



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:26 PM UTC

PDB ID : 8IUF / pdb_00008iuf
EMDB ID : EMD-35720
Title : Cryo-EM structure of Euglena gracilis super-complex I+III2+IV, composite
Authors : Wu, M.C.; Tian, H.T.; He, Z.X.; Hu, Y.Q.; Zhou, L.
Deposited on : 2023-03-24
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

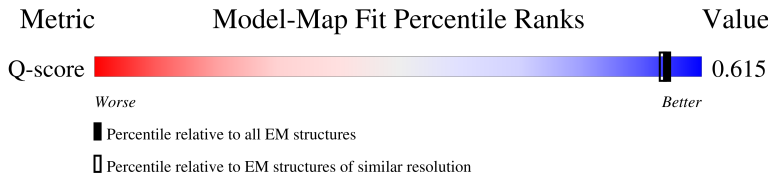
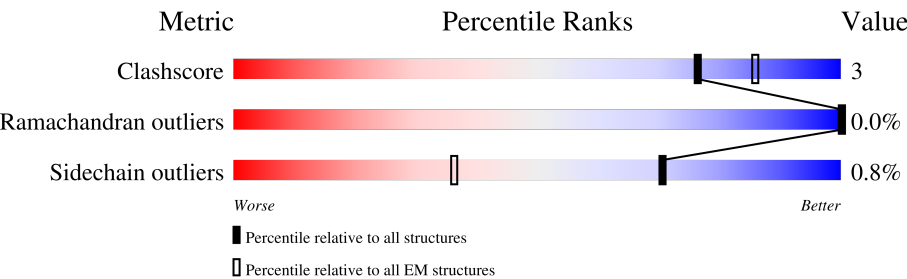
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 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	11740 (2.31 - 3.31)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	385	
2	1B	527	
3	2B	142	
4	4A	246	

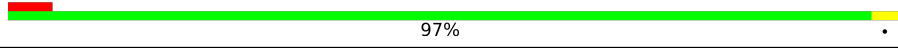
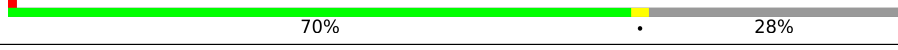
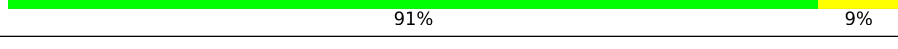
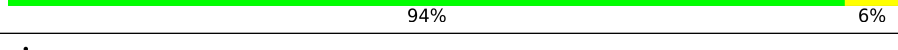
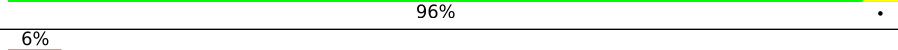
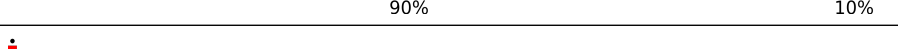
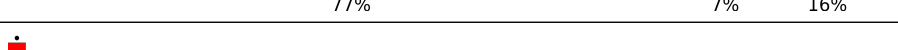
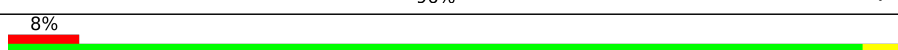
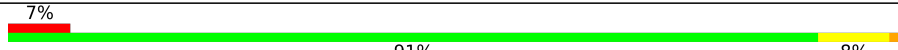
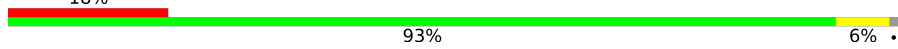
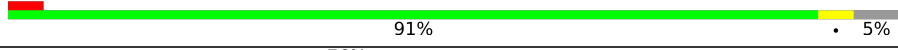
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Mol	Chain	Length	Quality of chain
5	4C	139	
6	4D	174	
7	4E	165	
8	4F	75	
9	4G	315	
10	4H	221	
11	4I	274	
12	4J	88	
13	4L	171	
14	5B	174	
15	5C	208	
16	6A	112	
17	6B	287	
18	7A	178	
19	7C	171	
20	A1	141	
21	A2	193	
22	A3	125	
23	A5	184	
24	A6	437	
25	A7	136	
26	A8	223	
27	A9	489	
28	AB	134	
29	AC	134	

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Mol	Chain	Length	Quality of chain
30	AL	281	
31	AM	198	
32	AN	287	
33	B2	145	
34	B3	62	
35	B4	171	
36	B5	140	
37	B6	91	
38	B7	97	
39	B8	176	
40	B9	158	
41	BL	144	
42	BM	112	
43	C1	495	
44	C2	196	
45	C3	161	
46	C4	185	
47	DC	179	
48	E1	483	
49	E2	472	
50	E3	594	
51	E4	368	
52	E5	290	
53	E6	371	
54	E7	246	

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Mol	Chain	Length	Quality of chain
55	E8	205	
56	E9	178	
57	EA	126	
58	EB	101	
59	EC	101	
60	ED	151	
61	FX	325	
62	G1	436	
63	G2	267	
64	G3	261	
65	N1	670	
66	N2	300	
67	N3	293	
67	N6	293	
68	N4	478	
69	N5	584	
70	QA	479	
70	Qa	479	
71	QB	474	
71	Qb	474	
72	QC	368	
72	Qc	368	
73	QD	243	
73	Qd	243	
74	QE	252	

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Mol	Chain	Length	Quality of chain
74	Qe	252	
75	QF	72	
75	Qf	72	
76	QG	228	
76	Qg	228	
77	QH	85	
77	Qh	85	
78	QI	70	
78	Qi	70	
79	QJ	154	
79	Qj	154	
80	QK	100	
80	Qk	100	
81	S2	395	
82	S3	277	
83	S4	208	
84	S5	122	
85	S6	147	
86	S7	207	
87	S8	212	
88	V1	526	
89	V2	225	
90	A	12	
90	B	12	

2 Entry composition [i](#)

There are 108 unique types of molecules in this entry. The entry contains 368218 atoms, of which 183093 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 NDUFS1a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1A	352	Total	C	H	N	O	S	0	0
			5501	1753	2700	488	537	23		

- Molecule 2 is a protein called NDUFS1b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1B	525	Total	C	H	N	O	S	1	0
			8357	2679	4159	743	765	11		

- Molecule 3 is a protein called ND2b.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2B	140	Total	C	H	N	O	S	0	0
			2059	712	989	172	183	3		

- Molecule 4 is a protein called COXEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4A	204	Total	C	H	N	O	S	0	0
			3220	1054	1608	267	285	6		

- Molecule 5 is a protein called COXEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4C	123	Total	C	H	N	O	S	0	0
			2049	670	1027	168	183	1		

- Molecule 6 is a protein called COXEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	4D	173	Total	C	H	N	O	S	0	0
			2708	863	1359	237	240	9		

- Molecule 7 is a protein called COXEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4E	160	Total	C	H	N	O	S	0	0
			2612	859	1279	220	247	7		

- Molecule 8 is a protein called COXEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4F	75	Total	C	H	N	O	S	0	0
			1246	418	626	98	103	1		

- Molecule 9 is a protein called COXEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4G	297	Total	C	H	N	O	S	0	0
			4691	1478	2340	408	457	8		

- Molecule 10 is a protein called COXEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4H	205	Total	C	H	N	O	S	0	0
			3250	1040	1644	260	306			

- Molecule 11 is a protein called COXEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4I	265	Total	C	H	N	O	S	0	0
			4224	1411	2046	374	388	5		

- Molecule 12 is a protein called COXEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	4J	88	Total	C	H	N	O	S	0	0
			1399	459	688	126	124	2		

- Molecule 13 is a protein called ND4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	4L	108	Total	C	H	N	O	S	0	0
			1768	606	878	133	145	6		

- Molecule 14 is a protein called COX5b-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	5B	157	Total	C	H	N	O	S	0	0
			2442	807	1184	208	237	6		

- Molecule 15 is a protein called COX5c.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	5C	196	Total	C	H	N	O	S	0	0
			3117	1026	1546	253	283	9		

- Molecule 16 is a protein called COX6a.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	6A	91	Total	C	H	N	O	S	0	0
			1497	498	747	128	120	4		

- Molecule 17 is a protein called COX6b-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	6B	282	Total	C	H	N	O	S	0	0
			4514	1455	2229	396	427	7		

- Molecule 18 is a protein called COX7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	7A	165	Total	C	H	N	O	S	0	0
			2603	838	1284	248	226	7		

- Molecule 19 is a protein called COX7c.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	7C	151	Total	C	H	N	O	S	0	0
			2437	821	1183	204	226	3		

- Molecule 20 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	A1	137	Total	C	H	N	O	S	0	0
			2097	684	1026	192	192	3		

- Molecule 21 is a protein called NDUFA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	A2	192	Total	C	H	N	O	S	0	0
			2967	942	1474	267	280	4		

- Molecule 22 is a protein called NDUFA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A3	124	Total	C	H	N	O	S	0	0
			2089	678	1039	191	175	6		

- Molecule 23 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	A5	154	Total	C	H	N	O	S	0	0
			2509	794	1248	221	244	2		

- Molecule 24 is a protein called NDUFA6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A6	423	Total	C	H	N	O	S	0	0
			6608	2091	3280	601	632	4		

- Molecule 25 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	A7	136	Total	C	H	N	O	S	0	0
			2272	735	1118	219	194	6		

- Molecule 26 is a protein called NDUFA8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	A8	223	Total	C	H	N	O	S	0	0
			3548	1160	1726	315	334	13		

- Molecule 27 is a protein called NDUFA9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	A9	484	Total	C	H	N	O	S	0	0
			7679	2449	3850	662	700	18		

- Molecule 28 is a protein called NDUFAB1-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	AB	88	Total	C	H	N	O	S	0	0
			1367	437	673	114	139	4		

- Molecule 29 is a protein called NDUFAB1-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	AC	92	Total	C	H	N	O	S	0	0
			1418	461	697	116	140	4		

- Molecule 30 is a protein called NDUFA12.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	AL	265	Total	C	H	N	O	S	0	0
			4409	1439	2172	414	379	5		

- Molecule 31 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	AM	184	Total	C	H	N	O	S	0	0
			2935	953	1448	264	263	7		

- Molecule 32 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	AN	287	Total	C	H	N	O	S	0	0
			4573	1501	2267	396	399	10		

- Molecule 33 is a protein called NDUF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	B2	105	Total	C	H	N	O	S	0	0
			1770	604	857	142	166	1		

- Molecule 34 is a protein called NDUF3.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	B3	61	Total	C	H	N	O	S	0	0
			758	292	309	88	68	1		

- Molecule 35 is a protein called NDUF4.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	B4	171	Total	C	H	N	O	S	0	0
			2735	885	1358	250	236	6		

- Molecule 36 is a protein called NDUFB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	B5	140	Total	C	H	N	O	S	0	0
			2181	708	1069	207	195	2		

- Molecule 37 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	B6	91	Total	C	H	N	O	S	0	0
			1520	509	747	132	128	4		

- Molecule 38 is a protein called NDUFB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	B7	97	Total	C	H	N	O	S	0	0
			1692	536	835	165	149	7		

- Molecule 39 is a protein called NDUFB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	B8	147	Total	C	H	N	O	S	0	0
			2351	804	1127	199	213	8		

- Molecule 40 is a protein called NDUFB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	B9	151	Total	C	H	N	O	S	0	0
			2443	795	1207	216	222	3		

- Molecule 41 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	BL	144	Total	C	H	N	O	S	0	0
			2406	786	1179	215	216	10		

- Molecule 42 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	BM	112	Total	C	H	N	O	S	0	0
			1737	577	827	164	167	2		

- Molecule 43 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	C1	495	Total	C	H	N	O	S	0	0
			7918	2635	3980	614	664	25		

- Molecule 44 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	C2	196	Total	C	H	N	O	S	0	0
			3232	1046	1647	262	272	5		

- Molecule 45 is a protein called Putative NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	C3	161	Total	C	H	N	O	S	0	0
			2791	935	1413	213	226	4		

- Molecule 46 is a protein called NDUFC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	C4	183	Total	C	H	N	O	S	0	0
			3062	1000	1517	268	271	6		

- Molecule 47 is a protein called COX4.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	DC	167	Total	C	H	N	O	S	0	0
			2728	887	1362	239	235	5		

- Molecule 48 is a protein called NDUEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	E1	450	Total	C	H	N	O	S	0	0
			7008	2244	3496	601	654	13		

- Molecule 49 is a protein called NDUEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	E2	466	Total	C	H	N	O	S	0	0
			7103	2286	3540	618	655	4		

- Molecule 50 is a protein called NDUEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	E3	432	Total	C	H	N	O	S	0	0
			6518	2071	3263	565	612	7		

- Molecule 51 is a protein called NDUEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	E4	351	Total	C	H	N	O	S	0	0
			5502	1774	2732	477	504	15		

- Molecule 52 is a protein called NDUEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	E5	276	Total	C	H	N	O	S	0	0
			4046	1265	2069	341	369	2		

- Molecule 53 is a protein called NDUEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	E6	342	Total	C	H	N	O	S	0	0
			5629	1839	2758	507	513	12		

- Molecule 54 is a protein called NDUEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	E7	246	Total	C	H	N	O	S	0	0
			3780	1205	1892	332	344	7		

- Molecule 55 is a protein called NDUEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	E8	205	Total	C	H	N	O	S	0	0
			3354	1100	1663	288	292	11		

- Molecule 56 is a protein called NDUEG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	E9	165	Total	C	H	N	O	S	0	0
			2436	779	1224	213	217	3		

- Molecule 57 is a protein called NDUEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	EA	124	Total	C	H	N	O	S	0	0
			1793	630	832	172	156	3		

- Molecule 58 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	EB	101	Total	C	H	N	O	S	0	0
			1405	473	631	150	144	7		

- Molecule 59 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	EC	85	Total	C	H	N	O	S	0	0
			1323	424	663	116	118	2		

- Molecule 60 is a protein called NDUEG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	ED	138	Total	C	H	N	O	S	0	0
			2273	736	1131	205	196	5		

- Molecule 61 is a protein called NDUFEX.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	FX	237	Total	C	H	N	O	S	0	0
			3816	1263	1849	338	359	7		

- Molecule 62 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	G1	426	Total	C	H	N	O	S	0	0
			6552	2115	3205	593	623	16		

- Molecule 63 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	G2	236	Total	C	H	N	O	S	0	0
			3650	1138	1846	323	338	5		

- Molecule 64 is a protein called NDUCA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	G3	261	Total	C	H	N	O	S	0	0
			3905	1226	1944	356	373	6		

- Molecule 65 is a protein called ND1.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	N1	310	Total	C	H	N	O	S	0	0
			5331	1783	2726	380	435	7		

- Molecule 66 is a protein called ND2a.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	N2	296	Total	C	H	N	O	S	0	0
			5101	1725	2589	362	418	7		

- Molecule 67 is a protein called ND3.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	N3	121	Total	C	H	N	O	S	0	0
			2094	720	1057	143	172	2		
67	N6	154	Total	C	H	N	O	S	0	0
			2642	857	1385	187	210	3		

- Molecule 68 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	N4	478	Total	C	H	N	O	S	0	0
			8215	2743	4214	582	663	13		

- Molecule 69 is a protein called ND5.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	N5	584	Total	C	H	N	O	S	0	0
			9869	3293	5032	711	808	25		

- Molecule 70 is a protein called MPP-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	QA	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		
70	Qa	476	Total	C	H	N	O	S	2	0
			7408	2367	3658	655	713	15		

- Molecule 71 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	QB	455	Total	C	H	N	O	S	0	0
			6889	2205	3431	585	665	3		
71	Qb	423	Total	C	H	N	O	S	0	0
			6408	2057	3192	540	616	3		

- Molecule 72 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	QC	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		
72	Qc	364	Total	C	H	N	O	S	0	0
			6039	2005	3064	463	494	13		

- Molecule 73 is a protein called Cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	QD	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		
73	Qd	241	Total	C	H	N	O	S	0	0
			3817	1261	1858	337	353	8		

- Molecule 74 is a protein called UQCRFS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	QE	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		
74	Qe	231	Total	C	H	N	O	S	0	0
			3571	1143	1776	310	330	12		

- Molecule 75 is a protein called UQCRH.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	QF	64	Total	C	H	N	O	S	0	0
			1014	325	499	91	93	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
75	Qf	64	Total	C	H	N	O	S	0	0
			1018	325	503	91	93	6		

- Molecule 76 is a protein called UQCRB.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	QG	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		
76	Qg	228	Total	C	H	N	O	S	0	0
			3802	1232	1870	341	351	8		

- Molecule 77 is a protein called UQCRQ.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	QH	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		
77	Qh	85	Total	C	H	N	O	S	0	0
			1393	447	692	131	120	3		

- Molecule 78 is a protein called UQCR9.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	QI	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		
78	Qi	70	Total	C	H	N	O	S	0	0
			742	290	293	77	81	1		

- Molecule 79 is a protein called UQCR10.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	QJ	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		
79	Qj	149	Total	C	H	N	O	S	0	0
			2418	781	1212	220	204	1		

- Molecule 80 is a protein called Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	QK	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
80	Qk	61	Total	C	H	N	O	S	0	0
			984	325	499	79	78	3		

- Molecule 81 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	S2	394	Total	C	H	N	O	S	0	0
			6274	2041	3101	541	569	22		

- Molecule 82 is a protein called NDUFS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	S3	248	Total	C	H	N	O	S	0	0
			3978	1307	1928	346	384	13		

- Molecule 83 is a protein called NDUFS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	S4	190	Total	C	H	N	O	S	0	0
			3038	956	1502	300	273	7		

- Molecule 84 is a protein called NDUFS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	S5	122	Total	C	H	N	O	S	0	0
			1886	625	895	173	188	5		

- Molecule 85 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	S6	147	Total	C	H	N	O	S	0	0
			2392	759	1192	225	208	8		

- Molecule 86 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	S7	201	Total	C	H	N	O	S	0	0
			3045	975	1500	272	284	14		

- Molecule 87 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
87	S8	182	Total	C	H	N	O	S	0	0
			2843	915	1392	245	275	16		

- Molecule 88 is a protein called NDUFV1.

Mol	Chain	Residues	Atoms						AltConf	Trace
88	V1	504	Total	C	H	N	O	S	0	0
			7724	2463	3827	680	727	27		

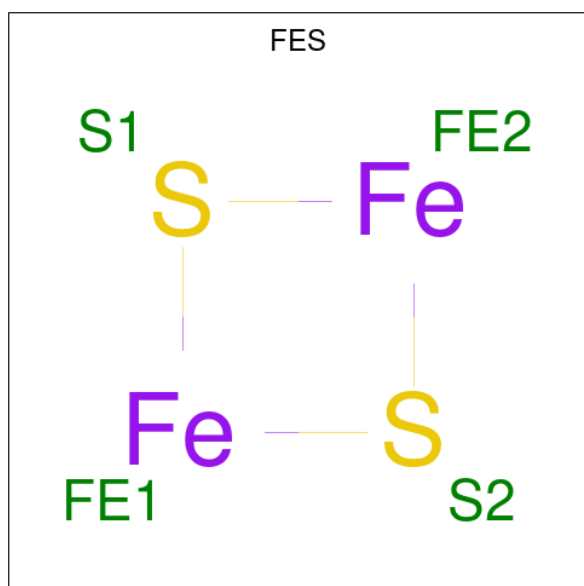
- Molecule 89 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
89	V2	225	Total	C	H	N	O	S	0	0
			3460	1124	1701	299	319	17		

- Molecule 90 is a protein called poly(UNK).

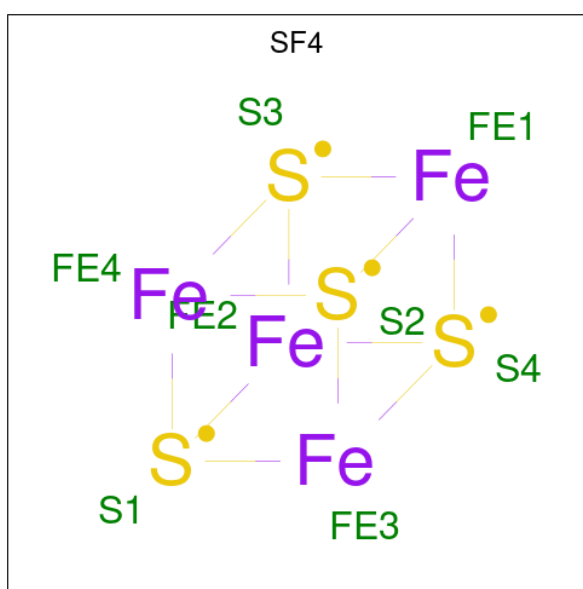
Mol	Chain	Residues	Atoms					AltConf	Trace
90	A	12	Total	C	H	N	O	0	0
			76	36	16	12	12		
90	B	12	Total	C	H	N	O	0	0
			76	36	16	12	12		

- Molecule 91 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
91	1A	1	Total	Fe	S	0
			4	2	2	
91	QE	1	Total	Fe	S	0
			4	2	2	
91	Qe	1	Total	Fe	S	0
			4	2	2	
91	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 92 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

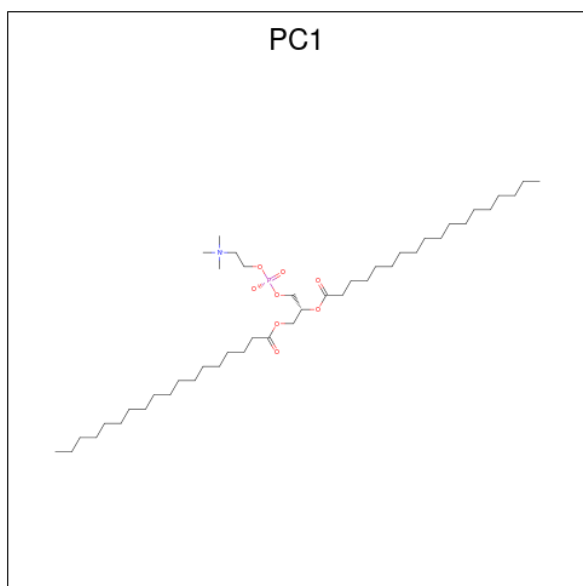


Mol	Chain	Residues	Atoms			AltConf
92	1A	1	Total	Fe	S	0
			8	4	4	
92	1A	1	Total	Fe	S	0
			8	4	4	
92	S7	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	S8	1	Total	Fe	S	0
			8	4	4	
92	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
93	1A	1	Total	K	0
			1	1	

- Molecule 94 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
94	4A	1	Total	C	H	N	O	P	0
			118	37	71	1	8	1	
94	4A	1	Total	C	H	N	O	P	0
			112	36	66	1	8	1	
94	4E	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	
94	7A	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	
94	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
94	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
94	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
94	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
94	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
94	AM	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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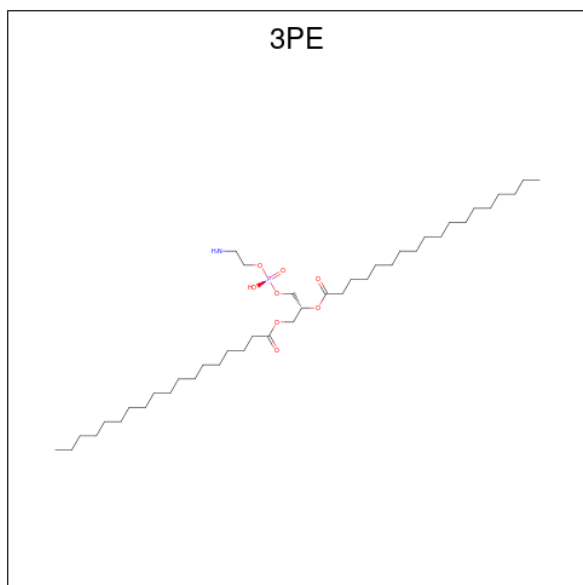
Mol	Chain	Residues	Atoms						AltConf
94	AM	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	AN	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	B8	1	Total 85	C 27	H 48	N 1	O 8	P 1	0
94	C1	1	Total 127	C 40	H 77	N 1	O 8	P 1	0
94	C3	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
94	E4	1	Total 130	C 41	H 79	N 1	O 8	P 1	0
94	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	E8	1	Total 73	C 23	H 40	N 1	O 8	P 1	0
94	E8	1	Total 64	C 20	H 34	N 1	O 8	P 1	0
94	E9	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
94	ED	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	ED	1	Total 97	C 31	H 56	N 1	O 8	P 1	0
94	G2	1	Total 88	C 28	H 50	N 1	O 8	P 1	0
94	N1	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
94	N1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
94	N3	1	Total 103	C 32	H 61	N 1	O 8	P 1	0
94	N4	1	Total 91	C 29	H 52	N 1	O 8	P 1	0
94	N4	1	Total 73	C 23	H 40	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
94	N4	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	N5	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	QC	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	QD	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
94	QI	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	Qc	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
94	Qc	1	Total 67	C 21	H 36	N 1	O 8	P 1	0
94	Qe	1	Total 82	C 26	H 46	N 1	O 8	P 1	0
94	Qg	1	Total 58	C 18	H 30	N 1	O 8	P 1	0
94	Qj	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

- Molecule 95 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



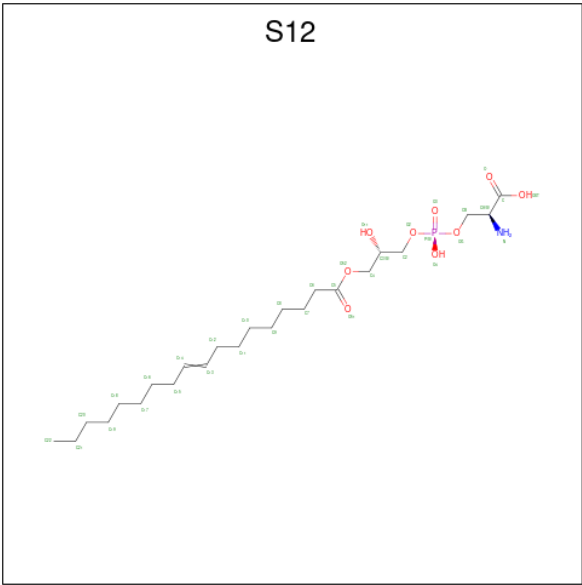
Mol	Chain	Residues	Atoms					AltConf	
95	4D	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	

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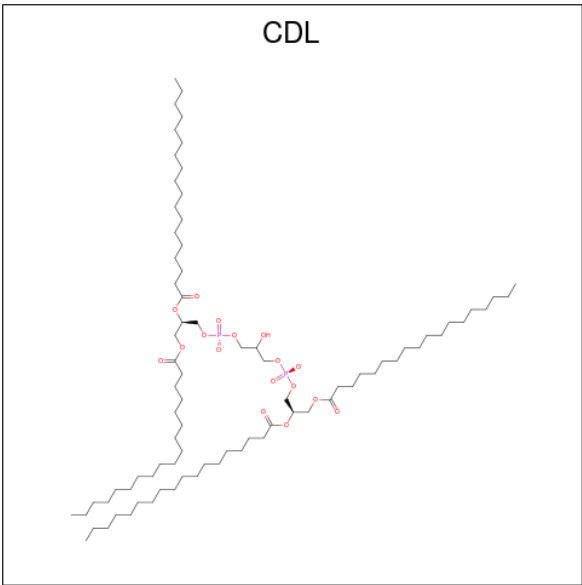
Mol	Chain	Residues	Atoms						AltConf
95	4D	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	7A	1	Total	C	H	N	O	P	0
			100	31	59	1	8	1	
95	B4	1	Total	C	H	N	O	P	0
			97	30	57	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	C1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
95	E9	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
95	N4	1	Total	C	H	N	O	P	0
			97	31	56	1	8	1	
95	N5	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 96 is O-[(S)-hydroxy{[(2S)-2-hydroxy-3-(octadec-9-enoyloxy)propyl]oxy}phosphoryl]-L-serine (CCD ID: S12) (formula: C₂₄H₄₆NO₉P).



Mol	Chain	Residues	Atoms						AltConf
96	4D	1	Total	C	H	N	O	P	0
			79	24	44	1	9	1	

- Molecule 97 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms					AltConf
97	4E	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	7C	1	Total	C	H	O	P	0
			220	71	130	17	2	
97	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	A9	1	Total	C	H	O	P	0
			136	45	72	17	2	
97	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
97	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
97	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	B3	1	Total	C	H	O	P	0
			139	46	74	17	2	
97	B8	1	Total	C	H	O	P	0
			157	51	87	17	2	
97	BM	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	C4	1	Total	C	H	O	P	0
			235	75	141	17	2	
97	C4	1	Total	C	H	O	P	0
			151	50	82	17	2	
97	C4	1	Total	C	H	O	P	0
			247	79	149	17	2	

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Mol	Chain	Residues	Atoms					AltConf
97	E4	1	Total	C	H	O	P	0
			163	53	91	17	2	
97	E6	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	
97	EA	1	Total	C	H	O	P	0
			121	40	62	17	2	
97	EA	1	Total	C	H	O	P	0
			109	36	54	17	2	
97	N1	1	Total	C	H	O	P	0
			154	51	84	17	2	
97	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
97	QC	1	Total	C	H	O	P	0
			112	37	56	17	2	
97	QD	1	Total	C	H	O	P	0
			151	50	82	17	2	
97	QH	1	Total	C	H	O	P	0
			175	57	99	17	2	
97	QH	1	Total	C	H	O	P	0
			124	41	64	17	2	
97	QJ	1	Total	C	H	O	P	0
			118	39	60	17	2	
97	Qc	1	Total	C	H	O	P	0
			106	35	52	17	2	
97	Qd	1	Total	C	H	O	P	0
			256	81	156	17	2	
97	Qe	1	Total	C	H	O	P	0
			124	41	64	17	2	
97	Qh	1	Total	C	H	O	P	0
			139	46	74	17	2	
97	Qj	1	Total	C	H	O	P	0
			88	29	40	17	2	

- Molecule 98 is ZINC ION (CCD ID: ZN) (formula: Zn).

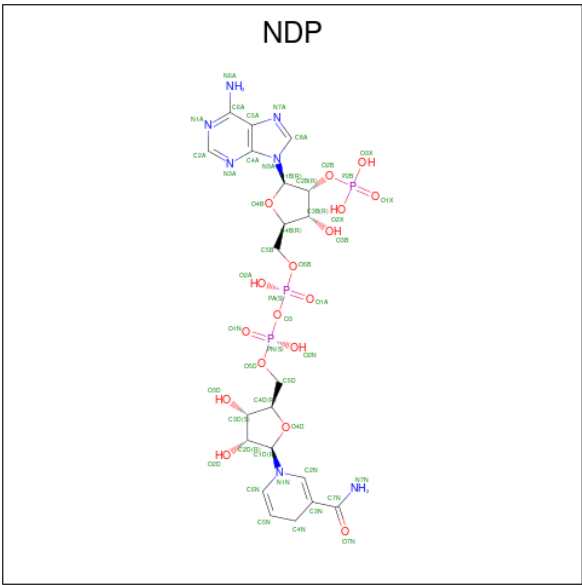
Mol	Chain	Residues	Atoms		AltConf
98	5B	1	Total	Zn	0
			1	1	
98	E7	1	Total	Zn	0
			1	1	

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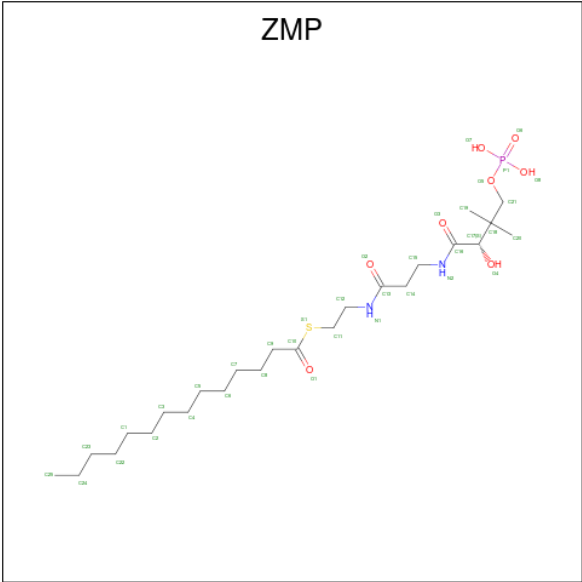
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
98	S6	1	1	1	0

- Molecule 99 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



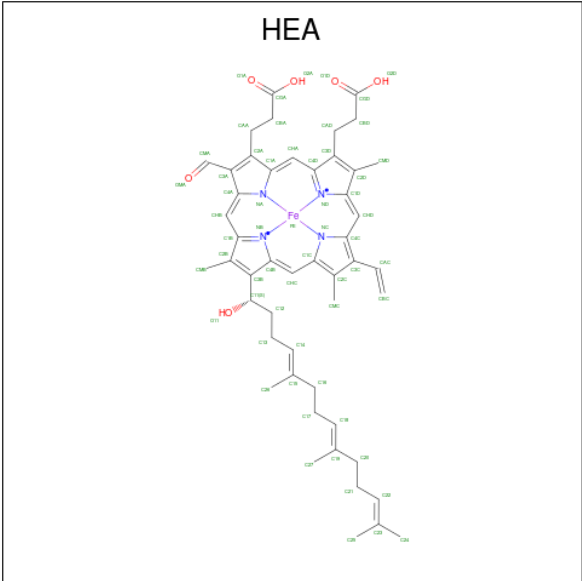
Mol	Chain	Residues	Atoms						AltConf
99	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 100 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
100	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
100	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 101 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
101	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
101	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

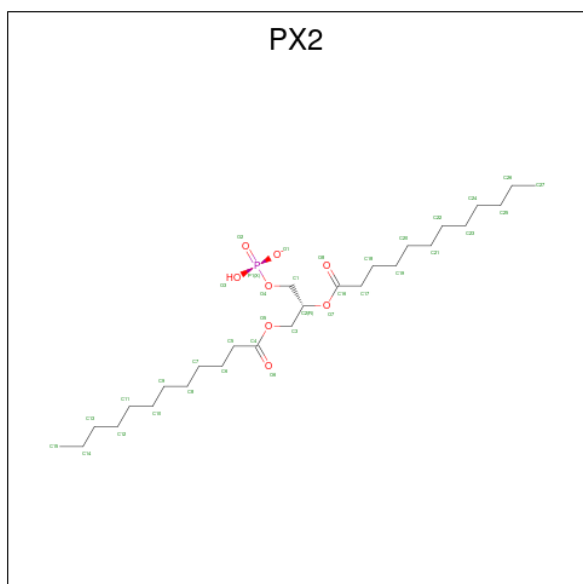
- Molecule 102 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
102	C1	1	Total	Cu	0
			1	1	
102	C2	2	Total	Cu	0
			2	2	

- Molecule 103 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
103	C1	1	Total	Mg	0
			1	1	

- Molecule 104 is 1,2-DILAULOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: C₂₇H₅₂O₈P).



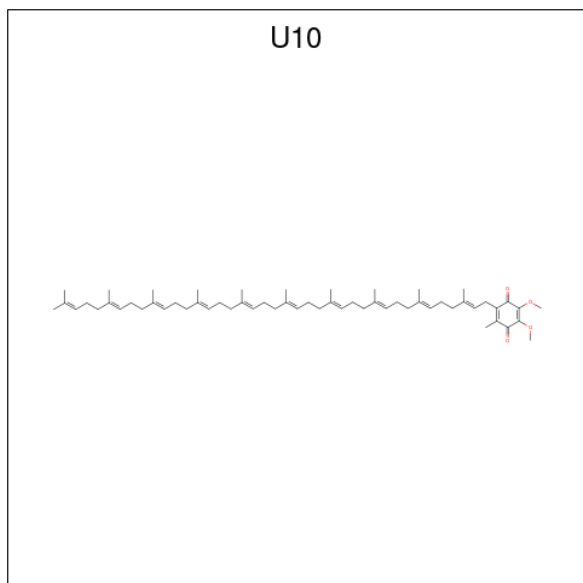
Mol	Chain	Residues	Atoms				AltConf
104	C2	1	Total	C	O	P	0
			36	27	8	1	

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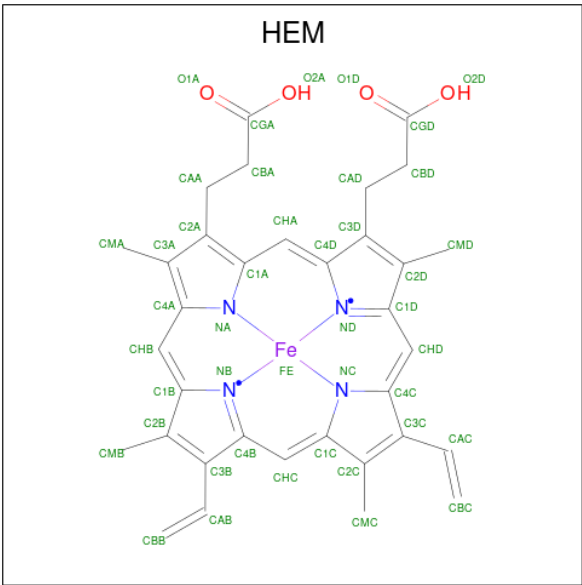
Mol	Chain	Residues	Atoms				AltConf
104	QJ	1	Total	C	O	P	0
			36	27	8	1	
104	QJ	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 105 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



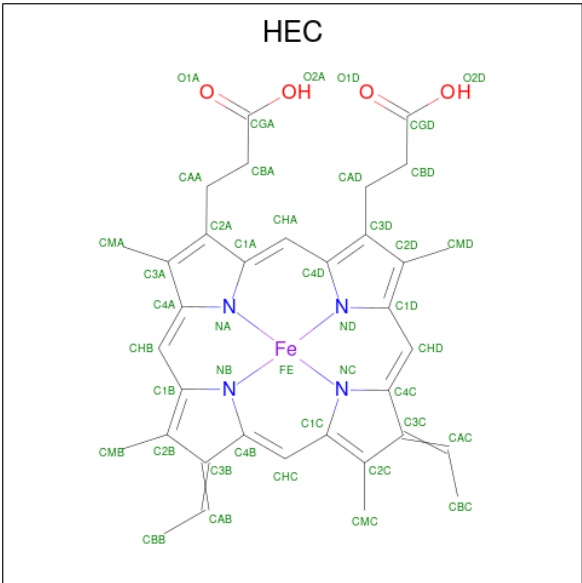
Mol	Chain	Residues	Atoms				AltConf
105	N4	1	Total	C	H	O	0
			98	39	55	4	

- Molecule 106 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



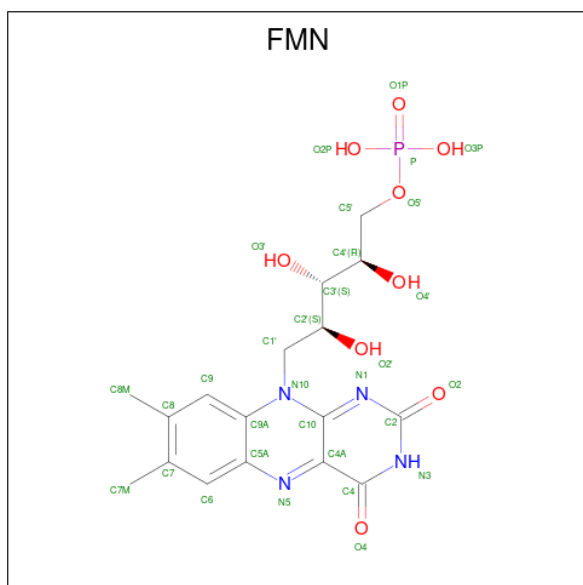
Mol	Chain	Residues	Atoms					AltConf
106	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
106	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
106	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
106	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 107 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
107	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
107	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 108 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

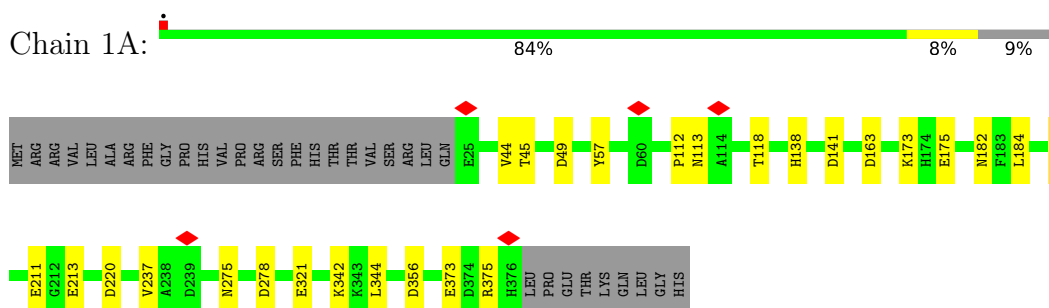


Mol	Chain	Residues	Atoms					AltConf
108	V1	1	Total	C	H	N	O	P
			50	17	19	4	9	1
								0

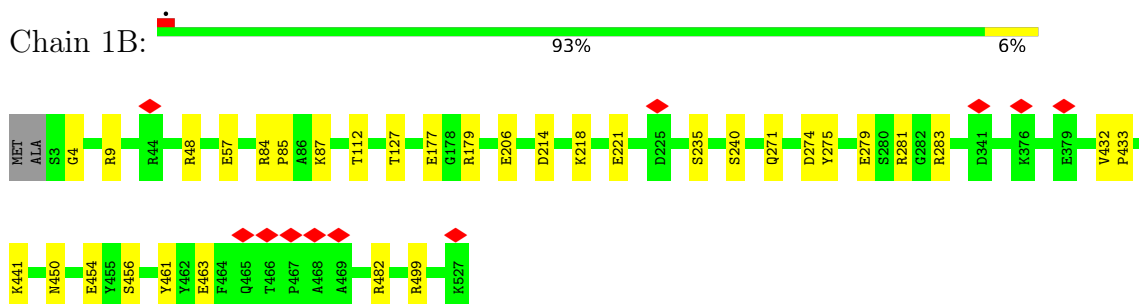
3 Residue-property plots

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

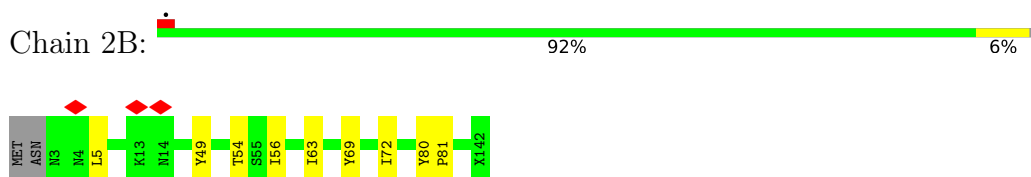
• Molecule 1: NDUFS1a



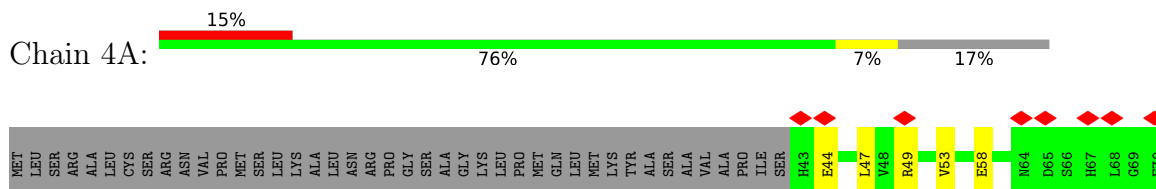
• Molecule 2: NDUFS1b

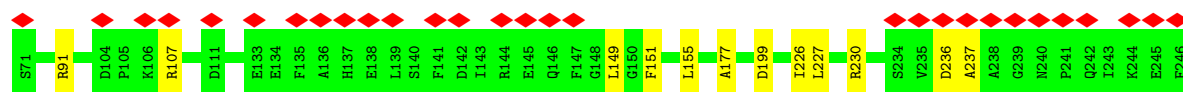


• Molecule 3: ND2b

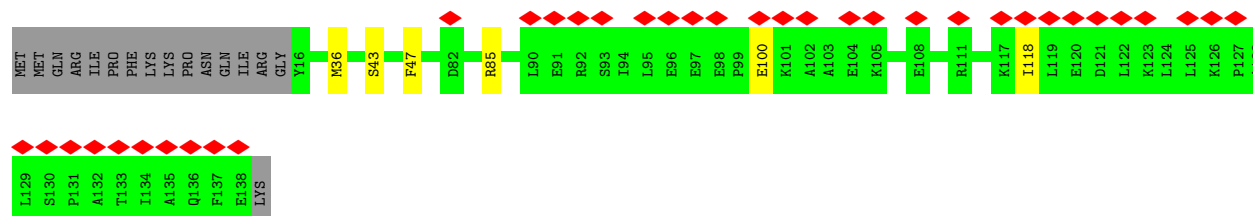
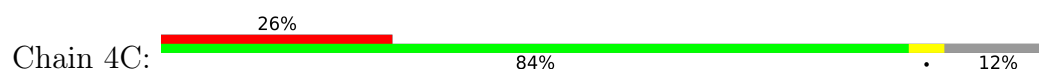


• Molecule 4: COXEG1

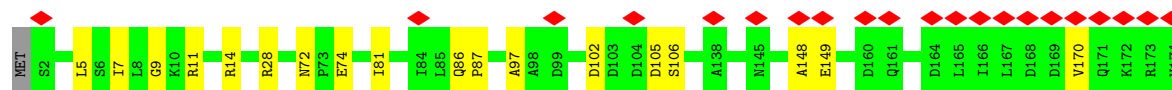
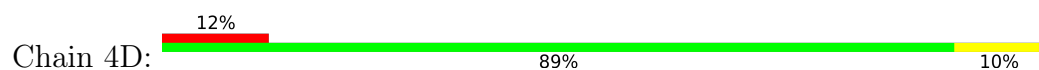




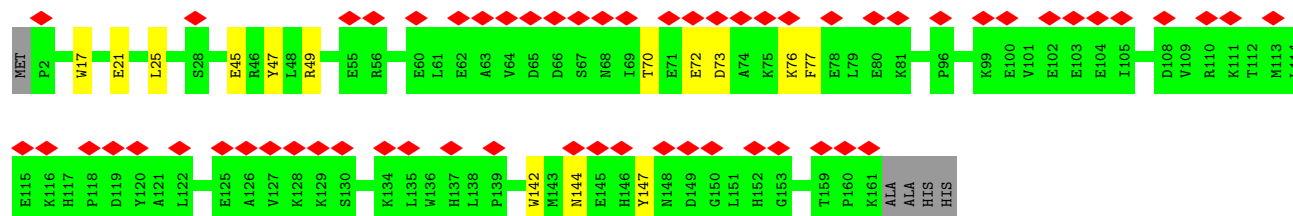
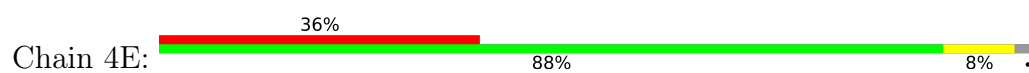
• Molecule 5: COXEG3



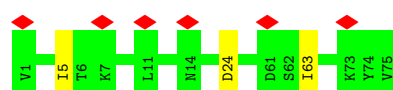
• Molecule 6: COXEG4



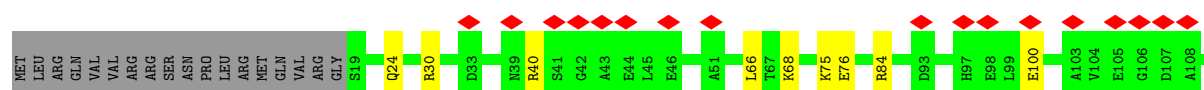
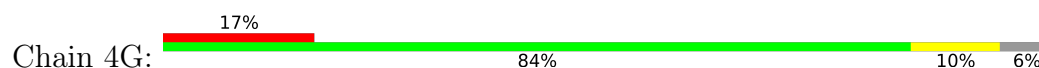
• Molecule 7: COXEG5

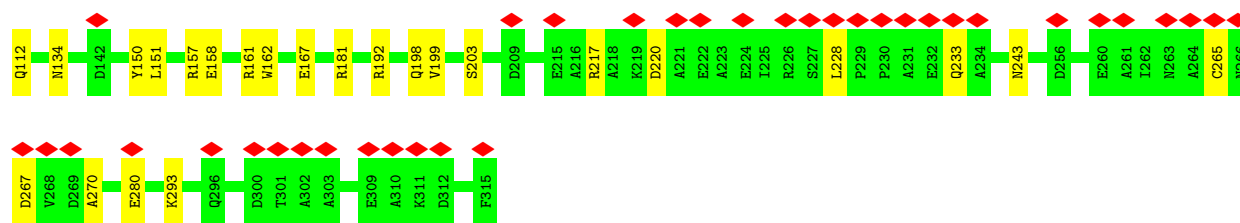


• Molecule 8: COXEG6

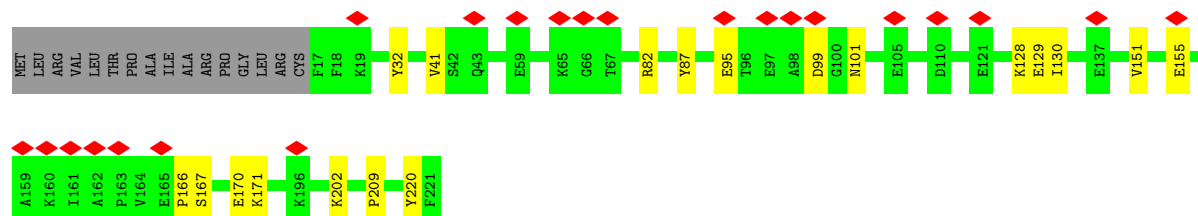
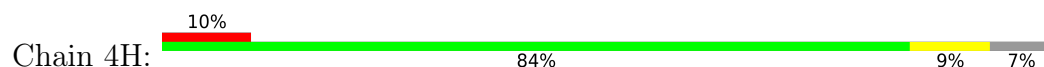


• Molecule 9: COXEG7

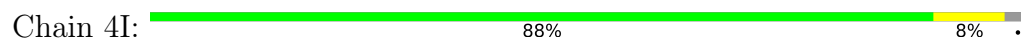




• Molecule 10: COXEG8



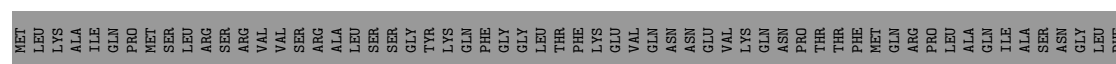
• Molecule 11: COXEG9



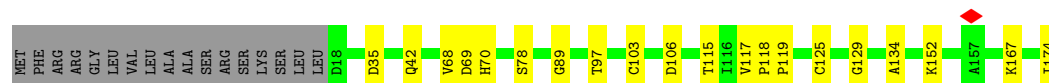
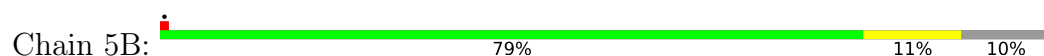
• Molecule 12: COXEG10



• Molecule 13: ND4L

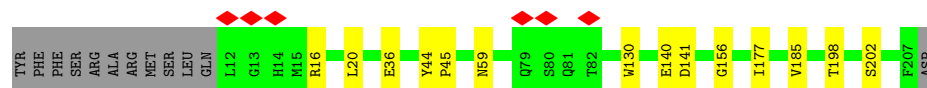


• Molecule 14: COX5b-2



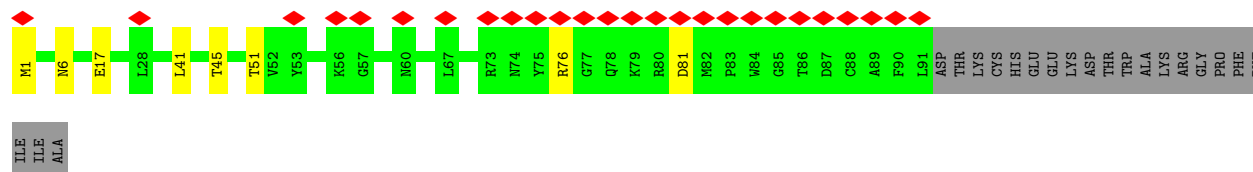
- Molecule 15: COX5c

Chain 5C: 

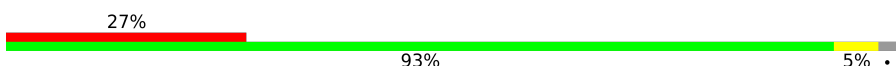


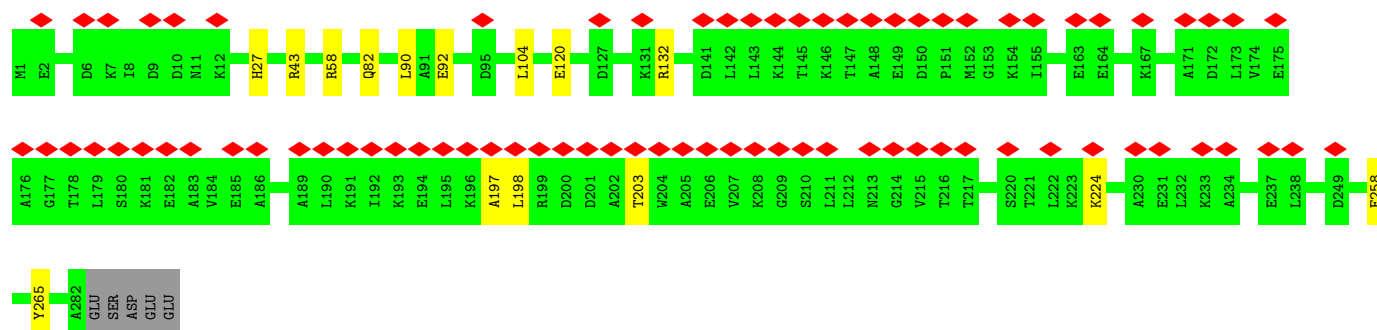
- Molecule 16: COX6a

Chain 6A: 



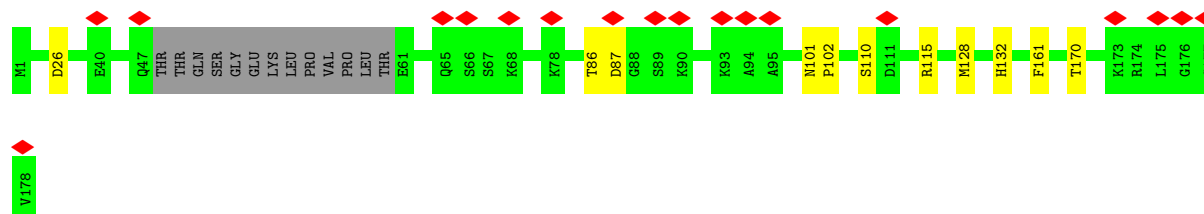
- Molecule 17: COX6b-1

Chain 6B: 



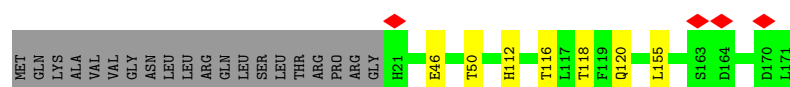
- Molecule 18: COX7a

Chain 7A: 

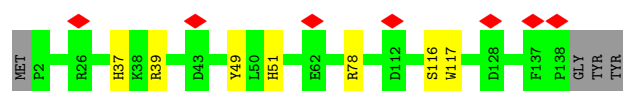


- Molecule 19: COX7c

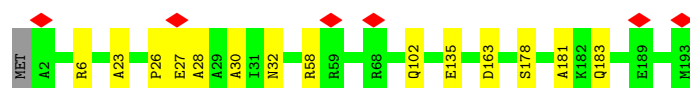
Chain 7C: 



- Molecule 20: NDUFA1



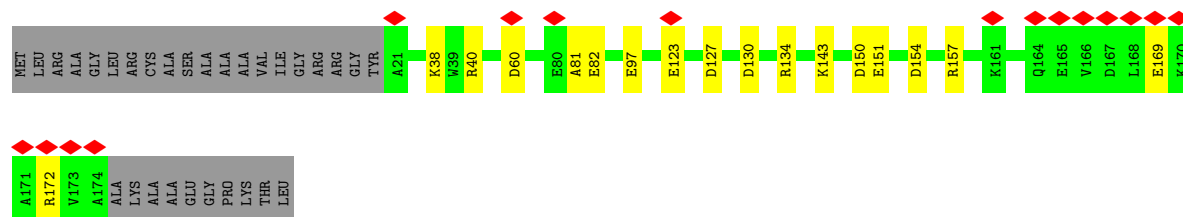
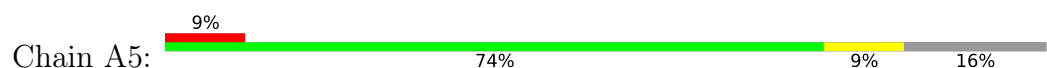
• Molecule 21: NDUFA2



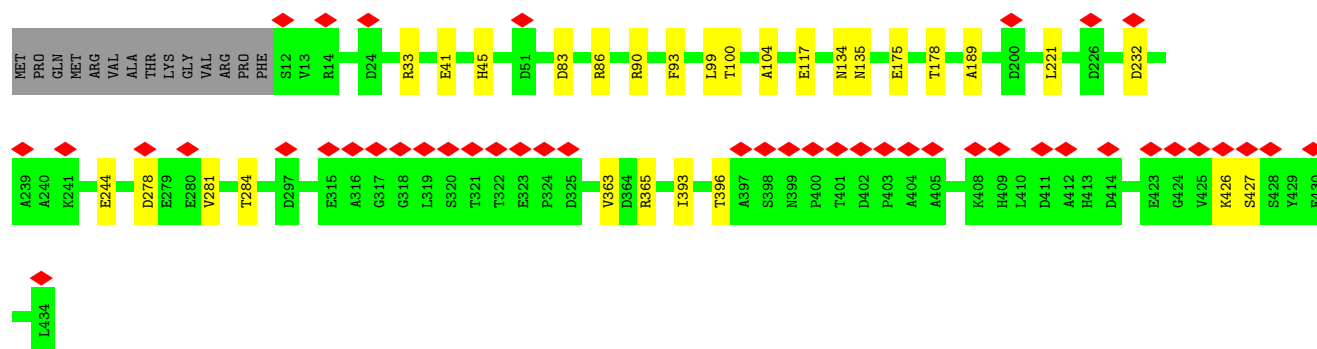
• Molecule 22: NDUFA3



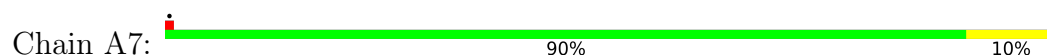
• Molecule 23: NDUFA5



• Molecule 24: NDUFA6

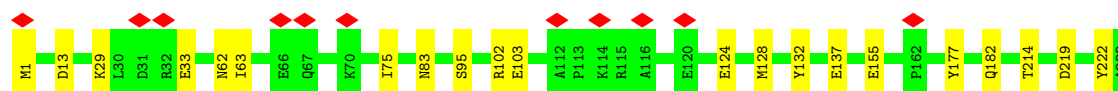


• Molecule 25: NDUFA7

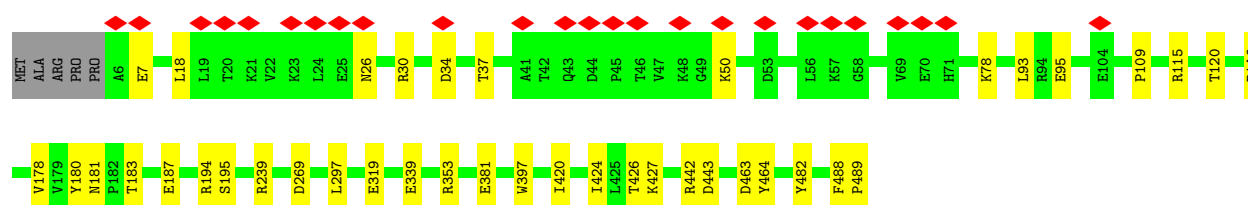




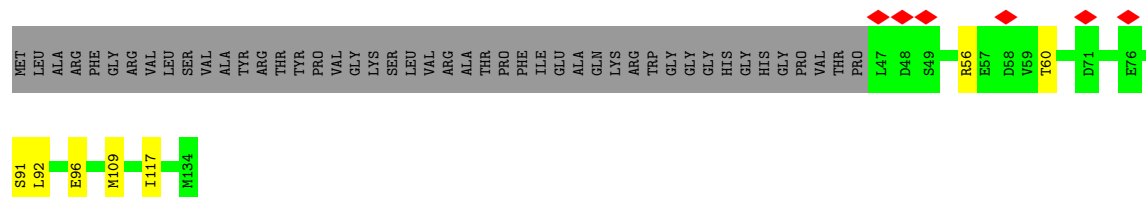
• Molecule 26: NDUFA8



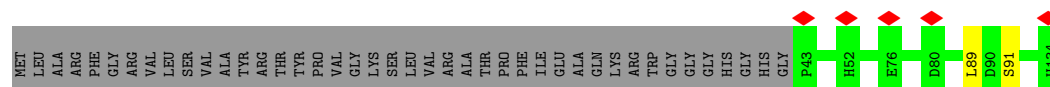
• Molecule 27: NDUFA9



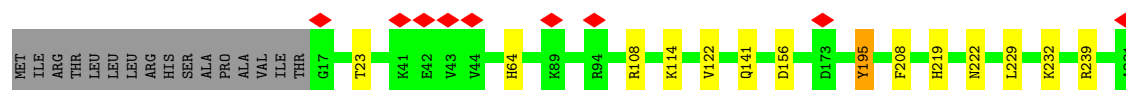
• Molecule 28: NDUFAB1-alpha



• Molecule 29: NDUFAB1-beta

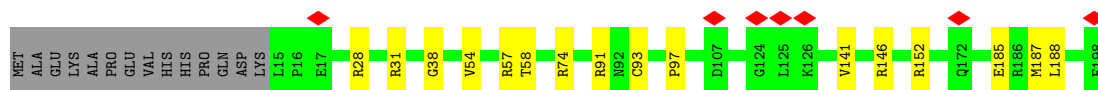


• Molecule 30: NDUFA12

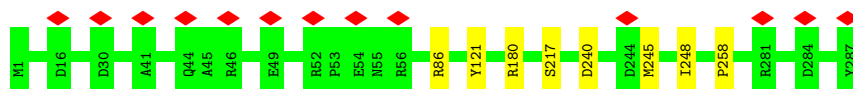


• Molecule 31: NDUFA13

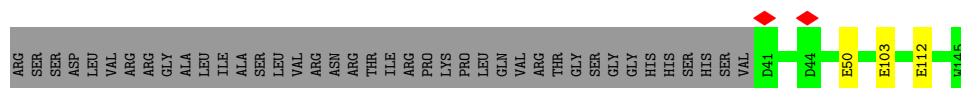




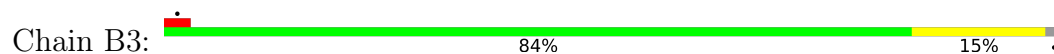
• Molecule 32: NDUFA11



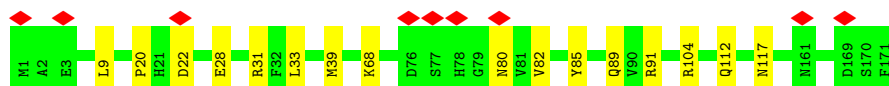
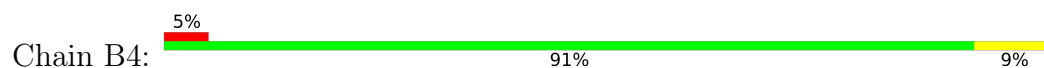
• Molecule 33: NDUFB2



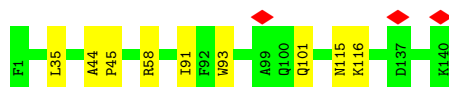
• Molecule 34: NDUFB3



• Molecule 35: NDUFB4



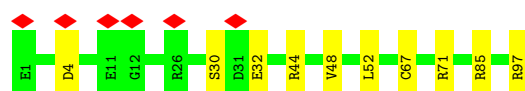
• Molecule 36: NDUFB5



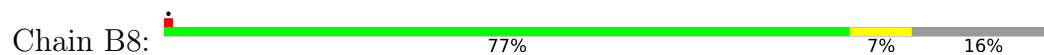
• Molecule 37: NDUFB6



• Molecule 38: NDUFB7



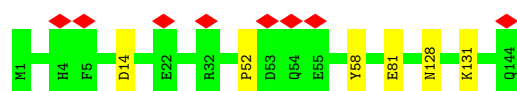
• Molecule 39: NDUFB8



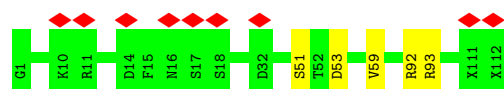
• Molecule 40: NDUFB9



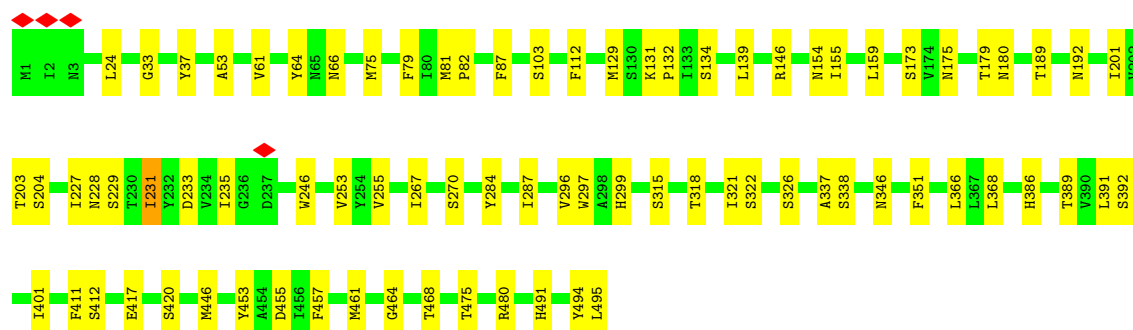
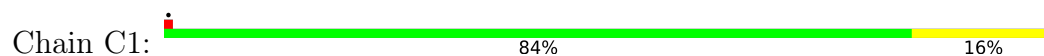
• Molecule 41: NDUFB10



• Molecule 42: NDUFB11



• Molecule 43: Cytochrome c oxidase subunit 1



• Molecule 44: Cytochrome c oxidase subunit 2

Chain C2:  88% 11% .



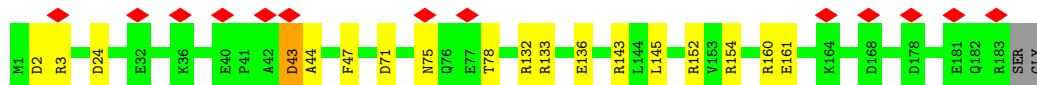
- Molecule 45: Putative NADH dehydrogenase subunit 6

Chain C3:  7% 91% 8% .



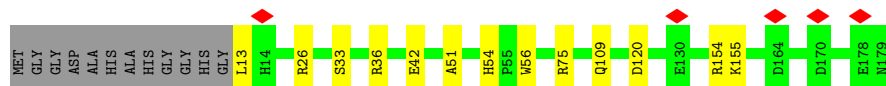
- Molecule 46: NDUFC2

Chain C4:  7% 89% 9% ..



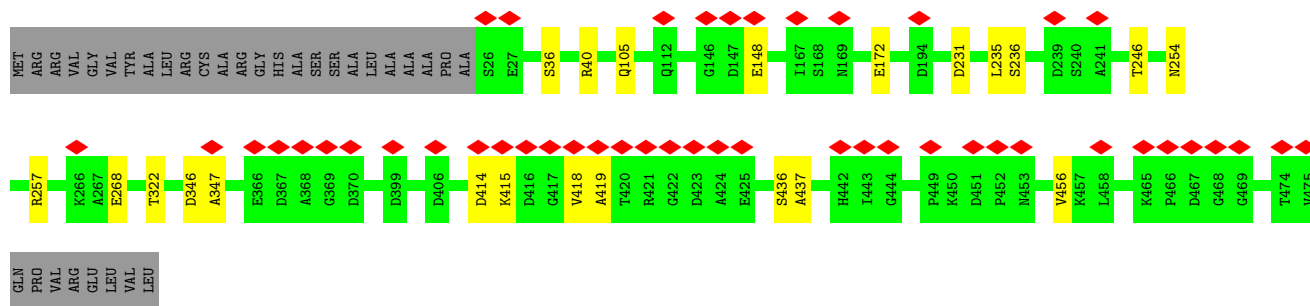
- Molecule 47: COX4

Chain DC:  86% 7% 7%

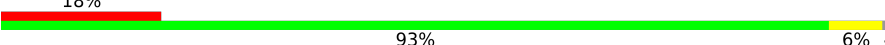


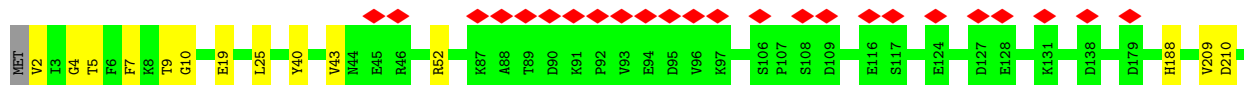
- Molecule 48: NDUEG1

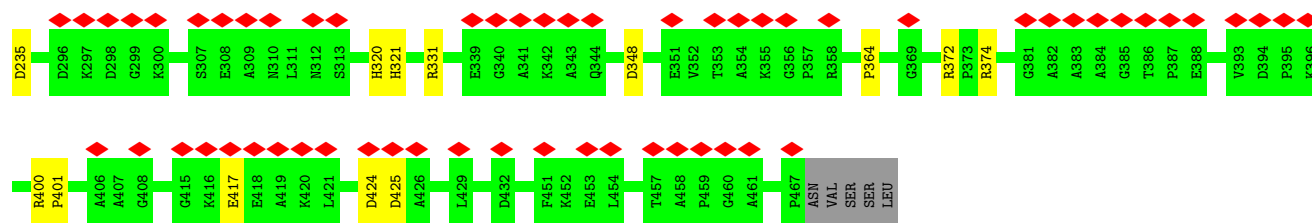
Chain E1:  10% 89% 5% 7%



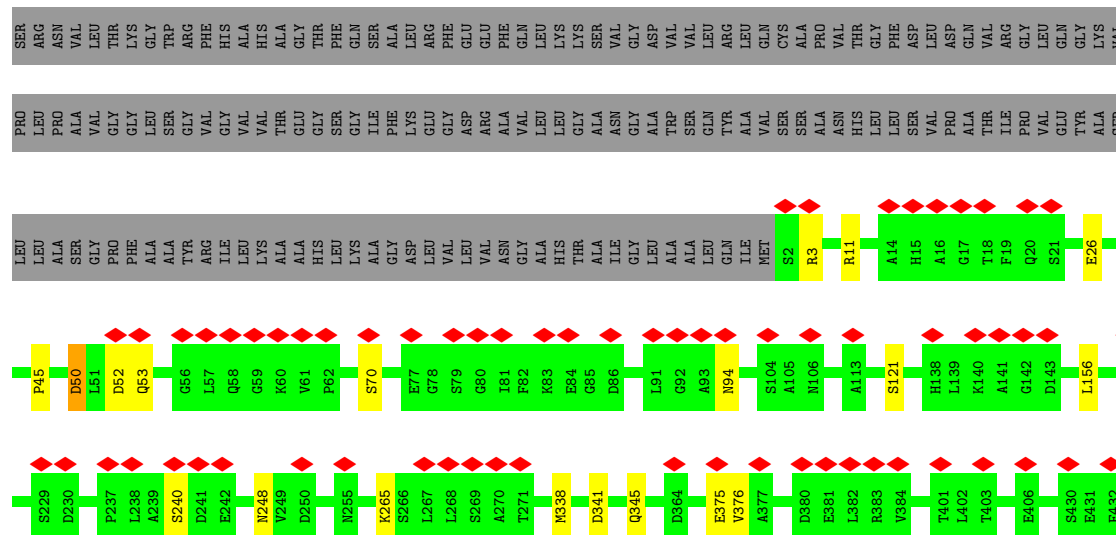
- Molecule 49: NDUEG2

Chain E2:  18% 93% 6% .

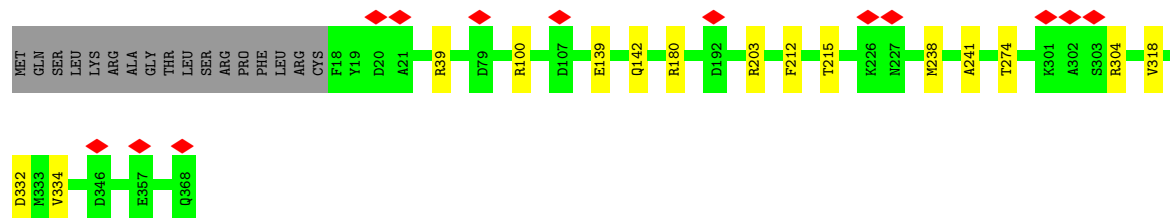




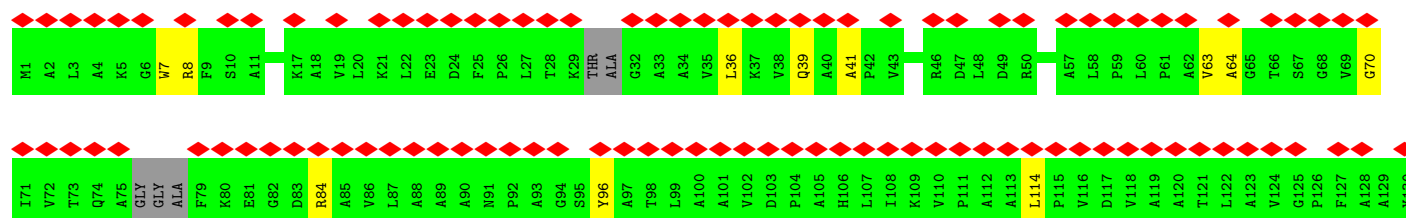
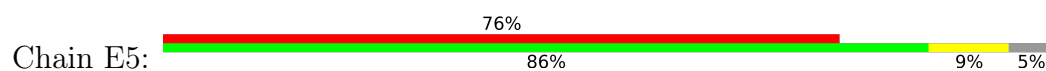
• Molecule 50: NDUEG3

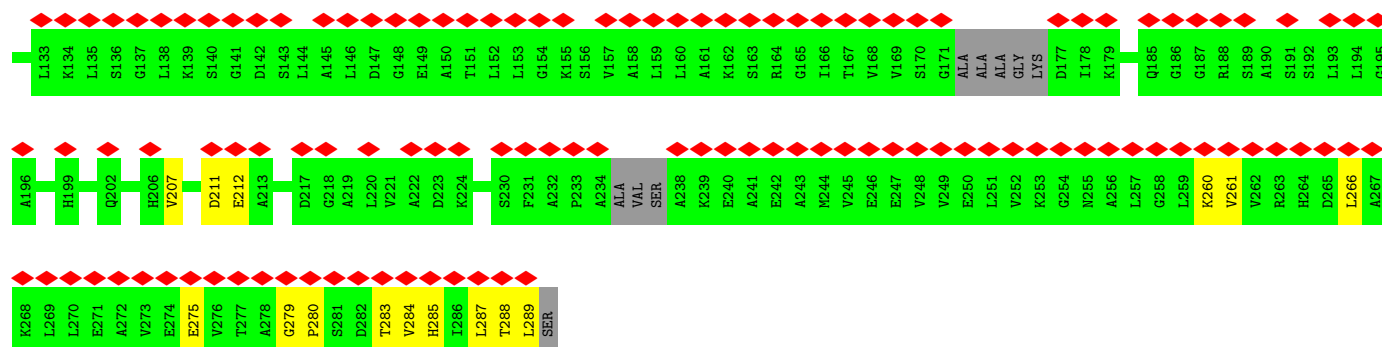


• Molecule 51: NDUEG4

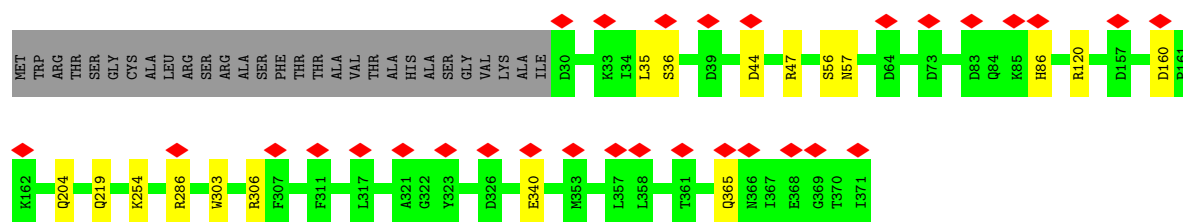
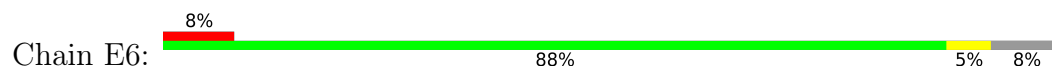


• Molecule 52: NDUEG5

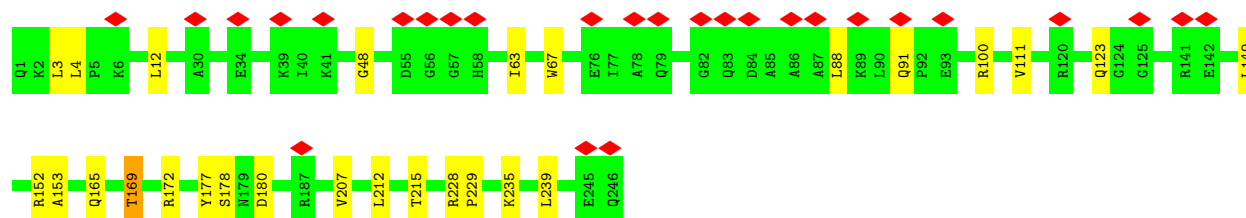




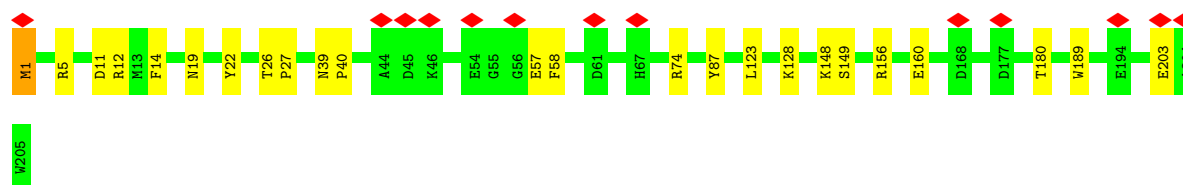
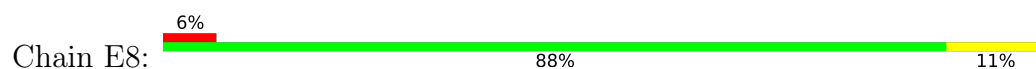
• Molecule 53: NDUEG6



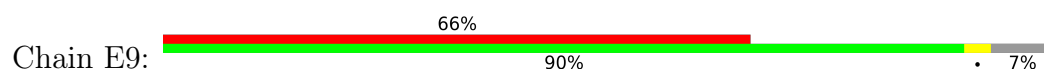
• Molecule 54: NDUEG7

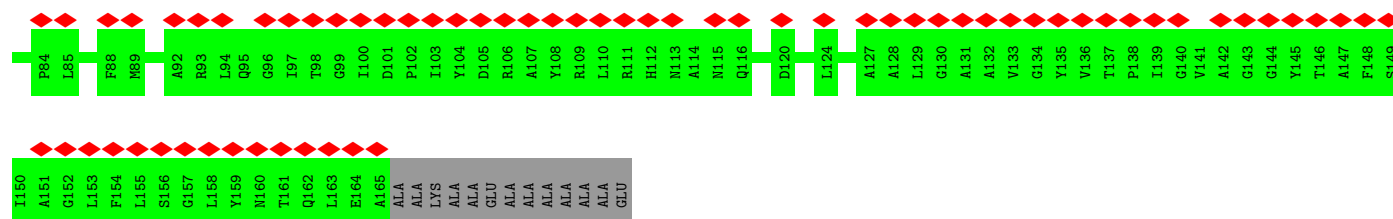


• Molecule 55: NDUEG8

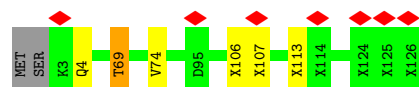


• Molecule 56: NDUEG9

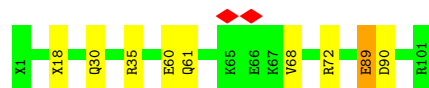




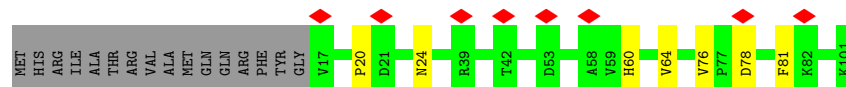
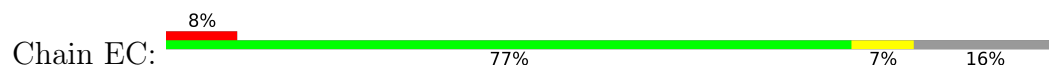
• Molecule 57: NDUEG10



• Molecule 58: NDUEG11



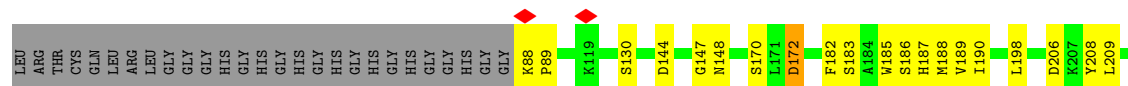
• Molecule 59: NDUEG11



• Molecule 60: NDUEG13



• Molecule 61: NDUFX



Chain G1:

89% 8%

NET
ALA
LYS
LEU
THR
TRP
LEU
LYS
ASN
LEU
L11
M12
T21
R28
S35
A36
E37
R38
D39
H105
R108
G112
R113
W114
F123
D124
F127
R133
W169
M184
A187
P205
K206
S207
E211
Q228
Q233
A246
D251
V278

R294
P295
A296
R297
D304
H321
E326
D339
Q354
A355
H356
R360
K370
D388
D389
R403
N413
Q416
R419
P420
V421
Y426
A436

Chain G2:

81% 7% 12%

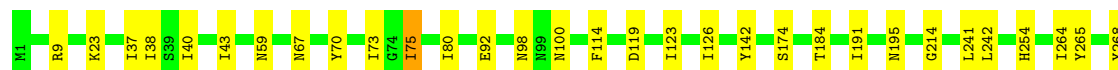
Chain G3: 94% 6%

Bar Label	Color	Red Diamond
X1	Green	Yes
I46	Green	Yes
K52	Green	Yes
E98	Yellow	No
I106	Green	Yes
L107	Green	Yes
V109	Green	Yes
R110	Yellow	No
P122	Yellow	No
I125	Yellow	No
I126	Green	No
S127	Yellow	No
P128	Yellow	No
V160	Yellow	No
E166	Green	Yes
V176	Yellow	No
P177	Yellow	No
A181	Green	Yes
E215	Yellow	No
E219	Yellow	No
G235	Yellow	No
T239	Yellow	No
K240	Yellow	No
R241	Yellow	No
A261	Green	No

Chain N1: 41% 5% 54%

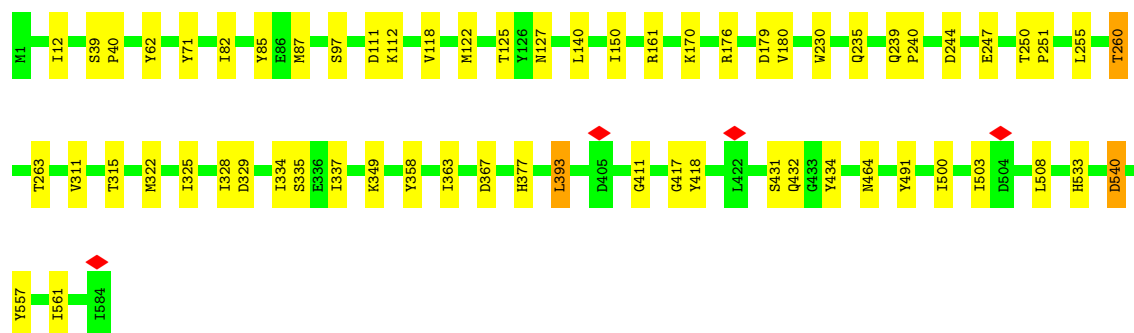
Sequence logo for Chain N1. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions 1 to 100. The color scale at the top indicates conservation levels: 41% (green), 5% (yellow), and 54% (red). The logo shows high conservation at positions 1-10, 20-30, and 40-50, with lower conservation at positions 60-70 and 80-90.

Position	Residue	Information Content (bits)
1	Met	1.4
2	Leu	1.3
3	Leu	1.2
4	Asn	1.1
5	Ser	1.0
6	Ser	0.9
7	Leu	0.8
8	Leu	0.7
9	Thr	0.6
10	Tyr	0.5
11	Thr	0.4
12	Leu	0.3
13	Leu	0.2
14	Asn	0.1
15	His	0.0
16	His	0.0
17	Leu	0.0
18	Leu	0.0
19	Leu	0.0
20	Leu	0.0
21	Leu	0.0
22	Leu	0.0
23	Leu	0.0
24	Leu	0.0
25	Leu	0.0
26	Leu	0.0
27	Leu	0.0
28	Leu	0.0
29	Leu	0.0
30	Leu	0.0
31	Leu	0.0
32	Leu	0.0
33	Leu	0.0
34	Leu	0.0
35	Leu	0.0
36	Leu	0.0
37	Leu	0.0
38	Leu	0.0
39	Leu	0.0
40	Leu	0.0
41	Leu	0.0
42	Leu	0.0
43	Leu	0.0
44	Leu	0.0
45	Leu	0.0
46	Leu	0.0
47	Leu	0.0
48	Leu	0.0
49	Leu	0.0
50	Leu	0.0
51	Leu	0.0
52	Leu	0.0
53	Leu	0.0
54	Leu	0.0
55	Leu	0.0
56	Leu	0.0
57	Leu	0.0
58	Leu	0.0
59	Leu	0.0
60	Leu	0.0
61	Leu	0.0
62	Leu	0.0
63	Leu	0.0
64	Leu	0.0
65	Leu	0.0
66	Leu	0.0
67	Leu	0.0
68	Leu	0.0
69	Leu	0.0
70	Leu	0.0
71	Leu	0.0
72	Leu	0.0
73	Leu	0.0
74	Leu	0.0
75	Leu	0.0
76	Leu	0.0
77	Leu	0.0
78	Leu	0.0
79	Leu	0.0
80	Leu	0.0
81	Leu	0.0
82	Leu	0.0
83	Leu	0.0
84	Leu	0.0
85	Leu	0.0
86	Leu	0.0
87	Leu	0.0
88	Leu	0.0
89	Leu	0.0
90	Leu	0.0
91	Leu	0.0
92	Leu	0.0
93	Leu	0.0
94	Leu	0.0
95	Leu	0.0
96	Leu	0.0
97	Leu	0.0
98	Leu	0.0
99	Leu	0.0
100	Leu	0.0





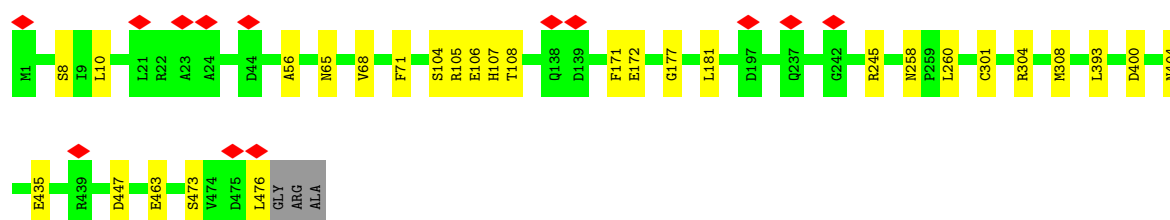
• Molecule 69: ND5



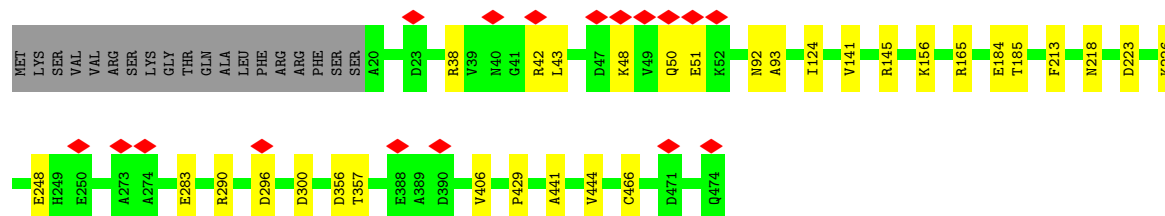
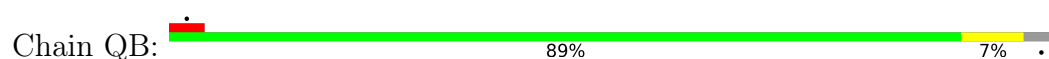
• Molecule 70: MPP-beta



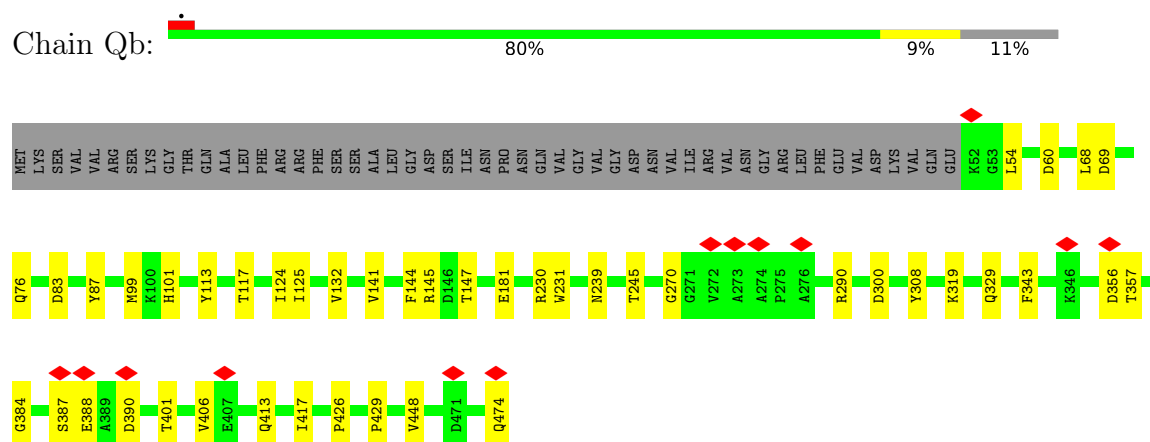
• Molecule 70: MPP-beta



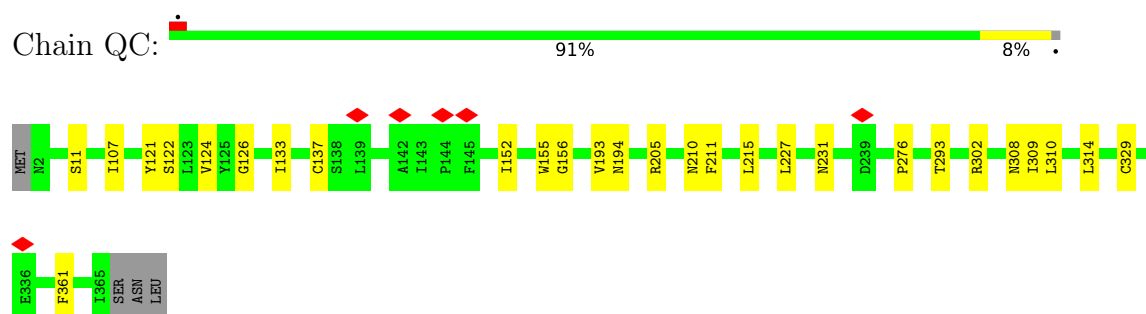
• Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



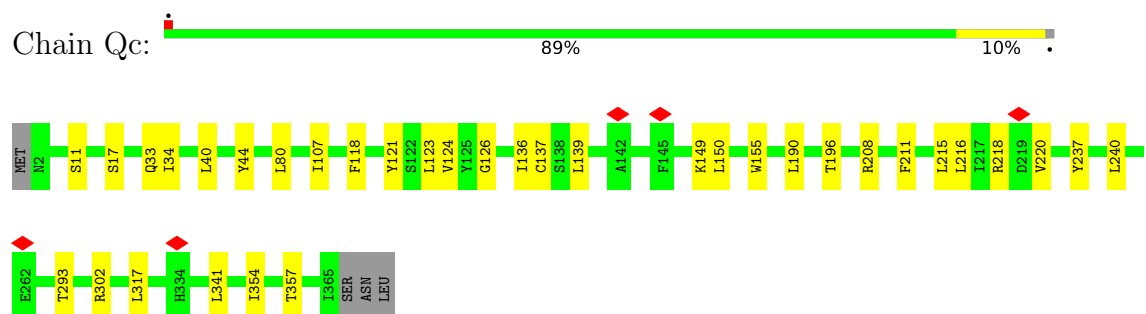
- Molecule 71: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



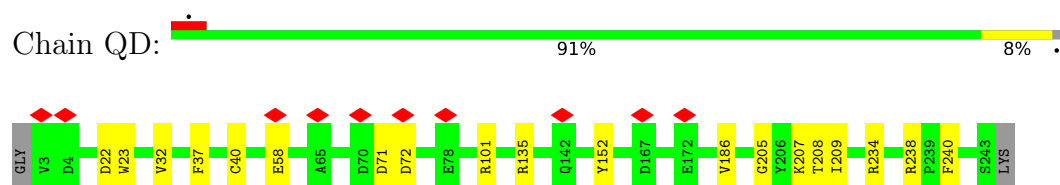
- Molecule 72: Cytochrome b



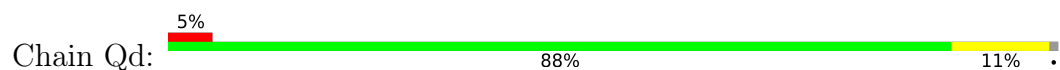
- Molecule 72: Cytochrome b

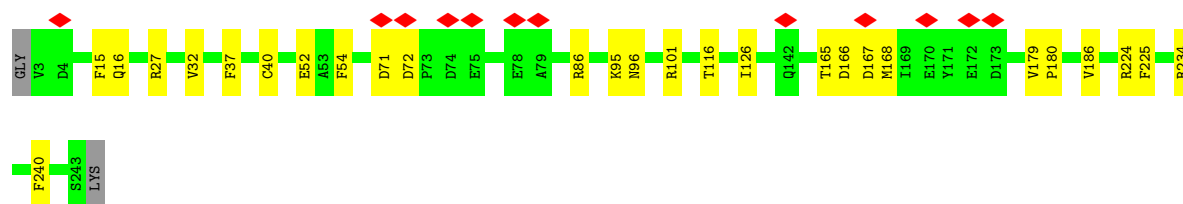


- Molecule 73: Cytochrome c1, heme protein

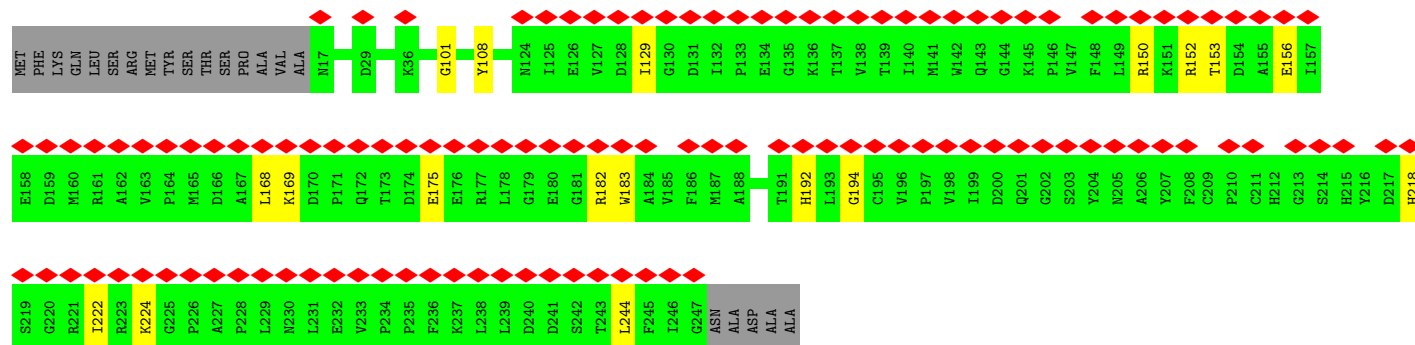
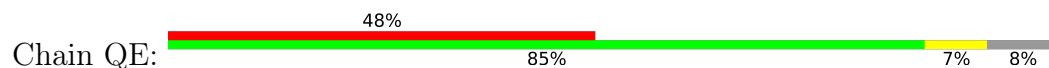


- Molecule 73: Cytochrome c1, heme protein

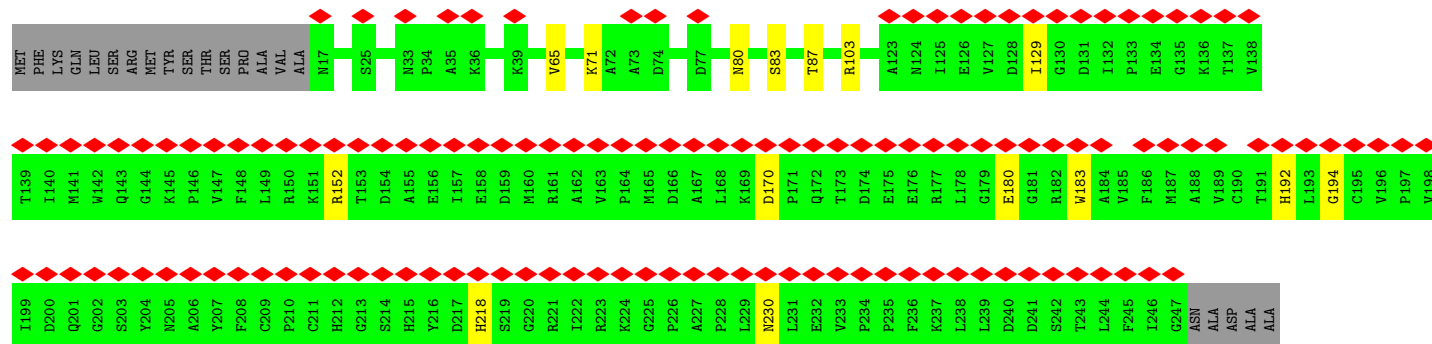
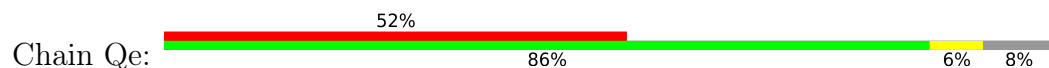




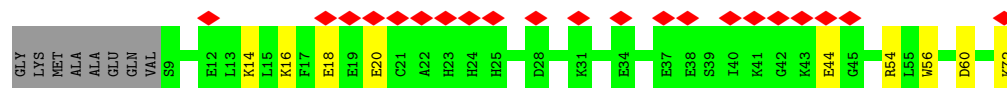
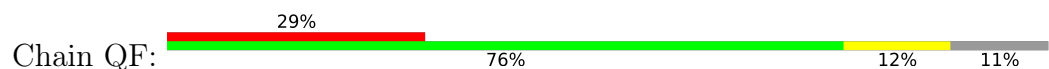
• Molecule 74: UQCRFS1



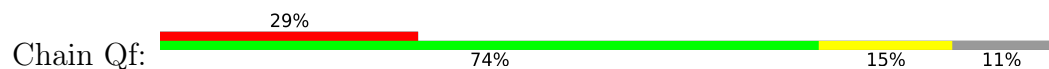
• Molecule 74: UQCRFS1

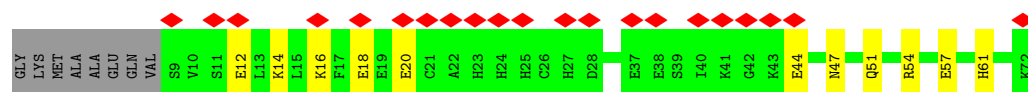


• Molecule 75: UQCRH



• Molecule 75: UQCRH

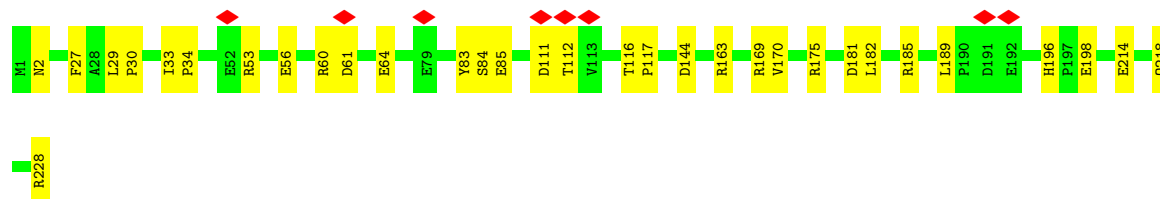




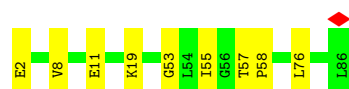
• Molecule 76: UQCRB



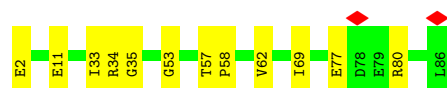
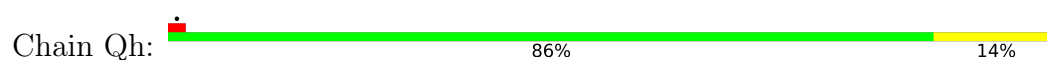
• Molecule 76: UQCRB



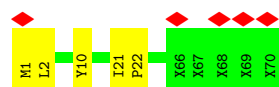
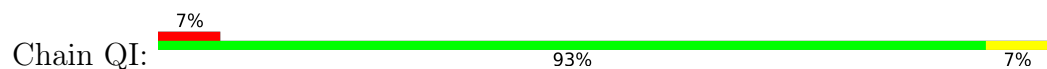
• Molecule 77: UQCRQ



• Molecule 77: UQCRQ

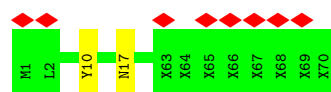


• Molecule 78: UQCR9

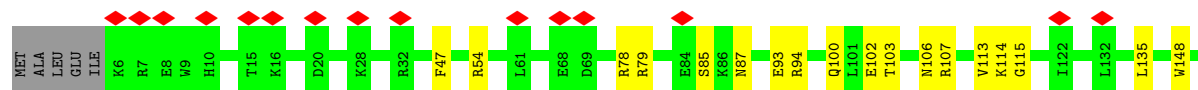
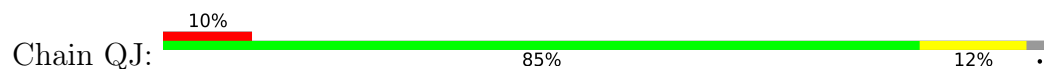


• Molecule 78: UQCR9

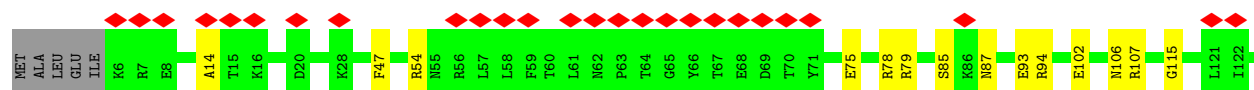
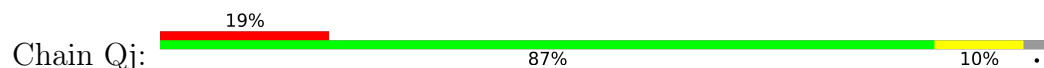




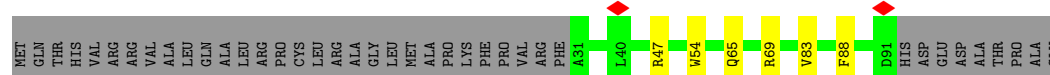
• Molecule 79: UQCR10



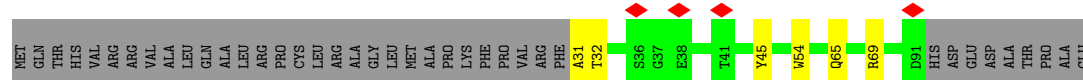
• Molecule 79: UQCR10



• Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial



• Molecule 80: Ubiquinol-cytochrome-C reductase complex subunit IX, mitochondrial

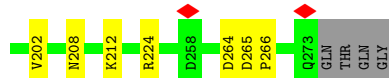
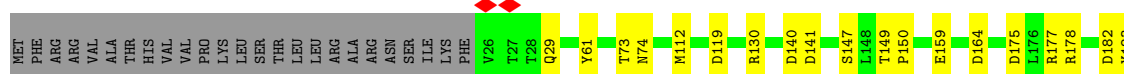
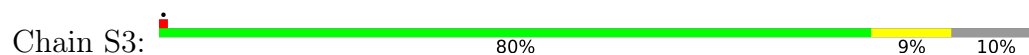


• Molecule 81: NDUFS2

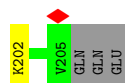
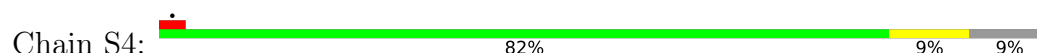




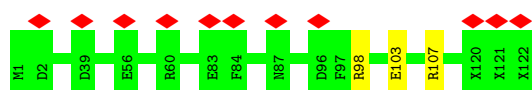
• Molecule 82: NDUFS3



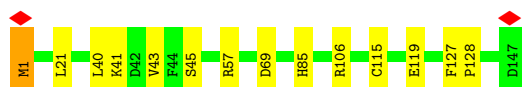
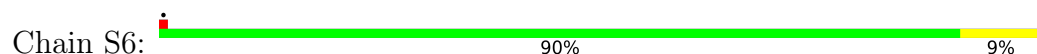
• Molecule 83: NDUFS4



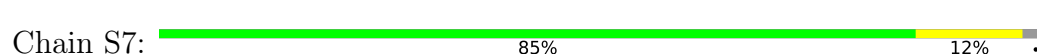
• Molecule 84: NDUFS5



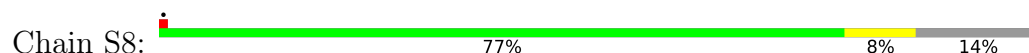
• Molecule 85: NDUFS6

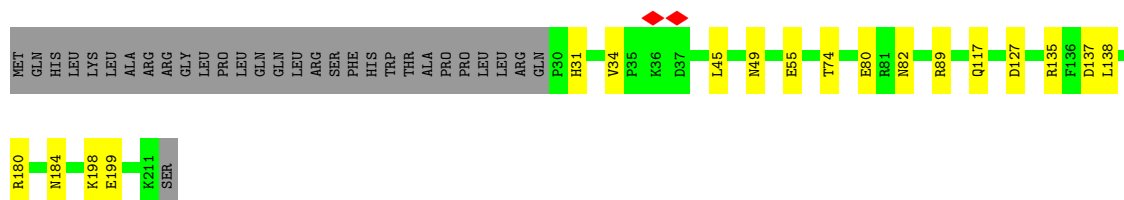


• Molecule 86: NDUFS7



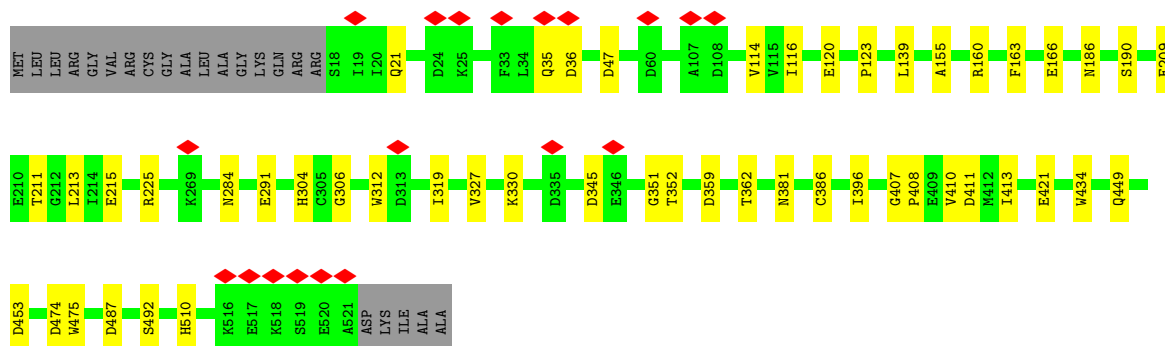
• Molecule 87: NDUFS8





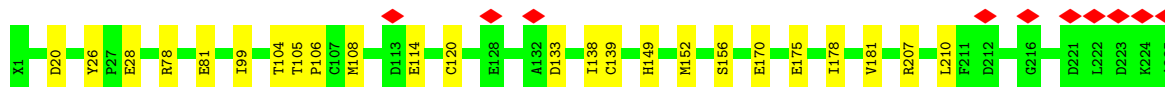
• Molecule 88: NDUFV1

Chain V1: 86% 10%



• Molecule 89: NDUFV2

Chain V2: 89% 11%



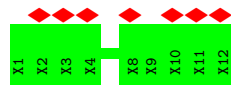
• Molecule 90: poly(UNK)

Chain A: 8% 100%



• Molecule 90: poly(UNK)

Chain B: 58% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	345048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	37.689	Depositor
Minimum map value	-25.803	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.049	Depositor
Recommended contour level	5	Depositor
Map size (Å)	537.60004, 537.60004, 537.60004	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U10, S12, HEA, PC1, FMN, NDP, SF4, HEM, K, CU, FES, 3PE, 2MR, MG, ZN, PX2, ZMP, CDL, 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	1A	0.28	0/2858	0.36	0/3878
2	1B	0.25	0/4306	0.30	0/5854
3	2B	0.28	0/958	0.36	0/1306
4	4A	0.18	0/1650	0.25	0/2235
5	4C	0.20	0/1051	0.27	0/1432
6	4D	0.21	0/1379	0.31	0/1867
7	4E	0.16	0/1376	0.26	0/1864
8	4F	0.19	0/641	0.28	0/867
9	4G	0.21	0/2391	0.28	0/3240
10	4H	0.20	0/1640	0.29	0/2224
11	4I	0.27	0/2255	0.32	0/3059
12	4J	0.25	0/736	0.29	0/1008
13	4L	0.26	0/924	0.30	0/1261
14	5B	0.29	0/1294	0.37	0/1759
15	5C	0.24	0/1616	0.30	0/2192
16	6A	0.19	0/777	0.28	0/1055
17	6B	0.20	0/2343	0.26	0/3174
18	7A	0.21	0/1359	0.30	0/1835
19	7C	0.25	0/1299	0.30	0/1777
20	A1	0.20	0/1108	0.28	0/1511
21	A2	0.22	0/1530	0.30	0/2089
22	A3	0.23	0/1079	0.30	0/1453
23	A5	0.23	0/1282	0.28	0/1737
24	A6	0.22	0/3395	0.28	0/4608
25	A7	0.25	0/1194	0.33	0/1619
26	A8	0.21	0/1879	0.27	0/2543
27	A9	0.25	0/3920	0.32	0/5335
28	AB	0.21	0/704	0.25	0/951
29	AC	0.25	0/736	0.28	0/1000
30	AL	0.25	0/2317	0.32	0/3136
31	AM	0.22	0/1533	0.26	0/2079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AN	0.22	0/2382	0.26	0/3249
33	B2	0.24	0/947	0.27	0/1291
34	B3	0.27	0/326	0.29	0/441
35	B4	0.25	0/1419	0.30	0/1922
36	B5	0.26	0/1111	0.32	0/1505
37	B6	0.24	0/803	0.29	0/1087
38	B7	0.23	0/877	0.27	0/1172
39	B8	0.25	0/1273	0.29	0/1733
40	B9	0.25	0/1274	0.32	0/1728
41	BL	0.25	0/1266	0.29	0/1710
42	BM	0.24	0/876	0.30	0/1192
43	C1	0.29	0/4054	0.38	0/5516
44	C2	0.26	0/1620	0.36	0/2207
45	C3	0.22	0/1416	0.31	0/1945
46	C4	0.24	0/1592	0.30	0/2158
47	DC	0.25	0/1410	0.31	0/1914
48	E1	0.21	0/3596	0.29	0/4879
49	E2	0.18	0/3658	0.26	0/4983
50	E3	0.19	0/3320	0.28	0/4520
51	E4	0.22	0/2850	0.27	0/3884
52	E5	0.14	0/2004	0.35	0/2721
53	E6	0.23	0/2954	0.29	0/4004
54	E7	0.22	0/1931	0.32	0/2618
55	E8	0.24	0/1747	0.31	0/2367
56	E9	0.13	0/1239	0.25	0/1690
57	EA	0.27	0/858	0.28	0/1163
58	EB	0.20	0/650	0.25	0/863
59	EC	0.19	0/676	0.30	0/925
60	ED	0.22	0/1176	0.29	0/1590
61	FX	0.29	0/2035	0.36	0/2763
62	G1	0.25	0/3443	0.33	0/4686
63	G2	0.23	0/1832	0.32	0/2476
64	G3	0.22	0/1957	0.34	0/2646
65	N1	0.24	0/2672	0.35	0/3639
66	N2	0.28	0/2582	0.36	0/3530
67	N3	0.26	0/1068	0.37	0/1456
67	N6	0.23	0/1275	0.35	0/1730
68	N4	0.27	0/4105	0.38	0/5594
69	N5	0.27	0/4963	0.38	0/6758
70	QA	0.23	0/3838	0.31	0/5193
70	Qa	0.22	0/3838	0.30	0/5193
71	QB	0.24	0/3532	0.31	0/4805
71	Qb	0.24	0/3288	0.30	0/4474

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
72	QC	0.26	0/3058	0.33	0/4178
72	Qc	0.27	0/3058	0.33	0/4178
73	QD	0.25	0/2027	0.31	0/2760
73	Qd	0.24	0/2027	0.33	0/2760
74	QE	0.18	0/1842	0.30	0/2502
74	Qe	0.17	0/1842	0.29	0/2502
75	QF	0.18	0/526	0.27	0/702
75	Qf	0.17	0/526	0.27	0/702
76	QG	0.28	0/1987	0.34	0/2696
76	Qg	0.27	0/1987	0.34	0/2696
77	QH	0.24	0/717	0.31	0/966
77	Qh	0.23	0/717	0.33	0/966
78	QI	0.25	0/251	0.28	0/340
78	Qi	0.22	0/251	0.27	0/340
79	QJ	0.20	0/1243	0.27	0/1693
79	Qj	0.19	0/1243	0.27	0/1693
80	QK	0.22	0/498	0.28	0/677
80	Qk	0.21	0/498	0.27	0/677
81	S2	0.29	0/3244	0.35	0/4403
82	S3	0.28	0/2112	0.37	0/2874
83	S4	0.24	0/1573	0.32	0/2107
84	S5	0.19	0/960	0.25	0/1291
85	S6	0.26	0/1232	0.32	0/1659
86	S7	0.28	0/1558	0.33	0/2120
87	S8	0.29	0/1485	0.33	0/2010
88	V1	0.22	0/3990	0.32	0/5394
89	V2	0.21	0/1787	0.30	0/2428
All	All	0.24	0/183502	0.31	0/249182

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2801	2700	2710	20	0
2	1B	4198	4159	4175	26	0
3	2B	1070	989	1009	6	0
4	4A	1612	1608	1617	12	0
5	4C	1022	1027	1029	6	0
6	4D	1349	1359	1363	11	0
7	4E	1333	1279	1283	8	0
8	4F	620	626	627	1	0
9	4G	2351	2340	2343	20	0
10	4H	1606	1644	1648	12	0
11	4I	2178	2046	2058	17	0
12	4J	711	688	689	1	0
13	4L	890	878	880	5	0
14	5B	1258	1184	1192	14	0
15	5C	1571	1546	1550	10	0
16	6A	750	747	749	9	0
17	6B	2285	2229	2239	14	0
18	7A	1319	1284	1295	9	0
19	7C	1254	1183	1190	4	0
20	A1	1071	1026	1030	5	0
21	A2	1493	1474	1478	10	0
22	A3	1050	1039	1041	4	0
23	A5	1261	1248	1251	9	0
24	A6	3328	3280	3293	23	0
25	A7	1154	1118	1123	14	0
26	A8	1822	1726	1736	25	0
27	A9	3829	3850	3857	27	0
28	AB	694	673	677	4	0
29	AC	721	697	702	2	0
30	AL	2237	2172	2180	11	0
31	AM	1487	1448	1452	17	0
32	AN	2306	2267	2275	6	0
33	B2	913	857	858	3	0
34	B3	449	309	312	6	0
35	B4	1377	1358	1364	10	0
36	B5	1112	1069	1075	8	0
37	B6	773	747	751	3	0
38	B7	857	835	841	6	0
39	B8	1224	1127	1136	9	0
40	B9	1236	1207	1212	11	0
41	BL	1227	1179	1185	4	0
42	BM	910	827	829	4	0
43	C1	3938	3980	3999	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	C2	1585	1647	1652	16	0
45	C3	1378	1413	1419	10	0
46	C4	1545	1517	1519	12	0
47	DC	1366	1362	1366	9	0
48	E1	3512	3496	3510	13	0
49	E2	3563	3540	3554	18	0
50	E3	3255	3263	3279	15	0
51	E4	2770	2732	2742	8	0
52	E5	1977	2069	2075	21	0
53	E6	2871	2758	2767	11	0
54	E7	1888	1892	1903	16	0
55	E8	1691	1663	1668	19	0
56	E9	1212	1224	1228	3	0
57	EA	961	832	835	5	0
58	EB	774	631	635	6	0
59	EC	660	663	666	5	0
60	ED	1142	1131	1134	5	0
61	FX	1967	1849	1858	28	0
62	G1	3347	3205	3222	29	0
63	G2	1804	1846	1850	12	0
64	G3	1961	1944	1950	13	0
65	N1	2605	2726	2729	25	0
66	N2	2512	2589	2592	31	0
67	N3	1037	1057	1057	11	0
67	N6	1257	1385	1385	13	0
68	N4	4001	4214	4224	27	0
69	N5	4837	5032	5046	38	0
70	QA	3750	3658	3668	23	0
70	Qa	3750	3658	3668	20	0
71	QB	3458	3431	3443	18	0
71	Qb	3216	3192	3204	27	0
72	QC	2975	3064	3076	16	0
72	Qc	2975	3064	3076	30	0
73	QD	1959	1858	1864	17	0
73	Qd	1959	1858	1865	25	0
74	QE	1795	1776	1780	12	0
74	Qe	1795	1776	1780	10	0
75	QF	515	499	505	5	0
75	Qf	515	503	509	5	0
76	QG	1932	1870	1880	21	0
76	Qg	1932	1870	1880	25	0
77	QH	701	692	694	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
77	Qh	701	692	694	13	0
78	QI	449	293	293	4	0
78	Qi	449	293	293	2	0
79	QJ	1206	1212	1216	14	0
79	Qj	1206	1212	1216	14	0
80	QK	485	499	500	6	0
80	Qk	485	499	500	6	0
81	S2	3173	3101	3114	28	0
82	S3	2050	1928	1936	16	0
83	S4	1536	1502	1505	15	0
84	S5	991	895	898	2	0
85	S6	1200	1192	1198	10	0
86	S7	1545	1500	1503	19	0
87	S8	1451	1392	1397	15	0
88	V1	3897	3827	3837	31	0
89	V2	1759	1701	1710	13	0
90	A	60	16	16	0	0
90	B	60	16	16	0	0
91	1A	4	0	0	0	0
91	QE	4	0	0	0	0
91	Qe	4	0	0	0	0
91	V2	4	0	0	0	0
92	1A	16	0	0	0	0
92	S7	8	0	0	1	0
92	S8	16	0	0	0	0
92	V1	8	0	0	0	0
93	1A	1	0	0	0	0
94	4A	93	137	137	0	0
94	4E	35	44	44	0	0
94	7A	36	46	46	0	0
94	A1	80	111	111	1	0
94	A9	66	80	80	0	0
94	AL	50	77	77	0	0
94	AM	97	148	148	1	0
94	AN	48	73	73	0	0
94	B5	108	176	176	3	0
94	B8	37	48	48	0	0
94	C1	50	77	77	0	0
94	C3	51	79	79	0	0
94	E4	51	79	79	0	0
94	E8	171	250	250	0	0
94	E9	35	44	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	ED	95	144	144	0	0
94	G2	38	50	50	0	0
94	N1	89	129	129	0	0
94	N3	42	61	61	0	0
94	N4	126	180	180	0	0
94	N5	36	46	46	0	0
94	QC	54	88	88	0	0
94	QD	31	36	36	0	0
94	QI	36	46	46	1	0
94	Qc	85	124	124	0	0
94	Qe	36	46	46	0	0
94	Qg	28	30	30	0	0
94	Qj	54	88	88	0	0
95	4D	86	126	126	0	0
95	7A	41	59	59	0	0
95	B4	40	57	57	1	0
95	C1	80	108	108	0	0
95	E9	51	82	82	0	0
95	N4	41	56	56	0	0
95	N5	51	82	82	0	0
96	4D	35	44	44	0	0
97	4E	72	91	91	0	0
97	7C	90	130	130	1	0
97	A3	58	60	60	1	0
97	A9	64	72	72	1	0
97	AL	132	152	152	0	0
97	AM	144	182	182	4	0
97	B3	65	74	74	1	0
97	B8	70	87	87	1	0
97	BM	58	60	60	0	0
97	C4	261	372	372	2	0
97	E4	72	91	91	2	0
97	E6	58	60	60	1	0
97	E7	68	80	80	0	0
97	EA	114	116	116	1	0
97	N1	70	84	84	1	0
97	N5	93	136	136	0	0
97	QC	56	56	56	0	0
97	QD	69	82	82	0	0
97	QH	136	163	163	2	0
97	QJ	58	60	60	1	0
97	Qc	54	52	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
97	Qd	100	156	156	2	0
97	Qe	60	64	64	0	0
97	Qh	65	74	74	0	0
97	Qj	48	40	40	1	0
98	5B	1	0	0	0	0
98	E7	1	0	0	0	0
98	S6	1	0	0	0	0
99	A9	48	26	26	0	0
100	AB	36	0	47	3	0
100	AC	36	0	47	7	0
101	C1	120	0	108	21	0
102	C1	1	0	0	0	0
102	C2	2	0	0	0	0
103	C1	1	0	0	0	0
104	C2	36	0	52	4	0
104	QJ	72	0	104	8	0
105	N4	43	55	55	4	0
106	QC	86	0	60	2	0
106	Qc	86	0	60	10	0
107	QD	43	0	31	5	0
107	Qd	43	0	32	6	0
108	V1	31	19	19	0	0
All	All	185125	183093	184288	1123	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 (1123) 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)
73:Qd:40:CYS:SG	107:Qd:301:HEC:HAC	1.36	1.63
73:QD:40:CYS:SG	107:QD:301:HEC:CAC	2.03	1.45
73:Qd:40:CYS:SG	107:Qd:301:HEC:CAC	2.07	1.43
101:C1:501:HEA:HBC1	101:C1:501:HEA:HHD	1.46	0.97
52:E5:287:LEU:O	52:E5:289:LEU:N	1.98	0.94
79:QJ:47:PHE:O	79:QJ:54:ARG:NH1	2.03	0.91
16:6A:76:ARG:NH1	17:6B:92:GLU:OE2	2.05	0.90
79:Qj:54:ARG:NH2	97:Qj:202:CDL:OB3	2.06	0.89
79:QJ:54:ARG:NH2	97:QJ:203:CDL:OB3	2.06	0.88
71:Qb:101:HIS:NE2	71:Qb:181:GLU:OE2	2.07	0.87
39:B8:25:ARG:NH1	39:B8:30:GLU:OE2	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:QG:60:ARG:NH1	79:Qj:93:GLU:OE2	2.08	0.86
58:EB:30:GLN:O	58:EB:35:ARG:NH2	2.09	0.86
73:Qd:224:ARG:NH1	77:Qh:33:ILE:O	2.09	0.86
47:DC:120:ASP:OD1	54:E7:123:GLN:NE2	2.08	0.85
79:Qj:47:PHE:O	79:Qj:54:ARG:NH1	2.09	0.85
76:QG:228:ARG:NH1	79:Qj:115:GLY:O	2.09	0.85
73:Qd:40:CYS:HG	107:Qd:301:HEC:HAC	1.06	0.85
74:Qe:170:ASP:OD2	74:Qe:230:ASN:ND2	2.09	0.84
88:V1:186:ASN:ND2	88:V1:190:SER:O	2.10	0.84
2:1B:48:ARG:NH1	21:A2:163:ASP:OD1	2.09	0.84
25:A7:46:ALA:O	31:AM:31:ARG:NH1	2.10	0.84
106:Qc:403:HEM:HMB1	106:Qc:403:HEM:HBB2	1.58	0.84
71:QB:290:ARG:NH1	71:QB:300:ASP:O	2.12	0.83
81:S2:187:ARG:NH1	81:S2:190:GLU:OE2	2.11	0.83
17:6B:58:ARG:NH2	45:C3:114:ASN:OD1	2.12	0.83
1:1A:275:ASN:ND2	1:1A:278:ASP:OD1	2.12	0.83
63:G2:126:GLU:OE2	63:G2:141:TYR:OH	1.97	0.83
86:S7:32:ARG:NH1	86:S7:35:GLU:OE1	2.12	0.82
43:C1:411:PHE:O	43:C1:412:SER:OG	1.98	0.82
69:N5:255:LEU:O	69:N5:260:THR:OG1	1.97	0.82
22:A3:22:ASN:OD1	22:A3:23:ARG:NH1	2.13	0.82
65:N1:424:ARG:NH1	67:N3:202:SER:OG	2.13	0.81
100:AC:201:ZMP:H12A	100:AC:201:ZMP:HN2	1.47	0.79
23:A5:169:GLU:OE2	23:A5:172:ARG:NH2	2.16	0.79
2:1B:235:SER:HG	2:1B:240:SER:HG	1.18	0.79
58:EB:89:GLU:N	58:EB:89:GLU:OE1	2.16	0.79
9:4G:161:ARG:NH2	16:6A:1:MET:O	2.16	0.79
4:4A:107:ARG:NH2	4:4A:177:ALA:O	2.17	0.78
13:4L:95:LYS:O	13:4L:103:ARG:NH2	2.16	0.78
43:C1:391:LEU:HD21	101:C1:501:HEA:HBC2	1.65	0.78
69:N5:161:ARG:NH1	69:N5:247:GLU:OE1	2.16	0.78
33:B2:50:GLU:O	60:ED:70:ARG:NH2	2.17	0.78
27:A9:442:ARG:NH2	65:N1:484:ILE:O	2.17	0.77
48:E1:254:ASN:OD1	48:E1:257:ARG:NH2	2.17	0.77
79:QJ:93:GLU:OE2	76:Qg:60:ARG:NH1	2.17	0.77
38:B7:30:SER:OG	38:B7:32:GLU:OE1	2.02	0.77
80:Qk:65:GLN:OE1	80:Qk:69:ARG:NH1	2.17	0.77
104:QJ:202:PX2:H34	104:QJ:202:PX2:H43	1.67	0.77
52:E5:41:ALA:O	52:E5:287:LEU:O	2.02	0.77
2:1B:221:GLU:OE2	49:E2:52:ARG:NH1	2.19	0.76
70:Qa:304:ARG:NH1	70:Qa:308:MET:SD	2.58	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:ED:58:ARG:NH1	60:ED:61:GLU:OE2	2.18	0.76
88:V1:421:GLU:OE2	88:V1:434:TRP:NE1	2.18	0.76
24:A6:33:ARG:NH2	24:A6:41:GLU:OE2	2.17	0.76
44:C2:108:GLU:OE1	44:C2:110:ARG:NH1	2.18	0.76
61:FX:185:TRP:O	61:FX:186:SER:OG	2.04	0.76
27:A9:120:THR:OG1	27:A9:195:SER:OG	1.96	0.75
48:E1:40:ARG:NH2	49:E2:235:ASP:OD1	2.19	0.75
24:A6:134:ASN:HD21	100:AB:201:ZMP:H25	1.50	0.75
60:ED:46:GLU:OE1	60:ED:49:ARG:NH1	2.20	0.75
2:1B:177:GLU:OE1	2:1B:179:ARG:NH1	2.20	0.75
50:E3:52:ASP:OD1	50:E3:240:SER:OG	2.04	0.75
76:Qg:163:ARG:NH2	76:Qg:214:GLU:OE2	2.20	0.74
70:QA:10:LEU:O	79:QJ:94:ARG:NH1	2.20	0.74
24:A6:45:HIS:NE2	24:A6:117:GLU:OE1	2.16	0.74
46:C4:47:PHE:O	46:C4:133:ARG:NH1	2.21	0.74
35:B4:85:TYR:OH	95:B4:201:3PE:O14	2.05	0.74
49:E2:364:PRO:O	49:E2:400:ARG:NH1	2.21	0.74
62:G1:416:GLN:OE1	62:G1:419:ARG:NH1	2.22	0.73
49:E2:4:GLY:O	49:E2:5:THR:OG1	2.06	0.73
16:6A:81:ASP:O	43:C1:228:ASN:ND2	2.20	0.73
15:5C:36:GLU:OE2	47:DC:26:ARG:NH1	2.22	0.73
53:E6:56:SER:OG	53:E6:57:ASN:ND2	2.22	0.73
76:QG:181:ASP:OD1	76:QG:185:ARG:NH1	2.22	0.72
2:1B:271:GLN:O	2:1B:499:ARG:NH2	2.23	0.72
9:4G:24:GLN:NE2	18:7A:26:ASP:OD1	2.23	0.72
7:4E:47:TYR:OH	17:6B:120:GLU:OE2	2.08	0.72
97:E6:401:CDL:OB7	62:G1:21:THR:OG1	2.06	0.72
62:G1:124:ASP:OD1	62:G1:403:ARG:NH2	2.23	0.72
71:Qb:356:ASP:O	71:Qb:357:THR:OG1	2.06	0.72
72:QC:205:ARG:NH2	72:QC:210:ASN:OD1	2.23	0.72
69:N5:170:LYS:NZ	69:N5:244:ASP:OD2	2.16	0.71
70:Qa:106:GLU:O	70:Qa:107:HIS:ND1	2.23	0.71
88:V1:35:GLN:N	88:V1:35:GLN:OE1	2.24	0.71
2:1B:454:GLU:OE2	21:A2:58:ARG:NH1	2.22	0.71
27:A9:443:ASP:OD2	65:N1:488:ASN:ND2	2.23	0.71
1:1A:211:GLU:OE1	89:V2:78:ARG:NH2	2.23	0.71
61:FX:190:ILE:O	61:FX:221:ASN:ND2	2.23	0.71
68:N4:67:ASN:N	68:N4:119:ASP:OD2	2.21	0.71
71:Qb:144:PHE:O	71:Qb:147:THR:OG1	2.09	0.71
56:E9:62:ARG:NH2	78:QI:1:MET:O	2.24	0.70
71:Qb:60:ASP:OD1	79:Qj:14:ALA:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A6:90:ARG:NH1	28:AB:96:GLU:OE2	2.25	0.70
55:E8:203:GLU:OE1	55:E8:203:GLU:N	2.23	0.70
46:C4:160:ARG:NH1	46:C4:161:GLU:OE2	2.25	0.70
4:4A:199:ASP:OD2	45:C3:149:THR:OG1	2.09	0.70
72:Qc:208:ARG:NH1	77:Qh:11:GLU:OE2	2.24	0.70
88:V1:411:ASP:OD2	88:V1:510:HIS:NE2	2.20	0.70
22:A3:5:GLU:OE1	25:A7:116:ARG:NH1	2.25	0.69
35:B4:28:GLU:OE1	35:B4:31:ARG:NH2	2.25	0.69
9:4G:228:LEU:O	9:4G:233:GLN:NE2	2.24	0.69
88:V1:449:GLN:NE2	88:V1:453:ASP:OD1	2.25	0.69
97:AM:202:CDL:OB3	87:S8:49:ASN:ND2	2.26	0.69
46:C4:132:ARG:NH1	46:C4:136:GLU:OE1	2.25	0.69
26:A8:13:ASP:OD1	36:B5:115:ASN:ND2	2.24	0.69
73:QD:40:CYS:SG	107:QD:301:HEC:C3C	2.81	0.69
70:QA:253:GLU:OE2	73:QD:238:ARG:NH1	2.26	0.69
21:A2:6:ARG:NH2	21:A2:135:GLU:OE1	2.26	0.68
46:C4:43:ASP:OD1	46:C4:43:ASP:N	2.26	0.68
62:G1:28:ARG:NH2	62:G1:37:GLU:OE2	2.26	0.68
43:C1:267:ILE:O	43:C1:270:SER:OG	2.10	0.68
49:E2:19:GLU:N	49:E2:19:GLU:OE1	2.26	0.68
61:FX:189:VAL:HG13	61:FX:221:ASN:HB2	1.74	0.68
67:N6:118:ASN:O	67:N6:120:ASN:ND2	2.26	0.68
6:4D:97:ALA:O	17:6B:43:ARG:NH2	2.26	0.68
9:4G:66:LEU:O	9:4G:198:GLN:NE2	2.26	0.68
101:C1:501:HEA:HHA	101:C1:501:HEA:CBA	2.24	0.68
11:4I:31:TRP:O	43:C1:480:ARG:NH2	2.27	0.68
24:A6:135:ASN:OD1	82:S3:212:LYS:NZ	2.27	0.67
26:A8:214:THR:OG1	26:A8:219:ASP:OD2	2.12	0.67
54:E7:207:VAL:O	55:E8:74:ARG:NH2	2.27	0.67
62:G1:211:GLU:OE2	63:G2:87:ARG:NH1	2.28	0.67
77:QH:57:THR:HG21	80:QK:54:TRP:HE1	1.59	0.67
10:4H:99:ASP:OD2	10:4H:101:ASN:ND2	2.28	0.67
71:QB:42:ARG:NH1	71:QB:43:LEU:O	2.28	0.67
71:QB:356:ASP:O	71:QB:357:THR:OG1	2.11	0.67
73:QD:101:ARG:NH2	74:Qe:194:GLY:O	2.28	0.67
76:QG:163:ARG:NH2	76:QG:214:GLU:OE2	2.28	0.67
31:AM:28:ARG:NH2	85:S6:21:LEU:O	2.26	0.67
27:A9:26:ASN:O	27:A9:26:ASN:ND2	2.27	0.67
73:Qd:40:CYS:SG	107:Qd:301:HEC:C3C	2.83	0.67
65:N1:394:GLN:OE1	65:N1:396:ARG:NH1	2.27	0.66
61:FX:275:LYS:O	61:FX:277:VAL:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:138:HIS:O	1:1A:173:LYS:NZ	2.27	0.66
37:B6:12:ASP:OD1	37:B6:13:PHE:N	2.29	0.66
76:Qg:53:ARG:NH2	76:Qg:56:GLU:OE2	2.29	0.66
81:S2:89:GLU:O	81:S2:93:GLU:N	2.26	0.66
18:7A:110:SER:O	18:7A:115:ARG:NH1	2.28	0.66
77:Qh:77:GLU:OE2	77:Qh:80:ARG:NH1	2.29	0.66
64:G3:235:GLY:O	67:N6:161:LYS:NZ	2.28	0.65
70:QA:41:GLU:OE1	70:QA:419:ARG:NH1	2.29	0.65
85:S6:41:LYS:O	85:S6:45:SER:OG	2.13	0.65
76:Qg:181:ASP:OD1	76:Qg:185:ARG:NH1	2.29	0.65
4:4A:47:LEU:O	4:4A:49:ARG:NH1	2.29	0.65
9:4G:75:LYS:O	9:4G:192:ARG:NH1	2.29	0.65
30:AL:141:GLN:NE2	87:S8:74:THR:O	2.29	0.65
24:A6:393:ILE:O	24:A6:396:THR:OG1	2.15	0.65
71:QB:145:ARG:NH1	71:QB:248:GLU:OE2	2.30	0.65
25:A7:129:ASP:OD2	51:E4:39:ARG:NH1	2.30	0.65
72:Qc:137:CYS:SG	72:Qc:155:TRP:NE1	2.70	0.65
38:B7:85:ARG:NH2	39:B8:130:GLY:O	2.30	0.65
61:FX:144:ASP:O	61:FX:147:GLY:N	2.28	0.65
62:G1:294:ARG:HG2	63:G2:181:VAL:HG21	1.78	0.65
5:4C:100:GLU:N	5:4C:100:GLU:OE1	2.29	0.64
70:Qa:400:ASP:O	70:Qa:404:ASN:ND2	2.31	0.64
16:6A:51:THR:OG1	45:C3:136:TYR:OH	2.15	0.64
74:Qe:180:GLU:OE1	74:Qe:183:TRP:N	2.29	0.64
62:G1:113:ARG:NH2	67:N6:166:TYR:OH	2.31	0.64
25:A7:105:SER:O	82:S3:130:ARG:NH1	2.31	0.64
77:Qh:57:THR:HG21	80:Qk:54:TRP:HE1	1.63	0.64
2:1B:283:ARG:NH2	50:E3:345:GLN:OE1	2.31	0.64
41:BL:81:GLU:OE2	42:BM:92:ARG:NH1	2.31	0.64
55:E8:156:ARG:NH2	55:E8:180:THR:O	2.31	0.64
71:Qb:329:GLN:NE2	71:Qb:401:THR:OG1	2.30	0.64
81:S2:153:SER:OG	81:S2:155:MET:O	2.16	0.63
26:A8:222:TYR:OH	57:EA:113:UNK:O	2.15	0.63
70:QA:447:ASP:OD2	78:QI:10:TYR:OH	2.14	0.63
73:QD:208:THR:HG22	104:QJ:201:PX2:H36	1.80	0.63
71:Qb:290:ARG:NH1	71:Qb:300:ASP:O	2.31	0.63
27:A9:239:ARG:NH2	27:A9:339:GLU:OE2	2.31	0.63
65:N1:586:SER:O	86:S7:114:GLN:NE2	2.32	0.63
11:4I:71:GLU:O	71:QB:38:ARG:NH2	2.32	0.62
22:A3:49:GLU:OE1	67:N3:291:ASN:ND2	2.32	0.62
69:N5:358:TYR:OH	69:N5:464:ASN:OD1	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:QJ:79:ARG:NH2	76:Qg:61:ASP:OD1	2.32	0.62
31:AM:152:ARG:NH2	31:AM:185:GLU:OE2	2.32	0.62
37:B6:66:ARG:NH1	41:BL:14:ASP:OD2	2.32	0.62
4:4A:236:ASP:OD1	4:4A:237:ALA:N	2.33	0.62
97:A3:201:CDL:O1	97:A3:201:CDL:OA3	2.17	0.62
27:A9:194:ARG:NH1	30:AL:219:HIS:O	2.32	0.62
74:QE:152:ARG:NH2	74:QE:218:HIS:O	2.32	0.62
6:4D:11:ARG:NH2	14:5B:70:HIS:O	2.32	0.62
15:5C:140:GLU:OE1	47:DC:26:ARG:NH2	2.32	0.62
31:AM:74:ARG:NH2	65:N1:516:TYR:O	2.33	0.62
48:E1:346:ASP:OD1	48:E1:347:ALA:N	2.32	0.62
50:E3:53:GLN:NE2	50:E3:94:ASN:OD1	2.33	0.62
23:A5:97:GLU:N	23:A5:97:GLU:OE1	2.33	0.62
73:Qd:27:ARG:NH1	73:Qd:54:PHE:O	2.33	0.62
54:E7:91:GLN:OE1	54:E7:91:GLN:N	2.32	0.61
72:QC:302:ARG:NH1	76:QG:33:ILE:O	2.29	0.61
9:4G:100:GLU:O	71:QB:48:LYS:NZ	2.32	0.61
81:S2:78:MET:HB2	81:S2:111:THR:HG21	1.82	0.61
43:C1:337:ALA:O	43:C1:338:SER:OG	2.17	0.61
48:E1:105:GLN:NE2	48:E1:236:SER:OG	2.32	0.61
66:N2:126:GLU:N	66:N2:126:GLU:OE1	2.32	0.61
88:V1:312:TRP:O	88:V1:330:LYS:NZ	2.33	0.61
89:V2:114:GLU:OE1	89:V2:114:GLU:N	2.32	0.61
24:A6:99:LEU:O	83:S4:47:GLN:NE2	2.29	0.61
25:A7:32:TRP:O	81:S2:187:ARG:NH2	2.30	0.61
31:AM:187:MET:O	84:S5:98:ARG:NH2	2.33	0.61
101:C1:502:HEA:H14	101:C1:502:HEA:O11	2.00	0.61
81:S2:111:THR:HG22	81:S2:147:TYR:OH	1.99	0.61
88:V1:351:GLY:O	88:V1:352:THR:OG1	2.13	0.61
27:A9:181:ASN:N	27:A9:187:GLU:OE1	2.34	0.61
87:S8:180:ARG:NH1	87:S8:184:ASN:OD1	2.33	0.61
75:Qf:57:GLU:O	75:Qf:61:HIS:ND1	2.33	0.61
100:AC:201:ZMP:O7	100:AC:201:ZMP:H20A	2.01	0.61
73:QD:37:PHE:HD2	107:QD:301:HEC:HAB	1.66	0.61
74:QE:108:TYR:HB2	104:QJ:201:PX2:H8	1.83	0.61
72:Qc:218:ARG:NH1	97:Qd:302:CDL:OB7	2.33	0.61
43:C1:368:LEU:HB3	101:C1:501:HEA:HMA	1.82	0.60
72:Qc:208:ARG:NH2	77:Qh:2:GLU:OE2	2.32	0.60
9:4G:158:GLU:OE2	9:4G:161:ARG:NH1	2.33	0.60
11:4I:155:GLU:N	11:4I:155:GLU:OE1	2.35	0.60
26:A8:1:MET:HE2	66:N2:195:ILE:HG21	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:QE:194:GLY:O	73:Qd:101:ARG:NH2	2.34	0.60
26:A8:102:ARG:NH2	31:AM:93:CYS:O	2.33	0.60
71:Qb:388:GLU:N	71:Qb:388:GLU:OE1	2.34	0.60
11:4I:217:GLU:OE2	11:4I:219:THR:OG1	2.20	0.60
27:A9:95:GLU:OE1	83:S4:137:LYS:NZ	2.34	0.60
2:1B:57:GLU:N	2:1B:57:GLU:OE1	2.33	0.60
21:A2:28:ALA:O	21:A2:32:ASN:ND2	2.35	0.60
26:A8:177:TYR:OH	65:N1:541:GLU:OE2	2.20	0.60
27:A9:319:GLU:OE1	27:A9:353:ARG:NH1	2.34	0.60
43:C1:392:SER:OG	101:C1:502:HEA:H131	2.01	0.60
66:N2:175:TYR:CG	66:N2:186:MET:HE1	2.37	0.60
66:N2:261:ASP:OD1	66:N2:262:PHE:N	2.34	0.60
43:C1:391:LEU:CD2	101:C1:501:HEA:HBC2	2.31	0.60
48:E1:414:ASP:OD1	48:E1:415:LYS:N	2.33	0.60
70:QA:73:GLU:OE1	70:QA:103:THR:OG1	2.12	0.60
9:4G:151:LEU:O	14:5B:152:LYS:NZ	2.35	0.59
73:QD:71:ASP:OD1	73:QD:72:ASP:N	2.32	0.59
81:S2:157:PRO:O	87:S8:89:ARG:NH2	2.34	0.59
13:4L:95:LYS:NZ	67:N6:39:GLU:OE2	2.35	0.59
27:A9:194:ARG:NH2	30:AL:222:ASN:O	2.33	0.59
32:AN:245:MET:O	46:C4:152:ARG:NH1	2.35	0.59
9:4G:76:GLU:OE2	9:4G:84:ARG:NH2	2.33	0.59
73:QD:58:GLU:N	73:QD:58:GLU:OE1	2.36	0.59
15:5C:16:ARG:NH2	15:5C:20:LEU:O	2.36	0.59
23:A5:40:ARG:NH2	23:A5:81:ALA:O	2.36	0.59
24:A6:426:LYS:O	24:A6:427:SER:OG	2.16	0.59
28:AB:92:LEU:HD13	100:AB:201:ZMP:H20A	1.84	0.59
68:N4:80:ILE:HD11	68:N4:337:ILE:HG23	1.85	0.59
70:QA:473:SER:OG	70:QA:475:ASP:OD1	2.19	0.59
82:S3:175:ASP:OD2	82:S3:177:ARG:NH1	2.35	0.59
1:1A:49:ASP:OD2	1:1A:118:THR:OG1	2.21	0.59
75:QF:16:LYS:NZ	75:QF:20:GLU:OE2	2.35	0.59
15:5C:156:GLY:O	44:C2:43:ARG:NH1	2.35	0.59
19:7C:118:THR:OG1	19:7C:120:GLN:NE2	2.36	0.59
43:C1:75:MET:HE3	101:C1:502:HEA:HMC3	1.84	0.58
43:C1:326:SER:HB2	101:C1:501:HEA:H202	1.85	0.58
82:S3:147:SER:OG	82:S3:159:GLU:OE1	2.18	0.58
6:4D:72:ASN:ND2	6:4D:74:GLU:OE2	2.36	0.58
35:B4:20:PRO:O	35:B4:22:ASP:N	2.36	0.58
74:QE:156:GLU:N	74:QE:156:GLU:OE1	2.36	0.58
9:4G:217:ARG:NH2	9:4G:220:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:QD:152:TYR:OH	75:QF:60:ASP:OD2	2.21	0.58
74:Qe:152:ARG:NH2	74:Qe:218:HIS:O	2.36	0.58
62:G1:133:ARG:NH2	63:G2:34:TYR:O	2.36	0.58
2:1B:283:ARG:NH1	50:E3:341:ASP:OD1	2.36	0.58
43:C1:346:ASN:ND2	43:C1:417:GLU:OE1	2.36	0.58
1:1A:195:CYS:O	1:1A:196:THR:OG1	2.15	0.58
68:N4:408:ASN:O	68:N4:412:SER:OG	2.22	0.58
10:4H:220:TYR:O	43:C1:491:HIS:NE2	2.33	0.58
69:N5:170:LYS:NZ	69:N5:540:ASP:OD1	2.36	0.58
106:Qc:403:HEM:HBB2	106:Qc:403:HEM:CMB	2.28	0.58
97:QH:102:CDL:OB4	97:QH:102:CDL:O1	2.17	0.57
76:Qg:144:ASP:OD2	76:Qg:175:ARG:NH1	2.37	0.57
89:V2:28:GLU:N	89:V2:28:GLU:OE1	2.37	0.57
82:S3:224:ARG:O	87:S8:117:GLN:NE2	2.36	0.57
53:E6:365:GLN:OE1	53:E6:365:GLN:N	2.34	0.57
70:Qa:172:GLU:OE2	73:Qd:234:ARG:NH2	2.35	0.57
32:AN:180:ARG:NH1	61:FX:206:ASP:OD1	2.33	0.57
53:E6:340:GLU:OE1	53:E6:340:GLU:N	2.38	0.57
73:Qd:71:ASP:OD1	73:Qd:72:ASP:N	2.37	0.57
27:A9:482:TYR:OH	67:N3:175:ASN:ND2	2.38	0.57
76:QG:61:ASP:OD1	79:Qj:79:ARG:NH2	2.37	0.57
56:E9:51:ALA:O	56:E9:55:ALA:N	2.38	0.57
61:FX:189:VAL:HA	61:FX:221:ASN:O	2.04	0.57
34:B3:5:ASN:ND2	60:ED:21:THR:OG1	2.37	0.57
43:C1:346:ASN:ND2	43:C1:420:SER:OG	2.38	0.57
83:S4:69:ARG:NH1	83:S4:143:PRO:O	2.38	0.57
26:A8:1:MET:HE1	66:N2:58:LEU:CD2	2.34	0.57
54:E7:165:GLN:O	54:E7:169:THR:OG1	2.21	0.57
68:N4:191:ILE:O	68:N4:195:ASN:ND2	2.38	0.56
27:A9:34:ASP:OD1	27:A9:37:THR:OG1	2.09	0.56
49:E2:188:HIS:O	49:E2:188:HIS:ND1	2.37	0.56
51:E4:180:ARG:NH2	51:E4:274:THR:OG1	2.37	0.56
66:N2:248:ILE:O	66:N2:252:ASN:ND2	2.33	0.56
35:B4:68:LYS:NZ	40:B9:129:GLN:O	2.35	0.56
51:E4:100:ARG:NH2	51:E4:139:GLU:O	2.38	0.56
70:QA:59:ARG:NH2	70:QA:341:ASP:OD1	2.39	0.56
88:V1:291:GLU:OE2	88:V1:304:HIS:NE2	2.30	0.56
48:E1:268:GLU:OE1	48:E1:322:THR:OG1	2.24	0.56
71:QB:93:ALA:O	71:QB:218:ASN:ND2	2.39	0.56
2:1B:112:THR:O	83:S4:155:ASN:ND2	2.39	0.56
17:6B:197:ALA:O	17:6B:203:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:G1:108:ARG:NH1	67:N3:288:ASN:OD1	2.38	0.56
24:A6:244:GLU:N	24:A6:244:GLU:OE1	2.35	0.56
16:6A:17:GLU:OE1	16:6A:17:GLU:N	2.39	0.56
24:A6:99:LEU:O	24:A6:100:THR:OG1	2.22	0.56
72:Qc:33:GLN:HG3	106:Qc:402:HEM:HBC2	1.88	0.56
101:C1:501:HEA:HBC1	101:C1:501:HEA:CHD	2.29	0.55
97:B8:302:CDL:OA4	55:E8:87:TYR:OH	2.19	0.55
54:E7:177:TYR:OH	54:E7:235:LYS:O	2.25	0.55
77:QH:57:THR:HG21	80:QK:54:TRP:NE1	2.20	0.55
73:Qd:37:PHE:HD2	107:Qd:301:HEC:HAB	1.71	0.55
89:V2:78:ARG:NH1	89:V2:81:GLU:OE1	2.39	0.55
14:5B:174:ILE:O	45:C3:12:ARG:NH2	2.40	0.55
39:B8:25:ARG:NH2	61:FX:172:ASP:OD2	2.39	0.55
50:E3:50:ASP:OD1	50:E3:50:ASP:N	2.39	0.55
66:N2:266:ASN:OD1	66:N2:267:LEU:N	2.39	0.55
87:S8:198:LYS:NZ	87:S8:199:GLU:OE2	2.40	0.55
79:QJ:115:GLY:O	76:Qg:228:ARG:NH1	2.40	0.55
74:QE:153:THR:OG1	74:QE:156:GLU:OE1	2.25	0.55
18:7A:128:MET:O	18:7A:132:HIS:N	2.35	0.55
66:N2:175:TYR:CD2	66:N2:186:MET:HE1	2.42	0.55
72:QC:137:CYS:SG	72:QC:155:TRP:NE1	2.79	0.55
72:Qc:302:ARG:NH1	76:Qg:33:ILE:O	2.33	0.55
3:2B:80:TYR:HB3	3:2B:81:PRO:HD3	1.89	0.55
82:S3:164:ASP:OD1	82:S3:178:ARG:NH1	2.40	0.55
29:AC:89:LEU:HD22	55:E8:1:MET:SD	2.47	0.54
55:E8:148:LYS:O	55:E8:149:SER:OG	2.16	0.54
2:1B:214:ASP:OD2	2:1B:218:LYS:NZ	2.40	0.54
18:7A:101:ASN:ND2	18:7A:102:PRO:O	2.40	0.54
25:A7:28:GLY:O	30:AL:64:HIS:NE2	2.38	0.54
100:AC:201:ZMP:H4A	40:B9:71:VAL:HG13	1.89	0.54
105:N4:504:U10:O5	105:N4:504:U10:H8	2.06	0.54
79:QJ:102:GLU:O	79:QJ:106:ASN:N	2.40	0.54
71:Qb:239:ASN:ND2	71:Qb:270:GLY:O	2.40	0.54
32:AN:86:ARG:NH1	32:AN:121:TYR:OH	2.40	0.54
54:E7:4:LEU:HD12	54:E7:4:LEU:O	2.07	0.54
81:S2:241:GLU:O	88:V1:492:SER:OG	2.20	0.54
20:A1:78:ARG:NH2	94:A1:202:PC1:O12	2.41	0.54
52:E5:7:TRP:O	52:E5:96:TYR:HB2	2.07	0.54
70:QA:1:MET:O	70:QA:2:THR:OG1	2.23	0.54
30:AL:108:ARG:NH1	65:N1:403:GLY:O	2.41	0.54
70:QA:296:GLU:OE1	76:Qg:218:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:N6:33:ILE:HA	67:N6:36:ILE:HG22	1.90	0.54
11:4I:15:ASP:OD2	70:QA:439:ARG:NH2	2.40	0.54
94:QI:101:PC1:H142	94:QI:101:PC1:O13	2.07	0.54
71:Qb:83:ASP:OD1	71:Qb:230:ARG:NH1	2.41	0.54
55:E8:14:PHE:O	55:E8:19:ASN:ND2	2.41	0.53
69:N5:97:SER:OG	69:N5:125:THR:HG21	2.08	0.53
76:QG:10:LEU:O	79:Qj:78:ARG:NH2	2.41	0.53
76:QG:182:LEU:HD11	76:QG:189:LEU:CD1	2.38	0.53
73:Qd:52:GLU:OE2	73:Qd:86:ARG:NE	2.39	0.53
73:Qd:95:LYS:O	73:Qd:96:ASN:C	2.50	0.53
62:G1:207:SER:OG	62:G1:233:GLY:O	2.25	0.53
105:N4:504:U10:H303	105:N4:504:U10:H261	1.89	0.53
10:4H:41:VAL:HG22	10:4H:129:GLU:OE1	2.08	0.53
52:E5:64:ALA:O	52:E5:96:TYR:N	2.41	0.53
105:N4:504:U10:C18	105:N4:504:U10:H151	2.39	0.53
83:S4:38:VAL:HG23	83:S4:39:ASN:H	1.74	0.53
85:S6:40:LEU:HA	85:S6:43:VAL:HG22	1.89	0.53
51:E4:241:ALA:O	51:E4:304:ARG:NH1	2.41	0.53
67:N3:249:ASP:O	67:N3:252:ILE:HG22	2.07	0.53
10:4H:87:TYR:OH	10:4H:128:LYS:NZ	2.39	0.53
11:4I:244:PHE:O	11:4I:247:ASN:ND2	2.37	0.53
49:E2:348:ASP:OD1	49:E2:372:ARG:NH2	2.41	0.53
74:QE:152:ARG:N	74:QE:182:ARG:O	2.41	0.53
72:Qc:190:LEU:CD2	106:Qc:403:HEM:HAA1	2.38	0.53
73:QD:37:PHE:CD2	107:QD:301:HEC:HAB	2.43	0.53
76:Qg:111:ASP:O	76:Qg:112:THR:OG1	2.25	0.53
45:C3:51:ILE:O	45:C3:55:ASN:ND2	2.40	0.53
72:QC:227:LEU:O	72:QC:231:ASN:ND2	2.42	0.53
73:Qd:234:ARG:HD2	74:Qe:65:VAL:HG21	1.91	0.53
77:Qh:53:GLY:O	77:Qh:57:THR:HG23	2.08	0.53
1:1A:375:ARG:NH1	24:A6:232:ASP:OD1	2.39	0.53
81:S2:48:PHE:HB3	86:S7:128:MET:HE2	1.91	0.53
81:S2:324:PRO:O	81:S2:345:SER:OG	2.26	0.53
1:1A:213:GLU:N	1:1A:213:GLU:OE1	2.42	0.53
101:C1:501:HEA:HHA	101:C1:501:HEA:HBA1	1.89	0.53
61:FX:170:SER:OG	61:FX:172:ASP:OD1	2.27	0.53
72:Qc:118:PHE:CE1	72:Qc:136:ILE:HD12	2.44	0.53
71:Qb:113:TYR:O	71:Qb:117:THR:OG1	2.17	0.52
9:4G:181:ARG:NH2	11:4I:188:GLU:OE2	2.42	0.52
42:BM:93:ARG:NH2	58:EB:18:UNK:O	2.43	0.52
65:N1:395:ARG:NH2	81:S2:190:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:C1:146:ARG:NH2	43:C1:229:SER:O	2.41	0.52
101:C1:501:HEA:HHA	101:C1:501:HEA:HBA2	1.91	0.52
71:Qb:406:VAL:HG22	71:Qb:429:PRO:HB2	1.90	0.52
52:E5:84:ARG:NH1	52:E5:114:LEU:O	2.38	0.52
88:V1:396:ILE:HB	88:V1:413:ILE:HD13	1.91	0.52
35:B4:112:GLN:O	35:B4:117:ASN:ND2	2.42	0.52
88:V1:410:VAL:O	88:V1:413:ILE:HG22	2.09	0.52
1:1A:141:ASP:OD2	1:1A:190:ASN:ND2	2.42	0.52
2:1B:127:THR:O	2:1B:127:THR:HG23	2.09	0.52
26:A8:103:GLU:OE2	26:A8:222:TYR:OH	2.27	0.52
65:N1:602:TYR:HA	65:N1:605:ILE:HG22	1.90	0.52
68:N4:403:SER:O	68:N4:406:ILE:HG22	2.08	0.52
2:1B:441:LYS:HG2	49:E2:25:LEU:HD11	1.92	0.52
62:G1:133:ARG:NH1	64:G3:215:GLU:OE2	2.42	0.52
68:N4:43:ILE:HD13	68:N4:472:LEU:HD21	1.92	0.52
62:G1:105:HIS:CE1	64:G3:241:ARG:HE	2.28	0.52
70:QA:172:GLU:OE2	73:QD:234:ARG:NH1	2.39	0.52
77:QH:53:GLY:O	77:QH:57:THR:HG23	2.10	0.52
89:V2:149:HIS:HB3	89:V2:170:GLU:HB3	1.92	0.52
27:A9:7:GLU:OE2	27:A9:30:ARG:NH2	2.42	0.51
34:B3:39:UNK:O	34:B3:40:UNK:CB	2.58	0.51
40:B9:150:GLY:O	63:G2:115:ARG:NH1	2.43	0.51
61:FX:130:SER:OG	62:G1:297:ARG:NH2	2.40	0.51
72:QC:152:ILE:O	72:QC:156:GLY:N	2.41	0.51
70:Qa:447:ASP:OD2	78:Qi:10:TYR:OH	2.26	0.51
71:Qb:54:LEU:HD21	71:Qb:426:PRO:HB2	1.92	0.51
73:Qd:37:PHE:CD2	107:Qd:301:HEC:HAB	2.45	0.51
82:S3:202:VAL:O	86:S7:170:ARG:NH1	2.37	0.51
13:4L:141:LEU:HB3	66:N2:116:VAL:HG11	1.90	0.51
43:C1:446:MET:HE2	43:C1:457:PHE:HB3	1.91	0.51
63:G2:135:GLN:OE1	63:G2:153:LYS:NZ	2.43	0.51
28:AB:56:ARG:O	28:AB:60:THR:HG23	2.10	0.51
17:6B:27:HIS:NE2	17:6B:265:TYR:O	2.40	0.51
24:A6:278:ASP:OD2	50:E3:3:ARG:NH2	2.43	0.51
39:B8:120:CYS:O	69:N5:417:GLY:O	2.28	0.51
104:QJ:202:PX2:H45	72:Qc:150:LEU:HD13	1.92	0.51
72:Qc:121:TYR:HA	106:Qc:402:HEM:HAD2	1.93	0.51
5:4C:85:ARG:NH2	17:6B:258:GLU:OE2	2.38	0.51
7:4E:144:ASN:OD1	7:4E:147:TYR:N	2.44	0.51
11:4I:239:GLN:NE2	11:4I:241:VAL:O	2.43	0.51
26:A8:62:ASN:ND2	26:A8:62:ASN:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Qf:14:LYS:NZ	75:Qf:18:GLU:OE2	2.43	0.51
73:QD:32:VAL:HG11	73:QD:186:VAL:CG1	2.40	0.51
74:QE:222:ILE:HD11	74:QE:224:LYS:O	2.10	0.51
69:N5:328:ILE:HG22	69:N5:328:ILE:O	2.11	0.51
107:QD:301:HEC:HHA	107:QD:301:HEC:HBD1	1.93	0.51
86:S7:90:GLU:HG2	86:S7:183:PRO:O	2.11	0.51
43:C1:453:TYR:CZ	43:C1:461:MET:HG3	2.46	0.51
104:C2:201:PX2:H16	104:C2:201:PX2:H40	1.93	0.51
53:E6:44:ASP:OD1	53:E6:47:ARG:NH2	2.44	0.51
86:S7:103:ARG:NH1	86:S7:104:TYR:OH	2.44	0.51
30:AL:232:LYS:O	30:AL:239:ARG:NH1	2.44	0.50
34:B3:23:ARG:NH2	55:E8:11:ASP:OD2	2.43	0.50
101:C1:501:HEA:HHH	101:C1:501:HEA:CBC	2.27	0.50
74:Qe:103:ARG:NH1	79:Qj:147:ARG:O	2.43	0.50
84:S5:103:GLU:O	84:S5:107:ARG:NH2	2.44	0.50
21:B2:281:ARG:NH1	21:A2:181:ALA:O	2.44	0.50
43:C1:464:GLY:O	43:C1:468:THR:HG23	2.11	0.50
61:FX:249:THR:N	61:FX:250:PRO:HD2	2.27	0.50
67:N6:52:GLY:HA3	67:N6:75:ILE:HD13	1.94	0.50
83:S4:38:VAL:HG23	83:S4:39:ASN:N	2.27	0.50
86:S7:99:TYR:OH	87:S8:82:ASN:ND2	2.44	0.50
72:Qc:211:PHE:CD2	72:Qc:215:LEU:HD12	2.46	0.50
51:E4:318:VAL:HG21	51:E4:334:VAL:HG21	1.92	0.50
79:Qj:85:SER:O	79:Qj:87:ASN:N	2.44	0.50
82:S3:140:ASP:OD1	82:S3:141:ASP:N	2.40	0.50
16:6A:6:ASN:OD1	18:7A:115:ARG:NH2	2.45	0.50
19:7C:116:THR:HG21	43:C1:53:ALA:HB1	1.94	0.50
28:AB:109:MET:HE1	28:AB:117:ILE:HD12	1.92	0.50
68:N4:98:ASN:OD1	68:N4:142:TYR:N	2.44	0.50
70:QA:129:ILE:O	70:QA:133:SER:OG	2.23	0.50
14:5B:119:PRO:O	14:5B:134:ALA:O	2.29	0.50
52:E5:260:LYS:C	52:E5:284:VAL:O	2.54	0.50
69:N5:239:GLN:N	69:N5:240:PRO:CD	2.75	0.50
72:QC:308:ASN:ND2	76:QG:48:ASP:OD2	2.40	0.50
53:E6:120:ARG:NH1	85:S6:69:ASP:OD2	2.45	0.50
73:Qd:32:VAL:HG11	73:Qd:186:VAL:CG2	2.41	0.50
74:QE:175:GLU:N	74:QE:175:GLU:OE1	2.45	0.50
81:S2:19:PRO:HB3	86:S7:128:MET:HE1	1.94	0.50
6:4D:86:GLN:N	6:4D:87:PRO:HD2	2.27	0.50
58:EB:60:GLU:OE2	58:EB:72:ARG:NH1	2.45	0.50
76:QG:131:ALA:O	80:QK:47:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A1:39:ARG:NH2	26:A8:155:GLU:OE2	2.41	0.49
57:EA:4:GLN:NE2	97:EA:201:CDL:OA9	2.45	0.49
79:QJ:85:SER:O	79:QJ:87:ASN:N	2.44	0.49
12:4J:11:ASN:O	12:4J:15:GLY:N	2.45	0.49
38:B7:44:ARG:HA	38:B7:48:VAL:CG1	2.42	0.49
40:B9:70:SER:OG	55:E8:5:ARG:NH2	2.45	0.49
43:C1:33:GLY:HA3	101:C1:502:HEA:H201	1.93	0.49
43:C1:318:THR:O	43:C1:321:ILE:HG22	2.12	0.49
44:C2:57:GLU:O	44:C2:61:THR:HG23	2.12	0.49
49:E2:374:ARG:NH2	59:EC:76:VAL:O	2.45	0.49
85:S6:127:PHE:N	85:S6:128:PRO:CD	2.76	0.49
43:C1:368:LEU:CB	101:C1:501:HEA:HMA	2.42	0.49
72:Qc:11:SER:OG	77:Qh:2:GLU:OE2	2.29	0.49
2:1B:4:GLY:O	2:1B:9:ARG:NH1	2.46	0.49
100:AC:201:ZMP:H9A	40:B9:89:LEU:HB3	1.95	0.49
36:B5:116:LYS:N	46:C4:24:ASP:OD2	2.45	0.49
75:Qf:16:LYS:NZ	75:Qf:20:GLU:OE2	2.46	0.49
18:7A:170:THR:HG22	43:C1:129:MET:HG2	1.94	0.49
26:A8:1:MET:HE3	66:N2:90:THR:OG1	2.12	0.49
39:B8:63:ASN:ND2	39:B8:65:THR:OG1	2.43	0.49
61:FX:188:MET:O	61:FX:221:ASN:O	2.31	0.49
81:S2:208:GLY:O	81:S2:261:ARG:NH2	2.38	0.49
1:1A:344:LEU:HD23	24:A6:363:VAL:HG13	1.95	0.49
44:C2:56:ILE:HG12	104:C2:201:PX2:H14	1.93	0.49
52:E5:7:TRP:HB2	52:E5:96:TYR:HB3	1.95	0.49
54:E7:212:LEU:O	54:E7:215:THR:OG1	2.25	0.49
71:Qb:68:LEU:O	71:Qb:245:THR:O	2.31	0.49
71:Qb:387:SER:OG	71:Qb:390:ASP:OD1	2.30	0.49
86:S7:79:PRO:HD3	86:S7:106:THR:HG23	1.93	0.49
97:A9:504:CDL:OB4	53:E6:303:TRP:NE1	2.40	0.49
49:E2:424:ASP:OD1	49:E2:425:ASP:N	2.45	0.49
50:E3:248:ASN:ND2	52:E5:212:GLU:O	2.46	0.49
68:N4:264:ILE:HG22	68:N4:265:TYR:N	2.28	0.49
70:QA:1:MET:HE2	70:QA:3:THR:HB	1.95	0.49
76:Qg:2:ASN:ND2	80:Qk:32:THR:OG1	2.45	0.49
46:C4:2:ASP:OD1	46:C4:3:ARG:N	2.46	0.49
72:Qc:196:THR:OG1	106:Qc:403:HEM:O1D	2.22	0.49
27:A9:183:THR:OG1	86:S7:32:ARG:NH2	2.46	0.49
21:A2:178:SER:O	21:A2:183:GLN:NE2	2.46	0.48
33:B2:112:GLU:OE1	39:B8:158:ARG:NH1	2.45	0.48
38:B7:67:CYS:SG	38:B7:71:ARG:NH1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:C2:80:TYR:O	44:C2:84:ILE:HG23	2.13	0.48
55:E8:26:THR:N	55:E8:27:PRO:CD	2.75	0.48
61:FX:212:LEU:HD13	61:FX:222:SER:HB3	1.95	0.48
75:Qf:44:GLU:OE1	75:Qf:44:GLU:N	2.47	0.48
74:QE:101:GLY:HA3	104:QJ:201:PX2:H48	1.95	0.48
76:Qg:198:GLU:O	80:Qk:31:ALA:N	2.47	0.48
89:V2:104:THR:HG22	89:V2:105:THR:H	1.78	0.48
1:1A:44:VAL:HG21	1:1A:57:TYR:HB2	1.95	0.48
26:A8:29:LYS:NZ	26:A8:33:GLU:OE2	2.43	0.48
43:C1:79:PHE:CE1	101:C1:502:HEA:H202	2.49	0.48
47:DC:154:ARG:O	47:DC:155:LYS:HB2	2.12	0.48
10:4H:155:GLU:OE1	10:4H:155:GLU:N	2.47	0.48
64:G3:239:THR:OG1	67:N6:161:LYS:NZ	2.47	0.48
65:N1:413:ASP:OD1	86:S7:76:SER:OG	2.25	0.48
71:QB:185:THR:HG21	71:QB:213:PHE:CE1	2.49	0.48
74:QE:129:ILE:HG21	74:QE:244:LEU:HB2	1.95	0.48
89:V2:20:ASP:OD1	89:V2:26:TYR:OH	2.30	0.48
30:AL:156:ASP:OD2	86:S7:190:TYR:OH	2.28	0.48
33:B2:103:GLU:OE2	38:B7:97:ARG:NH2	2.41	0.48
78:QI:1:MET:HE3	78:QI:1:MET:C	2.39	0.48
75:Qf:12:GLU:N	75:Qf:12:GLU:OE1	2.43	0.48
16:6A:41:LEU:O	16:6A:45:THR:OG1	2.31	0.48
66:N2:5:ASN:OD1	66:N2:6:ASN:ND2	2.47	0.48
88:V1:213:LEU:O	88:V1:213:LEU:HD23	2.13	0.48
1:1A:220:ASP:H	88:V1:381:ASN:ND2	2.12	0.48
14:5B:125:CYS:O	14:5B:129:GLY:N	2.40	0.48
36:B5:101:GLN:NE2	97:C4:203:CDL:OA9	2.47	0.48
64:G3:107:LEU:O	64:G3:110:ARG:NH1	2.46	0.48
88:V1:47:ASP:OD2	89:V2:207:ARG:NH2	2.42	0.48
4:4A:149:LEU:HD22	43:C1:229:SER:OG	2.14	0.48
11:4I:150:VAL:O	14:5B:97:THR:HA	2.14	0.48
43:C1:155:ILE:N	43:C1:155:ILE:HD12	2.28	0.48
61:FX:256:PHE:HB3	61:FX:282:PRO:HB3	1.96	0.48
81:S2:210:MET:SD	81:S2:214:ARG:NH1	2.87	0.48
6:4D:105:ASP:O	6:4D:106:SER:OG	2.22	0.48
66:N2:175:TYR:OH	66:N2:247:THR:HG21	2.14	0.48
75:QF:14:LYS:NZ	75:QF:18:GLU:OE2	2.44	0.48
76:Qg:116:THR:HG22	76:Qg:117:PRO:HD2	1.96	0.48
76:Qg:182:LEU:HD11	76:Qg:189:LEU:CD1	2.44	0.48
88:V1:21:GLN:NE2	88:V1:345:ASP:O	2.47	0.48
9:4G:265:CYS:O	9:4G:293:LYS:NZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:4H:166:PRO:O	10:4H:171:LYS:NZ	2.47	0.47
19:7C:112:HIS:O	19:7C:116:THR:HG23	2.14	0.47
21:A2:27:GLU:HA	21:A2:30:ALA:HB3	1.95	0.47
73:QD:240:PHE:HZ	76:QG:170:VAL:HG11	1.79	0.47
72:Qc:317:LEU:HD22	77:Qh:62:VAL:HG21	1.95	0.47
6:4D:102:ASP:OD1	17:6B:43:ARG:NH1	2.43	0.47
35:B4:104:ARG:NH2	39:B8:72:ASP:OD2	2.47	0.47
72:Qc:190:LEU:HD22	106:Qc:403:HEM:HAA1	1.95	0.47
85:S6:115:CYS:O	85:S6:119:GLU:HA	2.14	0.47
88:V1:319:ILE:HG12	88:V1:327:VAL:HG12	1.96	0.47
23:A5:38:LYS:NZ	62:G1:388:ASP:O	2.47	0.47
62:G1:251:ASP:N	62:G1:251:ASP:OD1	2.47	0.47
72:QC:121:TYR:HA	106:QC:401:HEM:HAD2	1.97	0.47
70:Qa:245:ARG:NH1	74:Qe:71:LYS:O	2.42	0.47
68:N4:420:CYS:SG	69:N5:180:VAL:HG22	2.54	0.47
77:Qh:57:THR:HG21	80:Qk:54:TRP:NE1	2.27	0.47
27:A9:18:LEU:O	27:A9:50:LYS:NZ	2.45	0.47
100:AC:201:ZMP:H25A	40:B9:100:ARG:HD2	1.97	0.47
51:E4:212:PHE:O	51:E4:215:THR:HG23	2.15	0.47
72:QC:124:VAL:O	72:QC:126:GLY:N	2.43	0.47
82:S3:182:ASP:OD1	82:S3:183:TYR:N	2.48	0.47
61:FX:212:LEU:CD1	61:FX:222:SER:HB3	2.44	0.47
67:N6:147:ILE:O	67:N6:150:MET:HG3	2.14	0.47
73:QD:207:LYS:HD3	104:QJ:201:PX2:H31	1.96	0.47
10:4H:82:ARG:NH1	14:5B:69:ASP:OD1	2.43	0.47
26:A8:124:GLU:OE1	26:A8:124:GLU:N	2.42	0.47
31:AM:141:VAL:O	31:AM:146:ARG:NH1	2.48	0.47
49:E2:320:HIS:O	49:E2:321:HIS:CG	2.68	0.47
55:E8:123:LEU:O	55:E8:128:LYS:NZ	2.48	0.47
75:QF:44:GLU:N	75:QF:44:GLU:OE1	2.48	0.47
79:Qj:102:GLU:O	79:Qj:106:ASN:N	2.46	0.47
88:V1:36:ASP:OD2	89:V2:210:LEU:N	2.41	0.47
2:1B:206:GLU:OE1	2:1B:482:ARG:NH1	2.43	0.47
6:4D:14:ARG:NH1	14:5B:106:ASP:OD1	2.45	0.47
27:A9:463:ASP:OD1	27:A9:464:TYR:N	2.44	0.47
41:BL:128:ASN:O	41:BL:131:LYS:NZ	2.47	0.47
69:N5:329:ASP:OD2	69:N5:335:SER:OG	2.33	0.47
2:1B:274:ASP:OD1	2:1B:274:ASP:N	2.48	0.47
8:4F:5:ILE:N	8:4F:24:ASP:OD1	2.47	0.47
24:A6:99:LEU:HD22	24:A6:104:ALA:HB1	1.97	0.47
46:C4:71:ASP:O	46:C4:75:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:E5:41:ALA:HB3	52:E5:289:LEU:HB3	1.97	0.47
56:E9:1:MET:N	56:E9:32:THR:OG1	2.42	0.47
61:FX:190:ILE:HG21	61:FX:198:LEU:HD11	1.97	0.47
69:N5:393:LEU:HD11	69:N5:432:GLN:HG2	1.96	0.47
89:V2:175:GLU:O	89:V2:178:ILE:HG13	2.15	0.47
31:AM:54:VAL:HG13	97:E4:401:CDL:C53	2.45	0.47
44:C2:120:VAL:HG12	44:C2:122:GLN:H	1.80	0.47
59:EC:60:HIS:O	59:EC:64:VAL:HG23	2.15	0.47
61:FX:144:ASP:OD1	61:FX:148:ASN:N	2.39	0.47
104:QJ:202:PX2:H38	72:Qc:149:LYS:HB2	1.97	0.47
80:QK:65:GLN:OE1	80:QK:69:ARG:NH1	2.48	0.47
72:Qc:80:LEU:HD23	106:Qc:402:HEM:HBC1	1.97	0.47
100:AC:201:ZMP:H4	100:AC:201:ZMP:H1A	1.37	0.46
49:E2:7:PHE:O	83:S4:157:ARG:NH2	2.46	0.46
50:E3:375:GLU:OE1	50:E3:375:GLU:N	2.42	0.46
52:E5:8:ARG:HA	52:E5:63:VAL:HA	1.97	0.46
64:G3:98:GLU:OE1	64:G3:98:GLU:N	2.44	0.46
82:S3:264:ASP:OD2	83:S4:151:ARG:NH1	2.48	0.46
1:1A:342:LYS:NZ	1:1A:373:GLU:OE1	2.44	0.46
20:A1:49:TYR:OH	26:A8:83:ASN:ND2	2.48	0.46
62:G1:127:PHE:CD1	64:G3:219:GLU:HG2	2.50	0.46
70:QA:465:ASP:OD1	70:QA:465:ASP:N	2.47	0.46
88:V1:407:GLY:O	88:V1:410:VAL:N	2.48	0.46
9:4G:30:ARG:NH2	9:4G:162:TRP:O	2.46	0.46
53:E6:160:ASP:OD1	53:E6:160:ASP:N	2.48	0.46
66:N2:164:SER:OG	66:N2:217:ASN:OD1	2.33	0.46
76:QG:112:THR:O	76:QG:112:THR:HG22	2.16	0.46
81:S2:105:VAL:HG21	81:S2:242:VAL:HG22	1.97	0.46
10:4H:202:LYS:NZ	43:C1:495:LEU:O	2.44	0.46
32:AN:248:ILE:O	46:C4:154:ARG:NH2	2.42	0.46
68:N4:43:ILE:HG22	68:N4:75:ILE:HG23	1.96	0.46
72:Qc:341:LEU:HD11	77:Qh:69:ILE:HG22	1.96	0.46
73:Qd:15:PHE:O	73:Qd:16:GLN:HB2	2.14	0.46
81:S2:308:GLU:OE1	81:S2:308:GLU:N	2.45	0.46
87:S8:135:ARG:NH1	87:S8:137:ASP:OD2	2.40	0.46
15:5C:141:ASP:OD1	47:DC:36:ARG:NH2	2.40	0.46
23:A5:154:ASP:OD1	23:A5:157:ARG:NH1	2.49	0.46
26:A8:1:MET:HE1	66:N2:58:LEU:HD23	1.97	0.46
43:C1:173:SER:O	43:C1:204:SER:OG	2.33	0.46
48:E1:246:THR:O	48:E1:436:SER:OG	2.32	0.46
69:N5:82:ILE:HG23	69:N5:87:MET:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Qd:165:THR:O	73:Qd:179:VAL:CG2	2.63	0.46
25:A7:78:ARG:HB3	25:A7:79:PRO:HD3	1.98	0.46
70:Qa:56:ALA:O	70:Qa:108:THR:HG23	2.16	0.46
3:2B:54:THR:HG21	97:C4:203:CDL:H792	1.97	0.46
24:A6:175:GLU:OE2	24:A6:178:THR:OG1	2.34	0.46
26:A8:182:GLN:OE1	31:AM:91:ARG:NH2	2.49	0.46
36:B5:58:ARG:HE	94:B5:201:PC1:H111	1.80	0.46
71:Qb:69:ASP:OD1	71:Qb:145:ARG:NH2	2.48	0.46
71:Qb:308:TYR:OH	71:Qb:474:GLN:NE2	2.48	0.46
5:4C:47:PHE:HZ	44:C2:71:ILE:HD11	1.80	0.46
14:5B:35:ASP:HA	14:5B:42:GLN:HG3	1.96	0.46
34:B3:22:MET:HE1	34:B3:34:ARG:HD2	1.98	0.46
46:C4:43:ASP:O	46:C4:44:ALA:HB3	2.15	0.46
70:QA:13:THR:O	71:QB:156:LYS:NZ	2.47	0.46
71:QB:50:GLN:O	71:QB:51:GLU:C	2.58	0.46
81:S2:197:GLN:HB3	87:S8:55:GLU:HG2	1.98	0.46
7:4E:72:GLU:O	7:4E:76:LYS:N	2.49	0.46
69:N5:363:ILE:O	69:N5:363:ILE:HG22	2.15	0.46
31:AM:57:ARG:NH2	97:AM:202:CDL:OA2	2.49	0.46
52:E5:207:VAL:HG22	52:E5:211:ASP:OD2	2.15	0.46
69:N5:230:TRP:CD1	69:N5:235:GLN:HB2	2.51	0.46
23:A5:127:ASP:OD1	25:A7:78:ARG:NH2	2.42	0.45
66:N2:171:ILE:N	66:N2:172:PRO:CD	2.80	0.45
69:N5:503:ILE:HD12	69:N5:508:LEU:HD11	1.97	0.45
70:QA:292:ARG:NH2	71:QB:184:GLU:OE1	2.46	0.45
72:Qc:34:ILE:HD13	106:Qc:402:HEM:HAB	1.98	0.45
72:Qc:124:VAL:O	72:Qc:126:GLY:N	2.43	0.45
83:S4:65:VAL:O	83:S4:139:ASN:N	2.45	0.45
2:1B:463:GLU:N	2:1B:463:GLU:OE1	2.43	0.45
4:4A:44:GLU:OE2	14:5B:167:LYS:NZ	2.46	0.45
62:G1:304:ASP:N	62:G1:304:ASP:OD1	2.48	0.45
67:N3:228:ILE:O	67:N3:228:ILE:HG22	2.16	0.45
9:4G:150:TYR:HA	16:6A:1:MET:SD	2.56	0.45
31:AM:54:VAL:HG13	97:E4:401:CDL:H532	1.98	0.45
71:Qb:384:GLY:CA	71:Qb:448:VAL:HG21	2.47	0.45
2:1B:235:SER:OG	2:1B:240:SER:OG	1.99	0.45
25:A7:126:ARG:NH2	31:AM:38:GLY:O	2.49	0.45
34:B3:58:UNK:O	34:B3:59:UNK:C	2.65	0.45
39:B8:150:GLU:OE1	39:B8:150:GLU:N	2.45	0.45
40:B9:114:GLY:O	69:N5:161:ARG:NH2	2.49	0.45
44:C2:38:ARG:O	44:C2:42:ASN:ND2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:N4:330:ASN:HB2	69:N5:71:TYR:OH	2.16	0.45
68:N4:354:TYR:O	68:N4:358:ASN:N	2.48	0.45
76:QG:224:ASP:HB3	70:Qa:301:CYS:SG	2.56	0.45
73:Qd:240:PHE:HZ	76:Qg:170:VAL:HG11	1.81	0.45
7:4E:77:PHE:O	17:6B:132:ARG:NH2	2.46	0.45
11:4I:92:PRO:HG2	11:4I:268:HIS:CE1	2.52	0.45
43:C1:155:ILE:O	43:C1:159:LEU:HG	2.17	0.45
69:N5:260:THR:O	69:N5:263:THR:N	2.46	0.45
82:S3:73:THR:O	82:S3:74:ASN:HB2	2.17	0.45
21:A2:26:PRO:O	21:A2:27:GLU:HB3	2.16	0.45
50:E3:265:LYS:HZ2	50:E3:265:LYS:HB3	1.82	0.45
52:E5:283:THR:HG23	52:E5:283:THR:O	2.17	0.45
65:N1:569:ARG:HD2	65:N1:605:ILE:HD13	1.99	0.45
70:Qa:258:ASN:ND2	70:Qa:260:LEU:O	2.49	0.45
1:1A:45:THR:O	1:1A:112:PRO:O	2.35	0.45
1:1A:45:THR:O	1:1A:113:ASN:HA	2.17	0.45
35:B4:9:LEU:HD11	61:FX:253:THR:HG21	1.99	0.45
54:E7:88:LEU:O	54:E7:152:ARG:NH1	2.43	0.45
59:EC:78:ASP:O	59:EC:81:PHE:HB2	2.17	0.45
61:FX:189:VAL:HA	61:FX:221:ASN:HB2	1.98	0.45
86:S7:122:GLY:HA2	92:S7:301:SF4:S4	2.56	0.45
26:A8:75:ILE:N	26:A8:137:GLU:OE2	2.37	0.45
77:QH:2:GLU:O	77:QH:8:VAL:HG21	2.17	0.45
88:V1:123:PRO:O	89:V2:106:PRO:HG2	2.16	0.45
2:1B:84:ARG:NH2	2:1B:279:GLU:OE1	2.50	0.45
97:AM:202:CDL:HB4	87:S8:45:LEU:HB3	1.99	0.45
43:C1:203:THR:HG23	43:C1:255:VAL:HG13	1.99	0.45
61:FX:183:SER:HA	61:FX:212:LEU:HD21	1.99	0.45
69:N5:118:VAL:HG12	69:N5:122:MET:HE2	1.98	0.45
72:QC:309:ILE:HG23	77:QH:55:ILE:HG22	1.98	0.45
73:Qd:225:PHE:CE1	74:Qe:87:THR:HG21	2.52	0.45
18:7A:86:THR:HG22	18:7A:87:ASP:N	2.32	0.44
94:AM:204:PC1:O14	62:G1:426:TYR:OH	2.29	0.44
44:C2:109:SER:HB3	44:C2:120:VAL:HG11	2.00	0.44
47:DC:33:SER:O	47:DC:36:ARG:NH1	2.50	0.44
54:E7:178:SER:OG	54:E7:180:ASP:OD1	2.34	0.44
64:G3:160:VAL:HB	64:G3:176:VAL:O	2.17	0.44
64:G3:176:VAL:HB	64:G3:177:PRO:HD3	1.99	0.44
65:N1:380:SER:O	65:N1:383:THR:OG1	2.33	0.44
106:QC:402:HEM:CMB	106:QC:402:HEM:HBB2	2.47	0.44
76:QG:126:CYS:SG	76:QG:127:LEU:N	2.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
97:QH:101:CDL:OB7	97:QH:101:CDL:HB31	2.17	0.44
26:A8:1:MET:SD	66:N2:57:ILE:HG22	2.57	0.44
27:A9:420:ILE:HG23	27:A9:424:ILE:HD11	1.98	0.44
43:C1:411:PHE:C	43:C1:412:SER:HG	2.13	0.44
74:QE:129:ILE:HB	74:QE:183:TRP:CZ2	2.52	0.44
86:S7:85:ALA:O	86:S7:88:ALA:N	2.43	0.44
88:V1:291:GLU:CD	88:V1:304:HIS:HE2	2.21	0.44
24:A6:93:PHE:CE1	100:AB:201:ZMP:H9A	2.53	0.44
25:A7:46:ALA:HB1	87:S8:198:LYS:HE2	1.99	0.44
46:C4:78:THR:HG22	68:N4:59:ASN:HB3	1.99	0.44
61:FX:221:ASN:C	61:FX:223:ARG:N	2.75	0.44
62:G1:105:HIS:HE1	64:G3:241:ARG:HE	1.65	0.44
66:N2:186:MET:HE3	66:N2:282:TRP:CZ2	2.51	0.44
76:QG:29:LEU:HA	76:QG:30:PRO:C	2.43	0.44
78:QI:21:ILE:HB	78:QI:22:PRO:HD3	2.00	0.44
25:A7:29:ASP:OD1	51:E4:203:ARG:NH2	2.49	0.44
42:BM:51:SER:OG	42:BM:53:ASP:OD1	2.35	0.44
43:C1:455:ASP:OD1	47:DC:109:GLN:NE2	2.44	0.44
57:EA:74:VAL:HG21	66:N2:15:SER:HA	1.99	0.44
61:FX:221:ASN:C	61:FX:223:ARG:H	2.25	0.44
66:N2:5:ASN:OD1	66:N2:6:ASN:N	2.49	0.44
69:N5:315:THR:HG22	69:N5:349:LYS:HG2	2.00	0.44
69:N5:337:ILE:HD11	69:N5:491:TYR:CD1	2.52	0.44
72:QC:122:SER:HB3	72:QC:133:ILE:HD11	1.99	0.44
70:Qa:463:GLU:OE1	70:Qa:463:GLU:N	2.51	0.44
71:Qb:87:TYR:O	71:Qb:230:ARG:NH2	2.48	0.44
82:S3:112:MET:HE1	83:S4:118:MET:SD	2.57	0.44
88:V1:407:GLY:N	88:V1:408:PRO:HD2	2.33	0.44
1:1A:175:GLU:OE1	85:S6:106:ARG:N	2.48	0.44
10:4H:209:PRO:HG2	43:C1:494:TYR:CD2	2.52	0.44
55:E8:189:TRP:CZ3	94:E9:202:PC1:H141	2.52	0.44
57:EA:106:UNK:O	57:EA:107:UNK:CB	2.65	0.44
5:4C:36:MET:HB3	104:C2:201:PX2:H34	2.00	0.44
6:4D:28:ARG:H	11:4I:167:HIS:CE1	2.36	0.44
9:4G:243:ASN:ND2	15:5C:59:ASN:OD1	2.38	0.44
25:A7:65:ASP:O	25:A7:68:ARG:NH1	2.40	0.44
30:AL:114:LYS:NZ	87:S8:80:GLU:OE2	2.40	0.44
52:E5:39:GLN:H	52:E5:70:GLY:HA2	1.83	0.44
52:E5:261:VAL:HA	52:E5:285:HIS:HA	1.99	0.44
53:E6:254:LYS:NZ	86:S7:40:LEU:O	2.49	0.44
68:N4:114:PHE:HB2	68:N4:126:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:N5:325:ILE:HD11	69:N5:334:ILE:HG12	1.99	0.44
70:QA:61:GLU:HG2	70:QA:68:VAL:HG12	2.00	0.44
79:QJ:78:ARG:NH1	76:Qg:64:GLU:OE2	2.50	0.44
81:S2:293:ALA:O	81:S2:297:THR:OG1	2.36	0.44
88:V1:474:ASP:OD1	88:V1:475:TRP:N	2.50	0.44
3:2B:69:TYR:HA	3:2B:72:ILE:HG22	1.98	0.44
27:A9:488:PHE:HB2	27:A9:489:PRO:HD3	2.00	0.44
35:B4:33:LEU:HD21	35:B4:39:MET:HB2	2.00	0.44
43:C1:66:ASN:OD1	43:C1:134:SER:HB3	2.18	0.44
66:N2:57:ILE:HG23	66:N2:279:ILE:CD1	2.48	0.44
11:4I:75:TRP:O	11:4I:78:SER:OG	2.32	0.44
27:A9:93:LEU:HB3	83:S4:141:SER:HB3	2.00	0.44
27:A9:426:THR:HG22	27:A9:427:LYS:N	2.33	0.44
48:E1:418:VAL:HG22	48:E1:419:ALA:H	1.82	0.44
52:E5:41:ALA:H	52:E5:289:LEU:HB3	1.82	0.44
52:E5:275:GLU:O	52:E5:279:GLY:N	2.51	0.44
77:QH:57:THR:OG1	77:QH:58:PRO:HD3	2.18	0.44
81:S2:33:GLU:HB2	81:S2:41:ARG:HB3	2.00	0.44
88:V1:359:ASP:O	88:V1:362:THR:HG22	2.18	0.44
48:E1:36:SER:O	48:E1:40:ARG:HG2	2.17	0.44
49:E2:331:ARG:NH1	49:E2:401:PRO:O	2.49	0.44
58:EB:60:GLU:HG3	58:EB:68:VAL:HG11	1.99	0.44
61:FX:182:PHE:O	61:FX:212:LEU:HD23	2.18	0.44
69:N5:62:TYR:HB3	69:N5:82:ILE:HB	1.99	0.44
69:N5:170:LYS:HZ1	69:N5:540:ASP:CG	2.25	0.44
69:N5:176:ARG:NH1	69:N5:179:ASP:OD2	2.51	0.44
71:Qb:99:MET:HE3	71:Qb:230:ARG:HG2	2.00	0.44
71:Qb:124:ILE:CG2	71:Qb:141:VAL:CG2	2.96	0.44
2:1B:84:ARG:NH1	2:1B:85:PRO:O	2.51	0.43
2:1B:461:TYR:O	21:A2:23:ALA:O	2.35	0.43
3:2B:56:ILE:HD12	66:N2:257:PHE:CZ	2.53	0.43
7:4E:45:GLU:OE2	7:4E:49:ARG:NH2	2.51	0.43
11:4I:263:PHE:O	11:4I:266:ARG:CG	2.66	0.43
20:A1:116:SER:OG	20:A1:117:TRP:N	2.50	0.43
24:A6:99:LEU:HD21	83:S4:50:GLN:HG3	1.99	0.43
24:A6:221:LEU:HD23	24:A6:221:LEU:C	2.43	0.43
27:A9:146:PRO:HA	27:A9:178:VAL:O	2.18	0.43
48:E1:148:GLU:OE1	48:E1:148:GLU:N	2.43	0.43
48:E1:172:GLU:OE1	50:E3:183:LYS:NZ	2.50	0.43
50:E3:45:PRO:HB2	50:E3:70:SER:HB2	2.00	0.43
65:N1:381:LEU:HA	65:N1:384:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:N1:506:TYR:CD1	65:N1:506:TYR:C	2.95	0.43
79:QJ:100:GLN:O	79:QJ:103:THR:OG1	2.33	0.43
81:S2:105:VAL:HG21	81:S2:242:VAL:CG2	2.48	0.43
26:A8:128:MET:HE2	26:A8:132:TYR:HE2	1.82	0.43
27:A9:297:LEU:HD11	27:A9:397:TRP:CZ2	2.52	0.43
47:DC:51:ALA:O	47:DC:75:ARG:NH2	2.44	0.43
79:QJ:107:ARG:NH2	76:Qg:27:PHE:O	2.39	0.43
70:Qa:104:SER:OG	70:Qa:105:ARG:N	2.49	0.43
88:V1:487:ASP:O	88:V1:492:SER:HA	2.18	0.43
2:1B:84:ARG:NH1	2:1B:87:LYS:O	2.51	0.43
4:4A:91:ARG:NH1	18:7A:132:HIS:O	2.51	0.43
7:4E:25:LEU:HD21	45:C3:135:LEU:HB2	1.98	0.43
26:A8:1:MET:HE2	66:N2:195:ILE:CG2	2.49	0.43
26:A8:128:MET:HE1	31:AM:97:PRO:HB3	1.99	0.43
50:E3:45:PRO:HD3	50:E3:121:SER:HB2	2.01	0.43
74:QE:150:ARG:NH2	74:QE:156:GLU:OE2	2.49	0.43
70:Qa:476:LEU:HD21	78:Qi:17:ASN:H	1.82	0.43
71:Qb:132:VAL:HG11	71:Qb:417:ILE:HG22	2.00	0.43
14:5B:117:VAL:HG22	14:5B:118:PRO:HD2	2.01	0.43
43:C1:24:LEU:HB3	43:C1:112:PHE:CZ	2.54	0.43
79:QJ:148:TRP:CG	104:QJ:202:PX2:H3	2.53	0.43
10:4H:167:SER:HB3	10:4H:170:GLU:HG2	2.00	0.43
24:A6:189:ALA:HB2	53:E6:219:GLN:HG3	2.00	0.43
27:A9:115:ARG:NH1	83:S4:97:GLU:OE2	2.51	0.43
34:B3:24:HIS:NE2	97:B3:101:CDL:OA7	2.44	0.43
43:C1:64:TYR:OH	101:C1:502:HEA:O2A	2.33	0.43
43:C1:322:SER:OG	43:C1:366:LEU:HD13	2.19	0.43
69:N5:322:MET:O	69:N5:325:ILE:HG22	2.17	0.43
70:QA:285:GLN:O	70:QA:386:ARG:NH2	2.52	0.43
43:C1:87:PHE:C	43:C1:87:PHE:CD1	2.97	0.43
43:C1:386:HIS:O	43:C1:389:THR:HG22	2.19	0.43
47:DC:54:HIS:HD2	47:DC:56:TRP:H	1.66	0.43
52:E5:260:LYS:HB2	52:E5:284:VAL:H	1.82	0.43
63:G2:144:ALA:HB1	64:G3:125:ILE:HD13	2.01	0.43
67:N3:234:GLY:HA2	81:S2:11:GLN:HB2	2.01	0.43
70:Qa:10:LEU:O	79:Qj:94:ARG:NH1	2.51	0.43
71:Qb:76:GLN:HB2	71:Qb:413:GLN:HG3	2.00	0.43
71:Qb:99:MET:HE1	71:Qb:231:TRP:HB2	2.01	0.43
5:4C:118:ILE:HD12	17:6B:198:LEU:HD12	2.00	0.43
62:G1:133:ARG:NH2	62:G1:339:ASP:OD1	2.51	0.43
23:A5:130:ASP:O	23:A5:134:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A9:109:PRO:HG3	83:S4:60:ARG:HB3	2.01	0.43
27:A9:381:GLU:OE2	62:G1:28:ARG:NH1	2.46	0.43
41:BL:52:PRO:HG3	41:BL:58:TYR:CZ	2.53	0.43
67:N3:255:ILE:HA	67:N3:258:ILE:HG22	2.00	0.43
4:4A:230:ARG:NH2	17:6B:104:LEU:O	2.51	0.43
5:4C:43:SER:OG	15:5C:185:VAL:HG12	2.18	0.43
15:5C:177:ILE:HG21	104:C2:201:PX2:H15	2.01	0.43
43:C1:189:THR:OG1	43:C1:192:ASN:ND2	2.52	0.43
70:QA:62:THR:O	70:QA:64:LYS:N	2.51	0.43
11:4I:263:PHE:O	11:4I:266:ARG:HG2	2.19	0.43
19:7C:46:GLU:O	19:7C:50:THR:OG1	2.36	0.43
21:A2:102:GLN:O	27:A9:78:LYS:NZ	2.41	0.43
32:AN:240:ASP:OD1	32:AN:240:ASP:N	2.51	0.43
62:G1:112:GLY:HA3	66:N2:27:VAL:HG11	2.01	0.43
66:N2:50:ILE:HD12	66:N2:62:ILE:HG21	2.01	0.43
72:Qc:40:LEU:HD13	106:Qc:402:HEM:HBA1	2.01	0.43
73:Qd:166:ASP:OD1	73:Qd:167:ASP:N	2.52	0.43
76:Qg:33:ILE:HB	76:Qg:34:PRO:HA	2.01	0.43
77:Qh:57:THR:OG1	77:Qh:58:PRO:HD3	2.18	0.43
20:A1:51:HIS:NE2	31:AM:188:LEU:O	2.40	0.42
37:B6:77:ASP:OD2	60:ED:125:TYR:OH	2.29	0.42
43:C1:146:ARG:NE	43:C1:233:ASP:OD2	2.46	0.42
61:FX:209:LEU:CD2	61:FX:222:SER:O	2.67	0.42
68:N4:92:GLU:OE2	68:N4:100:ASN:ND2	2.50	0.42
69:N5:127:ASN:HD22	69:N5:150:ILE:HD12	1.84	0.42
77:QH:76:LEU:HD21	80:QK:88:PHE:HA	1.99	0.42
83:S4:162:ARG:NE	83:S4:164:GLU:OE1	2.51	0.42
9:4G:68:LYS:NZ	9:4G:280:GLU:O	2.49	0.42
40:B9:59:SER:OG	55:E8:12:ARG:NH1	2.52	0.42
51:E4:238:MET:O	51:E4:304:ARG:NH1	2.52	0.42
59:EC:20:PRO:O	59:EC:24:ASN:ND2	2.47	0.42
61:FX:220:ARG:C	61:FX:221:ASN:OD1	2.62	0.42
69:N5:393:LEU:HD13	69:N5:393:LEU:O	2.19	0.42
71:QB:441:ALA:HA	71:QB:444:VAL:HG22	2.00	0.42
72:QC:11:SER:OG	77:QH:2:GLU:OE2	2.35	0.42
73:Qd:224:ARG:HE	97:Qd:302:CDL:H112	1.84	0.42
1:1A:175:GLU:H	85:S6:85:HIS:CE1	2.37	0.42
54:E7:111:VAL:O	54:E7:153:ALA:N	2.52	0.42
61:FX:88:LYS:N	61:FX:89:PRO:HD2	2.35	0.42
70:QA:1:MET:SD	71:QB:165:ARG:NH1	2.92	0.42
70:QA:365:LEU:HD12	70:QA:462:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4D:148:ALA:HB3	17:6B:258:GLU:HG2	2.01	0.42
17:6B:58:ARG:NH2	45:C3:116:ASN:OD1	2.52	0.42
43:C1:368:LEU:C	101:C1:501:HEA:HMA	2.45	0.42
45:C3:87:PHE:CE2	45:C3:91:LEU:HD11	2.54	0.42
62:G1:113:ARG:O	62:G1:114:TRP:HB2	2.19	0.42
64:G3:98:GLU:O	64:G3:122:PRO:HA	2.20	0.42
65:N1:534:LEU:HD11	67:N3:260:PHE:CE1	2.54	0.42
65:N1:660:LEU:HB3	65:N1:661:PRO:HD3	2.01	0.42
71:QB:406:VAL:HG22	71:QB:429:PRO:HB2	2.02	0.42
76:QG:27:PHE:O	79:Qj:107:ARG:NH2	2.44	0.42
72:Qc:136:ILE:O	72:Qc:139:LEU:HB2	2.19	0.42
81:S2:70:ASP:OD1	81:S2:81:GLU:CG	2.67	0.42
85:S6:1:MET:SD	85:S6:1:MET:N	2.79	0.42
86:S7:123:THR:HA	86:S7:151:CYS:HB3	2.00	0.42
100:AC:201:ZMP:H19A	40:B9:39:VAL:HG11	2.01	0.42
69:N5:418:TYR:O	69:N5:418:TYR:CD1	2.73	0.42
71:QB:124:ILE:HG23	71:QB:141:VAL:HG22	2.00	0.42
76:QG:136:ASP:OD1	76:QG:136:ASP:N	2.50	0.42
74:Qe:80:ASN:CG	74:Qe:83:SER:HG	2.27	0.42
4:4A:151:PHE:CZ	4:4A:155:LEU:HD11	2.54	0.42
9:4G:199:VAL:O	9:4G:203:SER:OG	2.34	0.42
43:C1:235:ILE:O	43:C1:235:ILE:HG13	2.19	0.42
45:C3:20:ILE:HB	45:C3:21:PRO:HD3	2.01	0.42
49:E2:4:GLY:C	49:E2:5:THR:HG1	2.16	0.42
49:E2:417:GLU:OE1	49:E2:417:GLU:N	2.51	0.42
61:FX:224:PHE:O	61:FX:228:LEU:HD12	2.20	0.42
64:G3:127:SER:HB3	64:G3:128:PRO:HD2	2.01	0.42
68:N4:214:GLY:HA3	68:N4:254:HIS:CE1	2.55	0.42
67:N6:19:SER:O	67:N6:20:LEU:HB3	2.19	0.42
76:QG:77:ALA:O	76:QG:81:GLY:N	2.44	0.42
76:QG:82:ASN:OD1	76:QG:82:ASN:N	2.52	0.42
76:QG:182:LEU:HD11	76:QG:189:LEU:HD13	2.01	0.42
3:2B:63:ILE:C	3:2B:63:ILE:HD12	2.45	0.42
15:5C:198:THR:OG1	15:5C:202:SER:O	2.31	0.42
26:A8:1:MET:HB3	66:N2:57:ILE:HB	2.01	0.42
52:E5:41:ALA:H	52:E5:289:LEU:N	2.18	0.42
69:N5:431:SER:HA	69:N5:434:TYR:CE2	2.54	0.42
71:Qb:60:ASP:OD1	71:Qb:60:ASP:N	2.52	0.42
73:Qd:32:VAL:HG11	73:Qd:186:VAL:HG21	2.02	0.42
1:1A:163:ASP:OD1	1:1A:163:ASP:N	2.52	0.42
1:1A:182:ASN:OD1	1:1A:237:VAL:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4G:30:ARG:NH1	9:4G:167:GLU:OE1	2.53	0.42
26:A8:63:ILE:O	26:A8:95:SER:OG	2.24	0.42
30:AL:208:PHE:HB2	86:S7:16:SER:O	2.19	0.42
43:C1:284:TYR:HA	43:C1:287:ILE:HG22	2.01	0.42
49:E2:9:THR:HG22	49:E2:10:GLY:N	2.34	0.42
66:N2:122:ILE:HD13	66:N2:178:ILE:HG12	2.02	0.42
67:N3:213:GLU:O	67:N3:215:GLY:N	2.52	0.42
68:N4:37:ILE:O	68:N4:40:ILE:HG22	2.19	0.42
68:N4:404:LEU:HD21	68:N4:415:LEU:HD12	2.02	0.42
69:N5:311:VAL:O	69:N5:315:THR:HG23	2.20	0.42
73:QD:205:GLY:O	73:QD:209:ILE:HG12	2.19	0.42
71:Qb:245:THR:OG1	71:Qb:413:GLN:HG2	2.19	0.42
86:S7:139:MET:HE3	86:S7:143:CYS:HB2	2.01	0.42
2:1B:275:TYR:O	2:1B:279:GLU:HG2	2.19	0.42
4:4A:53:VAL:HG13	4:4A:58:GLU:HB2	2.02	0.42
11:4I:127:ARG:HH11	14:5B:115:THR:HG1	1.68	0.42
25:A7:34:HIS:O	81:S2:142:LYS:NZ	2.49	0.42
101:C1:501:HEA:CBA	101:C1:501:HEA:CHA	2.92	0.42
67:N3:206:LYS:NZ	82:S3:208:ASN:O	2.52	0.42
72:QC:107:ILE:HG21	72:QC:293:THR:HG22	2.01	0.42
73:QD:135:ARG:HG2	75:QF:56:TRP:CE2	2.55	0.42
70:Qa:393:LEU:HD21	71:Qb:125:ILE:CD1	2.50	0.42
81:S2:135:TRP:O	81:S2:138:GLU:HG3	2.20	0.42
88:V1:163:PHE:HB3	88:V1:166:GLU:HB2	2.01	0.42
24:A6:83:ASP:OD1	24:A6:86:ARG:NH1	2.53	0.42
38:B7:4:ASP:OD1	38:B7:4:ASP:N	2.53	0.42
44:C2:63:LEU:HB2	44:C2:64:PRO:HD3	2.01	0.42
62:G1:294:ARG:CB	62:G1:295:PRO:HD3	2.50	0.42
69:N5:39:SER:HB3	69:N5:40:PRO:HD3	2.01	0.42
70:Qa:8:SER:O	79:Qj:94:ARG:NH2	2.52	0.42
72:Qc:357:THR:O	72:Qc:357:THR:HG23	2.19	0.42
79:Qj:75:GLU:OE1	79:Qj:75:GLU:N	2.48	0.42
2:1B:432:VAL:HB	2:1B:433:PRO:HD3	2.02	0.41
4:4A:149:LEU:HD23	43:C1:231:ILE:HG21	2.02	0.41
6:4D:5:LEU:O	6:4D:9:GLY:N	2.51	0.41
15:5C:44:TYR:N	15:5C:45:PRO:CD	2.83	0.41
31:AM:54:VAL:HB	31:AM:58:THR:HB	2.02	0.41
39:B8:45:PRO:HB3	39:B8:62:TRP:CE2	2.55	0.41
40:B9:63:GLU:OE1	55:E8:22:TYR:OH	2.34	0.41
48:E1:437:ALA:HB2	48:E1:456:VAL:HG22	2.01	0.41
65:N1:626:PHE:O	65:N1:629:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:QC:193:VAL:O	72:QC:194:ASN:CB	2.67	0.41
72:QC:276:PRO:HG3	80:QK:83:VAL:HG11	2.02	0.41
72:Qc:317:LEU:CD2	77:Qh:62:VAL:HG21	2.49	0.41
85:S6:57:ARG:NH2	87:S8:127:ASP:OD1	2.53	0.41
9:4G:267:ASP:HB2	9:4G:270:ALA:HB3	2.02	0.41
18:7A:161:PHE:CD2	45:C3:42:ILE:HD12	2.55	0.41
44:C2:71:ILE:O	44:C2:75:SER:OG	2.35	0.41
50:E3:11:ARG:NH2	50:E3:26:GLU:OE2	2.46	0.41
69:N5:111:ASP:OD1	69:N5:112:LYS:N	2.53	0.41
71:QB:92:ASN:O	71:QB:93:ALA:C	2.63	0.41
72:Qc:220:VAL:HG21	97:Qc:405:CDL:H322	2.01	0.41
88:V1:120:GLU:O	88:V1:160:ARG:NH1	2.52	0.41
88:V1:209:GLU:OE1	88:V1:211:THR:N	2.54	0.41
88:V1:215:GLU:OE2	88:V1:225:ARG:NE	2.42	0.41
1:1A:195:CYS:C	1:1A:196:THR:HG1	2.20	0.41
17:6B:82:GLN:HA	17:6B:90:LEU:HD11	2.01	0.41
26:A8:128:MET:HE1	31:AM:97:PRO:CB	2.50	0.41
36:B5:44:ALA:HB3	36:B5:45:PRO:HD3	2.02	0.41
55:E8:148:LYS:C	55:E8:149:SER:HG	2.20	0.41
62:G1:278:VAL:HB	62:G1:294:ARG:O	2.20	0.41
66:N2:104:ILE:O	66:N2:108:ILE:HG12	2.20	0.41
68:N4:305:MET:HE1	68:N4:336:MET:SD	2.60	0.41
69:N5:250:THR:N	69:N5:251:PRO:HD2	2.35	0.41
72:QC:211:PHE:CD2	72:QC:215:LEU:HD12	2.54	0.41
70:Qa:435:GLU:OE1	70:Qa:435:GLU:N	2.53	0.41
76:Qg:29:LEU:HA	76:Qg:30:PRO:C	2.45	0.41
81:S2:243:TYR:N	81:S2:244:PRO:HD2	2.34	0.41
36:B5:93:TRP:O	46:C4:143:ARG:NH2	2.38	0.41
44:C2:120:VAL:HG12	44:C2:121:ASP:N	2.35	0.41
54:E7:228:ARG:HB3	54:E7:229:PRO:HD3	2.03	0.41
63:G2:114:VAL:O	63:G2:114:VAL:HG13	2.20	0.41
79:QJ:79:ARG:NE	76:Qg:64:GLU:OE1	2.37	0.41
72:Qc:44:TYR:OH	72:Qc:123:LEU:O	2.37	0.41
73:Qd:165:THR:OG1	73:Qd:168:MET:SD	2.77	0.41
11:4I:264:HIS:O	11:4I:268:HIS:CD2	2.73	0.41
13:4L:141:LEU:HD11	67:N6:150:MET:HE1	2.03	0.41
23:A5:123:GLU:OE2	82:S3:61:TYR:OH	2.20	0.41
40:B9:21:SER:H	40:B9:112:ASN:ND2	2.19	0.41
54:E7:12:LEU:HD21	54:E7:212:LEU:HA	2.00	0.41
68:N4:9:ARG:NH2	68:N4:70:TYR:OH	2.53	0.41
68:N4:265:TYR:HB2	68:N4:268:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:V1:114:VAL:O	88:V1:155:ALA:HA	2.20	0.41
89:V2:99:ILE:HB	89:V2:138:ILE:HD13	2.03	0.41
9:4G:157:ARG:CZ	16:6A:1:MET:HG2	2.51	0.41
54:E7:48:GLY:O	54:E7:172:ARG:NH1	2.48	0.41
54:E7:100:ARG:HG3	54:E7:111:VAL:HG22	2.02	0.41
55:E8:39:ASN:N	55:E8:40:PRO:CD	2.84	0.41
62:G1:184:ASN:O	62:G1:205:PRO:HA	2.18	0.41
62:G1:421:VAL:HG21	81:S2:206:LYS:HD3	2.02	0.41
63:G2:132:SER:HB3	63:G2:133:PRO:HD2	2.02	0.41
65:N1:402:ASN:ND2	97:N1:701:CDL:O1	2.52	0.41
70:QA:1:MET:N	76:Qg:163:ARG:O	2.53	0.41
71:QB:223:ASP:OD1	71:QB:226:LYS:HG2	2.21	0.41
72:Qc:354:ILE:HD12	76:Qg:34:PRO:O	2.20	0.41
88:V1:284:ASN:ND2	88:V1:306:GLY:O	2.54	0.41
7:4E:17:TRP:CZ2	7:4E:21:GLU:HG3	2.56	0.41
97:7C:201:CDL:OB7	97:7C:201:CDL:HB31	2.20	0.41
43:C1:81:MET:HB2	43:C1:82:PRO:HD3	2.03	0.41
43:C1:351:PHE:HA	43:C1:401:ILE:HD11	2.03	0.41
50:E3:156:LEU:HD13	50:E3:184:LEU:HD22	2.02	0.41
54:E7:67:TRP:CZ2	54:E7:239:LEU:HD11	2.55	0.41
61:FX:208:TYR:HB3	61:FX:224:PHE:CZ	2.55	0.41
105:N4:504:U10:H151	105:N4:504:U10:H18	2.02	0.41
70:Qa:171:PHE:O	70:Qa:177:GLY:HA3	2.21	0.41
73:Qd:179:VAL:HB	73:Qd:180:PRO:HD3	2.02	0.41
74:Qe:129:ILE:HB	74:Qe:183:TRP:CZ2	2.55	0.41
86:S7:118:ILE:HG13	86:S7:139:MET:SD	2.61	0.41
4:4A:226:ILE:HG23	4:4A:227:LEU:N	2.36	0.41
24:A6:365:ARG:HG2	50:E3:338:MET:HB3	2.02	0.41
30:AL:23:THR:O	30:AL:23:THR:HG22	2.19	0.41
43:C1:129:MET:HB2	43:C1:154:ASN:OD1	2.21	0.41
44:C2:144:SER:CB	44:C2:178:CYS:O	2.69	0.41
52:E5:96:TYR:HA	52:E5:289:LEU:CD2	2.51	0.41
54:E7:12:LEU:HD21	54:E7:212:LEU:CB	2.50	0.41
55:E8:156:ARG:NH1	55:E8:160:GLU:OE1	2.54	0.41
62:G1:169:TRP:O	62:G1:187:ALA:HA	2.21	0.41
63:G2:192:GLU:OE1	63:G2:192:GLU:N	2.42	0.41
63:G2:215:ASN:O	63:G2:219:ILE:HG12	2.21	0.41
66:N2:88:ILE:HG21	67:N6:143:LEU:HD21	2.01	0.41
68:N4:241:LEU:O	68:N4:242:LEU:C	2.63	0.41
69:N5:328:ILE:HD11	69:N5:411:GLY:HA2	2.02	0.41
69:N5:557:TYR:O	69:N5:561:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:N6:45:ILE:HG23	67:N6:79:SER:HB3	2.02	0.41
67:N6:46:ILE:HD12	67:N6:46:ILE:N	2.35	0.41
70:QA:339:TYR:O	70:QA:341:ASP:N	2.53	0.41
72:Qc:237:TYR:HB3	72:Qc:240:LEU:HB2	2.02	0.41
73:Qd:116:THR:HG22	73:Qd:126:ILE:HD12	2.03	0.41
76:Qg:196:HIS:CE1	80:Qk:45:TYR:HB3	2.56	0.41
7:4E:70:THR:OG1	7:4E:73:ASP:OD1	2.32	0.41
13:4L:79:GLY:N	13:4L:80:PRO:HD2	2.36	0.41
23:A5:143:LYS:NZ	23:A5:151:GLU:OE2	2.46	0.41
43:C1:180:ASN:CB	43:C1:201:ILE:HD11	2.51	0.41
43:C1:227:ILE:HG22	43:C1:227:ILE:O	2.21	0.41
44:C2:5:ASN:HB3	44:C2:8:ILE:HG22	2.03	0.41
49:E2:40:TYR:HA	49:E2:43:VAL:HG22	2.03	0.41
62:G1:228:GLY:HA2	62:G1:246:ALA:HB1	2.02	0.41
66:N2:166:ILE:HG13	66:N2:166:ILE:O	2.20	0.41
69:N5:12:ILE:HG22	69:N5:122:MET:HE1	2.02	0.41
73:QD:22:ASP:O	73:QD:23:TRP:HB2	2.21	0.41
70:Qa:181:LEU:HD11	71:Qb:343:PHE:CE2	2.56	0.41
70:Qa:473:SER:OG	70:Qa:476:LEU:O	2.39	0.41
76:Qg:83:TYR:O	76:Qg:84:SER:C	2.64	0.41
81:S2:107:PHE:CZ	81:S2:150:VAL:HG11	2.56	0.41
82:S3:149:THR:N	82:S3:150:PRO:HD2	2.36	0.41
11:4I:146:PHE:CG	14:5B:89:GLY:HA2	2.56	0.41
52:E5:41:ALA:H	52:E5:289:LEU:H	1.68	0.41
53:E6:35:LEU:O	53:E6:36:SER:OG	2.27	0.41
65:N1:375:VAL:HG23	65:N1:445:TYR:CE2	2.55	0.41
65:N1:579:SER:OG	65:N1:645:ARG:NH1	2.54	0.41
65:N1:648:TYR:CD1	65:N1:648:TYR:C	2.99	0.41
72:Qc:216:LEU:O	72:Qc:220:VAL:HG23	2.21	0.41
6:4D:7:ILE:HG13	10:4H:151:VAL:HG21	2.04	0.40
10:4H:32:TYR:CE1	10:4H:130:ILE:HD11	2.56	0.40
22:A3:28:GLN:O	87:S8:31:HIS:NE2	2.54	0.40
29:AC:89:LEU:HD13	55:E8:1:MET:SD	2.61	0.40
30:AL:195:TYR:N	30:AL:195:TYR:CD1	2.88	0.40
94:B5:202:PC1:H281	42:BM:59:VAL:HG12	2.02	0.40
43:C1:61:VAL:O	43:C1:61:VAL:HG12	2.21	0.40
43:C1:296:VAL:O	43:C1:299:HIS:CD2	2.74	0.40
101:C1:502:HEA:HBA2	101:C1:502:HEA:CMA	2.52	0.40
63:G2:172:LEU:HD12	63:G2:172:LEU:N	2.36	0.40
76:QG:82:ASN:O	76:QG:83:TYR:C	2.63	0.40
87:S8:31:HIS:HB3	87:S8:34:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:450:ASN:HA	2:1B:456:SER:OG	2.21	0.40
3:2B:49:TYR:CG	66:N2:281:ILE:HG13	2.57	0.40
27:A9:442:ARG:NH1	65:N1:429:ASN:O	2.55	0.40
44:C2:121:ASP:OD1	44:C2:122:GLN:N	2.54	0.40
52:E5:279:GLY:N	52:E5:280:PRO:CD	2.84	0.40
65:N1:386:GLU:OE2	65:N1:640:ARG:NH1	2.54	0.40
68:N4:284:ASN:O	68:N4:287:ILE:HG22	2.21	0.40
68:N4:292:ASP:OD1	68:N4:293:THR:N	2.54	0.40
68:N4:317:ILE:HG13	68:N4:318:SER:N	2.36	0.40
77:Qh:34:ARG:O	77:Qh:35:GLY:C	2.64	0.40
88:V1:116:ILE:HG21	88:V1:139:LEU:HD11	2.03	0.40
1:1A:184:LEU:HD22	1:1A:321:GLU:HG3	2.04	0.40
24:A6:189:ALA:CB	53:E6:219:GLN:HG3	2.51	0.40
25:A7:45:PRO:HB2	81:S2:171:TYR:HD2	1.85	0.40
31:AM:54:VAL:HG12	97:AM:201:CDL:HA31	2.04	0.40
36:B5:35:LEU:HD22	94:B5:202:PC1:O32	2.21	0.40
58:EB:90:ASP:OD1	58:EB:90:ASP:N	2.54	0.40
59:EC:78:ASP:OD1	59:EC:78:ASP:N	2.53	0.40
72:QC:310:LEU:O	72:QC:314:LEU:HG	2.21	0.40
72:Qc:107:ILE:HG21	72:Qc:293:THR:HG22	2.03	0.40
82:S3:265:ASP:OD1	82:S3:266:PRO:HD2	2.21	0.40
14:5B:68:VAL:HG23	14:5B:68:VAL:O	2.21	0.40
24:A6:281:VAL:O	24:A6:284:THR:HG22	2.21	0.40
32:AN:258:PRO:HG2	36:B5:91:ILE:HG21	2.03	0.40
35:B4:80:ASN:O	35:B4:82:VAL:HG23	2.21	0.40
43:C1:37:TYR:CE1	43:C1:475:THR:HG21	2.56	0.40
43:C1:131:LYS:N	43:C1:132:PRO:HD3	2.37	0.40
43:C1:175:ASN:O	43:C1:179:THR:HG22	2.21	0.40
43:C1:246:TRP:O	43:C1:297:TRP:HB2	2.21	0.40
101:C1:501:HEA:HHB	101:C1:501:HEA:HMB1	1.85	0.40
55:E8:57:GLU:O	55:E8:58:PHE:CD1	2.74	0.40
57:EA:69:THR:OG1	66:N2:43:ASN:OD1	2.37	0.40
65:N1:433:ILE:HG13	65:N1:589:TYR:CZ	2.57	0.40
68:N4:9:ARG:HB2	68:N4:38:ILE:HG21	2.04	0.40
68:N4:73:ILE:HD12	68:N4:73:ILE:N	2.35	0.40
71:QB:296:ASP:OD1	77:QH:19:LYS:NZ	2.55	0.40
79:QJ:113:VAL:HG12	79:QJ:114:LYS:H	1.86	0.40
70:Qa:65:ASN:O	70:Qa:68:VAL:N	2.51	0.40
26:A8:102:ARG:HA	26:A8:128:MET:HE3	2.03	0.40
35:B4:89:GLN:NE2	35:B4:91:ARG:O	2.53	0.40
43:C1:103:SER:O	43:C1:175:ASN:OD1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:C2:60:TRP:C	44:C2:60:TRP:CD1	2.99	0.40
48:E1:418:VAL:HG13	48:E1:419:ALA:N	2.36	0.40
49:E2:209:VAL:HG23	49:E2:210:ASP:OD1	2.21	0.40
76:Qg:84:SER:O	76:Qg:85:GLU:C	2.65	0.40
89:V2:178:ILE:HA	89:V2:181:VAL:HG22	2.02	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	1A	350/385 (91%)	333 (95%)	17 (5%)	0	100	100
2	1B	523/527 (99%)	509 (97%)	14 (3%)	0	100	100
3	2B	112/142 (79%)	102 (91%)	10 (9%)	0	100	100
4	4A	202/246 (82%)	197 (98%)	5 (2%)	0	100	100
5	4C	121/139 (87%)	119 (98%)	2 (2%)	0	100	100
6	4D	171/174 (98%)	165 (96%)	6 (4%)	0	100	100
7	4E	158/165 (96%)	155 (98%)	3 (2%)	0	100	100
8	4F	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
9	4G	295/315 (94%)	288 (98%)	7 (2%)	0	100	100
10	4H	203/221 (92%)	195 (96%)	8 (4%)	0	100	100
11	4I	263/274 (96%)	256 (97%)	7 (3%)	0	100	100
12	4J	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
13	4L	106/171 (62%)	105 (99%)	1 (1%)	0	100	100
14	5B	155/174 (89%)	152 (98%)	3 (2%)	0	100	100
15	5C	194/208 (93%)	187 (96%)	7 (4%)	0	100	100
16	6A	89/112 (80%)	82 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	6B	280/287 (98%)	276 (99%)	4 (1%)	0	100	100
18	7A	161/178 (90%)	158 (98%)	3 (2%)	0	100	100
19	7C	149/171 (87%)	146 (98%)	3 (2%)	0	100	100
20	A1	135/141 (96%)	126 (93%)	9 (7%)	0	100	100
21	A2	190/193 (98%)	187 (98%)	3 (2%)	0	100	100
22	A3	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
23	A5	152/184 (83%)	147 (97%)	5 (3%)	0	100	100
24	A6	421/437 (96%)	396 (94%)	25 (6%)	0	100	100
25	A7	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
26	A8	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
27	A9	482/489 (99%)	462 (96%)	20 (4%)	0	100	100
28	AB	86/134 (64%)	86 (100%)	0	0	100	100
29	AC	90/134 (67%)	90 (100%)	0	0	100	100
30	AL	263/281 (94%)	249 (95%)	14 (5%)	0	100	100
31	AM	182/198 (92%)	178 (98%)	4 (2%)	0	100	100
32	AN	285/287 (99%)	279 (98%)	6 (2%)	0	100	100
33	B2	103/145 (71%)	103 (100%)	0	0	100	100
34	B3	32/62 (52%)	30 (94%)	2 (6%)	0	100	100
35	B4	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
36	B5	132/140 (94%)	130 (98%)	2 (2%)	0	100	100
37	B6	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
38	B7	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
39	B8	145/176 (82%)	142 (98%)	3 (2%)	0	100	100
40	B9	149/158 (94%)	143 (96%)	6 (4%)	0	100	100
41	BL	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
42	BM	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
43	C1	493/495 (100%)	474 (96%)	19 (4%)	0	100	100
44	C2	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
45	C3	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
46	C4	181/185 (98%)	175 (97%)	6 (3%)	0	100	100
47	DC	165/179 (92%)	156 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	E1	448/483 (93%)	431 (96%)	17 (4%)	0	100	100
49	E2	464/472 (98%)	447 (96%)	17 (4%)	0	100	100
50	E3	430/594 (72%)	419 (97%)	11 (3%)	0	100	100
51	E4	349/368 (95%)	339 (97%)	10 (3%)	0	100	100
52	E5	266/290 (92%)	246 (92%)	19 (7%)	1 (0%)	30	58
53	E6	340/371 (92%)	336 (99%)	4 (1%)	0	100	100
54	E7	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
55	E8	203/205 (99%)	190 (94%)	13 (6%)	0	100	100
56	E9	163/178 (92%)	149 (91%)	14 (9%)	0	100	100
57	EA	96/126 (76%)	91 (95%)	5 (5%)	0	100	100
58	EB	73/101 (72%)	73 (100%)	0	0	100	100
59	EC	83/101 (82%)	77 (93%)	6 (7%)	0	100	100
60	ED	136/151 (90%)	132 (97%)	4 (3%)	0	100	100
61	FX	235/325 (72%)	224 (95%)	11 (5%)	0	100	100
62	G1	424/436 (97%)	408 (96%)	16 (4%)	0	100	100
63	G2	234/267 (88%)	221 (94%)	13 (6%)	0	100	100
64	G3	253/261 (97%)	238 (94%)	15 (6%)	0	100	100
65	N1	308/670 (46%)	292 (95%)	16 (5%)	0	100	100
66	N2	294/300 (98%)	274 (93%)	20 (7%)	0	100	100
67	N3	119/293 (41%)	116 (98%)	2 (2%)	1 (1%)	16	41
67	N6	152/293 (52%)	145 (95%)	7 (5%)	0	100	100
68	N4	476/478 (100%)	462 (97%)	14 (3%)	0	100	100
69	N5	582/584 (100%)	560 (96%)	22 (4%)	0	100	100
70	QA	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
70	Qa	476/479 (99%)	462 (97%)	14 (3%)	0	100	100
71	QB	453/474 (96%)	443 (98%)	10 (2%)	0	100	100
71	Qb	421/474 (89%)	410 (97%)	11 (3%)	0	100	100
72	QC	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
72	Qc	362/368 (98%)	353 (98%)	9 (2%)	0	100	100
73	QD	239/243 (98%)	224 (94%)	15 (6%)	0	100	100
73	Qd	239/243 (98%)	215 (90%)	24 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	QE	229/252 (91%)	218 (95%)	11 (5%)	0	100	100
74	Qe	229/252 (91%)	215 (94%)	14 (6%)	0	100	100
75	QF	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
75	Qf	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
76	QG	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
76	Qg	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
77	QH	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
77	Qh	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
78	QI	28/70 (40%)	28 (100%)	0	0	100	100
78	Qi	28/70 (40%)	28 (100%)	0	0	100	100
79	QJ	147/154 (96%)	143 (97%)	4 (3%)	0	100	100
79	Qj	147/154 (96%)	138 (94%)	9 (6%)	0	100	100
80	QK	59/100 (59%)	58 (98%)	1 (2%)	0	100	100
80	Qk	59/100 (59%)	58 (98%)	1 (2%)	0	100	100
81	S2	391/395 (99%)	373 (95%)	18 (5%)	0	100	100
82	S3	246/277 (89%)	235 (96%)	11 (4%)	0	100	100
83	S4	188/208 (90%)	179 (95%)	9 (5%)	0	100	100
84	S5	110/122 (90%)	105 (96%)	5 (4%)	0	100	100
85	S6	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
86	S7	195/207 (94%)	187 (96%)	8 (4%)	0	100	100
87	S8	180/212 (85%)	174 (97%)	6 (3%)	0	100	100
88	V1	502/526 (95%)	477 (95%)	25 (5%)	0	100	100
89	V2	220/225 (98%)	212 (96%)	8 (4%)	0	100	100
All	All	22046/24488 (90%)	21217 (96%)	827 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
52	E5	288	THR
67	N3	214	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	310/340 (91%)	308 (99%)	2 (1%)	78	92
2	1B	453/454 (100%)	453 (100%)	0	100	100
3	2B	109/111 (98%)	108 (99%)	1 (1%)	70	89
4	4A	173/207 (84%)	173 (100%)	0	100	100
5	4C	112/127 (88%)	112 (100%)	0	100	100
6	4D	146/147 (99%)	143 (98%)	3 (2%)	47	78
7	4E	142/145 (98%)	141 (99%)	1 (1%)	76	91
8	4F	62/62 (100%)	61 (98%)	1 (2%)	55	82
9	4G	247/264 (94%)	244 (99%)	3 (1%)	63	86
10	4H	176/189 (93%)	175 (99%)	1 (1%)	78	92
11	4I	230/238 (97%)	228 (99%)	2 (1%)	70	89
12	4J	75/75 (100%)	74 (99%)	1 (1%)	61	85
13	4L	96/151 (64%)	96 (100%)	0	100	100
14	5B	134/148 (90%)	132 (98%)	2 (2%)	57	83
15	5C	167/178 (94%)	166 (99%)	1 (1%)	78	92
16	6A	79/97 (81%)	79 (100%)	0	100	100
17	6B	238/243 (98%)	237 (100%)	1 (0%)	84	94
18	7A	138/150 (92%)	138 (100%)	0	100	100
19	7C	135/152 (89%)	134 (99%)	1 (1%)	76	91
20	A1	115/118 (98%)	114 (99%)	1 (1%)	70	89
21	A2	159/160 (99%)	159 (100%)	0	100	100
22	A3	104/104 (100%)	104 (100%)	0	100	100
23	A5	134/152 (88%)	131 (98%)	3 (2%)	45	77
24	A6	346/358 (97%)	346 (100%)	0	100	100
25	A7	119/119 (100%)	119 (100%)	0	100	100
26	A8	196/196 (100%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	A9	420/424 (99%)	418 (100%)	2 (0%)	81	93
28	AB	79/114 (69%)	78 (99%)	1 (1%)	61	85
29	AC	80/111 (72%)	79 (99%)	1 (1%)	61	85
30	AL	228/242 (94%)	225 (99%)	3 (1%)	61	85
31	AM	156/168 (93%)	156 (100%)	0	100	100
32	AN	241/241 (100%)	240 (100%)	1 (0%)	84	94
33	B2	97/131 (74%)	97 (100%)	0	100	100
34	B3	30/31 (97%)	30 (100%)	0	100	100
35	B4	144/144 (100%)	144 (100%)	0	100	100
36	B5	108/108 (100%)	108 (100%)	0	100	100
37	B6	82/82 (100%)	82 (100%)	0	100	100
38	B7	93/93 (100%)	92 (99%)	1 (1%)	65	86
39	B8	127/148 (86%)	126 (99%)	1 (1%)	73	90
40	B9	132/139 (95%)	130 (98%)	2 (2%)	57	83
41	BL	132/132 (100%)	132 (100%)	0	100	100
42	BM	93/93 (100%)	93 (100%)	0	100	100
43	C1	438/438 (100%)	434 (99%)	4 (1%)	70	89
44	C2	178/178 (100%)	176 (99%)	2 (1%)	65	86
45	C3	155/155 (100%)	153 (99%)	2 (1%)	61	85
46	C4	166/167 (99%)	164 (99%)	2 (1%)	63	86
47	DC	148/153 (97%)	146 (99%)	2 (1%)	59	84
48	E1	381/404 (94%)	379 (100%)	2 (0%)	81	93
49	E2	379/385 (98%)	378 (100%)	1 (0%)	86	95
50	E3	339/460 (74%)	337 (99%)	2 (1%)	78	92
51	E4	302/317 (95%)	300 (99%)	2 (1%)	76	91
52	E5	200/205 (98%)	198 (99%)	2 (1%)	68	88
53	E6	293/314 (93%)	289 (99%)	4 (1%)	59	84
54	E7	192/192 (100%)	188 (98%)	4 (2%)	47	78
55	E8	179/179 (100%)	178 (99%)	1 (1%)	78	92
56	E9	115/118 (98%)	115 (100%)	0	100	100
57	EA	84/86 (98%)	83 (99%)	1 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	EB	70/70 (100%)	68 (97%)	2 (3%)	37	71
59	EC	73/86 (85%)	73 (100%)	0	100	100
60	ED	121/133 (91%)	119 (98%)	2 (2%)	53	81
61	FX	212/276 (77%)	209 (99%)	3 (1%)	59	84
62	G1	356/365 (98%)	348 (98%)	8 (2%)	45	77
63	G2	192/214 (90%)	189 (98%)	3 (2%)	55	82
64	G3	202/202 (100%)	202 (100%)	0	100	100
65	N1	295/639 (46%)	294 (100%)	1 (0%)	86	95
66	N2	285/289 (99%)	283 (99%)	2 (1%)	76	91
67	N3	116/281 (41%)	115 (99%)	1 (1%)	70	89
67	N6	147/281 (52%)	146 (99%)	1 (1%)	76	91
68	N4	455/455 (100%)	449 (99%)	6 (1%)	61	85
69	N5	546/546 (100%)	537 (98%)	9 (2%)	55	82
70	QA	400/401 (100%)	398 (100%)	2 (0%)	81	93
70	Qa	400/401 (100%)	399 (100%)	1 (0%)	86	95
71	QB	369/386 (96%)	367 (100%)	2 (0%)	81	93
71	Qb	342/386 (89%)	341 (100%)	1 (0%)	86	95
72	QC	337/341 (99%)	335 (99%)	2 (1%)	78	92
72	Qc	337/341 (99%)	336 (100%)	1 (0%)	86	95
73	QD	206/207 (100%)	206 (100%)	0	100	100
73	Qd	206/207 (100%)	206 (100%)	0	100	100
74	QE	193/209 (92%)	190 (98%)	3 (2%)	55	82
74	Qe	193/209 (92%)	192 (100%)	1 (0%)	81	93
75	QF	58/63 (92%)	56 (97%)	2 (3%)	32	66
75	Qf	58/63 (92%)	55 (95%)	3 (5%)	21	51
76	QG	207/207 (100%)	205 (99%)	2 (1%)	68	88
76	Qg	207/207 (100%)	206 (100%)	1 (0%)	81	93
77	QH	71/71 (100%)	70 (99%)	1 (1%)	59	84
77	Qh	71/71 (100%)	71 (100%)	0	100	100
78	QI	27/27 (100%)	26 (96%)	1 (4%)	30	63
78	Qi	27/27 (100%)	27 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	QJ	124/128 (97%)	123 (99%)	1 (1%)	73	90
79	Qj	124/128 (97%)	124 (100%)	0	100	100
80	QK	50/82 (61%)	50 (100%)	0	100	100
80	Qk	50/82 (61%)	50 (100%)	0	100	100
81	S2	335/336 (100%)	332 (99%)	3 (1%)	70	89
82	S3	224/250 (90%)	222 (99%)	2 (1%)	70	89
83	S4	159/172 (92%)	156 (98%)	3 (2%)	50	79
84	S5	102/102 (100%)	102 (100%)	0	100	100
85	S6	130/130 (100%)	129 (99%)	1 (1%)	73	90
86	S7	165/171 (96%)	162 (98%)	3 (2%)	51	80
87	S8	160/187 (86%)	159 (99%)	1 (1%)	78	92
88	V1	412/427 (96%)	411 (100%)	1 (0%)	87	96
89	V2	190/190 (100%)	184 (97%)	6 (3%)	34	68
All	All	19190/20883 (92%)	19041 (99%)	149 (1%)	70	90

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	191	ARG
1	1A	356	ASP
3	2B	5	LEU
6	4D	81	ILE
6	4D	149	GLU
6	4D	170	VAL
7	4E	142	TRP
8	4F	63	ILE
9	4G	40	ARG
9	4G	112	GLN
9	4G	134	ASN
10	4H	95	GLU
11	4I	18	LEU
11	4I	266	ARG
12	4J	29	THR
14	5B	78	SER
14	5B	103	CYS
15	5C	130	TRP
17	6B	224	LYS

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Mol	Chain	Res	Type
19	7C	155	LEU
20	A1	37	HIS
23	A5	60	ASP
23	A5	82	GLU
23	A5	150	ASP
27	A9	180	TYR
27	A9	269	ASP
28	AB	91	SER
29	AC	91	SER
30	AL	122	VAL
30	AL	195	TYR
30	AL	229	LEU
32	AN	217	SER
38	B7	52	LEU
39	B8	107	LEU
40	B9	21	SER
40	B9	130	GLN
43	C1	139	LEU
43	C1	231	ILE
43	C1	253	VAL
43	C1	315	SER
44	C2	75	SER
44	C2	144	SER
45	C3	125	LEU
45	C3	135	LEU
46	C4	43	ASP
46	C4	145	LEU
47	DC	13	LEU
47	DC	42	GLU
48	E1	231	ASP
48	E1	235	LEU
49	E2	2	VAL
50	E3	50	ASP
50	E3	376	VAL
51	E4	142	GLN
51	E4	332	ASP
52	E5	36	LEU
52	E5	266	LEU
53	E6	86	HIS
53	E6	204	GLN
53	E6	286	ARG
53	E6	306	ARG

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Mol	Chain	Res	Type
54	E7	3	LEU
54	E7	63	ILE
54	E7	149	LEU
54	E7	169	THR
55	E8	1	MET
57	EA	69	THR
58	EB	61	GLN
58	EB	89	GLU
60	ED	61	GLU
60	ED	146	LYS
61	FX	172	ASP
61	FX	187	HIS
61	FX	321	LYS
62	G1	28	ARG
62	G1	35	SER
62	G1	37	GLU
62	G1	123	PHE
62	G1	251	ASP
62	G1	321	HIS
62	G1	326	GLU
62	G1	413	ASN
63	G2	71	GLN
63	G2	74	VAL
63	G2	108	ARG
65	N1	378	LEU
66	N2	84	ILE
66	N2	155	SER
67	N3	258	ILE
68	N4	23	LYS
68	N4	75	ILE
68	N4	123	ILE
68	N4	174	SER
68	N4	184	THR
68	N4	390	LEU
69	N5	85	TYR
69	N5	140	LEU
69	N5	260	THR
69	N5	367	ASP
69	N5	377	HIS
69	N5	393	LEU
69	N5	500	ILE
69	N5	533	HIS

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Mol	Chain	Res	Type
69	N5	540	ASP
67	N6	108	TYR
70	QA	71	PHE
70	QA	476	LEU
71	QB	283	GLU
71	QB	466	CYS
72	QC	329	CYS
72	QC	361	PHE
74	QE	168	LEU
74	QE	169	LYS
74	QE	192	HIS
75	QF	54	ARG
75	QF	72	LYS
76	QG	126	CYS
76	QG	228	ARG
77	QH	11	GLU
78	QI	2	LEU
79	QJ	135	LEU
70	Qa	71	PHE
71	Qb	319	LYS
72	Qc	17	SER
74	Qe	192	HIS
75	Qf	47	ASN
75	Qf	51	GLN
75	Qf	54	ARG
76	Qg	169	ARG
81	S2	33	GLU
81	S2	147	TYR
81	S2	357	ARG
82	S3	29	GLN
82	S3	119	ASP
83	S4	16	ILE
83	S4	47	GLN
83	S4	202	LYS
85	S6	1	MET
86	S7	86	CYS
86	S7	116	ASP
86	S7	123	THR
87	S8	138	LEU
88	V1	386	CYS
89	V2	108	MET
89	V2	120	CYS

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Mol	Chain	Res	Type
89	V2	133	ASP
89	V2	139	CYS
89	V2	152	MET
89	V2	156	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (420) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	73	ASN
1	1A	80	ASN
1	1A	82	ASN
1	1A	128	GLN
2	1B	36	ASN
2	1B	95	HIS
2	1B	139	GLN
2	1B	149	ASN
2	1B	237	HIS
2	1B	315	ASN
2	1B	332	ASN
2	1B	344	GLN
2	1B	347	HIS
2	1B	387	HIS
2	1B	500	HIS
2	1B	507	HIS
3	2B	4	ASN
3	2B	37	ASN
3	2B	66	ASN
3	2B	112	ASN
4	4A	43	HIS
4	4A	60	GLN
4	4A	62	HIS
4	4A	67	HIS
4	4A	93	GLN
4	4A	131	GLN
4	4A	137	HIS
4	4A	161	HIS
4	4A	196	HIS
4	4A	240	ASN
4	4A	242	GLN
6	4D	37	GLN
6	4D	64	HIS
6	4D	94	GLN

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Mol	Chain	Res	Type
6	4D	118	HIS
7	4E	68	ASN
7	4E	146	HIS
9	4G	22	ASN
9	4G	112	GLN
9	4G	276	HIS
10	4H	25	ASN
10	4H	55	GLN
10	4H	199	HIS
11	4I	62	HIS
11	4I	74	ASN
11	4I	142	HIS
11	4I	153	ASN
11	4I	167	HIS
11	4I	254	GLN
11	4I	260	HIS
11	4I	264	HIS
13	4L	106	HIS
13	4L	159	GLN
14	5B	43	ASN
14	5B	131	HIS
15	5C	22	GLN
15	5C	120	GLN
16	6A	18	ASN
16	6A	60	ASN
16	6A	68	ASN
17	6B	64	GLN
17	6B	71	ASN
17	6B	83	GLN
17	6B	101	HIS
17	6B	252	HIS
18	7A	15	HIS
18	7A	31	ASN
18	7A	101	ASN
18	7A	106	HIS
18	7A	109	HIS
18	7A	132	HIS
19	7C	112	HIS
19	7C	120	GLN
19	7C	134	GLN
20	A1	42	ASN
20	A1	47	ASN

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Mol	Chain	Res	Type
20	A1	55	ASN
20	A1	60	ASN
20	A1	108	GLN
20	A1	121	HIS
20	A1	132	HIS
21	A2	12	HIS
21	A2	75	GLN
21	A2	113	HIS
21	A2	115	HIS
21	A2	123	ASN
21	A2	180	HIS
22	A3	28	GLN
22	A3	58	HIS
24	A6	74	GLN
24	A6	88	ASN
24	A6	107	HIS
24	A6	134	ASN
24	A6	161	ASN
24	A6	180	ASN
24	A6	205	HIS
24	A6	282	ASN
24	A6	336	GLN
25	A7	17	HIS
25	A7	56	GLN
25	A7	84	ASN
25	A7	92	GLN
25	A7	124	GLN
26	A8	23	HIS
26	A8	27	GLN
26	A8	52	HIS
26	A8	54	HIS
26	A8	83	ASN
26	A8	96	GLN
26	A8	203	HIS
27	A9	79	GLN
27	A9	159	ASN
27	A9	165	GLN
27	A9	174	GLN
27	A9	190	GLN
27	A9	200	ASN
27	A9	211	GLN
27	A9	242	HIS

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Mol	Chain	Res	Type
27	A9	288	ASN
27	A9	394	HIS
28	AB	52	HIS
29	AC	110	HIS
30	AL	20	GLN
30	AL	39	GLN
30	AL	107	GLN
30	AL	133	GLN
30	AL	183	HIS
30	AL	201	HIS
30	AL	217	ASN
30	AL	219	HIS
31	AM	104	GLN
31	AM	172	GLN
32	AN	20	HIS
32	AN	152	ASN
32	AN	154	GLN
32	AN	175	ASN
34	B3	5	ASN
35	B4	50	GLN
35	B4	69	GLN
36	B5	98	HIS
36	B5	100	GLN
37	B6	16	HIS
37	B6	19	ASN
37	B6	62	GLN
38	B7	78	GLN
39	B8	61	HIS
39	B8	63	ASN
39	B8	90	HIS
39	B8	91	GLN
39	B8	113	ASN
39	B8	121	HIS
39	B8	156	GLN
39	B8	165	HIS
40	B9	20	GLN
40	B9	112	ASN
40	B9	130	GLN
41	BL	4	HIS
41	BL	54	GLN
41	BL	128	ASN
42	BM	71	GLN

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Mol	Chain	Res	Type
42	BM	99	GLN
43	C1	7	HIS
43	C1	18	HIS
43	C1	192	ASN
43	C1	299	HIS
43	C1	386	HIS
43	C1	423	HIS
43	C1	439	HIS
43	C1	466	HIS
44	C2	105	ASN
44	C2	163	ASN
44	C2	167	ASN
45	C3	106	HIS
45	C3	124	HIS
45	C3	130	ASN
46	C4	75	ASN
46	C4	76	GLN
46	C4	95	ASN
46	C4	169	HIS
47	DC	29	GLN
47	DC	54	HIS
48	E1	61	GLN
48	E1	105	GLN
48	E1	177	GLN
48	E1	192	GLN
48	E1	198	GLN
48	E1	204	ASN
48	E1	227	HIS
49	E2	18	HIS
49	E2	20	GLN
49	E2	58	ASN
49	E2	99	GLN
49	E2	153	HIS
49	E2	169	HIS
49	E2	219	HIS
49	E2	321	HIS
49	E2	344	GLN
50	E3	13	HIS
50	E3	20	GLN
50	E3	99	GLN
50	E3	106	ASN
50	E3	160	GLN

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Mol	Chain	Res	Type
50	E3	186	GLN
50	E3	244	HIS
50	E3	303	ASN
50	E3	313	HIS
50	E3	333	ASN
50	E3	334	HIS
51	E4	162	HIS
52	E5	255	ASN
53	E6	49	GLN
53	E6	57	ASN
53	E6	214	GLN
53	E6	219	GLN
53	E6	222	GLN
53	E6	335	ASN
54	E7	1	GLN
54	E7	83	GLN
54	E7	99	HIS
54	E7	106	HIS
54	E7	163	ASN
54	E7	209	GLN
55	E8	19	ASN
55	E8	67	HIS
55	E8	89	HIS
56	E9	33	HIS
57	EA	4	GLN
58	EB	78	GLN
58	EB	99	ASN
59	EC	97	HIS
60	ED	38	ASN
60	ED	139	HIS
61	FX	95	HIS
61	FX	124	HIS
61	FX	133	GLN
61	FX	150	HIS
61	FX	203	HIS
61	FX	324	GLN
62	G1	105	HIS
62	G1	117	ASN
62	G1	142	GLN
62	G1	150	GLN
62	G1	191	HIS
62	G1	235	ASN

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Mol	Chain	Res	Type
62	G1	321	HIS
62	G1	391	HIS
62	G1	404	GLN
62	G1	413	ASN
63	G2	36	HIS
63	G2	71	GLN
64	G3	26	GLN
64	G3	174	GLN
64	G3	206	HIS
64	G3	210	ASN
64	G3	243	HIS
65	N1	402	ASN
65	N1	409	GLN
65	N1	440	ASN
65	N1	476	HIS
65	N1	487	ASN
65	N1	530	ASN
65	N1	650	ASN
66	N2	4	ASN
66	N2	6	ASN
66	N2	23	GLN
66	N2	70	ASN
66	N2	76	ASN
66	N2	82	HIS
66	N2	89	ASN
66	N2	206	ASN
66	N2	208	ASN
66	N2	209	HIS
66	N2	210	ASN
67	N3	172	ASN
67	N3	219	ASN
67	N3	264	ASN
67	N3	292	ASN
68	N4	26	ASN
68	N4	54	ASN
68	N4	59	ASN
68	N4	112	ASN
68	N4	140	ASN
68	N4	157	ASN
68	N4	177	ASN
68	N4	209	ASN
68	N4	231	HIS

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Mol	Chain	Res	Type
68	N4	254	HIS
68	N4	267	ASN
68	N4	304	HIS
68	N4	322	ASN
68	N4	339	HIS
68	N4	358	ASN
68	N4	359	ASN
68	N4	385	ASN
68	N4	422	ASN
68	N4	475	HIS
69	N5	95	ASN
69	N5	101	ASN
69	N5	127	ASN
69	N5	159	ASN
69	N5	160	ASN
69	N5	175	ASN
69	N5	202	ASN
69	N5	279	ASN
69	N5	377	HIS
69	N5	520	ASN
69	N5	572	HIS
67	N6	56	ASN
70	QA	30	ASN
70	QA	70	HIS
70	QA	167	HIS
70	QA	255	ASN
70	QA	268	GLN
70	QA	327	ASN
70	QA	398	GLN
71	QB	89	ASN
71	QB	159	GLN
71	QB	199	HIS
71	QB	289	HIS
71	QB	321	HIS
71	QB	329	GLN
71	QB	405	ASN
72	QC	33	GLN
72	QC	56	HIS
72	QC	194	ASN
72	QC	203	ASN
72	QC	204	ASN
72	QC	356	ASN

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Mol	Chain	Res	Type
73	QD	19	GLN
73	QD	50	HIS
74	QE	215	HIS
74	QE	218	HIS
76	QG	21	GLN
76	QG	96	HIS
76	QG	196	HIS
76	QG	205	HIS
77	QH	36	ASN
78	QI	4	ASN
78	QI	15	GLN
79	QJ	30	HIS
79	QJ	116	HIS
70	Qa	29	GLN
70	Qa	30	ASN
70	Qa	66	ASN
70	Qa	70	HIS
70	Qa	132	ASN
70	Qa	167	HIS
70	Qa	285	GLN
70	Qa	317	GLN
70	Qa	333	ASN
70	Qa	359	HIS
70	Qa	378	ASN
70	Qa	390	GLN
70	Qa	398	GLN
71	Qb	133	ASN
71	Qb	195	GLN
71	Qb	199	HIS
71	Qb	218	ASN
71	Qb	239	ASN
71	Qb	289	HIS
71	Qb	321	HIS
71	Qb	329	GLN
71	Qb	394	HIS
71	Qb	405	ASN
71	Qb	413	GLN
71	Qb	474	GLN
72	Qc	33	GLN
72	Qc	56	HIS
72	Qc	73	HIS
72	Qc	194	ASN

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Mol	Chain	Res	Type
72	Qc	203	ASN
72	Qc	204	ASN
72	Qc	352	HIS
73	Qd	14	HIS
73	Qd	19	GLN
74	Qe	112	GLN
74	Qe	192	HIS
76	Qg	2	ASN
76	Qg	16	ASN
76	Qg	21	GLN
76	Qg	96	HIS
76	Qg	125	HIS
76	Qg	133	HIS
76	Qg	196	HIS
77	Qh	18	GLN
78	Qi	15	GLN
79	Qj	10	HIS
81	S2	45	HIS
81	S2	64	GLN
81	S2	158	ASN
81	S2	199	ASN
81	S2	278	GLN
81	S2	309	ASN
81	S2	313	HIS
81	S2	372	GLN
82	S3	99	GLN
82	S3	173	HIS
82	S3	208	ASN
83	S4	39	ASN
84	S5	75	GLN
85	S6	85	HIS
86	S7	27	GLN
86	S7	31	GLN
86	S7	50	HIS
86	S7	93	GLN
86	S7	159	HIS
86	S7	169	ASN
87	S8	70	GLN
87	S8	76	HIS
87	S8	82	ASN
87	S8	208	GLN
88	V1	48	HIS

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Mol	Chain	Res	Type
88	V1	381	ASN
88	V1	382	GLN
88	V1	442	HIS
88	V1	502	ASN
89	V2	98	HIS
89	V2	122	HIS
89	V2	149	HIS
89	V2	183	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
81	2MR	S2	154	81	10,12,13	2.46	2 (20%)	5,13,15	0.99	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
81	2MR	S2	154	81	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	S2	154	2MR	CZ-NH2	5.37	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	S2	154	2MR	CZ-NE	5.00	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	S2	154	2MR	CG-CD-NE-CZ
81	S2	154	2MR	N-CA-CB-CG

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 116 ligands modelled in this entry, 8 are monoatomic - leaving 108 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	$\# Z > 2$
97	CDL	E7	301	-	67,67,99	0.37	0	73,79,111	0.33	0
97	CDL	AM	202	-	71,71,99	0.35	0	77,83,111	0.32	0
97	CDL	7C	201	-	89,89,99	0.32	0	95,101,111	0.31	0
95	3PE	E9	201	-	50,50,50	0.30	0	53,55,55	0.28	0
94	PC1	7A	201	-	35,35,53	0.37	0	41,43,61	0.38	0
94	PC1	E8	302	-	53,53,53	0.29	0	59,61,61	0.31	0
97	CDL	N5	603	-	92,92,99	0.31	0	98,104,111	0.31	0
94	PC1	A9	503	-	32,32,53	0.38	0	38,40,61	0.38	0
97	CDL	C4	201	-	93,93,99	0.32	0	99,105,111	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	PC1	QI	101	-	35,35,53	0.36	0	41,43,61	0.42	0
94	PC1	AM	203	-	48,48,53	0.30	0	54,56,61	0.33	0
104	PX2	QJ	201	-	35,35,35	1.00	3 (8%)	38,40,40	1.08	2 (5%)
92	SF4	1A	403	1	0,12,12	-	-	-	-	-
94	PC1	B5	201	-	53,53,53	0.29	0	59,61,61	0.34	0
94	PC1	N1	703	-	39,39,53	0.33	0	45,47,61	0.31	0
94	PC1	B8	301	-	36,36,53	0.35	0	42,44,61	0.49	0
100	ZMP	AB	201	28	30,35,36	0.80	1 (3%)	34,42,45	1.21	5 (14%)
107	HEC	QD	301	73	46,50,50	1.92	7 (15%)	58,82,82	1.88	7 (12%)
97	CDL	EA	201	-	58,58,99	0.40	0	64,70,111	0.39	0
97	CDL	Qc	405	-	53,53,99	0.41	0	59,65,111	0.36	0
94	PC1	ED	202	-	40,40,53	0.33	0	46,48,61	0.34	0
91	FES	V2	301	89	0,4,4	-	-	-	-	-
94	PC1	G2	301	-	37,37,53	0.35	0	43,45,61	0.32	0
105	U10	N4	504	-	43,43,63	2.44	18 (41%)	54,55,79	1.87	15 (27%)
94	PC1	N1	702	-	48,48,53	0.30	0	54,56,61	0.30	0
97	CDL	QC	403	-	55,55,99	0.41	0	61,67,111	0.34	0
94	PC1	Qc	401	-	53,53,53	0.30	0	59,61,61	0.34	0
97	CDL	B3	101	-	64,64,99	0.38	0	70,76,111	0.33	0
94	PC1	C3	201	-	50,50,53	0.31	0	56,58,61	0.31	0
92	SF4	1A	402	1	0,12,12	-	-	-	-	-
95	3PE	N5	602	-	50,50,50	0.32	0	53,55,55	0.36	0
92	SF4	S7	301	86	0,12,12	-	-	-	-	-
97	CDL	EA	202	-	54,54,99	0.40	0	60,66,111	0.36	0
94	PC1	Qg	301	-	27,27,53	0.40	0	33,35,61	0.36	0
91	FES	Qe	301	74	0,4,4	-	-	-	-	-
106	HEM	QC	402	72	50,50,50	1.37	8 (16%)	67,82,82	1.65	13 (19%)
95	3PE	C1	507	-	39,39,50	0.35	0	42,44,55	0.39	0
100	ZMP	AC	201	29	30,35,36	0.86	1 (3%)	34,42,45	1.08	3 (8%)
94	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.33	0
97	CDL	BM	201	-	57,57,99	0.39	0	63,69,111	0.36	0
97	CDL	Qe	302	-	59,59,99	0.38	0	65,71,111	0.34	0
97	CDL	A9	504	-	63,63,99	0.39	0	69,75,111	0.35	0
108	FMN	V1	601	-	33,33,33	0.37	0	48,50,50	0.36	0
94	PC1	Qc	404	-	30,30,53	0.40	0	36,38,61	0.46	0
94	PC1	AL	301	-	49,49,53	0.31	0	55,57,61	0.31	0
106	HEM	QC	401	72	50,50,50	1.34	9 (18%)	67,82,82	1.64	11 (16%)
95	3PE	B4	201	-	39,39,50	0.34	0	42,44,55	0.36	0
97	CDL	B8	302	-	69,69,99	0.35	0	75,81,111	0.32	0
107	HEC	Qd	301	73	46,50,50	1.92	8 (17%)	58,82,82	1.79	6 (10%)
94	PC1	N4	502	-	32,32,53	0.37	0	38,40,61	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
95	3PE	4D	201	-	34,34,50	0.37	0	37,39,55	0.35	0
97	CDL	C4	202	-	68,68,99	0.36	0	74,80,111	0.37	0
97	CDL	N1	701	-	69,69,99	0.37	0	75,81,111	0.33	0
92	SF4	V1	602	88	0,12,12	-	-	-		
94	PC1	N4	501	-	38,38,53	0.33	0	44,46,61	0.31	0
96	S12	4D	203	-	33,34,34	0.79	0	34,40,40	0.92	3 (8%)
106	HEM	Qc	402	72	50,50,50	1.35	9 (18%)	67,82,82	1.67	13 (19%)
94	PC1	AN	301	-	47,47,53	0.31	0	53,55,61	0.31	0
94	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.29	0
97	CDL	E6	401	-	57,57,99	0.39	0	63,69,111	0.46	0
104	PX2	C2	201	-	35,35,35	0.99	4 (11%)	38,40,40	1.10	2 (5%)
94	PC1	Qj	201	-	53,53,53	0.30	0	59,61,61	0.32	0
97	CDL	4E	202	-	71,71,99	0.36	0	77,83,111	0.34	0
95	3PE	4D	202	-	50,50,50	0.31	0	53,55,55	0.36	0
97	CDL	A3	201	-	57,57,99	0.39	0	63,69,111	0.37	0
94	PC1	N3	301	-	41,41,53	0.33	0	47,49,61	0.36	0
94	PC1	E8	303	-	32,32,53	0.37	0	38,40,61	0.38	0
94	PC1	A9	502	-	32,32,53	0.39	0	38,40,61	0.37	0
97	CDL	C4	203	-	97,97,99	0.32	0	103,109,111	0.34	0
94	PC1	C1	505	-	49,49,53	0.32	0	55,57,61	0.34	0
97	CDL	QH	102	-	59,59,99	0.38	0	65,71,111	0.35	0
94	PC1	A1	202	-	30,30,53	0.38	0	36,38,61	0.36	0
97	CDL	Qd	302	-	99,99,99	0.31	0	105,111,111	0.28	0
92	SF4	S8	302	87	0,12,12	-	-	-		
92	SF4	S8	301	87	0,12,12	-	-	-		
97	CDL	Qj	202	-	47,47,99	0.43	0	53,59,111	0.36	0
94	PC1	QD	303	-	30,30,53	0.39	0	36,38,61	0.40	0
94	PC1	E9	202	-	34,34,53	0.36	0	40,42,61	0.43	0
97	CDL	AL	303	-	63,63,99	0.38	0	69,75,111	0.33	0
91	FES	QE	301	74	0,4,4	-	-	-		
91	FES	1A	401	1	0,4,4	-	-	-		
94	PC1	N4	505	-	53,53,53	0.30	0	59,61,61	0.30	0
94	PC1	Qe	303	-	35,35,53	0.36	0	41,43,61	0.36	0
95	3PE	N4	503	-	40,40,50	0.35	0	43,45,55	0.33	0
97	CDL	E4	401	-	71,71,99	0.36	0	77,83,111	0.38	0
104	PX2	QJ	202	-	35,35,35	1.00	3 (8%)	38,40,40	1.11	2 (5%)
97	CDL	QH	101	-	75,75,99	0.35	0	81,87,111	0.33	0
106	HEM	Qc	403	72	50,50,50	1.35	7 (14%)	67,82,82	1.66	14 (20%)
95	3PE	C1	506	-	39,39,50	0.36	0	42,44,55	0.36	0
94	PC1	B5	202	-	53,53,53	0.30	0	59,61,61	0.30	0
94	PC1	4A	302	-	45,45,53	0.32	0	51,53,61	0.35	0
97	CDL	AL	302	-	67,67,99	0.37	0	73,79,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
94	PC1	QC	404	-	53,53,53	0.30	0	59,61,61	0.34	0
99	NDP	A9	501	-	51,52,52	0.46	0	71,80,80	0.45	0
97	CDL	Qh	101	-	64,64,99	0.38	0	70,76,111	0.33	0
94	PC1	4A	301	-	46,46,53	0.31	0	52,54,61	0.33	0
94	PC1	AM	204	-	47,47,53	0.31	0	53,55,61	0.27	0
97	CDL	QJ	203	-	57,57,99	0.40	0	63,69,111	0.32	0
97	CDL	QD	302	-	68,68,99	0.37	0	74,80,111	0.37	0
94	PC1	4E	201	-	34,34,53	0.36	0	40,42,61	0.36	0
101	HEA	C1	502	43	67,67,67	2.27	25 (37%)	81,103,103	2.42	24 (29%)
94	PC1	A1	201	-	48,48,53	0.32	0	54,56,61	0.37	0
95	3PE	7A	202	-	40,40,50	0.34	0	43,45,55	0.32	0
94	PC1	N5	601	-	35,35,53	0.35	0	41,43,61	0.32	0
101	HEA	C1	501	43	67,67,67	2.27	26 (38%)	81,103,103	2.41	30 (37%)
94	PC1	E4	402	-	50,50,53	0.29	0	56,58,61	0.30	0
94	PC1	ED	201	-	53,53,53	0.29	0	59,61,61	0.33	0
97	CDL	AM	201	-	71,71,99	0.35	0	77,83,111	0.33	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
97	CDL	E7	301	-	-	18/78/78/110	-
97	CDL	AM	202	-	-	20/82/82/110	-
97	CDL	7C	201	-	-	25/100/100/110	-
95	3PE	E9	201	-	-	9/54/54/54	-
94	PC1	7A	201	-	-	13/39/39/57	-
94	PC1	E8	302	-	-	13/57/57/57	-
97	CDL	N5	603	-	-	26/103/103/110	-
94	PC1	A9	503	-	-	6/36/36/57	-
97	CDL	C4	201	-	-	23/104/104/110	-
94	PC1	QI	101	-	-	2/39/39/57	-
94	PC1	AM	203	-	-	15/52/52/57	-
104	PX2	QJ	201	-	-	19/37/37/37	-
92	SF4	1A	403	1	-	-	0/6/5/5
94	PC1	B5	201	-	-	15/57/57/57	-
94	PC1	N1	703	-	-	17/43/43/57	-
94	PC1	B8	301	-	-	8/40/40/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
100	ZMP	AB	201	28	-	20/40/42/43	-
107	HEC	QD	301	73	-	9/14/54/54	-
97	CDL	EA	201	-	-	14/69/69/110	-
97	CDL	Qc	405	-	-	14/64/64/110	-
94	PC1	ED	202	-	-	16/44/44/57	-
91	FES	V2	301	89	-	-	0/1/1/1
94	PC1	G2	301	-	-	8/41/41/57	-
105	U10	N4	504	-	-	10/39/63/87	0/1/1/1
94	PC1	N1	702	-	-	15/52/52/57	-
97	CDL	QC	403	-	-	16/66/66/110	-
94	PC1	Qc	401	-	-	16/57/57/57	-
97	CDL	B3	101	-	-	9/75/75/110	-
94	PC1	C3	201	-	-	7/54/54/57	-
92	SF4	1A	402	1	-	-	0/6/5/5
95	3PE	N5	602	-	-	11/54/54/54	-
92	SF4	S7	301	86	-	-	0/6/5/5
97	CDL	EA	202	-	-	13/65/65/110	-
94	PC1	Qg	301	-	-	3/31/31/57	-
106	HEM	QC	402	72	-	6/14/54/54	-
91	FES	Qe	301	74	-	-	0/1/1/1
95	3PE	C1	507	-	-	10/43/43/54	-
100	ZMP	AC	201	29	-	18/40/42/43	-
94	PC1	E8	304	-	-	11/33/33/57	-
97	CDL	BM	201	-	-	6/68/68/110	-
97	CDL	Qe	302	-	-	9/70/70/110	-
97	CDL	A9	504	-	-	23/74/74/110	-
108	FMN	V1	601	-	-	3/18/18/18	0/3/3/3
94	PC1	Qc	404	-	-	13/34/34/57	-
94	PC1	AL	301	-	-	12/53/53/57	-
106	HEM	QC	401	72	-	8/14/54/54	-
95	3PE	B4	201	-	-	14/43/43/54	-
97	CDL	B8	302	-	-	12/80/80/110	-
107	HEC	Qd	301	73	-	11/14/54/54	-
94	PC1	N4	502	-	-	10/36/36/57	-
95	3PE	4D	201	-	-	9/38/38/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
97	CDL	C4	202	-	-	10/79/79/110	-
97	CDL	N1	701	-	-	23/80/80/110	-
92	SF4	V1	602	88	-	-	0/6/5/5
94	PC1	N4	501	-	-	12/42/42/57	-
96	S12	4D	203	-	-	13/38/38/38	-
106	HEM	Qc	402	72	-	7/14/54/54	-
94	PC1	AN	301	-	-	7/51/51/57	-
94	PC1	E8	301	-	-	13/57/57/57	-
97	CDL	E6	401	-	-	22/68/68/110	-
104	PX2	C2	201	-	-	20/37/37/37	-
94	PC1	Qj	201	-	-	15/57/57/57	-
97	CDL	4E	202	-	-	20/82/82/110	-
95	3PE	4D	202	-	-	21/54/54/54	-
97	CDL	A3	201	-	-	6/68/68/110	-
94	PC1	N3	301	-	-	7/45/45/57	-
94	PC1	E8	303	-	-	5/36/36/57	-
94	PC1	A9	502	-	-	13/36/36/57	-
97	CDL	C4	203	-	-	25/108/108/110	-
94	PC1	C1	505	-	-	10/53/53/57	-
97	CDL	QH	102	-	-	16/70/70/110	-
94	PC1	A1	202	-	-	7/34/34/57	-
97	CDL	Qd	302	-	-	28/110/110/110	-
92	SF4	S8	302	87	-	-	0/6/5/5
92	SF4	S8	301	87	-	-	0/6/5/5
97	CDL	Qj	202	-	-	20/58/58/110	-
94	PC1	QD	303	-	-	10/34/34/57	-
94	PC1	E9	202	-	-	8/38/38/57	-
97	CDL	AL	303	-	-	12/74/74/110	-
91	FES	QE	301	74	-	-	0/1/1/1
94	PC1	N4	505	-	-	13/57/57/57	-
91	FES	1A	401	1	-	-	0/1/1/1
94	PC1	Qe	303	-	-	5/39/39/57	-
95	3PE	N4	503	-	-	8/44/44/54	-
97	CDL	E4	401	-	-	14/82/82/110	-
104	PX2	QJ	202	-	-	24/37/37/37	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
97	CDL	QH	101	-	-	19/86/86/110	-
106	HEM	Qc	403	72	-	6/14/54/54	-
95	3PE	C1	506	-	-	15/43/43/54	-
94	PC1	B5	202	-	-	19/57/57/57	-
94	PC1	4A	302	-	-	20/49/49/57	-
97	CDL	AL	302	-	-	9/78/78/110	-
94	PC1	QC	404	-	-	8/57/57/57	-
99	NDP	A9	501	-	-	10/34/77/77	0/5/5/5
97	CDL	Qh	101	-	-	17/75/75/110	-
94	PC1	4A	301	-	-	7/50/50/57	-
94	PC1	AM	204	-	-	10/51/51/57	-
97	CDL	QJ	203	-	-	16/68/68/110	-
97	CDL	QD	302	-	-	14/79/79/110	-
94	PC1	4E	201	-	-	12/38/38/57	-
101	HEA	C1	502	43	-	18/36/76/76	-
94	PC1	A1	201	-	-	15/52/52/57	-
95	3PE	7A	202	-	-	7/44/44/54	-
94	PC1	N5	601	-	-	9/39/39/57	-
101	HEA	C1	501	43	-	18/36/76/76	-
94	PC1	E4	402	-	-	9/54/54/57	-
94	PC1	ED	201	-	-	10/57/57/57	-
97	CDL	AM	201	-	-	14/82/82/110	-

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
105	N4	504	U10	C6-C1	10.41	1.53	1.35
107	QD	301	HEC	CAC-C3C	7.09	1.58	1.35
107	Qd	301	HEC	CAC-C3C	7.06	1.57	1.35
107	QD	301	HEC	CAB-C3B	6.67	1.56	1.35
107	Qd	301	HEC	CAB-C3B	6.64	1.56	1.35
101	C1	502	HEA	C3B-C2B	5.33	1.46	1.34
101	C1	501	HEA	FE-ND	4.92	2.10	1.94
101	C1	502	HEA	FE-ND	4.92	2.10	1.94
101	C1	501	HEA	C3B-C2B	4.75	1.45	1.34
101	C1	501	HEA	FE-NB	4.65	2.09	1.94
105	N4	504	U10	C4-C3	4.60	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
101	C1	502	HEA	FE-NB	4.44	2.08	1.94
101	C1	502	HEA	FE-NC	4.44	2.09	1.95
101	C1	502	HEA	C4B-NB	-4.40	1.32	1.40
101	C1	501	HEA	FE-NC	4.29	2.09	1.95
101	C1	501	HEA	C11-C3B	-4.27	1.46	1.51
101	C1	501	HEA	CHA-C1A	4.24	1.46	1.38
101	C1	501	HEA	C3D-C2D	4.14	1.45	1.36
101	C1	502	HEA	C3A-C2A	4.11	1.46	1.37
101	C1	501	HEA	C1D-ND	-4.09	1.33	1.40
101	C1	502	HEA	C1D-ND	-3.93	1.33	1.40
101	C1	502	HEA	C3D-C2D	3.90	1.45	1.36
106	QC	402	HEM	C4D-ND	-3.82	1.33	1.40
106	QC	401	HEM	C4D-ND	-3.82	1.33	1.40
101	C1	502	HEA	C11-C3B	-3.81	1.46	1.51
101	C1	502	HEA	C4C-NC	-3.79	1.32	1.39
101	C1	501	HEA	C4B-NB	-3.75	1.33	1.40
106	Qc	402	HEM	C4D-ND	-3.69	1.33	1.40
101	C1	502	HEA	CHC-C4B	3.65	1.45	1.38
101	C1	501	HEA	C3A-C2A	3.61	1.45	1.37
106	Qc	403	HEM	C4D-ND	-3.58	1.34	1.40
107	QD	301	HEC	CBC-CAC	-3.50	1.36	1.49
107	Qd	301	HEC	CBC-CAC	-3.50	1.36	1.49
101	C1	502	HEA	CHA-C1A	3.49	1.45	1.38
101	C1	501	HEA	CHC-C4B	3.48	1.45	1.38
101	C1	501	HEA	CHD-C1D	3.42	1.45	1.38
101	C1	501	HEA	CHD-C4C	3.41	1.47	1.39
100	AC	201	ZMP	C9-C10	-3.41	1.47	1.50
106	QC	402	HEM	C1B-NB	-3.34	1.34	1.40
101	C1	502	HEA	C1B-NB	-3.26	1.32	1.38
101	C1	502	HEA	C1C-NC	-3.20	1.33	1.39
106	QC	401	HEM	C1B-NB	-3.18	1.34	1.40
101	C1	501	HEA	C1C-NC	-3.17	1.33	1.39
106	Qc	403	HEM	C1B-NB	-3.16	1.34	1.40
101	C1	502	HEA	CHD-C1D	3.13	1.44	1.38
106	Qc	403	HEM	C1C-C2C	-3.12	1.39	1.45
101	C1	501	HEA	C4C-NC	-3.12	1.33	1.39
101	C1	501	HEA	C1B-NB	-3.08	1.32	1.38
101	C1	501	HEA	C1A-NA	3.04	1.45	1.39
106	Qc	402	HEM	C1B-NB	-3.01	1.35	1.40
106	QC	402	HEM	C1C-C2C	-3.01	1.39	1.45
101	C1	501	HEA	CHA-C4D	3.01	1.46	1.39
104	QJ	202	PX2	O7-C2	-2.99	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
100	AB	201	ZMP	C9-C10	-2.91	1.48	1.50
106	Qc	402	HEM	C1C-C2C	-2.91	1.39	1.45
104	QJ	201	PX2	O7-C2	-2.87	1.39	1.46
105	N4	504	U10	C7-C6	2.85	1.56	1.51
101	C1	502	HEA	CHC-C1C	2.85	1.45	1.39
101	C1	501	HEA	C4D-ND	-2.83	1.33	1.38
106	QC	401	HEM	C1C-C2C	-2.82	1.39	1.45
106	QC	402	HEM	C1D-ND	-2.81	1.33	1.38
105	N4	504	U10	C7-C8	2.81	1.55	1.50
104	C2	201	PX2	O7-C2	-2.77	1.40	1.46
106	Qc	403	HEM	C1D-ND	-2.76	1.33	1.38
105	N4	504	U10	C31-C29	2.74	1.56	1.51
106	Qc	402	HEM	C1D-ND	-2.73	1.33	1.38
101	C1	502	HEA	C4D-ND	-2.72	1.33	1.38
105	N4	504	U10	C6-C5	2.69	1.54	1.46
101	C1	502	HEA	CHB-C4A	2.69	1.43	1.38
101	C1	502	HEA	O2D-CGD	-2.68	1.22	1.30
106	QC	401	HEM	C1D-ND	-2.67	1.33	1.38
101	C1	502	HEA	CHA-C4D	2.65	1.45	1.39
101	C1	502	HEA	CHB-C1B	2.63	1.45	1.39
101	C1	502	HEA	CHD-C4C	2.63	1.45	1.39
105	N4	504	U10	C16-C14	2.61	1.56	1.51
101	C1	501	HEA	C4B-C3B	2.61	1.49	1.44
101	C1	501	HEA	O2D-CGD	-2.59	1.22	1.30
101	C1	502	HEA	C1A-NA	2.59	1.44	1.39
105	N4	504	U10	O5-C5	-2.57	1.17	1.23
101	C1	502	HEA	C4A-NA	2.55	1.44	1.39
101	C1	502	HEA	O2A-CGA	-2.54	1.22	1.30
101	C1	501	HEA	O2A-CGA	-2.54	1.22	1.30
106	Qc	403	HEM	FE-NB	2.54	2.02	1.94
107	QD	301	HEC	CBB-CAB	-2.54	1.40	1.49
106	Qc	402	HEM	C3C-C4C	-2.49	1.41	1.46
106	Qc	402	HEM	FE-ND	2.48	2.02	1.94
107	Qd	301	HEC	CBB-CAB	-2.44	1.40	1.49
106	QC	402	HEM	FE-NB	2.40	2.02	1.94
106	QC	401	HEM	C3C-C4C	-2.39	1.41	1.46
104	QJ	201	PX2	O5-C3	-2.37	1.39	1.45
106	Qc	403	HEM	C4B-NB	-2.37	1.34	1.38
105	N4	504	U10	O3-C3M	-2.35	1.40	1.45
106	Qc	402	HEM	FE-NB	2.34	2.02	1.94
101	C1	501	HEA	CHB-C1B	2.33	1.44	1.39
106	QC	401	HEM	FE-NB	2.32	2.02	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
104	QJ	202	PX2	O5-C4	2.32	1.40	1.33
107	QD	301	HEC	C3D-C2D	-2.32	1.32	1.38
107	Qd	301	HEC	C3D-C2D	-2.31	1.32	1.38
105	N4	504	U10	C26-C24	2.30	1.56	1.51
106	QC	401	HEM	C4B-NB	-2.30	1.34	1.38
101	C1	501	HEA	C4A-NA	2.30	1.43	1.39
106	QC	402	HEM	C4B-NB	-2.28	1.34	1.38
104	QJ	201	PX2	O5-C4	2.26	1.39	1.33
101	C1	501	HEA	CHC-C1C	2.23	1.44	1.39
105	N4	504	U10	O2-C2	-2.22	1.18	1.23
104	C2	201	PX2	O5-C3	-2.22	1.40	1.45
105	N4	504	U10	C27-C28	2.21	1.57	1.50
105	N4	504	U10	C21-C19	2.21	1.55	1.51
106	QC	402	HEM	C3C-C4C	-2.18	1.42	1.46
104	C2	201	PX2	O5-C4	2.17	1.39	1.33
107	QD	301	HEC	C3C-C2C	-2.16	1.33	1.41
107	QD	301	HEC	C3B-C2B	-2.16	1.33	1.41
106	Qc	402	HEM	C4B-NB	-2.16	1.34	1.38
107	Qd	301	HEC	C3C-C2C	-2.15	1.33	1.41
104	C2	201	PX2	O7-C16	2.15	1.40	1.34
107	Qd	301	HEC	CMD-C2D	2.13	1.55	1.50
105	N4	504	U10	C36-C34	2.11	1.56	1.50
106	QC	401	HEM	C1A-C2A	-2.10	1.40	1.44
106	QC	402	HEM	FE-ND	2.09	2.01	1.94
104	QJ	202	PX2	O5-C3	-2.09	1.40	1.45
106	Qc	402	HEM	FE-NA	2.09	2.02	1.95
106	QC	401	HEM	FE-ND	2.07	2.01	1.94
105	N4	504	U10	C11-C9	2.07	1.55	1.51
107	Qd	301	HEC	C3B-C2B	-2.06	1.34	1.41
105	N4	504	U10	C32-C33	2.06	1.56	1.50
101	C1	501	HEA	CMB-C2B	-2.04	1.46	1.50
106	Qc	403	HEM	FE-ND	2.03	2.01	1.94
105	N4	504	U10	C12-C13	2.03	1.56	1.50
105	N4	504	U10	O4-C4M	-2.00	1.40	1.45

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
107	QD	301	HEC	CBB-CAB-C3B	-8.44	110.57	127.43
107	Qd	301	HEC	CBB-CAB-C3B	-8.36	110.73	127.43
107	QD	301	HEC	CBC-CAC-C3C	-6.82	113.80	127.43
107	Qd	301	HEC	CBC-CAC-C3C	-6.81	113.81	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	C1	502	HEA	CAD-CBD-CGD	-6.63	96.09	113.67
101	C1	501	HEA	C2B-C1B-NB	5.86	116.68	109.90
101	C1	502	HEA	C3C-C2C-C1C	-5.84	100.28	107.17
101	C1	501	HEA	CAD-CBD-CGD	-5.50	99.07	113.67
101	C1	501	HEA	C3D-C4D-ND	5.43	115.60	110.35
101	C1	502	HEA	C3C-C4C-NC	5.34	114.29	109.80
106	Qc	402	HEM	CHC-C4B-NB	5.28	130.10	124.42
101	C1	501	HEA	C3C-C2C-C1C	-5.26	100.97	107.17
101	C1	501	HEA	CAA-CBA-CGA	-5.21	99.85	113.67
101	C1	502	HEA	CAA-CBA-CGA	-5.15	100.01	113.67
106	QC	401	HEM	CHC-C4B-NB	5.14	129.96	124.42
101	C1	502	HEA	C3D-C4D-ND	5.10	115.28	110.35
101	C1	502	HEA	C1D-C2D-C3D	-5.08	101.63	106.98
101	C1	502	HEA	C13-C12-C11	-5.01	106.40	114.39
101	C1	502	HEA	C2D-C1D-ND	4.98	115.57	109.84
106	QC	402	HEM	CHC-C4B-NB	4.97	129.77	124.42
106	Qc	402	HEM	CHD-C4C-NC	4.87	129.75	124.45
101	C1	502	HEA	C2B-C1B-NB	4.76	115.40	109.90
105	N4	504	U10	C7-C6-C5	4.59	123.85	118.52
106	QC	401	HEM	CHD-C4C-NC	4.58	129.44	124.45
106	Qc	403	HEM	CHC-C4B-NB	4.54	129.31	124.42
101	C1	502	HEA	C3B-C4B-NB	4.51	115.02	109.84
101	C1	501	HEA	C3C-C4C-NC	4.50	113.59	109.80
101	C1	501	HEA	C3B-C4B-NB	4.46	114.97	109.84
101	C1	501	HEA	C1D-C2D-C3D	-4.41	102.34	106.98
101	C1	501	HEA	CHB-C1B-C2B	-4.35	118.16	125.03
104	C2	201	PX2	O7-C16-C17	4.33	120.85	111.48
101	C1	501	HEA	C2D-C1D-ND	4.27	114.74	109.84
101	C1	501	HEA	C13-C12-C11	-4.26	107.59	114.39
106	QC	402	HEM	CHD-C4C-NC	4.22	129.04	124.45
105	N4	504	U10	C15-C14-C16	4.17	122.47	115.23
104	QJ	201	PX2	O7-C16-C17	4.16	120.48	111.48
106	QC	402	HEM	CHB-C1B-NB	4.15	129.50	124.37
101	C1	501	HEA	CHA-C4D-C3D	-4.14	118.74	124.77
101	C1	502	HEA	CHB-C1B-C2B	-4.11	118.55	125.03
105	N4	504	U10	C7-C6-C1	-4.10	117.86	124.89
106	Qc	403	HEM	CHD-C4C-NC	3.99	128.80	124.45
105	N4	504	U10	C30-C29-C31	3.98	122.14	115.23
104	QJ	202	PX2	O7-C16-C17	3.96	120.04	111.48
101	C1	501	HEA	C2C-C1C-NC	3.93	116.45	110.14
106	Qc	402	HEM	CHB-C1B-NB	3.92	129.22	124.37
105	N4	504	U10	C15-C14-C13	-3.79	113.90	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
106	Qc	403	HEM	CHB-C1B-NB	3.74	129.00	124.37
101	C1	502	HEA	C4B-C3B-C2B	-3.72	101.19	107.44
101	C1	501	HEA	C4B-C3B-C2B	-3.68	101.25	107.44
101	C1	502	HEA	C2C-C1C-NC	3.64	115.98	110.14
106	QC	401	HEM	CHB-C1B-NB	3.59	128.81	124.37
101	C1	501	HEA	CHC-C4B-NB	-3.44	120.11	124.37
105	N4	504	U10	C22-C23-C24	-3.35	119.95	127.62
101	C1	502	HEA	CHA-C4D-C3D	-3.30	119.96	124.77
106	Qc	403	HEM	CHA-C4D-ND	3.24	128.38	124.37
106	Qc	403	HEM	C4D-ND-C1D	3.20	108.99	105.21
106	QC	401	HEM	CHA-C4D-ND	3.15	128.26	124.37
106	Qc	403	HEM	CHD-C1D-ND	3.14	127.80	124.42
106	Qc	402	HEM	CHA-C4D-ND	3.10	128.20	124.37
104	QJ	202	PX2	O5-C4-C5	3.01	121.02	111.83
106	QC	402	HEM	C4D-ND-C1D	3.00	108.77	105.21
106	Qc	402	HEM	C4D-ND-C1D	2.95	108.70	105.21
106	Qc	403	HEM	CHA-C1A-NA	2.93	129.18	123.86
106	Qc	402	HEM	C1B-NB-C4B	2.93	108.68	105.21
100	AC	201	ZMP	C20-C18-C21	2.88	112.98	108.22
100	AB	201	ZMP	C14-C13-N1	2.88	121.59	116.34
107	QD	301	HEC	O1D-CGD-CBD	-2.88	113.97	123.09
106	QC	401	HEM	C4D-ND-C1D	2.87	108.60	105.21
100	AB	201	ZMP	C15-C14-C13	-2.86	107.63	112.39
106	QC	401	HEM	C1B-NB-C4B	2.84	108.56	105.21
107	Qd	301	HEC	O1D-CGD-CBD	-2.83	114.10	123.09
96	4D	203	S12	OG-CB-CA	2.83	110.53	108.06
105	N4	504	U10	C7-C8-C9	-2.82	121.97	126.83
101	C1	501	HEA	CAA-C2A-C1A	2.77	130.48	124.85
106	QC	401	HEM	CHA-C1A-NA	2.75	128.85	123.86
105	N4	504	U10	C27-C28-C29	-2.75	121.33	127.62
106	QC	402	HEM	CHD-C1D-ND	2.73	127.36	124.42
101	C1	501	HEA	C13-C14-C15	-2.73	121.37	127.62
106	QC	402	HEM	CHA-C4D-ND	2.73	127.75	124.37
106	Qc	402	HEM	CHA-C1A-NA	2.72	128.79	123.86
101	C1	501	HEA	CMB-C2B-C1B	-2.71	120.80	125.03
104	QJ	201	PX2	O5-C4-C5	2.69	120.05	111.83
105	N4	504	U10	C25-C24-C26	2.69	119.89	115.23
106	QC	402	HEM	CHA-C1A-NA	2.67	128.71	123.86
105	N4	504	U10	C20-C19-C21	2.66	119.84	115.23
101	C1	501	HEA	CMB-C2B-C3B	2.65	135.40	130.28
96	4D	203	S12	O4-P-O3	2.62	124.65	112.44
105	N4	504	U10	C10-C9-C11	2.62	119.77	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
101	C1	502	HEA	CMB-C2B-C1B	-2.61	120.96	125.03
101	C1	501	HEA	C1B-C2B-C3B	-2.59	103.79	106.80
104	C2	201	PX2	O5-C4-C5	2.58	119.72	111.83
107	QD	301	HEC	O1A-CGA-CBA	-2.58	114.92	123.09
101	C1	501	HEA	C17-C18-C19	-2.56	121.76	127.62
106	Qc	403	HEM	C2A-C1A-NA	-2.56	107.31	110.15
101	C1	502	HEA	C1B-C2B-C3B	-2.55	103.85	106.80
101	C1	502	HEA	CMB-C2B-C3B	2.54	135.19	130.28
100	AB	201	ZMP	O1-C10-C9	-2.52	121.07	123.98
106	QC	402	HEM	CHB-C1B-C2B	-2.50	119.84	126.95
101	C1	502	HEA	C27-C19-C18	-2.50	117.21	123.63
101	C1	501	HEA	CMD-C2D-C1D	2.48	128.91	125.03
106	Qc	403	HEM	CHB-C1B-C2B	-2.45	119.98	126.95
106	Qc	403	HEM	CAD-CBD-CGD	-2.45	107.17	113.67
106	QC	402	HEM	C2A-C1A-NA	-2.45	107.43	110.15
101	C1	501	HEA	C4D-C3D-C2D	-2.42	103.37	106.89
101	C1	501	HEA	C27-C19-C20	2.42	119.42	115.23
101	C1	502	HEA	O1D-CGD-CBD	-2.41	115.44	123.09
106	QC	402	HEM	C1B-NB-C4B	2.40	108.05	105.21
101	C1	502	HEA	OMA-CMA-C3A	-2.36	120.30	125.62
106	QC	401	HEM	CHD-C1D-ND	2.33	126.94	124.42
105	N4	504	U10	C6-C1-C2	2.32	121.00	119.17
101	C1	502	HEA	O1A-CGA-CBA	-2.31	115.77	123.09
106	QC	402	HEM	C1C-CHC-C4B	-2.30	121.13	126.02
107	QD	301	HEC	CHC-C4B-NB	2.29	126.94	124.45
101	C1	502	HEA	C13-C14-C15	-2.29	122.39	127.62
106	Qc	403	HEM	C1B-NB-C4B	2.25	107.87	105.21
101	C1	501	HEA	C3A-C2A-C1A	-2.24	104.93	107.05
106	QC	402	HEM	O2A-CGA-CBA	2.22	121.03	114.00
107	QD	301	HEC	CMD-C2D-C1D	-2.22	122.04	125.42
107	Qd	301	HEC	O1A-CGA-CBA	-2.22	116.05	123.09
101	C1	501	HEA	CHC-C1C-C2C	-2.22	120.98	127.43
106	Qc	402	HEM	CHD-C1D-ND	2.22	126.81	124.42
106	Qc	402	HEM	C1C-CHC-C4B	-2.21	121.32	126.02
100	AB	201	ZMP	O2-C13-C14	-2.21	118.02	122.02
107	QD	301	HEC	O2A-CGA-O1A	2.20	128.99	123.33
100	AC	201	ZMP	C15-C14-C13	-2.20	108.73	112.39
106	Qc	403	HEM	O2A-CGA-CBA	2.19	120.93	114.00
106	Qc	403	HEM	C1C-CHC-C4B	-2.17	121.42	126.02
100	AB	201	ZMP	C12-N1-C13	2.16	126.84	122.82
101	C1	502	HEA	CMC-C2C-C3C	2.14	131.59	126.55
106	QC	401	HEM	O2A-CGA-CBA	2.14	120.76	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
106	QC	401	HEM	C1C-CHC-C4B	-2.13	121.49	126.02
106	Qc	402	HEM	CHB-C1B-C2B	-2.12	120.92	126.95
106	Qc	402	HEM	C3B-C4B-NB	-2.12	107.95	109.47
101	C1	501	HEA	O1D-CGD-CBD	-2.12	116.38	123.09
106	QC	402	HEM	C4A-CHB-C1B	-2.11	121.29	126.25
101	C1	501	HEA	CMC-C2C-C3C	2.10	131.49	126.55
107	Qd	301	HEC	O2A-CGA-O1A	2.10	128.73	123.33
107	Qd	301	HEC	CHC-C4B-NB	2.09	126.73	124.45
105	N4	504	U10	C17-C18-C19	-2.09	122.85	127.62
106	Qc	403	HEM	C4A-CHB-C1B	-2.08	121.35	126.25
96	4D	203	S12	O52-C5-O51	-2.07	118.46	123.63
101	C1	501	HEA	C27-C19-C18	-2.06	118.35	123.63
106	Qc	402	HEM	O2A-CGA-CBA	2.05	120.48	114.00
105	N4	504	U10	C10-C9-C8	-2.04	118.39	123.63
100	AC	201	ZMP	C14-C13-N1	2.03	120.05	116.34
101	C1	502	HEA	C17-C18-C19	-2.03	122.97	127.62
101	C1	501	HEA	C1C-CHC-C4B	2.02	131.00	126.25
105	N4	504	U10	C32-C33-C34	-2.02	120.91	127.64
106	Qc	402	HEM	O2D-CGD-CBD	2.01	120.36	114.00
106	QC	401	HEM	CHB-C1B-C2B	-2.00	121.25	126.95

There are no chirality outliers.

All (1281) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
94	4A	301	PC1	C11-O13-P-O12
94	4A	301	PC1	C11-O13-P-O11
94	4A	301	PC1	C1-O11-P-O14
94	4A	301	PC1	C1-O11-P-O13
94	4A	302	PC1	C11-O13-P-O14
94	4A	302	PC1	C11-O13-P-O11
94	4A	302	PC1	C1-O11-P-O12
94	4A	302	PC1	C1-O11-P-O13
94	4A	302	PC1	O21-C2-C3-O31
94	4E	201	PC1	C11-O13-P-O12
94	4E	201	PC1	C11-O13-P-O11
94	4E	201	PC1	C1-O11-P-O12
94	4E	201	PC1	C1-O11-P-O14
94	4E	201	PC1	C1-O11-P-O13
94	4E	201	PC1	O21-C2-C3-O31
94	7A	201	PC1	C11-O13-P-O12
94	7A	201	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
94	7A	201	PC1	C11-O13-P-O11
94	A1	201	PC1	C11-O13-P-O14
94	A1	201	PC1	C11-O13-P-O11
94	A1	202	PC1	C11-O13-P-O12
94	A1	202	PC1	C11-O13-P-O14
94	A1	202	PC1	C11-O13-P-O11
94	A1	202	PC1	C1-O11-P-O12
94	A1	202	PC1	C1-O11-P-O13
94	A9	502	PC1	C1-O11-P-O12
94	A9	502	PC1	C1-O11-P-O14
94	A9	502	PC1	C1-O11-P-O13
94	A9	503	PC1	C1-O11-P-O12
94	A9	503	PC1	C1-O11-P-O13
94	A9	503	PC1	O13-C11-C12-N
94	AM	203	PC1	C1-O11-P-O14
94	AM	204	PC1	C1-O11-P-O12
94	AM	204	PC1	C1-O11-P-O14
94	AM	204	PC1	C1-O11-P-O13
94	AN	301	PC1	C1-O11-P-O12
94	AN	301	PC1	C1-O11-P-O14
94	AN	301	PC1	C1-O11-P-O13
94	B5	201	PC1	C11-O13-P-O12
94	B5	201	PC1	C11-O13-P-O14
94	B5	201	PC1	C11-O13-P-O11
94	B5	201	PC1	C1-O11-P-O12
94	B5	201	PC1	C1-O11-P-O13
94	B5	202	PC1	C1-O11-P-O12
94	B5	202	PC1	C1-O11-P-O14
94	B5	202	PC1	C1-O11-P-O13
94	C1	505	PC1	C1-O11-P-O12
94	C1	505	PC1	C1-O11-P-O14
94	C1	505	PC1	C1-O11-P-O13
94	E4	402	PC1	C11-O13-P-O12
94	E4	402	PC1	C11-O13-P-O11
94	E8	301	PC1	C11-O13-P-O11
94	E8	301	PC1	C1-O11-P-O12
94	E8	301	PC1	C1-O11-P-O14
94	E8	301	PC1	C1-O11-P-O13
94	E8	303	PC1	C1-O11-P-O13
94	E8	304	PC1	C11-O13-P-O12
94	E8	304	PC1	C11-O13-P-O14
94	E8	304	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
94	E8	304	PC1	C1-O11-P-O13
94	E8	304	PC1	C2-C1-O11-P
94	E9	202	PC1	C11-O13-P-O12
94	E9	202	PC1	C11-O13-P-O14
94	E9	202	PC1	C11-O13-P-O11
94	E9	202	PC1	C1-O11-P-O12
94	E9	202	PC1	C1-O11-P-O14
94	E9	202	PC1	C1-O11-P-O13
94	ED	202	PC1	C11-O13-P-O12
94	ED	202	PC1	C11-O13-P-O11
94	ED	202	PC1	C1-O11-P-O14
94	ED	202	PC1	C1-O11-P-O13
94	G2	301	PC1	C11-O13-P-O11
94	N1	702	PC1	C1-O11-P-O12
94	N1	702	PC1	C1-O11-P-O14
94	N1	702	PC1	C1-O11-P-O13
94	N1	703	PC1	C11-O13-P-O12
94	N1	703	PC1	C11-O13-P-O14
94	N1	703	PC1	C11-O13-P-O11
94	N1	703	PC1	C1-O11-P-O14
94	N1	703	PC1	C1-O11-P-O13
94	N1	703	PC1	O13-C11-C12-N
94	N1	703	PC1	C2-C1-O11-P
94	N1	703	PC1	O21-C2-C3-O31
94	N4	501	PC1	C11-O13-P-O14
94	N4	501	PC1	C11-O13-P-O11
94	N4	501	PC1	C1-O11-P-O12
94	N4	501	PC1	C1-O11-P-O13
94	N4	502	PC1	C11-O13-P-O12
94	N4	502	PC1	C1-O11-P-O13
94	N4	505	PC1	C11-O13-P-O12
94	N4	505	PC1	C11-O13-P-O14
94	N4	505	PC1	C11-O13-P-O11
94	N5	601	PC1	C11-O13-P-O11
94	N5	601	PC1	C1-O11-P-O14
94	N5	601	PC1	C1-O11-P-O13
94	QC	404	PC1	C1-O11-P-O14
94	QC	404	PC1	C1-O11-P-O13
94	QD	303	PC1	C1-O11-P-O12
94	QD	303	PC1	C1-O11-P-O14
94	QD	303	PC1	C1-O11-P-O13
94	QI	101	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
94	Qc	401	PC1	C1-O11-P-O12
94	Qc	401	PC1	C1-O11-P-O14
94	Qc	401	PC1	C1-O11-P-O13
94	Qc	401	PC1	O13-C11-C12-N
94	Qc	404	PC1	C11-O13-P-O12
94	Qc	404	PC1	C11-O13-P-O14
94	Qc	404	PC1	C11-O13-P-O11
94	Qg	301	PC1	C1-O11-P-O12
94	Qg	301	PC1	C1-O11-P-O14
94	Qg	301	PC1	C1-O11-P-O13
94	Qj	201	PC1	C11-O13-P-O12
94	Qj	201	PC1	C11-O13-P-O14
94	Qj	201	PC1	C11-O13-P-O11
94	Qj	201	PC1	C1-O11-P-O14
95	4D	201	3PE	C1-O11-P-O13
95	4D	201	3PE	C11-O13-P-O11
95	4D	201	3PE	C11-O13-P-O12
95	4D	201	3PE	C11-O13-P-O14
95	4D	202	3PE	C1-O11-P-O12
95	4D	202	3PE	C1-O11-P-O13
95	4D	202	3PE	C11-O13-P-O11
95	4D	202	3PE	O13-C11-C12-N
95	7A	202	3PE	C11-O13-P-O11
95	7A	202	3PE	C11-O13-P-O12
95	B4	201	3PE	C11-O13-P-O11
95	B4	201	3PE	C11-O13-P-O14
95	B4	201	3PE	O13-C11-C12-N
95	C1	506	3PE	C11-O13-P-O11
95	C1	506	3PE	C11-O13-P-O12
95	C1	506	3PE	C11-O13-P-O14
95	C1	506	3PE	C2-C1-O11-P
95	E9	201	3PE	C11-O13-P-O11
95	E9	201	3PE	C11-O13-P-O14
95	E9	201	3PE	O13-C11-C12-N
95	N4	503	3PE	C11-O13-P-O11
95	N4	503	3PE	C11-O13-P-O12
95	N4	503	3PE	C11-O13-P-O14
95	N5	602	3PE	C11-O13-P-O11
95	N5	602	3PE	C11-O13-P-O12
95	N5	602	3PE	C11-O13-P-O14
95	N5	602	3PE	O13-C11-C12-N
96	4D	203	S12	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
96	4D	203	S12	OXT-C-CA-CB
96	4D	203	S12	CA-CB-OG-P
97	4E	202	CDL	CA2-OA2-PA1-OA3
97	4E	202	CDL	CA2-OA2-PA1-OA4
97	4E	202	CDL	CA2-OA2-PA1-OA5
97	7C	201	CDL	CA2-OA2-PA1-OA3
97	7C	201	CDL	CA2-OA2-PA1-OA5
97	7C	201	CDL	CB2-OB2-PB2-OB3
97	7C	201	CDL	CB2-OB2-PB2-OB4
97	7C	201	CDL	CB2-OB2-PB2-OB5
97	A9	504	CDL	O1-C1-CA2-OA2
97	A9	504	CDL	CA2-OA2-PA1-OA5
97	A9	504	CDL	CA3-OA5-PA1-OA2
97	A9	504	CDL	CA3-OA5-PA1-OA3
97	A9	504	CDL	CA3-OA5-PA1-OA4
97	A9	504	CDL	CB2-OB2-PB2-OB3
97	A9	504	CDL	CB2-OB2-PB2-OB4
97	A9	504	CDL	CB2-OB2-PB2-OB5
97	A9	504	CDL	CB3-OB5-PB2-OB2
97	AM	201	CDL	CB2-OB2-PB2-OB3
97	AM	201	CDL	CB2-OB2-PB2-OB4
97	AM	201	CDL	CB3-OB5-PB2-OB2
97	AM	201	CDL	CB3-OB5-PB2-OB4
97	AM	202	CDL	CA2-OA2-PA1-OA4
97	AM	202	CDL	CA2-OA2-PA1-OA5
97	AM	202	CDL	CA3-OA5-PA1-OA2
97	AM	202	CDL	CA3-OA5-PA1-OA4
97	B3	101	CDL	CA3-OA5-PA1-OA4
97	B8	302	CDL	CA2-OA2-PA1-OA4
97	B8	302	CDL	CA2-OA2-PA1-OA5
97	B8	302	CDL	CA3-OA5-PA1-OA3
97	B8	302	CDL	CA3-OA5-PA1-OA4
97	B8	302	CDL	CB2-OB2-PB2-OB4
97	B8	302	CDL	CB2-OB2-PB2-OB5
97	B8	302	CDL	CB3-OB5-PB2-OB2
97	B8	302	CDL	CB3-OB5-PB2-OB3
97	BM	201	CDL	CA3-OA5-PA1-OA2
97	C4	201	CDL	CA2-OA2-PA1-OA3
97	C4	201	CDL	CA2-OA2-PA1-OA5
97	C4	201	CDL	CA3-OA5-PA1-OA2
97	C4	201	CDL	CB3-OB5-PB2-OB2
97	C4	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
97	C4	201	CDL	CB3-OB5-PB2-OB4
97	C4	202	CDL	CA3-OA5-PA1-OA2
97	C4	202	CDL	CA3-OA5-PA1-OA3
97	C4	202	CDL	CA3-OA5-PA1-OA4
97	C4	202	CDL	CB2-OB2-PB2-OB4
97	C4	202	CDL	CB2-OB2-PB2-OB5
97	C4	203	CDL	CA2-OA2-PA1-OA3
97	C4	203	CDL	CA2-OA2-PA1-OA4
97	C4	203	CDL	CA2-OA2-PA1-OA5
97	E4	401	CDL	CB2-OB2-PB2-OB3
97	E4	401	CDL	CB2-OB2-PB2-OB4
97	E4	401	CDL	CB2-OB2-PB2-OB5
97	E4	401	CDL	CB3-OB5-PB2-OB2
97	E4	401	CDL	CB3-OB5-PB2-OB4
97	E6	401	CDL	CA3-OA5-PA1-OA2
97	E6	401	CDL	CA3-OA5-PA1-OA3
97	E6	401	CDL	CA4-CA3-OA5-PA1
97	E6	401	CDL	OA6-CA4-CA6-OA8
97	E7	301	CDL	C1-CA2-OA2-PA1
97	E7	301	CDL	CA2-OA2-PA1-OA3
97	E7	301	CDL	CA2-OA2-PA1-OA4
97	E7	301	CDL	CA2-OA2-PA1-OA5
97	E7	301	CDL	CA3-OA5-PA1-OA2
97	E7	301	CDL	CA3-OA5-PA1-OA4
97	EA	201	CDL	O1-C1-CA2-OA2
97	EA	201	CDL	CB2-C1-CA2-OA2
97	EA	201	CDL	CA3-OA5-PA1-OA2
97	EA	201	CDL	CA3-OA5-PA1-OA3
97	EA	201	CDL	CA3-OA5-PA1-OA4
97	EA	201	CDL	CB3-OB5-PB2-OB2
97	EA	201	CDL	CB3-OB5-PB2-OB4
97	EA	202	CDL	CB3-OB5-PB2-OB2
97	N1	701	CDL	CA2-OA2-PA1-OA4
97	N1	701	CDL	CA2-OA2-PA1-OA5
97	N1	701	CDL	CB3-OB5-PB2-OB2
97	N1	701	CDL	CB3-OB5-PB2-OB4
97	N5	603	CDL	CA3-OA5-PA1-OA2
97	N5	603	CDL	CA3-OA5-PA1-OA4
97	N5	603	CDL	CB2-OB2-PB2-OB3
97	N5	603	CDL	CB2-OB2-PB2-OB4
97	QC	403	CDL	CB3-OB5-PB2-OB3
97	QD	302	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
97	QD	302	CDL	CB3-OB5-PB2-OB3
97	QD	302	CDL	CB3-OB5-PB2-OB4
97	QH	101	CDL	CB2-OB2-PB2-OB3
97	QH	101	CDL	CB2-OB2-PB2-OB4
97	QH	101	CDL	CB2-OB2-PB2-OB5
97	QH	101	CDL	CB3-OB5-PB2-OB3
97	QH	102	CDL	CA3-OA5-PA1-OA4
97	QH	102	CDL	CB2-OB2-PB2-OB5
97	QJ	203	CDL	CA3-OA5-PA1-OA2
97	QJ	203	CDL	CA3-OA5-PA1-OA4
97	QJ	203	CDL	CB2-OB2-PB2-OB3
97	QJ	203	CDL	CB2-OB2-PB2-OB4
97	QJ	203	CDL	CB2-OB2-PB2-OB5
97	QJ	203	CDL	CB3-OB5-PB2-OB2
97	QJ	203	CDL	CB3-OB5-PB2-OB3
97	Qc	405	CDL	CA3-OA5-PA1-OA2
97	Qc	405	CDL	CA3-OA5-PA1-OA3
97	Qc	405	CDL	CA3-OA5-PA1-OA4
97	Qc	405	CDL	CB2-OB2-PB2-OB4
97	Qc	405	CDL	CB2-OB2-PB2-OB5
97	Qc	405	CDL	CB3-OB5-PB2-OB4
97	Qd	302	CDL	CA2-OA2-PA1-OA4
97	Qd	302	CDL	CA2-OA2-PA1-OA5
97	Qd	302	CDL	CA3-OA5-PA1-OA3
97	Qd	302	CDL	CA3-OA5-PA1-OA4
97	Qd	302	CDL	CB2-OB2-PB2-OB3
97	Qd	302	CDL	CB3-OB5-PB2-OB2
97	Qd	302	CDL	CB3-OB5-PB2-OB3
97	Qe	302	CDL	CA3-OA5-PA1-OA2
97	Qe	302	CDL	CB3-OB5-PB2-OB2
97	Qe	302	CDL	CB3-OB5-PB2-OB3
97	Qe	302	CDL	CB3-OB5-PB2-OB4
97	Qh	101	CDL	CA2-OA2-PA1-OA3
97	Qh	101	CDL	CA3-OA5-PA1-OA2
97	Qh	101	CDL	CA3-OA5-PA1-OA3
97	Qh	101	CDL	CA3-OA5-PA1-OA4
97	Qh	101	CDL	CB3-OB5-PB2-OB2
97	Qh	101	CDL	CB3-OB5-PB2-OB3
97	Qj	202	CDL	CA3-OA5-PA1-OA2
97	Qj	202	CDL	CA3-OA5-PA1-OA3
97	Qj	202	CDL	CB2-OB2-PB2-OB3
97	Qj	202	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
97	Qj	202	CDL	CB3-OB5-PB2-OB3
99	A9	501	NDP	C5D-O5D-PN-O3
99	A9	501	NDP	C5D-O5D-PN-O1N
100	AB	201	ZMP	C16-C17-C18-C21
100	AB	201	ZMP	O1-C10-S1-C11
100	AB	201	ZMP	C7-C8-C9-C10
100	AC	201	ZMP	C19-C18-C21-O5
100	AC	201	ZMP	C20-C18-C21-O5
100	AC	201	ZMP	C17-C18-C21-O5
101	C1	501	HEA	C1A-C2A-CAA-CBA
101	C1	501	HEA	C3A-C2A-CAA-CBA
101	C1	501	HEA	C2A-C3A-CMA-OMA
101	C1	501	HEA	C4A-C3A-CMA-OMA
101	C1	501	HEA	C2D-C3D-CAD-CBD
101	C1	501	HEA	C4D-C3D-CAD-CBD
101	C1	502	HEA	C2A-C3A-CMA-OMA
101	C1	502	HEA	C4A-C3A-CMA-OMA
101	C1	502	HEA	C11-C12-C13-C14
101	C1	502	HEA	C13-C14-C15-C16
101	C1	502	HEA	C13-C14-C15-C26
101	C1	502	HEA	C17-C18-C19-C20
101	C1	502	HEA	C17-C18-C19-C27
104	C2	201	PX2	C1-O4-P1-O1
104	C2	201	PX2	C1-O4-P1-O2
104	C2	201	PX2	C1-O4-P1-O3
104	QJ	201	PX2	C1-O4-P1-O1
104	QJ	201	PX2	C1-O4-P1-O2
104	QJ	201	PX2	C1-O4-P1-O3
104	QJ	202	PX2	C1-O4-P1-O1
104	QJ	202	PX2	C1-O4-P1-O2
104	QJ	202	PX2	C1-O4-P1-O3
104	QJ	202	PX2	C17-C16-O7-C2
105	N4	504	U10	C1-C6-C7-C8
105	N4	504	U10	C5-C6-C7-C8
106	QC	401	HEM	C2C-C3C-CAC-CBC
106	QC	401	HEM	C4C-C3C-CAC-CBC
107	QD	301	HEC	C2B-C3B-CAB-CBB
107	Qd	301	HEC	C2B-C3B-CAB-CBB
107	Qd	301	HEC	C4B-C3B-CAB-CBB
107	Qd	301	HEC	C2C-C3C-CAC-CBC
108	V1	601	FMN	C5'-O5'-P-O2P
108	V1	601	FMN	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
96	4D	203	S12	O51-C5-O52-C4
104	QJ	202	PX2	O8-C16-O7-C2
100	AB	201	ZMP	C14-C13-N1-C12
100	AC	201	ZMP	C14-C13-N1-C12
101	C1	502	HEA	C3A-C2A-CAA-CBA
96	4D	203	S12	C6-C5-O52-C4
101	C1	501	HEA	C17-C18-C19-C27
101	C1	501	HEA	C17-C18-C19-C20
101	C1	502	HEA	C1A-C2A-CAA-CBA
94	A1	201	PC1	C11-C12-N-C13
97	EA	202	CDL	O1-C1-CA2-OA2
97	QH	101	CDL	O1-C1-CA2-OA2
100	AC	201	ZMP	C3-C4-C5-C6
105	N4	504	U10	C30-C29-C31-C32
105	N4	504	U10	C28-C29-C31-C32
101	C1	501	HEA	C19-C20-C21-C22
101	C1	502	HEA	C15-C16-C17-C18
101	C1	502	HEA	C19-C20-C21-C22
97	Qh	101	CDL	CA4-CA3-OA5-PA1
101	C1	502	HEA	C21-C22-C23-C25
100	AB	201	ZMP	O2-C13-N1-C12
100	AC	201	ZMP	O2-C13-N1-C12
97	QH	101	CDL	CB2-C1-CA2-OA2
97	QH	102	CDL	CB2-C1-CA2-OA2
94	7A	201	PC1	C11-C12-N-C15
94	Qc	404	PC1	C11-C12-N-C13
100	AC	201	ZMP	C1-C2-C3-C4
97	AL	303	CDL	O1-C1-CB2-OB2
97	AM	202	CDL	O1-C1-CB2-OB2
97	QH	102	CDL	O1-C1-CA2-OA2
94	B8	301	PC1	C27-C28-C29-C2A
97	B3	101	CDL	CA7-C31-C32-C33
97	E7	301	CDL	OB5-CB3-CB4-OB6
94	C1	505	PC1	O21-C2-C3-O31
95	4D	202	3PE	O21-C2-C3-O31
97	C4	201	CDL	CB7-C71-C72-C73
94	G2	301	PC1	C11-C12-N-C15
94	C1	505	PC1	C21-C22-C23-C24
94	ED	202	PC1	C21-C22-C23-C24
97	AL	302	CDL	CB5-C51-C52-C53
101	C1	502	HEA	C21-C22-C23-C24
97	AM	202	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
94	A9	502	PC1	C2-C3-O31-C31
94	A1	201	PC1	C22-C23-C24-C25
97	N1	701	CDL	O1-C1-CA2-OA2
97	C4	203	CDL	CA5-C11-C12-C13
97	QH	101	CDL	CA5-C11-C12-C13
104	QJ	202	PX2	C4-C5-C6-C7
97	AL	303	CDL	CA2-C1-CB2-OB2
97	N1	701	CDL	CB2-C1-CA2-OA2
104	QJ	202	PX2	C17-C18-C19-C20
94	4A	302	PC1	C11-C12-N-C13
94	4A	302	PC1	C11-C12-N-C14
94	7A	201	PC1	C11-C12-N-C13
94	A1	201	PC1	C11-C12-N-C14
94	E4	402	PC1	C11-C12-N-C13
94	Qc	404	PC1	C11-C12-N-C14
94	QI	101	PC1	C32-C33-C34-C35
104	QJ	201	PX2	C4-C5-C6-C7
97	AM	201	CDL	C53-C54-C55-C56
97	QH	102	CDL	C1-CB2-OB2-PB2
97	Qc	405	CDL	C1-CA2-OA2-PA1
106	QC	401	HEM	C2A-CAA-CBA-CGA
106	Qc	402	HEM	C2A-CAA-CBA-CGA
97	AL	303	CDL	CB7-C71-C72-C73
95	4D	202	3PE	C27-C28-C29-C2A
94	4A	302	PC1	C11-C12-N-C15
94	A1	201	PC1	C11-C12-N-C15
94	E8	302	PC1	C11-C12-N-C14
94	AM	203	PC1	C24-C25-C26-C27
97	Qd	302	CDL	C75-C76-C77-C78
95	B4	201	3PE	C31-C32-C33-C34
94	ED	201	PC1	C28-C29-C2A-C2B
97	N1	701	CDL	C11-C12-C13-C14
94	A9	503	PC1	C32-C33-C34-C35
94	B5	202	PC1	C2E-C2F-C2G-C2H
96	4D	203	S12	C16-C17-C18-C19
97	4E	202	CDL	C62-C63-C64-C65
94	E9	202	PC1	C32-C33-C34-C35
96	4D	203	S12	C18-C19-C20-C21
97	N1	701	CDL	C13-C14-C15-C16
104	QJ	201	PX2	C6-C7-C8-C9
100	AC	201	ZMP	S1-C11-C12-N1
100	AB	201	ZMP	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
104	QJ	202	PX2	C21-C22-C23-C24
94	B5	201	PC1	C26-C27-C28-C29
97	4E	202	CDL	C56-C57-C58-C59
100	AC	201	ZMP	C22-C1-C2-C3
94	N4	505	PC1	C35-C36-C37-C38
94	AM	203	PC1	C25-C26-C27-C28
94	B5	202	PC1	C2C-C2D-C2E-C2F
101	C1	502	HEA	C27-C19-C20-C21
94	QC	404	PC1	C2-C3-O31-C31
97	E6	401	CDL	CA7-C31-C32-C33
97	B3	101	CDL	C51-C52-C53-C54
94	N4	505	PC1	C22-C23-C24-C25
96	4D	203	S12	C15-C16-C17-C18
104	QJ	202	PX2	C6-C7-C8-C9
97	N1	701	CDL	CB3-CB4-CB6-OB8
97	Qh	101	CDL	CA3-CA4-CA6-OA8
96	4D	203	S12	C11-C10-C9-C8
104	QJ	201	PX2	C10-C11-C12-C13
94	7A	201	PC1	C31-C32-C33-C34
94	ED	201	PC1	C21-C22-C23-C24
95	C1	506	3PE	C31-C32-C33-C34
97	A3	201	CDL	CA5-C11-C12-C13
100	AB	201	ZMP	C1-C2-C3-C4
104	QJ	201	PX2	C20-C21-C22-C23
94	E4	402	PC1	C33-C34-C35-C36
94	7A	201	PC1	C11-C12-N-C14
94	ED	202	PC1	C11-C12-N-C13
94	Qc	404	PC1	C11-C12-N-C15
104	QJ	201	PX2	C5-C6-C7-C8
97	Qd	302	CDL	C1-CB2-OB2-PB2
94	AM	204	PC1	C23-C24-C25-C26
94	A1	201	PC1	C31-C32-C33-C34
94	B5	201	PC1	C31-C32-C33-C34
94	AM	204	PC1	C2C-C2D-C2E-C2F
97	AL	302	CDL	C32-C33-C34-C35
104	QJ	202	PX2	C22-C23-C24-C25
97	QH	101	CDL	C41-C42-C43-C44
97	4E	202	CDL	C31-C32-C33-C34
94	N3	301	PC1	C26-C27-C28-C29
94	N4	505	PC1	C32-C33-C34-C35
97	E4	401	CDL	C37-C38-C39-C40
104	QJ	201	PX2	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
97	QJ	203	CDL	C12-C13-C14-C15
97	AL	303	CDL	C51-C52-C53-C54
95	7A	202	3PE	C36-C37-C38-C39
100	AB	201	ZMP	C13-C14-C15-N2
104	C2	201	PX2	C11-C10-C9-C8
94	E9	202	PC1	C22-C23-C24-C25
94	N1	702	PC1	C2B-C2C-C2D-C2E
95	C1	507	3PE	C36-C37-C38-C39
97	QH	102	CDL	C51-C52-C53-C54
97	C4	203	CDL	CA7-C31-C32-C33
97	7C	201	CDL	C43-C44-C45-C46
97	N5	603	CDL	C42-C43-C44-C45
94	N1	703	PC1	C22-C23-C24-C25
95	N5	602	3PE	C35-C36-C37-C38
101	C1	501	HEA	C27-C19-C20-C21
106	QC	402	HEM	C2C-C3C-CAC-CBC
106	Qc	403	HEM	C2C-C3C-CAC-CBC
94	AM	203	PC1	C11-C12-N-C13
94	B5	202	PC1	C11-C12-N-C13
94	E4	402	PC1	C11-C12-N-C14
94	E4	402	PC1	C11-C12-N-C15
94	E8	302	PC1	C11-C12-N-C15
94	ED	201	PC1	C11-C12-N-C14
94	ED	202	PC1	C11-C12-N-C14
94	G2	301	PC1	C11-C12-N-C13
94	G2	301	PC1	C11-C12-N-C14
94	N1	702	PC1	C11-C12-N-C15
94	N3	301	PC1	C11-C12-N-C15
94	Qc	401	PC1	C11-C12-N-C13
94	Qe	303	PC1	C11-C12-N-C15
97	AL	302	CDL	C35-C36-C37-C38
104	QJ	201	PX2	C7-C8-C9-C10
97	7C	201	CDL	C12-C13-C14-C15
94	Qj	201	PC1	C2D-C2E-C2F-C2G
95	4D	202	3PE	C21-C22-C23-C24
97	N5	603	CDL	CA7-C31-C32-C33
97	QC	403	CDL	OA5-CA3-CA4-OA6
97	Qd	302	CDL	OA5-CA3-CA4-OA6
94	AM	203	PC1	C39-C3A-C3B-C3C
101	C1	501	HEA	C15-C16-C17-C18
105	N4	504	U10	C24-C26-C27-C28
97	E6	401	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
94	4A	301	PC1	C27-C28-C29-C2A
94	4E	201	PC1	C21-C22-C23-C24
94	E4	402	PC1	O21-C2-C3-O31
97	AL	303	CDL	OB6-CB4-CB6-OB8
97	QD	302	CDL	OA6-CA4-CA6-OA8
104	C2	201	PX2	C5-C6-C7-C8
95	C1	506	3PE	C33-C34-C35-C36
104	QJ	201	PX2	C21-C22-C23-C24
97	4E	202	CDL	C1-CB2-OB2-PB2
97	A3	201	CDL	C1-CA2-OA2-PA1
97	AL	302	CDL	CB4-CB3-OB5-PB2
97	EA	201	CDL	C1-CB2-OB2-PB2
94	N4	505	PC1	C37-C38-C39-C3A
106	Qc	403	HEM	C4D-C3D-CAD-CBD
97	A9	504	CDL	CB2-C1-CA2-OA2
97	EA	202	CDL	CB2-C1-CA2-OA2
97	B3	101	CDL	O1-C1-CB2-OB2
95	N5	602	3PE	C2C-C2D-C2E-C2F
97	B8	302	CDL	C58-C59-C60-C61
97	QH	101	CDL	C51-C52-C53-C54
97	A3	201	CDL	C71-C72-C73-C74
94	AL	301	PC1	C31-C32-C33-C34
94	G2	301	PC1	C21-C22-C23-C24
97	AM	202	CDL	C33-C34-C35-C36
97	C4	201	CDL	C59-C60-C61-C62
94	Qj	201	PC1	C3A-C3B-C3C-C3D
94	AN	301	PC1	C35-C36-C37-C38
94	N1	702	PC1	C37-C38-C39-C3A
94	E8	302	PC1	C11-C12-N-C13
94	ED	202	PC1	C11-C12-N-C15
100	AB	201	ZMP	O3-C16-C17-O4
100	AB	201	ZMP	C22-C1-C2-C3
104	QJ	202	PX2	C19-C20-C21-C22
97	AM	201	CDL	C56-C57-C58-C59
95	E9	201	3PE	C27-C28-C29-C2A
95	C1	506	3PE	O11-C1-C2-C3
97	QD	302	CDL	OA5-CA3-CA4-CA6
97	QJ	203	CDL	OB5-CB3-CB4-CB6
97	Qh	101	CDL	OB5-CB3-CB4-CB6
97	EA	202	CDL	C53-C54-C55-C56
94	B5	202	PC1	C21-C22-C23-C24
97	Qe	302	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
94	B5	202	PC1	C24-C25-C26-C27
97	Qd	302	CDL	C33-C34-C35-C36
100	AB	201	ZMP	C1-C22-C23-C24
94	4A	302	PC1	C38-C39-C3A-C3B
94	ED	201	PC1	C24-C25-C26-C27
97	N5	603	CDL	C17-C18-C19-C20
100	AB	201	ZMP	C6-C7-C8-C9
94	4A	302	PC1	C1-C2-C3-O31
94	4E	201	PC1	C1-C2-C3-O31
94	A9	502	PC1	C1-C2-C3-O31
94	B5	202	PC1	C1-C2-C3-O31
94	C1	505	PC1	C1-C2-C3-O31
94	E4	402	PC1	C1-C2-C3-O31
94	QC	404	PC1	C1-C2-C3-O31
97	AL	302	CDL	CA3-CA4-CA6-OA8
97	E6	401	CDL	CA3-CA4-CA6-OA8
97	QH	102	CDL	CA3-CA4-CA6-OA8
104	QJ	201	PX2	C1-C2-C3-O5
97	C4	201	CDL	C51-C52-C53-C54
95	7A	202	3PE	C23-C24-C25-C26
97	4E	202	CDL	CA5-C11-C12-C13
97	C4	201	CDL	C14-C15-C16-C17
94	AM	203	PC1	C11-C12-N-C14
94	B5	202	PC1	C11-C12-N-C15
94	ED	201	PC1	C11-C12-N-C15
94	N1	702	PC1	C11-C12-N-C13
94	N3	301	PC1	C11-C12-N-C14
94	AM	204	PC1	C27-C28-C29-C2A
97	QD	302	CDL	CA5-C11-C12-C13
104	QJ	201	PX2	C19-C20-C21-C22
104	QJ	201	PX2	C23-C24-C25-C26
104	QJ	202	PX2	C9-C10-C11-C12
94	ED	201	PC1	C25-C26-C27-C28
95	4D	202	3PE	C38-C39-C3A-C3B
97	A9	504	CDL	CB6-CB4-OB6-CB5
97	C4	203	CDL	C76-C77-C78-C79
104	C2	201	PX2	C4-C5-C6-C7
104	C2	201	PX2	C16-C17-C18-C19
97	7C	201	CDL	C39-C40-C41-C42
95	N5	602	3PE	O11-C1-C2-O21
97	QH	101	CDL	C35-C36-C37-C38
97	BM	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
100	AC	201	ZMP	C6-C7-C8-C9
97	C4	201	CDL	C61-C62-C63-C64
104	QJ	201	PX2	C18-C19-C20-C21
94	A1	201	PC1	C21-C22-C23-C24
97	A3	201	CDL	C52-C53-C54-C55
94	ED	202	PC1	O21-C2-C3-O31
97	Qh	101	CDL	OA6-CA4-CA6-OA8
104	QJ	201	PX2	O7-C2-C3-O5
95	4D	202	3PE	C3A-C3B-C3C-C3D
106	Qc	403	HEM	C2D-C3D-CAD-CBD
94	Qc	401	PC1	C11-C12-N-C14
94	B8	301	PC1	C24-C25-C26-C27
94	AM	203	PC1	C37-C38-C39-C3A
94	Qc	401	PC1	C27-C28-C29-C2A
101	C1	501	HEA	C3B-C11-C12-C13
101	C1	502	HEA	C3B-C11-C12-C13
95	4D	202	3PE	C23-C24-C25-C26
95	N4	503	3PE	C36-C37-C38-C39
94	E8	302	PC1	C22-C23-C24-C25
94	N1	703	PC1	C27-C28-C29-C2A
94	Qj	201	PC1	C22-C23-C24-C25
97	N5	603	CDL	CB5-C51-C52-C53
94	QD	303	PC1	C22-C23-C24-C25
94	AM	204	PC1	C31-C32-C33-C34
94	E8	302	PC1	C39-C3A-C3B-C3C
95	N4	503	3PE	C22-C23-C24-C25
97	E6	401	CDL	C51-C52-C53-C54
104	QJ	202	PX2	C11-C12-C13-C14
94	C3	201	PC1	C3E-C3F-C3G-C3H
94	N3	301	PC1	C2-C1-O11-P
94	N5	601	PC1	C22-C23-C24-C25
94	E8	302	PC1	O11-C1-C2-C3
95	4D	202	3PE	O11-C1-C2-C3
95	N5	602	3PE	O11-C1-C2-C3
97	E7	301	CDL	OA5-CA3-CA4-CA6
97	E7	301	CDL	OB5-CB3-CB4-CB6
97	QC	403	CDL	OA5-CA3-CA4-CA6
97	Qd	302	CDL	OA5-CA3-CA4-CA6
97	Qd	302	CDL	OB5-CB3-CB4-CB6
104	C2	201	PX2	O4-C1-C2-C3
104	QJ	201	PX2	O4-C1-C2-C3
94	B8	301	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
94	E4	402	PC1	C28-C29-C2A-C2B
94	E8	302	PC1	C2D-C2E-C2F-C2G
94	B5	202	PC1	C11-C12-N-C14
94	N1	702	PC1	C11-C12-N-C14
94	N3	301	PC1	C11-C12-N-C13
94	Qe	303	PC1	C11-C12-N-C13
100	AC	201	ZMP	N2-C16-C17-C18
94	E8	301	PC1	C24-C25-C26-C27
94	Qc	401	PC1	C3C-C3D-C3E-C3F
94	QC	404	PC1	C2B-C2C-C2D-C2E
97	7C	201	CDL	C34-C35-C36-C37
97	C4	203	CDL	C38-C39-C40-C41
104	C2	201	PX2	C12-C13-C14-C15
97	4E	202	CDL	C33-C34-C35-C36
95	4D	202	3PE	C32-C33-C34-C35
97	N1	701	CDL	CA7-C31-C32-C33
97	BM	201	CDL	C71-C72-C73-C74
94	N4	501	PC1	C1-C2-C3-O31
94	QD	303	PC1	C1-C2-C3-O31
95	4D	202	3PE	C1-C2-C3-O31
95	B4	201	3PE	C1-C2-C3-O31
97	AM	202	CDL	CA3-CA4-CA6-OA8
97	E7	301	CDL	CB3-CB4-CB6-OB8
97	QD	302	CDL	CA3-CA4-CA6-OA8
97	QH	102	CDL	CB3-CB4-CB6-OB8
95	4D	202	3PE	C24-C25-C26-C27
94	Qj	201	PC1	C37-C38-C39-C3A
94	A1	202	PC1	C21-C22-C23-C24
104	QJ	201	PX2	C17-C18-C19-C20
101	C1	501	HEA	C18-C19-C20-C21
97	A9	504	CDL	C15-C16-C17-C18
94	AM	203	PC1	C3C-C3D-C3E-C3F
95	B4	201	3PE	C33-C34-C35-C36
94	B5	201	PC1	O11-C1-C2-O21
94	N1	703	PC1	O11-C1-C2-O21
97	4E	202	CDL	OB5-CB3-CB4-OB6
97	QJ	203	CDL	OB5-CB3-CB4-OB6
97	Qd	302	CDL	OB5-CB3-CB4-OB6
97	Qj	202	CDL	OB5-CB3-CB4-OB6
104	QJ	201	PX2	O4-C1-C2-O7
97	A3	201	CDL	C11-C12-C13-C14
94	Qc	401	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
97	E6	401	CDL	CB4-CB3-OB5-PB2
94	E8	302	PC1	C2A-C2B-C2C-C2D
94	ED	202	PC1	C24-C25-C26-C27
94	N1	702	PC1	C2C-C2D-C2E-C2F
94	B5	202	PC1	O21-C2-C3-O31
94	N4	501	PC1	O21-C2-C3-O31
97	4E	202	CDL	OA6-CA4-CA6-OA8
97	E4	401	CDL	OA6-CA4-CA6-OA8
97	QH	102	CDL	OB6-CB4-CB6-OB8
97	Qj	202	CDL	OA6-CA4-CA6-OA8
97	Qc	405	CDL	C11-C12-C13-C14
94	E8	302	PC1	C31-C32-C33-C34
97	BM	201	CDL	CA5-C11-C12-C13
95	4D	202	3PE	C34-C35-C36-C37
97	7C	201	CDL	C58-C59-C60-C61
94	AL	301	PC1	C28-C29-C2A-C2B
104	C2	201	PX2	C5-C4-O5-C3
104	C2	201	PX2	C18-C19-C20-C21
94	AM	203	PC1	C11-C12-N-C15
94	E8	304	PC1	C11-C12-N-C15
94	ED	201	PC1	C11-C12-N-C13
94	E8	301	PC1	C31-C32-C33-C34
97	B8	302	CDL	C32-C31-CA7-OA8
97	C4	203	CDL	C19-C20-C21-C22
97	B3	101	CDL	CA2-C1-CB2-OB2
94	7A	201	PC1	O11-C1-C2-C3
94	B8	301	PC1	O11-C1-C2-C3
97	EA	202	CDL	OB5-CB3-CB4-CB6
97	N1	701	CDL	OB5-CB3-CB4-CB6
97	QD	302	CDL	OB5-CB3-CB4-CB6
97	QH	101	CDL	OA5-CA3-CA4-CA6
97	Qj	202	CDL	OB5-CB3-CB4-CB6
107	Qd	301	HEC	C4D-C3D-CAD-CBD
97	AM	201	CDL	C1-CA2-OA2-PA1
104	C2	201	PX2	O5-C4-C5-C6
104	C2	201	PX2	O6-C4-O5-C3
94	C3	201	PC1	C3F-C3G-C3H-C3I
97	N5	603	CDL	CA5-C11-C12-C13
100	AB	201	ZMP	C2-C3-C4-C5
106	QC	401	HEM	C2B-C3B-CAB-CBB
106	Qc	402	HEM	C2B-C3B-CAB-CBB
106	Qc	402	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
94	Qc	401	PC1	C11-C12-N-C15
94	Qe	303	PC1	C11-C12-N-C14
97	N5	603	CDL	C81-C82-C83-C84
97	C4	203	CDL	C21-C22-C23-C24
97	E7	301	CDL	C32-C33-C34-C35
94	7A	201	PC1	O11-C1-C2-O21
94	B8	301	PC1	O11-C1-C2-O21
95	C1	506	3PE	O11-C1-C2-O21
97	E7	301	CDL	OA5-CA3-CA4-OA6
97	N1	701	CDL	OB5-CB3-CB4-OB6
97	QD	302	CDL	OB5-CB3-CB4-OB6
97	Qh	101	CDL	OB5-CB3-CB4-OB6
104	C2	201	PX2	O4-C1-C2-O7
94	Qc	401	PC1	C33-C34-C35-C36
94	C1	505	PC1	C3B-C3C-C3D-C3E
94	AM	203	PC1	C1-C2-C3-O31
94	N1	703	PC1	C1-C2-C3-O31
97	E4	401	CDL	CA3-CA4-CA6-OA8
97	N1	701	CDL	C14-C15-C16-C17
104	C2	201	PX2	C9-C10-C11-C12
94	E8	301	PC1	C12-C11-O13-P
94	E8	304	PC1	C12-C11-O13-P
94	N1	703	PC1	C12-C11-O13-P
95	C1	507	3PE	C12-C11-O13-P
100	AB	201	ZMP	C16-C17-C18-C19
100	AB	201	ZMP	C16-C17-C18-C20
100	AC	201	ZMP	C16-C17-C18-C19
95	B4	201	3PE	C21-C22-C23-C24
97	N1	701	CDL	CA5-C11-C12-C13
94	A9	502	PC1	O21-C2-C3-O31
94	AM	203	PC1	O21-C2-C3-O31
94	QC	404	PC1	O21-C2-C3-O31
95	B4	201	3PE	O21-C2-C3-O31
97	A9	504	CDL	OB6-CB4-CB6-OB8
97	AL	302	CDL	OA6-CA4-CA6-OA8
97	AM	202	CDL	OA6-CA4-CA6-OA8
97	C4	201	CDL	OB6-CB4-CB6-OB8
97	EA	202	CDL	OA6-CA4-CA6-OA8
97	QH	102	CDL	OA6-CA4-CA6-OA8
94	E8	304	PC1	C11-C12-N-C13
95	B4	201	3PE	C25-C26-C27-C28
94	A1	201	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
94	N5	601	PC1	O31-C31-C32-C33
94	B5	202	PC1	C3B-C3C-C3D-C3E
94	ED	202	PC1	C22-C23-C24-C25
95	4D	201	3PE	C2-C1-O11-P
97	AM	202	CDL	CB4-CB3-OB5-PB2
94	C1	505	PC1	C36-C37-C38-C39
94	A9	502	PC1	C31-C32-C33-C34
94	4A	302	PC1	O13-C11-C12-N
94	7A	201	PC1	O13-C11-C12-N
94	A9	502	PC1	O13-C11-C12-N
94	AN	301	PC1	O13-C11-C12-N
94	B8	301	PC1	O13-C11-C12-N
94	E8	301	PC1	O13-C11-C12-N
94	E8	303	PC1	O13-C11-C12-N
94	E8	304	PC1	O13-C11-C12-N
94	N4	501	PC1	O13-C11-C12-N
94	N4	502	PC1	O13-C11-C12-N
94	QD	303	PC1	O13-C11-C12-N
94	Qc	404	PC1	O13-C11-C12-N
96	4D	203	S12	N-CA-CB-OG
99	A9	501	NDP	PN-O3-PA-O1A
97	7C	201	CDL	C54-C55-C56-C57
97	AM	202	CDL	C17-C18-C19-C20
97	Qd	302	CDL	C60-C61-C62-C63
94	AL	301	PC1	C11-C12-N-C14
100	AC	201	ZMP	O3-C16-C17-O4
94	N4	505	PC1	C23-C24-C25-C26
94	B5	201	PC1	O11-C1-C2-C3
94	N1	703	PC1	O11-C1-C2-C3
94	Qe	303	PC1	O11-C1-C2-C3
97	4E	202	CDL	OB5-CB3-CB4-CB6
97	C4	202	CDL	OB5-CB3-CB4-CB6
94	ED	202	PC1	C35-C36-C37-C38
100	AB	201	ZMP	C19-C18-C21-O5
95	7A	202	3PE	C3C-C3D-C3E-C3F
100	AC	201	ZMP	C2-C3-C4-C5
97	E4	401	CDL	C31-C32-C33-C34
95	B4	201	3PE	C2-C3-O31-C31
94	A9	502	PC1	C2-C1-O11-P
94	AM	203	PC1	C2-C1-O11-P
97	QC	403	CDL	CA4-CA3-OA5-PA1
97	QH	102	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
108	V1	601	FMN	C4'-C5'-O5'-P
107	QD	301	HEC	C4B-C3B-CAB-CBB
107	QD	301	HEC	C4C-C3C-CAC-CBC
107	Qd	301	HEC	C4C-C3C-CAC-CBC
94	E8	302	PC1	O11-C1-C2-O21
94	Qe	303	PC1	O11-C1-C2-O21
95	4D	202	3PE	O11-C1-C2-O21
97	C4	201	CDL	OA5-CA3-CA4-OA6
97	E6	401	CDL	OA5-CA3-CA4-OA6
97	EA	202	CDL	OB5-CB3-CB4-OB6
97	QD	302	CDL	OA5-CA3-CA4-OA6
97	QH	101	CDL	OA5-CA3-CA4-OA6
94	AL	301	PC1	C11-C12-N-C15
104	C2	201	PX2	C21-C22-C23-C24
104	QJ	202	PX2	C11-C10-C9-C8
107	Qd	301	HEC	C1A-C2A-CAA-CBA
94	QD	303	PC1	O21-C2-C3-O31
97	E7	301	CDL	OB6-CB4-CB6-OB8
97	N1	701	CDL	OB6-CB4-CB6-OB8
97	N5	603	CDL	OB6-CB4-CB6-OB8
94	E8	303	PC1	C1-C2-C3-O31
94	N3	301	PC1	C1-C2-C3-O31
97	AL	303	CDL	CB3-CB4-CB6-OB8
97	C4	201	CDL	CB3-CB4-CB6-OB8
97	EA	201	CDL	CB3-CB4-CB6-OB8
97	EA	202	CDL	CA3-CA4-CA6-OA8
97	N5	603	CDL	CB3-CB4-CB6-OB8
104	C2	201	PX2	C6-C7-C8-C9
107	Qd	301	HEC	C3A-C2A-CAA-CBA
97	C4	203	CDL	C73-C74-C75-C76
94	ED	201	PC1	C3B-C3C-C3D-C3E
94	B5	202	PC1	C25-C26-C27-C28
94	4A	302	PC1	C11-O13-P-O12
94	4E	201	PC1	C11-O13-P-O14
94	7A	201	PC1	C1-O11-P-O14
94	A1	201	PC1	C1-O11-P-O12
94	A1	201	PC1	C1-O11-P-O14
94	A1	201	PC1	C1-O11-P-O13
94	E8	301	PC1	C11-O13-P-O14
94	E8	303	PC1	C1-O11-P-O14
94	E8	304	PC1	C1-O11-P-O14
94	ED	202	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
94	G2	301	PC1	C11-O13-P-O14
94	N1	703	PC1	C1-O11-P-O12
94	N4	501	PC1	C11-O13-P-O12
94	N4	502	PC1	C11-O13-P-O14
94	N4	502	PC1	C11-O13-P-O11
94	N4	502	PC1	C1-O11-P-O14
94	N4	505	PC1	C11-C12-N-C13
94	N5	601	PC1	C11-O13-P-O14
94	N5	601	PC1	C1-O11-P-O12
94	QC	404	PC1	C1-O11-P-O12
94	Qc	404	PC1	C1-O11-P-O12
94	Qc	404	PC1	C1-O11-P-O14
94	Qc	404	PC1	C1-O11-P-O13
95	4D	201	3PE	C1-O11-P-O12
95	4D	201	3PE	C1-O11-P-O14
95	4D	202	3PE	C11-O13-P-O14
95	7A	202	3PE	C11-O13-P-O14
95	C1	506	3PE	C1-O11-P-O14
95	C1	507	3PE	C11-O13-P-O11
95	C1	507	3PE	C11-O13-P-O12
95	C1	507	3PE	C11-O13-P-O14
96	4D	203	S12	CB-OG-P-O3
97	7C	201	CDL	CA2-OA2-PA1-OA4
97	A9	504	CDL	CA2-OA2-PA1-OA3
97	A9	504	CDL	CB3-OB5-PB2-OB3
97	AL	303	CDL	CA2-OA2-PA1-OA3
97	AM	201	CDL	CB2-OB2-PB2-OB5
97	AM	202	CDL	CB3-OB5-PB2-OB3
97	B3	101	CDL	CA2-OA2-PA1-OA3
97	B8	302	CDL	CA3-OA5-PA1-OA2
97	BM	201	CDL	CA3-OA5-PA1-OA3
97	C4	201	CDL	CA2-OA2-PA1-OA4
97	C4	201	CDL	CA3-OA5-PA1-OA3
97	EA	201	CDL	CB3-OB5-PB2-OB3
97	EA	202	CDL	CA3-OA5-PA1-OA3
97	EA	202	CDL	CB3-OB5-PB2-OB4
97	N5	603	CDL	CA2-OA2-PA1-OA3
97	N5	603	CDL	CA2-OA2-PA1-OA4
97	N5	603	CDL	CA2-OA2-PA1-OA5
97	N5	603	CDL	CA3-OA5-PA1-OA3
97	N5	603	CDL	CB2-OB2-PB2-OB5
97	QH	101	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
97	QH	101	CDL	CB3-OB5-PB2-OB4
97	QH	102	CDL	CA3-OA5-PA1-OA2
97	QH	102	CDL	CA3-OA5-PA1-OA3
97	QH	102	CDL	CB2-OB2-PB2-OB3
97	QH	102	CDL	CB3-OB5-PB2-OB3
97	Qc	405	CDL	CB3-OB5-PB2-OB2
97	Qd	302	CDL	CA3-OA5-PA1-OA2
97	Qd	302	CDL	CB2-OB2-PB2-OB4
97	Qd	302	CDL	CB2-OB2-PB2-OB5
97	Qh	101	CDL	CB3-OB5-PB2-OB4
97	Qj	202	CDL	CB2-OB2-PB2-OB4
97	Qj	202	CDL	CB3-OB5-PB2-OB2
97	Qj	202	CDL	CB3-OB5-PB2-OB4
99	A9	501	NDP	C5D-O5D-PN-O2N
107	QD	301	HEC	C2C-C3C-CAC-CBC
97	C4	203	CDL	C80-C81-C82-C83
95	N4	503	3PE	O31-C31-C32-C33
94	AL	301	PC1	C2-C1-O11-P
94	B5	201	PC1	C2-C1-O11-P
95	N5	602	3PE	C2-C1-O11-P
97	7C	201	CDL	CA4-CA3-OA5-PA1
97	AL	303	CDL	CB4-CB3-OB5-PB2
97	AM	202	CDL	C1-CB2-OB2-PB2
97	C4	203	CDL	CA4-CA3-OA5-PA1
97	EA	202	CDL	C1-CA2-OA2-PA1
97	N5	603	CDL	CB4-CB3-OB5-PB2
97	QD	302	CDL	C1-CA2-OA2-PA1
97	Qc	405	CDL	CA4-CA3-OA5-PA1
97	Qd	302	CDL	C59-C60-C61-C62
97	Qd	302	CDL	C56-C57-C58-C59
101	C1	502	HEA	C20-C21-C22-C23
97	C4	203	CDL	C54-C55-C56-C57
97	C4	202	CDL	C71-C72-C73-C74
94	AM	204	PC1	C25-C26-C27-C28
94	C3	201	PC1	C36-C37-C38-C39
94	A9	502	PC1	C1-C2-O21-C21
94	AN	301	PC1	C1-C2-O21-C21
94	N4	501	PC1	C3-C2-O21-C21
94	Qj	201	PC1	C3-C2-O21-C21
97	A9	504	CDL	CA6-CA4-OA6-CA5
97	Qj	202	CDL	CA6-CA4-OA6-CA5
97	Qj	202	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
94	4A	302	PC1	C3A-C3B-C3C-C3D
94	Qj	201	PC1	C11-C12-N-C13
97	AM	202	CDL	OA5-CA3-CA4-CA6
94	4A	301	PC1	C2A-C2B-C2C-C2D
94	C1	505	PC1	C37-C38-C39-C3A
94	N4	501	PC1	C31-C32-C33-C34
97	C4	202	CDL	OB5-CB3-CB4-OB6
97	N5	603	CDL	OA5-CA3-CA4-OA6
94	B5	201	PC1	C25-C26-C27-C28
97	4E	202	CDL	C71-C72-C73-C74
99	A9	501	NDP	O4D-C4D-C5D-O5D
94	B5	202	PC1	C35-C36-C37-C38
94	Qj	201	PC1	C27-C28-C29-C2A
95	4D	202	3PE	C2A-C2B-C2C-C2D
97	QH	101	CDL	C34-C35-C36-C37
97	E4	401	CDL	CB7-C71-C72-C73
94	QD	303	PC1	C2-C1-O11-P
97	A9	504	CDL	CA4-CA3-OA5-PA1
95	4D	201	3PE	O21-C2-C3-O31
97	EA	201	CDL	OB6-CB4-CB6-OB8
97	E6	401	CDL	O1-C1-CA2-OA2
94	B5	202	PC1	C3C-C3D-C3E-C3F
94	N4	505	PC1	C34-C35-C36-C37
97	QD	302	CDL	CA4-CA6-OA8-CA7
95	C1	506	3PE	C35-C36-C37-C38
94	4A	302	PC1	C26-C27-C28-C29
97	A9	504	CDL	CB3-CB4-CB6-OB8
94	AM	203	PC1	C29-C2A-C2B-C2C
97	N1	701	CDL	C31-C32-C33-C34
99	A9	501	NDP	PA-O3-PN-O1N
97	AL	302	CDL	C32-C31-CA7-OA8
97	QJ	203	CDL	C32-C31-CA7-OA8
99	A9	501	NDP	O4D-C1D-N1N-C6N
97	AM	201	CDL	C15-C16-C17-C18
95	B4	201	3PE	C34-C35-C36-C37
97	C4	203	CDL	C78-C79-C80-C81
97	C4	203	CDL	C53-C54-C55-C56
94	E8	304	PC1	C11-C12-N-C14
94	C3	201	PC1	C3A-C3B-C3C-C3D
104	C2	201	PX2	C17-C18-C19-C20
96	4D	203	S12	C3-C2-O2-P
100	AB	201	ZMP	S1-C11-C12-N1

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Mol	Chain	Res	Type	Atoms
97	A9	504	CDL	OA5-CA3-CA4-OA6
97	AM	201	CDL	OB5-CB3-CB4-OB6
97	E6	401	CDL	OA5-CA3-CA4-CA6
94	B5	201	PC1	C3E-C3F-C3G-C3H
106	QC	402	HEM	C4C-C3C-CAC-CBC
106	Qc	402	HEM	C4B-C3B-CAB-CBB
106	Qc	403	HEM	C4C-C3C-CAC-CBC
104	C2	201	PX2	C20-C21-C22-C23
95	4D	201	3PE	C23-C24-C25-C26
97	C4	203	CDL	C34-C35-C36-C37
97	N5	603	CDL	C32-C33-C34-C35
94	E8	303	PC1	O21-C2-C3-O31
94	4E	201	PC1	C23-C24-C25-C26
100	AB	201	ZMP	C4-C5-C6-C7
94	B8	301	PC1	O22-C21-C22-C23
94	B5	202	PC1	C36-C37-C38-C39
95	C1	506	3PE	C26-C27-C28-C29
97	4E	202	CDL	CA4-CA3-OA5-PA1
97	QC	403	CDL	CB4-CB3-OB5-PB2
97	E4	401	CDL	C35-C36-C37-C38
94	AL	301	PC1	C11-C12-N-C13
106	QC	401	HEM	C3D-CAD-CBD-CGD
107	Qd	301	HEC	C3D-CAD-CBD-CGD
106	QC	401	HEM	CAD-CBD-CGD-O1D
100	AC	201	ZMP	N2-C16-C17-O4
95	N4	503	3PE	C23-C24-C25-C26
94	A1	201	PC1	C1-C2-O21-C21
94	AL	301	PC1	C1-C2-O21-C21
94	B8	301	PC1	C3-C2-O21-C21
94	QD	303	PC1	C3-C2-O21-C21
94	Qc	404	PC1	C1-C2-O21-C21
95	C1	506	3PE	C3-C2-O21-C21
97	7C	201	CDL	CA3-CA4-OA6-CA5
97	7C	201	CDL	CB3-CB4-OB6-CB5
97	AM	202	CDL	CA6-CA4-OA6-CA5
97	AM	202	CDL	CB3-CB4-OB6-CB5
97	E6	401	CDL	CB6-CB4-OB6-CB5
97	QC	403	CDL	CB3-CB4-OB6-CB5
97	QH	101	CDL	CB3-CB4-OB6-CB5
97	QJ	203	CDL	CB3-CB4-OB6-CB5
97	Qh	101	CDL	CB3-CB4-OB6-CB5
97	Qj	202	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
94	7A	201	PC1	C33-C34-C35-C36
94	Qc	401	PC1	C2E-C2F-C2G-C2H
97	Qd	302	CDL	C35-C36-C37-C38
94	AM	204	PC1	C26-C27-C28-C29
95	4D	202	3PE	C36-C37-C38-C39
97	C4	203	CDL	C41-C42-C43-C44
106	QC	402	HEM	CAD-CBD-CGD-O2D
94	E8	302	PC1	C35-C36-C37-C38
106	Qc	402	HEM	CAD-CBD-CGD-O1D
107	Qd	301	HEC	CAD-CBD-CGD-O1D
94	4A	302	PC1	C29-C2A-C2B-C2C
97	7C	201	CDL	C1-CA2-OA2-PA1
97	E7	301	CDL	CA4-CA3-OA5-PA1
97	Qc	405	CDL	C1-CB2-OB2-PB2
101	C1	501	HEA	O11-C11-C12-C13
101	C1	502	HEA	O11-C11-C12-C13
106	QC	402	HEM	CAD-CBD-CGD-O1D
95	C1	507	3PE	O11-C1-C2-C3
97	AM	201	CDL	OB5-CB3-CB4-CB6
97	C4	201	CDL	OA5-CA3-CA4-CA6
105	N4	504	U10	C26-C27-C28-C29
94	N1	702	PC1	C23-C24-C25-C26
97	A9	504	CDL	OA6-CA4-CA6-OA8
106	Qc	402	HEM	CAD-CBD-CGD-O2D
107	QD	301	HEC	CAD-CBD-CGD-O1D
94	E8	301	PC1	C32-C33-C34-C35
97	C4	201	CDL	C13-C14-C15-C16
106	QC	401	HEM	CAD-CBD-CGD-O2D
104	QJ	202	PX2	C5-C6-C7-C8
94	7A	201	PC1	O21-C21-C22-C23
94	N1	702	PC1	O31-C31-C32-C33
97	7C	201	CDL	C32-C31-CA7-OA8
97	4E	202	CDL	C64-C65-C66-C67
95	B4	201	3PE	C29-C2A-C2B-C2C
97	E4	401	CDL	C41-C42-C43-C44
95	7A	202	3PE	C37-C38-C39-C3A
105	N4	504	U10	C12-C11-C9-C10
105	N4	504	U10	C20-C19-C21-C22
94	G2	301	PC1	C2-C1-O11-P
95	E9	201	3PE	C2-C1-O11-P
97	E4	401	CDL	C1-CB2-OB2-PB2
97	N1	701	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
97	7C	201	CDL	C53-C54-C55-C56
97	C4	203	CDL	C83-C84-C85-C86
94	AM	203	PC1	C27-C28-C29-C2A
94	ED	202	PC1	C1-C2-C3-O31
94	N5	601	PC1	C1-C2-C3-O31
97	QC	403	CDL	CA3-CA4-CA6-OA8
104	QJ	202	PX2	C23-C24-C25-C26
99	A9	501	NDP	C3D-C4D-C5D-O5D
94	4A	301	PC1	C28-C29-C2A-C2B
107	QD	301	HEC	CAD-CBD-CGD-O2D
94	AL	301	PC1	C2D-C2E-C2F-C2G
97	QC	403	CDL	OB5-CB3-CB4-OB6
104	QJ	202	PX2	O4-C1-C2-O7
94	E8	302	PC1	C3C-C3D-C3E-C3F
95	E9	201	3PE	C2C-C2D-C2E-C2F
104	QJ	202	PX2	C20-C21-C22-C23
107	Qd	301	HEC	CAD-CBD-CGD-O2D
94	Qj	201	PC1	C39-C3A-C3B-C3C
97	Qe	302	CDL	C14-C15-C16-C17
97	Qc	405	CDL	C52-C51-CB5-OB6
97	N5	603	CDL	C58-C59-C60-C61
107	QD	301	HEC	C1A-C2A-CAA-CBA
106	Qc	403	HEM	CAD-CBD-CGD-O1D
97	AL	302	CDL	C72-C73-C74-C75
97	C4	201	CDL	C77-C78-C79-C80
94	Qj	201	PC1	C28-C29-C2A-C2B
97	AM	202	CDL	CA2-C1-CB2-OB2
94	N4	505	PC1	C11-C12-N-C15
94	Qj	201	PC1	C11-C12-N-C14
101	C1	501	HEA	C11-C12-C13-C14
104	QJ	202	PX2	O7-C2-C3-O5
97	N1	701	CDL	CB5-C51-C52-C53
101	C1	501	HEA	CAD-CBD-CGD-O1D
105	N4	504	U10	C18-C19-C21-C22
97	AL	303	CDL	CA4-CA3-OA5-PA1
97	EA	201	CDL	CB4-CB3-OB5-PB2
97	EA	202	CDL	C1-CB2-OB2-PB2
97	QD	302	CDL	CB4-CB3-OB5-PB2
97	Qd	302	CDL	CA4-CA3-OA5-PA1
97	Qe	302	CDL	CA4-CA3-OA5-PA1
95	4D	202	3PE	C35-C36-C37-C38
95	B4	201	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
95	N4	503	3PE	C31-C32-C33-C34
97	Qe	302	CDL	C16-C17-C18-C19
107	QD	301	HEC	C3A-C2A-CAA-CBA
94	AM	204	PC1	O21-C21-C22-C23
95	E9	201	3PE	C29-C2A-C2B-C2C
94	4A	302	PC1	C24-C25-C26-C27
97	Qh	101	CDL	C52-C51-CB5-OB6
97	E6	401	CDL	CB5-C51-C52-C53
94	C3	201	PC1	C1-C2-O21-C21
94	C3	201	PC1	C3-C2-O21-C21
94	Qc	401	PC1	C3-C2-O21-C21
97	AM	202	CDL	CB6-CB4-OB6-CB5
97	E6	401	CDL	CB3-CB4-OB6-CB5
97	Qd	302	CDL	C51-C52-C53-C54
101	C1	501	HEA	CAD-CBD-CGD-O2D
106	QC	402	HEM	CAA-CBA-CGA-O2A
97	7C	201	CDL	C16-C17-C18-C19
97	C4	203	CDL	O1-C1-CA2-OA2
106	QC	402	HEM	CAA-CBA-CGA-O1A
97	QH	101	CDL	CA4-CA3-OA5-PA1
97	QJ	203	CDL	CA4-CA3-OA5-PA1
94	QC	404	PC1	O11-C1-C2-O21
94	N4	505	PC1	C11-C12-N-C14
94	Qj	201	PC1	C11-C12-N-C15
97	4E	202	CDL	CA3-CA4-CA6-OA8
97	4E	202	CDL	CB3-CB4-CB6-OB8
104	QJ	202	PX2	C1-C2-C3-O5
106	QC	401	HEM	C4B-C3B-CAB-CBB
106	Qc	402	HEM	C4C-C3C-CAC-CBC
97	QC	403	CDL	C51-C52-C53-C54
95	C1	507	3PE	C26-C27-C28-C29
100	AC	201	ZMP	C16-C17-C18-C20
95	N5	602	3PE	C23-C24-C25-C26
94	A9	502	PC1	C32-C33-C34-C35
97	C4	201	CDL	C38-C39-C40-C41
94	ED	201	PC1	C27-C28-C29-C2A
97	E7	301	CDL	C12-C11-CA5-OA6
97	AL	303	CDL	C53-C54-C55-C56
97	B8	302	CDL	C32-C31-CA7-OA9
97	QC	403	CDL	OA6-CA4-CA6-OA8
97	QH	101	CDL	OA6-CA4-CA6-OA8
95	C1	506	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
97	C4	202	CDL	C12-C11-CA5-OA6
97	E6	401	CDL	C12-C11-CA5-OA6
97	A9	504	CDL	OA5-CA3-CA4-CA6
97	A9	504	CDL	OB5-CB3-CB4-CB6
97	N5	603	CDL	OA5-CA3-CA4-CA6
97	QJ	203	CDL	OA5-CA3-CA4-CA6
105	N4	504	U10	C25-C24-C26-C27
97	E6	401	CDL	C32-C31-CA7-OA8
94	G2	301	PC1	C24-C25-C26-C27
97	C4	203	CDL	C39-C40-C41-C42
97	N1	701	CDL	C72-C71-CB7-OB8
94	E8	302	PC1	C36-C37-C38-C39
97	Qd	302	CDL	C1-CA2-OA2-PA1
107	Qd	301	HEC	C2D-C3D-CAD-CBD
97	C4	201	CDL	CA4-CA6-OA8-CA7
94	N4	502	PC1	O31-C31-C32-C33
97	EA	201	CDL	C52-C51-CB5-OB6
95	C1	506	3PE	C27-C28-C29-C2A
97	4E	202	CDL	C61-C62-C63-C64
94	4A	302	PC1	C36-C37-C38-C39
94	4A	302	PC1	O21-C21-C22-C23
94	N4	502	PC1	O21-C21-C22-C23
97	QC	403	CDL	C33-C34-C35-C36
97	7C	201	CDL	C72-C71-CB7-OB8
97	AL	303	CDL	C12-C11-CA5-OA6
97	E7	301	CDL	C32-C31-CA7-OA8
97	QC	403	CDL	C32-C31-CA7-OA8
100	AC	201	ZMP	O3-C16-C17-C18
96	4D	203	S12	OXT-C-CA-N
97	Qc	405	CDL	C52-C53-C54-C55
94	N1	702	PC1	O21-C21-C22-C23
94	N1	703	PC1	C32-C33-C34-C35
94	N4	505	PC1	C33-C34-C35-C36
94	E8	301	PC1	C29-C2A-C2B-C2C
97	Qd	302	CDL	C71-C72-C73-C74
95	C1	506	3PE	C34-C35-C36-C37
97	7C	201	CDL	C17-C18-C19-C20
97	N5	603	CDL	C41-C42-C43-C44
94	A9	503	PC1	O21-C21-C22-C23
94	ED	202	PC1	O21-C21-C22-C23
95	C1	507	3PE	O21-C21-C22-C23
95	4D	202	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
94	C1	505	PC1	C33-C34-C35-C36
106	Qc	403	HEM	CAD-CBD-CGD-O2D
97	4E	202	CDL	C12-C11-CA5-OA6
104	QJ	202	PX2	O5-C4-C5-C6
97	7C	201	CDL	OA6-CA4-CA6-OA8
97	E4	401	CDL	OB6-CB4-CB6-OB8
97	Qj	202	CDL	OB6-CB4-CB6-OB8
97	Qd	302	CDL	C54-C55-C56-C57
94	4E	201	PC1	O21-C21-C22-C23
94	A9	502	PC1	O31-C31-C32-C33
94	E8	301	PC1	O21-C21-C22-C23
94	Qc	401	PC1	O31-C31-C32-C33
97	7C	201	CDL	C12-C11-CA5-OA6
97	AM	201	CDL	C12-C11-CA5-OA6
97	B3	101	CDL	C72-C71-CB7-OB8
97	N1	701	CDL	C52-C51-CB5-OB6
97	QC	403	CDL	C72-C71-CB7-OB8
104	QJ	202	PX2	O7-C16-C17-C18
94	B5	202	PC1	C27-C28-C29-C2A
95	E9	201	3PE	C2B-C2C-C2D-C2E
97	Qj	202	CDL	C72-C71-CB7-OB8
94	N5	601	PC1	O32-C31-C32-C33
101	C1	501	HEA	CAA-CBA-CGA-O2A
100	AB	201	ZMP	C20-C18-C21-O5
100	AC	201	ZMP	C16-C17-C18-C21
104	C2	201	PX2	O6-C4-C5-C6
94	AL	301	PC1	O31-C31-C32-C33
94	N1	702	PC1	C2A-C2B-C2C-C2D
94	A1	201	PC1	C24-C25-C26-C27
94	B5	202	PC1	C34-C35-C36-C37
94	A1	201	PC1	C3-C2-O21-C21
94	AL	301	PC1	C3-C2-O21-C21
94	Qc	401	PC1	C1-C2-O21-C21
94	Qc	404	PC1	C3-C2-O21-C21
97	7C	201	CDL	CA6-CA4-OA6-CA5
97	AM	202	CDL	CA3-CA4-OA6-CA5
97	QC	403	CDL	CB6-CB4-OB6-CB5
97	QJ	203	CDL	CB6-CB4-OB6-CB5
97	Qh	101	CDL	CB6-CB4-OB6-CB5
97	Qj	202	CDL	CB6-CB4-OB6-CB5
97	Qj	202	CDL	C11-C12-C13-C14
97	N5	603	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
97	A3	201	CDL	C32-C31-CA7-OA8
107	QD	301	HEC	C4D-C3D-CAD-CBD
97	E6	401	CDL	C52-C51-CB5-OB6
97	QD	302	CDL	C52-C51-CB5-OB6
97	AL	302	CDL	CA4-CA3-OA5-PA1
97	Qe	302	CDL	C52-C51-CB5-OB6
95	N5	602	3PE	C29-C2A-C2B-C2C
94	B5	201	PC1	C3C-C3D-C3E-C3F
97	E6	401	CDL	C52-C51-CB5-OB7
95	C1	507	3PE	O11-C1-C2-O21
97	C4	201	CDL	C43-C44-C45-C46
94	N1	703	PC1	C33-C34-C35-C36
97	Qh	101	CDL	C54-C55-C56-C57
97	N5	603	CDL	C12-C11-CA5-OA6
97	QJ	203	CDL	C72-C71-CB7-OB8
97	4E	202	CDL	C12-C11-CA5-OA7
97	E6	401	CDL	C32-C31-CA7-OA9
97	EA	201	CDL	C52-C51-CB5-OB7
97	AM	202	CDL	C22-C23-C24-C25
94	N4	501	PC1	C33-C34-C35-C36
97	C4	203	CDL	C16-C17-C18-C19
94	AL	301	PC1	C2A-C2B-C2C-C2D
97	C4	202	CDL	C12-C11-CA5-OA7
97	A9	504	CDL	C13-C14-C15-C16
94	B5	201	PC1	C3B-C3C-C3D-C3E
94	N1	702	PC1	O22-C21-C22-C23
97	E6	401	CDL	C12-C11-CA5-OA7
97	N1	701	CDL	C72-C73-C74-C75
97	C4	201	CDL	C39-C40-C41-C42
97	C4	203	CDL	C22-C23-C24-C25
97	Qd	302	CDL	C81-C82-C83-C84
99	A9	501	NDP	O4B-C4B-C5B-O5B
94	4A	302	PC1	O22-C21-C22-C23
94	A9	503	PC1	O22-C21-C22-C23
94	ED	202	PC1	O22-C21-C22-C23
95	C1	507	3PE	O22-C21-C22-C23
97	7C	201	CDL	C72-C71-CB7-OB9
97	B3	101	CDL	C72-C71-CB7-OB9
97	E7	301	CDL	C12-C11-CA5-OA7
97	E7	301	CDL	C32-C31-CA7-OA9
94	AN	301	PC1	C3A-C3B-C3C-C3D
94	N3	301	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
97	Qc	405	CDL	OA6-CA4-CA6-OA8
97	AM	201	CDL	C13-C14-C15-C16
101	C1	502	HEA	CAA-CBA-CGA-O2A
94	E8	301	PC1	O22-C21-C22-C23
94	N4	502	PC1	O22-C21-C22-C23
94	N4	502	PC1	O32-C31-C32-C33
97	AL	303	CDL	C12-C11-CA5-OA7
97	N1	701	CDL	C72-C71-CB7-OB9
97	QC	403	CDL	C32-C31-CA7-OA9
94	B5	201	PC1	O31-C31-C32-C33
97	C4	203	CDL	C52-C51-CB5-OB6
97	QH	101	CDL	C12-C11-CA5-OA6
95	E9	201	3PE	C38-C39-C3A-C3B
97	B3	101	CDL	C35-C36-C37-C38
97	EA	202	CDL	C73-C74-C75-C76
97	Qj	202	CDL	CA3-CA4-CA6-OA8
100	AB	201	ZMP	N2-C16-C17-O4
94	ED	201	PC1	C32-C33-C34-C35
94	A9	502	PC1	O32-C31-C32-C33
94	Qc	401	PC1	O32-C31-C32-C33
97	Qj	202	CDL	C72-C71-CB7-OB9
94	N4	501	PC1	O21-C21-C22-C23
97	N1	701	CDL	C52-C51-CB5-OB7
97	QC	403	CDL	C72-C71-CB7-OB9
104	QJ	202	PX2	O8-C16-C17-C18
94	AM	203	PC1	C3D-C3E-C3F-C3G
94	4A	302	PC1	C23-C24-C25-C26
94	QD	303	PC1	O31-C31-C32-C33
97	N5	603	CDL	C52-C51-CB5-OB6
94	N1	702	PC1	O11-C1-C2-C3
97	AM	201	CDL	C12-C11-CA5-OA7
95	B4	201	3PE	O31-C31-C32-C33
97	E6	401	CDL	C71-C72-C73-C74
97	C4	203	CDL	C15-C16-C17-C18
97	Qd	302	CDL	C19-C20-C21-C22
97	BM	201	CDL	C52-C51-CB5-OB6
97	QH	102	CDL	C52-C51-CB5-OB6
97	Qh	101	CDL	C12-C11-CA5-OA6
99	A9	501	NDP	PN-O3-PA-O2A
94	4E	201	PC1	O22-C21-C22-C23
94	AL	301	PC1	O32-C31-C32-C33
94	Qc	404	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
94	A1	202	PC1	O31-C31-C32-C33
94	C3	201	PC1	O21-C21-C22-C23
97	C4	203	CDL	C52-C51-CB5-OB7
104	QJ	202	PX2	O6-C4-C5-C6

There are no ring outliers.

40 monomers are involved in 102 short contacts:

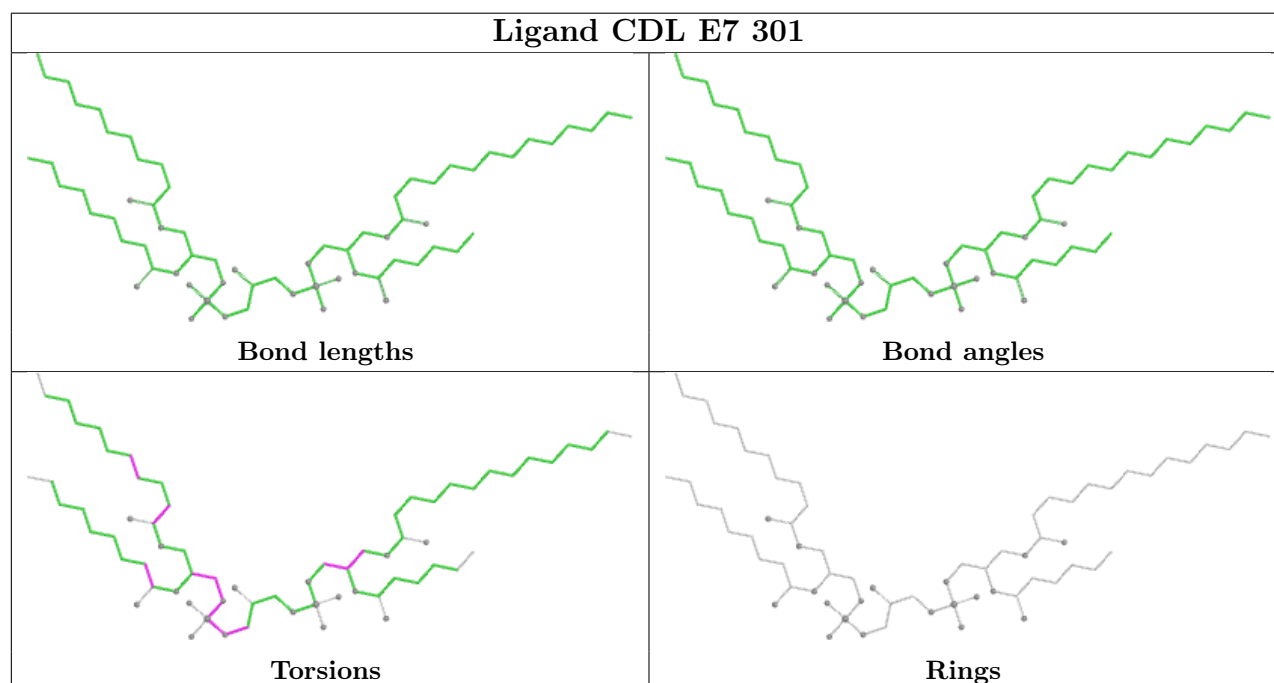
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AM	202	CDL	3	0
97	7C	201	CDL	1	0
94	QI	101	PC1	1	0
104	QJ	201	PX2	4	0
94	B5	201	PC1	1	0
100	AB	201	ZMP	3	0
107	QD	301	HEC	5	0
97	EA	201	CDL	1	0
97	Qc	405	CDL	1	0
105	N4	504	U10	4	0
97	B3	101	CDL	1	0
92	S7	301	SF4	1	0
106	QC	402	HEM	1	0
100	AC	201	ZMP	7	0
97	A9	504	CDL	1	0
106	QC	401	HEM	1	0
95	B4	201	3PE	1	0
97	B8	302	CDL	1	0
107	Qd	301	HEC	6	0
97	N1	701	CDL	1	0
106	Qc	402	HEM	5	0
97	E6	401	CDL	1	0
104	C2	201	PX2	4	0
97	A3	201	CDL	1	0
97	C4	203	CDL	2	0
97	QH	102	CDL	1	0
94	A1	202	PC1	1	0
97	Qd	302	CDL	2	0
97	Qj	202	CDL	1	0
94	E9	202	PC1	1	0
97	E4	401	CDL	2	0
104	QJ	202	PX2	4	0
97	QH	101	CDL	1	0

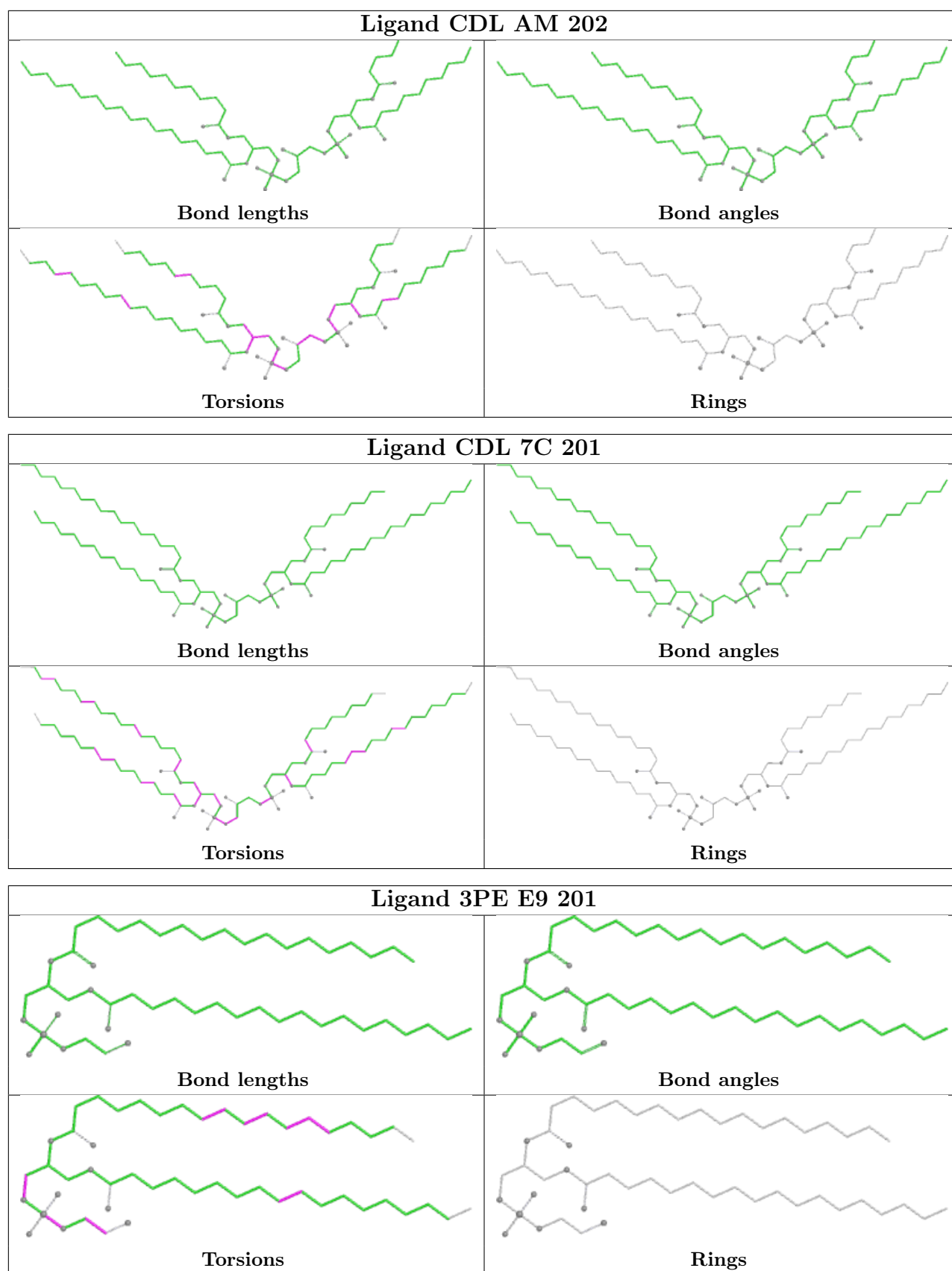
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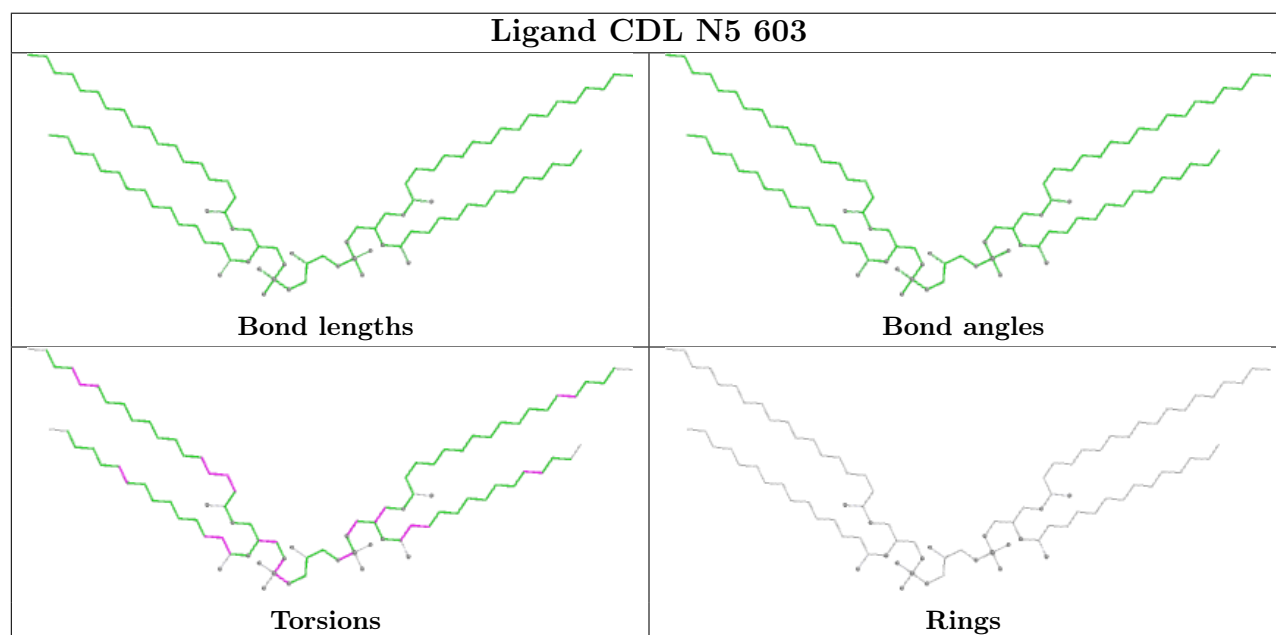
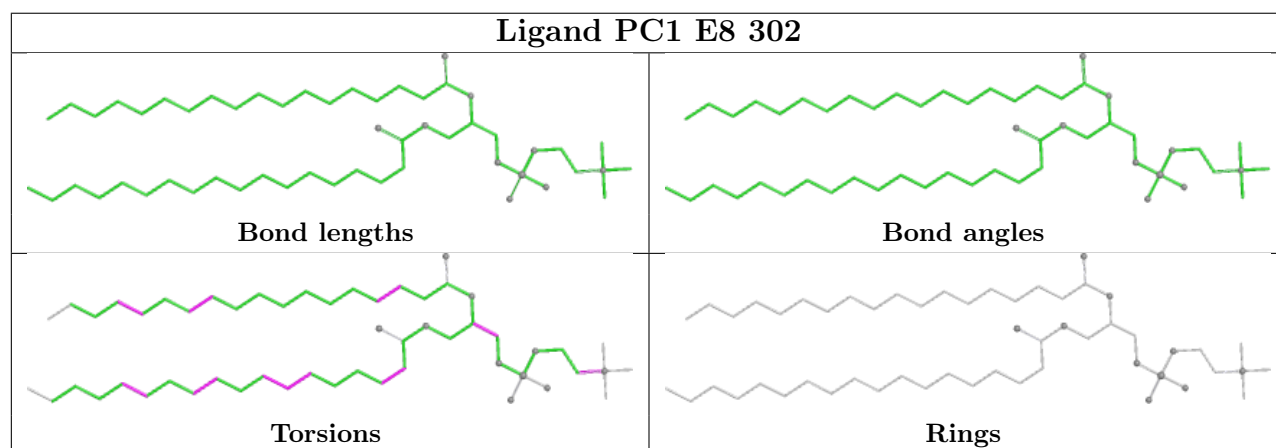
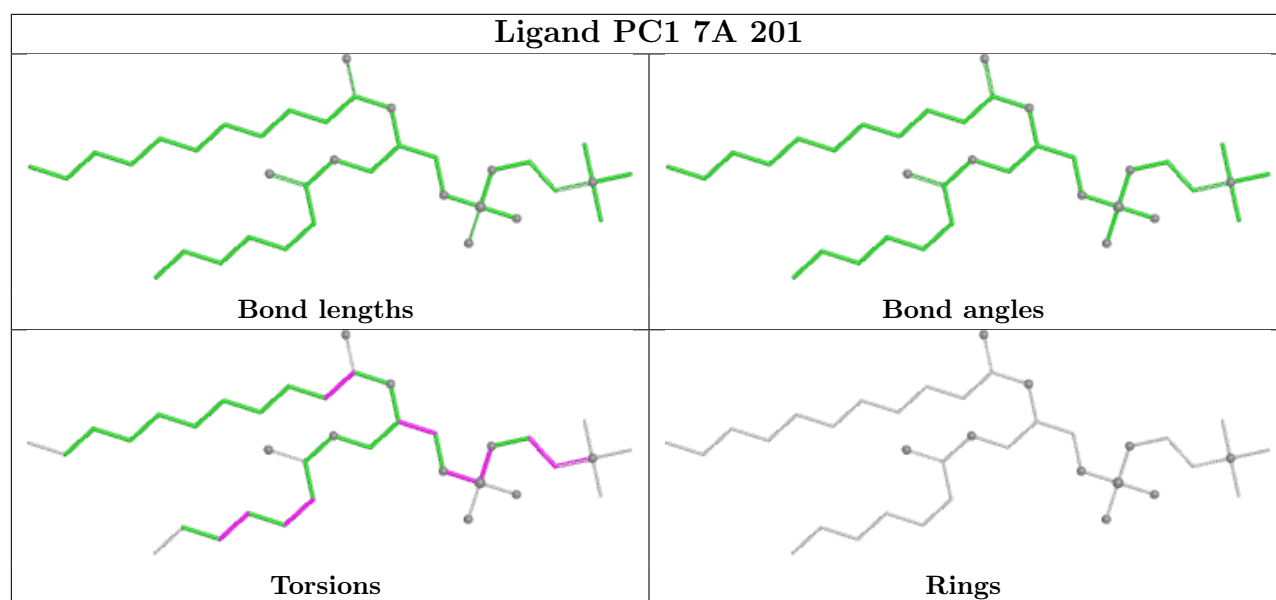
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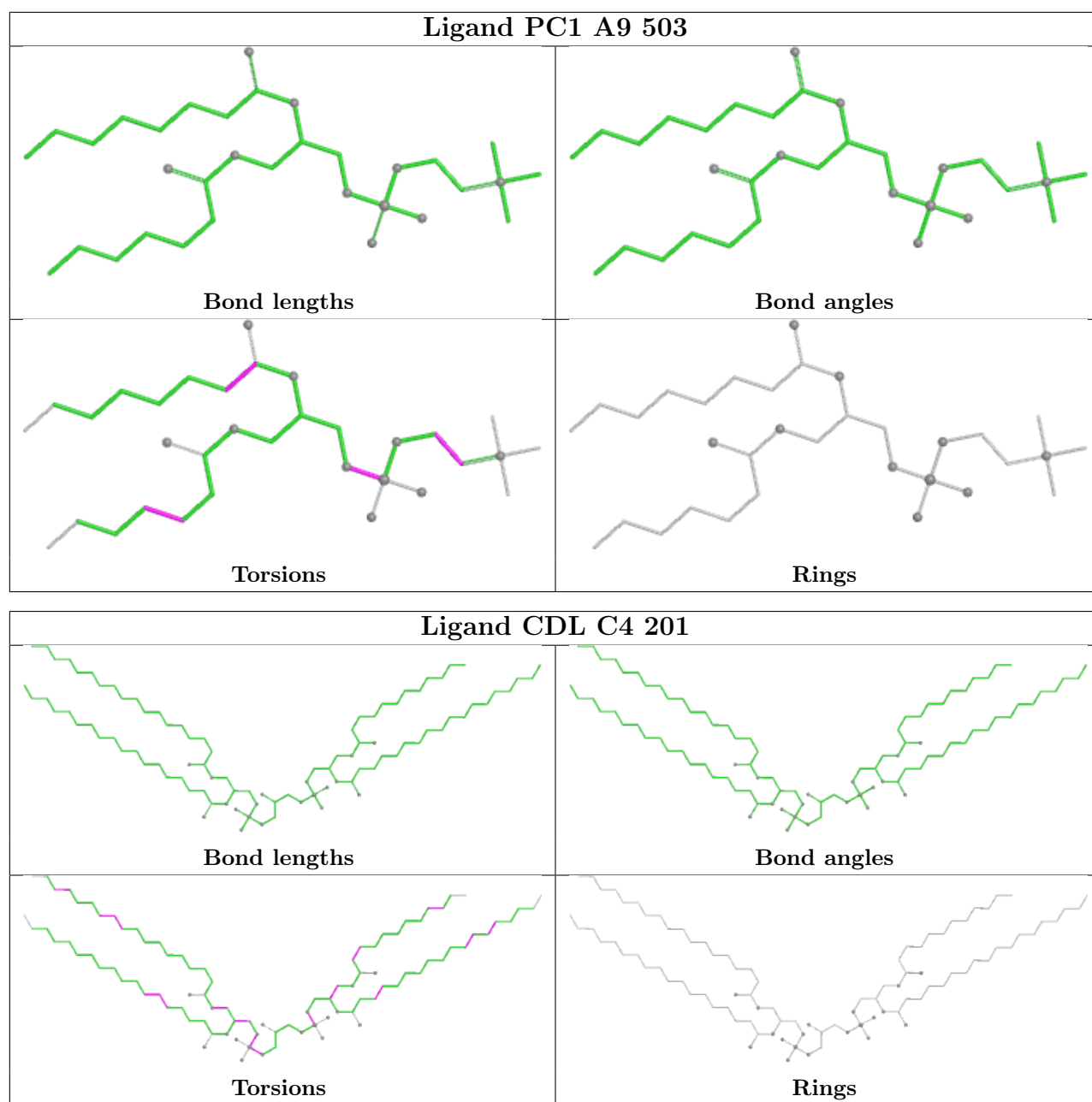
Mol	Chain	Res	Type	Clashes	Symm-Clashes
106	Qc	403	HEM	5	0
94	B5	202	PC1	2	0
94	AM	204	PC1	1	0
97	QJ	203	CDL	1	0
101	C1	502	HEA	7	0
101	C1	501	HEA	14	0
97	AM	201	CDL	1	0

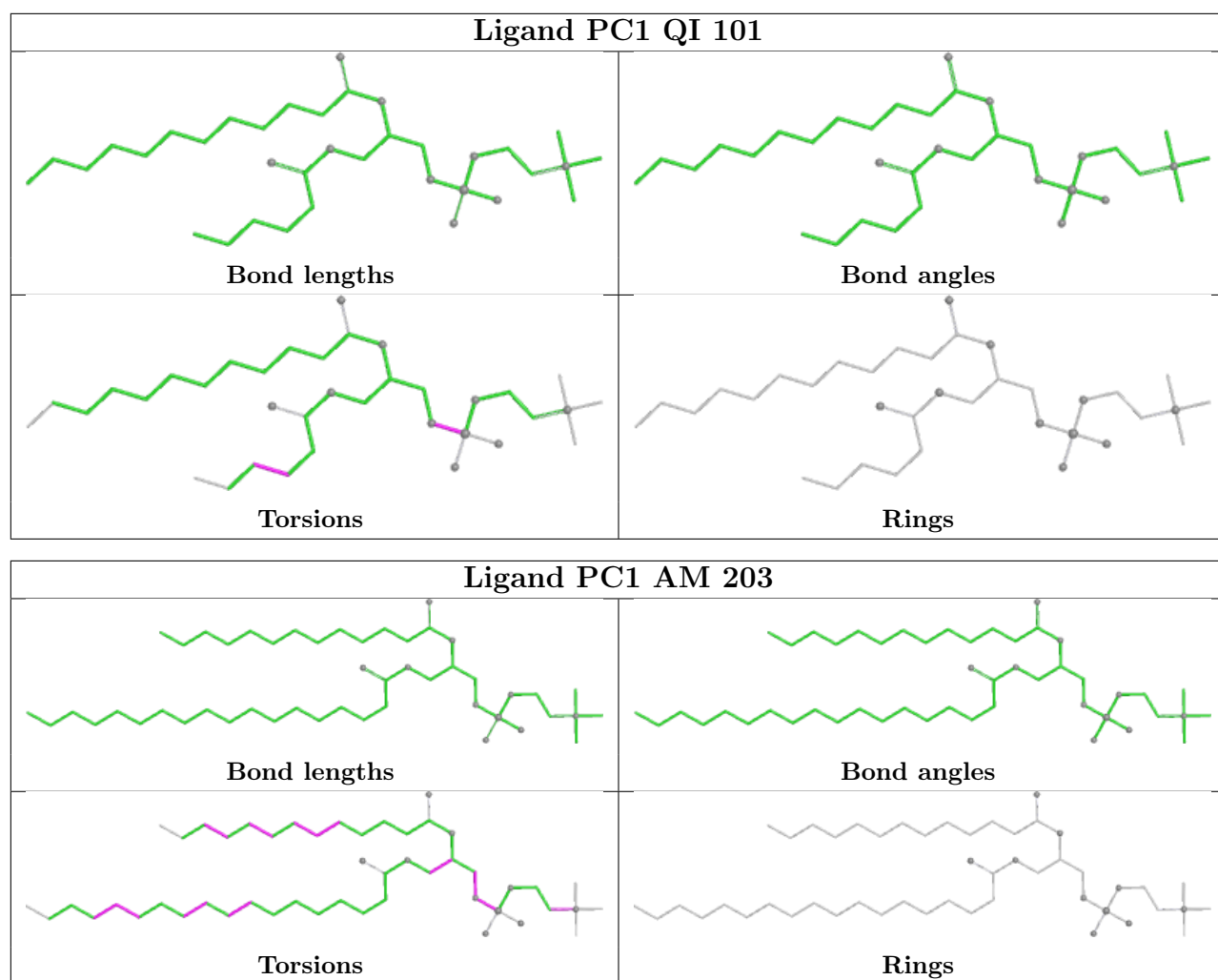
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

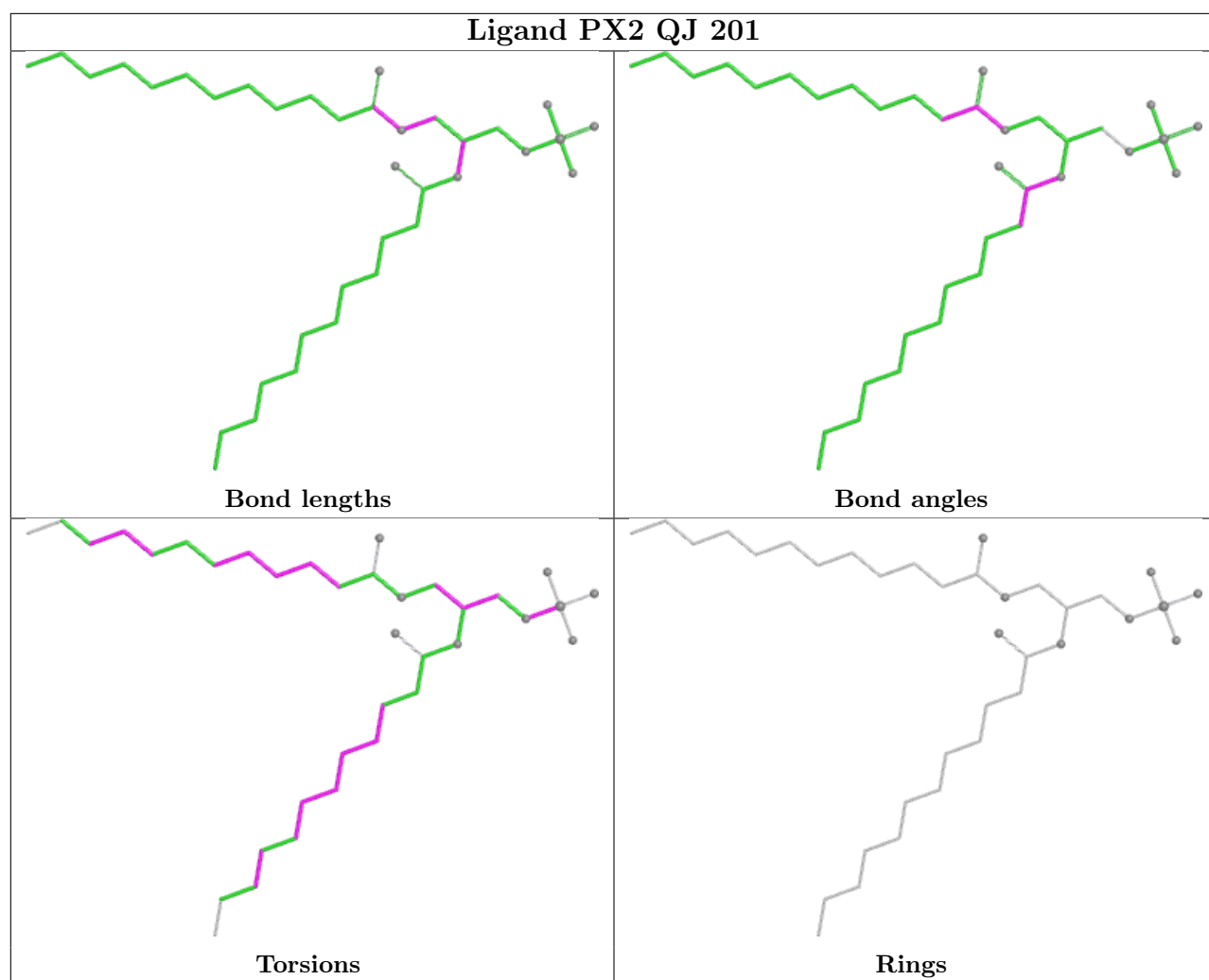


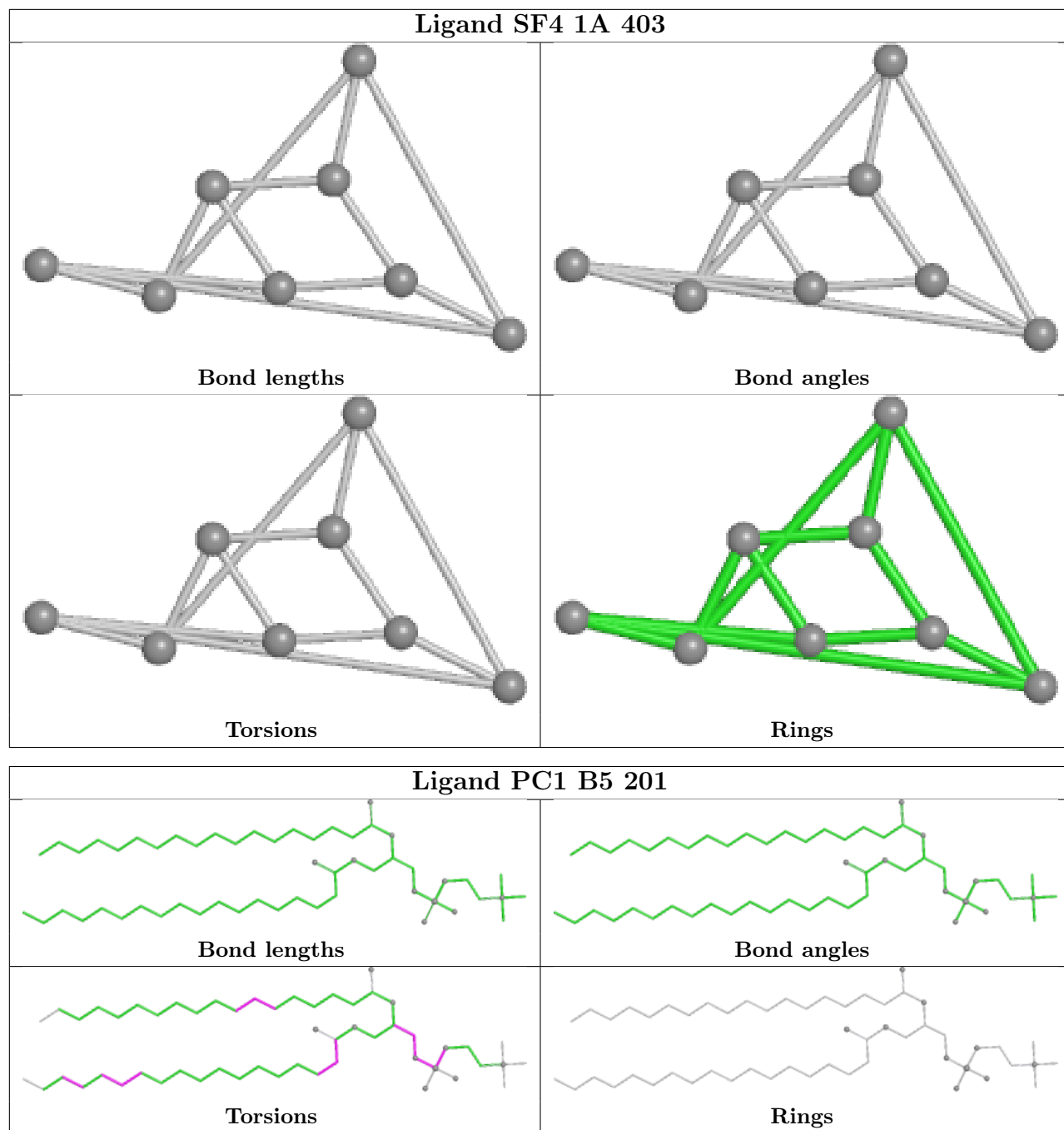


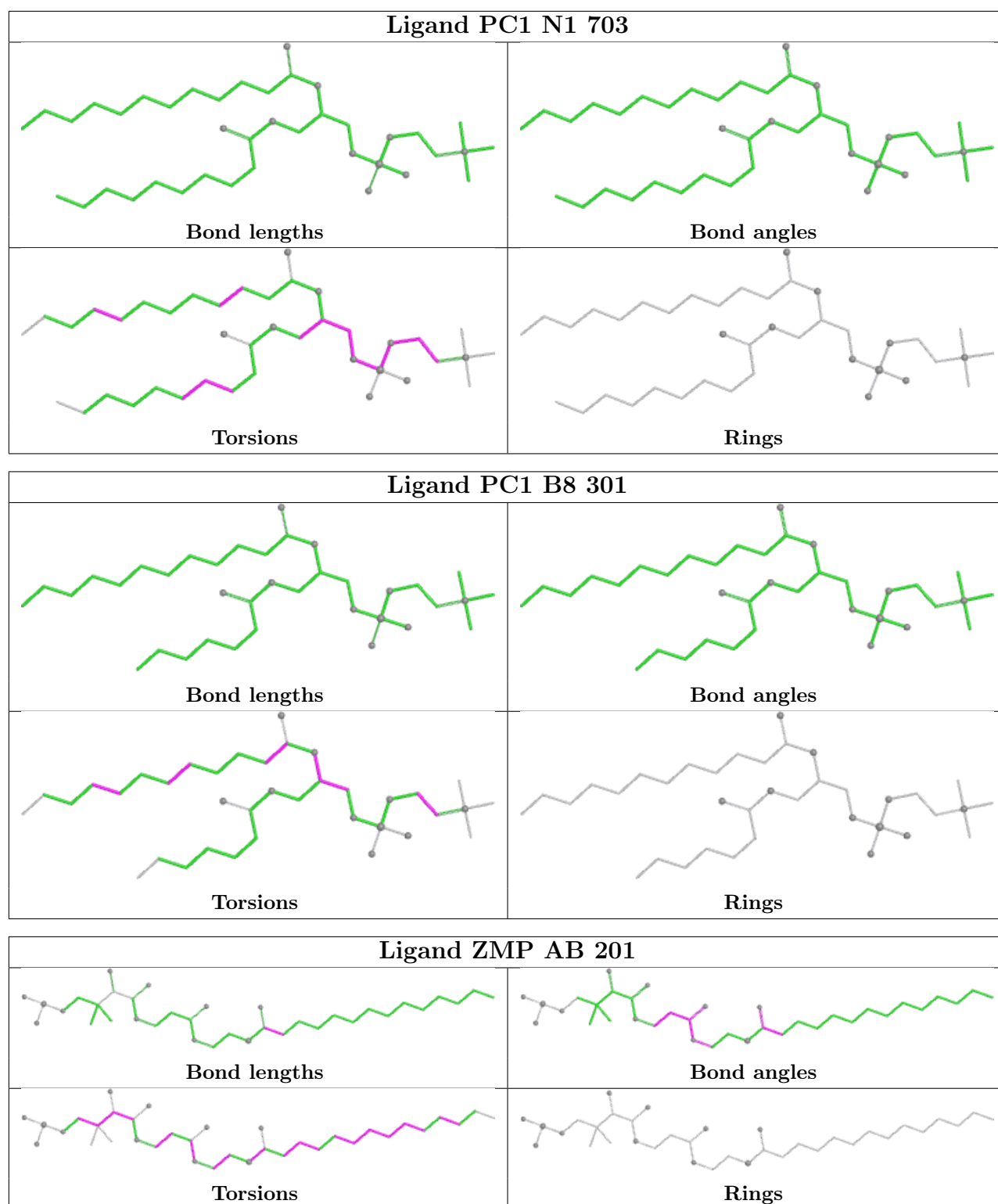




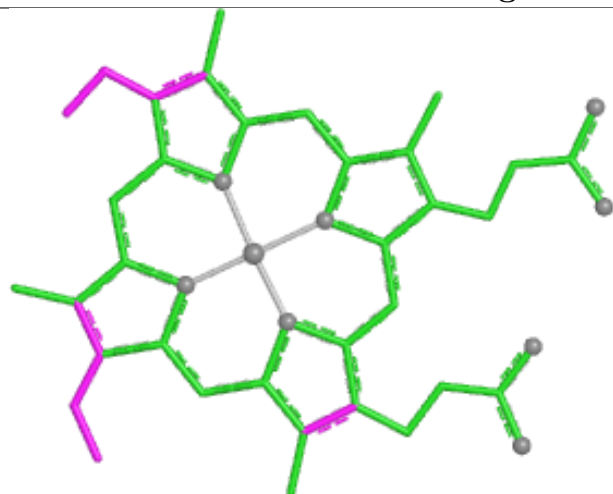




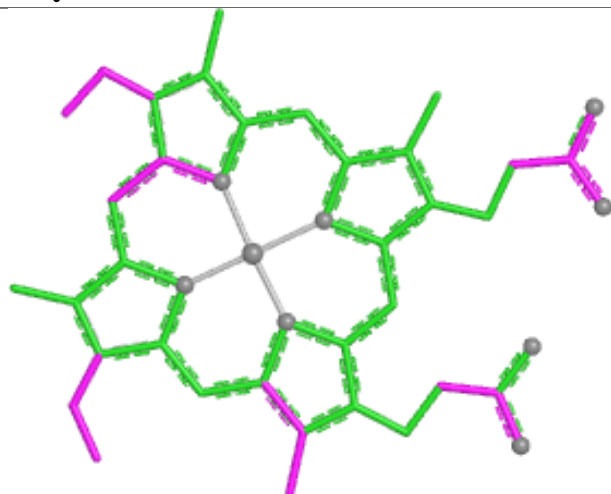




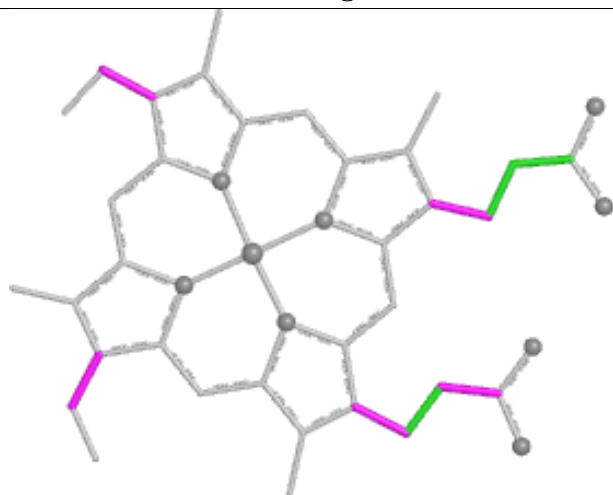
Ligand HEC QD 301



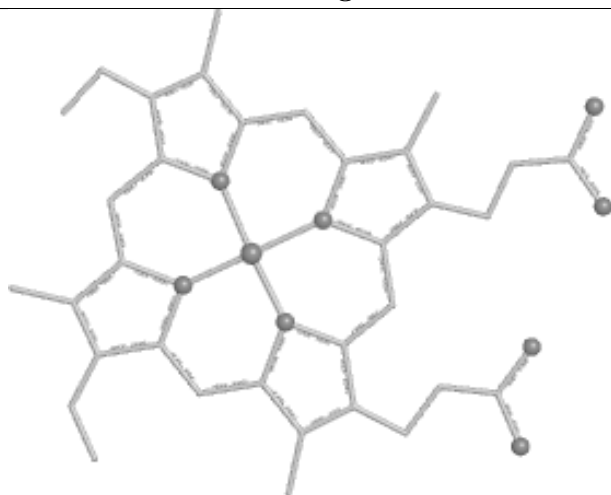
Bond lengths



Bond angles

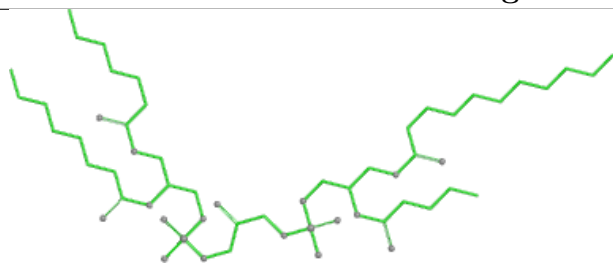


Torsions

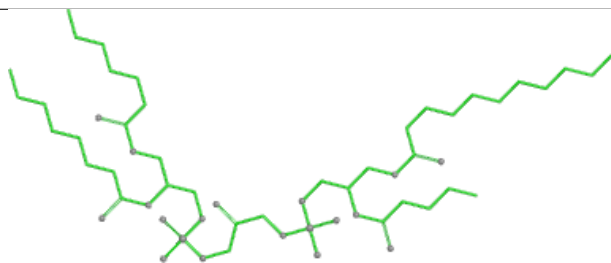


Rings

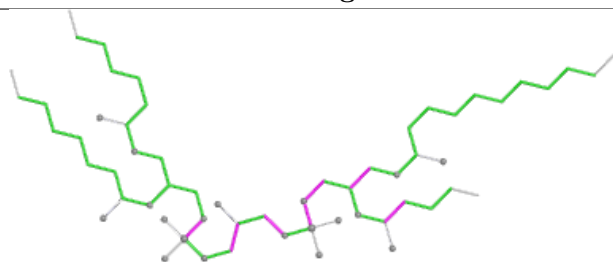
Ligand CDL EA 201



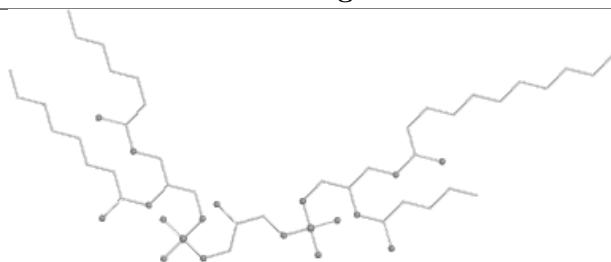
Bond lengths



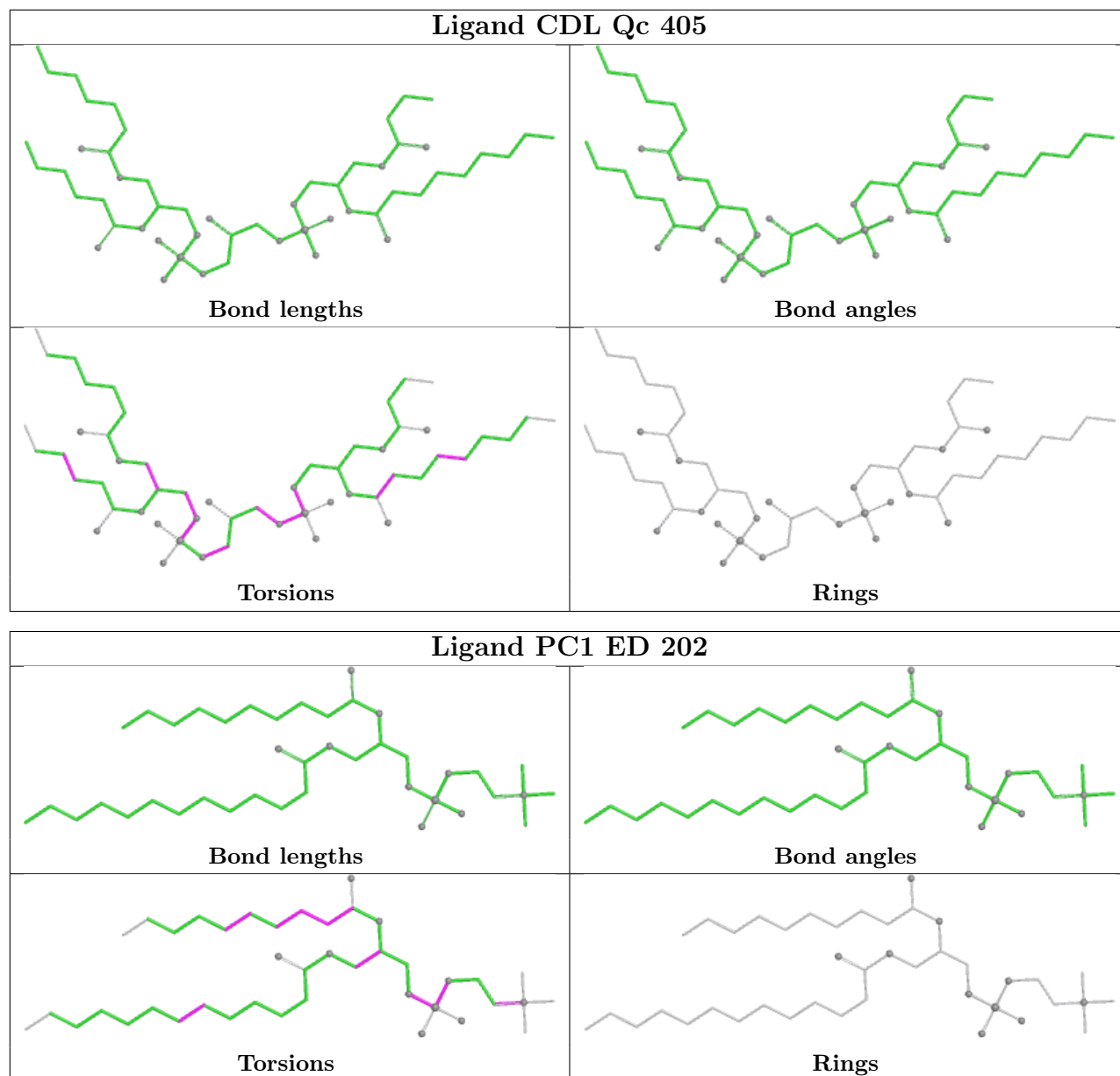
Bond angles

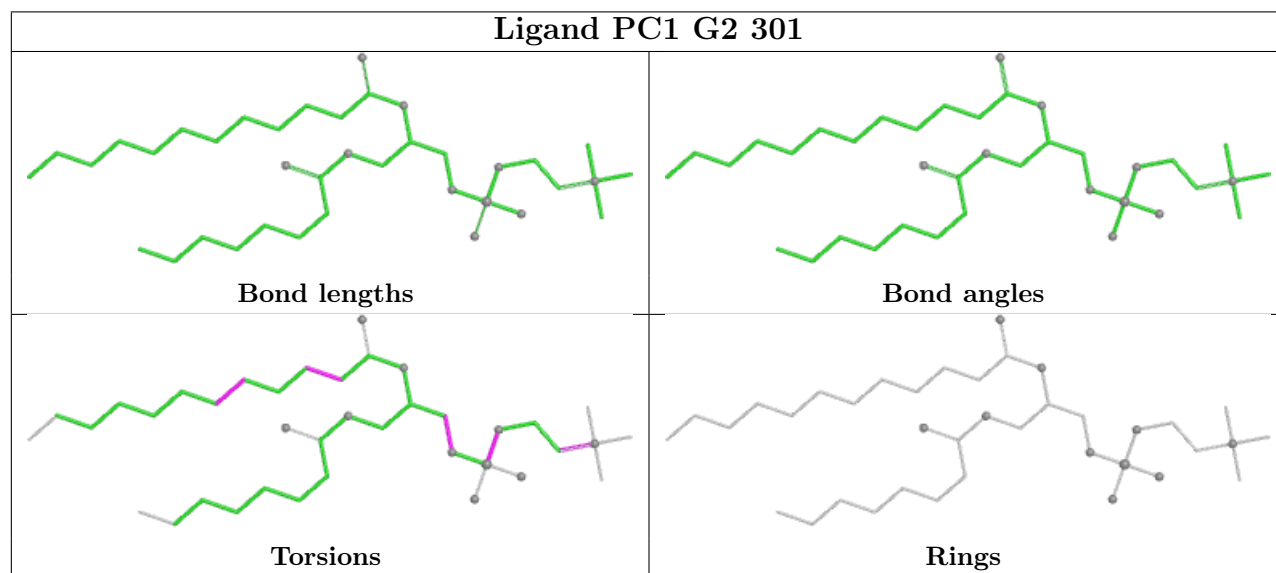
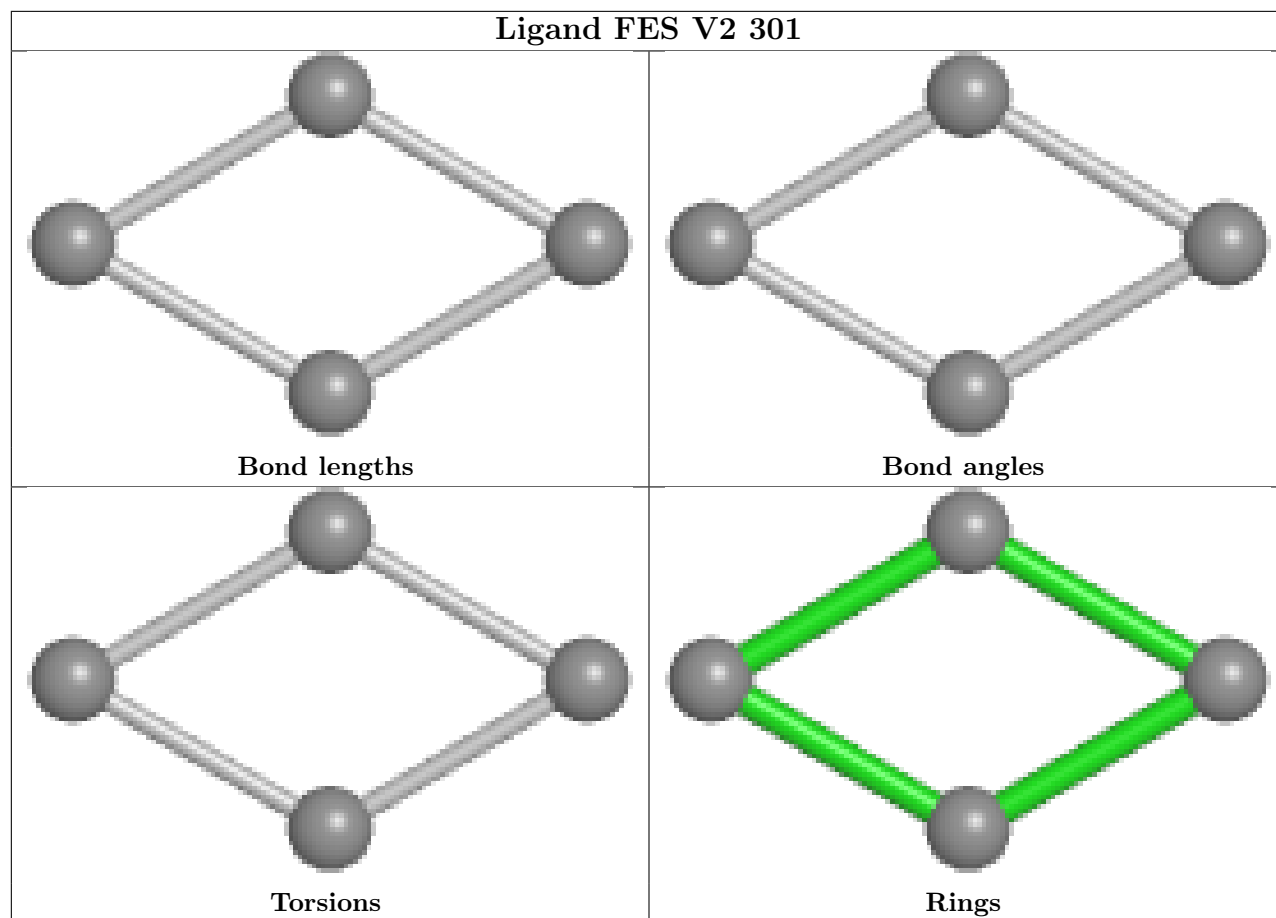


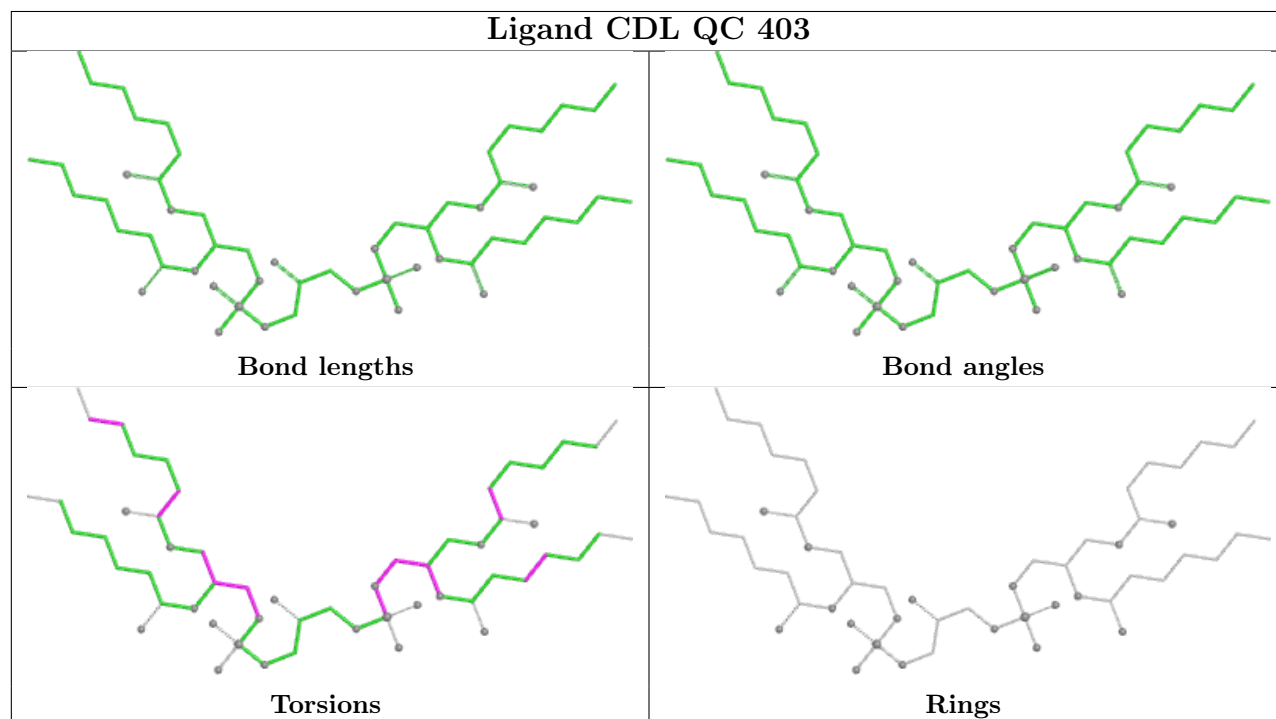
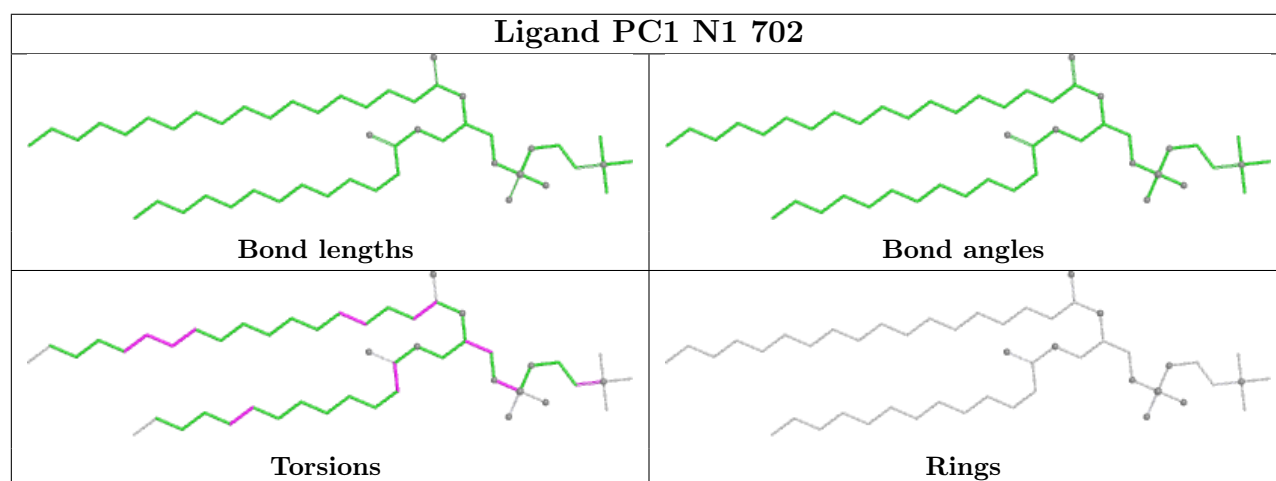
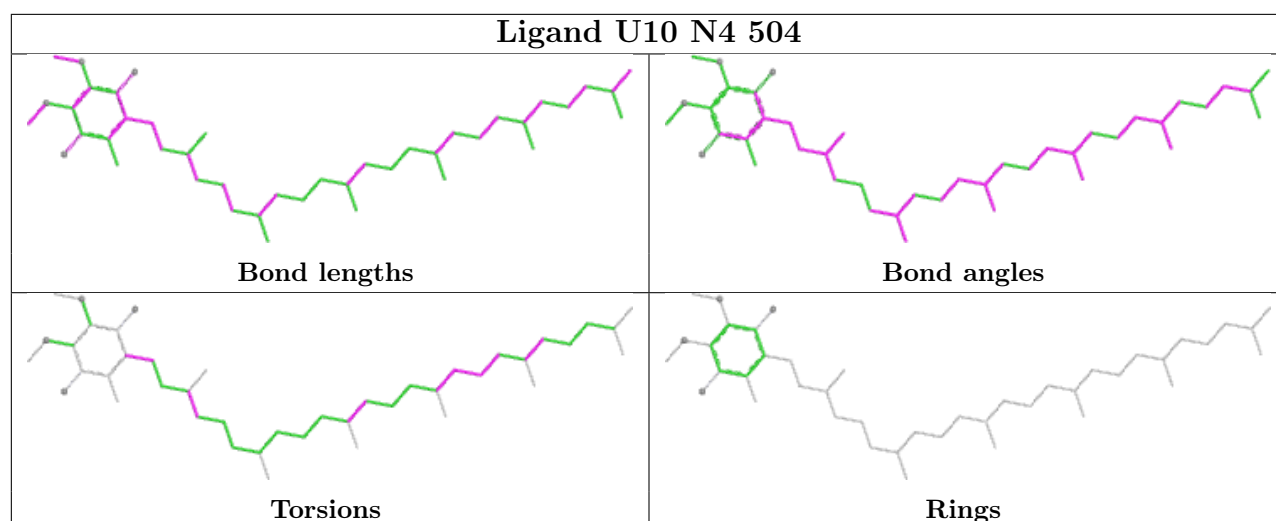
Torsions

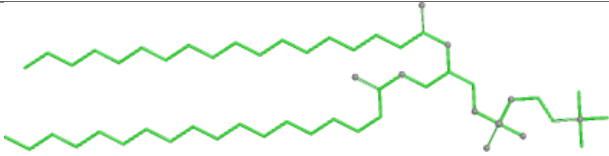
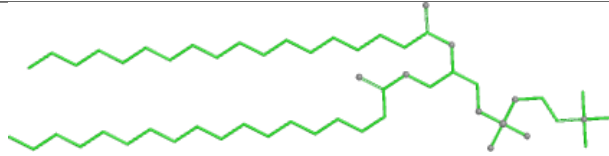
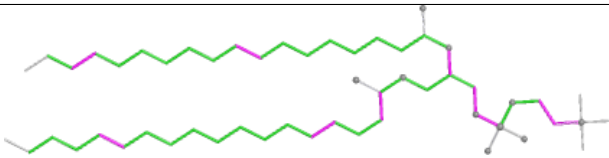
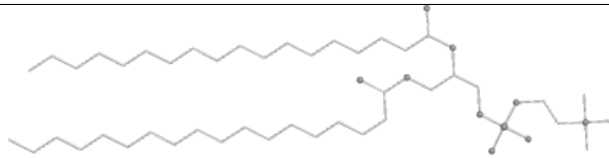


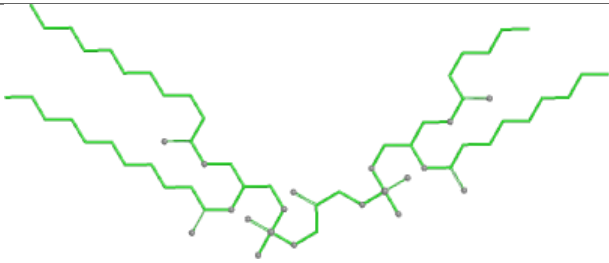
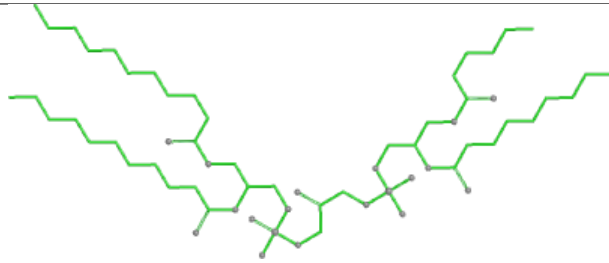
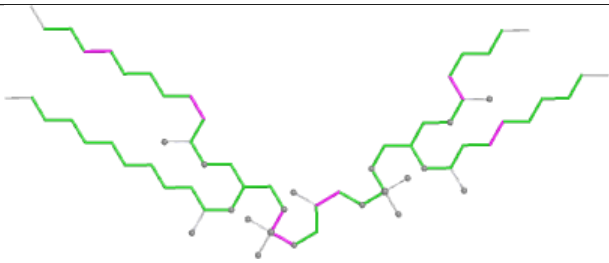
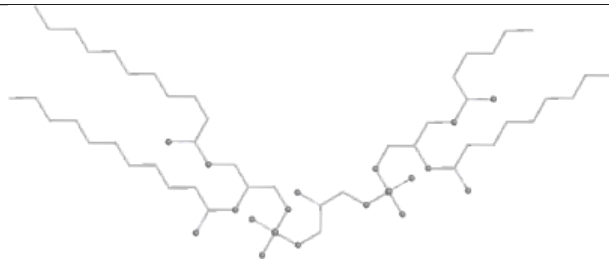
Rings

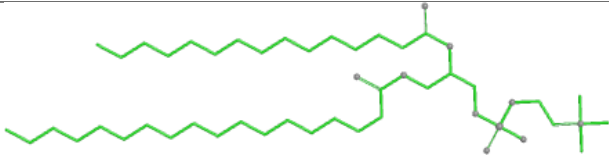
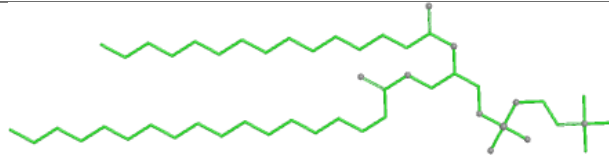
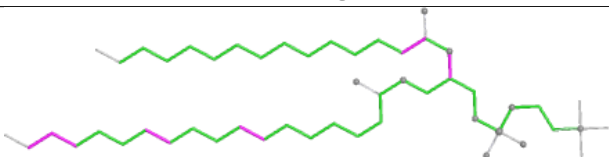
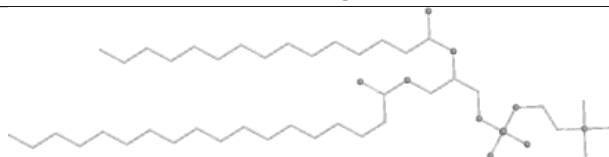


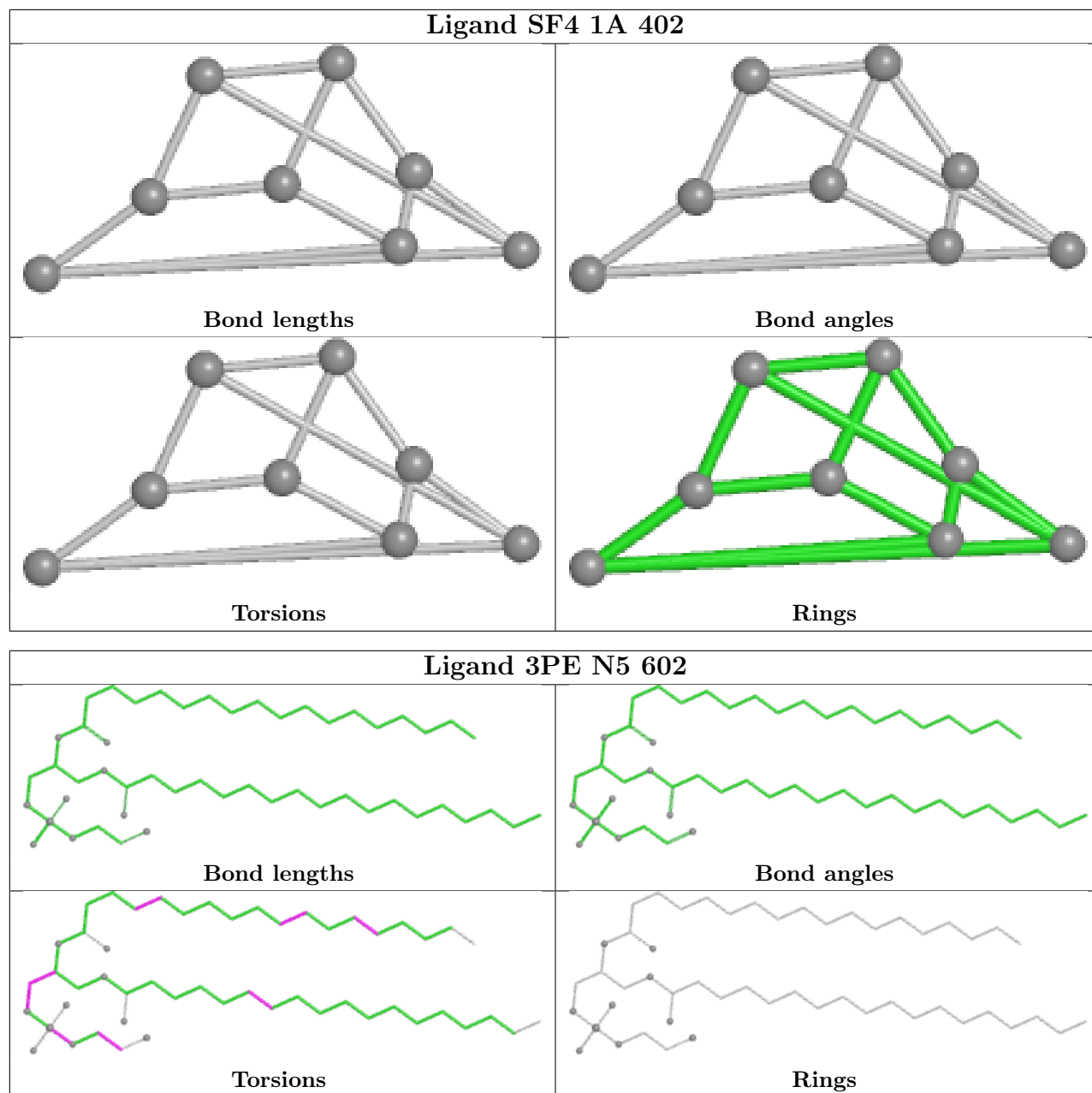


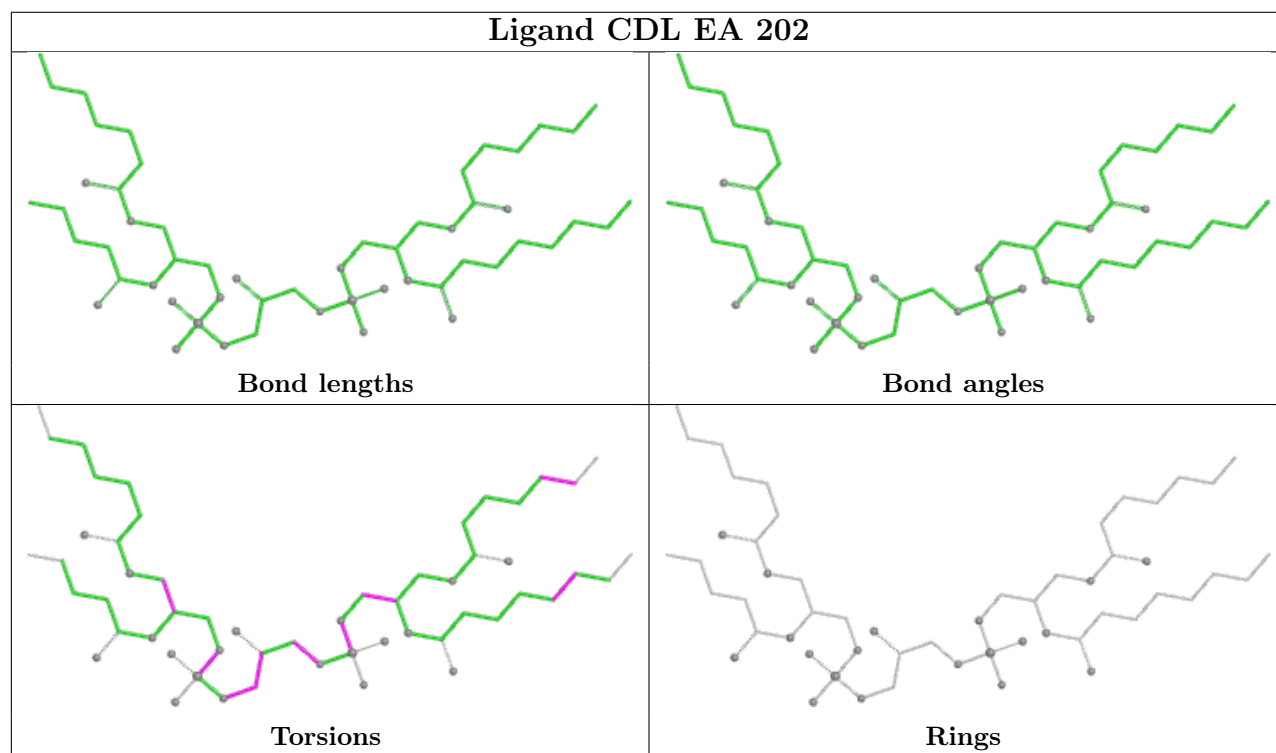
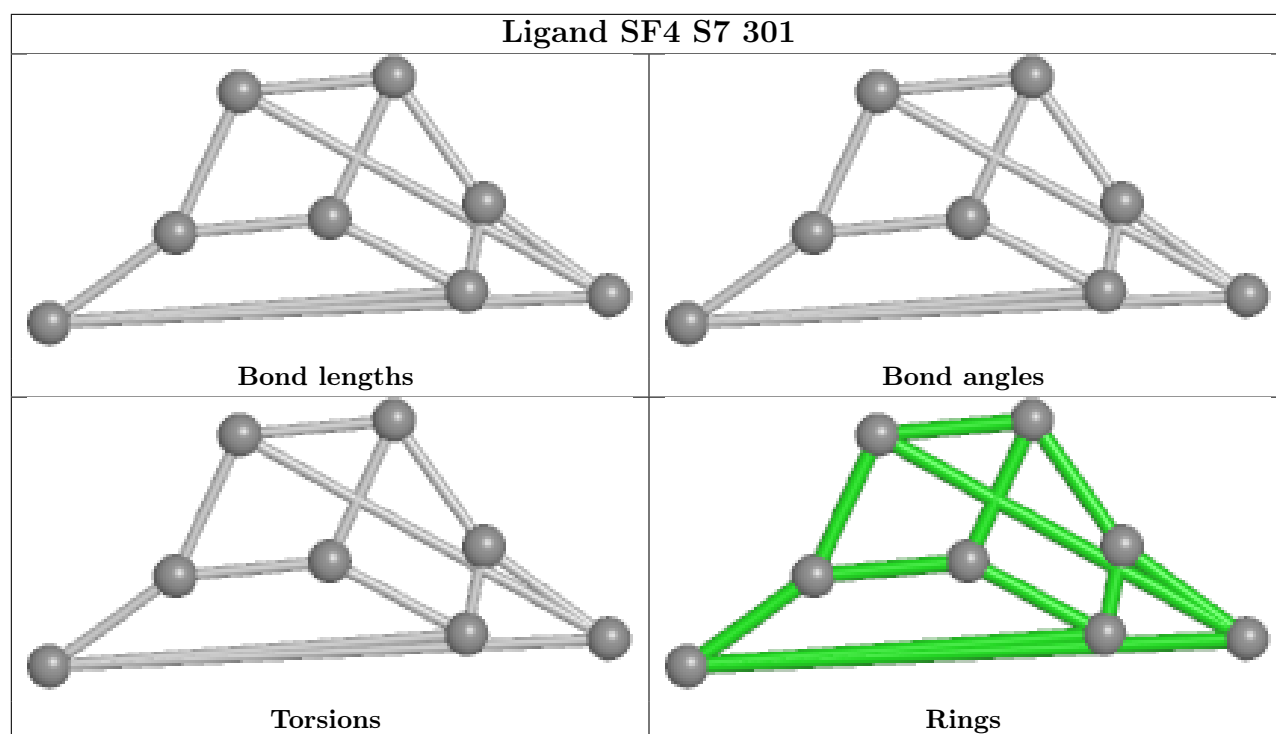


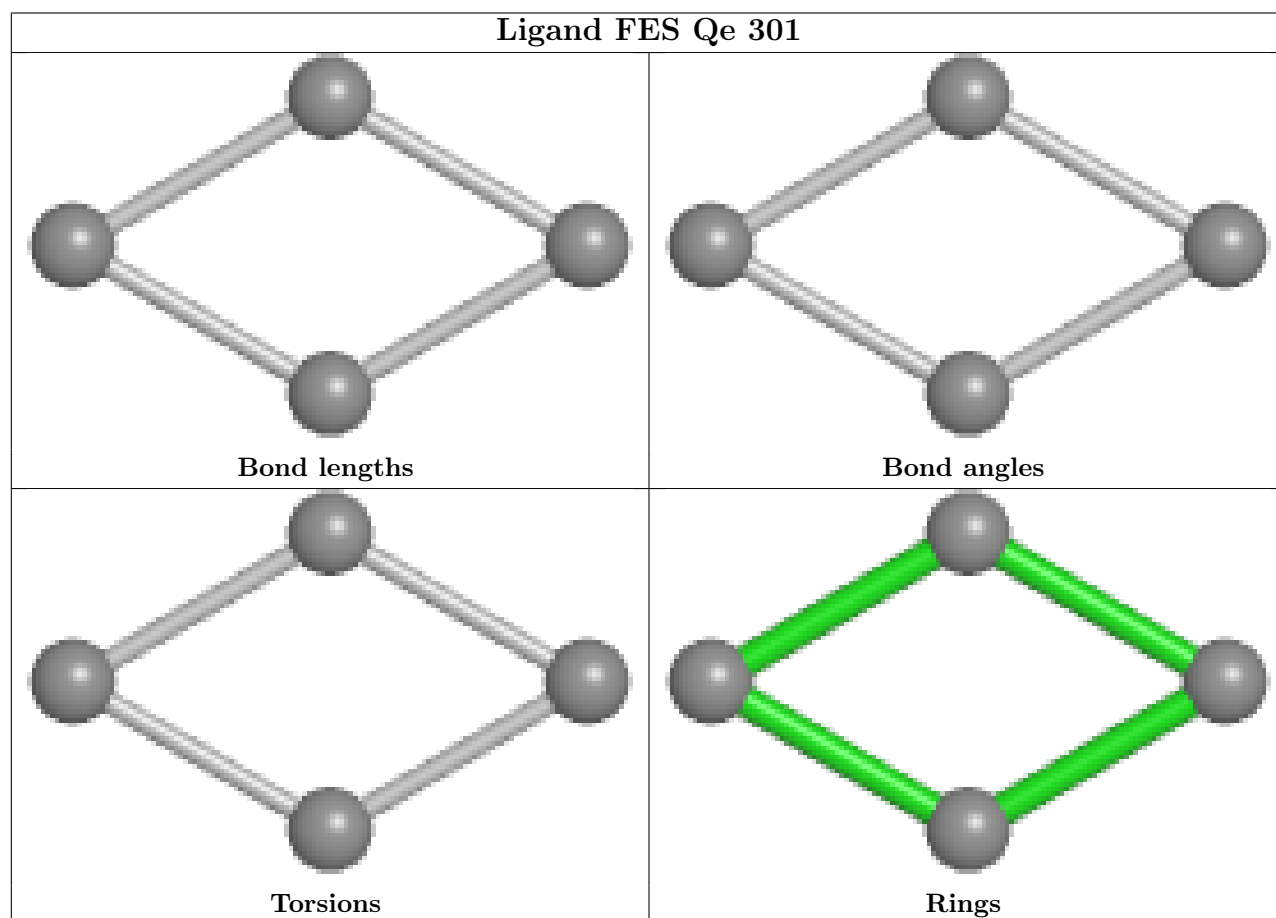
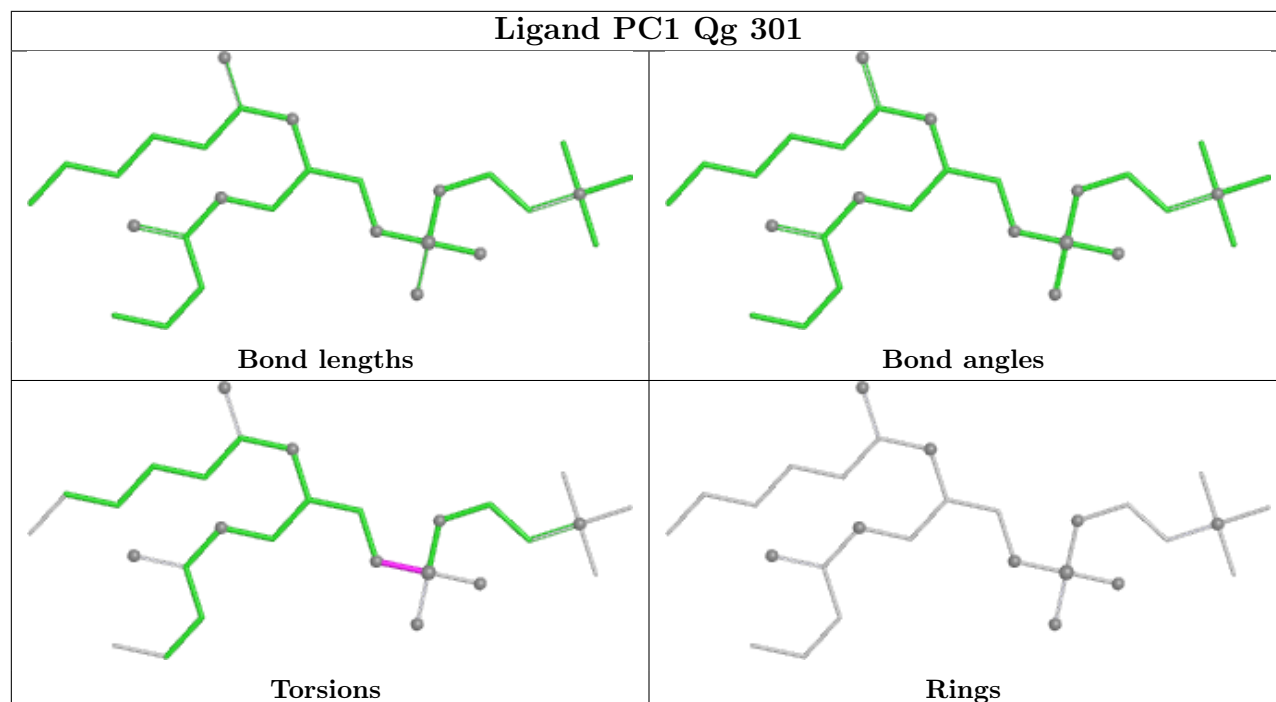
Ligand PC1 Qc 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL B3 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

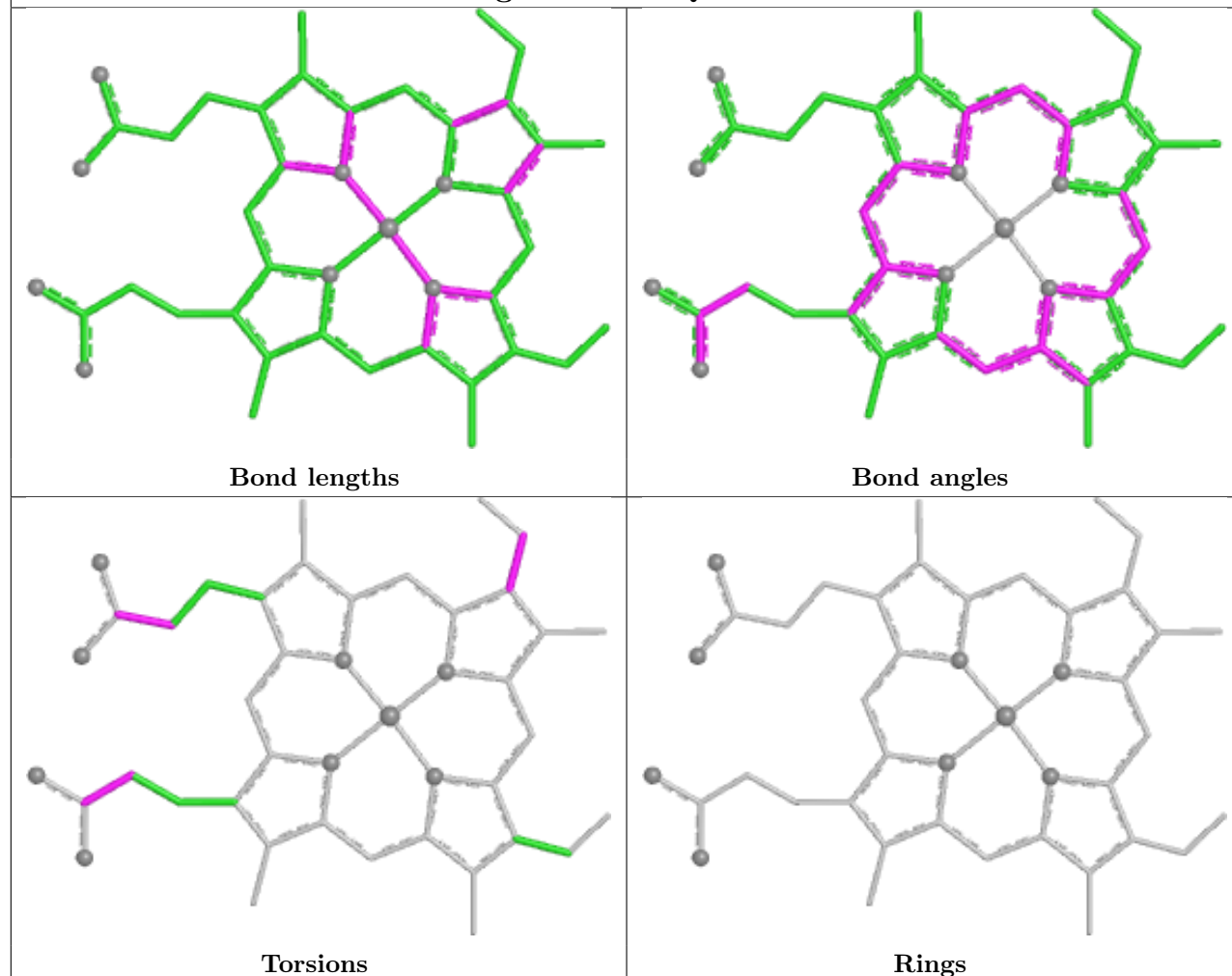
Ligand PC1 C3 201	
 Bond lengths	 Bond angles
 Torsions	 Rings



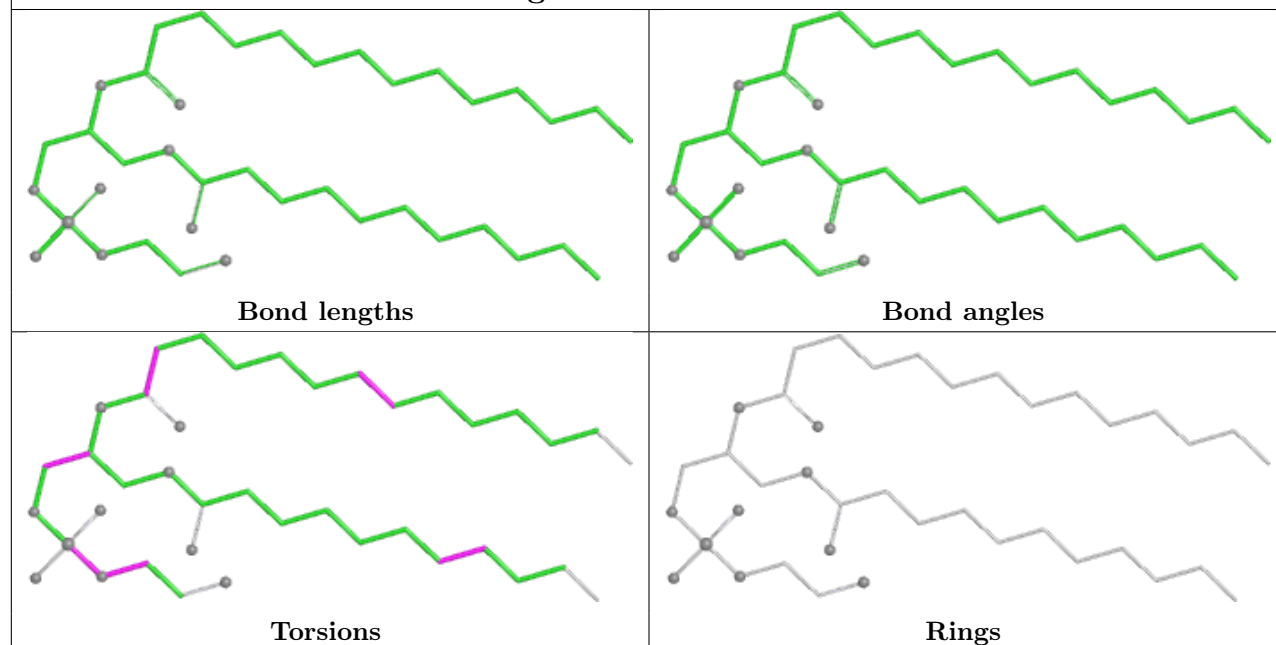


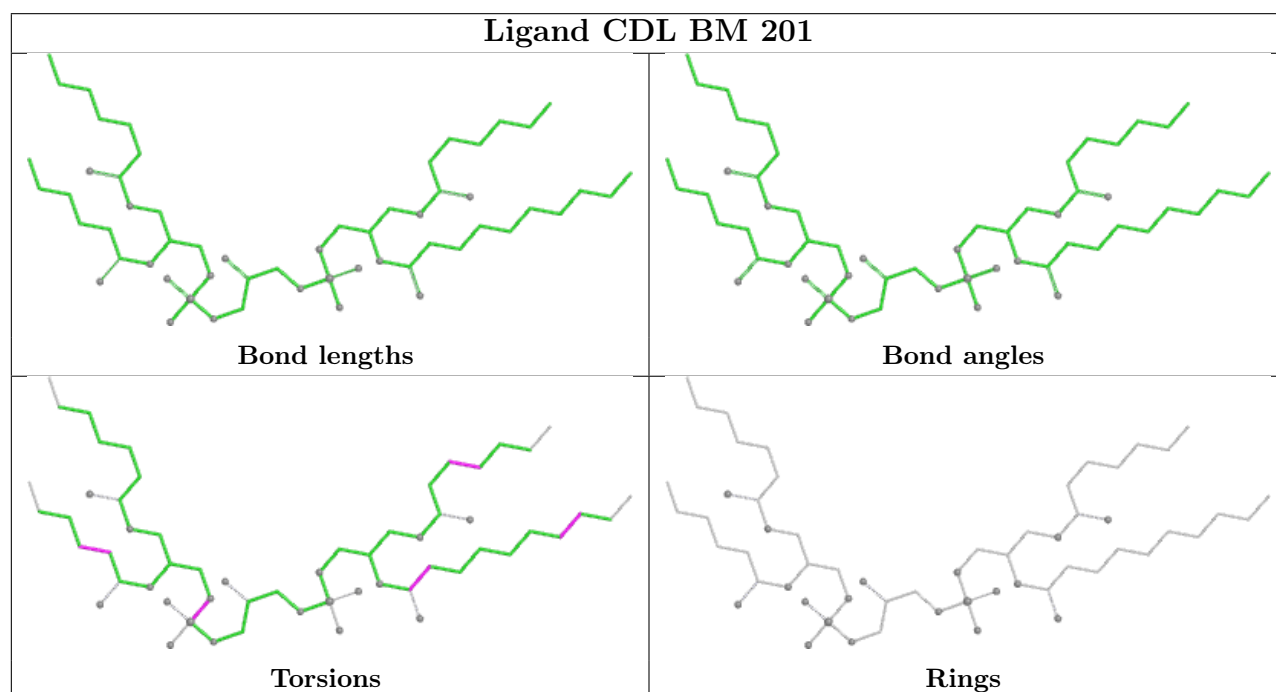
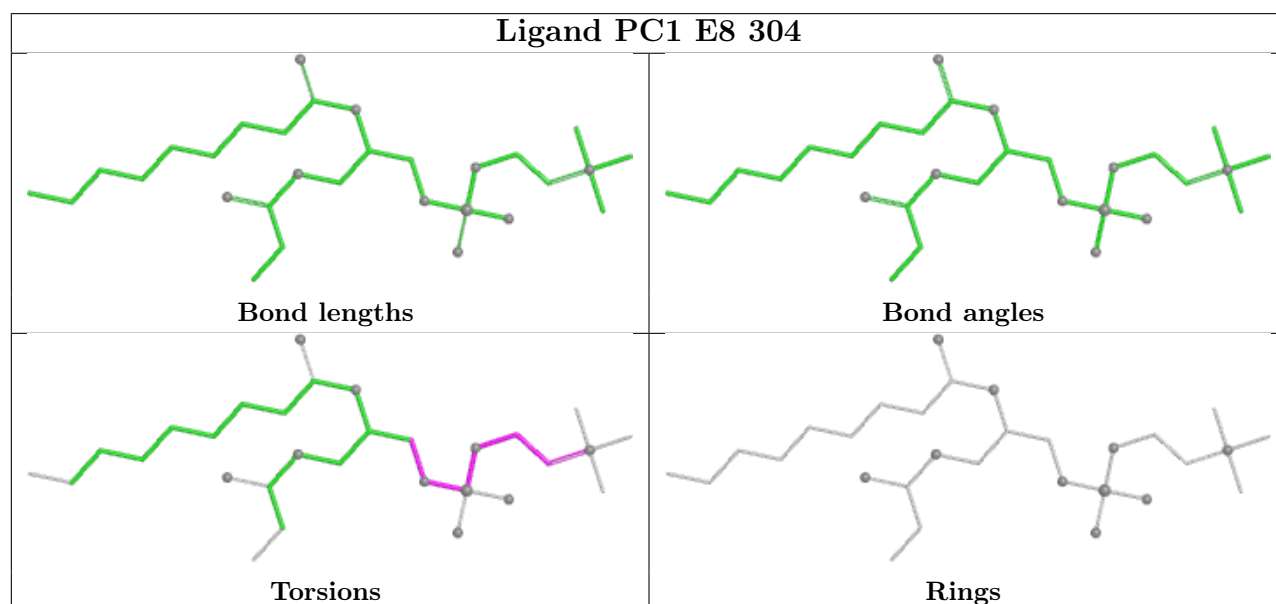
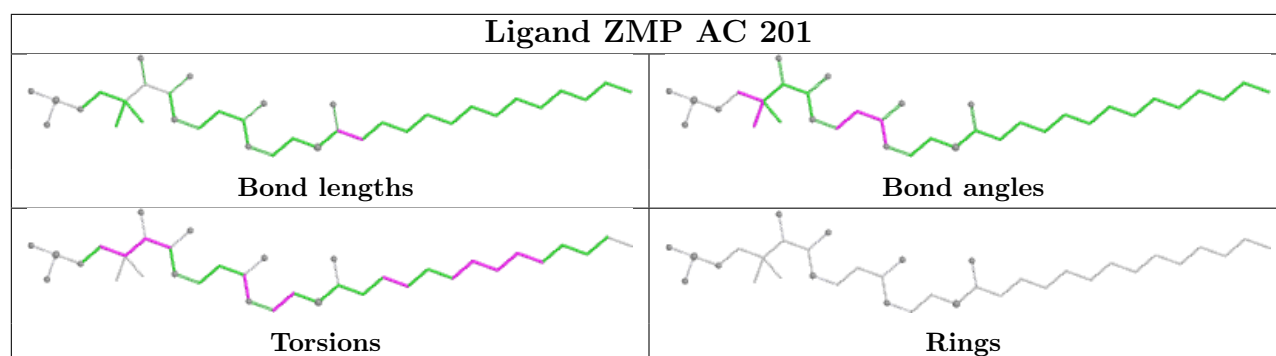


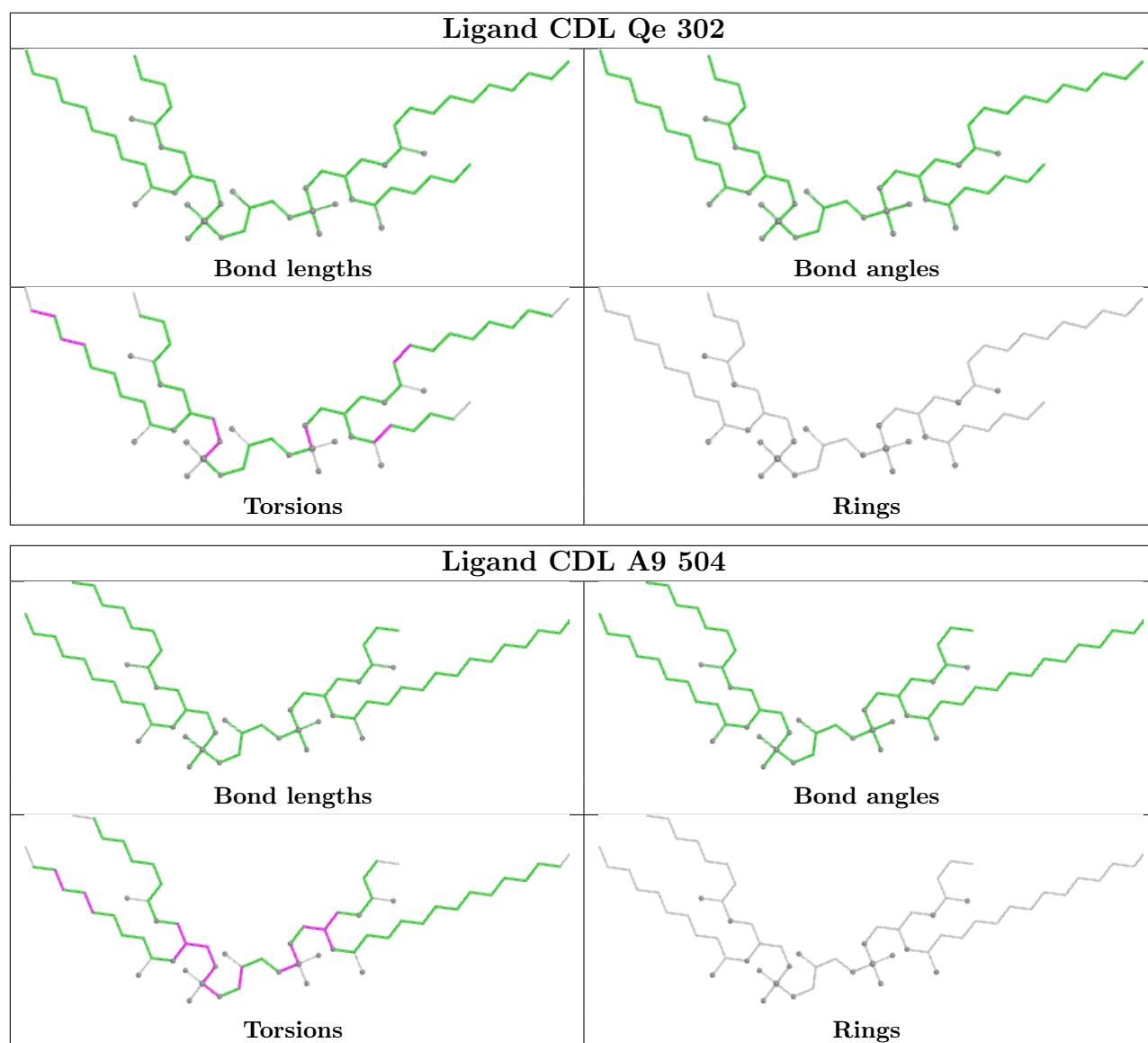
Ligand HEM QC 402

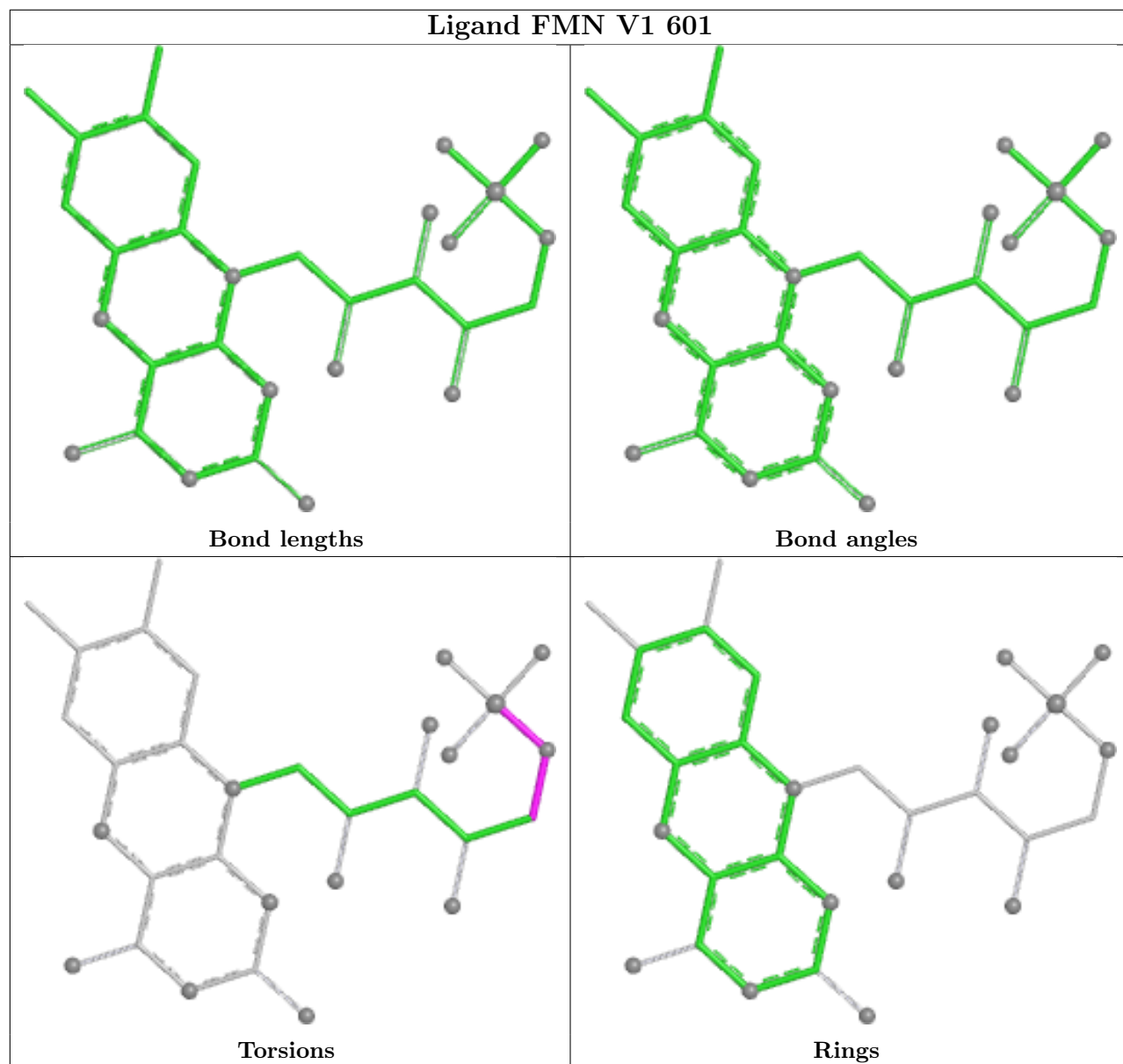


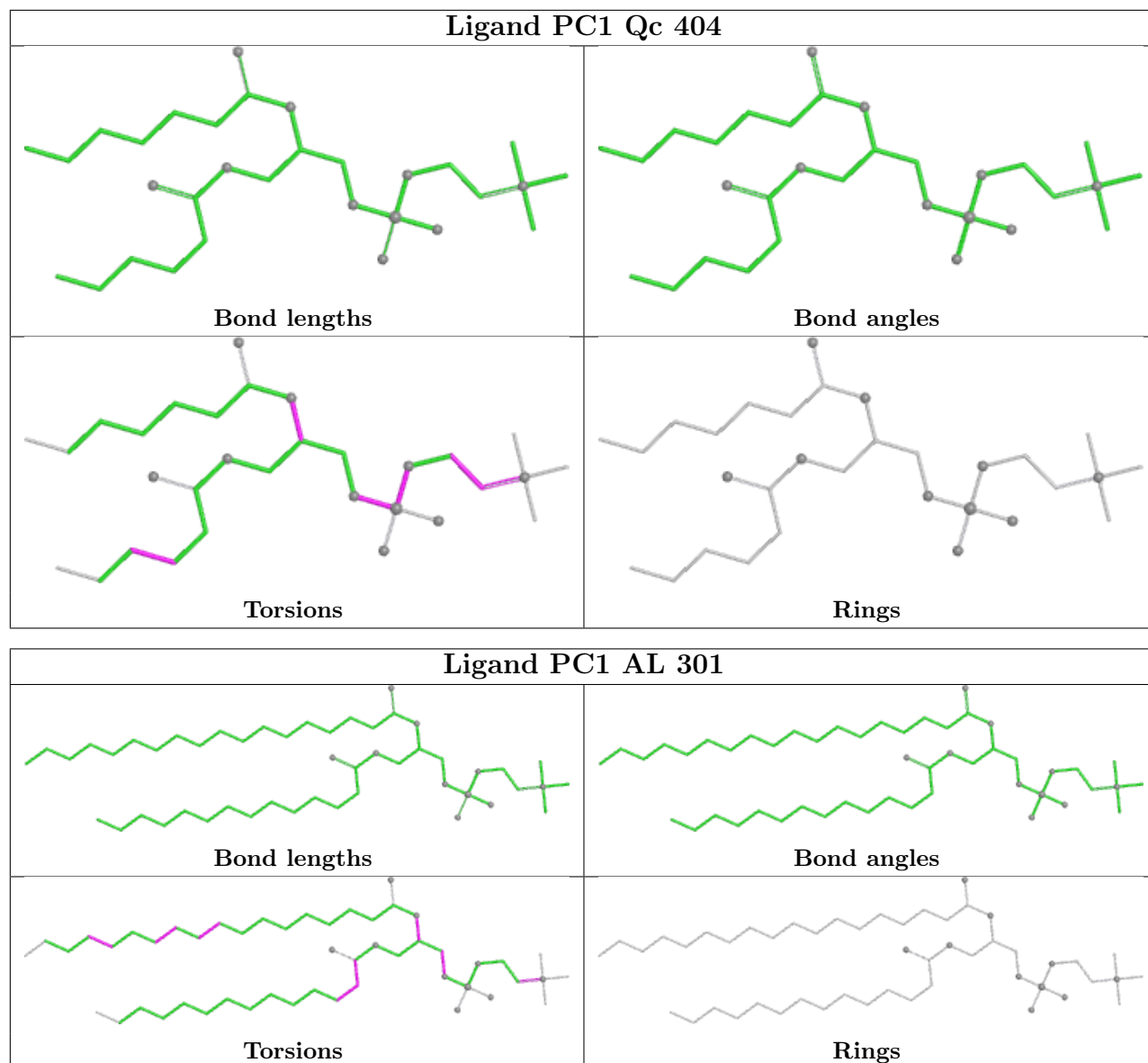
Ligand 3PE C1 507



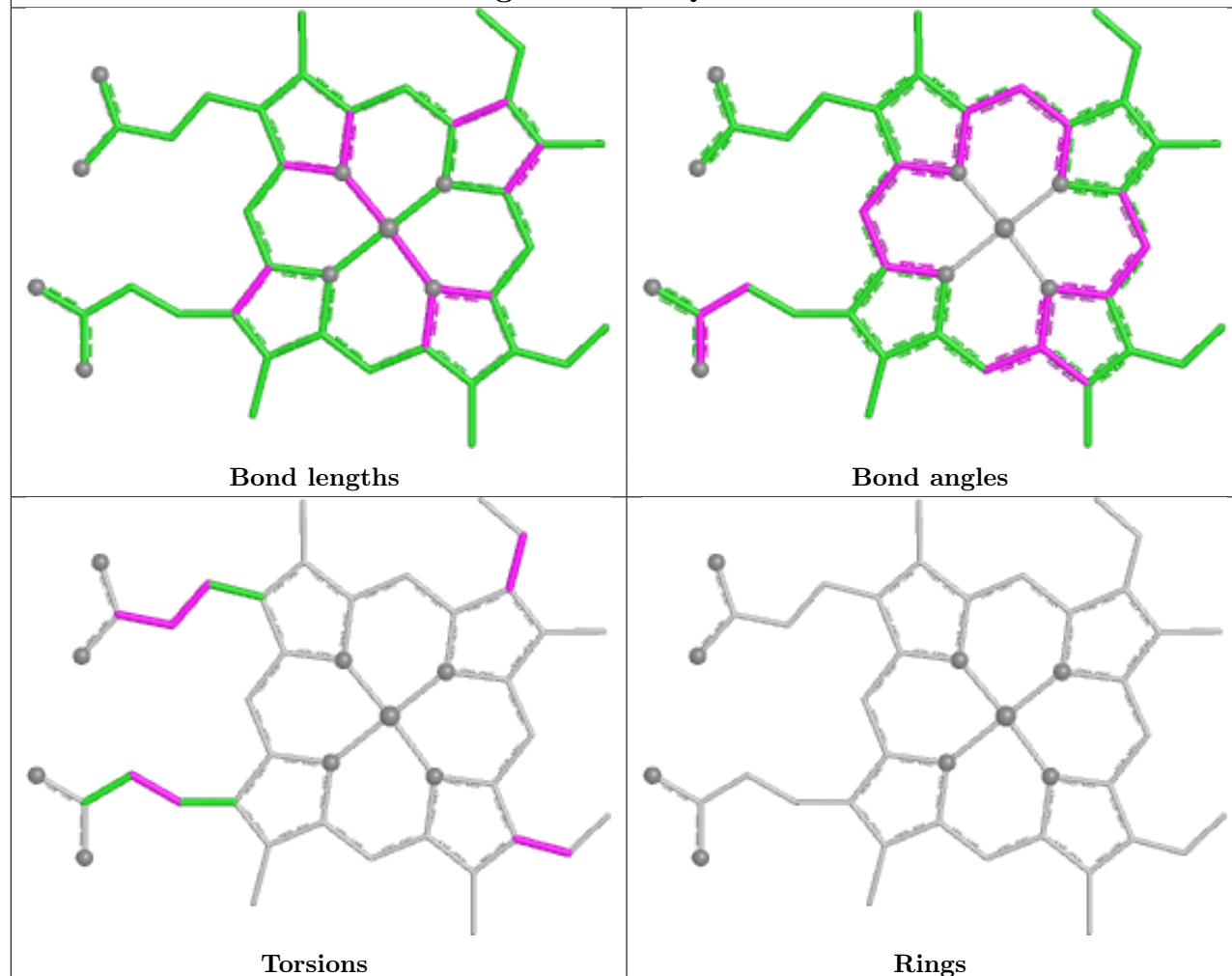




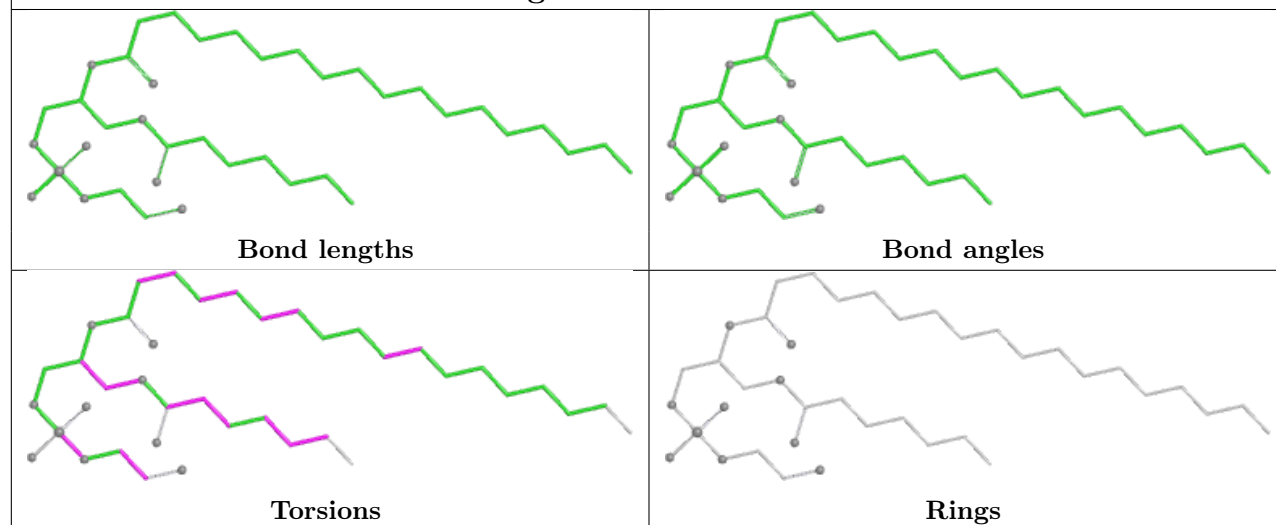




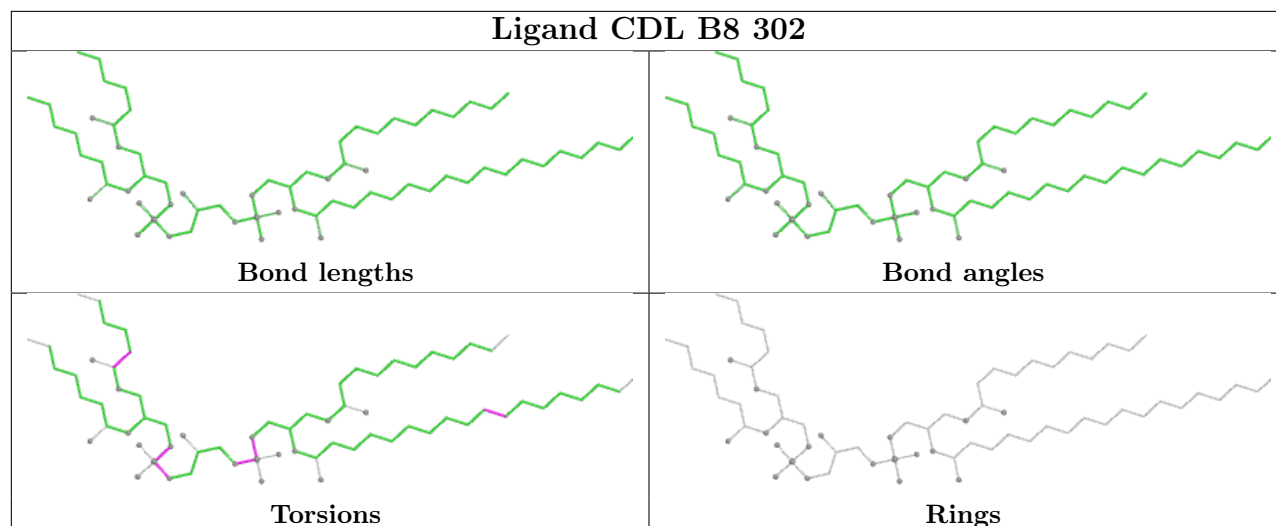
Ligand HEM QC 401



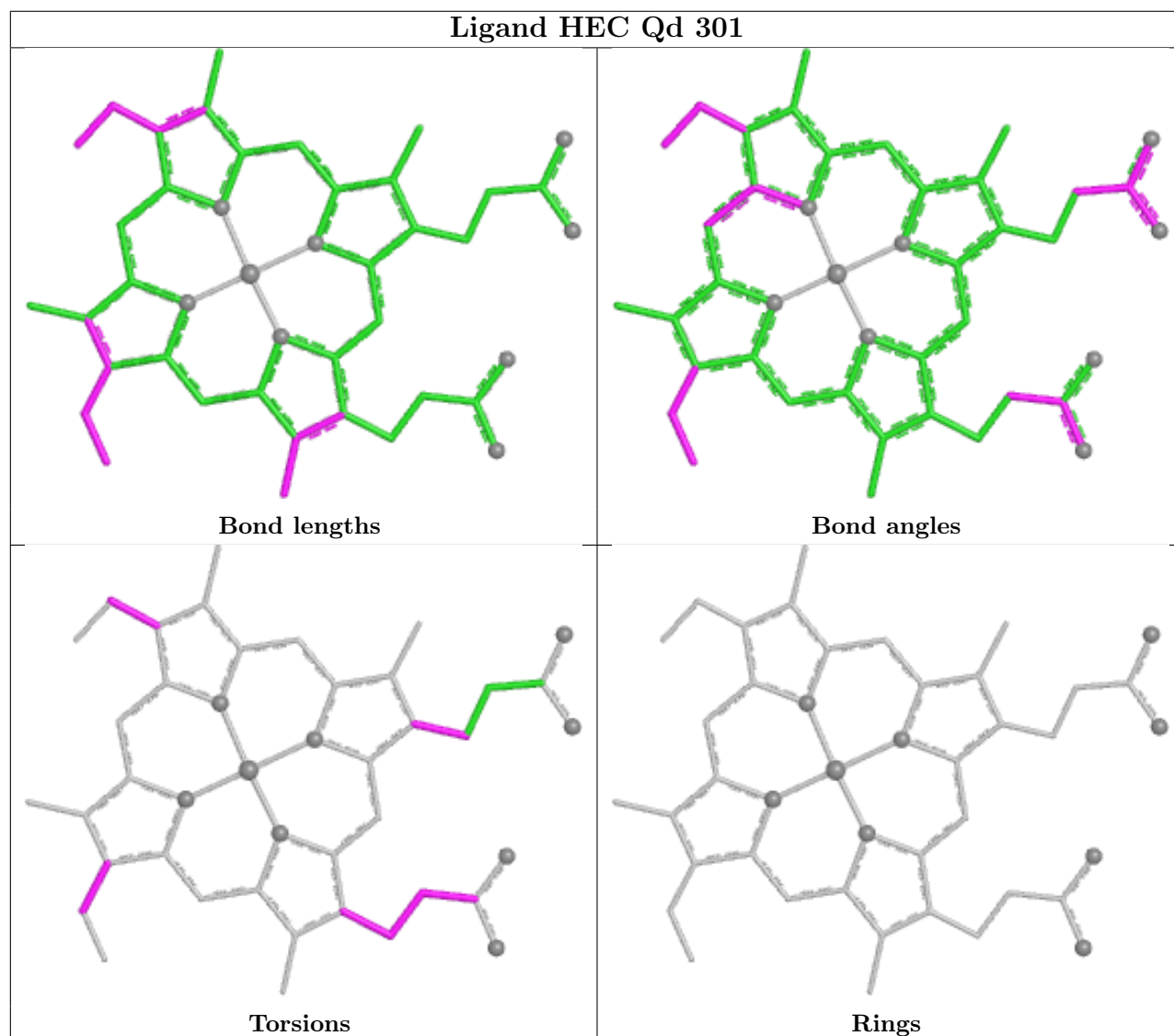
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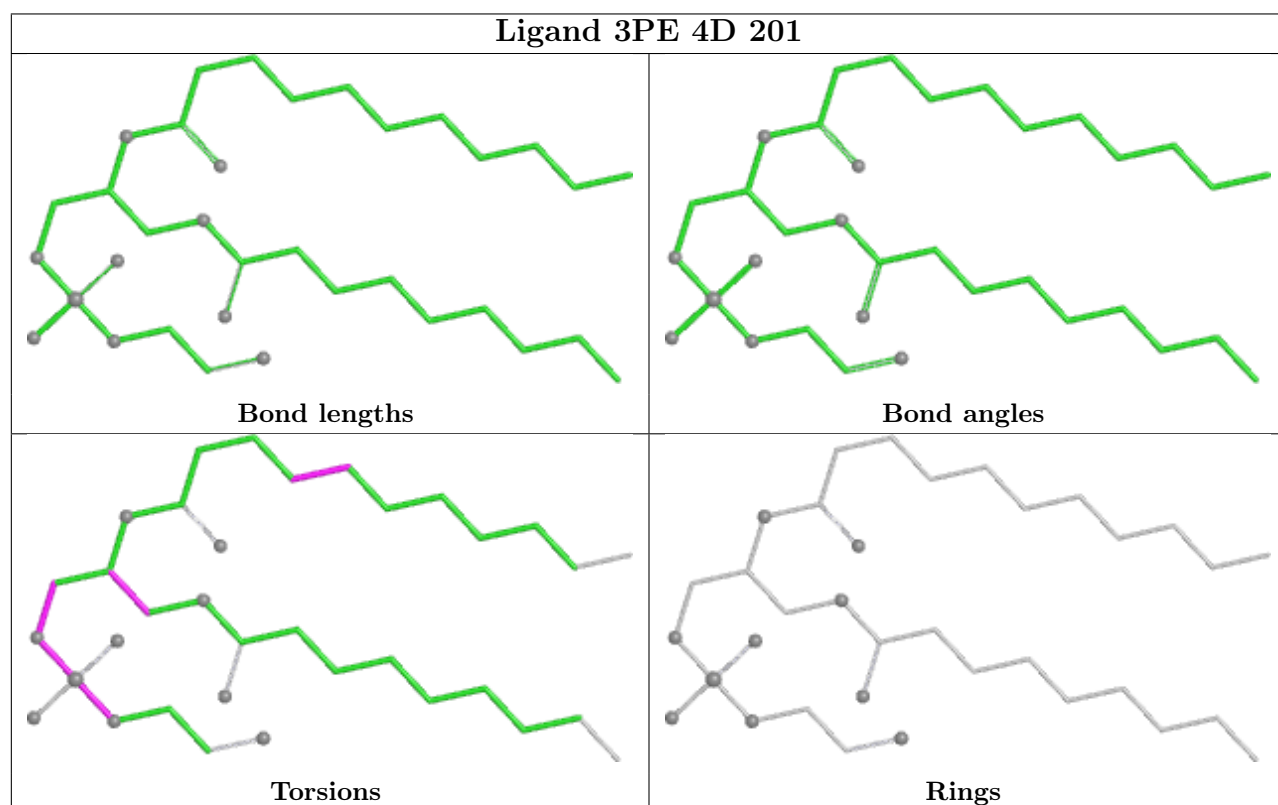
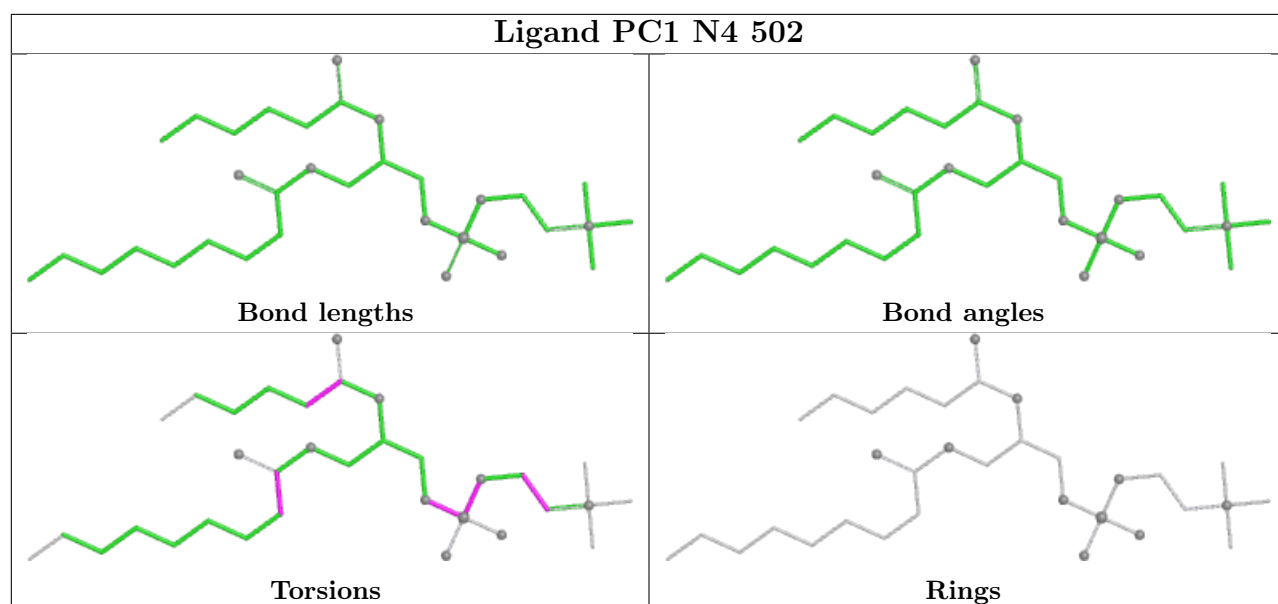


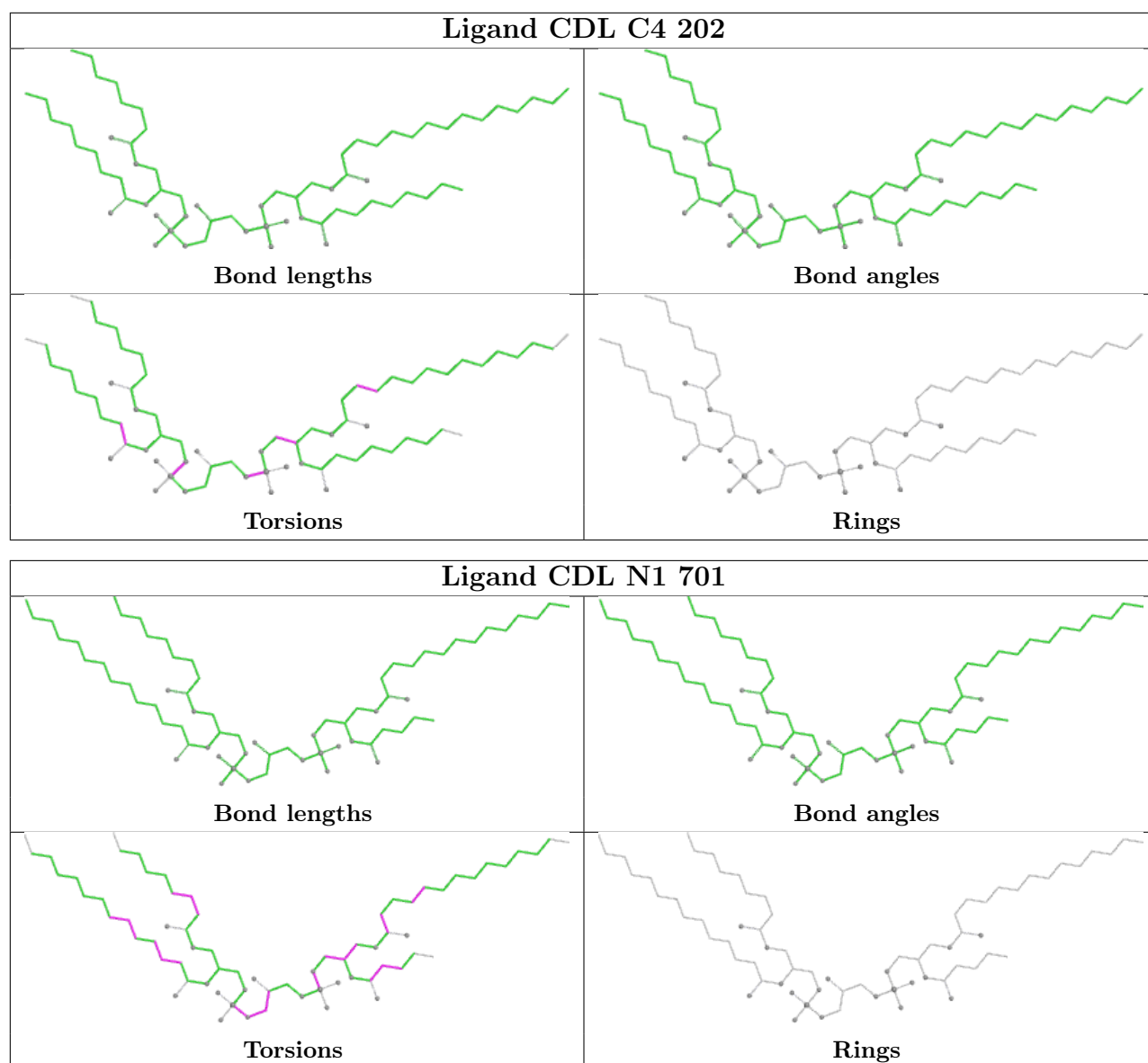
Ligand CDL B8 302

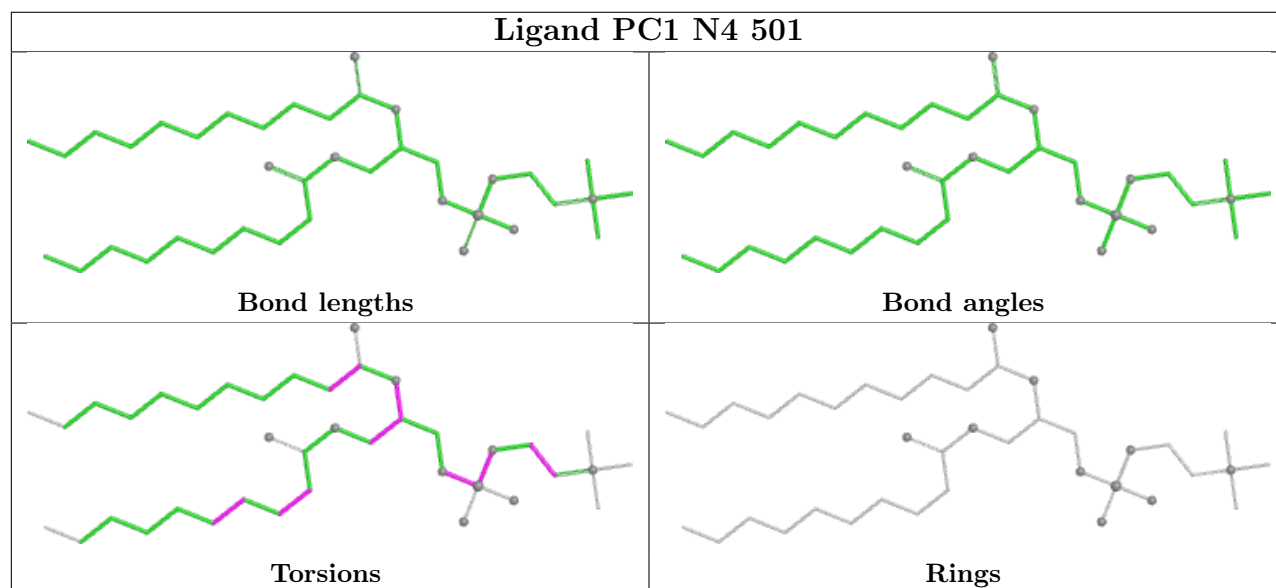
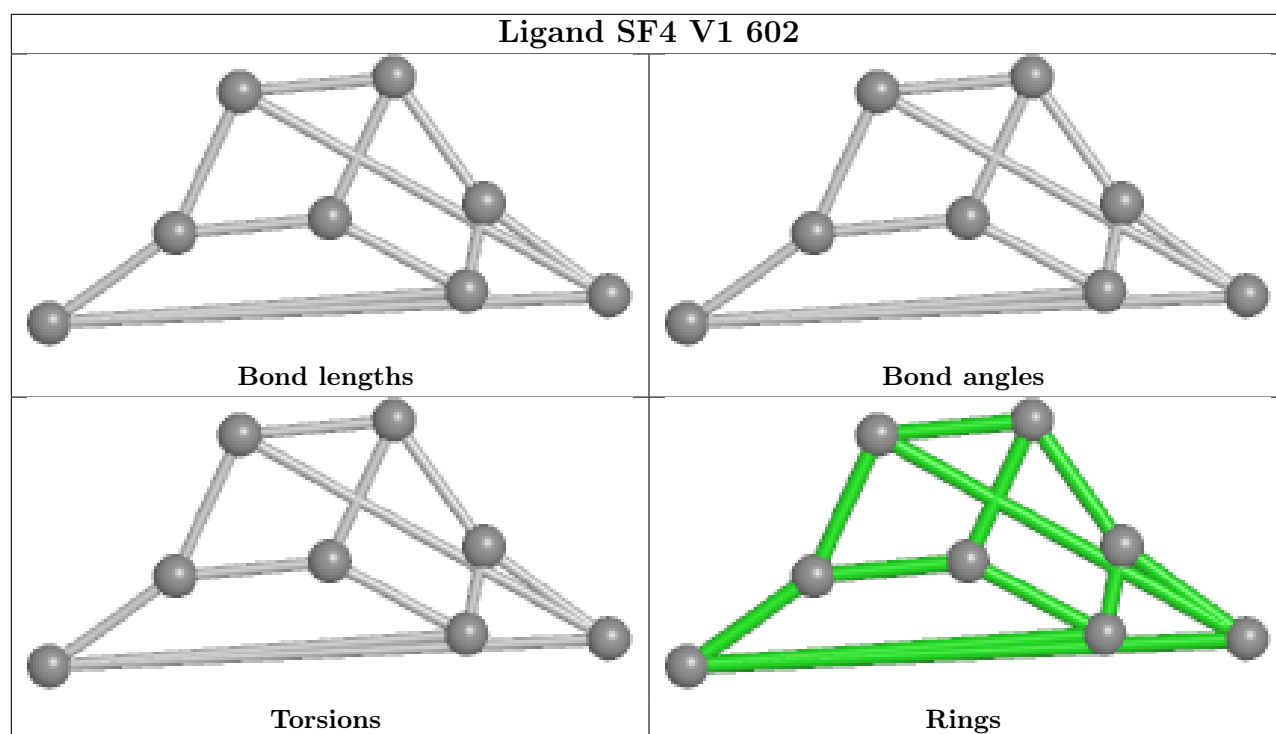


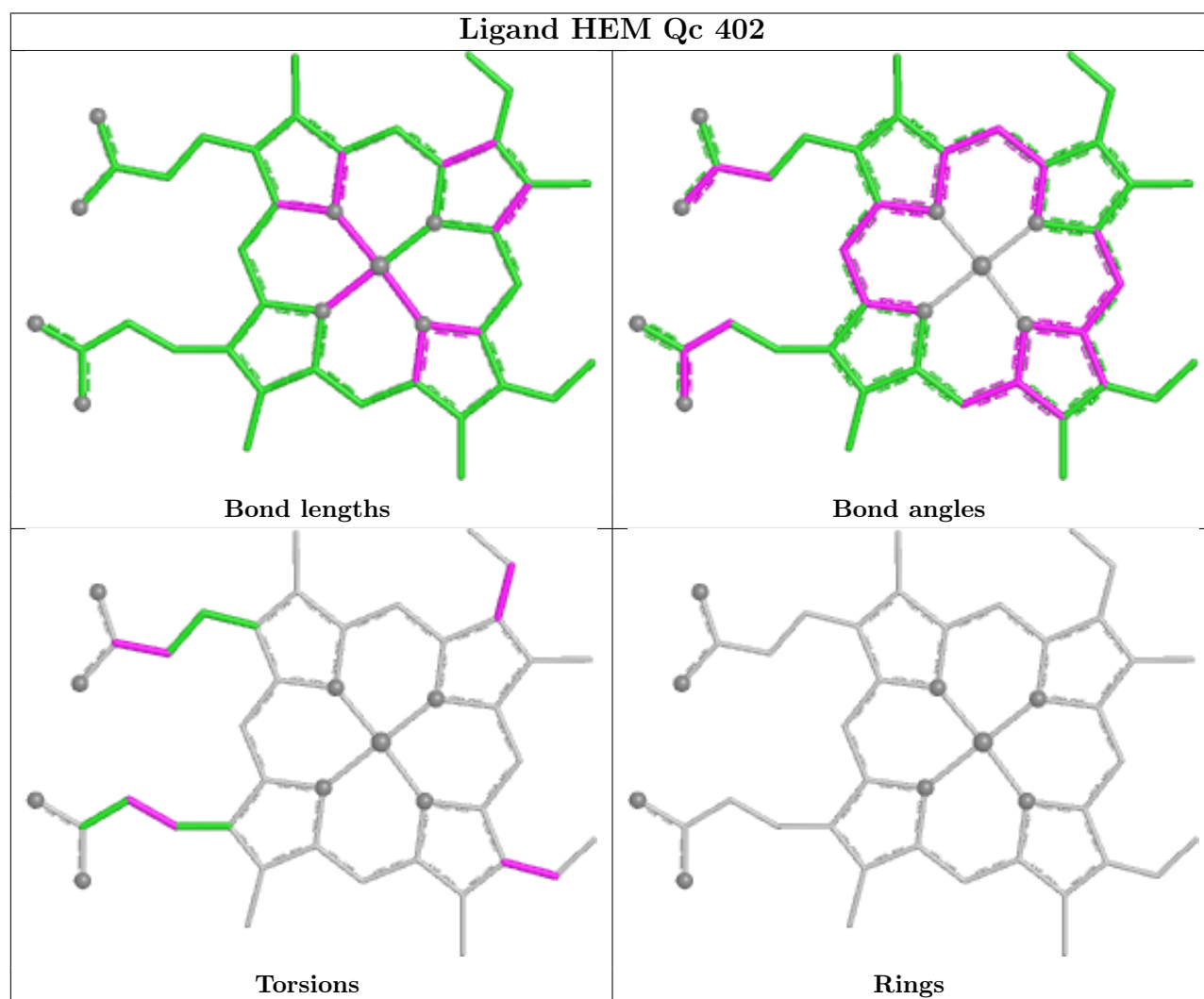
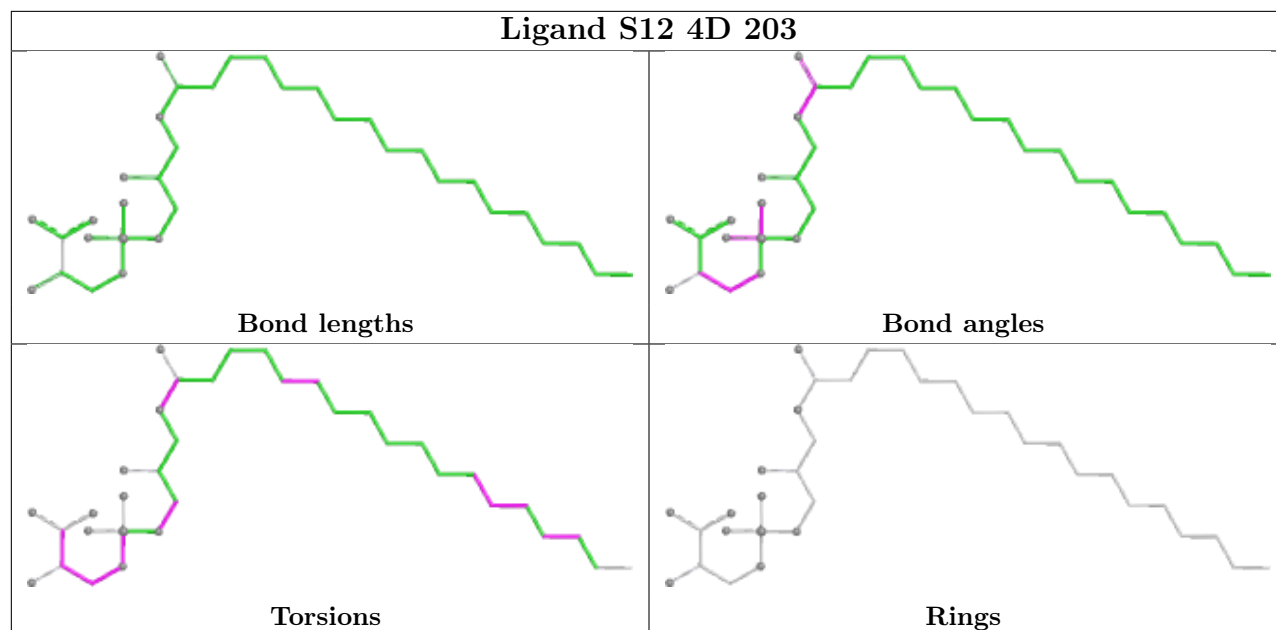
Ligand HEC Qd 301

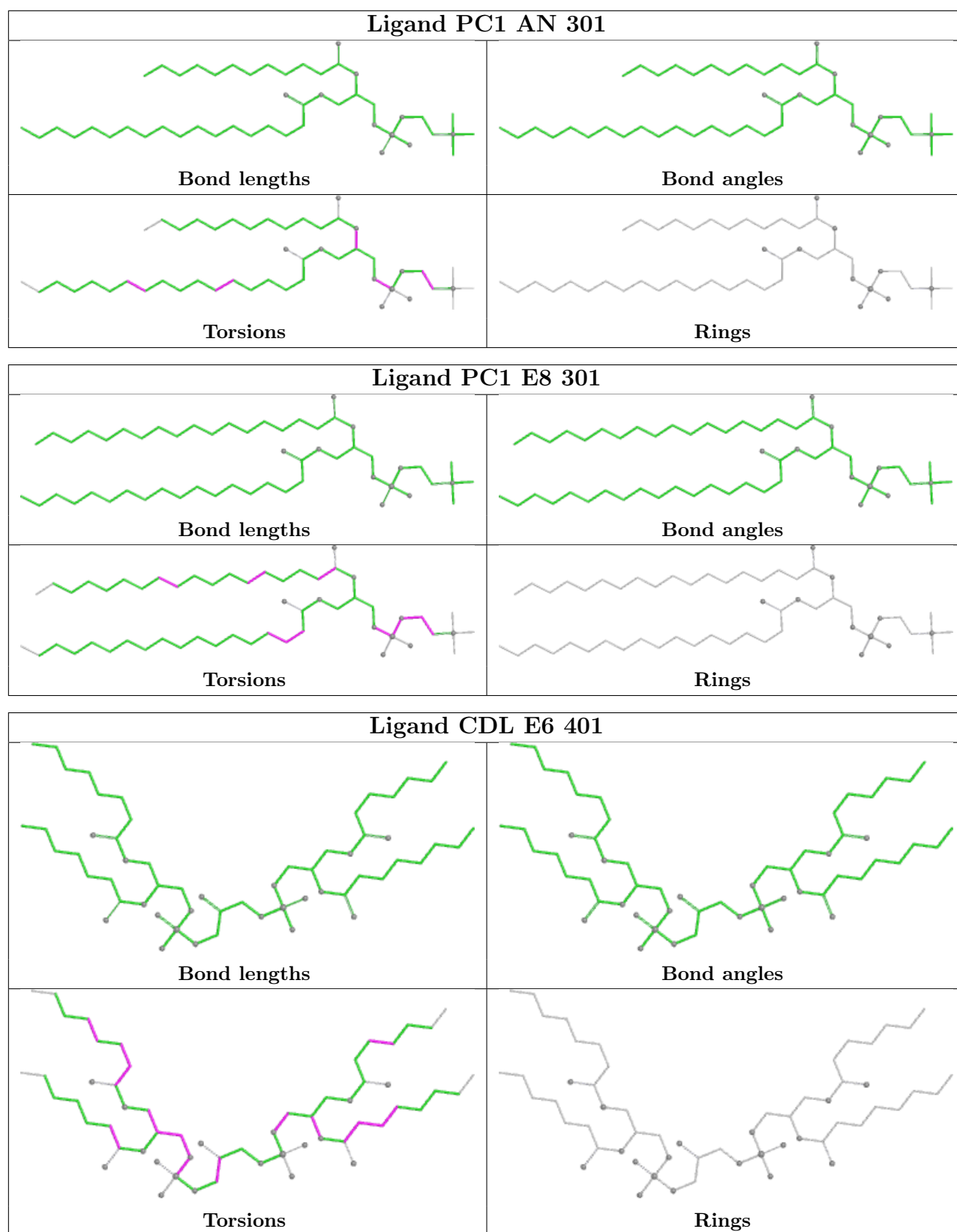


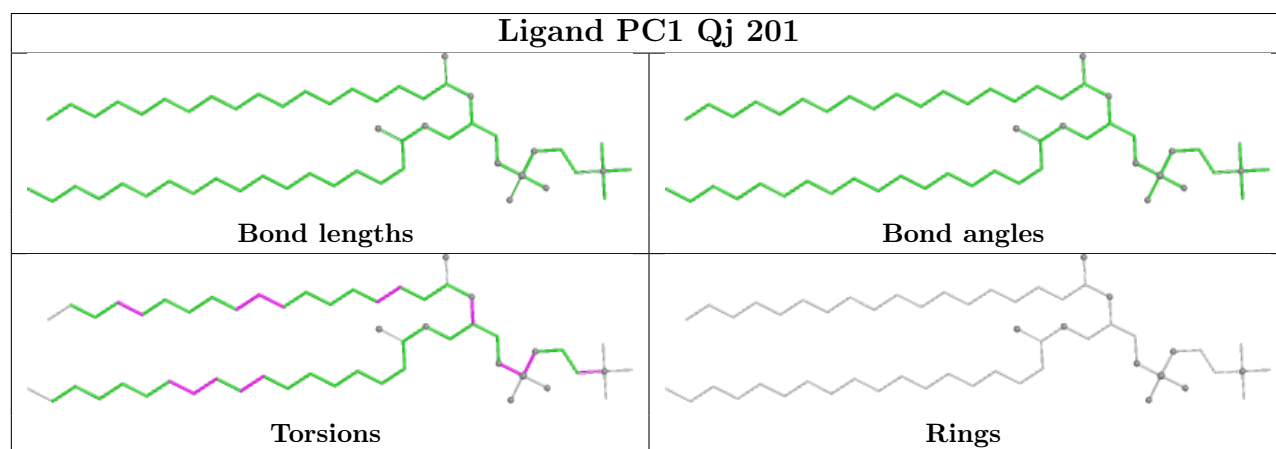
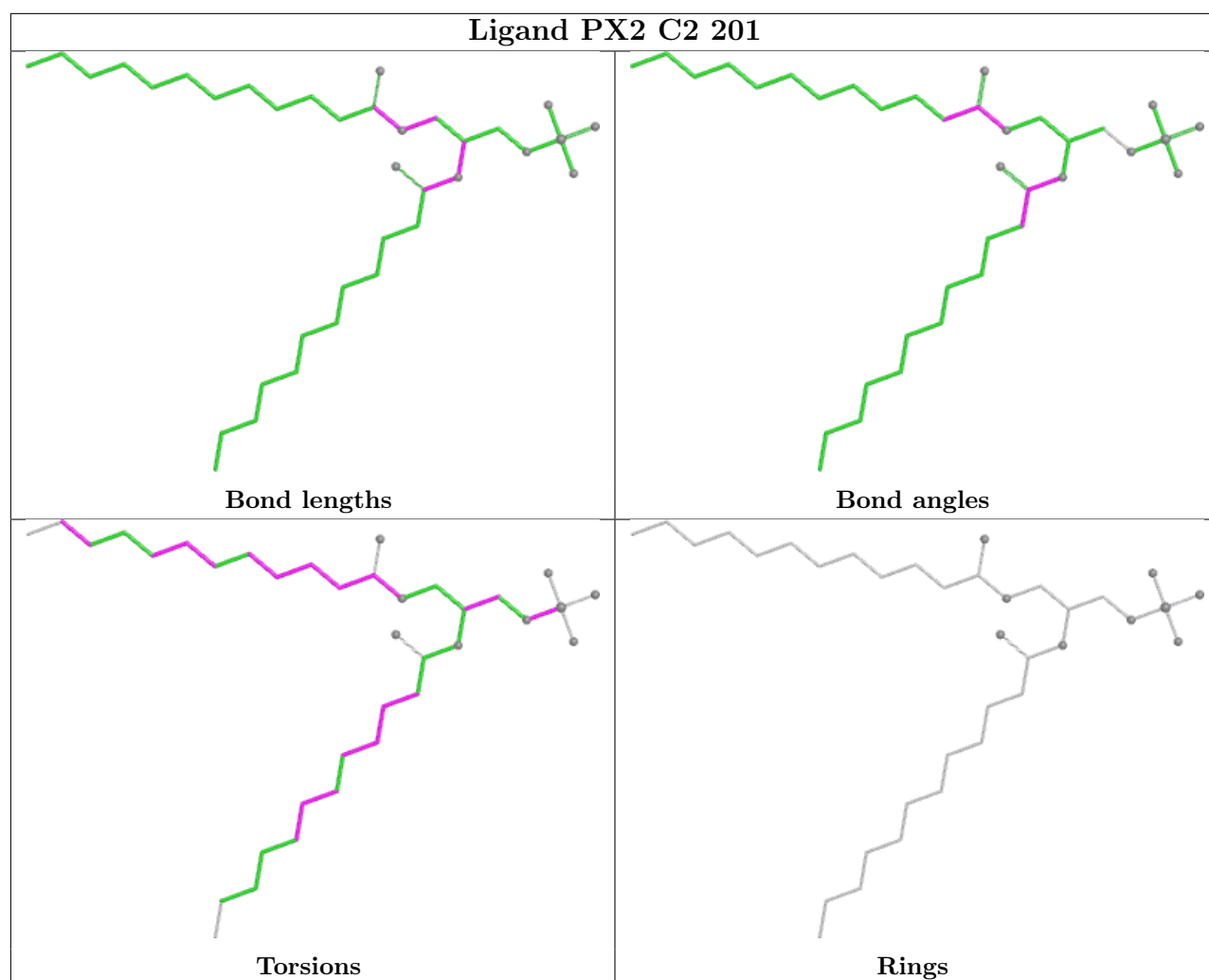


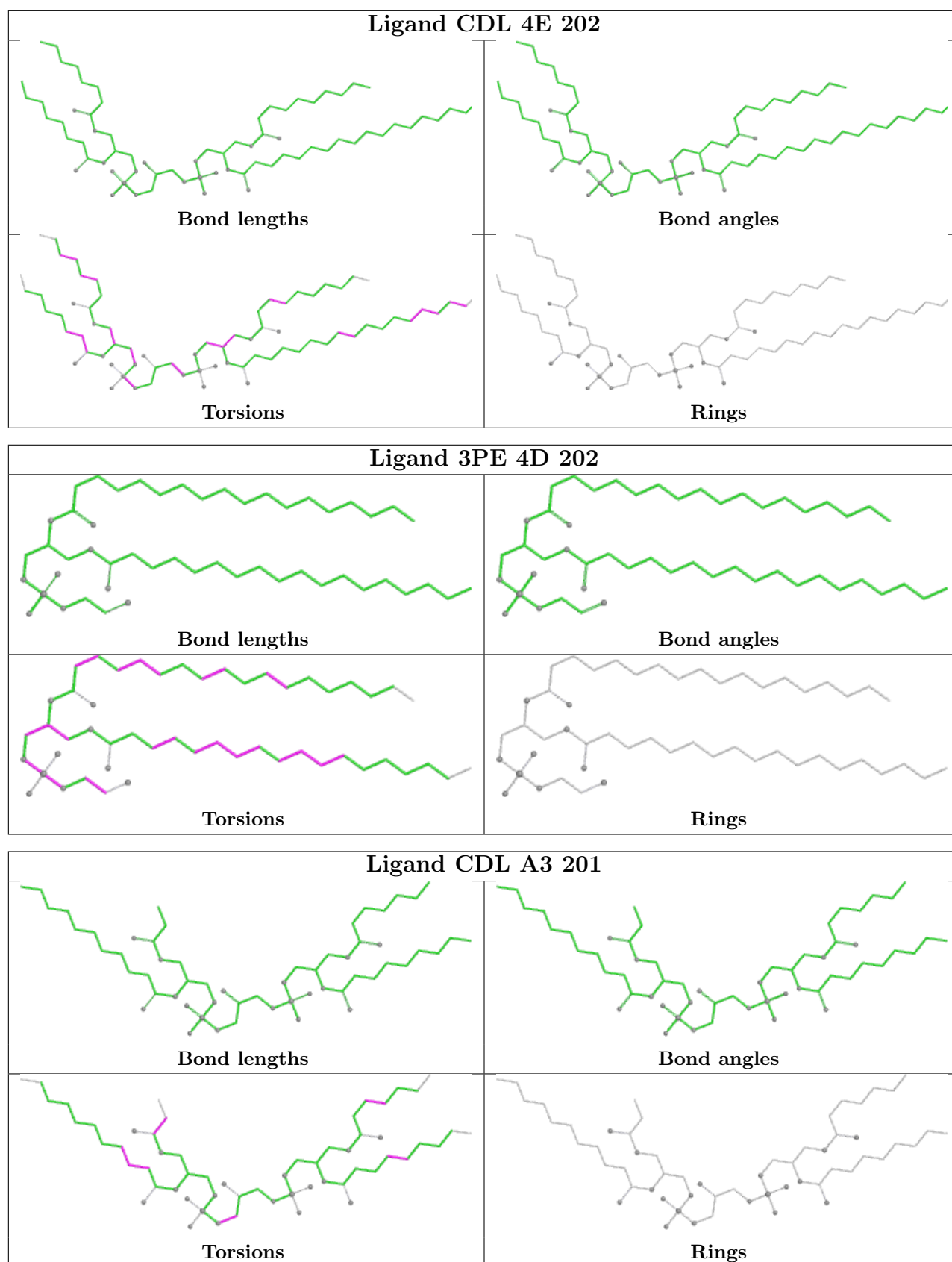


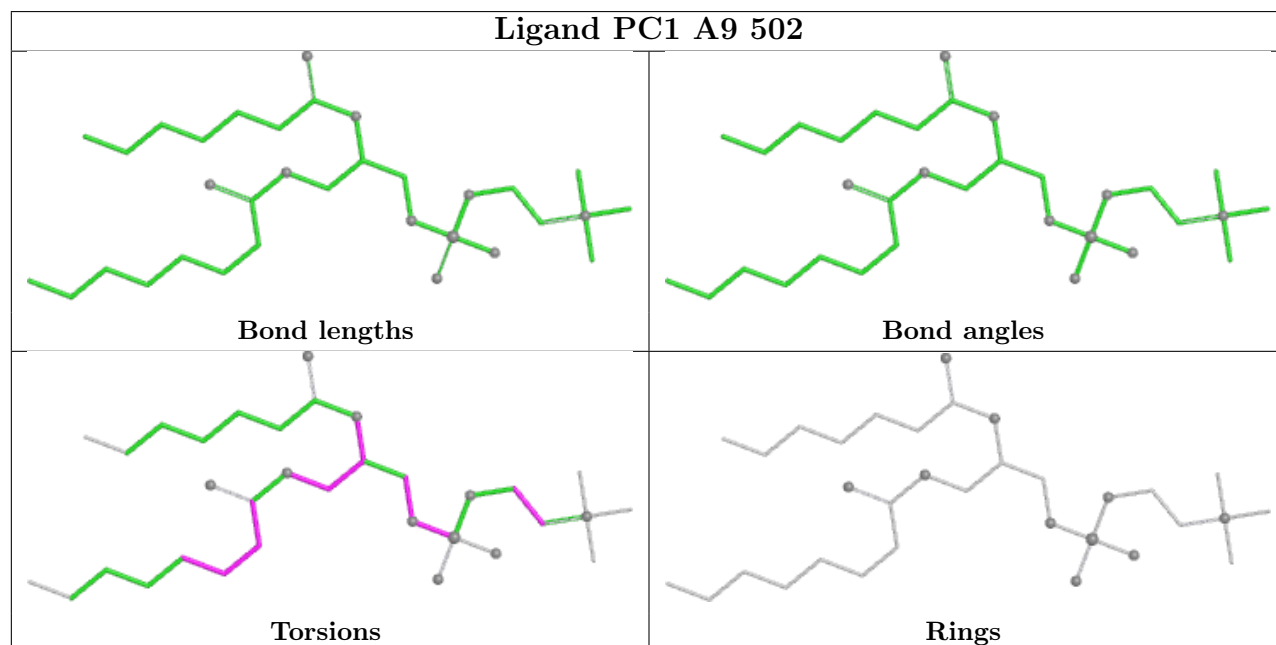
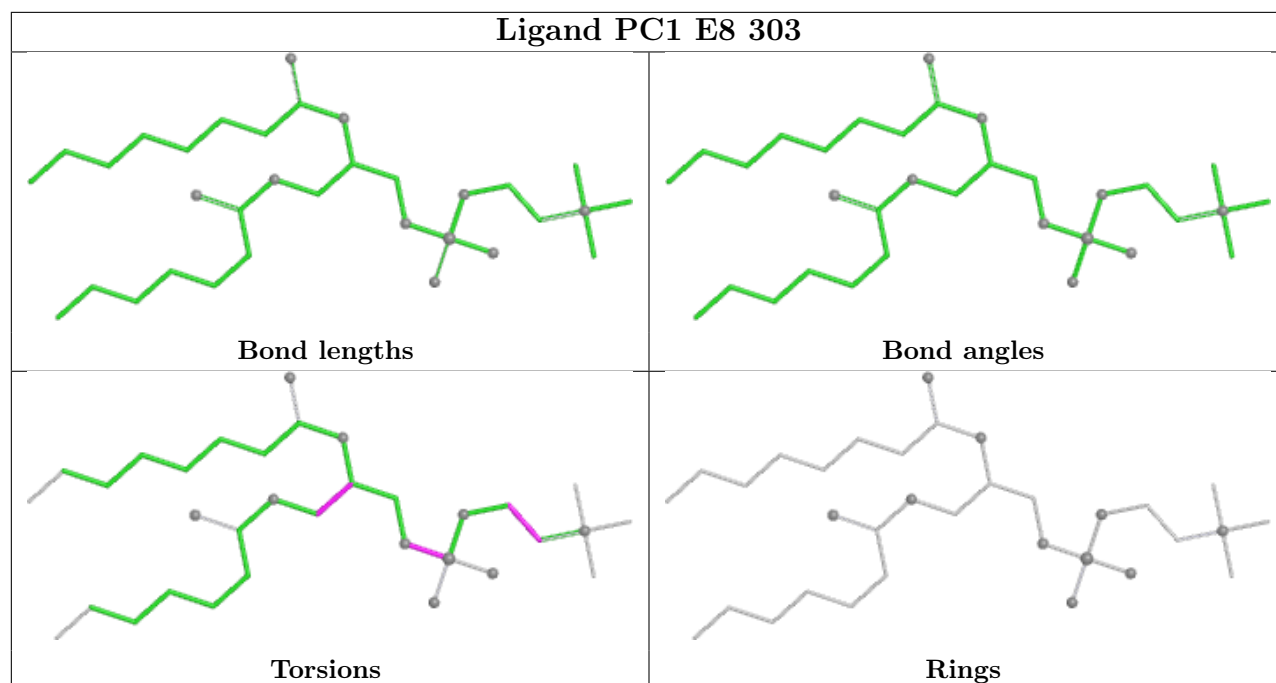
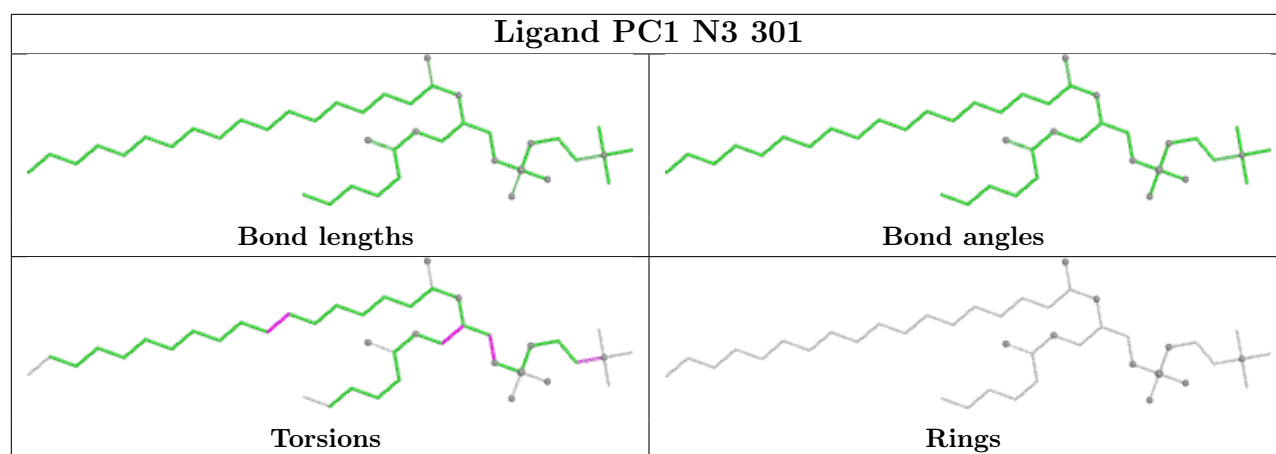


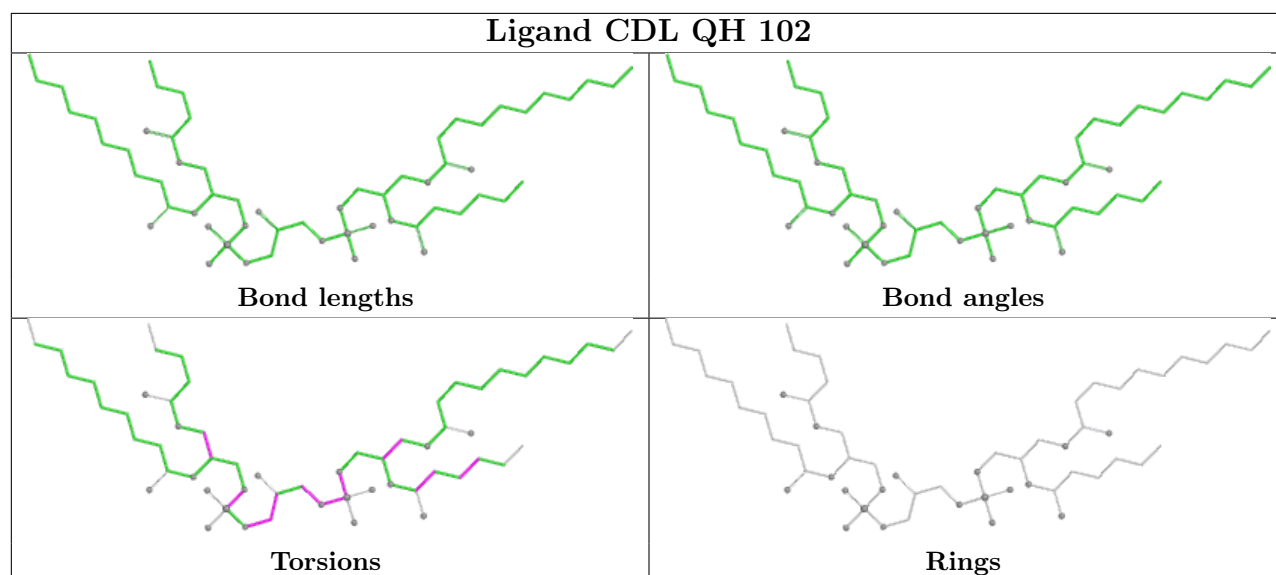
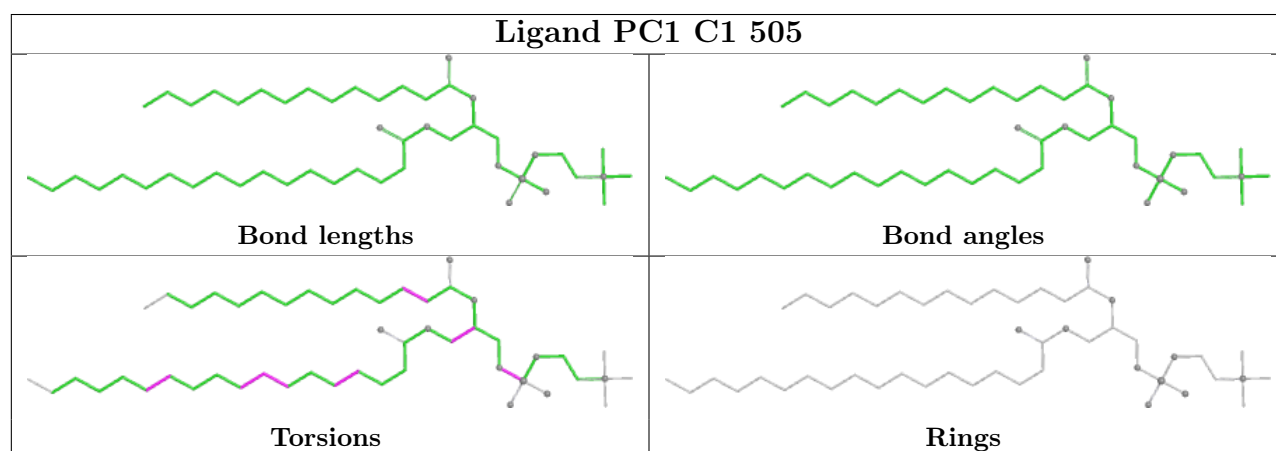
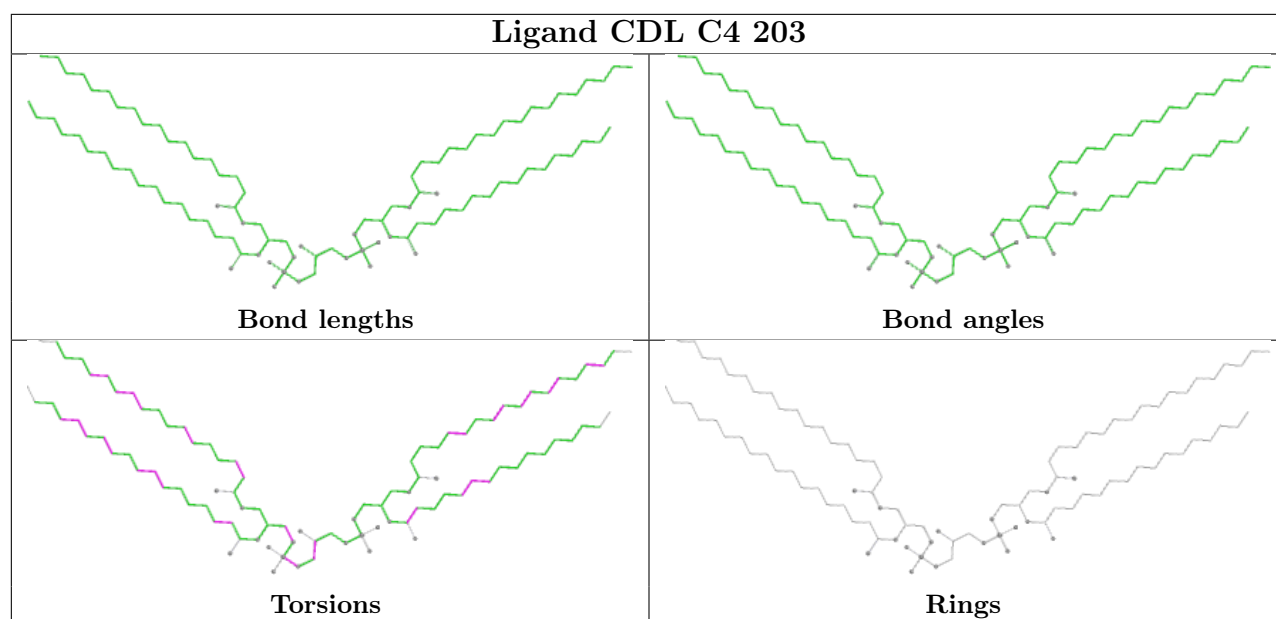


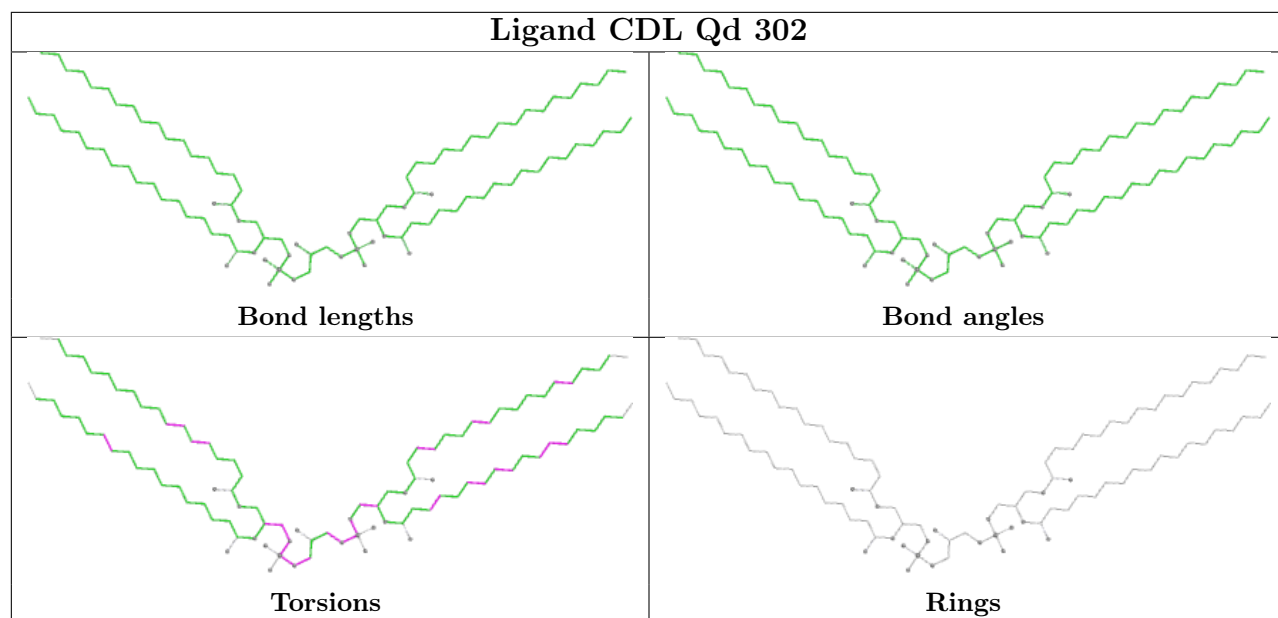
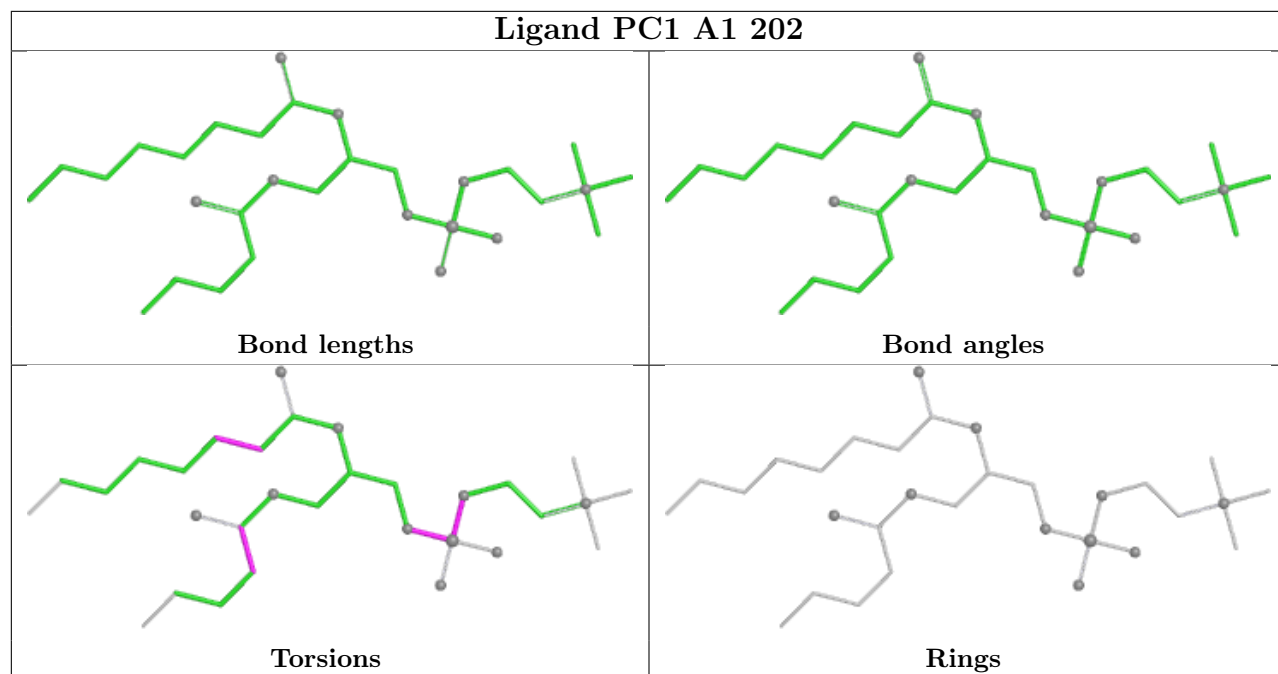


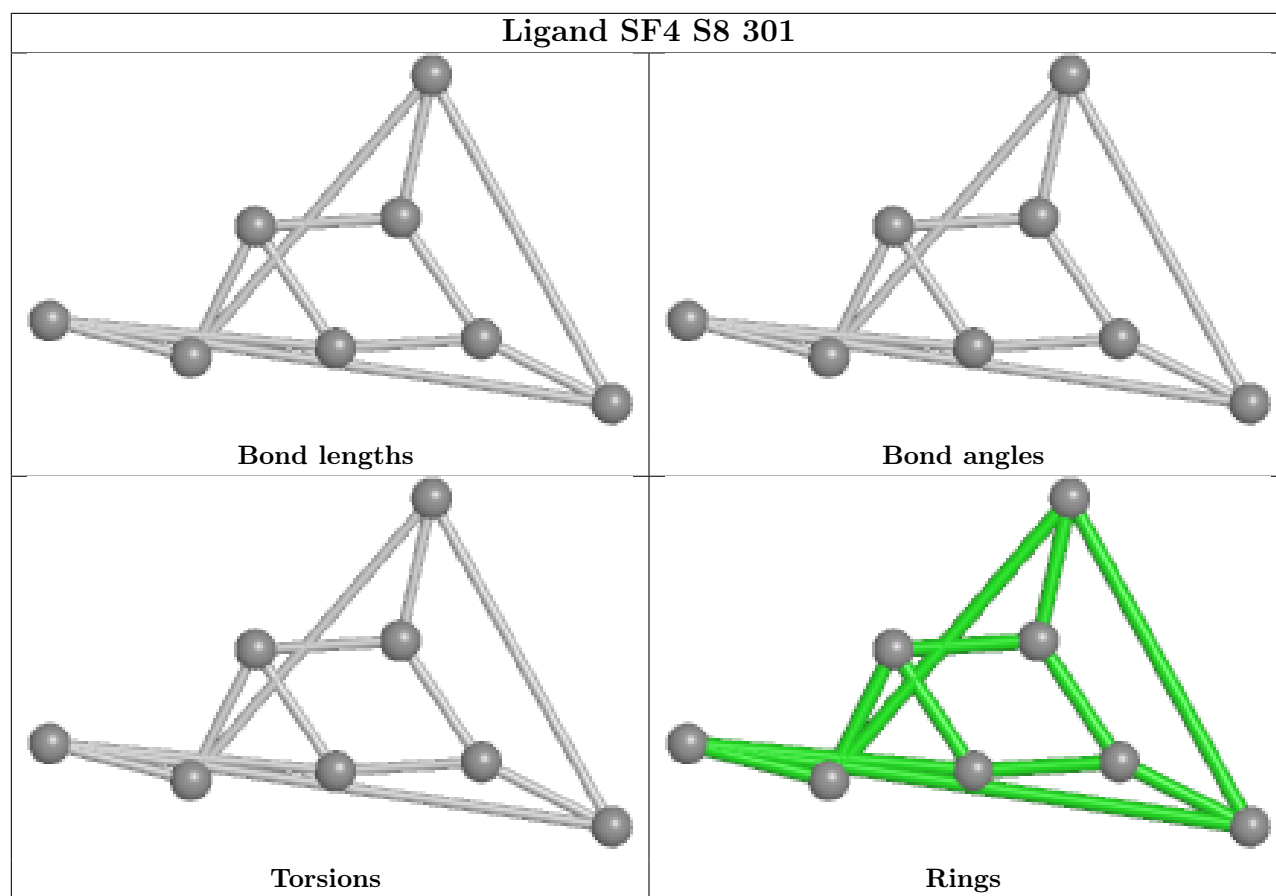
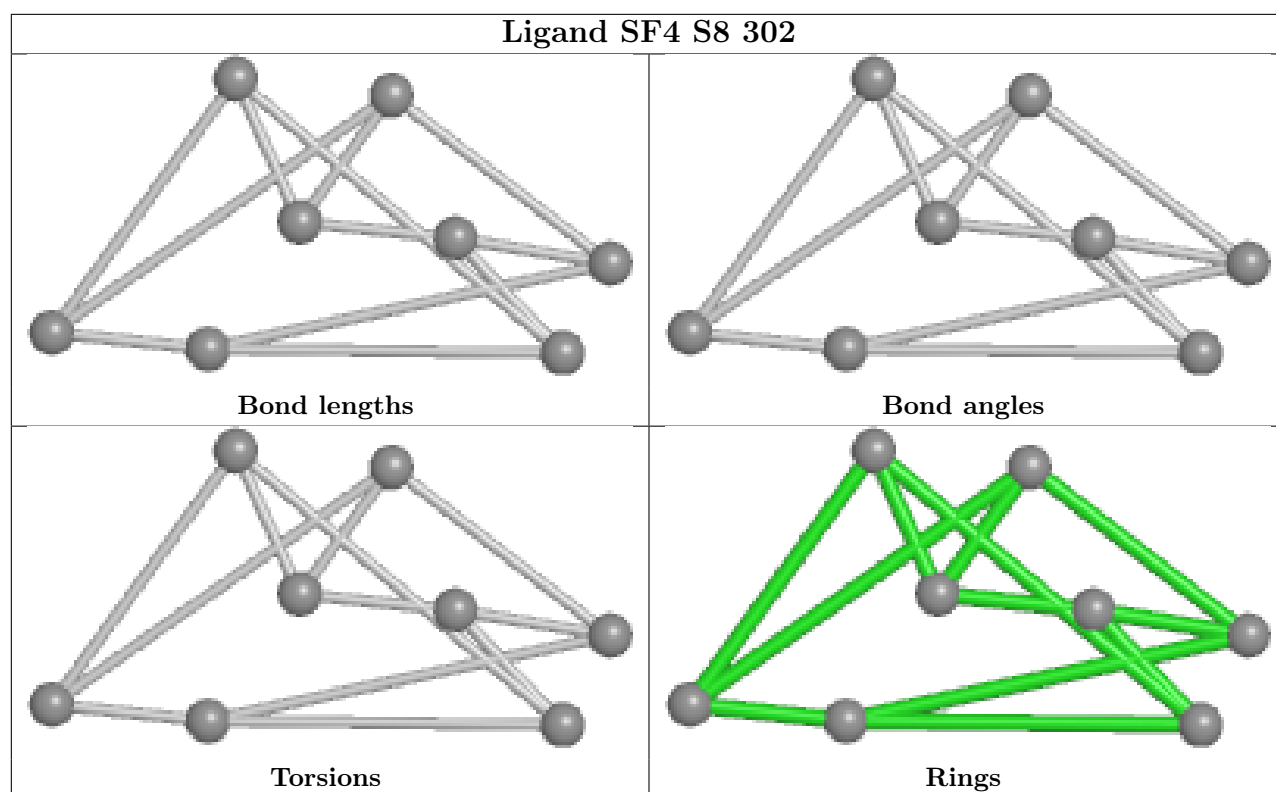


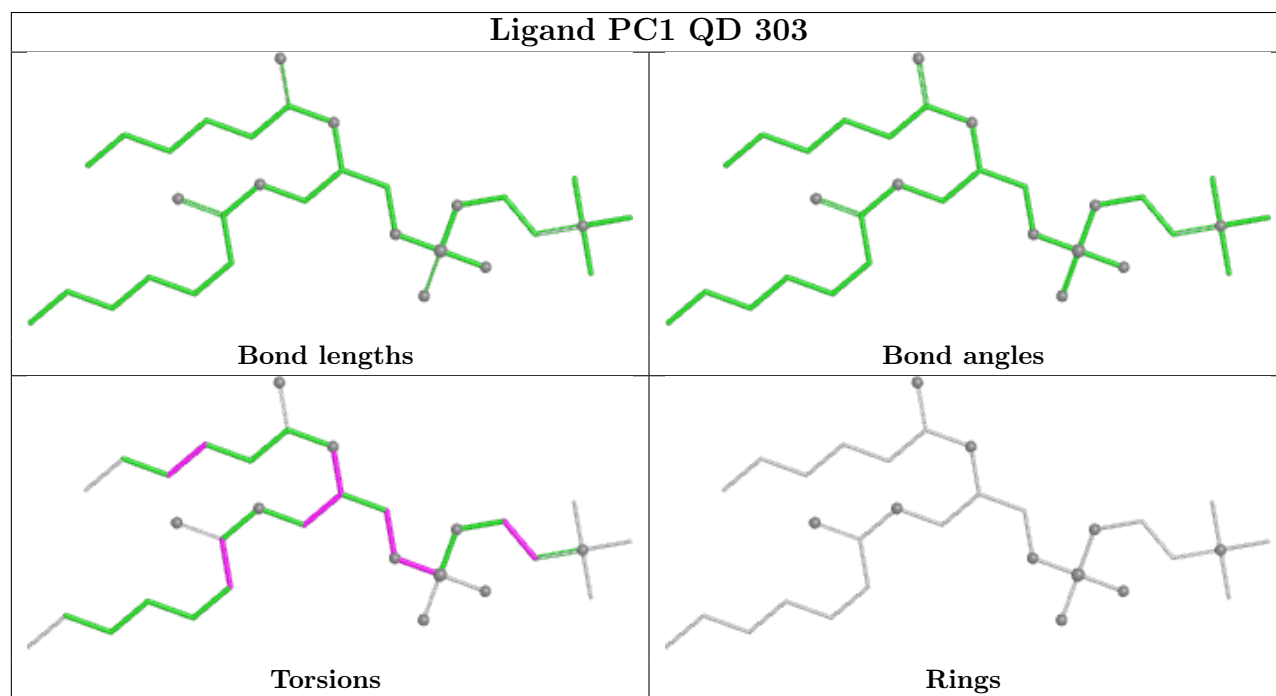
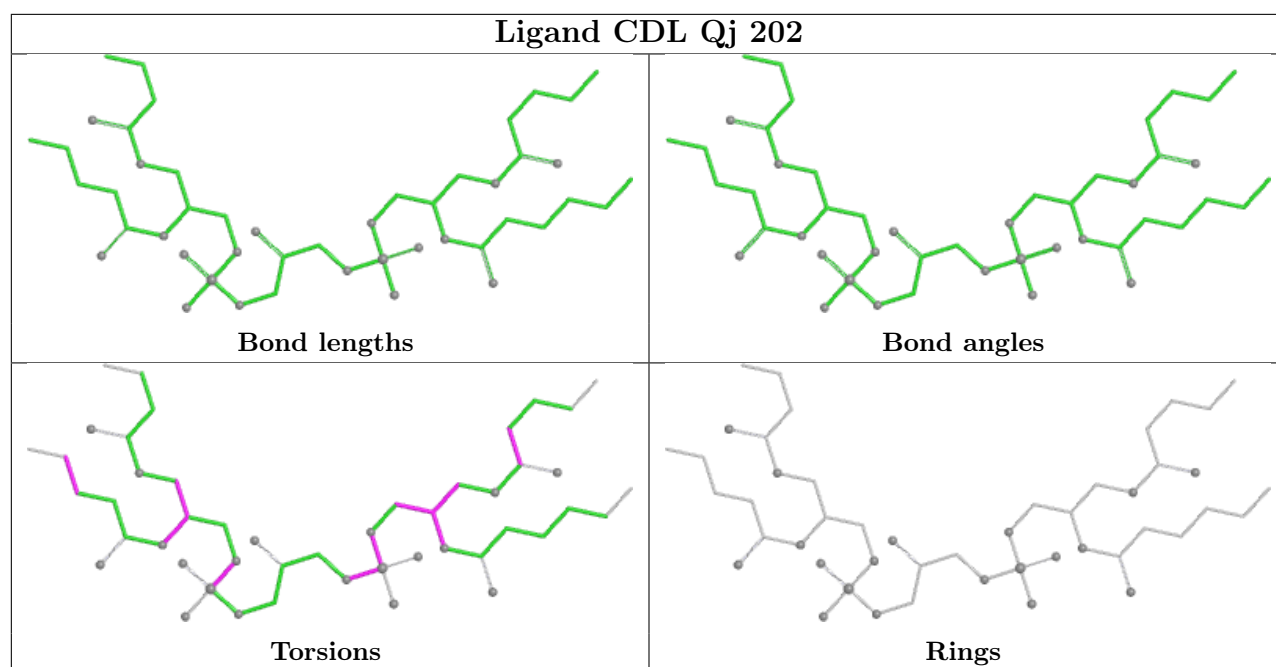


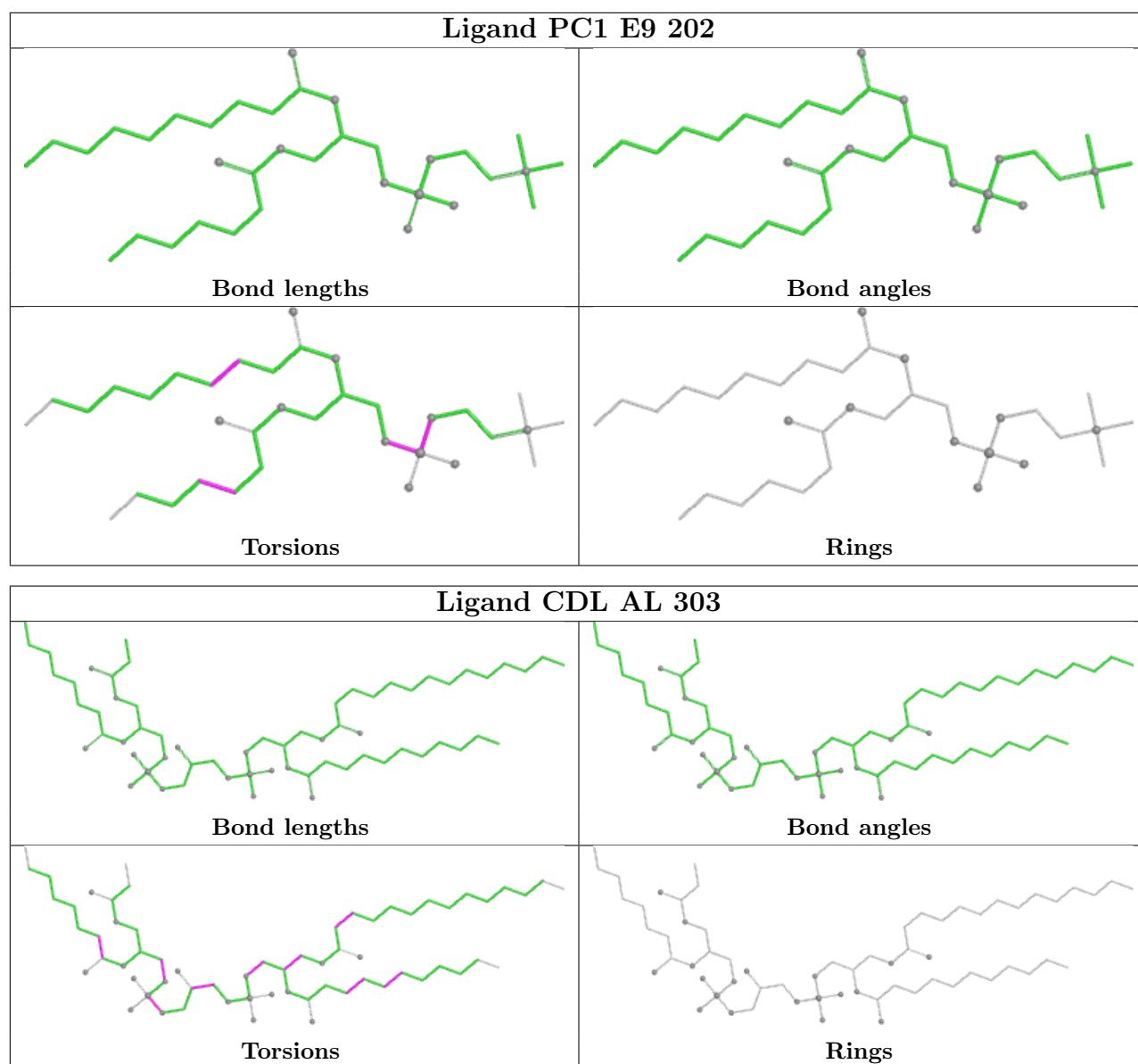


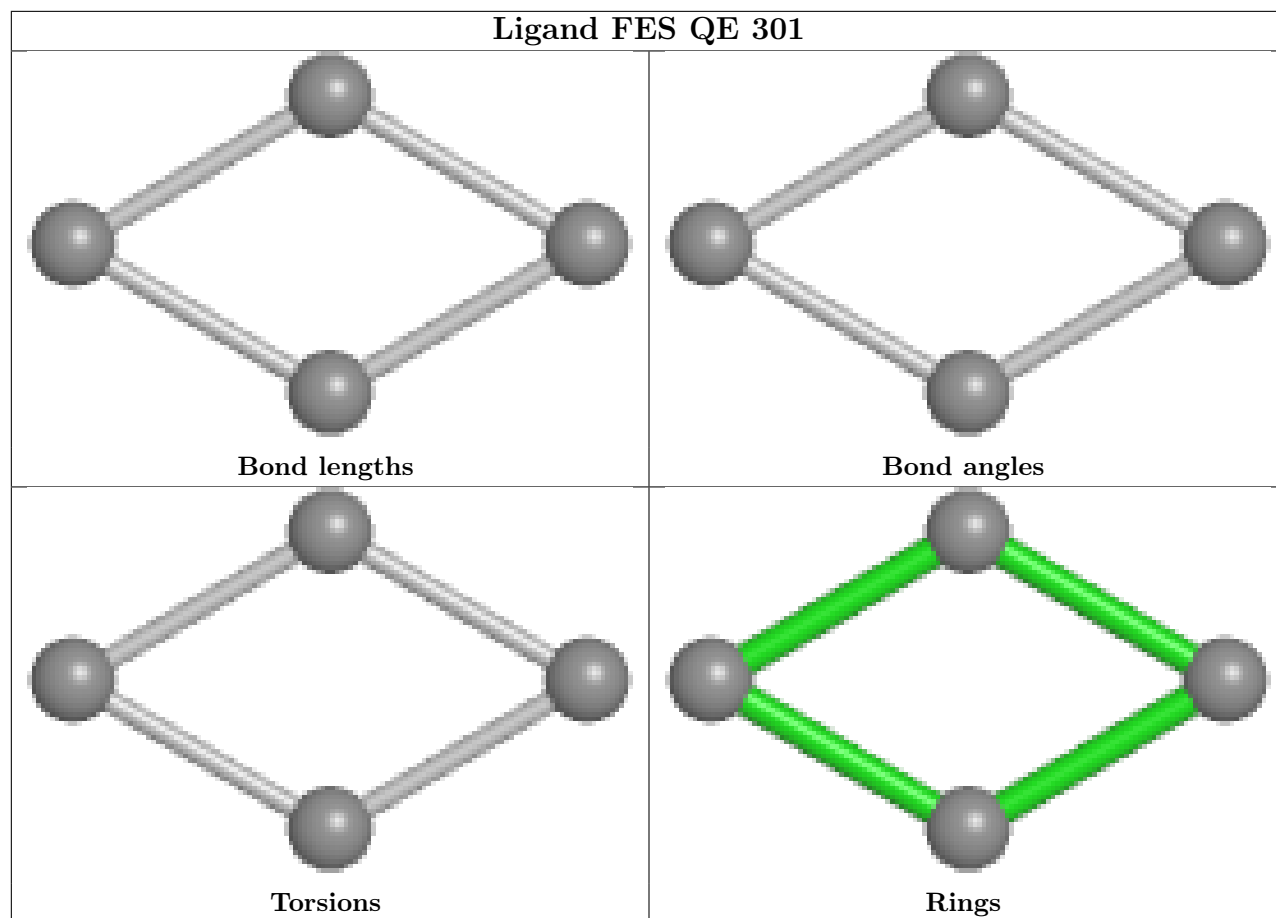


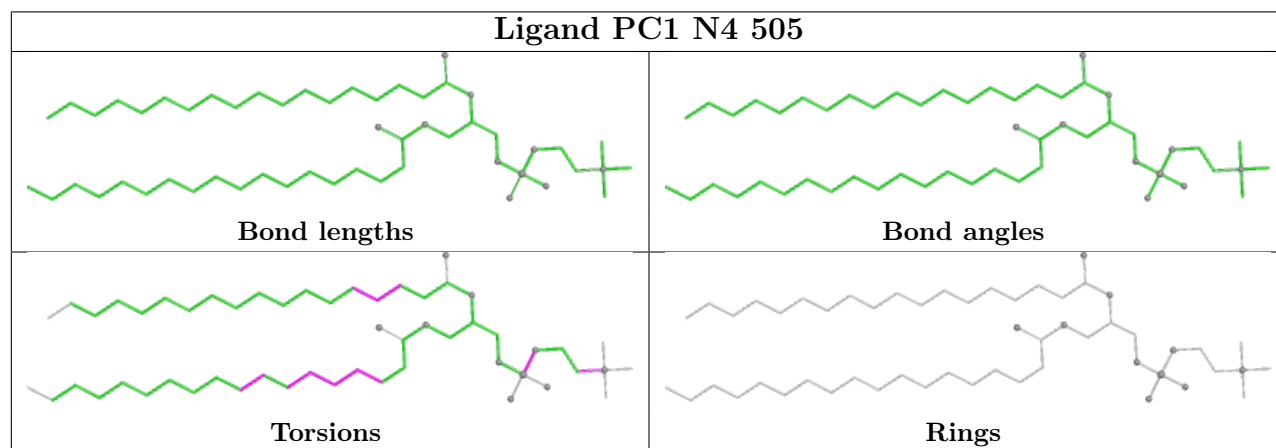
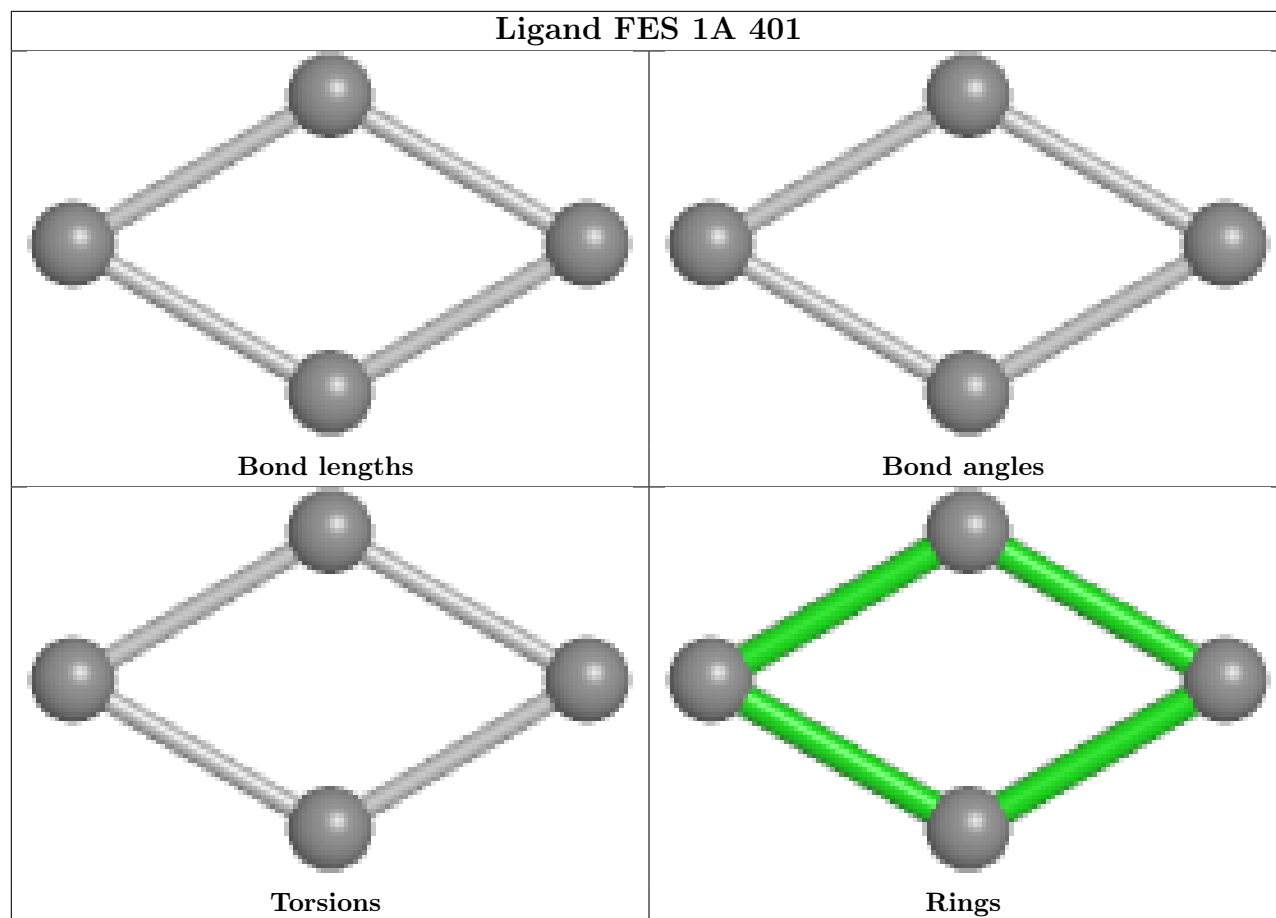


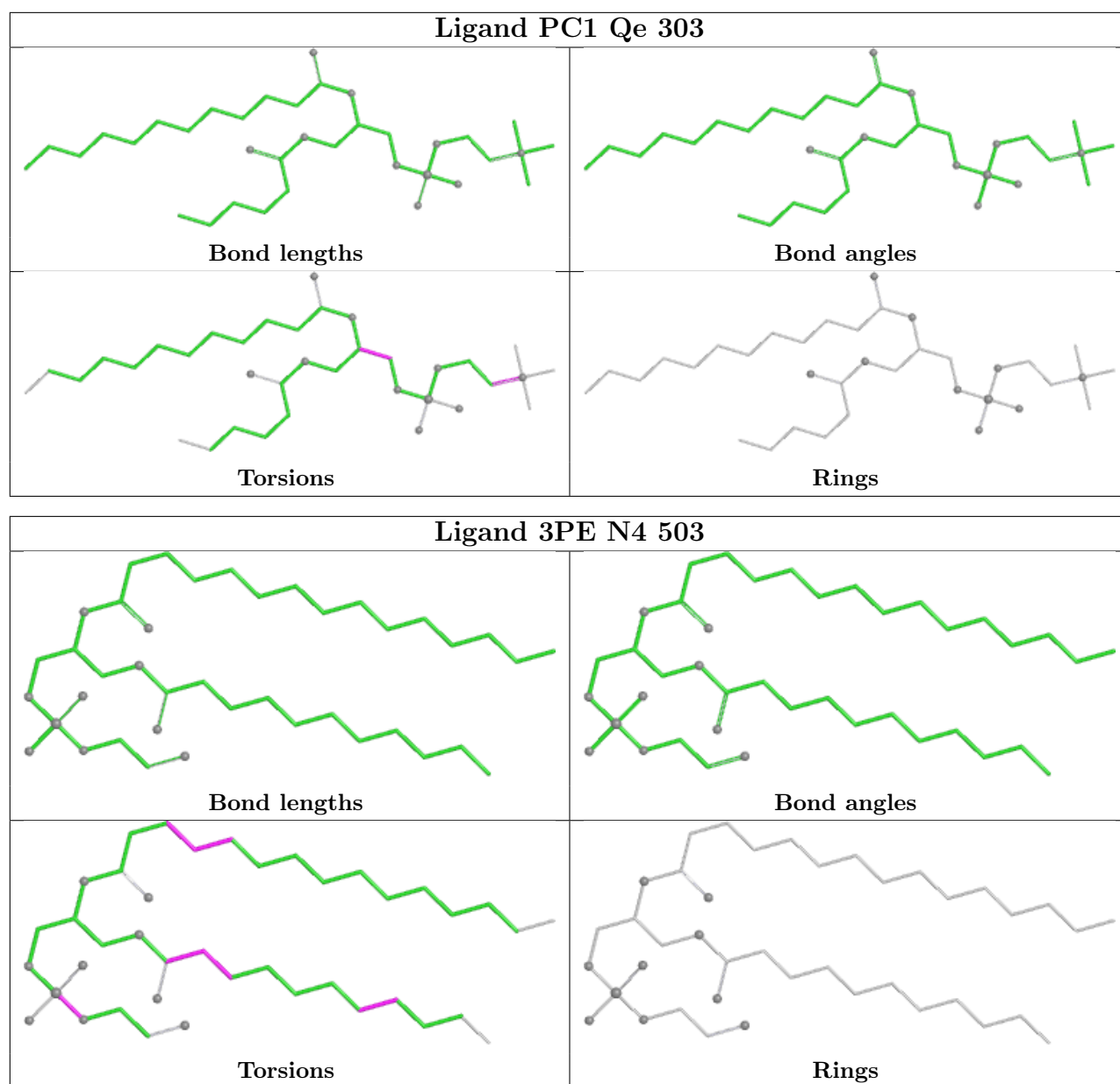


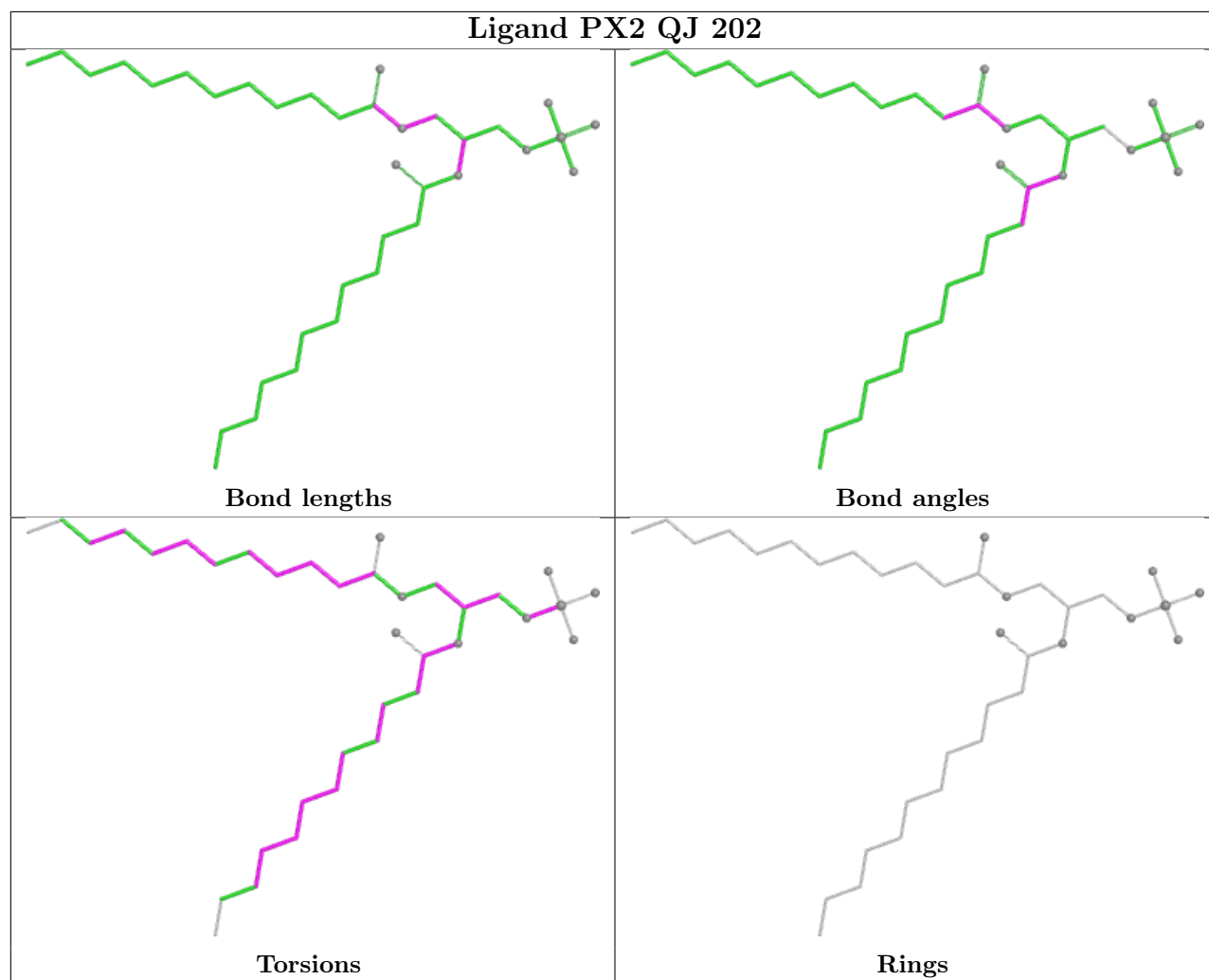
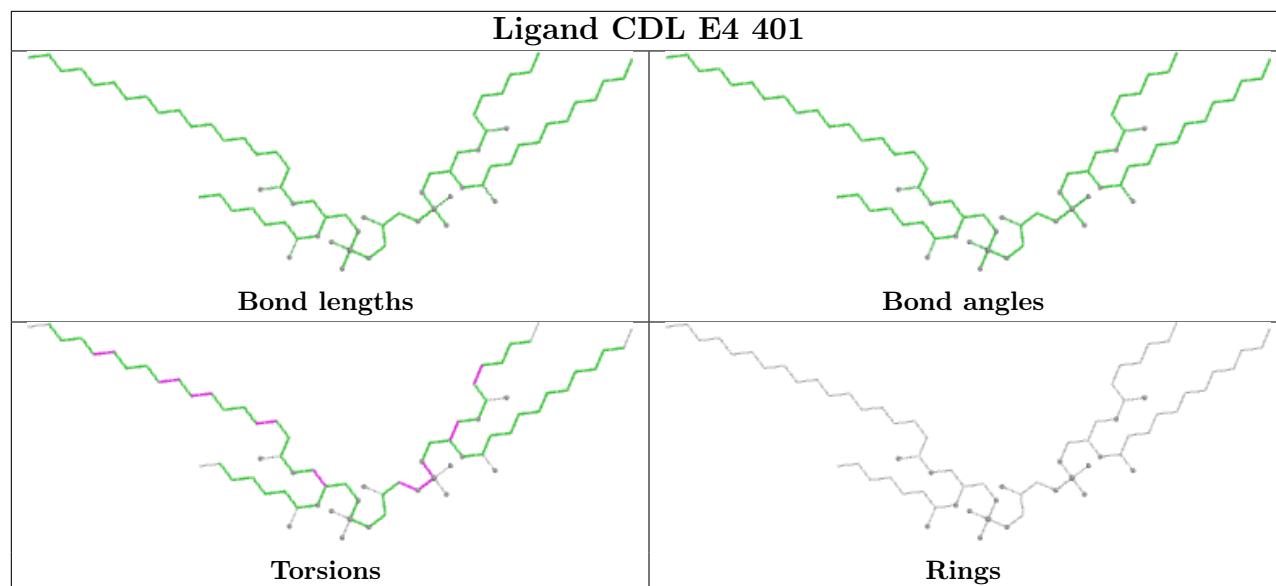


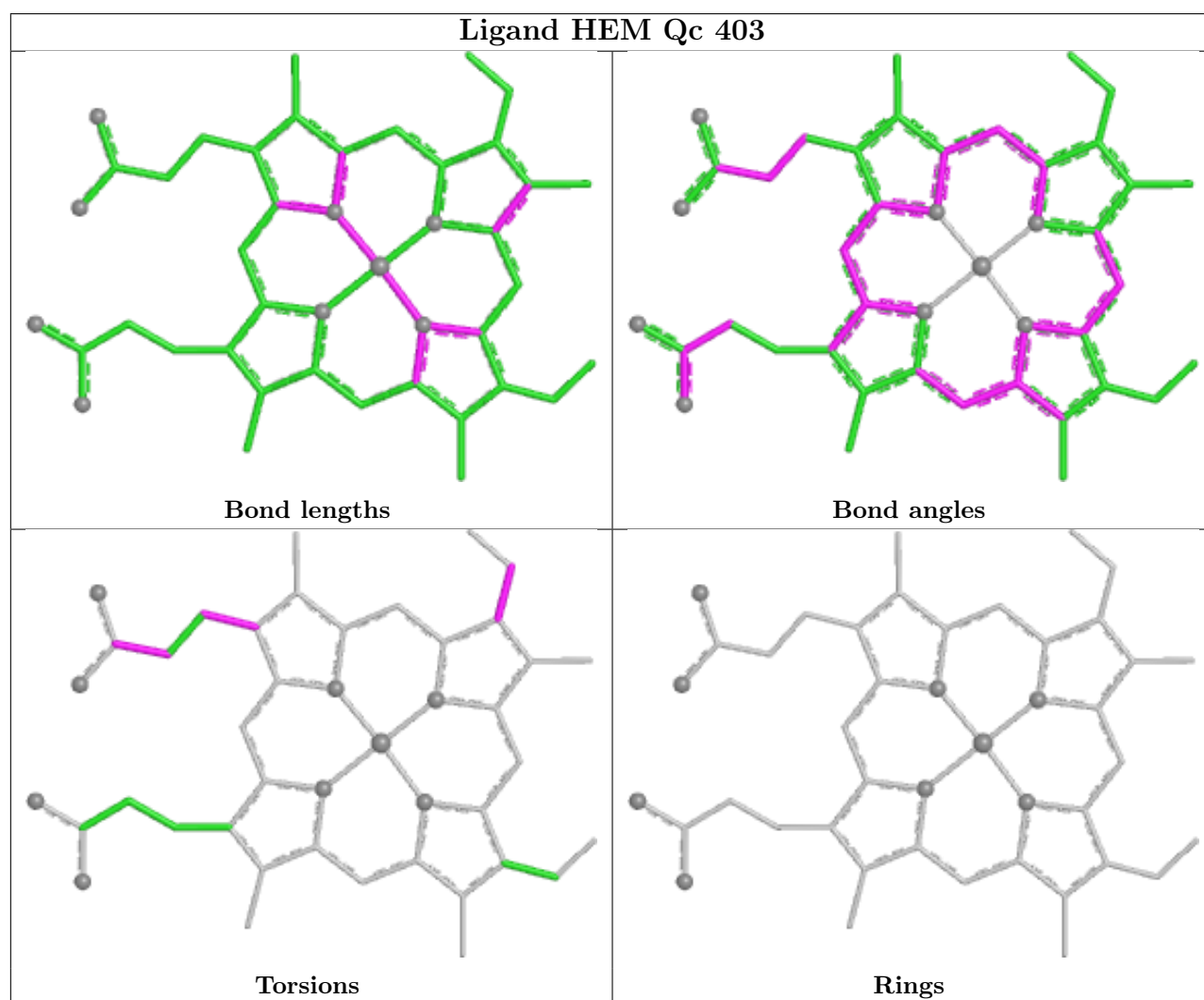
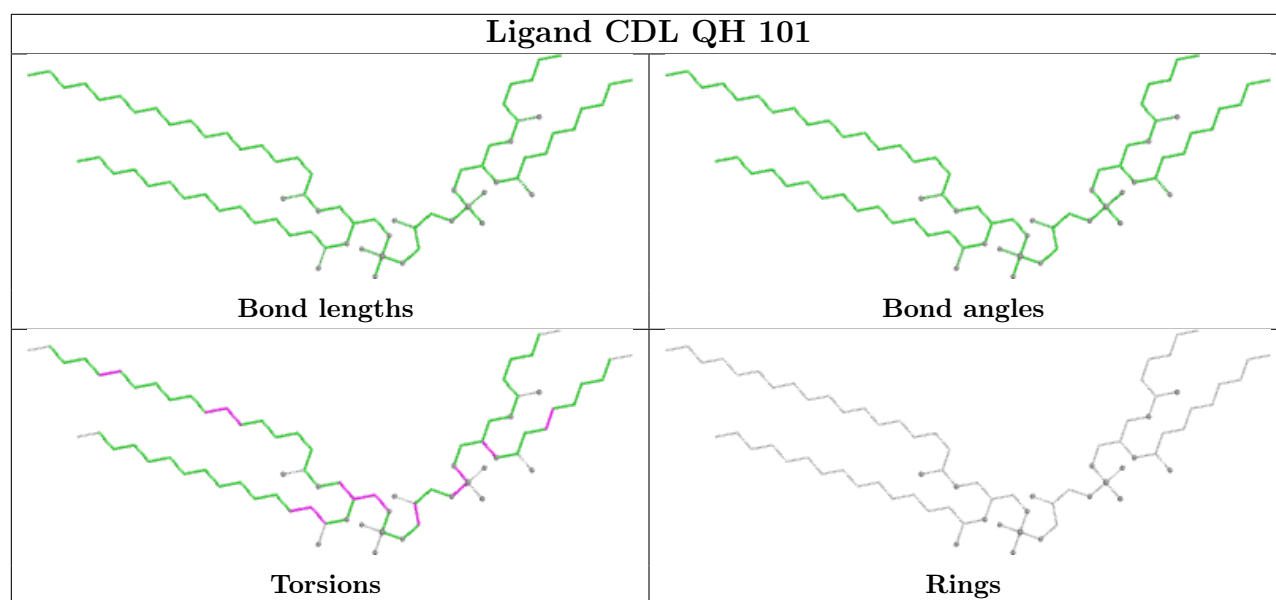


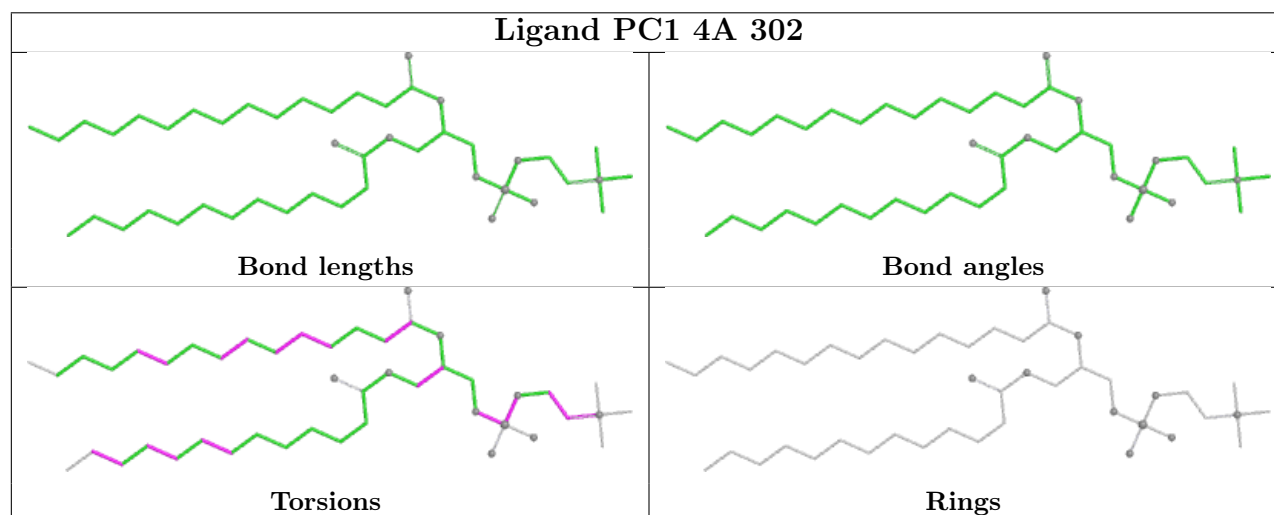
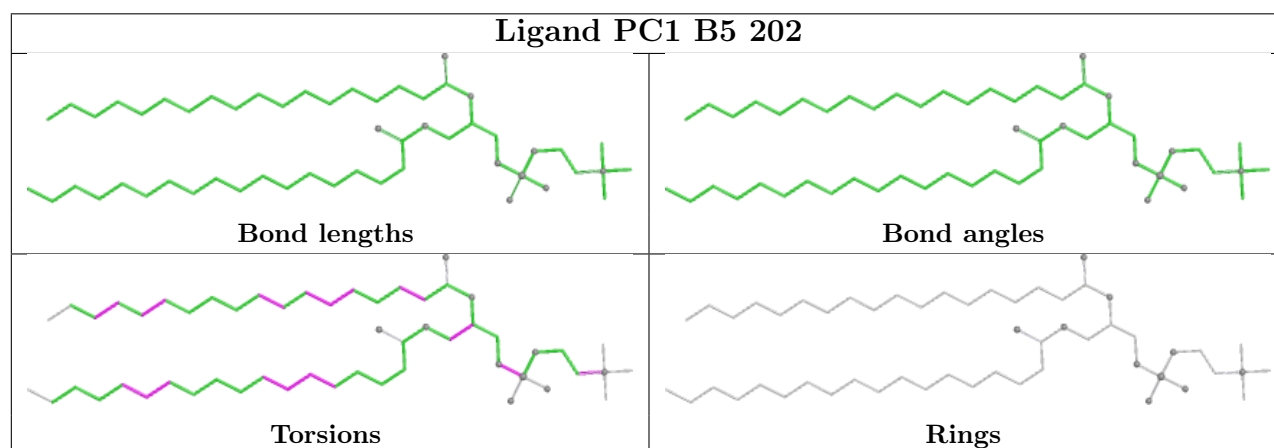
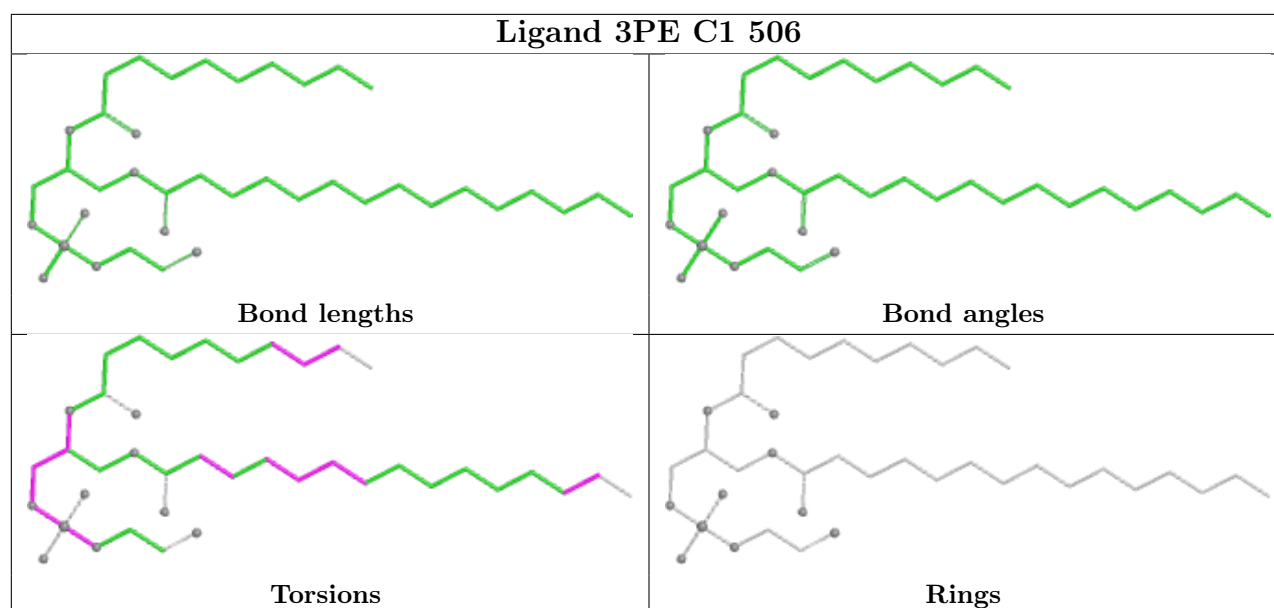


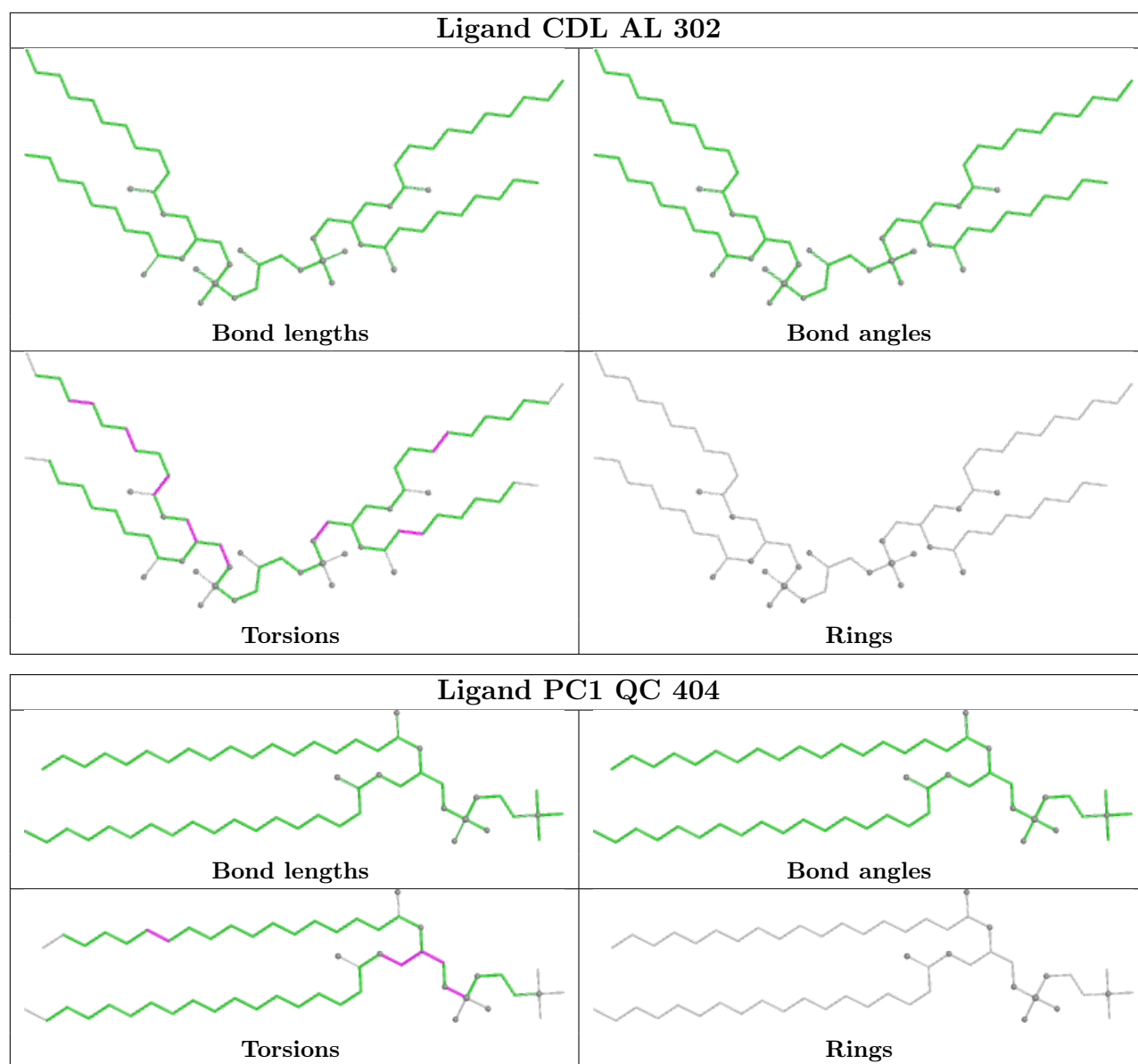


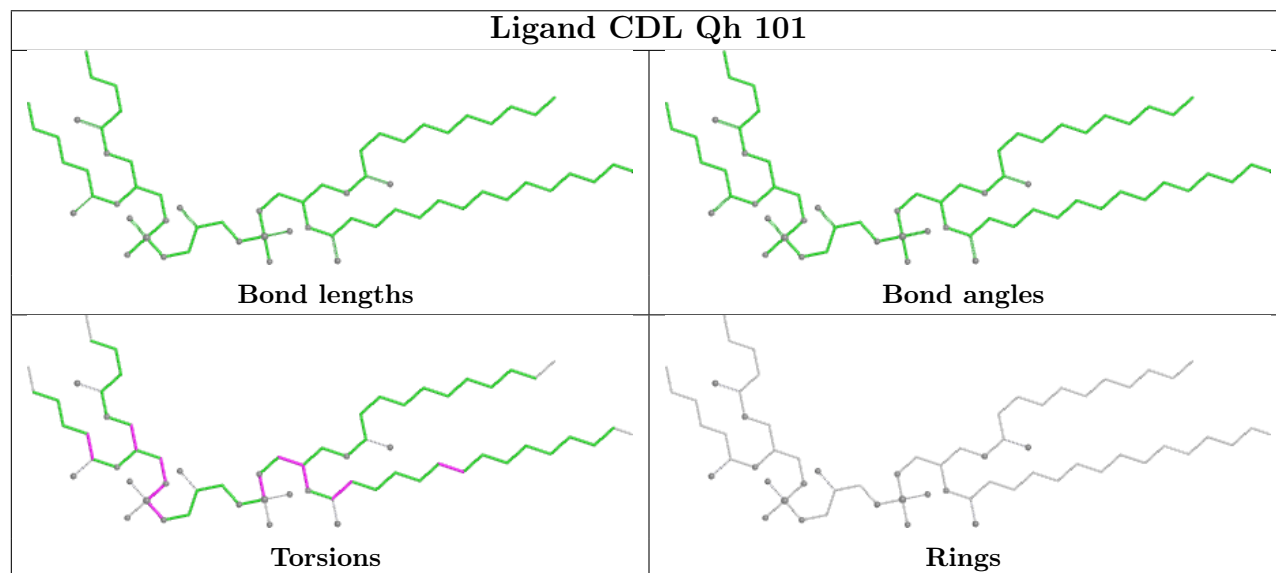
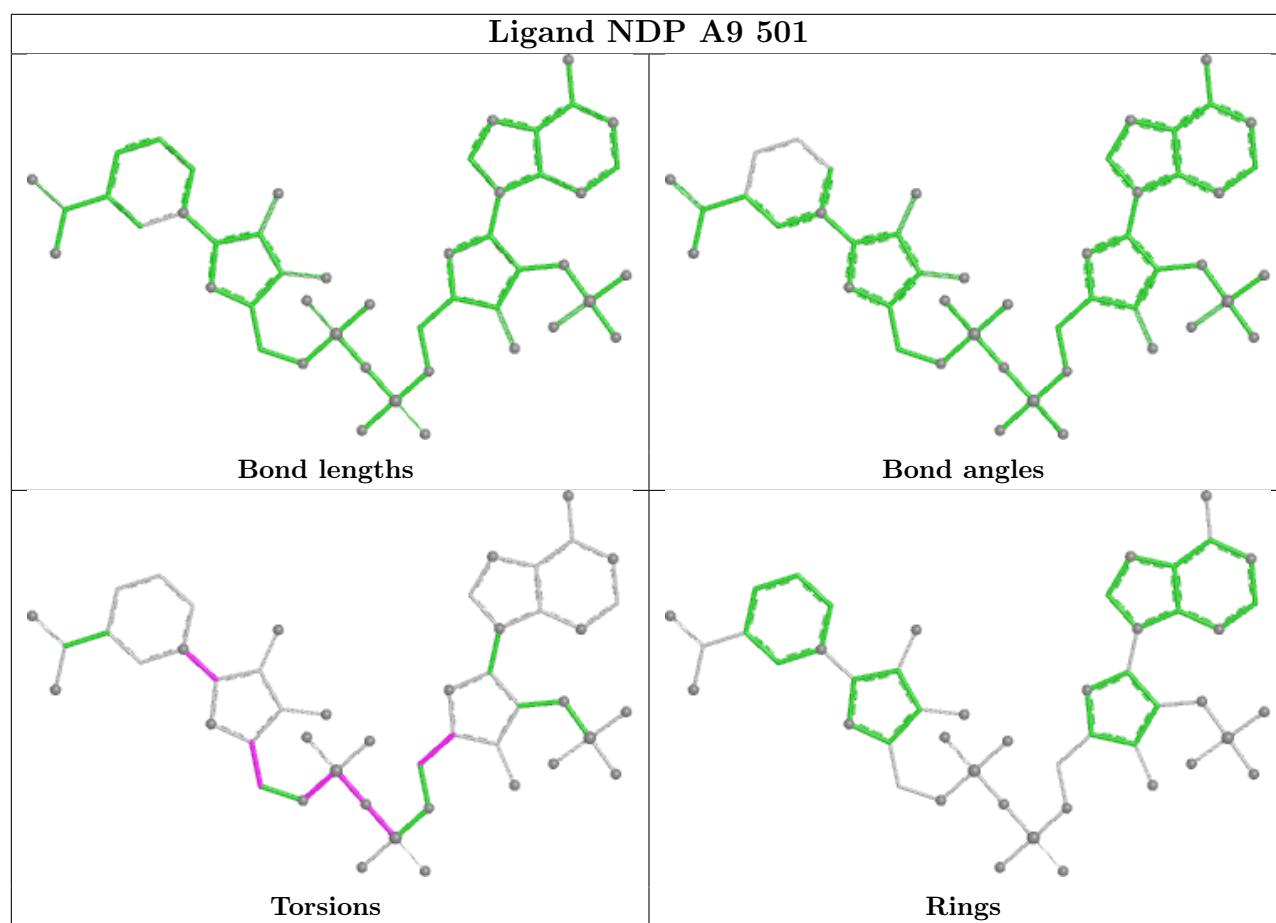


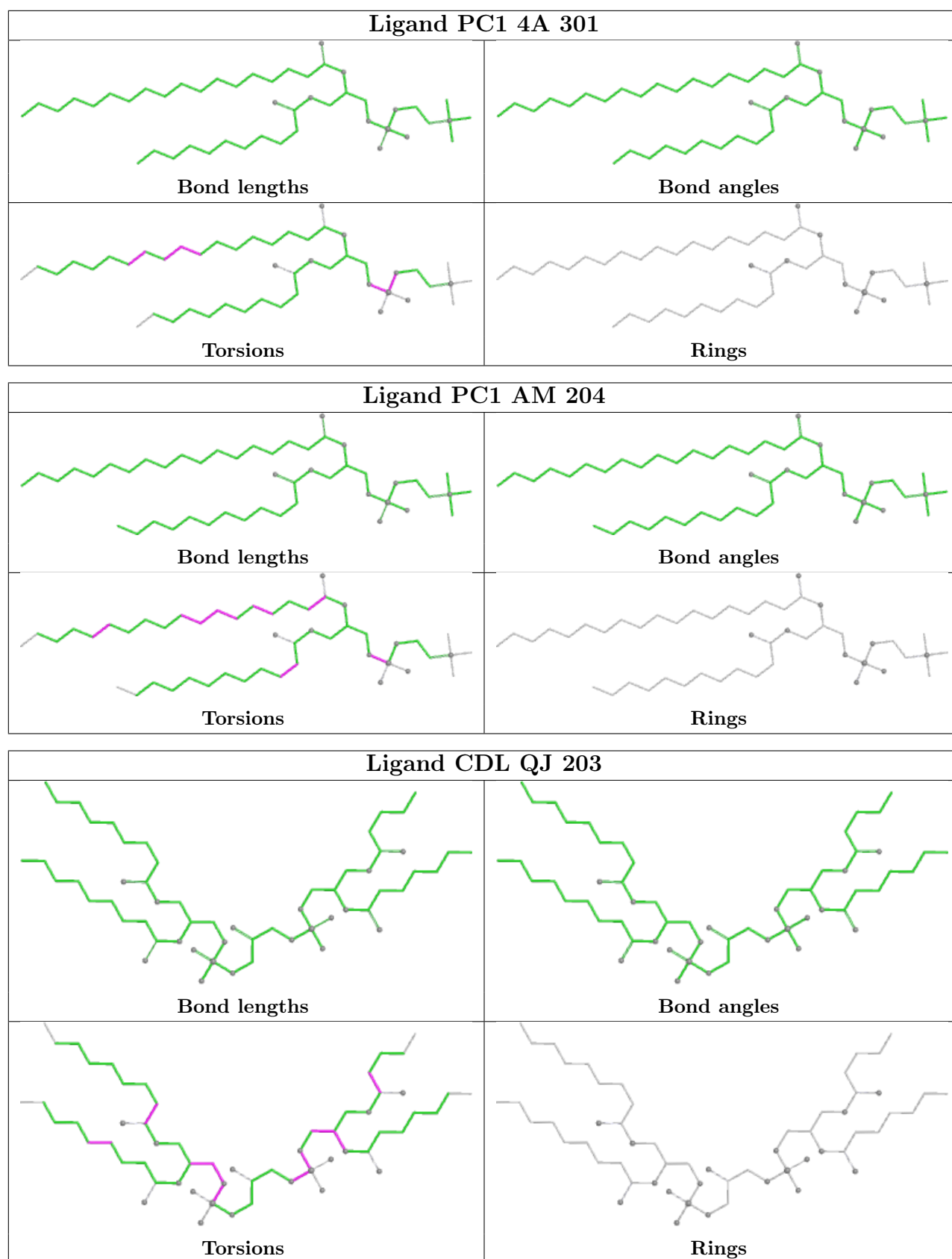


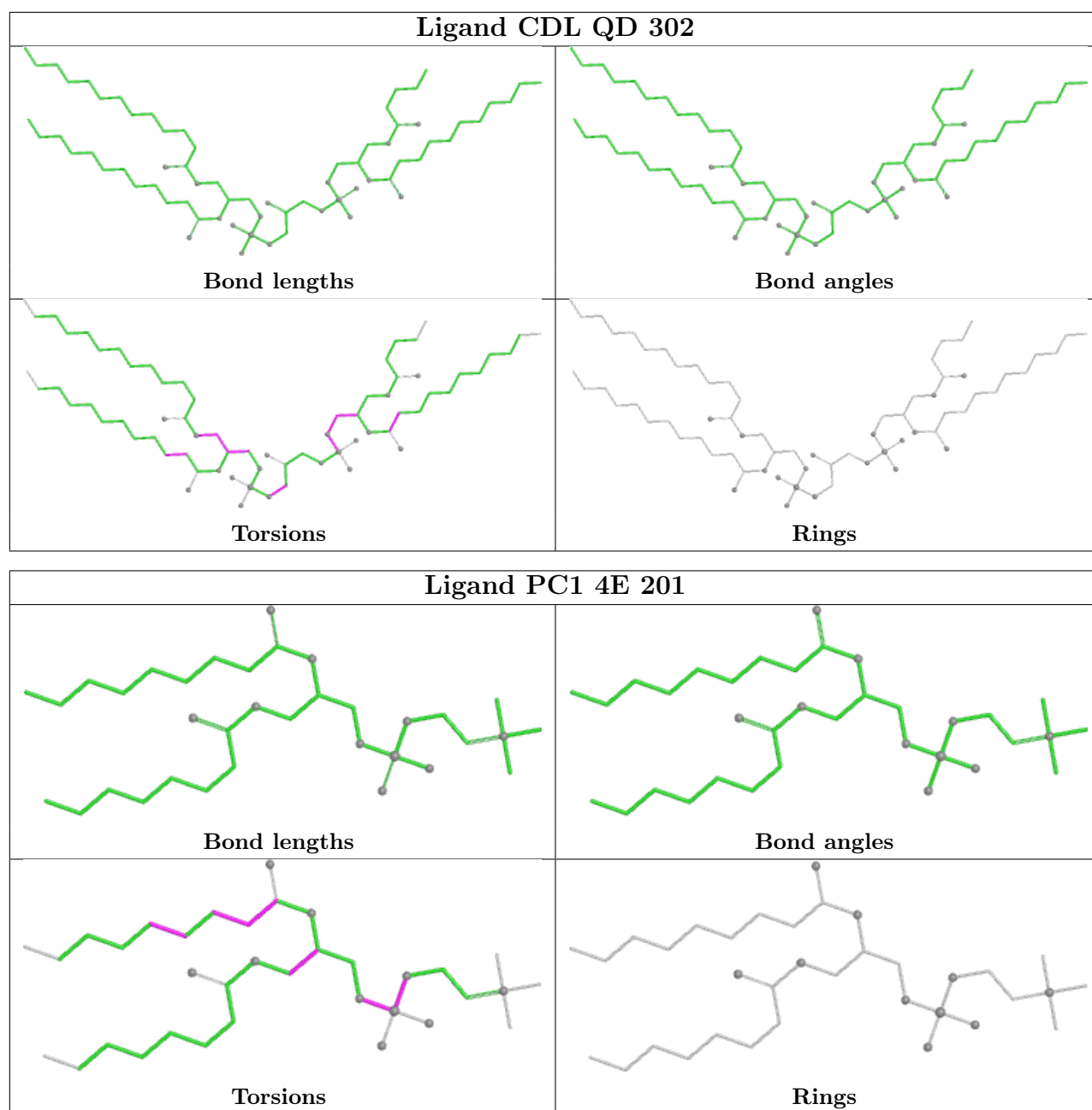


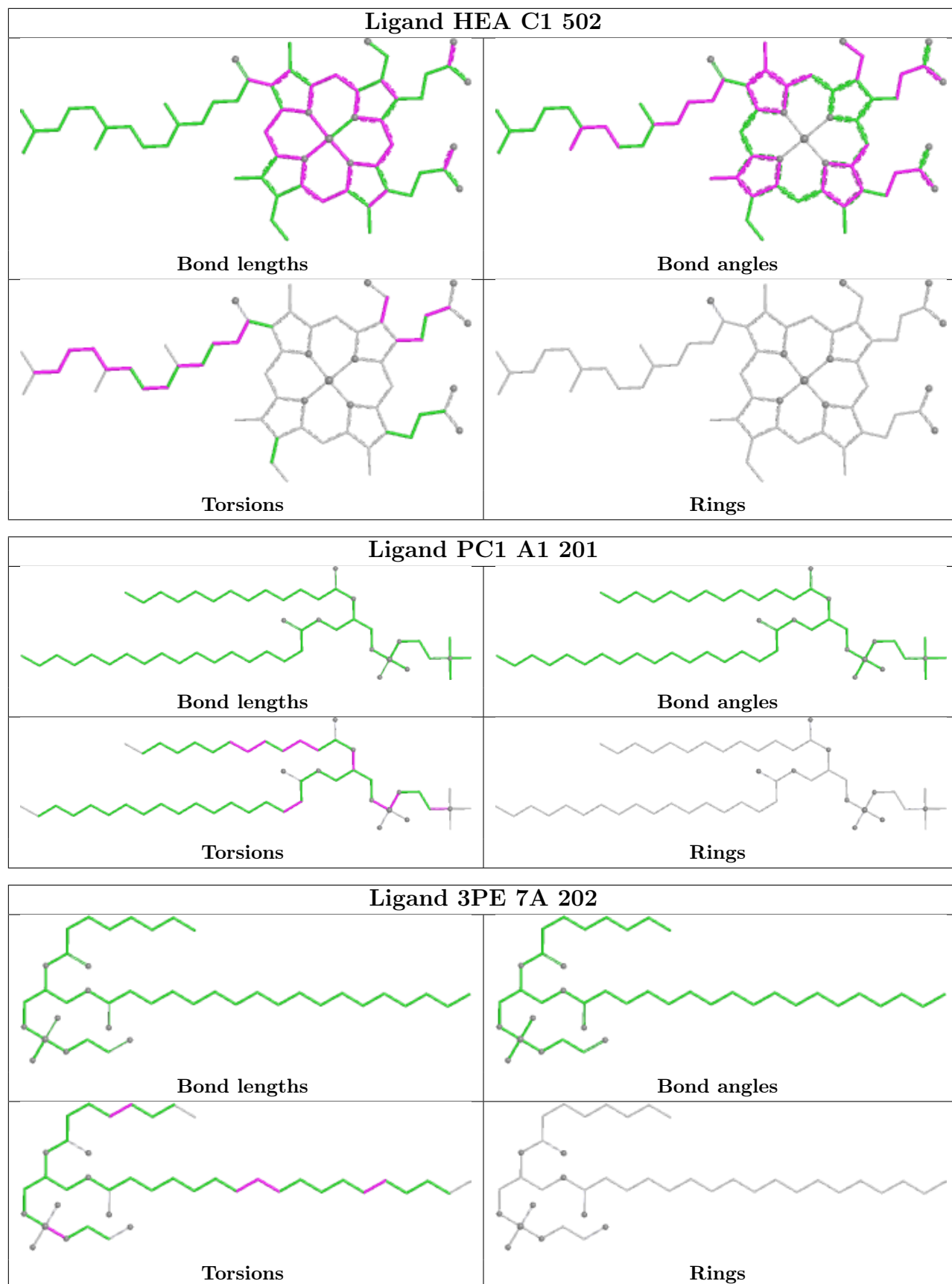


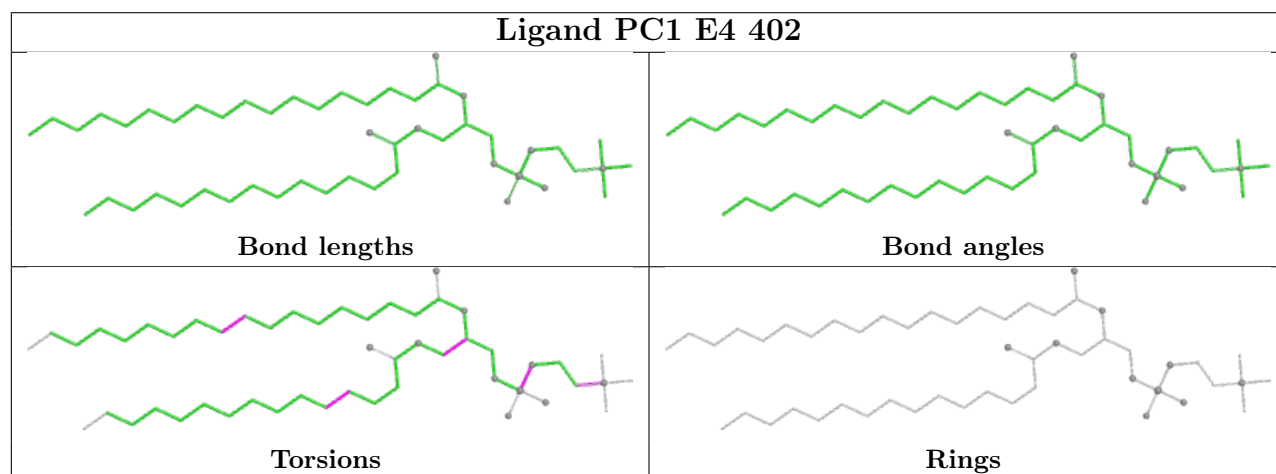
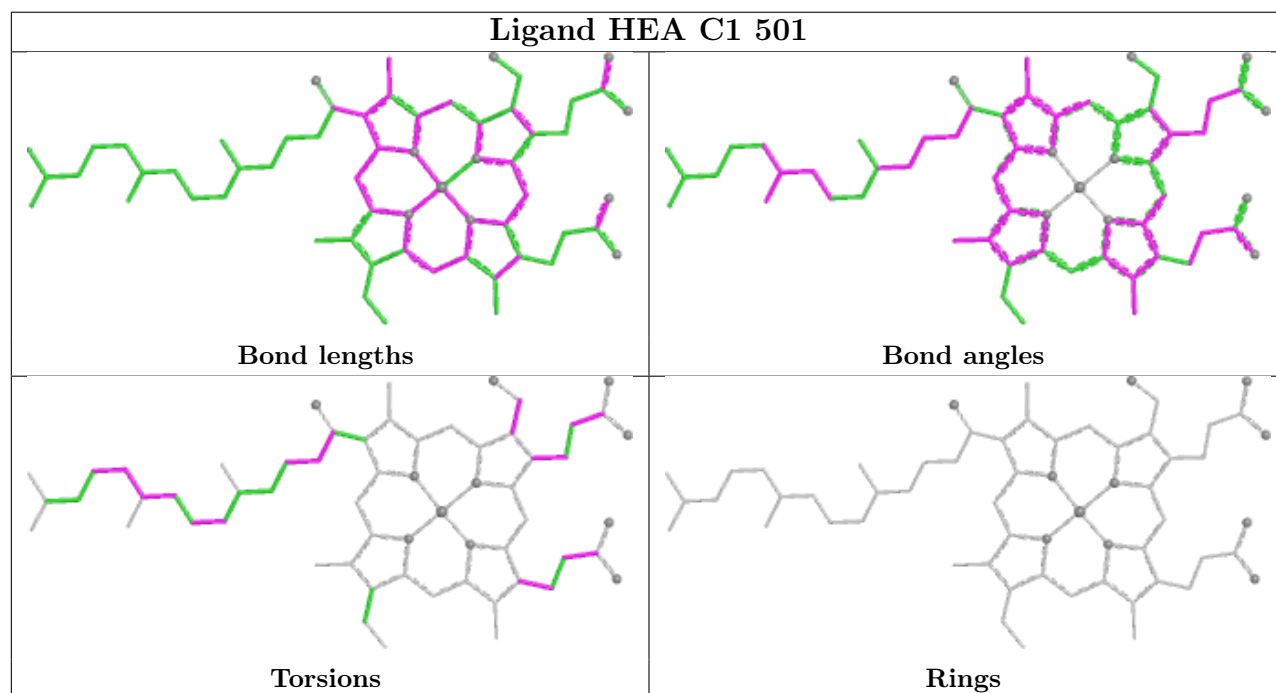
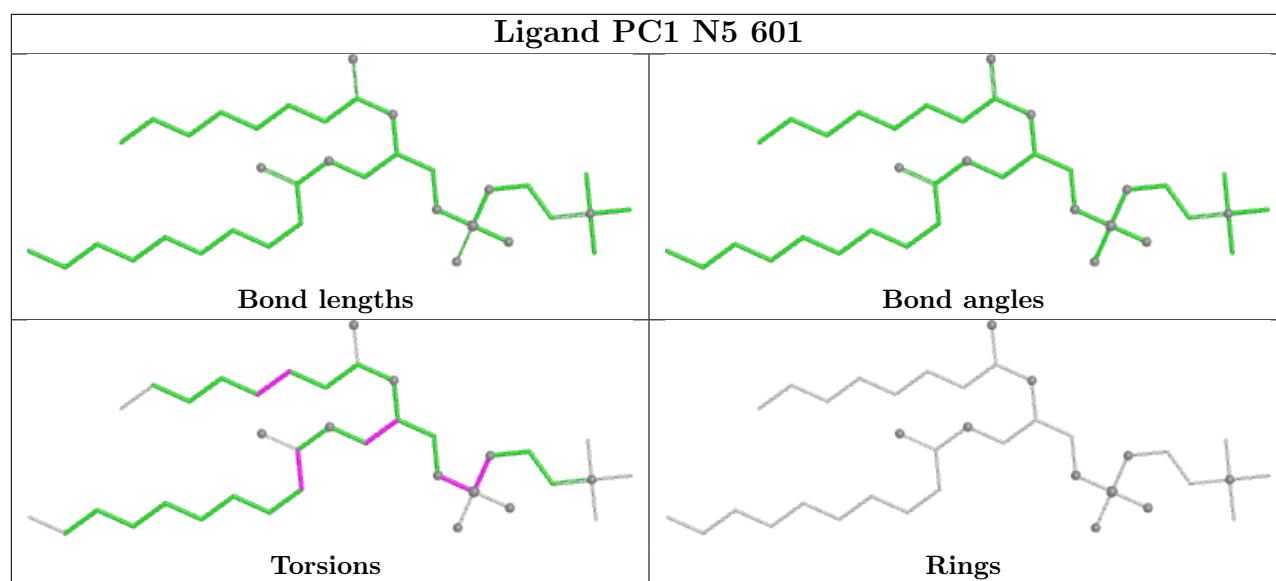


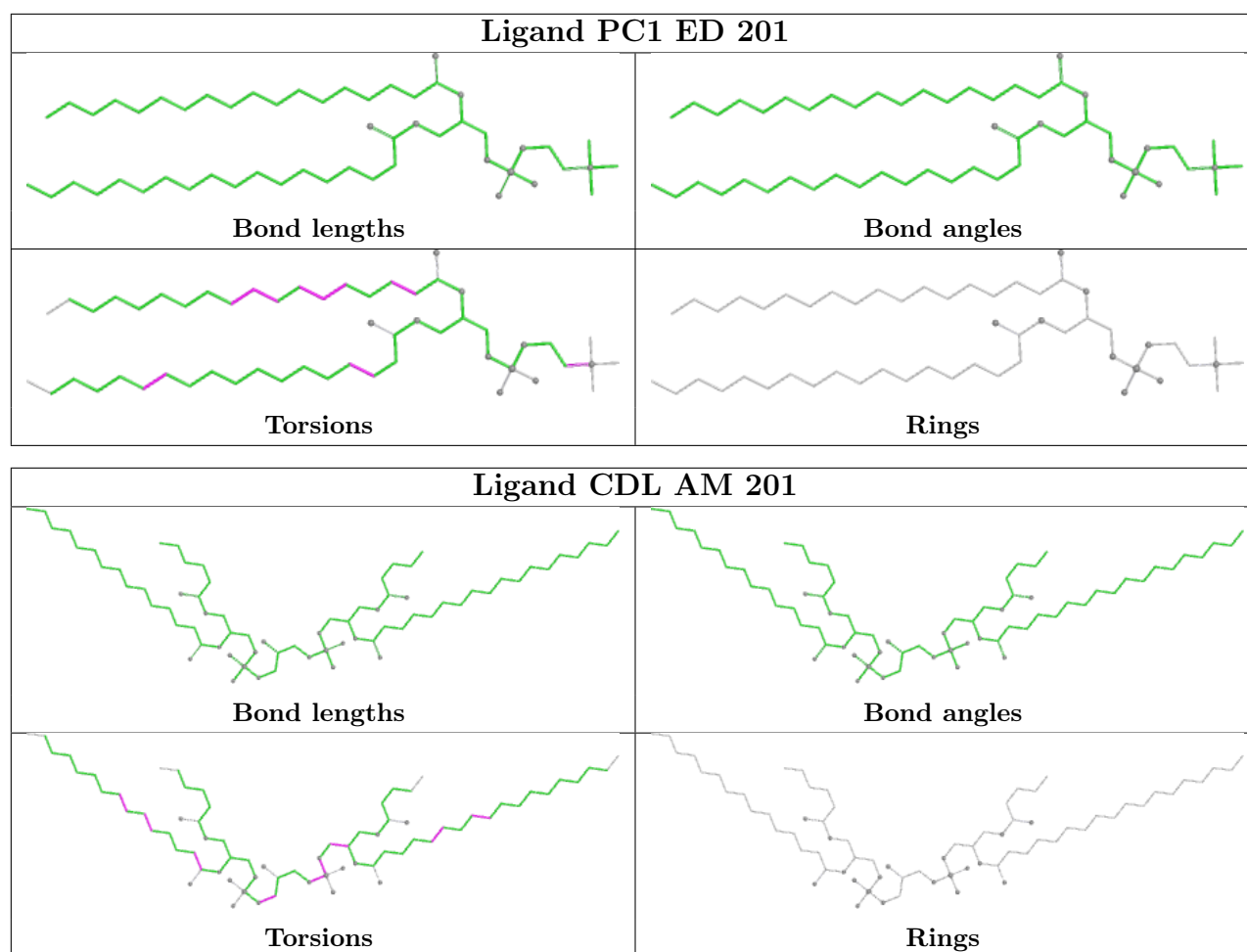












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

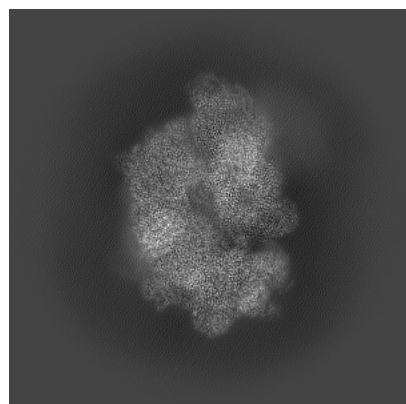
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35720. These allow visual inspection of the internal detail of the map and identification of artifacts.

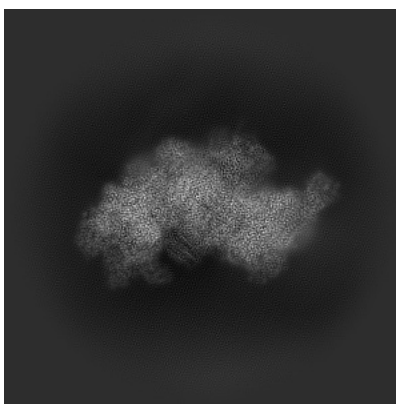
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

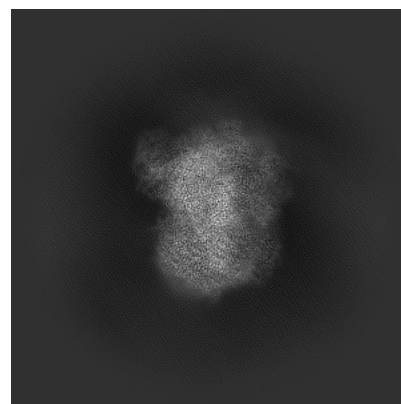
6.1.1 Primary map



X

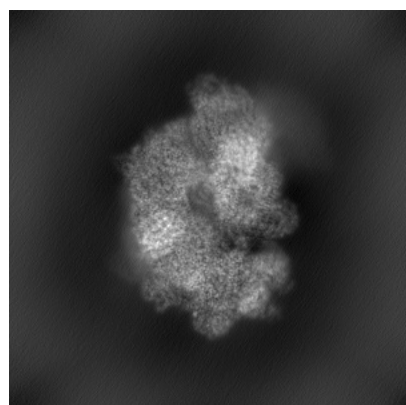


Y

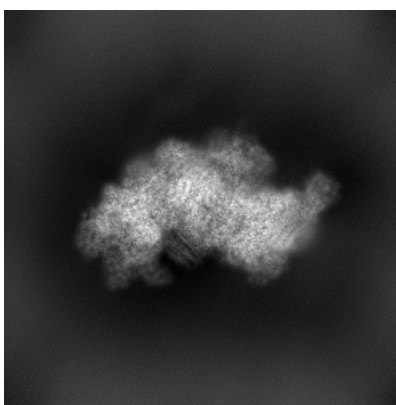


Z

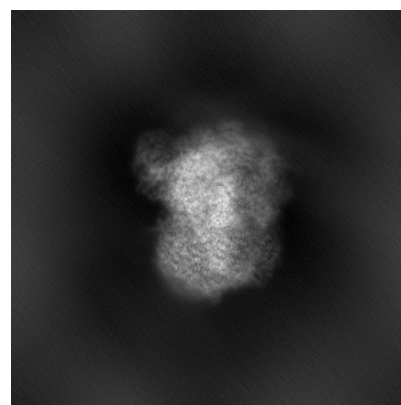
6.1.2 Raw map



X



Y

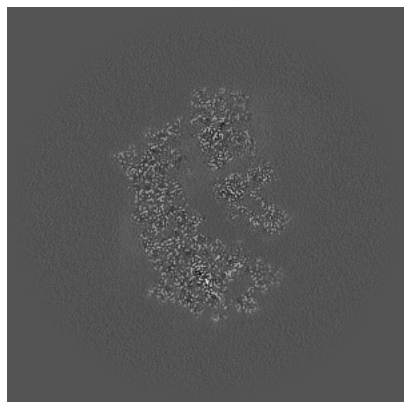


Z

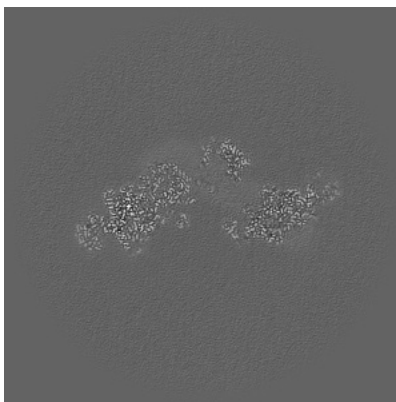
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

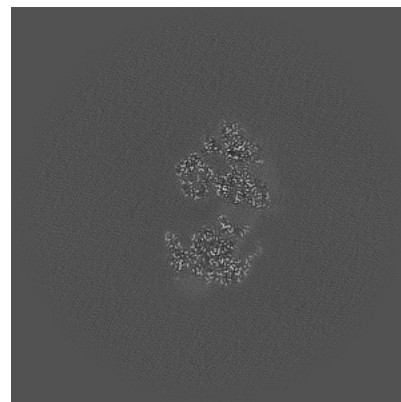
6.2.1 Primary map



X Index: 224

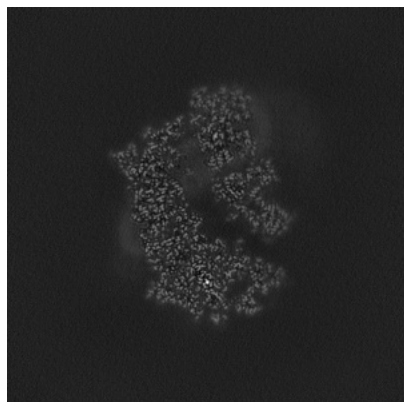


Y Index: 224

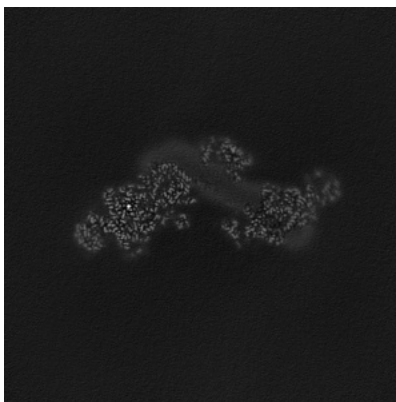


Z Index: 224

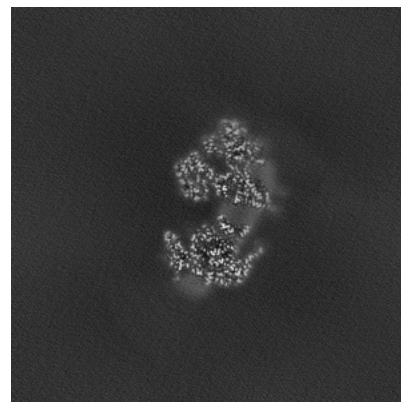
6.2.2 Raw map



X Index: 224



Y Index: 224

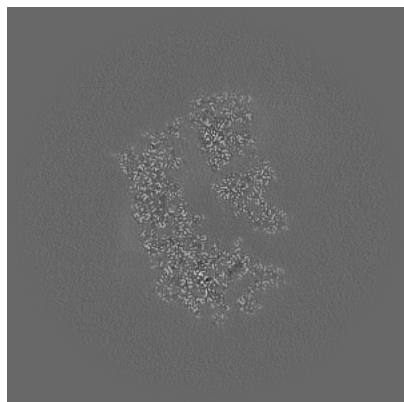


Z Index: 224

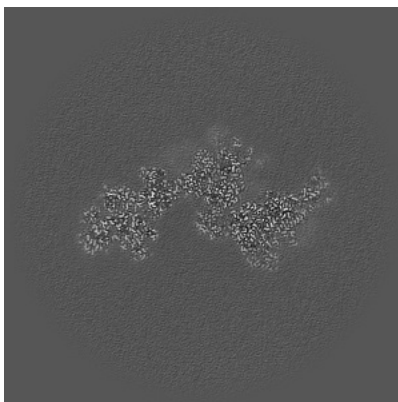
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

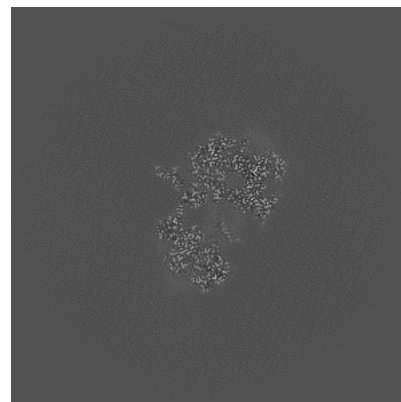
6.3.1 Primary map



X Index: 222

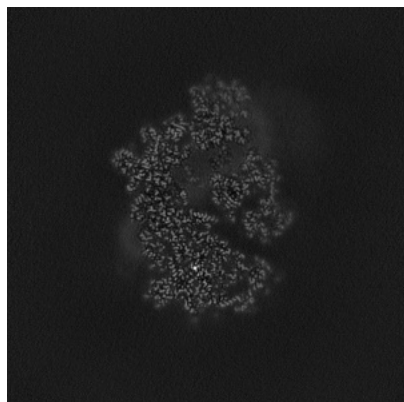


Y Index: 237

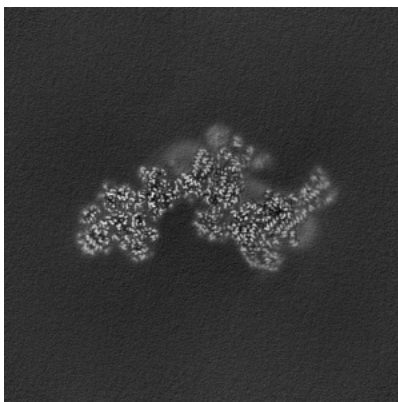


Z Index: 257

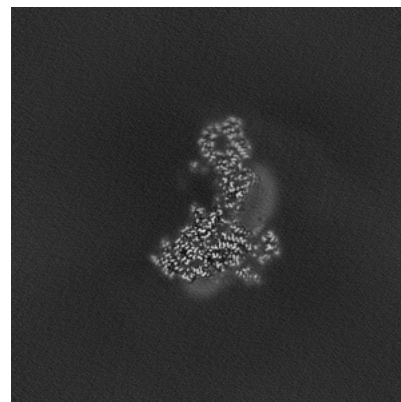
6.3.2 Raw map



X Index: 229



Y Index: 237

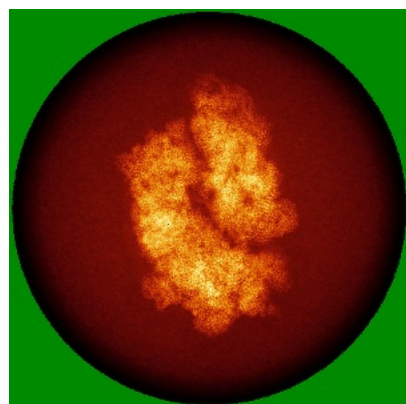


Z Index: 206

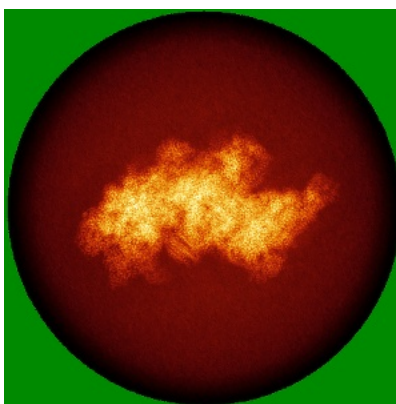
The images above show the largest variance slices of the map in three orthogonal directions.

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

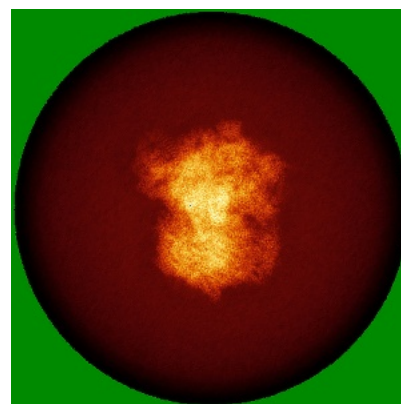
6.4.1 Primary map



X

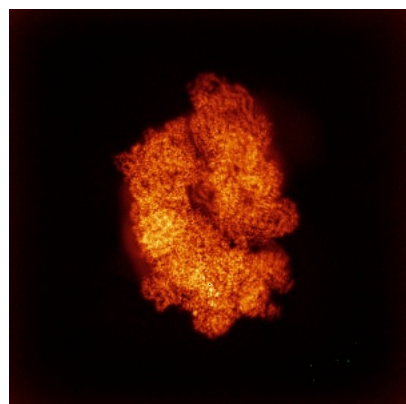


Y

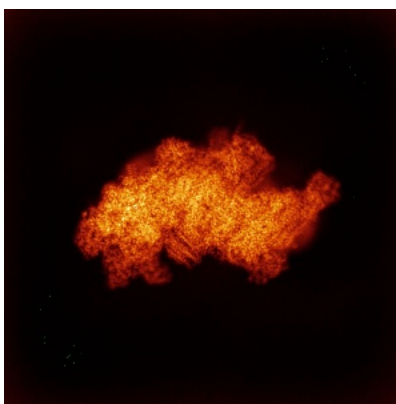


Z

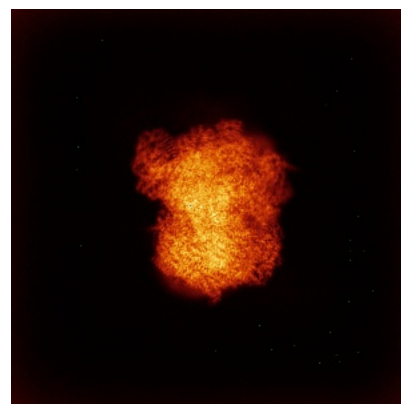
6.4.2 Raw map



X



Y

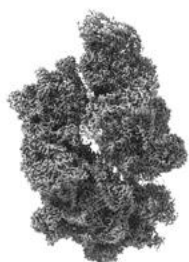


Z

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](#)

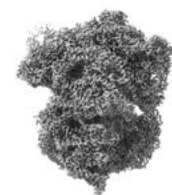
6.5.1 Primary map



X



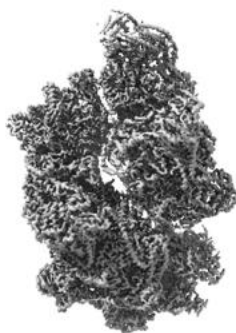
Y



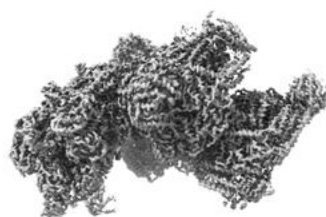
Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

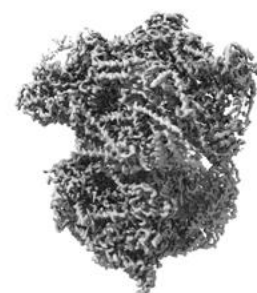
6.5.2 Raw map



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.

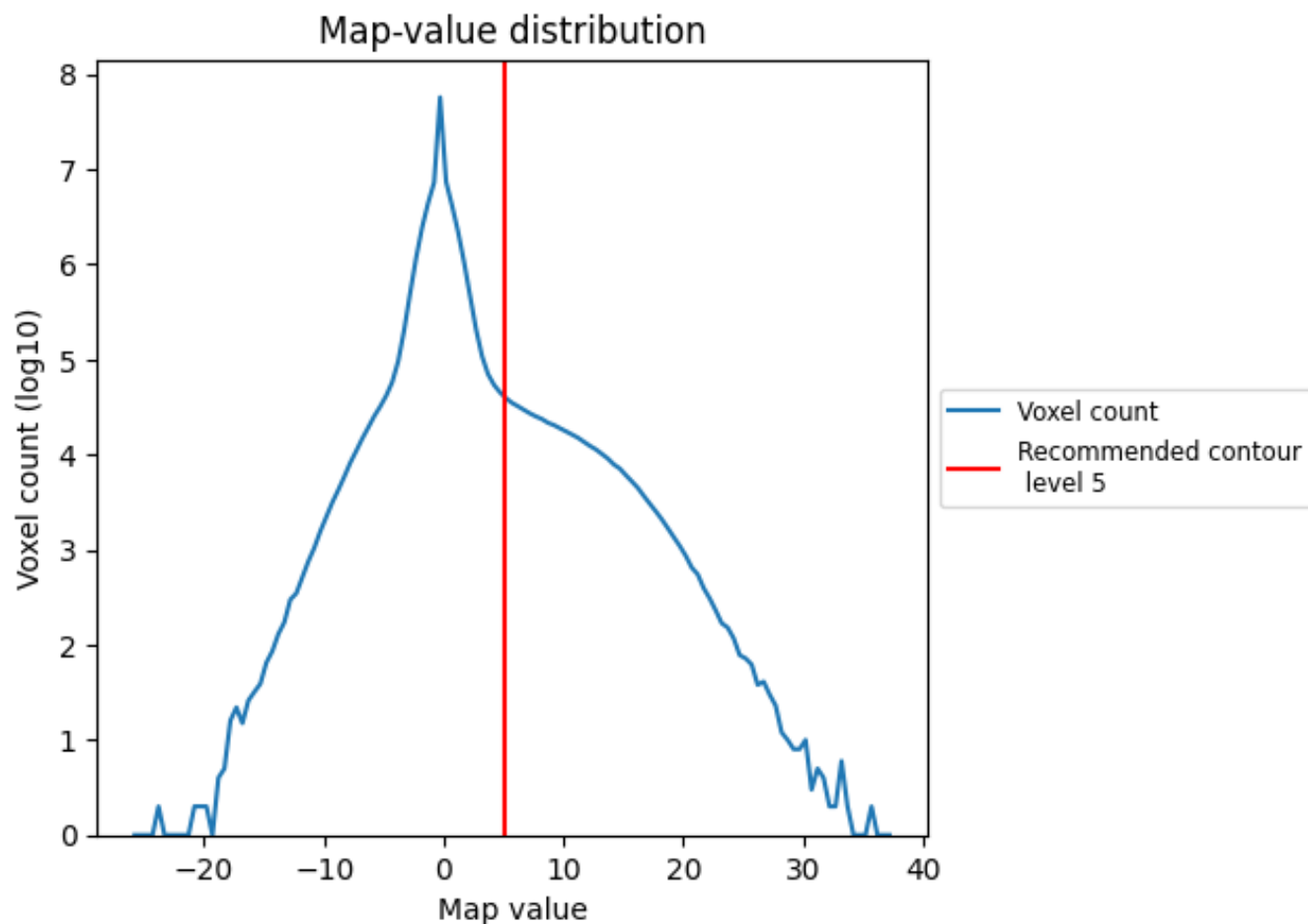
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

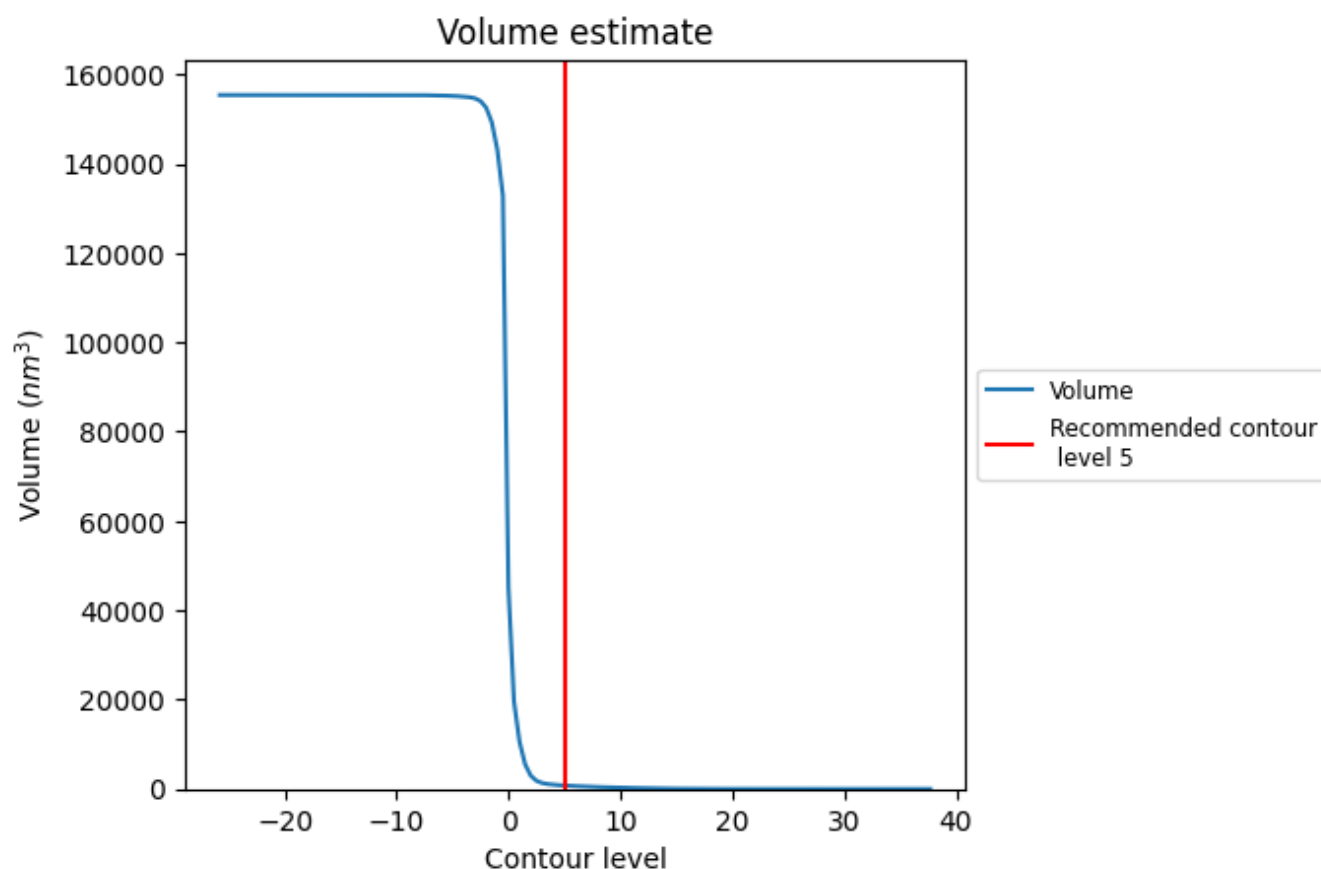
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

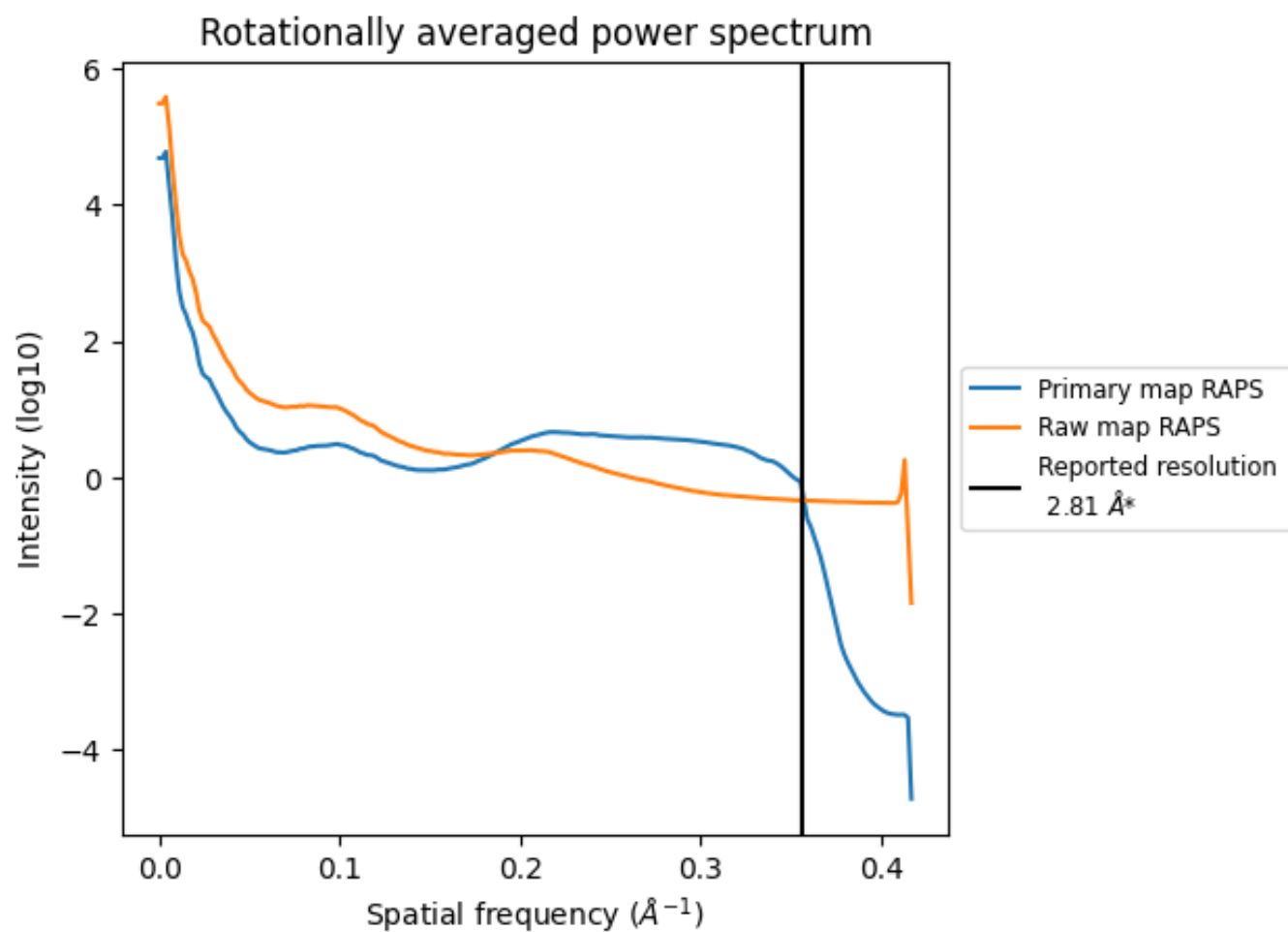
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm^3 ; this corresponds to an approximate mass of 696 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

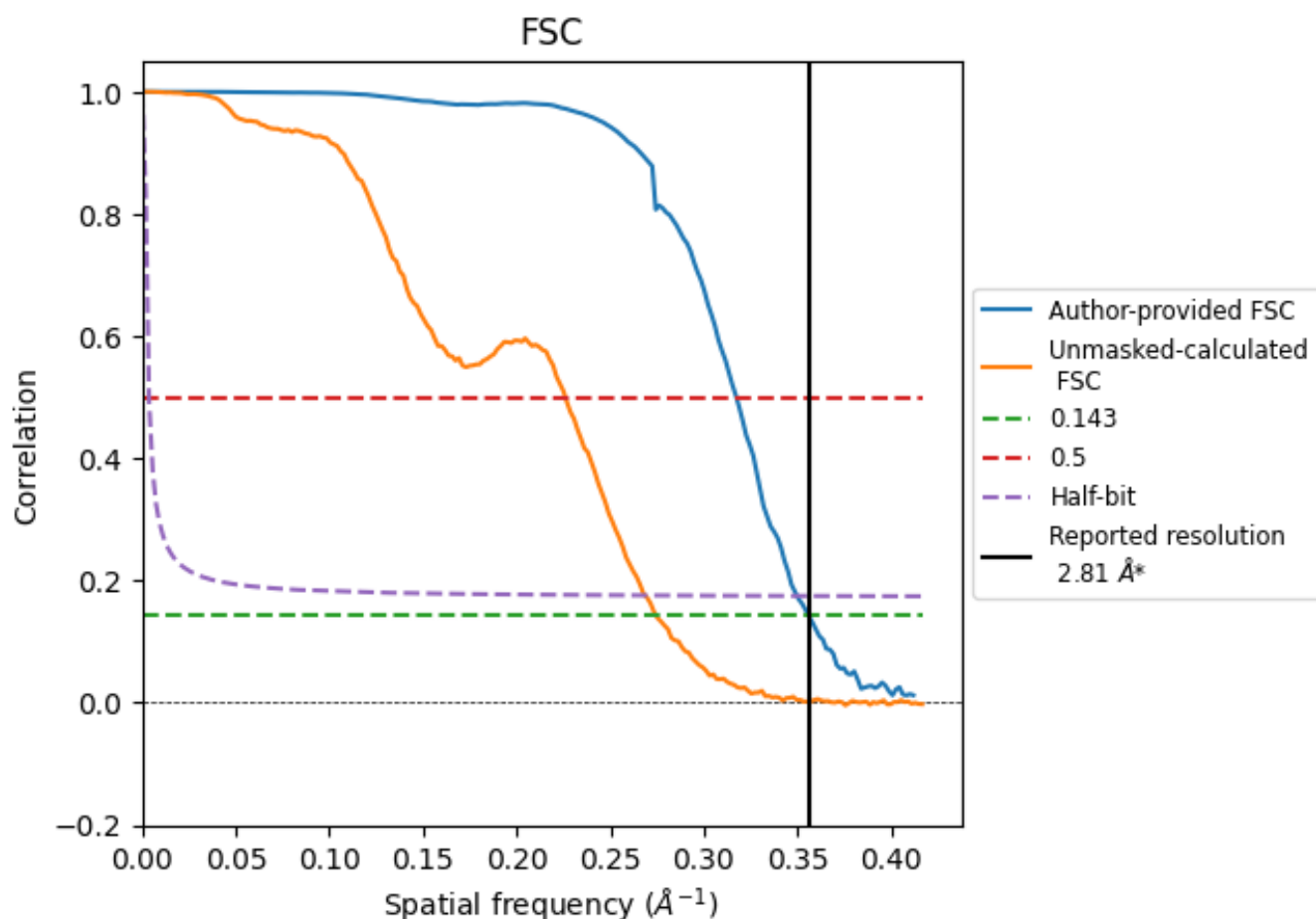


*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

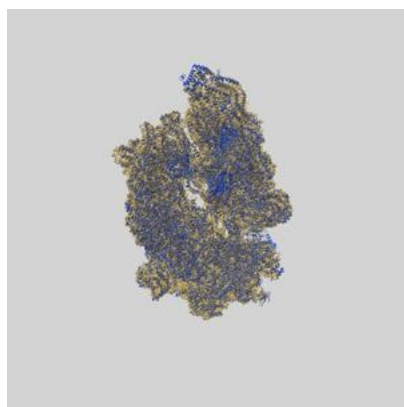
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.15	2.86
Unmasked-calculated*	3.64	4.42	3.72

*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 3.64 differs from the reported value 2.81 by more than 10 %

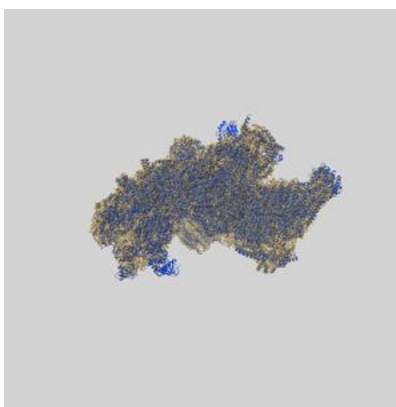
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35720 and PDB model 8IUF. Per-residue inclusion information can be found in section [3](#) on page [34](#).

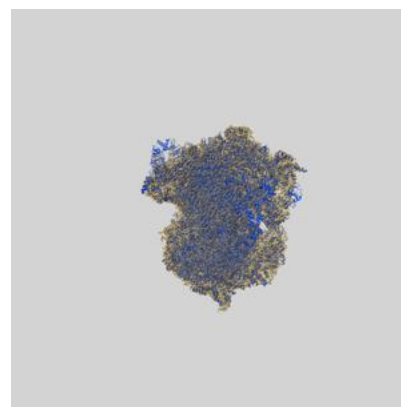
9.1 Map-model overlay [i](#)



X



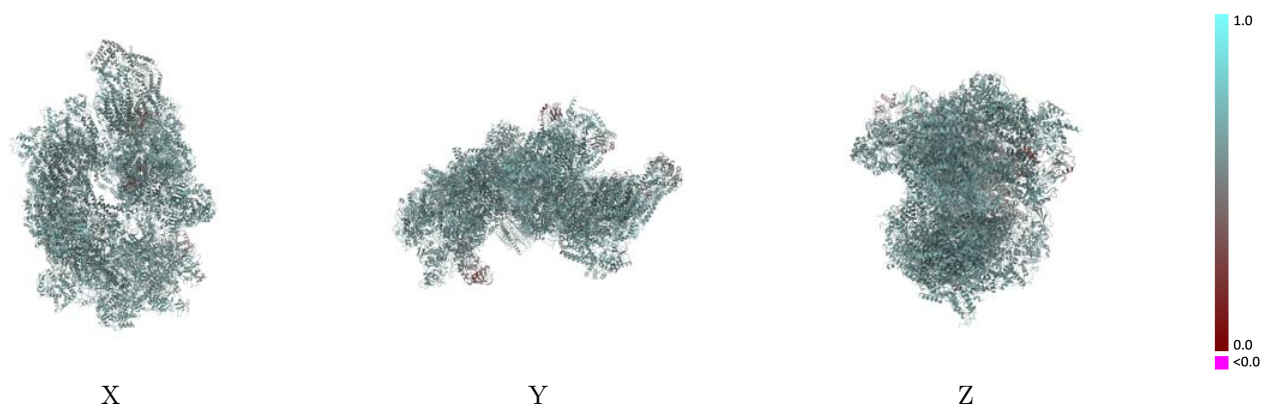
Y



Z

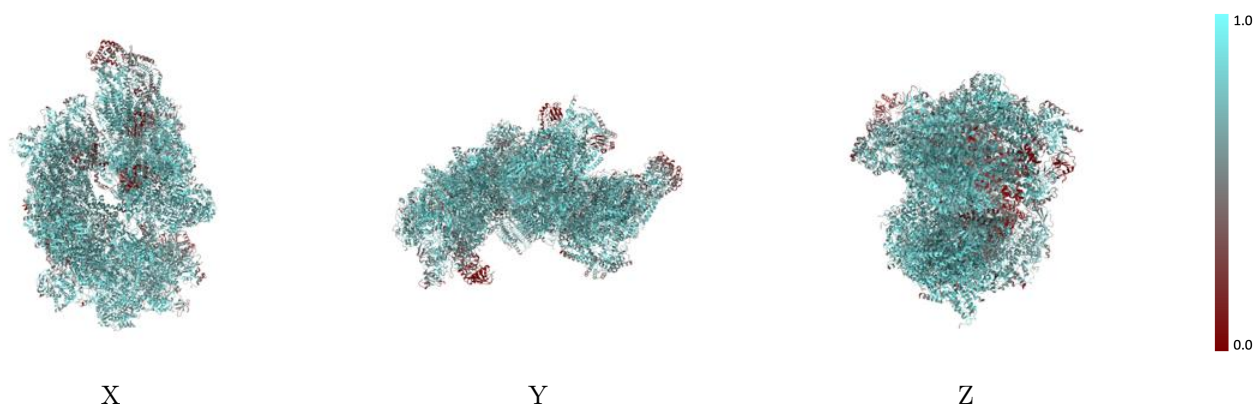
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



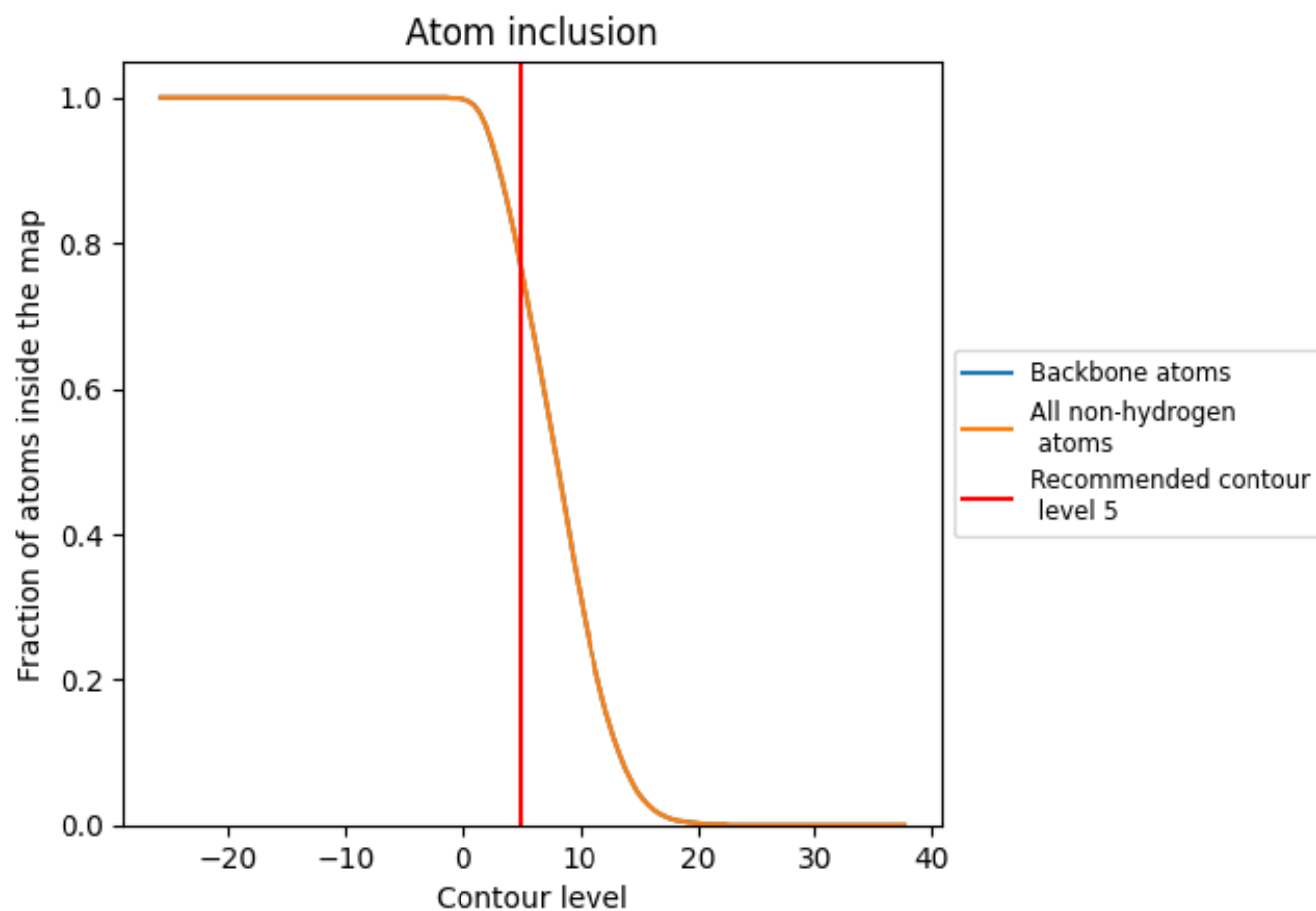
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.6150
1A	 0.8550	 0.6330
1B	 0.8450	 0.6320
2B	 0.8700	 0.6340
4A	 0.5880	 0.5830
4C	 0.6060	 0.5810
4D	 0.7000	 0.6030
4E	 0.4990	 0.5490
4F	 0.7000	 0.6000
4G	 0.6870	 0.5950
4H	 0.6790	 0.5990
4I	 0.8560	 0.6340
4J	 0.8180	 0.6340
4L	 0.8470	 0.6390
5B	 0.8410	 0.6250
5C	 0.8040	 0.6290
6A	 0.5940	 0.5900
6B	 0.6180	 0.5810
7A	 0.7190	 0.6040
7C	 0.8060	 0.6320
A	 0.7830	 0.5880
A1	 0.7270	 0.6080
A2	 0.7790	 0.6190
A3	 0.7690	 0.6180
A5	 0.7290	 0.6020
A6	 0.7320	 0.6040
A7	 0.8480	 0.6340
A8	 0.7610	 0.6100
A9	 0.8050	 0.6270
AB	 0.7370	 0.6110
AC	 0.7760	 0.6180
AL	 0.8060	 0.6260
AM	 0.7200	 0.6070
AN	 0.7820	 0.6210
B	 0.4830	 0.5890



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Chain	Atom inclusion	Q-score
B2	 0.8220	 0.6330
B3	 0.8270	 0.6210
B4	 0.8160	 0.6230
B5	 0.7880	 0.6140
B6	 0.8060	 0.6260
B7	 0.8000	 0.6190
B8	 0.8520	 0.6370
B9	 0.8490	 0.6380
BL	 0.8130	 0.6240
BM	 0.7830	 0.6260
C1	 0.8750	 0.6310
C2	 0.8730	 0.6370
C3	 0.7520	 0.6070
C4	 0.7590	 0.6160
DC	 0.8190	 0.6340
E1	 0.7540	 0.6050
E2	 0.6510	 0.5910
E3	 0.6600	 0.5970
E4	 0.7730	 0.6130
E5	 0.2040	 0.4480
E6	 0.7370	 0.6030
E7	 0.6880	 0.5990
E8	 0.7530	 0.6190
E9	 0.2920	 0.5490
EA	 0.8140	 0.6240
EB	 0.7810	 0.6150
EC	 0.6560	 0.5810
ED	 0.7470	 0.6080
FX	 0.8370	 0.6340
G1	 0.8310	 0.6310
G2	 0.7730	 0.6120
G3	 0.7790	 0.6130
N1	 0.8130	 0.6220
N2	 0.8780	 0.6340
N3	 0.8190	 0.6330
N4	 0.8440	 0.6260
N5	 0.8410	 0.6260
N6	 0.7910	 0.6220
QA	 0.8070	 0.6340
QB	 0.8080	 0.6280
QC	 0.8330	 0.6320
QD	 0.8120	 0.6290

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Chain	Atom inclusion	Q-score
QE	 0.4290	 0.5270
QF	 0.5600	 0.5730
QG	 0.8650	 0.6400
QH	 0.7660	 0.6270
QI	 0.7880	 0.6240
QJ	 0.6980	 0.6130
QK	 0.7810	 0.6290
Qa	 0.7860	 0.6220
Qb	 0.8110	 0.6290
Qc	 0.8130	 0.6280
Qd	 0.7880	 0.6210
Qe	 0.3790	 0.5130
Qf	 0.5530	 0.5610
Qg	 0.8430	 0.6350
Qh	 0.7750	 0.6260
Qi	 0.7550	 0.6070
Qj	 0.6260	 0.5940
Qk	 0.7470	 0.6280
S2	 0.8960	 0.6420
S3	 0.8590	 0.6340
S4	 0.8190	 0.6330
S5	 0.7280	 0.6060
S6	 0.8710	 0.6290
S7	 0.9050	 0.6400
S8	 0.8840	 0.6400
V1	 0.7860	 0.6110
V2	 0.7950	 0.6140