	0.64	1 (2%)	43,45,55	0.52	0
53	UQ1	3g	401	-	18,18,18	1.02	1 (5%)	22,25,25	1.04	2 (9%)
59	CDL	2o	201	-	85,85,99	0.31	0	91,97,111	0.42	0
59	CDL	3L	701	-	84,84,99	0.31	0	90,96,111	0.44	0
53	UQ1	3G	401	-	18,18,18	0.95	2 (11%)	22,25,25	1.33	4 (18%)
59	CDL	4g	202	-	65,65,99	0.35	0	69,76,111	0.47	0
61	HEC	3c	302	15	50,50,50	1.45	10 (20%)	68,82,82	1.48	10 (14%)
59	CDL	3h	403	-	84,84,99	0.32	0	90,96,111	0.48	1 (1%)
60	PC1	3A	501	-	37,37,53	0.32	0	43,45,61	0.36	0
56	F3S	2n	303	2	0,9,9	-	-	-		
52	FAD	2m	701	1	56,58,58	0.72	3 (5%)	81,89,89	0.98	4 (4%)
59	CDL	3g	404	-	88,88,99	0.30	0	94,100,111	0.42	0
58	PEE	4W	201	-	50,50,50	0.74	2 (4%)	53,55,55	0.56	0
59	CDL	2t	102	-	65,65,99	0.36	0	71,77,111	0.48	0
59	CDL	3g	403	-	69,69,99	0.35	0	75,81,111	0.53	0
59	CDL	4e	203	-	95,95,99	0.31	0	101,107,111	0.47	0
59	CDL	3G	403	-	99,99,99	0.29	0	105,111,111	0.46	0
59	CDL	4S	102	-	99,99,99	0.29	0	105,111,111	0.44	1 (0%)
59	CDL	4e	202	-	49,49,99	0.41	0	55,61,111	0.62	1 (1%)
59	CDL	4j	301	-	50,50,99	0.41	0	52,60,111	0.58	0
58	PEE	40	302	-	46,46,50	0.81	2 (4%)	49,51,55	0.61	0
59	CDL	4j	302	-	87,87,99	0.30	0	93,99,111	0.33	0
59	CDL	4E	202	-	45,45,99	0.40	0	51,57,111	0.52	0
59	CDL	3g	405	-	89,89,99	0.31	0	95,101,111	0.41	0
59	CDL	4Q	903	-	74,74,99	0.32	0	80,86,111	0.42	0
59	CDL	4z	304	-	85,85,99	0.30	0	91,97,111	0.53	1 (1%)
59	CDL	3L	702	-	80,80,99	0.32	0	86,92,111	0.41	0
58	PEE	4l	201	-	37,37,50	0.82	2 (5%)	39,42,55	0.69	1 (2%)
59	CDL	3L	703	-	92,92,99	0.30	0	98,104,111	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	CDL	3i	201	-	50,50,99	0.40	0	56,62,111	0.48	0
64	CUA	4N	201	39	0,1,1	-	-	-		
59	CDL	4K	201	-	89,89,99	0.30	0	95,101,111	0.38	0
58	PEE	41	302	-	43,43,50	0.78	2 (4%)	46,48,55	0.54	0
59	CDL	2P	203	-	80,80,99	0.31	0	86,92,111	0.34	0
60	PC1	3f	101	-	45,45,53	0.31	0	51,53,61	0.36	0
58	PEE	2O	201	-	38,38,50	0.63	1 (2%)	41,43,55	0.45	0
55	SF4	2N	303	2	0,12,12	-	-	-		
58	PEE	40	303	-	34,34,50	0.66	1 (2%)	36,39,55	0.45	0
60	PC1	2R	202	-	53,53,53	0.28	0	59,61,61	0.50	1 (1%)
59	CDL	3l	701	-	99,99,99	0.29	0	105,111,111	0.47	0
59	CDL	2Q	101	-	99,99,99	0.28	0	105,111,111	0.37	0
58	PEE	2T	103	-	44,44,50	0.79	2 (4%)	46,49,55	0.53	0
59	CDL	4F	202	-	99,99,99	0.30	0	105,111,111	0.42	0
58	PEE	2o	203	-	23,23,50	0.36	0	24,27,55	0.35	0
59	CDL	3I	203	-	62,62,99	0.36	0	68,74,111	0.43	0
67	HEA	4Q	907	42	66,67,67	1.36	7 (10%)	78,103,103	2.43	28 (35%)
54	FES	2N	302	2	0,4,4	-	-	-		
58	PEE	4d	101	-	50,50,50	0.75	2 (4%)	53,55,55	0.46	0
59	CDL	4s	102	-	99,99,99	0.29	0	105,111,111	0.47	1 (0%)
63	LPP	4g	201	-	38,38,43	0.25	0	42,43,48	0.44	0
60	PC1	3H	402	-	32,32,53	0.37	0	38,40,61	0.58	0
58	PEE	2p	203	-	23,23,50	0.38	0	26,28,55	0.41	0
59	CDL	3G	404	-	74,74,99	0.33	0	80,86,111	0.45	0
60	PC1	2P	201	-	34,34,53	0.34	0	40,42,61	0.41	0
60	PC1	2T	101	-	53,53,53	0.28	0	59,61,61	0.30	0
59	CDL	4o	501	-	92,92,99	0.30	0	98,104,111	0.41	0
59	CDL	3H	404	-	88,88,99	0.31	0	94,100,111	0.39	0
59	CDL	3e	201	-	70,70,99	0.34	0	76,82,111	0.48	0
62	HEM	3g	408	19	50,50,50	1.46	8 (16%)	66,82,82	1.52	11 (16%)
59	CDL	4W	202	-	72,72,99	0.34	0	78,84,111	0.40	0
67	HEA	4Q	908	42,68	66,67,67	1.38	6 (9%)	78,103,103	2.37	29 (37%)
58	PEE	4Q	901	-	35,35,50	0.84	2 (5%)	38,40,55	0.71	1 (2%)
58	PEE	3C	301	-	29,29,50	0.74	1 (3%)	32,34,55	0.62	0
62	HEM	3G	405	19	50,50,50	1.43	7 (14%)	66,82,82	1.37	9 (13%)
58	PEE	4R	201	-	42,42,50	0.83	2 (4%)	45,47,55	0.65	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
59	CDL	3l	702	-	-	14/91/91/110	-
67	HEA	4q	907	42	-	6/36/76/76	-
55	SF4	2n	302	2	-	-	0/6/5/5
59	CDL	4f	201	-	-	26/102/102/110	-
59	CDL	3I	201	-	-	14/75/75/110	-
56	F3S	2N	304	2	-	-	0/3/3/3
54	FES	3h	404	20	-	-	0/1/1/1
59	CDL	4M	201	-	-	22/85/85/110	-
59	CDL	4L	201	-	-	21/104/104/110	-
53	UQ1	2p	201	-	-	1/9/33/33	0/1/1/1
58	PEE	4z	302	-	-	22/47/47/54	-
60	PC1	3a	501	-	-	15/57/57/57	-
59	CDL	4m	201	-	-	23/110/110/110	-
60	PC1	4F	201	-	-	15/57/57/57	-
58	PEE	2P	202	-	-	15/49/49/54	-
59	CDL	3i	202	-	-	24/86/86/110	-
58	PEE	4Z	302	-	-	20/54/54/54	-
59	CDL	3D	201	-	-	26/94/94/110	-
60	PC1	2R	201	-	-	16/57/57/57	-
59	CDL	3D	202	-	-	10/110/110/110	-
59	CDL	2q	101	-	-	32/110/110/110	-
59	CDL	4Q	902	-	-	32/105/105/110	-
63	LPP	4z	301	-	-	10/39/39/45	-
58	PEE	4S	101	-	-	3/30/30/54	-
58	PEE	40	304	-	-	7/34/34/54	-
62	HEM	3g	407	19	-	7/14/54/54	-
59	CDL	3H	405	-	-	23/94/94/110	-
53	UQ1	2N	301	-	-	1/9/33/33	0/1/1/1
58	PEE	2r	203	-	-	8/42/42/54	-
59	CDL	4t	201	-	-	22/71/71/110	-
59	CDL	4U	501	-	-	21/82/82/110	-
60	PC1	3H	401	-	-	10/37/37/57	-
59	CDL	3I	202	-	-	24/91/91/110	-
58	PEE	40	301	-	-	19/48/48/54	-
54	FES	2n	301	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PC1	2o	202	-	-	12/42/42/57	-
59	CDL	3e	202	-	-	27/87/87/110	-
60	PC1	3h	402	-	-	10/44/44/57	-
63	LPP	4Z	301	-	-	5/45/45/45	-
58	PEE	4q	902	-	-	14/43/43/54	-
63	LPP	4C	101	-	-	8/45/45/45	-
60	PC1	2r	201	-	-	7/57/57/57	-
59	CDL	3g	406	-	-	24/68/68/110	-
60	PC1	2r	202	-	-	12/55/55/57	-
58	PEE	4q	901	-	-	13/40/40/54	-
60	PC1	3h	401	-	-	13/43/43/57	-
58	PEE	4D	101	-	-	5/43/43/54	-
52	FAD	2M	701	1	-	8/34/50/50	0/6/6/6
59	CDL	4J	301	-	-	22/68/68/110	-
59	CDL	2p	204	-	-	14/84/84/110	-
67	HEA	4q	908	42,68	-	8/36/76/76	-
59	CDL	4z	303	-	-	16/103/103/110	-
59	CDL	4E	201	-	-	11/99/99/110	-
58	PEE	4s	101	-	-	9/50/50/54	-
58	PEE	3H	403	-	-	11/49/49/54	-
59	CDL	4Z	303	-	-	20/58/58/110	-
59	CDL	4O	501	-	-	24/107/107/110	-
62	HEM	3G	406	19	-	6/14/54/54	-
54	FES	3H	406	20	-	-	0/1/1/1
60	PC1	4e	201	-	-	10/57/57/57	-
59	CDL	41	304	-	-	21/102/102/110	-
58	PEE	3c	301	-	-	13/36/36/54	-
59	CDL	3E	201	-	-	37/103/103/110	-
58	PEE	41	301	-	-	9/48/48/54	-
59	CDL	2T	104	-	-	18/81/81/110	-
58	PEE	3f	102	-	-	13/41/41/54	-
58	PEE	4w	201	-	-	12/54/54/54	-
53	UQ1	3g	402	-	-	1/9/33/33	0/1/1/1
59	CDL	2O	203	-	-	24/77/77/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PC1	2T	102	-	-	8/48/48/57	-
58	PEE	41	303	-	-	12/39/39/54	-
58	PEE	2t	101	-	-	10/45/45/54	-
53	UQ1	3G	402	-	-	1/9/33/33	0/1/1/1
59	CDL	4q	903	-	-	28/103/103/110	-
60	PC1	2p	202	-	-	2/44/44/57	-
58	PEE	2O	202	-	-	16/44/44/54	-
53	UQ1	3g	401	-	-	4/9/33/33	0/1/1/1
59	CDL	2o	201	-	-	18/96/96/110	-
59	CDL	3L	701	-	-	25/95/95/110	-
61	HEC	3c	302	15	1/1/3/7	5/14/54/54	-
53	UQ1	3G	401	-	-	4/9/33/33	0/1/1/1
59	CDL	4g	202	-	-	18/75/75/110	-
59	CDL	3h	403	-	-	24/95/95/110	-
60	PC1	3A	501	-	-	7/40/40/57	-
58	PEE	3C	301	-	-	3/33/33/54	-
56	F3S	2n	303	2	-	-	0/3/3/3
52	FAD	2m	701	1	-	8/34/50/50	0/6/6/6
59	CDL	3g	404	-	-	10/99/99/110	-
58	PEE	4W	201	-	-	9/54/54/54	-
59	CDL	2t	102	-	-	9/76/76/110	-
59	CDL	3g	403	-	-	25/80/80/110	-
59	CDL	4e	203	-	-	8/106/106/110	-
59	CDL	3G	403	-	-	19/110/110/110	-
59	CDL	4S	102	-	-	17/110/110/110	-
59	CDL	4e	202	-	-	15/60/60/110	-
59	CDL	4j	301	-	-	16/59/59/110	-
58	PEE	40	302	-	-	15/50/50/54	-
59	CDL	4j	302	-	-	22/98/98/110	-
59	CDL	4E	202	-	-	12/55/55/110	-
59	CDL	3g	405	-	-	18/100/100/110	-
59	CDL	4Q	903	-	-	15/84/84/110	-
59	CDL	4z	304	-	-	23/96/96/110	-
59	CDL	3L	702	-	-	17/91/91/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PEE	4l	201	-	-	16/41/41/54	-
59	CDL	3L	703	-	-	32/103/103/110	-
59	CDL	3i	201	-	-	19/61/61/110	-
59	CDL	4K	201	-	-	26/100/100/110	-
58	PEE	41	302	-	-	13/47/47/54	-
59	CDL	2P	203	-	-	17/91/91/110	-
60	PC1	3f	101	-	-	8/49/49/57	-
58	PEE	2O	201	-	-	15/42/42/54	-
58	PEE	40	303	-	-	12/38/38/54	-
55	SF4	2N	303	2	-	-	0/6/5/5
60	PC1	2R	202	-	-	14/57/57/57	-
59	CDL	3l	701	-	-	24/110/110/110	-
59	CDL	2Q	101	-	-	29/110/110/110	-
58	PEE	2T	103	-	-	12/48/48/54	-
59	CDL	4F	202	-	-	31/110/110/110	-
58	PEE	2o	203	-	-	8/26/26/54	-
59	CDL	3I	203	-	-	22/73/73/110	-
67	HEA	4Q	907	42	-	6/36/76/76	-
58	PEE	4d	101	-	-	6/54/54/54	-
59	CDL	4s	102	-	-	14/110/110/110	-
54	FES	2N	302	2	-	-	0/1/1/1
63	LPP	4g	201	-	-	8/40/40/45	-
60	PC1	3H	402	-	-	16/36/36/57	-
58	PEE	2p	203	-	-	8/27/27/54	-
59	CDL	3G	404	-	-	12/85/85/110	-
60	PC1	2P	201	-	-	0/38/38/57	-
60	PC1	2T	101	-	-	8/57/57/57	-
59	CDL	4o	501	-	-	19/103/103/110	-
59	CDL	3H	404	-	-	23/99/99/110	-
59	CDL	3e	201	-	-	14/81/81/110	-
62	HEM	3g	408	19	-	6/14/54/54	-
59	CDL	4W	202	-	-	22/83/83/110	-
67	HEA	4Q	908	42,68	-	8/36/76/76	-
58	PEE	4Q	901	-	-	13/39/39/54	-
61	HEC	3C	302	15	1/1/3/7	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	HEM	3G	405	19	-	7/14/54/54	-
58	PEE	4R	201	-	-	12/46/46/54	-

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	4q	908	HEA	C3B-C2B	4.59	1.45	1.34
67	4Q	908	HEA	C3B-C2B	4.58	1.45	1.34
67	4Q	907	HEA	C3B-C2B	4.49	1.44	1.34
67	4q	907	HEA	C3B-C2B	4.47	1.44	1.34
67	4Q	908	HEA	C3A-C2A	4.01	1.45	1.36
67	4q	908	HEA	C3A-C2A	3.96	1.45	1.36
67	4Q	907	HEA	C3D-C2D	3.89	1.45	1.36
62	3g	407	HEM	CBB-CAB	3.87	1.49	1.30
67	4q	907	HEA	C3D-C2D	3.87	1.44	1.36
62	3G	405	HEM	CBB-CAB	3.86	1.49	1.30
62	3g	408	HEM	CBC-CAC	3.83	1.49	1.30
62	3G	406	HEM	CBC-CAC	3.83	1.49	1.30
62	3G	406	HEM	CBB-CAB	3.77	1.49	1.30
62	3g	408	HEM	CBB-CAB	3.77	1.49	1.30
67	4Q	907	HEA	C3A-C2A	3.75	1.44	1.36
62	3G	406	HEM	FE-NA	3.74	2.07	1.95
67	4q	907	HEA	C3A-C2A	3.72	1.44	1.36
67	4Q	908	HEA	C3D-C2D	3.68	1.44	1.36
58	3H	403	PEE	C18-C19	3.63	1.52	1.31
62	3G	405	HEM	CBC-CAC	3.62	1.48	1.30
58	4z	302	PEE	C39-C38	3.61	1.52	1.31
67	4q	908	HEA	C3D-C2D	3.61	1.44	1.36
62	3g	407	HEM	CBC-CAC	3.59	1.48	1.30
58	4Z	302	PEE	C39-C38	3.59	1.52	1.31
58	40	302	PEE	C39-C38	3.57	1.52	1.31
58	4D	101	PEE	C18-C19	3.56	1.52	1.31
58	4s	101	PEE	C39-C38	3.55	1.52	1.31
58	4q	902	PEE	C18-C19	3.55	1.52	1.31
58	3C	301	PEE	C19-C18	3.53	1.52	1.28
58	40	302	PEE	C18-C19	3.52	1.52	1.31
58	4s	101	PEE	C18-C19	3.52	1.52	1.31
58	4R	201	PEE	C19-C18	3.51	1.52	1.28
58	4w	201	PEE	C39-C38	3.51	1.52	1.31
58	4q	901	PEE	C19-C18	3.51	1.52	1.28
58	2O	202	PEE	C39-C38	3.51	1.52	1.31
58	3f	102	PEE	C39-C38	3.50	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	3c	301	PEE	C18-C19	3.50	1.52	1.31
58	2T	103	PEE	C18-C19	3.49	1.52	1.31
58	41	301	PEE	C39-C38	3.49	1.52	1.31
58	4q	901	PEE	C39-C38	3.48	1.52	1.31
58	40	301	PEE	C39-C38	3.48	1.51	1.31
58	41	303	PEE	C39-C38	3.48	1.51	1.31
58	2O	201	PEE	C39-C38	3.47	1.51	1.31
58	40	303	PEE	C18-C19	3.47	1.51	1.31
58	4R	201	PEE	C39-C38	3.46	1.51	1.31
58	4W	201	PEE	C39-C38	3.45	1.51	1.31
58	4Z	302	PEE	C18-C19	3.45	1.51	1.31
58	4d	101	PEE	C39-C38	3.45	1.51	1.31
58	4q	902	PEE	C39-C38	3.44	1.51	1.31
58	4W	201	PEE	C18-C19	3.44	1.51	1.31
58	4z	302	PEE	C18-C19	3.44	1.51	1.31
58	4l	201	PEE	C18-C19	3.42	1.51	1.31
58	4Q	901	PEE	C19-C18	3.42	1.51	1.28
58	4d	101	PEE	C18-C19	3.41	1.51	1.31
58	4w	201	PEE	C18-C19	3.40	1.51	1.31
58	2P	202	PEE	C18-C19	3.39	1.51	1.31
58	2P	202	PEE	C39-C38	3.39	1.51	1.31
58	40	301	PEE	C18-C19	3.38	1.51	1.31
58	41	302	PEE	C39-C38	3.38	1.51	1.31
58	41	301	PEE	C18-C19	3.38	1.51	1.31
61	3c	302	HEC	CBC-CAC	-3.38	1.36	1.51
58	2t	101	PEE	C39-C38	3.37	1.51	1.31
58	41	302	PEE	C18-C19	3.36	1.51	1.31
58	2T	103	PEE	C39-C38	3.32	1.51	1.31
58	2r	203	PEE	C39-C38	3.32	1.51	1.31
58	3H	403	PEE	C39-C38	3.31	1.50	1.31
61	3C	302	HEC	CBC-CAC	-3.30	1.36	1.51
62	3G	405	HEM	FE-ND	3.14	2.04	1.94
61	3C	302	HEC	CAB-C3B	3.09	1.59	1.51
62	3g	407	HEM	FE-NC	3.08	2.05	1.95
62	3g	407	HEM	FE-ND	3.06	2.04	1.94
61	3C	302	HEC	CAC-C3C	3.04	1.58	1.51
53	3g	401	UQ1	C3-C4	-3.02	1.40	1.48
58	4l	201	PEE	C38-C39	3.01	1.52	1.29
58	4Q	901	PEE	C38-C39	3.01	1.52	1.29
67	4q	908	HEA	C4B-C3B	3.00	1.49	1.44
52	2M	701	FAD	C4-N3	-3.00	1.33	1.38
67	4Q	908	HEA	C4B-C3B	2.99	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2N	301	UQ1	C3-C4	-2.92	1.40	1.48
52	2m	701	FAD	C4-N3	-2.86	1.33	1.38
62	3g	408	HEM	FE-NA	2.83	2.04	1.95
62	3G	405	HEM	FE-NB	2.82	2.03	1.94
53	2p	201	UQ1	C3-C4	-2.81	1.40	1.48
62	3g	407	HEM	FE-NB	2.81	2.03	1.94
61	3c	302	HEC	CAC-C3C	2.81	1.58	1.51
62	3G	406	HEM	FE-ND	2.79	2.03	1.94
62	3g	408	HEM	FE-ND	2.76	2.03	1.94
53	3G	402	UQ1	C3-C4	-2.70	1.41	1.48
53	3g	402	UQ1	C3-C4	-2.68	1.41	1.48
67	4Q	907	HEA	C1D-ND	-2.67	1.35	1.40
67	4q	907	HEA	C1D-ND	-2.66	1.35	1.40
62	3G	405	HEM	FE-NC	2.66	2.04	1.95
62	3g	408	HEM	FE-NB	2.65	2.03	1.94
62	3g	408	HEM	FE-NC	2.59	2.03	1.95
62	3G	406	HEM	FE-NB	2.54	2.02	1.94
53	2p	201	UQ1	C2-C1	-2.51	1.41	1.48
61	3C	302	HEC	CBB-CAB	-2.48	1.40	1.51
53	3g	402	UQ1	C2-C1	-2.48	1.41	1.48
62	3G	405	HEM	FE-NA	2.47	2.03	1.95
61	3c	302	HEC	CAB-C3B	2.46	1.57	1.51
61	3C	302	HEC	C3D-C2D	-2.40	1.31	1.36
53	3G	402	UQ1	C2-C1	-2.40	1.42	1.48
67	4Q	908	HEA	C1D-ND	-2.36	1.36	1.40
67	4q	908	HEA	C1D-ND	-2.36	1.36	1.40
61	3c	302	HEC	C3D-C2D	-2.30	1.31	1.36
61	3c	302	HEC	CBB-CAB	-2.29	1.41	1.51
53	3G	401	UQ1	C3-C4	-2.28	1.42	1.48
61	3C	302	HEC	FE-ND	2.27	2.01	1.94
61	3C	302	HEC	FE-NB	2.26	2.01	1.94
53	2N	301	UQ1	C2-C1	-2.24	1.42	1.48
61	3c	302	HEC	C4C-C3C	-2.23	1.40	1.44
61	3C	302	HEC	CMD-C2D	2.20	1.55	1.50
67	4Q	907	HEA	C4A-NA	-2.20	1.35	1.39
67	4q	908	HEA	C1C-C2C	2.20	1.48	1.43
62	3g	408	HEM	CMC-C2C	2.19	1.55	1.50
67	4q	907	HEA	C4A-NA	-2.19	1.35	1.39
62	3G	406	HEM	C4D-ND	-2.18	1.36	1.40
52	2m	701	FAD	C9A-N10	-2.16	1.37	1.41
61	3c	302	HEC	C4B-NB	-2.16	1.36	1.40
67	4Q	907	HEA	C1C-C2C	2.15	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	4Q	908	HEA	C1C-C2C	2.15	1.48	1.43
53	3G	401	UQ1	C2-C1	-2.15	1.42	1.48
67	4q	907	HEA	C4B-NB	-2.14	1.36	1.40
61	3c	302	HEC	CMB-C2B	2.13	1.55	1.50
67	4Q	907	HEA	C4B-NB	-2.13	1.36	1.40
62	3g	407	HEM	C2A-C3A	-2.12	1.33	1.38
61	3c	302	HEC	CMD-C2D	2.11	1.55	1.50
61	3C	302	HEC	C4B-C3B	2.10	1.48	1.45
67	4q	907	HEA	C1C-C2C	2.10	1.48	1.43
62	3g	407	HEM	FE-NA	2.10	2.02	1.95
62	3G	405	HEM	C2A-C3A	-2.09	1.33	1.38
52	2m	701	FAD	C4X-C10	-2.08	1.38	1.44
62	3G	406	HEM	CMC-C2C	2.07	1.55	1.50
62	3G	406	HEM	C1B-NB	-2.04	1.36	1.40
61	3c	302	HEC	C1C-C2C	2.03	1.48	1.43
62	3g	408	HEM	C2A-C3A	-2.03	1.33	1.38
52	2M	701	FAD	C9A-N10	-2.02	1.37	1.41
67	4q	908	HEA	C4D-C3D	2.00	1.48	1.45

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	3C	302	HEC	CAB-C3B-C4B	10.29	138.17	124.81
61	3C	302	HEC	CAB-C3B-C2B	-7.23	115.17	127.53
67	4Q	907	HEA	C3A-C2A-C1A	-6.80	100.59	107.08
67	4q	908	HEA	C3A-C2A-C1A	-6.79	100.60	107.08
67	4q	907	HEA	C3A-C2A-C1A	-6.75	100.63	107.08
67	4Q	908	HEA	C3A-C2A-C1A	-6.73	100.65	107.08
62	3G	406	HEM	C4A-NA-C1A	6.16	111.38	105.35
67	4q	908	HEA	C2A-C1A-NA	5.20	115.38	110.32
52	2m	701	FAD	C4-N3-C2	-5.16	116.11	125.64
67	4q	907	HEA	CAA-CBA-CGA	-5.16	102.50	113.60
67	4Q	908	HEA	C2A-C1A-NA	5.14	115.33	110.32
52	2M	701	FAD	C4-N3-C2	-5.14	116.14	125.64
67	4Q	907	HEA	CAA-CBA-CGA	-5.13	102.57	113.60
62	3g	408	HEM	C4A-NA-C1A	4.90	110.14	105.35
67	4Q	907	HEA	CMC-C2C-C3C	4.64	137.82	126.59
67	4Q	908	HEA	C3D-C4D-ND	4.63	114.84	110.36
67	4q	907	HEA	C3D-C4D-ND	4.62	114.83	110.36
67	4q	907	HEA	CMC-C2C-C3C	4.61	137.76	126.59
67	4q	908	HEA	C3D-C4D-ND	4.60	114.81	110.36
67	4Q	907	HEA	C3D-C4D-ND	4.57	114.78	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	4q	907	HEA	C2A-C1A-NA	4.55	114.75	110.32
67	4q	908	HEA	CAD-CBD-CGD	-4.53	103.85	113.60
67	4Q	907	HEA	C2A-C1A-NA	4.53	114.73	110.32
67	4Q	908	HEA	CAD-CBD-CGD	-4.51	103.89	113.60
67	4q	908	HEA	CMC-C2C-C3C	4.49	137.46	126.59
67	4Q	908	HEA	CMC-C2C-C3C	4.47	137.41	126.59
67	4Q	908	HEA	C13-C12-C11	-4.44	107.68	114.35
67	4q	908	HEA	C13-C12-C11	-4.42	107.70	114.35
67	4Q	907	HEA	CMB-C2B-C1B	-4.27	118.54	125.04
67	4Q	908	HEA	CMB-C2B-C1B	-4.26	118.55	125.04
67	4q	908	HEA	CMB-C2B-C1B	-4.24	118.59	125.04
67	4q	908	HEA	CMC-C2C-C1C	-4.23	118.92	125.37
67	4q	907	HEA	CMD-C2D-C1D	-4.23	118.59	125.04
67	4Q	907	HEA	CMD-C2D-C1D	-4.23	118.60	125.04
67	4q	907	HEA	CMB-C2B-C1B	-4.21	118.62	125.04
67	4Q	908	HEA	CMC-C2C-C1C	-4.20	118.97	125.37
67	4Q	908	HEA	CAA-CBA-CGA	-4.17	104.63	113.60
67	4q	908	HEA	CAA-CBA-CGA	-4.16	104.65	113.60
67	4Q	907	HEA	CMC-C2C-C1C	-4.16	119.03	125.37
61	3c	302	HEC	CAC-C3C-C2C	4.15	133.51	126.86
61	3c	302	HEC	CAB-C3B-C4B	4.14	130.18	124.81
67	4q	907	HEA	CMC-C2C-C1C	-4.09	119.13	125.37
62	3G	406	HEM	C2A-C1A-NA	-4.07	105.60	110.15
62	3g	408	HEM	C1B-NB-C4B	4.04	109.25	105.07
67	4Q	907	HEA	OMA-CMA-C3A	-4.02	116.59	125.69
61	3c	302	HEC	CAC-C3C-C4C	-4.01	119.35	124.92
67	4q	907	HEA	OMA-CMA-C3A	-4.01	116.62	125.69
67	4Q	907	HEA	CHA-C4D-C3D	-4.00	118.96	124.84
67	4q	908	HEA	CHA-C1A-C2A	-3.99	118.47	124.94
67	4Q	908	HEA	CHA-C1A-C2A	-3.97	118.50	124.94
67	4q	907	HEA	CHA-C4D-C3D	-3.95	119.03	124.84
67	4Q	908	HEA	CHA-C4D-C3D	-3.90	119.11	124.84
67	4q	908	HEA	CHA-C4D-C3D	-3.89	119.13	124.84
67	4q	908	HEA	CMD-C2D-C1D	-3.88	119.14	125.04
62	3G	405	HEM	C4C-NC-C1C	3.87	109.14	105.35
67	4Q	908	HEA	CMD-C2D-C1D	-3.80	119.25	125.04
62	3G	406	HEM	C1B-NB-C4B	3.77	108.96	105.07
62	3g	407	HEM	C4A-NA-C1A	3.74	109.01	105.35
67	4Q	907	HEA	CHA-C1A-C2A	-3.72	118.90	124.94
67	4q	907	HEA	CHA-C1A-C2A	-3.69	118.96	124.94
67	4Q	907	HEA	CMB-C2B-C3B	3.66	137.32	130.34
67	4q	907	HEA	CMB-C2B-C3B	3.65	137.30	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	4Q	907	HEA	C4D-C3D-C2D	-3.60	101.65	106.90
61	3c	302	HEC	O1D-CGD-CBD	-3.57	111.61	123.08
67	4q	907	HEA	C4D-C3D-C2D	-3.52	101.76	106.90
62	3g	408	HEM	C2A-C1A-NA	-3.50	106.23	110.15
67	4Q	908	HEA	C4D-C3D-C2D	-3.50	101.80	106.90
67	4q	908	HEA	C4D-C3D-C2D	-3.50	101.80	106.90
62	3g	407	HEM	C4C-NC-C1C	3.49	108.77	105.35
67	4q	907	HEA	C13-C12-C11	-3.44	109.18	114.35
67	4Q	907	HEA	C13-C12-C11	-3.42	109.22	114.35
67	4q	907	HEA	C3C-C2C-C1C	-3.36	103.11	107.16
67	4q	907	HEA	CMD-C2D-C3D	3.35	135.21	126.12
67	4Q	907	HEA	C3C-C2C-C1C	-3.33	103.15	107.16
67	4Q	907	HEA	CMD-C2D-C3D	3.30	135.08	126.12
62	3G	405	HEM	C1B-NB-C4B	3.30	108.48	105.07
52	2M	701	FAD	C4X-C4-N3	3.28	121.51	113.19
62	3G	405	HEM	C4A-NA-C1A	3.24	108.52	105.35
52	2m	701	FAD	C4X-C4-N3	3.22	121.37	113.19
67	4q	908	HEA	C17-C18-C19	-3.18	120.00	127.66
62	3g	407	HEM	C2A-C1A-NA	-3.16	106.62	110.15
67	4Q	908	HEA	C17-C18-C19	-3.15	120.06	127.66
61	3C	302	HEC	CHC-C4B-NB	-3.14	120.51	124.37
53	3G	401	UQ1	O3-C3-C4	3.13	127.13	116.56
67	4q	908	HEA	CMD-C2D-C3D	3.11	134.57	126.12
67	4q	908	HEA	OMA-CMA-C3A	-3.11	118.65	125.69
62	3g	407	HEM	C1B-NB-C4B	3.10	108.28	105.07
67	4Q	908	HEA	CMD-C2D-C3D	3.10	134.52	126.12
67	4Q	908	HEA	OMA-CMA-C3A	-3.09	118.69	125.69
67	4Q	908	HEA	CMB-C2B-C3B	3.05	136.16	130.34
59	4e	202	CDL	OB8-CB6-CB4	3.05	117.31	108.43
67	4q	908	HEA	CMB-C2B-C3B	3.04	136.14	130.34
62	3G	406	HEM	CAD-CBD-CGD	-2.95	107.26	113.60
61	3c	302	HEC	O1A-CGA-CBA	-2.94	113.62	123.08
62	3G	405	HEM	C2A-C1A-NA	-2.94	106.86	110.15
62	3g	408	HEM	C4D-ND-C1D	2.94	108.11	105.07
62	3g	408	HEM	CAD-CBD-CGD	-2.94	107.27	113.60
67	4Q	907	HEA	C17-C18-C19	-2.94	120.59	127.66
67	4q	908	HEA	C3C-C2C-C1C	-2.94	103.62	107.16
67	4Q	908	HEA	C3C-C2C-C1C	-2.94	103.62	107.16
61	3C	302	HEC	O1A-CGA-CBA	-2.91	113.73	123.08
67	4q	907	HEA	C17-C18-C19	-2.88	120.72	127.66
67	4Q	908	HEA	C26-C15-C16	2.88	120.11	115.27
53	3G	401	UQ1	O2-C2-C1	2.87	126.27	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	3G	406	HEM	C4D-ND-C1D	2.86	108.03	105.07
67	4q	907	HEA	C13-C14-C15	-2.84	120.81	127.66
67	4q	908	HEA	C26-C15-C16	2.82	120.02	115.27
67	4Q	907	HEA	C13-C14-C15	-2.81	120.88	127.66
53	3G	401	UQ1	O2-C2-C3	-2.81	113.05	123.64
62	3g	407	HEM	C4D-ND-C1D	2.79	107.95	105.07
62	3G	406	HEM	C3A-C4A-NA	-2.77	105.86	110.08
61	3C	302	HEC	C2B-C1B-NB	2.76	113.18	109.88
61	3C	302	HEC	O1D-CGD-CBD	-2.74	114.29	123.08
59	4z	304	CDL	OB8-CB6-CB4	-2.72	100.51	108.43
67	4q	908	HEA	C27-C19-C20	2.71	119.84	115.27
52	2M	701	FAD	C4X-C10-N10	2.71	120.45	116.48
67	4Q	908	HEA	C27-C19-C20	2.70	119.82	115.27
67	4q	907	HEA	C26-C15-C16	2.70	119.82	115.27
67	4q	907	HEA	CHB-C1B-C2B	-2.70	120.76	124.98
67	4Q	907	HEA	C26-C15-C16	2.69	119.80	115.27
62	3G	405	HEM	C4D-ND-C1D	2.68	107.84	105.07
53	3G	401	UQ1	O3-C3-C2	-2.67	113.58	123.64
67	4q	908	HEA	CHB-C1B-C2B	-2.66	120.83	124.98
67	4Q	908	HEA	CHB-C1B-C2B	-2.64	120.85	124.98
52	2m	701	FAD	C4X-C10-N10	2.64	120.34	116.48
67	4q	907	HEA	CHB-C4A-NA	2.62	127.28	124.44
67	4Q	907	HEA	CHB-C1B-C2B	-2.61	120.91	124.98
67	4Q	907	HEA	CHB-C4A-NA	2.58	127.23	124.44
60	2r	201	PC1	O31-C3-C2	2.57	115.91	108.43
61	3c	302	HEC	CAA-CBA-CGA	-2.54	108.13	113.60
61	3c	302	HEC	CMB-C2B-C1B	2.54	128.91	125.04
67	4Q	907	HEA	C25-C23-C24	2.50	120.14	114.60
67	4q	907	HEA	C25-C23-C24	2.49	120.11	114.60
52	2M	701	FAD	O4-C4-C4X	-2.43	120.14	126.60
62	3g	408	HEM	C3D-C4D-ND	-2.43	107.46	110.17
62	3g	407	HEM	CAA-CBA-CGA	-2.43	108.37	113.60
60	3H	401	PC1	O31-C3-C2	-2.43	101.37	108.43
62	3g	408	HEM	C3A-C4A-NA	-2.39	106.44	110.08
52	2m	701	FAD	O4-C4-C4X	-2.37	120.30	126.60
62	3g	407	HEM	C3A-C4A-NA	-2.37	106.47	110.08
67	4q	908	HEA	C13-C14-C15	-2.35	121.99	127.66
61	3C	302	HEC	CHC-C4B-C3B	2.35	129.74	125.33
59	2T	104	CDL	CB6-CB4-CB3	-2.34	106.25	111.79
67	4Q	908	HEA	C13-C14-C15	-2.33	122.04	127.66
67	4Q	907	HEA	CAD-CBD-CGD	-2.33	108.58	113.60
67	4q	907	HEA	C2B-C1B-NB	2.33	112.68	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	3c	302	HEC	C3C-C4C-NC	2.33	112.75	110.15
67	4Q	907	HEA	C2B-C1B-NB	2.33	112.67	109.88
67	4q	907	HEA	CAD-CBD-CGD	-2.32	108.61	113.60
53	3g	401	UQ1	O2-C2-C1	2.31	124.37	116.56
67	4q	908	HEA	C25-C23-C24	2.31	119.70	114.60
61	3C	302	HEC	C2A-C1A-NA	-2.30	108.08	110.32
62	3G	406	HEM	CAA-CBA-CGA	-2.29	108.67	113.60
62	3G	405	HEM	CAA-CBA-CGA	-2.29	108.68	113.60
67	4q	907	HEA	C1B-C2B-C3B	-2.28	104.08	106.80
62	3g	407	HEM	C2B-C1B-NB	-2.25	107.17	109.84
58	3H	403	PEE	O3-C3-C2	2.24	114.96	108.43
62	3g	408	HEM	CMD-C2D-C1D	2.24	128.45	125.04
67	4Q	908	HEA	C25-C23-C24	2.23	119.54	114.60
62	3g	408	HEM	CAA-CBA-CGA	-2.23	108.80	113.60
67	4Q	907	HEA	C1B-C2B-C3B	-2.23	104.13	106.80
62	3g	407	HEM	C3D-C4D-ND	-2.23	107.69	110.17
62	3G	406	HEM	CMD-C2D-C1D	2.21	128.41	125.04
67	4q	907	HEA	C21-C22-C23	-2.21	120.20	127.75
67	4Q	908	HEA	C4B-C3B-C2B	-2.20	103.66	107.41
67	4Q	908	HEA	C21-C22-C23	-2.19	120.25	127.75
62	3g	407	HEM	CMD-C2D-C1D	2.19	128.38	125.04
58	4l	201	PEE	C37-C38-C39	-2.19	113.66	131.07
67	4Q	907	HEA	C21-C22-C23	-2.19	120.27	127.75
67	4q	908	HEA	C4B-C3B-C2B	-2.18	103.68	107.41
67	4q	908	HEA	C21-C22-C23	-2.18	120.29	127.75
67	4Q	907	HEA	CAA-C2A-C1A	2.17	128.99	124.89
62	3G	405	HEM	C3D-C4D-ND	-2.16	107.76	110.17
58	4Q	901	PEE	C37-C38-C39	-2.15	113.95	131.07
62	3G	405	HEM	CMD-C2D-C1D	2.15	128.32	125.04
62	3G	406	HEM	O1D-CGD-CBD	-2.15	116.17	123.08
62	3g	408	HEM	O1D-CGD-CBD	-2.14	116.20	123.08
67	4q	908	HEA	C2B-C1B-NB	2.14	112.44	109.88
67	4Q	908	HEA	C2B-C1B-NB	2.14	112.44	109.88
67	4q	907	HEA	CAA-C2A-C1A	2.13	128.91	124.89
61	3C	302	HEC	CHB-C1B-C2B	-2.13	121.65	124.98
67	4q	908	HEA	CHB-C1B-NB	2.13	126.73	124.42
60	2R	201	PC1	O31-C3-C2	2.13	114.62	108.43
62	3g	408	HEM	C4C-NC-C1C	2.12	107.42	105.35
61	3C	302	HEC	CMB-C2B-C1B	2.12	128.26	125.04
67	4Q	908	HEA	CHB-C1B-NB	2.11	126.71	124.42
61	3C	302	HEC	CAA-CBA-CGA	-2.11	109.06	113.60
59	4z	303	CDL	OA8-CA6-CA4	2.10	114.55	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	4q	907	HEA	O1A-CGA-CBA	-2.10	116.34	123.08
67	4Q	907	HEA	O1A-CGA-CBA	-2.09	116.38	123.08
59	4s	102	CDL	OB8-CB6-CB4	-2.08	102.38	108.43
67	4q	908	HEA	C3B-C4B-NB	2.08	112.30	109.84
67	4Q	908	HEA	C3B-C4B-NB	2.07	112.30	109.84
61	3c	302	HEC	CAB-C3B-C2B	-2.07	123.98	127.53
62	3g	407	HEM	CHC-C1C-NC	2.06	126.66	124.44
59	3h	403	CDL	OB8-CB6-CB4	-2.04	102.49	108.43
61	3c	302	HEC	C2B-C1B-NB	2.04	112.32	109.88
53	3g	401	UQ1	O3-C3-C4	-2.03	109.69	116.56
62	3G	405	HEM	C3A-C4A-NA	-2.02	107.00	110.08
59	4S	102	CDL	OB8-CB6-CB4	-2.02	102.56	108.43
67	4Q	908	HEA	CHC-C1C-C2C	-2.01	121.57	127.24
60	2R	202	PC1	O31-C3-C2	-2.00	102.60	108.43
61	3C	302	HEC	C4A-NA-C1A	2.00	107.31	105.35
67	4q	908	HEA	CHC-C1C-C2C	-2.00	121.58	127.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
61	3C	302	HEC	NA
61	3c	302	HEC	NA

All (1914) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	2M	701	FAD	N10-C1'-C2'-O2'
52	2M	701	FAD	N10-C1'-C2'-C3'
52	2m	701	FAD	N10-C1'-C2'-O2'
52	2m	701	FAD	N10-C1'-C2'-C3'
58	2O	201	PEE	C1-O3P-P-O2P
58	2O	202	PEE	C11-C10-O2-C2
58	2O	202	PEE	C4-O4P-P-O1P
58	2P	202	PEE	C1-O3P-P-O2P
58	2P	202	PEE	C1-O3P-P-O1P
58	2T	103	PEE	C37-C38-C39-C40
58	2o	203	PEE	C1-O3P-P-O2P
58	2o	203	PEE	C1-O3P-P-O1P
58	2o	203	PEE	O4P-C4-C5-N
58	2p	203	PEE	C1-O3P-P-O2P
58	2p	203	PEE	C1-O3P-P-O1P
58	2p	203	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
58	2r	203	PEE	C1-O3P-P-O2P
58	2r	203	PEE	C1-O3P-P-O1P
58	2r	203	PEE	C1-O3P-P-O4P
58	2r	203	PEE	C4-O4P-P-O1P
58	2t	101	PEE	C1-O3P-P-O1P
58	2t	101	PEE	C37-C38-C39-C40
58	3H	403	PEE	C1-O3P-P-O2P
58	3H	403	PEE	C1-O3P-P-O1P
58	3H	403	PEE	C4-O4P-P-O1P
58	3c	301	PEE	C1-O3P-P-O1P
58	3c	301	PEE	C4-O4P-P-O2P
58	3c	301	PEE	C4-O4P-P-O1P
58	3f	102	PEE	C1-O3P-P-O2P
58	3f	102	PEE	C1-O3P-P-O1P
58	3f	102	PEE	C4-O4P-P-O1P
58	40	301	PEE	C1-O3P-P-O2P
58	40	301	PEE	C1-O3P-P-O1P
58	40	302	PEE	C1-O3P-P-O2P
58	40	302	PEE	C1-O3P-P-O1P
58	40	302	PEE	C1-O3P-P-O4P
58	40	302	PEE	C4-O4P-P-O2P
58	40	302	PEE	C4-O4P-P-O1P
58	40	303	PEE	C1-O3P-P-O1P
58	40	304	PEE	C3-C2-O2-C10
58	40	304	PEE	O4P-C4-C5-N
58	41	301	PEE	C18-C19-C20-C21
58	41	302	PEE	C1-O3P-P-O1P
58	41	303	PEE	C3-C2-O2-C10
58	41	303	PEE	O4P-C4-C5-N
58	4Q	901	PEE	O4P-C4-C5-N
58	4Q	901	PEE	C37-C38-C39-C40
58	4R	201	PEE	C1-O3P-P-O2P
58	4R	201	PEE	C1-O3P-P-O1P
58	4S	101	PEE	C4-O4P-P-O1P
58	4W	201	PEE	C1-O3P-P-O1P
58	4Z	302	PEE	C1-O3P-P-O2P
58	4Z	302	PEE	C1-O3P-P-O1P
58	4Z	302	PEE	C1-O3P-P-O4P
58	4Z	302	PEE	C4-O4P-P-O2P
58	4Z	302	PEE	C4-O4P-P-O1P
58	4l	201	PEE	C1-O3P-P-O2P
58	4l	201	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
58	4l	201	PEE	O4P-C4-C5-N
58	4q	902	PEE	C4-O4P-P-O1P
58	4s	101	PEE	C4-O4P-P-O1P
58	4w	201	PEE	C1-O3P-P-O1P
58	4z	302	PEE	C1-O3P-P-O2P
58	4z	302	PEE	C1-O3P-P-O1P
58	4z	302	PEE	C1-O3P-P-O4P
58	4z	302	PEE	C4-O4P-P-O2P
58	4z	302	PEE	C4-O4P-P-O1P
59	2O	203	CDL	CA3-OA5-PA1-OA3
59	2O	203	CDL	CB2-OB2-PB2-OB4
59	2O	203	CDL	CB3-OB5-PB2-OB4
59	2P	203	CDL	O1-C1-CA2-OA2
59	2P	203	CDL	O1-C1-CB2-OB2
59	2P	203	CDL	CA3-OA5-PA1-OA3
59	2Q	101	CDL	CB3-OB5-PB2-OB4
59	2T	104	CDL	O1-C1-CA2-OA2
59	2T	104	CDL	CB2-C1-CA2-OA2
59	2T	104	CDL	CB2-OB2-PB2-OB4
59	2o	201	CDL	O1-C1-CB2-OB2
59	2o	201	CDL	CA3-OA5-PA1-OA3
59	2o	201	CDL	CB2-OB2-PB2-OB3
59	2o	201	CDL	CB3-OB5-PB2-OB2
59	2o	201	CDL	CB3-OB5-PB2-OB3
59	2o	201	CDL	CB3-OB5-PB2-OB4
59	2p	204	CDL	O1-C1-CA2-OA2
59	2p	204	CDL	O1-C1-CB2-OB2
59	2p	204	CDL	OA5-CA3-CA4-OA6
59	2q	101	CDL	CB3-OB5-PB2-OB4
59	2t	102	CDL	O1-C1-CA2-OA2
59	2t	102	CDL	CB2-C1-CA2-OA2
59	2t	102	CDL	CB2-OB2-PB2-OB4
59	3D	201	CDL	O1-C1-CA2-OA2
59	3D	201	CDL	CA3-OA5-PA1-OA3
59	3D	201	CDL	CA3-OA5-PA1-OA4
59	3E	201	CDL	CA2-OA2-PA1-OA4
59	3E	201	CDL	CA3-OA5-PA1-OA3
59	3E	201	CDL	CB2-OB2-PB2-OB4
59	3G	403	CDL	CB2-OB2-PB2-OB3
59	3G	404	CDL	CB2-C1-CA2-OA2
59	3G	404	CDL	CA2-OA2-PA1-OA3
59	3H	404	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
59	3H	404	CDL	CA2-OA2-PA1-OA4
59	3H	404	CDL	CA3-OA5-PA1-OA4
59	3H	405	CDL	C1-CB2-OB2-PB2
59	3H	405	CDL	CB3-OB5-PB2-OB3
59	3I	201	CDL	CB2-C1-CA2-OA2
59	3I	202	CDL	CB2-C1-CA2-OA2
59	3I	202	CDL	CB2-OB2-PB2-OB5
59	3I	202	CDL	CB3-OB5-PB2-OB3
59	3I	203	CDL	CA3-OA5-PA1-OA4
59	3I	203	CDL	CB3-OB5-PB2-OB4
59	3L	701	CDL	CB2-C1-CA2-OA2
59	3L	701	CDL	CA2-OA2-PA1-OA4
59	3L	701	CDL	CA3-OA5-PA1-OA3
59	3L	702	CDL	CA3-OA5-PA1-OA3
59	3L	703	CDL	OB6-CB4-CB6-OB8
59	3e	201	CDL	CB2-OB2-PB2-OB4
59	3e	201	CDL	CB3-OB5-PB2-OB2
59	3e	201	CDL	CB3-OB5-PB2-OB3
59	3e	201	CDL	CB3-OB5-PB2-OB4
59	3e	202	CDL	CA2-OA2-PA1-OA4
59	3e	202	CDL	CA3-OA5-PA1-OA3
59	3e	202	CDL	CB2-OB2-PB2-OB4
59	3e	202	CDL	C51-CB5-OB6-CB4
59	3g	403	CDL	CA2-C1-CB2-OB2
59	3g	403	CDL	C11-CA5-OA6-CA4
59	3g	403	CDL	CB2-OB2-PB2-OB3
59	3g	404	CDL	CA2-OA2-PA1-OA3
59	3g	404	CDL	C1-CB2-OB2-PB2
59	3g	404	CDL	CB2-OB2-PB2-OB4
59	3g	405	CDL	O1-C1-CA2-OA2
59	3g	405	CDL	CA3-OA5-PA1-OA4
59	3g	406	CDL	CA2-OA2-PA1-OA4
59	3g	406	CDL	CA3-OA5-PA1-OA2
59	3g	406	CDL	CA3-OA5-PA1-OA3
59	3g	406	CDL	CA3-OA5-PA1-OA4
59	3h	403	CDL	O1-C1-CB2-OB2
59	3h	403	CDL	CA2-OA2-PA1-OA3
59	3h	403	CDL	CA3-OA5-PA1-OA4
59	3h	403	CDL	CB2-OB2-PB2-OB4
59	3i	201	CDL	CB2-C1-CA2-OA2
59	3i	201	CDL	CB2-OB2-PB2-OB4
59	3i	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
59	3i	202	CDL	O1-C1-CA2-OA2
59	3i	202	CDL	CA2-OA2-PA1-OA3
59	3i	202	CDL	CA2-OA2-PA1-OA4
59	3i	202	CDL	CA2-OA2-PA1-OA5
59	3i	202	CDL	CA3-OA5-PA1-OA4
59	3i	202	CDL	CB3-OB5-PB2-OB3
59	3l	701	CDL	CA2-OA2-PA1-OA3
59	3l	702	CDL	CA3-OA5-PA1-OA3
59	41	304	CDL	O1-C1-CB2-OB2
59	41	304	CDL	CA2-OA2-PA1-OA4
59	4E	202	CDL	CA3-OA5-PA1-OA3
59	4F	202	CDL	CA2-OA2-PA1-OA4
59	4F	202	CDL	CB2-OB2-PB2-OB3
59	4J	301	CDL	CA3-OA5-PA1-OA3
59	4J	301	CDL	CA3-OA5-PA1-OA4
59	4J	301	CDL	C11-CA5-OA6-CA4
59	4J	301	CDL	CB3-CB4-OB6-CB5
59	4J	301	CDL	CB6-CB4-OB6-CB5
59	4K	201	CDL	O1-C1-CB2-OB2
59	4K	201	CDL	CA2-C1-CB2-OB2
59	4K	201	CDL	CA2-OA2-PA1-OA4
59	4L	201	CDL	CA2-OA2-PA1-OA3
59	4L	201	CDL	CB2-OB2-PB2-OB4
59	4M	201	CDL	CA2-OA2-PA1-OA4
59	4M	201	CDL	CB2-OB2-PB2-OB3
59	4M	201	CDL	CB2-OB2-PB2-OB4
59	4M	201	CDL	CB3-OB5-PB2-OB3
59	4O	501	CDL	CA2-OA2-PA1-OA3
59	4O	501	CDL	CA2-OA2-PA1-OA4
59	4O	501	CDL	CA2-OA2-PA1-OA5
59	4O	501	CDL	CB2-OB2-PB2-OB4
59	4Q	902	CDL	O1-C1-CA2-OA2
59	4Q	902	CDL	CA2-OA2-PA1-OA3
59	4Q	902	CDL	CA2-OA2-PA1-OA4
59	4Q	902	CDL	CA2-OA2-PA1-OA5
59	4Q	902	CDL	C11-CA5-OA6-CA4
59	4Q	902	CDL	CB2-OB2-PB2-OB3
59	4Q	902	CDL	CB3-OB5-PB2-OB4
59	4Q	902	CDL	C51-CB5-OB6-CB4
59	4Q	903	CDL	O1-C1-CB2-OB2
59	4Q	903	CDL	CA2-C1-CB2-OB2
59	4Q	903	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
59	4Q	903	CDL	CA3-OA5-PA1-OA3
59	4Q	903	CDL	CA3-OA5-PA1-OA4
59	4S	102	CDL	CA3-OA5-PA1-OA3
59	4U	501	CDL	O1-C1-CB2-OB2
59	4U	501	CDL	CA2-OA2-PA1-OA3
59	4U	501	CDL	CA4-CA3-OA5-PA1
59	4U	501	CDL	CB2-OB2-PB2-OB3
59	4W	202	CDL	O1-C1-CA2-OA2
59	4Z	303	CDL	O1-C1-CA2-OA2
59	4e	202	CDL	CB3-OB5-PB2-OB4
59	4e	202	CDL	CB4-CB6-OB8-CB7
59	4f	201	CDL	CA2-OA2-PA1-OA4
59	4f	201	CDL	CB2-OB2-PB2-OB3
59	4f	201	CDL	CB4-CB3-OB5-PB2
59	4g	202	CDL	O1-C1-CA2-OA2
59	4j	301	CDL	CA2-OA2-PA1-OA3
59	4j	301	CDL	OA5-CA3-CA4-OA6
59	4j	302	CDL	CA2-OA2-PA1-OA3
59	4j	302	CDL	CA3-OA5-PA1-OA3
59	4j	302	CDL	CB2-OB2-PB2-OB4
59	4m	201	CDL	CA2-OA2-PA1-OA4
59	4m	201	CDL	CA3-OA5-PA1-OA4
59	4m	201	CDL	CB2-OB2-PB2-OB3
59	4m	201	CDL	CB2-OB2-PB2-OB4
59	4m	201	CDL	CB3-OB5-PB2-OB3
59	4o	501	CDL	O1-C1-CB2-OB2
59	4o	501	CDL	CA2-OA2-PA1-OA3
59	4o	501	CDL	CB2-OB2-PB2-OB4
59	4q	903	CDL	O1-C1-CA2-OA2
59	4q	903	CDL	CA2-C1-CB2-OB2
59	4s	102	CDL	CA3-OA5-PA1-OA3
59	4t	201	CDL	O1-C1-CB2-OB2
59	4t	201	CDL	CA2-OA2-PA1-OA3
59	4t	201	CDL	CA4-CA3-OA5-PA1
59	4z	303	CDL	CA3-OA5-PA1-OA2
59	4z	303	CDL	CA3-OA5-PA1-OA3
59	4z	303	CDL	CA3-OA5-PA1-OA4
60	2T	101	PC1	O13-C11-C12-N
60	2T	102	PC1	C1-O11-P-O14
60	2o	202	PC1	C11-O13-P-O14
60	2o	202	PC1	C1-O11-P-O12
60	2o	202	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
60	3A	501	PC1	C1-O11-P-O12
60	3A	501	PC1	C1-O11-P-O14
60	3H	401	PC1	C11-O13-P-O12
60	3H	401	PC1	C1-O11-P-O14
60	3H	402	PC1	C1-O11-P-O14
60	3H	402	PC1	O13-C11-C12-N
60	3H	402	PC1	C22-C21-O21-C2
60	3f	101	PC1	C1-O11-P-O14
60	3h	401	PC1	C11-O13-P-O12
60	3h	401	PC1	C11-O13-P-O14
60	3h	401	PC1	C1-O11-P-O14
60	3h	402	PC1	C1-O11-P-O14
60	3h	402	PC1	O13-C11-C12-N
60	4F	201	PC1	C22-C21-O21-C2
60	4e	201	PC1	C11-O13-P-O12
60	4e	201	PC1	C22-C21-O21-C2
61	3C	302	HEC	C2C-C3C-CAC-CBC
62	3G	405	HEM	C2C-C3C-CAC-CBC
62	3G	405	HEM	C4C-C3C-CAC-CBC
62	3g	407	HEM	C2C-C3C-CAC-CBC
62	3g	407	HEM	C4C-C3C-CAC-CBC
63	4C	101	LPP	C6-O5-P1-O3
63	4C	101	LPP	C6-O5-P1-O4
63	4Z	301	LPP	C6-O5-P1-O2
63	4Z	301	LPP	C6-O5-P1-O4
63	4g	201	LPP	C6-O5-P1-O3
63	4g	201	LPP	C6-O5-P1-O4
63	4z	301	LPP	C6-O5-P1-O2
63	4z	301	LPP	C6-O5-P1-O4
67	4Q	907	HEA	C2A-C3A-CMA-OMA
67	4Q	907	HEA	C4A-C3A-CMA-OMA
67	4Q	908	HEA	C2A-C3A-CMA-OMA
67	4Q	908	HEA	C4A-C3A-CMA-OMA
67	4q	907	HEA	C2A-C3A-CMA-OMA
67	4q	907	HEA	C4A-C3A-CMA-OMA
67	4q	908	HEA	C2A-C3A-CMA-OMA
67	4q	908	HEA	C4A-C3A-CMA-OMA
61	3c	302	HEC	C2C-C3C-CAC-CBC
61	3C	302	HEC	C4C-C3C-CAC-CBC
59	3e	202	CDL	OB7-CB5-OB6-CB4
59	4J	301	CDL	OA7-CA5-OA6-CA4
59	4Q	902	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
59	4Q	902	CDL	OB7-CB5-OB6-CB4
60	3H	402	PC1	O22-C21-O21-C2
60	4F	201	PC1	O22-C21-O21-C2
60	4e	201	PC1	O22-C21-O21-C2
59	3E	201	CDL	C71-CB7-OB8-CB6
61	3c	302	HEC	C4C-C3C-CAC-CBC
59	3I	202	CDL	C11-CA5-OA6-CA4
59	3g	405	CDL	C11-CA5-OA6-CA4
59	3i	202	CDL	C11-CA5-OA6-CA4
59	4q	903	CDL	C11-CA5-OA6-CA4
59	4t	201	CDL	C11-CA5-OA6-CA4
58	2O	202	PEE	C37-C38-C39-C40
58	2O	201	PEE	O4-C10-O2-C2
58	2O	202	PEE	O4-C10-O2-C2
59	4m	201	CDL	OA9-CA7-OA8-CA6
59	4z	303	CDL	OA9-CA7-OA8-CA6
59	3G	403	CDL	O1-C1-CB2-OB2
59	3I	202	CDL	O1-C1-CA2-OA2
59	3L	703	CDL	O1-C1-CA2-OA2
59	3g	403	CDL	O1-C1-CB2-OB2
59	3h	403	CDL	O1-C1-CA2-OA2
59	3l	701	CDL	O1-C1-CA2-OA2
59	4O	501	CDL	O1-C1-CB2-OB2
59	4z	303	CDL	O1-C1-CB2-OB2
59	4z	304	CDL	O1-C1-CA2-OA2
59	4K	201	CDL	C31-CA7-OA8-CA6
59	4m	201	CDL	C31-CA7-OA8-CA6
60	2r	201	PC1	C32-C31-O31-C3
59	3E	201	CDL	OB9-CB7-OB8-CB6
58	2O	201	PEE	C11-C10-O2-C2
58	2o	203	PEE	C11-C10-O2-C2
59	3E	201	CDL	C11-CA5-OA6-CA4
59	3G	403	CDL	C11-CA5-OA6-CA4
60	2R	202	PC1	C22-C21-O21-C2
60	3a	501	PC1	C22-C21-O21-C2
59	4z	303	CDL	C31-CA7-OA8-CA6
59	3g	403	CDL	OA7-CA5-OA6-CA4
59	3I	203	CDL	C1-CB2-OB2-PB2
59	4F	202	CDL	CB4-CB3-OB5-PB2
59	4q	903	CDL	CB4-CB3-OB5-PB2
67	4Q	907	HEA	C15-C16-C17-C18
67	4q	907	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
58	4q	901	PEE	C31-C30-O3-C3
59	2O	203	CDL	C71-CB7-OB8-CB6
59	3D	201	CDL	C31-CA7-OA8-CA6
59	41	304	CDL	C31-CA7-OA8-CA6
59	3E	201	CDL	C51-CB5-OB6-CB4
59	2O	203	CDL	CB2-C1-CA2-OA2
59	2P	203	CDL	CB2-C1-CA2-OA2
59	2P	203	CDL	CA2-C1-CB2-OB2
59	2p	204	CDL	CA2-C1-CB2-OB2
59	3D	201	CDL	CB2-C1-CA2-OA2
59	3G	403	CDL	CA2-C1-CB2-OB2
59	3I	202	CDL	CA2-C1-CB2-OB2
59	3g	405	CDL	CB2-C1-CA2-OA2
59	3g	406	CDL	CA2-C1-CB2-OB2
59	3h	403	CDL	CB2-C1-CA2-OA2
59	3h	403	CDL	CA2-C1-CB2-OB2
59	3i	202	CDL	CB2-C1-CA2-OA2
59	41	304	CDL	CA2-C1-CB2-OB2
59	4Q	902	CDL	CB2-C1-CA2-OA2
59	4U	501	CDL	CA2-C1-CB2-OB2
59	4Z	303	CDL	CB2-C1-CA2-OA2
59	4q	903	CDL	CB2-C1-CA2-OA2
59	4t	201	CDL	CA2-C1-CB2-OB2
59	4z	303	CDL	CA2-C1-CB2-OB2
59	4z	304	CDL	CB2-C1-CA2-OA2
58	2o	203	PEE	O4-C10-O2-C2
59	3I	202	CDL	OA7-CA5-OA6-CA4
59	3i	202	CDL	OA7-CA5-OA6-CA4
59	4t	201	CDL	OA7-CA5-OA6-CA4
59	4K	201	CDL	OA9-CA7-OA8-CA6
58	4Q	901	PEE	C31-C30-O3-C3
59	3g	405	CDL	C31-CA7-OA8-CA6
60	2R	201	PC1	C32-C31-O31-C3
60	3H	402	PC1	C32-C31-O31-C3
60	2r	201	PC1	O32-C31-O31-C3
59	2o	201	CDL	OB5-CB3-CB4-OB6
59	3G	403	CDL	OB5-CB3-CB4-OB6
59	3H	405	CDL	OB5-CB3-CB4-OB6
59	3g	406	CDL	O1-C1-CB2-OB2
59	4j	301	CDL	O1-C1-CB2-OB2
59	2P	203	CDL	OB6-CB4-CB6-OB8
59	4W	202	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
60	3h	402	PC1	O21-C2-C3-O31
59	3I	201	CDL	C31-CA7-OA8-CA6
59	3E	201	CDL	OA7-CA5-OA6-CA4
59	3g	405	CDL	OA7-CA5-OA6-CA4
59	4q	903	CDL	OA7-CA5-OA6-CA4
58	4z	302	PEE	C11-C10-O2-C2
59	2o	201	CDL	C71-CB7-OB8-CB6
59	2T	104	CDL	CB5-C51-C52-C53
59	3i	202	CDL	CA7-C31-C32-C33
59	4j	301	CDL	C31-CA7-OA8-CA6
59	2Q	101	CDL	C72-C73-C74-C75
59	3h	403	CDL	C1-CB2-OB2-PB2
58	3C	301	PEE	C16-C17-C18-C19
59	2Q	101	CDL	C51-CB5-OB6-CB4
59	3L	701	CDL	C11-CA5-OA6-CA4
58	4Q	901	PEE	O5-C30-O3-C3
53	3G	401	UQ1	C2-C3-O3-CM3
53	3g	401	UQ1	C3-C2-O2-CM2
60	3H	402	PC1	O32-C31-O31-C3
60	2R	201	PC1	C31-C32-C33-C34
59	2O	203	CDL	O1-C1-CB2-OB2
59	3E	201	CDL	O1-C1-CA2-OA2
59	3G	404	CDL	O1-C1-CA2-OA2
59	3I	201	CDL	O1-C1-CA2-OA2
59	3I	202	CDL	O1-C1-CB2-OB2
59	3L	701	CDL	O1-C1-CA2-OA2
59	3e	202	CDL	O1-C1-CA2-OA2
59	3i	201	CDL	O1-C1-CA2-OA2
59	4E	202	CDL	O1-C1-CB2-OB2
59	4F	202	CDL	O1-C1-CA2-OA2
59	4M	201	CDL	O1-C1-CA2-OA2
59	4e	202	CDL	O1-C1-CB2-OB2
59	4f	201	CDL	O1-C1-CA2-OA2
59	4m	201	CDL	O1-C1-CA2-OA2
59	4q	903	CDL	O1-C1-CB2-OB2
59	3E	201	CDL	OB7-CB5-OB6-CB4
59	3G	403	CDL	OA7-CA5-OA6-CA4
60	2R	202	PC1	O22-C21-O21-C2
60	3a	501	PC1	O22-C21-O21-C2
59	3D	201	CDL	OA9-CA7-OA8-CA6
59	3g	405	CDL	OA9-CA7-OA8-CA6
59	41	304	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
58	2P	202	PEE	C17-C18-C19-C20
58	4z	302	PEE	C37-C38-C39-C40
58	4q	901	PEE	O5-C30-O3-C3
60	2R	201	PC1	O32-C31-O31-C3
58	2O	201	PEE	C1-O3P-P-O4P
58	2P	202	PEE	C1-O3P-P-O4P
58	2T	103	PEE	C4-O4P-P-O3P
58	2o	203	PEE	C1-O3P-P-O4P
58	2r	203	PEE	C4-O4P-P-O3P
58	2t	101	PEE	C1-O3P-P-O4P
58	3H	403	PEE	C1-O3P-P-O4P
58	3H	403	PEE	C4-O4P-P-O3P
58	3c	301	PEE	C4-O4P-P-O3P
58	3f	102	PEE	C1-O3P-P-O4P
58	3f	102	PEE	C4-O4P-P-O3P
58	40	301	PEE	C1-O3P-P-O4P
58	40	302	PEE	C4-O4P-P-O3P
58	4R	201	PEE	C1-O3P-P-O4P
58	4W	201	PEE	C1-O3P-P-O4P
58	4Z	302	PEE	C4-O4P-P-O3P
58	4l	201	PEE	C1-O3P-P-O4P
58	4s	101	PEE	C4-O4P-P-O3P
58	4w	201	PEE	C1-O3P-P-O4P
58	4z	302	PEE	C4-O4P-P-O3P
59	2O	203	CDL	CA3-OA5-PA1-OA2
59	2O	203	CDL	CB2-OB2-PB2-OB5
59	2O	203	CDL	CB3-OB5-PB2-OB2
59	2T	104	CDL	CB2-OB2-PB2-OB5
59	2o	201	CDL	CA3-OA5-PA1-OA2
59	2p	204	CDL	CA3-OA5-PA1-OA2
59	2t	102	CDL	CB2-OB2-PB2-OB5
59	3D	201	CDL	CA3-OA5-PA1-OA2
59	3D	202	CDL	CB3-OB5-PB2-OB2
59	3E	201	CDL	CA2-OA2-PA1-OA5
59	3E	201	CDL	CB2-OB2-PB2-OB5
59	3G	403	CDL	CB2-OB2-PB2-OB5
59	3G	404	CDL	CA2-OA2-PA1-OA5
59	3H	404	CDL	CA2-OA2-PA1-OA5
59	3H	404	CDL	CA3-OA5-PA1-OA2
59	3H	405	CDL	CA3-OA5-PA1-OA2
59	3H	405	CDL	CB3-OB5-PB2-OB2
59	3I	202	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
59	3I	202	CDL	CB3-OB5-PB2-OB2
59	3I	203	CDL	CA3-OA5-PA1-OA2
59	3I	203	CDL	CB3-OB5-PB2-OB2
59	3L	701	CDL	CA2-OA2-PA1-OA5
59	3L	702	CDL	CA2-OA2-PA1-OA5
59	3L	702	CDL	CA3-OA5-PA1-OA2
59	3L	703	CDL	CB3-OB5-PB2-OB2
59	3e	201	CDL	CB2-OB2-PB2-OB5
59	3e	202	CDL	CA2-OA2-PA1-OA5
59	3e	202	CDL	CB2-OB2-PB2-OB5
59	3g	404	CDL	CB2-OB2-PB2-OB5
59	3g	405	CDL	CA3-OA5-PA1-OA2
59	3g	406	CDL	CA2-OA2-PA1-OA5
59	3h	403	CDL	CA3-OA5-PA1-OA2
59	3h	403	CDL	CB2-OB2-PB2-OB5
59	3i	201	CDL	CB2-OB2-PB2-OB5
59	3i	202	CDL	CA3-OA5-PA1-OA2
59	3i	202	CDL	CB2-OB2-PB2-OB5
59	3i	202	CDL	CB3-OB5-PB2-OB2
59	3l	702	CDL	CA2-OA2-PA1-OA5
59	3l	702	CDL	CA3-OA5-PA1-OA2
59	41	304	CDL	CA2-OA2-PA1-OA5
59	41	304	CDL	CA3-OA5-PA1-OA2
59	41	304	CDL	CB2-OB2-PB2-OB5
59	41	304	CDL	CB3-OB5-PB2-OB2
59	4E	202	CDL	CA2-OA2-PA1-OA5
59	4F	202	CDL	CA2-OA2-PA1-OA5
59	4F	202	CDL	CB3-OB5-PB2-OB2
59	4J	301	CDL	CA3-OA5-PA1-OA2
59	4K	201	CDL	CA2-OA2-PA1-OA5
59	4K	201	CDL	CA3-OA5-PA1-OA2
59	4K	201	CDL	CB2-OB2-PB2-OB5
59	4L	201	CDL	CA2-OA2-PA1-OA5
59	4L	201	CDL	CB2-OB2-PB2-OB5
59	4M	201	CDL	CA2-OA2-PA1-OA5
59	4M	201	CDL	CA3-OA5-PA1-OA2
59	4M	201	CDL	CB2-OB2-PB2-OB5
59	4O	501	CDL	CB2-OB2-PB2-OB5
59	4O	501	CDL	CB3-OB5-PB2-OB2
59	4Q	902	CDL	CA3-OA5-PA1-OA2
59	4Q	902	CDL	CB3-OB5-PB2-OB2
59	4S	102	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
59	4S	102	CDL	CA3-OA5-PA1-OA2
59	4S	102	CDL	CB3-OB5-PB2-OB2
59	4U	501	CDL	CA2-OA2-PA1-OA5
59	4Z	303	CDL	CA3-OA5-PA1-OA2
59	4Z	303	CDL	CB3-OB5-PB2-OB2
59	4e	202	CDL	CA2-OA2-PA1-OA5
59	4e	202	CDL	CB3-OB5-PB2-OB2
59	4f	201	CDL	CA2-OA2-PA1-OA5
59	4f	201	CDL	CB3-OB5-PB2-OB2
59	4j	301	CDL	CA2-OA2-PA1-OA5
59	4j	301	CDL	CA3-OA5-PA1-OA2
59	4j	302	CDL	CA2-OA2-PA1-OA5
59	4j	302	CDL	CB2-OB2-PB2-OB5
59	4m	201	CDL	CA2-OA2-PA1-OA5
59	4m	201	CDL	CA3-OA5-PA1-OA2
59	4m	201	CDL	CB2-OB2-PB2-OB5
59	4o	501	CDL	CB2-OB2-PB2-OB5
59	4o	501	CDL	CB3-OB5-PB2-OB2
59	4q	903	CDL	CA2-OA2-PA1-OA5
59	4q	903	CDL	CA3-OA5-PA1-OA2
59	4s	102	CDL	CA2-OA2-PA1-OA5
59	4s	102	CDL	CA3-OA5-PA1-OA2
59	4s	102	CDL	CB3-OB5-PB2-OB2
59	4t	201	CDL	CA2-OA2-PA1-OA5
59	4t	201	CDL	CA3-OA5-PA1-OA2
59	4z	304	CDL	CA3-OA5-PA1-OA2
59	4z	304	CDL	CB3-OB5-PB2-OB2
60	2o	202	PC1	C1-O11-P-O13
60	3A	501	PC1	C1-O11-P-O13
60	3H	401	PC1	C11-O13-P-O11
60	3H	401	PC1	C1-O11-P-O13
60	3a	501	PC1	C1-O11-P-O13
60	3f	101	PC1	C1-O11-P-O13
60	3h	401	PC1	C11-O13-P-O11
60	3h	401	PC1	C1-O11-P-O13
60	4F	201	PC1	C11-O13-P-O11
60	3h	402	PC1	C32-C31-O31-C3
59	2O	203	CDL	CA2-C1-CB2-OB2
59	2o	201	CDL	CA2-C1-CB2-OB2
59	2p	204	CDL	CB2-C1-CA2-OA2
59	3E	201	CDL	CB2-C1-CA2-OA2
59	3L	703	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
59	3e	202	CDL	CB2-C1-CA2-OA2
59	3l	701	CDL	CB2-C1-CA2-OA2
59	4E	202	CDL	CA2-C1-CB2-OB2
59	4F	202	CDL	CB2-C1-CA2-OA2
59	4M	201	CDL	CB2-C1-CA2-OA2
59	4O	501	CDL	CA2-C1-CB2-OB2
59	4W	202	CDL	CB2-C1-CA2-OA2
59	4e	202	CDL	CA2-C1-CB2-OB2
59	4f	201	CDL	CB2-C1-CA2-OA2
59	4g	202	CDL	CB2-C1-CA2-OA2
59	4j	301	CDL	CA2-C1-CB2-OB2
59	4m	201	CDL	CB2-C1-CA2-OA2
59	4o	501	CDL	CA2-C1-CB2-OB2
58	40	301	PEE	O4-C10-O2-C2
59	3I	202	CDL	CA7-C31-C32-C33
58	40	301	PEE	C11-C10-O2-C2
59	2q	101	CDL	C51-CB5-OB6-CB4
59	2P	203	CDL	C59-C60-C61-C62
60	2T	102	PC1	C22-C23-C24-C25
60	3f	101	PC1	C22-C23-C24-C25
58	2t	101	PEE	C40-C41-C42-C43
59	3g	405	CDL	CA6-CA4-OA6-CA5
59	4J	301	CDL	CA6-CA4-OA6-CA5
59	4t	201	CDL	CA6-CA4-OA6-CA5
58	4z	302	PEE	O4-C10-O2-C2
59	2Q	101	CDL	OB7-CB5-OB6-CB4
58	4z	302	PEE	C30-C31-C32-C33
59	2o	201	CDL	C1-CB2-OB2-PB2
59	3G	404	CDL	C1-CB2-OB2-PB2
59	3g	403	CDL	C1-CB2-OB2-PB2
59	3h	403	CDL	CA4-CA3-OA5-PA1
58	4D	101	PEE	C17-C18-C19-C20
58	2o	203	PEE	C12-C13-C14-C15
60	2R	201	PC1	C39-C3A-C3B-C3C
59	2O	203	CDL	O1-C1-CA2-OA2
58	4w	201	PEE	C11-C12-C13-C14
59	3D	201	CDL	C13-C14-C15-C16
59	3g	403	CDL	OA6-CA4-CA6-OA8
60	2T	102	PC1	C2B-C2C-C2D-C2E
60	2r	202	PC1	C32-C33-C34-C35
60	3f	101	PC1	C2B-C2C-C2D-C2E
59	3I	203	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
60	2r	202	PC1	C22-C23-C24-C25
60	2R	201	PC1	C2E-C2F-C2G-C2H
58	40	302	PEE	C30-C31-C32-C33
59	4o	501	CDL	OA5-CA3-CA4-CA6
59	2Q	101	CDL	C59-C60-C61-C62
58	2O	201	PEE	O4P-C4-C5-N
58	41	302	PEE	O4P-C4-C5-N
58	4z	302	PEE	O4P-C4-C5-N
58	41	303	PEE	C31-C32-C33-C34
59	4L	201	CDL	C82-C83-C84-C85
60	2R	202	PC1	C31-C32-C33-C34
59	2o	201	CDL	OB9-CB7-OB8-CB6
59	3I	201	CDL	OA9-CA7-OA8-CA6
59	3D	201	CDL	C12-C13-C14-C15
58	2O	201	PEE	C31-C30-O3-C3
59	3L	701	CDL	C71-CB7-OB8-CB6
59	2O	203	CDL	OB9-CB7-OB8-CB6
59	4F	202	CDL	C51-C52-C53-C54
59	2q	101	CDL	OB7-CB5-OB6-CB4
59	3L	701	CDL	OA7-CA5-OA6-CA4
60	2R	201	PC1	C34-C35-C36-C37
59	3g	406	CDL	C11-CA5-OA6-CA4
59	4F	202	CDL	C51-CB5-OB6-CB4
59	4j	302	CDL	C11-CA5-OA6-CA4
59	2T	104	CDL	C34-C35-C36-C37
59	4j	301	CDL	OA9-CA7-OA8-CA6
59	2Q	101	CDL	C13-C14-C15-C16
59	4J	301	CDL	O1-C1-CA2-OA2
58	4Q	901	PEE	C11-C12-C13-C14
60	2R	201	PC1	C36-C37-C38-C39
59	4j	302	CDL	OA7-CA5-OA6-CA4
58	2O	202	PEE	C13-C14-C15-C16
59	3E	201	CDL	C20-C21-C22-C23
59	4Q	902	CDL	C21-C22-C23-C24
59	2Q	101	CDL	CB5-C51-C52-C53
59	3L	703	CDL	C15-C16-C17-C18
58	4q	902	PEE	C31-C30-O3-C3
59	3h	403	CDL	C71-CB7-OB8-CB6
58	40	302	PEE	C11-C10-O2-C2
59	3D	201	CDL	C11-CA5-OA6-CA4
59	2Q	101	CDL	C36-C37-C38-C39
59	4j	302	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
58	2T	103	PEE	C18-C19-C20-C21
58	2O	201	PEE	O5-C30-O3-C3
60	3h	402	PC1	O32-C31-O31-C3
59	4M	201	CDL	C12-C11-CA5-OA6
53	3G	401	UQ1	C3-C2-O2-CM2
59	3g	406	CDL	OA7-CA5-OA6-CA4
59	4z	304	CDL	C31-CA7-OA8-CA6
59	4f	201	CDL	C52-C53-C54-C55
59	3D	201	CDL	C71-C72-C73-C74
59	2P	203	CDL	CA5-C11-C12-C13
59	2Q	101	CDL	C17-C18-C19-C20
60	3f	101	PC1	C23-C24-C25-C26
58	40	302	PEE	C12-C13-C14-C15
59	3I	203	CDL	C77-C78-C79-C80
60	2T	102	PC1	C23-C24-C25-C26
58	40	304	PEE	C11-C10-O2-C2
58	41	303	PEE	C11-C10-O2-C2
58	4Z	302	PEE	C11-C10-O2-C2
58	4s	101	PEE	C11-C10-O2-C2
59	3G	403	CDL	C51-CB5-OB6-CB4
59	3H	404	CDL	C11-CA5-OA6-CA4
59	3i	201	CDL	C11-CA5-OA6-CA4
59	4K	201	CDL	C11-CA5-OA6-CA4
59	4W	202	CDL	C11-CA5-OA6-CA4
59	4e	202	CDL	C51-CB5-OB6-CB4
59	4j	302	CDL	C51-CB5-OB6-CB4
59	4z	304	CDL	C51-CB5-OB6-CB4
60	2o	202	PC1	C22-C21-O21-C2
59	3I	203	CDL	OB5-CB3-CB4-OB6
59	3g	403	CDL	OB5-CB3-CB4-OB6
58	40	301	PEE	C36-C37-C38-C39
58	41	303	PEE	O4-C10-O2-C2
59	3D	201	CDL	OA7-CA5-OA6-CA4
59	4F	202	CDL	OB7-CB5-OB6-CB4
59	4z	304	CDL	OB7-CB5-OB6-CB4
60	2o	202	PC1	O22-C21-O21-C2
59	4J	301	CDL	CB7-C71-C72-C73
58	4q	901	PEE	C31-C32-C33-C34
59	2Q	101	CDL	C63-C64-C65-C66
58	3c	301	PEE	O2-C2-C3-O3
59	2Q	101	CDL	C16-C17-C18-C19
58	4Z	302	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
58	4z	302	PEE	C35-C36-C37-C38
60	3h	401	PC1	C32-C31-O31-C3
58	40	304	PEE	O4-C10-O2-C2
59	3i	201	CDL	OA7-CA5-OA6-CA4
59	4K	201	CDL	OA7-CA5-OA6-CA4
59	4e	202	CDL	OB7-CB5-OB6-CB4
59	4j	302	CDL	OB7-CB5-OB6-CB4
59	2Q	101	CDL	C11-CA5-OA6-CA4
59	4e	203	CDL	C51-CB5-OB6-CB4
52	2M	701	FAD	C2'-C3'-C4'-O4'
58	2O	202	PEE	C4-O4P-P-O3P
58	4q	902	PEE	C4-O4P-P-O3P
59	2P	203	CDL	CA3-OA5-PA1-OA2
59	2Q	101	CDL	CB3-OB5-PB2-OB2
59	2T	104	CDL	CA3-OA5-PA1-OA2
59	2o	201	CDL	CB2-OB2-PB2-OB5
59	3D	201	CDL	CA2-OA2-PA1-OA5
59	3I	203	CDL	CA2-OA2-PA1-OA5
59	3e	202	CDL	CB3-OB5-PB2-OB2
59	3g	403	CDL	CB2-OB2-PB2-OB5
59	3g	405	CDL	CA2-OA2-PA1-OA5
59	3g	406	CDL	CB2-OB2-PB2-OB5
59	3l	701	CDL	CB3-OB5-PB2-OB2
59	4E	202	CDL	CA3-OA5-PA1-OA2
59	4F	202	CDL	CB2-OB2-PB2-OB5
59	4Q	902	CDL	CB2-OB2-PB2-OB5
59	4U	501	CDL	CA3-OA5-PA1-OA2
59	4W	202	CDL	CB3-OB5-PB2-OB2
59	4Z	303	CDL	CA2-OA2-PA1-OA5
59	4f	201	CDL	CB2-OB2-PB2-OB5
59	4g	202	CDL	CB3-OB5-PB2-OB2
59	4q	903	CDL	CB2-OB2-PB2-OB5
59	4z	304	CDL	CA2-OA2-PA1-OA5
60	2T	102	PC1	C1-O11-P-O13
60	2r	201	PC1	C1-O11-P-O13
60	3H	402	PC1	C1-O11-P-O13
60	3h	402	PC1	C1-O11-P-O13
60	4e	201	PC1	C11-O13-P-O11
59	3h	403	CDL	C1-CA2-OA2-PA1
59	4K	201	CDL	C74-C75-C76-C77
58	4Z	302	PEE	O3P-C1-C2-C3
58	4z	302	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
59	2O	203	CDL	OB5-CB3-CB4-CB6
59	2Q	101	CDL	OB5-CB3-CB4-CB6
59	2o	201	CDL	OB5-CB3-CB4-CB6
59	2q	101	CDL	OB5-CB3-CB4-CB6
59	3L	701	CDL	OA5-CA3-CA4-CA6
59	3L	701	CDL	OB5-CB3-CB4-CB6
59	3L	702	CDL	OB5-CB3-CB4-CB6
59	3e	202	CDL	OB5-CB3-CB4-CB6
59	3i	201	CDL	OB5-CB3-CB4-CB6
59	4E	202	CDL	OB5-CB3-CB4-CB6
59	4F	202	CDL	OB5-CB3-CB4-CB6
59	4L	201	CDL	OA5-CA3-CA4-CA6
59	4M	201	CDL	OA5-CA3-CA4-CA6
59	4Q	902	CDL	OB5-CB3-CB4-CB6
59	4S	102	CDL	OB5-CB3-CB4-CB6
59	4U	501	CDL	OA5-CA3-CA4-CA6
59	4U	501	CDL	OB5-CB3-CB4-CB6
59	4f	201	CDL	OB5-CB3-CB4-CB6
59	4j	301	CDL	OA5-CA3-CA4-CA6
59	4j	302	CDL	OA5-CA3-CA4-CA6
59	4s	102	CDL	OB5-CB3-CB4-CB6
59	4t	201	CDL	OA5-CA3-CA4-CA6
60	2T	101	PC1	O11-C1-C2-C3
58	4Q	901	PEE	C31-C32-C33-C34
59	2Q	101	CDL	C80-C81-C82-C83
59	41	304	CDL	CA4-CA6-OA8-CA7
59	4K	201	CDL	CA4-CA6-OA8-CA7
53	3G	401	UQ1	C4-C3-O3-CM3
53	3g	401	UQ1	C1-C2-O2-CM2
59	2Q	101	CDL	C76-C77-C78-C79
59	3E	201	CDL	C37-C38-C39-C40
59	3L	703	CDL	C71-CB7-OB8-CB6
59	3H	404	CDL	CB2-C1-CA2-OA2
59	4J	301	CDL	CB2-C1-CA2-OA2
59	3H	404	CDL	OA7-CA5-OA6-CA4
59	2P	203	CDL	C56-C57-C58-C59
58	4q	902	PEE	O5-C30-O3-C3
59	3L	701	CDL	OB9-CB7-OB8-CB6
59	4M	201	CDL	O1-C1-CB2-OB2
58	4q	902	PEE	C1-C2-C3-O3
59	3G	403	CDL	CA3-CA4-CA6-OA8
59	3I	203	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
59	3L	701	CDL	C72-C73-C74-C75
59	3L	703	CDL	CB3-CB4-CB6-OB8
59	3e	202	CDL	CA3-CA4-CA6-OA8
59	3g	403	CDL	CA3-CA4-CA6-OA8
59	4J	301	CDL	CB3-CB4-CB6-OB8
59	4W	202	CDL	CA3-CA4-CA6-OA8
60	2R	202	PC1	C1-C2-C3-O31
60	3h	402	PC1	C1-C2-C3-O31
63	4g	201	LPP	C6-C7-C8-O27
59	3D	201	CDL	C12-C11-CA5-OA6
59	4Q	902	CDL	C52-C51-CB5-OB6
59	2q	101	CDL	C59-C60-C61-C62
58	4q	902	PEE	C12-C13-C14-C15
60	2R	201	PC1	C2C-C2D-C2E-C2F
58	41	301	PEE	C36-C37-C38-C39
59	3l	701	CDL	C64-C65-C66-C67
58	2T	103	PEE	C11-C10-O2-C2
59	4U	501	CDL	C11-CA5-OA6-CA4
59	4f	201	CDL	CB5-C51-C52-C53
63	4g	201	LPP	C11-C12-C13-C14
59	2q	101	CDL	C71-CB7-OB8-CB6
59	3D	202	CDL	C31-CA7-OA8-CA6
58	2O	201	PEE	C31-C32-C33-C34
59	4j	301	CDL	C77-C78-C79-C80
59	3E	201	CDL	CB3-CB4-OB6-CB5
59	4Q	902	CDL	CB3-CB4-OB6-CB5
59	4W	202	CDL	OA7-CA5-OA6-CA4
59	4M	201	CDL	C56-C57-C58-C59
63	4Z	301	LPP	C6-O5-P1-O3
63	4z	301	LPP	C6-O5-P1-O3
59	4E	201	CDL	C75-C76-C77-C78
59	4F	202	CDL	C71-CB7-OB8-CB6
63	4g	201	LPP	C30-C29-O27-C8
59	2T	104	CDL	OA5-CA3-CA4-OA6
59	3L	702	CDL	OA5-CA3-CA4-OA6
59	4J	301	CDL	OB5-CB3-CB4-OB6
59	4O	501	CDL	OA5-CA3-CA4-OA6
59	4W	202	CDL	OB5-CB3-CB4-OB6
60	2o	202	PC1	O11-C1-C2-O21
59	4o	501	CDL	C32-C31-CA7-OA8
59	3L	703	CDL	C64-C65-C66-C67
59	4q	903	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
59	4f	201	CDL	C51-C52-C53-C54
59	3L	703	CDL	C55-C56-C57-C58
59	3G	403	CDL	C53-C54-C55-C56
59	4F	202	CDL	C74-C75-C76-C77
59	3L	701	CDL	C72-C71-CB7-OB8
59	3g	405	CDL	C12-C11-CA5-OA6
59	3g	406	CDL	C32-C31-CA7-OA8
60	3H	402	PC1	O21-C2-C3-O31
59	4z	304	CDL	C55-C56-C57-C58
59	4E	201	CDL	C79-C80-C81-C82
59	4j	301	CDL	C73-C74-C75-C76
59	3L	701	CDL	C32-C31-CA7-OA8
59	4O	501	CDL	C32-C31-CA7-OA8
59	3h	403	CDL	OB9-CB7-OB8-CB6
59	3I	202	CDL	C40-C41-C42-C43
59	4F	202	CDL	C37-C38-C39-C40
59	4E	201	CDL	C31-CA7-OA8-CA6
59	4M	201	CDL	CA2-C1-CB2-OB2
58	40	302	PEE	O4-C10-O2-C2
59	3g	403	CDL	C51-CB5-OB6-CB4
59	2q	101	CDL	C31-CA7-OA8-CA6
59	4K	201	CDL	C71-CB7-OB8-CB6
59	4q	903	CDL	C71-CB7-OB8-CB6
59	4q	903	CDL	C75-C76-C77-C78
58	4z	302	PEE	C36-C37-C38-C39
58	40	301	PEE	C12-C13-C14-C15
58	2O	202	PEE	O3P-C1-C2-C3
58	2T	103	PEE	O3P-C1-C2-C3
58	2t	101	PEE	O3P-C1-C2-C3
58	3c	301	PEE	O3P-C1-C2-C3
59	2T	104	CDL	OB5-CB3-CB4-CB6
59	3D	201	CDL	OA5-CA3-CA4-CA6
59	3E	201	CDL	OA5-CA3-CA4-CA6
59	3G	403	CDL	OB5-CB3-CB4-CB6
59	3H	405	CDL	OA5-CA3-CA4-CA6
59	3H	405	CDL	OB5-CB3-CB4-CB6
59	3I	203	CDL	OB5-CB3-CB4-CB6
59	3e	201	CDL	OA5-CA3-CA4-CA6
59	3g	403	CDL	OB5-CB3-CB4-CB6
59	3g	406	CDL	OA5-CA3-CA4-CA6
59	3i	202	CDL	OB5-CB3-CB4-CB6
59	3l	701	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
59	4g	202	CDL	OB5-CB3-CB4-CB6
59	4m	201	CDL	OA5-CA3-CA4-CA6
59	4z	304	CDL	OB5-CB3-CB4-CB6
59	2q	101	CDL	CB5-C51-C52-C53
59	3H	405	CDL	CA5-C11-C12-C13
58	40	303	PEE	O4P-C4-C5-N
59	3I	202	CDL	C71-CB7-OB8-CB6
59	4J	301	CDL	C12-C11-CA5-OA6
59	3L	703	CDL	C62-C63-C64-C65
52	2m	701	FAD	C2'-C3'-C4'-O4'
59	4L	201	CDL	C31-CA7-OA8-CA6
59	3D	201	CDL	C52-C53-C54-C55
59	4O	501	CDL	C19-C20-C21-C22
58	4Z	302	PEE	C14-C15-C16-C17
59	2p	204	CDL	C71-CB7-OB8-CB6
59	3g	405	CDL	C11-C12-C13-C14
58	2O	201	PEE	C1-C2-C3-O3
58	2P	202	PEE	C1-C2-C3-O3
59	2P	203	CDL	CB3-CB4-CB6-OB8
59	3D	201	CDL	CA3-CA4-CA6-OA8
59	3E	201	CDL	CA3-CA4-CA6-OA8
59	4K	201	CDL	CB3-CB4-CB6-OB8
59	4g	202	CDL	CA3-CA4-CA6-OA8
60	2T	102	PC1	C1-C2-C3-O31
60	2r	202	PC1	C1-C2-C3-O31
60	3H	402	PC1	C1-C2-C3-O31
60	3f	101	PC1	C1-C2-C3-O31
58	4d	101	PEE	C17-C18-C19-C20
59	4z	304	CDL	OA9-CA7-OA8-CA6
60	2r	201	PC1	C39-C3A-C3B-C3C
59	2q	101	CDL	C13-C14-C15-C16
58	2O	201	PEE	C4-O4P-P-O3P
58	3c	301	PEE	C1-O3P-P-O4P
58	40	301	PEE	C4-O4P-P-O3P
58	4S	101	PEE	C4-O4P-P-O3P
59	2q	101	CDL	CB3-OB5-PB2-OB2
59	3E	201	CDL	CA3-OA5-PA1-OA2
59	3H	405	CDL	CA2-OA2-PA1-OA5
59	3H	405	CDL	CB2-OB2-PB2-OB5
59	3I	203	CDL	CB2-OB2-PB2-OB5
59	3g	404	CDL	CA2-OA2-PA1-OA5
59	3h	403	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
59	3l	701	CDL	CA2-OA2-PA1-OA5
59	4M	201	CDL	CB3-OB5-PB2-OB2
59	4U	501	CDL	CB2-OB2-PB2-OB5
59	4j	302	CDL	CA3-OA5-PA1-OA2
59	4m	201	CDL	CB3-OB5-PB2-OB2
60	2o	202	PC1	C11-O13-P-O11
58	4q	902	PEE	C11-C12-C13-C14
59	4F	202	CDL	C32-C33-C34-C35
59	2O	203	CDL	C56-C57-C58-C59
59	3L	703	CDL	C16-C17-C18-C19
58	2O	202	PEE	O3P-C1-C2-O2
58	40	302	PEE	O3P-C1-C2-O2
58	4Z	302	PEE	O3P-C1-C2-O2
59	2O	203	CDL	OB5-CB3-CB4-OB6
59	3E	201	CDL	OA5-CA3-CA4-OA6
59	3I	201	CDL	OB5-CB3-CB4-OB6
59	3L	701	CDL	OB5-CB3-CB4-OB6
59	3e	202	CDL	OB5-CB3-CB4-OB6
59	3g	406	CDL	OA5-CA3-CA4-OA6
59	3l	702	CDL	OA5-CA3-CA4-OA6
59	4Q	902	CDL	OB5-CB3-CB4-OB6
59	4S	102	CDL	OB5-CB3-CB4-OB6
59	4U	501	CDL	OA5-CA3-CA4-OA6
59	4g	202	CDL	OB5-CB3-CB4-OB6
59	4s	102	CDL	OB5-CB3-CB4-OB6
60	3a	501	PC1	O11-C1-C2-O21
59	3H	405	CDL	O1-C1-CA2-OA2
58	4Q	901	PEE	C33-C34-C35-C36
59	3L	703	CDL	OB9-CB7-OB8-CB6
58	2P	202	PEE	O2-C2-C3-O3
58	3f	102	PEE	O2-C2-C3-O3
58	40	301	PEE	O2-C2-C3-O3
59	3G	403	CDL	OA6-CA4-CA6-OA8
59	3I	203	CDL	OB6-CB4-CB6-OB8
59	3g	403	CDL	OB6-CB4-CB6-OB8
59	4K	201	CDL	OB6-CB4-CB6-OB8
63	4g	201	LPP	O9-C7-C8-O27
58	2O	201	PEE	C33-C34-C35-C36
59	4L	201	CDL	C11-CA5-OA6-CA4
63	4z	301	LPP	C12-C13-C14-C15
58	2T	103	PEE	O4-C10-O2-C2
59	4L	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
59	3L	701	CDL	C18-C19-C20-C21
59	2O	203	CDL	C1-CB2-OB2-PB2
59	2P	203	CDL	CA4-CA3-OA5-PA1
59	3D	201	CDL	CB4-CB3-OB5-PB2
59	3G	403	CDL	C1-CB2-OB2-PB2
59	3H	404	CDL	CA4-CA3-OA5-PA1
59	3H	404	CDL	C1-CB2-OB2-PB2
59	3I	202	CDL	CB4-CB3-OB5-PB2
59	3g	404	CDL	CA4-CA3-OA5-PA1
59	41	304	CDL	C1-CB2-OB2-PB2
59	4F	202	CDL	C1-CB2-OB2-PB2
59	4J	301	CDL	C1-CA2-OA2-PA1
59	4K	201	CDL	CA4-CA3-OA5-PA1
59	4e	202	CDL	C1-CA2-OA2-PA1
60	2r	202	PC1	C2-C1-O11-P
60	4F	201	PC1	C2-C1-O11-P
59	3L	703	CDL	C12-C13-C14-C15
60	4F	201	PC1	C11-C12-N-C14
59	3L	703	CDL	CA5-C11-C12-C13
58	4z	302	PEE	C38-C39-C40-C41
59	3L	703	CDL	C53-C54-C55-C56
59	4K	201	CDL	C17-C18-C19-C20
59	4z	303	CDL	CA7-C31-C32-C33
58	4Z	302	PEE	O4-C10-O2-C2
59	2T	104	CDL	C11-CA5-OA6-CA4
59	2q	101	CDL	C11-CA5-OA6-CA4
59	3i	201	CDL	C51-CB5-OB6-CB4
60	3a	501	PC1	C32-C33-C34-C35
58	3c	301	PEE	C18-C19-C20-C21
58	40	301	PEE	C18-C19-C20-C21
58	40	303	PEE	C18-C19-C20-C21
58	4l	201	PEE	C18-C19-C20-C21
58	4q	901	PEE	C38-C39-C40-C41
58	4q	902	PEE	C18-C19-C20-C21
60	2R	201	PC1	C26-C27-C28-C29
58	40	302	PEE	O3P-C1-C2-C3
59	2p	204	CDL	OA5-CA3-CA4-CA6
59	3H	404	CDL	OA5-CA3-CA4-CA6
59	3I	201	CDL	OB5-CB3-CB4-CB6
59	3L	703	CDL	OB5-CB3-CB4-CB6
59	3e	202	CDL	OA5-CA3-CA4-CA6
59	3h	403	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
59	3l	702	CDL	OB5-CB3-CB4-CB6
59	41	304	CDL	OB5-CB3-CB4-CB6
59	4J	301	CDL	OB5-CB3-CB4-CB6
59	4Q	902	CDL	OA5-CA3-CA4-CA6
59	4W	202	CDL	OB5-CB3-CB4-CB6
59	4Z	303	CDL	OB5-CB3-CB4-CB6
59	4q	903	CDL	OA5-CA3-CA4-CA6
59	4t	201	CDL	OB5-CB3-CB4-CB6
59	3H	404	CDL	O1-C1-CB2-OB2
58	2P	202	PEE	C31-C32-C33-C34
58	4w	201	PEE	C43-C44-C45-C46
59	2Q	101	CDL	C41-C42-C43-C44
58	3H	403	PEE	C18-C19-C20-C21
59	2q	101	CDL	OB9-CB7-OB8-CB6
58	4Z	302	PEE	C20-C21-C22-C23
52	2M	701	FAD	C2'-C3'-C4'-C5'
59	2q	101	CDL	C16-C17-C18-C19
58	41	302	PEE	C31-C30-O3-C3
59	2Q	101	CDL	C71-CB7-OB8-CB6
59	4Q	902	CDL	C71-CB7-OB8-CB6
59	3H	404	CDL	C71-CB7-OB8-CB6
63	4z	301	LPP	C13-C14-C15-C16
59	3D	201	CDL	CA6-CA4-OA6-CA5
59	4Z	303	CDL	CB3-CB4-OB6-CB5
59	4q	903	CDL	CB3-CB4-OB6-CB5
59	4z	304	CDL	CB3-CB4-OB6-CB5
60	4e	201	PC1	C3-C2-O21-C21
62	3G	406	HEM	C2B-C3B-CAB-CBB
62	3g	408	HEM	C2B-C3B-CAB-CBB
58	4s	101	PEE	O4-C10-O2-C2
59	3e	201	CDL	C32-C33-C34-C35
59	3D	201	CDL	C71-CB7-OB8-CB6
59	4F	202	CDL	C31-CA7-OA8-CA6
59	4t	201	CDL	C31-CA7-OA8-CA6
59	4O	501	CDL	C62-C63-C64-C65
58	40	301	PEE	C1-C2-C3-O3
59	3L	701	CDL	CB3-CB4-CB6-OB8
59	3i	201	CDL	CB4-CB3-OB5-PB2
59	4e	202	CDL	CB4-CB3-OB5-PB2
59	4f	201	CDL	C1-CB2-OB2-PB2
60	4F	201	PC1	C1-C2-C3-O31
60	4e	201	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
59	4W	202	CDL	C51-CB5-OB6-CB4
59	2T	104	CDL	C51-C52-C53-C54
58	3c	301	PEE	O3P-C1-C2-O2
59	2T	104	CDL	OB5-CB3-CB4-OB6
59	3D	201	CDL	OA5-CA3-CA4-OA6
59	3H	405	CDL	OA5-CA3-CA4-OA6
59	3e	201	CDL	OA5-CA3-CA4-OA6
59	3i	201	CDL	OB5-CB3-CB4-OB6
59	3l	701	CDL	OB5-CB3-CB4-OB6
59	41	304	CDL	OB5-CB3-CB4-OB6
59	4E	202	CDL	OB5-CB3-CB4-OB6
59	4M	201	CDL	OA5-CA3-CA4-OA6
59	4Q	902	CDL	OA5-CA3-CA4-OA6
59	4Z	303	CDL	OB5-CB3-CB4-OB6
59	4m	201	CDL	OA5-CA3-CA4-OA6
59	4o	501	CDL	OA5-CA3-CA4-OA6
59	4t	201	CDL	OB5-CB3-CB4-OB6
60	2T	101	PC1	O11-C1-C2-O21
58	4Q	901	PEE	C16-C17-C18-C19
58	4q	901	PEE	C16-C17-C18-C19
59	3g	403	CDL	C71-C72-C73-C74
59	2Q	101	CDL	OA7-CA5-OA6-CA4
59	3G	403	CDL	OB7-CB5-OB6-CB4
59	3i	201	CDL	C53-C54-C55-C56
59	3D	202	CDL	OA9-CA7-OA8-CA6
59	4F	202	CDL	OB9-CB7-OB8-CB6
59	4L	201	CDL	OA9-CA7-OA8-CA6
60	3h	401	PC1	O32-C31-O31-C3
63	4g	201	LPP	O28-C29-O27-C8
59	3I	201	CDL	C71-C72-C73-C74
58	4q	902	PEE	O2-C2-C3-O3
59	3D	201	CDL	OA6-CA4-CA6-OA8
59	3E	201	CDL	OA6-CA4-CA6-OA8
59	3E	201	CDL	OB6-CB4-CB6-OB8
60	2r	202	PC1	O21-C2-C3-O31
59	2p	204	CDL	OB9-CB7-OB8-CB6
59	4E	201	CDL	OA9-CA7-OA8-CA6
52	2M	701	FAD	C5B-O5B-PA-O3P
52	2m	701	FAD	C5B-O5B-PA-O3P
58	4l	201	PEE	C11-C10-O2-C2
59	3e	202	CDL	C11-CA5-OA6-CA4
59	4Z	303	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
58	4w	201	PEE	C15-C16-C17-C18
59	2P	203	CDL	C71-CB7-OB8-CB6
59	4e	203	CDL	OB7-CB5-OB6-CB4
58	2T	103	PEE	C16-C17-C18-C19
59	4L	201	CDL	C72-C73-C74-C75
60	2R	201	PC1	C38-C39-C3A-C3B
59	4q	903	CDL	OB9-CB7-OB8-CB6
60	3H	402	PC1	C22-C23-C24-C25
58	40	301	PEE	C11-C12-C13-C14
58	40	303	PEE	C31-C30-O3-C3
58	4R	201	PEE	C4-O4P-P-O3P
58	4l	201	PEE	C4-O4P-P-O3P
59	4o	501	CDL	CA2-OA2-PA1-OA5
59	3l	702	CDL	O1-C1-CB2-OB2
58	4l	201	PEE	C2-C1-O3P-P
59	3G	404	CDL	CA4-CA3-OA5-PA1
59	3e	201	CDL	CA4-CA3-OA5-PA1
59	3g	406	CDL	CA4-CA3-OA5-PA1
59	3g	406	CDL	C1-CB2-OB2-PB2
59	3g	406	CDL	CB4-CB3-OB5-PB2
59	3i	201	CDL	C1-CB2-OB2-PB2
59	4E	202	CDL	C1-CA2-OA2-PA1
59	4K	201	CDL	C1-CB2-OB2-PB2
59	4L	201	CDL	C1-CB2-OB2-PB2
59	4q	903	CDL	C1-CB2-OB2-PB2
59	4s	102	CDL	CB4-CB3-OB5-PB2
59	4K	201	CDL	OB9-CB7-OB8-CB6
58	2O	202	PEE	C4-O4P-P-O2P
58	2r	203	PEE	C4-O4P-P-O2P
58	2t	101	PEE	C1-O3P-P-O2P
58	3H	403	PEE	C4-O4P-P-O2P
58	3c	301	PEE	C1-O3P-P-O2P
58	3f	102	PEE	C4-O4P-P-O2P
58	4S	101	PEE	C4-O4P-P-O2P
58	4W	201	PEE	C1-O3P-P-O2P
58	4q	902	PEE	C4-O4P-P-O2P
58	4s	101	PEE	C4-O4P-P-O2P
58	4w	201	PEE	C1-O3P-P-O2P
59	2O	203	CDL	CA3-OA5-PA1-OA4
59	2Q	101	CDL	CB3-OB5-PB2-OB3
59	2T	104	CDL	CB2-OB2-PB2-OB3
59	2o	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
59	2o	201	CDL	CB2-OB2-PB2-OB4
59	2p	204	CDL	CA3-OA5-PA1-OA3
59	2q	101	CDL	CB3-OB5-PB2-OB3
59	2t	102	CDL	CB2-OB2-PB2-OB3
59	3D	202	CDL	CB3-OB5-PB2-OB3
59	3D	202	CDL	CB3-OB5-PB2-OB4
59	3G	403	CDL	CB2-OB2-PB2-OB4
59	3G	404	CDL	CA2-OA2-PA1-OA4
59	3H	405	CDL	CA3-OA5-PA1-OA3
59	3H	405	CDL	CB3-OB5-PB2-OB4
59	3I	202	CDL	CA3-OA5-PA1-OA3
59	3I	202	CDL	CB2-OB2-PB2-OB4
59	3I	202	CDL	CB3-OB5-PB2-OB4
59	3I	203	CDL	CA3-OA5-PA1-OA3
59	3L	702	CDL	CA2-OA2-PA1-OA3
59	3L	702	CDL	CA3-OA5-PA1-OA4
59	3L	703	CDL	CA2-OA2-PA1-OA3
59	3L	703	CDL	CB3-OB5-PB2-OB3
59	3L	703	CDL	CB3-OB5-PB2-OB4
59	3g	404	CDL	CA2-OA2-PA1-OA4
59	3g	405	CDL	CA3-OA5-PA1-OA3
59	3g	406	CDL	CB2-OB2-PB2-OB3
59	3h	403	CDL	CA2-OA2-PA1-OA4
59	3i	202	CDL	CA3-OA5-PA1-OA3
59	3i	202	CDL	CB2-OB2-PB2-OB3
59	3i	202	CDL	CB3-OB5-PB2-OB4
59	3l	701	CDL	CB3-OB5-PB2-OB3
59	3l	701	CDL	CB3-OB5-PB2-OB4
59	3l	702	CDL	CA2-OA2-PA1-OA3
59	3l	702	CDL	CA3-OA5-PA1-OA4
59	41	304	CDL	CA3-OA5-PA1-OA3
59	41	304	CDL	CB2-OB2-PB2-OB3
59	41	304	CDL	CB3-OB5-PB2-OB3
59	4E	202	CDL	CA2-OA2-PA1-OA3
59	4F	202	CDL	CB2-OB2-PB2-OB4
59	4F	202	CDL	CB3-OB5-PB2-OB3
59	4K	201	CDL	CA3-OA5-PA1-OA3
59	4K	201	CDL	CB2-OB2-PB2-OB3
59	4L	201	CDL	CA2-OA2-PA1-OA4
59	4M	201	CDL	CA2-OA2-PA1-OA3
59	4M	201	CDL	CA3-OA5-PA1-OA3
59	4M	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
59	4O	501	CDL	CB3-OB5-PB2-OB3
59	4Q	902	CDL	CA3-OA5-PA1-OA3
59	4S	102	CDL	CA2-OA2-PA1-OA3
59	4S	102	CDL	CB3-OB5-PB2-OB3
59	4U	501	CDL	CA2-OA2-PA1-OA4
59	4U	501	CDL	CA3-OA5-PA1-OA3
59	4U	501	CDL	CA3-OA5-PA1-OA4
59	4W	202	CDL	CB3-OB5-PB2-OB3
59	4W	202	CDL	CB3-OB5-PB2-OB4
59	4Z	303	CDL	CA3-OA5-PA1-OA3
59	4Z	303	CDL	CB3-OB5-PB2-OB3
59	4e	202	CDL	CA2-OA2-PA1-OA3
59	4f	201	CDL	CB2-OB2-PB2-OB4
59	4f	201	CDL	CB3-OB5-PB2-OB3
59	4g	202	CDL	CB3-OB5-PB2-OB3
59	4g	202	CDL	CB3-OB5-PB2-OB4
59	4j	301	CDL	CA3-OA5-PA1-OA3
59	4j	302	CDL	CA2-OA2-PA1-OA4
59	4j	302	CDL	CA3-OA5-PA1-OA4
59	4m	201	CDL	CA2-OA2-PA1-OA3
59	4m	201	CDL	CA3-OA5-PA1-OA3
59	4o	501	CDL	CB3-OB5-PB2-OB3
59	4q	903	CDL	CA2-OA2-PA1-OA3
59	4q	903	CDL	CA3-OA5-PA1-OA3
59	4s	102	CDL	CA2-OA2-PA1-OA3
59	4s	102	CDL	CB3-OB5-PB2-OB3
59	4t	201	CDL	CA2-OA2-PA1-OA4
59	4t	201	CDL	CA3-OA5-PA1-OA3
59	4t	201	CDL	CA3-OA5-PA1-OA4
59	4z	304	CDL	CA3-OA5-PA1-OA3
59	4z	304	CDL	CB3-OB5-PB2-OB3
60	2o	202	PC1	C1-O11-P-O14
60	3H	401	PC1	C11-O13-P-O14
60	3H	401	PC1	C1-O11-P-O12
60	3H	402	PC1	C1-O11-P-O12
60	3a	501	PC1	C1-O11-P-O12
60	3a	501	PC1	C1-O11-P-O14
60	3h	401	PC1	C1-O11-P-O12
60	3h	402	PC1	C1-O11-P-O12
60	4F	201	PC1	C11-O13-P-O14
60	4F	201	PC1	C11-C12-N-C13
60	4e	201	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
59	3H	404	CDL	CB7-C71-C72-C73
59	3H	405	CDL	CB7-C71-C72-C73
59	4f	201	CDL	C32-C33-C34-C35
59	3I	202	CDL	OB5-CB3-CB4-CB6
60	2o	202	PC1	O11-C1-C2-C3
58	41	302	PEE	C11-C12-C13-C14
59	4Q	902	CDL	C76-C77-C78-C79
58	4R	201	PEE	C16-C17-C18-C19
59	3L	703	CDL	C54-C55-C56-C57
58	4R	201	PEE	C5-C4-O4P-P
58	4W	201	PEE	C5-C4-O4P-P
58	4l	201	PEE	C5-C4-O4P-P
58	4w	201	PEE	C5-C4-O4P-P
52	2M	701	FAD	O3'-C3'-C4'-O4'
59	4O	501	CDL	C76-C77-C78-C79
59	3g	405	CDL	C71-CB7-OB8-CB6
59	4U	501	CDL	OA7-CA5-OA6-CA4
58	2T	103	PEE	O3P-C1-C2-O2
58	2t	101	PEE	O3P-C1-C2-O2
58	4z	302	PEE	O3P-C1-C2-O2
59	2Q	101	CDL	OB5-CB3-CB4-OB6
59	3G	403	CDL	OA5-CA3-CA4-OA6
59	3H	404	CDL	OA5-CA3-CA4-OA6
59	3H	404	CDL	OB5-CB3-CB4-OB6
59	3I	202	CDL	OB5-CB3-CB4-OB6
59	3L	701	CDL	OA5-CA3-CA4-OA6
59	3L	702	CDL	OB5-CB3-CB4-OB6
59	3L	703	CDL	OB5-CB3-CB4-OB6
59	3g	403	CDL	OA5-CA3-CA4-OA6
59	3h	403	CDL	OA5-CA3-CA4-OA6
59	3h	403	CDL	OB5-CB3-CB4-OB6
59	3i	202	CDL	OB5-CB3-CB4-OB6
59	4L	201	CDL	OA5-CA3-CA4-OA6
59	4M	201	CDL	OB5-CB3-CB4-OB6
59	4U	501	CDL	OB5-CB3-CB4-OB6
59	4q	903	CDL	OA5-CA3-CA4-OA6
59	4t	201	CDL	OA5-CA3-CA4-OA6
59	4z	304	CDL	OB5-CB3-CB4-OB6
60	3h	401	PC1	O11-C1-C2-O21
58	40	301	PEE	C32-C33-C34-C35
58	4Z	302	PEE	C36-C37-C38-C39
59	4Q	903	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
59	2O	203	CDL	C51-CB5-OB6-CB4
59	3D	201	CDL	OB9-CB7-OB8-CB6
59	3L	702	CDL	O1-C1-CB2-OB2
60	3a	501	PC1	C11-C12-N-C15
59	3l	701	CDL	C74-C75-C76-C77
58	2O	202	PEE	C1-C2-C3-O3
58	3c	301	PEE	C1-C2-C3-O3
59	3E	201	CDL	CB3-CB4-CB6-OB8
60	2R	201	PC1	O13-C11-C12-N
60	2r	201	PC1	O13-C11-C12-N
60	3H	401	PC1	O13-C11-C12-N
60	3h	401	PC1	O13-C11-C12-N
63	4z	301	LPP	C32-C33-C34-C35
58	2O	202	PEE	O2-C2-C3-O3
59	4J	301	CDL	OB6-CB4-CB6-OB8
60	2R	202	PC1	O21-C2-C3-O31
60	2T	102	PC1	O21-C2-C3-O31
60	3f	101	PC1	O21-C2-C3-O31
59	3L	702	CDL	C35-C36-C37-C38
60	2R	202	PC1	C39-C3A-C3B-C3C
63	4Z	301	LPP	C14-C15-C16-C17
59	2q	101	CDL	OA9-CA7-OA8-CA6
58	2P	202	PEE	C16-C17-C18-C19
58	2P	202	PEE	C2-C1-O3P-P
58	2T	103	PEE	C2-C1-O3P-P
59	41	304	CDL	CA4-CA3-OA5-PA1
59	4g	202	CDL	CB4-CB3-OB5-PB2
59	4j	302	CDL	C1-CB2-OB2-PB2
60	4e	201	PC1	C2-C1-O11-P
59	2Q	101	CDL	C31-CA7-OA8-CA6
58	4q	901	PEE	C11-C12-C13-C14
60	2r	202	PC1	C3B-C3C-C3D-C3E
59	2q	101	CDL	C77-C78-C79-C80
59	3I	202	CDL	OB9-CB7-OB8-CB6
58	2O	202	PEE	C40-C41-C42-C43
59	4E	201	CDL	C72-C73-C74-C75
59	3E	201	CDL	C16-C17-C18-C19
60	3A	501	PC1	C11-C12-N-C15
60	4F	201	PC1	C11-C12-N-C15
60	2T	101	PC1	C3C-C3D-C3E-C3F
59	3H	404	CDL	OB9-CB7-OB8-CB6
59	2q	101	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
58	2P	202	PEE	C38-C39-C40-C41
58	41	303	PEE	C36-C37-C38-C39
58	4W	201	PEE	C18-C19-C20-C21
58	4W	201	PEE	C38-C39-C40-C41
58	4s	101	PEE	C38-C39-C40-C41
59	3I	203	CDL	C71-CB7-OB8-CB6
59	4f	201	CDL	C31-CA7-OA8-CA6
63	4C	101	LPP	C36-C37-C38-C39
60	2r	202	PC1	C23-C24-C25-C26
58	40	301	PEE	C1-C2-O2-C10
59	3G	404	CDL	CA6-CA4-OA6-CA5
59	4S	102	CDL	CB6-CB4-OB6-CB5
59	4e	202	CDL	CB3-CB4-OB6-CB5
60	2R	202	PC1	C1-C2-O21-C21
60	4F	201	PC1	C3-C2-O21-C21
60	2R	201	PC1	C3C-C3D-C3E-C3F
59	4F	202	CDL	OA9-CA7-OA8-CA6
59	4K	201	CDL	C81-C82-C83-C84
59	4L	201	CDL	C78-C79-C80-C81
58	2P	202	PEE	C36-C37-C38-C39
58	4W	201	PEE	C36-C37-C38-C39
52	2M	701	FAD	C4'-C5'-O5'-P
58	40	301	PEE	C2-C1-O3P-P
58	4R	201	PEE	C2-C1-O3P-P
59	2p	204	CDL	C1-CA2-OA2-PA1
59	3D	202	CDL	CA4-CA3-OA5-PA1
59	3E	201	CDL	C1-CA2-OA2-PA1
59	3E	201	CDL	C1-CB2-OB2-PB2
59	3I	201	CDL	C1-CB2-OB2-PB2
59	3I	201	CDL	CB4-CB3-OB5-PB2
59	3L	702	CDL	C1-CB2-OB2-PB2
59	3e	202	CDL	C1-CA2-OA2-PA1
59	3e	202	CDL	C1-CB2-OB2-PB2
59	3g	405	CDL	CB4-CB3-OB5-PB2
59	3g	406	CDL	C1-CA2-OA2-PA1
59	3i	202	CDL	CB4-CB3-OB5-PB2
59	3l	702	CDL	CA4-CA3-OA5-PA1
59	4O	501	CDL	CB4-CB3-OB5-PB2
59	4S	102	CDL	CB4-CB3-OB5-PB2
59	4j	301	CDL	CA4-CA3-OA5-PA1
59	4o	501	CDL	CB4-CB3-OB5-PB2
59	4z	303	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
60	2R	202	PC1	C2-C1-O11-P
59	3L	702	CDL	C78-C79-C80-C81
59	4J	301	CDL	C79-C80-C81-C82
59	4O	501	CDL	C53-C54-C55-C56
58	41	302	PEE	O5-C30-O3-C3
59	2q	101	CDL	OB5-CB3-CB4-OB6
59	3e	202	CDL	OA5-CA3-CA4-OA6
59	3l	702	CDL	OB5-CB3-CB4-OB6
59	4F	202	CDL	OB5-CB3-CB4-OB6
59	4f	201	CDL	OB5-CB3-CB4-OB6
59	4j	302	CDL	OA5-CA3-CA4-OA6
59	3h	403	CDL	C19-C20-C21-C22
59	4L	201	CDL	OB7-CB5-OB6-CB4
59	4z	304	CDL	CB7-C71-C72-C73
60	2R	202	PC1	C35-C36-C37-C38
59	3l	701	CDL	C51-CB5-OB6-CB4
58	2T	103	PEE	C38-C39-C40-C41
58	3H	403	PEE	C38-C39-C40-C41
58	40	302	PEE	C38-C39-C40-C41
58	40	303	PEE	C16-C17-C18-C19
58	4q	902	PEE	C38-C39-C40-C41
58	4s	101	PEE	C18-C19-C20-C21
58	2O	201	PEE	O2-C2-C3-O3
59	4g	202	CDL	OA6-CA4-CA6-OA8
58	2O	202	PEE	C1-O3P-P-O4P
58	2P	202	PEE	C4-O4P-P-O3P
58	2o	203	PEE	C4-O4P-P-O3P
58	3C	301	PEE	C4-O4P-P-O3P
58	40	304	PEE	C4-O4P-P-O3P
58	41	303	PEE	C4-O4P-P-O3P
58	4q	902	PEE	C1-O3P-P-O4P
59	2P	203	CDL	CB2-OB2-PB2-OB5
59	2T	104	CDL	CA2-OA2-PA1-OA5
59	2p	204	CDL	CB2-OB2-PB2-OB5
59	2t	102	CDL	CA2-OA2-PA1-OA5
59	3D	202	CDL	CA2-OA2-PA1-OA5
59	3E	201	CDL	CB3-OB5-PB2-OB2
59	3G	403	CDL	CB3-OB5-PB2-OB2
59	3G	404	CDL	CB2-OB2-PB2-OB5
59	3I	201	CDL	CB2-OB2-PB2-OB5
59	3L	701	CDL	CA3-OA5-PA1-OA2
59	3L	703	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
59	3L	703	CDL	CB2-OB2-PB2-OB5
59	3e	201	CDL	CA2-OA2-PA1-OA5
59	3e	202	CDL	CA3-OA5-PA1-OA2
59	3g	403	CDL	CB3-OB5-PB2-OB2
59	3i	201	CDL	CB3-OB5-PB2-OB2
59	3l	701	CDL	CB2-OB2-PB2-OB5
59	4E	201	CDL	CA2-OA2-PA1-OA5
59	4E	202	CDL	CB3-OB5-PB2-OB2
59	4K	201	CDL	CB3-OB5-PB2-OB2
59	4Q	903	CDL	CA2-OA2-PA1-OA5
59	4Q	903	CDL	CB2-OB2-PB2-OB5
59	4W	202	CDL	CA2-OA2-PA1-OA5
59	4W	202	CDL	CB2-OB2-PB2-OB5
59	4e	203	CDL	CA2-OA2-PA1-OA5
59	4g	202	CDL	CA2-OA2-PA1-OA5
59	4g	202	CDL	CB2-OB2-PB2-OB5
59	4j	302	CDL	CB3-OB5-PB2-OB2
59	4q	903	CDL	CB3-OB5-PB2-OB2
59	4z	303	CDL	CA2-OA2-PA1-OA5
59	4z	303	CDL	CB2-OB2-PB2-OB5
60	2R	201	PC1	C11-O13-P-O11
60	2R	202	PC1	C11-O13-P-O11
60	2r	201	PC1	C11-O13-P-O11
60	2r	202	PC1	C11-O13-P-O11
60	3H	402	PC1	C11-O13-P-O11
60	4F	201	PC1	C1-O11-P-O13
60	4e	201	PC1	C1-O11-P-O13
59	4U	501	CDL	CA5-C11-C12-C13
52	2m	701	FAD	O4B-C4B-C5B-O5B
59	3l	701	CDL	C34-C35-C36-C37
59	3l	701	CDL	C71-C72-C73-C74
59	3L	703	CDL	C56-C57-C58-C59
59	4E	201	CDL	CA3-CA4-CA6-OA8
61	3c	302	HEC	C2B-C3B-CAB-CBB
58	3f	102	PEE	C36-C37-C38-C39
58	40	302	PEE	C36-C37-C38-C39
58	4q	902	PEE	C36-C37-C38-C39
59	2Q	101	CDL	OB9-CB7-OB8-CB6
59	2q	101	CDL	C12-C13-C14-C15
59	4f	201	CDL	C55-C56-C57-C58
59	3i	201	CDL	C32-C31-CA7-OA8
59	3L	703	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
59	4L	201	CDL	C51-CB5-OB6-CB4
59	3i	201	CDL	C32-C31-CA7-OA9
53	2N	301	UQ1	C4-C3-O3-CM3
59	3D	201	CDL	C12-C11-CA5-OA7
59	3g	406	CDL	C32-C31-CA7-OA9
58	41	301	PEE	C12-C13-C14-C15
58	2t	101	PEE	C32-C33-C34-C35
58	3f	102	PEE	C31-C30-O3-C3
52	2m	701	FAD	C4'-C5'-O5'-P
58	2p	203	PEE	C2-C1-O3P-P
59	3I	202	CDL	C1-CA2-OA2-PA1
59	3L	702	CDL	CA4-CA3-OA5-PA1
59	3g	403	CDL	CB4-CB3-OB5-PB2
59	4Q	903	CDL	CB4-CB3-OB5-PB2
59	4U	501	CDL	C1-CB2-OB2-PB2
59	4W	202	CDL	CB4-CB3-OB5-PB2
59	4t	201	CDL	C1-CB2-OB2-PB2
59	4z	304	CDL	CB4-CB3-OB5-PB2
60	2T	101	PC1	C2-C1-O11-P
60	3A	501	PC1	C2-C1-O11-P
58	2O	202	PEE	C36-C37-C38-C39
58	41	303	PEE	C38-C39-C40-C41
58	4R	201	PEE	C38-C39-C40-C41
58	4Z	302	PEE	C16-C17-C18-C19
58	4q	901	PEE	C36-C37-C38-C39
58	4w	201	PEE	C18-C19-C20-C21
59	3H	405	CDL	CB2-C1-CA2-OA2
59	2T	104	CDL	OA7-CA5-OA6-CA4
59	3I	203	CDL	C73-C74-C75-C76
59	3L	702	CDL	C71-CB7-OB8-CB6
60	2R	202	PC1	C32-C31-O31-C3
60	2r	202	PC1	C32-C31-O31-C3
52	2m	701	FAD	O3'-C3'-C4'-O4'
59	3I	203	CDL	OB9-CB7-OB8-CB6
59	4z	304	CDL	C54-C55-C56-C57
52	2m	701	FAD	C2'-C3'-C4'-C5'
58	40	301	PEE	C31-C32-C33-C34
59	2P	203	CDL	OB9-CB7-OB8-CB6
58	4w	201	PEE	C16-C17-C18-C19
67	4Q	908	HEA	CAD-CBD-CGD-O1D
67	4q	908	HEA	CAD-CBD-CGD-O1D
59	4O	501	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
59	2q	101	CDL	C17-C18-C19-C20
60	3a	501	PC1	C22-C23-C24-C25
58	4q	902	PEE	O3P-C1-C2-O2
58	4w	201	PEE	O3P-C1-C2-O2
59	4m	201	CDL	OB5-CB3-CB4-OB6
59	3E	201	CDL	C40-C41-C42-C43
59	4Q	902	CDL	OB9-CB7-OB8-CB6
59	4S	102	CDL	C22-C23-C24-C25
67	4Q	907	HEA	CAA-CBA-CGA-O1A
59	2t	102	CDL	C33-C34-C35-C36
59	4f	201	CDL	OA9-CA7-OA8-CA6
58	41	301	PEE	C38-C39-C40-C41
59	4m	201	CDL	O1-C1-CB2-OB2
59	4o	501	CDL	O1-C1-CA2-OA2
67	4q	907	HEA	CAA-CBA-CGA-O1A
59	2p	204	CDL	OB6-CB4-CB6-OB8
59	3L	701	CDL	OB6-CB4-CB6-OB8
59	3L	701	CDL	C1-CB2-OB2-PB2
59	3e	201	CDL	CB4-CB3-OB5-PB2
59	3l	702	CDL	C1-CB2-OB2-PB2
59	4O	501	CDL	C1-CA2-OA2-PA1
59	4j	301	CDL	C1-CA2-OA2-PA1
59	4j	302	CDL	CB4-CB3-OB5-PB2
59	4o	501	CDL	C32-C31-CA7-OA9
60	3a	501	PC1	C11-C12-N-C14
58	4W	201	PEE	C16-C17-C18-C19
58	4s	101	PEE	C36-C37-C38-C39
58	4w	201	PEE	C36-C37-C38-C39
59	2q	101	CDL	OA7-CA5-OA6-CA4
59	4W	202	CDL	OB7-CB5-OB6-CB4
59	3g	403	CDL	C53-C54-C55-C56
60	4F	201	PC1	C33-C34-C35-C36
61	3c	302	HEC	C4B-C3B-CAB-CBB
59	3i	201	CDL	C51-C52-C53-C54
59	4F	202	CDL	C52-C53-C54-C55
59	4z	303	CDL	C76-C77-C78-C79
52	2M	701	FAD	O4B-C4B-C5B-O5B
59	3E	201	CDL	C52-C53-C54-C55
59	3H	404	CDL	CA2-C1-CB2-OB2
59	3g	403	CDL	CB3-CB4-CB6-OB8
59	3l	702	CDL	CA2-C1-CB2-OB2
59	4m	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
59	4o	501	CDL	CB2-C1-CA2-OA2
63	4C	101	LPP	C6-C7-C8-O27
59	3g	403	CDL	OB7-CB5-OB6-CB4
59	3L	703	CDL	C52-C53-C54-C55
59	3H	404	CDL	C19-C20-C21-C22
61	3C	302	HEC	CAD-CBD-CGD-O1D
62	3G	406	HEM	CAA-CBA-CGA-O2A
62	3g	408	HEM	CAA-CBA-CGA-O2A
58	40	303	PEE	O5-C30-O3-C3
59	3E	201	CDL	C14-C15-C16-C17
62	3g	407	HEM	CAA-CBA-CGA-O2A
67	4Q	907	HEA	CAA-CBA-CGA-O2A
67	4q	907	HEA	CAA-CBA-CGA-O2A
59	3g	404	CDL	CA6-CA4-OA6-CA5
59	4E	202	CDL	CB6-CB4-OB6-CB5
59	4s	102	CDL	CB6-CB4-OB6-CB5
60	2R	202	PC1	C3-C2-O21-C21
59	4s	102	CDL	C12-C13-C14-C15
60	2T	101	PC1	C3B-C3C-C3D-C3E
58	4D	101	PEE	C16-C17-C18-C19
58	4l	201	PEE	C16-C17-C18-C19
58	4w	201	PEE	C38-C39-C40-C41
62	3G	406	HEM	CAA-CBA-CGA-O1A
62	3g	408	HEM	CAA-CBA-CGA-O1A
58	40	303	PEE	C1-O3P-P-O4P
59	4t	201	CDL	OA9-CA7-OA8-CA6
59	3e	202	CDL	C17-C18-C19-C20
59	4e	203	CDL	C75-C76-C77-C78
59	3L	701	CDL	C1-CA2-OA2-PA1
59	4Q	903	CDL	CA4-CA3-OA5-PA1
58	40	303	PEE	O3P-C1-C2-O2
59	2t	102	CDL	OA5-CA3-CA4-OA6
60	4F	201	PC1	C3A-C3B-C3C-C3D
59	4O	501	CDL	OA5-CA3-CA4-CA6
58	2P	202	PEE	C18-C19-C20-C21
58	3c	301	PEE	C16-C17-C18-C19
58	40	302	PEE	C18-C19-C20-C21
58	4R	201	PEE	C36-C37-C38-C39
58	4d	101	PEE	C16-C17-C18-C19
58	2O	202	PEE	C31-C32-C33-C34
62	3g	408	HEM	CAD-CBD-CGD-O2D
60	2R	201	PC1	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
62	3G	406	HEM	CAD-CBD-CGD-O2D
67	4Q	908	HEA	CAD-CBD-CGD-O2D
67	4q	908	HEA	CAD-CBD-CGD-O2D
59	3L	703	CDL	C36-C37-C38-C39
58	4l	201	PEE	O4-C10-O2-C2
59	3e	202	CDL	OA7-CA5-OA6-CA4
59	4Z	303	CDL	OB7-CB5-OB6-CB4
59	3l	701	CDL	C33-C34-C35-C36
58	4Q	901	PEE	O2-C2-C3-O3
63	4C	101	LPP	O9-C7-C8-O27
58	4R	201	PEE	C31-C30-O3-C3
59	41	304	CDL	C71-CB7-OB8-CB6
62	3g	407	HEM	CAA-CBA-CGA-O1A
59	4g	202	CDL	C51-CB5-OB6-CB4
59	2q	101	CDL	C80-C81-C82-C83
59	3E	201	CDL	C74-C75-C76-C77
60	3a	501	PC1	C29-C2A-C2B-C2C
59	3L	702	CDL	CA2-C1-CB2-OB2
59	3e	201	CDL	CA2-C1-CB2-OB2
59	3g	406	CDL	CB2-C1-CA2-OA2
59	4O	501	CDL	CB2-C1-CA2-OA2
62	3G	405	HEM	CAA-CBA-CGA-O1A
62	3G	406	HEM	CAD-CBD-CGD-O1D
67	4q	908	HEA	C1A-C2A-CAA-CBA
67	4Q	908	HEA	C26-C15-C16-C17
67	4q	908	HEA	C26-C15-C16-C17
59	3L	701	CDL	C32-C31-CA7-OA9
59	3G	403	CDL	C72-C73-C74-C75
59	4F	202	CDL	C36-C37-C38-C39
59	4O	501	CDL	C31-C32-C33-C34
62	3G	405	HEM	CAA-CBA-CGA-O2A
62	3g	408	HEM	CAD-CBD-CGD-O1D
59	4Q	902	CDL	C52-C51-CB5-OB7
59	3g	405	CDL	OB9-CB7-OB8-CB6
59	41	304	CDL	C19-C20-C21-C22
59	4q	903	CDL	C76-C77-C78-C79
60	4F	201	PC1	C39-C3A-C3B-C3C
61	3C	302	HEC	CAD-CBD-CGD-O2D
59	2P	203	CDL	C55-C56-C57-C58
59	4Z	303	CDL	CB4-CB3-OB5-PB2
63	4z	301	LPP	C12-C11-O9-C7
59	3H	405	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
59	3I	201	CDL	C52-C53-C54-C55
61	3C	302	HEC	CAA-CBA-CGA-O2A
59	4f	201	CDL	C16-C17-C18-C19
59	3I	203	CDL	C76-C77-C78-C79
62	3G	405	HEM	C3D-CAD-CBD-CGD
62	3g	407	HEM	C3D-CAD-CBD-CGD
67	4Q	908	HEA	C1A-C2A-CAA-CBA
59	2Q	101	CDL	OA9-CA7-OA8-CA6
58	41	303	PEE	C32-C33-C34-C35
59	2q	101	CDL	C55-C56-C57-C58
58	41	302	PEE	C36-C37-C38-C39
58	4d	101	PEE	C38-C39-C40-C41
58	4z	302	PEE	C18-C19-C20-C21
58	4W	201	PEE	O3P-C1-C2-O2
58	40	301	PEE	C2-C3-O3-C30
60	2R	202	PC1	O32-C31-O31-C3
59	2q	101	CDL	C18-C19-C20-C21
60	3H	401	PC1	O11-C1-C2-C3
60	3h	401	PC1	O11-C1-C2-C3
59	2T	104	CDL	C31-C32-C33-C34
59	4z	303	CDL	C71-CB7-OB8-CB6
58	3c	301	PEE	O4P-C4-C5-N
58	2t	101	PEE	C38-C39-C40-C41
59	3G	403	CDL	C31-C32-C33-C34
59	3L	701	CDL	C52-C51-CB5-OB6
59	4L	201	CDL	C64-C65-C66-C67
59	2t	102	CDL	CA4-CA3-OA5-PA1
59	4e	202	CDL	CA4-CA3-OA5-PA1
59	3e	202	CDL	CA2-C1-CB2-OB2
59	4g	202	CDL	CA2-C1-CB2-OB2
59	3i	201	CDL	OB7-CB5-OB6-CB4
59	3l	701	CDL	C71-CB7-OB8-CB6
59	4e	203	CDL	C79-C80-C81-C82
60	2p	202	PC1	C22-C21-O21-C2
62	3g	407	HEM	CAD-CBD-CGD-O2D
58	2O	201	PEE	C36-C37-C38-C39
58	2r	203	PEE	C38-C39-C40-C41
58	3f	102	PEE	C38-C39-C40-C41
58	4Z	302	PEE	C38-C39-C40-C41
59	3L	702	CDL	C51-C52-C53-C54
59	4M	201	CDL	C55-C56-C57-C58
63	4C	101	LPP	C6-O5-P1-O2

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Mol	Chain	Res	Type	Atoms
63	4g	201	LPP	C6-O5-P1-O2
58	2O	201	PEE	C2-C3-O3-C30
59	3L	703	CDL	C13-C14-C15-C16
63	4z	301	LPP	C14-C15-C16-C17
60	2T	102	PC1	C11-O13-P-O11
60	3f	101	PC1	C11-O13-P-O11
60	3A	501	PC1	C11-C12-N-C14
60	3a	501	PC1	C11-C12-N-C13
59	4M	201	CDL	C12-C11-CA5-OA7
59	4Q	903	CDL	C71-CB7-OB8-CB6
59	4f	201	CDL	C54-C55-C56-C57
58	41	301	PEE	C35-C36-C37-C38
62	3G	405	HEM	CAD-CBD-CGD-O2D
59	3g	406	CDL	O1-C1-CA2-OA2
60	2R	201	PC1	O21-C21-C22-C23
58	2r	203	PEE	C36-C37-C38-C39
58	2t	101	PEE	C36-C37-C38-C39
58	3H	403	PEE	C36-C37-C38-C39
58	40	301	PEE	C38-C39-C40-C41
58	41	301	PEE	C16-C17-C18-C19
58	41	302	PEE	C18-C19-C20-C21
58	41	302	PEE	C38-C39-C40-C41
58	4d	101	PEE	C18-C19-C20-C21
58	4l	201	PEE	C36-C37-C38-C39
58	4s	101	PEE	C16-C17-C18-C19
58	3f	102	PEE	C3-C2-O2-C10
59	3L	703	CDL	OB7-CB5-OB6-CB4
59	3l	701	CDL	OB7-CB5-OB6-CB4
59	2q	101	CDL	C76-C77-C78-C79
59	3H	404	CDL	C37-C38-C39-C40
58	4Q	901	PEE	O3-C30-C31-C32
59	4L	201	CDL	C58-C59-C60-C61
59	4Q	902	CDL	C19-C20-C21-C22
60	4F	201	PC1	C28-C29-C2A-C2B
61	3c	302	HEC	CAD-CBD-CGD-O1D
63	4C	101	LPP	C30-C31-C32-C33
53	3g	401	UQ1	C4-C3-O3-CM3
58	2O	201	PEE	C38-C39-C40-C41
58	2T	103	PEE	C36-C37-C38-C39
58	3H	403	PEE	C16-C17-C18-C19
58	40	301	PEE	C16-C17-C18-C19
58	4Q	901	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
59	4S	102	CDL	C53-C54-C55-C56
59	2Q	101	CDL	CA3-CA4-CA6-OA8
67	4Q	907	HEA	C12-C11-C3B-C2B
67	4q	907	HEA	C12-C11-C3B-C2B
59	4Q	902	CDL	C51-C52-C53-C54
59	3G	404	CDL	OB5-CB3-CB4-OB6
59	4S	102	CDL	C12-C13-C14-C15
67	4Q	908	HEA	C4D-C3D-CAD-CBD
67	4q	908	HEA	C4D-C3D-CAD-CBD
58	41	303	PEE	C34-C35-C36-C37
58	4z	302	PEE	C34-C35-C36-C37
62	3G	406	HEM	C4C-C3C-CAC-CBC
62	3g	408	HEM	C4C-C3C-CAC-CBC
59	4j	302	CDL	C31-CA7-OA8-CA6
59	3G	404	CDL	C32-C31-CA7-OA8
62	3G	405	HEM	CAD-CBD-CGD-O1D
62	3g	407	HEM	CAD-CBD-CGD-O1D
59	2q	101	CDL	C54-C55-C56-C57
59	3H	405	CDL	C11-C12-C13-C14
58	4D	101	PEE	C18-C19-C20-C21
58	4z	302	PEE	C16-C17-C18-C19
59	3L	702	CDL	OB9-CB7-OB8-CB6
60	3H	402	PC1	O21-C21-C22-C23
59	2Q	101	CDL	C55-C56-C57-C58
58	40	303	PEE	O3P-C1-C2-C3
58	4R	201	PEE	O3P-C1-C2-C3
58	4l	201	PEE	O3P-C1-C2-C3
59	2T	104	CDL	OA5-CA3-CA4-CA6
59	3l	702	CDL	OA5-CA3-CA4-CA6
59	4F	202	CDL	OA5-CA3-CA4-CA6
59	4K	201	CDL	C15-C16-C17-C18
58	40	304	PEE	O2-C10-C11-C12
59	3g	403	CDL	C12-C11-CA5-OA6
59	3i	202	CDL	C32-C31-CA7-OA8
59	41	304	CDL	C12-C11-CA5-OA6
59	4O	501	CDL	C52-C51-CB5-OB6
59	4e	203	CDL	C52-C51-CB5-OB6
58	2p	203	PEE	O2-C2-C3-O3
58	3C	301	PEE	O2-C2-C3-O3
59	2Q	101	CDL	OA6-CA4-CA6-OA8
59	3H	405	CDL	OB6-CB4-CB6-OB8
59	4E	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
58	4Z	302	PEE	C10-C11-C12-C13
60	2r	202	PC1	O32-C31-O31-C3
59	4m	201	CDL	OA7-CA5-OA6-CA4
58	4l	201	PEE	C11-C12-C13-C14
58	4z	302	PEE	C11-C12-C13-C14
58	2p	203	PEE	O2-C10-C11-C12
58	41	303	PEE	O2-C10-C11-C12
59	3I	201	CDL	C32-C31-CA7-OA8
59	3I	202	CDL	C32-C31-CA7-OA8
59	3g	403	CDL	C52-C51-CB5-OB6
59	4F	202	CDL	C12-C11-CA5-OA6
59	4K	201	CDL	C12-C11-CA5-OA6
59	4z	304	CDL	C72-C71-CB7-OB8
59	2q	101	CDL	C63-C64-C65-C66
60	3A	501	PC1	C11-C12-N-C13
59	3l	701	CDL	C31-CA7-OA8-CA6
58	41	302	PEE	C11-C10-O2-C2
58	4q	901	PEE	C11-C10-O2-C2
59	2O	203	CDL	C72-C71-CB7-OB8
59	2Q	101	CDL	C72-C71-CB7-OB8
59	3E	201	CDL	C52-C51-CB5-OB6
59	4Z	303	CDL	C32-C31-CA7-OA8
58	41	301	PEE	C14-C15-C16-C17
59	4F	202	CDL	C76-C77-C78-C79
58	4q	901	PEE	O4-C10-O2-C2
59	4g	202	CDL	OB7-CB5-OB6-CB4
58	2O	202	PEE	C38-C39-C40-C41
58	4d	101	PEE	C36-C37-C38-C39
59	2q	101	CDL	C72-C71-CB7-OB8
59	3E	201	CDL	C12-C11-CA5-OA6
59	4E	201	CDL	C52-C51-CB5-OB6
59	4o	501	CDL	C52-C51-CB5-OB6
59	4O	501	CDL	C15-C16-C17-C18
63	4C	101	LPP	C11-C12-C13-C14
59	3E	201	CDL	C72-C71-CB7-OB8
59	3e	202	CDL	C12-C11-CA5-OA6
59	3g	404	CDL	C32-C31-CA7-OA8
59	4f	201	CDL	C12-C11-CA5-OA6
59	4g	202	CDL	C32-C31-CA7-OA8
59	4j	302	CDL	OA9-CA7-OA8-CA6
59	4Q	903	CDL	C51-CB5-OB6-CB4
59	4m	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
59	3L	703	CDL	C39-C40-C41-C42
60	2o	202	PC1	C32-C33-C34-C35
58	4Z	302	PEE	C18-C19-C20-C21
58	4l	201	PEE	C31-C32-C33-C34
60	4e	201	PC1	C28-C29-C2A-C2B
59	3g	405	CDL	C71-C72-C73-C74
60	3a	501	PC1	C2B-C2C-C2D-C2E
67	4Q	908	HEA	C14-C15-C16-C17
59	4Z	303	CDL	C72-C71-CB7-OB8
59	4z	304	CDL	C12-C11-CA5-OA6
59	4o	501	CDL	C76-C77-C78-C79
59	3L	701	CDL	C72-C71-CB7-OB9
59	3D	202	CDL	C51-C52-C53-C54
59	3I	203	CDL	CB2-C1-CA2-OA2
59	4L	201	CDL	C84-C85-C86-C87
59	3g	403	CDL	C12-C11-CA5-OA7
58	2p	203	PEE	C1-C2-C3-O3
58	4Z	302	PEE	O3-C30-C31-C32
58	4q	901	PEE	O3-C30-C31-C32
59	2O	203	CDL	C32-C31-CA7-OA8
59	4U	501	CDL	C52-C51-CB5-OB6
59	3L	703	CDL	C38-C39-C40-C41
59	4f	201	CDL	C71-C72-C73-C74
58	4q	901	PEE	O5-C30-C31-C32
59	2Q	101	CDL	C72-C71-CB7-OB9
60	2R	201	PC1	O22-C21-C22-C23
59	2o	201	CDL	C52-C51-CB5-OB6
59	3g	406	CDL	C52-C51-CB5-OB6
59	3i	202	CDL	C52-C51-CB5-OB6
59	4S	102	CDL	C52-C51-CB5-OB6
59	4W	202	CDL	C32-C31-CA7-OA8
60	2T	101	PC1	O21-C21-C22-C23
60	3a	501	PC1	O21-C21-C22-C23
60	3a	501	PC1	O22-C21-C22-C23
67	4q	908	HEA	C14-C15-C16-C17
59	4o	501	CDL	C62-C63-C64-C65
59	3l	702	CDL	C35-C36-C37-C38
53	2p	201	UQ1	C6-C7-C8-C9
53	3G	401	UQ1	C6-C7-C8-C9
53	3G	402	UQ1	C6-C7-C8-C9
53	3g	401	UQ1	C6-C7-C8-C9
53	3g	402	UQ1	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
58	2T	103	PEE	C4-O4P-P-O1P
58	41	301	PEE	C1-O3P-P-O1P
58	4D	101	PEE	C1-O3P-P-O1P
59	2P	203	CDL	CA3-OA5-PA1-OA4
59	2T	104	CDL	CA3-OA5-PA1-OA3
59	2p	204	CDL	CB2-OB2-PB2-OB3
59	3D	201	CDL	CA2-OA2-PA1-OA3
59	3H	405	CDL	CA2-OA2-PA1-OA3
59	3H	405	CDL	CB2-OB2-PB2-OB3
59	3I	203	CDL	CA2-OA2-PA1-OA3
59	3I	203	CDL	CB2-OB2-PB2-OB3
59	3L	703	CDL	CB2-OB2-PB2-OB3
59	3e	202	CDL	CB3-OB5-PB2-OB3
59	3g	405	CDL	CA2-OA2-PA1-OA3
59	3g	406	CDL	CB2-OB2-PB2-OB4
59	3i	201	CDL	CB3-OB5-PB2-OB3
59	3i	202	CDL	CB2-OB2-PB2-OB4
59	3l	701	CDL	CB2-OB2-PB2-OB3
59	4E	201	CDL	CA2-OA2-PA1-OA3
59	4F	202	CDL	CA3-OA5-PA1-OA3
59	4Q	902	CDL	CB2-OB2-PB2-OB4
59	4Q	903	CDL	CA2-OA2-PA1-OA3
59	4S	102	CDL	CA3-OA5-PA1-OA4
59	4W	202	CDL	CA2-OA2-PA1-OA3
59	4Z	303	CDL	CA2-OA2-PA1-OA3
59	4e	202	CDL	CA3-OA5-PA1-OA3
59	4e	203	CDL	CA2-OA2-PA1-OA3
59	4f	201	CDL	CA3-OA5-PA1-OA3
59	4j	301	CDL	CA2-OA2-PA1-OA4
59	4j	301	CDL	CB2-OB2-PB2-OB3
59	4j	302	CDL	CB3-OB5-PB2-OB3
59	4q	903	CDL	CB2-OB2-PB2-OB3
59	4q	903	CDL	CB2-OB2-PB2-OB4
59	4s	102	CDL	CA3-OA5-PA1-OA4
59	4t	201	CDL	CB2-OB2-PB2-OB3
59	4z	303	CDL	CA2-OA2-PA1-OA3
59	4z	304	CDL	CA2-OA2-PA1-OA3
60	2R	202	PC1	C11-O13-P-O14
60	2r	201	PC1	C1-O11-P-O14
60	2r	202	PC1	C11-O13-P-O14
59	3I	202	CDL	C34-C35-C36-C37
59	4e	203	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
58	4Q	901	PEE	O5-C30-C31-C32
59	3I	202	CDL	C32-C31-CA7-OA9
59	4z	304	CDL	C72-C71-CB7-OB9
60	2o	202	PC1	C2-C3-O31-C31
59	4Q	902	CDL	C32-C31-CA7-OA8
58	41	302	PEE	O3P-C1-C2-C3
58	4d	101	PEE	O4P-C4-C5-N
58	4q	901	PEE	O4P-C4-C5-N
59	3i	202	CDL	C32-C31-CA7-OA9
63	4Z	301	LPP	C32-C33-C34-C35
58	40	303	PEE	O2-C10-C11-C12
59	4q	903	CDL	C32-C31-CA7-OA8
59	2O	203	CDL	C32-C33-C34-C35
60	2p	202	PC1	O22-C21-O21-C2
63	4z	301	LPP	O10-C11-O9-C7
59	4L	201	CDL	C71-C72-C73-C74
59	2q	101	CDL	C72-C71-CB7-OB9
59	4S	102	CDL	C72-C73-C74-C75
58	2p	203	PEE	O4-C10-C11-C12
60	3h	401	PC1	O32-C31-C32-C33
58	40	303	PEE	C11-C10-O2-C2
58	3H	403	PEE	C3-C2-O2-C10
58	3f	102	PEE	C1-C2-O2-C10
59	3g	403	CDL	CA3-CA4-OA6-CA5
59	4E	202	CDL	CA3-CA4-OA6-CA5
59	4q	903	CDL	CA3-CA4-OA6-CA5
58	4R	201	PEE	O5-C30-O3-C3
59	3l	701	CDL	OB9-CB7-OB8-CB6
58	2P	202	PEE	O4-C10-C11-C12
59	3E	201	CDL	C72-C71-CB7-OB9
59	3G	404	CDL	C32-C31-CA7-OA9
59	3g	406	CDL	C52-C51-CB5-OB7
59	3h	403	CDL	C52-C51-CB5-OB7
59	3h	403	CDL	C72-C71-CB7-OB9
59	4J	301	CDL	C12-C11-CA5-OA7
59	4O	501	CDL	C52-C51-CB5-OB7
59	4W	202	CDL	C32-C31-CA7-OA9
59	4F	202	CDL	C16-C17-C18-C19
59	4s	102	CDL	C22-C23-C24-C25
58	41	301	PEE	O2-C10-C11-C12
59	3I	203	CDL	C52-C51-CB5-OB6
59	3h	403	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
59	4q	903	CDL	CB4-CB6-OB8-CB7
58	3f	102	PEE	O5-C30-O3-C3
59	2O	203	CDL	C32-C31-CA7-OA9
59	4g	202	CDL	C32-C31-CA7-OA9
60	3H	402	PC1	O32-C31-C32-C33
58	2P	202	PEE	O2-C10-C11-C12
59	3I	201	CDL	C52-C51-CB5-OB6
59	3e	201	CDL	C72-C71-CB7-OB8
59	3e	202	CDL	C72-C71-CB7-OB8
60	3H	401	PC1	O21-C21-C22-C23
60	3h	402	PC1	O21-C21-C22-C23
59	3D	202	CDL	C16-C17-C18-C19
59	4s	102	CDL	C53-C54-C55-C56
59	3l	701	CDL	C81-C82-C83-C84
59	4Z	303	CDL	C72-C71-CB7-OB9
59	4o	501	CDL	C52-C51-CB5-OB7
59	4z	303	CDL	CB4-CB6-OB8-CB7
58	4l	201	PEE	O3-C30-C31-C32
59	3H	404	CDL	C72-C71-CB7-OB8
59	3H	405	CDL	C52-C51-CB5-OB6
59	4W	202	CDL	C12-C11-CA5-OA6
60	3H	402	PC1	O31-C31-C32-C33
59	2q	101	CDL	CB2-C1-CA2-OA2
59	4W	202	CDL	CA2-C1-CB2-OB2
58	41	302	PEE	C13-C14-C15-C16
58	4D	101	PEE	C22-C23-C24-C25
59	4j	302	CDL	C78-C79-C80-C81
58	4Z	302	PEE	O5-C30-C31-C32
59	3E	201	CDL	C12-C11-CA5-OA7
59	3e	202	CDL	C72-C71-CB7-OB9
59	41	304	CDL	C12-C11-CA5-OA7
59	4E	201	CDL	C52-C51-CB5-OB7
59	4K	201	CDL	C12-C11-CA5-OA7
59	4f	201	CDL	C12-C11-CA5-OA7
59	4Q	903	CDL	OB7-CB5-OB6-CB4
59	2q	101	CDL	C39-C40-C41-C42
58	4Q	901	PEE	O3P-C1-C2-O2
59	3D	202	CDL	OB5-CB3-CB4-OB6
58	40	304	PEE	O4-C10-C11-C12
58	41	303	PEE	O4-C10-C11-C12
59	3E	201	CDL	C52-C51-CB5-OB7
59	4F	202	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
59	4W	202	CDL	C12-C11-CA5-OA7
59	4Z	303	CDL	C32-C31-CA7-OA9
59	4Z	303	CDL	C52-C51-CB5-OB7
59	2q	101	CDL	C72-C73-C74-C75
59	3D	201	CDL	C14-C15-C16-C17
59	4S	102	CDL	C19-C20-C21-C22
59	4z	303	CDL	C31-C32-C33-C34
58	41	302	PEE	O2-C10-C11-C12
58	4z	302	PEE	O3-C30-C31-C32
59	3H	404	CDL	C52-C51-CB5-OB6
59	4J	301	CDL	C72-C71-CB7-OB8
59	4Z	303	CDL	C52-C51-CB5-OB6
59	4t	201	CDL	C52-C51-CB5-OB6
60	3h	401	PC1	O31-C31-C32-C33
58	4q	901	PEE	C10-C11-C12-C13
59	4J	301	CDL	CA7-C31-C32-C33
58	4z	302	PEE	O5-C30-C31-C32
59	3H	404	CDL	C52-C51-CB5-OB7
59	3e	202	CDL	C12-C11-CA5-OA7
59	3g	403	CDL	C52-C51-CB5-OB7
59	3g	404	CDL	C32-C31-CA7-OA9
59	3i	202	CDL	C52-C51-CB5-OB7
59	4Q	903	CDL	CB4-CB6-OB8-CB7
59	4U	501	CDL	C52-C51-CB5-OB7
59	4m	201	CDL	C32-C31-CA7-OA9
59	4t	201	CDL	C52-C51-CB5-OB7
59	3h	403	CDL	C72-C71-CB7-OB8
58	41	302	PEE	O4-C10-C11-C12
59	2O	203	CDL	C72-C71-CB7-OB9
59	2o	201	CDL	C52-C51-CB5-OB7
59	3H	405	CDL	C52-C51-CB5-OB7
59	3I	201	CDL	C32-C31-CA7-OA9
59	4J	301	CDL	C72-C71-CB7-OB9
59	4Q	902	CDL	C32-C31-CA7-OA9
60	3h	402	PC1	O22-C21-C22-C23
59	4e	202	CDL	C31-CA7-OA8-CA6
59	4g	202	CDL	O1-C1-CB2-OB2
59	3l	701	CDL	C12-C11-CA5-OA6
59	4Q	902	CDL	C12-C11-CA5-OA6
58	40	303	PEE	O4-C10-C11-C12
59	4z	304	CDL	C12-C11-CA5-OA7
60	2T	101	PC1	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
60	2r	202	PC1	C28-C29-C2A-C2B
59	3e	201	CDL	C72-C71-CB7-OB9
59	4q	903	CDL	C32-C31-CA7-OA9
60	3H	401	PC1	O22-C21-C22-C23
60	3H	402	PC1	O22-C21-C22-C23
59	3l	701	CDL	C32-C33-C34-C35
59	2O	203	CDL	C52-C51-CB5-OB6
63	4z	301	LPP	O9-C11-C12-C13

There are no ring outliers.

63 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	4q	907	HEA	5	0
59	4f	201	CDL	4	0
54	3h	404	FES	1	0
59	4M	201	CDL	1	0
59	4L	201	CDL	1	0
53	2p	201	UQ1	1	0
58	4z	302	PEE	1	0
59	4m	201	CDL	3	0
60	4F	201	PC1	2	0
59	3i	202	CDL	2	0
58	4Z	302	PEE	2	0
60	2R	201	PC1	1	0
61	3C	302	HEC	4	0
59	2q	101	CDL	7	0
59	4Q	902	CDL	2	0
58	40	304	PEE	1	0
62	3g	407	HEM	7	0
59	3H	405	CDL	1	0
59	4t	201	CDL	1	0
59	3I	202	CDL	1	0
59	3e	202	CDL	2	0
60	3h	402	PC1	1	0
63	4C	101	LPP	1	0
60	2r	201	PC1	2	0
59	2p	204	CDL	1	0
67	4q	908	HEA	6	0
59	4z	303	CDL	1	0
59	4Z	303	CDL	1	0
54	3H	406	FES	1	0

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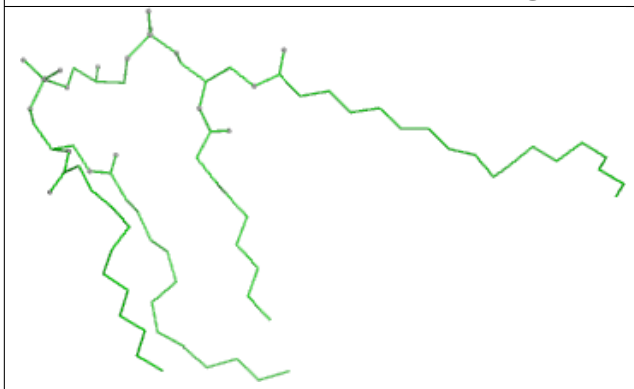
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	3c	301	PEE	1	0
58	41	301	PEE	1	0
59	2O	203	CDL	2	0
60	2T	102	PC1	3	0
58	41	303	PEE	1	0
59	4q	903	CDL	3	0
58	2O	202	PEE	1	0
53	3g	401	UQ1	4	0
53	3G	401	UQ1	5	0
59	4g	202	CDL	1	0
61	3c	302	HEC	6	0
59	3h	403	CDL	2	0
59	3g	404	CDL	1	0
59	2t	102	CDL	2	0
59	3g	403	CDL	2	0
59	4e	203	CDL	3	0
59	4e	202	CDL	2	0
59	4j	301	CDL	1	0
59	4j	302	CDL	1	0
59	4E	202	CDL	2	0
58	4l	201	PEE	2	0
59	3L	703	CDL	5	0
59	3i	201	CDL	1	0
59	4K	201	CDL	1	0
60	3f	101	PC1	1	0
58	2O	201	PEE	1	0
59	3l	701	CDL	7	0
58	2T	103	PEE	1	0
67	4Q	907	HEA	4	0
59	4o	501	CDL	4	0
59	3H	404	CDL	1	0
59	3e	201	CDL	3	0
67	4Q	908	HEA	5	0
62	3G	405	HEM	4	0

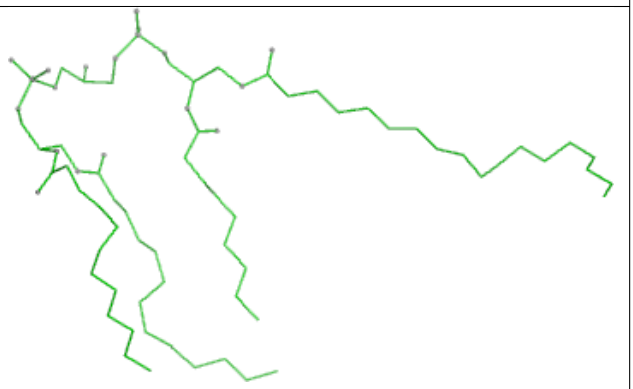
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

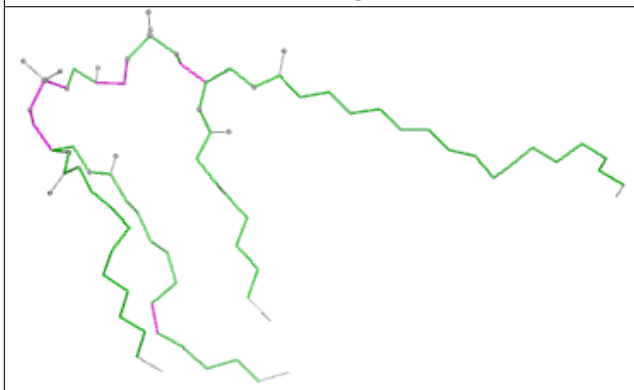
Ligand CDL 3l 702



Bond lengths



Bond angles

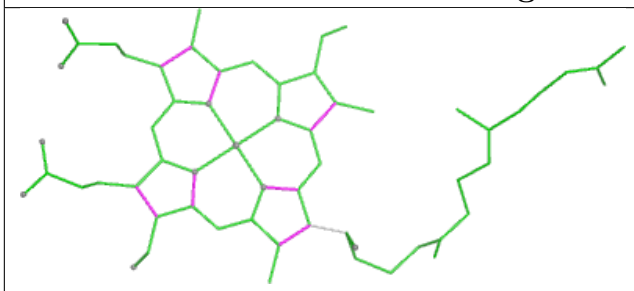


Torsions

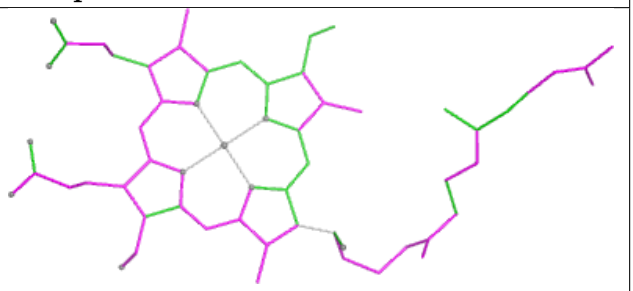


Rings

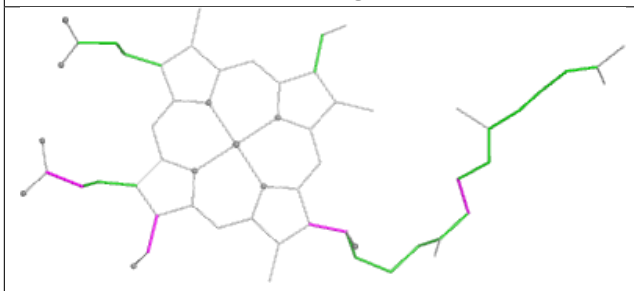
Ligand HEA 4q 907



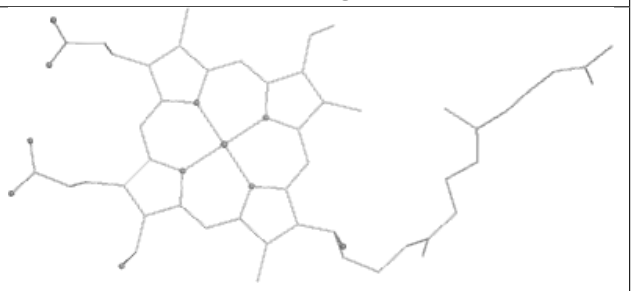
Bond lengths



Bond angles

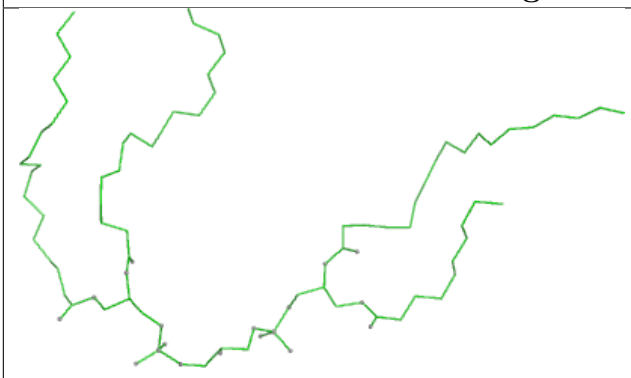


Torsions



Rings

Ligand CDL 4f 201



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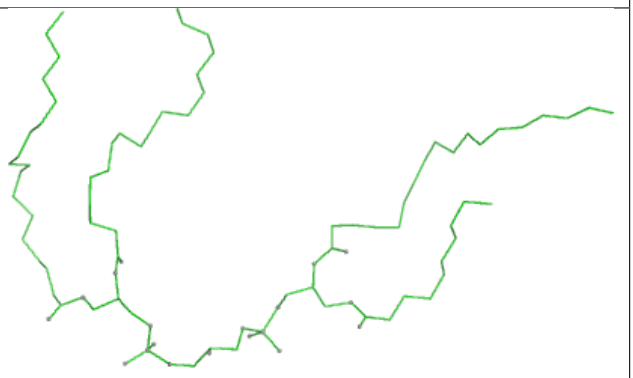
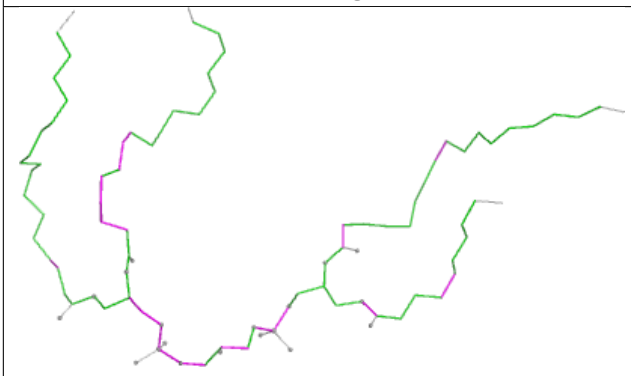


Bond angles

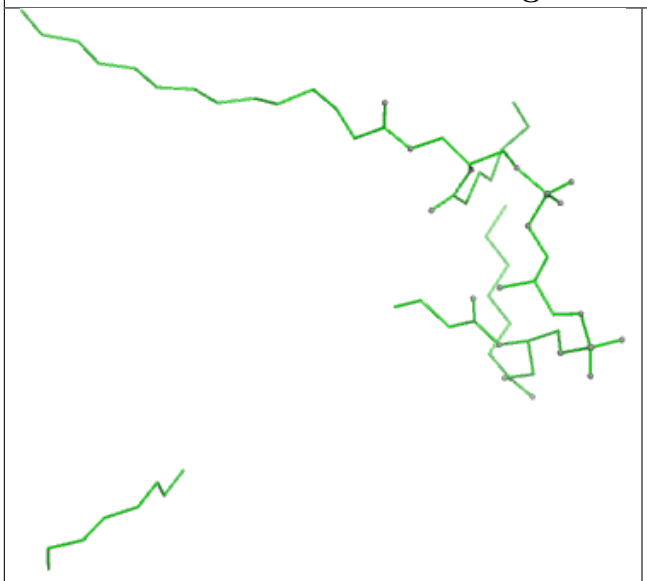


Torsions



Rings

Ligand CDL 3I 201



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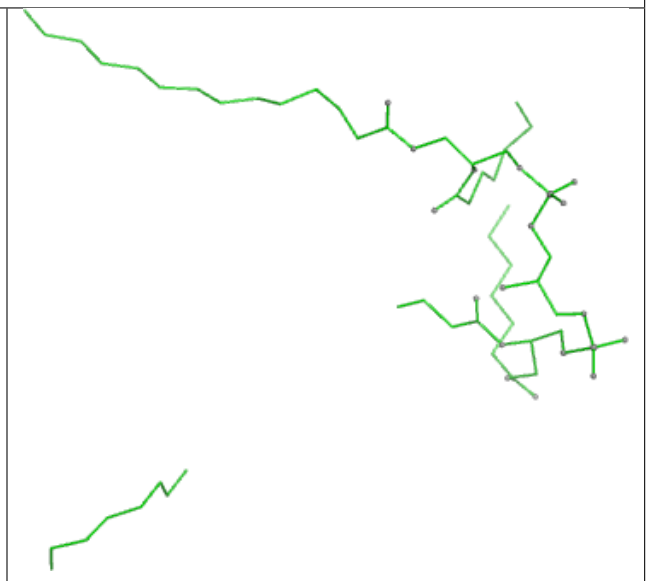
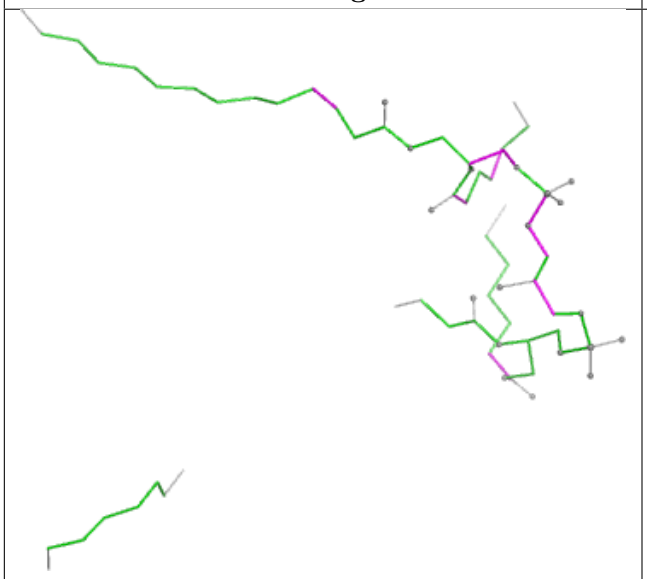


Bond angles



Torsions



Rings

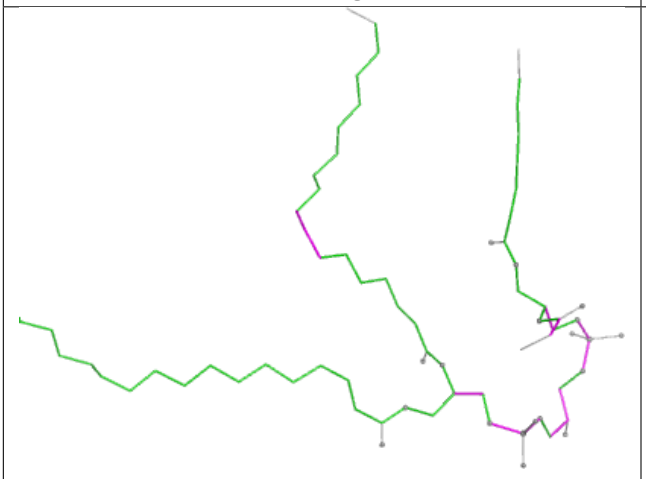
Ligand CDL 4M 201



Bond lengths



Bond angles



Torsions



Rings

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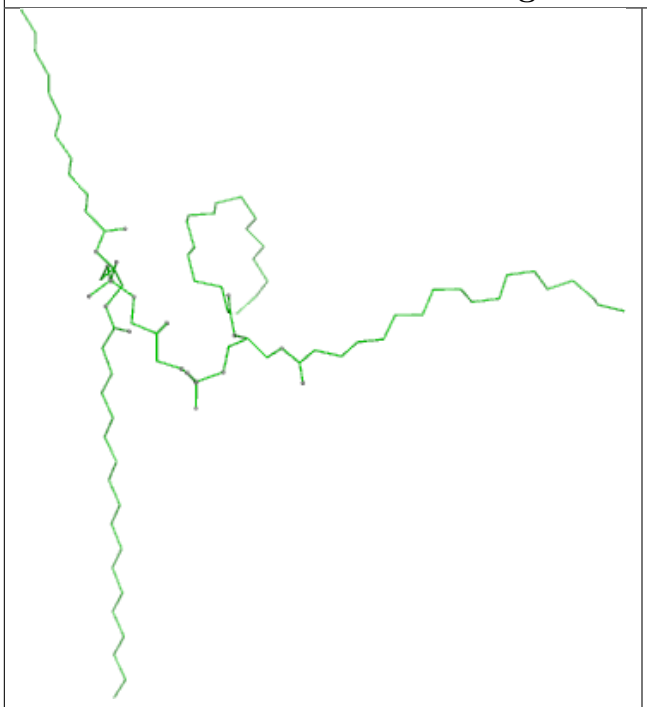

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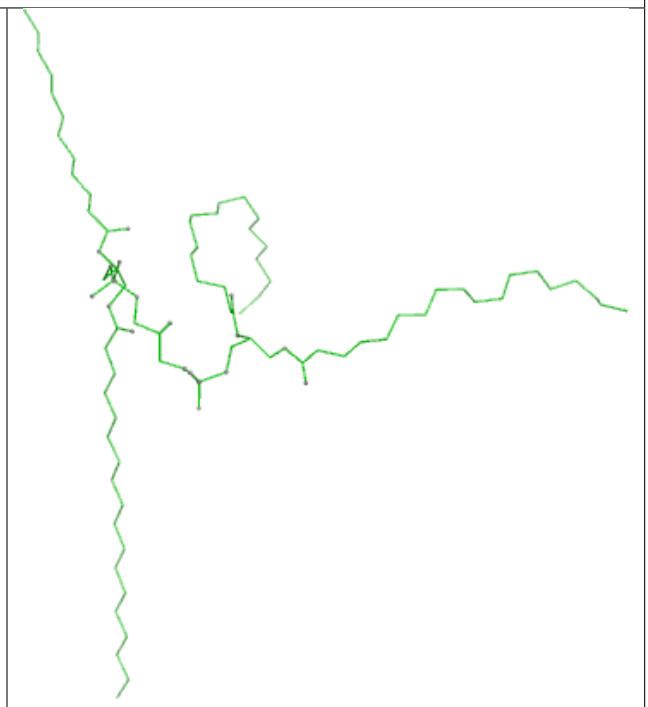
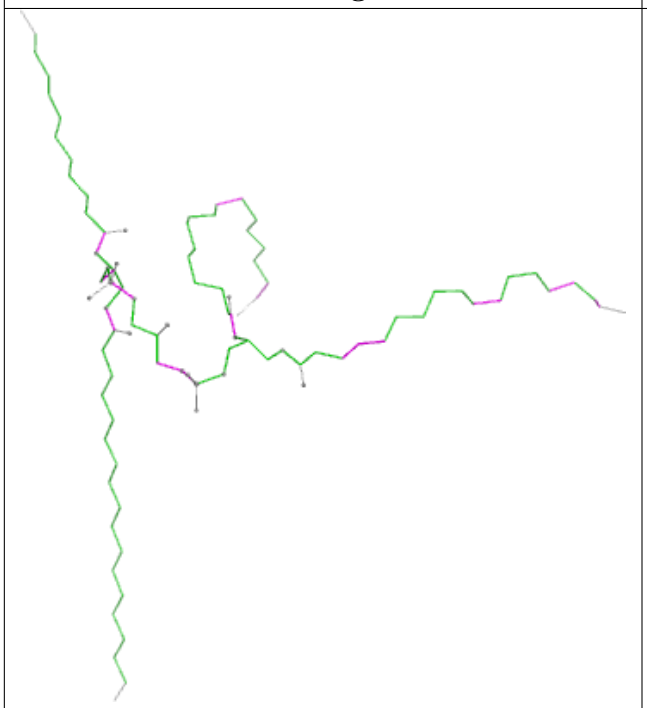


Bond angles

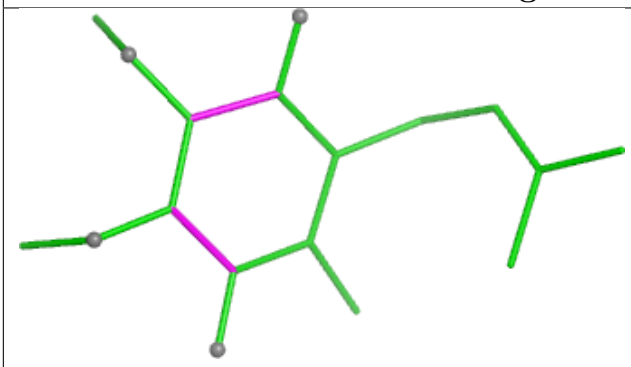


Torsions



Rings

Ligand UQ1 2p 201



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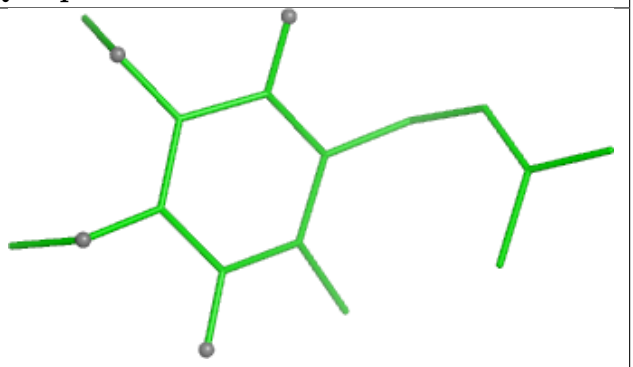

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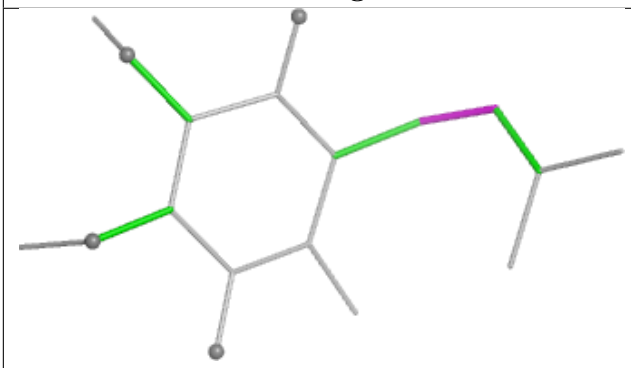

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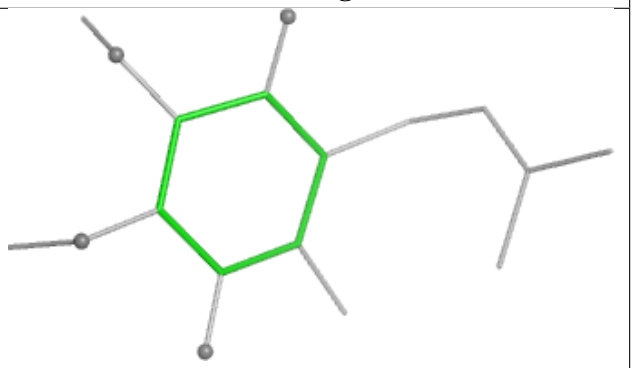
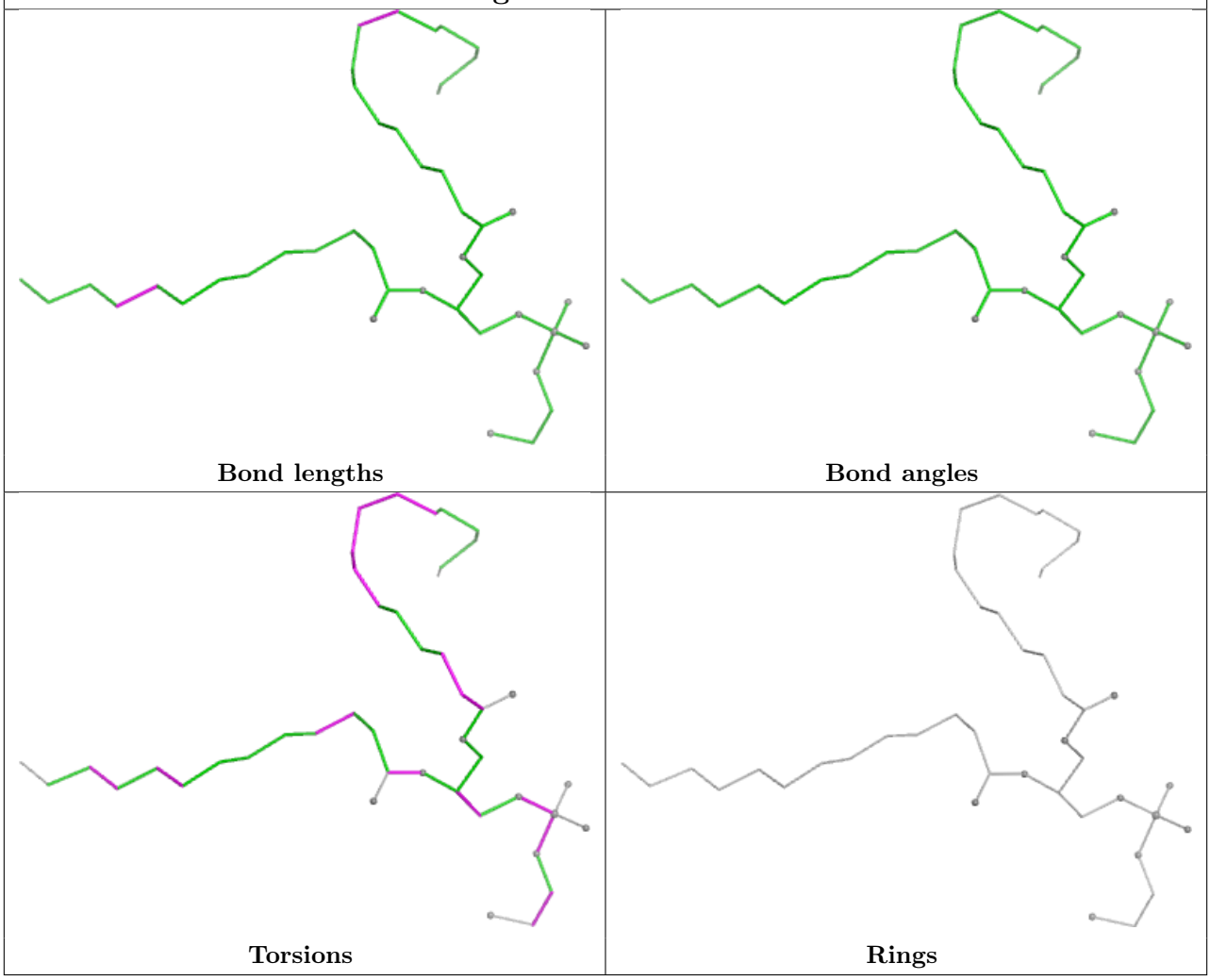
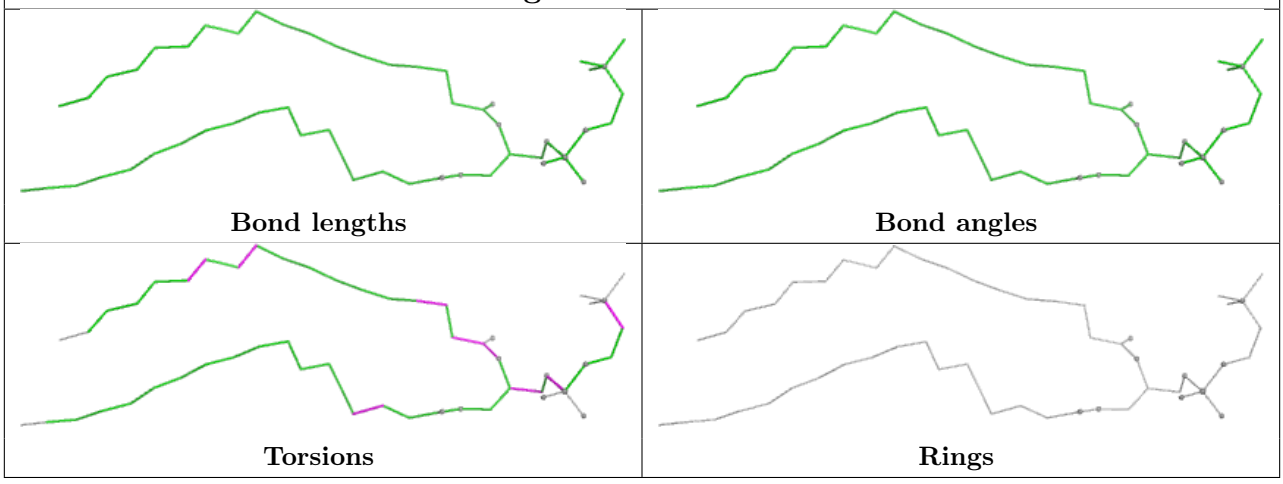


Rings

Ligand PEE 4z 302



Ligand PC1 3a 501



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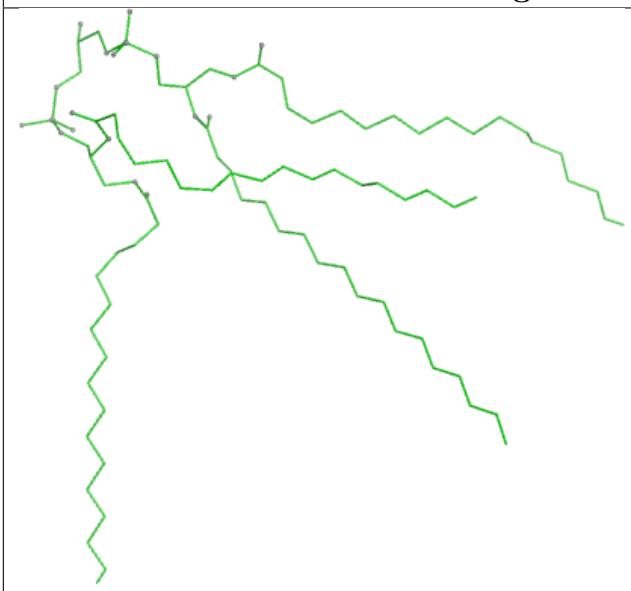

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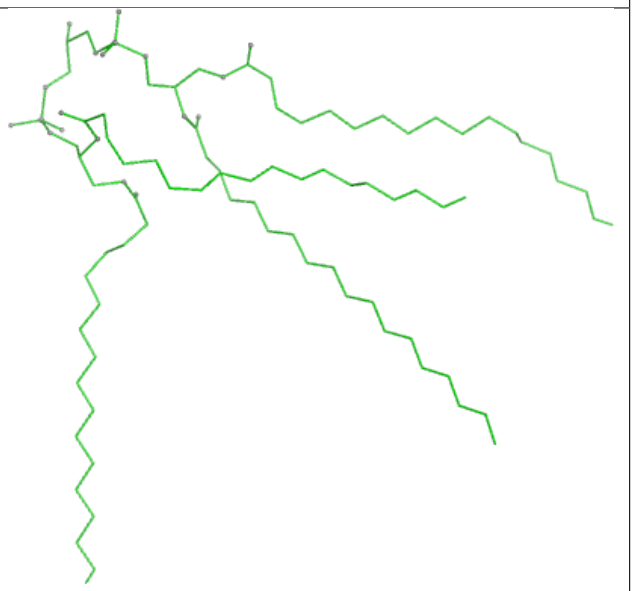

Bond angles



Torsions



Rings

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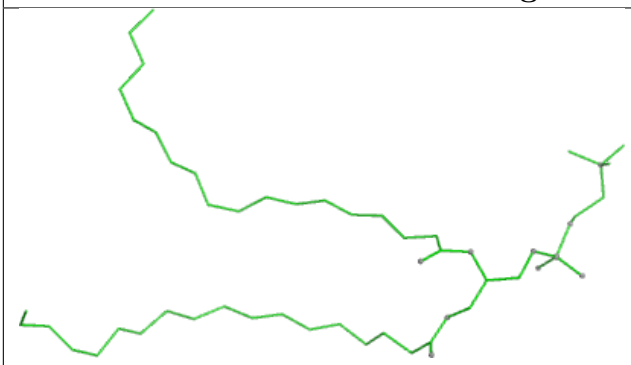

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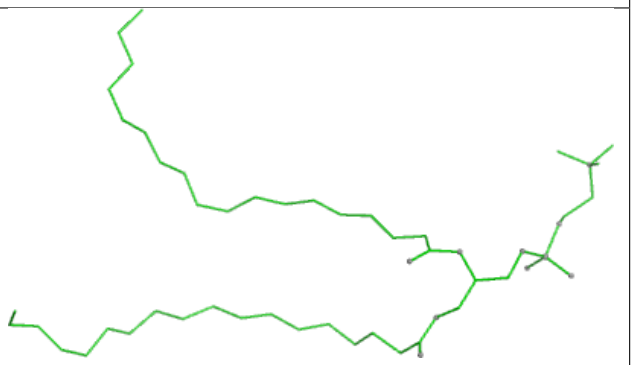
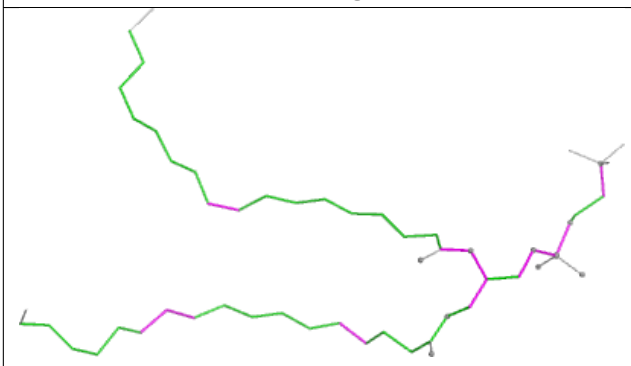


Bond angles

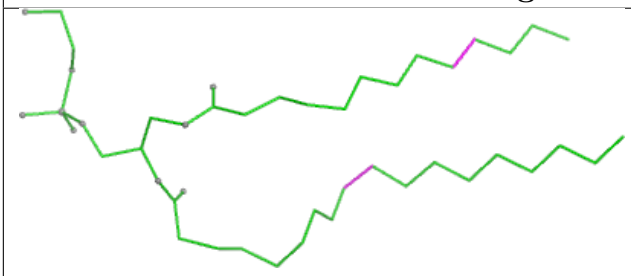


Torsions



Rings

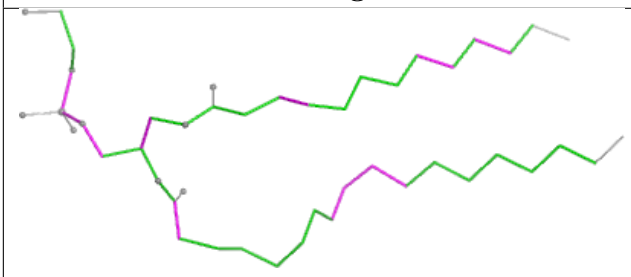
Ligand PEE 2P 202



Bond lengths



Bond angles



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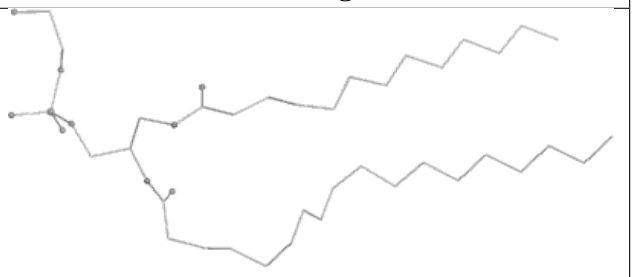
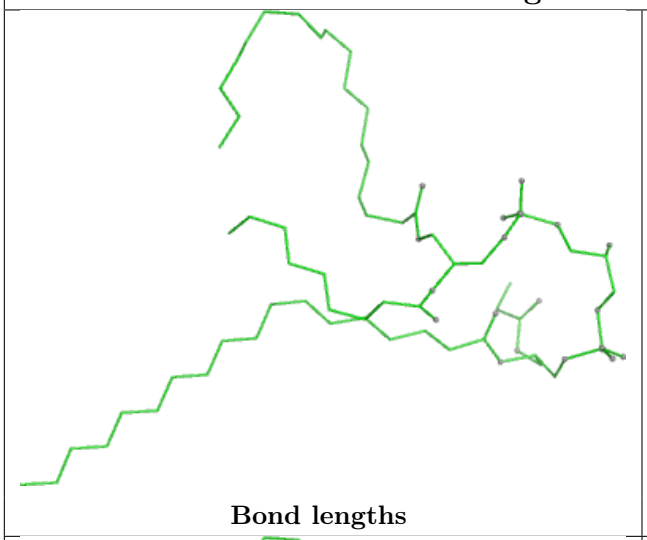


Rings

Ligand CDL 3i 202



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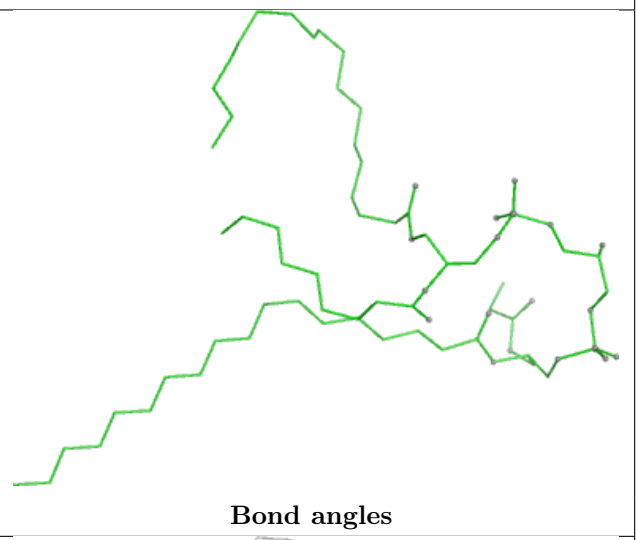
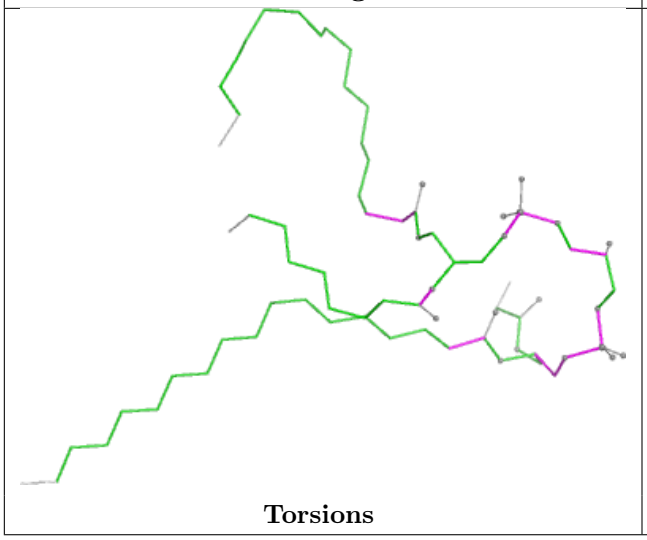


Bond angles



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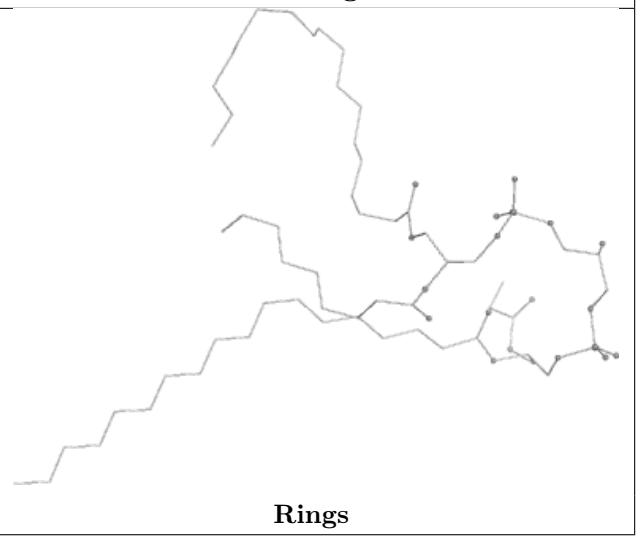
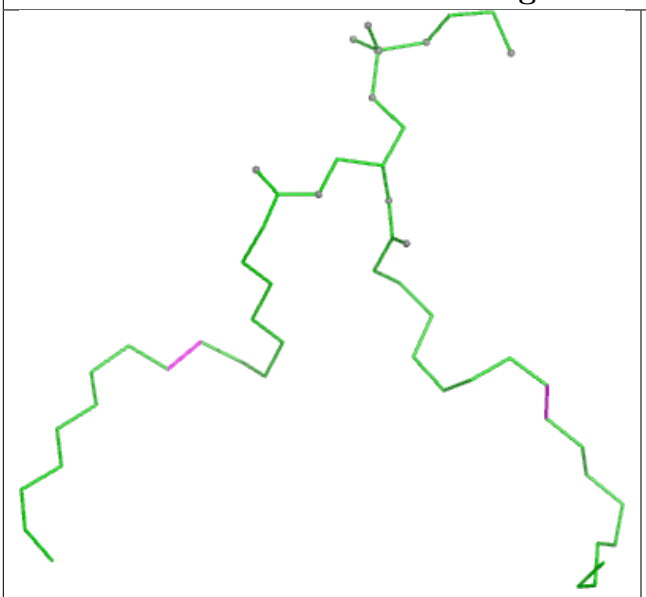


Rings

Ligand PEE 4Z 302



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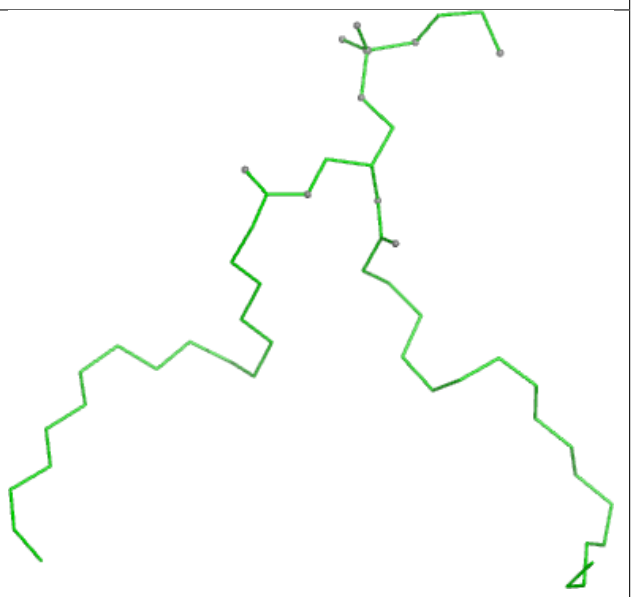

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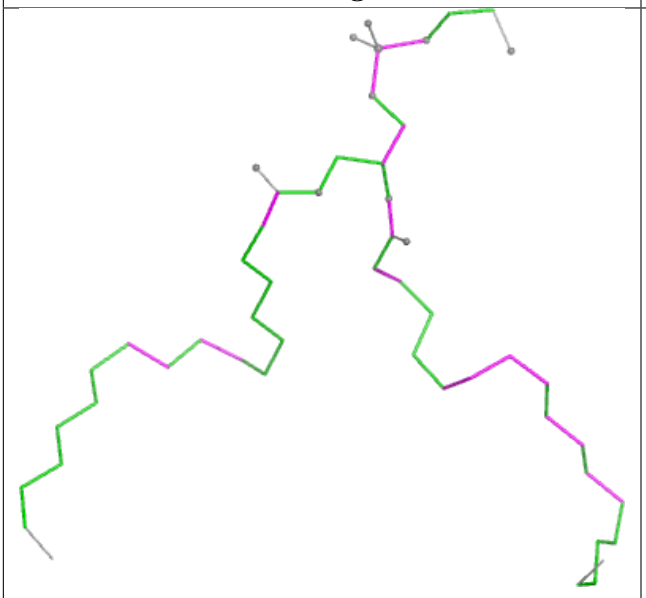

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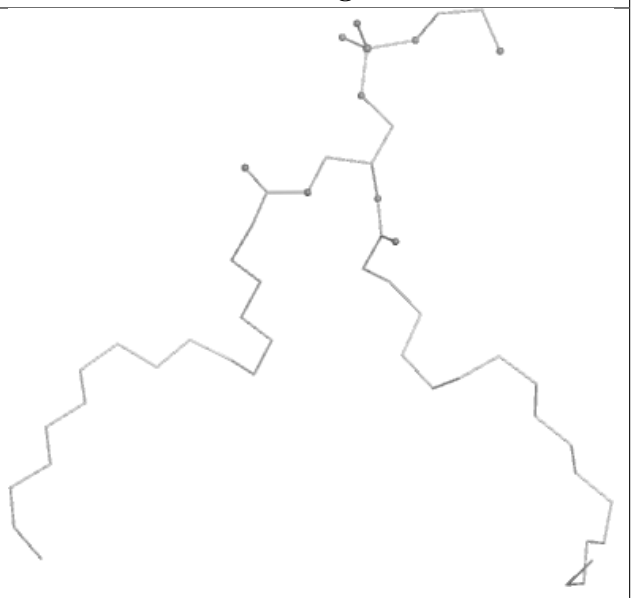
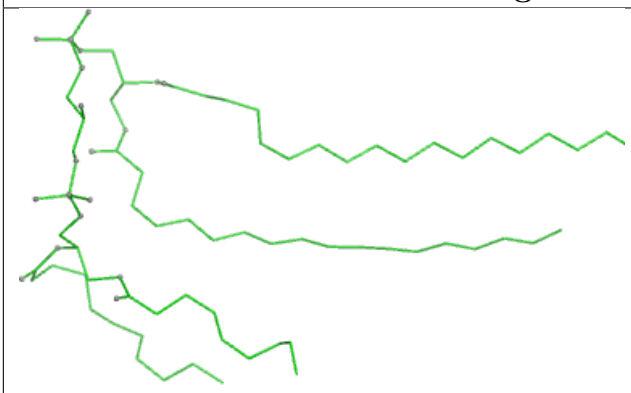


Rings

Ligand CDL 3D 201



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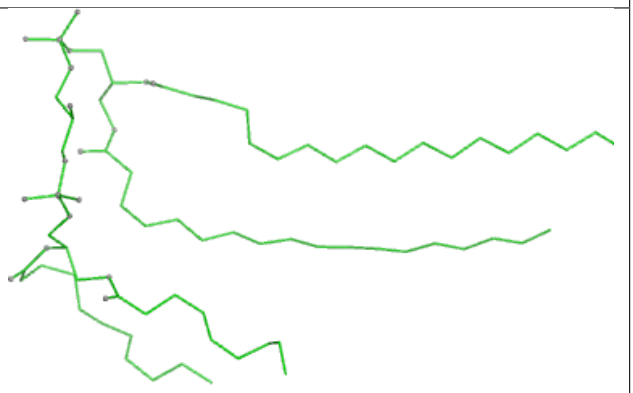
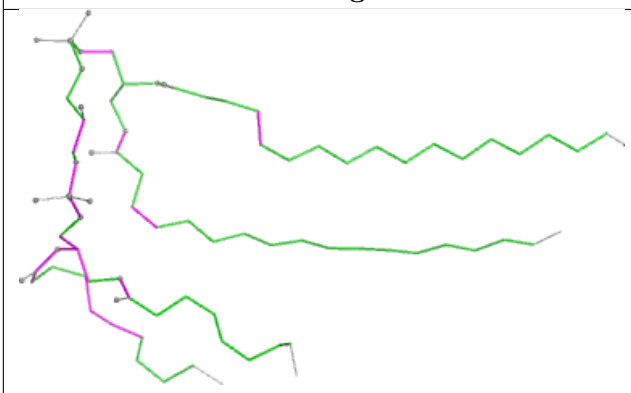


Bond angles

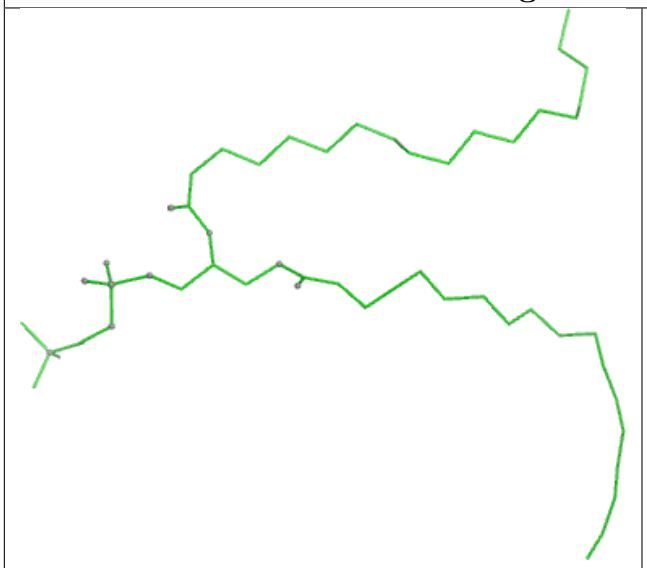


Torsions



Rings

Ligand PC1 2R 201



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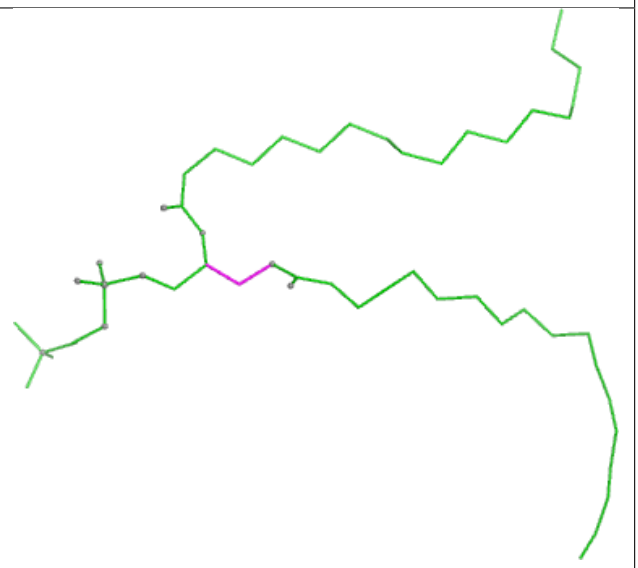

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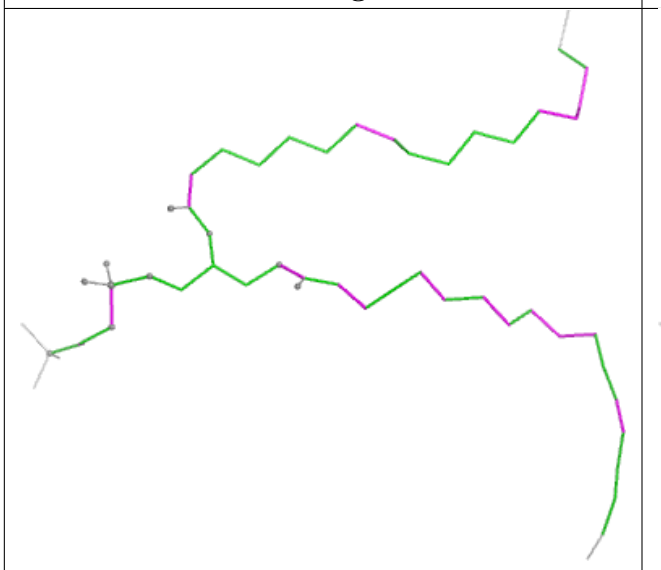
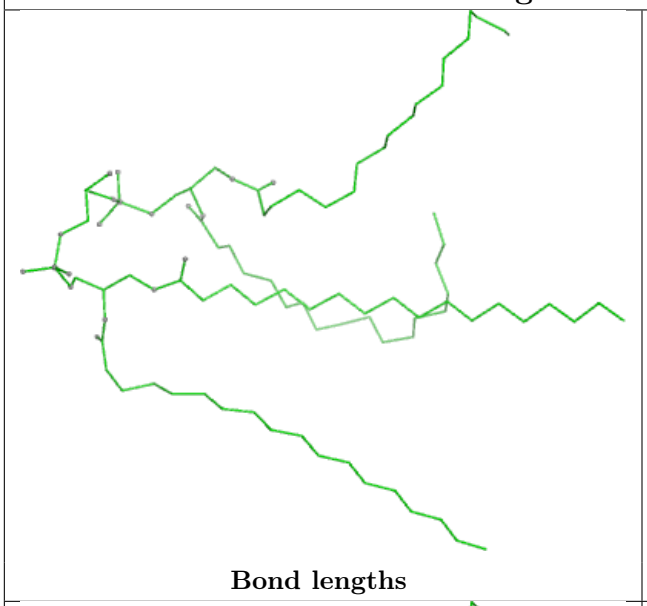


Torsions



Rings

Ligand CDL 3D 202



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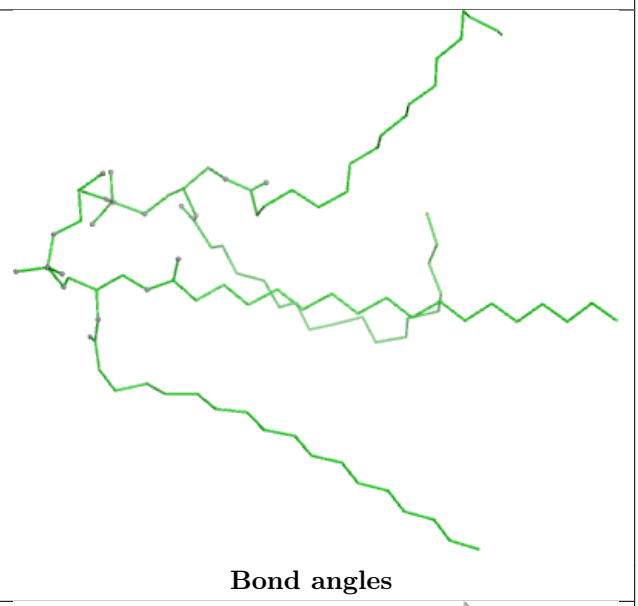

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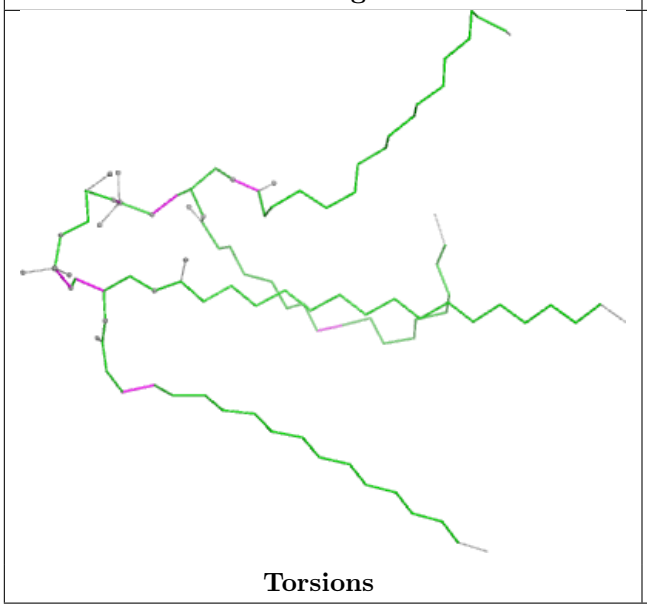
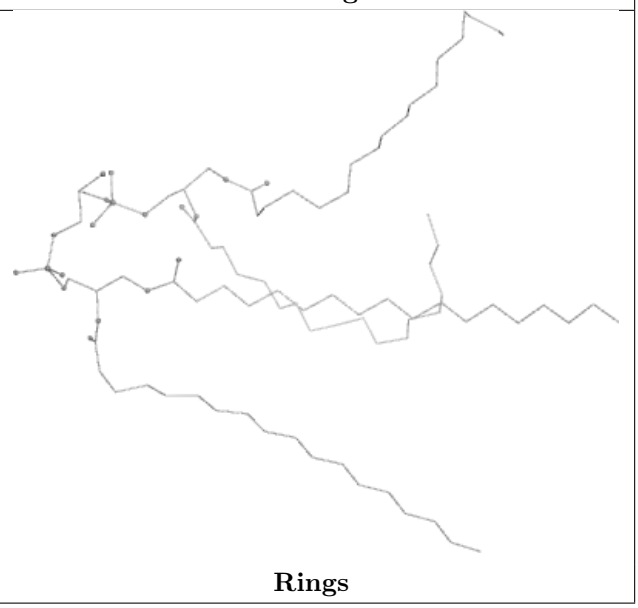
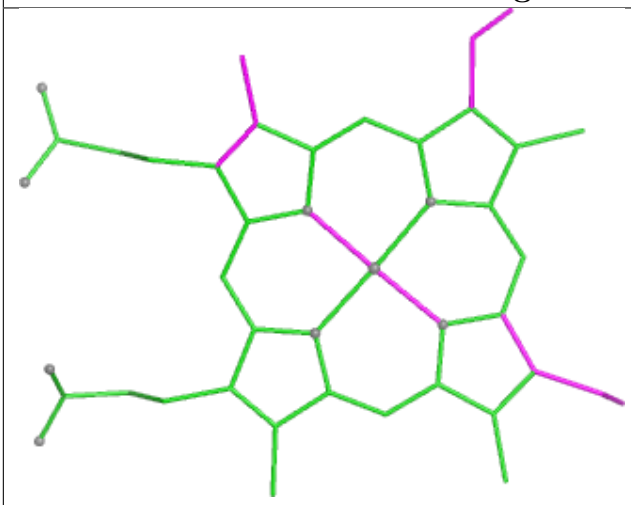


Torsions



Rings

Ligand HEC 3C 302



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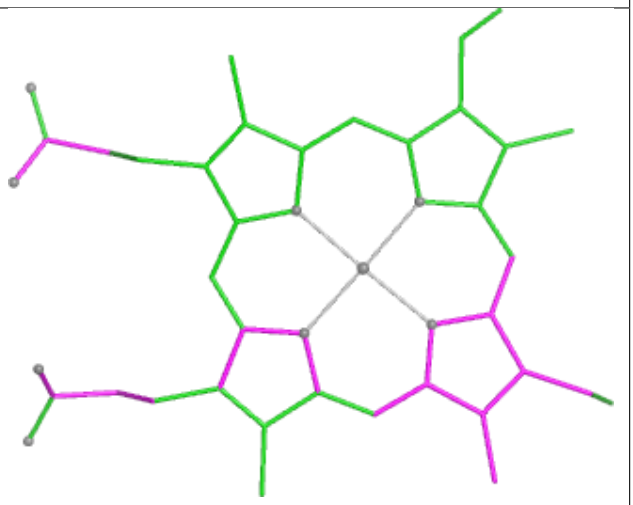
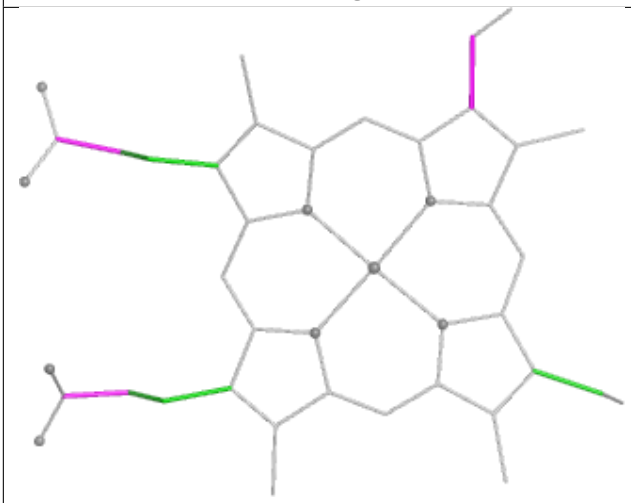


Bond angles



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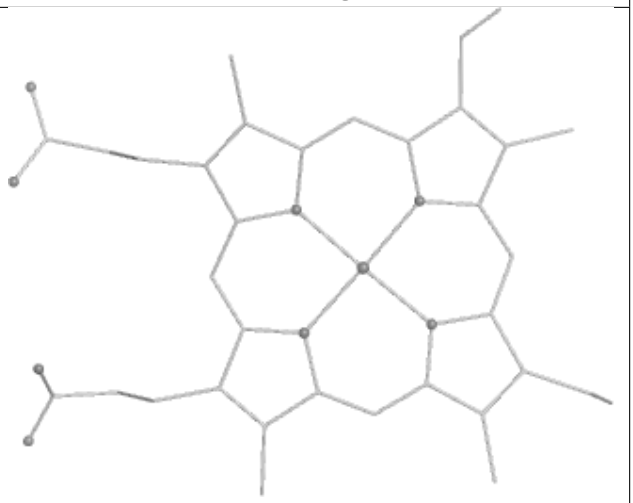
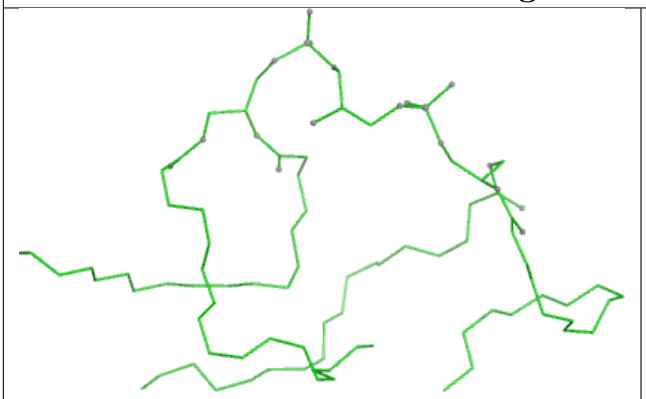


Rings

Ligand CDL 2q 101



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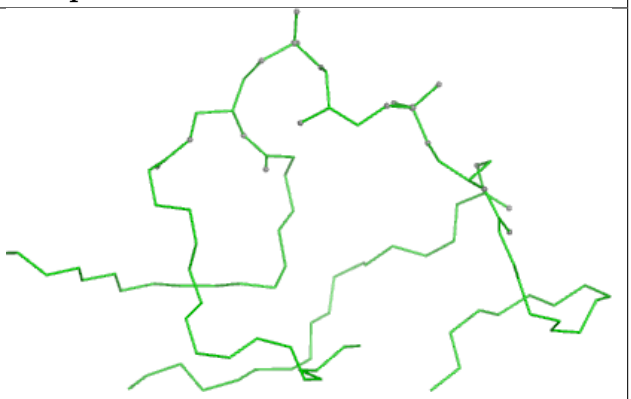
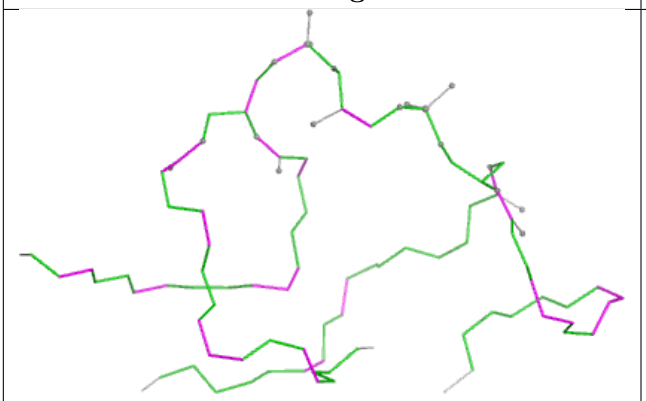


Bond angles

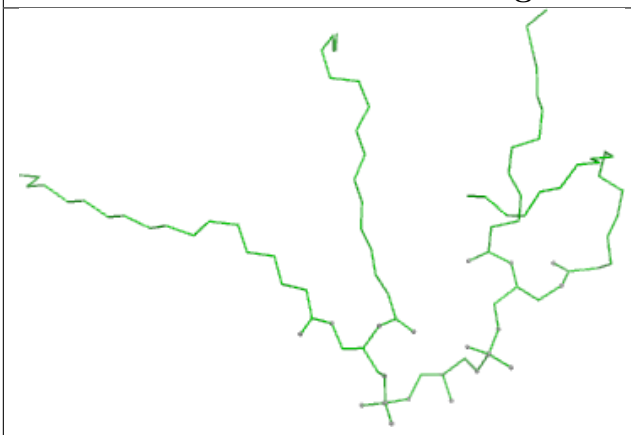


Torsions



Rings

Ligand CDL 4Q 902



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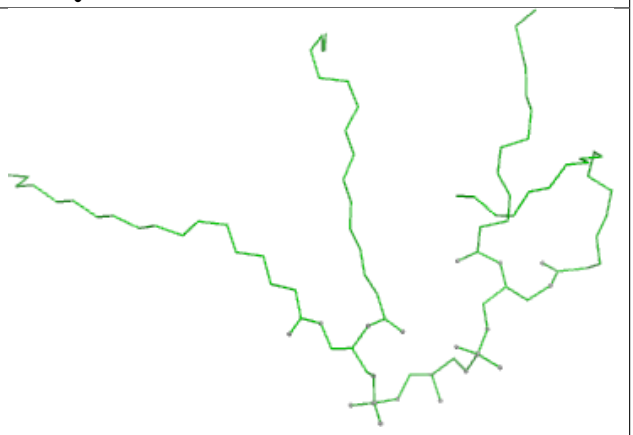
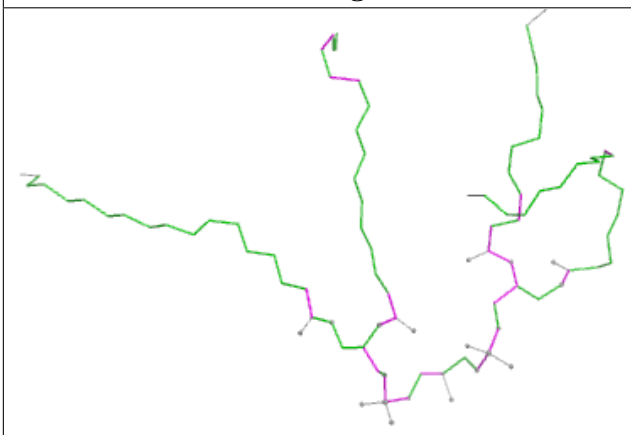


Bond angles

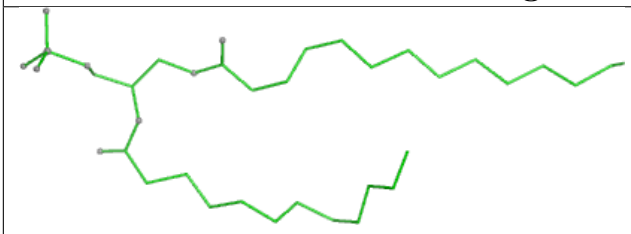


Torsions



Rings

Ligand LPP 4z 301



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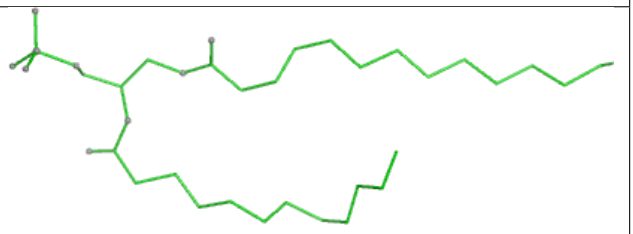
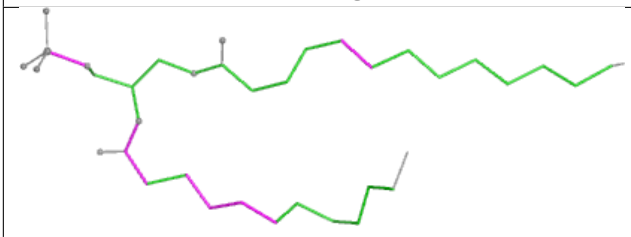
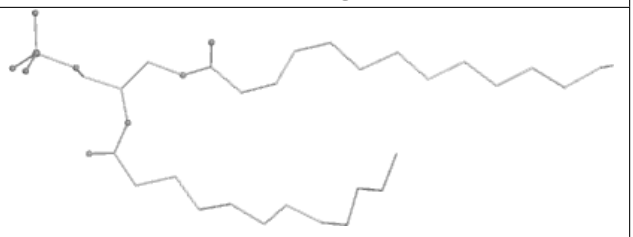


Bond angles

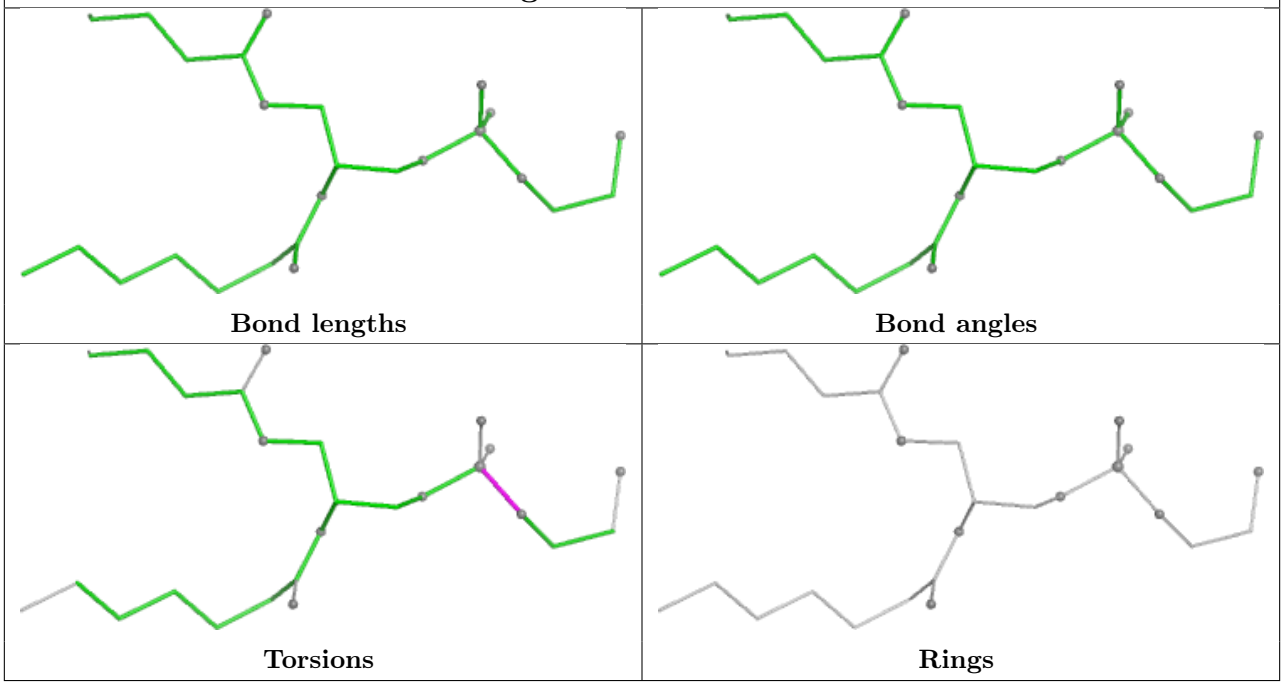


Torsions

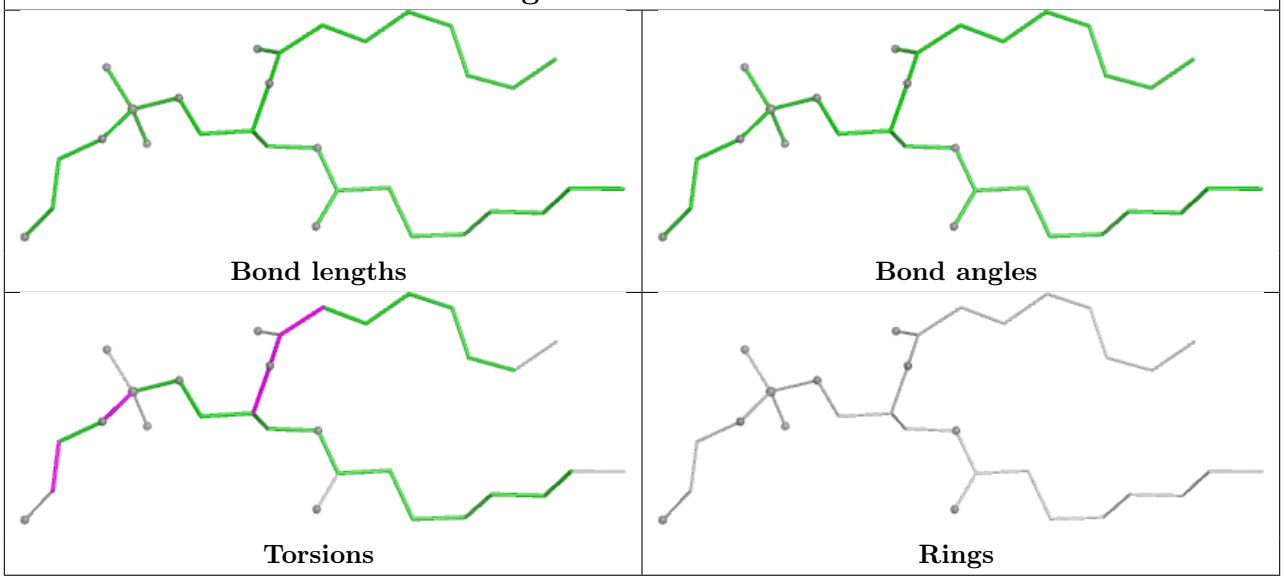


Rings

Ligand PEE 4S 101



Ligand PEE 40 304



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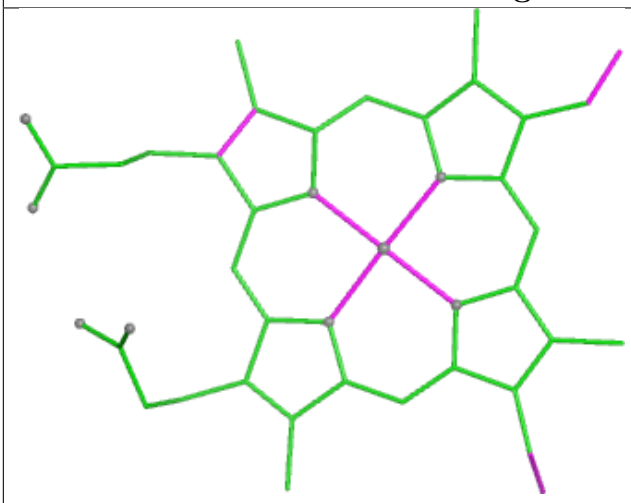

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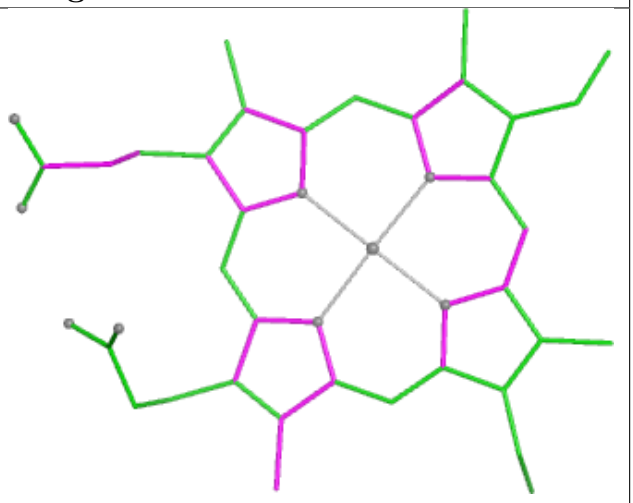
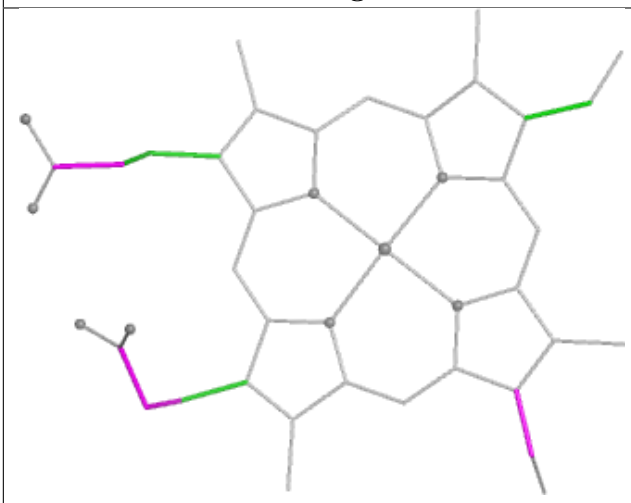


Bond angles



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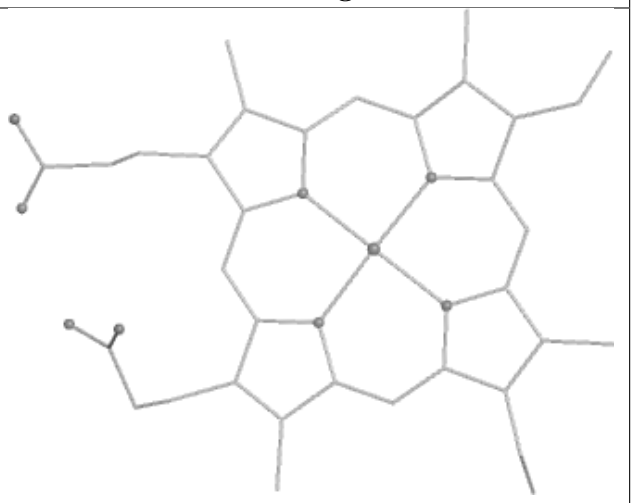
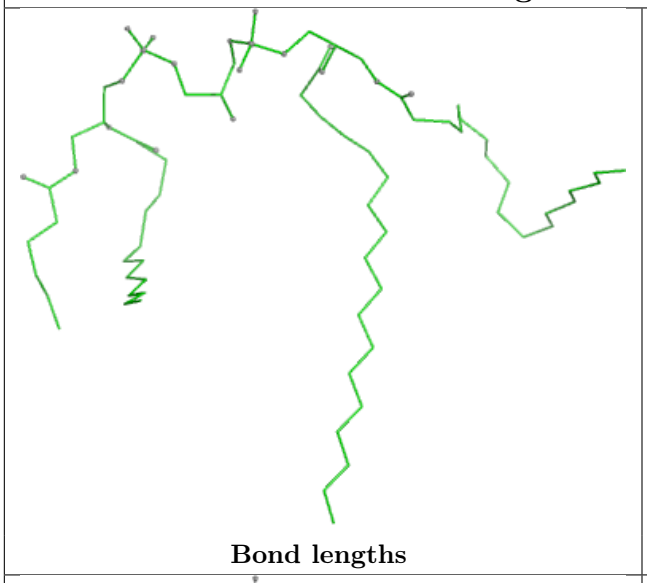


Rings

Ligand CDL 3H 405



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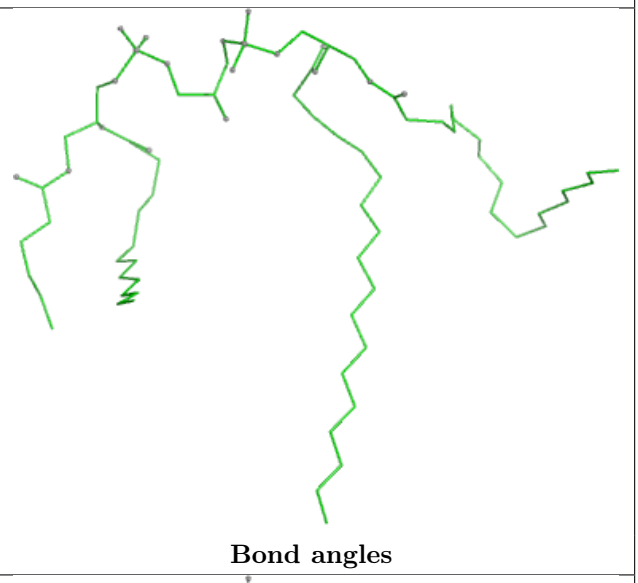

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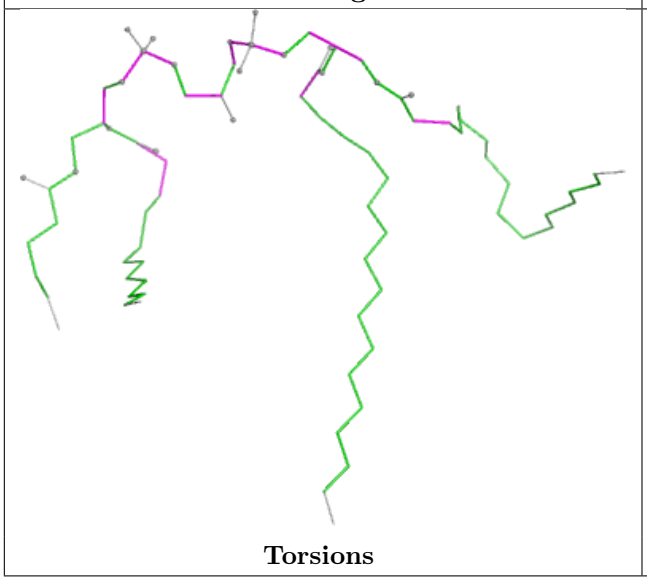

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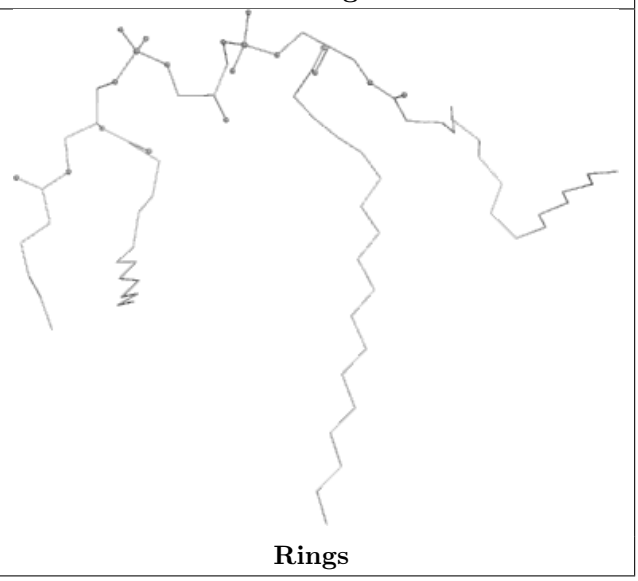
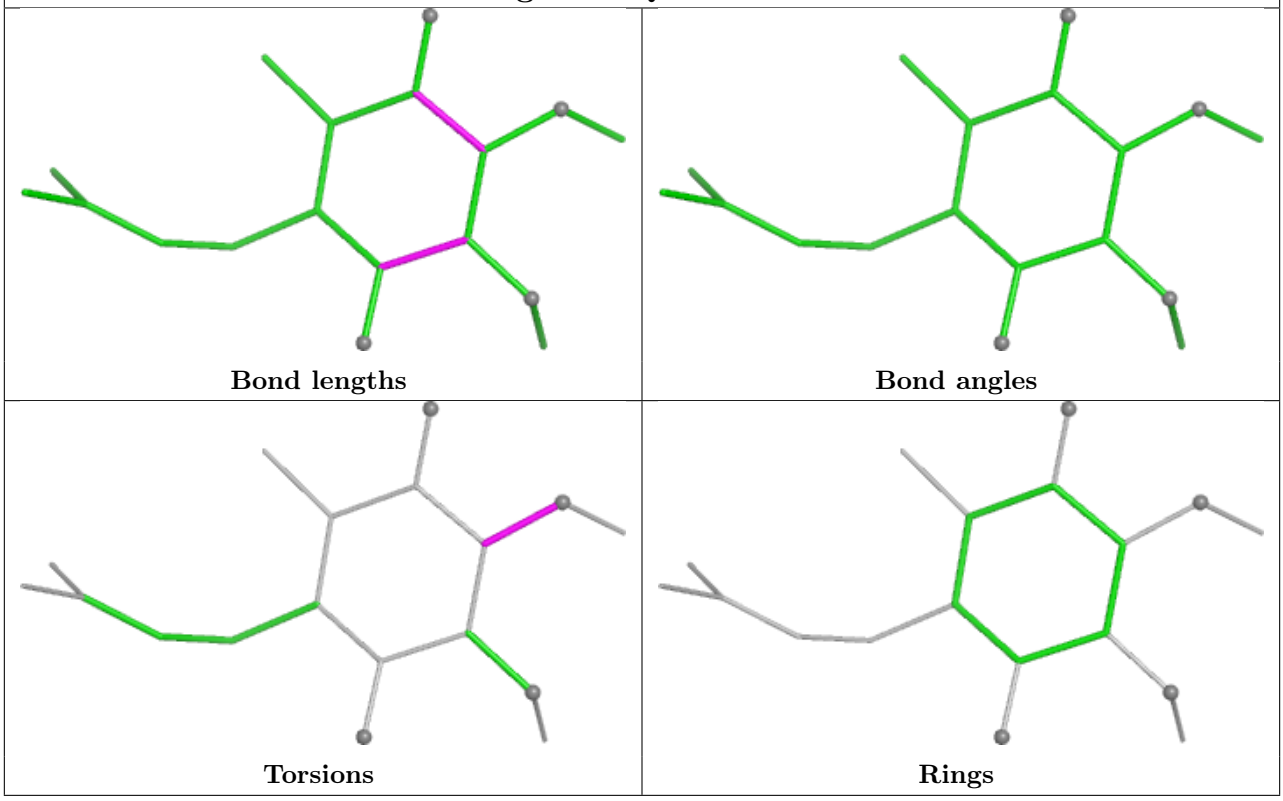


Rings

Ligand UQ1 2N 301



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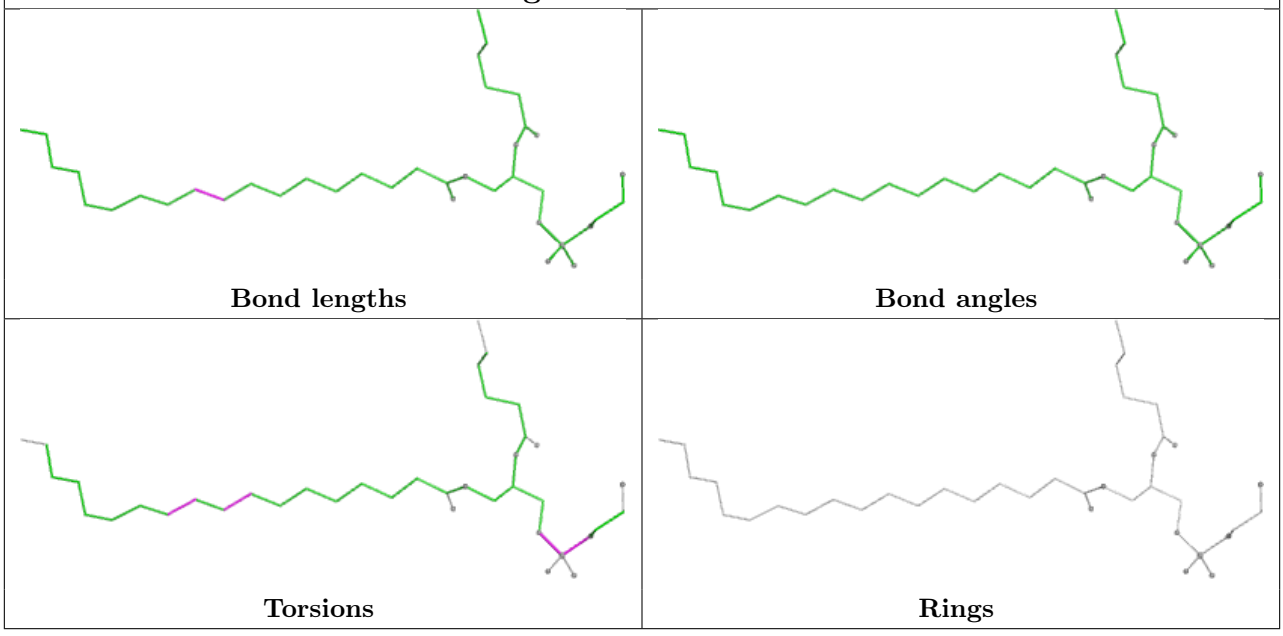

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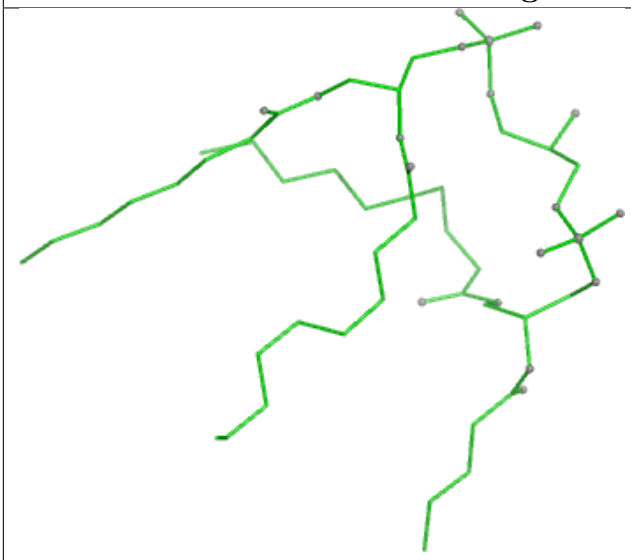

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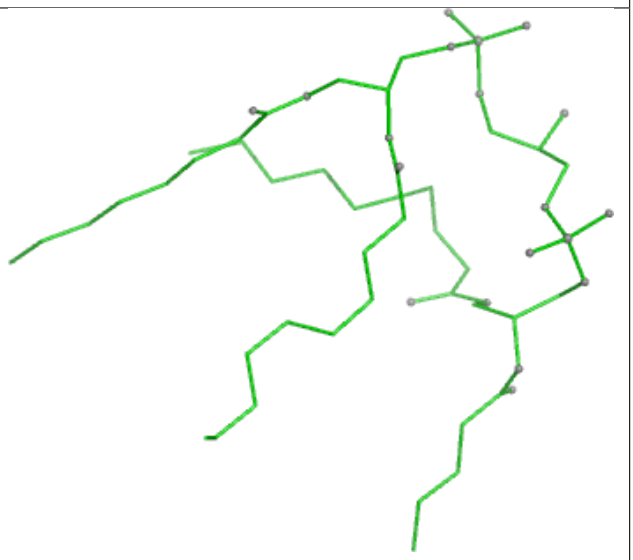
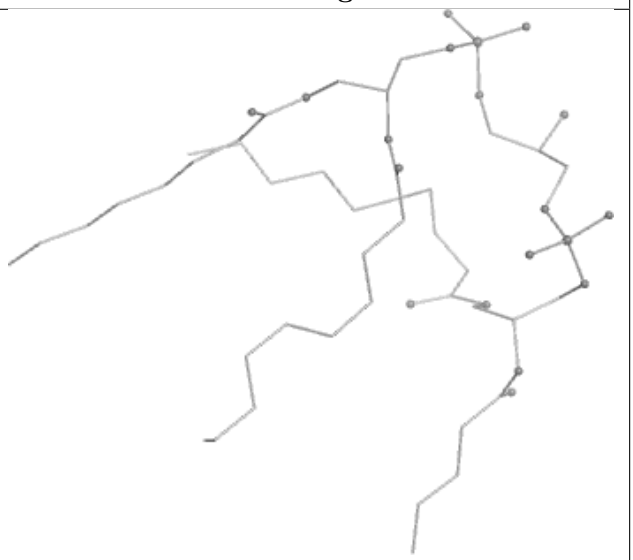


Bond angles

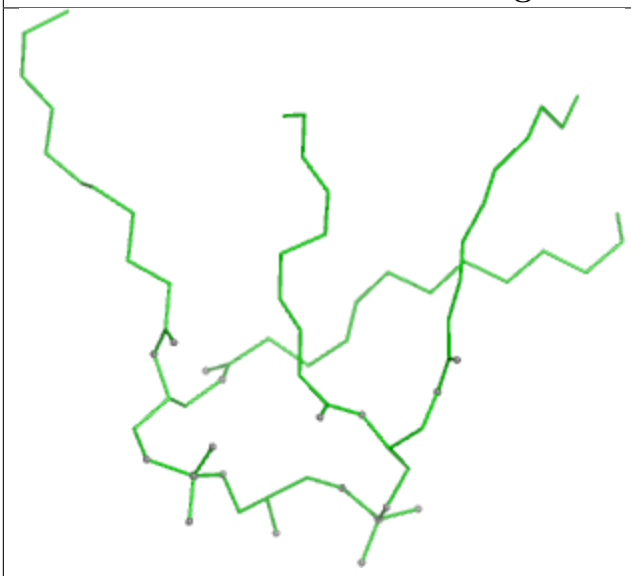


Torsions



Rings

Ligand CDL 4U 501



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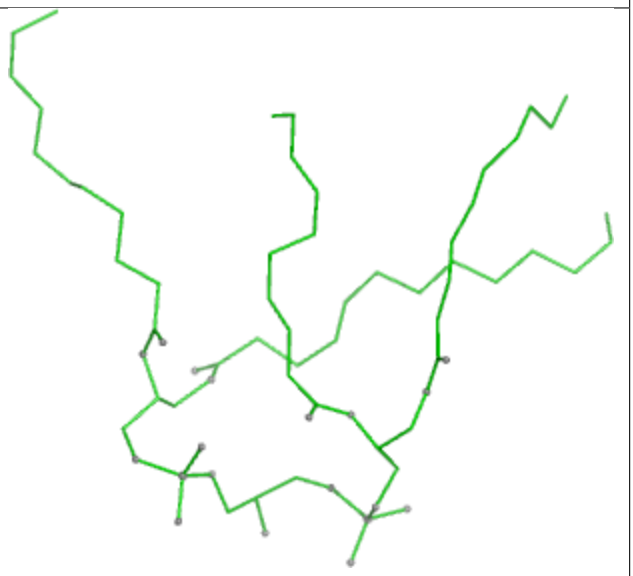
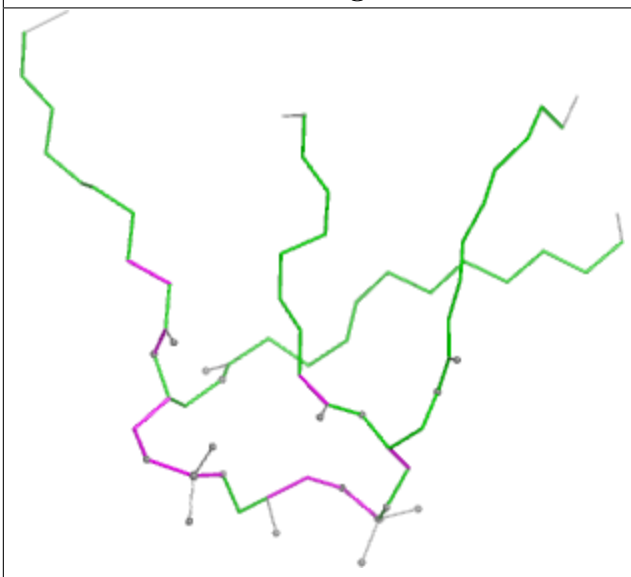


Bond angles



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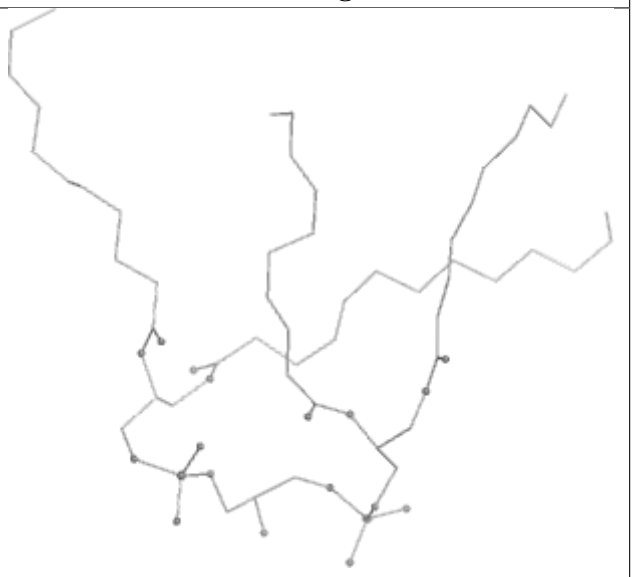
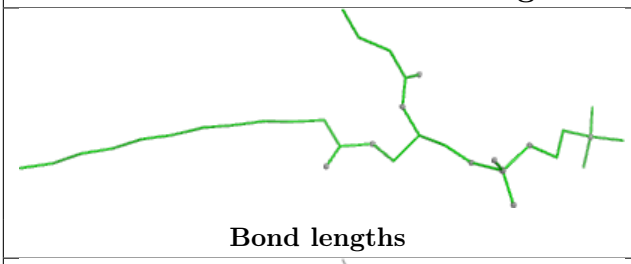


Rings

Ligand PC1 3H 401



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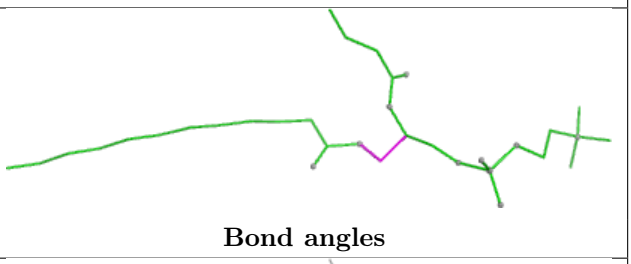
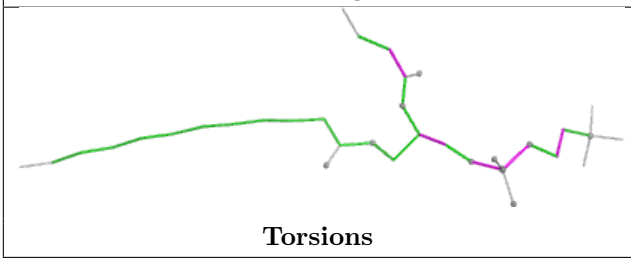


Bond angles



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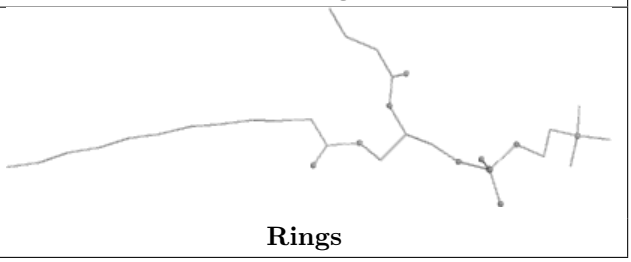
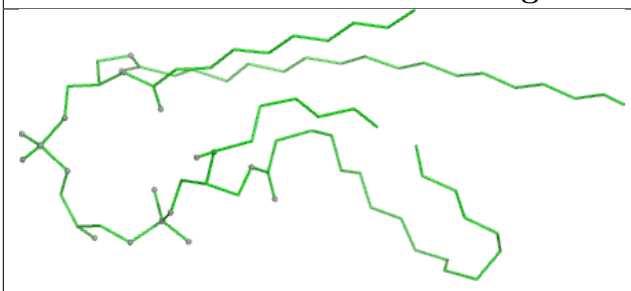


Rings

Ligand CDL 3I 202



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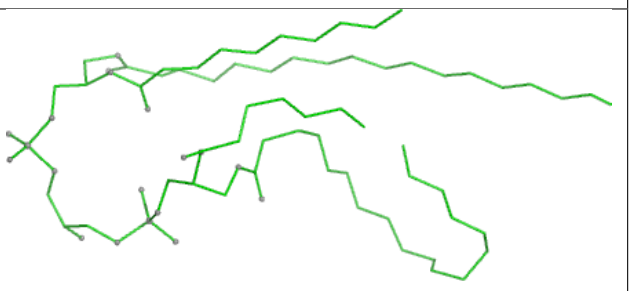

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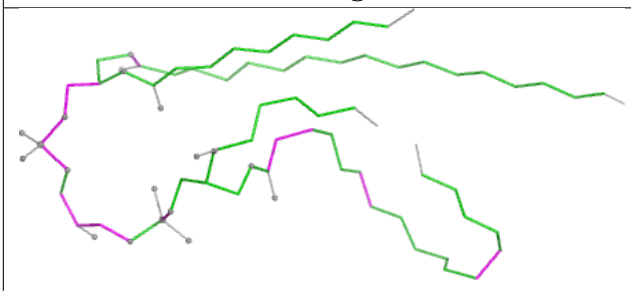

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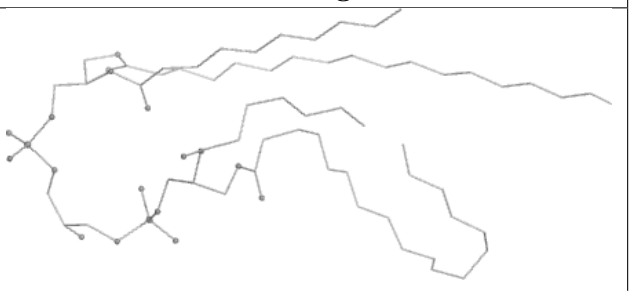
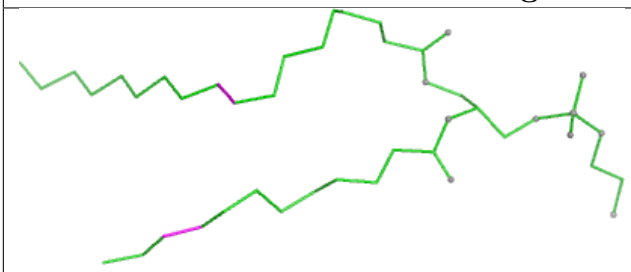


Rings

Ligand PEE 40 301



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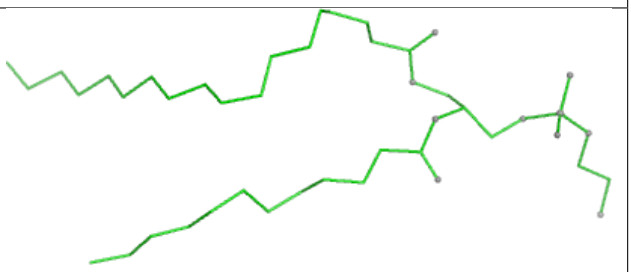

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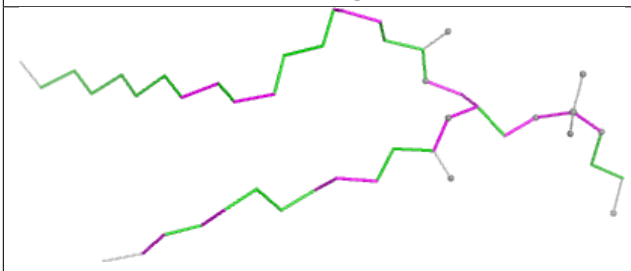

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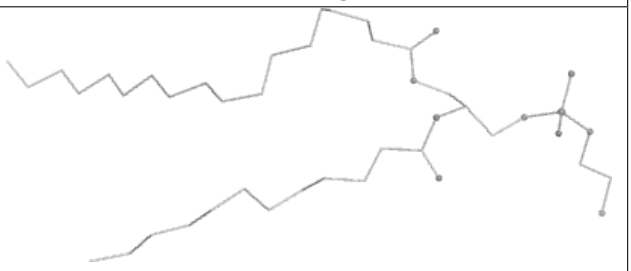
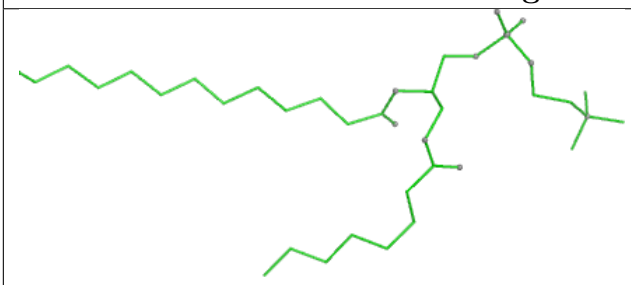


Rings

Ligand PC1 2o 202



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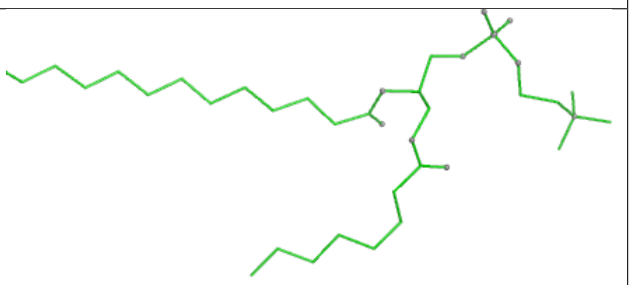

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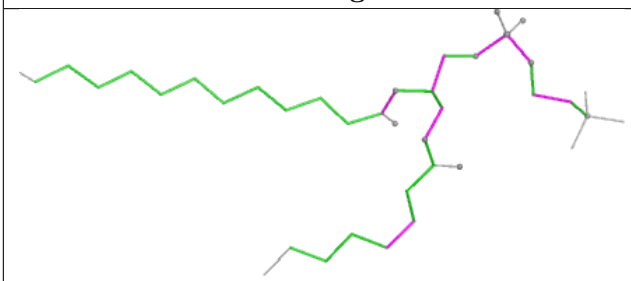
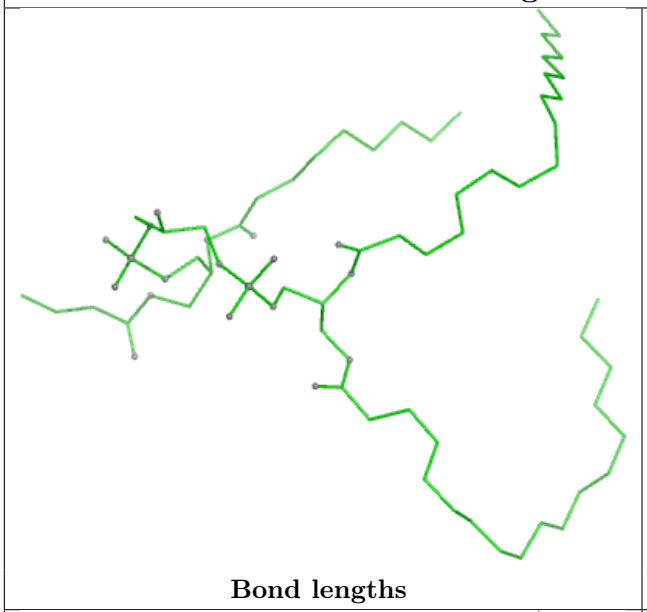


Torsions



Rings

Ligand CDL 3e 202



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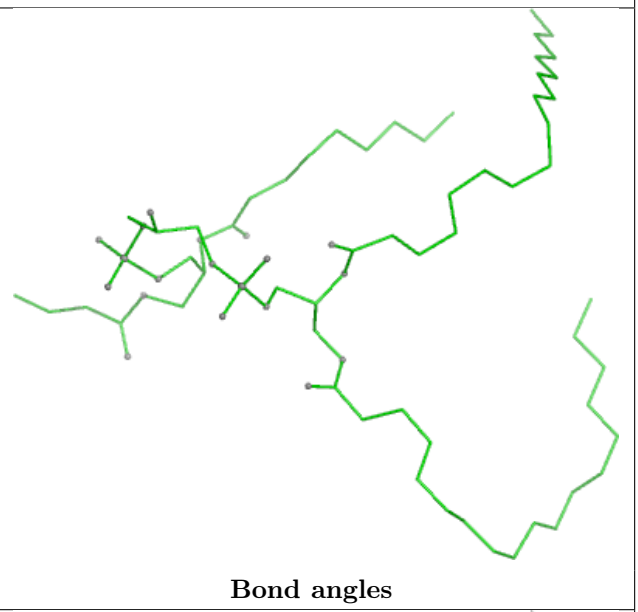

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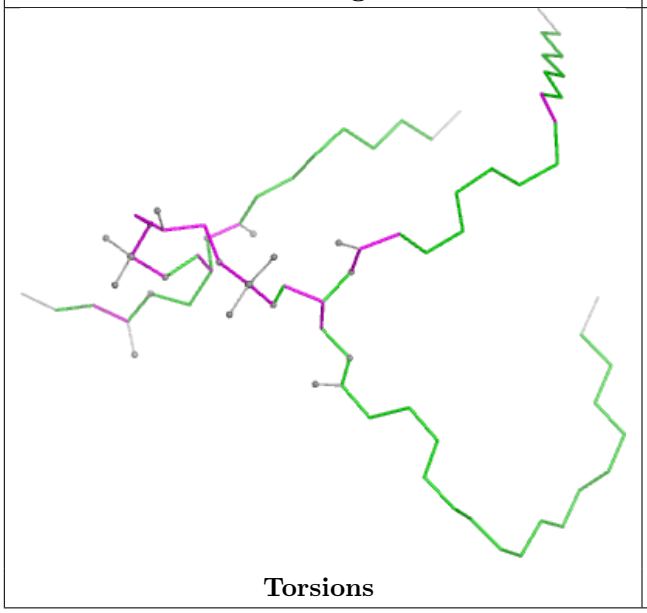

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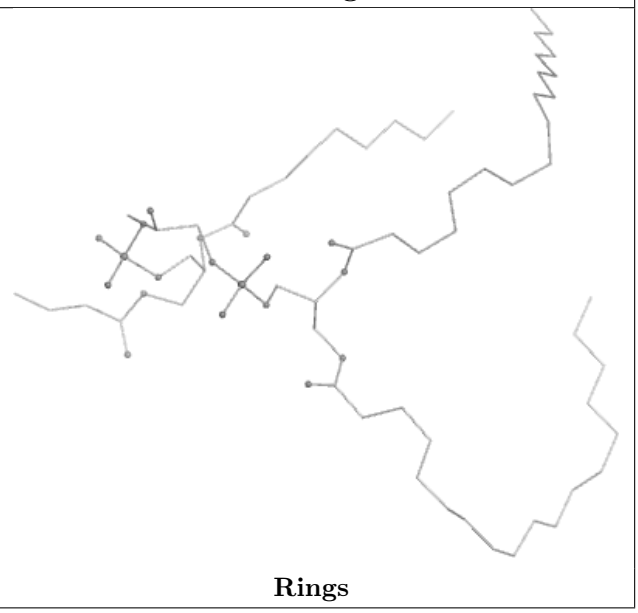
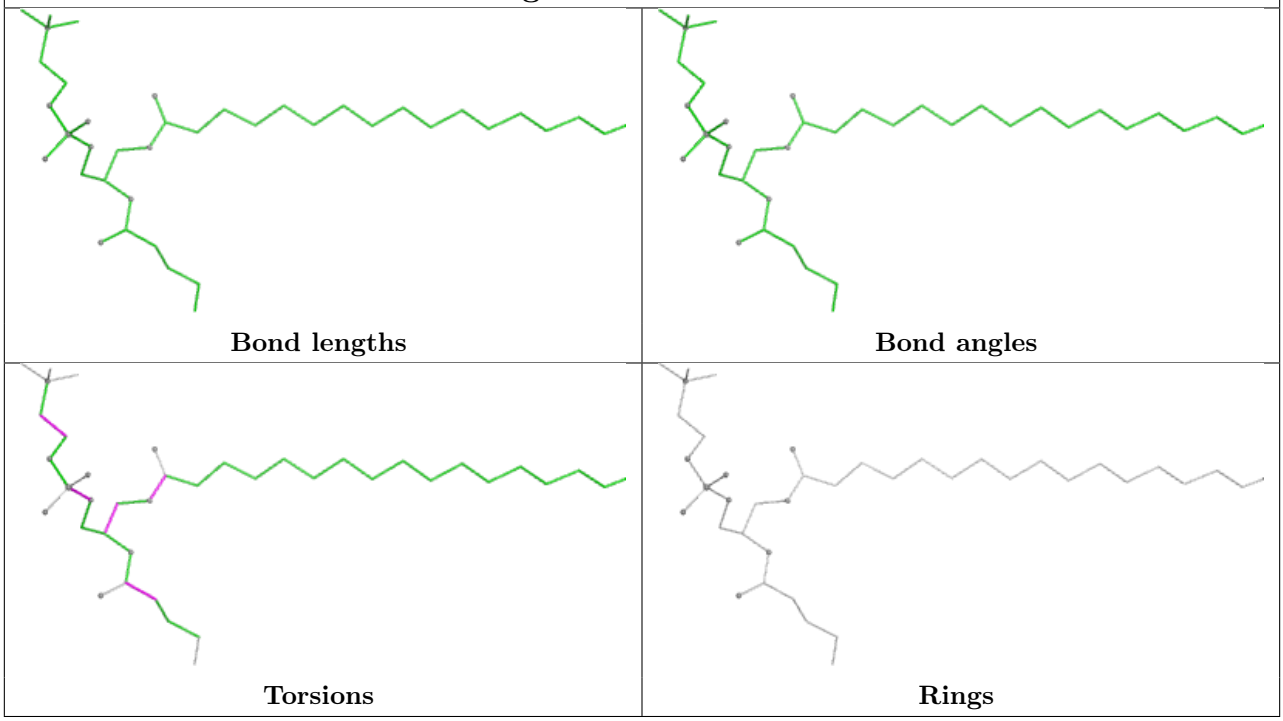
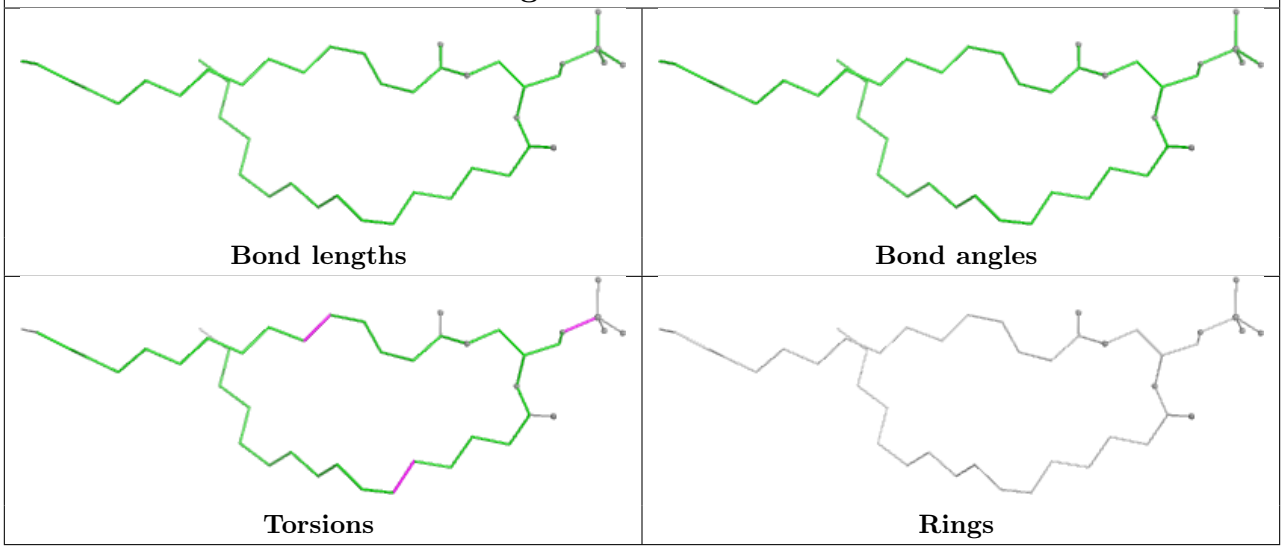


Rings

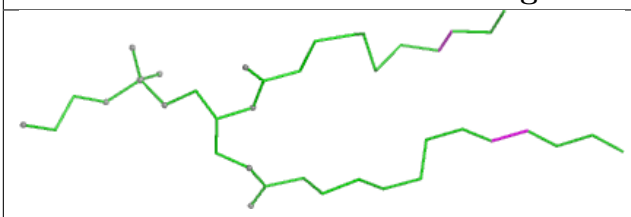
Ligand PC1 3h 402



Ligand LPP 4Z 301



Ligand PEE 4q 902



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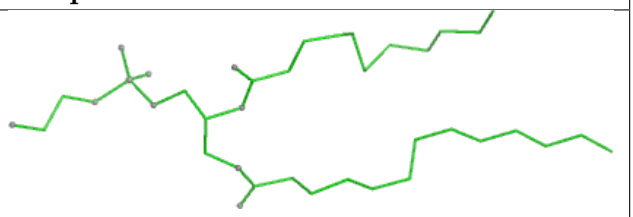
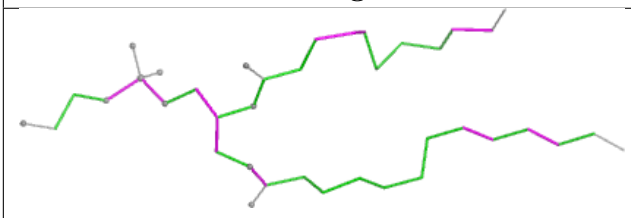


Bond angles



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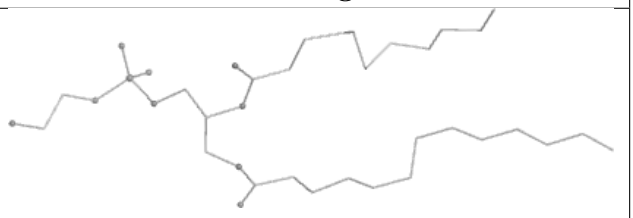


Rings

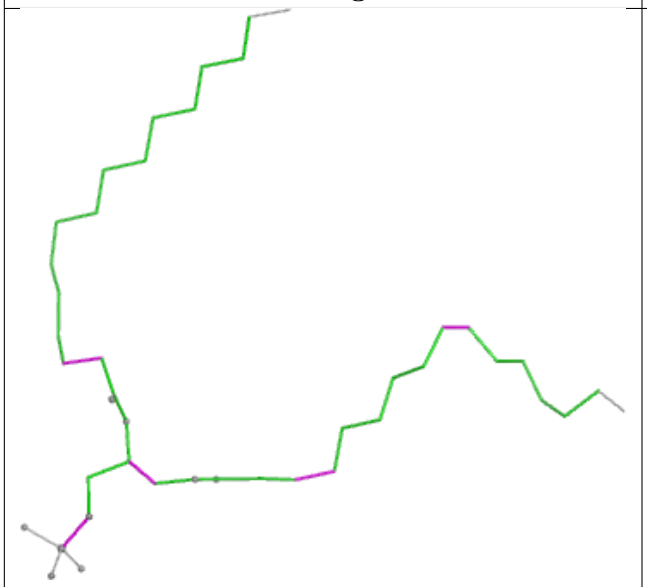
Ligand LPP 4C 101



Bond lengths



Bond angles

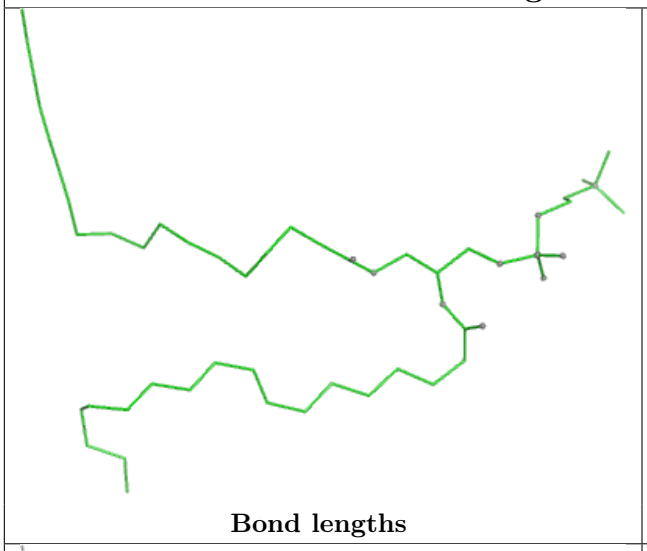


Torsions



Rings

Ligand PC1 2r 201



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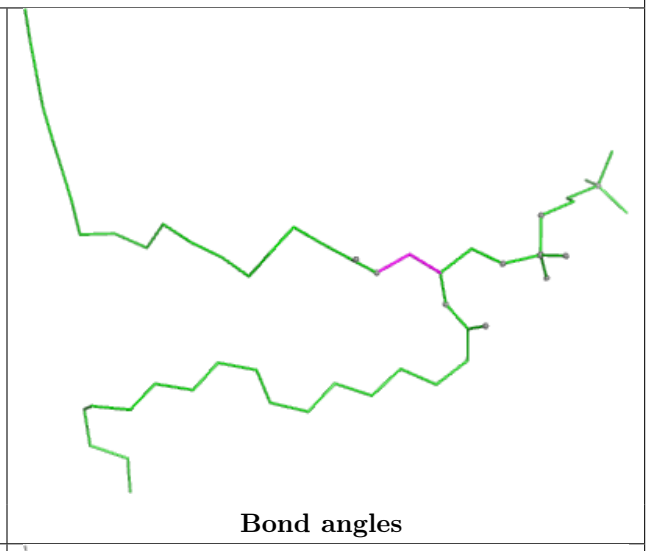
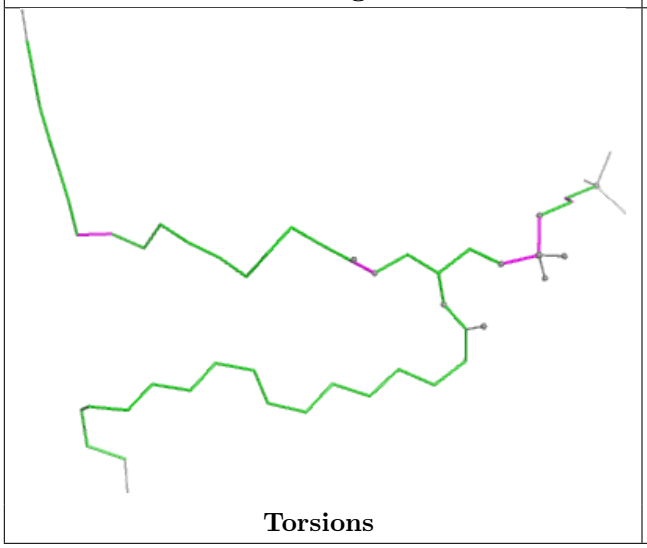


Bond angles



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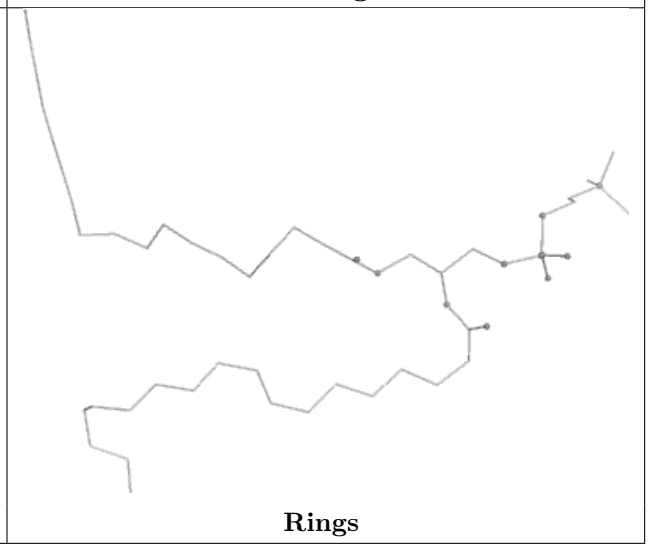
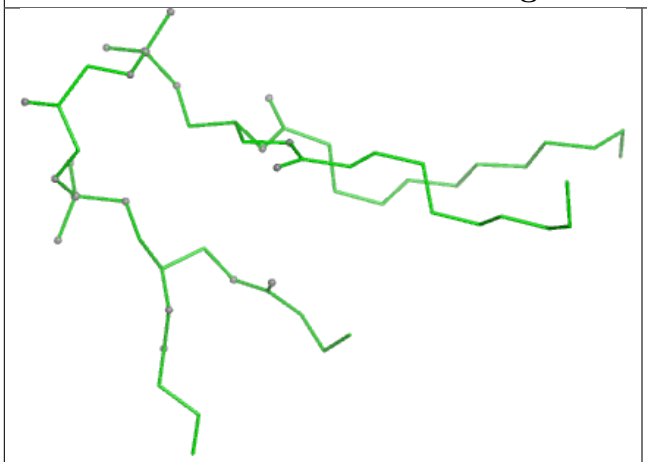


Rings

Ligand CDL 3g 406



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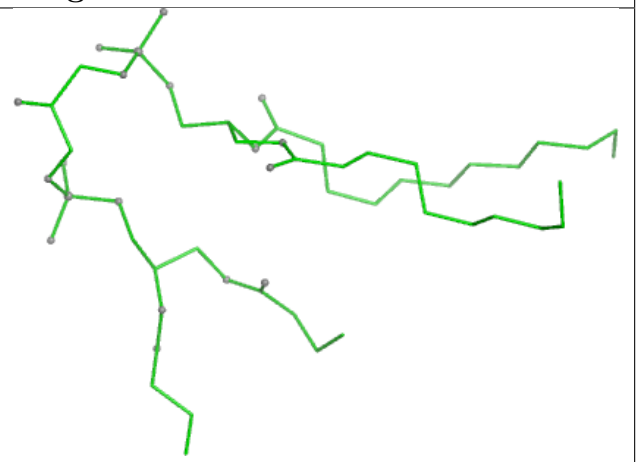
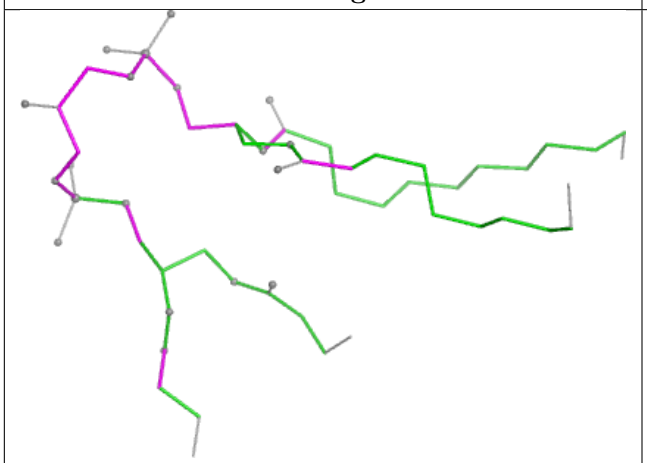


Bond angles



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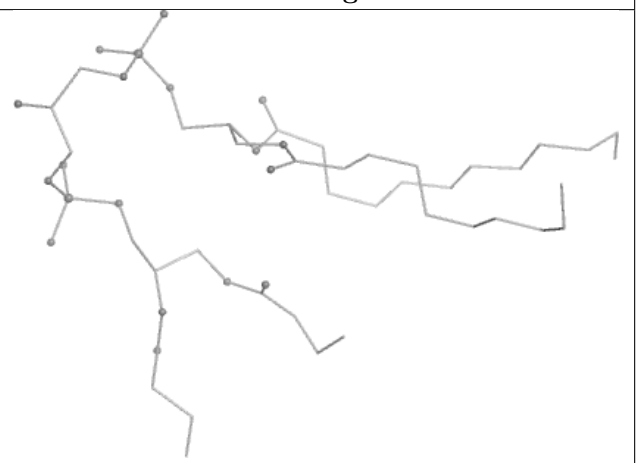
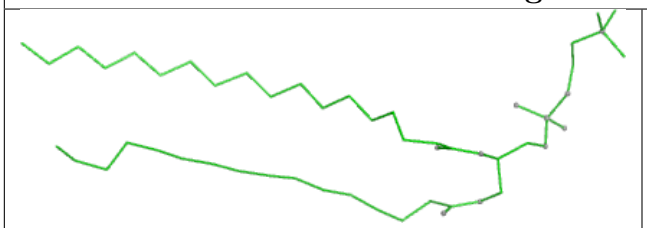
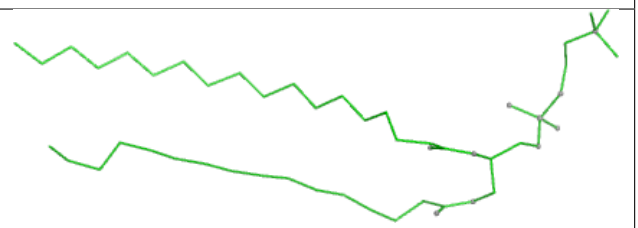


Rings

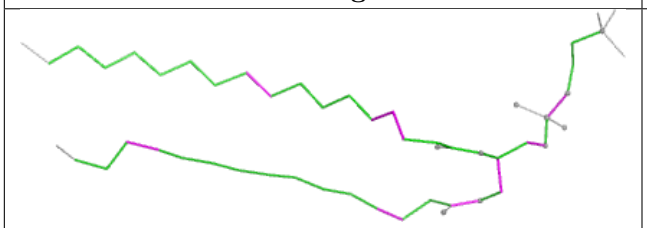
Ligand PC1 2r 202



Bond lengths



Bond angles



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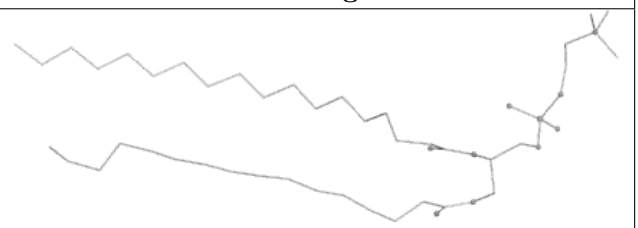
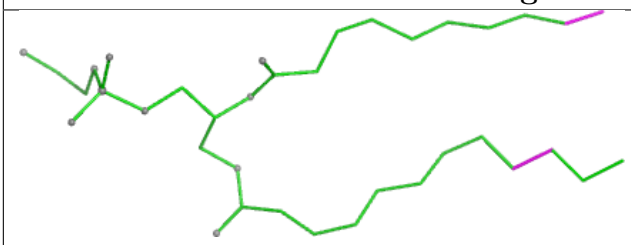
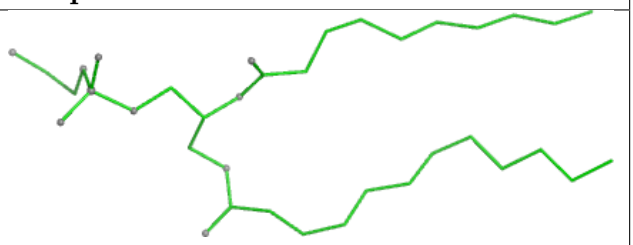


Rings

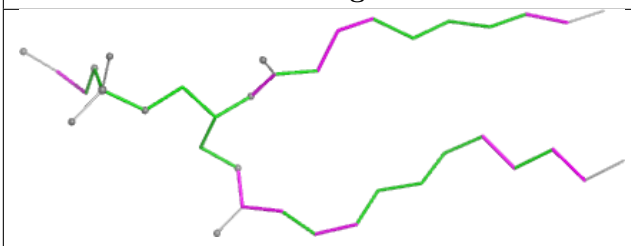
Ligand PEE 4q 901



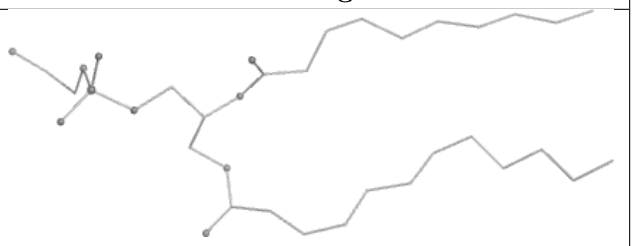
Bond lengths



Bond angles

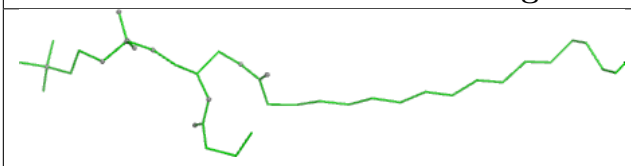


Torsions



Rings

Ligand PC1 3h 401



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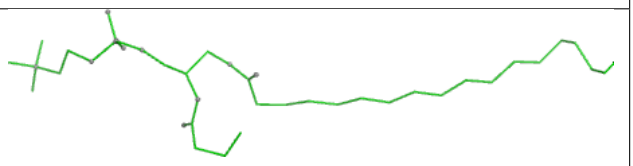

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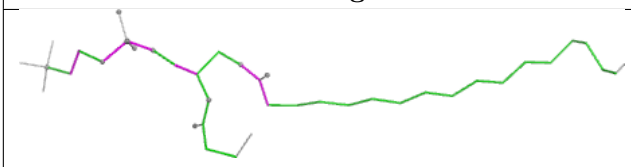
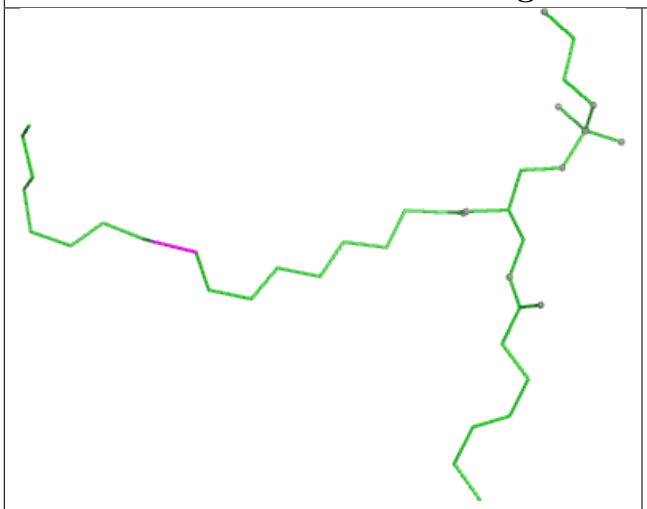


Torsions



Rings

Ligand PEE 4D 101



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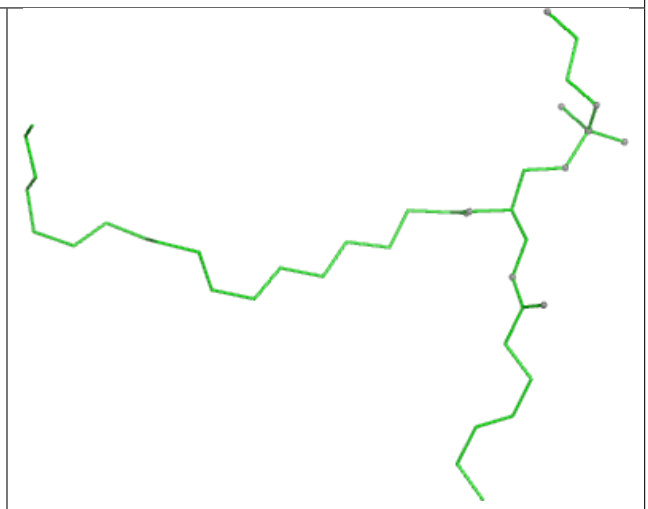

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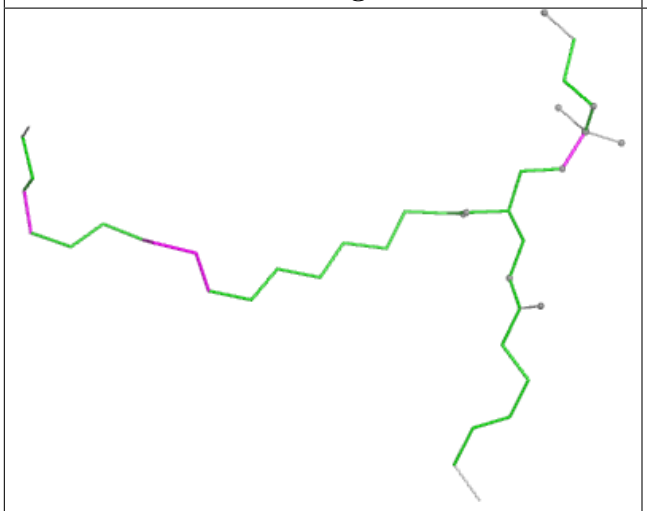


Torsions

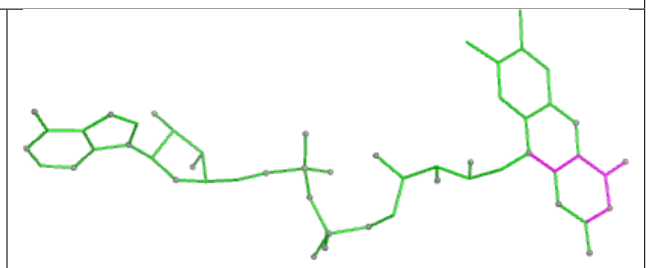


Rings

Ligand FAD 2M 701



Bond lengths



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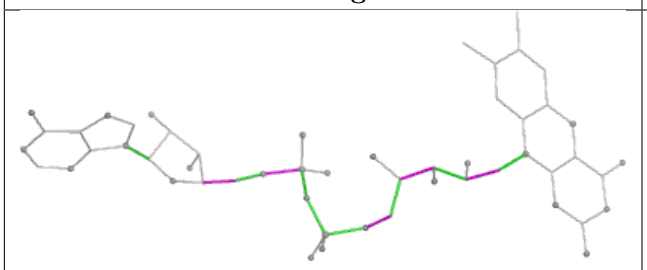

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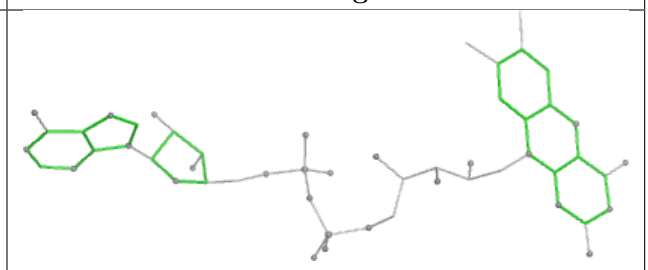
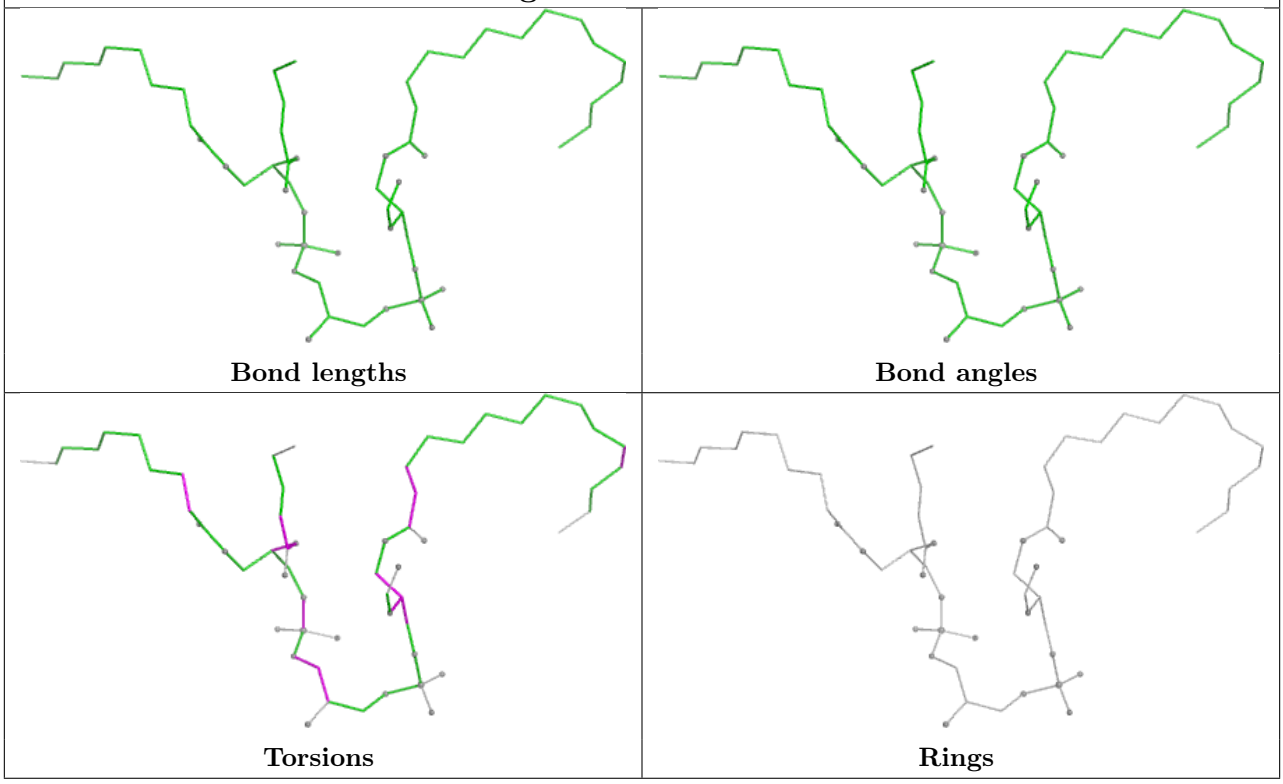
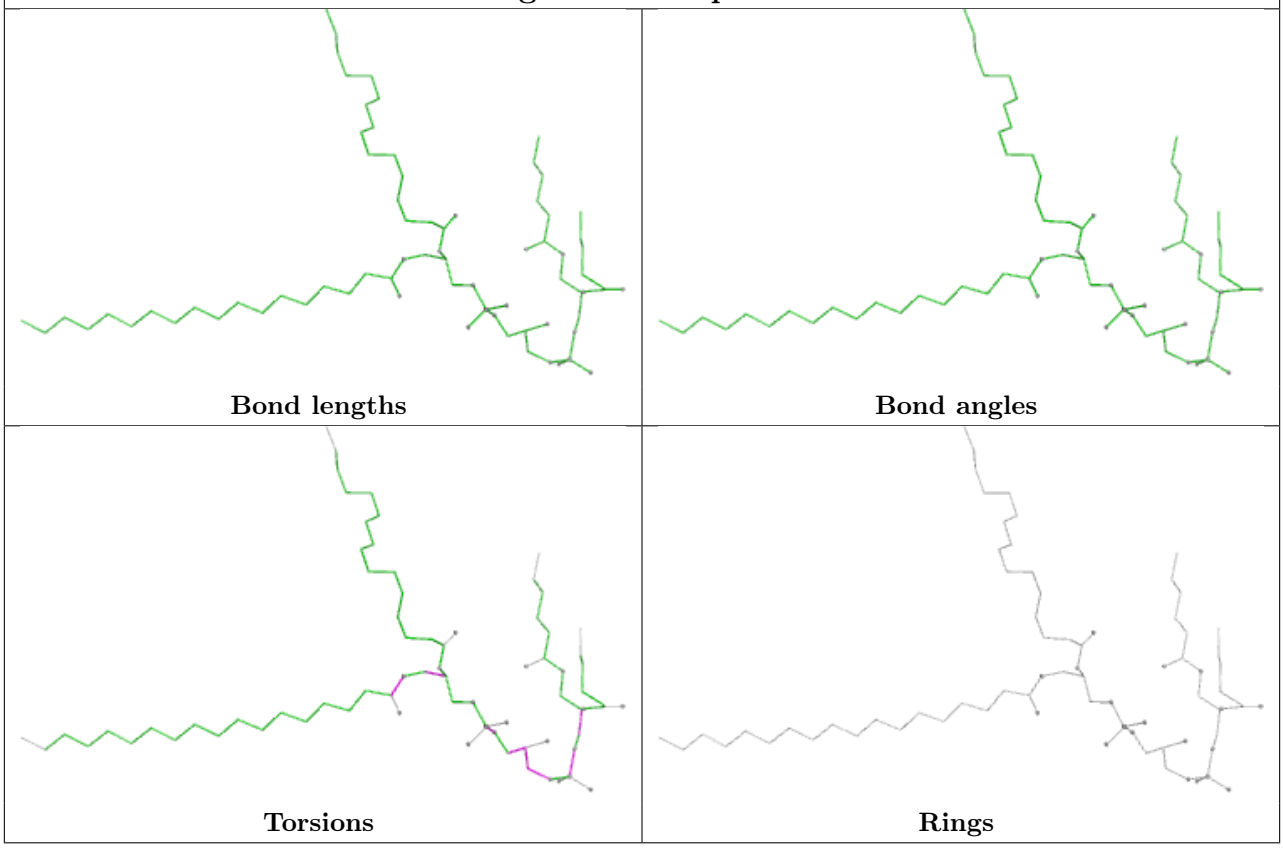


Rings

Ligand CDL 4J 301



Ligand CDL 2p 204



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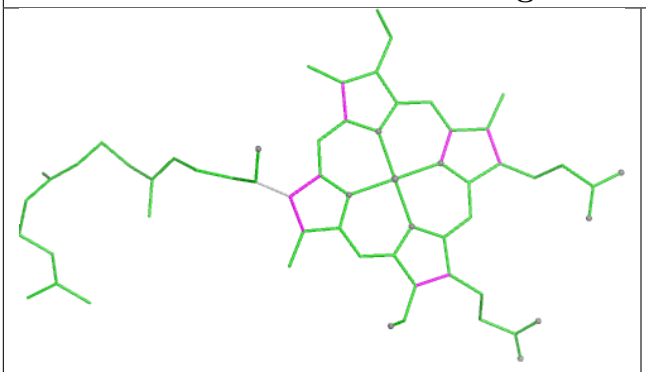
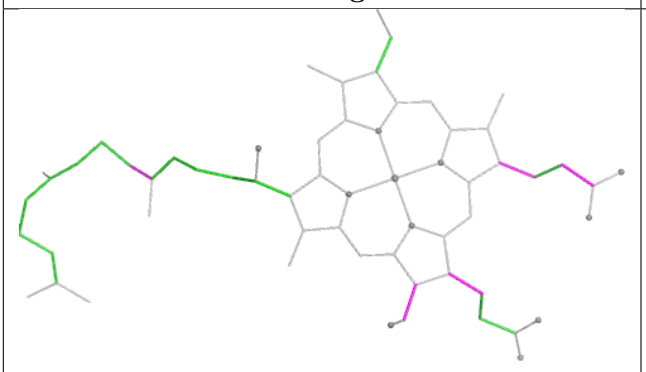


Bond lengths



Bond angles



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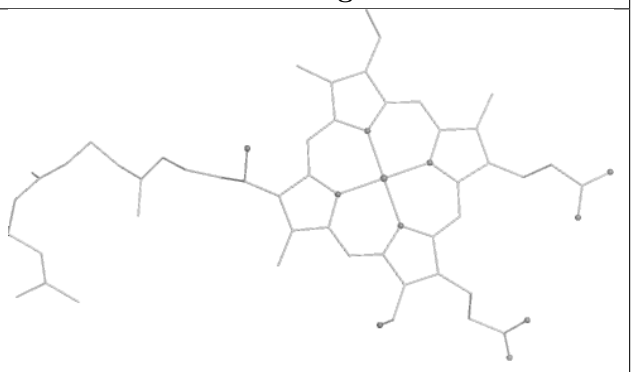
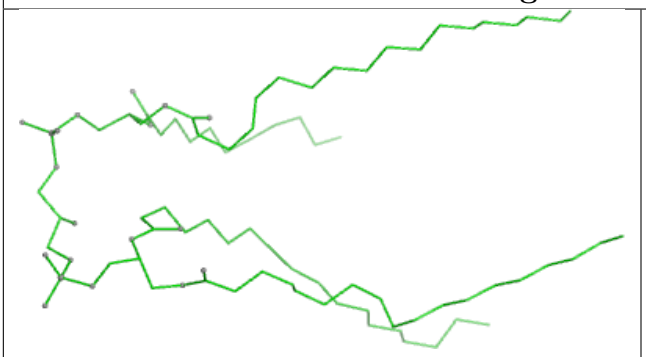


Rings

Ligand CDL 4z 303



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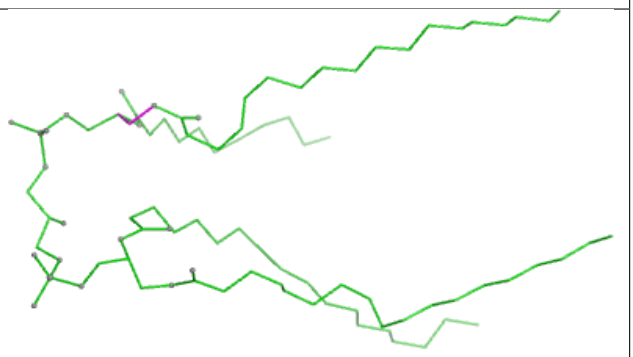

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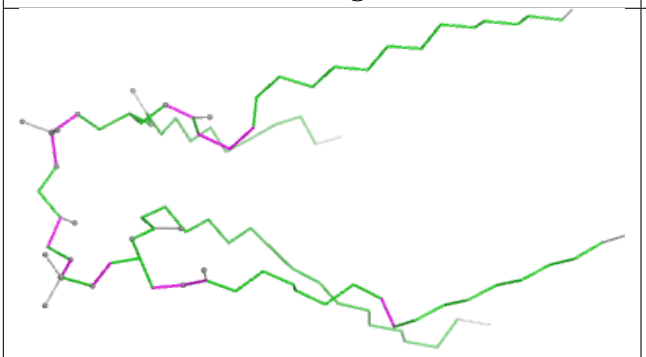

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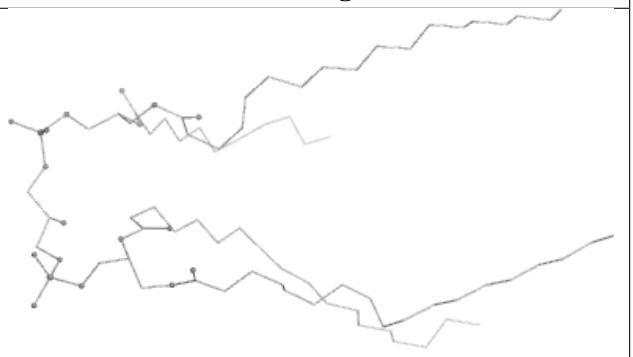
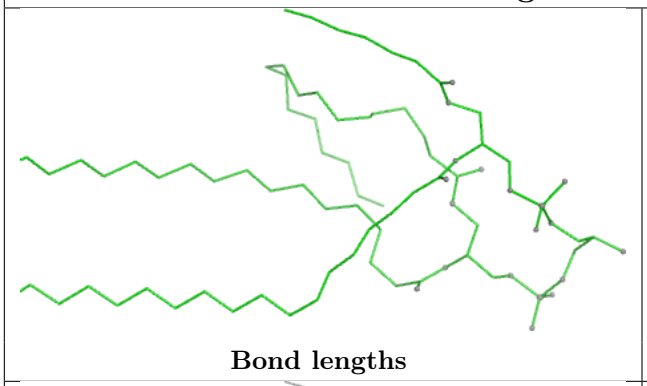


Rings

Ligand CDL 4E 201



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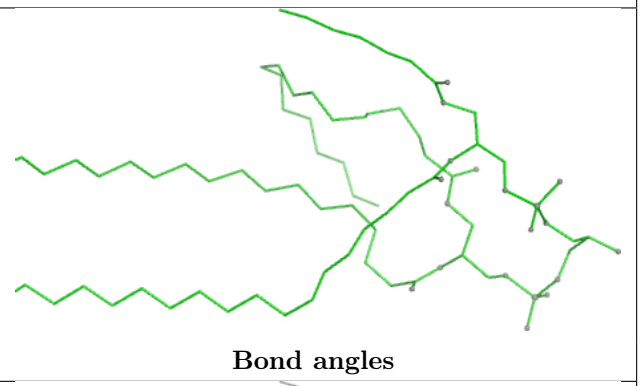

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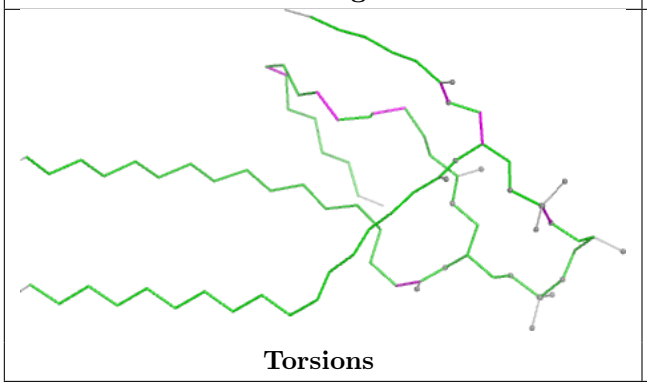

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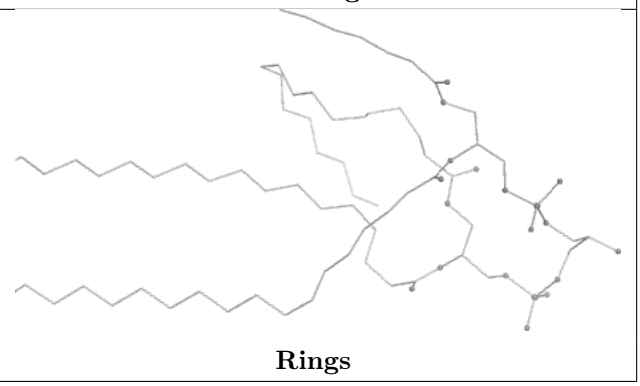
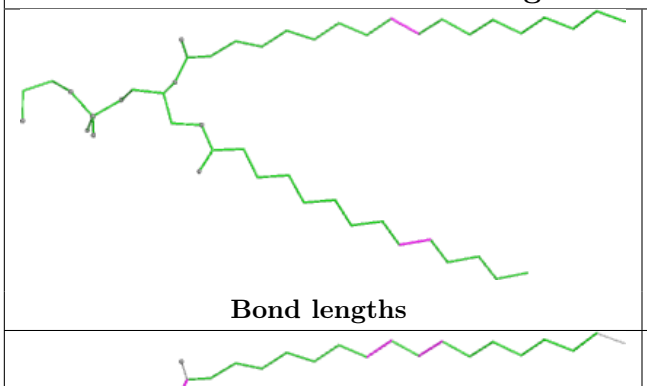


Rings

Ligand PEE 4s 101



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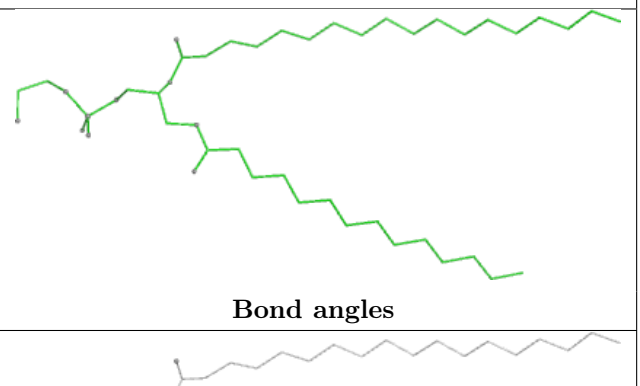

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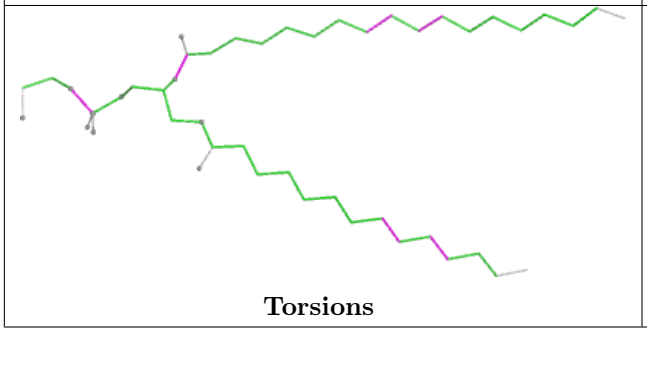

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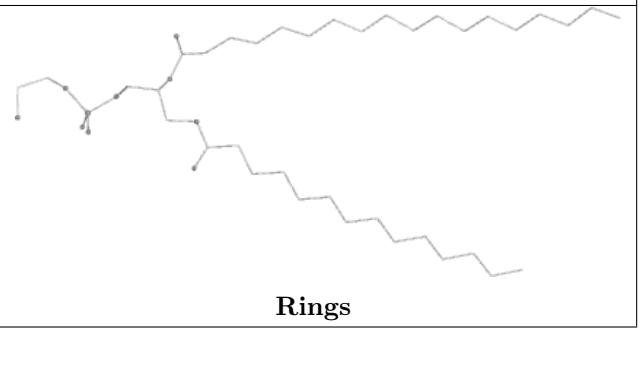
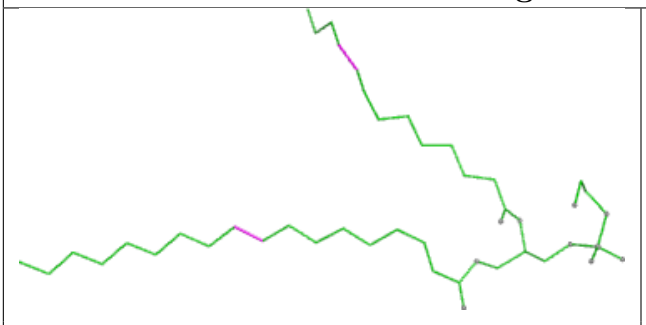


Rings

Ligand PEE 3H 403



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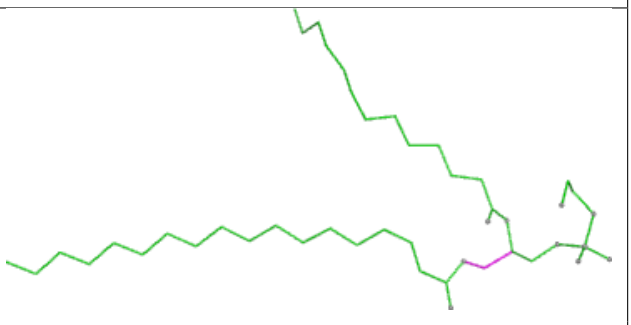
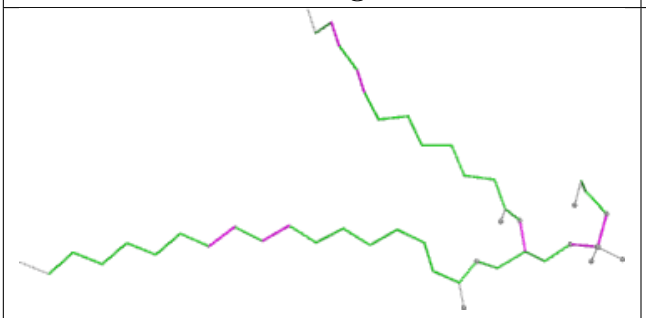


Bond angles



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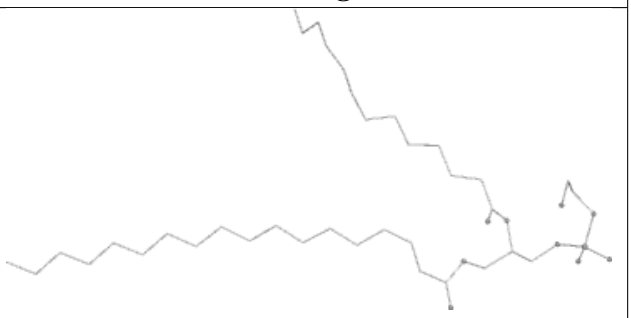
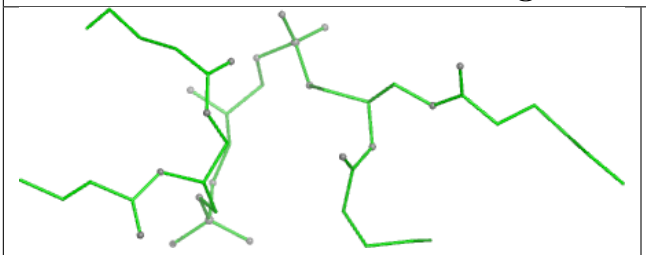


Rings

Ligand CDL 4Z 303



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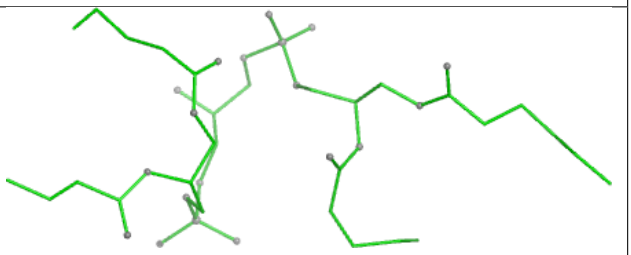

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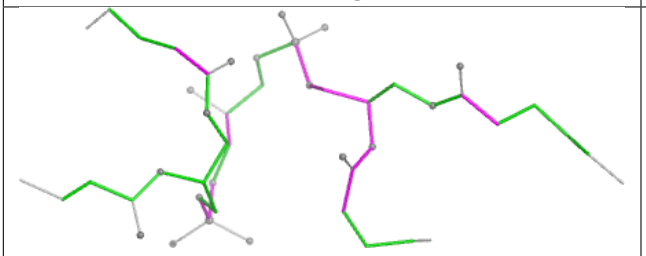

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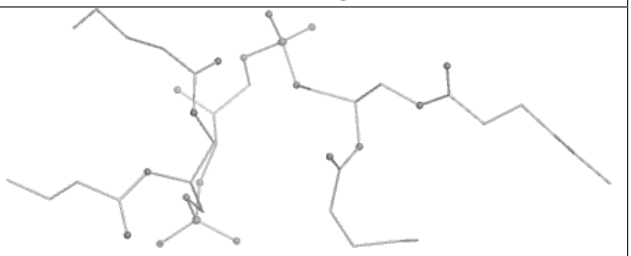

Rings

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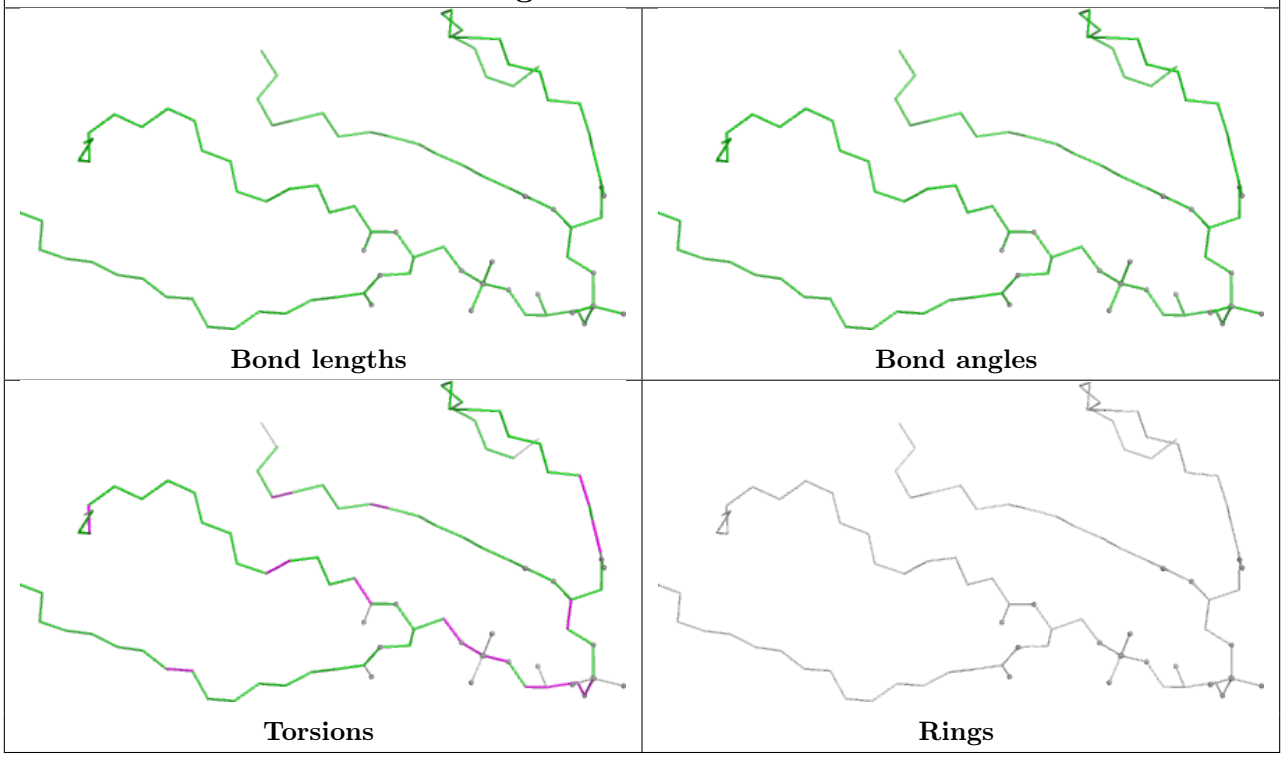

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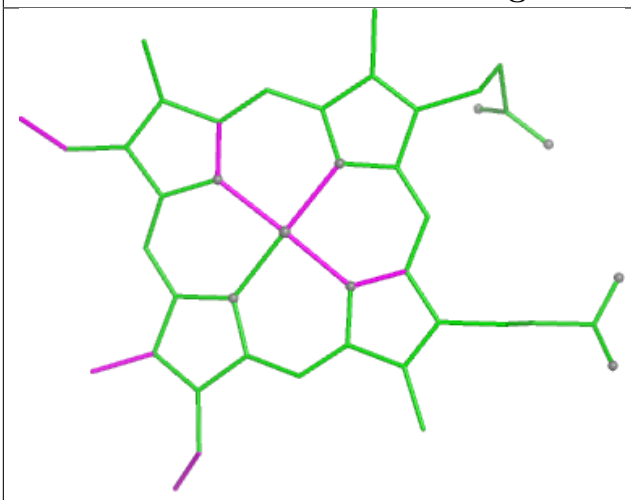

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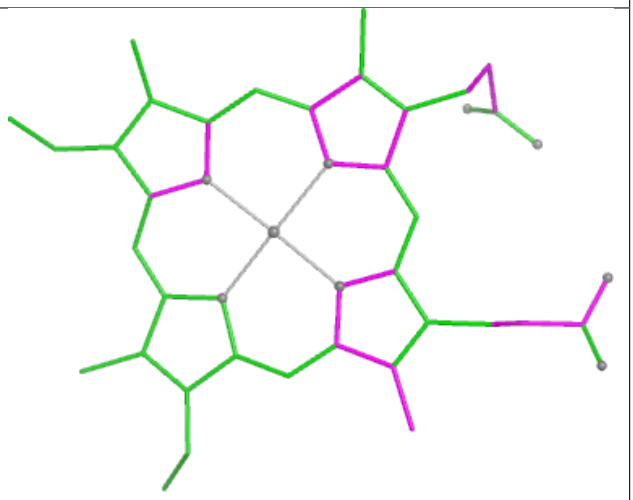
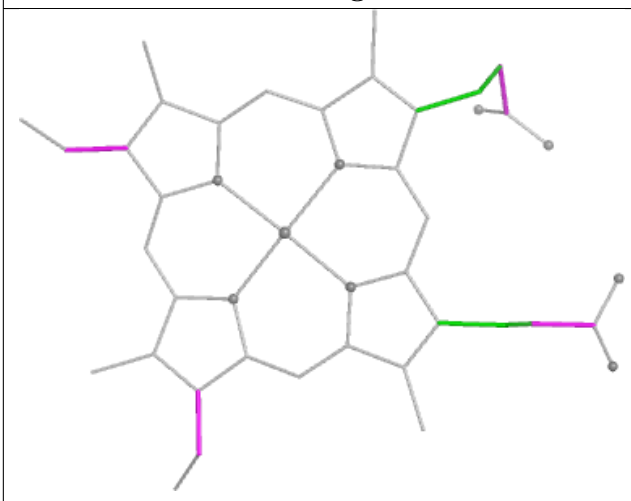


Bond angles



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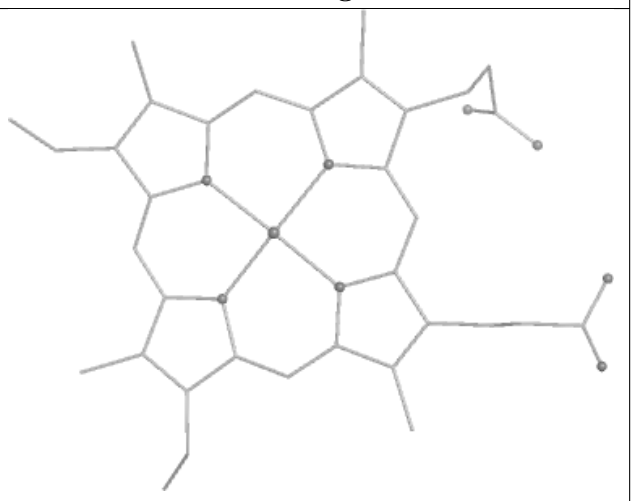
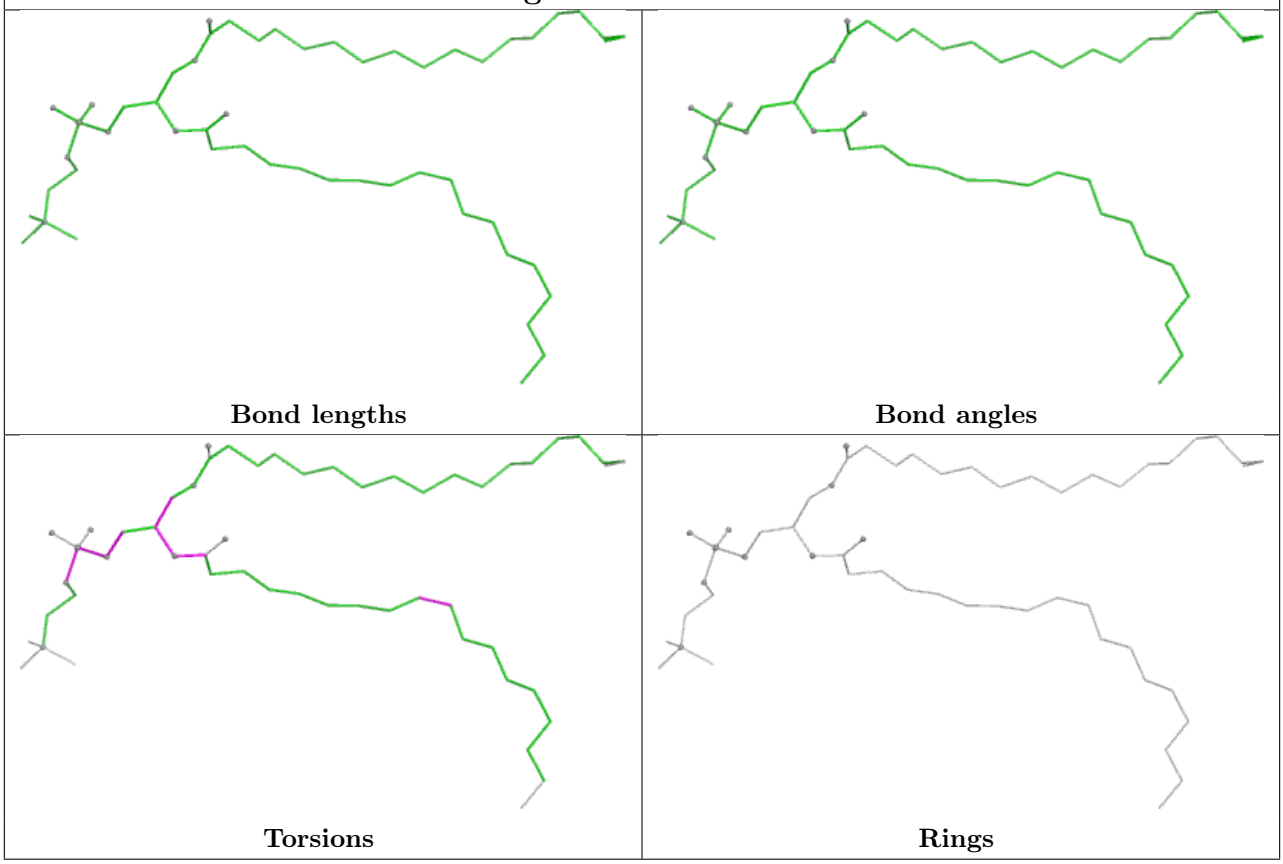
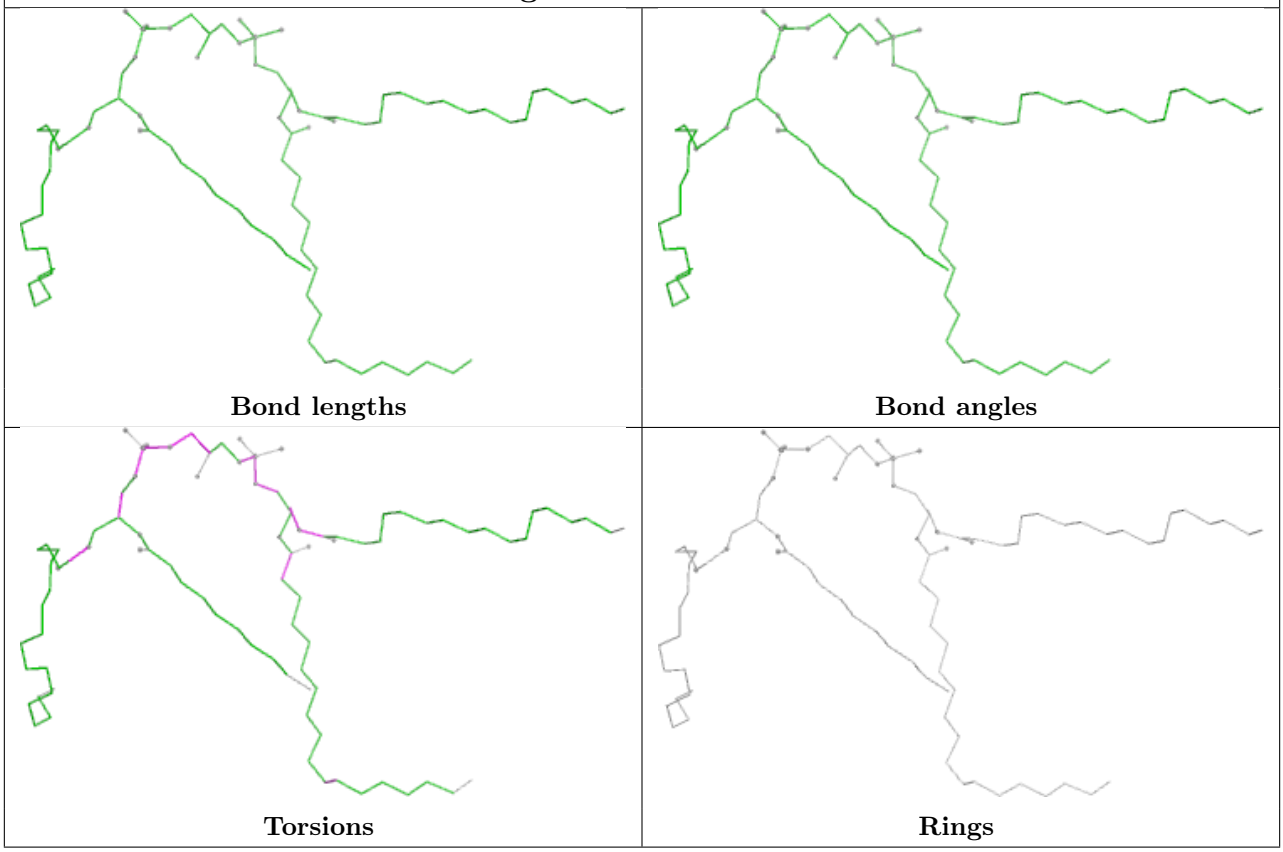


Rings

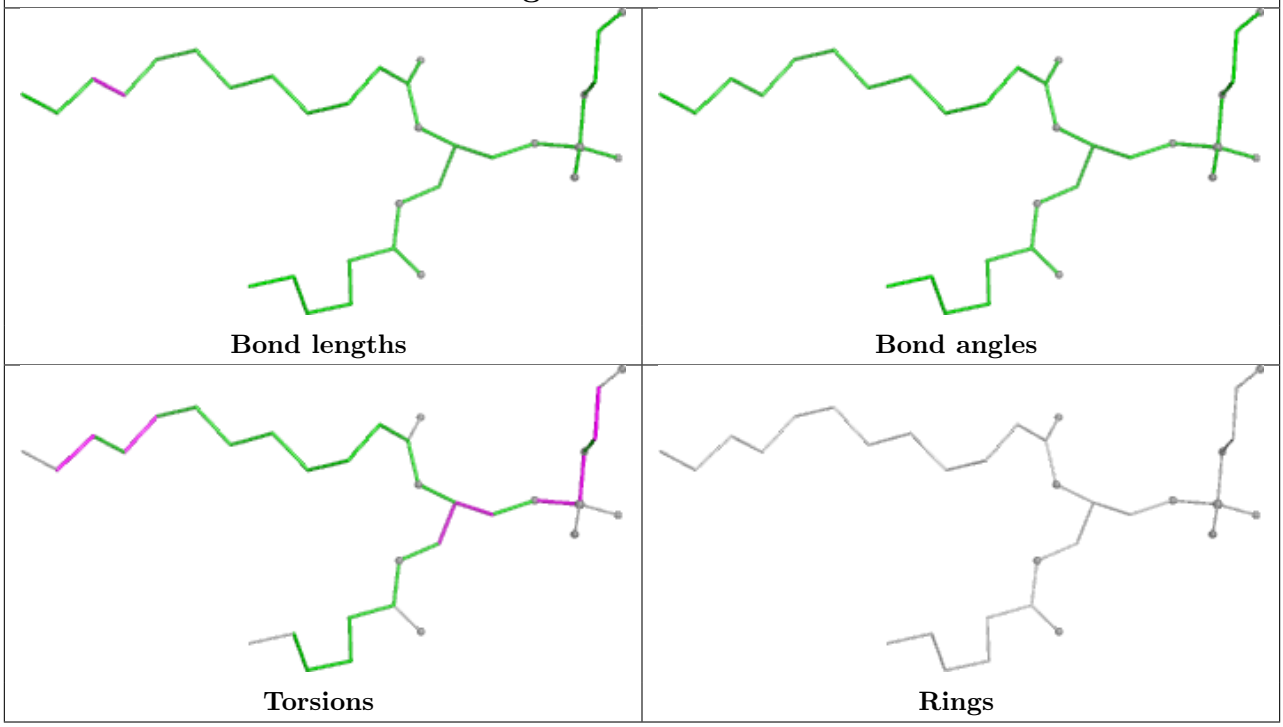
Ligand PC1 4e 201



Ligand CDL 41 304



Ligand PEE 3c 301



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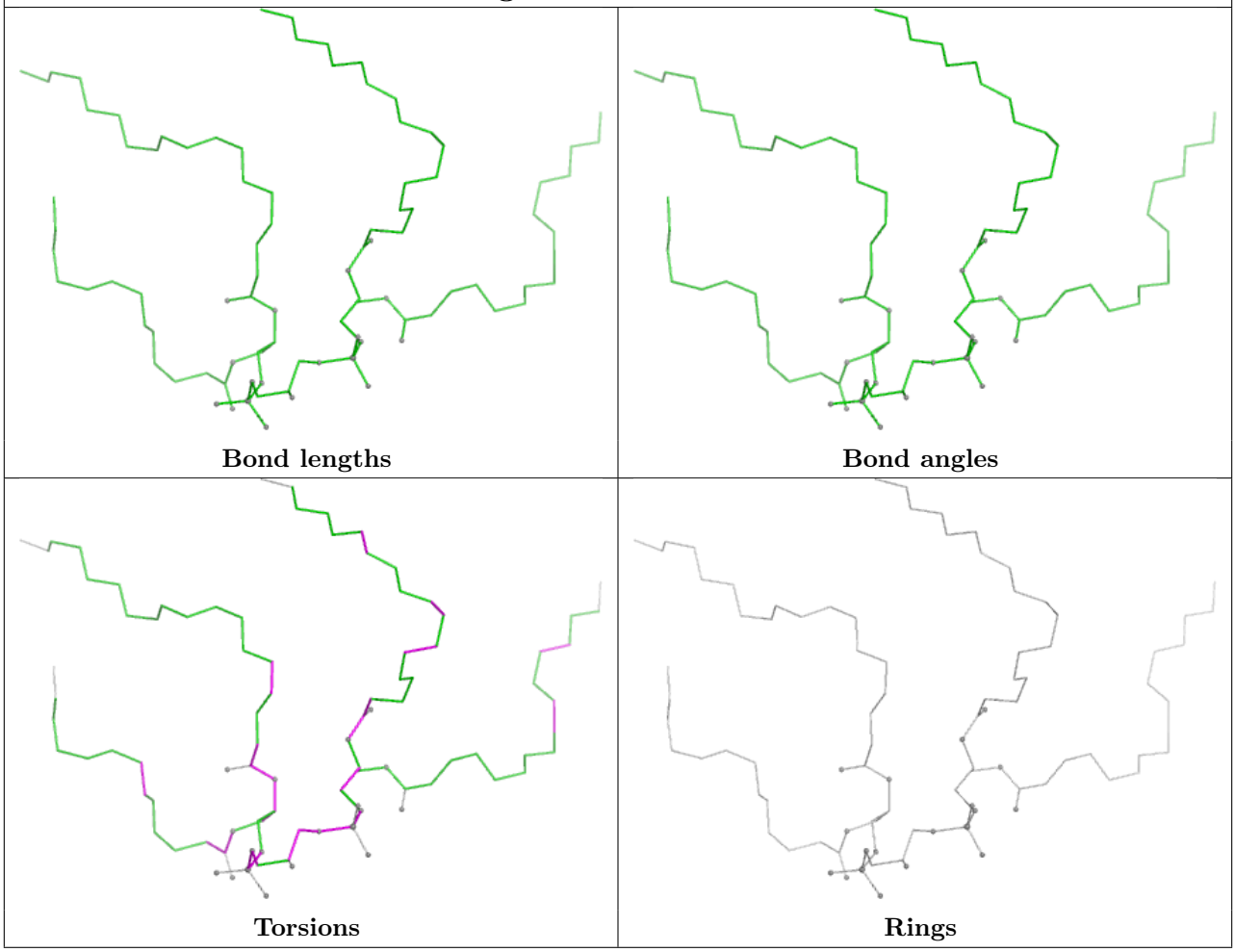

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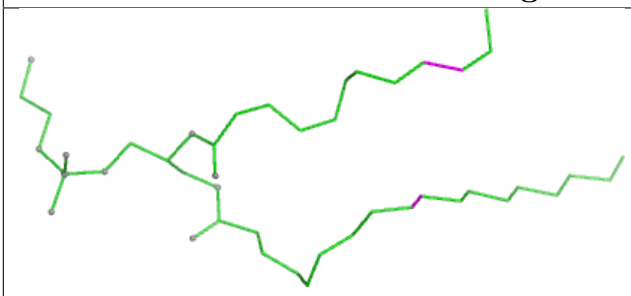

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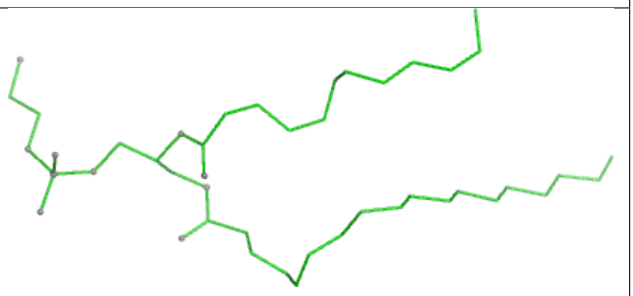
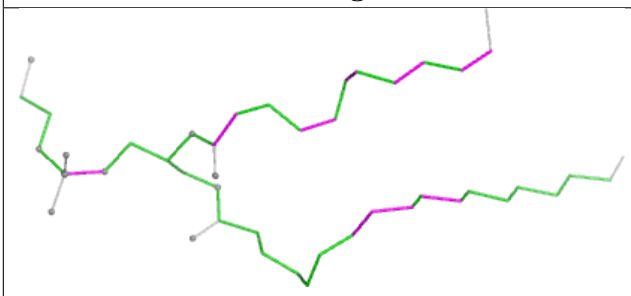


Bond angles



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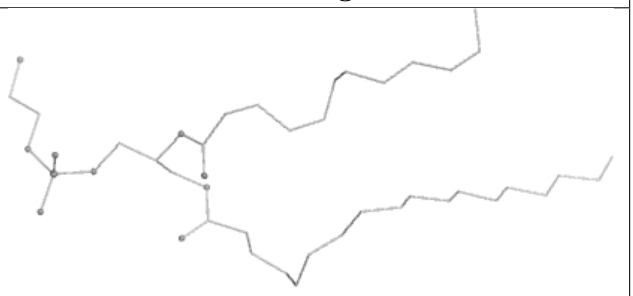
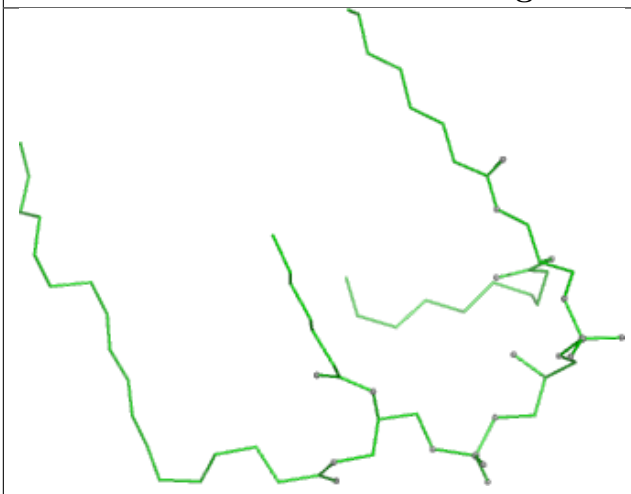


Rings

Ligand CDL 2T 104



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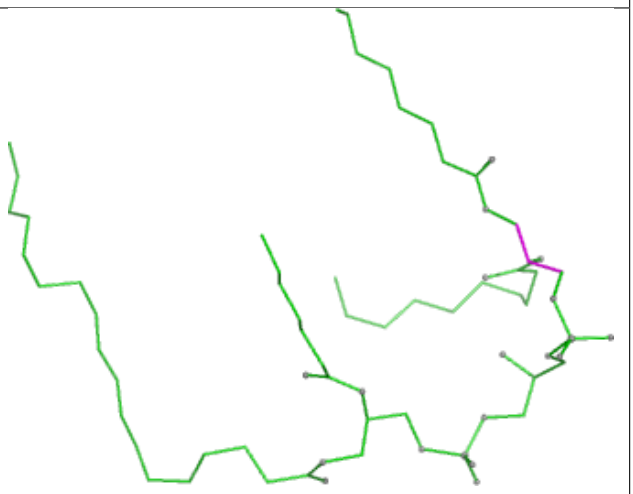
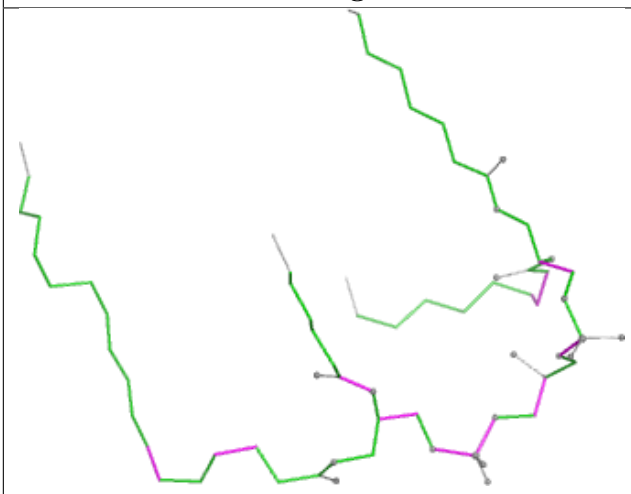


Bond angles

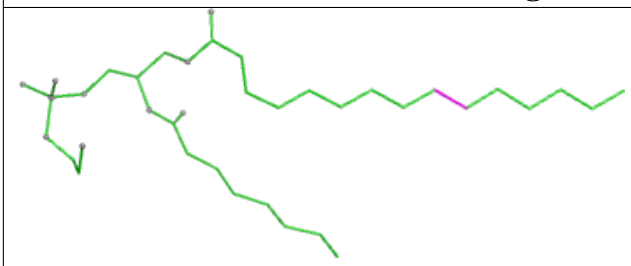


Torsions



Rings

Ligand PEE 3f 102



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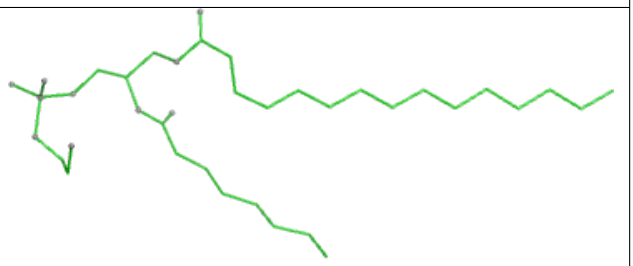
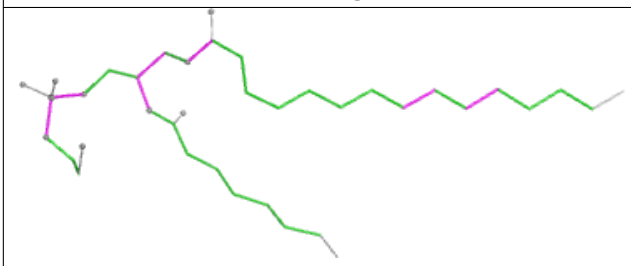


Bond angles



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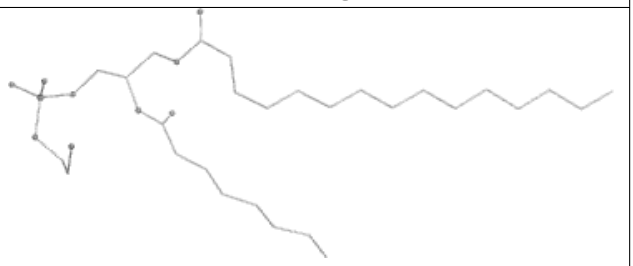
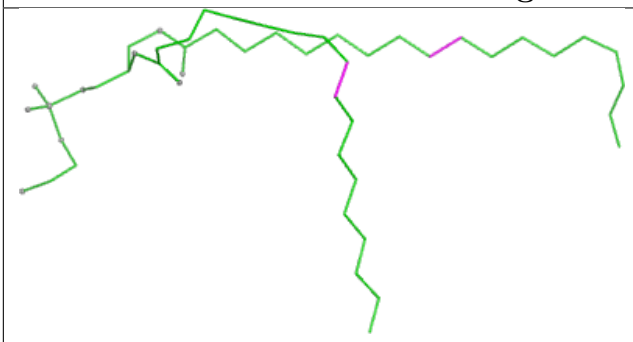
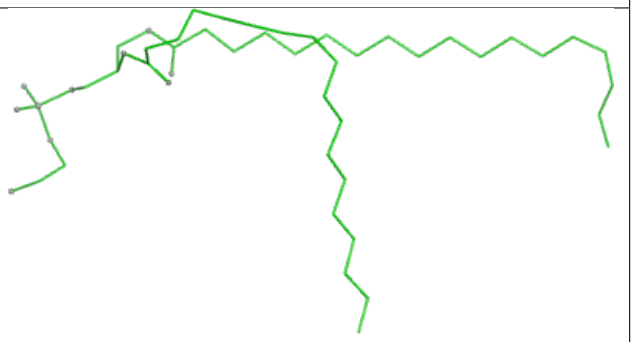


Rings

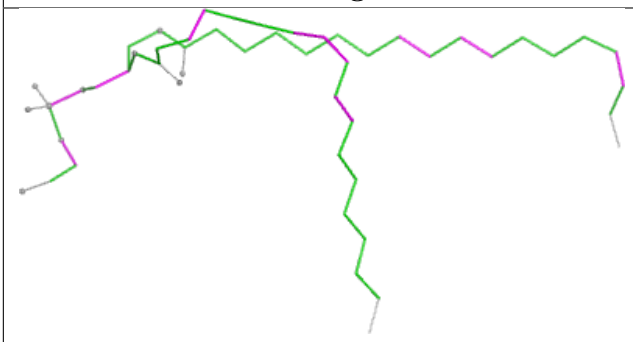
Ligand PEE 4w 201



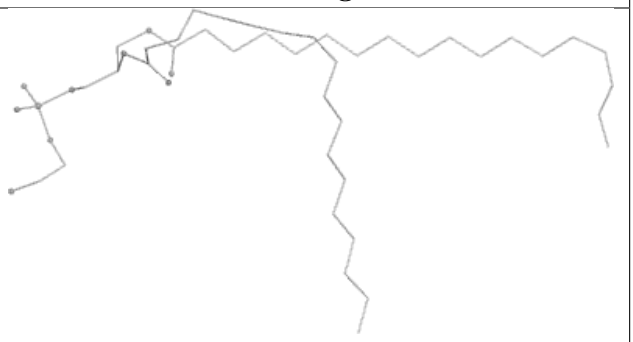
Bond lengths



Bond angles

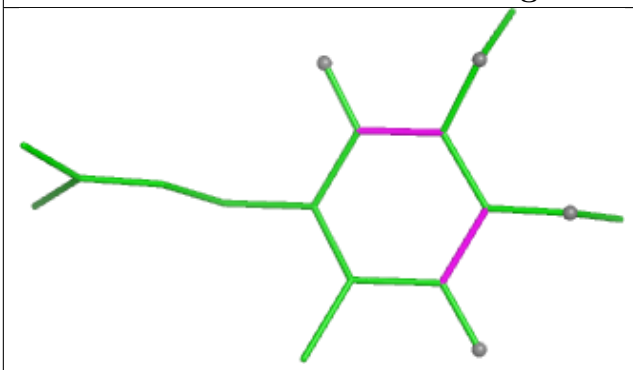


Torsions



Rings

Ligand UQ1 3g 402



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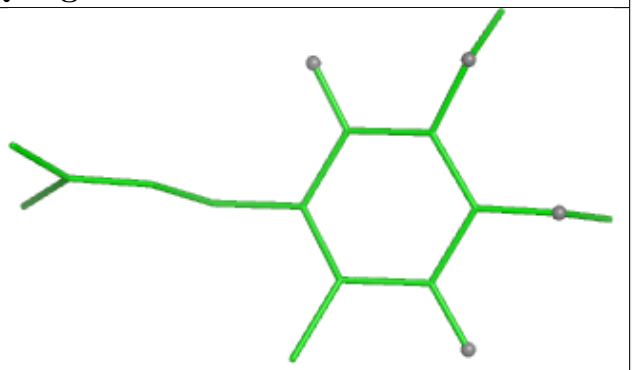
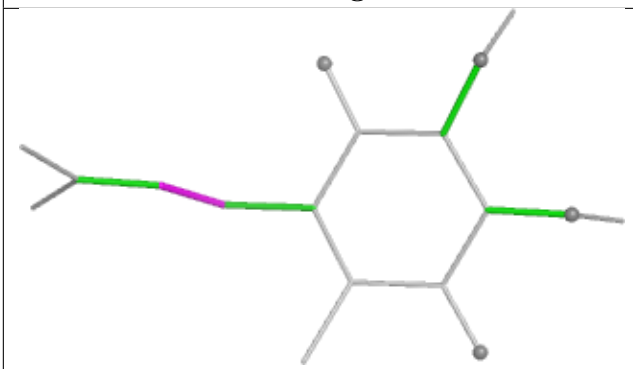


Bond angles



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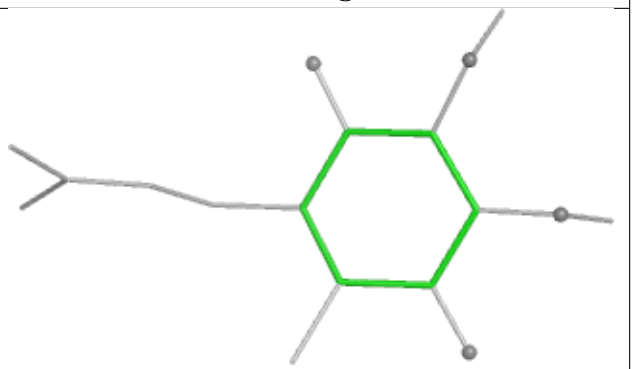
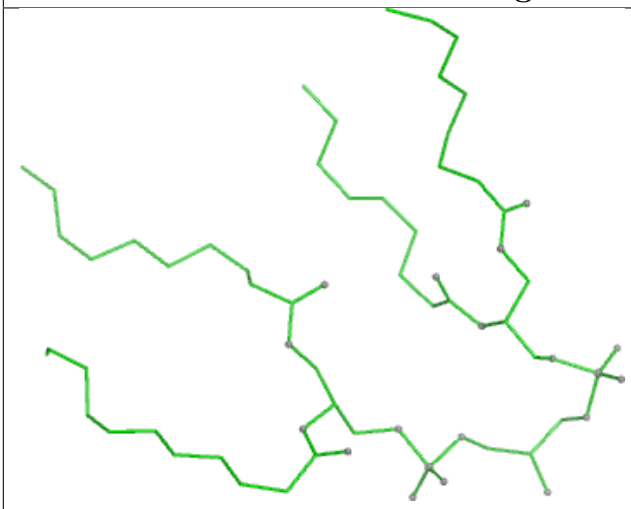


Rings

Ligand CDL 2O 203



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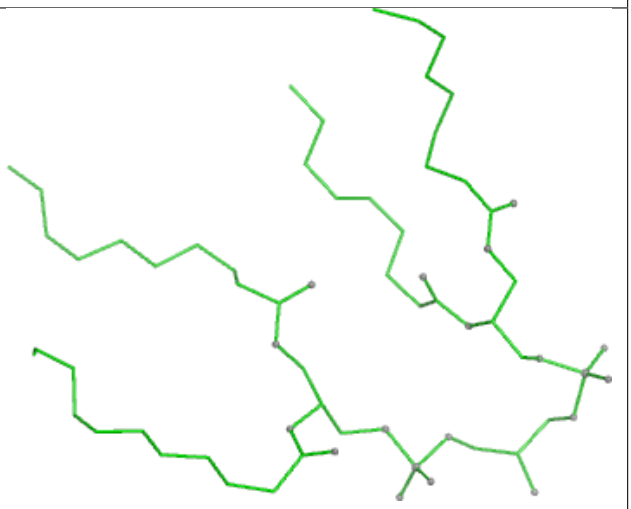

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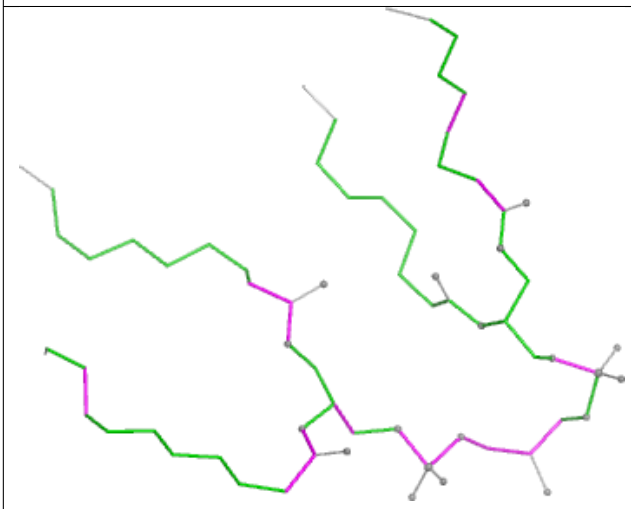

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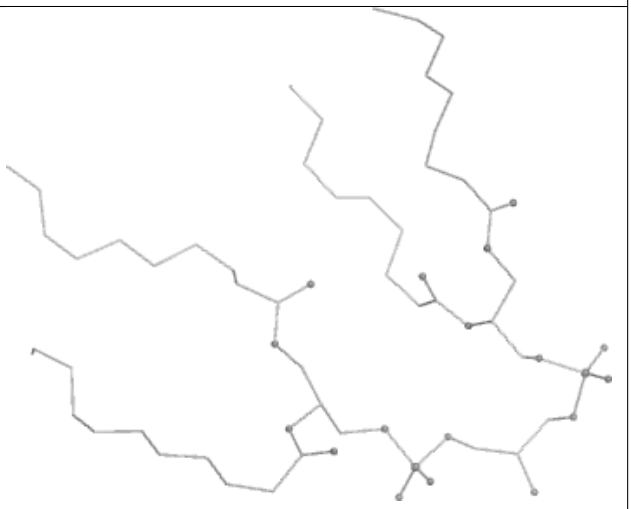
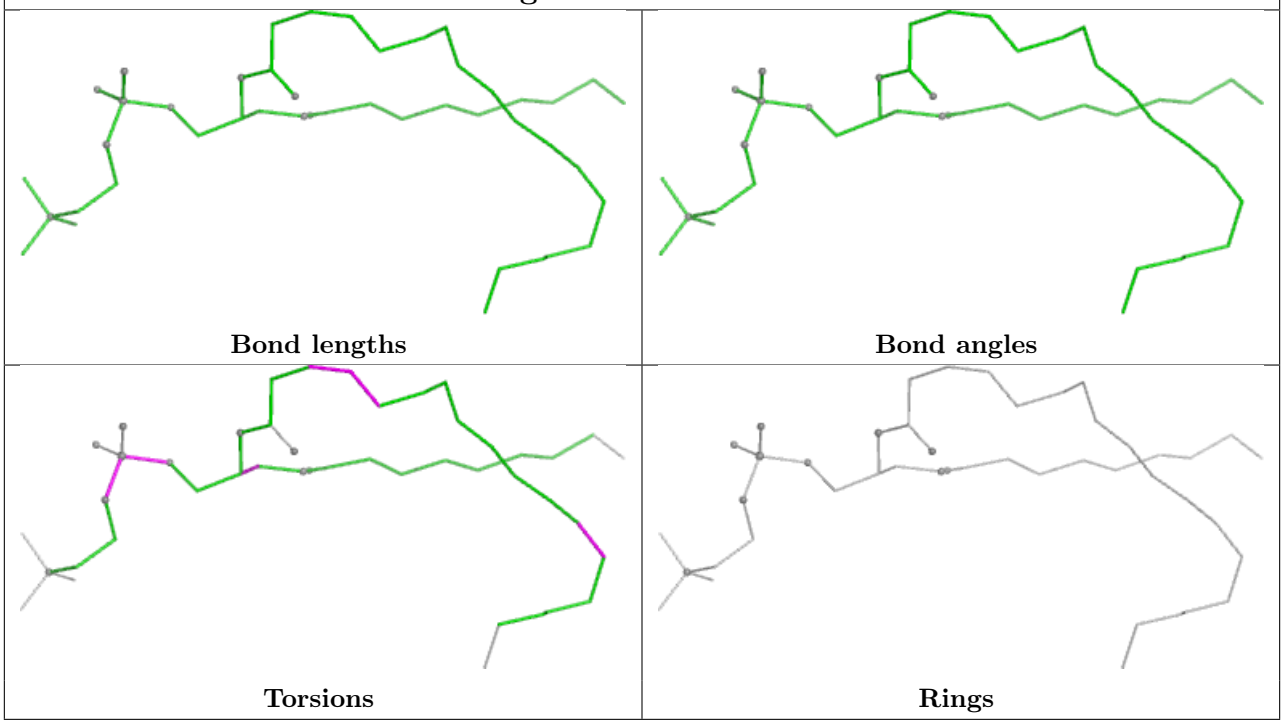
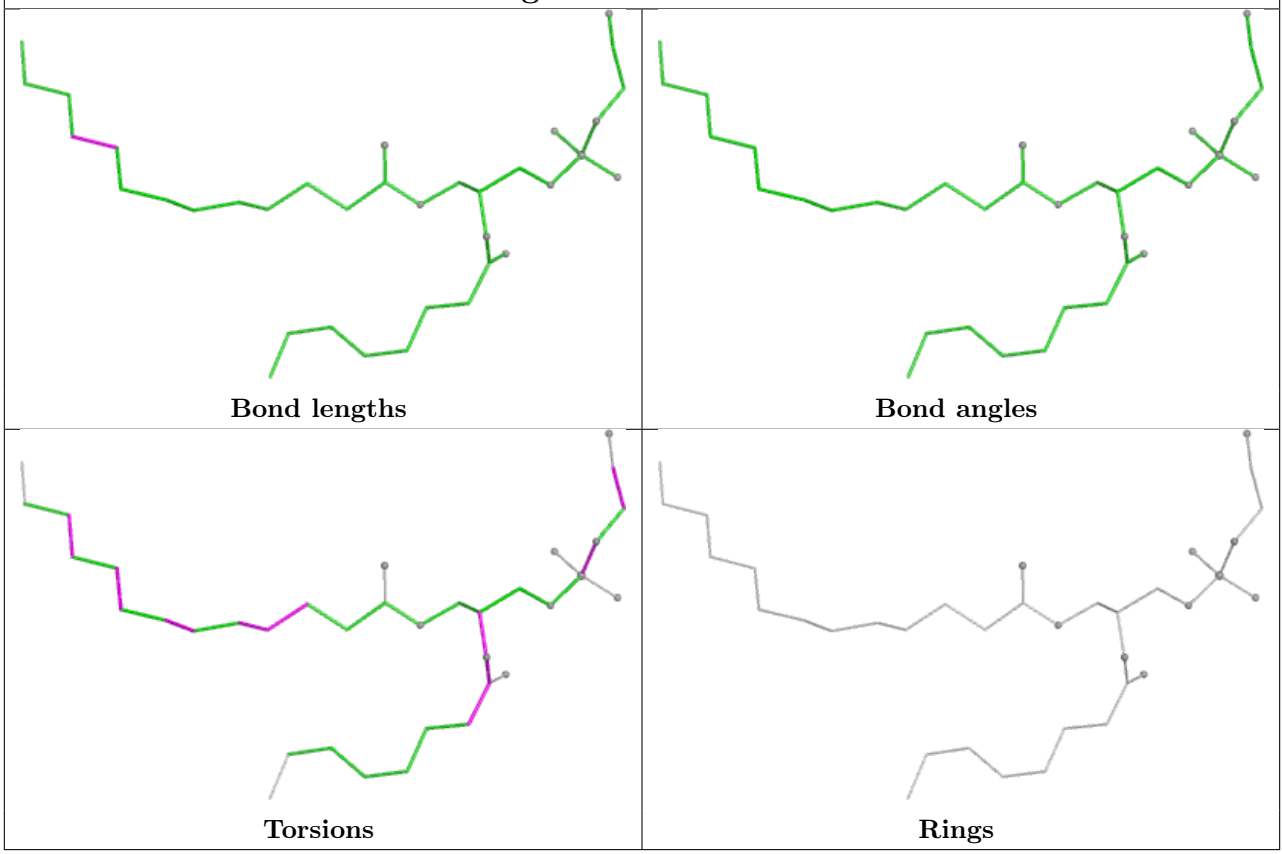


Rings

Ligand PC1 2T 102



Ligand PEE 41 303



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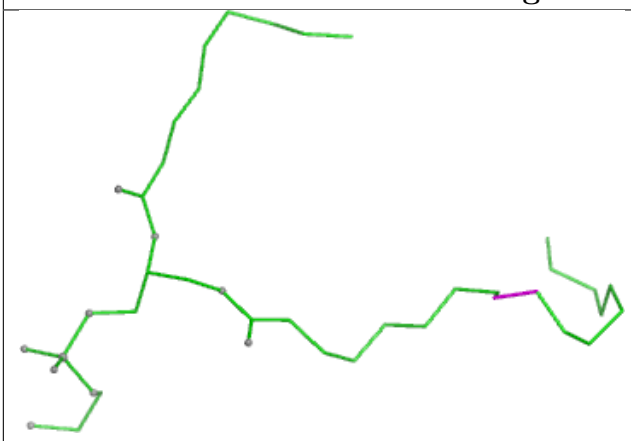

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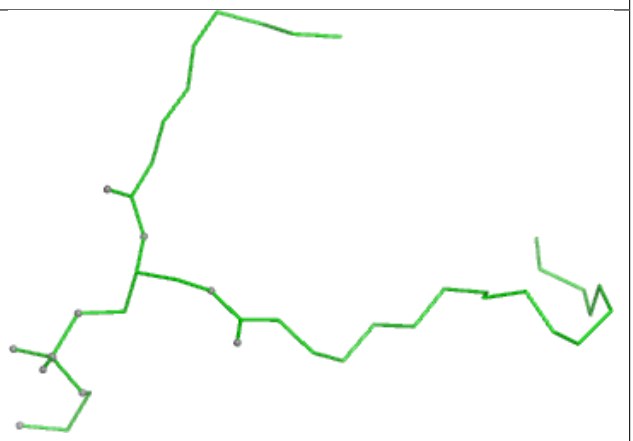
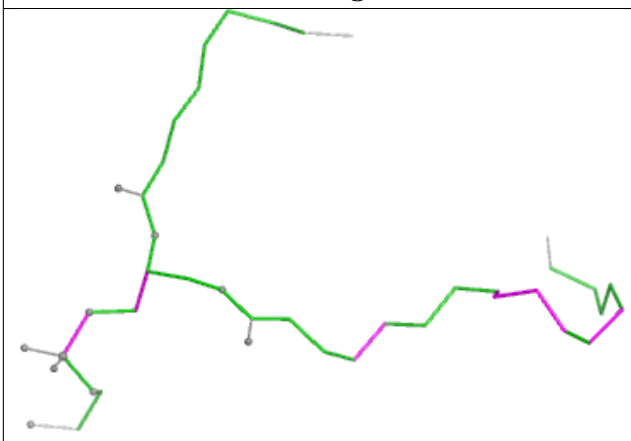


Bond angles



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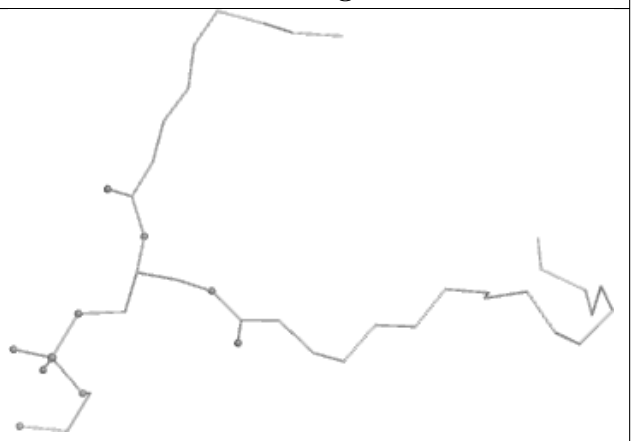
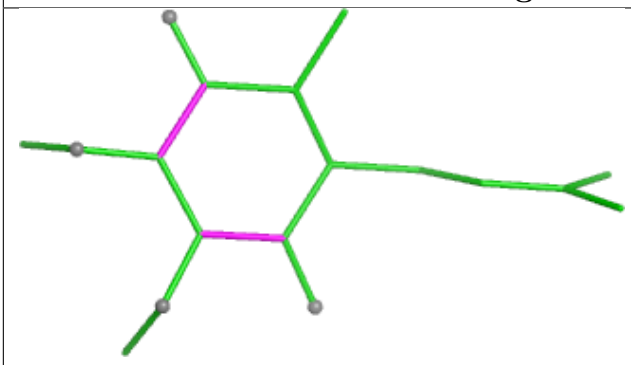


Rings

Ligand UQ1 3G 402



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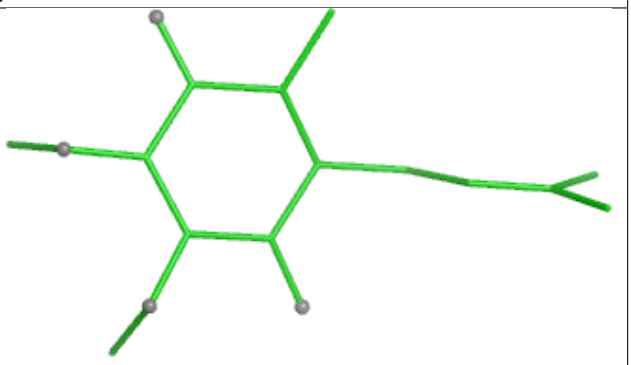

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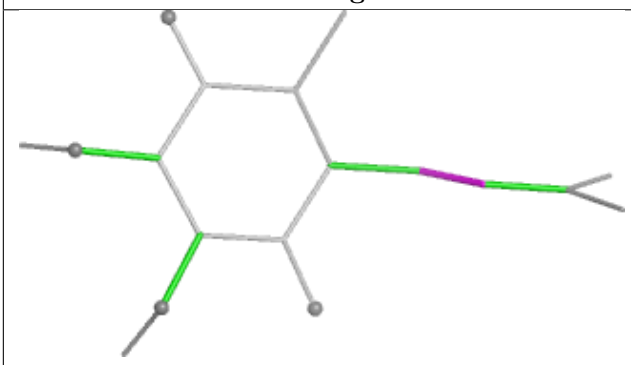

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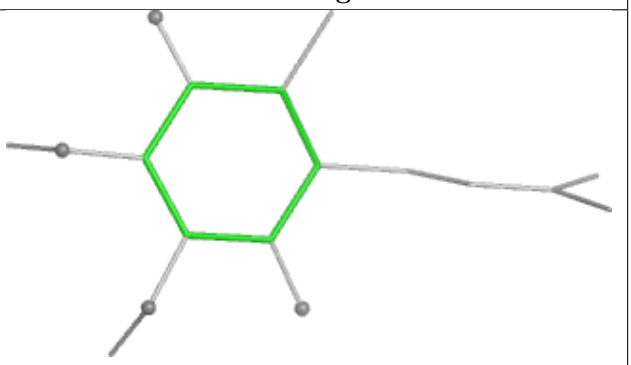
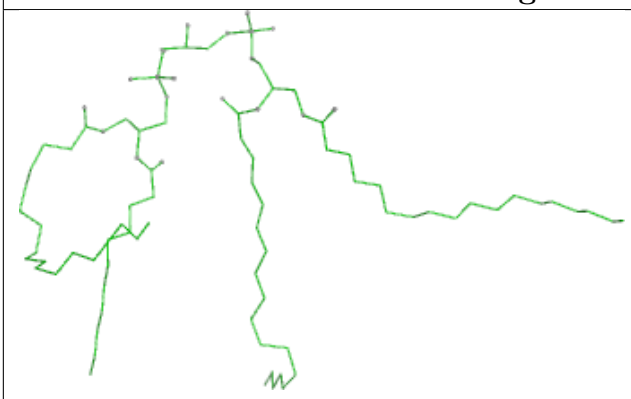


Rings

Ligand CDL 4q 903



Bond lengths



Bond angles

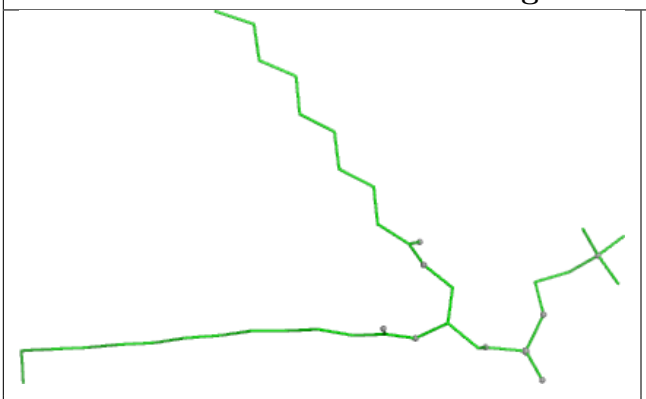


Torsions



Rings

Ligand PC1 2p 202



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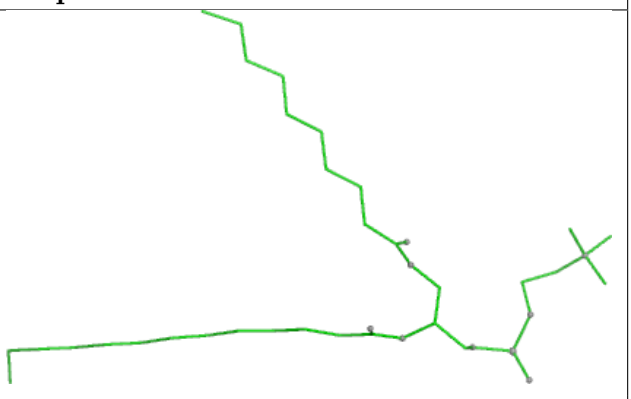


Bond angles

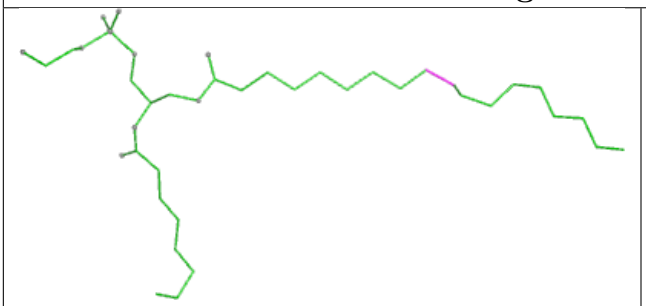


Torsions



Rings

Ligand PEE 2O 202



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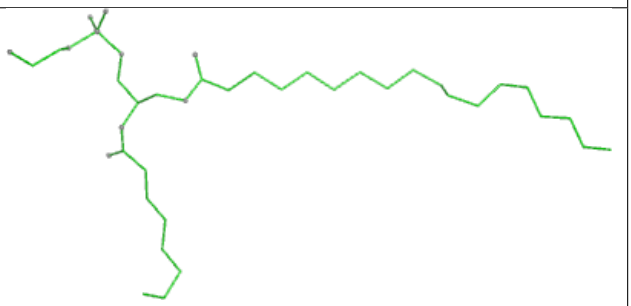
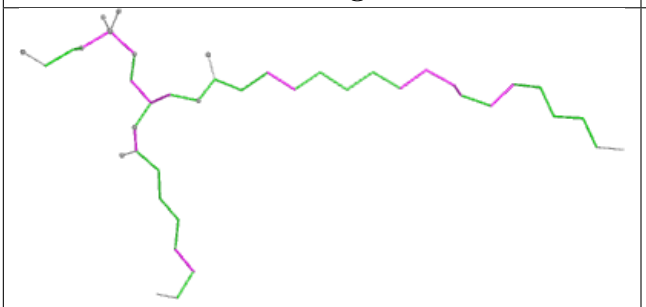


Bond angles



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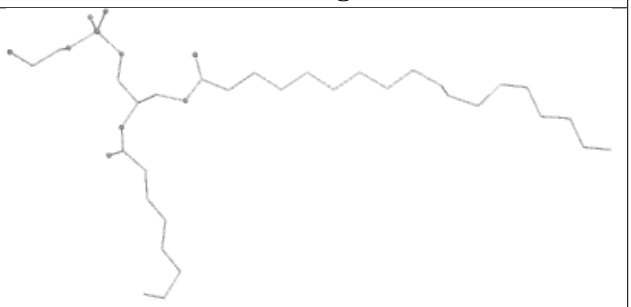
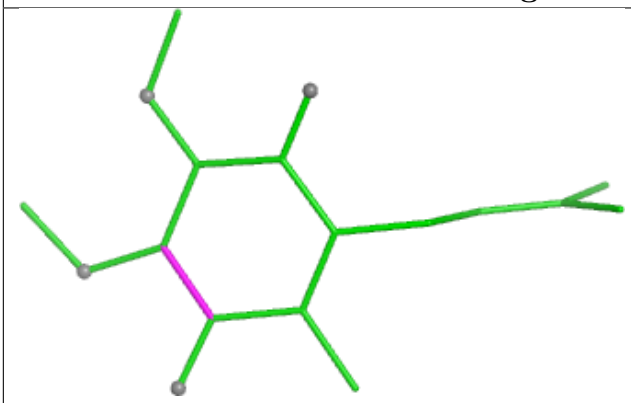


Rings

Ligand UQ1 3g 401



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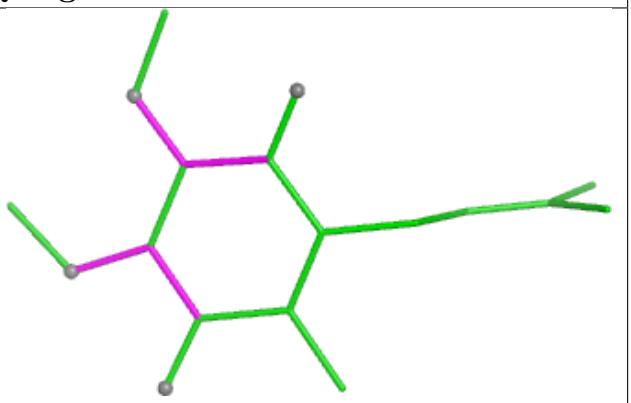

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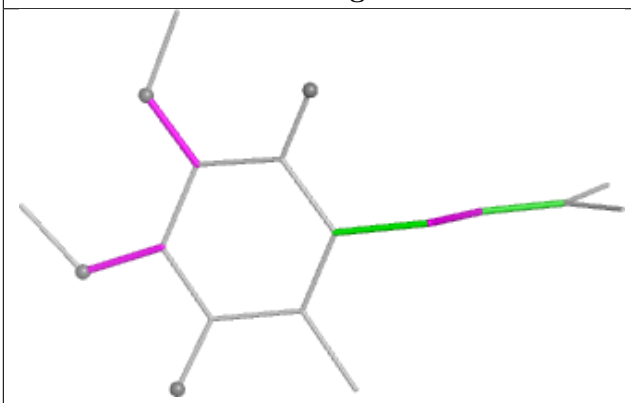

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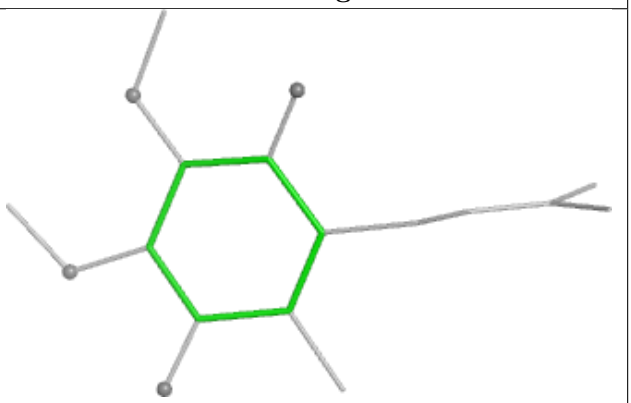
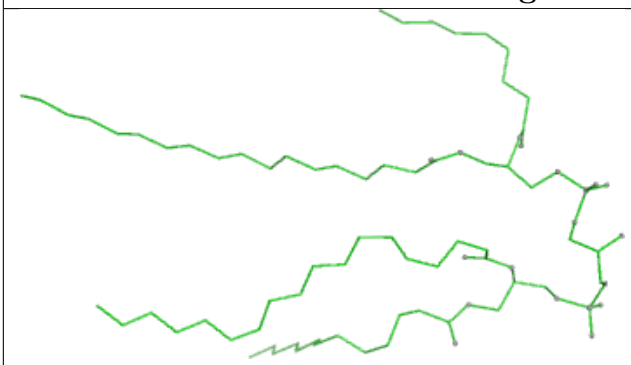


Rings

Ligand CDL 2o 201



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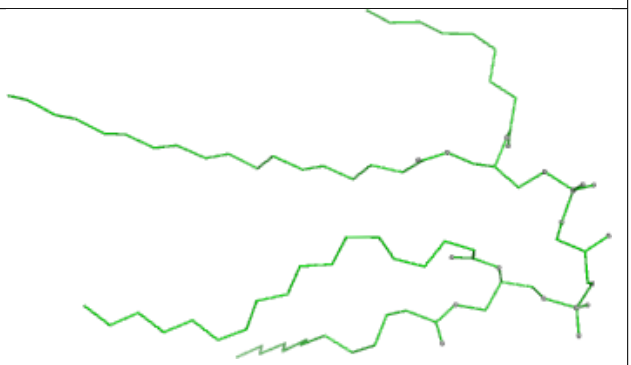
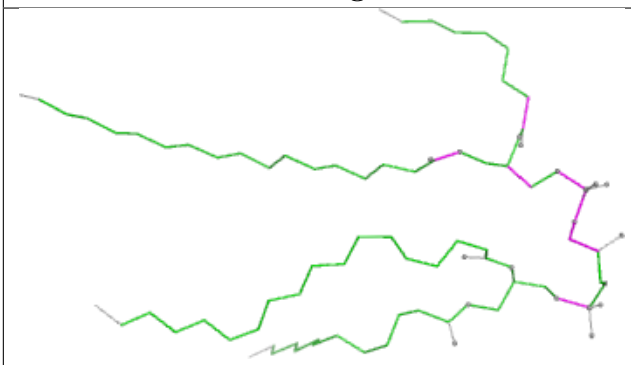


Bond angles

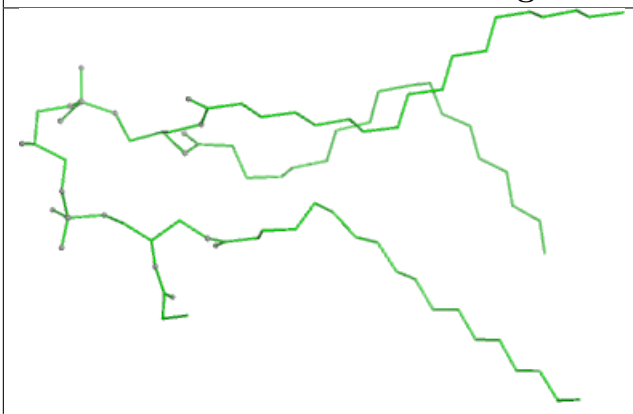


Torsions



Rings

Ligand CDL 3L 701



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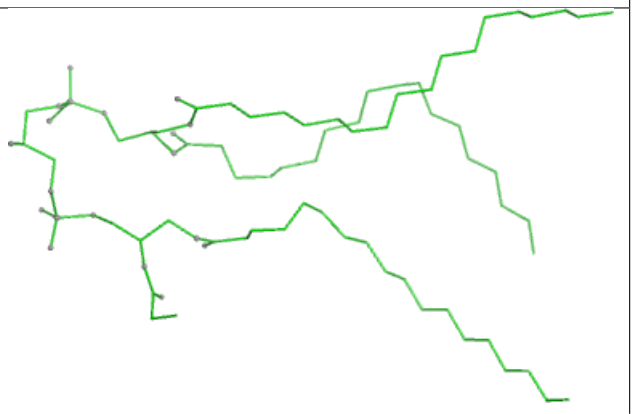
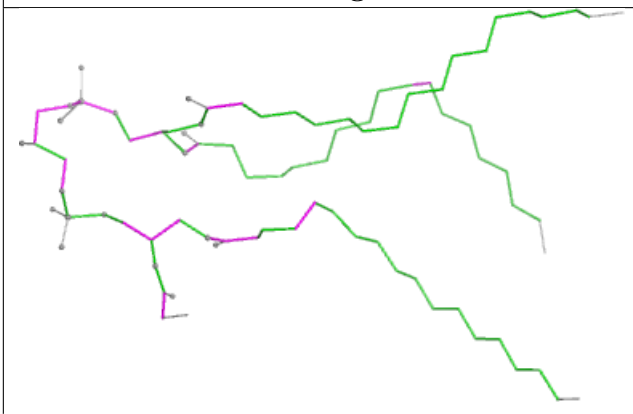


Bond angles

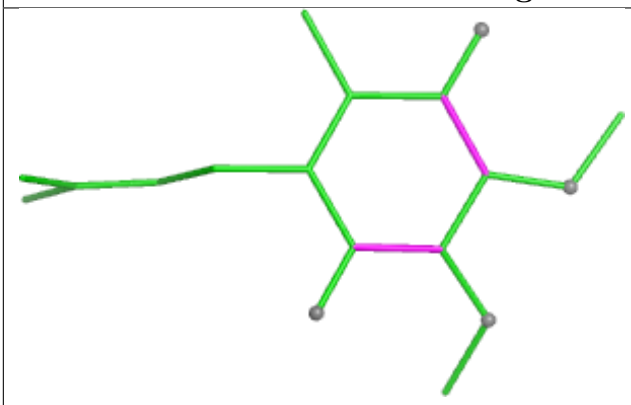


Torsions



Rings

Ligand UQ1 3G 401



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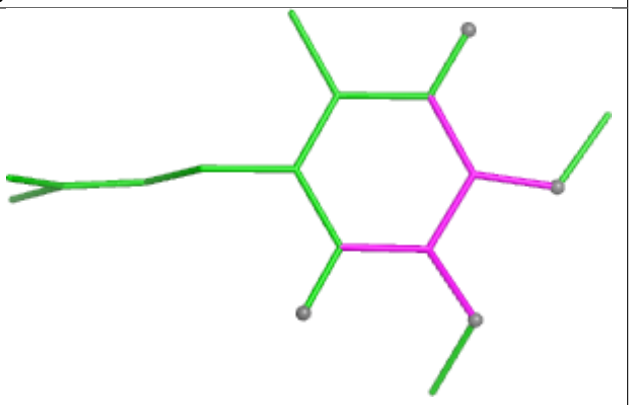

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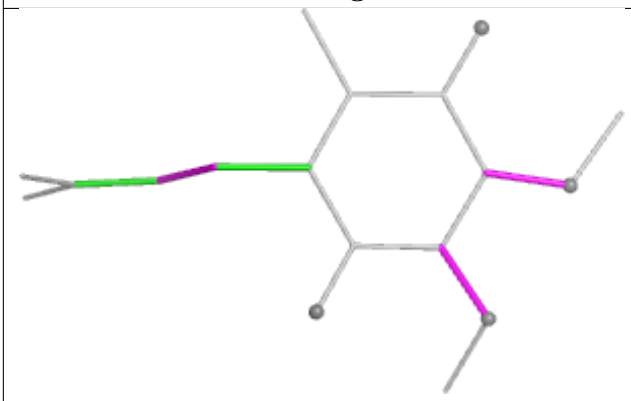

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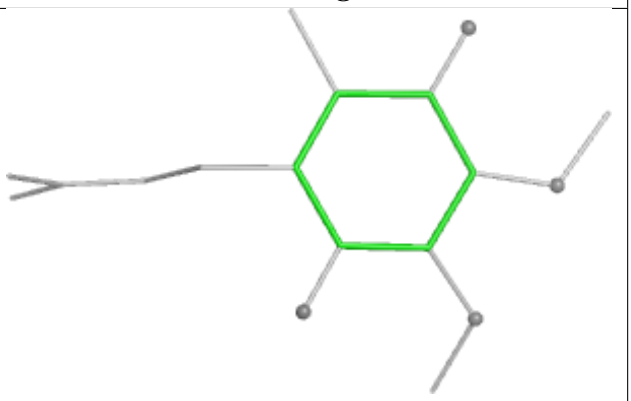
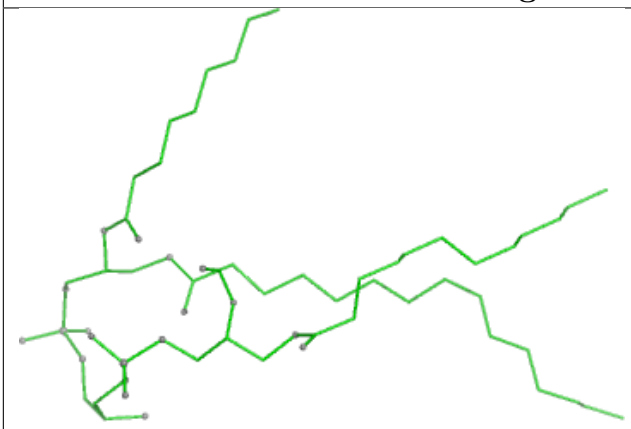


Rings

Ligand CDL 4g 202



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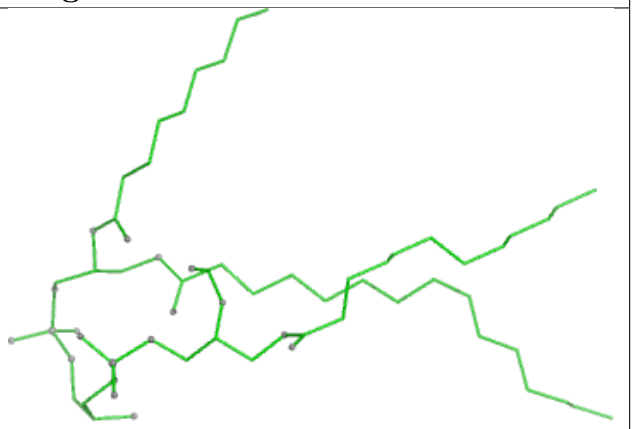
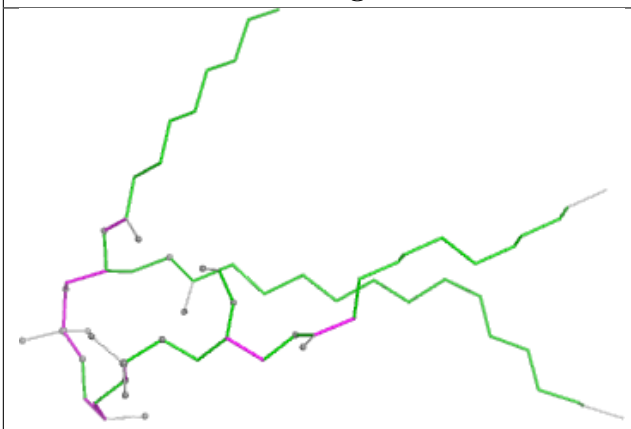


Bond angles

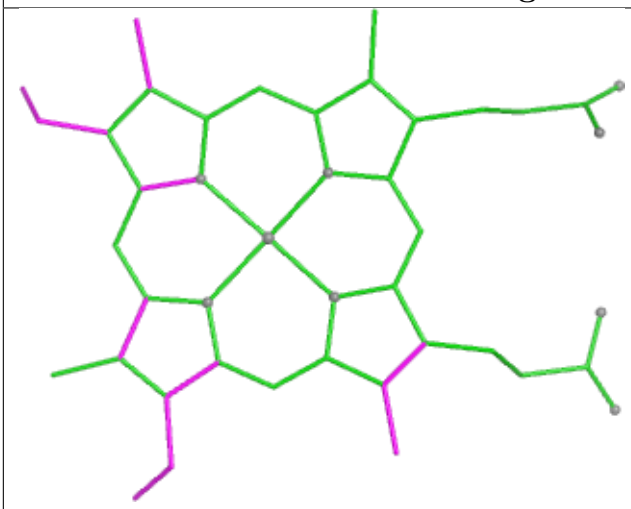


Torsions



Rings

Ligand HEC 3c 302



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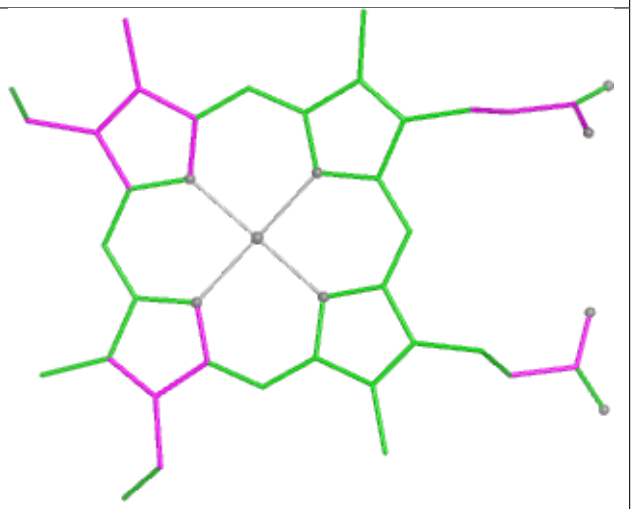
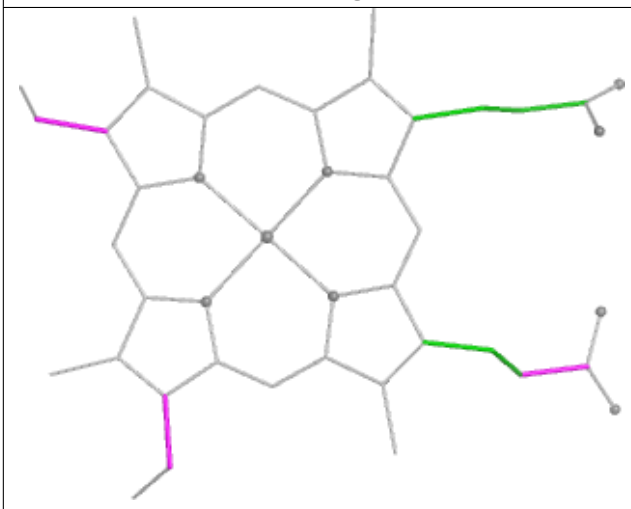


Bond angles



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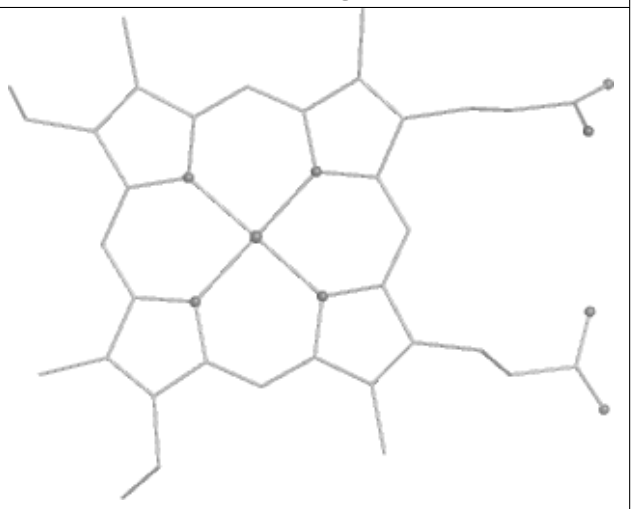
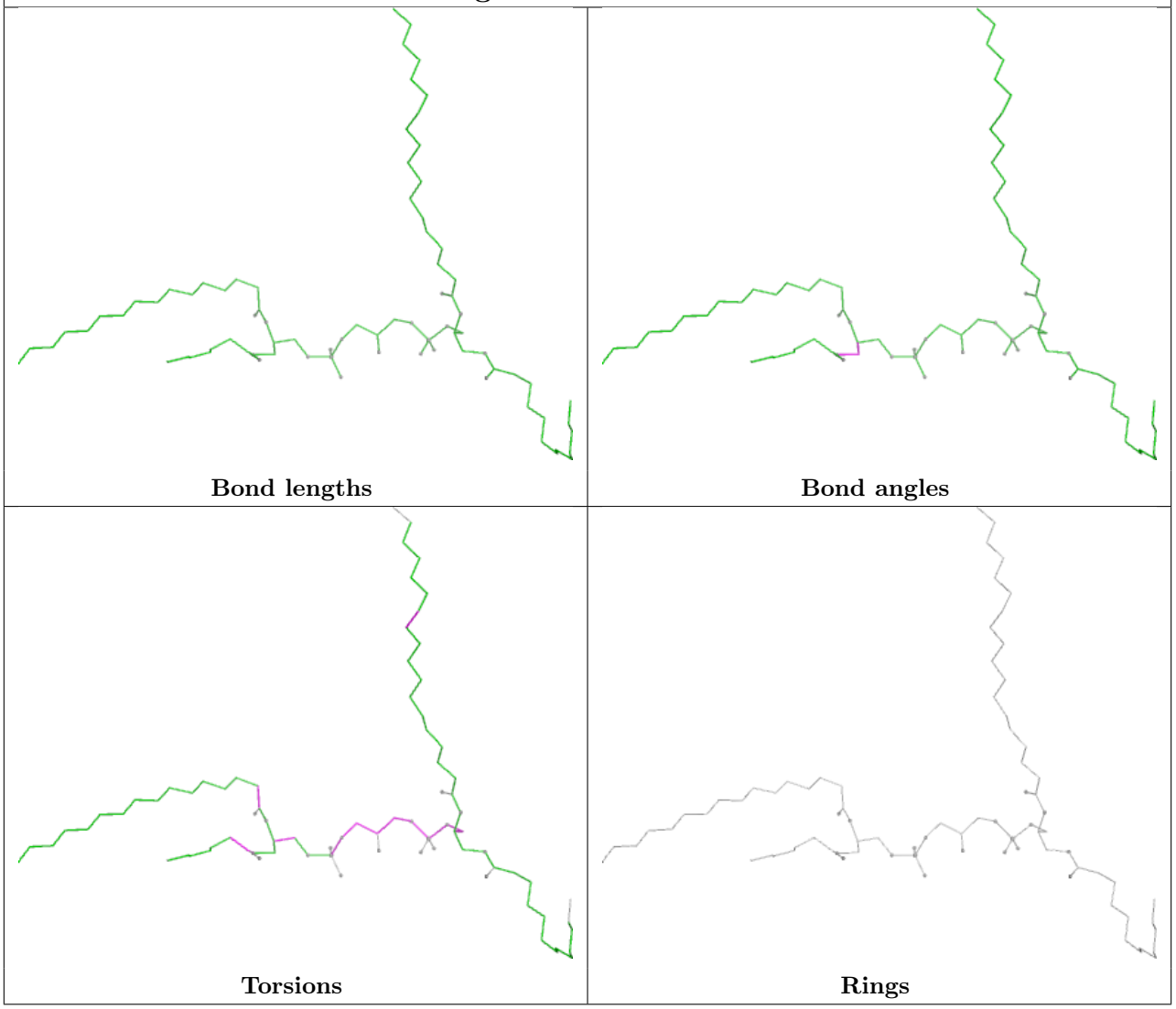
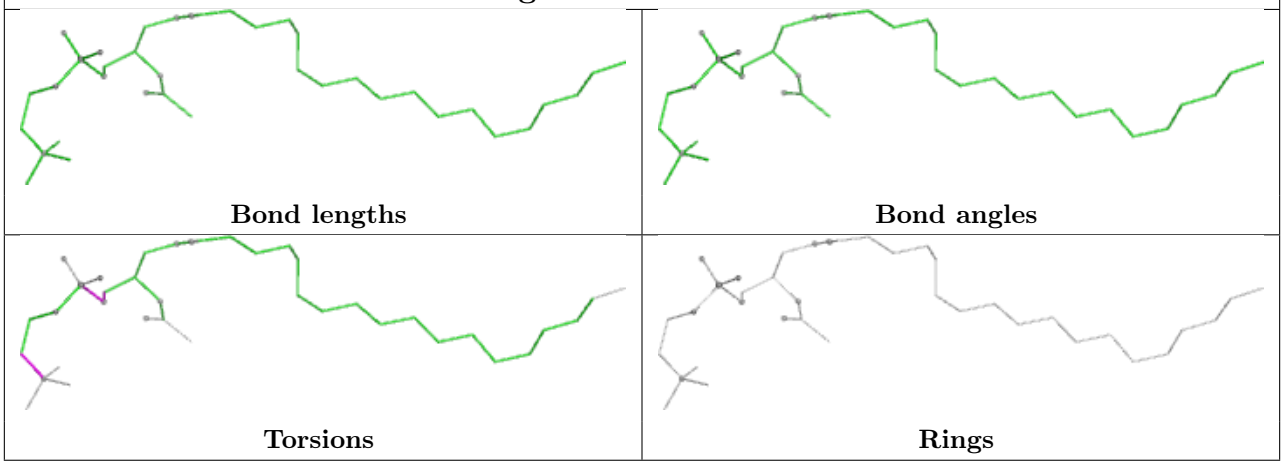


Rings

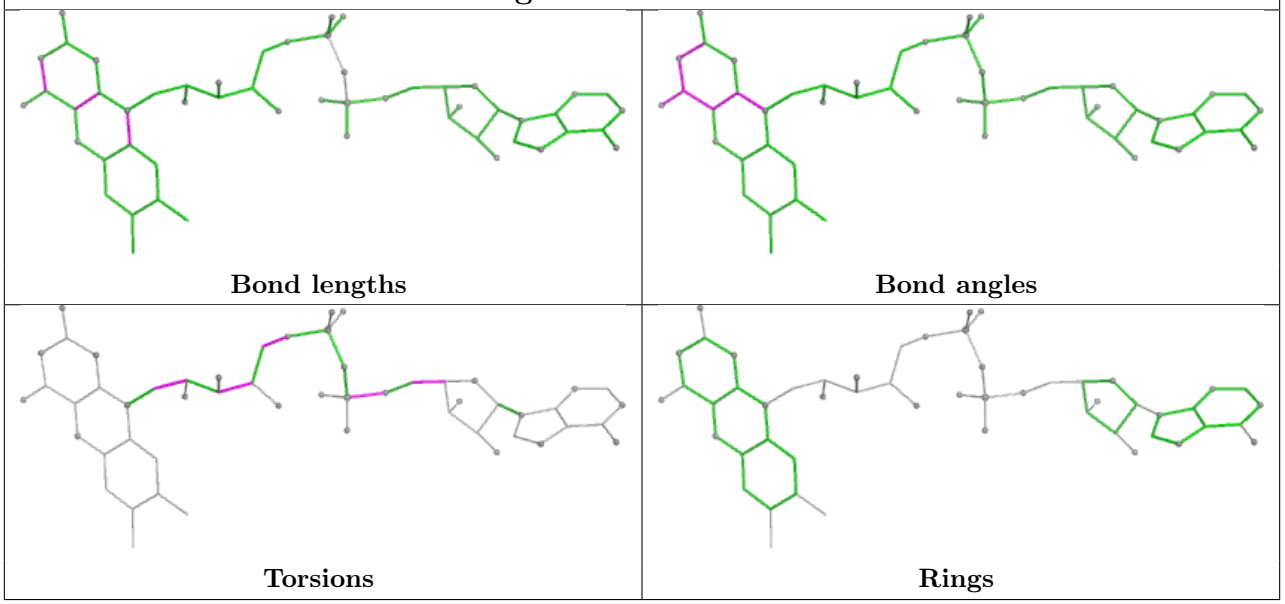
Ligand CDL 3h 403



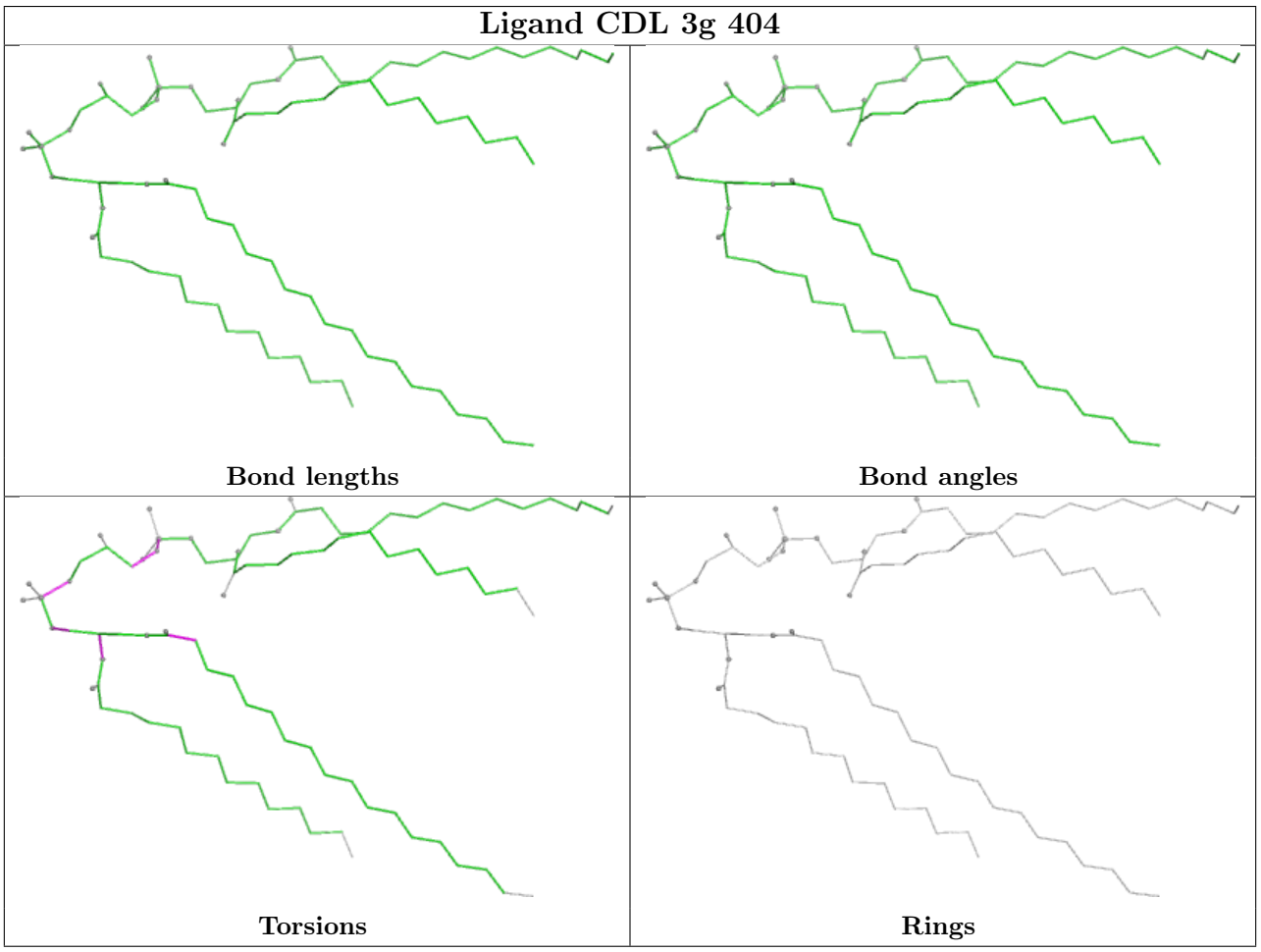
Ligand PC1 3A 501



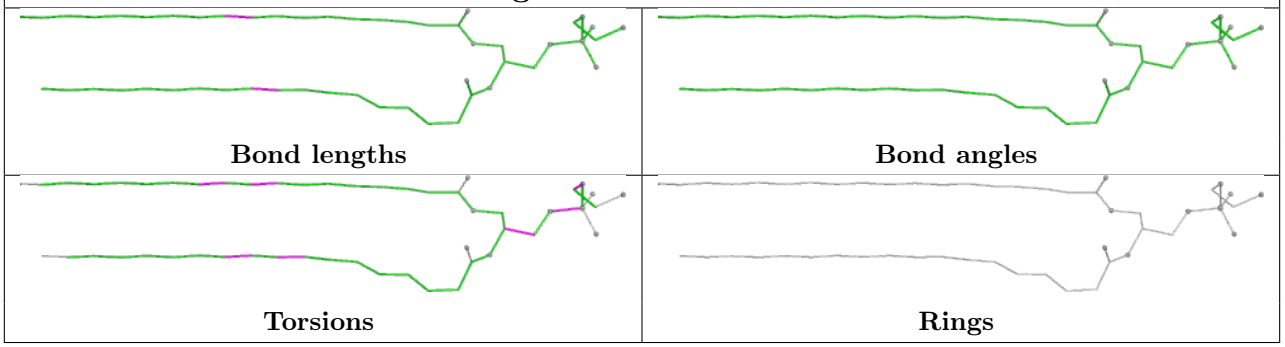
Ligand FAD 2m 701



Ligand CDL 3g 404



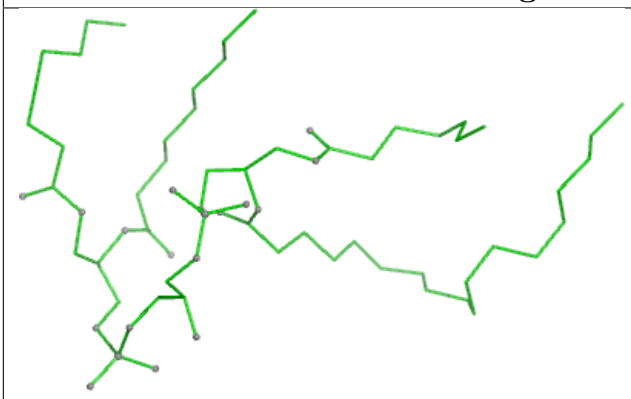
Ligand PEE 4W 201



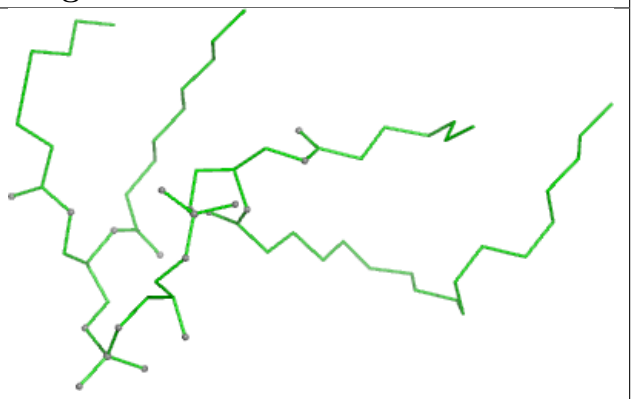
Ligand CDL 2t 102



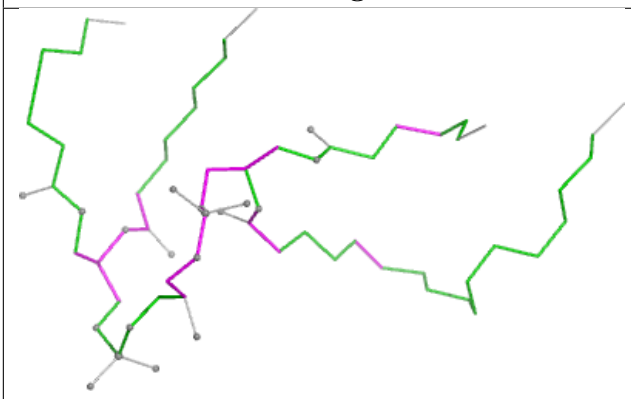
Ligand CDL 3g 403



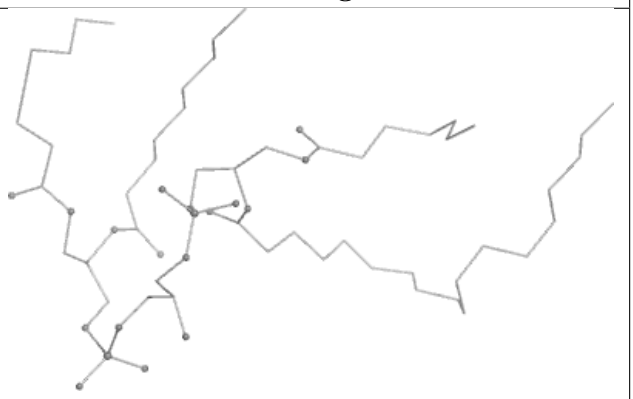
Bond lengths



Bond angles

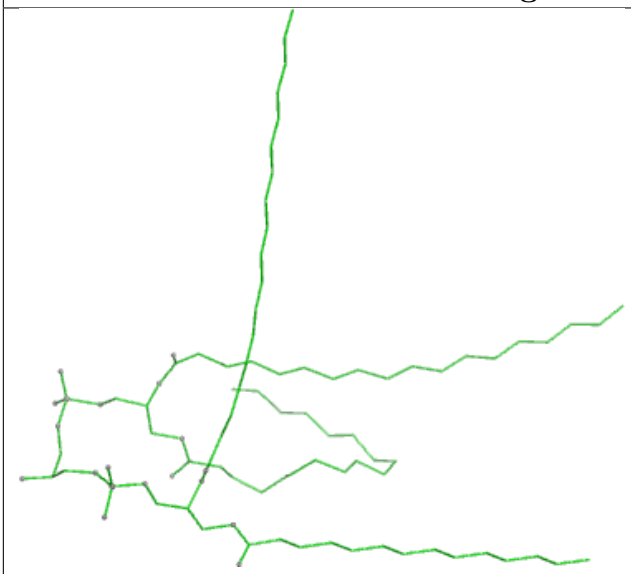


Torsions



Rings

Ligand CDL 4e 203



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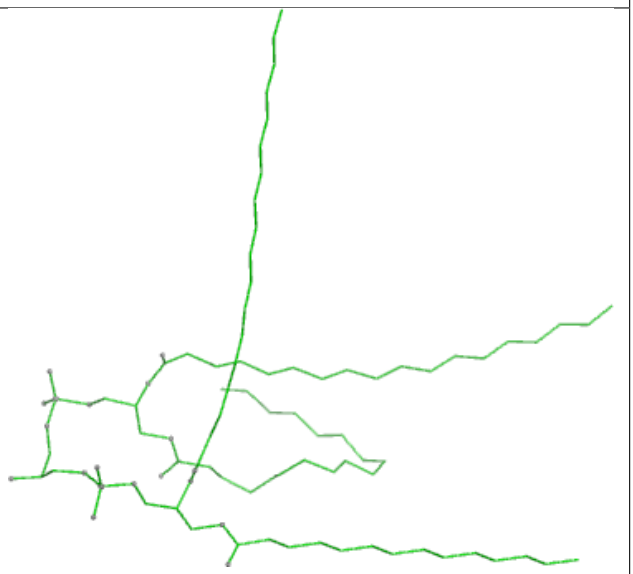
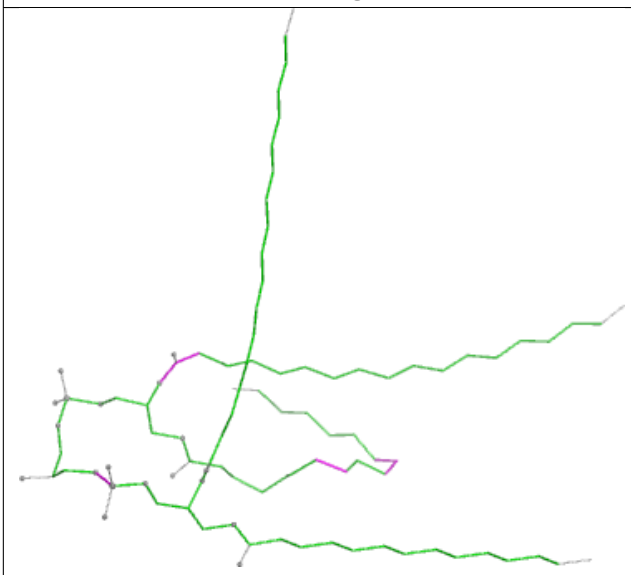


Bond angles

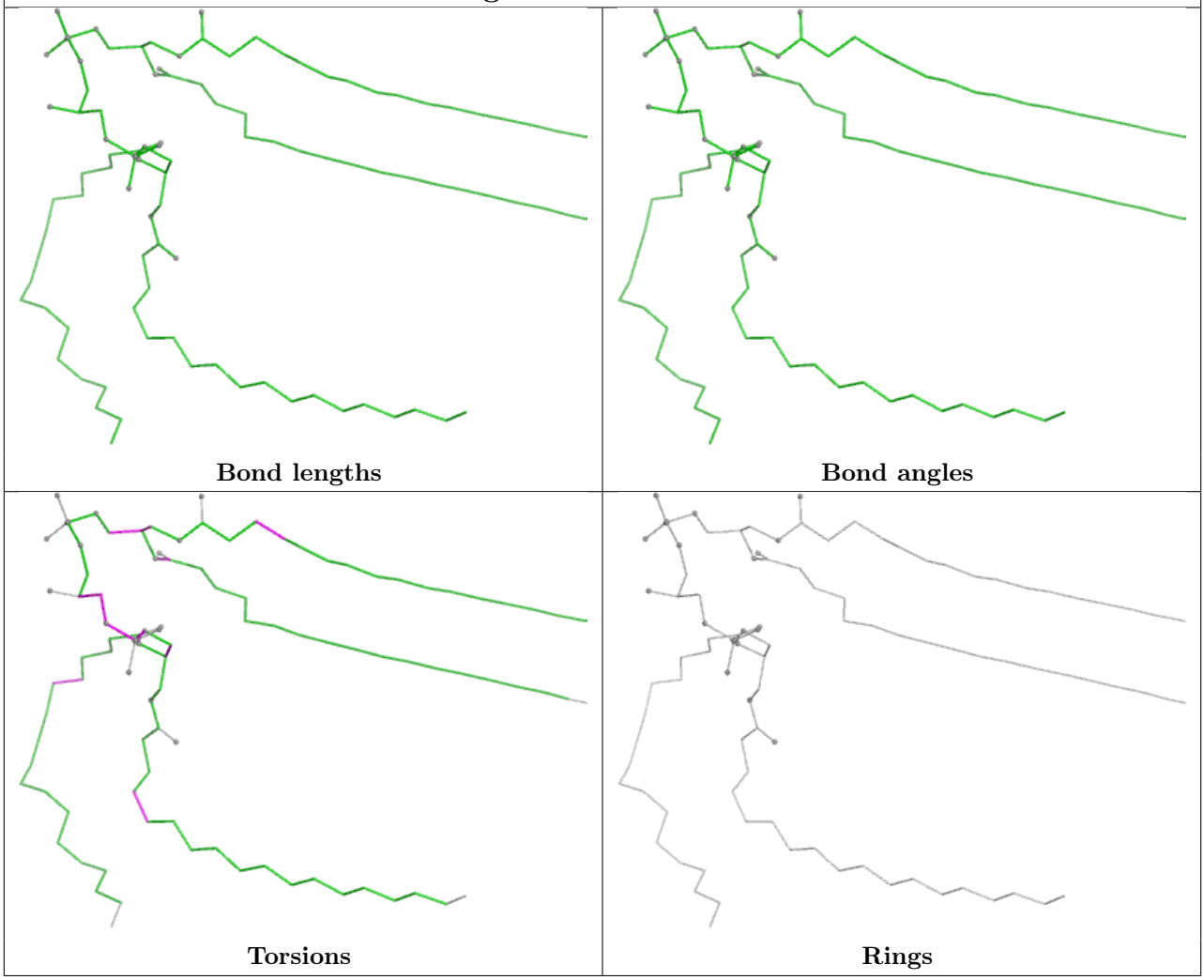


Torsions

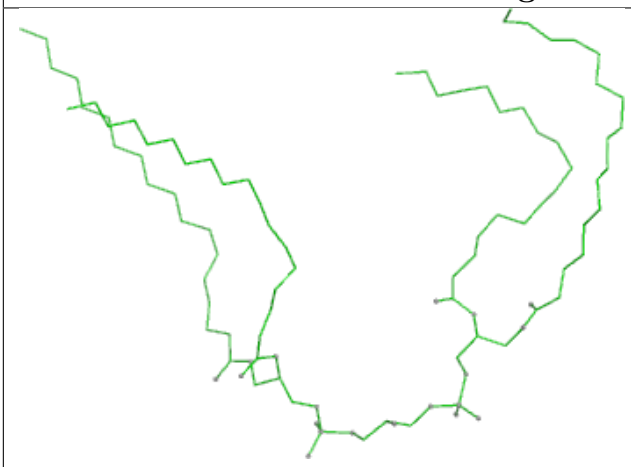


Rings

Ligand CDL 3G 403



Ligand CDL 4S 102



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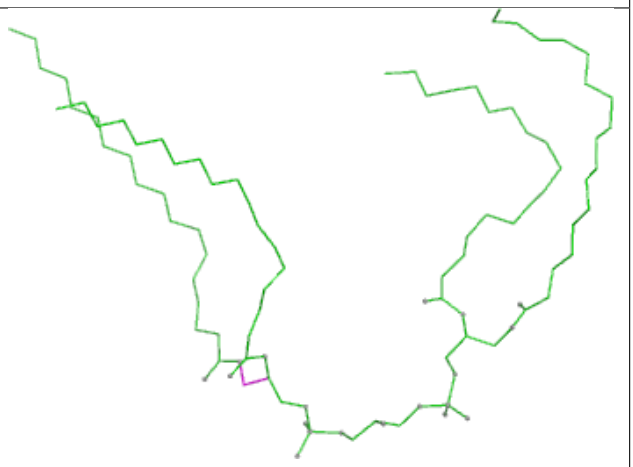

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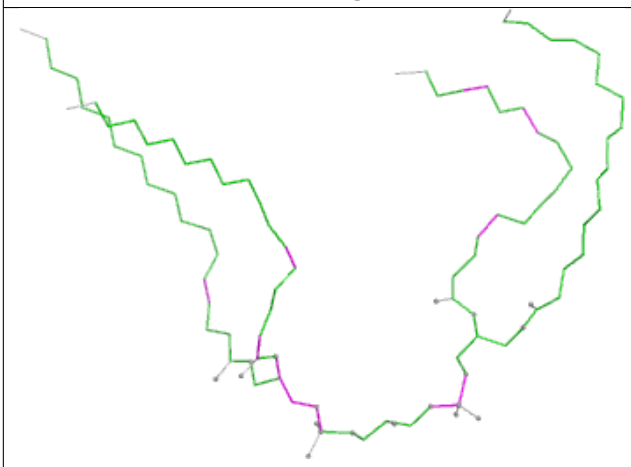
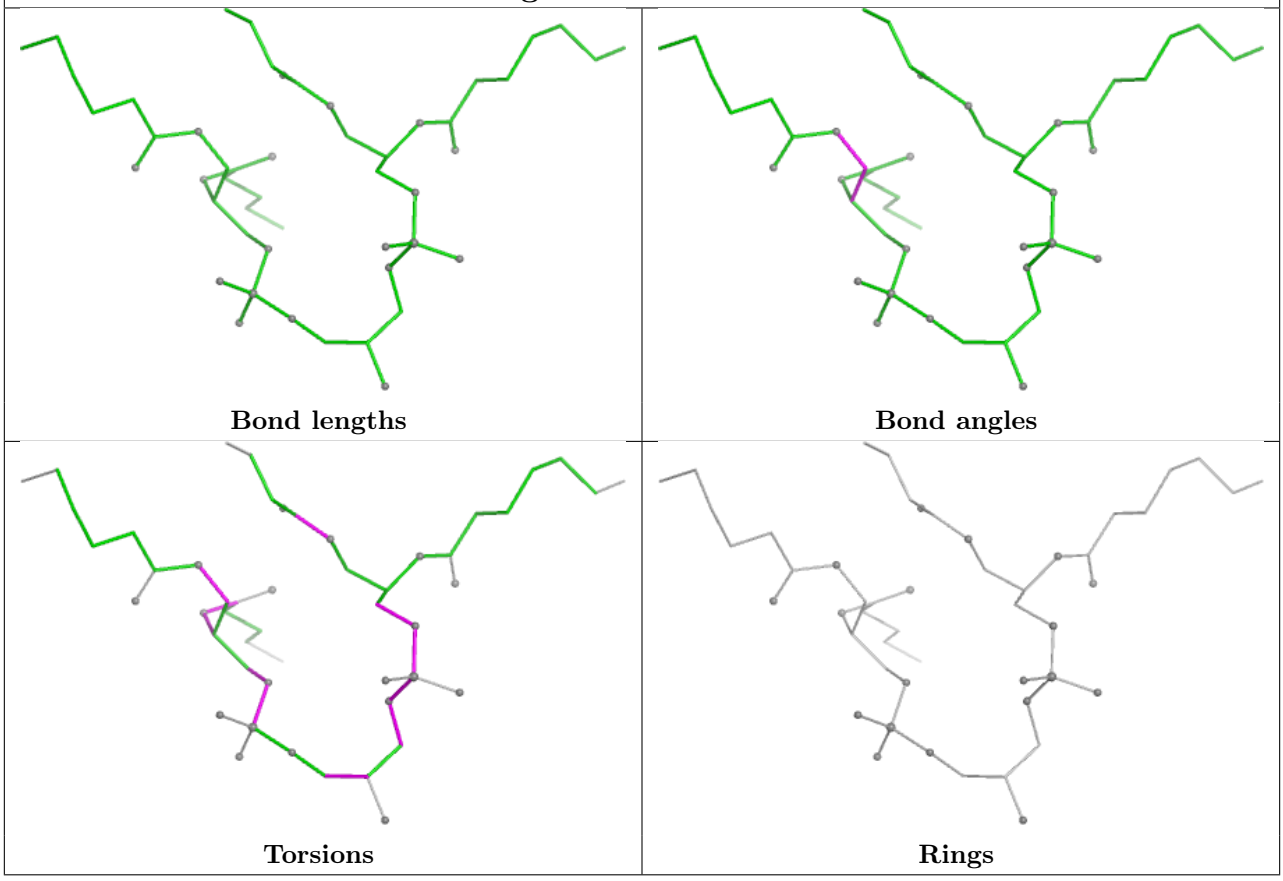


Torsions



Rings

Ligand CDL 4e 202



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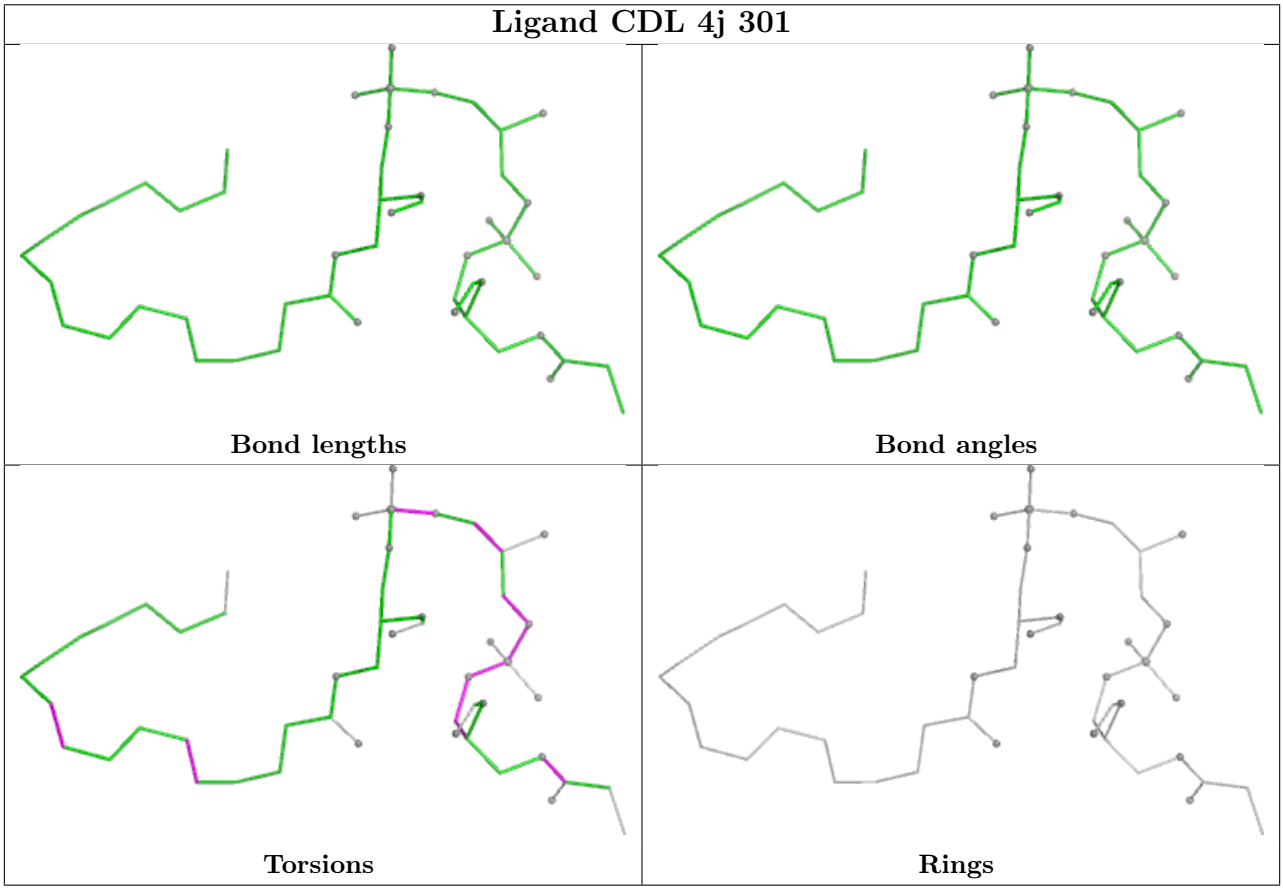
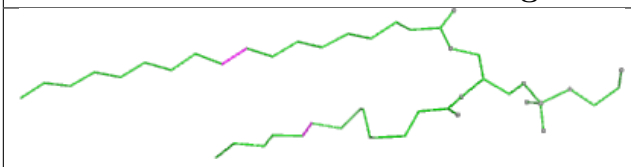


Ligand PEE 40 302



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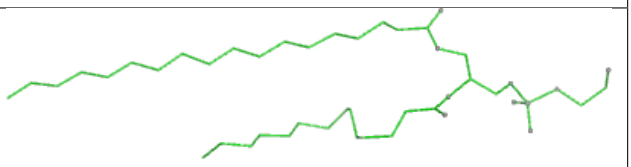

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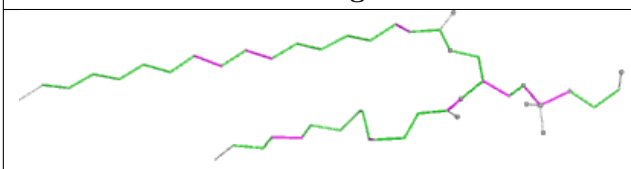
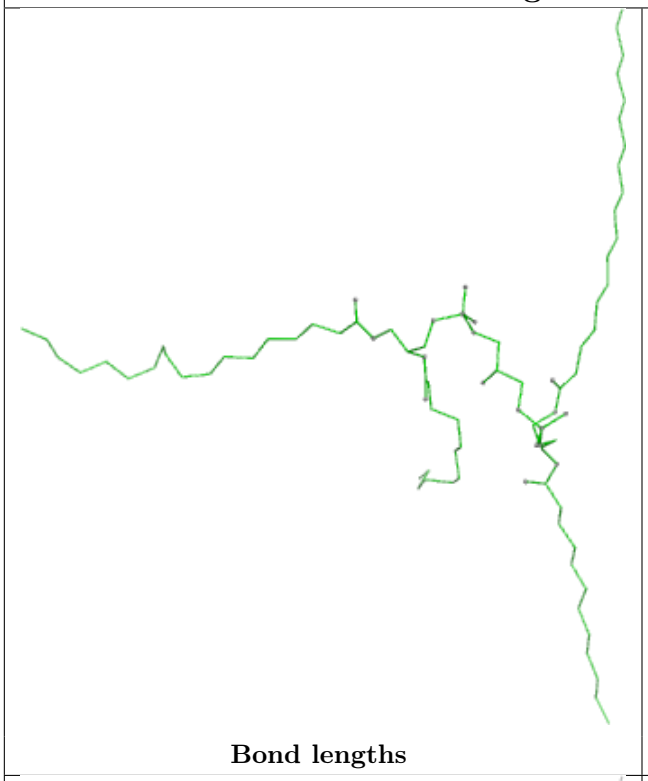


Torsions



Rings

Ligand CDL 4j 302



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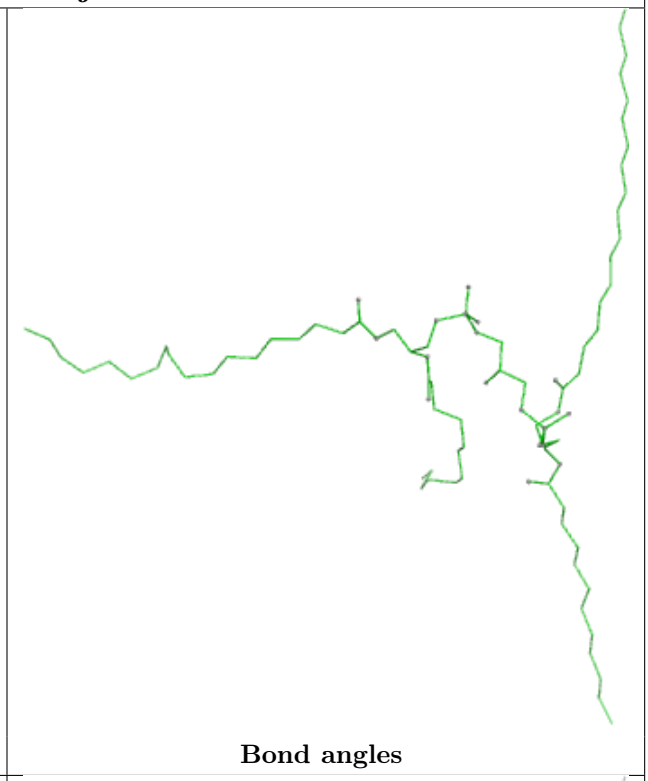

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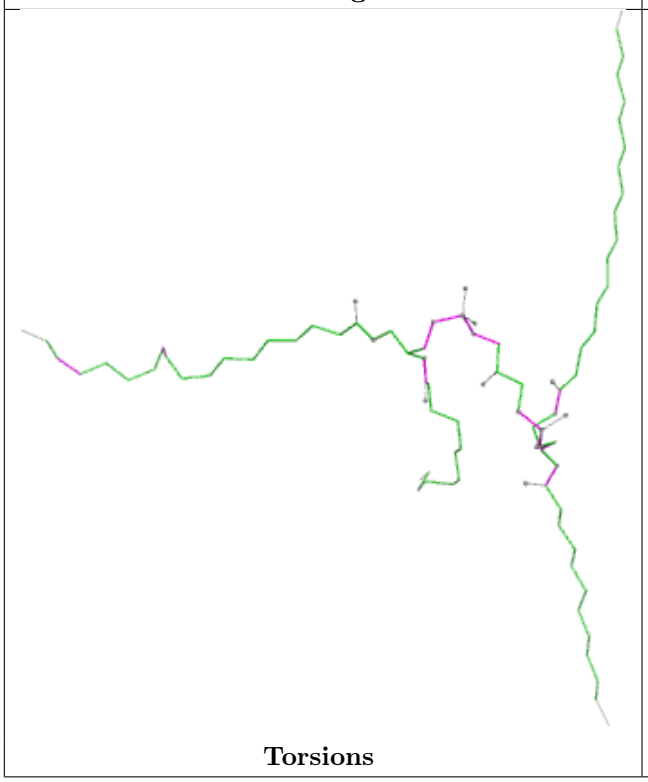

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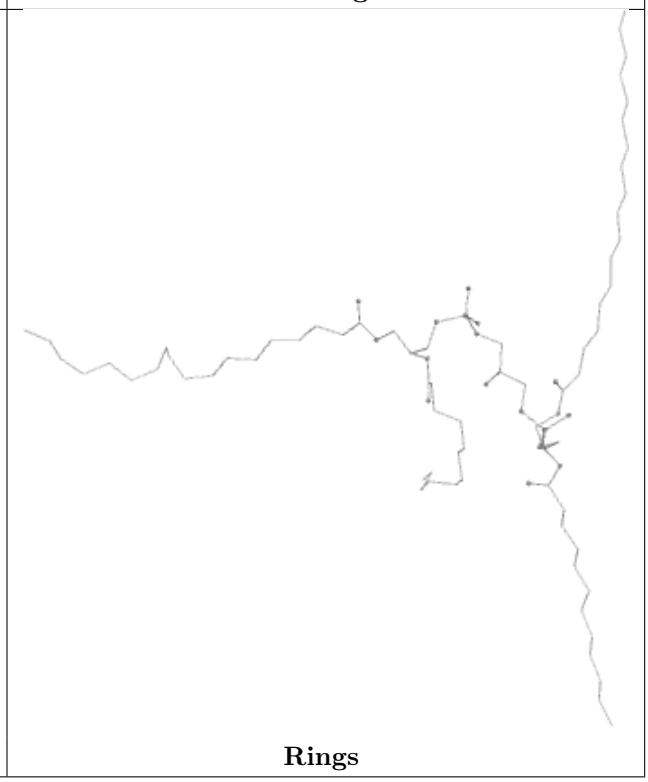
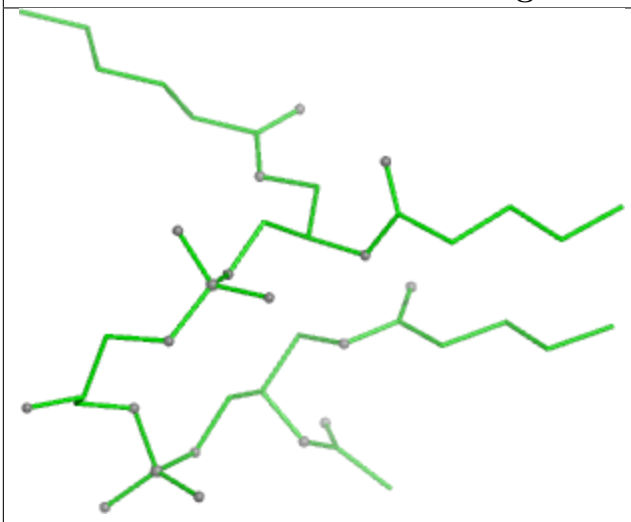


Rings

Ligand CDL 4E 202



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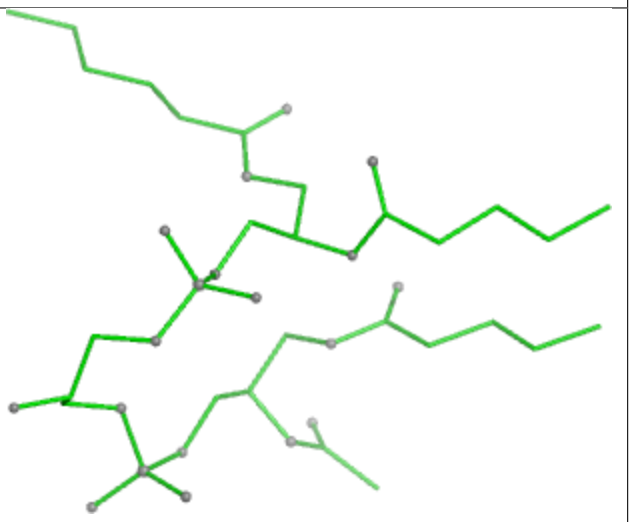

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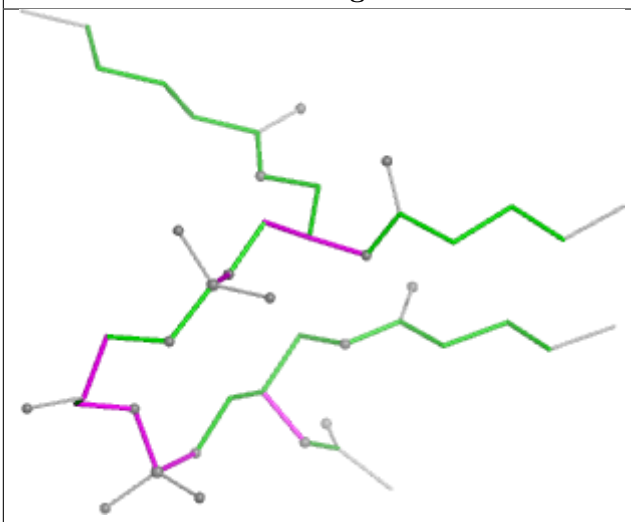

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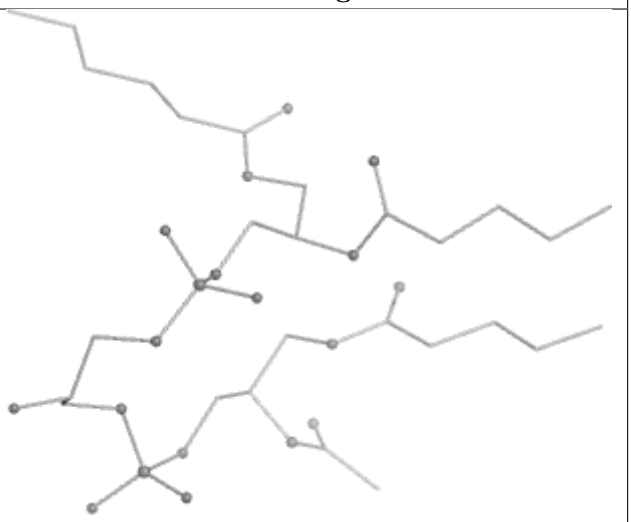
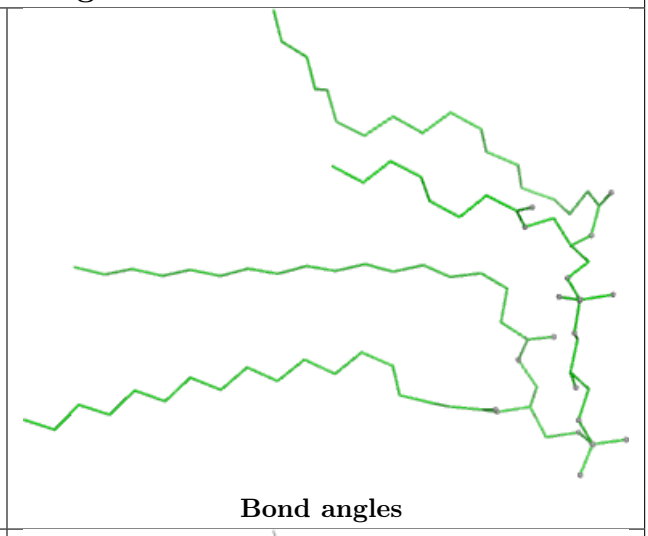


Rings

Ligand CDL 3g 405



Bond lengths



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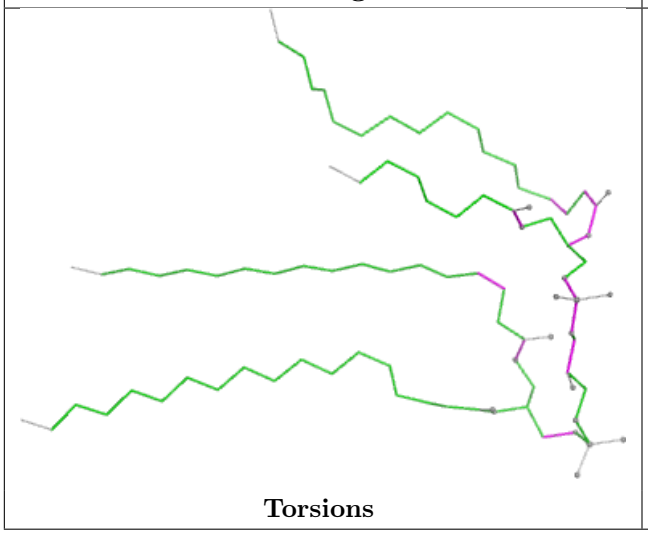

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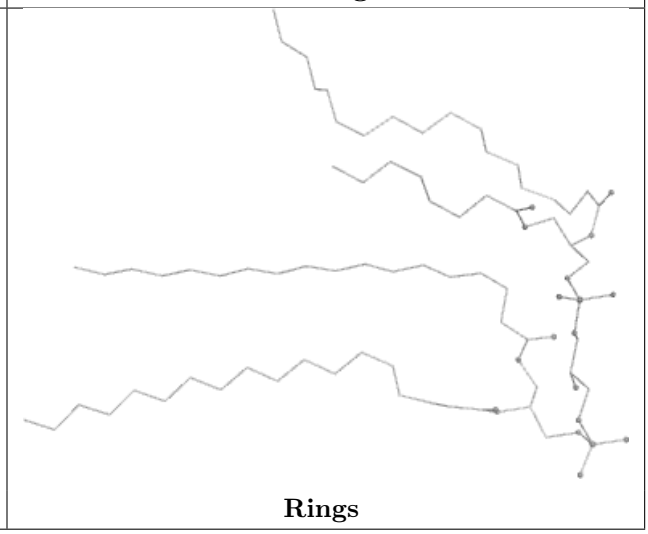
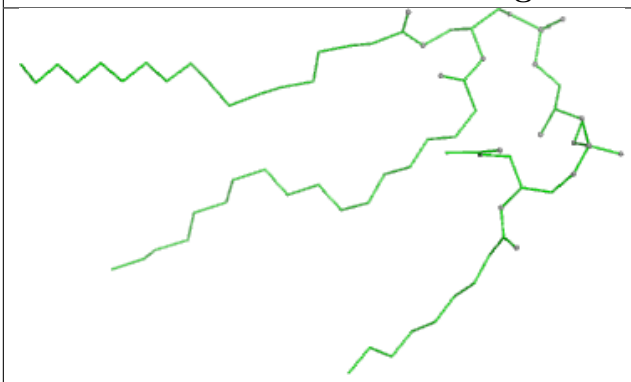


Rings

Ligand CDL 4Q 903



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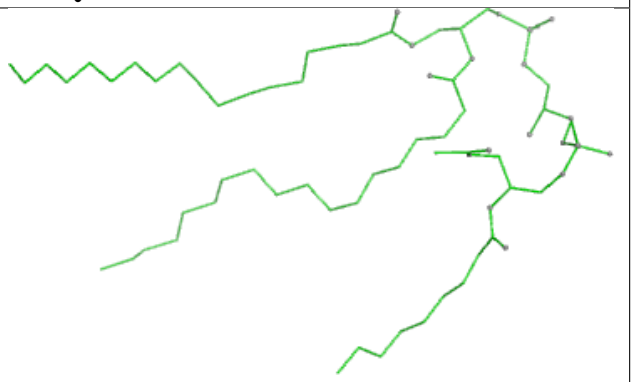

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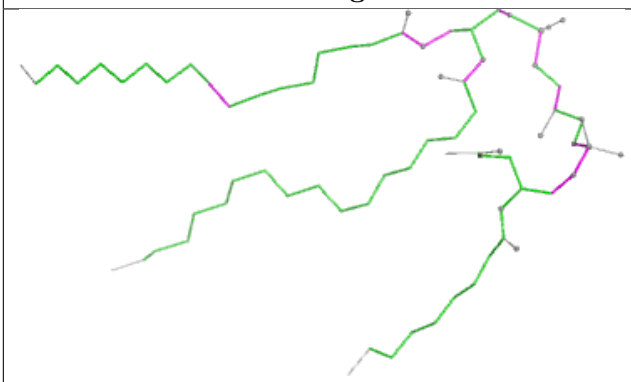

Torsions



Rings

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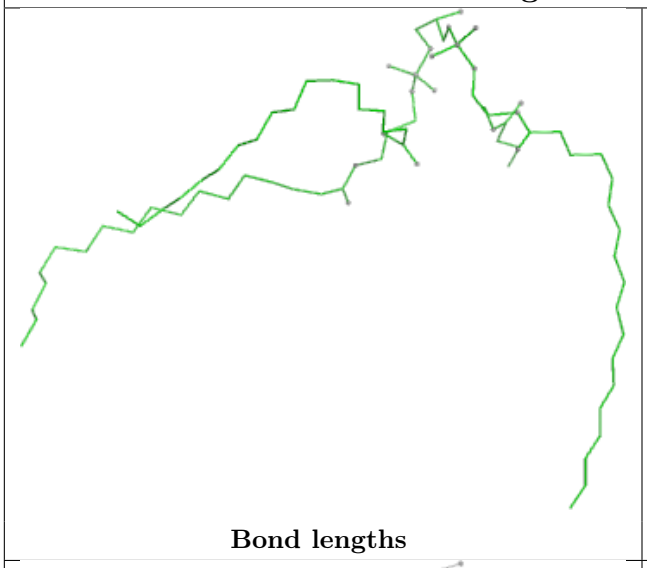

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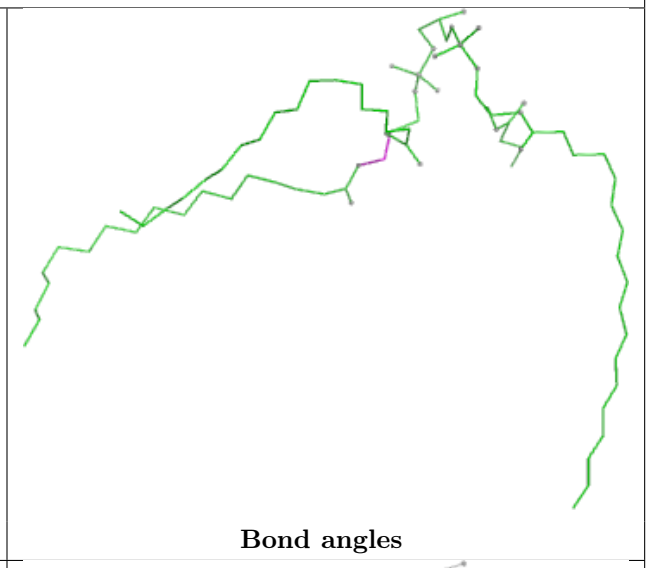

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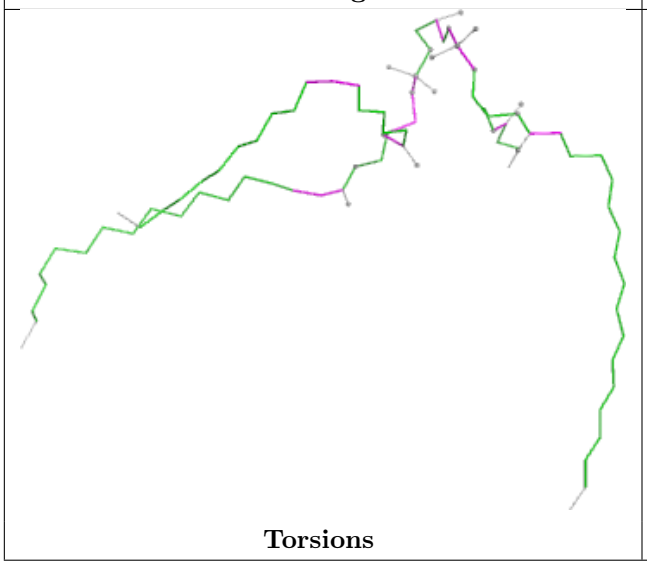

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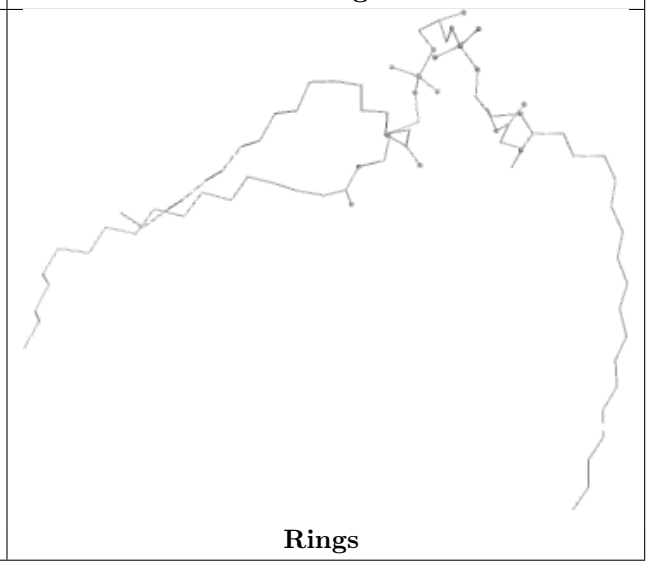
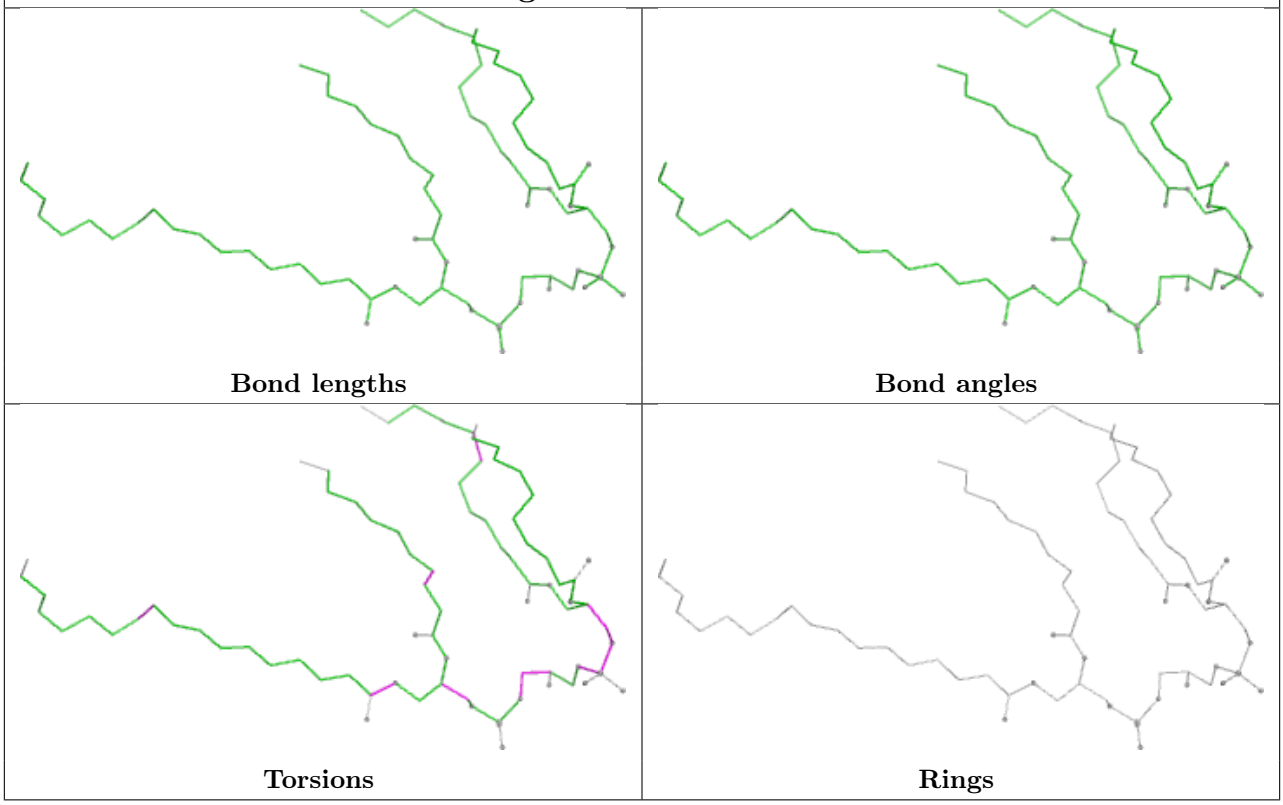
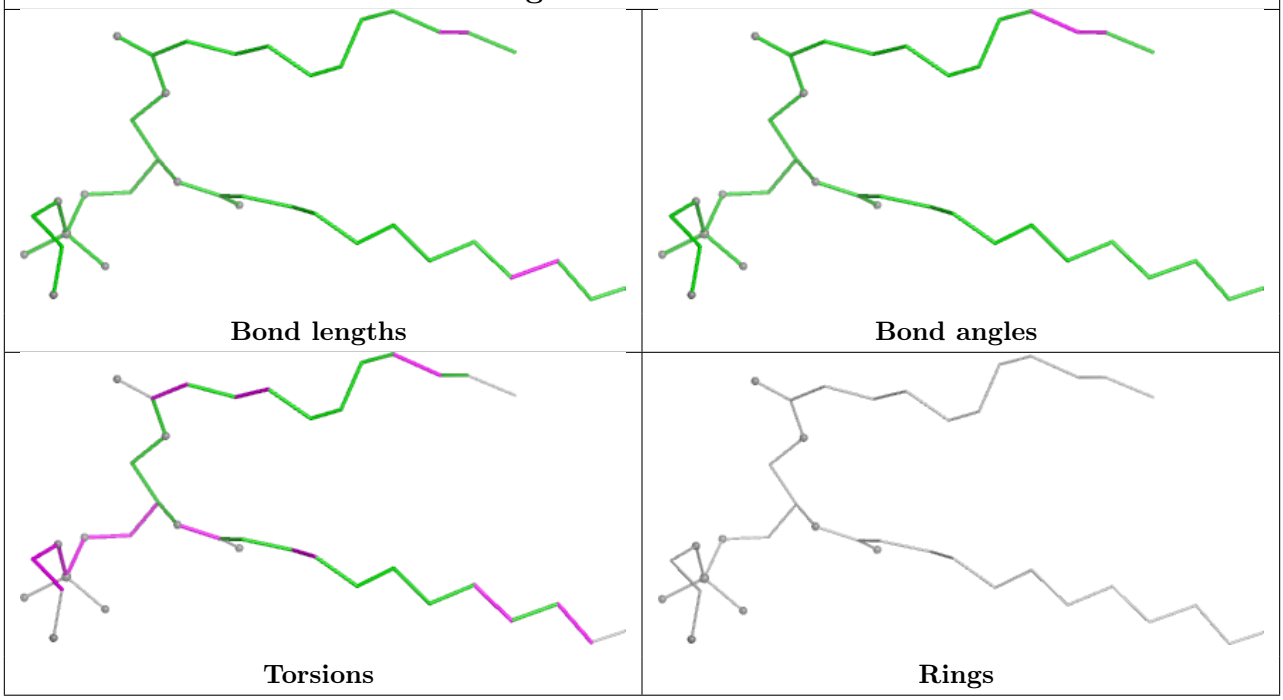


Rings

Ligand CDL 3L 702



Ligand PEE 4l 201



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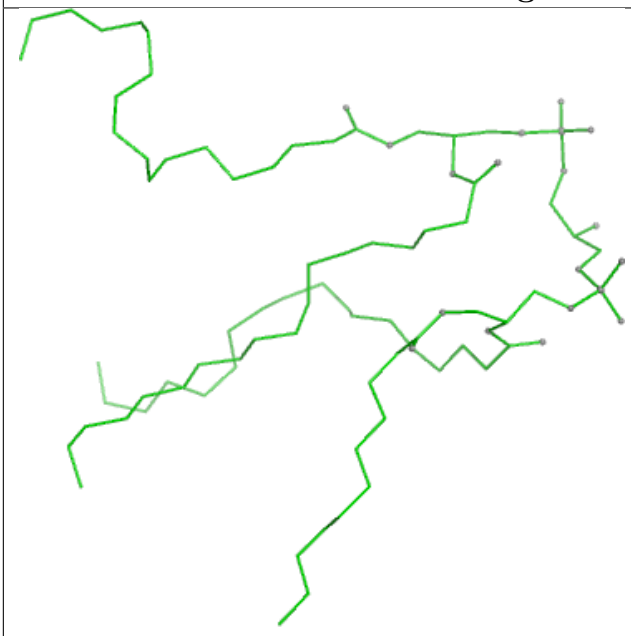

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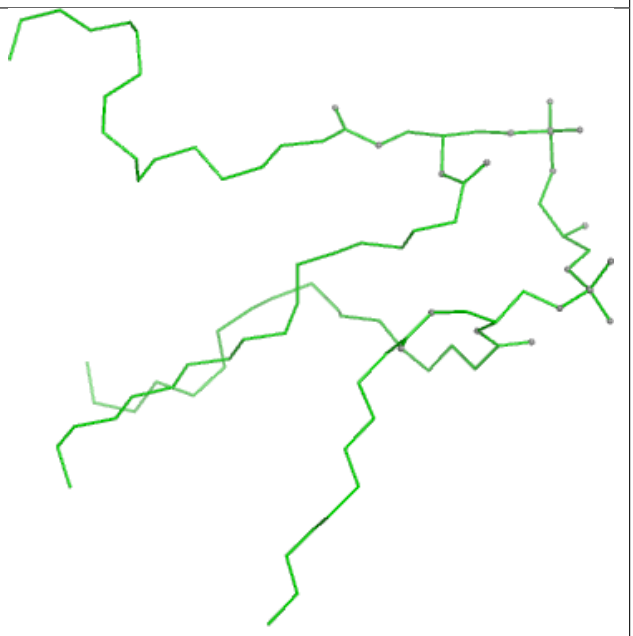
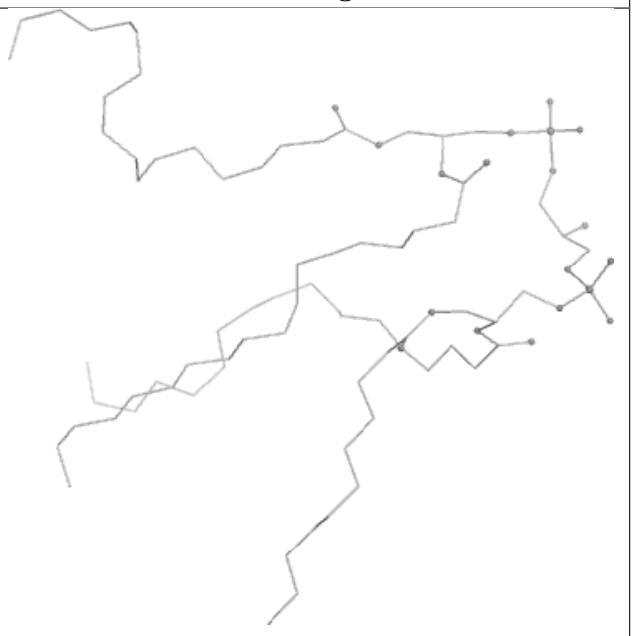


Bond angles



Torsions



Rings

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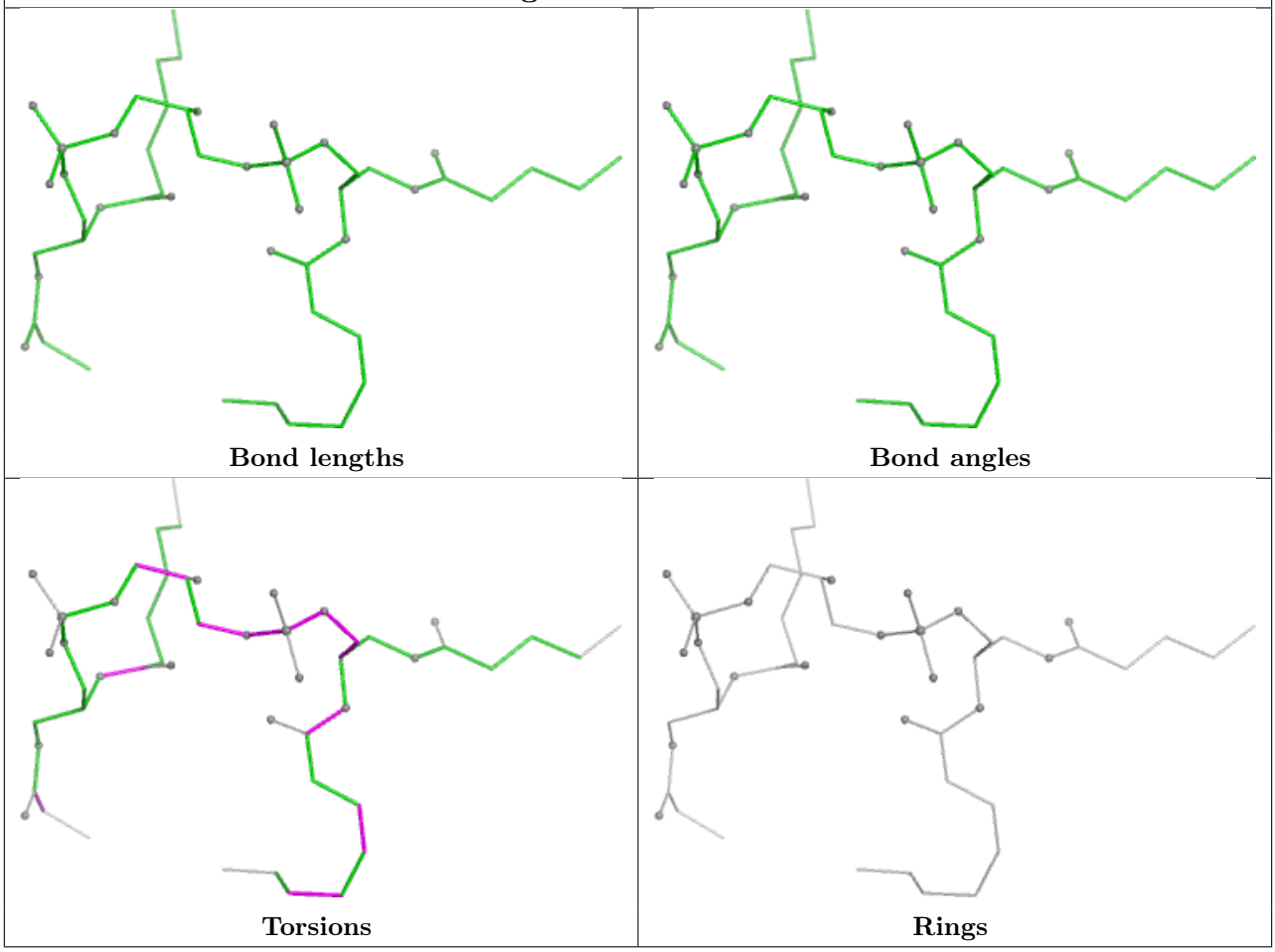

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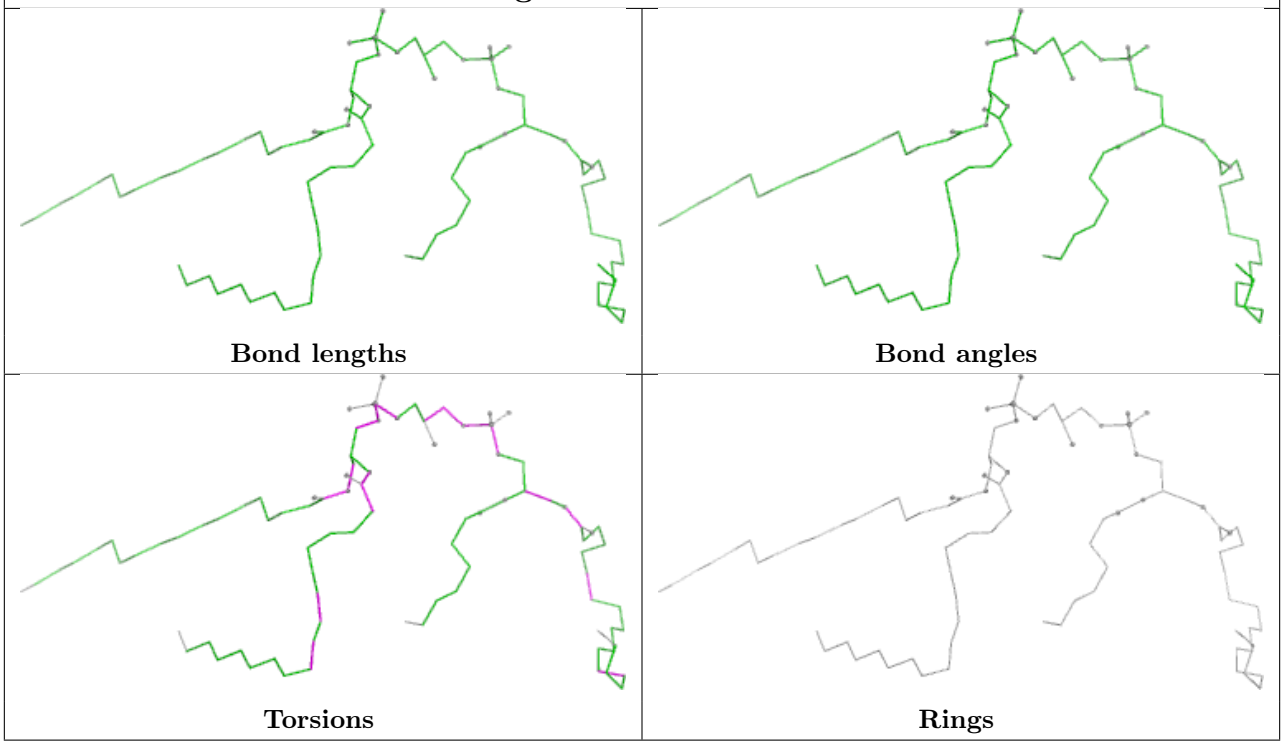
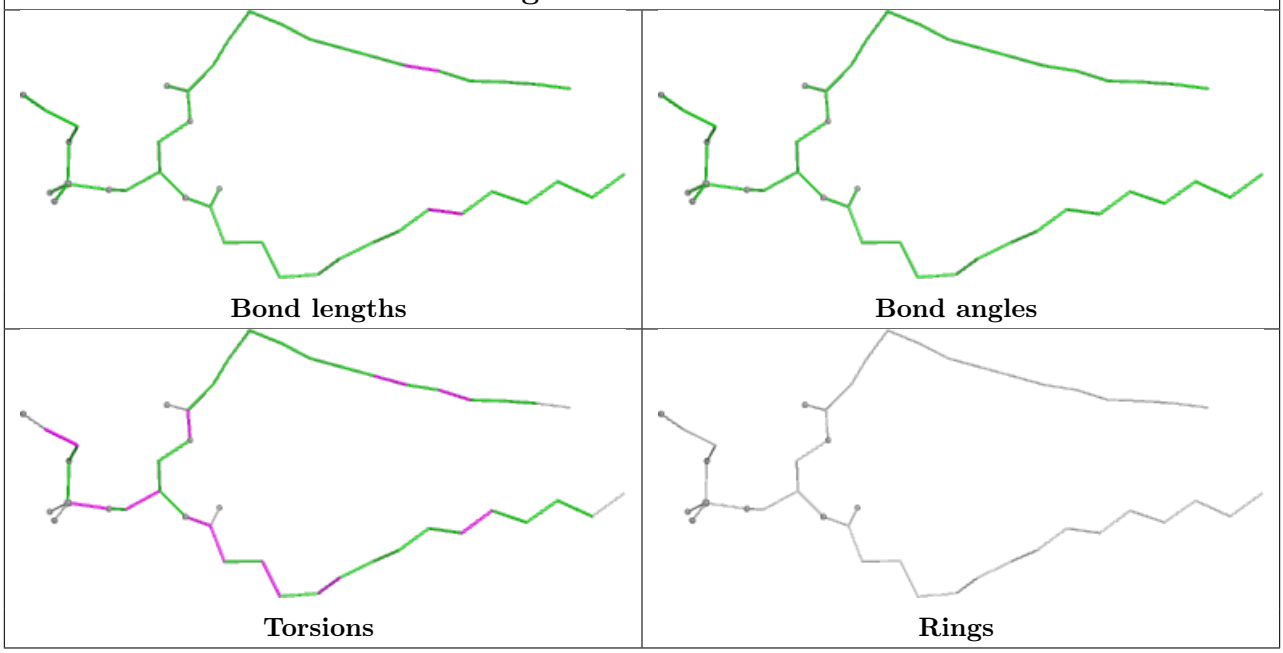


Ligand PEE 41 302



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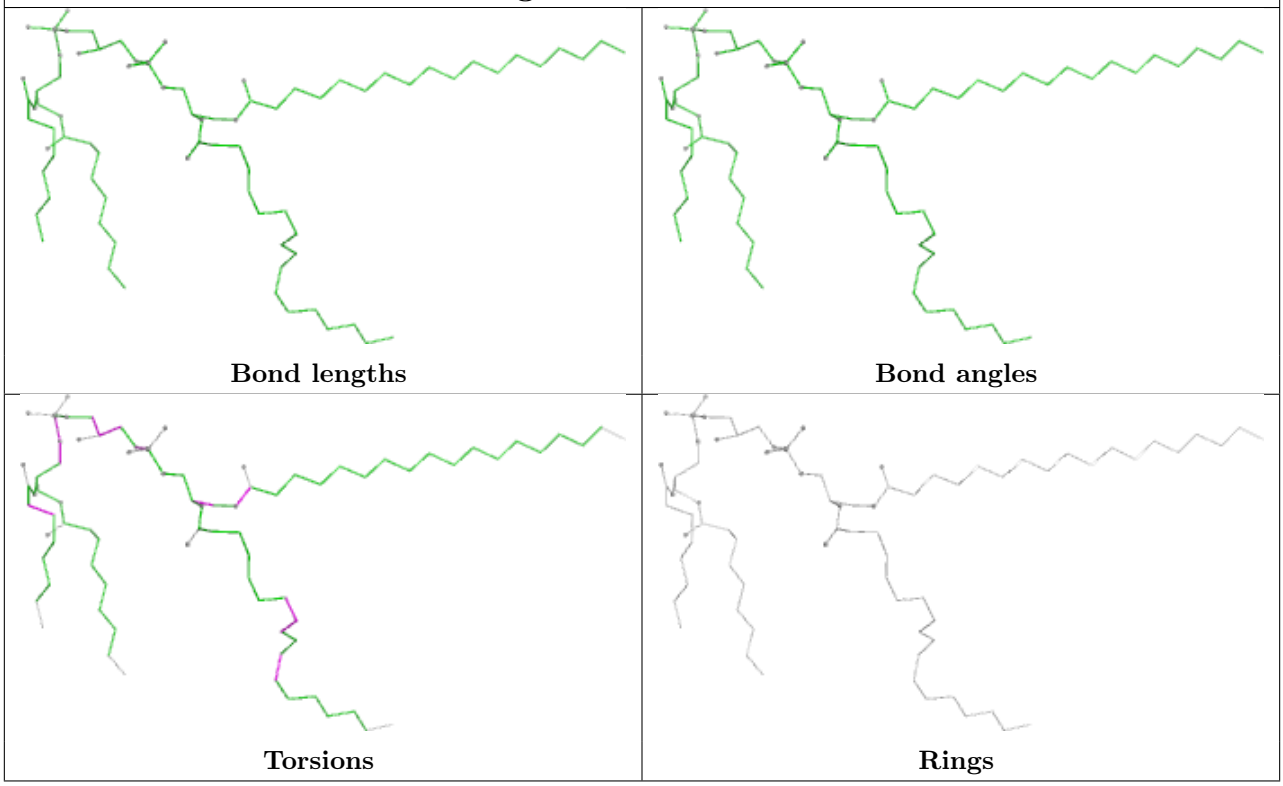

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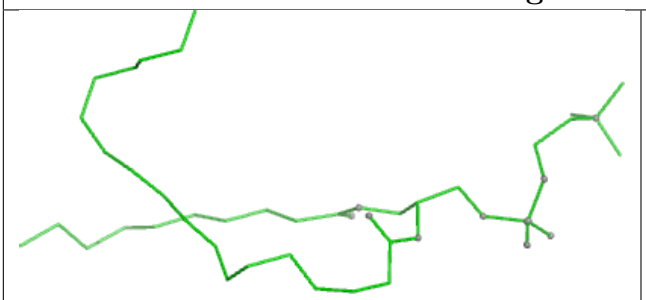

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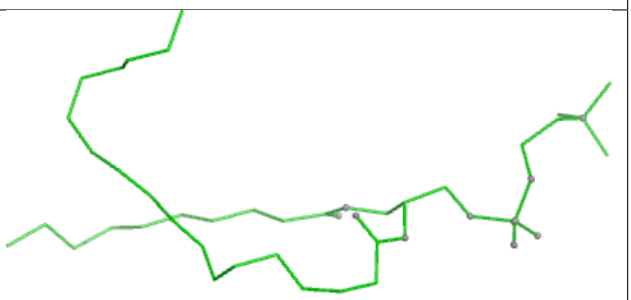
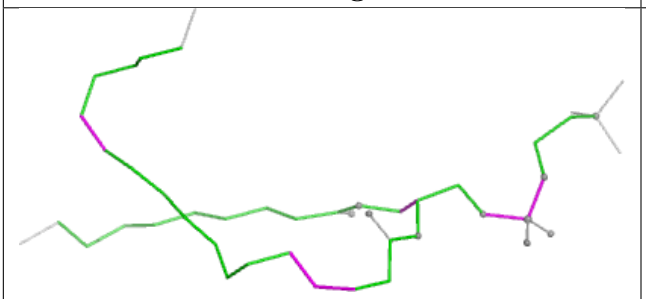


Bond angles

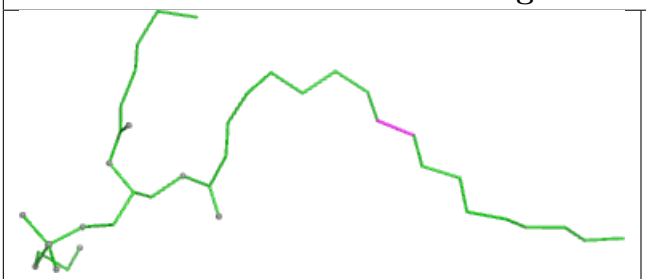


Torsions



Rings

Ligand PEE 2O 201



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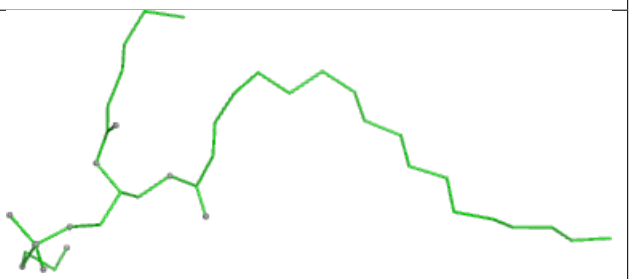

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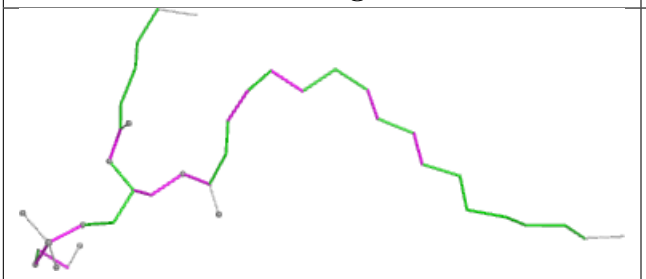

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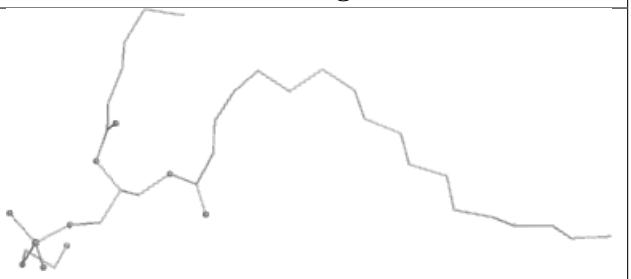
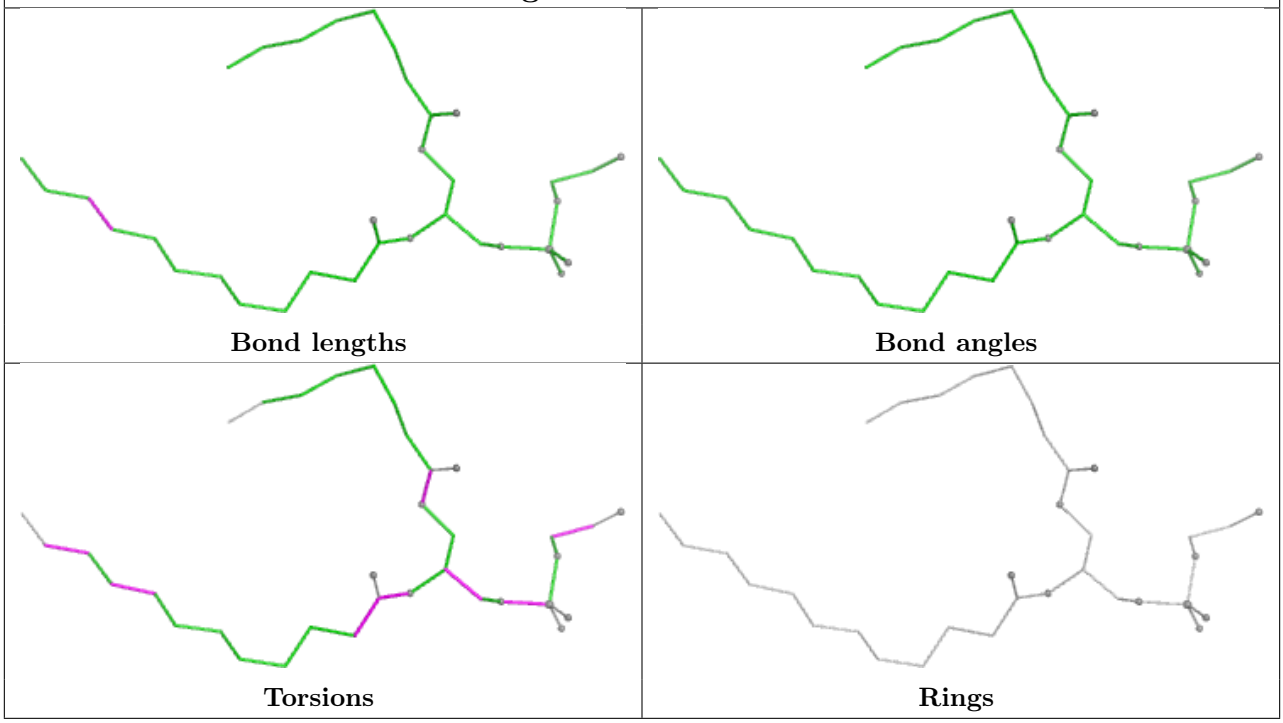
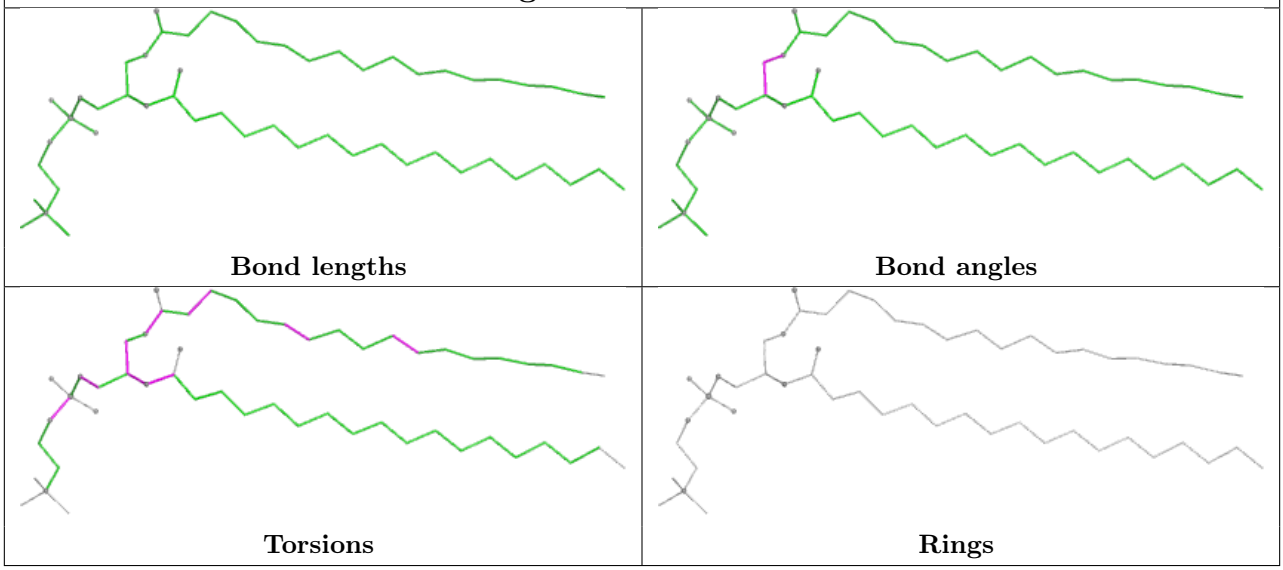


Rings

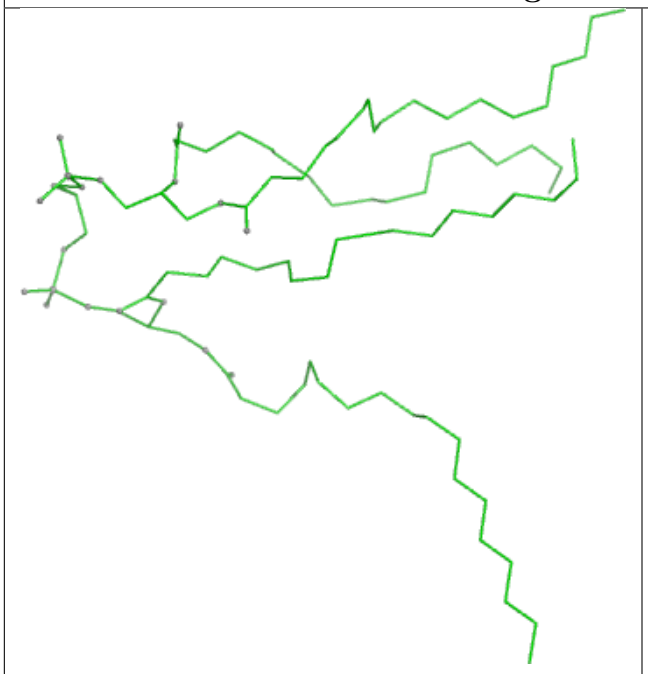
Ligand PEE 40 303



Ligand PC1 2R 202



Ligand CDL 3l 701



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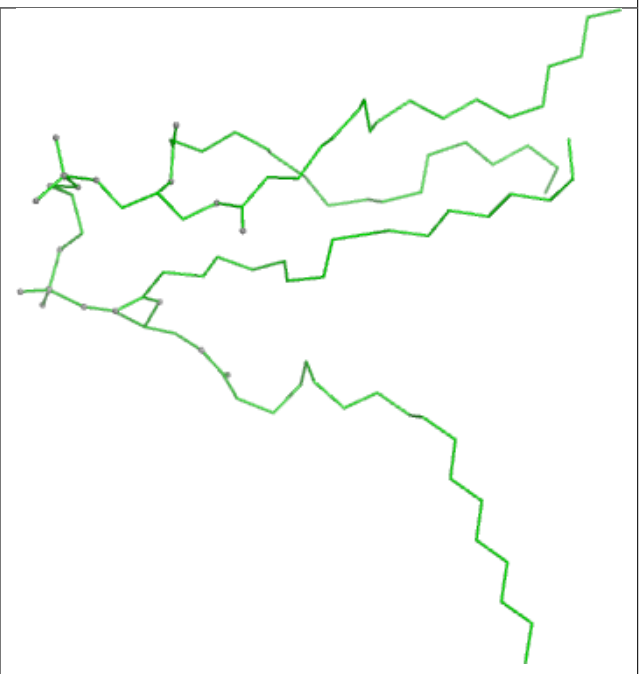
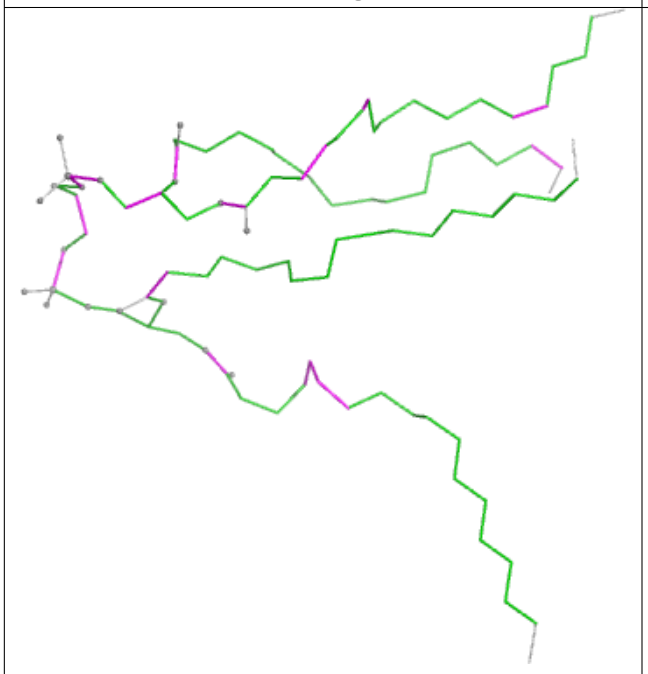


Bond angles



Torsions



Rings

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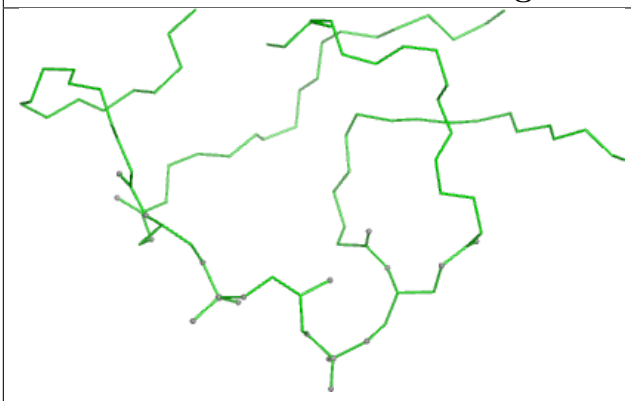

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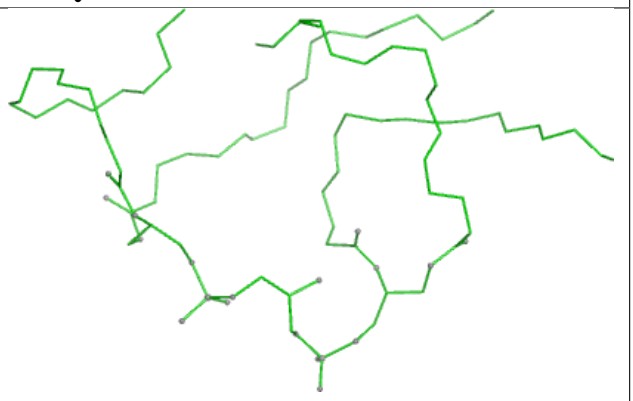
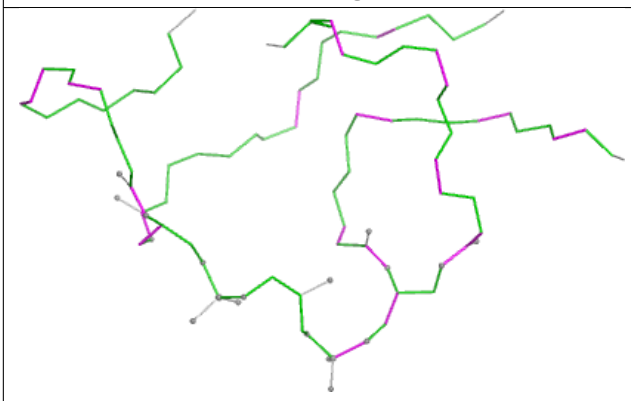


Bond angles

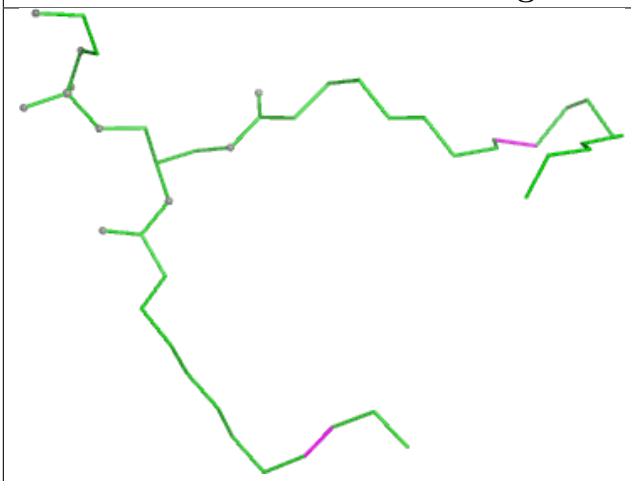


Torsions



Rings

Ligand PEE 2T 103



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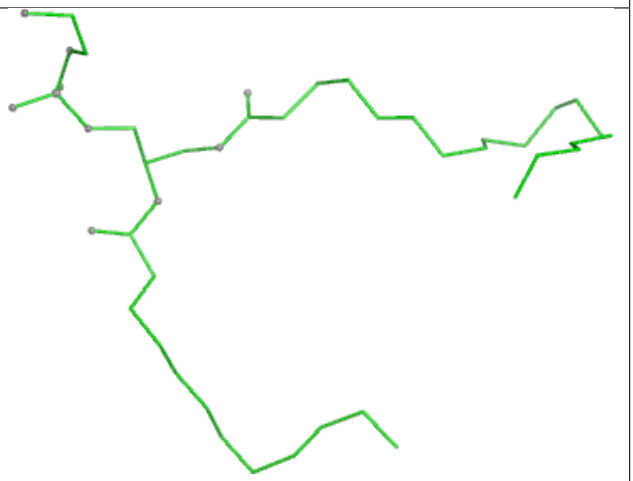

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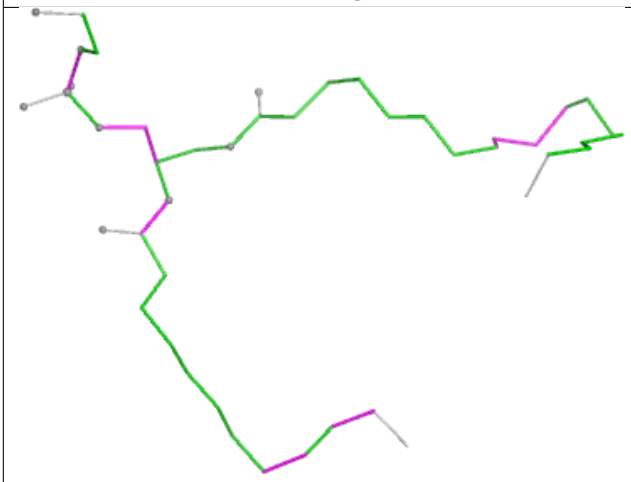
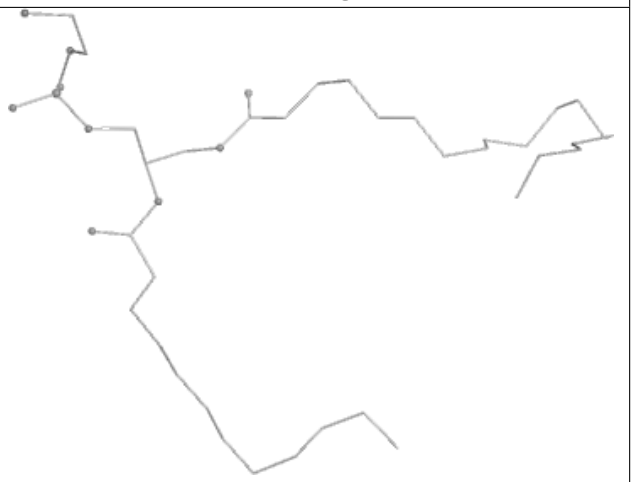
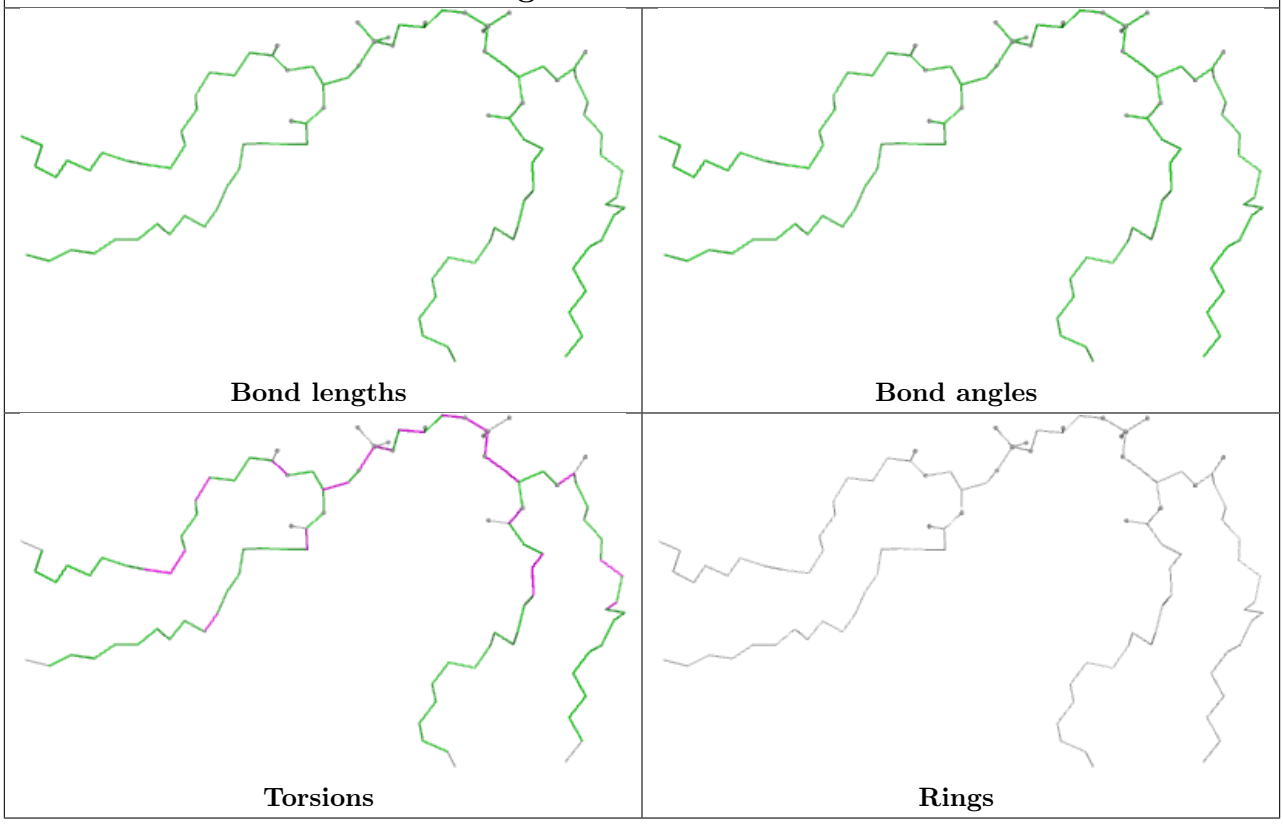


Torsions

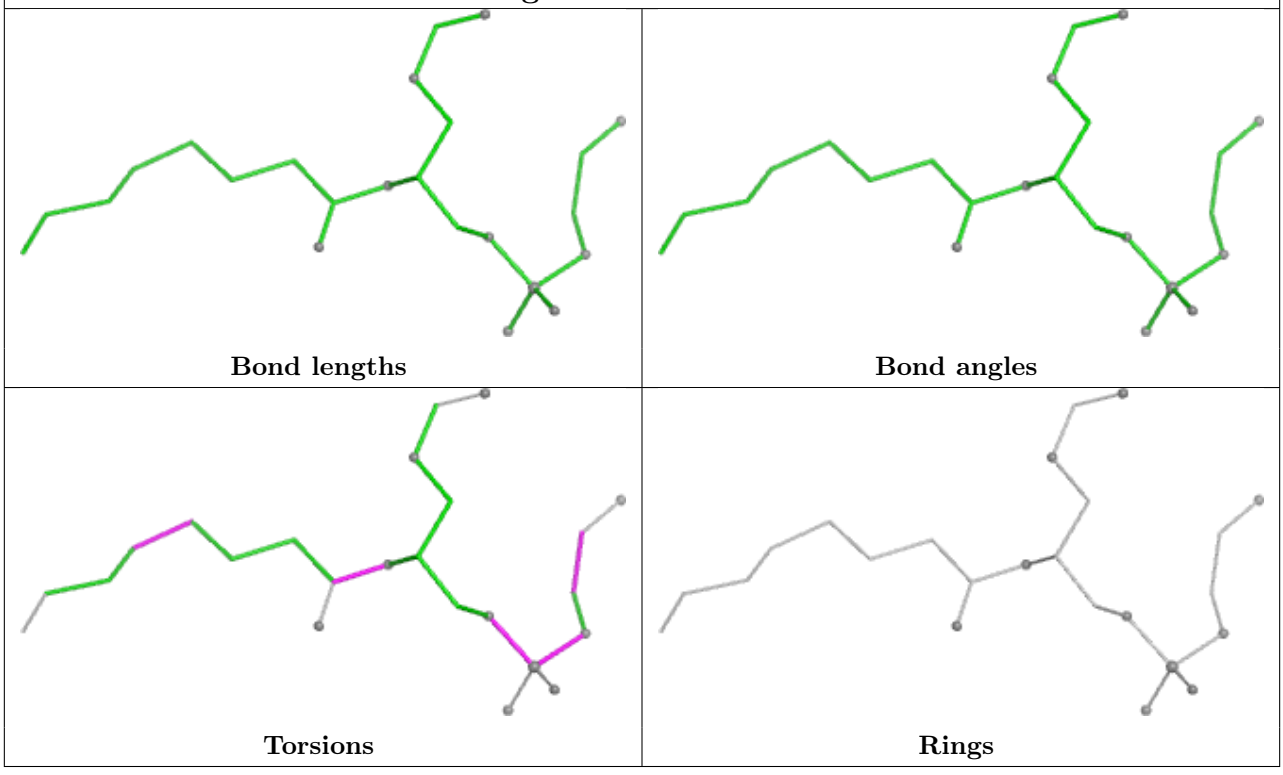


Rings

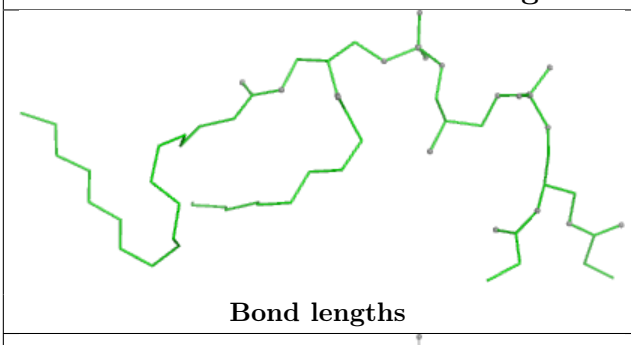
Ligand CDL 4F 202



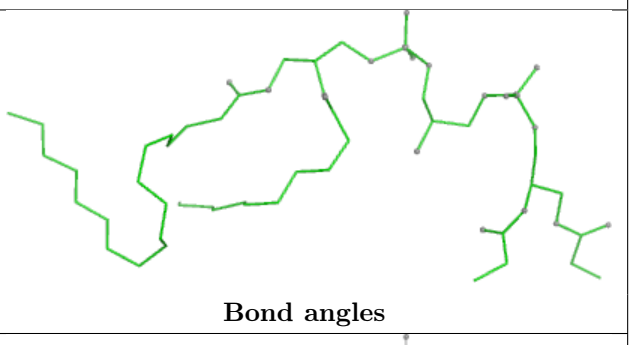
Ligand PEE 2o 203



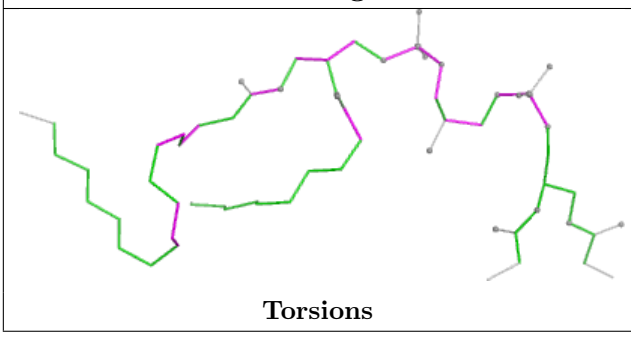
Ligand CDL 3I 203



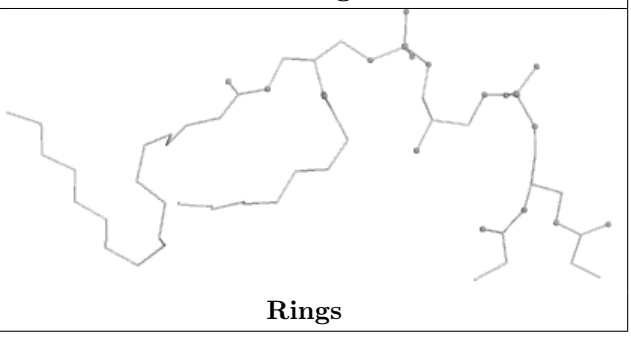
Bond lengths



Bond angles

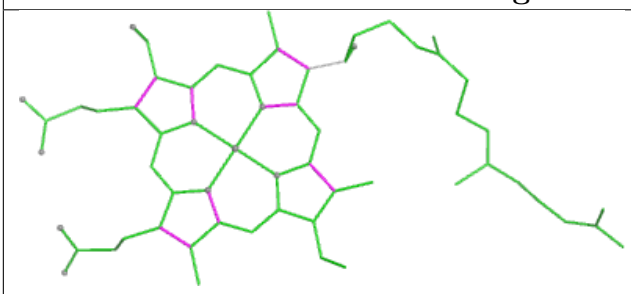


Torsions



Rings

Ligand HEA 4Q 907



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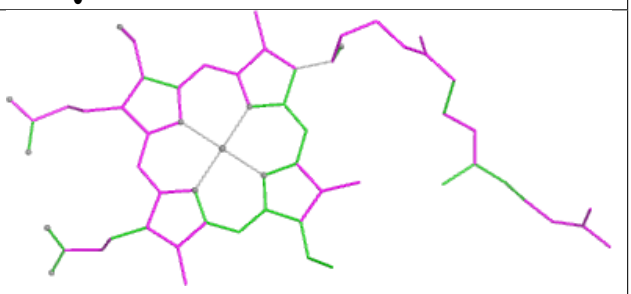
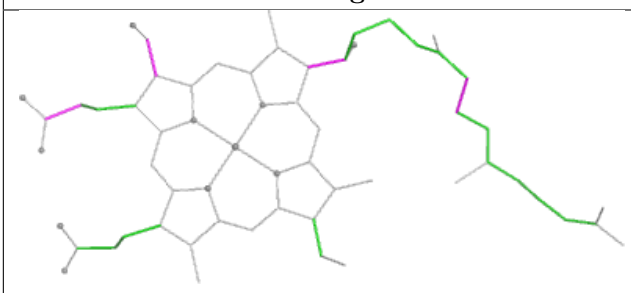


Bond angles



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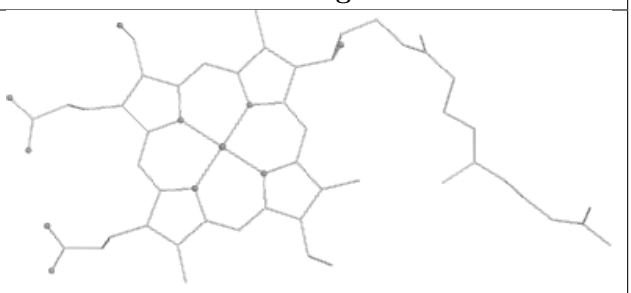
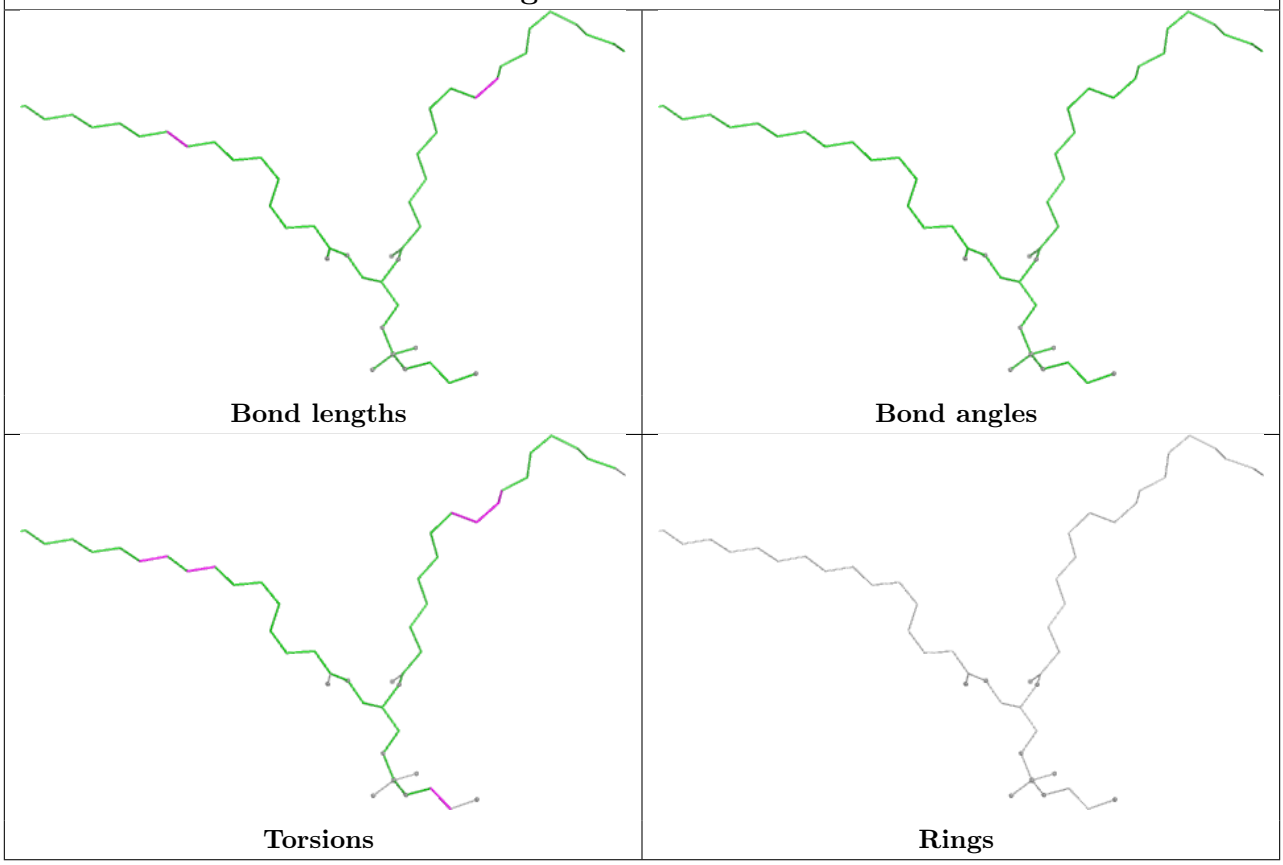
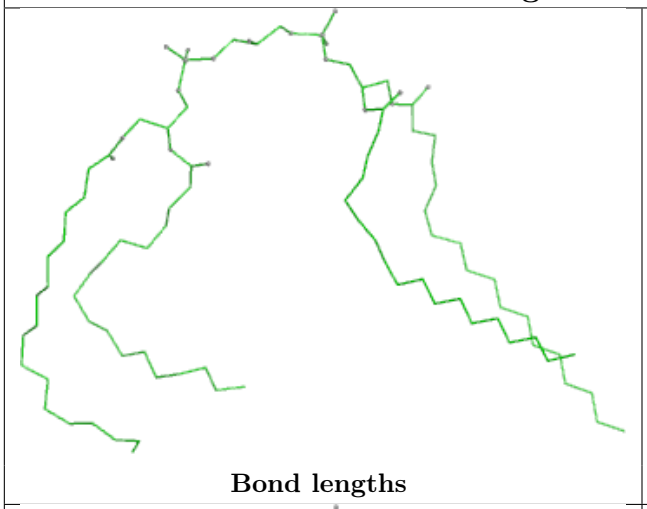


Rings

Ligand PEE 4d 101



Ligand CDL 4s 102



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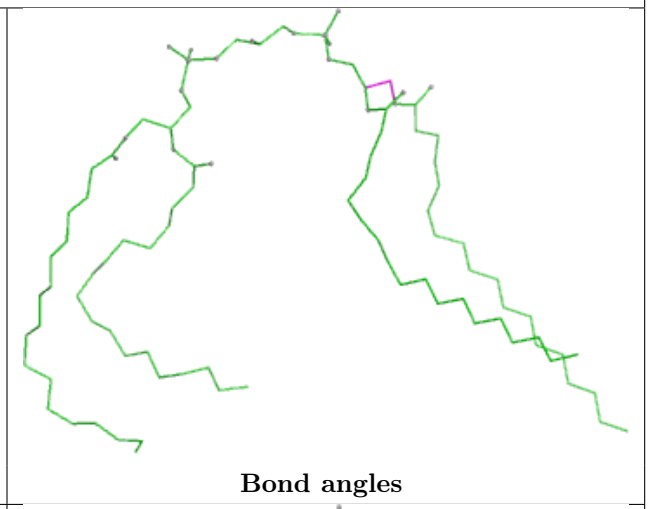
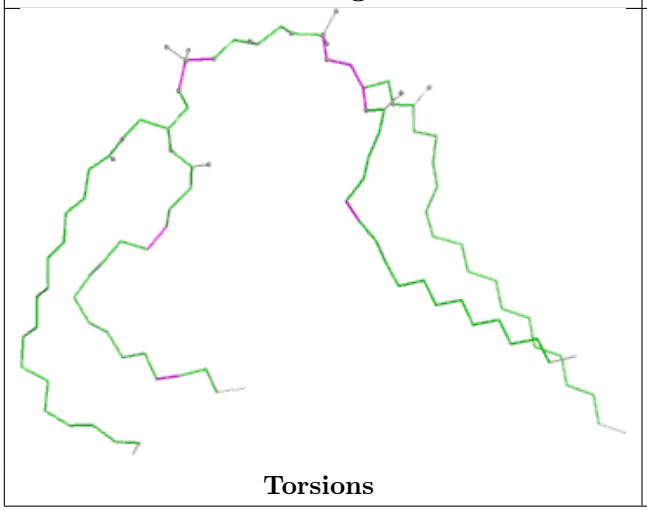


Bond angles



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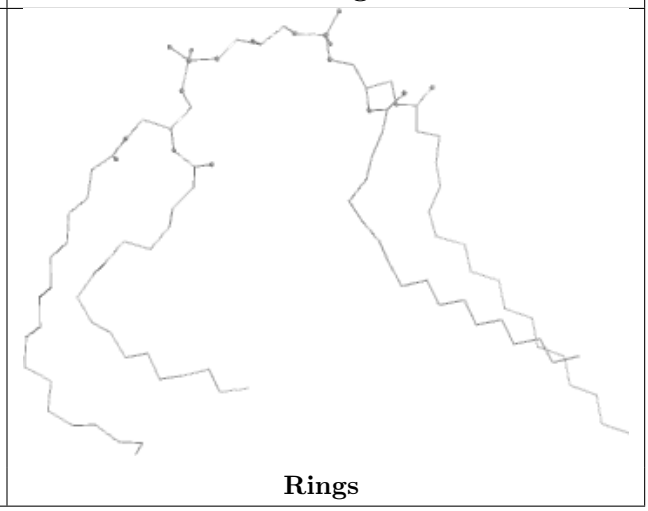
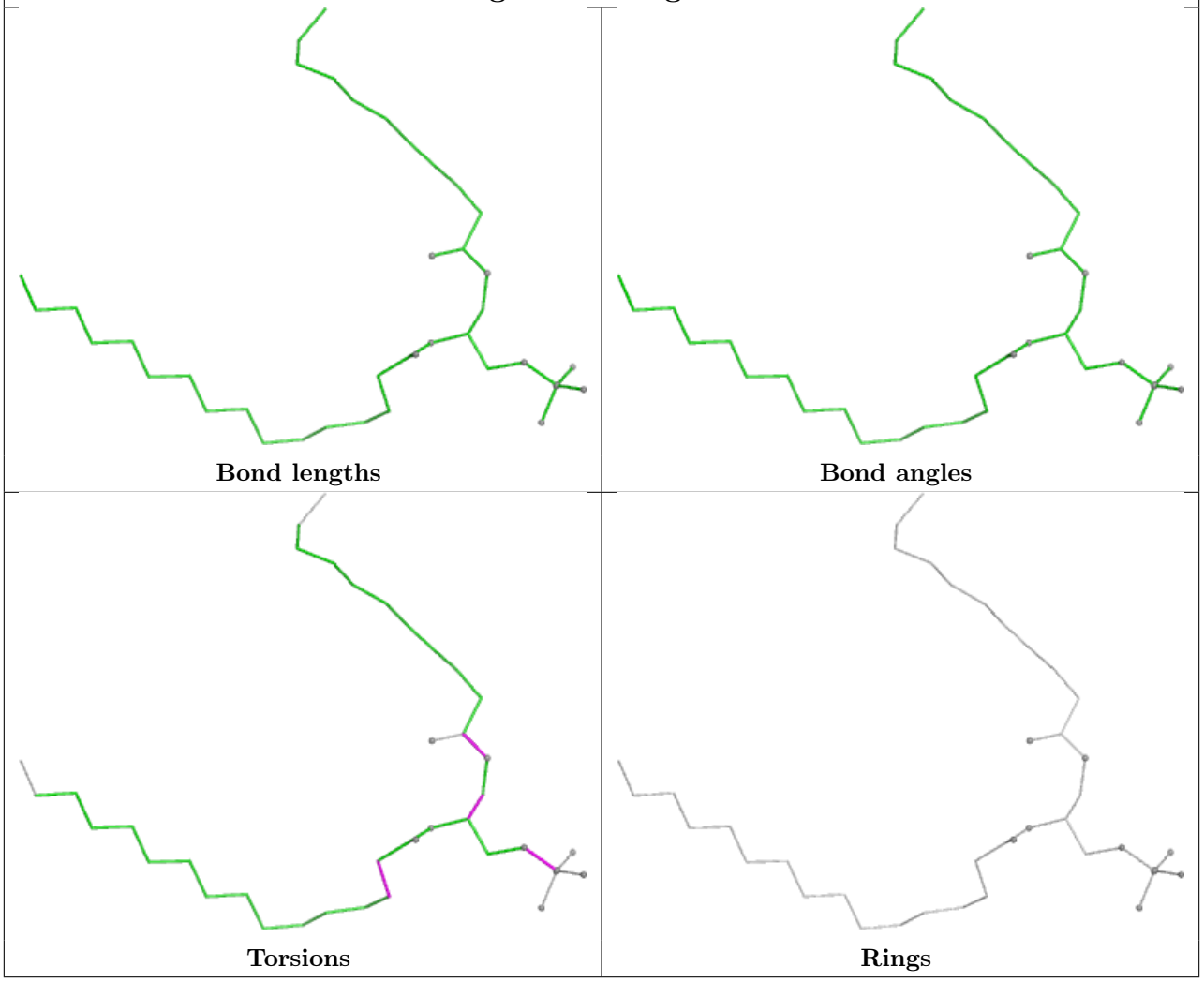
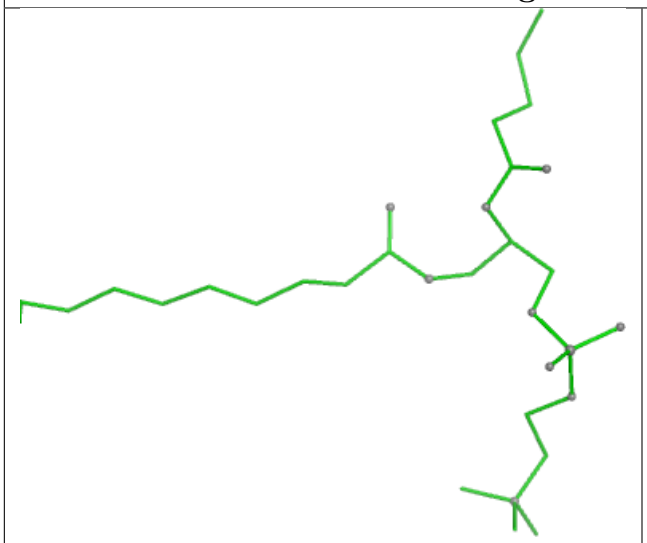


Rings

Ligand LPP 4g 201



Ligand PC1 3H 402



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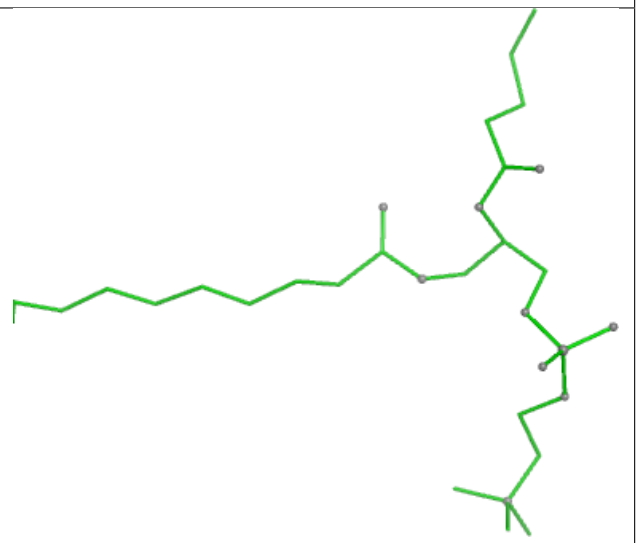
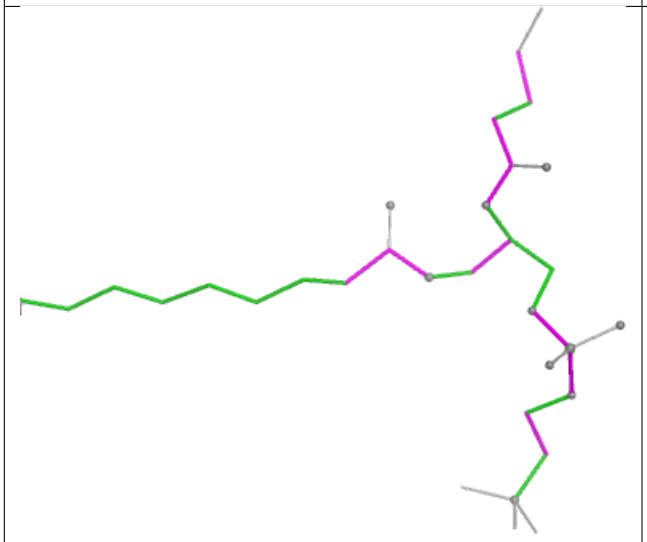


Bond angles



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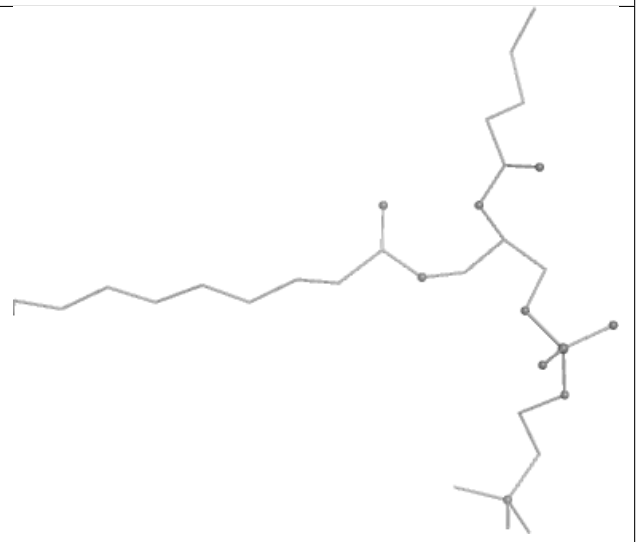
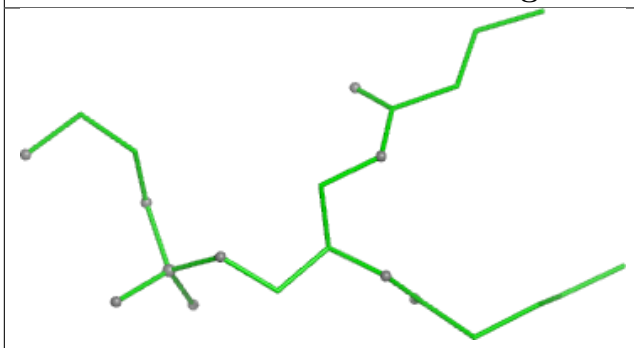


Rings

Ligand PEE 2p 203



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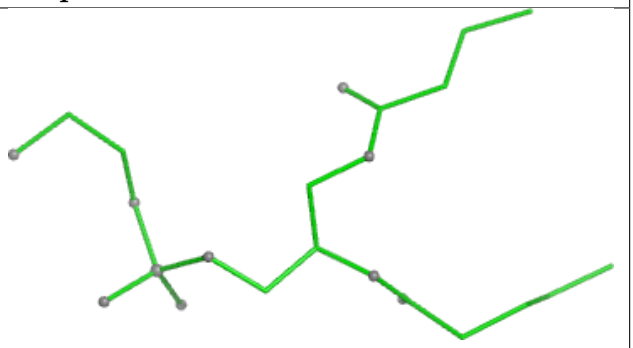
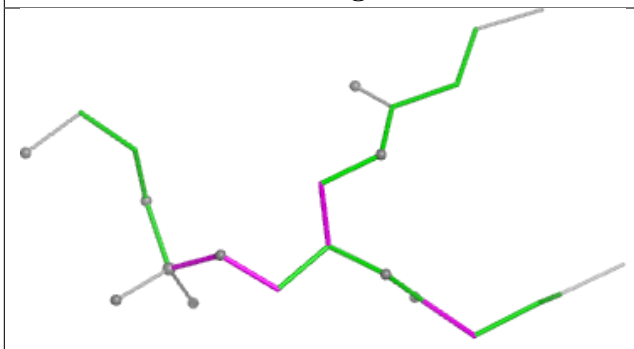


Bond angles



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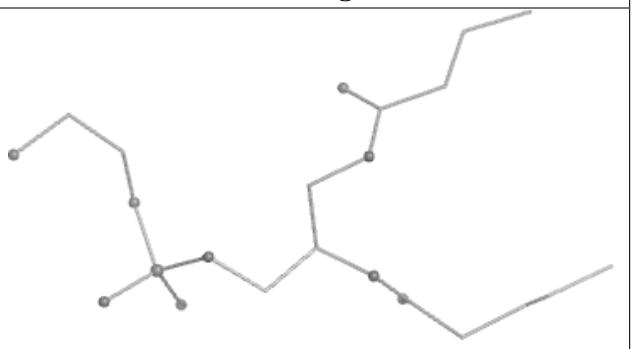
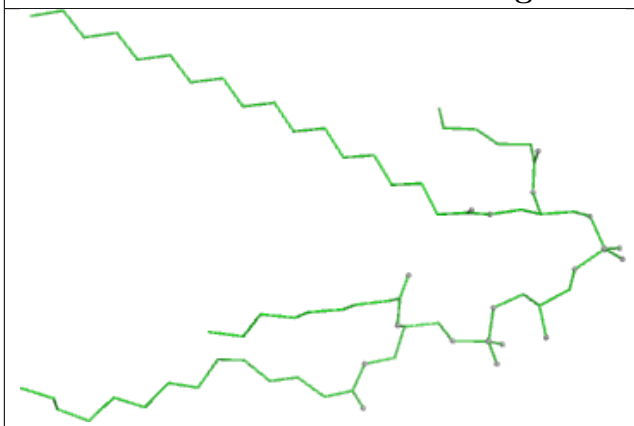


Rings

Ligand CDL 3G 404



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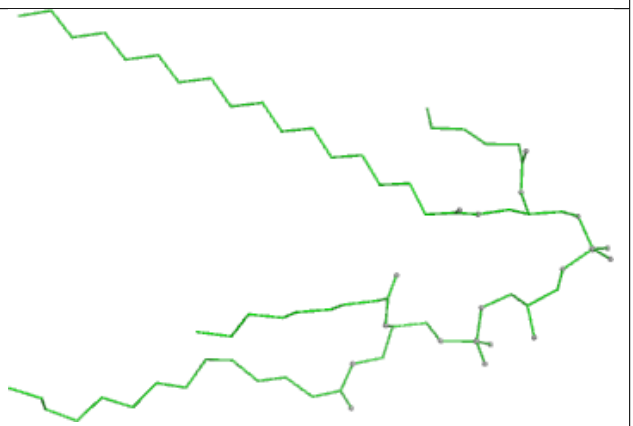
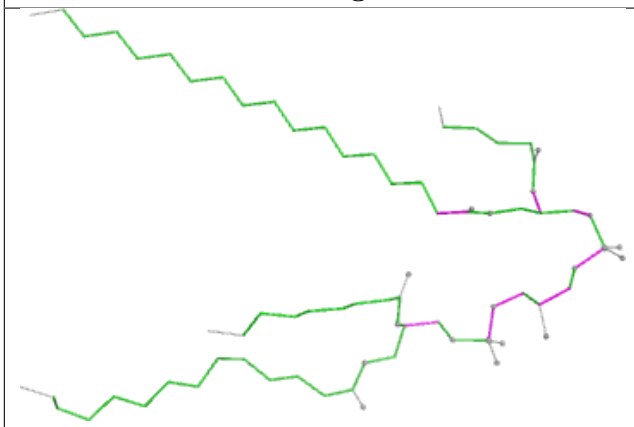


Bond angles



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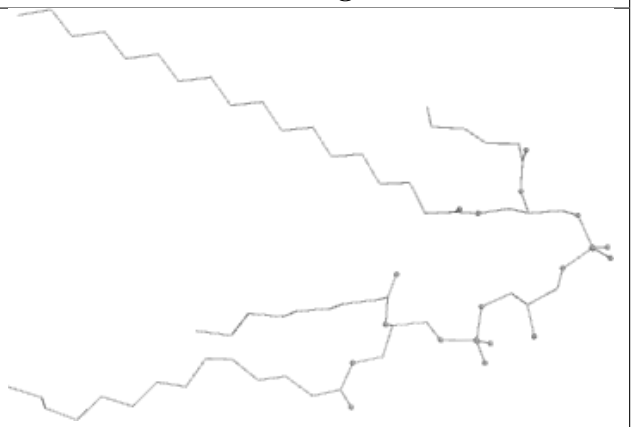
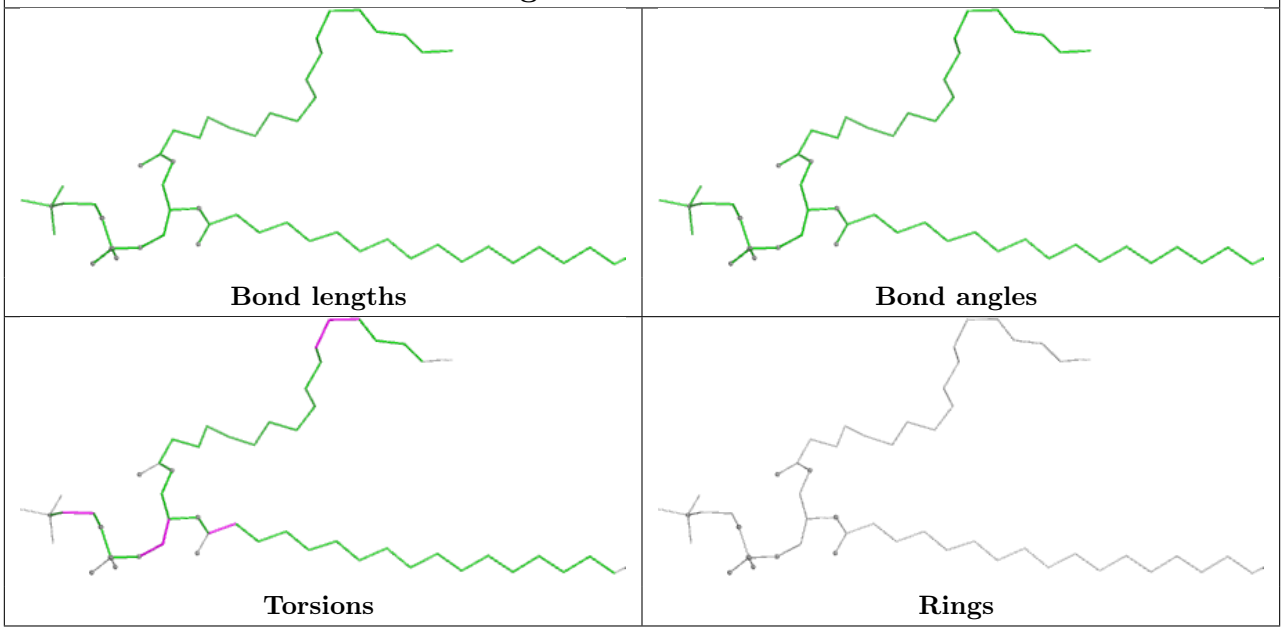
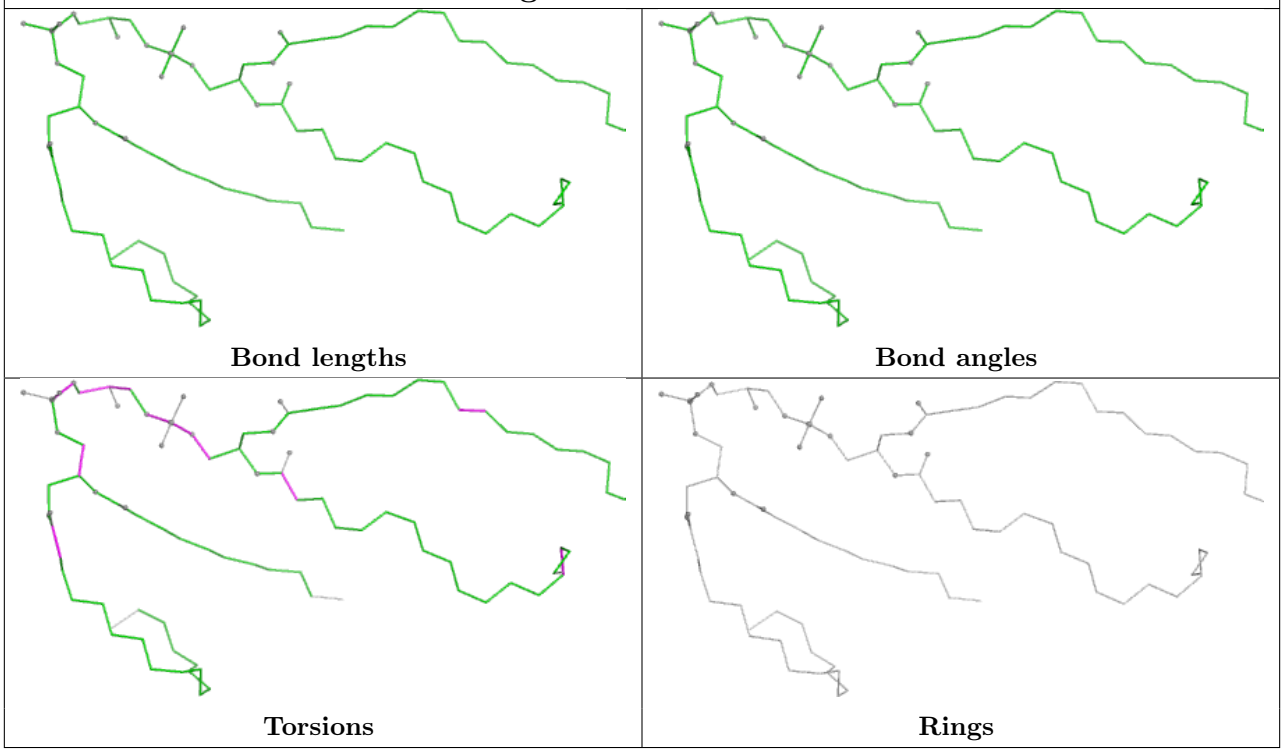


Rings

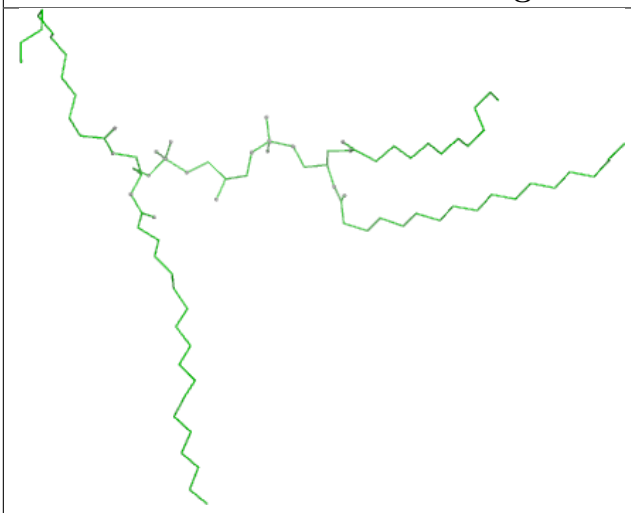
Ligand PC1 2T 101



Ligand CDL 4o 501



Ligand CDL 3H 404



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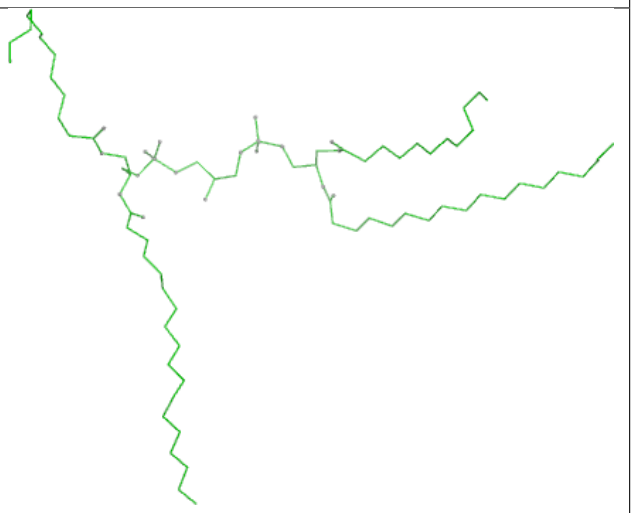
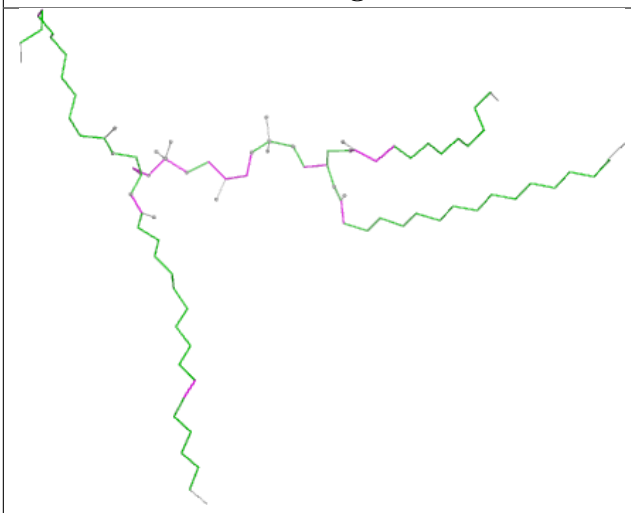


Bond angles



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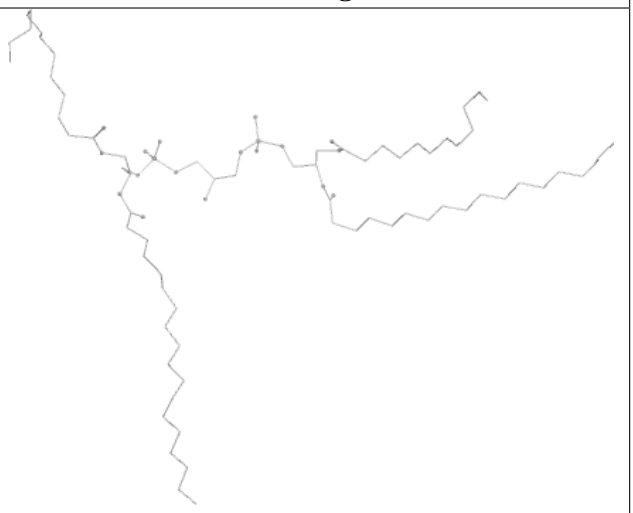
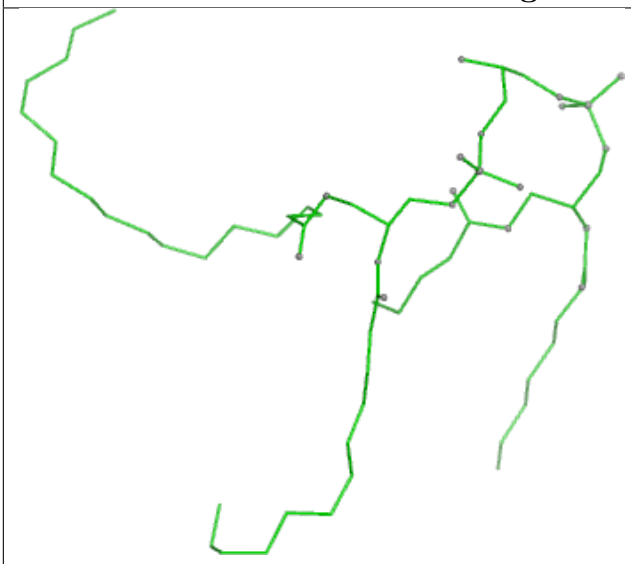


Rings

Ligand CDL 3e 201



Bond lengths



Bond angles

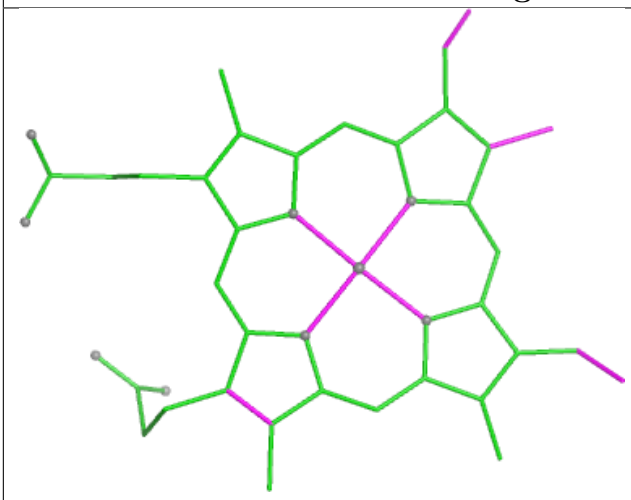


Torsions



Rings

Ligand HEM 3g 408



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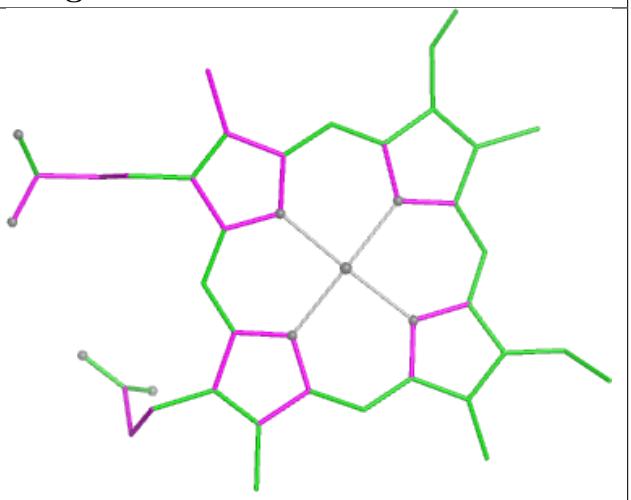
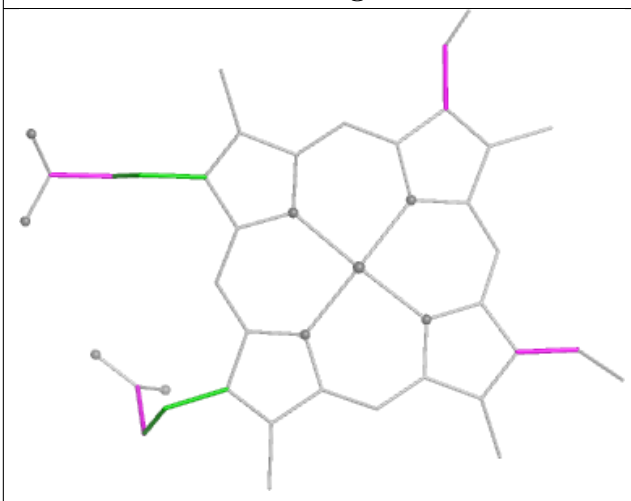


Bond angles



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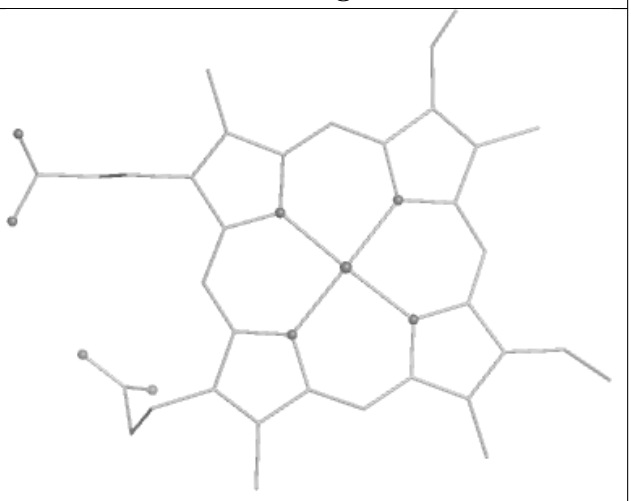
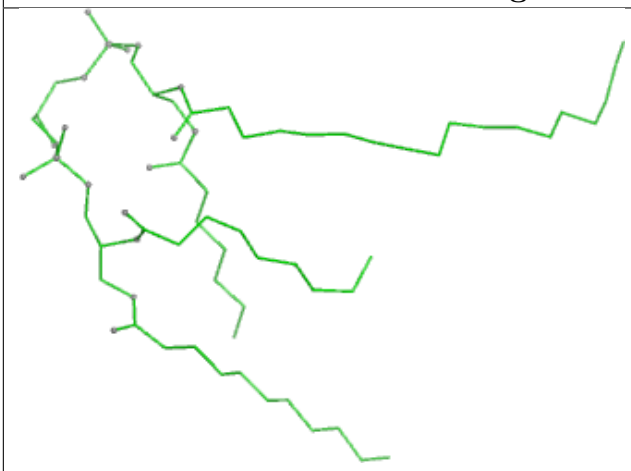


Rings

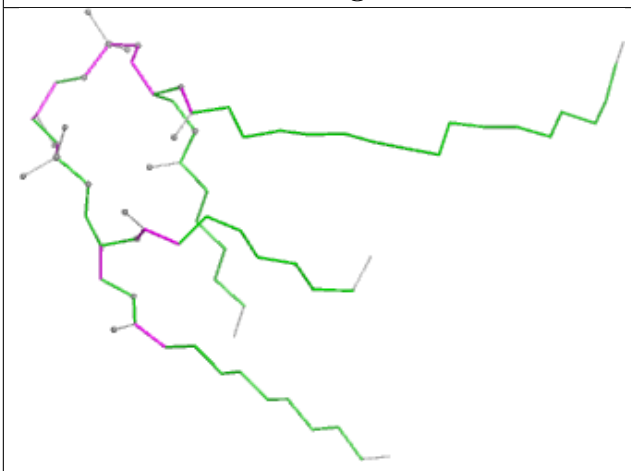
Ligand CDL 4W 202



Bond lengths



Bond angles

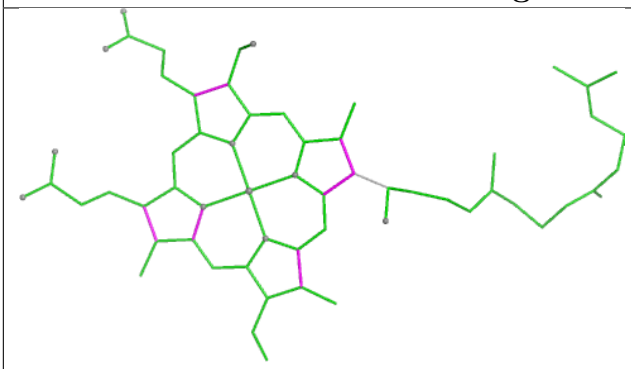


Torsions



Rings

Ligand HEA 4Q 908



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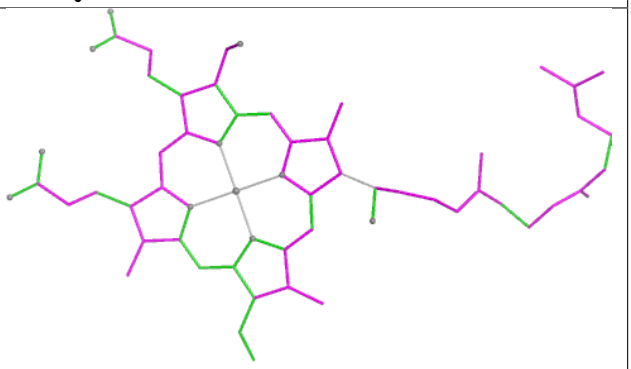
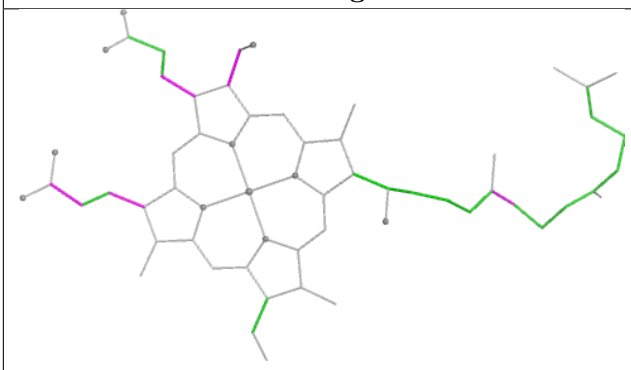


Bond angles



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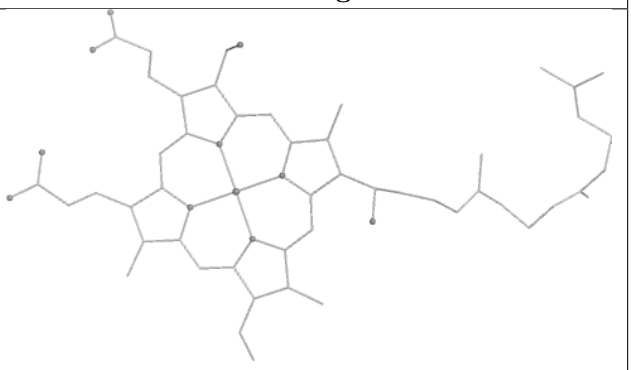
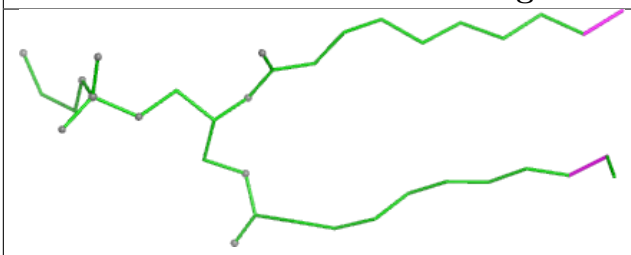


Rings

Ligand PEE 4Q 901



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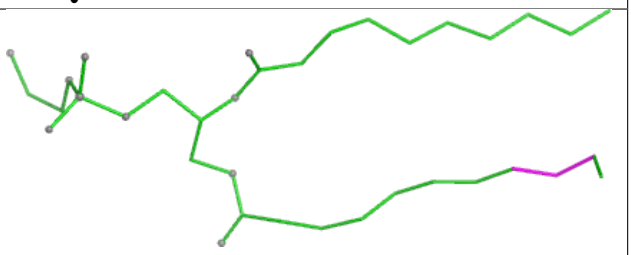
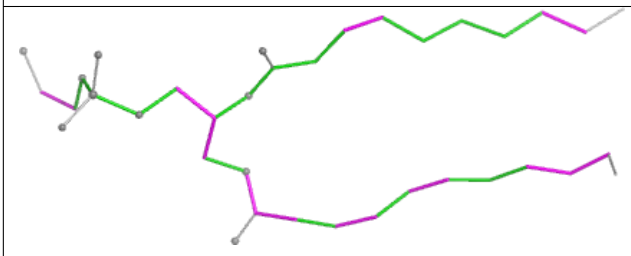


Bond angles



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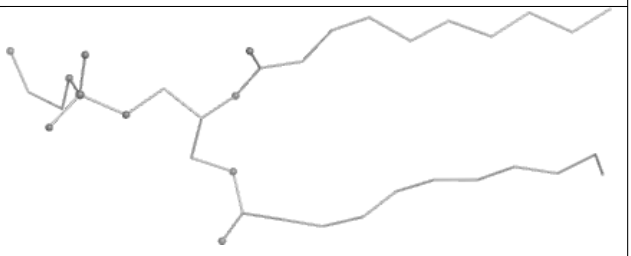
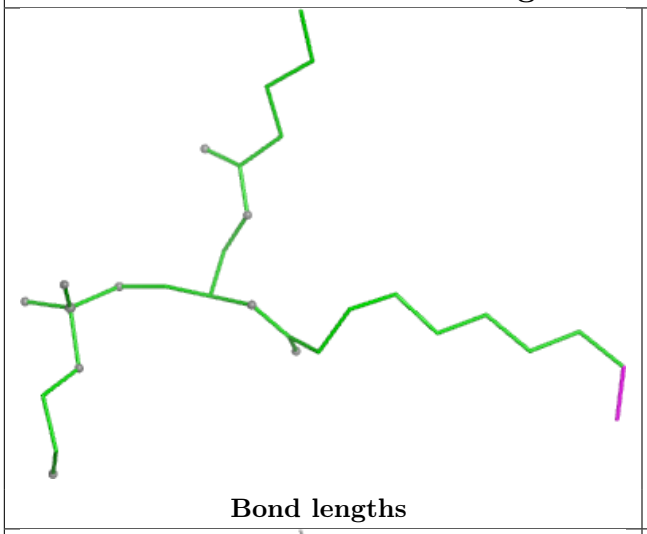


Rings

Ligand PEE 3C 301



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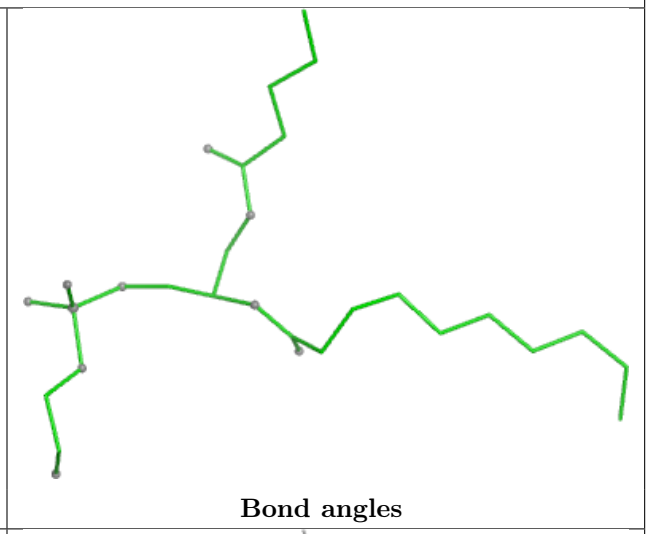
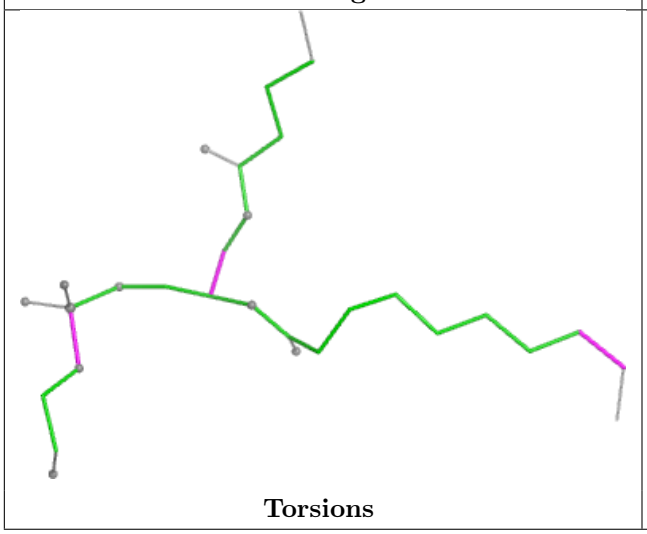


Bond angles



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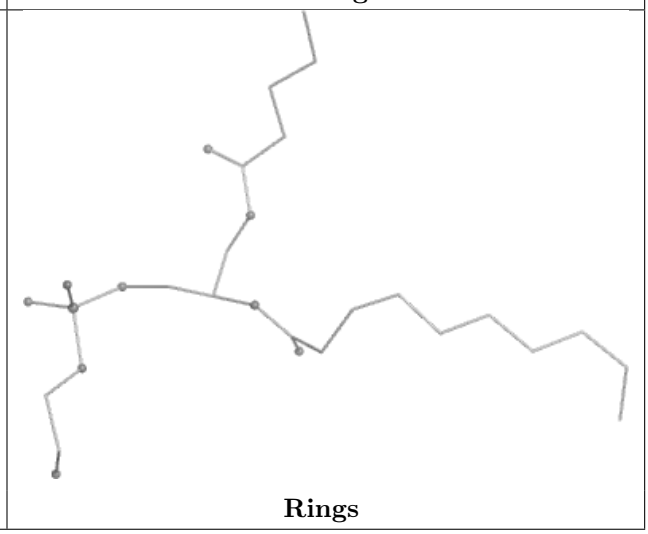
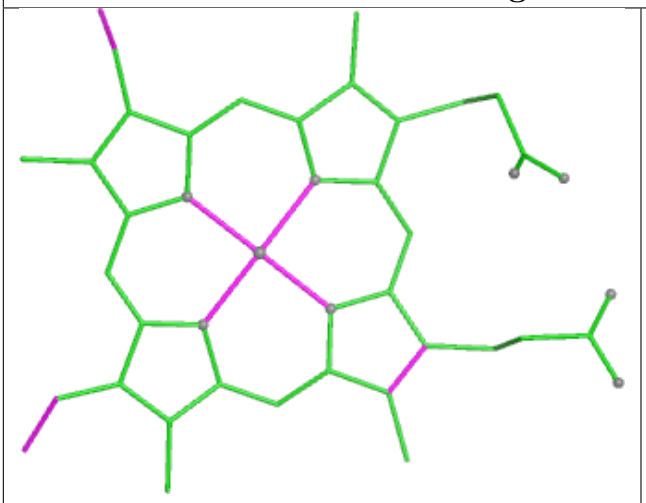


Rings

Ligand HEM 3G 405



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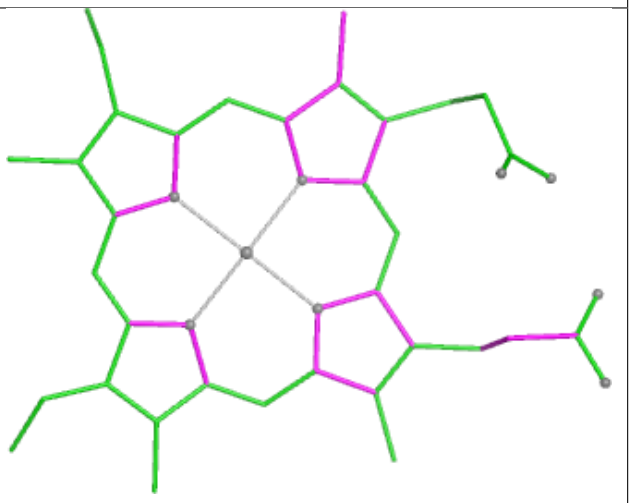
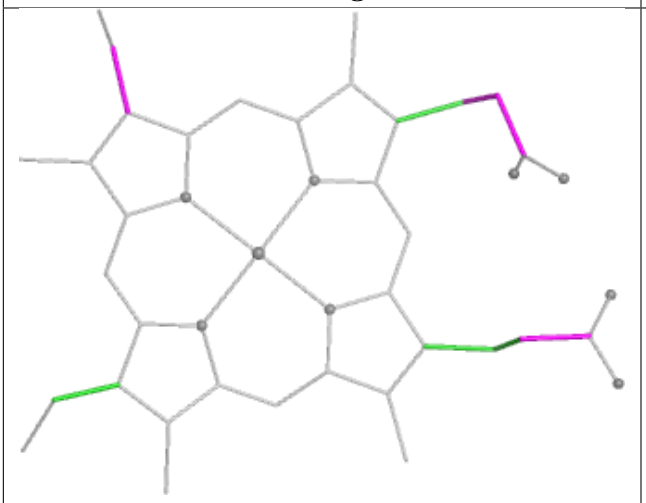


Bond angles



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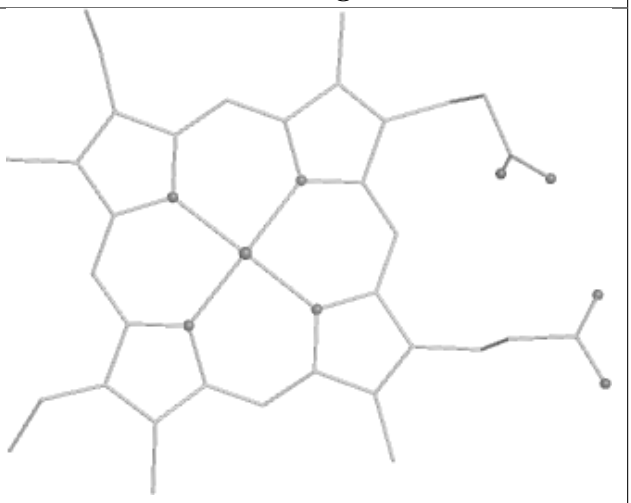
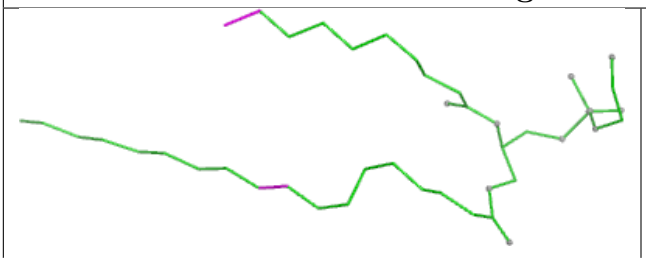


Rings

Ligand PEE 4R 201



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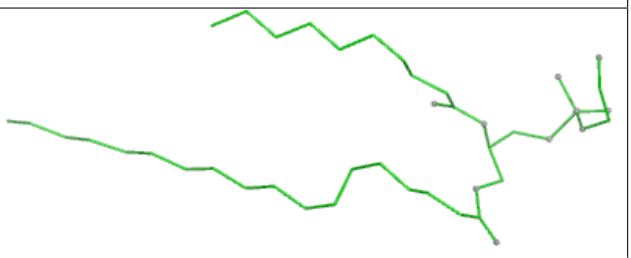
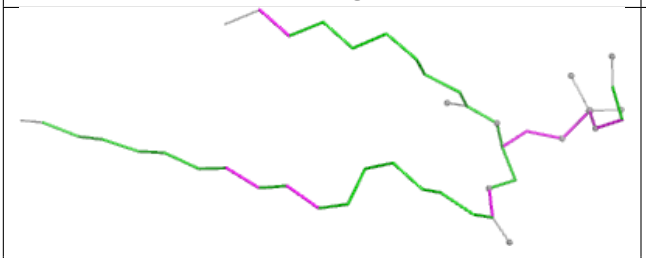
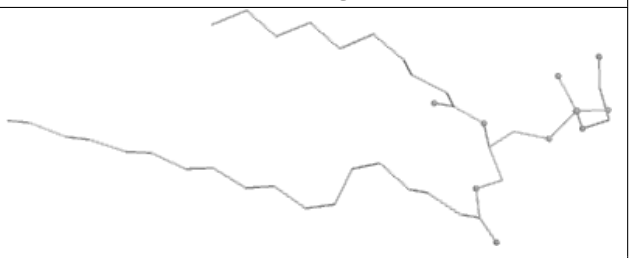


Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	30	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	30	73:ALA	C	81:GLY	N	8.69

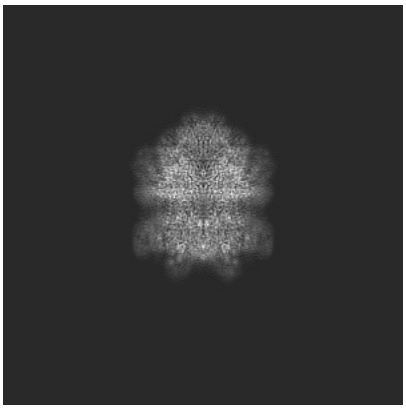
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50403. These allow visual inspection of the internal detail of the map and identification of artifacts.

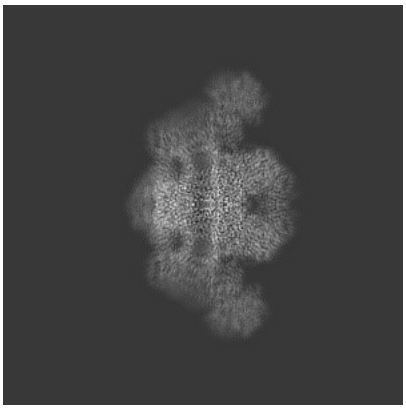
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

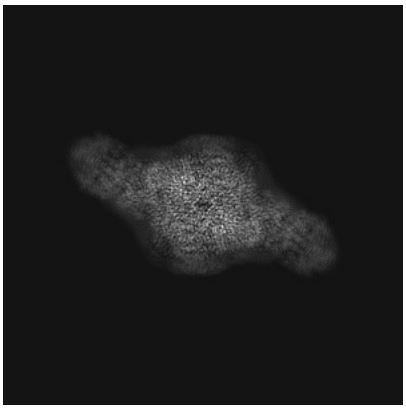
6.1.1 Primary map



X

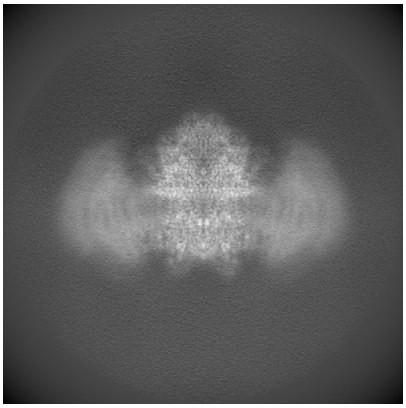


Y

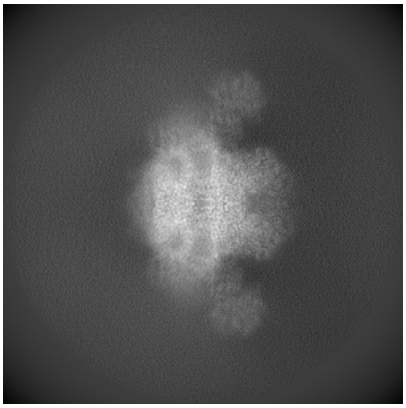


Z

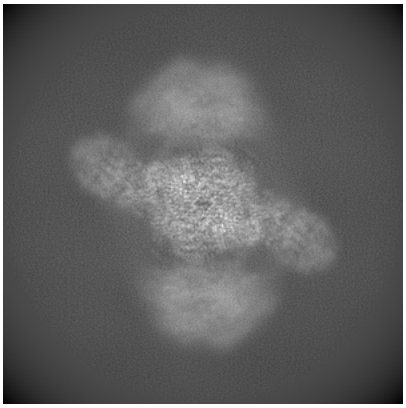
6.1.2 Raw map



X



Y



Z

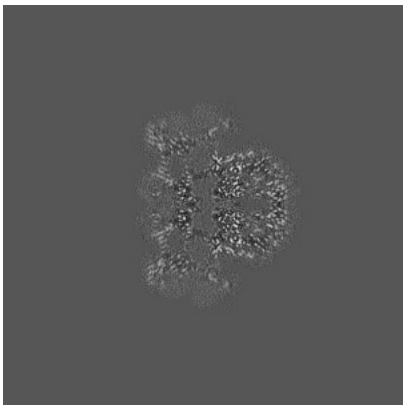
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

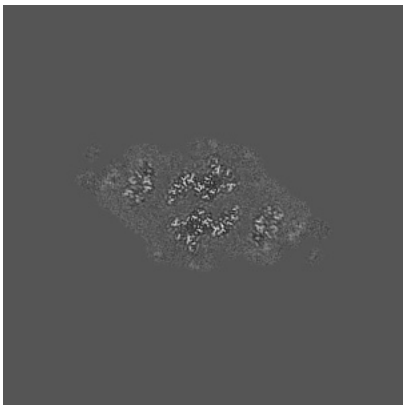
6.2.1 Primary map



X Index: 250

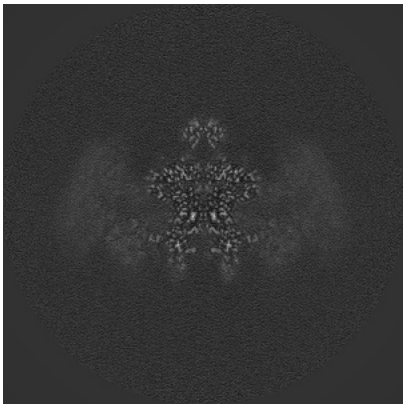


Y Index: 250

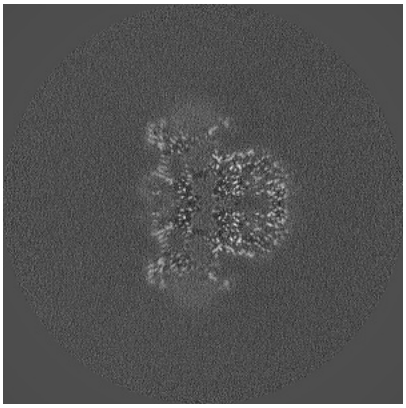


Z Index: 250

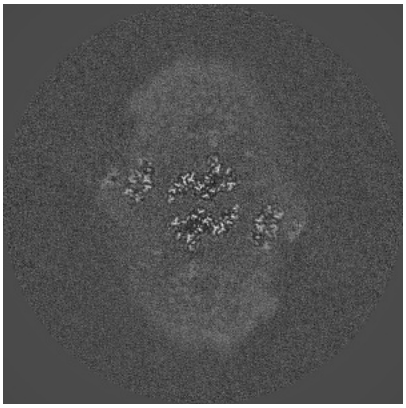
6.2.2 Raw map



X Index: 250



Y Index: 250

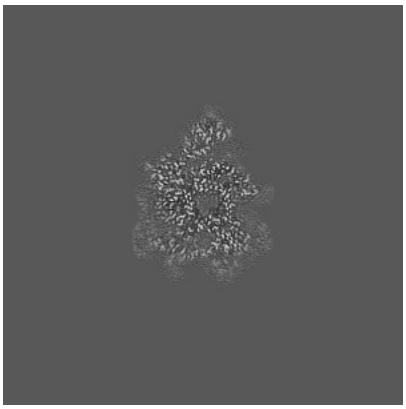


Z Index: 250

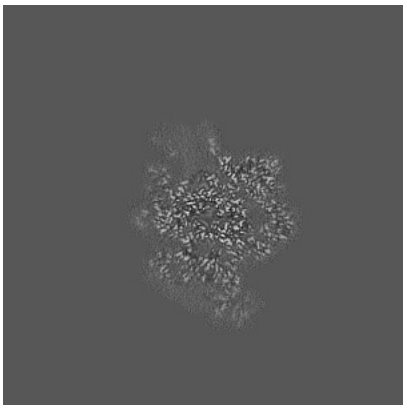
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

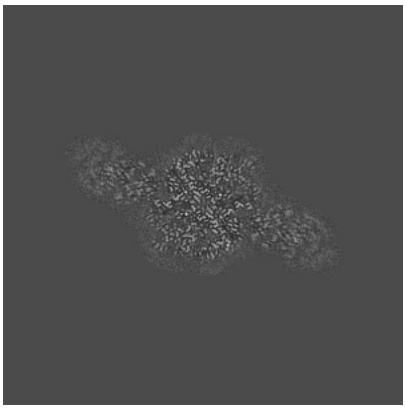
6.3.1 Primary map



X Index: 237

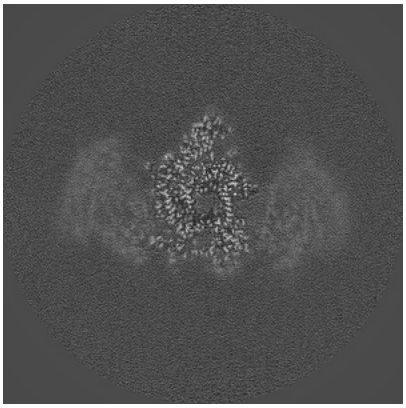


Y Index: 267

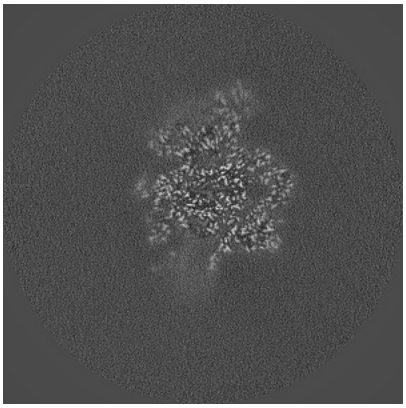


Z Index: 268

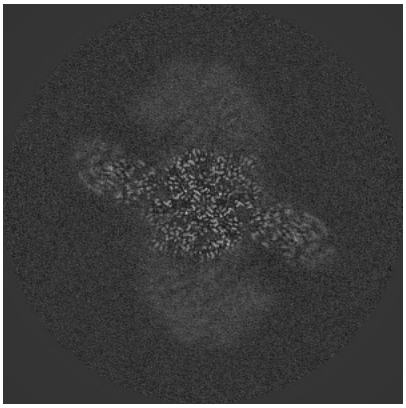
6.3.2 Raw map



X Index: 235



Y Index: 233

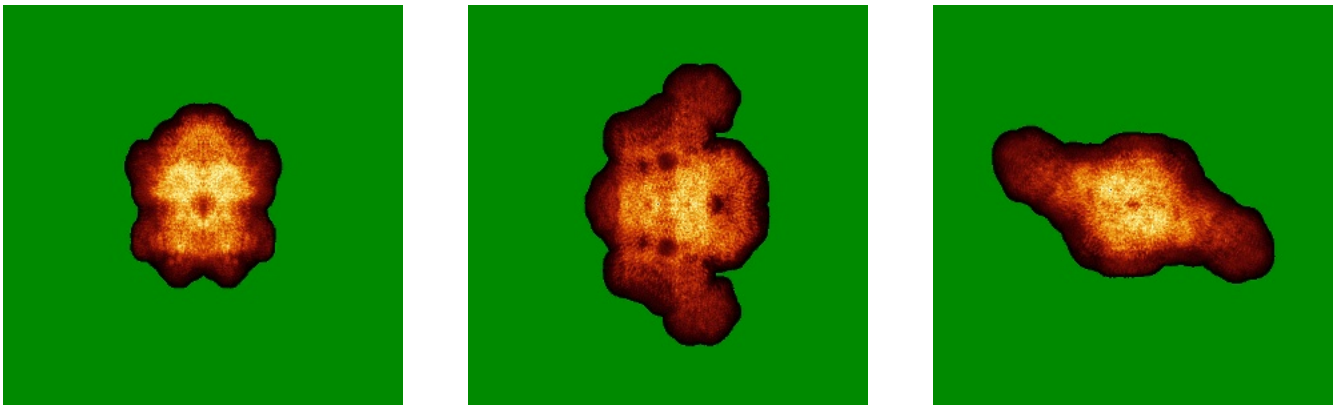


Z Index: 268

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

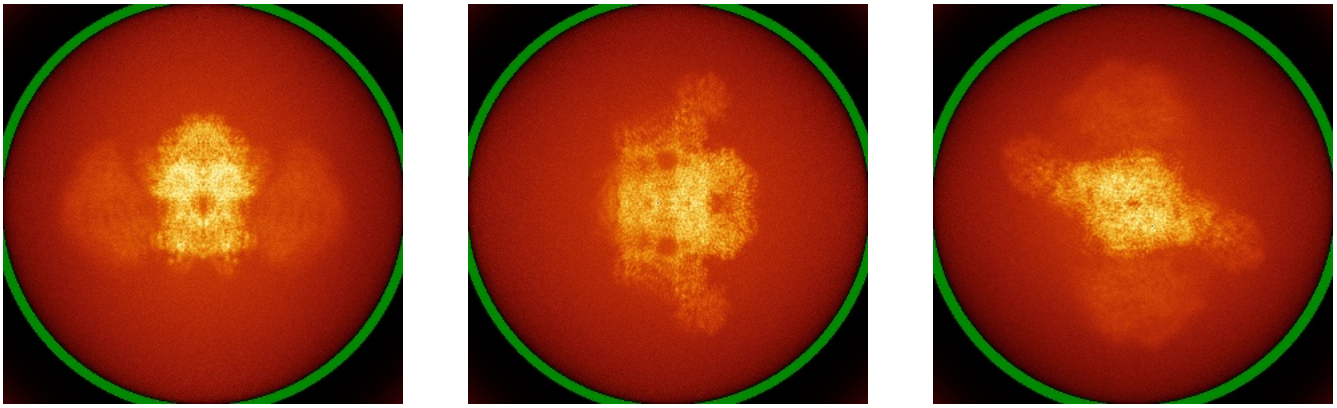
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

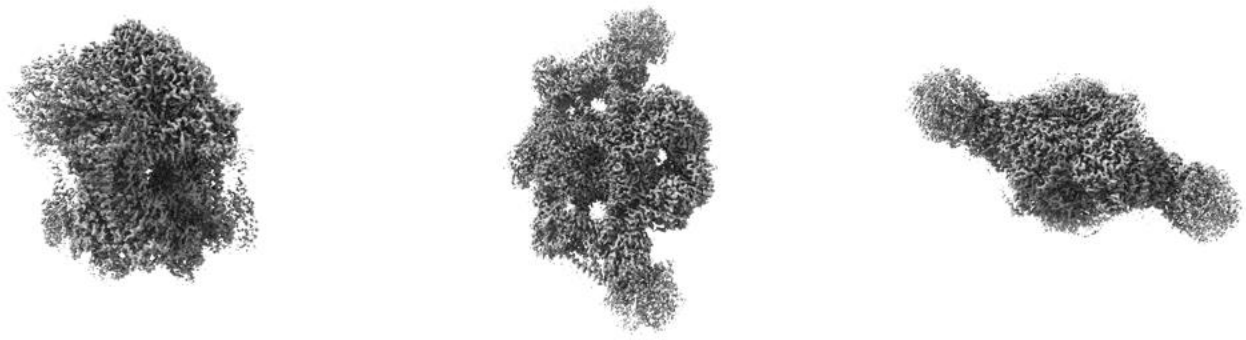


X Y Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

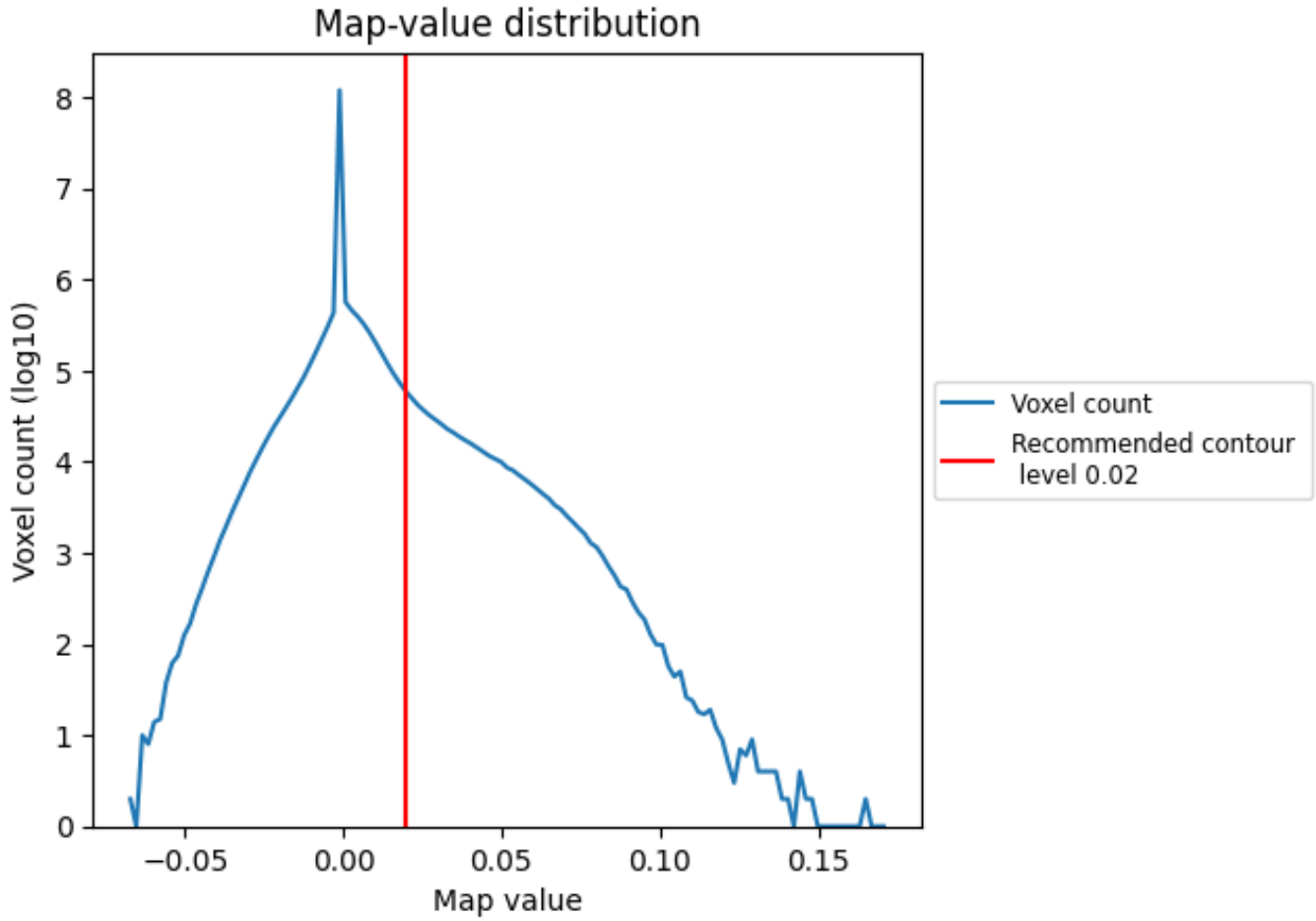
6.6 Mask visualisation (i)

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

7 Map analysis

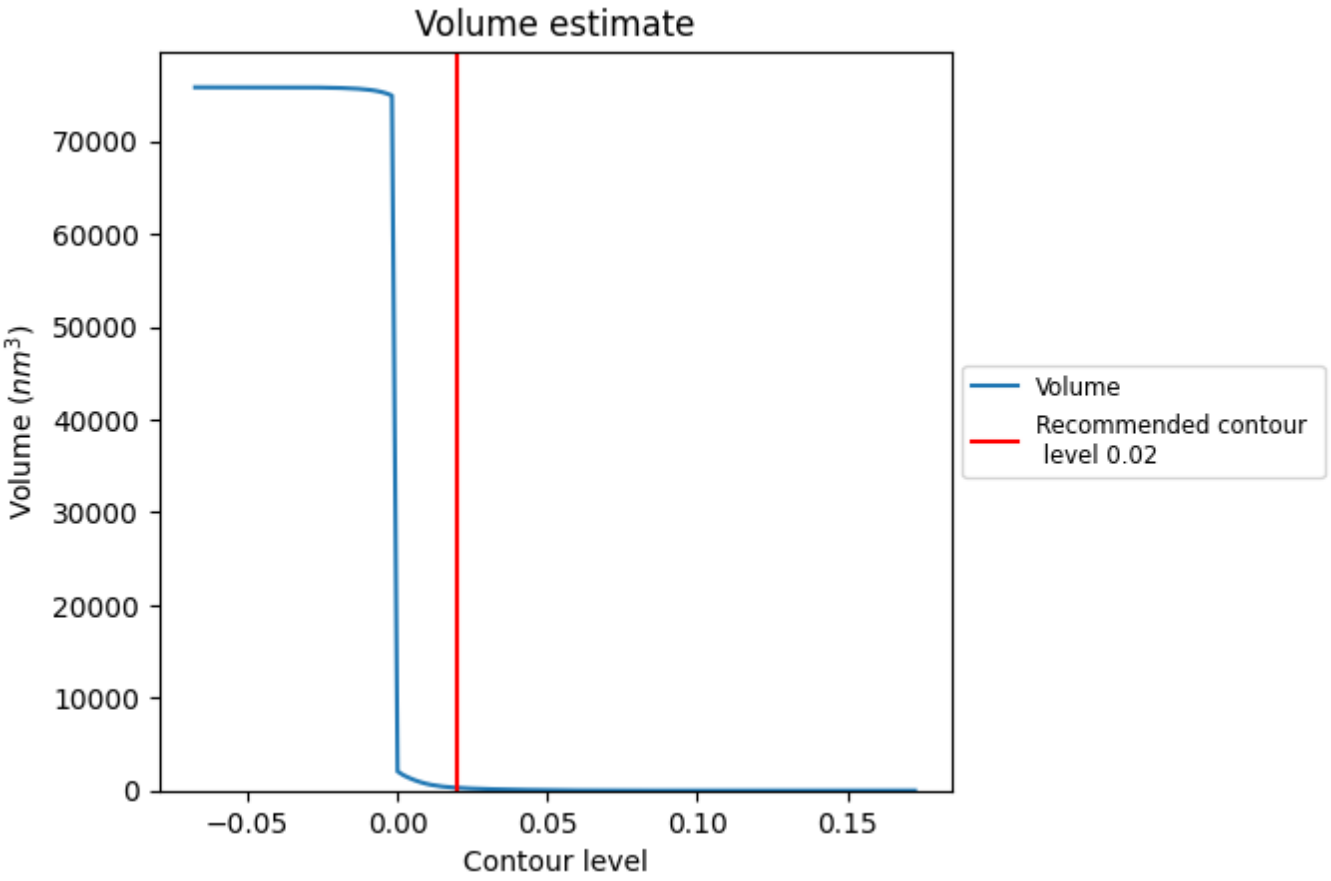
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

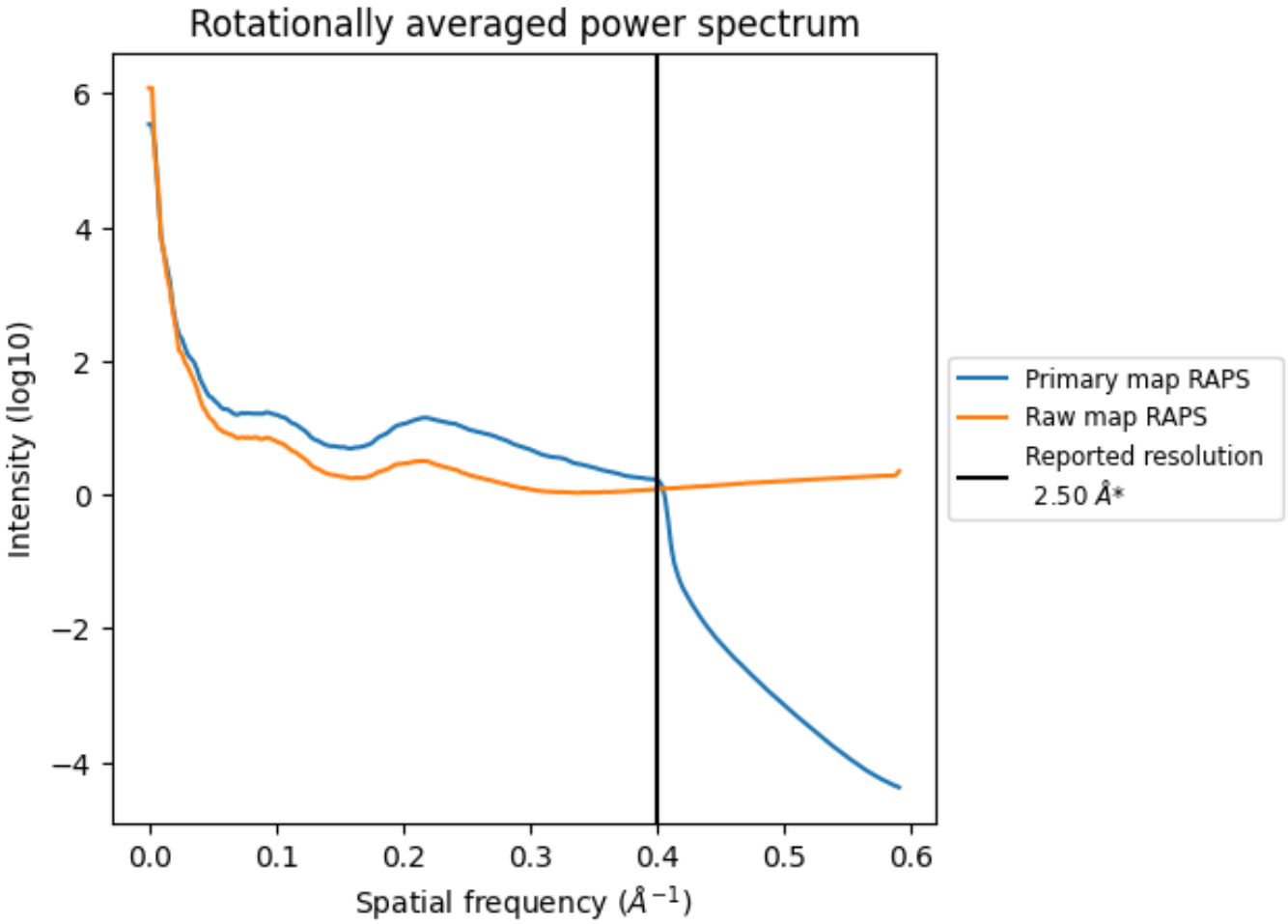
7.2 Volume estimate



The volume at the recommended contour level is 300 nm^3; this corresponds to an approximate mass of 271 kDa.

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

7.3 Rotationally averaged power spectrum (i)

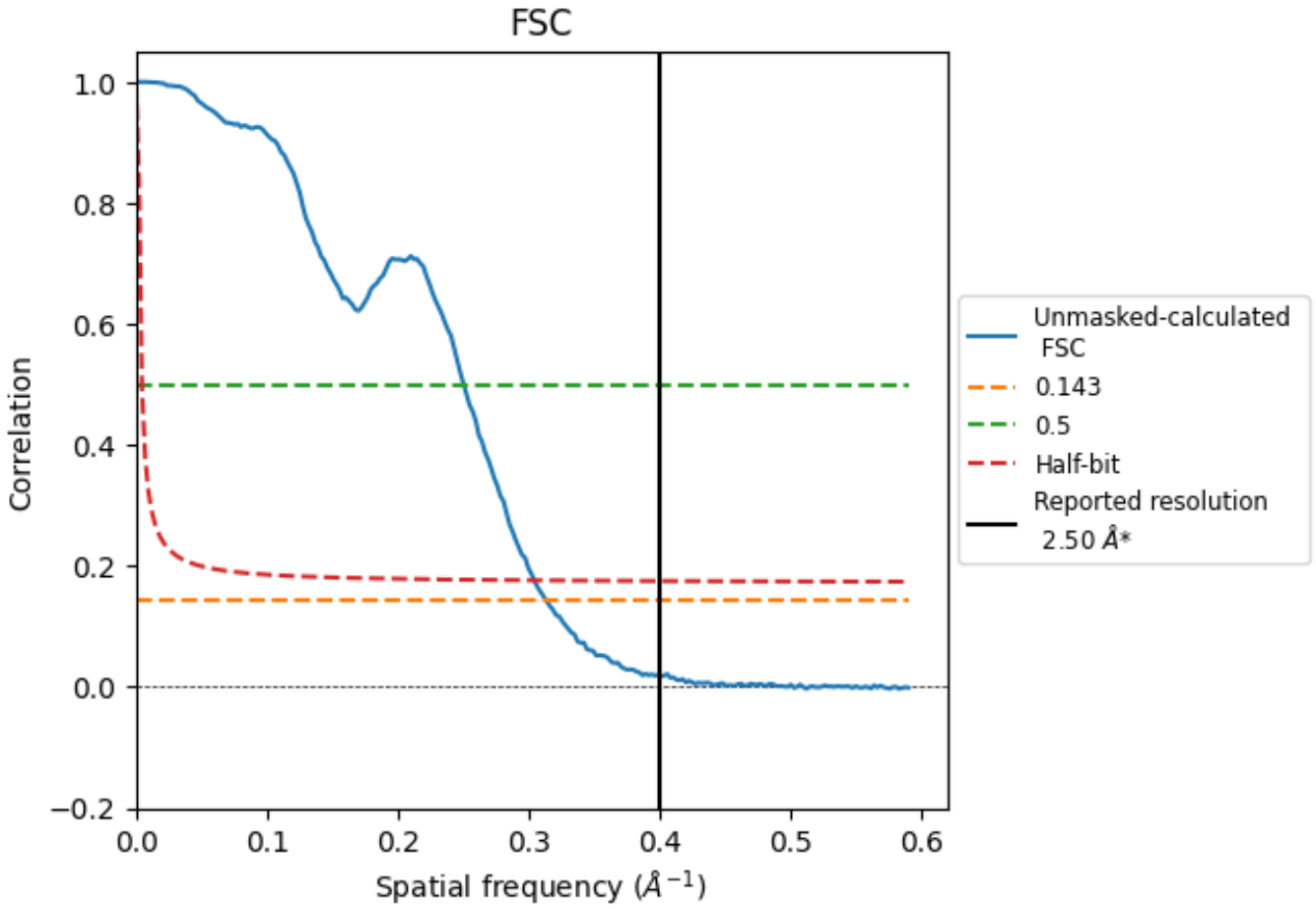


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

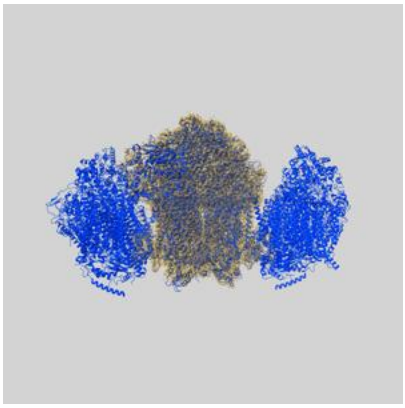
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.99	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.5 by more than 10 %

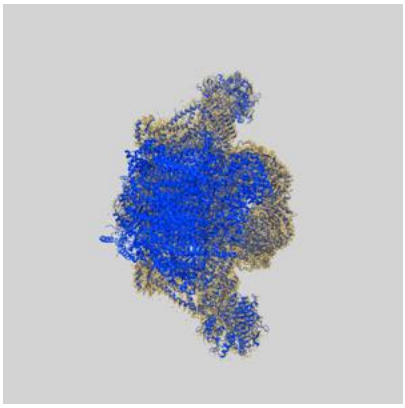
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50403 and PDB model 9FQ7. Per-residue inclusion information can be found in section 3 on page 32.

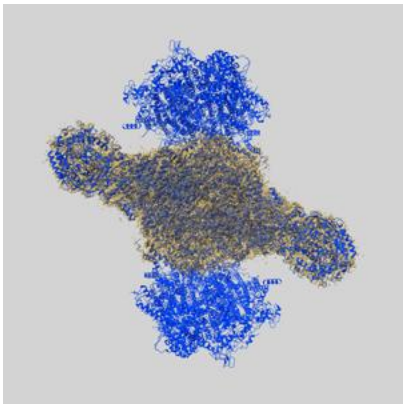
9.1 Map-model overlay



X



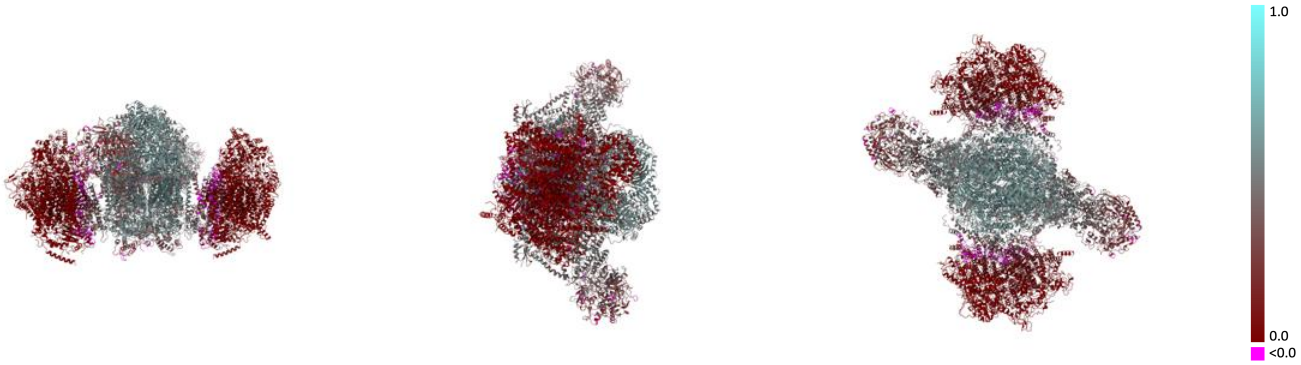
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

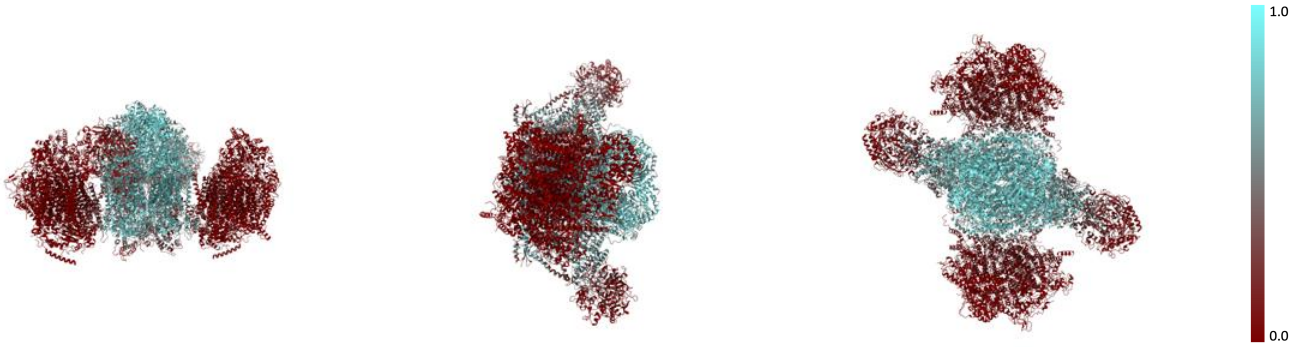
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

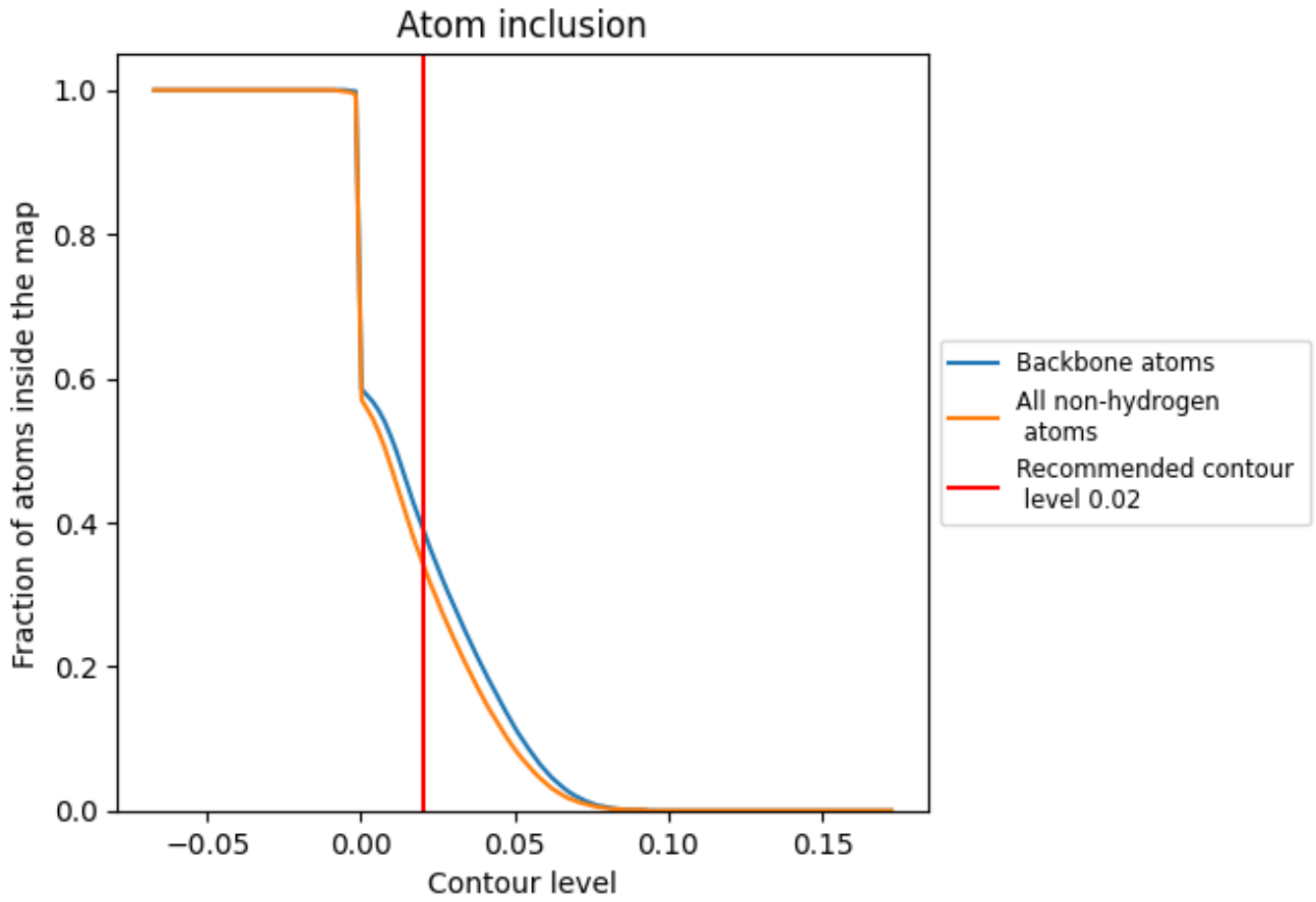
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 39% of all backbone atoms, 34% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3440	0.2760
2M	0.1330	0.2740
2N	0.3560	0.3680
2O	0.6730	0.4980
2P	0.6050	0.4880
2Q	0.5500	0.4370
2R	0.6300	0.4740
2S	0.6240	0.4770
2T	0.6430	0.4960
2U	0.4150	0.3900
2V	0.3670	0.3800
2m	0.1310	0.2860
2n	0.3680	0.3720
2o	0.6880	0.5050
2p	0.6390	0.5030
2q	0.5560	0.4470
2r	0.5950	0.4780
2s	0.6460	0.4760
2t	0.6790	0.5040
2u	0.4200	0.4020
2v	0.4200	0.4110
30	0.2220	0.2470
31	0.1960	0.2440
3A	0.8110	0.5670
3B	0.8090	0.5660
3C	0.8610	0.5990
3D	0.8220	0.5810
3E	0.8140	0.5750
3F	0.8970	0.6110
3G	0.8870	0.6240
3H	0.7290	0.5430
3I	0.8170	0.5850
3J	0.6480	0.5000
3K	0.8240	0.6060
3L	0.5730	0.4820



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Chain	Atom inclusion	Q-score
3a	0.8070	0.5650
3b	0.8050	0.5610
3c	0.8540	0.5970
3d	0.8750	0.6130
3e	0.8250	0.5680
3f	0.8820	0.5990
3g	0.8600	0.6140
3h	0.7870	0.5650
3i	0.8450	0.5950
3j	0.6290	0.4780
3k	0.8130	0.6010
3l	0.5860	0.4810
40	0.0000	-0.0020
41	0.0000	-0.0010
4A	0.0130	0.0850
4B	0.0380	0.0870
4C	0.0960	0.2500
4D	0.0750	0.2040
4E	0.0000	0.0000
4F	0.0510	0.0910
4G	0.0340	0.1010
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	0.0100
4O	0.0000	-0.0010
4P	0.0010	0.0130
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	0.0010	0.0090
4X	0.0000	0.0000
4Y	0.0000	0.0000
4Z	0.0460	0.1300
4a	0.0220	0.0930
4b	0.0310	0.0670

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Chain	Atom inclusion	Q-score
4c	0.0670	0.2310
4d	0.0340	0.1560
4e	0.0000	-0.0000
4f	0.0210	0.0700
4g	0.0250	0.0950
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	0.0100
4o	0.0000	-0.0030
4p	0.0010	0.0090
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	0.0010	0.0140
4x	0.0000	0.0000
4y	0.0000	0.0000
4z	0.0280	0.1170