



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:31 PM UTC

PDB ID : 7TGH / pdb_00007tgh
EMDB ID : EMD-25882
Title : Cryo-EM structure of respiratory super-complex CI+III2 from Tetrahymena thermophila
Authors : Zhou, L.; Maldonado, M.; Padavannil, A.; Guo, F.; Letts, J.A.
Deposited on : 2022-01-07
Resolution : 2.60 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

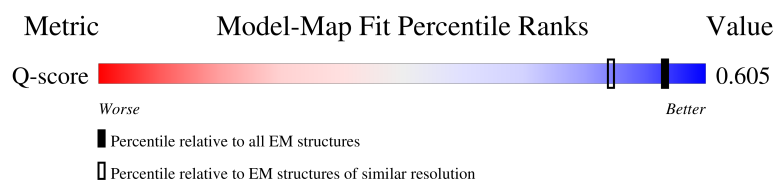
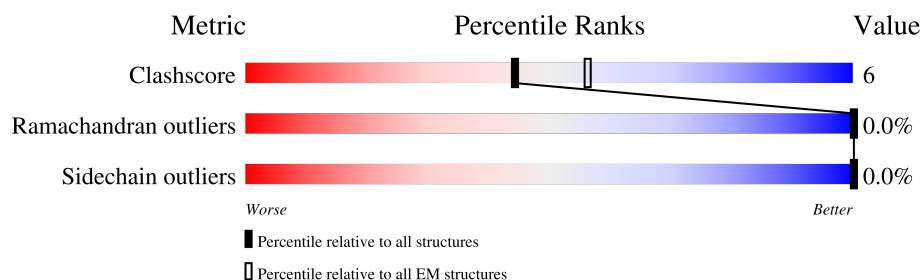
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



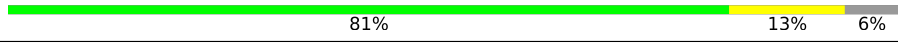
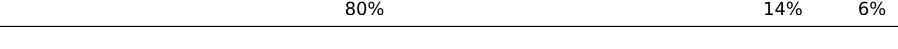
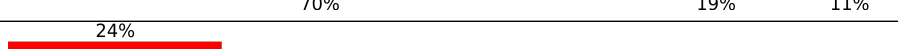
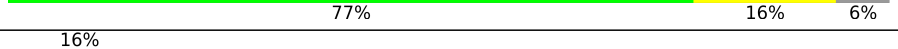
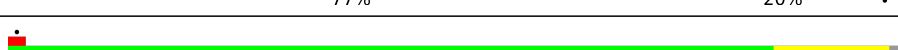
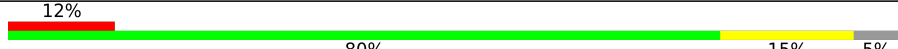
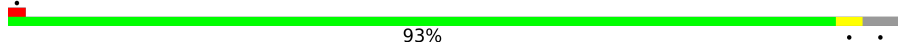
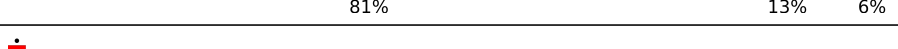
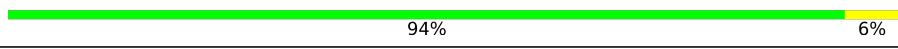
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	1	284	 75%25%
2	1B	59	 80%20%
3	2	360	 84%15%
4	2B	178	 87%13%

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Mol	Chain	Length	Quality of chain
5	3	121	
6	3A	482	
6	3a	482	
7	3B	513	
7	3b	513	
8	3C	426	
8	3c	426	
9	3D	319	
9	3d	319	
10	3E	269	
10	3e	269	
11	3F	90	
11	3f	90	
12	3G	328	
12	3g	328	
13	3H	130	
13	3h	130	
14	3I	119	
14	3i	119	
15	3J	62	
15	3j	62	
16	3M	19	
17	3l	24	
18	3m	17	
19	4	505	

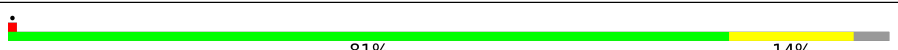
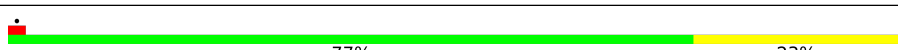
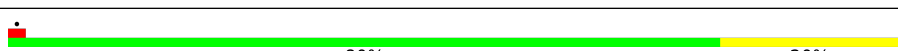
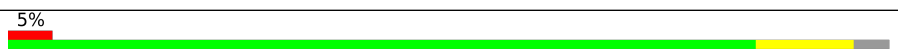
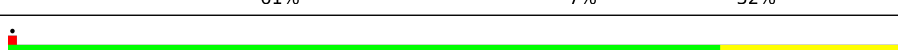
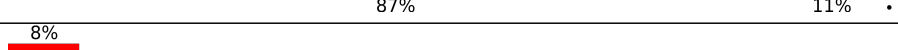
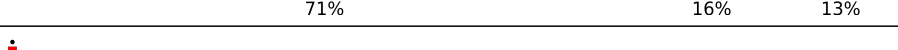
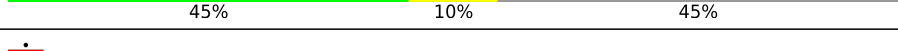
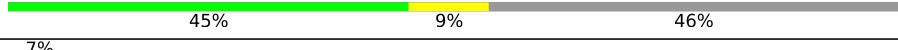
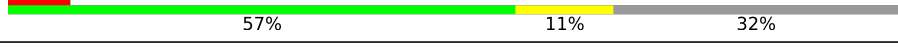
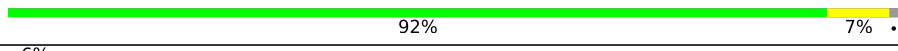
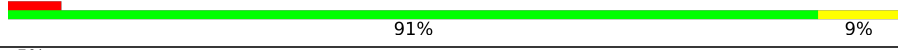
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Mol	Chain	Length	Quality of chain
20	4L	116	
21	5	750	
22	5B	100	
23	6	255	
24	A2	103	
25	A5	206	
26	A6	172	
27	A7	282	
28	A9	362	
29	AB	138	
30	AC	133	
31	AL	194	
32	AM	175	
33	B7	120	
34	B8	207	
35	BL	188	
36	C	209	
37	C1	257	
38	C2	233	
39	C3	346	
40	TD	73	
41	J1	317	
42	FX	172	
43	T2	333	
44	T1	516	

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Mol	Chain	Length	Quality of chain
45	A1	94	
46	X1	150	
47	T6	144	
48	T5	205	
49	R	124	
50	S1	718	
51	S2	442	
52	S3	198	
53	S4	185	
54	S6	132	
55	S7	162	
56	S8	236	
57	B9	189	
58	TX	166	
59	A8	238	
60	TB	113	
61	V1	474	
62	V2	274	
63	B6	129	
64	BM	214	
65	C4	102	
66	AN	231	
67	B4	108	
68	T4	212	
69	T8	135	

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Mol	Chain	Length	Quality of chain
70	B2	126	
71	T3	311	
72	P1	251	
73	B3	83	
74	TA	102	
75	S5	94	
76	TC	93	
77	P2	189	
78	A3	135	
79	T9	135	
80	TE	71	
81	T7	143	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
93	SF4	S1	802	-	-	X	-
93	SF4	S8	302	-	-	X	-

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 153366 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	284	Total	C	N	O	S	0	0
			2313	1586	335	379	13		

- Molecule 2 is a protein called NADH dehydrogenase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	59	Total	C	N	O	S	0	0
			516	362	78	73	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1B	49	VAL	LEU	conflict	UNP Q09FB0
1B	56	THR	SER	conflict	UNP Q09FB0

- Molecule 3 is a protein called Ymf65.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	359	Total	C	N	O	S	0	0
			3065	2129	435	494	7		

- Molecule 4 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2B	178	Total	C	N	O	S	0	0
			1483	1015	215	248	5		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	120	Total	C	N	O	S	0	0
			1017	705	142	166	4		

- Molecule 6 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3A	453	Total	C	N	O	S	0	0
			3511	2210	598	697	6		
6	3a	451	Total	C	N	O	S	0	0
			3495	2199	595	695	6		

- Molecule 7 is a protein called Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3B	479	Total	C	N	O	S	0	0
			3826	2426	667	728	5		
7	3b	478	Total	C	N	O	S	0	0
			3815	2420	663	727	5		

- Molecule 8 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3C	426	Total	C	N	O	S	0	0
			3590	2417	541	610	22		
8	3c	426	Total	C	N	O	S	0	0
			3589	2417	541	609	22		

- Molecule 9 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3D	295	Total	C	N	O	S	0	0
			2488	1627	418	430	13		
9	3d	285	Total	C	N	O	S	0	0
			2403	1569	405	416	13		

- Molecule 10 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3E	230	Total	C	N	O	S	0	0
			1846	1178	325	334	9		
10	3e	104	Total	C	N	O	S	0	0
			882	567	162	152	1		

- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3F	89	Total	C	N	O	S	0	0
			703	439	125	130	9		
11	3f	75	Total	C	N	O	S	0	0
			597	374	105	109	9		

- Molecule 12 is a protein called UQCRB.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3G	307	Total	C	N	O	S	0	0
			2595	1676	450	463	6		
12	3g	317	Total	C	N	O	S	0	0
			2682	1738	464	474	6		

- Molecule 13 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3H	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
13	3h	124	Total	C	N	O	S	0	0
			1046	669	190	179	8		

- Molecule 14 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3I	114	Total	C	N	O	S	0	0
			971	651	161	158	1		
14	3i	111	Total	C	N	O	S	0	0
			948	638	157	152	1		

- Molecule 15 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3J	58	Total	C	N	O	S	0	0
			501	341	79	79	2		
15	3j	51	Total	C	N	O	S	0	0
			443	306	65	70	2		

- Molecule 16 is a protein called UNK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3M	19	Total	C	N	O	S	0	0
			150	94	27	27	2		

- Molecule 17 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	3l	24	Total	C	N	O	0	0
			124	74	24	26		

- Molecule 18 is a protein called UNK3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	3m	17	Total	C	N	O	0	0
			121	78	25	18		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	505	Total	C	N	O	S	0	0
			4170	2859	601	692	18		

- Molecule 20 is a protein called Ymf58.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4L	116	Total	C	N	O	S	0	0
			957	648	142	163	4		

- Molecule 21 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	587	Total	C	N	O	S	0	0
			4844	3313	696	819	16		

- Molecule 22 is a protein called Ymf57.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5B	100	Total	C	N	O	S	0	0
			888	620	128	137	3		

- Molecule 23 is a protein called Ymf62.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	244	Total	C	N	O	S	0	0
			2076	1419	295	358	4		

- Molecule 24 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A2	92	Total	C	N	O	S	0	0
			765	486	136	141	2		

- Molecule 25 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A5	155	Total	C	N	O	S	0	0
			1307	838	219	244	6		

- Molecule 26 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A6	172	Total	C	N	O	S	0	0
			1421	903	253	257	8		

- Molecule 27 is a protein called NDUA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A7	281	Total	C	N	O	S	0	0
			2339	1473	412	452	2		

- Molecule 28 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A9	338	Total	C	N	O	S	0	0
			2718	1737	475	494	12		

- Molecule 29 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	AB	112	Total	C	N	O	0	0
			926	586	158	182		

- Molecule 30 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AC	98	Total	C	N	O	S	0	0
			806	513	134	158	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AL	193	Total	C	N	O	S	0	0
			1612	1019	303	285	5		

- Molecule 32 is a protein called NDUA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AM	160	Total	C	N	O	S	0	0
			1349	858	256	227	8		

- Molecule 33 is a protein called NDUB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B7	115	Total	C	N	O	S	0	0
			937	593	162	176	6		

- Molecule 34 is a protein called NDUB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B8	169	Total	C	N	O	S	0	0
			1408	904	238	260	6		

- Molecule 35 is a protein called NDUB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BL	175	Total	C	N	O	S	0	0
			1461	925	264	268	4		

- Molecule 36 is a protein called UNK4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C	209	Total	C	N	O	S	0	0
			1045	627	209	209			

- Molecule 37 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C1	229	Total	C	N	O	S	0	0
			1769	1110	304	350	5		

- Molecule 38 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C2	223	Total	C	N	O	S	0	0
			1624	1020	294	303	7		

- Molecule 39 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C3	346	Total	C	N	O	S	0	0
			2804	1766	481	549	8		

- Molecule 40 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	TD	71	Total	C	N	O	S	0	0
			608	399	108	101			

- Molecule 41 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	J1	262	Total	C	N	O	S	0	0
			2146	1361	396	386	3		

- Molecule 42 is a protein called 2 iron, 2 sulfur cluster-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	FX	146	Total	C	N	O	S	0	0
			1162	722	207	223	10		

- Molecule 43 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T2	271	Total	C	N	O	S	0	0
			2117	1347	362	407	1		

- Molecule 44 is a protein called Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	T1	481	Total	C	N	O	S	0	0
			3884	2492	662	717	13		

- Molecule 45 is a protein called NDUA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	A1	92	Total	C	N	O	0	0
			799	526	138	135		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	X1	149	Total	C	N	O	0	0
			1227	800	213	214		

- Molecule 47 is a protein called NDUTT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	T6	109	Total	C	N	O	S	0	0
			903	562	161	174	6		

- Molecule 48 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T5	134	Total	C	N	O	S	0	0
			1088	699	193	194	2		

- Molecule 49 is a protein called UNK5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R	124	Total	C	N	O	S	0	0
			943	613	160	167	3		

- Molecule 50 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S1	687	Total	C	N	O	S	0	0
			5394	3404	933	1029	28		

- Molecule 51 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S2	442	Total	C	N	O	S	0	0
			3599	2291	624	660	24		

- Molecule 52 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S3	198	Total	C	N	O	S	0	0
			1681	1096	267	312	6		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S4	177	Total	C	N	O	S	0	0
			1463	928	257	269	9		

- Molecule 54 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S6	90	Total	C	N	O	S	0	0
			722	456	128	134	4		

- Molecule 55 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S7	162	Total	C	N	O	S	0	0
			1286	827	221	227	11		

- Molecule 56 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	S8	218	Total	C	N	O	S	0	0
			1812	1155	299	347	11		

- Molecule 57 is a protein called NDUB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B9	186	Total	C	N	O	S	0	0
			1579	1021	252	302	4		

- Molecule 58 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	TX	144	Total	C	N	O	S	0	0
			1206	767	205	227	7		

- Molecule 59 is a protein called NDUA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	A8	132	Total	C	N	O	S	0	0
			1075	676	180	208	11		

- Molecule 60 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	TB	96	Total	C	N	O		0	0
			801	515	139	147			

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	V1	442	Total	C	N	O	S	0	0
			3410	2146	600	640	24		

- Molecule 62 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	V2	231	Total	C	N	O	S	0	0
			1858	1173	318	357	10		

- Molecule 63 is a protein called NDUB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	B6	70	Total	C	N	O	S	0	0
			596	400	98	94	4		

- Molecule 64 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BM	145	Total	C	N	O	S	0	0
			1163	737	195	226	5		

- Molecule 65 is a protein called NDUC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	C4	101	Total	C	N	O	S	0	0
			842	548	138	149	7		

- Molecule 66 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AN	231	Total	C	N	O	S	0	0
			1879	1219	317	336	7		

- Molecule 67 is a protein called NDUB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	B4	108	Total	C	N	O	S	0	0
			898	601	138	157	2		

- Molecule 68 is a protein called NDUTT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	T4	170	Total	C	N	O	S	0	0
			1408	918	242	245	3		

- Molecule 69 is a protein called NDUTT8.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	T8	129	Total	C	N	O	S	0	0
			1064	691	189	184			

- Molecule 70 is a protein called NDUB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	B2	118	Total	C	N	O	S	0	0
			955	615	165	172	3		

- Molecule 71 is a protein called NDUTT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	T3	305	Total	C	N	O	S	0	0
			2442	1555	426	455	6		

- Molecule 72 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	P1	228	Total	C	N	O	S	0	0
			1896	1235	320	336	5		

- Molecule 73 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	B3	68	Total	C	N	O	S	0	0
			594	392	104	97	1		

- Molecule 74 is a protein called NDUTT10.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	TA	102	Total	C	N	O	S	0	0
			854	553	141	155	5		

- Molecule 75 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	S5	85	Total	C	N	O	S	0	0
			693	440	118	129	6		

- Molecule 76 is a protein called NDUTT12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	TC	91	Total	C	N	O	S	0	0
			781	491	145	144	1		

- Molecule 77 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	P2	167	Total	C	N	O	S	0	0
			1414	926	225	258	5		

- Molecule 78 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	A3	127	Total	C	N	O	S	0	0
			1065	691	193	178	3		

- Molecule 79 is a protein called NDUTT9.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	T9	132	Total	C	N	O	S	0	0
			1066	670	185	201	10		

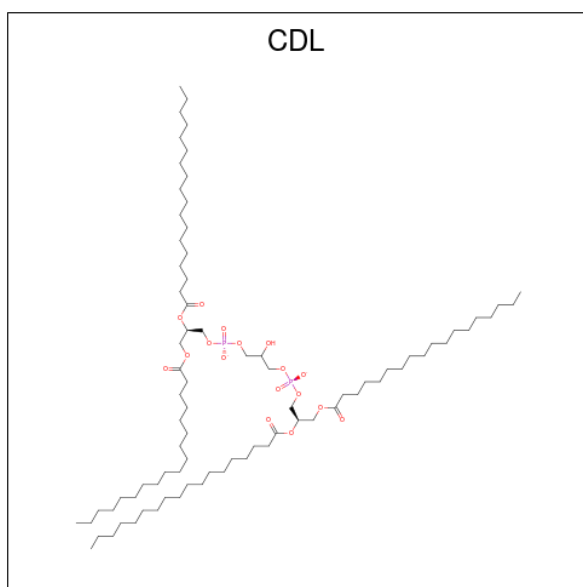
- Molecule 80 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	TE	49	Total	C	N	O	S	0	0
			413	277	63	71	2		

- Molecule 81 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	T7	142	Total	C	N	O	S	0	0
			1187	770	202	209	6		

- Molecule 82 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
82	1	1	Total	C	O	P	0
			50	31	17	2	
82	2B	1	Total	C	O	P	0
			53	34	17	2	
82	3	1	Total	C	O	P	0
			44	25	17	2	
82	3B	1	Total	C	O	P	0
			78	59	17	2	
82	3C	1	Total	C	O	P	0
			65	46	17	2	
82	3G	1	Total	C	O	P	0
			66	47	17	2	
82	3H	1	Total	C	O	P	0
			62	43	17	2	

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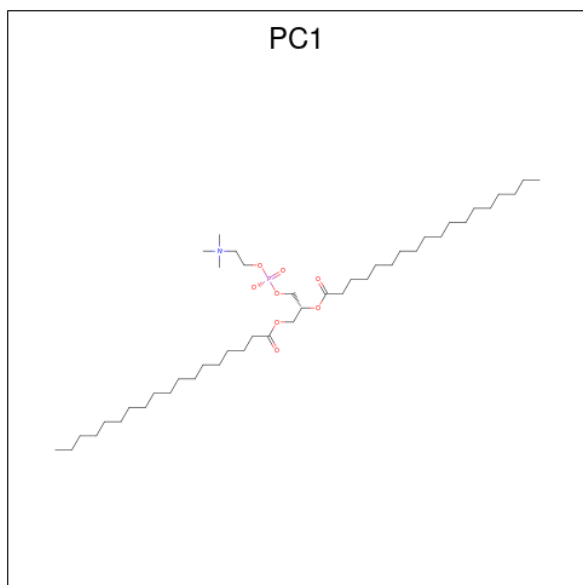
Mol	Chain	Residues	Atoms				AltConf
82	3H	1	Total	C	O	P	0
			66	47	17	2	
82	3I	1	Total	C	O	P	0
			71	52	17	2	
82	3I	1	Total	C	O	P	0
			37	18	17	2	
82	3b	1	Total	C	O	P	0
			68	49	17	2	
82	3c	1	Total	C	O	P	0
			64	45	17	2	
82	3c	1	Total	C	O	P	0
			56	37	17	2	
82	3i	1	Total	C	O	P	0
			71	52	17	2	
82	5	1	Total	C	O	P	0
			90	71	17	2	
82	5	1	Total	C	O	P	0
			96	77	17	2	
82	AL	1	Total	C	O	P	0
			53	34	17	2	
82	AM	1	Total	C	O	P	0
			62	43	17	2	
82	B8	1	Total	C	O	P	0
			45	26	17	2	
82	TD	1	Total	C	O	P	0
			66	47	17	2	
82	T1	1	Total	C	O	P	0
			55	36	17	2	
82	A1	1	Total	C	O	P	0
			53	34	17	2	
82	R	1	Total	C	O	P	0
			84	65	17	2	
82	BM	1	Total	C	O	P	0
			86	67	17	2	
82	C4	1	Total	C	O	P	0
			98	79	17	2	
82	AN	1	Total	C	O	P	0
			53	34	17	2	
82	B4	1	Total	C	O	P	0
			40	21	17	2	
82	P2	1	Total	C	O	P	0
			82	63	17	2	

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Mol	Chain	Residues	Atoms				AltConf
82	T7	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 83 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
83	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
83	3	1	Total	C	N	O	P	0
			31	21	1	8	1	
83	3C	1	Total	C	N	O	P	0
			46	36	1	8	1	
83	3C	1	Total	C	N	O	P	0
			44	34	1	8	1	
83	3C	1	Total	C	N	O	P	0
			29	19	1	8	1	
83	3E	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	3E	1	Total	C	N	O	P	0
			24	14	1	8	1	
83	3F	1	Total	C	N	O	P	0
			22	12	1	8	1	
83	3I	1	Total	C	N	O	P	0
			32	22	1	8	1	
83	3I	1	Total	C	N	O	P	0
			46	36	1	8	1	

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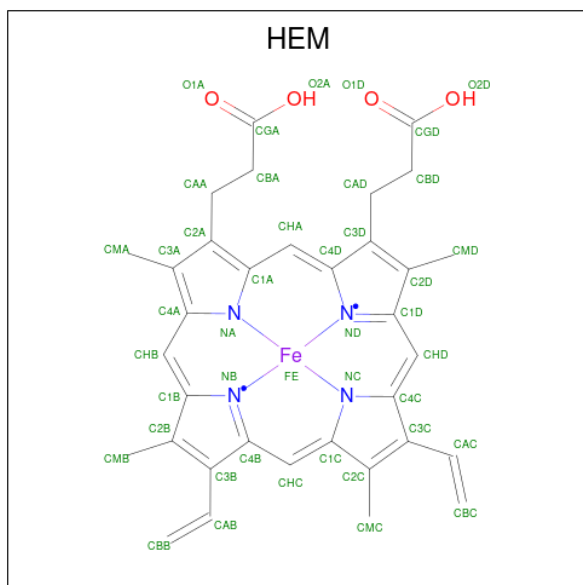
Mol	Chain	Residues	Atoms					AltConf
83	3J	1	Total	C	N	O	P	0
			37	27	1	8	1	
83	3b	1	Total	C	N	O	P	0
			30	20	1	8	1	
83	3c	1	Total	C	N	O	P	0
			31	21	1	8	1	
83	3c	1	Total	C	N	O	P	0
			38	28	1	8	1	
83	3e	1	Total	C	N	O	P	0
			50	40	1	8	1	
83	3g	1	Total	C	N	O	P	0
			33	23	1	8	1	
83	3j	1	Total	C	N	O	P	0
			36	26	1	8	1	
83	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	5	1	Total	C	N	O	P	0
			39	29	1	8	1	
83	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	6	1	Total	C	N	O	P	0
			39	29	1	8	1	
83	6	1	Total	C	N	O	P	0
			54	44	1	8	1	
83	AM	1	Total	C	N	O	P	0
			30	20	1	8	1	
83	J1	1	Total	C	N	O	P	0
			40	30	1	8	1	
83	T1	1	Total	C	N	O	P	0
			26	16	1	8	1	
83	X1	1	Total	C	N	O	P	0
			49	39	1	8	1	
83	B6	1	Total	C	N	O	P	0
			52	42	1	8	1	
83	C4	1	Total	C	N	O	P	0
			32	22	1	8	1	
83	AN	1	Total	C	N	O	P	0
			36	26	1	8	1	
83	B2	1	Total	C	N	O	P	0
			48	38	1	8	1	
83	P1	1	Total	C	N	O	P	0
			40	30	1	8	1	

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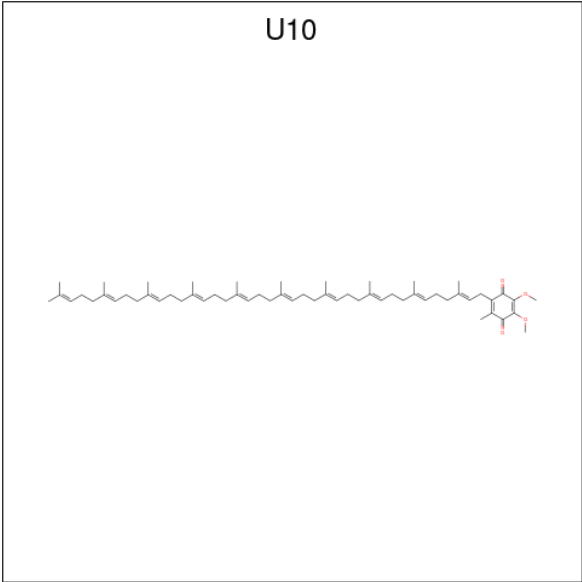
Mol	Chain	Residues	Atoms					AltConf
83	TC	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 84 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



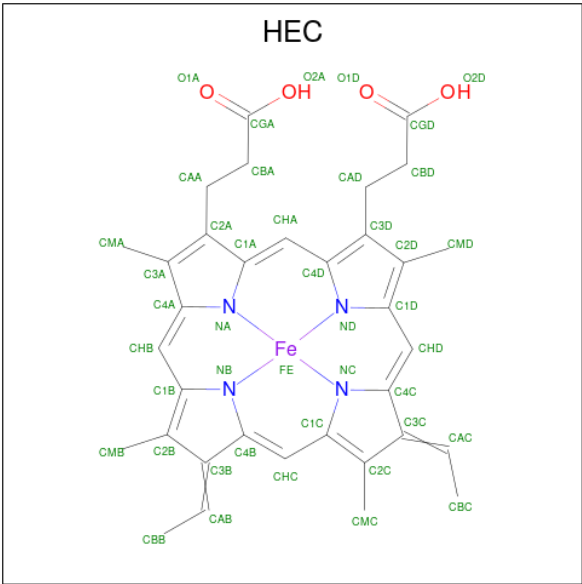
Mol	Chain	Residues	Atoms					AltConf
84	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	3c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	3c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 85 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



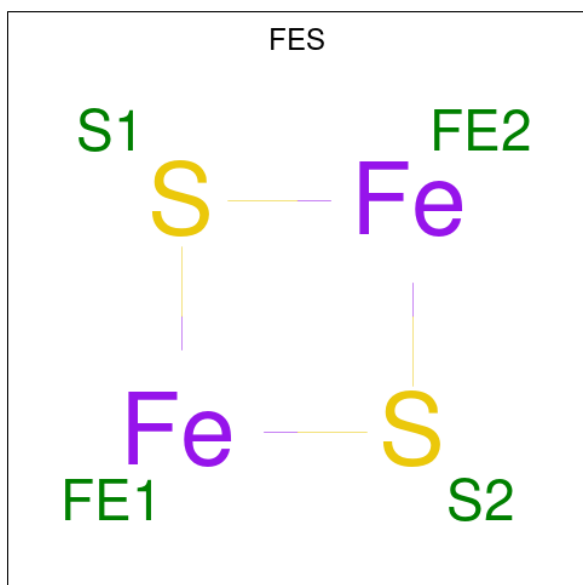
Mol	Chain	Residues	Atoms		AltConf
85	3C	1	Total	C	0
			26	26	
85	3H	1	Total	C	O
			29	25	4
85	5B	1	Total	C	O
			63	59	4

- Molecule 86 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



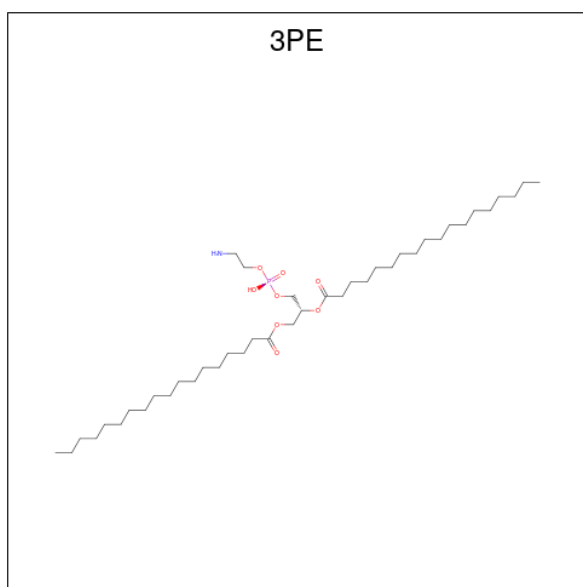
Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total 43	C 34	Fe 1	N 4	O 4	0
86	3d	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 87 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
87	3E	1	Total	Fe	S	0
			4	2	2	
87	FX	1	Total	Fe	S	0
			4	2	2	
87	S1	1	Total	Fe	S	0
			4	2	2	
87	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 88 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
88	3E	1	Total	C	N	O	P	0
			34	24	1	8	1	
88	3d	1	Total	C	N	O	P	0
			47	37	1	8	1	
88	4	1	Total	C	N	O	P	0
			47	37	1	8	1	
88	4	1	Total	C	N	O	P	0
			36	26	1	8	1	
88	5	1	Total	C	N	O	P	0
			37	27	1	8	1	
88	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
88	5B	1	Total	C	N	O	P	0
			24	14	1	8	1	
88	B8	1	Total	C	N	O	P	0
			36	26	1	8	1	
88	S8	1	Total	C	N	O	P	0
			41	31	1	8	1	
88	C4	1	Total	C	N	O	P	0
			51	41	1	8	1	
88	AN	1	Total	C	N	O	P	0
			45	35	1	8	1	
88	AN	1	Total	C	N	O	P	0
			35	25	1	8	1	
88	T4	1	Total	C	N	O	P	0
			25	15	1	8	1	
88	T8	1	Total	C	N	O	P	0
			39	29	1	8	1	

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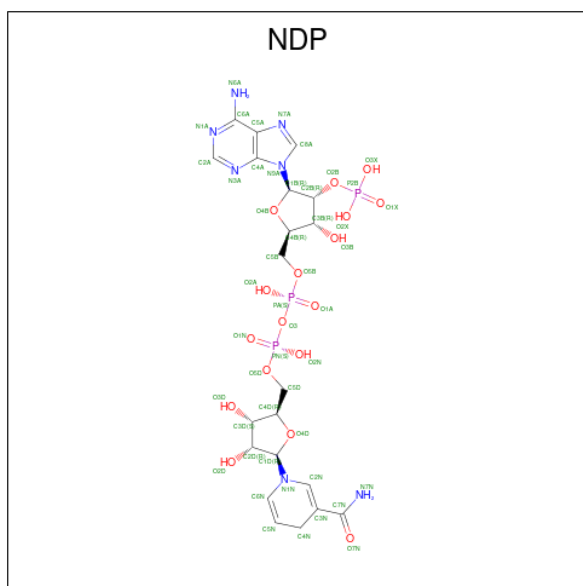
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Mol	Chain	Residues	Atoms					AltConf
88	P1	1	Total	C	N	O	P	0
			47	37	1	8	1	
88	TA	1	Total	C	N	O	P	0
			26	16	1	8	1	
88	A3	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
89	3F	1	Total	Zn	0
			1	1	
89	A9	1	Total	Zn	0
			1	1	
89	S6	1	Total	Zn	0
			1	1	

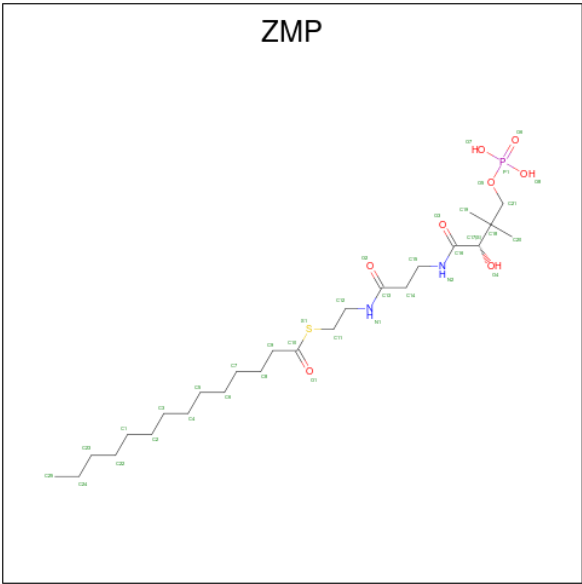
- Molecule 90 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
90	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

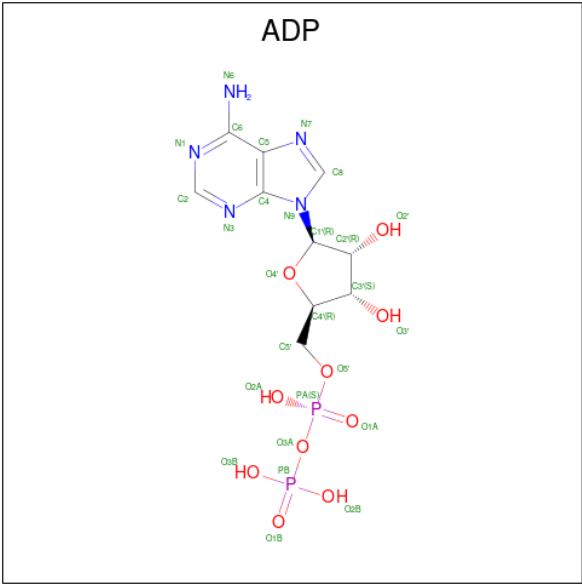
- Molecule 91 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alan

yl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



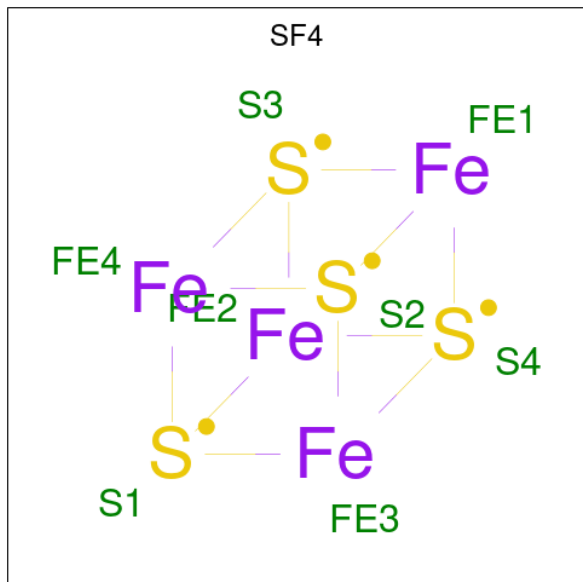
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	AB	1	34	23	2	7	1	0

- Molecule 92 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



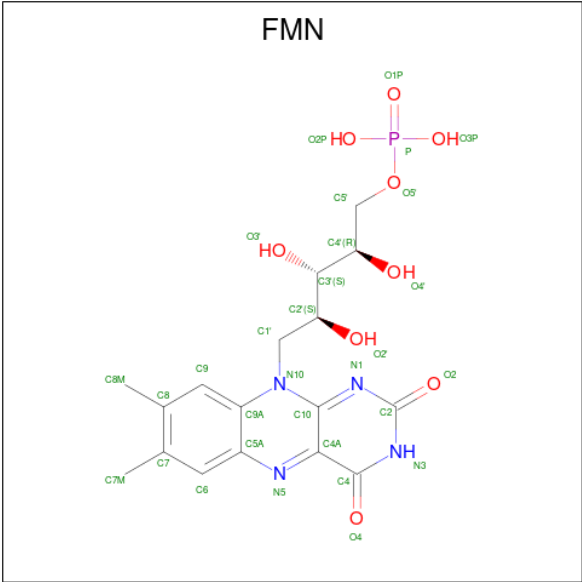
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	B8	1	27	10	5	10	2	0

- Molecule 93 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
93	S1	1	Total	Fe	S	0
			8	4	4	
93	S1	1	Total	Fe	S	0
			8	4	4	
93	S7	1	Total	Fe	S	0
			8	4	4	
93	S8	1	Total	Fe	S	0
			8	4	4	
93	S8	1	Total	Fe	S	0
			8	4	4	
93	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 94 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).

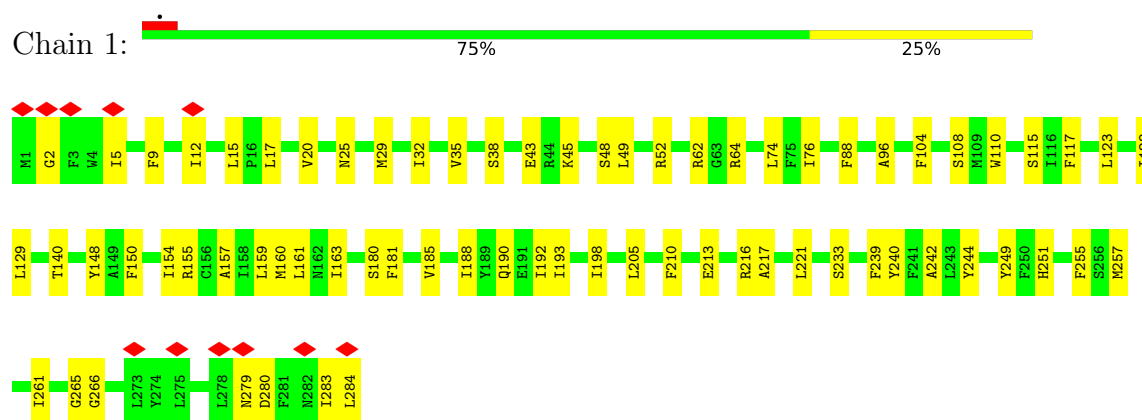


Mol	Chain	Residues	Atoms					AltConf
94	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

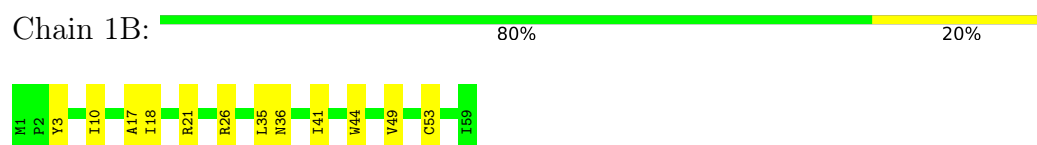
3 Residue-property plots

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

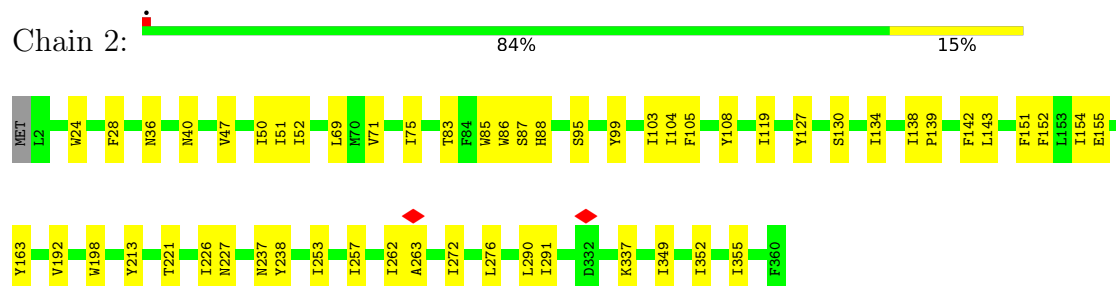
• Molecule 1: NADH-ubiquinone oxidoreductase chain 1



• Molecule 2: NADH dehydrogenase subunit 1

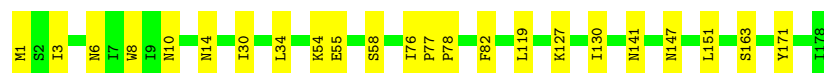


• Molecule 3: Ymf65

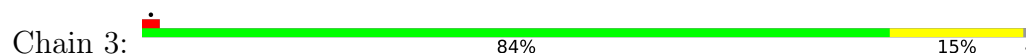


• Molecule 4: NADH dehydrogenase subunit 2

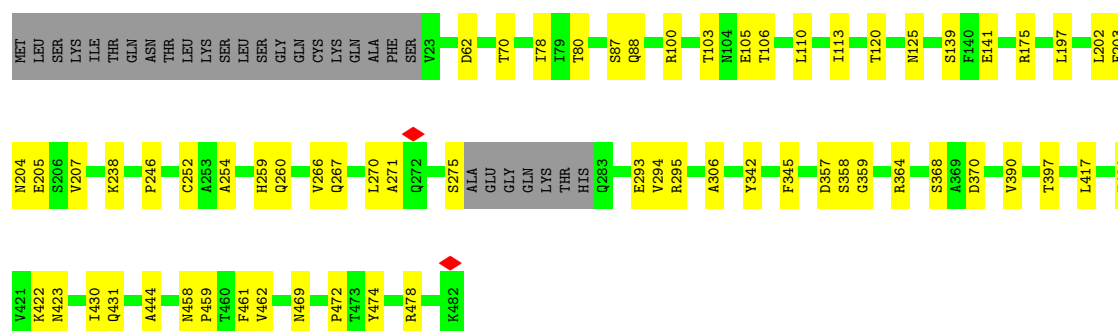
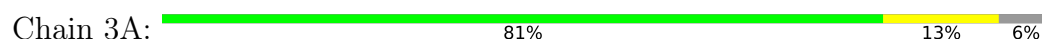




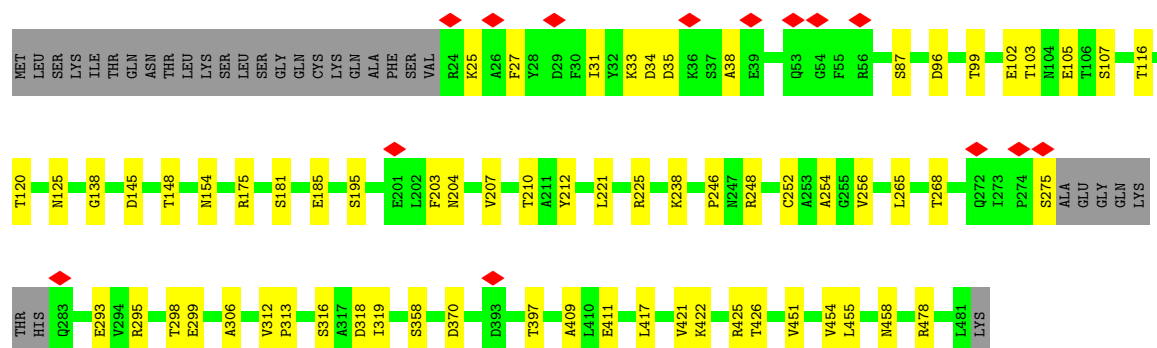
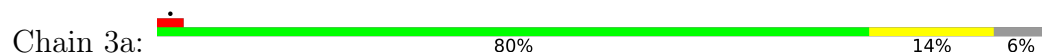
- Molecule 5: NADH-ubiquinone oxidoreductase chain 3



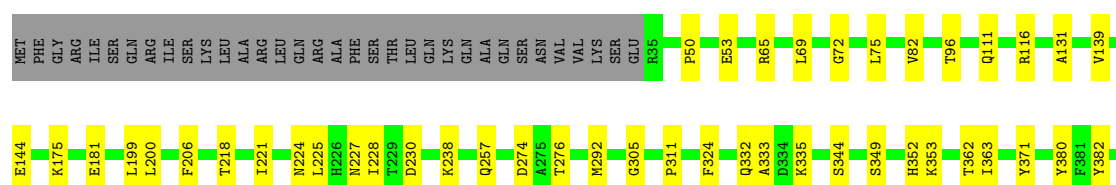
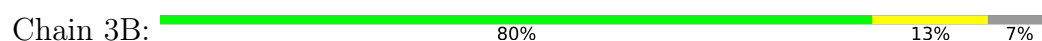
- Molecule 6: M16 family peptidase, putative



- Molecule 6: M16 family peptidase, putative



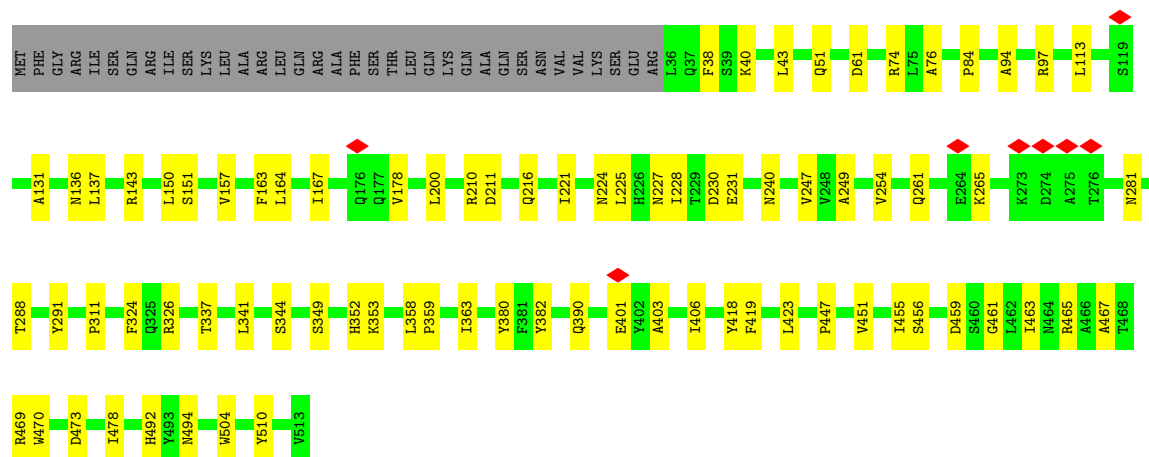
- Molecule 7: Peptidase M16 inactive domain protein





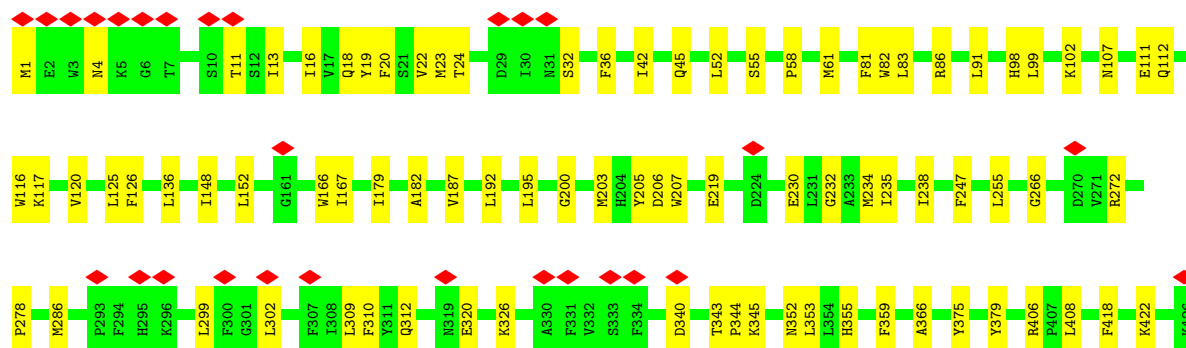
• Molecule 7: Peptidase M16 inactive domain protein

Chain 3b: 78% 16% 7%



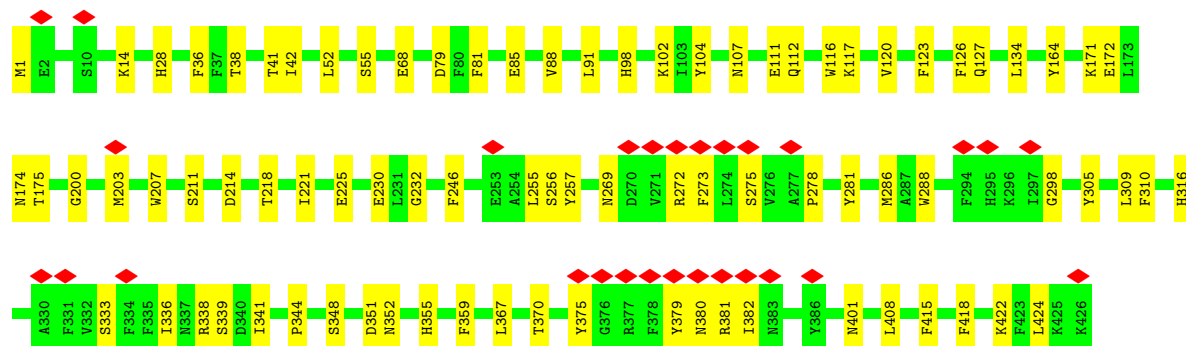
• Molecule 8: Apocytochrome b

Chain 3C: 7% 80% 20%



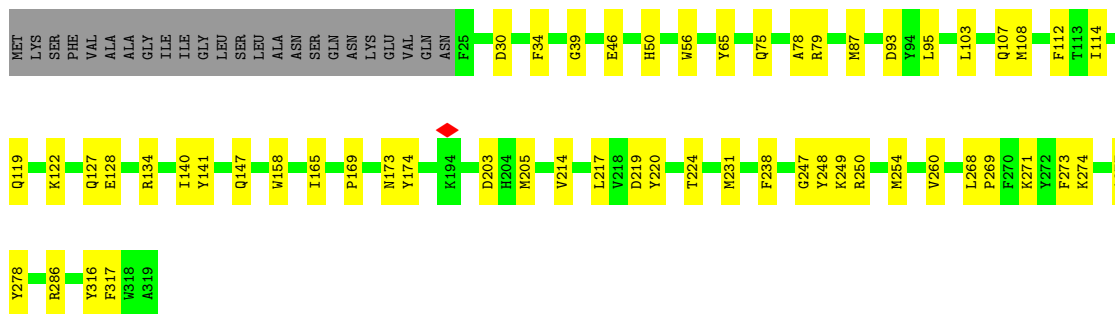
• Molecule 8: Apocytochrome b

Chain 3c: 7% 80% 20%



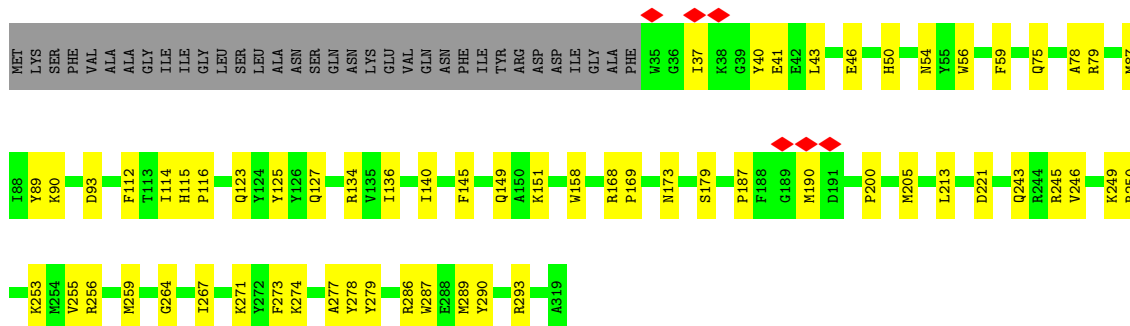
- Molecule 9: Cytochrome protein c1

Chain 3D: 



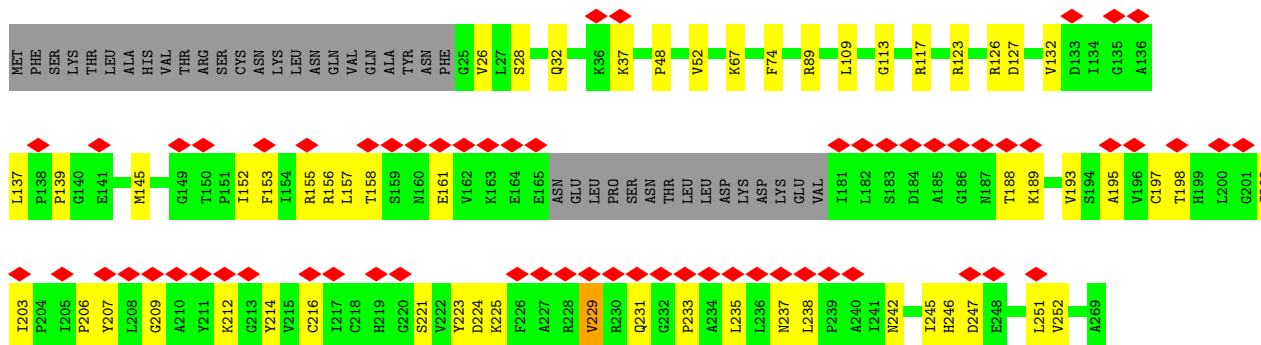
- Molecule 9: Cytochrome protein c1

Chain 3d: 



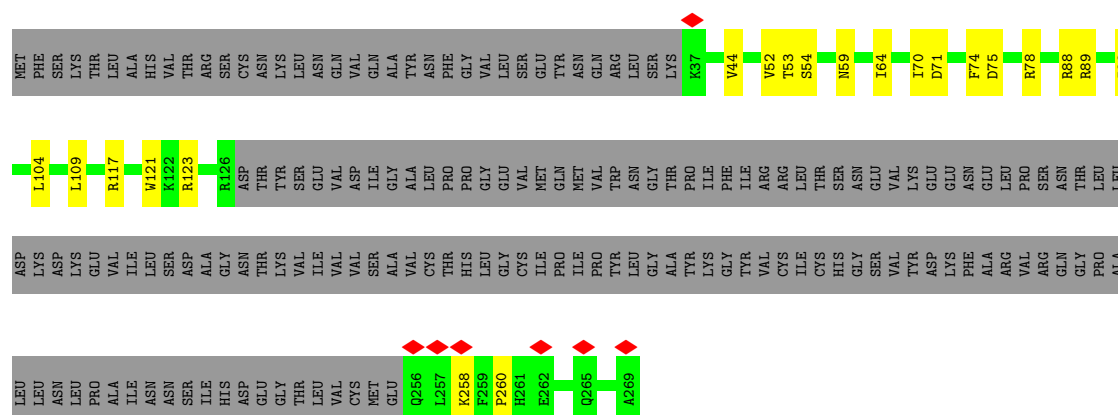
- Molecule 10: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain 3E: 

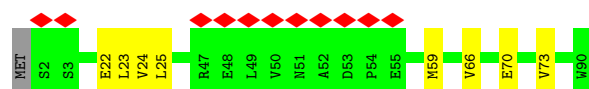
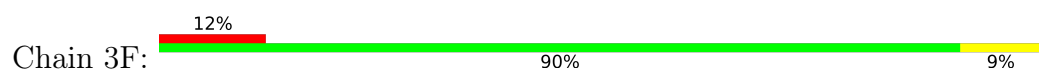


- Molecule 10: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

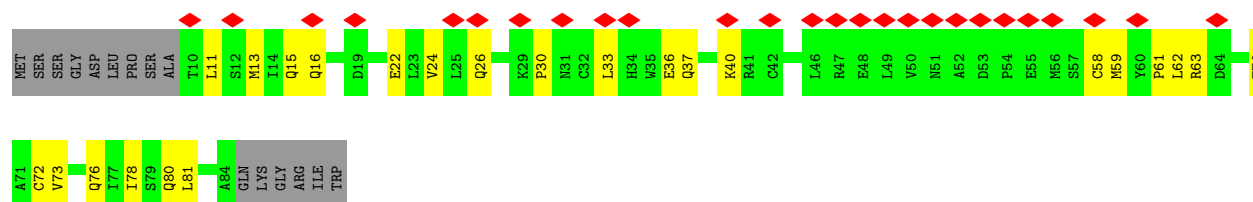
Chain 3e: 



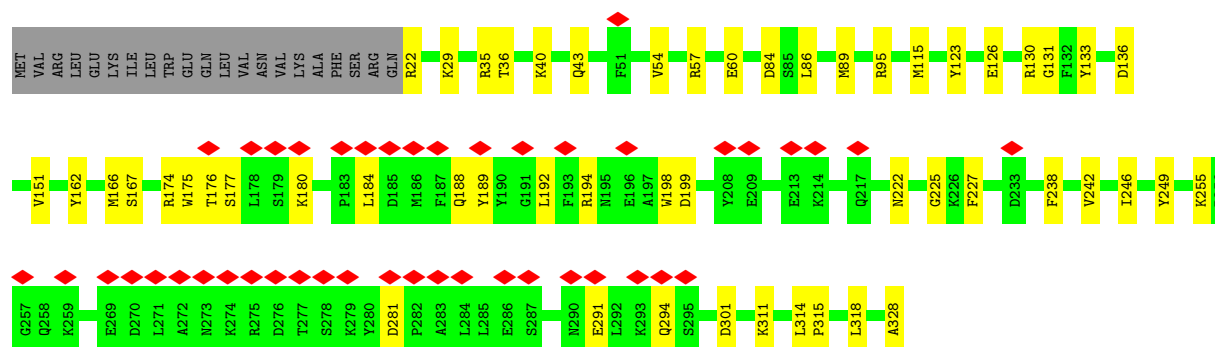
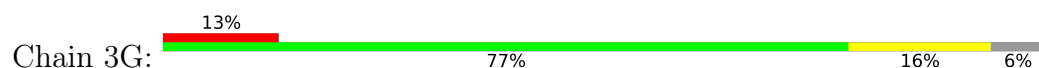
• Molecule 11: Ubiquinol-cytochrome C reductase hinge protein



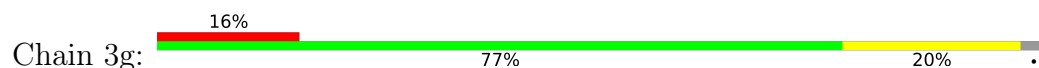
• Molecule 11: Ubiquinol-cytochrome C reductase hinge protein

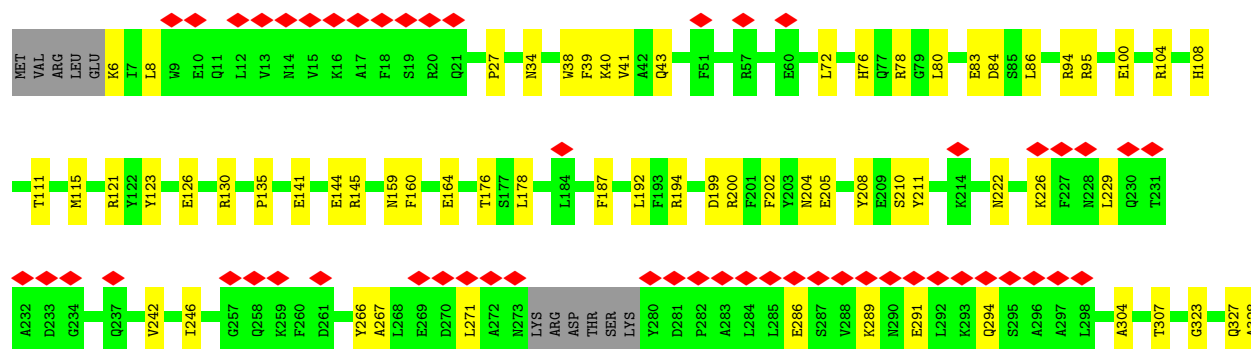


• Molecule 12: UQCRB

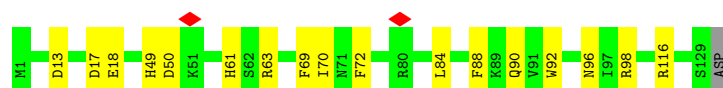


• Molecule 12: UQCRB

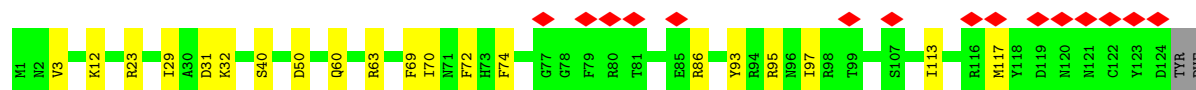
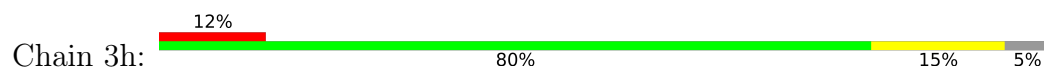




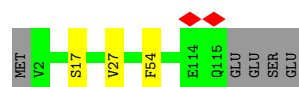
- Molecule 13: Transmembrane protein, putative



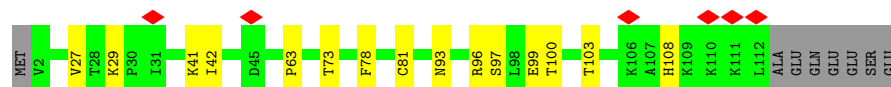
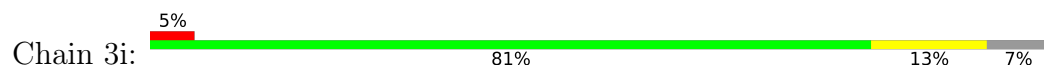
- Molecule 13: Transmembrane protein, putative



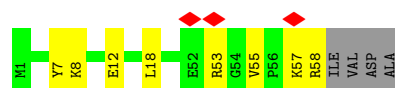
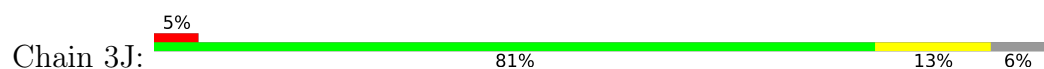
- Molecule 14: Transmembrane protein, putative



- Molecule 14: Transmembrane protein, putative

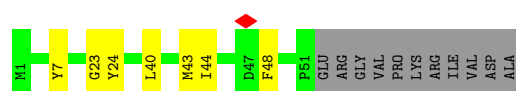


- Molecule 15: Transmembrane protein, putative



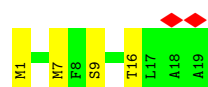
- Molecule 15: Transmembrane protein, putative

Chain 3j:  71% 11% 18%



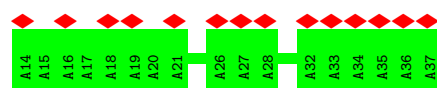
- Molecule 16: UNK1

Chain 3M:  11% 79% 21%

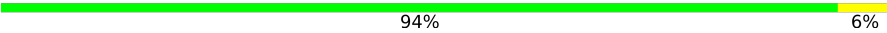


- Molecule 17: UNK2

Chain 3l:  58% 100%



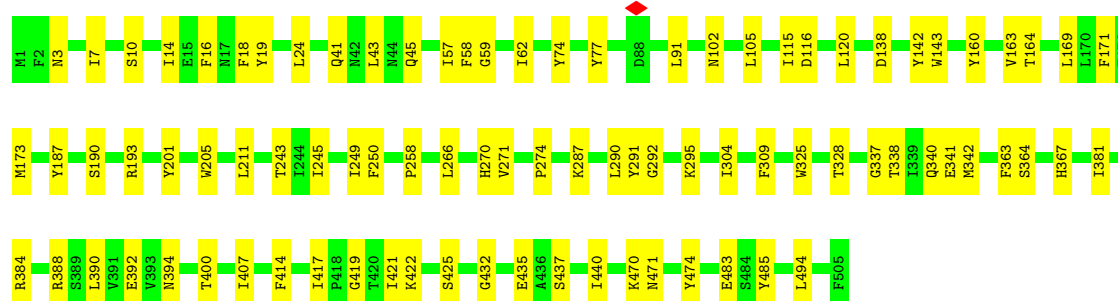
- Molecule 18: UNK3

Chain 3m:  94% 6%



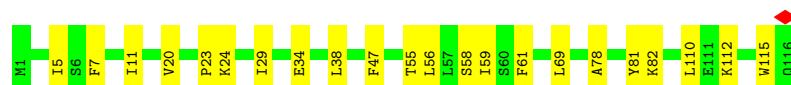
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4

Chain 4:  83% 17%



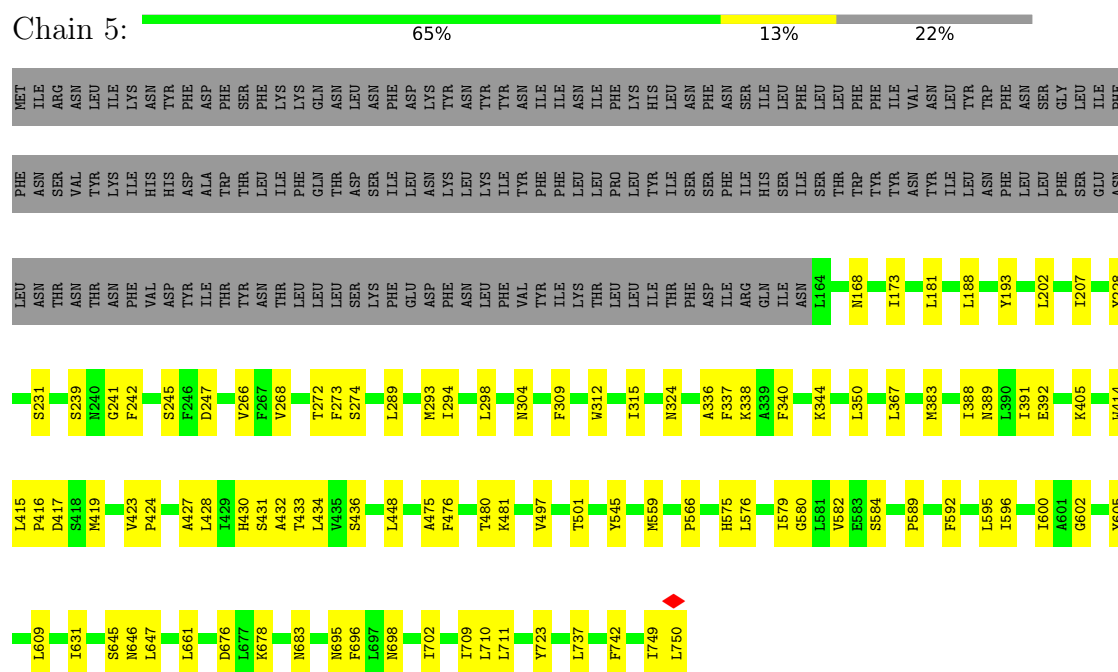
- Molecule 20: Ymf58

Chain 4L:  81% 19%



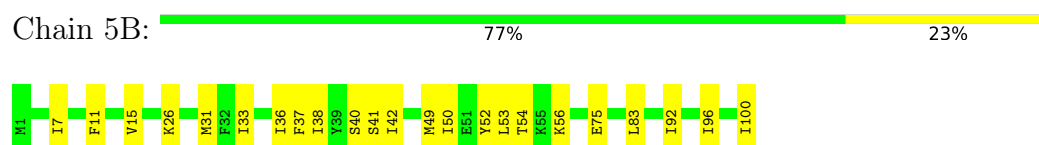
- Molecule 21: NADH dehydrogenase subunit 5

Chain 5:



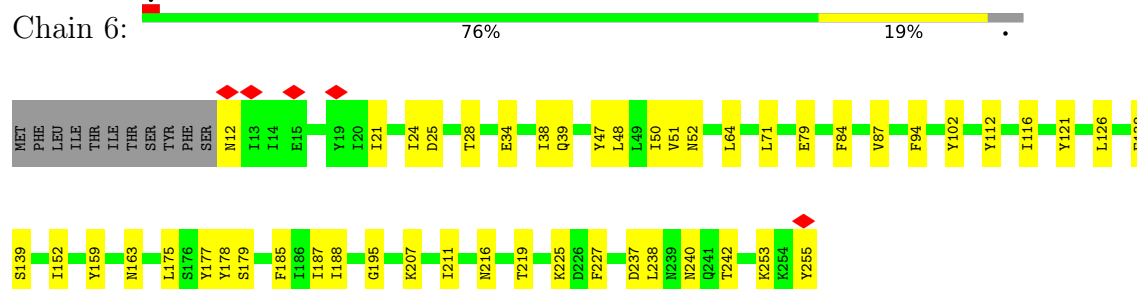
- Molecule 22: Ymf57

Chain 5B:



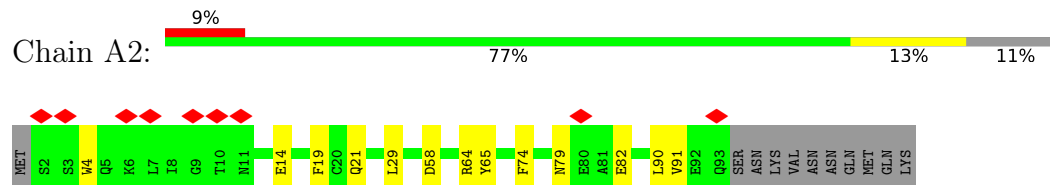
- Molecule 23: Ymf62

Chain 6:



- Molecule 24: Ribosomal protein L51/S25/CI-B8 domain protein

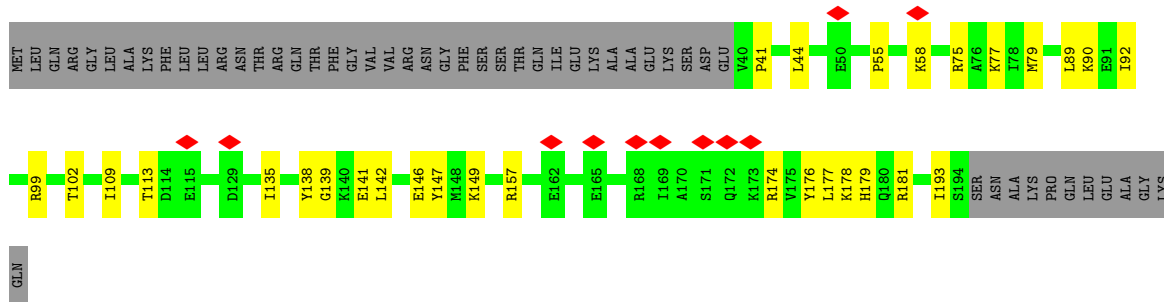
Chain A2:



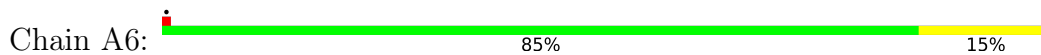
- Molecule 25: ETC complex I subunit motif protein

Chain A5:

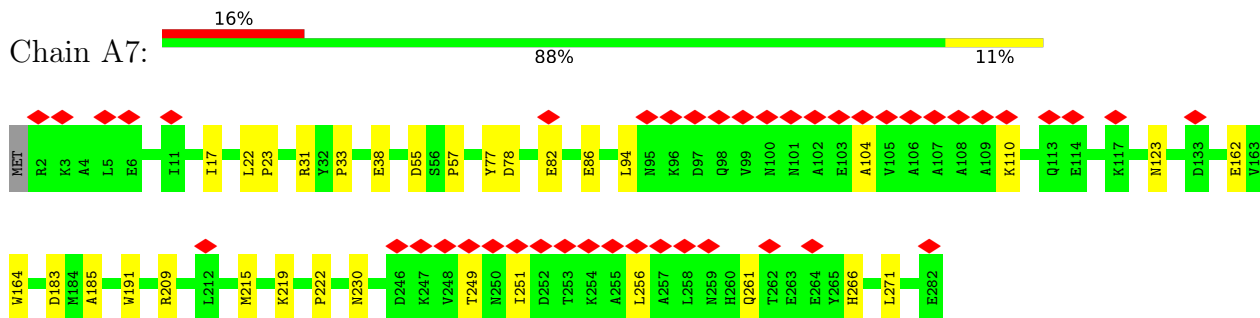




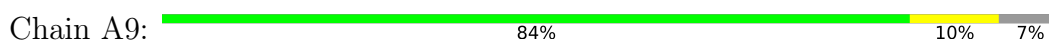
- Molecule 26: NADH dehydrogenase, putative



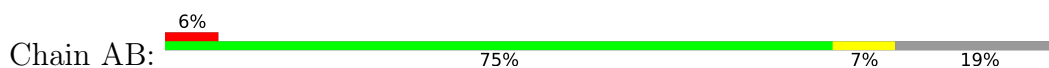
- Molecule 27: NDUA7



- Molecule 28: NAD-dependent epimerase/dehydratase family protein

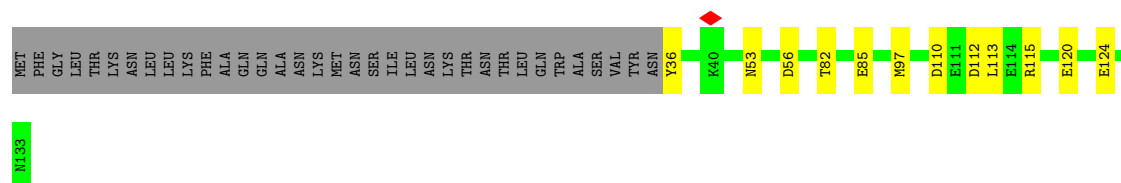


- Molecule 29: Acyl carrier protein



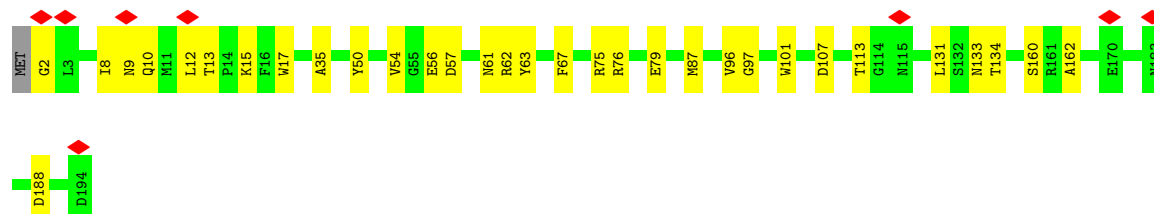
- Molecule 30: Acyl carrier protein





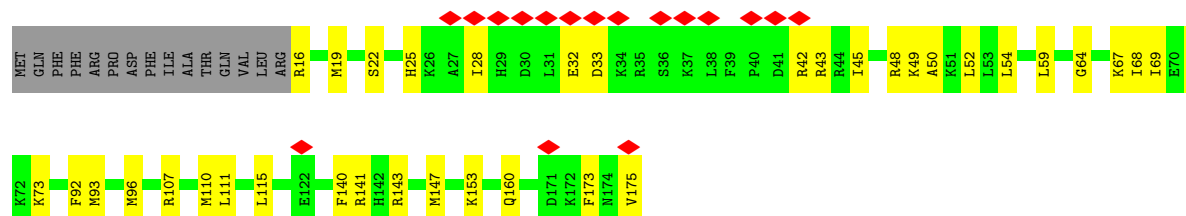
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL: 83% 16%



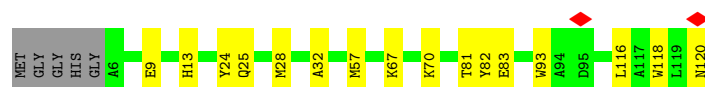
- Molecule 32: NDUA13

Chain AM: 10% 70% 21% 9%



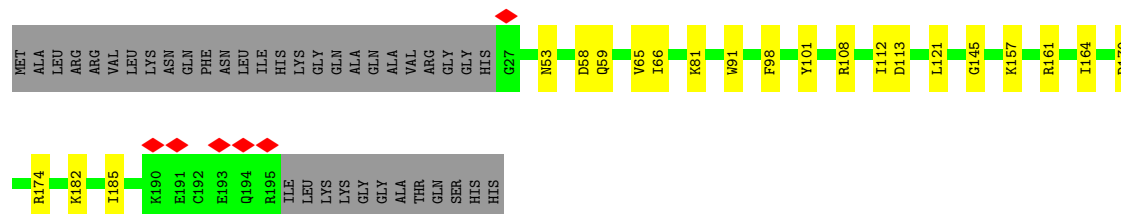
- Molecule 33: NDUB7

Chain B7: 82% 13%



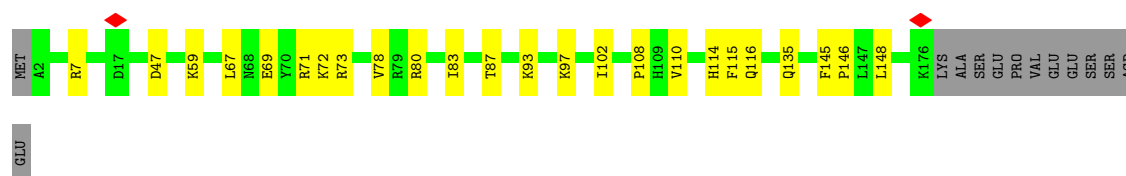
- Molecule 34: NDUB8

Chain B8: 71% 10% 18%

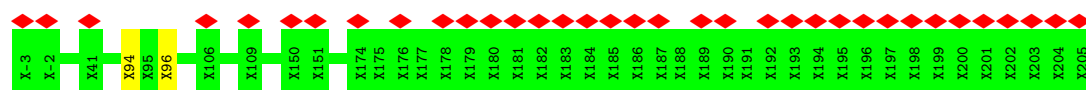


- Molecule 35: NDUB10

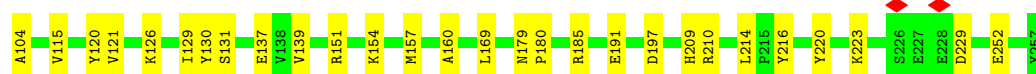
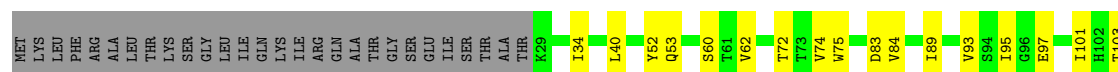
Chain BL: 80% 13% 7%



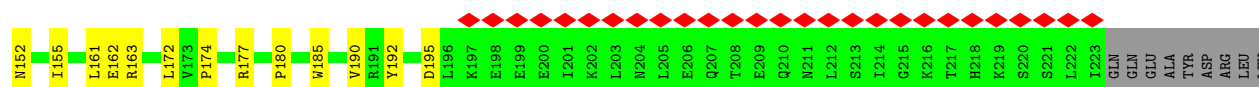
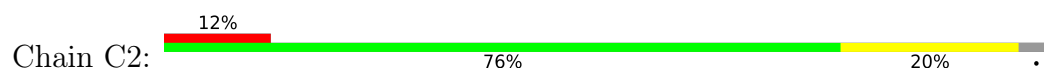
- Molecule 36: UNK4



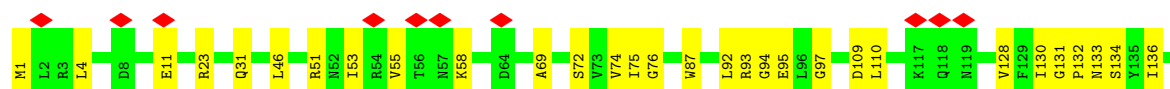
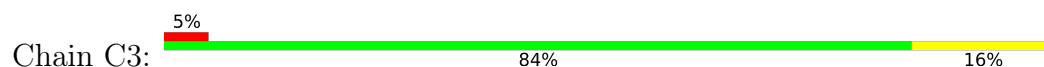
- Molecule 37: Gamma-carbonic anhydrase



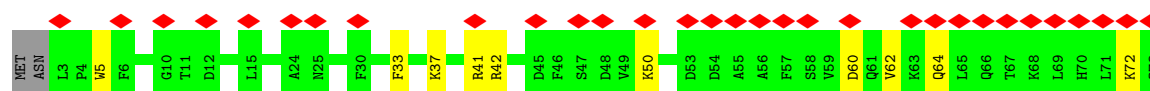
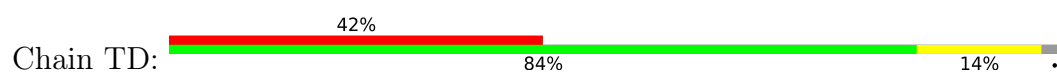
- Molecule 38: Gamma-carbonic anhydrase



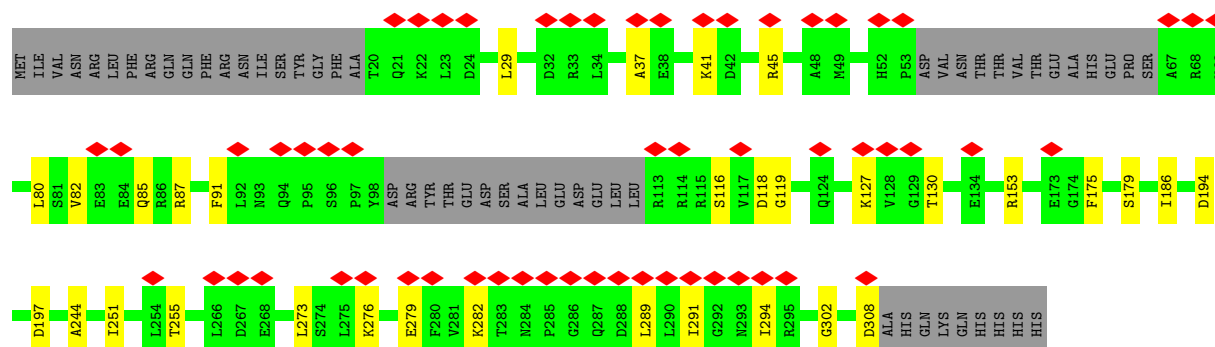
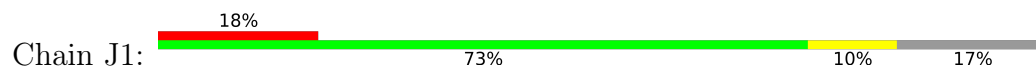
- Molecule 39: Transcription factor apf protein, putative



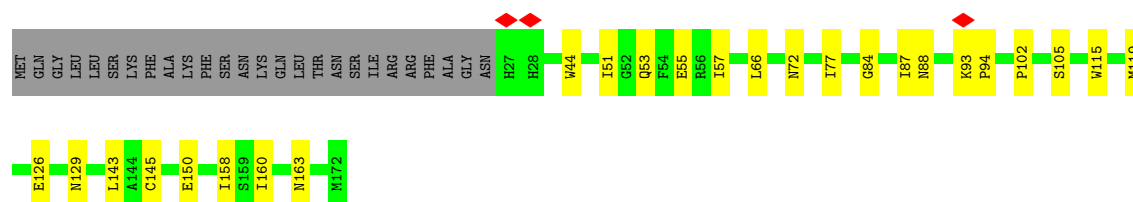
- Molecule 40: Transmembrane protein, putative



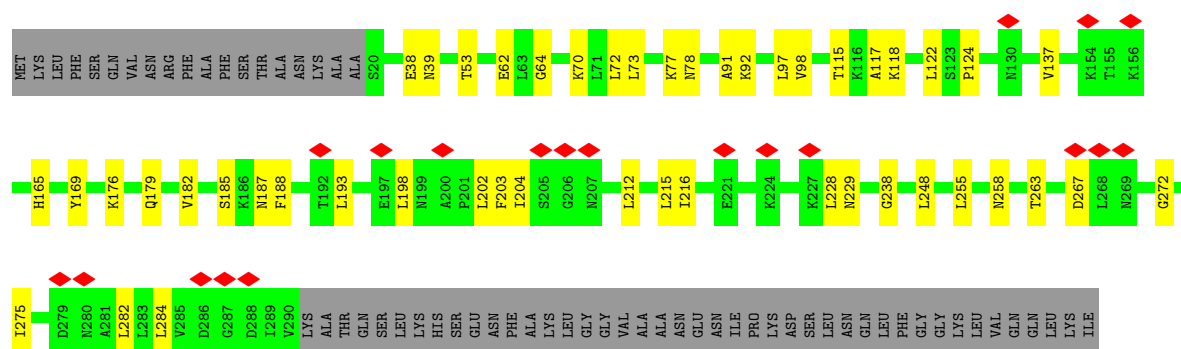
• Molecule 41: DnaJ domain protein



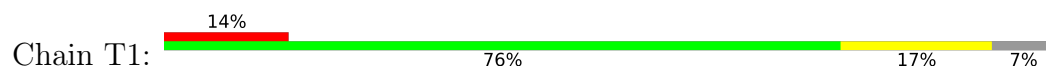
• Molecule 42: 2 iron, 2 sulfur cluster-binding protein



• Molecule 43: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

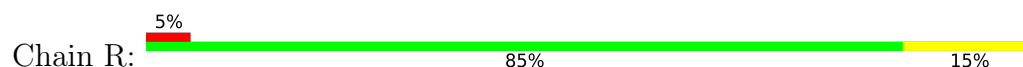


• Molecule 44: Lipid-A-disaccharide synthase

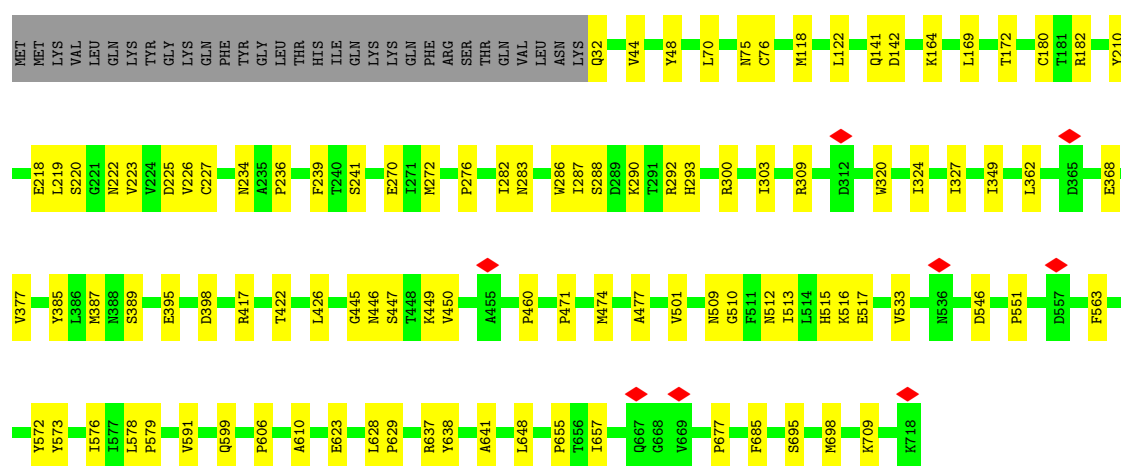
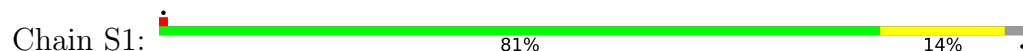




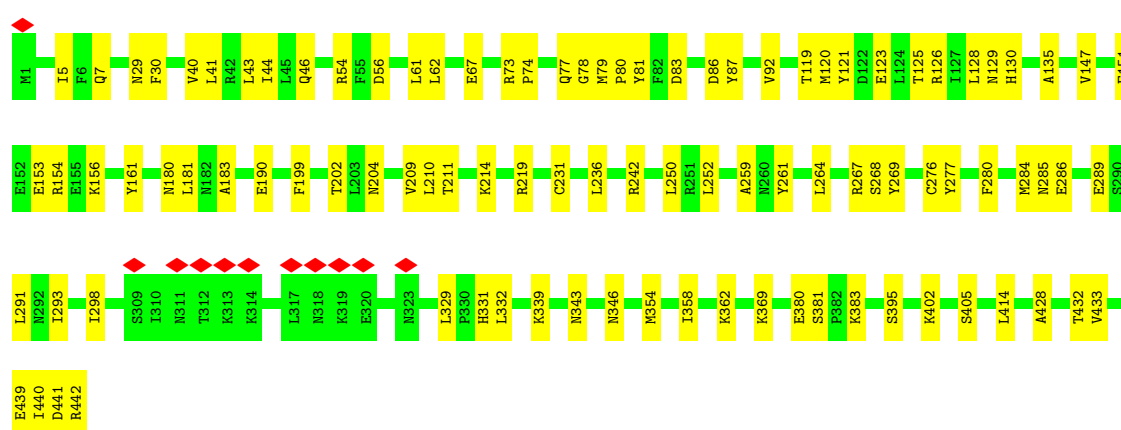
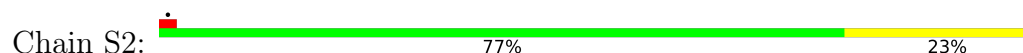
• Molecule 49: UNK5



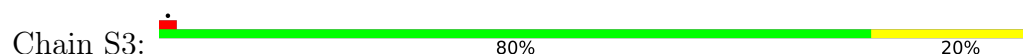
• Molecule 50: NADH-ubiquinone oxidoreductase 75 kDa subunit

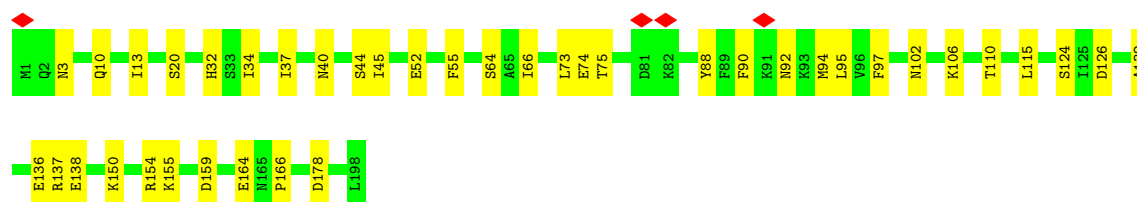


• Molecule 51: NADH dehydrogenase subunit 7

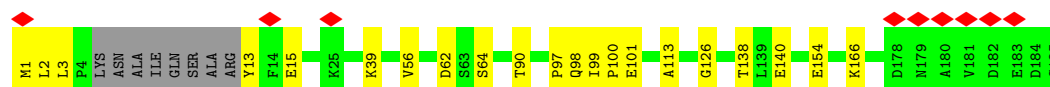
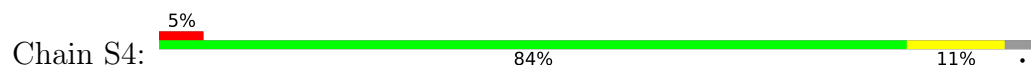


• Molecule 52: NADH dehydrogenase subunit 9

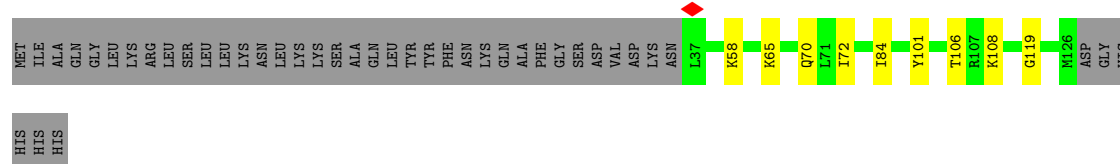




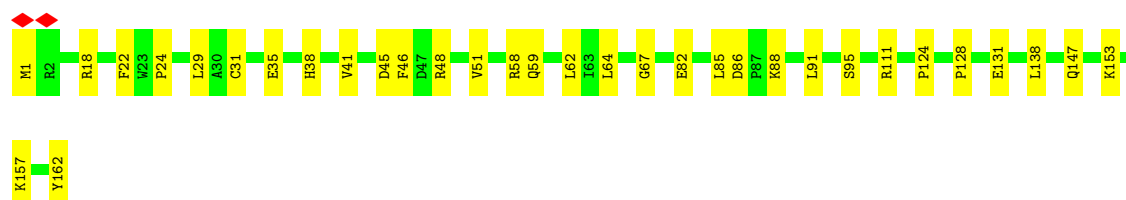
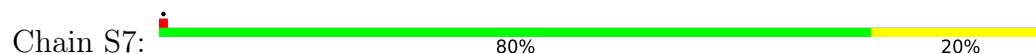
- Molecule 53: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



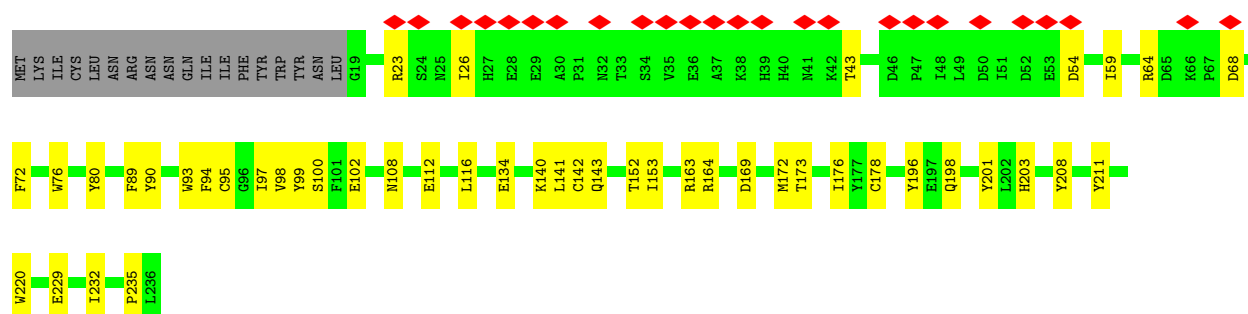
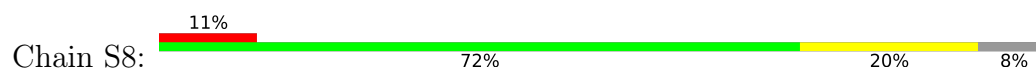
- Molecule 54: Zinc-finger protein



- Molecule 55: NADH dehydrogenase subunit 10



- Molecule 56: NADH-ubiquinone oxidoreductase 1, chain, putative



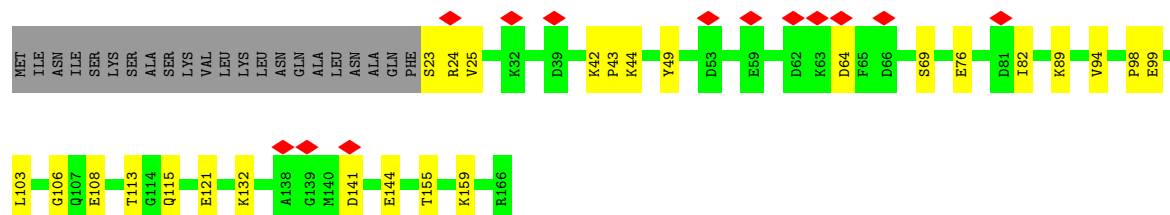
- Molecule 57: NDUB9

Chain B9: 

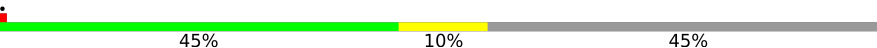


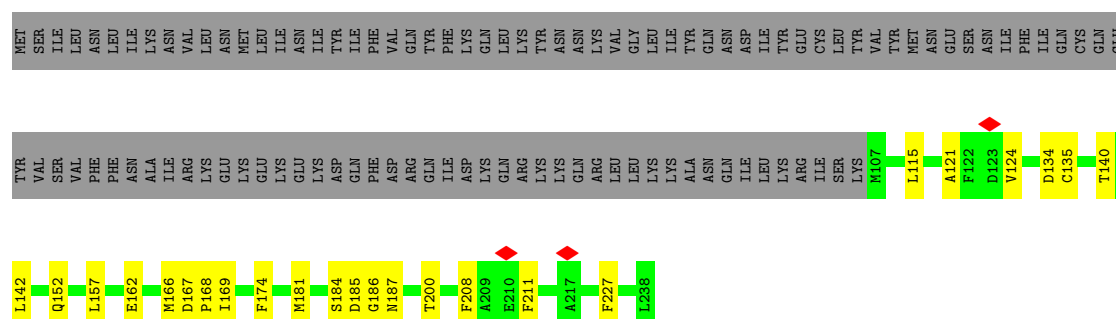
• Molecule 58: Thioredoxin

Chain TX: 



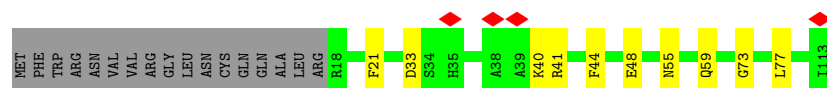
• Molecule 59: NDUA8

Chain A8: 



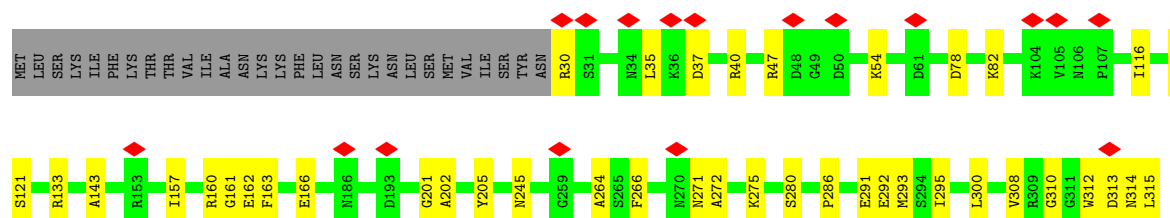
• Molecule 60: Transmembrane protein, putative

Chain TB: 



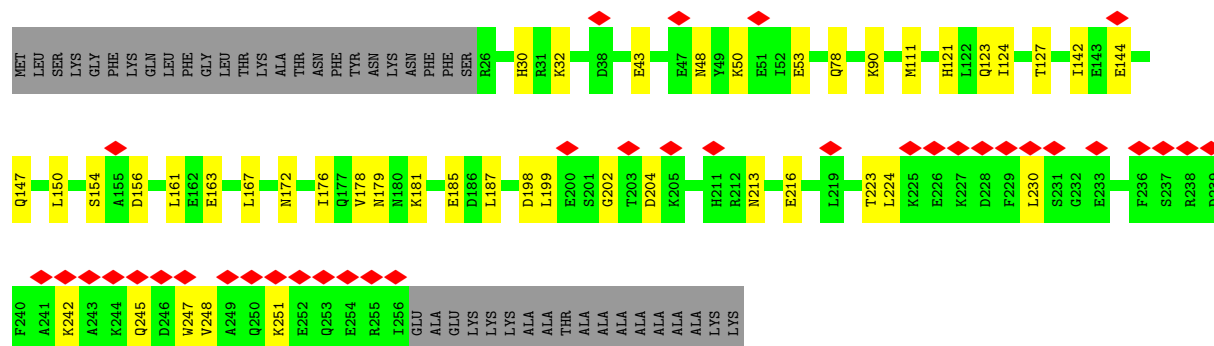
• Molecule 61: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1: 

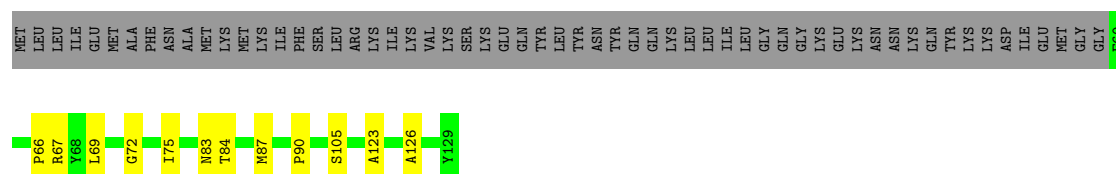




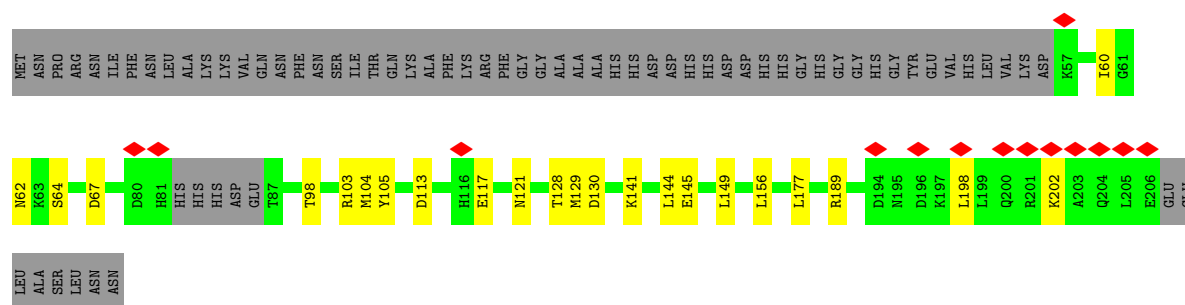
- Molecule 62: NADH-ubiquinone oxidoreductase 24 kDa subunit



- Molecule 63: NDUB6



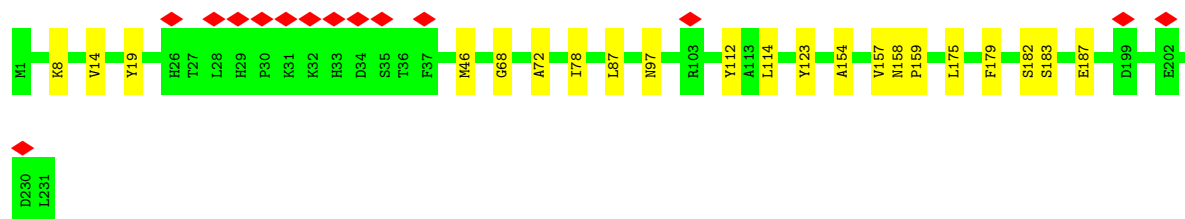
- Molecule 64: Transmembrane protein, putative



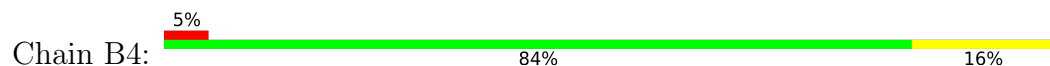
- Molecule 65: NDUC2



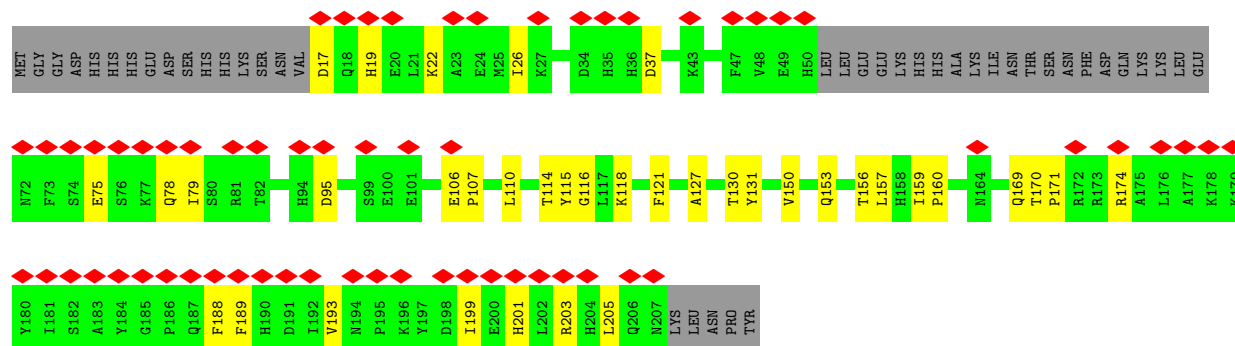
- Molecule 66: Transmembrane protein, putative



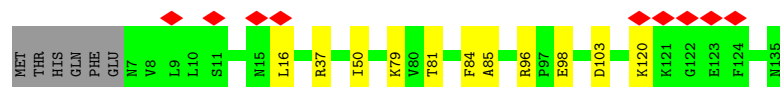
- Molecule 67: NDUB4



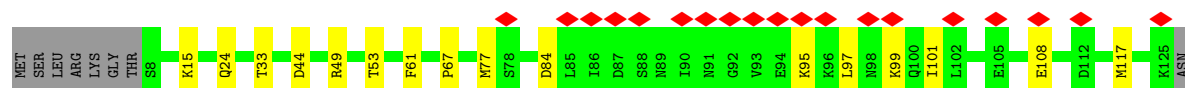
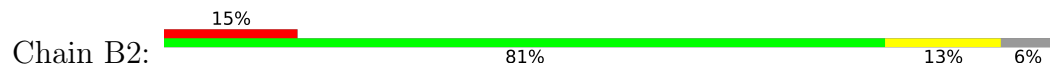
- Molecule 68: NDUTT4



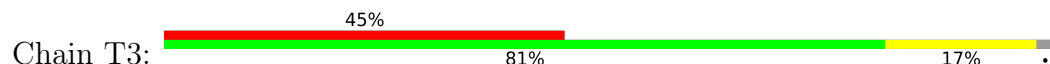
- Molecule 69: NDUTT8

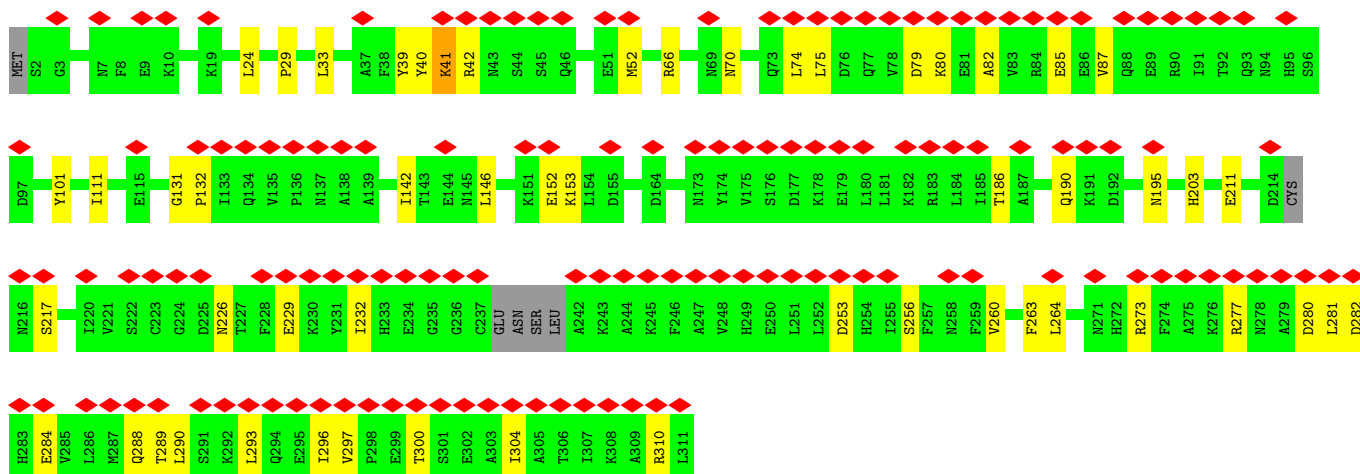


- Molecule 70: NDUB2

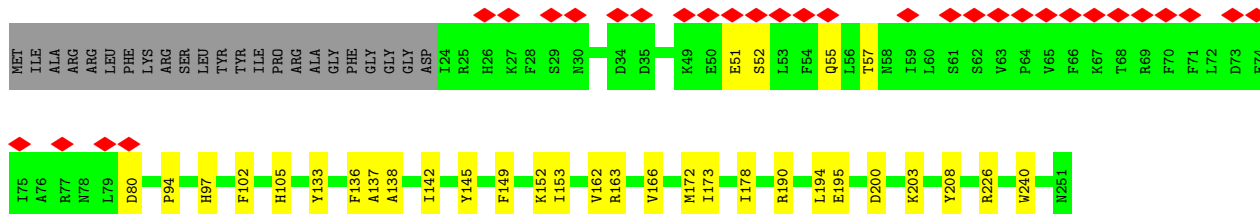
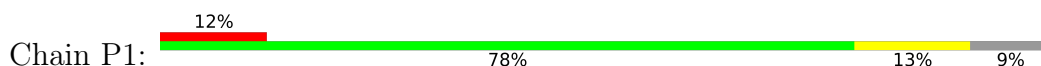


- Molecule 71: NDUTT3





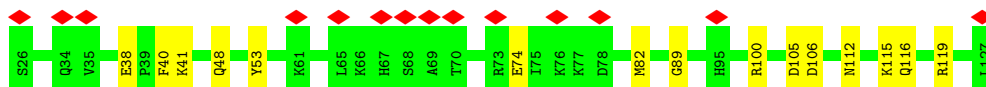
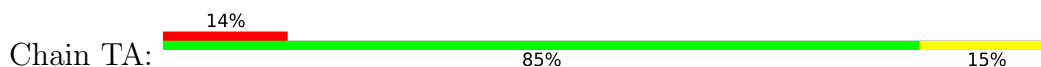
- Molecule 72: Transmembrane protein, putative



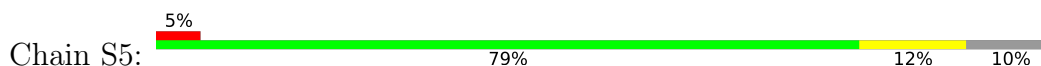
- Molecule 73: Transmembrane protein, putative



- Molecule 74: NDUTT10

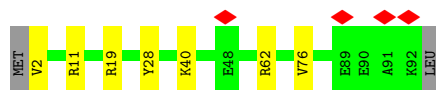


- Molecule 75: GRAM domain protein



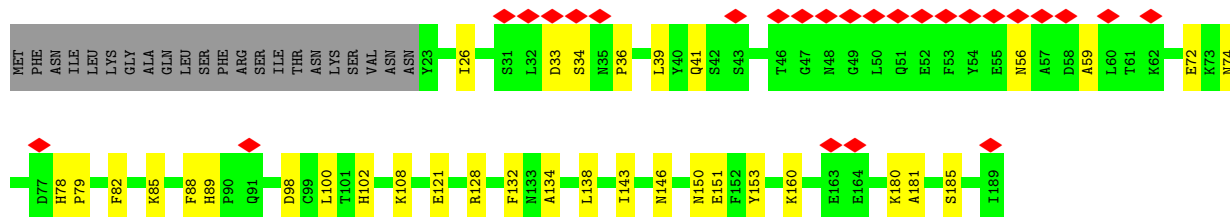
- Molecule 76: NDUTT12

Chain TC:  90% 8%



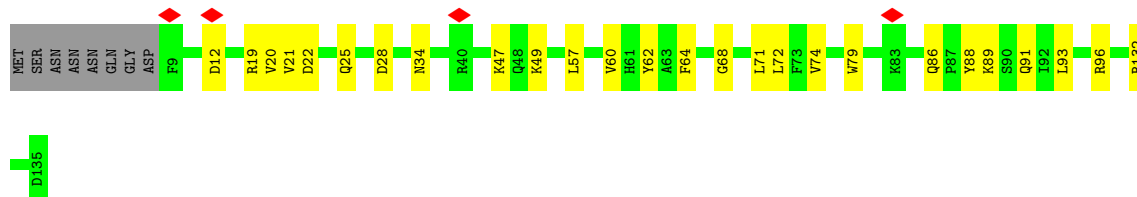
- Molecule 77: NDUPH2

Chain P2:  14% 70% 18% 12%



- Molecule 78: Transmembrane protein, putative

Chain A3:  75% 19% 6%



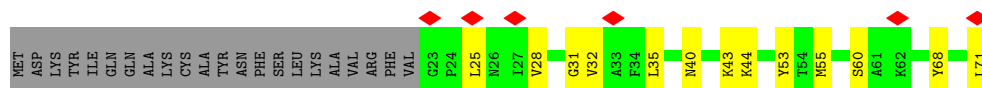
- Molecule 79: NDUTT9

Chain T9:  7% 83% 15%



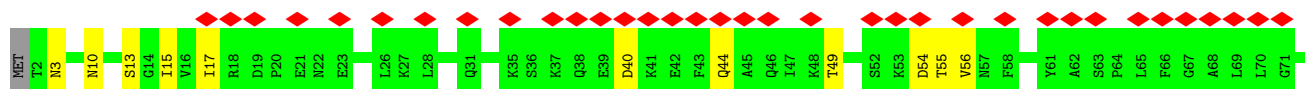
- Molecule 80: Transmembrane protein, putative

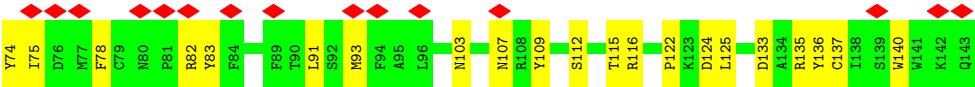
Chain TE:  8% 51% 18% 31%



- Molecule 81: Transmembrane protein, putative

Chain T7:  35% 77% 22%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203834	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 ($e^-/\text{\AA}^2$)	66.69	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	58616	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	32.050	Depositor
Minimum map value	-15.499	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.092	Depositor
Recommended contour level	6	Depositor
Map size (Å)	501.0, 501.0, 501.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, ZMP, SF4, NDP, 3PE, PC1, ZN, FES, FMN, HEM, HEC, ADP, U10

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	1	0.14	0/2384	0.33	0/3244
2	1B	0.12	0/536	0.25	0/727
3	2	0.15	0/3165	0.33	0/4302
4	2B	0.14	0/1520	0.31	0/2058
5	3	0.14	0/1051	0.28	0/1429
6	3A	0.11	0/3563	0.25	0/4827
6	3a	0.11	0/3547	0.26	0/4806
7	3B	0.13	0/3912	0.28	0/5313
7	3b	0.13	0/3901	0.30	0/5299
8	3C	0.13	0/3716	0.29	0/5046
8	3c	0.13	0/3715	0.30	1/5046 (0.0%)
9	3D	0.13	0/2579	0.29	0/3491
9	3d	0.13	0/2491	0.28	0/3371
10	3E	0.13	0/1893	0.30	0/2566
10	3e	0.13	0/909	0.25	0/1226
11	3F	0.12	0/717	0.31	0/969
11	3f	0.15	0/608	0.35	0/823
12	3G	0.12	0/2670	0.28	0/3602
12	3g	0.12	0/2759	0.31	0/3724
13	3H	0.13	0/1133	0.31	0/1524
13	3h	0.12	0/1077	0.30	0/1448
14	3I	0.12	0/1005	0.29	0/1365
14	3i	0.12	0/982	0.32	0/1334
15	3J	0.14	0/522	0.31	0/712
15	3j	0.17	0/463	0.35	0/634
16	3M	0.10	0/151	0.33	0/198
17	3l	0.16	0/123	0.22	0/170
18	3m	0.09	0/122	0.24	0/162
19	4	0.16	0/4303	0.33	0/5844
20	4L	0.16	0/982	0.31	0/1335
21	5	0.14	0/4997	0.30	0/6794
22	5B	0.14	0/915	0.35	0/1224

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	6	0.13	0/2137	0.27	0/2906
24	A2	0.10	0/780	0.26	0/1054
25	A5	0.12	0/1336	0.28	0/1797
26	A6	0.13	0/1459	0.26	0/1965
27	A7	0.10	0/2400	0.24	0/3259
28	A9	0.11	0/2789	0.26	0/3777
29	AB	0.09	0/942	0.24	0/1272
30	AC	0.11	0/822	0.27	0/1114
31	AL	0.11	0/1667	0.28	0/2256
32	AM	0.13	0/1379	0.27	0/1841
33	B7	0.13	0/964	0.30	0/1302
34	B8	0.12	0/1445	0.26	0/1952
35	BL	0.12	0/1489	0.27	0/2000
37	C1	0.12	0/1806	0.28	0/2461
38	C2	0.12	0/1653	0.29	0/2257
39	C3	0.11	0/2865	0.27	0/3877
40	TD	0.10	0/626	0.23	0/844
41	J1	0.09	0/2194	0.22	0/2954
42	FX	0.11	0/1186	0.30	0/1607
43	T2	0.10	0/2160	0.23	0/2937
44	T1	0.12	0/3975	0.28	0/5380
45	A1	0.12	0/827	0.27	0/1122
46	X1	0.11	0/1261	0.25	0/1698
47	T6	0.10	0/923	0.26	0/1239
48	T5	0.15	0/1113	0.35	0/1507
49	R	0.14	0/962	0.32	0/1302
50	S1	0.12	0/5502	0.30	0/7454
51	S2	0.14	0/3681	0.31	0/4969
52	S3	0.12	0/1718	0.30	0/2319
53	S4	0.11	0/1505	0.28	0/2035
54	S6	0.11	0/739	0.31	0/1000
55	S7	0.14	0/1319	0.36	0/1789
56	S8	0.14	0/1867	0.31	0/2538
57	B9	0.11	0/1627	0.25	0/2203
58	TX	0.10	0/1235	0.25	0/1662
59	A8	0.12	0/1099	0.26	0/1477
60	TB	0.11	0/825	0.26	0/1115
61	V1	0.11	0/3485	0.29	0/4713
62	V2	0.11	0/1895	0.29	0/2559
63	B6	0.13	0/623	0.26	0/850
64	BM	0.13	0/1187	0.29	0/1605
65	C4	0.11	0/865	0.26	0/1165
66	AN	0.09	0/1935	0.22	0/2616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
67	B4	0.13	0/935	0.27	0/1277
68	T4	0.10	0/1447	0.25	0/1957
69	T8	0.12	0/1091	0.28	0/1479
70	B2	0.13	0/980	0.29	0/1318
71	T3	0.11	0/2488	0.29	0/3367
72	P1	0.11	0/1951	0.30	0/2642
73	B3	0.12	0/613	0.31	0/829
74	TA	0.10	0/877	0.28	0/1181
75	S5	0.10	0/710	0.24	0/959
76	TC	0.09	0/803	0.22	0/1082
77	P2	0.11	0/1454	0.26	0/1970
78	A3	0.11	0/1103	0.26	0/1491
79	T9	0.11	0/1088	0.27	0/1458
80	TE	0.10	0/425	0.27	0/573
81	T7	0.11	0/1223	0.30	0/1648
All	All	0.12	0/151866	0.29	1/205593 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3c	382	ILE	N-CA-C	-6.04	106.61	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2313	0	2361	63	0
2	1B	516	0	528	12	0
3	2	3065	0	3141	45	0
4	2B	1483	0	1554	20	0
5	3	1017	0	1014	18	0
6	3A	3511	0	3507	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3a	3495	0	3485	43	0
7	3B	3826	0	3728	49	0
7	3b	3815	0	3715	55	0
8	3C	3590	0	3482	70	0
8	3c	3589	0	3483	67	0
9	3D	2488	0	2343	40	0
9	3d	2403	0	2265	48	0
10	3E	1846	0	1806	46	0
10	3e	882	0	843	20	0
11	3F	703	0	702	5	0
11	3f	597	0	599	17	0
12	3G	2595	0	2520	38	0
12	3g	2682	0	2611	48	0
13	3H	1098	0	1040	17	0
13	3h	1046	0	999	20	0
14	3I	971	0	986	3	0
14	3i	948	0	967	12	0
15	3J	501	0	503	11	0
15	3j	443	0	439	6	0
16	3M	150	0	160	6	0
17	3l	124	0	120	0	0
18	3m	121	0	133	2	0
19	4	4170	0	4223	71	0
20	4L	957	0	987	17	0
21	5	4844	0	4892	84	0
22	5B	888	0	917	17	0
23	6	2076	0	2071	46	0
24	A2	765	0	755	7	0
25	A5	1307	0	1317	21	0
26	A6	1421	0	1382	21	0
27	A7	2339	0	2237	25	0
28	A9	2718	0	2649	25	0
29	AB	926	0	902	6	0
30	AC	806	0	784	7	0
31	AL	1612	0	1511	23	0
32	AM	1349	0	1375	40	0
33	B7	937	0	881	13	0
34	B8	1408	0	1357	21	0
35	BL	1461	0	1467	22	0
36	C	1045	0	216	1	0
37	C1	1769	0	1721	34	0
38	C2	1624	0	1566	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	C3	2804	0	2727	40	0
40	TD	608	0	605	10	0
41	J1	2146	0	2110	25	0
42	FX	1162	0	1120	18	0
43	T2	2117	0	2109	29	0
44	T1	3884	0	3827	54	0
45	A1	799	0	792	16	0
46	X1	1227	0	1208	13	0
47	T6	903	0	851	12	0
48	T5	1088	0	1107	22	0
49	R	943	0	950	18	0
50	S1	5394	0	5345	69	0
51	S2	3599	0	3552	72	0
52	S3	1681	0	1679	27	0
53	S4	1463	0	1397	17	0
54	S6	722	0	714	6	0
55	S7	1286	0	1283	27	0
56	S8	1812	0	1688	39	0
57	B9	1579	0	1482	17	0
58	TX	1206	0	1155	18	0
59	A8	1075	0	1022	16	0
60	TB	801	0	763	8	0
61	V1	3410	0	3357	42	0
62	V2	1858	0	1842	28	0
63	B6	596	0	583	9	0
64	BM	1163	0	1120	18	0
65	C4	842	0	828	7	0
66	AN	1879	0	1818	17	0
67	B4	898	0	819	13	0
68	T4	1408	0	1392	27	0
69	T8	1064	0	1095	13	0
70	B2	955	0	930	14	0
71	T3	2442	0	2438	37	0
72	P1	1896	0	1854	25	0
73	B3	594	0	589	9	0
74	TA	854	0	839	15	0
75	S5	693	0	669	14	0
76	TC	781	0	734	9	0
77	P2	1414	0	1378	23	0
78	A3	1065	0	997	23	0
79	T9	1066	0	1023	16	0
80	TE	413	0	418	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	T7	1187	0	1137	23	0
82	1	50	0	44	1	0
82	2B	53	0	50	0	0
82	3	44	0	32	0	0
82	3B	78	0	103	5	0
82	3C	65	0	74	4	0
82	3G	66	0	79	2	0
82	3H	128	0	144	3	0
82	3I	108	0	104	2	0
82	3b	68	0	80	3	0
82	3c	120	0	128	2	0
82	3i	71	0	86	3	0
82	5	186	0	272	14	0
82	A1	53	0	50	0	0
82	AL	53	0	50	3	0
82	AM	62	0	68	7	0
82	AN	53	0	50	3	0
82	B4	40	0	20	1	0
82	B8	45	0	34	1	0
82	BM	86	0	119	9	0
82	C4	98	0	149	6	0
82	P2	82	0	111	3	0
82	R	84	0	115	3	0
82	T1	55	0	54	3	0
82	T7	48	0	40	1	0
82	TD	66	0	76	2	0
83	1	36	0	46	0	0
83	3	31	0	36	0	0
83	3C	119	0	166	6	0
83	3E	78	0	110	8	0
83	3F	22	0	18	0	0
83	3I	78	0	107	0	0
83	3J	37	0	48	4	0
83	3b	30	0	34	1	0
83	3c	69	0	86	2	0
83	3e	50	0	77	2	0
83	3g	33	0	40	2	0
83	3j	36	0	46	1	0
83	5	147	0	228	10	0
83	6	93	0	140	6	0
83	AM	30	0	34	2	0
83	AN	36	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	B2	48	0	73	7	0
83	B6	52	0	81	3	0
83	C4	32	0	38	1	0
83	J1	40	0	54	1	0
83	P1	40	0	54	0	0
83	T1	26	0	26	0	0
83	TC	42	0	61	4	0
83	X1	49	0	75	2	0
84	3C	86	0	60	2	0
84	3c	86	0	60	7	0
85	3C	26	0	35	4	0
85	3H	29	0	33	0	0
85	5B	63	0	90	7	0
86	3D	43	0	30	0	0
86	3d	43	0	30	1	0
87	3E	4	0	0	0	0
87	FX	4	0	0	0	0
87	S1	4	0	0	0	0
87	V2	4	0	0	1	0
88	3E	34	0	42	0	0
88	3d	47	0	68	3	0
88	4	83	0	114	2	0
88	5	72	0	92	2	0
88	5B	24	0	22	0	0
88	A3	45	0	64	4	0
88	AN	80	0	111	5	0
88	B8	36	0	46	3	0
88	C4	51	0	82	3	0
88	P1	47	0	71	4	0
88	S8	41	0	59	1	0
88	T4	25	0	24	3	0
88	T8	39	0	55	0	0
88	TA	26	0	26	0	0
89	3F	1	0	0	0	0
89	A9	1	0	0	0	0
89	S6	1	0	0	0	0
90	A9	48	0	26	1	0
91	AB	34	0	40	4	0
92	B8	27	0	12	1	0
93	S1	16	0	0	2	0
93	S7	8	0	0	1	0
93	S8	16	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	V1	8	0	0	0	0
94	V1	31	0	19	1	0
All	All	153366	0	150757	1931	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 6.

All (1931) 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)
32:AM:16:ARG:N	32:AM:22:SER:HG	1.46	1.14
7:3b:418:TYR:HD2	7:3b:455:ILE:HD13	1.39	0.87
53:S4:98:GLN:HG3	53:S4:99:ILE:HD12	1.58	0.85
10:3E:202:CYS:CB	10:3E:216:CYS:SG	2.64	0.84
12:3g:80:LEU:HD12	12:3g:84:ASP:HB2	1.60	0.83
19:4:394:ASN:HD21	34:B8:58:ASP:HA	1.42	0.83
72:P1:200:ASP:HA	72:P1:203:LYS:HE3	1.59	0.82
10:3E:202:CYS:HB3	10:3E:216:CYS:SG	2.20	0.81
7:3B:418:TYR:HD2	7:3B:455:ILE:HD13	1.46	0.80
56:S8:142:CYS:HB3	93:S8:302:SF4:S3	2.20	0.80
28:A9:102:ASN:HD22	28:A9:105:ASP:HB2	1.47	0.79
1:1:217:ALA:HB2	2:1B:21:ARG:HA	1.65	0.78
1:1:216:ARG:HD2	2:1B:17:ALA:HB1	1.66	0.78
12:3g:267:ALA:HB3	12:3g:289:LYS:HE3	1.64	0.78
11:3f:70:GLU:HA	11:3f:73:VAL:HG22	1.64	0.77
82:BM:301:CDL:H802	82:BM:301:CDL:H751	1.67	0.77
3:2:36:ASN:ND2	78:A3:28:ASP:OD2	2.18	0.76
8:3c:207:TRP:HE1	84:3c:503:HEM:HBA2	1.48	0.76
71:T3:226:ASN:HB3	71:T3:229:GLU:HG2	1.69	0.75
81:T7:74:TYR:O	81:T7:78:PHE:HB2	1.86	0.75
19:4:169:LEU:HD21	69:T8:84:PHE:HB2	1.69	0.75
8:3C:266:GLY:O	18:3m:14:ARG:NH2	2.20	0.74
11:3F:25:LEU:HD23	11:3F:73:VAL:HG21	1.70	0.74
35:BL:83:ILE:HD12	48:T5:150:VAL:HG21	1.69	0.74
11:3f:22:GLU:O	11:3f:26:GLN:NE2	2.21	0.74
12:3G:315:PRO:HD2	12:3G:318:LEU:HD12	1.69	0.74
28:A9:54:MET:HE1	28:A9:201:VAL:HG21	1.68	0.74
26:A6:114:GLU:HG3	52:S3:154:ARG:HG2	1.69	0.73
12:3g:6:LYS:HE2	12:3g:8:LEU:HD21	1.68	0.73
83:B6:201:PC1:H2B1	83:B6:201:PC1:H381	1.68	0.73
88:4:601:3PE:H2E1	49:R:64:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A5:77:LYS:HE3	25:A5:135:ILE:HG21	1.71	0.73
10:3E:28:SER:O	10:3E:32:GLN:NE2	2.22	0.72
50:S1:118:MET:HE2	50:S1:122:LEU:HG	1.72	0.72
37:C1:137:GLU:OE1	37:C1:154:LYS:NZ	2.23	0.72
71:T3:39:TYR:HB3	71:T3:52:MET:HE1	1.70	0.72
19:4:258:PRO:HG3	19:4:266:LEU:HD22	1.71	0.72
40:TD:60:ASP:O	40:TD:64:GLN:NE2	2.23	0.71
49:R:15:LYS:HD3	49:R:17:LYS:H	1.55	0.71
8:3c:278:PRO:HG3	8:3c:286:MET:HG3	1.73	0.71
47:T6:124:ASN:OD1	69:T8:96:ARG:NH1	2.23	0.71
62:V2:121:HIS:HD2	62:V2:123:GLN:HE21	1.36	0.71
6:3A:246:PRO:HG2	6:3A:275:SER:HA	1.72	0.70
7:3B:397:MET:SD	7:3B:507:ASN:ND2	2.64	0.70
9:3D:103:LEU:O	9:3D:107:GLN:NE2	2.25	0.70
37:C1:93:VAL:HG12	37:C1:121:VAL:H	1.56	0.70
44:T1:282:VAL:HG11	44:T1:324:ALA:HB1	1.72	0.70
50:S1:70:LEU:O	53:S4:166:LYS:NZ	2.23	0.70
8:3C:278:PRO:HG3	8:3C:286:MET:HG3	1.74	0.70
19:4:169:LEU:HD23	69:T8:81:THR:HA	1.73	0.69
10:3e:98:ILE:HA	14:3i:73:THR:HG21	1.74	0.69
11:3f:11:LEU:O	11:3f:15:GLN:NE2	2.25	0.69
55:S7:46:PHE:HB3	55:S7:51:VAL:HB	1.75	0.69
62:V2:224:LEU:HD12	62:V2:230:LEU:HD21	1.73	0.69
72:P1:80:ASP:OD2	77:P2:74:ASN:ND2	2.26	0.69
83:B2:201:PC1:H3F2	82:P2:201:CDL:H561	1.74	0.68
32:AM:43:ARG:NH2	56:S8:54:ASP:OD2	2.26	0.68
3:2:257:ILE:HD13	3:2:262:ILE:HD12	1.74	0.68
6:3a:87:SER:HA	7:3b:423:LEU:HD22	1.76	0.68
51:S2:128:LEU:HD23	51:S2:154:ARG:HB2	1.76	0.68
51:S2:129:ASN:OD1	51:S2:383:LYS:NZ	2.26	0.68
72:P1:142:ILE:HD13	88:P1:402:3PE:H281	1.76	0.68
52:S3:88:TYR:O	52:S3:92:ASN:ND2	2.27	0.68
10:3E:74:PHE:O	13:3H:63:ARG:NH1	2.27	0.68
6:3A:88:GLN:NE2	7:3B:420:ASN:OD1	2.27	0.67
10:3E:155:ARG:HH22	10:3E:225:LYS:HE3	1.59	0.67
82:3c:505:CDL:H372	82:3c:505:CDL:H712	1.76	0.67
11:3F:24:VAL:HG12	11:3F:73:VAL:HG22	1.76	0.67
15:3J:18:LEU:HD22	83:3J:101:PC1:H242	1.76	0.67
51:S2:44:ILE:HB	51:S2:56:ASP:HB3	1.76	0.67
25:A5:174:ARG:HD3	53:S4:1:MET:HB3	1.75	0.67
26:A6:44:THR:O	26:A6:55:LYS:NZ	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3A:100:ARG:NH2	6:3A:357:ASP:OD1	2.28	0.67
7:3b:418:TYR:CD2	7:3b:455:ILE:HD13	2.26	0.67
21:5:683:ASN:HA	34:B8:112:ILE:HA	1.77	0.67
83:5:807:PC1:H3H1	88:P1:402:3PE:H2E2	1.77	0.67
15:3J:18:LEU:HB2	83:3J:101:PC1:H222	1.77	0.66
7:3b:143:ARG:NH1	7:3b:216:GLN:O	2.27	0.66
50:S1:276:PRO:HG3	50:S1:287:ILE:HG12	1.78	0.66
10:3E:229:VAL:H	10:3E:237:ASN:HD22	1.44	0.66
30:AC:112:ASP:OD1	30:AC:115:ARG:NH2	2.28	0.66
71:T3:41:LYS:O	71:T3:42:ARG:HD3	1.96	0.66
35:BL:80:ARG:NH2	48:T5:149:LEU:O	2.29	0.66
62:V2:144:GLU:O	62:V2:147:GLN:NE2	2.29	0.66
3:2:151:PHE:O	3:2:155:GLU:HG2	1.95	0.66
7:3B:349:SER:HB3	7:3B:352:HIS:HB2	1.77	0.66
16:3M:1:MET:HE3	8:3c:175:THR:HG21	1.78	0.66
7:3B:418:TYR:CD2	7:3B:455:ILE:HD13	2.29	0.66
10:3E:198:THR:OG1	10:3E:235:LEU:O	2.12	0.66
38:C2:174:PRO:HG2	38:C2:177:ARG:HG3	1.76	0.66
50:S1:75:ASN:OD1	50:S1:76:CYS:N	2.29	0.66
37:C1:139:VAL:HB	37:C1:157:MET:HG2	1.77	0.65
55:S7:95:SER:N	93:S7:201:SF4:S3	2.68	0.65
8:3c:269:ASN:O	8:3c:272:ARG:NH1	2.28	0.65
9:3d:54:ASN:ND2	9:3d:173:ASN:OD1	2.29	0.65
27:A7:266:HIS:NE2	56:S8:229:GLU:OE2	2.25	0.65
78:A3:28:ASP:OD1	78:A3:34:ASN:ND2	2.24	0.65
9:3d:273:PHE:O	9:3d:277:ALA:HB3	1.97	0.65
47:T6:99:ARG:NH1	65:C4:99:LYS:O	2.23	0.65
51:S2:329:LEU:HB2	51:S2:332:LEU:HD23	1.79	0.65
61:V1:120:GLU:O	61:V1:160:ARG:NH1	2.30	0.65
27:A7:22:LEU:HD12	27:A7:23:PRO:HD2	1.78	0.65
11:3f:78:ILE:HG22	11:3f:81:LEU:HD12	1.79	0.65
12:3g:222:ASN:ND2	12:3g:226:LYS:O	2.30	0.65
37:C1:220:TYR:OH	38:C2:27:ASP:OD2	2.13	0.65
8:3C:152:LEU:HD12	8:3C:299:LEU:HD13	1.78	0.65
9:3d:293:ARG:NH1	12:3g:304:ALA:O	2.30	0.65
24:A2:79:ASN:ND2	24:A2:82:GLU:OE1	2.30	0.65
61:V1:411:ASP:OD1	61:V1:444:ARG:NH2	2.30	0.65
61:V1:245:ASN:ND2	94:V1:501:FMN:O2	2.30	0.65
68:T4:201:HIS:O	68:T4:205:LEU:HB2	1.96	0.65
51:S2:73:ARG:HB3	51:S2:77:GLN:HB2	1.79	0.65
27:A7:31:ARG:NH2	56:S8:116:LEU:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:61:PHE:HB2	5:3:64:LEU:HD12	1.78	0.64
66:AN:175:LEU:HD21	88:AN:301:3PE:H3B1	1.80	0.64
5:3:76:THR:HA	5:3:79:PHE:HD2	1.62	0.64
3:2:276:LEU:O	3:2:337:LYS:NZ	2.31	0.64
15:3J:7:TYR:OH	12:3g:194:ARG:NH1	2.31	0.64
4:2B:76:ILE:HG22	4:2B:78:PRO:HD2	1.80	0.64
1:1:108:SER:HA	1:1:257:MET:HE1	1.80	0.64
32:AM:16:ARG:N	32:AM:22:SER:OG	2.25	0.64
8:3C:366:ALA:HB1	83:3C:604:PC1:H2B2	1.79	0.64
3:2:227:ASN:HB3	47:T6:37:GLU:HB3	1.80	0.64
1:1:45:LYS:HB3	45:A1:16:THR:HG22	1.79	0.64
82:3B:701:CDL:H571	8:3c:1:MET:HE2	1.79	0.64
8:3C:272:ARG:NH2	9:3D:39:GLY:O	2.31	0.64
26:A6:63:PHE:CZ	26:A6:67:ILE:HD11	2.33	0.64
3:2:50:ILE:HG13	3:2:51:ILE:HD12	1.79	0.64
88:3d:402:3PE:H332	10:3e:109:LEU:HD11	1.80	0.64
11:3f:76:GLN:O	11:3f:80:GLN:HG3	1.97	0.64
12:3g:84:ASP:HA	12:3g:115:MET:HE3	1.79	0.64
12:3G:174:ARG:NH1	12:3G:175:TRP:O	2.30	0.63
19:4:435:GLU:HG3	35:BL:114:HIS:CD2	2.33	0.63
8:3C:61:MET:HG3	9:3d:123:GLN:HB2	1.80	0.63
9:3D:273:PHE:O	9:3D:277:ALA:HB3	1.98	0.63
21:5:661:LEU:HD11	83:5:802:PC1:H3C2	1.80	0.63
8:3C:353:LEU:HD21	82:3H:202:CDL:H132	1.80	0.63
9:3D:205:MET:HG3	11:3F:59:MET:HE3	1.80	0.63
83:B6:201:PC1:H2I1	82:BM:301:CDL:H361	1.79	0.63
27:A7:215:MET:HB3	27:A7:271:LEU:HB3	1.81	0.63
1:1:64:ARG:NH1	82:AL:301:CDL:OA3	2.32	0.63
8:3c:38:THR:HG21	84:3c:503:HEM:HAB	1.80	0.63
61:V1:121:SER:HB2	61:V1:205:TYR:HD1	1.64	0.63
68:T4:106:GLU:O	68:T4:169:GLN:NE2	2.31	0.63
6:3A:80:THR:OG1	6:3A:259:HIS:ND1	2.25	0.62
43:T2:229:ASN:O	43:T2:258:ASN:ND2	2.32	0.62
73:B3:18:HIS:O	73:B3:22:GLU:HG2	1.99	0.62
1:1:160:MET:HA	1:1:163:ILE:HG22	1.79	0.62
38:C2:36:ASP:OD1	39:C3:23:ARG:NH1	2.32	0.62
6:3a:212:TYR:HH	6:3a:358:SER:HG	1.47	0.62
21:5:181:LEU:HD13	21:5:294:ILE:HG21	1.82	0.62
23:6:47:TYR:OH	82:AN:304:CDL:OA4	2.17	0.62
12:3G:291:GLU:HA	12:3G:294:GLN:HG2	1.82	0.62
6:3a:116:THR:O	6:3a:175:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A9:280:SER:HB3	28:A9:346:ILE:HD12	1.81	0.62
66:AN:97:ASN:O	76:TC:19:ARG:NH2	2.32	0.62
19:4:419:GLY:HA3	82:BM:301:CDL:H392	1.82	0.62
73:B3:32:LEU:HD21	77:P2:180:LYS:HG3	1.79	0.62
24:A2:21:GLN:NE2	50:S1:655:PRO:O	2.32	0.62
37:C1:210:ARG:NH2	37:C1:252:GLU:O	2.33	0.62
75:S5:35:MET:HE1	76:TC:76:VAL:HG21	1.80	0.62
21:5:181:LEU:HA	21:5:294:ILE:HD13	1.81	0.62
22:5B:49:MET:HA	22:5B:53:LEU:HD12	1.82	0.61
44:T1:178:PHE:HE2	44:T1:180:TYR:HB3	1.64	0.61
8:3C:42:ILE:HG13	8:3C:91:LEU:HD21	1.82	0.61
10:3E:48:PRO:HB3	10:3E:67:LYS:HD2	1.82	0.61
7:3b:358:LEU:HD23	13:3h:32:LYS:HG3	1.82	0.61
14:3i:93:ASN:OD1	14:3i:96:ARG:NH1	2.33	0.61
32:AM:48:ARG:NH2	82:AM:202:CDL:OA9	2.34	0.61
7:3b:337:THR:HG22	7:3b:341:LEU:HD12	1.81	0.61
9:3d:114:ILE:HB	9:3d:134:ARG:HG2	1.82	0.61
5:3:76:THR:HA	5:3:79:PHE:CD2	2.35	0.61
56:S8:64:ARG:HH22	74:TA:40:PHE:HB2	1.64	0.61
34:B8:65:VAL:HG13	34:B8:66:ILE:HG13	1.83	0.61
83:6:302:PC1:H2D1	83:TC:101:PC1:H271	1.82	0.61
25:A5:146:GLU:HA	25:A5:149:LYS:HE2	1.82	0.61
41:J1:276:LYS:HG2	41:J1:289:LEU:HD11	1.83	0.61
79:T9:66:LEU:O	79:T9:69:LYS:HB3	2.00	0.61
80:TE:40:ASN:OD1	80:TE:44:LYS:NZ	2.34	0.61
10:3E:214:TYR:HB3	10:3E:223:TYR:HB2	1.82	0.61
11:3f:11:LEU:HB3	11:3f:15:GLN:HE22	1.65	0.61
43:T2:228:LEU:HD11	43:T2:282:LEU:HD22	1.81	0.61
6:3a:417:LEU:O	6:3a:421:VAL:HG23	2.01	0.61
28:A9:25:ARG:NH2	28:A9:153:ASN:O	2.26	0.61
1:1:154:ILE:HG13	5:3:57:ILE:HG21	1.82	0.60
88:3d:402:3PE:H361	14:3i:78:PHE:HA	1.82	0.60
19:4:363:PHE:HB2	19:4:425:SER:HB3	1.83	0.60
23:6:24:ILE:O	23:6:28:THR:OG1	2.18	0.60
34:B8:157:LYS:HA	34:B8:161:ARG:HD2	1.83	0.60
51:S2:87:TYR:CG	55:S7:31:CYS:HB3	2.34	0.60
44:T1:178:PHE:HB3	44:T1:196:SER:HB3	1.83	0.60
61:V1:312:TRP:NE1	61:V1:334:ASP:OD1	2.31	0.60
78:A3:19:ARG:HH12	78:A3:21:VAL:HA	1.66	0.60
82:3C:603:CDL:H111	13:3H:96:ASN:HB3	1.83	0.60
37:C1:103:THR:HG22	37:C1:115:VAL:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:J1:153:ARG:NH2	42:FX:55:GLU:OE1	2.35	0.60
50:S1:445:GLY:HA3	50:S1:450:VAL:HG21	1.83	0.60
55:S7:153:LYS:HD2	55:S7:162:TYR:HB2	1.83	0.60
71:T3:40:TYR:O	71:T3:101:TYR:OH	2.20	0.60
22:5B:38:ILE:O	22:5B:42:ILE:HG12	2.02	0.60
39:C3:182:ILE:HD11	39:C3:194:ILE:HD12	1.82	0.60
44:T1:28:ASP:OD1	44:T1:29:LEU:N	2.35	0.60
12:3g:176:THR:HG22	12:3g:178:LEU:H	1.67	0.60
23:6:225:LYS:HE3	39:C3:275:LEU:HD12	1.83	0.60
54:S6:72:ILE:HG12	54:S6:119:GLY:HA3	1.84	0.60
37:C1:179:ASN:HB3	37:C1:180:PRO:HD3	1.84	0.60
7:3b:473:ASP:OD1	10:3e:89:ARG:NH1	2.35	0.60
31:AL:2:GLY:N	82:AL:301:CDL:OA4	2.35	0.60
50:S1:387:MET:HE3	50:S1:474:MET:HE2	1.84	0.60
79:T9:122:GLN:NE2	79:T9:126:ASP:OD1	2.34	0.60
19:4:115:ILE:HD12	19:4:120:LEU:HD11	1.84	0.59
21:5:497:VAL:HG21	21:5:595:LEU:HD21	1.84	0.59
50:S1:218:GLU:OE2	50:S1:709:LYS:NZ	2.35	0.59
72:P1:94:PRO:O	72:P1:163:ARG:NH2	2.35	0.59
83:3g:401:PC1:H251	83:3g:401:PC1:H341	1.84	0.59
71:T3:256:SER:HA	71:T3:260:VAL:HB	1.84	0.59
74:TA:112:ASN:O	74:TA:116:GLN:NE2	2.32	0.59
6:3a:458:ASN:OD1	6:3a:478:ARG:NH1	2.35	0.59
19:4:432:GLY:HA3	35:BL:115:PHE:CE1	2.38	0.59
21:5:750:LEU:HD23	68:T4:150:VAL:HG13	1.84	0.59
23:6:39:GLN:OE1	76:TC:28:TYR:OH	2.19	0.59
28:A9:127:LEU:HG	28:A9:308:ASN:HD21	1.66	0.59
34:B8:170:ASP:OD2	34:B8:174:ARG:NH1	2.36	0.59
1:1:279:ASN:OD1	81:T7:103:ASN:ND2	2.34	0.59
61:V1:37:ASP:HA	61:V1:40:ARG:HD3	1.83	0.59
64:BM:128:THR:HG22	64:BM:130:ASP:H	1.67	0.59
88:T4:301:3PE:H232	82:P2:201:CDL:H802	1.84	0.59
8:3C:55:SER:HB3	10:3E:117:ARG:HH21	1.67	0.59
52:S3:94:MET:HB3	52:S3:115:LEU:HB2	1.83	0.59
20:4L:61:PHE:HB2	23:6:177:TYR:OH	2.03	0.59
31:AL:131:LEU:O	31:AL:134:THR:OG1	2.18	0.59
32:AM:111:LEU:HD13	75:S5:71:LEU:HD21	1.85	0.59
48:T5:122:ARG:NH2	60:TB:73:GLY:O	2.34	0.59
66:AN:14:VAL:HG13	66:AN:19:TYR:HB3	1.84	0.59
1:1:155:ARG:HD3	1:1:221:LEU:HD12	1.85	0.59
8:3C:219:GLU:OE2	13:3H:49:HIS:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:S6:108:LYS:HG2	62:V2:32:LYS:HG3	1.85	0.59
83:TC:101:PC1:H121	83:TC:101:PC1:H2	1.84	0.59
82:5:805:CDL:H721	82:R:201:CDL:H171	1.85	0.59
9:3d:246:VAL:HG23	9:3d:250:ARG:HD2	1.85	0.59
23:6:12:ASN:ND2	41:J1:308:ASP:OD2	2.36	0.59
63:B6:67:ARG:NH2	64:BM:121:ASN:OD1	2.33	0.59
9:3D:46:GLU:HB3	9:3D:50:HIS:HB3	1.85	0.58
63:B6:72:GLY:HA2	63:B6:75:ILE:HD12	1.84	0.58
68:T4:131:TYR:HB2	88:T4:301:3PE:H221	1.85	0.58
6:3A:423:ASN:HD22	6:3A:431:GLN:H	1.50	0.58
8:3c:88:VAL:HG22	84:3c:502:HEM:HBC2	1.84	0.58
28:A9:28:GLN:O	28:A9:157:ARG:NH1	2.36	0.58
38:C2:7:MET:HG2	69:T8:50:ILE:HG13	1.86	0.58
48:T5:59:GLN:HB2	63:B6:126:ALA:HB3	1.84	0.58
58:TX:23:SER:N	58:TX:69:SER:O	2.36	0.58
13:3h:23:ARG:HG2	13:3h:29:ILE:HG12	1.84	0.58
50:S1:227:CYS:CB	93:S1:802:SF4:S2	2.91	0.58
60:TB:33:ASP:OD2	60:TB:59:GLN:NE2	2.36	0.58
1:1:52:ARG:HE	56:S8:102:GLU:HB3	1.69	0.58
13:3h:113:ILE:HG22	13:3h:117:MET:HE2	1.86	0.58
23:6:242:THR:HG23	51:S2:214:LYS:HG3	1.85	0.58
44:T1:87:VAL:HG13	44:T1:95:MET:HG3	1.84	0.58
59:A8:134:ASP:OD2	74:TA:119:ARG:NH2	2.36	0.58
82:AM:202:CDL:H531	82:AM:202:CDL:H122	1.86	0.58
71:T3:75:LEU:HD12	71:T3:87:VAL:HG13	1.84	0.58
77:P2:39:LEU:HD11	77:P2:88:PHE:HB2	1.85	0.58
82:3b:602:CDL:H342	83:3j:101:PC1:H332	1.86	0.58
32:AM:45:ILE:HD13	74:TA:74:GLU:HG2	1.86	0.58
6:3A:458:ASN:OD1	6:3A:478:ARG:NH1	2.37	0.58
78:A3:68:GLY:O	78:A3:72:LEU:HG	2.04	0.58
15:3J:8:LYS:O	15:3J:12:GLU:HG3	2.04	0.58
15:3J:8:LYS:NZ	12:3g:8:LEU:HD22	2.19	0.58
19:4:18:PHE:HB2	19:4:160:TYR:CE2	2.39	0.58
21:5:676:ASP:OD2	35:BL:87:THR:OG1	2.22	0.58
40:TD:42:ARG:NH1	45:A1:43:ASP:OD2	2.36	0.58
44:T1:113:SER:OG	44:T1:117:ASP:OD2	2.21	0.58
6:3A:204:ASN:OD1	6:3A:364:ARG:NH1	2.36	0.58
21:5:247:ASP:OD2	21:5:304:ASN:ND2	2.35	0.58
41:J1:153:ARG:NH1	41:J1:179:SER:O	2.36	0.58
44:T1:92:HIS:HE2	82:T1:602:CDL:HA32	1.69	0.58
61:V1:40:ARG:NH2	62:V2:223:THR:OG1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C3:279:GLU:OE1	52:S3:44:SER:OG	2.22	0.58
7:3b:363:ILE:HB	7:3b:382:TYR:HB3	1.86	0.57
9:3d:190:MET:HE1	11:3f:59:MET:HE3	1.86	0.57
32:AM:49:LYS:NZ	82:AM:202:CDL:OB3	2.36	0.57
10:3E:247:ASP:HB3	10:3E:251:LEU:H	1.70	0.57
28:A9:279:LEU:HB3	28:A9:346:ILE:HD11	1.86	0.57
59:A8:208:PHE:O	59:A8:211:PHE:HB3	2.04	0.57
34:B8:121:LEU:HD22	34:B8:164:ILE:HG23	1.86	0.57
44:T1:370:GLN:O	44:T1:433:ARG:NH1	2.37	0.57
58:TX:24:ARG:HE	58:TX:25:VAL:H	1.51	0.57
81:T7:124:ASP:OD1	81:T7:125:LEU:N	2.37	0.57
10:3E:237:ASN:OD1	10:3E:238:LEU:N	2.36	0.57
21:5:207:ILE:HD11	21:5:293:MET:HE1	1.86	0.57
25:A5:181:ARG:NH1	50:S1:48:TYR:OH	2.37	0.57
52:S3:155:LYS:NZ	52:S3:159:ASP:O	2.37	0.57
11:3f:36:GLU:HG3	11:3f:40:LYS:NZ	2.19	0.57
6:3a:265:LEU:O	6:3a:268:THR:OG1	2.21	0.57
34:B8:112:ILE:O	34:B8:174:ARG:NH2	2.38	0.57
7:3B:276:THR:HB	41:J1:45:ARG:HG2	1.86	0.57
8:3C:235:ILE:HG23	83:3E:302:PC1:H2H1	1.86	0.57
12:3G:36:THR:HG22	12:3G:40:LYS:HE3	1.87	0.57
33:B7:67:LYS:NZ	68:T4:95:ASP:OD1	2.37	0.57
70:B2:24:GLN:HB2	70:B2:33:THR:HB	1.87	0.57
12:3g:27:PRO:HA	12:3g:204:ASN:HA	1.85	0.57
82:5:805:CDL:H431	48:T5:134:LEU:HD11	1.87	0.57
23:6:79:GLU:HB2	32:AM:147:MET:HE2	1.86	0.57
35:BL:78:VAL:HG21	35:BL:102:ILE:HD11	1.85	0.57
39:C3:266:GLU:HA	39:C3:269:VAL:HG22	1.87	0.57
61:V1:30:ARG:NH2	61:V1:292:GLU:OE2	2.37	0.57
62:V2:48:ASN:ND2	62:V2:78:GLN:OE1	2.37	0.57
31:AL:76:ARG:NH2	31:AL:107:ASP:OD1	2.37	0.57
50:S1:349:ILE:HD11	50:S1:591:VAL:HG23	1.86	0.57
1:1:180:SER:HB3	1:1:185:VAL:HG11	1.85	0.57
23:6:126:LEU:HD22	82:AN:304:CDL:H322	1.87	0.57
28:A9:297:ILE:HG22	28:A9:307:PHE:HZ	1.69	0.57
82:C4:401:CDL:H761	82:C4:401:CDL:H572	1.87	0.57
43:T2:248:LEU:HD12	43:T2:284:LEU:HD21	1.87	0.56
51:S2:153:GLU:HG3	51:S2:202:THR:HG21	1.86	0.56
1:1:115:SER:OG	1:1:117:PHE:O	2.22	0.56
26:A6:32:ARG:HH11	28:A9:361:GLU:HG3	1.69	0.56
88:3d:402:3PE:H362	14:3i:81:CYS:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3g:83:GLU:OE1	12:3g:145:ARG:NE	2.35	0.56
64:BM:141:LYS:O	64:BM:145:GLU:HG3	2.06	0.56
66:AN:8:LYS:NZ	66:AN:182:SER:O	2.37	0.56
68:T4:188:PHE:HZ	68:T4:205:LEU:HD11	1.71	0.56
71:T3:33:LEU:HD13	72:P1:97:HIS:HB2	1.85	0.56
13:3h:93:TYR:HA	13:3h:97:ILE:HB	1.87	0.56
26:A6:82:ALA:O	26:A6:86:MET:HG3	2.06	0.56
8:3c:79:ASP:OD1	9:3d:253:LYS:NZ	2.38	0.56
19:4:290:LEU:HD11	19:4:342:MET:HE1	1.86	0.56
83:5:807:PC1:H3B2	72:P1:137:ALA:HB1	1.86	0.56
51:S2:67:GLU:OE2	51:S2:402:LYS:NZ	2.38	0.56
21:5:241:GLY:O	35:BL:72:LYS:NZ	2.39	0.56
25:A5:176:TYR:HA	53:S4:2:LEU:HB2	1.88	0.56
32:AM:54:LEU:HD12	56:S8:76:TRP:HZ3	1.71	0.56
71:T3:142:ILE:HG12	71:T3:146:LEU:HD12	1.87	0.56
16:3M:9:SER:HB2	8:3c:174:ASN:HB3	1.87	0.56
12:3g:40:LYS:O	12:3g:43:GLN:HG3	2.06	0.56
19:4:142:TYR:OH	37:C1:197:ASP:OD1	2.23	0.56
44:T1:185:LYS:HE3	44:T1:187:ILE:HD11	1.87	0.56
32:AM:143:ARG:HD3	45:A1:92:LEU:HB3	1.88	0.56
50:S1:141:GLN:HG2	51:S2:358:ILE:HG23	1.88	0.56
3:2:138:ILE:HG13	3:2:139:PRO:HD3	1.88	0.56
7:3b:265:LYS:HA	7:3b:265:LYS:HE3	1.88	0.56
9:3d:46:GLU:HB3	9:3d:50:HIS:HB3	1.88	0.56
9:3d:286:ARG:NH2	10:3e:75:ASP:OD2	2.36	0.56
14:3i:27:VAL:O	14:3i:29:LYS:NZ	2.36	0.56
21:5:337:PHE:HD2	88:B8:601:3PE:H221	1.69	0.56
50:S1:599:GLN:HE22	50:S1:637:ARG:NH2	2.03	0.56
50:S1:606:PRO:HB2	50:S1:610:ALA:HB3	1.88	0.56
3:2:134:ILE:O	3:2:138:ILE:HG12	2.06	0.55
7:3B:200:LEU:HD21	7:3B:305:GLY:HA3	1.88	0.55
82:3B:701:CDL:H832	8:3C:20:PHE:HE1	1.72	0.55
33:B7:70:LYS:NZ	68:T4:95:ASP:OD1	2.39	0.55
68:T4:75:GLU:HG2	68:T4:78:GLN:H	1.70	0.55
11:3f:30:PRO:HA	11:3f:33:LEU:HG	1.87	0.55
21:5:702:ILE:HG12	72:P1:136:PHE:HE1	1.70	0.55
23:6:38:ILE:HD11	83:6:301:PC1:H351	1.87	0.55
27:A7:185:ALA:HA	27:A7:191:TRP:HE3	1.71	0.55
31:AL:87:MET:HG2	55:S7:138:LEU:HD11	1.88	0.55
39:C3:154:SER:HB3	39:C3:173:GLU:HG2	1.88	0.55
43:T2:39:ASN:ND2	43:T2:78:ASN:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:T2:62:GLU:HG3	50:S1:449:LYS:HD3	1.86	0.55
53:S4:13:TYR:CE2	53:S4:15:GLU:HB3	2.42	0.55
4:2B:77:PRO:HA	4:2B:82:PHE:CG	2.41	0.55
7:3B:200:LEU:HD22	7:3B:380:TYR:HD1	1.71	0.55
8:3C:352:ASN:HB3	8:3C:355:HIS:HB3	1.87	0.55
6:3a:246:PRO:HG2	6:3a:275:SER:HB2	1.88	0.55
7:3b:224:ASN:HA	7:3b:227:ASN:HB2	1.87	0.55
9:3d:78:ALA:HB1	9:3d:112:PHE:HZ	1.72	0.55
56:S8:72:PHE:HE1	78:A3:47:LYS:HE2	1.71	0.55
5:3:44:GLU:HG2	51:S2:29:ASN:HB2	1.87	0.55
6:3A:113:ILE:HG12	6:3A:175:ARG:HD2	1.88	0.55
19:4:338:THR:HG23	19:4:367:HIS:HE2	1.70	0.55
21:5:312:TRP:CZ2	21:5:405:LYS:HG3	2.42	0.55
50:S1:164:LYS:O	50:S1:172:THR:OG1	2.22	0.55
77:P2:41:GLN:HB3	77:P2:160:LYS:HB2	1.89	0.55
10:3E:52:VAL:HG22	14:3I:27:VAL:HG11	1.88	0.55
32:AM:67:LYS:O	32:AM:71:ILE:HD12	2.07	0.55
74:TA:105:ASP:OD1	78:A3:88:TYR:OH	2.20	0.55
7:3B:473:ASP:OD1	10:3E:89:ARG:NH1	2.39	0.55
8:3c:344:PRO:HG3	8:3c:408:LEU:HD12	1.89	0.55
35:BL:97:LYS:HD2	48:T5:61:ALA:HA	1.88	0.55
1:1:140:THR:HG1	1:1:244:TYR:HH	1.55	0.55
10:3e:104:LEU:HD11	83:3e:301:PC1:H321	1.89	0.55
26:A6:115:LEU:HD12	91:AB:201:ZMP:H4	1.88	0.55
34:B8:145:GLY:HA2	35:BL:108:PRO:HG3	1.88	0.55
57:B9:76:MET:HE3	57:B9:89:TYR:HB3	1.87	0.55
57:B9:145:ARG:NH2	60:TB:55:ASN:OD1	2.36	0.55
66:AN:157:VAL:HG12	66:AN:158:ASN:H	1.72	0.55
1:1:110:TRP:HB3	2:1B:3:TYR:HB3	1.89	0.55
8:3c:107:ASN:HA	8:3c:112:GLN:HE21	1.71	0.55
41:J1:244:ALA:HB2	83:J1:400:PC1:H232	1.88	0.55
83:AM:201:PC1:H31	56:S8:90:TYR:HD1	1.72	0.55
40:TD:72:LYS:HD2	40:TD:72:LYS:O	2.07	0.55
51:S2:30:PHE:HB3	51:S2:43:LEU:HB3	1.88	0.55
3:2:263:ALA:HB2	3:2:349:ILE:HD11	1.88	0.55
23:6:138:PHE:HZ	75:S5:48:HIS:HB3	1.72	0.55
37:C1:60:SER:OG	37:C1:75:TRP:O	2.24	0.55
46:X1:22:PRO:HG3	65:C4:54:MET:HG2	1.89	0.55
1:1:280:ASP:HA	81:T7:3:ASN:HB2	1.89	0.54
19:4:91:LEU:HD21	79:T9:1:MET:HB2	1.88	0.54
39:C3:93:ARG:NH2	39:C3:95:GLU:OE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S7:24:PRO:HB3	55:S7:62:LEU:HD23	1.87	0.54
67:B4:42:LEU:HD13	67:B4:67:VAL:HG11	1.88	0.54
88:T4:301:3PE:H2	82:P2:201:CDL:H731	1.89	0.54
8:3C:112:GLN:NE2	8:3C:206:ASP:OD2	2.39	0.54
12:3g:78:ARG:HH22	13:3h:95:ARG:HH22	1.55	0.54
82:5:805:CDL:H121	82:R:201:CDL:H362	1.90	0.54
67:B4:119:ASP:OD1	67:B4:120:ASN:N	2.37	0.54
11:3F:66:VAL:O	11:3F:70:GLU:HG2	2.07	0.54
8:3c:55:SER:HB3	10:3e:117:ARG:HH21	1.70	0.54
20:4L:7:PHE:O	20:4L:11:ILE:HG12	2.08	0.54
51:S2:125:THR:HB	51:S2:161:TYR:OH	2.08	0.54
58:TX:43:PRO:HB3	58:TX:76:GLU:HG3	1.89	0.54
83:3C:606:PC1:H261	88:AN:302:3PE:H242	1.89	0.54
10:3E:246:HIS:NE2	15:3J:55:VAL:O	2.30	0.54
8:3c:380:ASN:OD1	8:3c:381:ARG:N	2.40	0.54
20:4L:69:LEU:HD11	23:6:195:GLY:HA3	1.89	0.54
25:A5:89:LEU:HD11	25:A5:102:THR:HB	1.90	0.54
38:C2:162:GLU:OE2	60:TB:41:ARG:NH1	2.40	0.54
19:4:337:GLY:O	19:4:341:GLU:HG2	2.06	0.54
46:X1:148:ILE:HG22	46:X1:149:ARG:HG3	1.90	0.54
51:S2:211:THR:O	51:S2:277:TYR:OH	2.25	0.54
4:2B:34:LEU:HD12	4:2B:151:LEU:HB3	1.88	0.54
19:4:62:ILE:HD11	49:R:67:VAL:HG21	1.90	0.54
23:6:25:ASP:OD2	75:S5:64:ASN:ND2	2.41	0.54
27:A7:55:ASP:O	51:S2:343:ASN:ND2	2.40	0.54
39:C3:55:VAL:HG23	39:C3:58:LYS:HE2	1.89	0.54
47:T6:36:MET:O	47:T6:37:GLU:HG2	2.08	0.54
4:2B:10:ASN:ND2	65:C4:70:GLN:OE1	2.41	0.54
7:3b:344:SER:HB3	7:3b:353:LYS:HA	1.88	0.54
50:S1:142:ASP:OD1	51:S2:362:LYS:NZ	2.40	0.54
71:T3:203:HIS:ND1	71:T3:211:GLU:OE2	2.37	0.54
4:2B:58:SER:O	37:C1:52:TYR:OH	2.25	0.54
10:3e:70:ILE:HD11	12:3g:121:ARG:HD2	1.89	0.54
10:3e:74:PHE:O	13:3h:63:ARG:NH1	2.41	0.54
70:B2:77:MET:HG3	83:B2:201:PC1:H231	1.88	0.54
1:1:25:ASN:OD1	5:3:12:ASN:ND2	2.40	0.54
9:3D:286:ARG:HB3	13:3H:61:HIS:HB2	1.89	0.54
10:3E:221:SER:HB2	10:3E:233:PRO:HD2	1.90	0.54
83:3E:302:PC1:H371	83:3E:302:PC1:H3C2	1.90	0.54
12:3g:242:VAL:O	12:3g:246:ILE:HG12	2.07	0.54
19:4:10:SER:O	19:4:14:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:5:805:CDL:H441	82:BM:301:CDL:H531	1.90	0.54
41:J1:294:ILE:HG22	41:J1:308:ASP:HB2	1.89	0.54
7:3B:492:HIS:CD2	7:3B:494:ASN:HB3	2.43	0.54
6:3a:422:LYS:HD2	12:3g:327:GLN:HB3	1.89	0.54
21:5:711:LEU:HD22	82:5:803:CDL:H621	1.90	0.54
61:V1:280:SER:HA	61:V1:286:PRO:HB3	1.90	0.54
72:P1:152:LYS:HG2	72:P1:153:ILE:HG13	1.89	0.54
1:1:104:PHE:HD1	1:1:129:LEU:HD13	1.73	0.53
9:3D:274:LYS:O	9:3D:278:TYR:HB2	2.07	0.53
26:A6:17:GLN:HB3	26:A6:19:ASN:O	2.07	0.53
27:A7:251:ILE:HD12	27:A7:256:LEU:HD11	1.89	0.53
41:J1:29:LEU:HD12	41:J1:80:LEU:HD12	1.90	0.53
71:T3:203:HIS:HB2	71:T3:211:GLU:HG3	1.89	0.53
12:3g:100:GLU:OE2	12:3g:104:ARG:NH1	2.41	0.53
38:C2:46:HIS:HE2	38:C2:70:SER:HG	1.51	0.53
50:S1:510:GLY:O	50:S1:512:ASN:ND2	2.42	0.53
1:1:261:ILE:HA	1:1:266:GLY:HA2	1.90	0.53
1:1:283:ILE:HG22	1:1:284:LEU:HD12	1.89	0.53
21:5:268:VAL:O	21:5:272:THR:OG1	2.24	0.53
83:5:801:PC1:H152	83:5:801:PC1:H31	1.88	0.53
32:AM:50:ALA:HB2	56:S8:80:TYR:HB2	1.90	0.53
37:C1:74:VAL:HG22	37:C1:95:ILE:HD12	1.90	0.53
43:T2:179:GLN:O	50:S1:446:ASN:ND2	2.37	0.53
61:V1:443:PHE:HB3	61:V1:446:GLU:HB2	1.90	0.53
74:TA:106:ASP:HB3	81:T7:115:THR:CG2	2.37	0.53
8:3c:352:ASN:HB3	8:3c:355:HIS:HB3	1.90	0.53
21:5:274:SER:OG	21:5:645:SER:OG	2.26	0.53
31:AL:9:ASN:OD1	31:AL:10:GLN:N	2.42	0.53
88:B8:601:3PE:H3A1	88:B8:601:3PE:H282	1.91	0.53
43:T2:198:LEU:HD13	43:T2:212:LEU:HD23	1.91	0.53
44:T1:109:VAL:O	44:T1:112:SER:OG	2.25	0.53
50:S1:227:CYS:HB2	93:S1:802:SF4:S2	2.47	0.53
61:V1:368:ILE:HG13	61:V1:439:LEU:HB2	1.90	0.53
15:3j:43:MET:HE3	15:3j:48:PHE:HE2	1.73	0.53
21:5:480:THR:HG22	21:5:609:LEU:HD11	1.91	0.53
21:5:575:HIS:O	21:5:579:ILE:HG13	2.08	0.53
28:A9:292:ASP:OD1	28:A9:293:ILE:HD12	2.09	0.53
44:T1:178:PHE:CE2	44:T1:180:TYR:HB3	2.43	0.53
80:TE:28:VAL:O	80:TE:32:VAL:HG23	2.09	0.53
8:3C:136:LEU:HD11	8:3C:182:ALA:HA	1.90	0.53
30:AC:82:THR:HB	30:AC:85:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:TA:106:ASP:OD1	81:T7:116:ARG:NE	2.42	0.53
77:P2:33:ASP:OD1	77:P2:34:SER:N	2.41	0.53
8:3C:18:GLN:O	8:3C:22:VAL:HG22	2.08	0.53
21:5:419:MET:SD	21:5:430:HIS:NE2	2.82	0.53
44:T1:92:HIS:NE2	82:T1:602:CDL:HA32	2.23	0.53
44:T1:270:ALA:HB1	44:T1:362:LEU:HD13	1.90	0.53
48:T5:73:LEU:HD22	48:T5:78:LEU:HD12	1.91	0.53
61:V1:266:PHE:HB3	61:V1:292:GLU:HG3	1.89	0.53
77:P2:85:LYS:HB2	77:P2:98:ASP:HB2	1.90	0.53
7:3B:69:LEU:O	7:3B:72:GLY:N	2.36	0.53
9:3d:200:PRO:HA	9:3d:205:MET:SD	2.48	0.53
19:4:287:LYS:HD2	19:4:364:SER:HB2	1.91	0.53
50:S1:546:ASP:HB3	50:S1:569:GLU:HB2	1.90	0.53
62:V2:50:LYS:O	62:V2:53:GLU:HG3	2.09	0.53
71:T3:277:ARG:NH1	71:T3:282:ASP:OD2	2.42	0.53
8:3C:272:ARG:NH1	9:3D:203:ASP:OD2	2.41	0.53
6:3a:33:LYS:O	7:3b:465:ARG:NH1	2.42	0.53
41:J1:279:GLU:HA	41:J1:282:LYS:HD2	1.91	0.53
8:3C:61:MET:HE1	8:3C:266:GLY:HA3	1.91	0.53
12:3G:281:ASP:OD1	12:3G:281:ASP:N	2.41	0.53
13:3H:98:ARG:NE	82:3H:202:CDL:OA4	2.35	0.53
9:3d:75:GLN:O	9:3d:79:ARG:HG2	2.09	0.53
23:6:159:TYR:O	23:6:163:ASN:ND2	2.42	0.53
50:S1:599:GLN:HE22	50:S1:637:ARG:HH22	1.55	0.53
51:S2:369:LYS:HD2	52:S3:75:THR:HG21	1.91	0.53
53:S4:62:ASP:OD1	53:S4:64:SER:OG	2.23	0.53
1:1:43:GLU:HA	2:1B:18:ILE:HD13	1.91	0.52
8:3C:247:PHE:HB3	83:AN:303:PC1:H321	1.91	0.52
82:3b:602:CDL:HA21	83:3e:301:PC1:H2	1.90	0.52
32:AM:140:PHE:CG	75:S5:52:GLN:HG2	2.43	0.52
39:C3:11:GLU:OE2	46:X1:70:ARG:NH2	2.42	0.52
43:T2:72:LEU:HD21	43:T2:115:THR:HG21	1.91	0.52
49:R:69:VAL:HG23	49:R:101:PRO:HB3	1.91	0.52
51:S2:126:ARG:HG3	51:S2:130:HIS:HD2	1.74	0.52
61:V1:35:LEU:O	61:V1:40:ARG:NH1	2.36	0.52
75:S5:74:TYR:OH	75:S5:79:ASP:OD1	2.23	0.52
6:3A:105:GLU:OE2	6:3A:238:LYS:NZ	2.42	0.52
8:3c:85:GLU:OE1	9:3d:245:ARG:NH2	2.42	0.52
23:6:139:SER:O	76:TC:40:LYS:NZ	2.38	0.52
39:C3:130:ILE:HG21	39:C3:136:ILE:HD11	1.91	0.52
39:C3:131:GLY:O	39:C3:134:SER:OG	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:B9:167:GLU:OE2	69:T8:37:ARG:NH1	2.42	0.52
8:3c:28:HIS:HB3	8:3c:207:TRP:HH2	1.73	0.52
19:4:74:TYR:OH	67:B4:134:PHE:O	2.25	0.52
53:S4:1:MET:SD	53:S4:138:THR:OG1	2.67	0.52
61:V1:264:ALA:HA	61:V1:272:ALA:HB1	1.90	0.52
19:4:14:ILE:O	19:4:160:TYR:OH	2.22	0.52
19:4:24:LEU:HD22	19:4:59:GLY:HA3	1.91	0.52
21:5:338:LYS:HD3	21:5:414:TRP:HA	1.91	0.52
27:A7:77:TYR:HB2	52:S3:20:SER:HB3	1.89	0.52
39:C3:1:MET:HG3	39:C3:4:LEU:H	1.73	0.52
7:3B:507:ASN:HB3	7:3B:511:TYR:HD2	1.74	0.52
9:3D:220:TYR:HD2	9:3D:224:THR:HB	1.75	0.52
13:3H:116:ARG:HH21	66:AN:46:MET:HG2	1.74	0.52
44:T1:372:PRO:HG3	44:T1:433:ARG:HA	1.92	0.52
5:3:92:GLU:HG3	23:6:178:TYR:HB3	1.91	0.52
21:5:419:MET:HE3	21:5:481:LYS:HE2	1.92	0.52
33:B7:28:MET:HE3	33:B7:32:ALA:HB2	1.90	0.52
34:B8:81:LYS:HE2	82:B8:603:CDL:HA62	1.91	0.52
47:T6:115:TYR:OH	69:T8:103:ASP:OD1	2.22	0.52
69:T8:81:THR:O	69:T8:85:ALA:HB3	2.10	0.52
72:P1:162:VAL:HG21	72:P1:178:ILE:HG13	1.92	0.52
77:P2:78:HIS:HD2	77:P2:79:PRO:HD2	1.75	0.52
6:3A:358:SER:OG	6:3A:359:GLY:N	2.41	0.52
10:3E:155:ARG:HH12	10:3E:225:LYS:HG3	1.74	0.52
10:3e:88:ARG:NH2	13:3h:70:ILE:HG12	2.24	0.52
19:4:414:PHE:O	19:4:422:LYS:NZ	2.42	0.52
49:R:6:TRP:CE3	79:T9:60:PHE:HB2	2.44	0.52
3:2:99:TYR:CE2	3:2:139:PRO:HB2	2.45	0.52
6:3A:368:SER:OG	6:3A:370:ASP:OD1	2.22	0.52
9:3D:134:ARG:HH12	9:3D:141:TYR:H	1.58	0.52
12:3G:123:TYR:HA	12:3G:126:GLU:HB3	1.92	0.52
38:C2:107:LYS:HZ1	39:C3:110:LEU:HB3	1.75	0.52
43:T2:38:GLU:HB2	43:T2:263:THR:HG22	1.92	0.52
55:S7:58:ARG:HA	55:S7:85:LEU:HD13	1.92	0.52
8:3C:343:THR:O	12:3G:35:ARG:NH2	2.37	0.52
8:3c:338:ARG:HD3	12:3g:211:TYR:CE1	2.44	0.52
12:3g:123:TYR:HA	12:3g:126:GLU:HB3	1.92	0.52
14:3i:41:LYS:HG3	14:3i:42:ILE:HD12	1.91	0.52
44:T1:214:ASN:O	44:T1:250:GLN:NE2	2.42	0.52
69:T8:81:THR:O	69:T8:85:ALA:CB	2.58	0.52
4:2B:54:LYS:NZ	42:FX:84:GLY:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3C:375:TYR:O	8:3C:379:TYR:HB2	2.10	0.51
8:3c:418:PHE:HZ	12:3g:86:LEU:HD13	1.73	0.51
21:5:388:ILE:HG23	88:5:804:3PE:H362	1.90	0.51
22:5B:37:PHE:O	22:5B:41:SER:HB2	2.10	0.51
37:C1:104:ALA:N	37:C1:131:SER:OG	2.42	0.51
44:T1:269:LEU:HD22	44:T1:285:LEU:HD22	1.92	0.51
9:3D:169:PRO:O	9:3D:174:TYR:HB2	2.10	0.51
10:3E:157:LEU:N	10:3E:189:LYS:O	2.43	0.51
21:5:579:ILE:HA	21:5:696:PHE:HZ	1.75	0.51
24:A2:14:GLU:OE1	24:A2:64:ARG:NH1	2.44	0.51
49:R:6:TRP:HE1	79:T9:67:PRO:HG3	1.75	0.51
1:1:62:ARG:NH1	82:1:301:CDL:OB4	2.36	0.51
1:1:159:LEU:HD11	1:1:221:LEU:HB2	1.91	0.51
4:2B:30:ILE:HD13	82:C4:401:CDL:H631	1.92	0.51
8:3C:1:MET:O	8:3c:14:LYS:NZ	2.43	0.51
6:3a:451:VAL:HA	6:3a:454:VAL:HG12	1.93	0.51
8:3c:126:PHE:HE1	84:3c:502:HEM:HBC1	1.75	0.51
82:5:803:CDL:H601	82:5:803:CDL:H562	1.93	0.51
44:T1:18:ILE:HD12	44:T1:38:LEU:HD21	1.92	0.51
45:A1:65:LYS:HE2	45:A1:91:LEU:HD21	1.92	0.51
56:S8:93:TRP:CD1	56:S8:97:ILE:HD13	2.45	0.51
61:V1:406:ASP:HB2	61:V1:409:GLU:HG3	1.90	0.51
82:3G:401:CDL:H121	82:3G:401:CDL:H772	1.93	0.51
7:3b:157:VAL:HG11	7:3b:254:VAL:HG23	1.92	0.51
11:3f:36:GLU:HG3	11:3f:40:LYS:HZ2	1.74	0.51
21:5:737:LEU:HD23	68:T4:130:THR:HG23	1.93	0.51
39:C3:74:VAL:HG22	39:C3:92:LEU:HD13	1.93	0.51
42:FX:57:ILE:HD12	42:FX:72:ASN:HB3	1.93	0.51
70:B2:15:LYS:NZ	77:P2:143:ILE:O	2.44	0.51
72:P1:173:ILE:HD13	72:P1:194:LEU:HD21	1.91	0.51
7:3b:224:ASN:O	7:3b:224:ASN:ND2	2.43	0.51
8:3c:415:PHE:HD2	12:3g:39:PHE:HB3	1.75	0.51
26:A6:99:TYR:HB2	91:AB:201:ZMP:H14	1.90	0.51
39:C3:187:PRO:HG2	39:C3:189:GLN:HE22	1.76	0.51
46:X1:92:TYR:O	46:X1:96:ILE:HG12	2.11	0.51
59:A8:140:THR:HG22	59:A8:142:LEU:H	1.76	0.51
6:3A:342:TYR:HB2	6:3A:345:PHE:HD2	1.74	0.51
8:3C:58:PRO:HB2	8:3C:179:ILE:HG12	1.93	0.51
25:A5:177:LEU:HB2	53:S4:2:LEU:HD13	1.93	0.51
35:BL:59:LYS:NZ	35:BL:135:GLN:OE1	2.44	0.51
37:C1:214:LEU:O	38:C2:45:ARG:NH2	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:T5:185:LYS:HA	48:T5:188:ILE:HG22	1.91	0.51
62:V2:248:VAL:HG23	62:V2:251:LYS:NZ	2.26	0.51
21:5:337:PHE:CD2	88:B8:601:3PE:H221	2.45	0.51
22:5B:31:MET:HE3	82:B4:201:CDL:H711	1.93	0.51
32:AM:48:ARG:HH22	81:T7:78:PHE:HD1	1.57	0.51
43:T2:64:GLY:O	43:T2:118:LYS:NZ	2.44	0.51
47:T6:142:PHE:O	79:T9:117:ARG:NH1	2.43	0.51
52:S3:10:GLN:HA	52:S3:13:ILE:HD12	1.92	0.51
52:S3:34:ILE:HG12	52:S3:110:THR:HB	1.93	0.51
1:1:239:PHE:HD2	76:TC:2:VAL:HG22	1.76	0.51
3:2:151:PHE:O	3:2:154:ILE:HG22	2.11	0.51
7:3B:111:GLN:HB2	7:3B:139:VAL:HG11	1.93	0.51
6:3a:145:ASP:OD2	6:3a:148:THR:OG1	2.27	0.51
83:5:807:PC1:H2E2	83:5:807:PC1:H352	1.92	0.51
23:6:185:PHE:O	23:6:188:ILE:HG22	2.11	0.51
25:A5:92:ILE:O	25:A5:99:ARG:NH1	2.36	0.51
29:AB:60:LYS:HG3	29:AB:132:LEU:HD11	1.91	0.51
43:T2:176:LYS:HB2	43:T2:179:GLN:HG3	1.93	0.51
44:T1:54:PRO:HA	44:T1:57:GLN:HB3	1.93	0.51
51:S2:41:LEU:HB2	51:S2:437:PHE:CZ	2.45	0.51
9:3d:93:ASP:N	9:3d:136:ILE:O	2.44	0.51
19:4:201:TYR:O	19:4:205:TRP:HE3	1.94	0.51
31:AL:57:ASP:OD2	31:AL:61:ASN:ND2	2.44	0.51
32:AM:73:LYS:HG3	74:TA:100:ARG:HD3	1.92	0.51
32:AM:92:PHE:O	32:AM:96:MET:HG3	2.11	0.51
38:C2:192:TYR:OH	38:C2:195:ASP:OD1	2.27	0.51
52:S3:66:ILE:HD12	52:S3:95:LEU:HD23	1.93	0.51
57:B9:102:ASP:O	57:B9:105:MET:HG3	2.11	0.51
73:B3:45:LYS:HG2	77:P2:121:GLU:HG2	1.93	0.51
1:1:192:ILE:HG22	1:1:193:ILE:HG23	1.92	0.50
23:6:34:GLU:OE2	45:A1:93:ARG:NH2	2.44	0.50
30:AC:36:TYR:N	64:BM:117:GLU:O	2.44	0.50
37:C1:216:TYR:HB2	38:C2:24:LEU:HD13	1.92	0.50
56:S8:23:ARG:HD3	56:S8:26:ILE:HG22	1.92	0.50
3:2:99:TYR:CD2	3:2:139:PRO:HB2	2.46	0.50
6:3A:266:VAL:HG13	6:3A:270:LEU:HD12	1.93	0.50
8:3C:98:HIS:O	8:3C:102:LYS:HG2	2.12	0.50
8:3C:320:GLU:HG3	9:3D:317:PHE:CG	2.46	0.50
6:3a:203:PHE:HE2	6:3a:306:ALA:HB2	1.77	0.50
7:3b:461:GLY:O	7:3b:465:ARG:NE	2.37	0.50
21:5:742:PHE:HD2	83:B2:201:PC1:H282	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C3:132:PRO:HD2	39:C3:149:MET:HB3	1.92	0.50
50:S1:368:GLU:HB3	50:S1:533:VAL:HG22	1.92	0.50
61:V1:407:TYR:OH	61:V1:452:ASP:OD2	2.28	0.50
1:1:43:GLU:OE1	1:1:249:TYR:OH	2.18	0.50
3:2:352:ILE:HA	3:2:355:ILE:HD12	1.93	0.50
6:3A:62:ASP:HB3	7:3B:82:VAL:HG23	1.92	0.50
9:3d:179:SER:HB3	9:3d:213:LEU:HD12	1.94	0.50
10:3e:258:LYS:NZ	10:3e:260:PRO:HB3	2.26	0.50
21:5:698:ASN:HB3	33:B7:118:TRP:CZ2	2.46	0.50
28:A9:352:ARG:NH1	28:A9:353:GLY:O	2.44	0.50
41:J1:175:PHE:CZ	41:J1:186:ILE:HG21	2.46	0.50
44:T1:346:PHE:HE1	44:T1:365:GLU:HG2	1.76	0.50
50:S1:447:SER:HA	50:S1:677:PRO:HA	1.92	0.50
51:S2:151:PHE:HA	51:S2:154:ARG:HG2	1.93	0.50
56:S8:152:THR:HB	56:S8:169:ASP:OD2	2.11	0.50
70:B2:95:LYS:O	70:B2:99:LYS:HG2	2.11	0.50
71:T3:79:ASP:OD1	71:T3:80:LYS:N	2.44	0.50
77:P2:134:ALA:HB1	77:P2:138:LEU:HD21	1.93	0.50
4:2B:55:GLU:HB3	4:2B:130:ILE:HG21	1.93	0.50
7:3b:94:ALA:HB2	7:3b:240:ASN:HB3	1.92	0.50
9:3d:123:GLN:NE2	9:3d:125:TYR:HB2	2.26	0.50
19:4:193:ARG:NH1	42:FX:87:ILE:O	2.44	0.50
19:4:421:ILE:HD11	19:4:494:LEU:HD23	1.92	0.50
51:S2:440:ILE:O	51:S2:442:ARG:NH1	2.45	0.50
82:C4:401:CDL:H511	82:C4:401:CDL:H311	1.93	0.50
12:3g:95:ARG:NH2	13:3h:50:ASP:O	2.44	0.50
12:3g:130:ARG:O	13:3h:86:ARG:NH1	2.43	0.50
33:B7:116:LEU:HD12	33:B7:120:ASN:HA	1.92	0.50
44:T1:357:PRO:HB2	44:T1:363:VAL:HG22	1.92	0.50
51:S2:276:CYS:SG	51:S2:432:THR:HG21	2.52	0.50
56:S8:143:GLN:HB2	56:S8:153:ILE:HD12	1.92	0.50
58:TX:103:LEU:HD23	58:TX:108:GLU:HA	1.92	0.50
10:3E:197:CYS:SG	10:3E:223:TYR:OH	2.69	0.50
6:3a:203:PHE:O	6:3a:207:VAL:HG13	2.11	0.50
21:5:596:ILE:HG13	34:B8:101:TYR:HE2	1.77	0.50
83:6:302:PC1:H3A1	83:6:302:PC1:H362	1.94	0.50
32:AM:160:GLN:NE2	80:TE:53:TYR:O	2.44	0.50
38:C2:107:LYS:HZ1	39:C3:133:ASN:HD22	1.60	0.50
48:T5:149:LEU:HG	48:T5:150:VAL:H	1.77	0.50
6:3a:451:VAL:O	6:3a:455:LEU:HD23	2.12	0.50
37:C1:72:THR:HG23	37:C1:93:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BM:113:ASP:OD1	64:BM:113:ASP:N	2.44	0.50
7:3B:65:ARG:NH1	7:3B:257:GLN:OE1	2.45	0.50
10:3E:158:THR:HG23	10:3E:161:GLU:H	1.76	0.50
12:3G:162:TYR:HA	12:3G:166:MET:HG2	1.93	0.50
9:3d:277:ALA:HB1	13:3h:70:ILE:O	2.12	0.50
19:4:417:ILE:HG21	82:BM:301:CDL:H411	1.94	0.50
19:4:485:TYR:HB2	64:BM:144:LEU:HD13	1.94	0.50
21:5:173:ILE:HG22	82:BM:301:CDL:H273	1.92	0.50
21:5:338:LYS:NZ	21:5:417:ASP:OD2	2.31	0.50
31:AL:160:SER:HB3	50:S1:270:GLU:HG2	1.93	0.50
50:S1:327:ILE:HD11	50:S1:576:ILE:HG21	1.94	0.50
59:A8:181:MET:HE3	59:A8:186:GLY:HA2	1.93	0.50
61:V1:161:GLY:N	61:V1:201:GLY:O	2.44	0.50
61:V1:316:LEU:HD21	61:V1:364:PRO:HG3	1.92	0.50
62:V2:242:LYS:HA	62:V2:245:GLN:HG2	1.92	0.50
71:T3:74:LEU:HB3	71:T3:232:ILE:HD13	1.94	0.50
3:2:83:THR:HB	3:2:87:SER:HA	1.93	0.50
8:3C:238:ILE:HD12	83:3C:606:PC1:H341	1.94	0.50
9:3d:221:ASP:O	14:3i:108:HIS:ND1	2.45	0.50
51:S2:119:THR:OG1	51:S2:259:ALA:O	2.27	0.50
62:V2:121:HIS:CD2	62:V2:123:GLN:HE21	2.25	0.50
8:3C:83:LEU:HD11	83:3E:302:PC1:H372	1.94	0.49
13:3H:69:PHE:HB2	13:3H:72:PHE:HB2	1.94	0.49
7:3b:97:ARG:O	7:3b:281:ASN:ND2	2.40	0.49
85:5B:202:U10:O2	34:B8:91:TRP:NE1	2.41	0.49
26:A6:164:TYR:HE1	50:S1:324:ILE:HD12	1.77	0.49
50:S1:320:TRP:HZ3	50:S1:578:LEU:HD13	1.77	0.49
61:V1:291:GLU:HG2	61:V1:295:ILE:HD12	1.92	0.49
1:1:2:GLY:HA2	1:1:5:ILE:HG12	1.92	0.49
1:1:74:LEU:HD13	1:1:242:ALA:HB2	1.94	0.49
7:3b:200:LEU:HD23	7:3b:380:TYR:HD1	1.77	0.49
12:3g:192:LEU:HG	83:3g:401:PC1:H262	1.93	0.49
19:4:437:SER:HB3	19:4:440:ILE:HB	1.94	0.49
83:6:301:PC1:H292	83:TC:101:PC1:H2C1	1.93	0.49
31:AL:12:LEU:HA	31:AL:17:TRP:HE1	1.77	0.49
32:AM:59:LEU:HD11	74:TA:89:GLY:HA3	1.93	0.49
48:T5:142:LYS:HB3	82:BM:301:CDL:HA21	1.94	0.49
61:V1:320:PRO:HG2	61:V1:325:VAL:HG11	1.93	0.49
7:3b:419:PHE:CE1	7:3b:455:ILE:HD11	2.47	0.49
12:3g:108:HIS:O	12:3g:111:THR:HG22	2.13	0.49
21:5:600:ILE:HD12	21:5:710:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A6:63:PHE:O	26:A6:67:ILE:HG12	2.12	0.49
41:J1:87:ARG:NH1	58:TX:121:GLU:OE1	2.41	0.49
42:FX:158:ILE:HD12	42:FX:160:ILE:HD11	1.94	0.49
78:A3:86:GLN:HA	78:A3:89:LYS:HD2	1.94	0.49
78:A3:91:GLN:HG3	78:A3:96:ARG:HD3	1.94	0.49
9:3D:214:VAL:HG22	9:3D:217:LEU:HD12	1.93	0.49
12:3G:192:LEU:O	12:3G:198:TRP:NE1	2.46	0.49
15:3J:8:LYS:HZ1	12:3g:8:LEU:HD22	1.76	0.49
82:5:805:CDL:H412	82:5:805:CDL:H371	1.93	0.49
26:A6:44:THR:OG1	41:J1:197:ASP:OD2	2.28	0.49
32:AM:93:MET:HE2	59:A8:115:LEU:HD21	1.94	0.49
37:C1:185:ARG:NH2	57:B9:150:MET:HE2	2.27	0.49
71:T3:284:GLU:O	71:T3:288:GLN:HG2	2.12	0.49
81:T7:82:ARG:NH2	81:T7:83:TYR:OH	2.45	0.49
10:3E:26:VAL:N	83:3E:304:PC1:O14	2.44	0.49
9:3d:40:TYR:HB3	9:3d:43:LEU:HD21	1.93	0.49
10:3e:44:VAL:HG21	12:3g:135:PRO:HG3	1.93	0.49
12:3g:8:LEU:HD13	12:3g:202:PHE:HZ	1.76	0.49
26:A6:52:ALA:HB1	26:A6:105:ILE:HG21	1.94	0.49
27:A7:209:ARG:NH2	51:S2:190:GLU:OE1	2.45	0.49
52:S3:132:ALA:O	52:S3:136:GLU:HB2	2.13	0.49
62:V2:176:ILE:HG12	62:V2:187:LEU:HD11	1.94	0.49
70:B2:97:LEU:O	70:B2:101:ILE:HG12	2.12	0.49
11:3f:33:LEU:O	11:3f:37:GLN:HG2	2.12	0.49
51:S2:199:PHE:HA	51:S2:202:THR:HG22	1.93	0.49
62:V2:178:VAL:HG21	62:V2:199:LEU:HD11	1.94	0.49
3:2:52:ILE:HB	46:X1:78:PHE:HB3	1.93	0.49
7:3B:224:ASN:O	7:3B:224:ASN:ND2	2.43	0.49
10:3E:113:GLY:HA3	83:3E:302:PC1:H342	1.94	0.49
10:3E:224:ASP:HB3	10:3E:231:GLN:CD	2.36	0.49
6:3a:411:GLU:HG3	7:3b:84:PRO:HD2	1.95	0.49
8:3c:111:GLU:HG2	8:3c:112:GLN:OE1	2.13	0.49
9:3d:290:TYR:HE1	10:3e:52:VAL:HG12	1.77	0.49
26:A6:112:GLY:HA2	91:AB:201:ZMP:H4A	1.94	0.49
58:TX:64:ASP:OD2	58:TX:115:GLN:NE2	2.43	0.49
88:A3:201:3PE:H222	88:A3:201:3PE:H272	1.94	0.49
79:T9:97:ASP:OD1	79:T9:97:ASP:N	2.42	0.49
12:3G:222:ASN:ND2	12:3G:225:GLY:O	2.39	0.49
23:6:253:LYS:HB2	32:AM:16:ARG:NH2	2.27	0.49
27:A7:230:ASN:HB3	27:A7:261:GLN:H	1.76	0.49
31:AL:13:THR:HG22	31:AL:15:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AM:107:ARG:HG2	32:AM:110:MET:HE2	1.94	0.49
32:AM:173:PHE:O	32:AM:175:VAL:HG23	2.13	0.49
43:T2:53:THR:OG1	43:T2:92:LYS:NZ	2.38	0.49
44:T1:115:LEU:HD12	44:T1:143:LEU:HD23	1.94	0.49
51:S2:86:ASP:HA	51:S2:436:VAL:HG11	1.93	0.49
61:V1:313:ASP:O	61:V1:360:LYS:NZ	2.46	0.49
66:AN:179:PHE:HB2	88:AN:301:3PE:H382	1.95	0.49
82:3c:505:CDL:HB21	12:3g:130:ARG:HH22	1.78	0.49
22:5B:52:TYR:HA	22:5B:56:LYS:HB2	1.95	0.49
23:6:50:ILE:HD11	82:AN:304:CDL:H352	1.95	0.49
33:B7:83:GLU:OE2	34:B8:113:ASP:HA	2.12	0.49
50:S1:283:ASN:HB2	50:S1:286:TRP:O	2.13	0.49
51:S2:153:GLU:OE2	51:S2:156:LYS:NZ	2.33	0.49
72:P1:80:ASP:HB2	77:P2:102:HIS:CE1	2.48	0.49
3:2:28:PHE:HB3	88:A3:201:3PE:H252	1.95	0.49
7:3b:492:HIS:CD2	7:3b:494:ASN:HB3	2.47	0.49
8:3c:123:PHE:O	8:3c:127:GLN:HG2	2.13	0.49
28:A9:163:SER:OG	28:A9:183:GLU:OE2	2.30	0.49
39:C3:69:ALA:O	39:C3:72:SER:OG	2.28	0.49
51:S2:346:ASN:O	61:V1:465:ARG:NH2	2.46	0.49
55:S7:45:ASP:HB3	55:S7:48:ARG:HG3	1.94	0.49
9:3D:114:ILE:HB	9:3D:134:ARG:HG2	1.94	0.48
23:6:21:ILE:HG12	75:S5:64:ASN:HB3	1.95	0.48
32:AM:96:MET:HG2	59:A8:157:LEU:HD21	1.94	0.48
42:FX:93:LYS:NZ	42:FX:150:GLU:OE2	2.46	0.48
62:V2:43:GLU:OE2	62:V2:90:LYS:NZ	2.46	0.48
3:2:71:VAL:O	3:2:75:ILE:HG12	2.13	0.48
8:3c:126:PHE:CE1	84:3c:502:HEM:HBC1	2.48	0.48
12:3g:41:VAL:HB	12:3g:211:TYR:CE2	2.48	0.48
23:6:84:PHE:O	23:6:87:VAL:HG22	2.12	0.48
42:FX:51:ILE:HG13	42:FX:53:GLN:HG3	1.94	0.48
44:T1:261:ASN:HD21	44:T1:264:LYS:HE2	1.78	0.48
3:2:238:TYR:OH	75:S5:48:HIS:O	2.31	0.48
6:3A:103:THR:H	6:3A:106:THR:HG1	1.60	0.48
12:3G:227:PHE:CE2	12:3G:238:PHE:HB2	2.48	0.48
16:3M:9:SER:OG	8:3c:172:GLU:OE2	2.24	0.48
8:3c:36:PHE:CD2	8:3c:230:GLU:HB3	2.48	0.48
19:4:266:LEU:HG	19:4:270:HIS:HD2	1.77	0.48
19:4:432:GLY:HA3	35:BL:115:PHE:CZ	2.48	0.48
85:5B:202:U10:H322	85:5B:202:U10:H301	1.53	0.48
42:FX:87:ILE:HG13	42:FX:88:ASN:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:T6:127:LYS:NZ	69:T8:98:GLU:OE2	2.46	0.48
77:P2:36:PRO:HG3	77:P2:89:HIS:HE1	1.78	0.48
6:3A:252:CYS:HB2	6:3A:417:LEU:HD11	1.95	0.48
6:3A:293:GLU:HA	6:3A:461:PHE:O	2.13	0.48
8:3C:234:MET:HE3	8:3C:238:ILE:HD11	1.96	0.48
12:3G:84:ASP:HA	12:3G:115:MET:HE3	1.95	0.48
7:3b:230:ASP:OD1	7:3b:231:GLU:N	2.46	0.48
82:3b:602:CDL:HA4	82:3b:602:CDL:HA22	1.93	0.48
20:4L:23:PRO:HG3	23:6:112:TYR:CD2	2.48	0.48
54:S6:106:THR:OG1	54:S6:108:LYS:O	2.31	0.48
71:T3:24:LEU:HB3	72:P1:94:PRO:HB3	1.95	0.48
71:T3:226:ASN:O	71:T3:229:GLU:HG2	2.12	0.48
72:P1:138:ALA:O	72:P1:142:ILE:HG12	2.13	0.48
7:3B:206:PHE:HD1	7:3B:292:MET:HE1	1.77	0.48
10:3E:209:GLY:HA3	10:3E:212:LYS:HE3	1.96	0.48
7:3b:390:GLN:NE2	7:3b:510:TYR:O	2.40	0.48
19:4:24:LEU:CD2	19:4:59:GLY:HA3	2.43	0.48
82:5:803:CDL:H782	73:B3:56:LEU:HD11	1.93	0.48
43:T2:73:LEU:HD11	43:T2:97:LEU:HD21	1.94	0.48
51:S2:87:TYR:CD1	55:S7:31:CYS:HB3	2.49	0.48
61:V1:275:LYS:HE2	61:V1:353:ALA:HB2	1.96	0.48
74:TA:115:LYS:O	78:A3:132:ARG:NH2	2.45	0.48
9:3d:43:LEU:HD11	9:3d:169:PRO:HG3	1.95	0.48
11:3f:24:VAL:HG12	11:3f:73:VAL:HG12	1.95	0.48
43:T2:185:SER:OG	43:T2:187:ASN:O	2.27	0.48
54:S6:84:ILE:HD11	54:S6:101:TYR:HB3	1.96	0.48
5:3:73:VAL:HA	5:3:76:THR:HG22	1.95	0.48
8:3C:36:PHE:CD2	8:3C:230:GLU:HB3	2.49	0.48
21:5:289:LEU:HD22	21:5:428:LEU:HD12	1.95	0.48
27:A7:94:LEU:HD11	27:A7:104:ALA:HB1	1.95	0.48
37:C1:53:GLN:NE2	37:C1:252:GLU:OE2	2.47	0.48
37:C1:126:LYS:NZ	38:C2:152:ASN:OD1	2.29	0.48
51:S2:126:ARG:HG3	51:S2:130:HIS:CD2	2.49	0.48
4:2B:3:ILE:HD11	4:2B:6:ASN:HA	1.96	0.48
9:3D:79:ARG:NH1	9:3D:219:ASP:O	2.46	0.48
12:3G:255:LYS:HD3	58:TX:42:LYS:HZ1	1.79	0.48
8:3c:52:LEU:HD11	8:3c:81:PHE:HA	1.96	0.48
27:A7:162:GLU:HG3	52:S3:106:LYS:HZ2	1.78	0.48
44:T1:339:THR:HB	44:T1:344:GLU:HG3	1.96	0.48
50:S1:303:ILE:HG22	50:S1:579:PRO:HB3	1.95	0.48
51:S2:414:LEU:HD12	51:S2:433:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:S8:134:GLU:O	56:S8:164:ARG:NH1	2.46	0.48
58:TX:141:ASP:OD1	58:TX:141:ASP:N	2.46	0.48
5:3:101:PHE:CG	83:X1:201:PC1:H3D2	2.49	0.48
7:3B:116:ARG:NE	7:3B:181:GLU:OE2	2.43	0.48
8:3C:107:ASN:HB3	8:3C:112:GLN:HG2	1.96	0.48
10:3E:245:ILE:HG12	10:3E:252:VAL:HG22	1.94	0.48
7:3b:326:ARG:HG2	7:3b:418:TYR:HB2	1.96	0.48
32:AM:48:ARG:NH1	74:TA:74:GLU:OE2	2.47	0.48
38:C2:59:PHE:HB3	38:C2:77:LEU:HB2	1.94	0.48
42:FX:126:GLU:HG3	42:FX:143:LEU:HD12	1.95	0.48
44:T1:359:ASN:HD22	44:T1:377:SER:HB2	1.79	0.48
45:A1:47:ARG:NH2	59:A8:185:ASP:O	2.47	0.48
50:S1:563:PHE:CE1	50:S1:578:LEU:HD12	2.48	0.48
51:S2:231:CYS:HA	51:S2:236:LEU:HD12	1.96	0.48
51:S2:442:ARG:NH2	52:S3:138:GLU:OE1	2.43	0.48
79:T9:9:SER:OG	79:T9:11:PHE:O	2.26	0.48
7:3B:206:PHE:CD1	7:3B:292:MET:HE1	2.49	0.48
10:3E:127:ASP:OD1	15:3J:58:ARG:NH2	2.38	0.48
10:3E:152:ILE:HA	10:3E:195:ALA:H	1.79	0.48
7:3b:137:LEU:HD13	7:3b:150:LEU:HD13	1.95	0.48
8:3c:351:ASP:N	8:3c:351:ASP:OD1	2.47	0.48
19:4:102:ASN:HB2	49:R:53:PHE:CZ	2.49	0.48
35:BL:93:LYS:HB3	48:T5:62:TYR:CE1	2.49	0.48
37:C1:191:GLU:HG2	57:B9:150:MET:HE1	1.95	0.48
38:C2:107:LYS:NZ	39:C3:133:ASN:HD22	2.12	0.48
50:S1:385:TYR:HA	50:S1:513:ILE:HD12	1.95	0.48
57:B9:108:ASP:OD2	57:B9:110:SER:OG	2.28	0.48
58:TX:49:TYR:HE1	58:TX:98:PRO:HB3	1.78	0.48
61:V1:163:PHE:HB3	61:V1:166:GLU:HB2	1.96	0.48
81:T7:75:ILE:HD13	81:T7:91:LEU:HD11	1.96	0.48
81:T7:122:PRO:HD2	81:T7:125:LEU:HD12	1.96	0.48
1:1:123:LEU:HD12	1:1:181:PHE:HD1	1.79	0.47
2:1B:26:ARG:O	51:S2:219:ARG:NH1	2.43	0.47
3:2:253:ILE:O	3:2:257:ILE:HG12	2.14	0.47
6:3a:313:PRO:O	6:3a:316:SER:OG	2.32	0.47
7:3b:113:LEU:HD11	7:3b:178:VAL:HG22	1.96	0.47
12:3g:34:ASN:ND2	12:3g:159:ASN:OD1	2.46	0.47
82:5:803:CDL:H552	82:5:803:CDL:H352	1.96	0.47
39:C3:94:GLY:HA2	39:C3:97:GLY:O	2.14	0.47
45:A1:78:PRO:HD3	75:S5:71:LEU:HD13	1.96	0.47
50:S1:239:PHE:CD2	56:S8:163:ARG:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S2:135:ALA:HB1	51:S2:147:VAL:HA	1.95	0.47
51:S2:395:SER:HB3	52:S3:74:GLU:HG3	1.96	0.47
6:3A:267:GLN:HG3	6:3A:271:ALA:HB2	1.95	0.47
7:3B:507:ASN:HB3	7:3B:511:TYR:CD2	2.49	0.47
9:3d:249:LYS:O	9:3d:253:LYS:HG2	2.14	0.47
83:5:802:PC1:H222	33:B7:57:MET:HE2	1.95	0.47
23:6:116:ILE:HG12	66:AN:87:LEU:HD13	1.94	0.47
24:A2:4:TRP:CE3	24:A2:91:VAL:HG21	2.49	0.47
27:A7:17:ILE:HD13	56:S8:94:PHE:CZ	2.49	0.47
27:A7:222:PRO:HB2	27:A7:249:THR:HG21	1.95	0.47
32:AM:140:PHE:HD1	75:S5:49:ARG:HG2	1.79	0.47
50:S1:219:LEU:HB3	50:S1:222:ASN:HD22	1.79	0.47
64:BM:189:ARG:NE	79:T9:10:GLU:OE1	2.35	0.47
72:P1:51:GLU:OE1	72:P1:57:THR:OG1	2.31	0.47
72:P1:80:ASP:HB2	77:P2:102:HIS:HE1	1.79	0.47
1:1:9:PHE:HD1	1:1:12:ILE:HD11	1.78	0.47
9:3D:316:TYR:HD2	12:3G:177:SER:HA	1.79	0.47
9:3d:243:GLN:HB2	9:3d:246:VAL:O	2.13	0.47
27:A7:33:PRO:HG2	27:A7:38:GLU:HG3	1.96	0.47
29:AB:66:ARG:NH2	29:AB:138:VAL:O	2.42	0.47
39:C3:194:ILE:HG12	39:C3:199:ARG:HD2	1.96	0.47
44:T1:107:ASN:HB3	44:T1:111:LYS:NZ	2.30	0.47
55:S7:1:MET:HE1	55:S7:162:TYR:HA	1.95	0.47
58:TX:99:GLU:HG2	58:TX:113:THR:HG22	1.96	0.47
77:P2:151:GLU:OE2	77:P2:153:TYR:OH	2.24	0.47
6:3A:459:PRO:O	6:3A:474:TYR:OH	2.27	0.47
9:3D:127:GLN:HB2	16:3M:16:THR:HB	1.96	0.47
6:3a:25:LYS:NZ	7:3b:459:ASP:OD2	2.41	0.47
8:3c:246:PHE:HB2	83:3c:506:PC1:H231	1.96	0.47
8:3c:341:ILE:HD12	8:3c:408:LEU:HD13	1.95	0.47
19:4:340:GLN:HG3	19:4:341:GLU:N	2.29	0.47
21:5:475:ALA:HA	21:5:605:TYR:HB3	1.96	0.47
82:5:805:CDL:H351	82:5:805:CDL:H392	1.96	0.47
22:5B:52:TYR:HH	29:AB:27:PHE:N	2.13	0.47
26:A6:50:VAL:HG13	39:C3:314:ALA:HB3	1.95	0.47
37:C1:120:TYR:O	37:C1:137:GLU:HA	2.15	0.47
50:S1:290:LYS:NZ	50:S1:685:PHE:O	2.44	0.47
52:S3:124:SER:OG	52:S3:136:GLU:OE1	2.20	0.47
81:T7:137:CYS:HB2	81:T7:140:TRP:HD1	1.78	0.47
3:2:99:TYR:CE1	3:2:103:ILE:HD11	2.49	0.47
7:3B:224:ASN:O	7:3B:228:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3C:126:PHE:HA	8:3C:192:LEU:HD11	1.96	0.47
8:3C:232:GLY:HA3	9:3D:271:LYS:HG3	1.95	0.47
8:3c:116:TRP:CD2	84:3c:503:HEM:HBC1	2.49	0.47
8:3c:333:SER:HB2	8:3c:339:SER:HA	1.97	0.47
23:6:64:LEU:HD21	83:TC:101:PC1:H242	1.96	0.47
32:AM:153:LYS:HE2	45:A1:49:TYR:HB3	1.96	0.47
39:C3:205:HIS:O	39:C3:208:GLU:HG3	2.14	0.47
77:P2:72:GLU:OE2	77:P2:132:PHE:N	2.43	0.47
81:T7:133:ASP:OD2	81:T7:135:ARG:NH2	2.43	0.47
6:3A:204:ASN:HA	6:3A:207:VAL:HG22	1.97	0.47
82:3C:603:CDL:H512	13:3H:92:TRP:CE2	2.49	0.47
12:3G:131:GLY:O	13:3H:90:GLN:NE2	2.42	0.47
8:3c:68:GLU:OE1	9:3d:90:LYS:NZ	2.40	0.47
9:3d:255:VAL:O	9:3d:259:MET:HG3	2.14	0.47
28:A9:214:LYS:HD3	28:A9:306:PHE:HZ	1.79	0.47
35:BL:116:GLN:O	67:B4:120:ASN:ND2	2.35	0.47
51:S2:199:PHE:HD2	51:S2:291:LEU:HD11	1.79	0.47
1:1:49:LEU:HB3	56:S8:100:SER:HB2	1.95	0.47
1:1:157:ALA:O	1:1:160:MET:HG3	2.15	0.47
6:3A:202:LEU:O	6:3A:205:GLU:HG2	2.15	0.47
8:3C:340:ASP:OD1	8:3C:340:ASP:N	2.48	0.47
8:3C:359:PHE:CE2	82:3C:603:CDL:H312	2.49	0.47
10:3E:37:LYS:HD2	58:TX:132:LYS:NZ	2.30	0.47
6:3a:138:GLY:HA3	6:3a:154:ASN:O	2.15	0.47
7:3b:61:ASP:N	7:3b:61:ASP:OD1	2.47	0.47
7:3b:403:ALA:HA	7:3b:467:ALA:HB3	1.97	0.47
7:3b:406:ILE:HD13	7:3b:463:ILE:HG21	1.97	0.47
13:3h:31:ASP:OD1	13:3h:31:ASP:N	2.47	0.47
21:5:388:ILE:HG12	88:5:804:3PE:H371	1.97	0.47
21:5:602:GLY:HA2	21:5:605:TYR:CE2	2.50	0.47
30:AC:120:GLU:O	30:AC:124:GLU:HG2	2.14	0.47
38:C2:117:ALA:HB3	38:C2:120:ILE:HD12	1.97	0.47
44:T1:377:SER:HB3	44:T1:410:VAL:HG22	1.97	0.47
48:T5:188:ILE:HD13	64:BM:202:LYS:HA	1.96	0.47
50:S1:551:PRO:HA	50:S1:573:TYR:HE2	1.79	0.47
51:S2:405:SER:HB2	51:S2:439:GLU:HG2	1.97	0.47
55:S7:64:LEU:HG	55:S7:91:LEU:HD22	1.96	0.47
56:S8:173:THR:HG21	56:S8:203:HIS:CD2	2.50	0.47
82:C4:401:CDL:H252	88:C4:402:3PE:H232	1.96	0.47
81:T7:15:ILE:HG23	81:T7:17:ILE:HD11	1.97	0.47
81:T7:54:ASP:OD1	81:T7:55:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:81:VAL:HB	23:6:178:TYR:CZ	2.49	0.47
85:3C:605:U10:H121	85:3C:605:U10:H101	1.60	0.47
12:3G:194:ARG:NH1	15:3j:7:TYR:OH	2.47	0.47
8:3c:338:ARG:NH1	12:3g:210:SER:HA	2.30	0.47
35:BL:148:LEU:HD12	64:BM:177:LEU:HD12	1.97	0.47
62:V2:142:ILE:HG22	62:V2:161:LEU:HD21	1.96	0.47
64:BM:64:SER:HB3	64:BM:67:ASP:HB2	1.96	0.47
4:2B:14:ASN:HB2	65:C4:70:GLN:HE21	1.80	0.47
14:3I:54:PHE:CZ	82:3I:604:CDL:H112	2.49	0.47
7:3b:311:PRO:HG3	7:3b:470:TRP:CZ2	2.50	0.47
7:3b:349:SER:HB3	7:3b:352:HIS:HB2	1.95	0.47
8:3c:211:SER:O	12:3g:94:ARG:NH2	2.48	0.47
43:T2:188:PHE:HA	50:S1:460:PRO:HG2	1.96	0.47
50:S1:32:GLN:HA	50:S1:44:VAL:O	2.15	0.47
51:S2:120:MET:HE2	51:S2:298:ILE:HG13	1.97	0.47
52:S3:37:ILE:HD12	52:S3:45:ILE:HD13	1.96	0.47
88:S8:303:3PE:H2B2	78:A3:62:TYR:HA	1.97	0.47
62:V2:154:SER:OG	62:V2:156:ASP:OD1	2.29	0.47
1:1:29:MET:O	1:1:32:ILE:HG22	2.15	0.47
6:3A:294:VAL:HB	6:3A:462:VAL:HG22	1.97	0.47
7:3B:175:LYS:HB2	7:3B:175:LYS:HE2	1.75	0.47
7:3B:419:PHE:CE1	7:3B:455:ILE:HD11	2.50	0.47
8:3C:32:SER:HB2	8:3C:207:TRP:HH2	1.79	0.47
82:3H:202:CDL:CB5	66:AN:114:LEU:HD21	2.45	0.47
27:A7:110:LYS:HA	27:A7:110:LYS:HD3	1.79	0.47
31:AL:96:VAL:HG12	56:S8:220:TRP:CE3	2.50	0.47
83:AM:201:PC1:H231	56:S8:89:PHE:HB2	1.96	0.47
38:C2:28:ARG:O	38:C2:31:CYS:HB2	2.15	0.47
38:C2:185:TRP:HB3	38:C2:190:VAL:HG22	1.97	0.47
43:T2:267:ASP:OD1	43:T2:267:ASP:N	2.46	0.47
1:1:150:PHE:HE2	5:3:57:ILE:HG23	1.79	0.46
2:1B:53:CYS:HB3	78:A3:74:VAL:HG11	1.97	0.46
3:2:192:VAL:HG22	3:2:272:ILE:HA	1.96	0.46
6:3A:420:THR:HG23	6:3A:430:ILE:HD12	1.96	0.46
10:3E:37:LYS:HD2	58:TX:132:LYS:HZ1	1.80	0.46
19:4:173:MET:HA	19:4:173:MET:HE3	1.98	0.46
21:5:579:ILE:O	34:B8:108:ARG:NH1	2.36	0.46
49:R:69:VAL:HG21	49:R:100:MET:SD	2.55	0.46
55:S7:86:ASP:OD1	55:S7:88:LYS:NZ	2.46	0.46
61:V1:133:ARG:HB3	61:V1:166:GLU:HG3	1.96	0.46
68:T4:170:THR:OG1	68:T4:171:PRO:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:205:LEU:HD23	2:1B:44:TRP:CE2	2.50	0.46
1:1:240:TYR:HD1	76:TC:2:VAL:HG21	1.79	0.46
11:3f:58:CYS:HB2	11:3f:61:PRO:HG2	1.96	0.46
19:4:384:ARG:HH12	19:4:483:GLU:CD	2.23	0.46
27:A7:78:ASP:HB2	27:A7:123:ASN:HB2	1.97	0.46
31:AL:162:ALA:HB3	50:S1:300:ARG:HA	1.96	0.46
49:R:100:MET:N	49:R:101:PRO:HD2	2.30	0.46
51:S2:46:GLN:HB3	51:S2:54:ARG:HB2	1.96	0.46
59:A8:181:MET:CE	59:A8:186:GLY:HA2	2.45	0.46
61:V1:116:ILE:HD11	61:V1:143:ALA:HB2	1.97	0.46
8:3C:32:SER:HB2	8:3C:207:TRP:CH2	2.51	0.46
8:3C:302:LEU:HD23	83:3C:604:PC1:H2I1	1.96	0.46
12:3G:95:ARG:NH2	13:3H:50:ASP:O	2.49	0.46
20:4L:78:ALA:O	20:4L:81:TYR:HB2	2.16	0.46
21:5:602:GLY:HA2	21:5:605:TYR:CZ	2.49	0.46
37:C1:83:ASP:OD1	37:C1:84:VAL:N	2.48	0.46
39:C3:152:THR:HB	39:C3:170:VAL:HG13	1.98	0.46
49:R:6:TRP:NE1	79:T9:67:PRO:HG3	2.31	0.46
51:S2:121:TYR:O	51:S2:125:THR:HG22	2.14	0.46
64:BM:60:ILE:HG22	64:BM:62:ASN:H	1.80	0.46
8:3C:86:ARG:HB3	83:3C:606:PC1:H332	1.97	0.46
12:3G:301:ASP:OD1	14:3I:17:SER:OG	2.33	0.46
7:3b:291:TYR:HD1	7:3b:478:ILE:HB	1.81	0.46
19:4:16:PHE:HB3	49:R:56:PHE:CE2	2.51	0.46
19:4:394:ASN:ND2	34:B8:58:ASP:HA	2.22	0.46
21:5:545:TYR:CZ	73:B3:48:THR:HG22	2.50	0.46
23:6:255:TYR:CE2	32:AM:19:MET:HE1	2.50	0.46
26:A6:78:THR:HG21	28:A9:343:GLU:HB3	1.97	0.46
8:3C:82:TRP:HZ2	83:3C:606:PC1:H11	1.80	0.46
19:4:328:THR:HG23	19:4:390:LEU:HB3	1.98	0.46
82:AL:301:CDL:H712	82:T1:602:CDL:H731	1.98	0.46
41:J1:37:ALA:O	41:J1:41:LYS:HG2	2.16	0.46
41:J1:119:GLY:O	42:FX:44:TRP:NE1	2.33	0.46
44:T1:204:VAL:O	44:T1:208:ILE:HG12	2.15	0.46
51:S2:250:LEU:HB2	51:S2:380:GLU:HB2	1.96	0.46
64:BM:98:THR:HA	64:BM:103:ARG:HG2	1.96	0.46
68:T4:118:LYS:HB2	68:T4:157:LEU:HD21	1.96	0.46
68:T4:156:THR:O	68:T4:160:PRO:HD3	2.16	0.46
7:3b:164:LEU:HD23	7:3b:167:ILE:HD11	1.97	0.46
9:3d:145:PHE:N	9:3d:149:GLN:OE1	2.43	0.46
19:4:400:THR:O	19:4:400:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:273:PHE:HB3	64:BM:105:TYR:CE1	2.50	0.46
82:5:805:CDL:H372	64:BM:156:LEU:HD11	1.97	0.46
39:C3:284:LYS:HB2	39:C3:287:TYR:CZ	2.51	0.46
50:S1:122:LEU:HD22	51:S2:354:MET:HG2	1.96	0.46
1:1:148:TYR:OH	51:S2:29:ASN:O	2.33	0.46
7:3B:363:ILE:HB	7:3B:382:TYR:HB3	1.97	0.46
9:3D:30:ASP:OD1	9:3D:30:ASP:N	2.45	0.46
28:A9:78:ALA:HB3	55:S7:147:GLN:HG2	1.97	0.46
37:C1:34:ILE:HD12	39:C3:46:LEU:HB3	1.96	0.46
56:S8:232:ILE:O	56:S8:235:PRO:HD2	2.15	0.46
61:V1:383:CYS:HB3	61:V1:425:ILE:HD12	1.97	0.46
66:AN:68:GLY:HA2	88:AN:301:3PE:H2C2	1.98	0.46
66:AN:154:ALA:HA	66:AN:159:PRO:HA	1.98	0.46
80:TE:60:SER:O	80:TE:71:LEU:HD12	2.16	0.46
1:1:233:SER:O	55:S7:59:GLN:NE2	2.49	0.46
3:2:221:THR:H	75:S5:2:SER:HB2	1.81	0.46
7:3B:324:PHE:CZ	7:3B:467:ALA:HB2	2.51	0.46
8:3C:45:GLN:HG2	84:3C:602:HEM:HBB2	1.97	0.46
6:3a:312:VAL:HG21	6:3a:318:ASP:HB2	1.98	0.46
11:3f:72:CYS:O	11:3f:76:GLN:NE2	2.49	0.46
21:5:245:SER:OG	21:5:247:ASP:OD1	2.33	0.46
49:R:79:MET:SD	49:R:82:ARG:NH2	2.88	0.46
55:S7:29:LEU:HB2	55:S7:67:GLY:HA3	1.97	0.46
57:B9:35:LYS:HE3	57:B9:35:LYS:HB3	1.72	0.46
73:B3:56:LEU:HA	73:B3:59:PRO:HG2	1.98	0.46
1:1:35:VAL:O	1:1:38:SER:OG	2.28	0.46
5:3:28:GLU:HA	5:3:31:TYR:CE1	2.51	0.46
8:3C:326:LYS:HB3	8:3C:340:ASP:HB2	1.97	0.46
6:3a:34:ASP:OD2	7:3b:469:ARG:NH1	2.48	0.46
12:3g:229:LEU:HD23	12:3g:266:TYR:CE1	2.51	0.46
33:B7:81:THR:HG21	70:B2:117:MET:SD	2.56	0.46
83:X1:201:PC1:H121	78:A3:93:LEU:HB3	1.97	0.46
71:T3:82:ALA:O	71:T3:85:GLU:HG3	2.16	0.46
1:1:157:ALA:O	1:1:161:LEU:HG	2.17	0.46
7:3B:332:GLN:NE2	7:3B:335:LYS:HD3	2.31	0.46
8:3c:200:GLY:O	8:3c:203:MET:HG2	2.16	0.46
9:3d:274:LYS:O	9:3d:278:TYR:HB2	2.15	0.46
13:3h:50:ASP:OD1	13:3h:50:ASP:N	2.49	0.46
21:5:383:MET:O	67:B4:113:GLN:NE2	2.22	0.46
21:5:389:ASN:HB2	21:5:392:GLU:HG2	1.97	0.46
26:A6:10:THR:HG22	26:A6:28:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:C2:61:HIS:CE1	57:B9:187:ASN:HB2	2.51	0.46
39:C3:58:LYS:HB3	39:C3:76:GLY:HA2	1.98	0.46
42:FX:115:TRP:O	42:FX:119:MET:HG3	2.16	0.46
43:T2:98:VAL:HG13	43:T2:204:ILE:HB	1.98	0.46
48:T5:125:TRP:CZ2	63:B6:90:PRO:HD3	2.51	0.46
62:V2:150:LEU:HD21	62:V2:163:GLU:HB2	1.98	0.46
68:T4:110:LEU:HB3	68:T4:114:THR:HG21	1.98	0.46
68:T4:116:GLY:HA2	83:B2:201:PC1:H372	1.98	0.46
3:2:127:TYR:O	3:2:130:SER:OG	2.26	0.45
3:2:237:ASN:HD22	76:TC:62:ARG:HA	1.80	0.45
7:3B:221:ILE:O	7:3B:225:LEU:HG	2.16	0.45
8:3C:166:TRP:CD2	8:3C:167:ILE:HG23	2.51	0.45
9:3d:43:LEU:HD23	9:3d:43:LEU:H	1.81	0.45
9:3d:56:TRP:HB2	9:3d:59:PHE:HD2	1.82	0.45
20:4L:5:ILE:HG12	20:4L:47:PHE:HE1	1.80	0.45
21:5:559:MET:HE2	21:5:609:LEU:HD23	1.98	0.45
26:A6:156:LYS:NZ	50:S1:623:GLU:OE2	2.48	0.45
66:AN:72:ALA:HB2	66:AN:112:TYR:CG	2.51	0.45
88:P1:402:3PE:H272	88:P1:402:3PE:H342	1.99	0.45
79:T9:55:ASP:OD2	79:T9:57:SER:OG	2.29	0.45
3:2:119:ILE:HD11	4:2B:141:ASN:HD22	1.81	0.45
10:3E:229:VAL:HG22	10:3E:237:ASN:HB2	1.99	0.45
8:3c:98:HIS:HE1	84:3c:503:HEM:C1A	2.33	0.45
9:3d:287:TRP:CD1	13:3h:60:GLN:HG3	2.52	0.45
21:5:576:LEU:HD23	21:5:579:ILE:HD12	1.98	0.45
92:B8:602:ADP:H5'2	57:B9:9:LYS:HD2	1.98	0.45
82:TD:101:CDL:HB22	45:A1:40:HIS:HE1	1.81	0.45
41:J1:116:SER:OG	41:J1:118:ASP:OD1	2.22	0.45
59:A8:184:SER:HB3	59:A8:227:PHE:CZ	2.52	0.45
71:T3:152:GLU:HG3	71:T3:153:LYS:HG3	1.97	0.45
3:2:108:TYR:OH	4:2B:147:ASN:OD1	2.14	0.45
8:3C:55:SER:HB3	10:3E:117:ARG:NH2	2.30	0.45
9:3D:147:GLN:HG3	9:3D:158:TRP:CD1	2.51	0.45
12:3G:176:THR:HG23	12:3G:188:GLN:HB2	1.98	0.45
6:3a:27:PHE:O	6:3a:31:ILE:HG12	2.16	0.45
6:3a:204:ASN:HA	6:3a:207:VAL:HG22	1.99	0.45
27:A7:82:GLU:HG3	27:A7:86:GLU:HB2	1.98	0.45
35:BL:71:ARG:HA	35:BL:71:ARG:HD2	1.79	0.45
44:T1:30:GLN:NE2	44:T1:361:GLU:OE2	2.48	0.45
44:T1:65:TYR:CG	44:T1:114:LEU:HD12	2.51	0.45
47:T6:69:LEU:C	47:T6:71:SER:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S4:97:PRO:HG2	53:S4:100:PRO:HA	1.98	0.45
71:T3:293:LEU:HA	71:T3:296:ILE:HB	1.97	0.45
12:3g:38:TRP:HA	12:3g:211:TYR:HE2	1.81	0.45
82:3i:201:CDL:HA32	82:3i:201:CDL:HB31	1.98	0.45
31:AL:188:ASP:OD1	43:T2:169:TYR:OH	2.34	0.45
82:AM:202:CDL:H122	82:AM:202:CDL:H512	1.97	0.45
51:S2:80:PRO:O	51:S2:83:ASP:HB2	2.16	0.45
61:V1:47:ARG:HA	61:V1:47:ARG:HD3	1.82	0.45
88:P1:402:3PE:H261	88:P1:402:3PE:H321	1.98	0.45
81:T7:56:VAL:HG21	81:T7:109:TYR:HB2	1.98	0.45
10:3E:132:VAL:HG21	10:3E:145:MET:HE1	1.99	0.45
10:3E:209:GLY:HA3	10:3E:212:LYS:HB3	1.97	0.45
6:3a:426:THR:OG1	12:3g:328:ALA:O	2.26	0.45
15:3j:40:LEU:O	15:3j:44:ILE:HD12	2.16	0.45
21:5:231:SER:O	63:B6:105:SER:OG	2.33	0.45
25:A5:75:ARG:O	25:A5:79:MET:HG2	2.16	0.45
33:B7:82:TYR:OH	70:B2:117:MET:O	2.30	0.45
50:S1:241:SER:HB2	50:S1:272:MET:HE2	1.98	0.45
51:S2:242:ARG:NH2	51:S2:286:GLU:OE2	2.46	0.45
61:V1:308:VAL:HG21	61:V1:315:LEU:HD12	1.97	0.45
72:P1:102:PHE:CE1	72:P1:105:HIS:HB2	2.51	0.45
1:1:213:GLU:OE2	1:1:251:HIS:NE2	2.44	0.45
35:BL:47:ASP:OD1	35:BL:47:ASP:N	2.50	0.45
38:C2:122:VAL:O	38:C2:140:SER:OG	2.31	0.45
44:T1:397:ILE:HD12	44:T1:440:TYR:CZ	2.52	0.45
50:S1:398:ASP:OD1	50:S1:398:ASP:N	2.44	0.45
51:S2:209:VAL:HG23	51:S2:210:LEU:HG	1.99	0.45
56:S8:176:ILE:HG13	56:S8:178:CYS:HB3	1.98	0.45
6:3A:120:THR:O	6:3A:125:ASN:HA	2.16	0.45
6:3a:252:CYS:HB2	6:3a:417:LEU:HD11	1.98	0.45
21:5:415:LEU:HB3	21:5:416:PRO:HD3	1.99	0.45
21:5:579:ILE:HA	21:5:696:PHE:CZ	2.52	0.45
31:AL:35:ALA:HB2	31:AL:79:GLU:HG2	1.98	0.45
37:C1:151:ARG:HD3	37:C1:169:LEU:HD12	1.98	0.45
44:T1:141:VAL:HG22	55:S7:157:LYS:HD2	1.98	0.45
48:T5:126:SER:HB3	60:TB:77:LEU:HD13	1.98	0.45
55:S7:1:MET:HE1	55:S7:162:TYR:HD1	1.81	0.45
58:TX:89:LYS:HG3	58:TX:94:VAL:HB	1.98	0.45
61:V1:295:ILE:HD13	61:V1:300:LEU:HD12	1.98	0.45
68:T4:19:HIS:ND1	70:B2:108:GLU:OE2	2.43	0.45
80:TE:25:LEU:HD23	80:TE:25:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:LYS:HA	1:1:45:LYS:HD2	1.70	0.45
8:3c:255:LEU:O	9:3d:37:ILE:HG13	2.15	0.45
10:3e:121:TRP:CZ3	10:3e:123:ARG:HG2	2.52	0.45
19:4:381:ILE:HD11	19:4:407:ILE:HD11	1.99	0.45
21:5:315:ILE:HD12	21:5:434:LEU:HD12	1.99	0.45
27:A7:57:PRO:HG3	51:S2:343:ASN:HB3	1.99	0.45
29:AB:60:LYS:HA	29:AB:132:LEU:HD21	1.99	0.45
37:C1:216:TYR:HD1	38:C2:28:ARG:HE	1.64	0.45
57:B9:146:PRO:HB3	57:B9:152:PHE:HD1	1.82	0.45
61:V1:116:ILE:HD12	61:V1:157:ILE:HG12	1.99	0.45
70:B2:61:PHE:HE1	73:B3:67:LEU:HD12	1.82	0.45
4:2B:1:MET:HE3	4:2B:8:TRP:CE3	2.52	0.45
7:3B:472:TRP:O	7:3B:474:LYS:NZ	2.41	0.45
8:3c:102:LYS:HD3	8:3c:102:LYS:HA	1.81	0.45
19:4:271:VAL:O	19:4:388:ARG:NH2	2.50	0.45
85:5B:202:U10:H402	34:B8:98:PHE:HE2	1.82	0.45
23:6:227:PHE:CD2	41:J1:194:ASP:HB3	2.52	0.45
27:A7:164:TRP:CD1	51:S2:252:LEU:HD13	2.52	0.45
52:S3:55:PHE:HA	52:S3:102:ASN:HD21	1.81	0.45
57:B9:72:ASP:O	57:B9:76:MET:HG3	2.17	0.45
68:T4:107:PRO:HD3	70:B2:84:ASP:HB3	1.98	0.45
71:T3:226:ASN:HB3	71:T3:229:GLU:CG	2.42	0.45
1:1:88:PHE:HB2	76:TC:11:ARG:HD3	1.99	0.45
8:3C:52:LEU:HD11	8:3C:81:PHE:HA	1.99	0.45
9:3D:250:ARG:O	9:3D:254:MET:HG2	2.17	0.45
12:3G:40:LYS:O	12:3G:43:GLN:HG3	2.16	0.45
19:4:62:ILE:HD13	19:4:62:ILE:HA	1.84	0.45
19:4:470:LYS:HG3	34:B8:59:GLN:HG2	1.99	0.45
21:5:324:ASN:HB2	21:5:336:ALA:HB2	1.99	0.45
21:5:501:THR:HG23	21:5:580:GLY:O	2.17	0.45
28:A9:306:PHE:HA	28:A9:311:LYS:NZ	2.32	0.45
32:AM:32:GLU:HG3	56:S8:43:THR:HG21	1.99	0.45
37:C1:223:LYS:HD2	38:C2:43:LEU:HD11	1.98	0.45
44:T1:53:GLY:O	44:T1:57:GLN:N	2.50	0.45
44:T1:213:GLN:HG3	44:T1:225:VAL:HG11	1.99	0.45
46:X1:18:LYS:NZ	46:X1:145:LYS:O	2.47	0.45
50:S1:182:ARG:HB3	50:S1:226:VAL:HG12	1.99	0.45
80:TE:31:GLY:O	80:TE:35:LEU:HD23	2.17	0.45
1:1:190:GLN:HB3	1:1:265:GLY:HA2	1.99	0.44
6:3A:260:GLN:HB3	71:T3:111:ILE:HD13	1.98	0.44
7:3B:292:MET:HE2	13:3H:61:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3G:136:ASP:OD2	58:TX:44:LYS:NZ	2.37	0.44
14:3i:97:SER:HB3	14:3i:100:THR:HG23	1.98	0.44
23:6:207:LYS:HE2	51:S2:7:GLN:HA	1.99	0.44
31:AL:113:THR:HG23	44:T1:431:LYS:HE2	2.00	0.44
38:C2:116:LEU:HD22	57:B9:152:PHE:HD2	1.82	0.44
38:C2:163:ARG:NH2	69:T8:16:LEU:O	2.42	0.44
44:T1:125:SER:HB3	44:T1:488:ALA:HB1	1.99	0.44
53:S4:90:THR:OG1	53:S4:101:GLU:OE1	2.32	0.44
56:S8:176:ILE:HG12	93:S8:301:SF4:S1	2.57	0.44
62:V2:198:ASP:HB3	62:V2:204:ASP:HA	1.98	0.44
1:1:104:PHE:CE1	1:1:129:LEU:HB3	2.52	0.44
7:3B:96:THR:HG21	7:3B:218:THR:HA	1.98	0.44
19:4:338:THR:HG23	19:4:367:HIS:NE2	2.32	0.44
28:A9:167:ALA:HA	28:A9:176:LEU:HB3	1.99	0.44
82:AM:202:CDL:H382	74:TA:82:MET:HA	1.98	0.44
37:C1:89:ILE:CG2	37:C1:93:VAL:HG21	2.46	0.44
38:C2:68:ASN:HB3	38:C2:86:GLY:H	1.82	0.44
43:T2:97:LEU:O	43:T2:203:PHE:HA	2.16	0.44
55:S7:38:HIS:O	55:S7:41:VAL:HG22	2.17	0.44
56:S8:140:LYS:N	93:S8:302:SF4:S1	2.80	0.44
61:V1:271:ASN:HB3	61:V1:293:MET:HE2	1.99	0.44
72:P1:52:SER:OG	72:P1:55:GLN:HG3	2.17	0.44
77:P2:82:PHE:HD2	77:P2:100:LEU:HB3	1.82	0.44
8:3C:187:VAL:HG21	85:3C:605:U10:H262	1.99	0.44
9:3D:87:MET:HE3	9:3D:140:ILE:HD13	2.00	0.44
12:3G:60:GLU:OE2	12:3G:249:TYR:OH	2.31	0.44
12:3G:189:TYR:CD2	12:3G:192:LEU:HB2	2.52	0.44
8:3c:68:GLU:HG3	9:3d:89:TYR:HB3	2.00	0.44
19:4:471:ASN:HB3	19:4:474:TYR:HD1	1.82	0.44
22:5B:36:ILE:O	22:5B:40:SER:HB2	2.17	0.44
25:A5:147:TYR:OH	39:C3:276:PRO:O	2.26	0.44
37:C1:160:ALA:HB3	38:C2:172:LEU:HD22	1.99	0.44
50:S1:220:SER:O	50:S1:223:VAL:HG12	2.17	0.44
63:B6:66:PRO:HG2	63:B6:69:LEU:HD12	1.99	0.44
71:T3:66:ARG:HD3	71:T3:277:ARG:HG2	1.99	0.44
5:3:67:PHE:HB3	5:3:71:TYR:CE2	2.53	0.44
9:3D:93:ASP:OD1	10:3E:123:ARG:NH2	2.39	0.44
12:3G:22:ARG:NH1	12:3G:199:ASP:O	2.49	0.44
15:3j:44:ILE:HA	15:3j:48:PHE:HD2	1.82	0.44
37:C1:209:HIS:CE1	38:C2:72:ILE:HG21	2.52	0.44
49:R:30:LEU:O	49:R:34:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S2:79:MET:HE3	51:S2:79:MET:HB3	1.82	0.44
52:S3:64:SER:HB3	52:S3:97:PHE:CE2	2.53	0.44
52:S3:64:SER:HB3	52:S3:97:PHE:CZ	2.52	0.44
56:S8:108:ASN:O	56:S8:112:GLU:N	2.50	0.44
82:C4:401:CDL:H332	82:C4:401:CDL:H531	2.00	0.44
10:3E:202:CYS:O	10:3E:203:ILE:HD13	2.17	0.44
11:3F:22:GLU:HG2	11:3F:23:LEU:N	2.32	0.44
9:3d:187:PRO:HD3	11:3f:62:LEU:HD22	2.00	0.44
14:3i:63:PRO:HB2	15:3j:24:TYR:OH	2.17	0.44
21:5:298:LEU:HD13	82:BM:301:CDL:H212	1.99	0.44
26:A6:156:LYS:HB3	26:A6:160:LEU:HD23	1.98	0.44
34:B8:182:LYS:O	34:B8:185:ILE:HG22	2.18	0.44
37:C1:40:LEU:HD23	37:C1:62:VAL:HB	1.99	0.44
51:S2:78:GLY:O	51:S2:81:TYR:HB2	2.17	0.44
52:S3:126:ASP:HA	52:S3:132:ALA:HB3	1.99	0.44
78:A3:64:PHE:HD1	88:A3:201:3PE:H392	1.83	0.44
7:3B:461:GLY:O	7:3B:465:ARG:HG3	2.18	0.44
83:3J:101:PC1:H322	12:3g:187:PHE:HE2	1.82	0.44
7:3b:210:ARG:HG3	7:3b:288:THR:OG1	2.17	0.44
8:3c:104:TYR:HB2	8:3c:359:PHE:CZ	2.53	0.44
23:6:175:LEU:O	23:6:179:SER:HB3	2.17	0.44
25:A5:138:TYR:O	25:A5:141:GLU:HB3	2.17	0.44
25:A5:157:ARG:NH1	52:S3:40:ASN:O	2.51	0.44
38:C2:52:ILE:HG22	38:C2:53:TYR:H	1.83	0.44
39:C3:31:GLN:NE2	78:A3:12:ASP:OD2	2.51	0.44
43:T2:182:VAL:HG22	50:S1:446:ASN:HB2	1.99	0.44
51:S2:151:PHE:HB3	55:S7:41:VAL:HG21	2.00	0.44
59:A8:200:THR:HG21	81:T7:136:TYR:HE1	1.83	0.44
65:C4:34:TYR:O	65:C4:38:MET:HG3	2.18	0.44
1:1:17:LEU:O	1:1:20:VAL:HG12	2.18	0.44
4:2B:163:SER:HB2	69:T8:79:LYS:HE2	1.98	0.44
7:3B:333:ALA:HB2	7:3B:362:THR:HA	1.99	0.44
82:3B:701:CDL:H852	8:3C:36:PHE:HD1	1.83	0.44
9:3D:316:TYR:CD2	12:3G:177:SER:HA	2.52	0.44
12:3G:180:LYS:HD3	82:3G:401:CDL:OA4	2.17	0.44
8:3c:42:ILE:HG13	8:3c:91:LEU:HD21	2.00	0.44
8:3c:232:GLY:HA3	9:3d:271:LYS:HG3	1.98	0.44
19:4:116:ASP:OD1	19:4:116:ASP:N	2.51	0.44
21:5:709:ILE:HD11	83:5:807:PC1:H281	2.00	0.44
25:A5:141:GLU:OE1	52:S3:52:GLU:HA	2.17	0.44
28:A9:214:LYS:HD3	28:A9:306:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:X1:80:SER:HB2	78:A3:28:ASP:HB2	1.99	0.44
47:T6:84:GLN:HG2	47:T6:85:THR:N	2.32	0.44
1:1:198:ILE:HG12	32:AM:64:GLY:HA3	1.99	0.44
12:3G:54:VAL:HG12	12:3G:57:ARG:HH22	1.83	0.44
8:3c:316:HIS:NE2	8:3c:401:ASN:O	2.47	0.44
22:5B:92:ILE:HD12	22:5B:92:ILE:HA	1.89	0.44
85:5B:202:U10:H371	85:5B:202:U10:H351	1.64	0.44
23:6:237:ASP:HB3	23:6:240:ASN:HB2	1.98	0.44
38:C2:49:ILE:HG23	38:C2:57:PRO:HG2	1.99	0.44
39:C3:281:GLU:O	39:C3:287:TYR:OH	2.27	0.44
44:T1:313:ASP:OD1	44:T1:317:ASN:ND2	2.47	0.44
50:S1:169:LEU:HD22	50:S1:293:HIS:CE1	2.53	0.44
51:S2:40:VAL:HG21	51:S2:62:LEU:HB2	2.00	0.44
71:T3:253:ASP:OD2	71:T3:273:ARG:NH1	2.46	0.44
7:3B:403:ALA:HA	7:3B:467:ALA:HB3	2.00	0.44
8:3C:125:LEU:HD22	8:3C:195:LEU:HD12	2.00	0.44
8:3C:418:PHE:HZ	12:3G:86:LEU:HD13	1.83	0.44
9:3D:214:VAL:O	9:3D:231:MET:HE1	2.18	0.44
10:3E:153:PHE:HB2	10:3E:193:VAL:HG23	1.99	0.44
10:3E:229:VAL:N	10:3E:237:ASN:HD22	2.14	0.44
8:3c:305:TYR:CZ	8:3c:309:LEU:HD11	2.53	0.44
19:4:77:TYR:OH	67:B4:138:THR:HG21	2.18	0.44
31:AL:56:GLU:OE1	31:AL:62:ARG:NH1	2.51	0.44
38:C2:180:PRO:HG2	60:TB:44:PHE:HE2	1.83	0.44
62:V2:124:ILE:HA	62:V2:176:ILE:HG22	2.00	0.44
67:B4:135:GLN:HG2	67:B4:137:TYR:CZ	2.53	0.44
72:P1:145:TYR:HA	72:P1:149:PHE:HB2	2.00	0.44
10:3E:139:PRO:HB3	10:3E:188:THR:HG21	2.00	0.43
6:3a:102:GLU:OE1	6:3a:107:SER:HA	2.18	0.43
7:3b:136:ASN:HD22	7:3b:151:SER:HB3	1.82	0.43
21:5:678:LYS:HA	35:BL:87:THR:HG21	2.00	0.43
21:5:749:ILE:O	21:5:750:LEU:HG	2.18	0.43
40:TD:5:TRP:HB2	45:A1:6:TYR:CD2	2.52	0.43
40:TD:33:PHE:O	40:TD:37:LYS:HG3	2.17	0.43
40:TD:50:LYS:HE3	40:TD:50:LYS:HB2	1.79	0.43
56:S8:95:CYS:HA	56:S8:99:TYR:CD2	2.53	0.43
57:B9:130:PHE:CZ	57:B9:132:PRO:HG3	2.53	0.43
66:AN:157:VAL:HG12	66:AN:158:ASN:N	2.33	0.43
71:T3:289:THR:HG23	71:T3:290:LEU:HD22	2.00	0.43
1:1:240:TYR:CD1	76:TC:2:VAL:HG21	2.53	0.43
2:1B:35:LEU:HG	23:6:238:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3B:492:HIS:HD2	7:3B:494:ASN:HB3	1.83	0.43
9:3D:128:GLU:HG3	16:3M:16:THR:HA	2.01	0.43
6:3a:35:ASP:OD1	6:3a:38:ALA:N	2.51	0.43
19:4:19:TYR:CD2	19:4:105:LEU:HD13	2.53	0.43
21:5:423:VAL:N	21:5:424:PRO:HD2	2.33	0.43
22:5B:50:ILE:O	22:5B:54:THR:HB	2.18	0.43
43:T2:124:PRO:HD3	43:T2:165:HIS:HB2	1.99	0.43
48:T5:175:ALA:O	48:T5:179:GLU:OE1	2.36	0.43
50:S1:180:CYS:SG	50:S1:182:ARG:HB2	2.57	0.43
51:S2:280:PHE:O	51:S2:284:MET:HG2	2.18	0.43
51:S2:339:LYS:HA	51:S2:339:LYS:HD3	1.85	0.43
68:T4:79:ILE:HG13	68:T4:174:ARG:HH11	1.83	0.43
70:B2:67:PRO:HG3	83:B2:201:PC1:H112	1.99	0.43
1:1:32:ILE:O	1:1:35:VAL:HG12	2.18	0.43
7:3b:211:ASP:OD2	10:3e:78:ARG:NH2	2.39	0.43
9:3d:127:GLN:HG3	18:3m:14:ARG:HD3	1.98	0.43
9:3d:151:LYS:HG2	9:3d:158:TRP:HB2	2.00	0.43
13:3h:69:PHE:HB2	13:3h:72:PHE:HB2	2.00	0.43
21:5:202:LEU:HB2	63:B6:84:THR:HG23	2.00	0.43
22:5B:33:ILE:O	22:5B:37:PHE:HB2	2.18	0.43
37:C1:130:TYR:CG	39:C3:149:MET:HE1	2.54	0.43
38:C2:41:GLU:HG3	38:C2:43:LEU:HG	2.00	0.43
46:X1:23:ARG:NH1	46:X1:30:GLU:OE1	2.38	0.43
61:V1:82:LYS:HB3	61:V1:82:LYS:HE3	1.80	0.43
1:1:185:VAL:O	1:1:188:ILE:HG12	2.18	0.43
3:2:24:TRP:HB2	88:A3:201:3PE:H2E2	2.00	0.43
10:3E:246:HIS:CD2	15:3J:57:LYS:HB2	2.54	0.43
6:3a:103:THR:C	6:3a:105:GLU:H	2.27	0.43
8:3c:273:PHE:CE2	8:3c:275:SER:HB2	2.53	0.43
12:3g:291:GLU:O	12:3g:294:GLN:HG3	2.19	0.43
19:4:325:TRP:O	34:B8:53:ASN:ND2	2.40	0.43
20:4L:82:LYS:HE2	23:6:102:TYR:OH	2.18	0.43
82:5:803:CDL:H371	82:5:803:CDL:H132	2.01	0.43
28:A9:275:MET:SD	28:A9:339:PRO:HG3	2.58	0.43
35:BL:67:LEU:HB3	35:BL:110:VAL:HG22	1.99	0.43
39:C3:200:GLN:O	39:C3:204:GLU:OE1	2.36	0.43
43:T2:272:GLY:HA2	43:T2:275:ILE:HG22	2.00	0.43
51:S2:40:VAL:HG11	51:S2:62:LEU:HB2	2.00	0.43
66:AN:182:SER:OG	66:AN:183:SER:N	2.50	0.43
1:1:43:GLU:HG3	2:1B:18:ILE:HG12	1.99	0.43
1:1:104:PHE:HE1	1:1:129:LEU:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:3B:69:LEU:HD11	7:3B:75:LEU:HD11	2.01	0.43
8:3C:148:ILE:O	8:3C:152:LEU:HD23	2.19	0.43
9:3D:119:GLN:HB2	9:3D:122:LYS:HB2	2.00	0.43
6:3a:120:THR:O	6:3a:125:ASN:HA	2.18	0.43
6:3a:313:PRO:O	6:3a:319:ILE:HD11	2.18	0.43
7:3b:51:GLN:O	7:3b:456:SER:OG	2.27	0.43
19:4:435:GLU:HG3	35:BL:114:HIS:CG	2.54	0.43
23:6:216:ASN:HA	23:6:219:THR:HG22	1.99	0.43
25:A5:139:GLY:O	25:A5:142:LEU:HB2	2.18	0.43
38:C2:33:LEU:HD23	38:C2:33:LEU:HA	1.90	0.43
42:FX:77:ILE:HA	42:FX:163:ASN:HD22	1.84	0.43
44:T1:449:PRO:HG2	44:T1:476:THR:HA	2.01	0.43
46:X1:2:SER:N	46:X1:149:ARG:H	2.16	0.43
51:S2:154:ARG:HG3	55:S7:38:HIS:HE1	1.84	0.43
71:T3:290:LEU:HD12	71:T3:304:ILE:HD12	2.01	0.43
8:3C:4:ASN:O	8:3c:14:LYS:NZ	2.47	0.43
8:3C:19:TYR:O	8:3C:23:MET:HB2	2.18	0.43
15:3J:18:LEU:HD13	83:3J:101:PC1:H222	2.01	0.43
6:3a:195:SER:OG	6:3a:225:ARG:NH1	2.33	0.43
83:3b:601:PC1:H232	15:3j:23:GLY:HA3	2.00	0.43
9:3d:93:ASP:OD1	10:3e:123:ARG:NH2	2.50	0.43
12:3g:72:LEU:CD1	12:3g:76:HIS:HE1	2.32	0.43
20:4L:24:LYS:HD3	20:4L:24:LYS:HA	1.71	0.43
21:5:272:THR:HG23	21:5:424:PRO:HG3	1.99	0.43
21:5:723:TYR:OH	77:P2:128:ARG:NH1	2.51	0.43
24:A2:58:ASP:HB3	24:A2:74:PHE:HE1	1.83	0.43
46:X1:44:VAL:HG11	78:A3:79:TRP:CH2	2.54	0.43
50:S1:142:ASP:OD2	53:S4:98:GLN:N	2.48	0.43
50:S1:389:SER:OG	50:S1:509:ASN:O	2.33	0.43
51:S2:181:LEU:HB3	51:S2:331:HIS:NE2	2.34	0.43
53:S4:113:ALA:HB3	53:S4:126:GLY:HA3	2.00	0.43
79:T9:112:PRO:C	79:T9:114:GLN:H	2.27	0.43
21:5:207:ILE:HG12	21:5:266:VAL:HG22	2.00	0.43
21:5:367:LEU:HD23	21:5:367:LEU:HA	1.88	0.43
21:5:582:VAL:HG12	21:5:584:SER:H	1.84	0.43
82:5:805:CDL:H671	82:BM:301:CDL:H121	2.01	0.43
22:5B:26:LYS:HD2	34:B8:66:ILE:HG23	2.00	0.43
23:6:48:LEU:O	23:6:52:ASN:HB2	2.18	0.43
25:A5:90:LYS:HD3	25:A5:90:LYS:HA	1.82	0.43
31:AL:54:VAL:HG12	31:AL:63:TYR:O	2.19	0.43
31:AL:54:VAL:HG11	31:AL:101:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:AL:96:VAL:HG23	31:AL:97:GLY:H	1.82	0.43
44:T1:75:PRO:HB2	44:T1:98:LEU:HD12	2.01	0.43
48:T5:82:GLU:OE1	48:T5:82:GLU:HA	2.19	0.43
48:T5:112:ARG:HG3	48:T5:122:ARG:HB2	2.01	0.43
77:P2:56:ASN:HB3	77:P2:59:ALA:HB3	2.00	0.43
78:A3:22:ASP:O	78:A3:25:GLN:NE2	2.45	0.43
4:2B:3:ILE:HD12	4:2B:8:TRP:CE2	2.53	0.43
6:3A:390:VAL:HB	6:3A:444:ALA:HB1	2.01	0.43
7:3B:311:PRO:HG3	7:3B:470:TRP:CZ2	2.53	0.43
82:3B:701:CDL:HB31	83:3c:501:PC1:H151	2.00	0.43
8:3C:117:LYS:HD2	8:3C:310:PHE:CE1	2.53	0.43
8:3C:207:TRP:CZ3	84:3C:601:HEM:HBD2	2.54	0.43
9:3D:277:ALA:HB1	13:3H:70:ILE:O	2.19	0.43
10:3E:137:LEU:O	10:3E:156:ARG:NH1	2.51	0.43
7:3b:76:ALA:O	7:3b:249:ALA:HA	2.19	0.43
19:4:392:GLU:HG2	67:B4:66:GLN:HB3	2.00	0.43
21:5:193:TYR:CD1	48:T5:121:PRO:HD3	2.53	0.43
21:5:309:PHE:HD1	21:5:350:LEU:HD23	1.83	0.43
21:5:589:PRO:HG2	85:5B:202:U10:H563	2.00	0.43
21:5:698:ASN:HB3	33:B7:118:TRP:CH2	2.54	0.43
28:A9:127:LEU:HG	28:A9:308:ASN:ND2	2.34	0.43
51:S2:92:VAL:HG11	51:S2:381:SER:HA	2.01	0.43
51:S2:441:ASP:O	51:S2:442:ARG:HG2	2.19	0.43
52:S3:32:HIS:NE2	52:S3:110:THR:OG1	2.29	0.43
52:S3:178:ASP:OD1	55:S7:111:ARG:NH1	2.51	0.43
68:T4:121:PHE:CG	68:T4:153:GLN:HG2	2.54	0.43
2:1B:36:ASN:O	2:1B:41:ILE:HG13	2.18	0.43
3:2:104:ILE:HG13	3:2:105:PHE:N	2.34	0.43
6:3A:203:PHE:HE2	6:3A:306:ALA:HB2	1.84	0.43
6:3A:397:THR:HG23	7:3B:131:ALA:HB1	2.01	0.43
6:3A:422:LYS:HB3	12:3G:328:ALA:OXT	2.19	0.43
13:3H:18:GLU:OE1	13:3h:40:SER:OG	2.25	0.43
8:3c:375:TYR:O	8:3c:379:TYR:HB2	2.18	0.43
8:3c:422:LYS:HA	8:3c:422:LYS:HD3	1.66	0.43
12:3g:160:PHE:CE1	12:3g:164:GLU:HG3	2.52	0.43
21:5:427:ALA:O	21:5:431:SER:OG	2.31	0.43
21:5:647:LEU:HD12	64:BM:104:MET:HE1	2.00	0.43
35:BL:145:PHE:HB3	35:BL:146:PRO:HD3	2.01	0.43
37:C1:97:GLU:HG3	38:C2:109:ALA:HB1	2.01	0.43
47:T6:89:TRP:CH2	47:T6:102:MET:HE3	2.53	0.43
50:S1:75:ASN:HB2	61:V1:382:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S3:73:LEU:HD13	52:S3:90:PHE:HZ	1.84	0.43
55:S7:124:PRO:HG2	56:S8:198:GLN:HG3	2.01	0.43
58:TX:155:THR:HA	58:TX:159:LYS:HB2	2.00	0.43
70:B2:49:ARG:HA	70:B2:49:ARG:HD2	1.87	0.43
3:2:85:TRP:O	3:2:88:HIS:HB2	2.18	0.43
3:2:95:SER:HB3	3:2:143:LEU:HD23	2.00	0.43
10:3E:207:TYR:HD1	10:3E:225:LYS:HZ1	1.66	0.43
6:3a:96:ASP:HB3	6:3a:248:ARG:HG2	2.01	0.43
19:4:266:LEU:HG	19:4:270:HIS:CD2	2.53	0.43
29:AB:87:ASN:HB2	29:AB:90:LYS:NZ	2.34	0.43
43:T2:193:LEU:HD23	43:T2:193:LEU:HA	1.90	0.43
45:A1:66:LEU:HB3	80:TE:68:TYR:OH	2.19	0.43
53:S4:138:THR:HG22	53:S4:140:GLU:H	1.84	0.43
68:T4:17:ASP:N	68:T4:17:ASP:OD1	2.52	0.43
71:T3:296:ILE:HG22	71:T3:297:VAL:HG13	2.00	0.43
1:1:76:ILE:HG21	55:S7:18:ARG:HH21	1.84	0.42
6:3A:139:SER:OG	6:3A:141:GLU:OE2	2.37	0.42
8:3C:255:LEU:HB2	9:3D:34:PHE:HD2	1.84	0.42
8:3C:344:PRO:HG3	8:3C:408:LEU:HD12	2.00	0.42
6:3a:238:LYS:HB3	6:3a:238:LYS:HE2	1.80	0.42
8:3c:288:TRP:HE1	8:3c:298:GLY:HA2	1.83	0.42
19:4:250:PHE:CE1	19:4:309:PHE:HB3	2.54	0.42
21:5:476:PHE:CE1	83:5:801:PC1:H322	2.54	0.42
39:C3:128:VAL:HG13	39:C3:145:SER:HB2	2.01	0.42
49:R:24:PHE:CE2	79:T9:64:GLY:HA2	2.54	0.42
50:S1:282:ILE:O	50:S1:283:ASN:OD1	2.37	0.42
50:S1:638:TYR:HE1	53:S4:39:LYS:HD3	1.83	0.42
59:A8:121:ALA:HA	59:A8:124:VAL:HG12	2.00	0.42
73:B3:17:LYS:HE3	73:B3:17:LYS:HB3	1.78	0.42
81:T7:10:ASN:HB3	81:T7:13:SER:HB2	2.01	0.42
1:1:9:PHE:CD1	1:1:12:ILE:HD11	2.53	0.42
1:1:160:MET:HE3	23:6:94:PHE:CG	2.54	0.42
2:1B:49:VAL:HG13	5:3:97:PHE:HE1	1.84	0.42
6:3A:70:THR:HG22	6:3A:78:ILE:HB	2.00	0.42
7:3B:274:ASP:OD2	7:3B:276:THR:OG1	2.38	0.42
6:3a:254:ALA:HB2	6:3a:417:LEU:HD13	2.01	0.42
7:3b:324:PHE:CZ	7:3b:467:ALA:HB2	2.54	0.42
8:3c:336:ILE:HD11	8:3c:341:ILE:HG22	2.01	0.42
23:6:71:LEU:HD21	83:6:301:PC1:H281	2.00	0.42
25:A5:58:LYS:HE2	25:A5:58:LYS:HB3	1.73	0.42
26:A6:126:HIS:CE1	26:A6:127:THR:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:AM:143:ARG:HH11	45:A1:92:LEU:HD22	1.84	0.42
38:C2:51:PRO:HB3	38:C2:56:VAL:HA	2.00	0.42
38:C2:155:ILE:HD13	38:C2:161:LEU:HD11	2.01	0.42
55:S7:22:PHE:CZ	55:S7:62:LEU:HB2	2.54	0.42
81:T7:107:ASN:C	81:T7:107:ASN:HD22	2.27	0.42
1:1:150:PHE:CE2	5:3:57:ILE:HG23	2.55	0.42
8:3C:11:THR:HG23	8:3C:16:ILE:HD11	2.00	0.42
6:3a:409:ALA:HB2	12:3g:323:GLY:C	2.44	0.42
7:3b:359:PRO:HD3	13:3h:32:LYS:HB2	2.01	0.42
23:6:47:TYR:O	23:6:51:VAL:HG22	2.19	0.42
23:6:152:ILE:HG21	32:AM:141:ARG:HG2	2.00	0.42
38:C2:108:VAL:HA	38:C2:136:CYS:O	2.19	0.42
44:T1:132:ASN:HB2	44:T1:135:PHE:HB3	2.01	0.42
44:T1:315:ALA:O	44:T1:318:ALA:HB3	2.20	0.42
51:S2:267:ARG:O	51:S2:289:GLU:HG2	2.19	0.42
68:T4:157:LEU:HD23	68:T4:157:LEU:HA	1.88	0.42
1:1:128:ILE:HG13	23:6:87:VAL:HG12	2.01	0.42
1:1:160:MET:HG2	23:6:94:PHE:CZ	2.55	0.42
7:3B:224:ASN:HA	7:3B:227:ASN:HB2	2.01	0.42
10:3E:229:VAL:HA	10:3E:237:ASN:HB2	2.00	0.42
20:4L:58:SER:HA	23:6:177:TYR:OH	2.20	0.42
26:A6:67:ILE:HD13	26:A6:67:ILE:HA	1.86	0.42
44:T1:315:ALA:O	44:T1:319:GLU:OE1	2.37	0.42
45:A1:82:THR:HG22	80:TE:43:LYS:HB2	2.01	0.42
51:S2:40:VAL:HB	51:S2:61:LEU:HB2	2.02	0.42
51:S2:269:TYR:CE1	51:S2:285:ASN:HB3	2.55	0.42
71:T3:70:ASN:O	71:T3:74:LEU:HG	2.20	0.42
78:A3:71:LEU:HA	78:A3:71:LEU:HD23	1.79	0.42
81:T7:112:SER:O	81:T7:116:ARG:HB2	2.19	0.42
1:1:257:MET:HG3	2:1B:10:ILE:HD11	2.01	0.42
3:2:69:LEU:HD13	46:X1:98:TRP:CD1	2.54	0.42
3:2:152:PHE:HB3	23:6:187:ILE:HG21	2.00	0.42
4:2B:127:LYS:HA	4:2B:127:LYS:HD3	1.73	0.42
6:3A:197:LEU:HD21	13:3h:3:VAL:HG21	2.01	0.42
7:3B:144:GLU:HG3	7:3B:371:TYR:HD1	1.84	0.42
8:3c:79:ASP:CG	9:3d:256:ARG:HH22	2.28	0.42
85:5B:202:U10:H562	85:5B:202:U10:H33	2.00	0.42
25:A5:178:LYS:HG3	25:A5:179:HIS:CD2	2.55	0.42
43:T2:203:PHE:HD2	43:T2:215:LEU:HD11	1.84	0.42
44:T1:380:ASN:N	44:T1:380:ASN:OD1	2.52	0.42
61:V1:54:LYS:HE2	61:V1:54:LYS:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:12:ILE:O	1:1:15:LEU:HB2	2.20	0.42
3:2:86:TRP:NE1	23:6:179:SER:O	2.52	0.42
7:3b:455:ILE:HG13	7:3b:456:SER:N	2.35	0.42
9:3d:264:GLY:O	9:3d:267:ILE:HG22	2.19	0.42
28:A9:39:SER:OG	28:A9:40:ILE:N	2.53	0.42
32:AM:25:HIS:HB2	32:AM:28:ILE:HD11	2.02	0.42
32:AM:45:ILE:HB	32:AM:48:ARG:HD2	2.01	0.42
41:J1:127:LYS:HB2	41:J1:130:THR:HG23	2.01	0.42
43:T2:122:LEU:HD22	43:T2:137:VAL:HG21	2.00	0.42
44:T1:115:LEU:HG	44:T1:146:GLN:HG2	2.01	0.42
58:TX:24:ARG:HH21	58:TX:25:VAL:HG23	1.84	0.42
66:AN:123:TYR:CD2	88:AN:301:3PE:H241	2.54	0.42
68:T4:127:ALA:HB2	83:B2:201:PC1:H3I3	2.01	0.42
71:T3:41:LYS:C	71:T3:42:ARG:HD3	2.44	0.42
81:T7:40:ASP:O	81:T7:44:GLN:HG2	2.19	0.42
3:2:75:ILE:HD12	88:C4:402:3PE:H12	2.01	0.42
3:2:99:TYR:HE1	3:2:103:ILE:HD11	1.85	0.42
5:3:7:ILE:H	5:3:7:ILE:HD12	1.85	0.42
6:3A:254:ALA:HB2	6:3A:417:LEU:HD13	2.01	0.42
82:3B:701:CDL:H861	8:3C:36:PHE:HB2	2.00	0.42
8:3C:13:ILE:HG22	8:3c:1:MET:HE1	2.02	0.42
9:3D:78:ALA:HB1	9:3D:112:PHE:HZ	1.85	0.42
6:3a:370:ASP:OD1	6:3a:370:ASP:N	2.53	0.42
12:3g:141:GLU:HA	12:3g:144:GLU:OE1	2.20	0.42
14:3i:99:GLU:O	14:3i:103:THR:HG23	2.19	0.42
85:5B:202:U10:H272	85:5B:202:U10:H251	1.62	0.42
26:A6:88:ASN:ND2	26:A6:133:LEU:O	2.50	0.42
41:J1:82:VAL:HB	41:J1:85:GLN:HB2	2.00	0.42
82:R:201:CDL:H732	64:BM:149:LEU:HB3	2.01	0.42
50:S1:225:ASP:OD2	50:S1:292:ARG:NH2	2.51	0.42
54:S6:58:LYS:HG2	54:S6:70:GLN:NE2	2.34	0.42
61:V1:162:GLU:HG2	62:V2:167:LEU:HD22	2.02	0.42
71:T3:280:ASP:OD1	71:T3:280:ASP:N	2.51	0.42
77:P2:181:ALA:HA	77:P2:185:SER:HB2	2.00	0.42
78:A3:28:ASP:O	78:A3:34:ASN:ND2	2.53	0.42
1:1:213:GLU:HG2	1:1:255:PHE:CD1	2.55	0.42
3:2:40:ASN:ND2	56:S8:68:ASP:HA	2.35	0.42
3:2:47:VAL:HG11	74:TA:48:GLN:OE1	2.20	0.42
85:3C:605:U10:H222	85:3C:605:U10:H261	1.79	0.42
9:3D:65:TYR:HE2	9:3D:248:TYR:H	1.67	0.42
7:3b:74:ARG:HB2	7:3b:247:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3c:134:LEU:HD11	8:3c:281:TYR:HE1	1.84	0.42
8:3c:367:LEU:HA	8:3c:370:THR:HG22	2.02	0.42
19:4:163:VAL:HG23	19:4:164:THR:HG23	2.02	0.42
19:4:243:THR:HG23	19:4:304:ILE:HD12	2.00	0.42
23:6:121:TYR:HB2	66:AN:78:ILE:HD13	2.02	0.42
32:AM:42:ARG:NH1	82:T7:201:CDL:HA31	2.34	0.42
36:C:94:UNK:C	36:C:96:UNK:N	2.82	0.42
41:J1:153:ARG:NH1	42:FX:72:ASN:O	2.52	0.42
42:FX:102:PRO:HG2	42:FX:129:ASN:OD1	2.20	0.42
42:FX:105:SER:HB3	42:FX:129:ASN:HB3	2.01	0.42
44:T1:201:HIS:CD2	44:T1:361:GLU:HG2	2.54	0.42
50:S1:477:ALA:HB2	50:S1:515:HIS:HA	2.02	0.42
52:S3:137:ARG:HG3	52:S3:150:LYS:HE3	2.02	0.42
67:B4:116:ASN:OD1	67:B4:117:ARG:HG2	2.20	0.42
72:P1:172:MET:HG2	72:P1:190:ARG:HA	2.01	0.42
77:P2:146:ASN:O	77:P2:150:ASN:N	2.52	0.42
1:1:48:SER:O	1:1:52:ARG:N	2.52	0.42
1:1:96:ALA:HA	83:6:302:PC1:H2B2	2.02	0.42
3:2:130:SER:HB3	3:2:163:TYR:CD2	2.54	0.42
3:2:213:TYR:CE1	20:4L:47:PHE:HE2	2.38	0.42
9:3D:56:TRP:NE1	9:3D:173:ASN:OD1	2.47	0.42
6:3a:96:ASP:OD1	6:3a:425:ARG:HD3	2.20	0.42
7:3b:261:GLN:O	7:3b:265:LYS:HG2	2.20	0.42
8:3c:348:SER:O	8:3c:352:ASN:HB2	2.20	0.42
9:3d:289:MET:HE2	10:3e:64:ILE:HD11	2.02	0.42
28:A9:292:ASP:OD1	28:A9:292:ASP:N	2.52	0.42
44:T1:271:PRO:HB2	44:T1:278:ILE:HA	2.01	0.42
45:A1:51:ARG:HA	45:A1:51:ARG:HD2	1.85	0.42
51:S2:123:GLU:OE2	51:S2:261:TYR:OH	2.22	0.42
56:S8:172:MET:HE2	56:S8:208:TYR:CE2	2.54	0.42
62:V2:172:ASN:HB2	62:V2:185:GLU:HG2	2.01	0.42
67:B4:119:ASP:CG	67:B4:120:ASN:N	2.78	0.42
71:T3:281:LEU:O	71:T3:284:GLU:HG3	2.20	0.42
4:2B:1:MET:SD	4:2B:10:ASN:HB3	2.60	0.42
7:3B:344:SER:HB3	7:3B:353:LYS:HA	2.02	0.42
8:3C:116:TRP:NE1	8:3C:312:GLN:HB2	2.35	0.42
8:3C:422:LYS:HB2	12:3G:151:VAL:HG11	2.02	0.42
10:3E:206:PRO:HB3	10:3E:214:TYR:CE1	2.55	0.42
13:3H:13:ASP:OD1	13:3H:13:ASP:N	2.49	0.42
9:3d:115:HIS:CG	9:3d:116:PRO:HD2	2.55	0.42
12:3g:205:GLU:OE2	12:3g:208:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:115:ILE:HG22	19:4:164:THR:HG22	2.00	0.42
22:5B:40:SER:OG	67:B4:92:VAL:HG12	2.19	0.42
31:AL:133:ASN:HB2	56:S8:201:TYR:CD1	2.55	0.42
32:AM:33:ASP:OD1	32:AM:33:ASP:N	2.50	0.42
32:AM:52:LEU:HD22	82:AM:202:CDL:H311	2.02	0.42
43:T2:70:LYS:HB2	43:T2:117:ALA:HA	2.01	0.42
48:T5:185:LYS:O	48:T5:188:ILE:HG22	2.20	0.42
50:S1:210:TYR:CE2	62:V2:30:HIS:HB2	2.55	0.42
59:A8:166:MET:HE1	59:A8:174:PHE:CG	2.55	0.42
63:B6:83:ASN:O	63:B6:87:MET:HG3	2.19	0.42
68:T4:22:LYS:O	68:T4:26:ILE:HG12	2.20	0.42
71:T3:131:GLY:HA2	71:T3:132:PRO:HD3	1.93	0.42
79:T9:66:LEU:HD23	79:T9:66:LEU:HA	1.88	0.42
6:3A:469:ASN:HD22	6:3a:210:THR:HA	1.83	0.41
9:3D:95:LEU:HD21	9:3D:238:PHE:HE1	1.85	0.41
9:3D:269:PRO:HG2	82:3I:603:CDL:H582	2.02	0.41
10:3e:71:ASP:OD1	10:3e:71:ASP:N	2.51	0.41
19:4:3:ASN:OD1	19:4:3:ASN:N	2.52	0.41
19:4:57:ILE:O	19:4:58:PHE:C	2.63	0.41
21:5:188:LEU:HD22	83:B6:201:PC1:H321	2.02	0.41
21:5:391:ILE:HG23	21:5:448:LEU:HD12	2.01	0.41
21:5:589:PRO:HB3	34:B8:98:PHE:CE1	2.55	0.41
28:A9:108:MET:HE3	44:T1:190:GLN:HA	2.01	0.41
32:AM:115:LEU:HD11	75:S5:63:LEU:HG	2.02	0.41
82:TD:101:CDL:HB22	45:A1:40:HIS:CE1	2.55	0.41
42:FX:93:LYS:HB3	42:FX:94:PRO:HD3	2.02	0.41
50:S1:219:LEU:HD23	50:S1:288:SER:HA	2.01	0.41
68:T4:159:ILE:HD13	68:T4:159:ILE:HA	1.95	0.41
71:T3:29:PRO:HA	71:T3:217:SER:HB3	2.01	0.41
5:3:97:PHE:CE2	78:A3:71:LEU:HD21	2.55	0.41
7:3B:238:LYS:HB3	7:3B:238:LYS:HE2	1.83	0.41
12:3G:133:TYR:CE1	13:3H:90:GLN:HG2	2.56	0.41
7:3b:447:PRO:O	7:3b:451:VAL:HG23	2.20	0.41
9:3d:41:GLU:O	11:3f:63:ARG:NH1	2.48	0.41
11:3f:13:MET:HA	11:3f:16:GLN:HG2	2.01	0.41
12:3g:271:LEU:HD12	12:3g:286:GLU:OE1	2.20	0.41
21:5:181:LEU:HA	21:5:294:ILE:CD1	2.49	0.41
27:A7:94:LEU:HD12	27:A7:94:LEU:HA	1.90	0.41
30:AC:110:ASP:OD1	57:B9:41:ARG:NH1	2.53	0.41
35:BL:7:ARG:NH1	66:AN:187:GLU:OE2	2.43	0.41
39:C3:87:TRP:HB3	39:C3:109:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C3:281:GLU:HA	39:C3:284:LYS:HE3	2.01	0.41
41:J1:273:LEU:HD22	41:J1:291:ILE:HD11	2.02	0.41
43:T2:91:ALA:HB2	43:T2:202:LEU:HD21	2.02	0.41
46:X1:49:ASN:HB3	46:X1:107:SER:OG	2.20	0.41
48:T5:181:GLN:HG3	64:BM:198:LEU:HD22	2.02	0.41
51:S2:428:ALA:O	51:S2:432:THR:HG23	2.19	0.41
61:V1:78:ASP:OD2	62:V2:247:TRP:NE1	2.54	0.41
62:V2:198:ASP:O	62:V2:202:GLY:N	2.52	0.41
67:B4:95:LEU:O	67:B4:99:VAL:HG23	2.20	0.41
81:T7:125:LEU:HD23	81:T7:125:LEU:HA	1.92	0.41
7:3B:230:ASP:N	7:3B:230:ASP:OD1	2.53	0.41
12:3G:242:VAL:O	12:3G:246:ILE:HG23	2.21	0.41
7:3b:40:LYS:HB3	7:3b:43:LEU:HD12	2.01	0.41
8:3c:221:ILE:HG22	8:3c:225:GLU:HG3	2.02	0.41
8:3c:225:GLU:O	9:3d:279:TYR:OH	2.32	0.41
19:4:41:GLN:HG2	19:4:43:LEU:H	1.85	0.41
21:5:695:ASN:HB3	33:B7:93:TRP:CZ3	2.55	0.41
22:5B:7:ILE:HD13	72:P1:208:TYR:HD1	1.85	0.41
32:AM:69:ILE:O	32:AM:73:LYS:HG2	2.20	0.41
35:BL:69:GLU:O	35:BL:73:ARG:HG2	2.21	0.41
48:T5:160:LEU:HD13	48:T5:167:ARG:HA	2.01	0.41
53:S4:3:LEU:HD23	53:S4:3:LEU:HA	1.84	0.41
71:T3:300:THR:O	71:T3:304:ILE:HG12	2.19	0.41
77:P2:36:PRO:HG3	77:P2:89:HIS:CE1	2.55	0.41
79:T9:83:LYS:HB3	79:T9:83:LYS:HE2	1.84	0.41
19:4:58:PHE:HZ	49:R:64:VAL:HB	1.86	0.41
19:4:211:LEU:HD23	19:4:211:LEU:HA	1.95	0.41
88:4:601:3PE:O11	88:4:601:3PE:N	2.46	0.41
20:4L:55:THR:O	20:4L:59:ILE:HG13	2.21	0.41
25:A5:41:PRO:HG2	25:A5:44:LEU:HD12	2.02	0.41
25:A5:55:PRO:HD3	74:TA:53:TYR:HE2	1.86	0.41
91:AB:201:ZMP:O2	91:AB:201:ZMP:N2	2.52	0.41
30:AC:53:ASN:HB3	30:AC:56:ASP:HB3	2.02	0.41
39:C3:51:ARG:O	39:C3:74:VAL:HB	2.20	0.41
52:S3:164:GLU:HG3	52:S3:166:PRO:HD3	2.01	0.41
1:1:210:PHE:HA	1:1:255:PHE:HE2	1.85	0.41
8:3C:99:LEU:HD11	8:3C:309:LEU:HD11	2.02	0.41
8:3C:235:ILE:HG12	83:3E:302:PC1:H2F2	2.03	0.41
7:3b:221:ILE:O	7:3b:225:LEU:HG	2.20	0.41
7:3b:224:ASN:O	7:3b:228:ILE:HG12	2.20	0.41
7:3b:492:HIS:HD2	7:3b:494:ASN:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:428:LEU:O	21:5:433:THR:OG1	2.32	0.41
21:5:592:PHE:HE2	34:B8:101:TYR:CD2	2.37	0.41
22:5B:96:ILE:HA	22:5B:100:ILE:HB	2.01	0.41
23:6:211:ILE:HG21	39:C3:243:GLU:HG2	2.02	0.41
25:A5:193:ILE:HB	50:S1:657:ILE:HD12	2.03	0.41
50:S1:516:LYS:HG3	50:S1:517:GLU:HG3	2.02	0.41
56:S8:59:ILE:HD12	56:S8:59:ILE:HA	1.94	0.41
62:V2:248:VAL:HG23	62:V2:251:LYS:HZ2	1.85	0.41
65:C4:92:PHE:HZ	75:S5:35:MET:HE3	1.85	0.41
6:3A:87:SER:HA	7:3B:423:LEU:HD22	2.02	0.41
7:3B:200:LEU:HD22	7:3B:380:TYR:CD1	2.55	0.41
8:3C:344:PRO:O	8:3C:406:ARG:HD3	2.20	0.41
10:3E:109:LEU:HD11	83:3E:302:PC1:H242	2.02	0.41
6:3a:293:GLU:OE1	6:3a:295:ARG:NH2	2.53	0.41
7:3b:163:PHE:O	7:3b:167:ILE:HG12	2.20	0.41
19:4:62:ILE:HD11	49:R:67:VAL:CG2	2.50	0.41
19:4:171:PHE:CE2	19:4:292:GLY:HA2	2.56	0.41
20:4L:56:LEU:HA	20:4L:59:ILE:HG13	2.03	0.41
20:4L:112:LYS:HE3	20:4L:115:TRP:CD2	2.55	0.41
83:5:807:PC1:H3H2	72:P1:138:ALA:HB2	2.01	0.41
31:AL:54:VAL:HG11	31:AL:101:TRP:CH2	2.55	0.41
33:B7:24:TYR:C	33:B7:25:GLN:HG2	2.45	0.41
41:J1:302:GLY:C	75:S5:72:PRO:HG3	2.46	0.41
42:FX:66:LEU:HD22	42:FX:145:CYS:HB3	2.01	0.41
43:T2:77:LYS:HD2	43:T2:238:GLY:HA2	2.01	0.41
44:T1:283:ASN:HB3	44:T1:287:ARG:HH21	1.86	0.41
50:S1:234:ASN:OD1	50:S1:236:PRO:HD2	2.20	0.41
50:S1:309:ARG:NH1	50:S1:572:TYR:O	2.52	0.41
50:S1:377:VAL:HG11	50:S1:385:TYR:HB3	2.01	0.41
56:S8:23:ARG:HE	56:S8:26:ILE:HA	1.84	0.41
59:A8:135:CYS:SG	59:A8:152:GLN:NE2	2.93	0.41
61:V1:376:LYS:HA	61:V1:390:THR:HB	2.01	0.41
62:V2:213:ASN:O	62:V2:216:GLU:HG2	2.20	0.41
67:B4:78:TYR:CZ	67:B4:84:TRP:HB3	2.55	0.41
72:P1:240:TRP:HB2	77:P2:26:ILE:HD13	2.02	0.41
78:A3:57:LEU:HD22	78:A3:60:VAL:HG21	2.03	0.41
5:3:36:GLN:OE1	55:S7:82:GLU:HG2	2.20	0.41
85:3C:605:U10:H172	85:3C:605:U10:H151	1.84	0.41
9:3D:165:ILE:HD12	9:3D:165:ILE:HA	1.92	0.41
6:3a:181:SER:O	6:3a:185:GLU:HG2	2.20	0.41
8:3c:424:LEU:HD23	8:3c:424:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3d:87:MET:HB2	9:3d:140:ILE:HB	2.03	0.41
9:3d:273:PHE:CE2	82:3i:201:CDL:H521	2.56	0.41
19:4:138:ASP:N	19:4:138:ASP:OD1	2.53	0.41
20:4L:34:GLU:O	20:4L:38:LEU:HG	2.20	0.41
21:5:646:ASN:ND2	70:B2:44:ASP:OD1	2.54	0.41
22:5B:75:GLU:OE1	22:5B:75:GLU:N	2.47	0.41
33:B7:9:GLU:OE2	33:B7:13:HIS:HD2	2.04	0.41
37:C1:93:VAL:HG12	37:C1:121:VAL:N	2.30	0.41
37:C1:101:ILE:HG12	37:C1:129:ILE:HB	2.03	0.41
40:TD:37:LYS:HB3	40:TD:37:LYS:HE2	1.93	0.41
40:TD:37:LYS:HB3	40:TD:41:ARG:HH12	1.86	0.41
40:TD:37:LYS:HB3	40:TD:41:ARG:NH1	2.36	0.41
41:J1:251:ILE:O	41:J1:255:THR:OG1	2.26	0.41
44:T1:133:GLU:HG2	44:T1:159:PHE:CE2	2.54	0.41
71:T3:263:PHE:HD2	71:T3:264:LEU:HD12	1.86	0.41
72:P1:166:VAL:HG22	72:P1:173:ILE:HG22	2.03	0.41
8:3C:24:THR:HB	8:3C:219:GLU:HG3	2.03	0.41
8:3C:117:LYS:H	8:3C:117:LYS:HG2	1.71	0.41
8:3C:120:VAL:HG11	8:3C:310:PHE:HB2	2.01	0.41
21:5:566:PRO:O	82:5:803:CDL:H251	2.21	0.41
25:A5:109:ILE:O	25:A5:113:THR:HG22	2.21	0.41
29:AB:93:LEU:HD22	29:AB:97:ASP:HB3	2.02	0.41
31:AL:8:ILE:H	31:AL:8:ILE:HD12	1.86	0.41
31:AL:15:LYS:HG3	31:AL:50:TYR:HB3	2.02	0.41
37:C1:229:ASP:HB3	78:A3:20:VAL:HG22	2.02	0.41
43:T2:216:ILE:HG12	43:T2:255:LEU:HD11	2.02	0.41
44:T1:230:LEU:HD23	44:T1:230:LEU:HA	1.89	0.41
48:T5:153:ARG:NH2	63:B6:123:ALA:O	2.53	0.41
50:S1:471:PRO:HB2	50:S1:501:VAL:HG22	2.02	0.41
50:S1:641:ALA:HB2	50:S1:648:LEU:HD11	2.03	0.41
51:S2:74:PRO:HD2	51:S2:77:GLN:HG3	2.02	0.41
54:S6:65:LYS:HG3	56:S8:211:TYR:CZ	2.55	0.41
59:A8:167:ASP:OD2	59:A8:169:ILE:HG22	2.20	0.41
3:2:40:ASN:HD22	56:S8:68:ASP:HA	1.86	0.41
3:2:198:TRP:CH2	20:4L:29:ILE:HG22	2.56	0.41
6:3A:295:ARG:NH2	6:3A:472:PRO:O	2.45	0.41
7:3B:199:LEU:HD12	7:3B:199:LEU:HA	1.89	0.41
7:3B:408:GLN:HA	7:3B:411:ILE:HD12	2.02	0.41
8:3C:111:GLU:HB2	8:3C:205:TYR:HE2	1.86	0.41
8:3C:310:PHE:CE2	12:3G:184:LEU:HG	2.56	0.41
9:3D:75:GLN:HG2	9:3D:108:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3D:247:GLY:C	9:3D:249:LYS:H	2.27	0.41
9:3D:260:VAL:HG12	83:3E:302:PC1:H2I2	2.03	0.41
13:3H:17:ASP:OD2	13:3h:12:LYS:NZ	2.42	0.41
6:3a:256:VAL:HG12	7:3b:38:PHE:HZ	1.86	0.41
8:3c:164:TYR:CZ	8:3c:171:LYS:HE3	2.55	0.41
8:3c:256:SER:OG	8:3c:257:TYR:N	2.53	0.41
8:3c:415:PHE:CD2	12:3g:39:PHE:HB3	2.55	0.41
9:3d:168:ARG:NE	86:3d:401:HEC:O2A	2.52	0.41
10:3e:52:VAL:HG22	14:3i:27:VAL:HG11	2.02	0.41
13:3h:74:PHE:HE2	82:3i:201:CDL:H751	1.86	0.41
14:3i:99:GLU:H	14:3i:99:GLU:CD	2.29	0.41
21:5:340:PHE:O	21:5:344:LYS:HG2	2.20	0.41
27:A7:164:TRP:HZ2	51:S2:268:SER:HB3	1.86	0.41
30:AC:97:MET:HG3	30:AC:113:LEU:HD22	2.03	0.41
39:C3:53:ILE:HD12	39:C3:75:ILE:HG12	2.02	0.41
41:J1:87:ARG:HG2	41:J1:91:PHE:CZ	2.56	0.41
44:T1:264:LYS:NZ	44:T1:304:ASP:O	2.54	0.41
49:R:113:ARG:HD2	49:R:116:ILE:HD11	2.03	0.41
50:S1:395:GLU:OE2	50:S1:417:ARG:NH1	2.53	0.41
53:S4:56:VAL:HG22	53:S4:154:GLU:HG3	2.03	0.41
55:S7:35:GLU:HG2	55:S7:128:PRO:O	2.21	0.41
57:B9:134:GLY:HA2	57:B9:137:SER:O	2.20	0.41
61:V1:327:MET:HE2	61:V1:443:PHE:HE2	1.86	0.41
62:V2:127:THR:HB	87:V2:300:FES:S2	2.61	0.41
83:C4:403:PC1:H232	69:T8:50:ILE:HG21	2.03	0.41
70:B2:53:THR:HG23	73:B3:59:PRO:HA	2.02	0.41
71:T3:229:GLU:HA	71:T3:232:ILE:HG22	2.03	0.41
81:T7:93:MET:HA	81:T7:93:MET:HE2	2.02	0.41
3:2:221:THR:HA	3:2:226:ILE:HD11	2.03	0.41
4:2B:77:PRO:HA	4:2B:82:PHE:CD1	2.56	0.41
8:3C:200:GLY:O	8:3C:203:MET:HG2	2.21	0.41
8:3C:345:LYS:O	12:3G:89:MET:HE2	2.21	0.41
8:3c:117:LYS:HB3	8:3c:310:PHE:CZ	2.55	0.41
10:3e:59:ASN:HA	12:3g:307:THR:HG22	2.02	0.41
12:3g:130:ARG:HH21	13:3h:95:ARG:HD3	1.85	0.41
19:4:190:SER:HB2	19:4:274:PRO:HD3	2.03	0.41
20:4L:20:VAL:HG21	22:5B:83:LEU:HB2	2.02	0.41
20:4L:110:LEU:HD23	20:4L:110:LEU:HA	1.93	0.41
83:5:801:PC1:H281	83:5:801:PC1:H3B1	2.02	0.41
22:5B:11:PHE:O	22:5B:15:VAL:HG23	2.21	0.41
27:A7:183:ASP:OD1	51:S2:204:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:J1:194:ASP:OD1	41:J1:194:ASP:N	2.54	0.41
45:A1:61:LYS:HA	45:A1:61:LYS:HD3	1.85	0.41
51:S2:264:LEU:HD13	51:S2:293:ILE:HG23	2.03	0.41
82:C4:401:CDL:H221	88:C4:402:3PE:H2H1	2.03	0.41
78:A3:49:LYS:HE3	78:A3:49:LYS:HB3	1.89	0.41
81:T7:49:THR:HG23	81:T7:112:SER:HB3	2.03	0.41
6:3A:110:LEU:HD23	6:3A:110:LEU:HA	1.84	0.40
82:3C:603:CDL:OB4	12:3G:130:ARG:NH1	2.55	0.40
10:3E:242:ASN:HA	15:3J:53:ARG:CZ	2.51	0.40
13:3H:84:LEU:HA	13:3H:88:PHE:HD2	1.86	0.40
7:3b:492:HIS:HD1	8:3c:218:THR:HB	1.86	0.40
19:4:45:GLN:HG3	60:TB:21:PHE:HA	2.03	0.40
21:5:239:SER:HB3	21:5:242:PHE:HB3	2.03	0.40
21:5:709:ILE:HD13	21:5:709:ILE:HA	1.91	0.40
24:A2:19:PHE:HB3	24:A2:29:LEU:HD23	2.02	0.40
24:A2:65:TYR:OH	24:A2:90:LEU:O	2.32	0.40
27:A7:219:LYS:HB3	27:A7:219:LYS:HE2	1.92	0.40
28:A9:124:GLY:HA3	90:A9:401:NDP:O3D	2.20	0.40
28:A9:293:ILE:O	28:A9:297:ILE:HG12	2.21	0.40
41:J1:153:ARG:NH2	42:FX:57:ILE:HD11	2.36	0.40
44:T1:204:VAL:HG12	44:T1:368:ALA:HB2	2.03	0.40
55:S7:131:GLU:HB3	56:S8:196:TYR:CE1	2.56	0.40
61:V1:310:GLY:HA3	61:V1:314:ASN:HD22	1.85	0.40
61:V1:313:ASP:OD1	61:V1:313:ASP:N	2.44	0.40
77:P2:108:LYS:HB2	77:P2:108:LYS:HE3	1.87	0.40
79:T9:3:LEU:HD13	79:T9:15:VAL:HG21	2.03	0.40
3:2:142:PHE:CE1	3:2:291:ILE:HA	2.56	0.40
6:3a:99:THR:HG21	6:3a:221:LEU:HA	2.03	0.40
8:3c:120:VAL:HG11	8:3c:310:PHE:HA	2.03	0.40
21:5:432:ALA:HA	21:5:436:SER:OG	2.21	0.40
21:5:433:THR:OG1	21:5:434:LEU:N	2.53	0.40
38:C2:107:LYS:NZ	39:C3:110:LEU:O	2.55	0.40
40:TD:62:VAL:HG21	59:A8:168:PRO:HB2	2.03	0.40
50:S1:695:SER:HB3	50:S1:698:MET:HB2	2.03	0.40
51:S2:180:ASN:ND2	51:S2:183:ALA:HB2	2.36	0.40
57:B9:175:ASP:OD1	57:B9:175:ASP:N	2.53	0.40
58:TX:82:ILE:HD12	58:TX:89:LYS:HB2	2.03	0.40
58:TX:106:GLY:HA3	58:TX:144:GLU:O	2.21	0.40
72:P1:195:GLU:HB3	72:P1:226:ARG:HH21	1.85	0.40
7:3B:392:LEU:O	7:3B:396:GLN:NE2	2.55	0.40
12:3G:311:LYS:HD2	12:3G:311:LYS:HA	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3a:298:THR:HG22	6:3a:299:GLU:N	2.37	0.40
6:3a:397:THR:HG23	7:3b:131:ALA:HB1	2.03	0.40
8:3c:214:ASP:OD1	8:3c:214:ASP:N	2.53	0.40
9:3d:79:ARG:HA	9:3d:79:ARG:HD3	1.93	0.40
10:3e:53:THR:O	10:3e:54:SER:HB3	2.22	0.40
19:4:142:TYR:CG	19:4:143:TRP:N	2.89	0.40
19:4:291:TYR:CZ	19:4:295:LYS:HE2	2.56	0.40
21:5:168:ASN:O	21:5:228:TYR:OH	2.34	0.40
31:AL:67:PHE:CE1	31:AL:75:ARG:HD2	2.57	0.40
44:T1:255:ARG:NH1	44:T1:261:ASN:O	2.54	0.40
47:T6:65:HIS:HA	47:T6:85:THR:HB	2.03	0.40
50:S1:628:LEU:HA	50:S1:629:PRO:HD3	1.89	0.40
53:S4:101:GLU:OE1	53:S4:101:GLU:N	2.55	0.40
61:V1:202:ALA:HB1	62:V2:111:MET:HB3	2.03	0.40
62:V2:179:ASN:O	62:V2:181:LYS:HG2	2.22	0.40
68:T4:189:PHE:O	68:T4:193:VAL:HG23	2.22	0.40
68:T4:199:ILE:O	68:T4:203:ARG:HG3	2.22	0.40
74:TA:38:GLU:O	74:TA:41:LYS:NZ	2.53	0.40
3:2:142:PHE:CZ	3:2:291:ILE:HG13	2.57	0.40
3:2:290:LEU:HD23	3:2:290:LEU:HA	1.92	0.40
10:3E:126:ARG:HH22	16:3M:7:MET:HE2	1.86	0.40
12:3G:314:LEU:HD23	12:3G:314:LEU:HA	1.95	0.40
7:3b:401:GLU:OE2	7:3b:504:TRP:N	2.54	0.40
8:3c:38:THR:HA	8:3c:41:THR:HG22	2.04	0.40
12:3g:199:ASP:OD1	12:3g:200:ARG:N	2.54	0.40
21:5:631:ILE:HD13	21:5:631:ILE:HA	1.93	0.40
32:AM:49:LYS:HD3	82:AM:202:CDL:H131	2.04	0.40
44:T1:206:ARG:NH1	44:T1:209:GLN:OE1	2.52	0.40
44:T1:303:ARG:NH1	44:T1:333:THR:OG1	2.54	0.40
47:T6:43:LEU:HD23	47:T6:43:LEU:HA	1.92	0.40
59:A8:162:GLU:N	59:A8:162:GLU:OE1	2.53	0.40
64:BM:129:MET:O	64:BM:129:MET:HG2	2.22	0.40
71:T3:186:THR:O	71:T3:190:GLN:HG2	2.21	0.40
80:TE:55:MET:HE3	80:TE:55:MET:HB2	2.01	0.40
4:2B:119:LEU:O	19:4:187:TYR:OH	2.37	0.40
4:2B:171:TYR:HA	65:C4:59:LEU:HD13	2.04	0.40
7:3B:50:PRO:HG2	7:3B:53:GLU:HG2	2.04	0.40
9:3D:231:MET:HE3	9:3D:231:MET:HB2	1.99	0.40
9:3D:268:LEU:HD23	9:3D:268:LEU:HA	1.83	0.40
12:3G:29:LYS:HD2	12:3G:167:SER:HB3	2.04	0.40
19:4:7:ILE:HG12	19:4:77:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:245:ILE:O	19:4:249:ILE:HG12	2.21	0.40
27:A7:17:ILE:HD12	56:S8:98:VAL:HG11	2.04	0.40
32:AM:64:GLY:O	32:AM:68:ILE:HG12	2.21	0.40
39:C3:250:MET:CE	51:S2:5:ILE:HD12	2.52	0.40
46:X1:139:ASP:HA	46:X1:144:LYS:HE3	2.02	0.40
49:R:45:PHE:O	49:R:49:LEU:HD23	2.22	0.40
50:S1:362:LEU:HD23	50:S1:362:LEU:HA	1.93	0.40
50:S1:422:THR:HA	50:S1:426:LEU:HB3	2.03	0.40
56:S8:141:LEU:HD23	56:S8:141:LEU:HA	1.94	0.40
60:TB:40:LYS:NZ	60:TB:48:GLU:OE2	2.53	0.40
68:T4:37:ASP:OD2	72:P1:133:TYR:OH	2.27	0.40
68:T4:115:TYR:HB3	83:B2:201:PC1:H322	2.02	0.40
69:T8:120:LYS:HA	69:T8:120:LYS:HD3	1.93	0.40
71:T3:195:ASN:ND2	71:T3:310:ARG:O	2.38	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	1	282/284 (99%)	272 (96%)	10 (4%)	0	100	100
2	1B	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
3	2	357/360 (99%)	349 (98%)	8 (2%)	0	100	100
4	2B	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
5	3	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
6	3A	449/482 (93%)	437 (97%)	12 (3%)	0	100	100
6	3a	447/482 (93%)	435 (97%)	12 (3%)	0	100	100
7	3B	477/513 (93%)	468 (98%)	9 (2%)	0	100	100
7	3b	476/513 (93%)	461 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	3C	424/426 (100%)	415 (98%)	9 (2%)	0	100	100
8	3c	424/426 (100%)	404 (95%)	20 (5%)	0	100	100
9	3D	293/319 (92%)	275 (94%)	18 (6%)	0	100	100
9	3d	283/319 (89%)	267 (94%)	16 (6%)	0	100	100
10	3E	226/269 (84%)	215 (95%)	10 (4%)	1 (0%)	30	51
10	3e	100/269 (37%)	91 (91%)	9 (9%)	0	100	100
11	3F	87/90 (97%)	86 (99%)	1 (1%)	0	100	100
11	3f	73/90 (81%)	73 (100%)	0	0	100	100
12	3G	305/328 (93%)	291 (95%)	14 (5%)	0	100	100
12	3g	313/328 (95%)	298 (95%)	15 (5%)	0	100	100
13	3H	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
13	3h	122/130 (94%)	108 (88%)	14 (12%)	0	100	100
14	3I	112/119 (94%)	106 (95%)	6 (5%)	0	100	100
14	3i	109/119 (92%)	101 (93%)	8 (7%)	0	100	100
15	3J	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
15	3j	49/62 (79%)	47 (96%)	2 (4%)	0	100	100
16	3M	17/19 (90%)	14 (82%)	3 (18%)	0	100	100
17	3l	22/24 (92%)	22 (100%)	0	0	100	100
18	3m	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
19	4	503/505 (100%)	481 (96%)	22 (4%)	0	100	100
20	4L	114/116 (98%)	114 (100%)	0	0	100	100
21	5	585/750 (78%)	576 (98%)	9 (2%)	0	100	100
22	5B	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
23	6	242/255 (95%)	228 (94%)	14 (6%)	0	100	100
24	A2	90/103 (87%)	90 (100%)	0	0	100	100
25	A5	153/206 (74%)	150 (98%)	3 (2%)	0	100	100
26	A6	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
27	A7	279/282 (99%)	274 (98%)	5 (2%)	0	100	100
28	A9	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
29	AB	110/138 (80%)	108 (98%)	2 (2%)	0	100	100
30	AC	96/133 (72%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	AL	191/194 (98%)	184 (96%)	7 (4%)	0	100	100
32	AM	158/175 (90%)	152 (96%)	6 (4%)	0	100	100
33	B7	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
34	B8	167/207 (81%)	166 (99%)	1 (1%)	0	100	100
35	BL	173/188 (92%)	167 (96%)	6 (4%)	0	100	100
37	C1	227/257 (88%)	213 (94%)	14 (6%)	0	100	100
38	C2	221/233 (95%)	209 (95%)	12 (5%)	0	100	100
39	C3	344/346 (99%)	337 (98%)	7 (2%)	0	100	100
40	TD	69/73 (94%)	68 (99%)	1 (1%)	0	100	100
41	J1	256/317 (81%)	253 (99%)	3 (1%)	0	100	100
42	FX	144/172 (84%)	142 (99%)	2 (1%)	0	100	100
43	T2	269/333 (81%)	259 (96%)	10 (4%)	0	100	100
44	T1	479/516 (93%)	465 (97%)	14 (3%)	0	100	100
45	A1	90/94 (96%)	87 (97%)	3 (3%)	0	100	100
46	X1	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
47	T6	107/144 (74%)	104 (97%)	3 (3%)	0	100	100
48	T5	132/205 (64%)	129 (98%)	3 (2%)	0	100	100
49	R	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
50	S1	685/718 (95%)	667 (97%)	18 (3%)	0	100	100
51	S2	440/442 (100%)	427 (97%)	13 (3%)	0	100	100
52	S3	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
53	S4	173/185 (94%)	166 (96%)	7 (4%)	0	100	100
54	S6	88/132 (67%)	87 (99%)	1 (1%)	0	100	100
55	S7	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
56	S8	216/236 (92%)	212 (98%)	4 (2%)	0	100	100
57	B9	184/189 (97%)	177 (96%)	7 (4%)	0	100	100
58	TX	142/166 (86%)	140 (99%)	2 (1%)	0	100	100
59	A8	130/238 (55%)	129 (99%)	1 (1%)	0	100	100
60	TB	94/113 (83%)	89 (95%)	5 (5%)	0	100	100
61	V1	440/474 (93%)	426 (97%)	14 (3%)	0	100	100
62	V2	229/274 (84%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	B6	68/129 (53%)	64 (94%)	4 (6%)	0	100	100
64	BM	141/214 (66%)	139 (99%)	2 (1%)	0	100	100
65	C4	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
66	AN	229/231 (99%)	226 (99%)	3 (1%)	0	100	100
67	B4	106/108 (98%)	103 (97%)	3 (3%)	0	100	100
68	T4	166/212 (78%)	164 (99%)	2 (1%)	0	100	100
69	T8	127/135 (94%)	124 (98%)	3 (2%)	0	100	100
70	B2	116/126 (92%)	112 (97%)	4 (3%)	0	100	100
71	T3	299/311 (96%)	294 (98%)	4 (1%)	1 (0%)	36	58
72	P1	226/251 (90%)	218 (96%)	8 (4%)	0	100	100
73	B3	66/83 (80%)	63 (96%)	3 (4%)	0	100	100
74	TA	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
75	S5	83/94 (88%)	80 (96%)	3 (4%)	0	100	100
76	TC	89/93 (96%)	87 (98%)	2 (2%)	0	100	100
77	P2	165/189 (87%)	164 (99%)	1 (1%)	0	100	100
78	A3	125/135 (93%)	122 (98%)	3 (2%)	0	100	100
79	T9	130/135 (96%)	126 (97%)	4 (3%)	0	100	100
80	TE	47/71 (66%)	47 (100%)	0	0	100	100
81	T7	140/143 (98%)	135 (96%)	5 (4%)	0	100	100
All	All	17880/19899 (90%)	17305 (97%)	573 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
71	T3	41	LYS
10	3E	229	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	1	250/250 (100%)	250 (100%)	0	100	100
2	1B	55/55 (100%)	55 (100%)	0	100	100
3	2	345/346 (100%)	345 (100%)	0	100	100
4	2B	170/170 (100%)	170 (100%)	0	100	100
5	3	111/112 (99%)	111 (100%)	0	100	100
6	3A	384/409 (94%)	384 (100%)	0	100	100
6	3a	382/409 (93%)	382 (100%)	0	100	100
7	3B	410/440 (93%)	410 (100%)	0	100	100
7	3b	409/440 (93%)	409 (100%)	0	100	100
8	3C	386/386 (100%)	386 (100%)	0	100	100
8	3c	386/386 (100%)	386 (100%)	0	100	100
9	3D	255/274 (93%)	255 (100%)	0	100	100
9	3d	247/274 (90%)	247 (100%)	0	100	100
10	3E	200/237 (84%)	200 (100%)	0	100	100
10	3e	92/237 (39%)	92 (100%)	0	100	100
11	3F	80/81 (99%)	80 (100%)	0	100	100
11	3f	69/81 (85%)	69 (100%)	0	100	100
12	3G	269/289 (93%)	269 (100%)	0	100	100
12	3g	278/289 (96%)	278 (100%)	0	100	100
13	3H	117/118 (99%)	117 (100%)	0	100	100
13	3h	112/118 (95%)	112 (100%)	0	100	100
14	3I	104/109 (95%)	104 (100%)	0	100	100
14	3i	102/109 (94%)	102 (100%)	0	100	100
15	3J	53/56 (95%)	53 (100%)	0	100	100
15	3j	47/56 (84%)	47 (100%)	0	100	100
16	3M	16/16 (100%)	16 (100%)	0	100	100
17	3l	1/1 (100%)	1 (100%)	0	100	100
18	3m	7/7 (100%)	7 (100%)	0	100	100
19	4	463/463 (100%)	463 (100%)	0	100	100
20	4L	108/108 (100%)	108 (100%)	0	100	100
21	5	533/694 (77%)	533 (100%)	0	100	100
22	5B	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	6	233/244 (96%)	233 (100%)	0	100	100
24	A2	82/93 (88%)	82 (100%)	0	100	100
25	A5	144/186 (77%)	144 (100%)	0	100	100
26	A6	154/154 (100%)	154 (100%)	0	100	100
27	A7	256/257 (100%)	256 (100%)	0	100	100
28	A9	288/311 (93%)	288 (100%)	0	100	100
29	AB	104/129 (81%)	104 (100%)	0	100	100
30	AC	88/119 (74%)	88 (100%)	0	100	100
31	AL	169/170 (99%)	169 (100%)	0	100	100
32	AM	142/156 (91%)	142 (100%)	0	100	100
33	B7	97/99 (98%)	97 (100%)	0	100	100
34	B8	151/180 (84%)	151 (100%)	0	100	100
35	BL	160/172 (93%)	160 (100%)	0	100	100
37	C1	194/218 (89%)	194 (100%)	0	100	100
38	C2	165/197 (84%)	165 (100%)	0	100	100
39	C3	309/309 (100%)	309 (100%)	0	100	100
40	TD	63/65 (97%)	63 (100%)	0	100	100
41	J1	220/270 (82%)	220 (100%)	0	100	100
42	FX	130/152 (86%)	130 (100%)	0	100	100
43	T2	230/280 (82%)	230 (100%)	0	100	100
44	T1	421/454 (93%)	421 (100%)	0	100	100
45	A1	87/89 (98%)	87 (100%)	0	100	100
46	X1	132/133 (99%)	132 (100%)	0	100	100
47	T6	97/131 (74%)	97 (100%)	0	100	100
48	T5	115/179 (64%)	115 (100%)	0	100	100
49	R	98/98 (100%)	98 (100%)	0	100	100
50	S1	588/617 (95%)	588 (100%)	0	100	100
51	S2	399/399 (100%)	399 (100%)	0	100	100
52	S3	191/191 (100%)	190 (100%)	1 (0%)	81	92
53	S4	157/163 (96%)	157 (100%)	0	100	100
54	S6	80/116 (69%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	S7	137/137 (100%)	137 (100%)	0	100	100
56	S8	197/215 (92%)	197 (100%)	0	100	100
57	B9	169/172 (98%)	169 (100%)	0	100	100
58	TX	128/147 (87%)	128 (100%)	0	100	100
59	A8	121/224 (54%)	120 (99%)	1 (1%)	73	88
60	TB	82/97 (84%)	82 (100%)	0	100	100
61	V1	362/392 (92%)	362 (100%)	0	100	100
62	V2	205/236 (87%)	205 (100%)	0	100	100
63	B6	64/117 (55%)	64 (100%)	0	100	100
64	BM	125/182 (69%)	125 (100%)	0	100	100
65	C4	88/89 (99%)	88 (100%)	0	100	100
66	AN	199/199 (100%)	199 (100%)	0	100	100
67	B4	94/94 (100%)	94 (100%)	0	100	100
68	T4	151/190 (80%)	151 (100%)	0	100	100
69	T8	116/122 (95%)	116 (100%)	0	100	100
70	B2	102/109 (94%)	102 (100%)	0	100	100
71	T3	267/275 (97%)	267 (100%)	0	100	100
72	P1	206/223 (92%)	206 (100%)	0	100	100
73	B3	63/74 (85%)	63 (100%)	0	100	100
74	TA	94/94 (100%)	94 (100%)	0	100	100
75	S5	76/83 (92%)	76 (100%)	0	100	100
76	TC	82/84 (98%)	82 (100%)	0	100	100
77	P2	158/178 (89%)	158 (100%)	0	100	100
78	A3	107/114 (94%)	107 (100%)	0	100	100
79	T9	118/121 (98%)	118 (100%)	0	100	100
80	TE	44/63 (70%)	44 (100%)	0	100	100
81	T7	124/125 (99%)	124 (100%)	0	100	100
All	All	15962/17605 (91%)	15960 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	S3	3	ASN

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Mol	Chain	Res	Type
59	A8	187	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (196) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	ASN
1	1	162	ASN
2	1B	36	ASN
3	2	116	HIS
3	2	188	ASN
4	2B	11	ASN
4	2B	117	GLN
4	2B	126	ASN
5	3	11	GLN
5	3	12	ASN
6	3A	88	GLN
7	3B	111	GLN
7	3B	226	HIS
7	3B	390	GLN
7	3B	420	ASN
8	3C	209	ASN
9	3D	80	ASN
9	3D	107	GLN
9	3D	243	GLN
10	3E	32	GLN
10	3E	91	GLN
10	3E	199	HIS
11	3F	37	GLN
11	3F	76	GLN
12	3G	156	ASN
12	3G	217	GLN
12	3G	258	GLN
12	3G	294	GLN
13	3H	42	ASN
13	3H	60	GLN
14	3I	67	GLN
6	3a	188	GLN
6	3a	310	GLN
6	3a	347	GLN
6	3a	431	GLN
6	3a	438	GLN
6	3a	446	GLN

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Mol	Chain	Res	Type
7	3b	170	ASN
7	3b	216	GLN
8	3c	209	ASN
9	3d	50	HIS
9	3d	183	HIS
9	3d	243	GLN
9	3d	300	HIS
9	3d	307	ASN
10	3e	39	HIS
10	3e	80	HIS
10	3e	91	GLN
11	3f	15	GLN
11	3f	76	GLN
12	3g	44	HIS
12	3g	230	GLN
13	3h	35	ASN
13	3h	60	GLN
13	3h	90	GLN
14	3i	43	ASN
14	3i	58	ASN
19	4	45	GLN
19	4	46	ASN
19	4	93	ASN
21	5	203	ASN
21	5	290	ASN
21	5	389	ASN
21	5	561	ASN
21	5	698	ASN
21	5	718	ASN
23	6	52	ASN
23	6	163	ASN
23	6	201	ASN
23	6	243	ASN
24	A2	5	GLN
25	A5	48	ASN
27	A7	21	GLN
27	A7	46	GLN
28	A9	131	ASN
28	A9	141	HIS
28	A9	155	ASN
28	A9	223	ASN
28	A9	359	ASN

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Mol	Chain	Res	Type
29	AB	28	GLN
29	AB	46	ASN
29	AB	78	ASN
29	AB	98	GLN
31	AL	61	ASN
31	AL	137	ASN
32	AM	160	GLN
33	B7	78	HIS
34	B8	69	ASN
34	B8	115	ASN
35	BL	114	HIS
35	BL	165	GLN
37	C1	186	ASN
38	C2	131	ASN
39	C3	31	GLN
39	C3	52	ASN
39	C3	112	ASN
39	C3	120	GLN
39	C3	133	ASN
39	C3	174	ASN
39	C3	189	GLN
39	C3	207	GLN
39	C3	242	HIS
40	TD	64	GLN
41	J1	71	GLN
41	J1	207	GLN
42	FX	28	HIS
42	FX	34	GLN
42	FX	70	GLN
42	FX	163	ASN
43	T2	47	ASN
43	T2	208	GLN
44	T1	150	HIS
44	T1	166	ASN
44	T1	214	ASN
44	T1	250	GLN
44	T1	359	ASN
44	T1	388	GLN
44	T1	435	HIS
44	T1	442	ASN
44	T1	450	GLN
44	T1	452	ASN

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Mol	Chain	Res	Type
44	T1	454	GLN
45	A1	68	HIS
45	A1	87	ASN
46	X1	82	ASN
46	X1	140	ASN
47	T6	107	GLN
49	R	3	ASN
49	R	11	ASN
50	S1	134	GLN
50	S1	371	GLN
50	S1	599	GLN
51	S2	22	GLN
51	S2	325	GLN
52	S3	2	GLN
52	S3	3	ASN
52	S3	187	GLN
53	S4	60	GLN
54	S6	64	HIS
54	S6	70	GLN
57	B9	164	ASN
57	B9	168	GLN
58	TX	29	ASN
58	TX	119	ASN
59	A8	119	GLN
59	A8	197	GLN
59	A8	230	ASN
60	TB	46	GLN
60	TB	59	GLN
60	TB	112	GLN
61	V1	168	ASN
61	V1	314	ASN
61	V1	418	GLN
61	V1	458	HIS
61	V1	460	GLN
61	V1	468	ASN
62	V2	113	ASN
62	V2	123	GLN
63	B6	70	HIS
64	BM	163	GLN
64	BM	166	ASN
64	BM	200	GLN
65	C4	98	GLN

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Mol	Chain	Res	Type
66	AN	97	ASN
66	AN	150	GLN
66	AN	208	GLN
67	B4	63	ASN
67	B4	139	ASN
68	T4	36	HIS
68	T4	50	HIS
68	T4	94	HIS
68	T4	158	HIS
68	T4	206	GLN
69	T8	104	GLN
70	B2	24	GLN
70	B2	42	ASN
70	B2	79	GLN
70	B2	109	HIS
71	T3	134	GLN
72	P1	58	ASN
72	P1	189	HIS
72	P1	192	GLN
72	P1	246	ASN
73	B3	78	GLN
75	S5	52	GLN
76	TC	36	ASN
76	TC	42	GLN
76	TC	83	HIS
77	P2	41	GLN
77	P2	74	ASN
77	P2	158	ASN
78	A3	35	ASN
79	T9	32	ASN
79	T9	100	GLN
79	T9	108	GLN
80	TE	66	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 3 are monoatomic - leaving 101 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	$\# Z > 2$
82	CDL	C4	401	-	97,97,99	0.30	0	103,109,111	0.33	0
82	CDL	TD	101	-	65,65,99	0.36	0	71,77,111	0.36	0
83	PC1	3I	602	-	45,45,53	0.32	0	51,53,61	0.30	0
83	PC1	X1	201	-	48,48,53	0.30	0	54,56,61	0.35	0
83	PC1	3j	101	-	35,35,53	0.34	0	41,43,61	0.33	0
82	CDL	1	301	-	49,49,99	0.41	0	55,61,111	0.35	0
82	CDL	3H	202	-	61,61,99	0.37	0	67,73,111	0.36	0
88	3PE	T4	301	-	24,24,50	0.42	0	27,29,55	0.37	0
83	PC1	3I	601	-	31,31,53	0.38	0	37,39,61	0.36	0
82	CDL	5	803	-	89,89,99	0.31	0	95,101,111	0.26	0
88	3PE	4	602	-	35,35,50	0.35	0	38,40,55	0.33	0
85	U10	5B	202	-	63,63,63	2.19	24 (38%)	78,79,79	1.72	22 (28%)
93	SF4	S8	302	56	0,12,12	-	-	-	-	-
82	CDL	T7	201	-	47,47,99	0.42	0	53,59,111	0.35	0
82	CDL	3I	604	-	36,36,99	0.43	0	42,48,111	0.39	0
82	CDL	5	805	-	95,95,99	0.31	0	101,107,111	0.36	0
82	CDL	B4	201	-	38,38,99	0.42	0	43,49,111	0.40	0
83	PC1	C4	403	-	31,31,53	0.37	0	37,39,61	0.41	0
91	ZMP	AB	201	29	28,33,36	0.72	1 (3%)	32,40,45	3.80	6 (18%)
92	ADP	B8	602	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
87	FES	FX	201	42	0,4,4	-	-	-	-	-
93	SF4	S7	201	55	0,12,12	-	-	-	-	-
87	FES	3E	301	10	0,4,4	-	-	-	-	-
82	CDL	B8	603	-	44,44,99	0.43	0	50,56,111	0.36	0
84	HEM	3C	602	8	50,50,50	1.30	7 (14%)	67,82,82	1.56	11 (16%)
88	3PE	T8	201	-	38,38,50	0.33	0	41,43,55	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	U10	3C	605	-	25,25,63	2.84	9 (36%)	24,29,79	1.99	8 (33%)
82	CDL	3G	401	-	65,65,99	0.36	0	71,77,111	0.32	0
82	CDL	A1	101	-	52,52,99	0.40	0	58,64,111	0.34	0
82	CDL	2B	201	-	52,52,99	0.40	0	58,64,111	0.33	0
82	CDL	3I	603	-	70,70,99	0.35	0	76,82,111	0.35	0
83	PC1	3C	604	-	45,45,53	0.31	0	51,53,61	0.31	0
82	CDL	T1	602	-	54,54,99	0.39	0	60,66,111	0.41	0
82	CDL	3i	201	-	70,70,99	0.35	0	76,82,111	0.34	0
93	SF4	V1	500	61	0,12,12	-	-	-		
83	PC1	TC	101	-	41,41,53	0.32	0	47,49,61	0.31	0
88	3PE	4	601	-	46,46,50	0.32	0	49,51,55	0.37	0
83	PC1	T1	601	-	25,25,53	0.40	0	31,33,61	0.38	0
87	FES	V2	300	62	0,4,4	-	-	-		
86	HEC	3d	401	9	46,50,50	1.92	10 (21%)	58,82,82	1.83	8 (13%)
88	3PE	A3	201	-	44,44,50	0.33	0	47,49,55	0.40	0
88	3PE	3E	303	-	33,33,50	0.37	0	36,38,55	0.34	0
88	3PE	B8	601	-	35,35,50	0.35	0	38,40,55	0.33	0
83	PC1	3E	304	-	23,23,53	0.41	0	29,31,61	0.38	0
83	PC1	5	807	-	53,53,53	0.29	0	59,61,61	0.30	0
83	PC1	3c	506	-	37,37,53	0.34	0	43,45,61	0.32	0
82	CDL	BM	301	-	85,85,99	0.32	0	91,97,111	0.31	0
88	3PE	5	804	-	36,36,50	0.34	0	39,41,55	0.31	0
83	PC1	3C	606	-	43,43,53	0.31	0	49,51,61	0.30	0
83	PC1	3g	401	-	32,32,53	0.36	0	38,40,61	0.36	0
93	SF4	S1	802	50	0,12,12	-	-	-		
82	CDL	3c	504	-	63,63,99	0.36	0	69,75,111	0.31	0
82	CDL	3c	505	-	55,55,99	0.38	0	61,67,111	0.33	0
85	U10	3H	201	-	29,29,63	2.72	13 (44%)	36,38,79	1.60	8 (22%)
88	3PE	P1	402	-	46,46,50	0.32	0	49,51,55	0.32	0
82	CDL	3C	603	-	64,64,99	0.36	0	70,76,111	0.35	0
84	HEM	3C	601	8	50,50,50	1.29	8 (16%)	67,82,82	1.68	12 (17%)
90	NDP	A9	401	-	51,52,52	0.35	0	71,80,80	0.37	0
88	3PE	5B	201	-	23,23,50	0.43	0	26,28,55	0.36	0
82	CDL	3B	701	-	77,77,99	0.33	0	83,89,111	0.31	0
94	FMN	V1	501	-	33,33,33	0.21	0	48,50,50	0.34	0
83	PC1	3J	101	-	36,36,53	0.36	0	42,44,61	0.40	0
87	FES	S1	803	50	0,4,4	-	-	-		
88	3PE	3d	402	-	46,46,50	0.32	0	49,51,55	0.39	0
83	PC1	AM	201	-	29,29,53	0.38	0	35,37,61	0.34	0
88	3PE	AN	301	-	44,44,50	0.32	0	47,49,55	0.32	0
88	3PE	5	806	-	34,34,50	0.35	0	37,39,55	0.32	0
82	CDL	P2	201	-	81,81,99	0.33	0	87,93,111	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	PC1	5	802	-	38,38,53	0.33	0	44,46,61	0.33	0
83	PC1	AN	303	-	35,35,53	0.35	0	41,43,61	0.39	0
88	3PE	TA	201	-	25,25,50	0.41	0	28,30,55	0.37	0
83	PC1	B6	201	-	51,51,53	0.29	0	57,59,61	0.30	0
82	CDL	3H	203	-	65,65,99	0.36	0	71,77,111	0.31	0
82	CDL	3b	602	-	67,67,99	0.36	0	73,79,111	0.37	0
84	HEM	3c	502	8	50,50,50	1.30	8 (16%)	67,82,82	1.60	10 (14%)
82	CDL	3	202	-	43,43,99	0.43	0	49,55,111	0.37	0
93	SF4	S1	801	50	0,12,12	-	-	-	-	-
83	PC1	B2	201	-	47,47,53	0.31	0	53,55,61	0.35	0
83	PC1	3E	302	-	53,53,53	0.29	0	59,61,61	0.32	0
86	HEC	3D	401	9	46,50,50	1.93	10 (21%)	58,82,82	1.80	8 (13%)
83	PC1	3e	301	-	49,49,53	0.31	0	55,57,61	0.30	0
83	PC1	6	302	-	53,53,53	0.29	0	59,61,61	0.31	0
88	3PE	C4	402	-	50,50,50	0.30	0	53,55,55	0.34	0
83	PC1	3c	501	-	30,30,53	0.38	0	36,38,61	0.45	0
83	PC1	3C	607	-	28,28,53	0.38	0	34,36,61	0.37	0
93	SF4	S8	301	56	0,12,12	-	-	-	-	-
82	CDL	R	201	-	83,83,99	0.32	0	89,95,111	0.31	0
84	HEM	3c	503	8	50,50,50	1.30	7 (14%)	67,82,82	1.61	15 (22%)
83	PC1	3b	601	-	29,29,53	0.39	0	35,37,61	0.48	0
83	PC1	3	201	-	30,30,53	0.37	0	36,38,61	0.36	0
83	PC1	6	301	-	38,38,53	0.33	0	44,46,61	0.33	0
88	3PE	S8	303	-	40,40,50	0.34	0	43,45,55	0.32	0
83	PC1	J1	400	-	39,39,53	0.33	0	45,47,61	0.35	0
88	3PE	AN	302	-	34,34,50	0.36	0	37,39,55	0.33	0
83	PC1	1	302	-	35,35,53	0.35	0	41,43,61	0.35	0
82	CDL	AN	304	-	52,52,99	0.39	0	58,64,111	0.35	0
83	PC1	3F	102	-	21,21,53	0.39	0	27,29,61	0.43	0
82	CDL	AM	202	-	61,61,99	0.37	0	67,73,111	0.31	0
83	PC1	5	801	-	53,53,53	0.29	0	59,61,61	0.28	0
83	PC1	P1	401	-	39,39,53	0.33	0	45,47,61	0.30	0
82	CDL	AL	301	-	52,52,99	0.40	0	58,64,111	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
82	CDL	C4	401	-	-	21/108/108/110	-
82	CDL	TD	101	-	-	14/76/76/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PC1	3I	602	-	-	7/49/49/57	-
83	PC1	X1	201	-	-	12/52/52/57	-
83	PC1	3j	101	-	-	5/39/39/57	-
82	CDL	1	301	-	-	11/60/60/110	-
82	CDL	3H	202	-	-	17/72/72/110	-
88	3PE	T4	301	-	-	4/28/28/54	-
83	PC1	3I	601	-	-	9/35/35/57	-
82	CDL	5	803	-	-	22/100/100/110	-
88	3PE	4	602	-	-	7/39/39/54	-
85	U10	5B	202	-	-	18/63/87/87	0/1/1/1
93	SF4	S8	302	56	-	-	0/6/5/5
82	CDL	T7	201	-	-	14/58/58/110	-
82	CDL	3I	604	-	-	6/44/44/110	-
82	CDL	5	805	-	-	20/106/106/110	-
82	CDL	B4	201	-	-	10/44/44/110	-
83	PC1	C4	403	-	-	13/35/35/57	-
91	ZMP	AB	201	29	-	8/38/40/43	-
92	ADP	B8	602	-	-	1/16/32/32	0/3/3/3
87	FES	FX	201	42	-	-	0/1/1/1
93	SF4	S7	201	55	-	-	0/6/5/5
87	FES	3E	301	10	-	-	0/1/1/1
82	CDL	B8	603	-	-	4/55/55/110	-
84	HEM	3C	602	8	-	5/14/54/54	-
88	3PE	T8	201	-	-	9/42/42/54	-
85	U10	3C	605	-	-	12/28/28/87	-
82	CDL	3G	401	-	-	19/76/76/110	-
82	CDL	A1	101	-	-	15/63/63/110	-
82	CDL	2B	201	-	-	9/63/63/110	-
82	CDL	3I	603	-	-	23/81/81/110	-
83	PC1	3C	604	-	-	14/49/49/57	-
82	CDL	T1	602	-	-	10/65/65/110	-
82	CDL	3i	201	-	-	15/81/81/110	-
93	SF4	V1	500	61	-	-	0/6/5/5
83	PC1	TC	101	-	-	7/45/45/57	-
88	3PE	4	601	-	-	6/50/50/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PC1	T1	601	-	-	11/29/29/57	-
87	FES	V2	300	62	-	-	0/1/1/1
86	HEC	3d	401	9	-	7/14/54/54	-
88	3PE	A3	201	-	-	6/48/48/54	-
88	3PE	3E	303	-	-	7/37/37/54	-
88	3PE	B8	601	-	-	8/39/39/54	-
83	PC1	3E	304	-	-	9/26/26/57	-
83	PC1	5	807	-	-	10/57/57/57	-
83	PC1	3c	506	-	-	13/41/41/57	-
82	CDL	BM	301	-	-	19/96/96/110	-
88	3PE	5	804	-	-	5/40/40/54	-
83	PC1	3C	606	-	-	6/47/47/57	-
83	PC1	3g	401	-	-	2/36/36/57	-
93	SF4	S1	802	50	-	-	0/6/5/5
82	CDL	3c	504	-	-	15/74/74/110	-
82	CDL	3c	505	-	-	16/66/66/110	-
85	U10	3H	201	-	-	6/23/47/87	0/1/1/1
88	3PE	P1	402	-	-	11/50/50/54	-
82	CDL	3C	603	-	-	20/75/75/110	-
84	HEM	3C	601	8	-	5/14/54/54	-
90	NDP	A9	401	-	-	3/34/77/77	0/5/5/5
88	3PE	5B	201	-	-	7/27/27/54	-
82	CDL	3B	701	-	-	23/88/88/110	-
94	FMN	V1	501	-	-	1/18/18/18	0/3/3/3
83	PC1	3J	101	-	-	16/40/40/57	-
87	FES	S1	803	50	-	-	0/1/1/1
88	3PE	3d	402	-	-	11/50/50/54	-
83	PC1	AM	201	-	-	12/33/33/57	-
88	3PE	AN	301	-	-	6/48/48/54	-
88	3PE	5	806	-	-	6/38/38/54	-
82	CDL	P2	201	-	-	20/92/92/110	-
83	PC1	5	802	-	-	7/42/42/57	-
83	PC1	AN	303	-	-	7/39/39/57	-
88	3PE	TA	201	-	-	5/29/29/54	-
83	PC1	B6	201	-	-	9/55/55/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	CDL	3H	203	-	-	11/76/76/110	-
82	CDL	3b	602	-	-	24/78/78/110	-
84	HEM	3c	502	8	-	7/14/54/54	-
82	CDL	3	202	-	-	7/54/54/110	-
93	SF4	S1	801	50	-	-	0/6/5/5
83	PC1	B2	201	-	-	15/51/51/57	-
83	PC1	3E	302	-	-	21/57/57/57	-
86	HEC	3D	401	9	-	7/14/54/54	-
83	PC1	3e	301	-	-	6/53/53/57	-
83	PC1	6	302	-	-	11/57/57/57	-
88	3PE	C4	402	-	-	14/54/54/54	-
83	PC1	3c	501	-	-	7/34/34/57	-
83	PC1	3C	607	-	-	9/32/32/57	-
93	SF4	S8	301	56	-	-	0/6/5/5
82	CDL	R	201	-	-	17/94/94/110	-
84	HEM	3c	503	8	-	9/14/54/54	-
83	PC1	3b	601	-	-	15/33/33/57	-
83	PC1	3	201	-	-	6/34/34/57	-
83	PC1	6	301	-	-	6/42/42/57	-
88	3PE	S8	303	-	-	8/44/44/54	-
83	PC1	J1	400	-	-	9/43/43/57	-
88	3PE	AN	302	-	-	8/38/38/54	-
83	PC1	1	302	-	-	12/39/39/57	-
82	CDL	AN	304	-	-	20/62/62/110	-
83	PC1	3F	102	-	-	8/23/23/57	-
82	CDL	AM	202	-	-	14/72/72/110	-
83	PC1	5	801	-	-	6/57/57/57	-
83	PC1	P1	401	-	-	15/43/43/57	-
82	CDL	AL	301	-	-	15/63/63/110	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	3H	201	U10	C6-C1	10.27	1.53	1.35
85	3C	605	U10	C6-C1	10.27	1.56	1.33
85	5B	202	U10	C6-C1	10.25	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3D	401	HEC	CAC-C3C	7.19	1.58	1.35
86	3d	401	HEC	CAC-C3C	7.18	1.58	1.35
86	3D	401	HEC	CAB-C3B	6.77	1.57	1.35
86	3d	401	HEC	CAB-C3B	6.76	1.57	1.35
85	3C	605	U10	C2-C1	-5.86	1.36	1.51
85	3H	201	U10	C4-C3	4.82	1.53	1.36
85	5B	202	U10	C4-C3	4.79	1.53	1.36
92	B8	602	ADP	C5-C4	4.68	1.47	1.39
84	3C	601	HEM	C4D-ND	-3.75	1.33	1.40
84	3c	503	HEM	C4D-ND	-3.66	1.33	1.40
84	3c	502	HEM	C4D-ND	-3.66	1.33	1.40
84	3C	602	HEM	C4D-ND	-3.65	1.33	1.40
86	3d	401	HEC	CBC-CAC	-3.44	1.36	1.49
86	3D	401	HEC	CBC-CAC	-3.41	1.36	1.49
84	3C	602	HEM	C1B-NB	-3.08	1.34	1.40
84	3C	601	HEM	C1B-NB	-3.07	1.34	1.40
84	3c	502	HEM	C1B-NB	-3.03	1.35	1.40
84	3c	503	HEM	C1B-NB	-2.99	1.35	1.40
85	5B	202	U10	C41-C39	2.98	1.57	1.51
85	5B	202	U10	C26-C24	2.85	1.57	1.51
85	3C	605	U10	C11-C9	2.78	1.57	1.51
84	3c	503	HEM	C1D-ND	-2.76	1.33	1.38
85	5B	202	U10	C31-C29	2.74	1.56	1.51
84	3C	602	HEM	C1D-ND	-2.72	1.33	1.38
85	5B	202	U10	C21-C19	2.71	1.56	1.51
84	3C	601	HEM	C1D-ND	-2.70	1.33	1.38
84	3c	502	HEM	C1D-ND	-2.69	1.33	1.38
92	B8	602	ADP	C5-C6	2.67	1.48	1.41
85	3H	201	U10	C7-C8	2.66	1.54	1.50
85	3C	605	U10	C16-C14	2.65	1.56	1.51
84	3c	503	HEM	C1C-C2C	-2.63	1.40	1.45
85	5B	202	U10	C7-C8	2.59	1.54	1.50
84	3c	502	HEM	C1C-C2C	-2.56	1.40	1.45
91	AB	201	ZMP	C9-C10	2.50	1.53	1.50
85	5B	202	U10	C36-C34	2.46	1.56	1.51
85	3C	605	U10	C21-C19	2.45	1.56	1.51
85	5B	202	U10	C46-C44	2.45	1.56	1.51
85	3H	201	U10	C11-C9	2.45	1.56	1.51
84	3C	601	HEM	C1C-C2C	-2.45	1.40	1.45
84	3C	602	HEM	C1C-C2C	-2.43	1.40	1.45
85	5B	202	U10	O5-C5	-2.42	1.18	1.23
85	3C	605	U10	C7-C8	2.42	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	3c	502	HEM	FE-NB	2.41	2.02	1.94
85	3H	201	U10	C6-C5	2.40	1.53	1.46
85	3H	201	U10	O5-C5	-2.40	1.18	1.23
84	3C	602	HEM	FE-NB	2.40	2.02	1.94
85	5B	202	U10	C51-C49	2.37	1.56	1.51
84	3c	503	HEM	FE-NB	2.36	2.02	1.94
85	5B	202	U10	C27-C28	2.33	1.57	1.50
85	3C	605	U10	C12-C13	2.31	1.57	1.50
92	B8	602	ADP	C5-N7	-2.30	1.34	1.39
86	3D	401	HEC	CBB-CAB	-2.30	1.41	1.49
86	3d	401	HEC	CBB-CAB	-2.30	1.41	1.49
84	3C	601	HEM	C3C-C4C	-2.30	1.42	1.46
85	5B	202	U10	C6-C5	2.28	1.52	1.46
85	3H	201	U10	O3-C3M	-2.28	1.40	1.45
85	5B	202	U10	O3-C3M	-2.27	1.40	1.45
85	5B	202	U10	O2-C2	-2.27	1.18	1.23
85	5B	202	U10	C16-C14	2.27	1.56	1.51
84	3C	601	HEM	FE-NB	2.26	2.01	1.94
85	5B	202	U10	C11-C9	2.25	1.55	1.51
86	3D	401	HEC	CMD-C2D	2.24	1.55	1.50
86	3d	401	HEC	CMD-C2D	2.24	1.55	1.50
85	5B	202	U10	C22-C23	2.24	1.57	1.50
85	3H	201	U10	O2-C2	-2.24	1.18	1.23
85	3H	201	U10	C16-C14	2.24	1.55	1.51
86	3D	401	HEC	C3D-C2D	-2.22	1.33	1.38
86	3d	401	HEC	C3D-C2D	-2.19	1.33	1.38
85	5B	202	U10	C42-C43	2.19	1.57	1.50
92	B8	602	ADP	C8-N7	2.17	1.35	1.31
85	5B	202	U10	C7-C6	2.17	1.55	1.51
84	3c	502	HEM	C4B-NB	-2.14	1.34	1.38
85	3H	201	U10	C7-C6	2.14	1.55	1.51
86	3D	401	HEC	CMB-C2B	2.14	1.55	1.50
85	3H	201	U10	C12-C13	2.14	1.56	1.50
85	5B	202	U10	C17-C18	2.12	1.56	1.50
86	3D	401	HEC	C3C-C2C	-2.11	1.34	1.41
86	3d	401	HEC	C3C-C2C	-2.11	1.34	1.41
85	3H	201	U10	C17-C18	2.10	1.56	1.50
85	3C	605	U10	C26-C24	2.10	1.57	1.51
85	5B	202	U10	C32-C33	2.10	1.56	1.50
84	3c	502	HEM	FE-ND	2.10	2.01	1.94
85	5B	202	U10	C12-C13	2.10	1.56	1.50
85	3H	201	U10	O4-C4M	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3D	401	HEC	CMA-C3A	2.08	1.55	1.50
86	3d	401	HEC	CMA-C3A	2.07	1.55	1.50
84	3c	503	HEM	FE-ND	2.06	2.01	1.94
85	5B	202	U10	O4-C4M	-2.06	1.40	1.45
85	3C	605	U10	C17-C18	2.05	1.56	1.50
84	3C	602	HEM	C4B-NB	-2.05	1.34	1.38
84	3C	602	HEM	FE-ND	2.05	2.01	1.94
86	3d	401	HEC	CMB-C2B	2.04	1.55	1.50
84	3c	503	HEM	C4B-NB	-2.03	1.34	1.38
84	3c	502	HEM	C3C-C4C	-2.03	1.42	1.46
84	3C	601	HEM	C4B-NB	-2.02	1.34	1.38
86	3d	401	HEC	C3B-C2B	-2.02	1.34	1.41
86	3D	401	HEC	C3B-C2B	-2.02	1.34	1.41
84	3C	601	HEM	FE-ND	2.00	2.01	1.94

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	AB	201	ZMP	C19-C18-C17	-12.73	87.07	108.77
91	AB	201	ZMP	C20-C18-C17	-11.76	88.73	108.77
86	3d	401	HEC	CBB-CAB-C3B	-8.72	110.00	127.43
86	3D	401	HEC	CBB-CAB-C3B	-8.54	110.37	127.43
91	AB	201	ZMP	C20-C18-C21	8.27	121.88	108.22
86	3D	401	HEC	CBC-CAC-C3C	-6.69	114.06	127.43
86	3d	401	HEC	CBC-CAC-C3C	-6.64	114.17	127.43
91	AB	201	ZMP	C19-C18-C21	5.91	117.98	108.22
92	B8	602	ADP	C5-C4-N3	-5.80	118.73	126.72
91	AB	201	ZMP	C20-C18-C19	5.33	119.84	109.20
84	3C	601	HEM	CHC-C4B-NB	4.85	129.64	124.42
84	3C	602	HEM	CHC-C4B-NB	4.75	129.54	124.42
84	3C	601	HEM	CHD-C4C-NC	4.72	129.59	124.45
84	3c	502	HEM	CHC-C4B-NB	4.69	129.47	124.42
92	B8	602	ADP	N3-C4-N9	4.66	135.09	127.17
84	3c	503	HEM	CHC-C4B-NB	4.46	129.22	124.42
84	3c	502	HEM	CHD-C4C-NC	4.36	129.20	124.45
84	3C	602	HEM	CHD-C4C-NC	4.02	128.84	124.45
85	3H	201	U10	C7-C8-C9	-3.89	120.13	126.83
84	3c	503	HEM	CHD-C4C-NC	3.86	128.65	124.45
84	3c	503	HEM	CHB-C1B-NB	3.71	128.95	124.37
84	3c	502	HEM	CHB-C1B-NB	3.66	128.90	124.37
92	B8	602	ADP	C2-N3-C4	3.65	120.75	111.83
84	3C	601	HEM	CHB-C1B-NB	3.64	128.87	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	3C	602	HEM	CHB-C1B-NB	3.62	128.85	124.37
92	B8	602	ADP	C4-C5-N7	-3.38	106.72	110.58
85	3C	605	U10	C1M-C1-C2	3.36	120.09	116.13
85	5B	202	U10	C27-C28-C29	-3.34	119.97	127.62
85	3C	605	U10	C17-C18-C19	-3.31	120.04	127.62
85	3C	605	U10	C25-C24-C26	3.28	119.99	116.13
84	3C	601	HEM	CHA-C4D-ND	3.26	128.40	124.37
85	3C	605	U10	C12-C13-C14	-3.26	120.16	127.62
84	3C	601	HEM	C1B-NB-C4B	3.24	109.04	105.21
85	5B	202	U10	C17-C18-C19	-3.22	120.24	127.62
85	3C	605	U10	C22-C23-C24	-3.22	120.25	127.62
85	5B	202	U10	C37-C38-C39	-3.20	120.30	127.62
85	3H	201	U10	C7-C6-C1	-3.19	119.41	124.89
84	3C	601	HEM	C4D-ND-C1D	3.15	108.94	105.21
92	B8	602	ADP	N3-C2-N1	-3.15	123.81	128.58
85	5B	202	U10	C7-C8-C9	-3.15	121.41	126.83
85	5B	202	U10	C32-C33-C34	-3.11	120.50	127.62
85	5B	202	U10	C10-C9-C11	3.10	120.60	115.23
85	5B	202	U10	C12-C13-C14	-3.09	120.56	127.62
85	5B	202	U10	C42-C43-C44	-3.08	120.57	127.62
85	3H	201	U10	C20-C19-C21	3.07	119.74	116.13
84	3c	503	HEM	C1B-NB-C4B	3.07	108.84	105.21
85	5B	202	U10	C47-C48-C49	-3.04	120.67	127.62
84	3C	602	HEM	C4D-ND-C1D	3.04	108.80	105.21
84	3c	503	HEM	C4D-ND-C1D	3.03	108.80	105.21
85	3H	201	U10	C17-C18-C19	-2.93	120.92	127.62
84	3c	502	HEM	C1B-NB-C4B	2.92	108.66	105.21
85	5B	202	U10	C22-C23-C24	-2.90	120.98	127.62
85	5B	202	U10	C35-C34-C36	2.90	120.26	115.23
85	5B	202	U10	C7-C6-C1	-2.88	119.95	124.89
85	3C	605	U10	C15-C14-C16	2.86	120.20	115.23
84	3C	602	HEM	C1B-NB-C4B	2.84	108.57	105.21
84	3c	502	HEM	C4D-ND-C1D	2.84	108.57	105.21
85	3C	605	U10	C20-C19-C21	2.83	120.14	115.23
84	3c	502	HEM	CHA-C4D-ND	2.83	127.86	124.37
86	3d	401	HEC	O1D-CGD-CBD	-2.82	114.15	123.09
85	5B	202	U10	C25-C24-C26	2.82	120.12	115.23
84	3C	602	HEM	CHA-C4D-ND	2.81	127.84	124.37
85	3H	201	U10	C1M-C1-C6	-2.80	119.85	124.45
86	3D	401	HEC	O1D-CGD-CBD	-2.80	114.21	123.09
84	3c	503	HEM	CHA-C1A-NA	2.79	128.92	123.86
85	5B	202	U10	C45-C44-C46	2.77	120.04	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	5B	202	U10	C1M-C1-C6	-2.77	119.89	124.45
84	3c	502	HEM	CHA-C1A-NA	2.75	128.85	123.86
85	5B	202	U10	C30-C29-C31	2.72	119.95	115.23
85	3H	201	U10	C12-C13-C14	-2.70	121.44	127.62
85	5B	202	U10	C20-C19-C21	2.69	119.89	115.23
91	AB	201	ZMP	O1-C10-C9	-2.68	120.89	123.98
85	3H	201	U10	C15-C14-C16	2.66	119.85	115.23
92	B8	602	ADP	C4-N9-C8	2.66	108.53	105.74
84	3C	602	HEM	CHA-C1A-NA	2.64	128.65	123.86
84	3c	503	HEM	CHA-C4D-ND	2.62	127.60	124.37
85	5B	202	U10	C15-C14-C16	2.61	119.76	115.23
85	5B	202	U10	C40-C39-C41	2.61	119.75	115.23
84	3C	602	HEM	CHD-C1D-ND	2.60	127.22	124.42
84	3C	601	HEM	CHA-C1A-NA	2.59	128.55	123.86
85	3C	605	U10	C10-C9-C11	2.57	119.69	115.23
84	3C	601	HEM	CHD-C1D-ND	2.55	127.17	124.42
85	5B	202	U10	C50-C49-C51	2.54	119.63	115.23
84	3c	503	HEM	C4A-CHB-C1B	-2.50	120.37	126.25
92	B8	602	ADP	C3'-C2'-C1'	2.49	106.17	101.46
84	3c	502	HEM	CHD-C1D-ND	2.48	127.09	124.42
85	3H	201	U10	C10-C9-C11	2.46	119.50	115.23
92	B8	602	ADP	C5-N7-C8	2.45	107.30	103.45
86	3D	401	HEC	CBD-CAD-C3D	2.40	119.17	112.53
86	3d	401	HEC	CHC-C4B-NB	2.36	127.02	124.45
84	3C	601	HEM	C1C-CHC-C4B	-2.35	121.03	126.02
84	3C	602	HEM	C1C-CHC-C4B	-2.30	121.13	126.02
84	3c	503	HEM	CHD-C1D-ND	2.28	126.88	124.42
84	3c	502	HEM	C1C-CHC-C4B	-2.27	121.19	126.02
84	3C	601	HEM	C4C-CHD-C1D	-2.27	121.20	126.02
86	3d	401	HEC	CMD-C2D-C1D	-2.25	121.99	125.42
84	3c	503	HEM	C3B-C4B-NB	-2.24	107.86	109.47
86	3D	401	HEC	O1A-CGA-CBA	-2.23	116.03	123.09
85	5B	202	U10	C56-C54-C55	2.22	119.70	114.59
86	3d	401	HEC	O1A-CGA-CBA	-2.22	116.05	123.09
86	3D	401	HEC	CHC-C4B-NB	2.18	126.83	124.45
85	5B	202	U10	C52-C53-C54	-2.17	120.41	127.64
84	3c	503	HEM	C1C-CHC-C4B	-2.15	121.44	126.02
84	3C	601	HEM	C3B-C4B-NB	-2.15	107.92	109.47
84	3c	502	HEM	CHB-C1B-C2B	-2.14	120.86	126.95
84	3c	503	HEM	C2A-C1A-NA	-2.14	107.78	110.15
84	3c	503	HEM	C4C-CHD-C1D	-2.14	121.48	126.02
84	3C	602	HEM	C2A-C1A-NA	-2.13	107.79	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	3c	503	HEM	CHB-C1B-C2B	-2.10	120.97	126.95
84	3C	601	HEM	C4A-CHB-C1B	-2.10	121.31	126.25
86	3D	401	HEC	CMD-C2D-C1D	-2.10	122.22	125.42
84	3C	602	HEM	CHB-C1B-C2B	-2.10	120.98	126.95
84	3c	503	HEM	CAD-CBD-CGD	-2.10	108.11	113.67
86	3D	401	HEC	O2A-CGA-O1A	2.08	128.68	123.33
86	3d	401	HEC	O2A-CGA-O1A	2.05	128.62	123.33
86	3d	401	HEC	CBD-CAD-C3D	2.01	118.09	112.53
92	B8	602	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (983) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	1	301	CDL	CB2-OB2-PB2-OB3
82	1	301	CDL	OB5-CB3-CB4-OB6
82	2B	201	CDL	CA2-OA2-PA1-OA3
82	2B	201	CDL	CA2-OA2-PA1-OA5
82	2B	201	CDL	CB2-OB2-PB2-OB4
82	2B	201	CDL	CB2-OB2-PB2-OB5
82	2B	201	CDL	CB3-OB5-PB2-OB4
82	3	202	CDL	CA3-OA5-PA1-OA2
82	3	202	CDL	CA3-OA5-PA1-OA3
82	3	202	CDL	CB3-OB5-PB2-OB2
82	3B	701	CDL	CA2-OA2-PA1-OA3
82	3B	701	CDL	CA2-OA2-PA1-OA5
82	3B	701	CDL	CA3-OA5-PA1-OA2
82	3B	701	CDL	CA3-OA5-PA1-OA4
82	3B	701	CDL	CB2-OB2-PB2-OB5
82	3B	701	CDL	CB3-OB5-PB2-OB2
82	3B	701	CDL	CB3-OB5-PB2-OB4
82	3C	603	CDL	CA2-OA2-PA1-OA3
82	3C	603	CDL	CA2-OA2-PA1-OA4
82	3C	603	CDL	CA2-OA2-PA1-OA5
82	3C	603	CDL	CB2-OB2-PB2-OB3
82	3C	603	CDL	CB2-OB2-PB2-OB4
82	3C	603	CDL	CB2-OB2-PB2-OB5
82	3C	603	CDL	CB3-OB5-PB2-OB2
82	3C	603	CDL	CB3-OB5-PB2-OB4
82	3G	401	CDL	CA3-OA5-PA1-OA2
82	3G	401	CDL	CA3-OA5-PA1-OA3
82	3G	401	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
82	3G	401	CDL	CB2-OB2-PB2-OB4
82	3G	401	CDL	CB2-OB2-PB2-OB5
82	3H	202	CDL	CA2-OA2-PA1-OA3
82	3H	202	CDL	CA3-OA5-PA1-OA3
82	3H	202	CDL	CB3-OB5-PB2-OB2
82	3H	202	CDL	CB3-OB5-PB2-OB3
82	3H	202	CDL	CB3-OB5-PB2-OB4
82	3H	203	CDL	CA2-OA2-PA1-OA4
82	3H	203	CDL	CA2-OA2-PA1-OA5
82	3H	203	CDL	CB2-OB2-PB2-OB3
82	3H	203	CDL	CB2-OB2-PB2-OB4
82	3H	203	CDL	CB2-OB2-PB2-OB5
82	3H	203	CDL	CB3-OB5-PB2-OB2
82	3H	203	CDL	CB3-OB5-PB2-OB3
82	3I	603	CDL	CA3-OA5-PA1-OA3
82	3I	603	CDL	CB2-OB2-PB2-OB3
82	3I	603	CDL	CB2-OB2-PB2-OB4
82	3I	603	CDL	CB2-OB2-PB2-OB5
82	3I	603	CDL	CB3-OB5-PB2-OB3
82	3I	604	CDL	CA3-OA5-PA1-OA2
82	3I	604	CDL	CA3-OA5-PA1-OA3
82	3b	602	CDL	CA2-OA2-PA1-OA4
82	3b	602	CDL	CA3-OA5-PA1-OA2
82	3b	602	CDL	CA3-OA5-PA1-OA4
82	3b	602	CDL	CB2-OB2-PB2-OB3
82	3b	602	CDL	CB2-OB2-PB2-OB4
82	3b	602	CDL	CB2-OB2-PB2-OB5
82	3c	504	CDL	CA2-OA2-PA1-OA3
82	3c	504	CDL	CA2-OA2-PA1-OA4
82	3c	504	CDL	CA2-OA2-PA1-OA5
82	3c	504	CDL	CA3-OA5-PA1-OA2
82	3c	504	CDL	CA3-OA5-PA1-OA3
82	3c	504	CDL	CB2-OB2-PB2-OB3
82	3c	504	CDL	CB2-OB2-PB2-OB5
82	3c	504	CDL	CB3-OB5-PB2-OB2
82	3c	504	CDL	CB3-OB5-PB2-OB3
82	3c	504	CDL	CB3-OB5-PB2-OB4
82	3c	505	CDL	CA2-OA2-PA1-OA3
82	3c	505	CDL	CA3-OA5-PA1-OA2
82	3c	505	CDL	CA3-OA5-PA1-OA3
82	3c	505	CDL	CB2-OB2-PB2-OB3
82	3c	505	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
82	3c	505	CDL	CB2-OB2-PB2-OB5
82	3i	201	CDL	CA2-OA2-PA1-OA3
82	3i	201	CDL	CA2-OA2-PA1-OA4
82	3i	201	CDL	CA3-OA5-PA1-OA2
82	3i	201	CDL	CA3-OA5-PA1-OA3
82	3i	201	CDL	CA3-OA5-PA1-OA4
82	3i	201	CDL	CB2-OB2-PB2-OB3
82	3i	201	CDL	CB3-OB5-PB2-OB3
82	3i	201	CDL	CB3-OB5-PB2-OB4
82	5	803	CDL	CA2-OA2-PA1-OA3
82	5	803	CDL	CA2-OA2-PA1-OA4
82	5	803	CDL	CA2-OA2-PA1-OA5
82	5	803	CDL	CA3-OA5-PA1-OA2
82	5	803	CDL	CA3-OA5-PA1-OA3
82	5	803	CDL	CB2-OB2-PB2-OB4
82	5	803	CDL	CB2-OB2-PB2-OB5
82	5	803	CDL	CB3-OB5-PB2-OB2
82	5	803	CDL	CB3-OB5-PB2-OB3
82	5	803	CDL	CB3-OB5-PB2-OB4
82	5	805	CDL	CA3-OA5-PA1-OA4
82	5	805	CDL	CB3-OB5-PB2-OB2
82	5	805	CDL	CB3-OB5-PB2-OB3
82	AL	301	CDL	CA2-OA2-PA1-OA4
82	AL	301	CDL	CA2-OA2-PA1-OA5
82	AL	301	CDL	CA3-OA5-PA1-OA2
82	AL	301	CDL	CA3-OA5-PA1-OA4
82	AL	301	CDL	CB2-OB2-PB2-OB3
82	AL	301	CDL	CB2-OB2-PB2-OB4
82	AL	301	CDL	CB2-OB2-PB2-OB5
82	AM	202	CDL	CA2-OA2-PA1-OA5
82	AM	202	CDL	CA3-OA5-PA1-OA2
82	AM	202	CDL	CA3-OA5-PA1-OA3
82	AM	202	CDL	CA3-OA5-PA1-OA4
82	B8	603	CDL	CB3-OB5-PB2-OB2
82	B8	603	CDL	CB3-OB5-PB2-OB3
82	B8	603	CDL	CB3-OB5-PB2-OB4
82	TD	101	CDL	CA2-OA2-PA1-OA3
82	TD	101	CDL	CA3-OA5-PA1-OA2
82	TD	101	CDL	CA3-OA5-PA1-OA4
82	TD	101	CDL	CB2-OB2-PB2-OB3
82	TD	101	CDL	CB2-OB2-PB2-OB4
82	TD	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
82	T1	602	CDL	CA3-OA5-PA1-OA2
82	T1	602	CDL	CA3-OA5-PA1-OA3
82	T1	602	CDL	CB3-OB5-PB2-OB3
82	A1	101	CDL	CA2-OA2-PA1-OA3
82	A1	101	CDL	CA2-OA2-PA1-OA4
82	A1	101	CDL	CA2-OA2-PA1-OA5
82	R	201	CDL	CA2-OA2-PA1-OA3
82	R	201	CDL	CA2-OA2-PA1-OA4
82	R	201	CDL	CA2-OA2-PA1-OA5
82	BM	301	CDL	CA2-OA2-PA1-OA4
82	BM	301	CDL	CA2-OA2-PA1-OA5
82	BM	301	CDL	CA3-OA5-PA1-OA2
82	BM	301	CDL	CA3-OA5-PA1-OA4
82	BM	301	CDL	CB2-OB2-PB2-OB3
82	BM	301	CDL	CB3-OB5-PB2-OB2
82	BM	301	CDL	CB3-OB5-PB2-OB3
82	BM	301	CDL	CB3-OB5-PB2-OB4
82	BM	301	CDL	OB5-CB3-CB4-OB6
82	C4	401	CDL	CA2-OA2-PA1-OA3
82	C4	401	CDL	CA2-OA2-PA1-OA4
82	C4	401	CDL	CA2-OA2-PA1-OA5
82	C4	401	CDL	CA3-OA5-PA1-OA2
82	C4	401	CDL	CA3-OA5-PA1-OA3
82	C4	401	CDL	CA3-OA5-PA1-OA4
82	C4	401	CDL	CB2-OB2-PB2-OB5
82	AN	304	CDL	CA2-OA2-PA1-OA3
82	AN	304	CDL	CA2-OA2-PA1-OA4
82	AN	304	CDL	CA2-OA2-PA1-OA5
82	AN	304	CDL	CA3-OA5-PA1-OA4
82	AN	304	CDL	CB2-OB2-PB2-OB3
82	AN	304	CDL	CB2-OB2-PB2-OB4
82	AN	304	CDL	CB2-OB2-PB2-OB5
82	AN	304	CDL	CB3-OB5-PB2-OB2
82	AN	304	CDL	CB3-OB5-PB2-OB3
82	B4	201	CDL	CB2-OB2-PB2-OB3
82	B4	201	CDL	CB3-OB5-PB2-OB2
82	B4	201	CDL	CB3-OB5-PB2-OB3
82	B4	201	CDL	CB3-OB5-PB2-OB4
82	P2	201	CDL	CA2-OA2-PA1-OA3
82	P2	201	CDL	CA2-OA2-PA1-OA4
82	P2	201	CDL	CA2-OA2-PA1-OA5
82	P2	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
82	P2	201	CDL	CB2-OB2-PB2-OB4
82	P2	201	CDL	CB2-OB2-PB2-OB5
82	P2	201	CDL	CB3-OB5-PB2-OB3
82	T7	201	CDL	CA2-OA2-PA1-OA3
82	T7	201	CDL	CA2-OA2-PA1-OA5
82	T7	201	CDL	CA3-OA5-PA1-OA2
82	T7	201	CDL	CA3-OA5-PA1-OA3
82	T7	201	CDL	CA3-OA5-PA1-OA4
82	T7	201	CDL	CB2-OB2-PB2-OB5
82	T7	201	CDL	CB3-OB5-PB2-OB2
82	T7	201	CDL	CB3-OB5-PB2-OB3
83	1	302	PC1	C11-O13-P-O14
83	1	302	PC1	C1-O11-P-O14
83	1	302	PC1	C1-O11-P-O13
83	3	201	PC1	C1-O11-P-O14
83	3C	604	PC1	C11-O13-P-O14
83	3C	604	PC1	C1-O11-P-O12
83	3C	604	PC1	C1-O11-P-O14
83	3C	606	PC1	C11-O13-P-O14
83	3C	607	PC1	C1-O11-P-O12
83	3E	302	PC1	C1-O11-P-O14
83	3E	302	PC1	C1-O11-P-O13
83	3E	304	PC1	C11-O13-P-O14
83	3E	304	PC1	C11-O13-P-O11
83	3E	304	PC1	C1-O11-P-O12
83	3E	304	PC1	C1-O11-P-O14
83	3E	304	PC1	C1-O11-P-O13
83	3I	601	PC1	C11-O13-P-O12
83	3I	601	PC1	C1-O11-P-O13
83	3J	101	PC1	C11-O13-P-O12
83	3J	101	PC1	C11-O13-P-O14
83	3J	101	PC1	C11-O13-P-O11
83	3J	101	PC1	C1-O11-P-O12
83	3J	101	PC1	C1-O11-P-O14
83	3J	101	PC1	C1-O11-P-O13
83	3b	601	PC1	C11-O13-P-O12
83	3c	506	PC1	C11-O13-P-O12
83	3c	506	PC1	C11-O13-P-O14
83	3c	506	PC1	C11-O13-P-O11
83	3c	506	PC1	C1-O11-P-O12
83	3c	506	PC1	C1-O11-P-O14
83	3c	506	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
83	3e	301	PC1	C11-O13-P-O11
83	3g	401	PC1	C11-O13-P-O11
83	3j	101	PC1	C11-O13-P-O12
83	3j	101	PC1	C11-O13-P-O11
83	5	801	PC1	C11-O13-P-O12
83	5	801	PC1	C11-O13-P-O14
83	5	801	PC1	C11-O13-P-O11
83	5	801	PC1	C1-O11-P-O12
83	5	802	PC1	C1-O11-P-O12
83	5	802	PC1	C1-O11-P-O13
83	5	807	PC1	C11-O13-P-O12
83	5	807	PC1	C1-O11-P-O14
83	5	807	PC1	C1-O11-P-O13
83	6	301	PC1	C11-O13-P-O14
83	6	301	PC1	C11-O13-P-O11
83	6	301	PC1	C1-O11-P-O12
83	6	301	PC1	C1-O11-P-O14
83	6	301	PC1	C1-O11-P-O13
83	6	302	PC1	C11-O13-P-O12
83	6	302	PC1	C11-O13-P-O11
83	AM	201	PC1	C11-O13-P-O14
83	AM	201	PC1	C11-O13-P-O11
83	AM	201	PC1	C1-O11-P-O12
83	AM	201	PC1	C1-O11-P-O14
83	AM	201	PC1	C1-O11-P-O13
83	J1	400	PC1	C11-O13-P-O12
83	J1	400	PC1	C1-O11-P-O13
83	T1	601	PC1	C11-O13-P-O12
83	T1	601	PC1	C11-O13-P-O14
83	T1	601	PC1	C1-O11-P-O14
83	T1	601	PC1	C1-O11-P-O13
83	X1	201	PC1	C1-O11-P-O12
83	X1	201	PC1	C1-O11-P-O13
83	C4	403	PC1	C11-O13-P-O14
83	C4	403	PC1	C11-O13-P-O11
83	B2	201	PC1	C11-O13-P-O11
83	B2	201	PC1	C1-O11-P-O12
83	B2	201	PC1	C1-O11-P-O14
83	B2	201	PC1	C1-O11-P-O13
83	P1	401	PC1	C11-O13-P-O12
83	P1	401	PC1	C11-O13-P-O14
83	P1	401	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
83	P1	401	PC1	C1-O11-P-O12
83	P1	401	PC1	C1-O11-P-O14
83	P1	401	PC1	C1-O11-P-O13
84	3C	601	HEM	C2B-C3B-CAB-CBB
84	3C	601	HEM	C2C-C3C-CAC-CBC
84	3C	601	HEM	C4C-C3C-CAC-CBC
84	3c	502	HEM	C2C-C3C-CAC-CBC
85	3C	605	U10	C6-C1-C2-C3
85	3C	605	U10	C23-C24-C26-C27
85	3C	605	U10	C25-C24-C26-C27
85	5B	202	U10	C19-C21-C22-C23
88	3E	303	3PE	C11-O13-P-O11
88	3E	303	3PE	C11-O13-P-O12
88	3E	303	3PE	C11-O13-P-O14
88	3d	402	3PE	C11-O13-P-O11
88	3d	402	3PE	C11-O13-P-O14
88	3d	402	3PE	O13-C11-C12-N
88	4	601	3PE	C1-O11-P-O13
88	4	602	3PE	C1-O11-P-O12
88	4	602	3PE	C1-O11-P-O13
88	4	602	3PE	C1-O11-P-O14
88	4	602	3PE	O13-C11-C12-N
88	5	804	3PE	O13-C11-C12-N
88	5	806	3PE	C1-O11-P-O12
88	5	806	3PE	C1-O11-P-O13
88	5	806	3PE	O13-C11-C12-N
88	5B	201	3PE	C1-O11-P-O13
88	5B	201	3PE	C11-O13-P-O11
88	5B	201	3PE	C11-O13-P-O14
88	B8	601	3PE	C1-O11-P-O13
88	B8	601	3PE	C1-O11-P-O14
88	B8	601	3PE	C11-O13-P-O11
88	B8	601	3PE	O13-C11-C12-N
88	S8	303	3PE	O13-C11-C12-N
88	C4	402	3PE	C1-O11-P-O12
88	C4	402	3PE	C1-O11-P-O13
88	C4	402	3PE	C1-O11-P-O14
88	C4	402	3PE	C11-O13-P-O11
88	C4	402	3PE	O13-C11-C12-N
88	AN	301	3PE	C1-O11-P-O13
88	AN	301	3PE	C1-O11-P-O14
88	AN	302	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
88	AN	302	3PE	O13-C11-C12-N
88	T4	301	3PE	C11-O13-P-O11
88	T4	301	3PE	C11-O13-P-O14
88	T8	201	3PE	C1-O11-P-O13
88	T8	201	3PE	C1-O11-P-O14
88	T8	201	3PE	O13-C11-C12-N
88	P1	402	3PE	C11-O13-P-O14
88	P1	402	3PE	O13-C11-C12-N
88	A3	201	3PE	O13-C11-C12-N
91	AB	201	ZMP	C19-C18-C21-O5
91	AB	201	ZMP	C20-C18-C21-O5
91	AB	201	ZMP	C17-C18-C21-O5
91	AB	201	ZMP	O1-C10-S1-C11
91	AB	201	ZMP	C9-C10-S1-C11
85	3C	605	U10	C12-C11-C9-C10
85	5B	202	U10	C30-C29-C31-C32
85	3C	605	U10	C12-C11-C9-C8
85	5B	202	U10	C28-C29-C31-C32
85	3C	605	U10	C1M-C1-C6-C7
85	3C	605	U10	C2-C1-C6-C7
85	3C	605	U10	C15-C14-C16-C17
85	5B	202	U10	C35-C34-C36-C37
85	3C	605	U10	C13-C14-C16-C17
85	5B	202	U10	C23-C24-C26-C27
85	5B	202	U10	C33-C34-C36-C37
85	5B	202	U10	C9-C11-C12-C13
85	5B	202	U10	C29-C31-C32-C33
85	5B	202	U10	C34-C36-C37-C38
82	3C	603	CDL	CA2-C1-CB2-OB2
82	R	201	CDL	CA2-C1-CB2-OB2
83	3E	304	PC1	C11-C12-N-C15
83	TC	101	PC1	C11-C12-N-C15
85	5B	202	U10	C25-C24-C26-C27
82	3C	603	CDL	O1-C1-CB2-OB2
82	R	201	CDL	O1-C1-CB2-OB2
85	5B	202	U10	C24-C26-C27-C28
85	5B	202	U10	C49-C51-C52-C53
83	3E	304	PC1	C11-C12-N-C14
83	3I	601	PC1	C11-C12-N-C15
83	6	302	PC1	C11-C12-N-C15
83	X1	201	PC1	C11-C12-N-C14
83	B6	201	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
83	B2	201	PC1	C11-C12-N-C14
83	TC	101	PC1	C11-C12-N-C14
82	5	805	CDL	CA5-C11-C12-C13
82	R	201	CDL	CA5-C11-C12-C13
82	3H	202	CDL	CA5-C11-C12-C13
88	5	806	3PE	C21-C22-C23-C24
82	3c	505	CDL	CA7-C31-C32-C33
82	P2	201	CDL	CB7-C71-C72-C73
83	3I	601	PC1	C11-C12-N-C14
83	3c	501	PC1	C11-C12-N-C15
83	6	302	PC1	C11-C12-N-C13
83	B2	201	PC1	C11-C12-N-C13
83	P1	401	PC1	C11-C12-N-C15
83	B6	201	PC1	C11-C12-N-C15
83	TC	101	PC1	C11-C12-N-C13
82	AN	304	CDL	C34-C35-C36-C37
88	S8	303	3PE	C2A-C2B-C2C-C2D
83	3E	302	PC1	C34-C35-C36-C37
88	A3	201	3PE	C22-C23-C24-C25
82	P2	201	CDL	C12-C13-C14-C15
82	AM	202	CDL	C34-C35-C36-C37
82	3C	603	CDL	C31-C32-C33-C34
83	3C	607	PC1	C11-C12-N-C14
83	3E	304	PC1	C11-C12-N-C13
83	X1	201	PC1	C11-C12-N-C13
83	P1	401	PC1	C11-C12-N-C14
82	P2	201	CDL	CA5-C11-C12-C13
82	3b	602	CDL	C52-C53-C54-C55
82	5	805	CDL	C72-C73-C74-C75
83	B6	201	PC1	C2D-C2E-C2F-C2G
83	B2	201	PC1	C3D-C3E-C3F-C3G
82	3I	603	CDL	C52-C53-C54-C55
82	P2	201	CDL	C52-C53-C54-C55
82	P2	201	CDL	C57-C58-C59-C60
83	1	302	PC1	C34-C35-C36-C37
83	3E	302	PC1	C26-C27-C28-C29
84	3c	503	HEM	C2C-C3C-CAC-CBC
83	3I	601	PC1	C11-C12-N-C13
83	3c	501	PC1	C11-C12-N-C13
83	3c	501	PC1	C11-C12-N-C14
83	3c	506	PC1	C11-C12-N-C14
83	6	302	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
83	X1	201	PC1	C11-C12-N-C15
83	B6	201	PC1	C11-C12-N-C14
83	B2	201	PC1	C11-C12-N-C15
83	P1	401	PC1	C11-C12-N-C13
82	A1	101	CDL	C51-C52-C53-C54
83	3E	302	PC1	C37-C38-C39-C3A
91	AB	201	ZMP	C2-C3-C4-C5
83	5	807	PC1	C21-C22-C23-C24
82	AM	202	CDL	OB5-CB3-CB4-OB6
82	TD	101	CDL	OB5-CB3-CB4-OB6
88	AN	302	3PE	C23-C24-C25-C26
82	AL	301	CDL	CA5-C11-C12-C13
83	B6	201	PC1	O21-C2-C3-O31
82	BM	301	CDL	C75-C76-C77-C78
83	B6	201	PC1	C25-C26-C27-C28
85	5B	202	U10	C43-C44-C46-C47
83	3I	602	PC1	C35-C36-C37-C38
83	3J	101	PC1	C35-C36-C37-C38
83	B2	201	PC1	C34-C35-C36-C37
83	TC	101	PC1	C25-C26-C27-C28
83	3	201	PC1	C11-C12-N-C14
83	C4	403	PC1	C11-C12-N-C15
83	AN	303	PC1	C11-C12-N-C15
82	3c	504	CDL	OB5-CB3-CB4-CB6
82	R	201	CDL	OB5-CB3-CB4-CB6
82	BM	301	CDL	C76-C77-C78-C79
83	3e	301	PC1	C2D-C2E-C2F-C2G
88	3E	303	3PE	C26-C27-C28-C29
83	3	201	PC1	C31-C32-C33-C34
83	6	302	PC1	C31-C32-C33-C34
82	3I	604	CDL	CB3-CB4-CB6-OB8
82	5	803	CDL	CB3-CB4-CB6-OB8
82	AM	202	CDL	CA3-CA4-CA6-OA8
88	T4	301	3PE	C1-C2-C3-O31
82	3b	602	CDL	C55-C56-C57-C58
88	3E	303	3PE	C24-C25-C26-C27
82	R	201	CDL	CB7-C71-C72-C73
83	3C	607	PC1	C11-C12-N-C13
83	3c	506	PC1	C11-C12-N-C13
83	T1	601	PC1	C11-C12-N-C13
85	5B	202	U10	C45-C44-C46-C47
85	5B	202	U10	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
82	3B	701	CDL	OA5-CA3-CA4-OA6
82	3B	701	CDL	OB5-CB3-CB4-OB6
82	3c	505	CDL	OB5-CB3-CB4-OB6
88	B8	601	3PE	O11-C1-C2-O21
82	5	805	CDL	C78-C79-C80-C81
82	C4	401	CDL	C74-C75-C76-C77
83	3E	302	PC1	C24-C25-C26-C27
82	P2	201	CDL	C37-C38-C39-C40
83	3C	606	PC1	O21-C2-C3-O31
83	C4	403	PC1	O21-C2-C3-O31
83	3	201	PC1	C11-C12-N-C13
85	3C	605	U10	C9-C11-C12-C13
82	3I	603	CDL	CA7-C31-C32-C33
85	5B	202	U10	C12-C11-C9-C10
83	6	302	PC1	C35-C36-C37-C38
82	3b	602	CDL	CA4-CA3-OA5-PA1
82	3c	504	CDL	C1-CB2-OB2-PB2
82	AL	301	CDL	CA4-CA3-OA5-PA1
88	TA	201	3PE	C2-C1-O11-P
82	5	805	CDL	C76-C77-C78-C79
82	BM	301	CDL	C35-C36-C37-C38
82	1	301	CDL	OB5-CB3-CB4-CB6
82	3H	202	CDL	OA5-CA3-CA4-CA6
82	3H	203	CDL	OB5-CB3-CB4-CB6
82	3b	602	CDL	OA5-CA3-CA4-CA6
82	5	803	CDL	OB5-CB3-CB4-CB6
82	AM	202	CDL	OB5-CB3-CB4-CB6
82	TD	101	CDL	OB5-CB3-CB4-CB6
82	BM	301	CDL	OB5-CB3-CB4-CB6
83	3C	607	PC1	C11-C12-N-C15
83	T1	601	PC1	C11-C12-N-C15
83	C4	403	PC1	C11-C12-N-C14
83	AN	303	PC1	C11-C12-N-C13
82	5	803	CDL	C17-C18-C19-C20
83	3b	601	PC1	C23-C24-C25-C26
88	C4	402	3PE	C38-C39-C3A-C3B
85	3C	605	U10	C1M-C1-C2-C3
82	A1	101	CDL	CA3-CA4-CA6-OA8
82	R	201	CDL	CA3-CA4-CA6-OA8
83	1	302	PC1	C1-C2-C3-O31
83	B6	201	PC1	C1-C2-C3-O31
83	C4	403	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
88	C4	402	3PE	C2F-C2G-C2H-C2I
83	3e	301	PC1	C2F-C2G-C2H-C2I
88	5	804	3PE	C31-C32-C33-C34
82	3b	602	CDL	OA5-CA3-CA4-OA6
82	3c	504	CDL	OB5-CB3-CB4-OB6
82	R	201	CDL	OB5-CB3-CB4-OB6
82	AN	304	CDL	OB5-CB3-CB4-OB6
82	T7	201	CDL	OB5-CB3-CB4-OB6
88	S8	303	3PE	O11-C1-C2-O21
82	3I	603	CDL	C54-C55-C56-C57
82	C4	401	CDL	C1-CB2-OB2-PB2
84	3C	601	HEM	C3D-CAD-CBD-CGD
84	3c	503	HEM	C3D-CAD-CBD-CGD
82	BM	301	CDL	C38-C39-C40-C41
82	3H	202	CDL	OB6-CB4-CB6-OB8
82	3I	603	CDL	OA6-CA4-CA6-OA8
82	5	803	CDL	OB6-CB4-CB6-OB8
82	R	201	CDL	OA6-CA4-CA6-OA8
83	3C	604	PC1	O21-C2-C3-O31
83	3I	602	PC1	C11-C12-N-C15
83	3j	101	PC1	C11-C12-N-C13
82	BM	301	CDL	O1-C1-CB2-OB2
82	B4	201	CDL	O1-C1-CA2-OA2
82	3I	603	CDL	C31-C32-C33-C34
83	3C	606	PC1	C36-C37-C38-C39
82	3b	602	CDL	C33-C34-C35-C36
88	P1	402	3PE	C37-C38-C39-C3A
82	C4	401	CDL	C35-C36-C37-C38
82	C4	401	CDL	OB5-CB3-CB4-CB6
83	3b	601	PC1	O11-C1-C2-C3
83	X1	201	PC1	O11-C1-C2-C3
88	S8	303	3PE	O11-C1-C2-C3
82	A1	101	CDL	C1-CB2-OB2-PB2
83	B2	201	PC1	C22-C23-C24-C25
91	AB	201	ZMP	C5-C6-C7-C8
83	J1	400	PC1	O31-C31-C32-C33
84	3C	602	HEM	C2B-C3B-CAB-CBB
84	3c	502	HEM	C2B-C3B-CAB-CBB
82	3H	203	CDL	OB5-CB3-CB4-OB6
82	5	803	CDL	OB5-CB3-CB4-OB6
83	3J	101	PC1	O11-C1-C2-O21
82	3B	701	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
85	3C	605	U10	C19-C21-C22-C23
84	3C	601	HEM	C4B-C3B-CAB-CBB
84	3c	502	HEM	C4C-C3C-CAC-CBC
82	AL	301	CDL	C52-C51-CB5-OB6
83	J1	400	PC1	C12-C11-O13-P
82	3B	701	CDL	OA6-CA4-CA6-OA8
82	3I	604	CDL	OB6-CB4-CB6-OB8
82	3b	602	CDL	OB6-CB4-CB6-OB8
82	A1	101	CDL	OA6-CA4-CA6-OA8
83	1	302	PC1	O21-C2-C3-O31
88	3d	402	3PE	O21-C2-C3-O31
88	T4	301	3PE	O21-C2-C3-O31
83	6	302	PC1	C36-C37-C38-C39
88	4	602	3PE	C36-C37-C38-C39
83	3b	601	PC1	C22-C23-C24-C25
88	P1	402	3PE	C2C-C2D-C2E-C2F
83	3I	602	PC1	C11-C12-N-C13
83	3J	101	PC1	C11-C12-N-C14
83	3J	101	PC1	C11-C12-N-C15
83	3j	101	PC1	C11-C12-N-C14
83	AM	201	PC1	C11-C12-N-C14
83	AM	201	PC1	C11-C12-N-C15
82	A1	101	CDL	CA4-CA3-OA5-PA1
83	P1	401	PC1	C2-C1-O11-P
88	S8	303	3PE	C2-C1-O11-P
83	1	302	PC1	O13-C11-C12-N
83	3C	604	PC1	O13-C11-C12-N
83	3E	302	PC1	O13-C11-C12-N
83	3E	304	PC1	O13-C11-C12-N
83	3F	102	PC1	O13-C11-C12-N
83	3b	601	PC1	O13-C11-C12-N
83	3e	301	PC1	O13-C11-C12-N
83	5	802	PC1	O13-C11-C12-N
83	J1	400	PC1	O13-C11-C12-N
83	B2	201	PC1	O13-C11-C12-N
88	P1	402	3PE	C26-C27-C28-C29
82	TD	101	CDL	O1-C1-CA2-OA2
82	AM	202	CDL	C33-C34-C35-C36
83	3c	506	PC1	C11-C12-N-C15
82	3B	701	CDL	OB5-CB3-CB4-CB6
82	3c	505	CDL	OB5-CB3-CB4-CB6
82	B4	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
82	T7	201	CDL	OB5-CB3-CB4-CB6
83	3J	101	PC1	O11-C1-C2-C3
85	3H	201	U10	C18-C19-C21-C22
82	5	805	CDL	C13-C14-C15-C16
82	AN	304	CDL	C33-C34-C35-C36
82	3b	602	CDL	C51-C52-C53-C54
82	5	805	CDL	C36-C37-C38-C39
82	3G	401	CDL	C1-CA2-OA2-PA1
82	B4	201	CDL	C1-CA2-OA2-PA1
83	X1	201	PC1	C2-C1-O11-P
83	TC	101	PC1	C2-C1-O11-P
88	A3	201	3PE	C2-C1-O11-P
86	3D	401	HEC	C4B-C3B-CAB-CBB
86	3d	401	HEC	C4C-C3C-CAC-CBC
82	3C	603	CDL	OB5-CB3-CB4-OB6
82	3H	202	CDL	OA5-CA3-CA4-OA6
82	C4	401	CDL	OB5-CB3-CB4-OB6
82	B4	201	CDL	OB5-CB3-CB4-OB6
83	3b	601	PC1	O11-C1-C2-O21
82	5	803	CDL	C56-C57-C58-C59
83	3	201	PC1	C11-C12-N-C15
83	3b	601	PC1	C11-C12-N-C14
82	AM	202	CDL	OA6-CA4-CA6-OA8
82	1	301	CDL	CB3-CB4-CB6-OB8
82	3I	603	CDL	CA3-CA4-CA6-OA8
83	3C	604	PC1	C1-C2-C3-O31
83	3C	606	PC1	C1-C2-C3-O31
88	3d	402	3PE	C1-C2-C3-O31
82	3I	603	CDL	C56-C57-C58-C59
82	3G	401	CDL	C55-C56-C57-C58
82	5	803	CDL	C22-C23-C24-C25
85	3H	201	U10	C5-C4-O4-C4M
82	P2	201	CDL	C11-C12-C13-C14
82	1	301	CDL	CB2-OB2-PB2-OB4
82	1	301	CDL	CB2-OB2-PB2-OB5
82	2B	201	CDL	CA2-OA2-PA1-OA4
82	2B	201	CDL	CB3-OB5-PB2-OB2
82	3	202	CDL	CB3-OB5-PB2-OB3
82	3B	701	CDL	CA3-OA5-PA1-OA3
82	3B	701	CDL	CB2-OB2-PB2-OB3
82	3B	701	CDL	CB3-OB5-PB2-OB3
82	3C	603	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
82	3C	603	CDL	CA3-OA5-PA1-OA3
82	3C	603	CDL	CA3-OA5-PA1-OA4
82	3G	401	CDL	CA2-OA2-PA1-OA3
82	3G	401	CDL	CA2-OA2-PA1-OA4
82	3G	401	CDL	CA2-OA2-PA1-OA5
82	3G	401	CDL	CA3-OA5-PA1-OA4
82	3H	202	CDL	CA2-OA2-PA1-OA4
82	3H	202	CDL	CA2-OA2-PA1-OA5
82	3H	202	CDL	CA3-OA5-PA1-OA2
82	3H	203	CDL	CA2-OA2-PA1-OA3
82	3I	603	CDL	CA3-OA5-PA1-OA2
82	3I	604	CDL	CA3-OA5-PA1-OA4
82	3b	602	CDL	CA2-OA2-PA1-OA3
82	3b	602	CDL	CA2-OA2-PA1-OA5
82	3b	602	CDL	CA3-OA5-PA1-OA3
82	3c	504	CDL	CA3-OA5-PA1-OA4
82	3c	504	CDL	CB2-OB2-PB2-OB4
82	3c	505	CDL	CA2-OA2-PA1-OA4
82	3c	505	CDL	CA2-OA2-PA1-OA5
82	3c	505	CDL	CA3-OA5-PA1-OA4
82	3i	201	CDL	CA2-OA2-PA1-OA5
82	3i	201	CDL	CB3-OB5-PB2-OB2
82	5	803	CDL	CA3-OA5-PA1-OA4
82	5	805	CDL	CA2-OA2-PA1-OA3
82	5	805	CDL	CA2-OA2-PA1-OA4
82	5	805	CDL	CA2-OA2-PA1-OA5
82	5	805	CDL	CA3-OA5-PA1-OA2
82	5	805	CDL	CA3-OA5-PA1-OA3
82	5	805	CDL	CB3-OB5-PB2-OB4
82	AL	301	CDL	CA3-OA5-PA1-OA3
82	TD	101	CDL	CA2-OA2-PA1-OA5
82	T1	602	CDL	CA3-OA5-PA1-OA4
82	T1	602	CDL	CB3-OB5-PB2-OB2
82	A1	101	CDL	CB3-OB5-PB2-OB2
82	A1	101	CDL	CB3-OB5-PB2-OB3
82	A1	101	CDL	CB3-OB5-PB2-OB4
82	R	201	CDL	CB3-OB5-PB2-OB3
82	BM	301	CDL	CA3-OA5-PA1-OA3
82	C4	401	CDL	CB2-OB2-PB2-OB3
82	AN	304	CDL	CA3-OA5-PA1-OA2
82	AN	304	CDL	CA3-OA5-PA1-OA3
82	AN	304	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
82	B4	201	CDL	CB2-OB2-PB2-OB5
82	P2	201	CDL	CB3-OB5-PB2-OB4
82	T7	201	CDL	CA2-OA2-PA1-OA4
82	T7	201	CDL	CB2-OB2-PB2-OB3
82	T7	201	CDL	CB3-OB5-PB2-OB4
83	1	302	PC1	C11-O13-P-O11
83	1	302	PC1	C1-O11-P-O12
83	3	201	PC1	C1-O11-P-O13
83	3C	604	PC1	C1-O11-P-O13
83	3C	606	PC1	C1-O11-P-O14
83	3C	607	PC1	C11-O13-P-O14
83	3C	607	PC1	C1-O11-P-O14
83	3C	607	PC1	C1-O11-P-O13
83	3E	302	PC1	C1-O11-P-O12
83	3E	302	PC1	C11-C12-N-C13
83	3F	102	PC1	C11-O13-P-O12
83	3F	102	PC1	C11-O13-P-O14
83	3F	102	PC1	C11-O13-P-O11
83	3F	102	PC1	C1-O11-P-O12
83	3I	601	PC1	C11-O13-P-O14
83	3I	601	PC1	C11-O13-P-O11
83	3I	601	PC1	C1-O11-P-O14
83	3b	601	PC1	C11-O13-P-O11
83	3c	501	PC1	C11-O13-P-O12
83	3e	301	PC1	C11-O13-P-O14
83	3g	401	PC1	C11-O13-P-O14
83	5	801	PC1	C1-O11-P-O13
83	5	802	PC1	C11-O13-P-O14
83	5	802	PC1	C1-O11-P-O14
83	5	807	PC1	C11-O13-P-O14
83	5	807	PC1	C11-O13-P-O11
83	5	807	PC1	C1-O11-P-O12
83	AM	201	PC1	C11-O13-P-O12
83	J1	400	PC1	C11-O13-P-O14
83	J1	400	PC1	C11-O13-P-O11
83	J1	400	PC1	C1-O11-P-O14
83	T1	601	PC1	C11-O13-P-O11
83	T1	601	PC1	C1-O11-P-O12
83	T1	601	PC1	C11-C12-N-C14
83	C4	403	PC1	C11-O13-P-O12
83	C4	403	PC1	C11-C12-N-C13
83	AN	303	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
86	3D	401	HEC	C2B-C3B-CAB-CBB
86	3d	401	HEC	C2B-C3B-CAB-CBB
86	3d	401	HEC	C2C-C3C-CAC-CBC
88	3E	303	3PE	O13-C11-C12-N
88	3d	402	3PE	C11-O13-P-O12
88	4	601	3PE	C1-O11-P-O14
88	4	602	3PE	C11-O13-P-O14
88	5	804	3PE	C11-O13-P-O14
88	5B	201	3PE	C1-O11-P-O14
88	5B	201	3PE	C11-O13-P-O12
88	B8	601	3PE	C11-O13-P-O14
88	C4	402	3PE	C11-O13-P-O14
88	AN	302	3PE	C11-O13-P-O11
88	T8	201	3PE	C1-O11-P-O12
83	3E	302	PC1	C3A-C3B-C3C-C3D
82	2B	201	CDL	CA4-CA3-OA5-PA1
82	3B	701	CDL	C1-CB2-OB2-PB2
82	3C	603	CDL	C1-CB2-OB2-PB2
82	3G	401	CDL	C1-CB2-OB2-PB2
82	3c	505	CDL	C1-CA2-OA2-PA1
82	R	201	CDL	C1-CB2-OB2-PB2
83	5	802	PC1	C2-C1-O11-P
83	C4	403	PC1	C2-C1-O11-P
88	3d	402	3PE	C2-C1-O11-P
88	5	804	3PE	C2-C1-O11-P
88	A3	201	3PE	C23-C24-C25-C26
83	3E	302	PC1	C27-C28-C29-C2A
82	3b	602	CDL	C72-C73-C74-C75
83	6	302	PC1	C3C-C3D-C3E-C3F
88	TA	201	3PE	O32-C31-C32-C33
83	3I	602	PC1	C11-C12-N-C14
83	3b	601	PC1	C11-C12-N-C13
82	AN	304	CDL	OB5-CB3-CB4-CB6
83	3C	606	PC1	C23-C24-C25-C26
82	5	803	CDL	C14-C15-C16-C17
83	B2	201	PC1	C25-C26-C27-C28
82	C4	401	CDL	CA5-C11-C12-C13
82	3I	604	CDL	C1-CA2-OA2-PA1
82	5	805	CDL	C52-C51-CB5-OB6
83	3I	602	PC1	C26-C27-C28-C29
83	6	302	PC1	C25-C26-C27-C28
82	R	201	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
88	T8	201	3PE	C27-C28-C29-C2A
82	3b	602	CDL	CB3-CB4-CB6-OB8
88	T8	201	3PE	C1-C2-C3-O31
82	R	201	CDL	C33-C34-C35-C36
82	1	301	CDL	C72-C71-CB7-OB8
82	T1	602	CDL	C72-C71-CB7-OB8
84	3c	503	HEM	C2B-C3B-CAB-CBB
83	3j	101	PC1	C11-C12-N-C15
82	5	803	CDL	CA5-C11-C12-C13
88	TA	201	3PE	O31-C31-C32-C33
83	3I	601	PC1	C31-C32-C33-C34
82	T1	602	CDL	C1-CA2-OA2-PA1
88	4	601	3PE	C2-C1-O11-P
82	AM	202	CDL	C11-C12-C13-C14
82	C4	401	CDL	C20-C21-C22-C23
88	AN	301	3PE	C36-C37-C38-C39
82	3C	603	CDL	OB5-CB3-CB4-CB6
84	3C	602	HEM	C4B-C3B-CAB-CBB
84	3c	503	HEM	C4C-C3C-CAC-CBC
83	AM	201	PC1	O31-C31-C32-C33
83	3E	302	PC1	C11-C12-N-C15
83	3J	101	PC1	C11-C12-N-C13
83	AM	201	PC1	C11-C12-N-C13
88	S8	303	3PE	C27-C28-C29-C2A
83	3I	602	PC1	C21-C22-C23-C24
83	B2	201	PC1	C23-C24-C25-C26
82	T7	201	CDL	CA4-CA3-OA5-PA1
85	3H	201	U10	C20-C19-C21-C22
84	3C	602	HEM	C2A-CAA-CBA-CGA
88	AN	301	3PE	C1-C2-C3-O31
82	AM	202	CDL	C12-C13-C14-C15
83	5	802	PC1	C22-C23-C24-C25
82	3i	201	CDL	CA6-CA4-OA6-CA5
82	5	805	CDL	CB3-CB4-OB6-CB5
88	4	601	3PE	C1-C2-O21-C21
88	A3	201	3PE	C1-C2-O21-C21
88	C4	402	3PE	C23-C24-C25-C26
90	A9	401	NDP	O4D-C1D-N1N-C6N
82	BM	301	CDL	C34-C35-C36-C37
82	3G	401	CDL	CB7-C71-C72-C73
82	3G	401	CDL	OA5-CA3-CA4-OA6
88	C4	402	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
82	3H	202	CDL	C32-C33-C34-C35
82	3B	701	CDL	CA4-CA3-OA5-PA1
82	AM	202	CDL	CA4-CA3-OA5-PA1
82	B8	603	CDL	CA4-CA3-OA5-PA1
82	T1	602	CDL	CB4-CB3-OB5-PB2
82	C4	401	CDL	CA4-CA3-OA5-PA1
83	3C	604	PC1	C2-C1-O11-P
83	3J	101	PC1	C2-C1-O11-P
85	3H	201	U10	C15-C14-C16-C17
82	C4	401	CDL	C38-C39-C40-C41
83	3E	302	PC1	C39-C3A-C3B-C3C
82	3b	602	CDL	OB5-CB3-CB4-CB6
88	B8	601	3PE	O11-C1-C2-C3
83	1	302	PC1	C32-C33-C34-C35
82	1	301	CDL	OB6-CB4-CB6-OB8
83	3E	302	PC1	C2E-C2F-C2G-C2H
83	3C	604	PC1	C11-C12-N-C14
83	3F	102	PC1	C11-C12-N-C15
83	3b	601	PC1	C11-C12-N-C15
82	3B	701	CDL	CA2-C1-CB2-OB2
82	3C	603	CDL	C12-C13-C14-C15
84	3c	502	HEM	CAD-CBD-CGD-O2D
83	B6	201	PC1	C34-C35-C36-C37
86	3d	401	HEC	CAA-CBA-CGA-O2A
84	3C	602	HEM	CAA-CBA-CGA-O1A
84	3C	602	HEM	CAA-CBA-CGA-O2A
82	5	803	CDL	C12-C13-C14-C15
82	3	202	CDL	C1-CB2-OB2-PB2
82	3H	203	CDL	CB4-CB3-OB5-PB2
94	V1	501	FMN	C4'-C5'-O5'-P
91	AB	201	ZMP	C1-C2-C3-C4
84	3c	502	HEM	C3D-CAD-CBD-CGD
83	P1	401	PC1	C33-C34-C35-C36
83	5	807	PC1	C1-C2-C3-O31
85	5B	202	U10	C44-C46-C47-C48
83	X1	201	PC1	C38-C39-C3A-C3B
82	TD	101	CDL	OA5-CA3-CA4-OA6
82	3b	602	CDL	C32-C31-CA7-OA8
83	5	801	PC1	C22-C23-C24-C25
83	3J	101	PC1	C23-C24-C25-C26
88	C4	402	3PE	C36-C37-C38-C39
86	3D	401	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
82	3B	701	CDL	OA5-CA3-CA4-CA6
83	3b	601	PC1	O21-C2-C3-O31
88	AN	301	3PE	O21-C2-C3-O31
82	AM	202	CDL	CB4-CB3-OB5-PB2
82	TD	101	CDL	C1-CA2-OA2-PA1
88	4	601	3PE	O31-C31-C32-C33
90	A9	401	NDP	C2D-C1D-N1N-C6N
84	3c	503	HEM	CAA-CBA-CGA-O2A
86	3d	401	HEC	CAA-CBA-CGA-O1A
82	R	201	CDL	C11-C12-C13-C14
82	3G	401	CDL	C72-C71-CB7-OB8
83	3E	302	PC1	C11-C12-N-C14
84	3c	502	HEM	CAD-CBD-CGD-O1D
83	3c	506	PC1	C22-C23-C24-C25
88	4	602	3PE	O21-C21-C22-C23
82	3C	603	CDL	CA3-CA4-OA6-CA5
82	3C	603	CDL	CA6-CA4-OA6-CA5
82	3I	603	CDL	CA3-CA4-OA6-CA5
82	3I	603	CDL	CA6-CA4-OA6-CA5
82	TD	101	CDL	CA3-CA4-OA6-CA5
82	C4	401	CDL	CA6-CA4-OA6-CA5
83	3J	101	PC1	C3-C2-O21-C21
83	3b	601	PC1	C3-C2-O21-C21
83	X1	201	PC1	C3-C2-O21-C21
83	AN	303	PC1	C3-C2-O21-C21
82	C4	401	CDL	C63-C64-C65-C66
82	3H	202	CDL	C11-C12-C13-C14
82	3I	603	CDL	O1-C1-CB2-OB2
84	3c	503	HEM	CAA-CBA-CGA-O1A
86	3D	401	HEC	CAA-CBA-CGA-O1A
82	AN	304	CDL	C1-CA2-OA2-PA1
83	3c	506	PC1	C2-C1-O11-P
82	3b	602	CDL	OB5-CB3-CB4-OB6
83	3c	501	PC1	O11-C1-C2-O21
88	3d	402	3PE	O11-C1-C2-O21
84	3c	502	HEM	C4B-C3B-CAB-CBB
84	3c	503	HEM	C4B-C3B-CAB-CBB
82	3I	603	CDL	C73-C74-C75-C76
88	TA	201	3PE	C12-C11-O13-P
82	3I	603	CDL	C58-C59-C60-C61
82	AN	304	CDL	C37-C38-C39-C40
83	AN	303	PC1	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
82	3I	603	CDL	C72-C71-CB7-OB8
82	P2	201	CDL	C52-C51-CB5-OB6
88	5B	201	3PE	O21-C21-C22-C23
82	3I	603	CDL	OB5-CB3-CB4-CB6
82	A1	101	CDL	OB5-CB3-CB4-CB6
82	3B	701	CDL	CA7-C31-C32-C33
83	3C	604	PC1	C31-C32-C33-C34
83	T1	601	PC1	O21-C21-C22-C23
82	3c	505	CDL	C1-CB2-OB2-PB2
82	3	202	CDL	C12-C11-CA5-OA6
82	3G	401	CDL	C52-C51-CB5-OB6
82	AL	301	CDL	C72-C71-CB7-OB8
83	X1	201	PC1	O31-C31-C32-C33
88	5	806	3PE	O31-C31-C32-C33
83	B6	201	PC1	C27-C28-C29-C2A
83	3c	506	PC1	O31-C31-C32-C33
83	AM	201	PC1	O21-C21-C22-C23
83	P1	401	PC1	O31-C31-C32-C33
88	P1	402	3PE	O31-C31-C32-C33
83	6	302	PC1	C34-C35-C36-C37
83	1	302	PC1	O31-C31-C32-C33
83	3b	601	PC1	O21-C21-C22-C23
82	C4	401	CDL	C60-C61-C62-C63
83	3C	604	PC1	C11-C12-N-C13
88	AN	301	3PE	C22-C23-C24-C25
88	P1	402	3PE	C29-C2A-C2B-C2C
83	B2	201	PC1	O31-C31-C32-C33
83	P1	401	PC1	O21-C21-C22-C23
82	3G	401	CDL	C62-C63-C64-C65
88	3E	303	3PE	C31-C32-C33-C34
82	BM	301	CDL	C52-C51-CB5-OB6
88	C4	402	3PE	C2C-C2D-C2E-C2F
82	3b	602	CDL	C72-C71-CB7-OB8
82	3i	201	CDL	C52-C51-CB5-OB6
82	A1	101	CDL	C52-C51-CB5-OB6
83	C4	403	PC1	O21-C21-C22-C23
88	AN	302	3PE	O21-C21-C22-C23
82	3H	202	CDL	CB3-CB4-CB6-OB8
83	3E	302	PC1	C1-C2-C3-O31
83	3F	102	PC1	C11-C12-N-C13
83	5	807	PC1	C3A-C3B-C3C-C3D
82	3c	505	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
83	3C	607	PC1	O21-C21-C22-C23
88	T8	201	3PE	O31-C31-C32-C33
82	TD	101	CDL	OA6-CA4-CA6-OA8
83	5	807	PC1	O21-C2-C3-O31
88	S8	303	3PE	O21-C2-C3-O31
83	3E	302	PC1	C3C-C3D-C3E-C3F
82	1	301	CDL	C12-C11-CA5-OA6
82	2B	201	CDL	C72-C71-CB7-OB8
82	P2	201	CDL	C72-C71-CB7-OB8
88	AN	302	3PE	O31-C31-C32-C33
83	TC	101	PC1	C2C-C2D-C2E-C2F
88	P1	402	3PE	C3A-C3B-C3C-C3D
88	TA	201	3PE	C21-C22-C23-C24
82	T1	602	CDL	C12-C11-CA5-OA6
82	A1	101	CDL	C57-C58-C59-C60
88	4	601	3PE	C26-C27-C28-C29
82	3i	201	CDL	CA3-CA4-OA6-CA5
82	5	805	CDL	CB6-CB4-OB6-CB5
82	C4	401	CDL	CA3-CA4-OA6-CA5
83	3J	101	PC1	C1-C2-O21-C21
83	3c	501	PC1	C1-C2-O21-C21
83	3c	501	PC1	C3-C2-O21-C21
83	X1	201	PC1	C1-C2-O21-C21
83	C4	403	PC1	C1-C2-O21-C21
83	C4	403	PC1	C3-C2-O21-C21
83	AN	303	PC1	C1-C2-O21-C21
88	3d	402	3PE	C1-C2-O21-C21
88	3d	402	3PE	C3-C2-O21-C21
85	3H	201	U10	C3-C4-O4-C4M
88	S8	303	3PE	C25-C26-C27-C28
90	A9	401	NDP	O4B-C4B-C5B-O5B
92	B8	602	ADP	O4'-C4'-C5'-O5'
88	C4	402	3PE	C29-C2A-C2B-C2C
82	R	201	CDL	C34-C35-C36-C37
83	3E	302	PC1	C22-C23-C24-C25
83	AN	303	PC1	O21-C21-C22-C23
88	P1	402	3PE	O32-C31-C32-C33
82	AN	304	CDL	C35-C36-C37-C38
88	P1	402	3PE	C22-C23-C24-C25
82	AL	301	CDL	C1-CA2-OA2-PA1
86	3D	401	HEC	C4C-C3C-CAC-CBC
86	3d	401	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
83	J1	400	PC1	O32-C31-C32-C33
88	5	806	3PE	O32-C31-C32-C33
83	3E	302	PC1	C2D-C2E-C2F-C2G
88	C4	402	3PE	C33-C34-C35-C36
82	5	805	CDL	OB5-CB3-CB4-OB6
82	3H	202	CDL	C72-C73-C74-C75
88	3d	402	3PE	C23-C24-C25-C26
82	3I	603	CDL	C11-C12-C13-C14
82	AL	301	CDL	C52-C51-CB5-OB7
82	A1	101	CDL	C52-C51-CB5-OB7
83	T1	601	PC1	O22-C21-C22-C23
83	P1	401	PC1	O22-C21-C22-C23
83	P1	401	PC1	O32-C31-C32-C33
85	3H	201	U10	C2-C3-O3-C3M
83	3E	302	PC1	C3D-C3E-C3F-C3G
82	3G	401	CDL	C52-C51-CB5-OB7
82	P2	201	CDL	C16-C17-C18-C19
82	3B	701	CDL	CB7-C71-C72-C73
83	3e	301	PC1	C33-C34-C35-C36
88	B8	601	3PE	C26-C27-C28-C29
83	AM	201	PC1	O22-C21-C22-C23
83	C4	403	PC1	O22-C21-C22-C23
88	P1	402	3PE	C32-C33-C34-C35
82	3G	401	CDL	C32-C31-CA7-OA8
82	3I	603	CDL	C52-C51-CB5-OB6
88	A3	201	3PE	O21-C21-C22-C23
83	3b	601	PC1	C21-C22-C23-C24
82	3	202	CDL	C12-C11-CA5-OA7
82	3I	603	CDL	C72-C71-CB7-OB9
82	3c	505	CDL	C72-C71-CB7-OB9
83	B2	201	PC1	O32-C31-C32-C33
85	5B	202	U10	C31-C32-C33-C34
83	TC	101	PC1	C29-C2A-C2B-C2C
86	3d	401	HEC	CAD-CBD-CGD-O2D
82	3b	602	CDL	C72-C71-CB7-OB9
82	AL	301	CDL	C72-C71-CB7-OB9
83	X1	201	PC1	O32-C31-C32-C33
88	T8	201	3PE	O32-C31-C32-C33
88	T8	201	3PE	O21-C2-C3-O31
82	B4	201	CDL	CB2-C1-CA2-OA2
88	5	804	3PE	C34-C35-C36-C37
82	P2	201	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
82	P2	201	CDL	C72-C71-CB7-OB9
88	5B	201	3PE	O22-C21-C22-C23
83	3C	604	PC1	O21-C21-C22-C23
83	3I	602	PC1	O31-C31-C32-C33
82	3i	201	CDL	CB3-CB4-CB6-OB8
82	3i	201	CDL	C52-C51-CB5-OB7
82	BM	301	CDL	C52-C51-CB5-OB7
83	3C	607	PC1	O22-C21-C22-C23
83	3b	601	PC1	O22-C21-C22-C23
88	AN	302	3PE	O32-C31-C32-C33
88	AN	302	3PE	O22-C21-C22-C23
83	3C	604	PC1	C11-C12-N-C15
83	3F	102	PC1	C11-C12-N-C14
86	3D	401	HEC	CAD-CBD-CGD-O2D
83	1	302	PC1	O32-C31-C32-C33
82	3B	701	CDL	C12-C11-CA5-OA6
82	T1	602	CDL	C12-C11-CA5-OA7
82	AN	304	CDL	CA5-C11-C12-C13
82	5	805	CDL	C37-C38-C39-C40
83	3E	302	PC1	C2B-C2C-C2D-C2E
86	3D	401	HEC	CAD-CBD-CGD-O1D
83	3c	506	PC1	O32-C31-C32-C33
82	3B	701	CDL	C32-C31-CA7-OA8
82	1	301	CDL	C12-C13-C14-C15
82	1	301	CDL	C12-C11-CA5-OA7
82	3H	202	CDL	C72-C71-CB7-OB8
83	6	301	PC1	O31-C31-C32-C33
84	3c	503	HEM	CAD-CBD-CGD-O2D
83	3C	604	PC1	O22-C21-C22-C23
82	5	803	CDL	C59-C60-C61-C62
84	3c	503	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

75 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	C4	401	CDL	6	0
82	TD	101	CDL	2	0
83	X1	201	PC1	2	0
83	3j	101	PC1	1	0
82	1	301	CDL	1	0
82	3H	202	CDL	3	0

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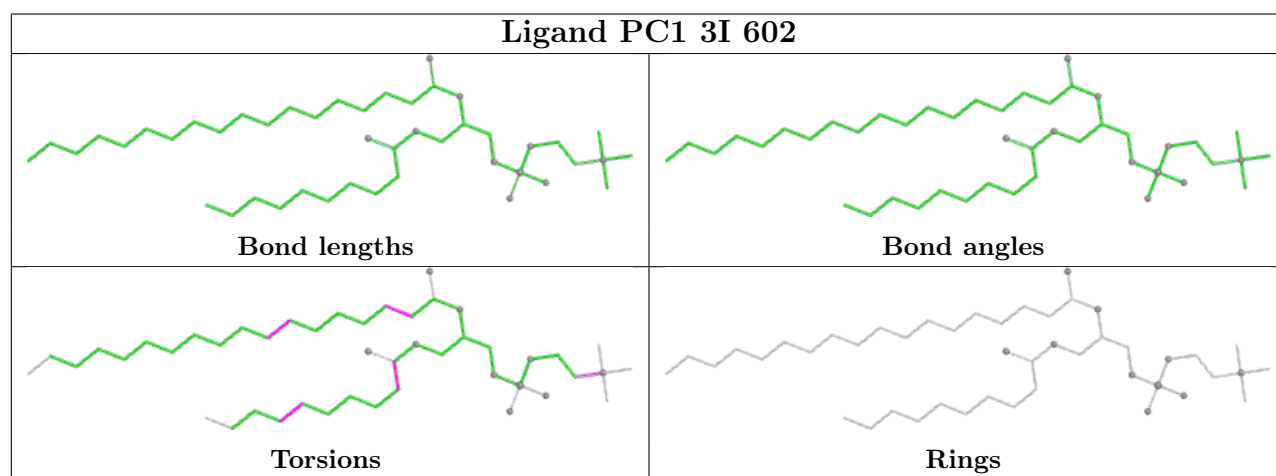
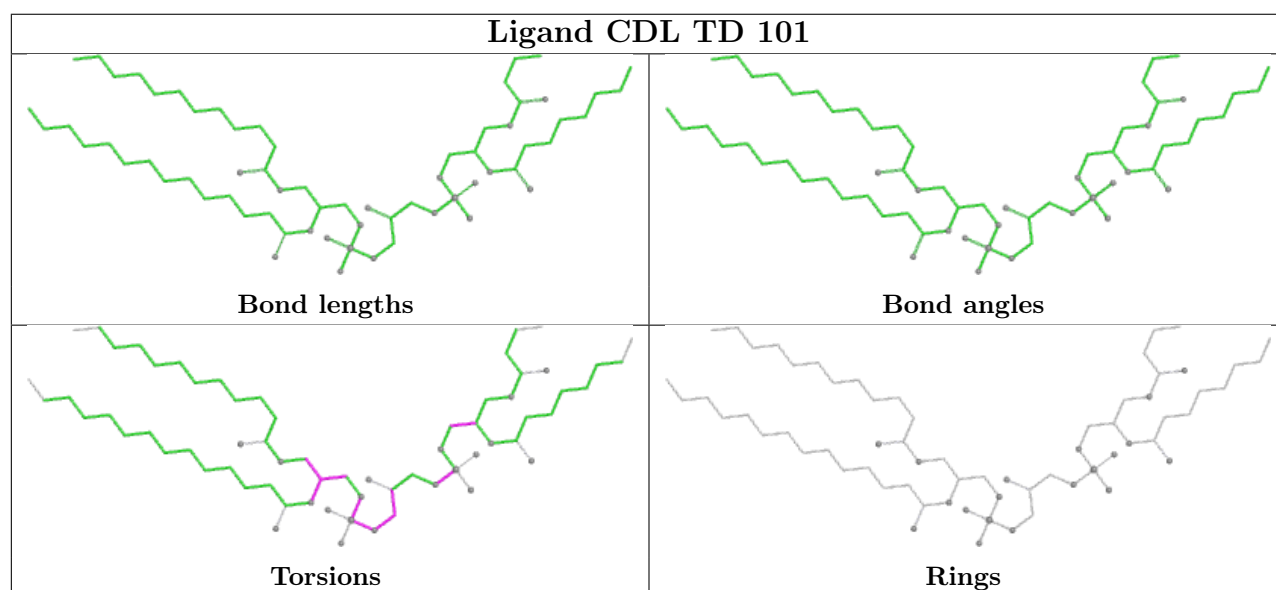
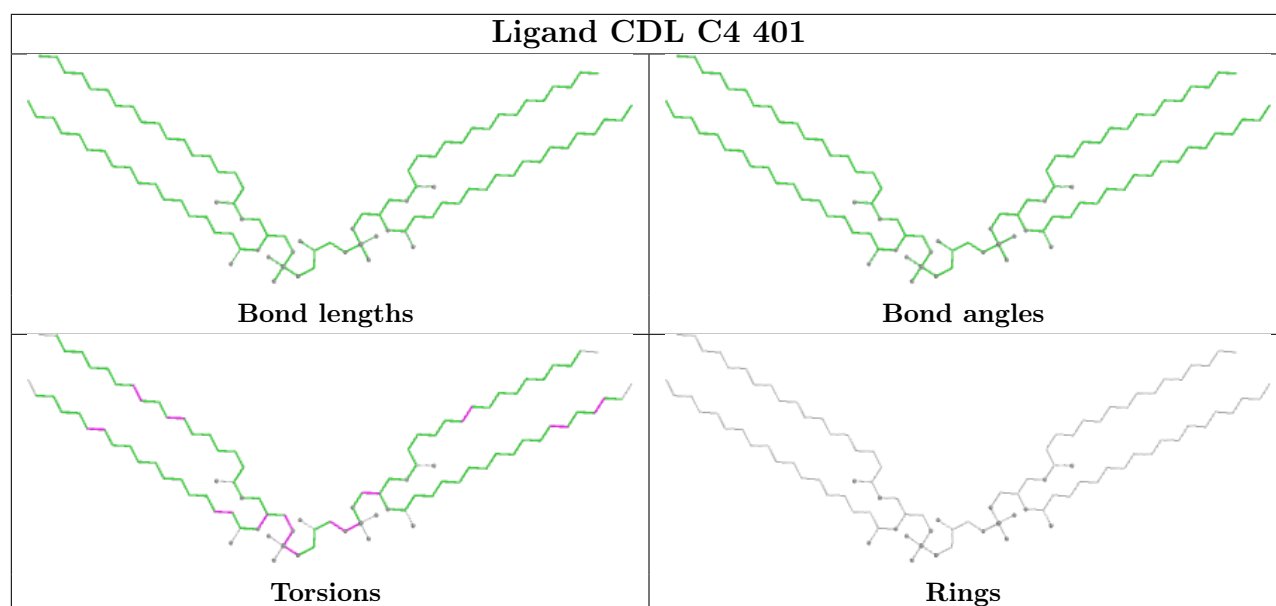
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	T4	301	3PE	3	0
82	5	803	CDL	6	0
85	5B	202	U10	7	0
93	S8	302	SF4	2	0
82	T7	201	CDL	1	0
82	3I	604	CDL	1	0
82	5	805	CDL	8	0
82	B4	201	CDL	1	0
83	C4	403	PC1	1	0
91	AB	201	ZMP	4	0
92	B8	602	ADP	1	0
93	S7	201	SF4	1	0
82	B8	603	CDL	1	0
84	3C	602	HEM	1	0
85	3C	605	U10	4	0
82	3G	401	CDL	2	0
82	3I	603	CDL	1	0
83	3C	604	PC1	2	0
82	T1	602	CDL	3	0
82	3i	201	CDL	3	0
83	TC	101	PC1	4	0
88	4	601	3PE	2	0
87	V2	300	FES	1	0
86	3d	401	HEC	1	0
88	A3	201	3PE	4	0
88	B8	601	3PE	3	0
83	3E	304	PC1	1	0
83	5	807	PC1	5	0
83	3c	506	PC1	1	0
82	BM	301	CDL	9	0
88	5	804	3PE	2	0
83	3C	606	PC1	4	0
83	3g	401	PC1	2	0
93	S1	802	SF4	2	0
82	3c	505	CDL	2	0
88	P1	402	3PE	4	0
82	3C	603	CDL	4	0
84	3C	601	HEM	1	0
90	A9	401	NDP	1	0
82	3B	701	CDL	5	0
94	V1	501	FMN	1	0
83	3J	101	PC1	4	0

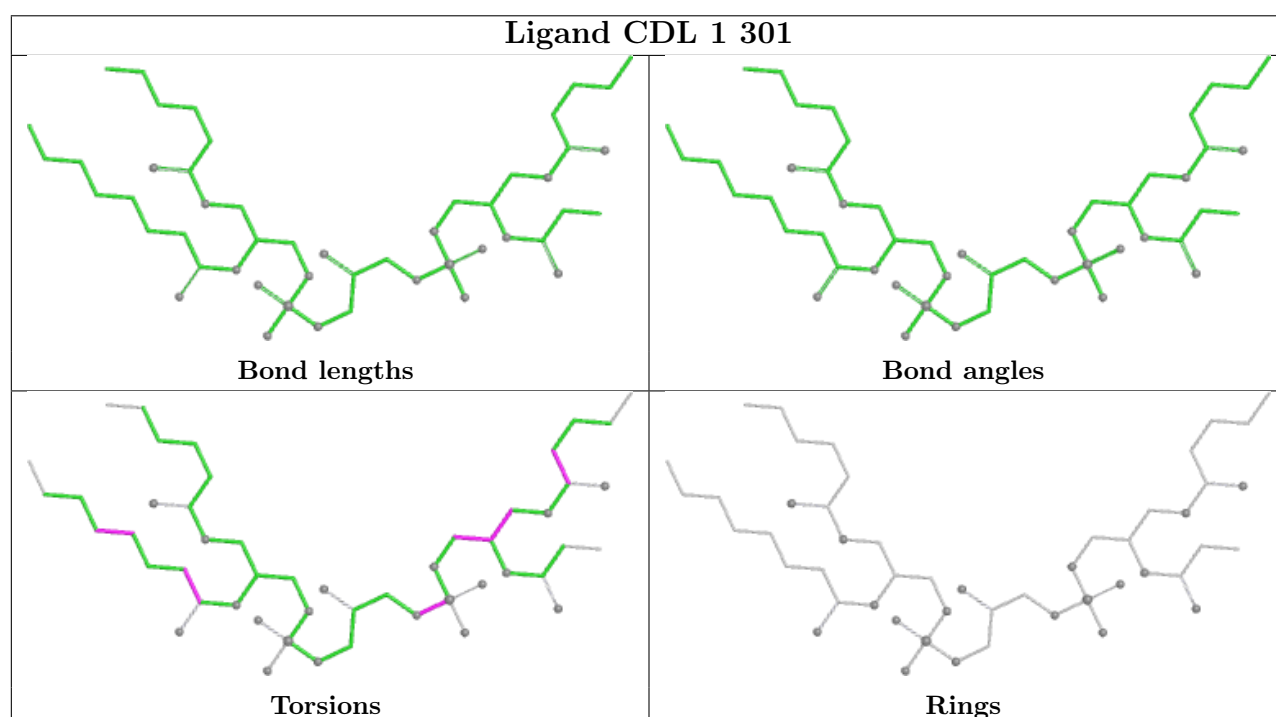
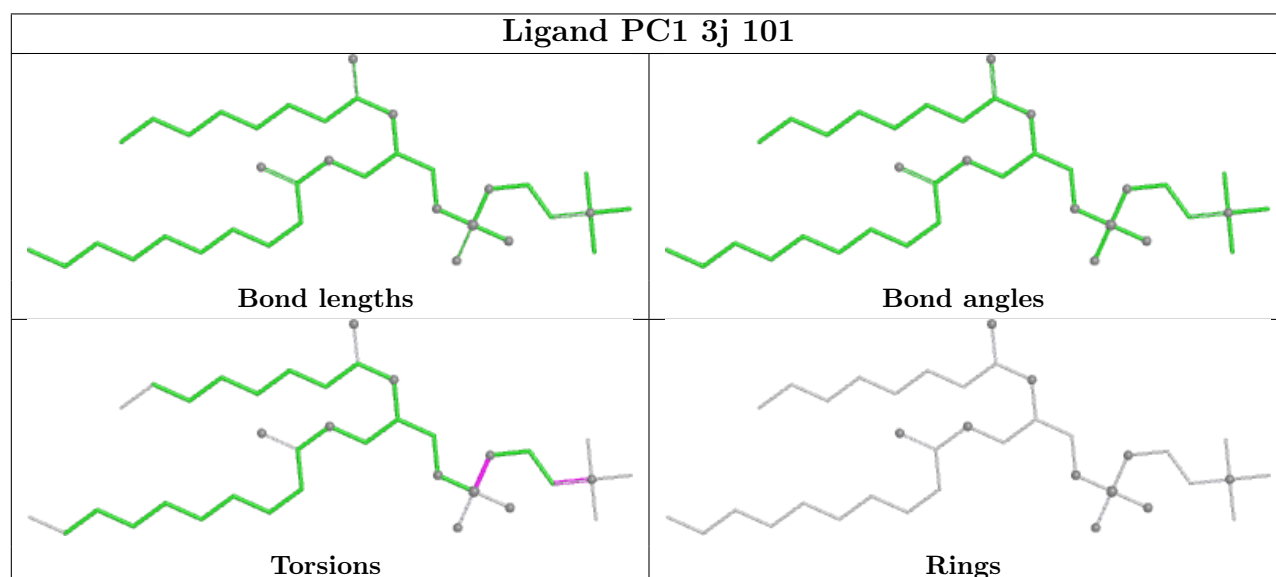
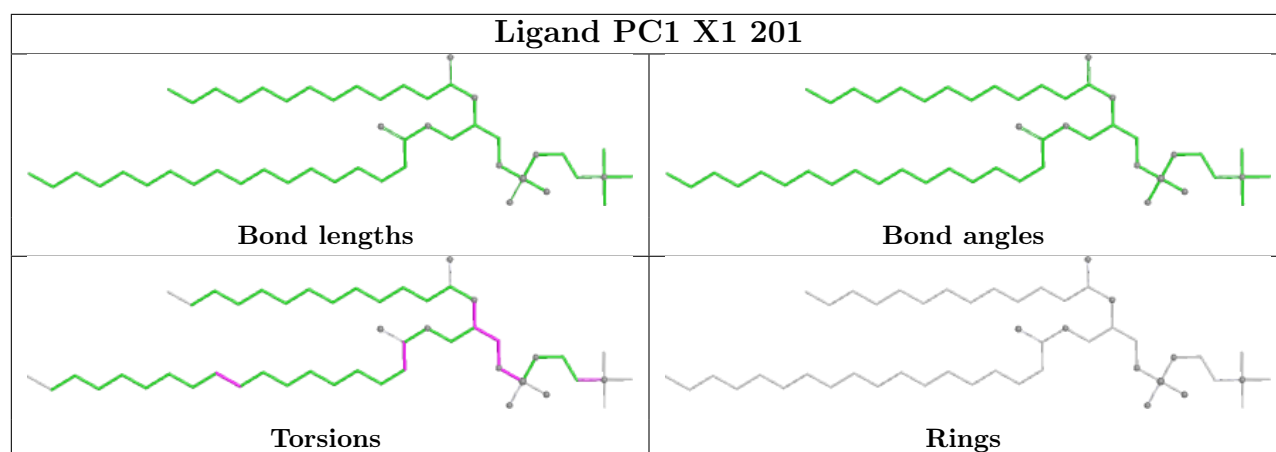
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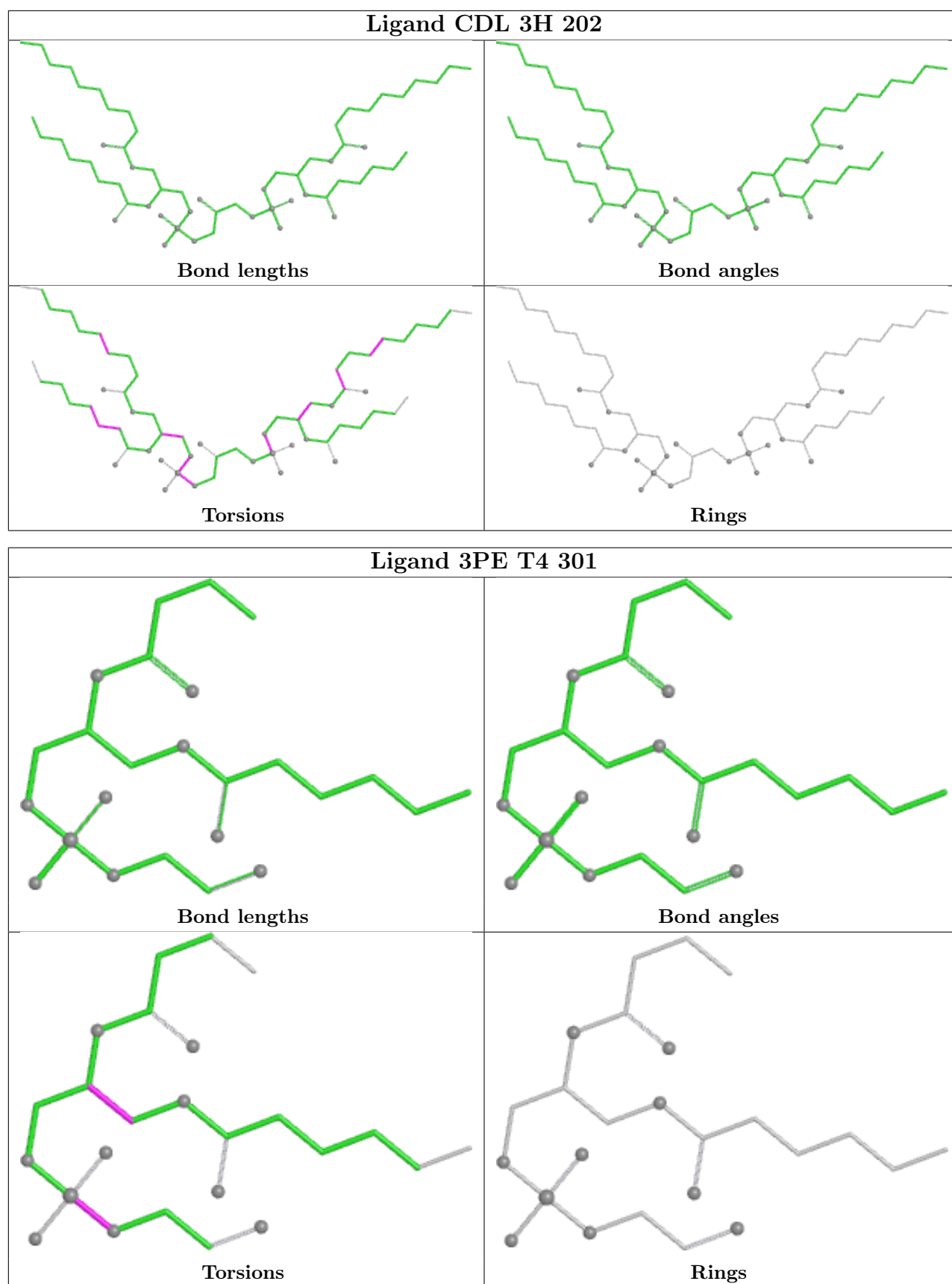
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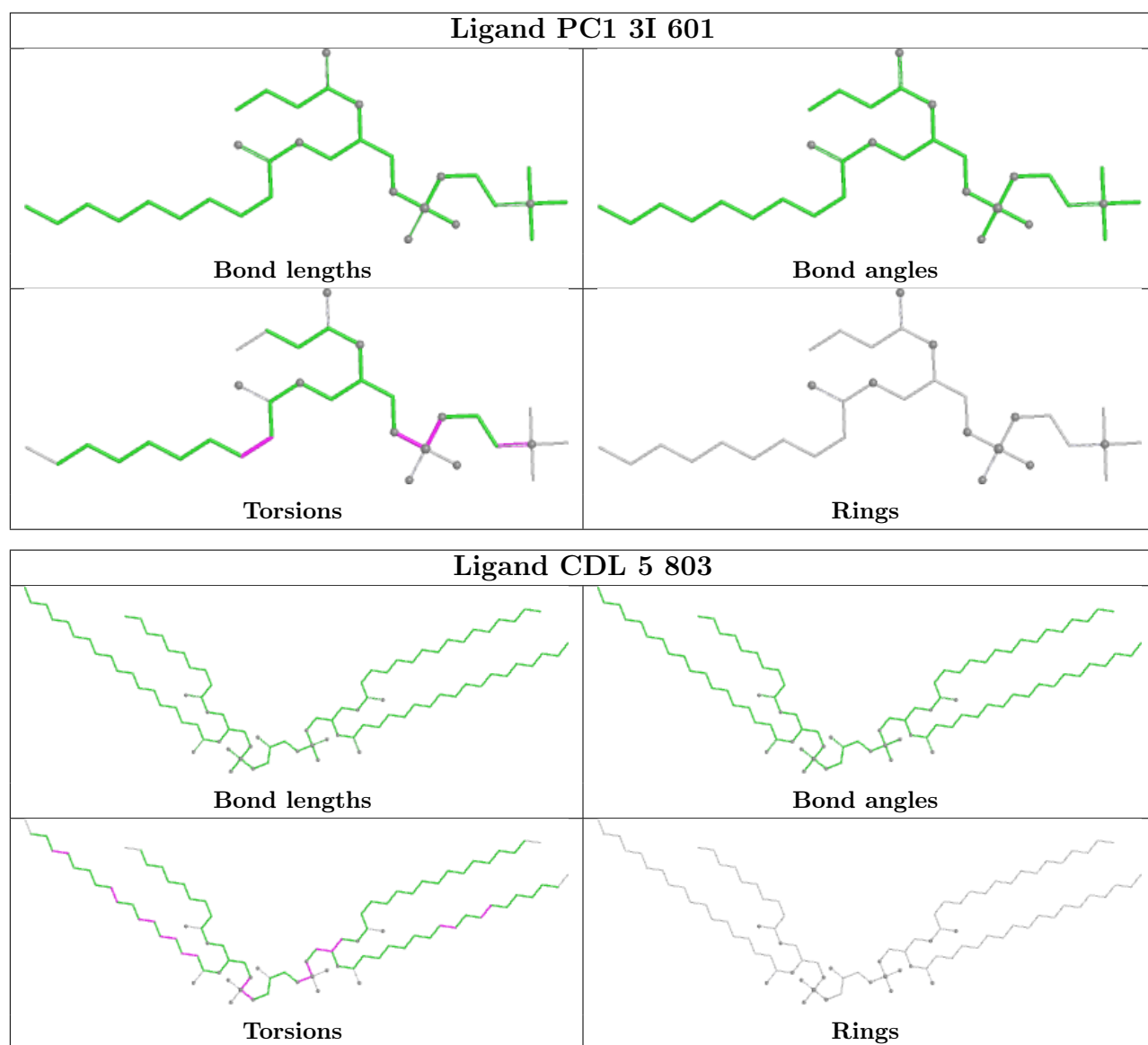
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	3d	402	3PE	3	0
83	AM	201	PC1	2	0
88	AN	301	3PE	4	0
82	P2	201	CDL	3	0
83	5	802	PC1	2	0
83	AN	303	PC1	1	0
83	B6	201	PC1	3	0
82	3b	602	CDL	3	0
84	3c	502	HEM	3	0
83	B2	201	PC1	7	0
83	3E	302	PC1	7	0
83	3e	301	PC1	2	0
83	6	302	PC1	3	0
88	C4	402	3PE	3	0
83	3c	501	PC1	1	0
93	S8	301	SF4	1	0
82	R	201	CDL	3	0
84	3c	503	HEM	4	0
83	3b	601	PC1	1	0
83	6	301	PC1	3	0
88	S8	303	3PE	1	0
83	J1	400	PC1	1	0
88	AN	302	3PE	1	0
82	AN	304	CDL	3	0
82	AM	202	CDL	7	0
83	5	801	PC1	3	0
82	AL	301	CDL	3	0

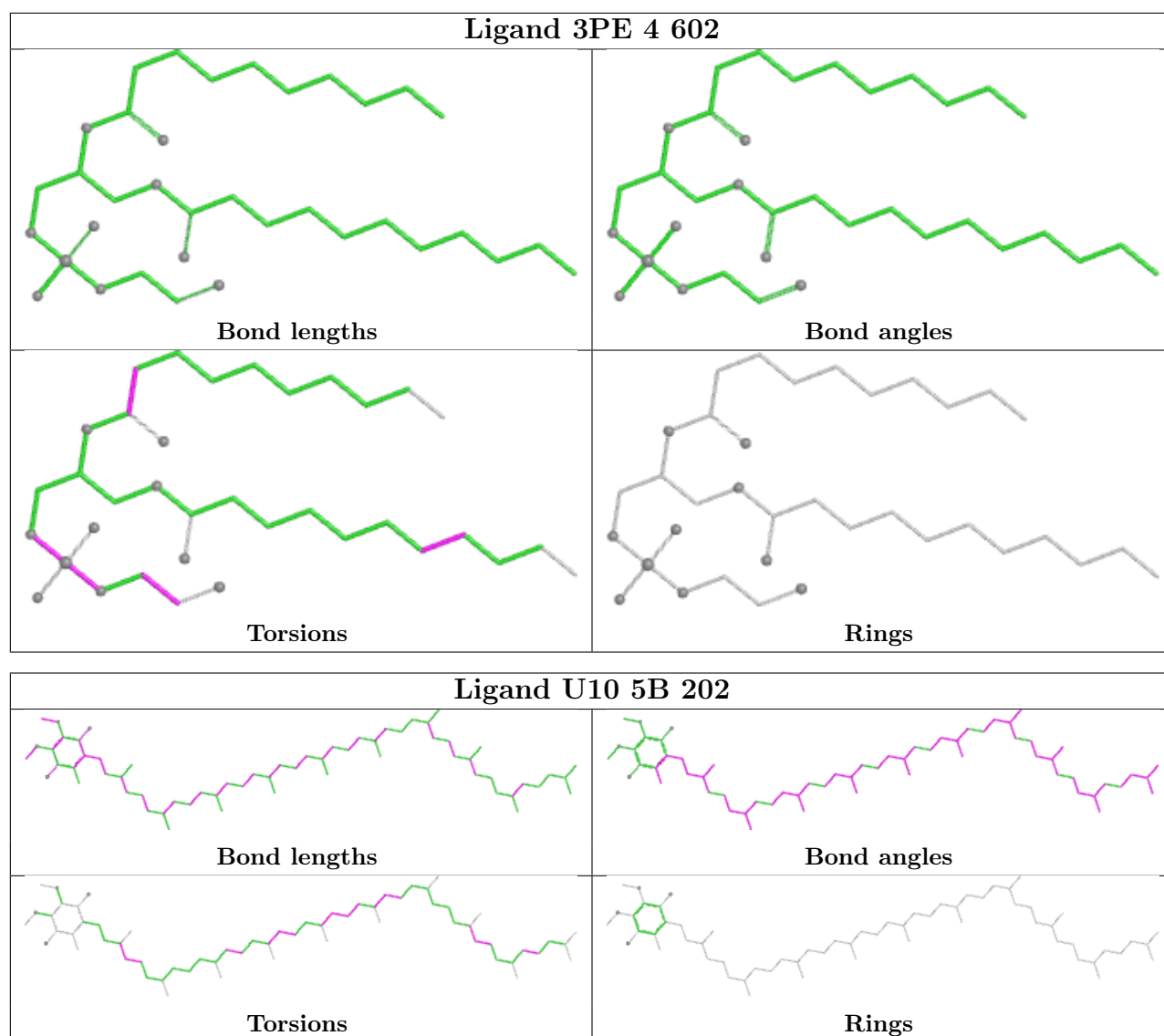
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

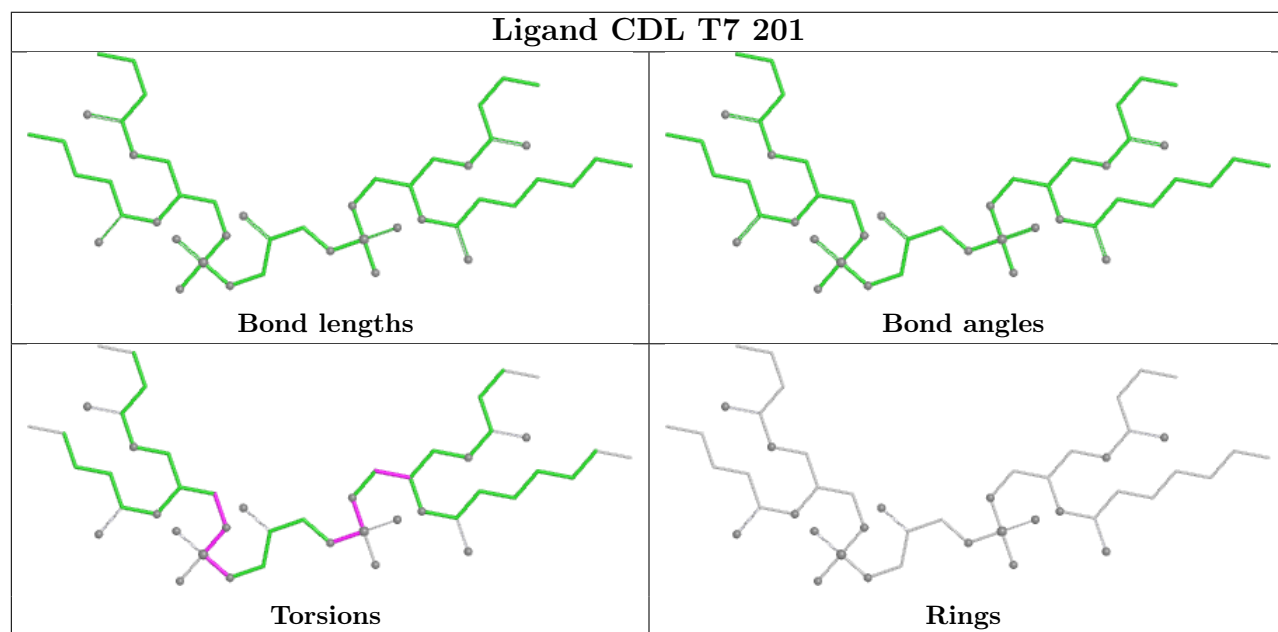
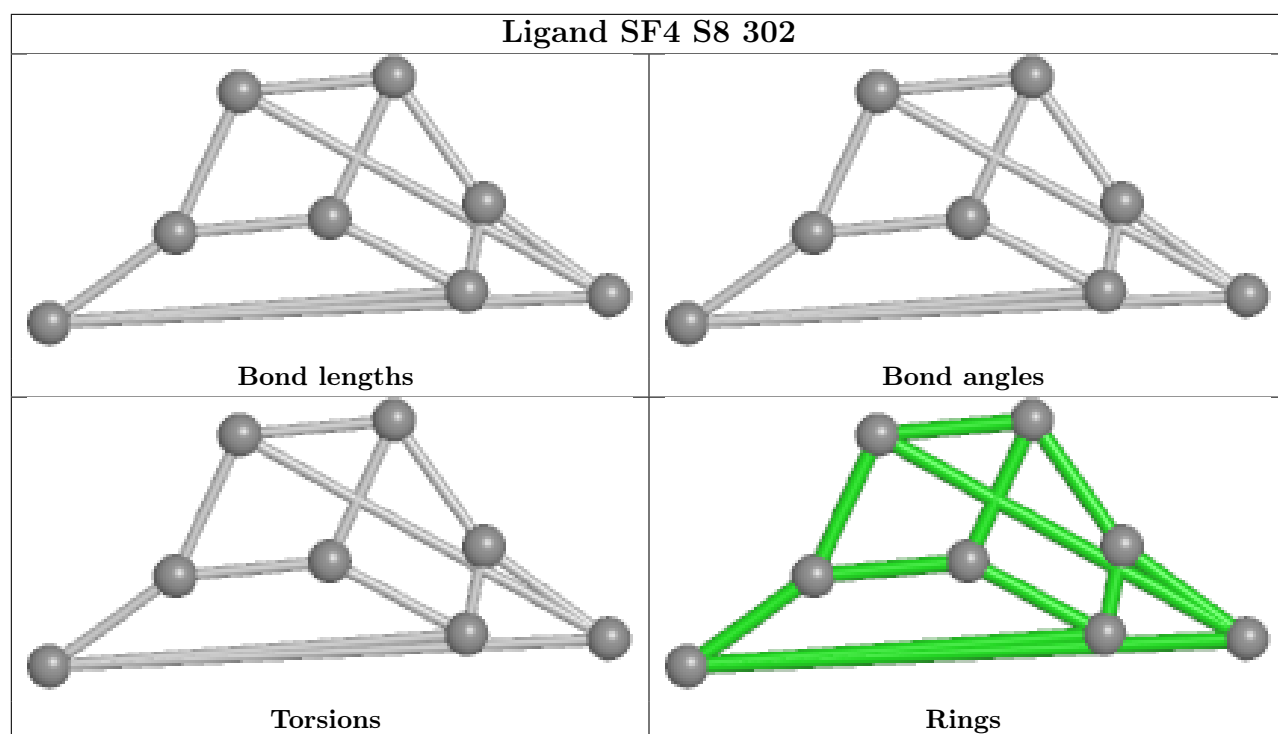


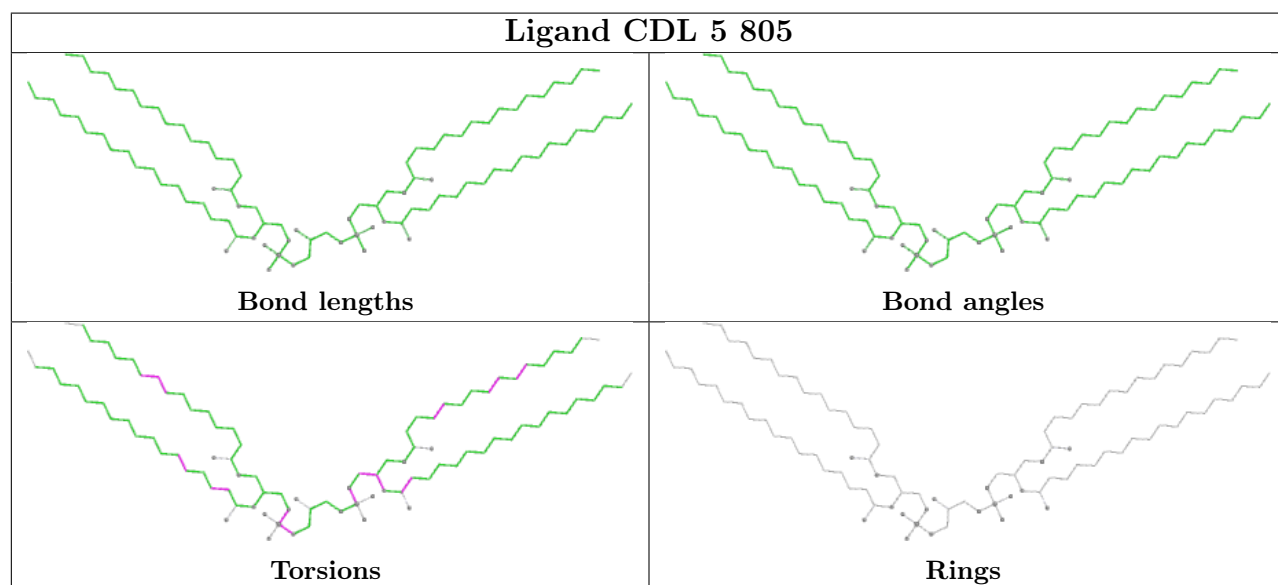
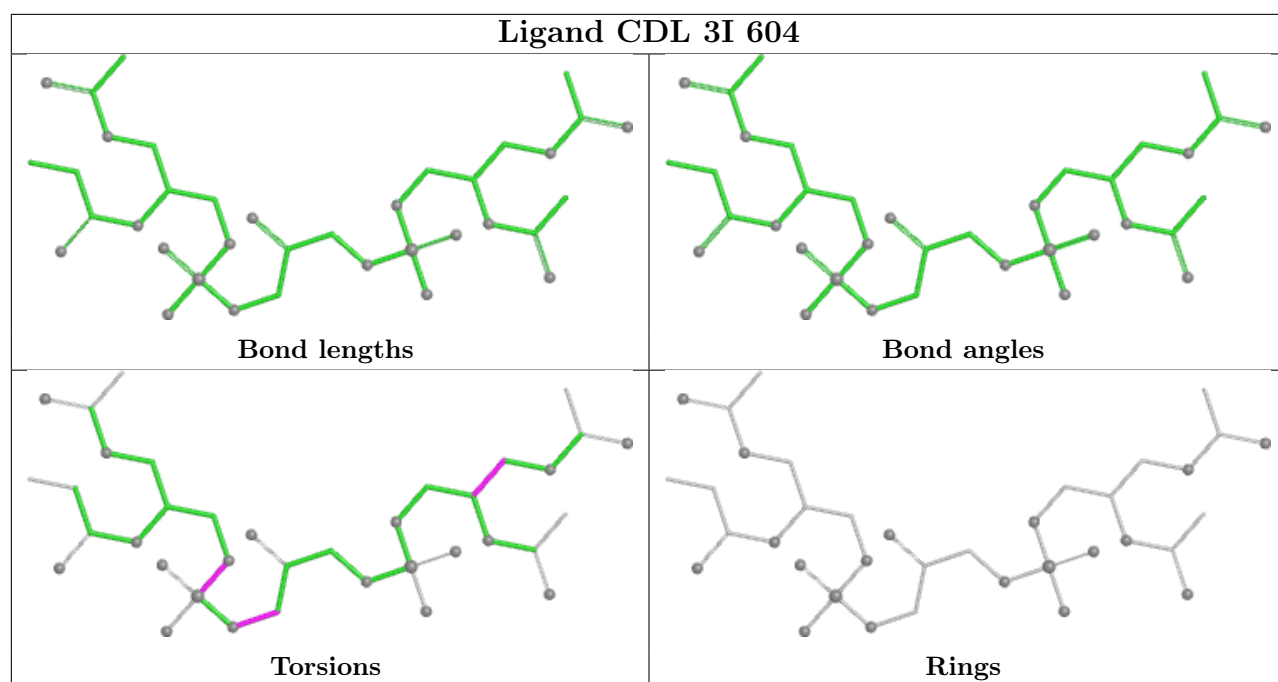


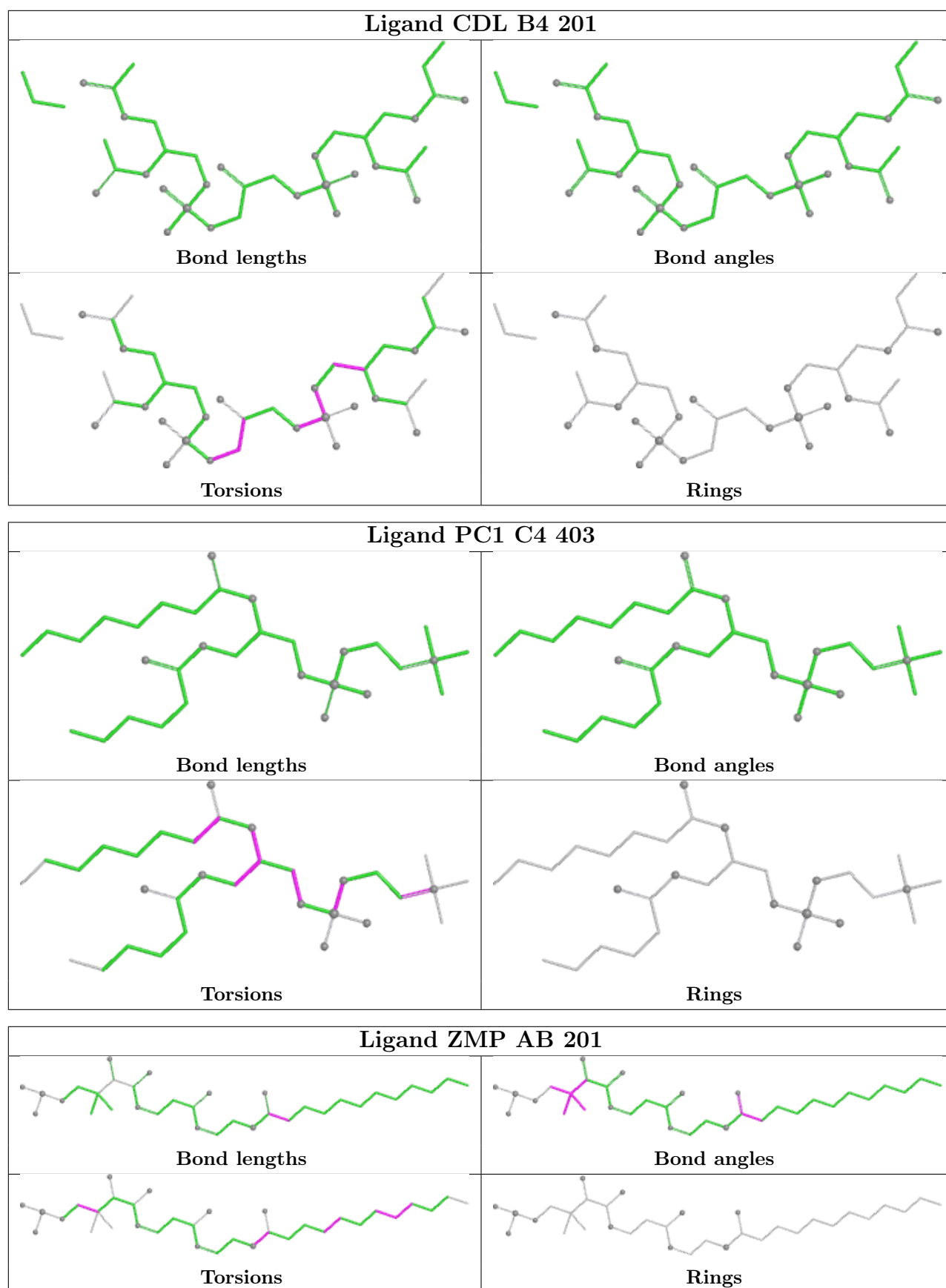


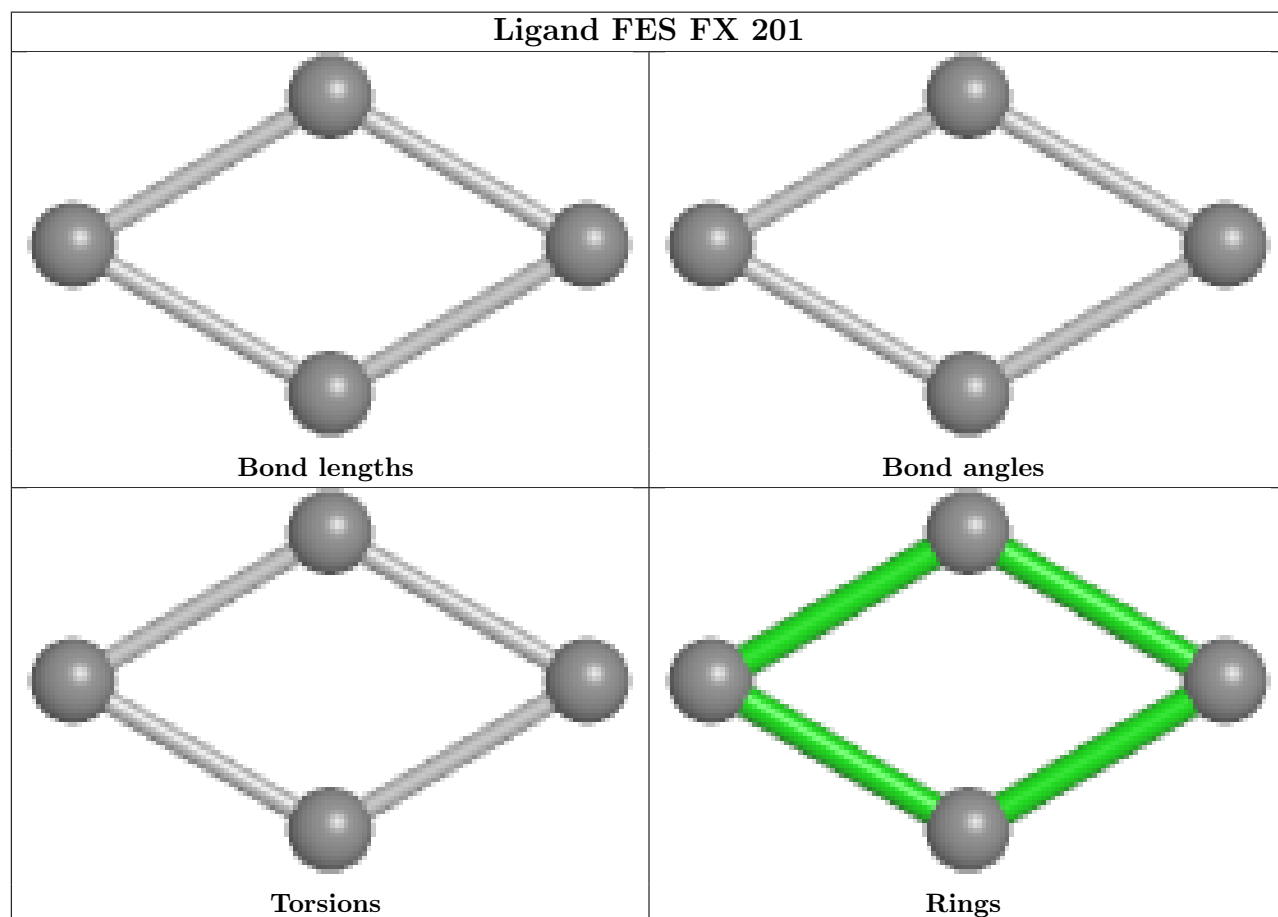
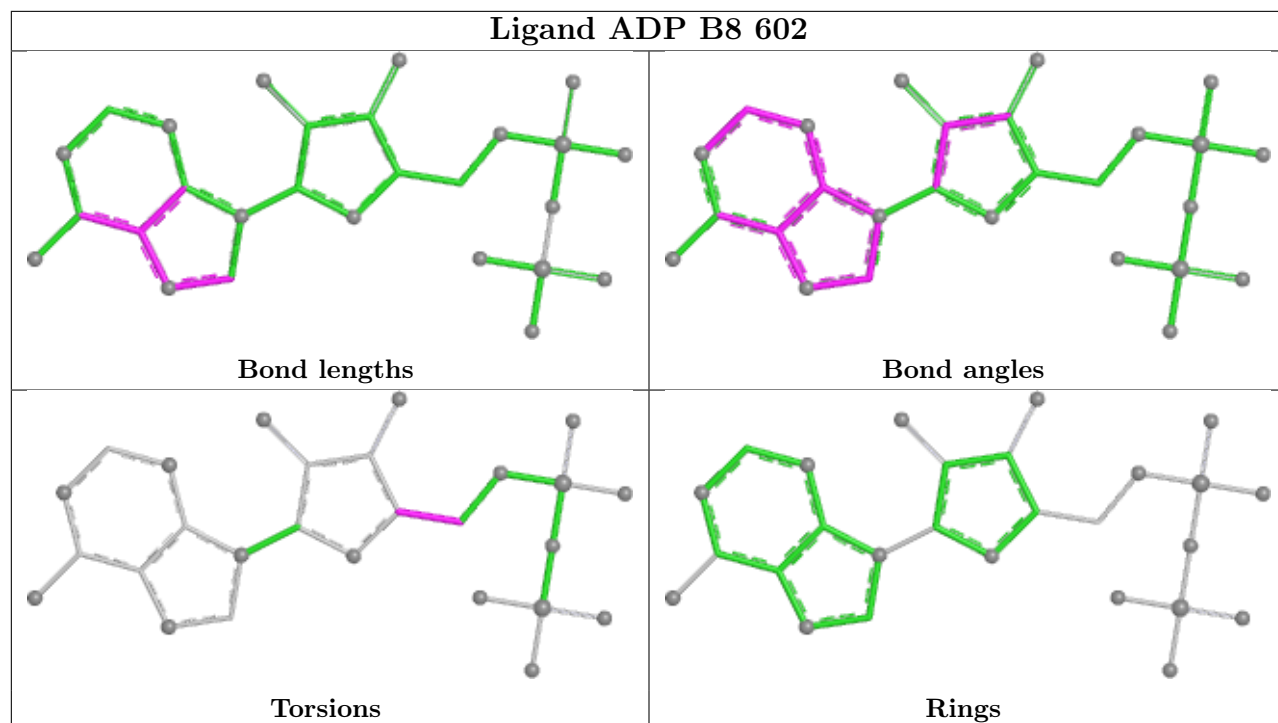


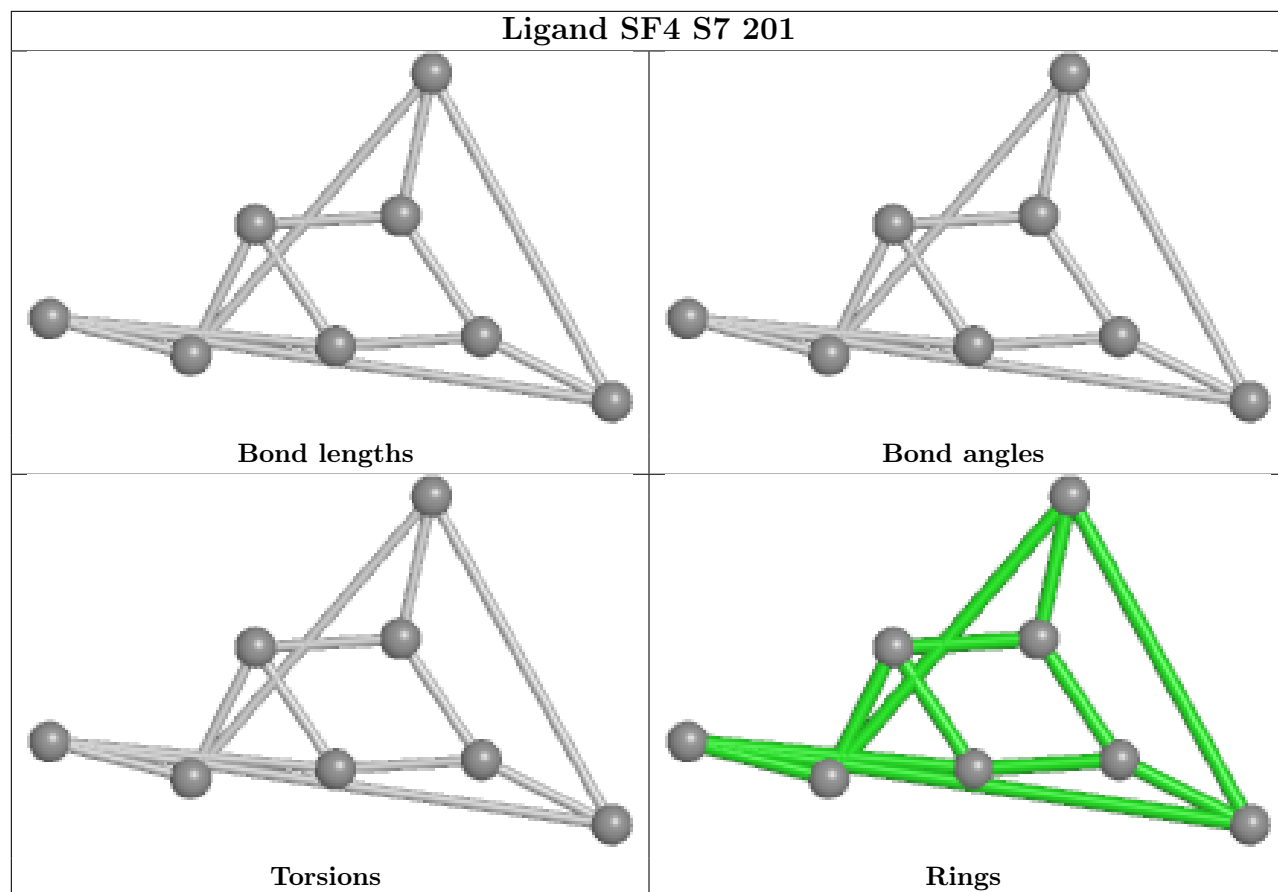


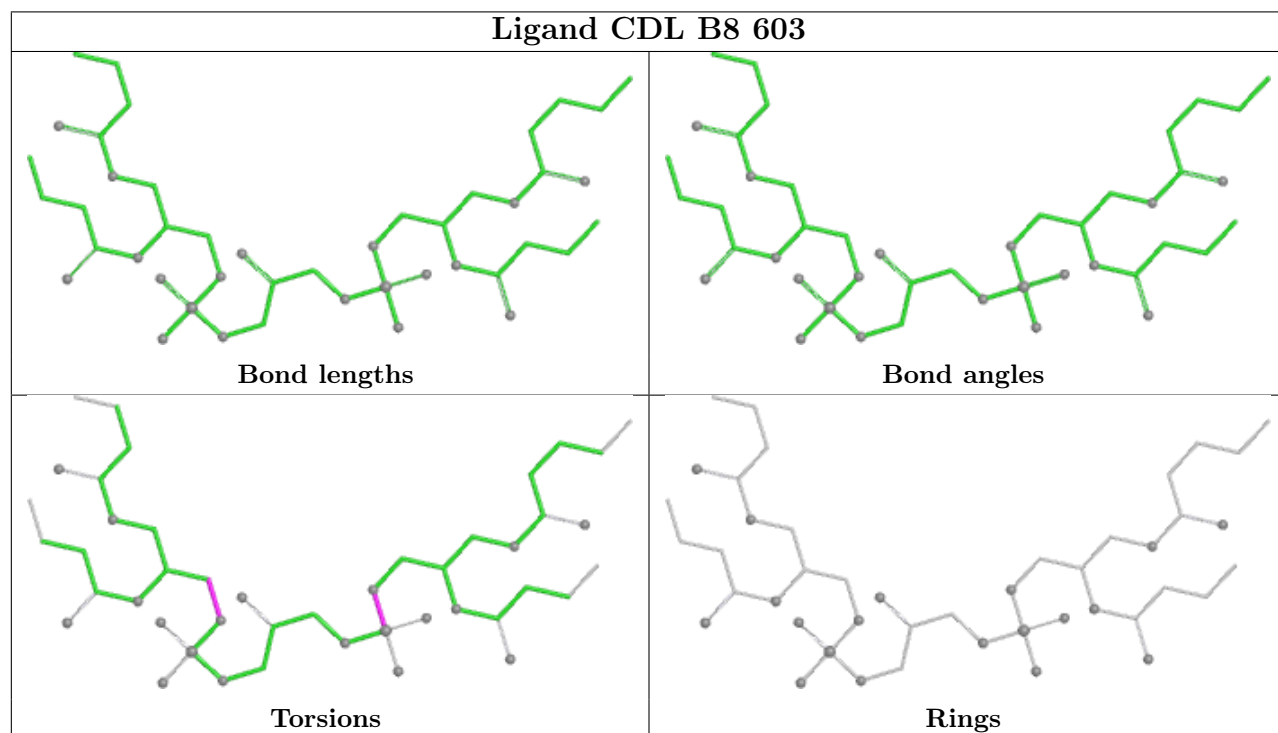
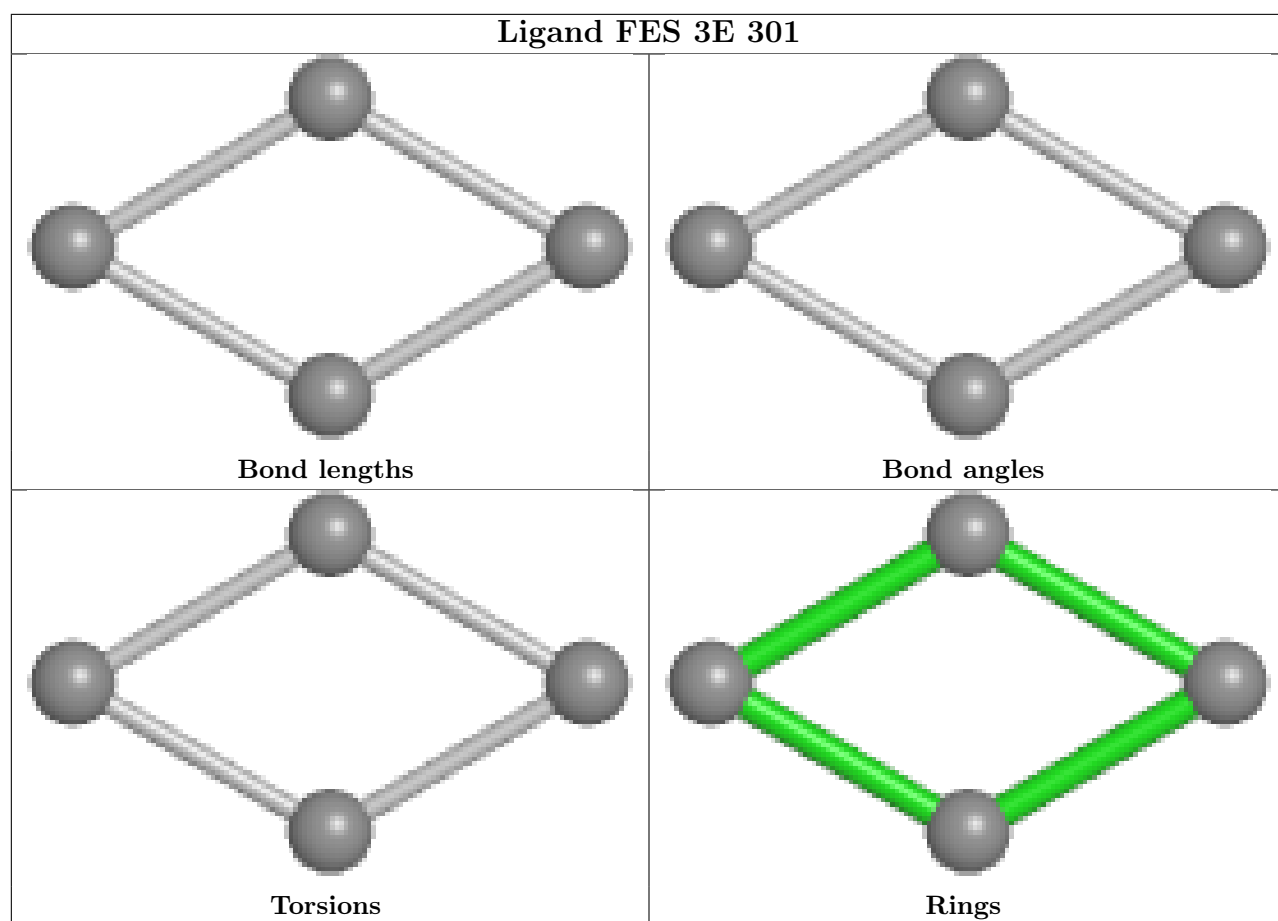




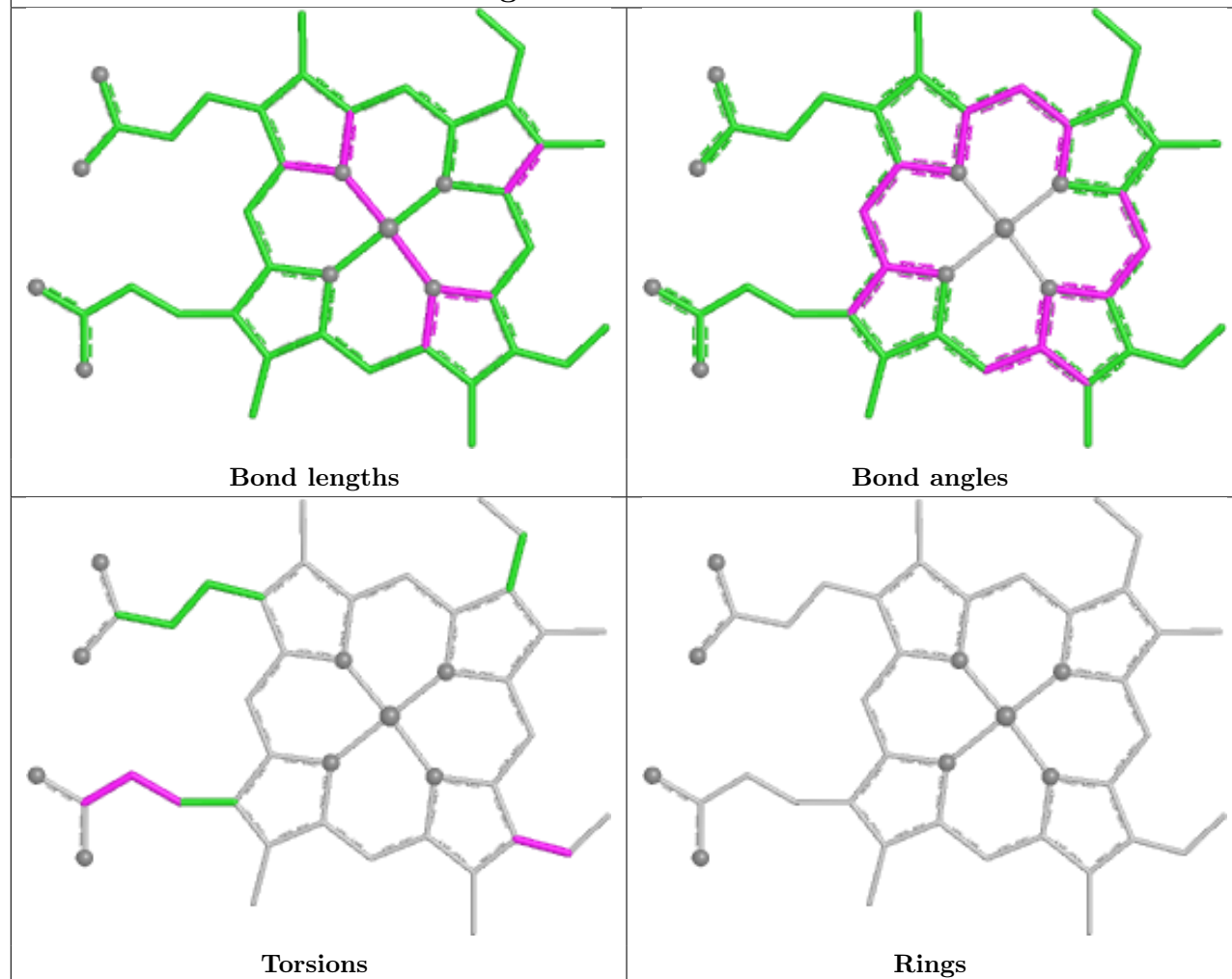




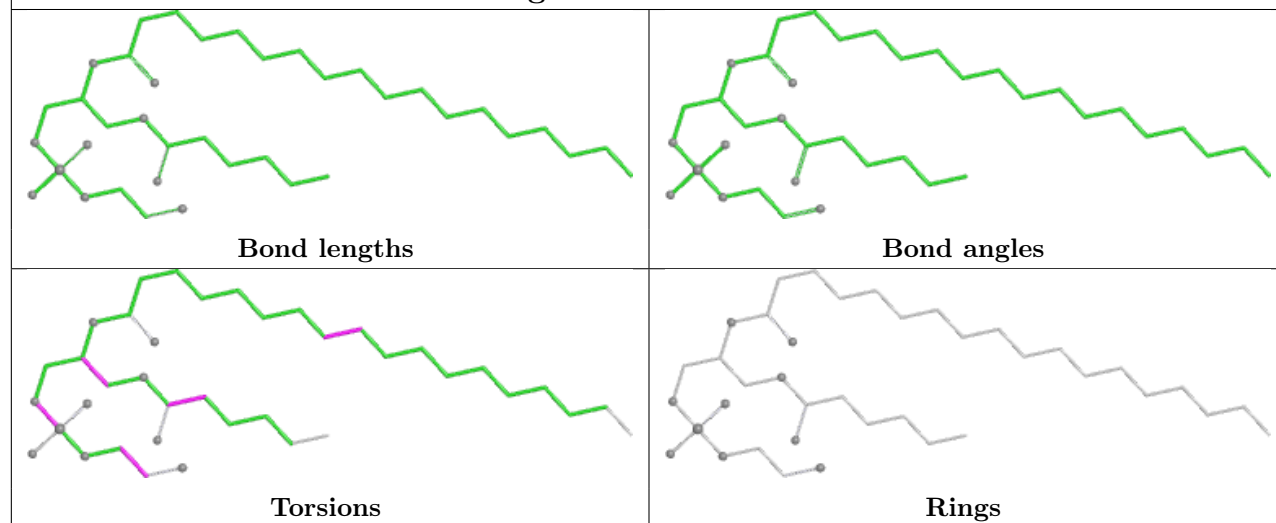


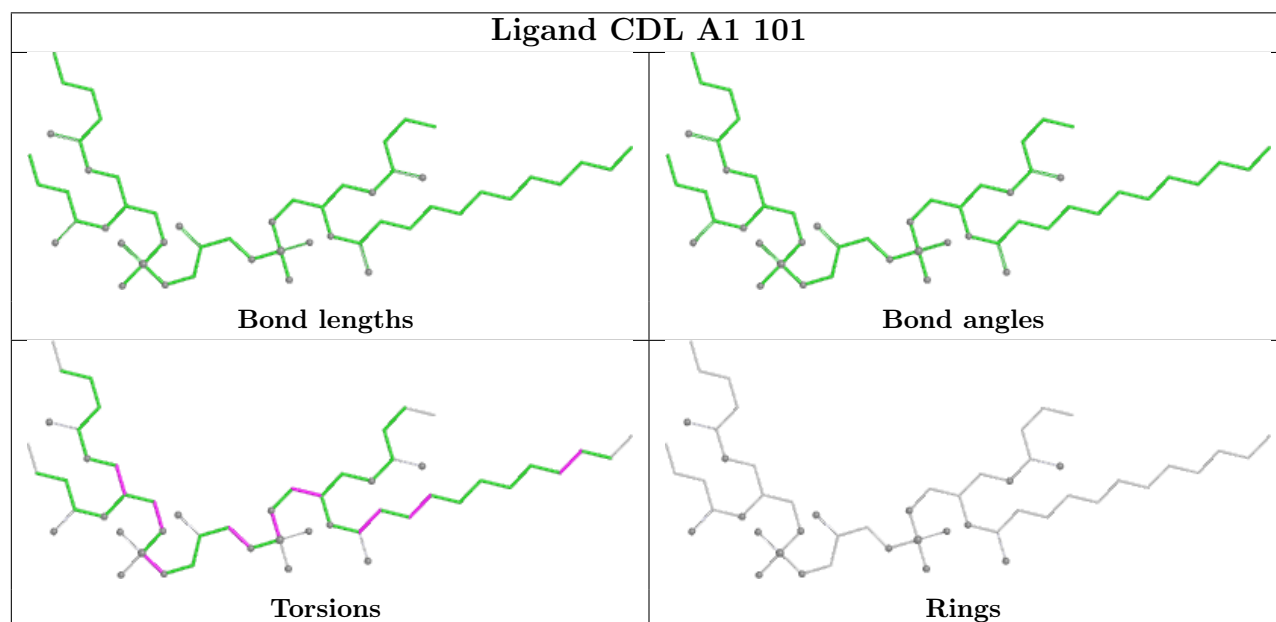
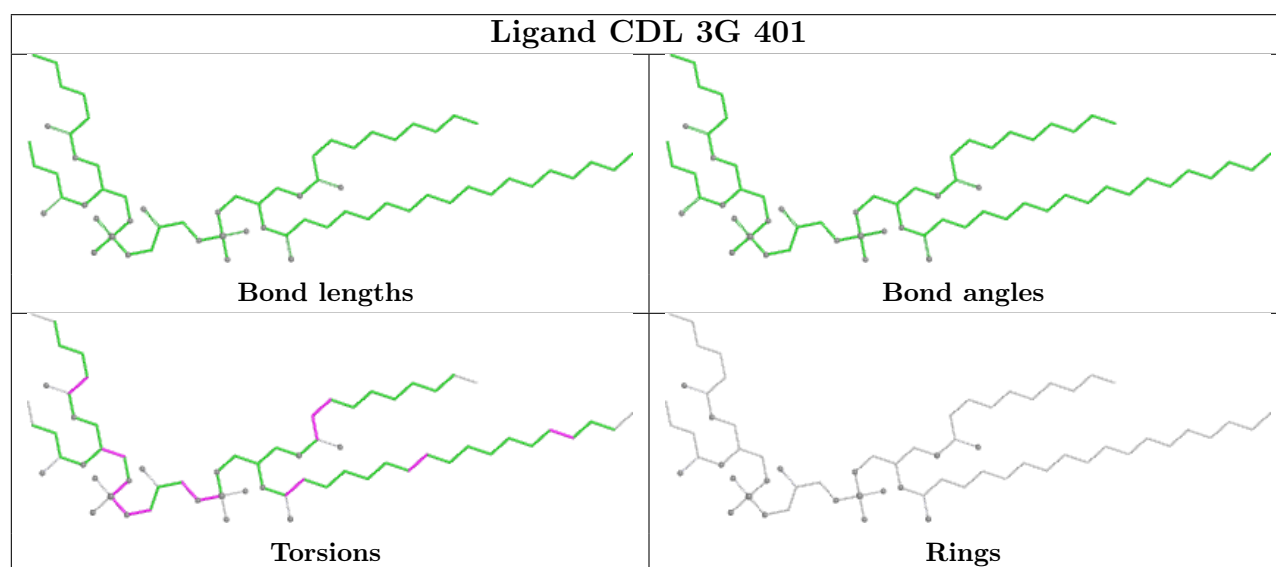
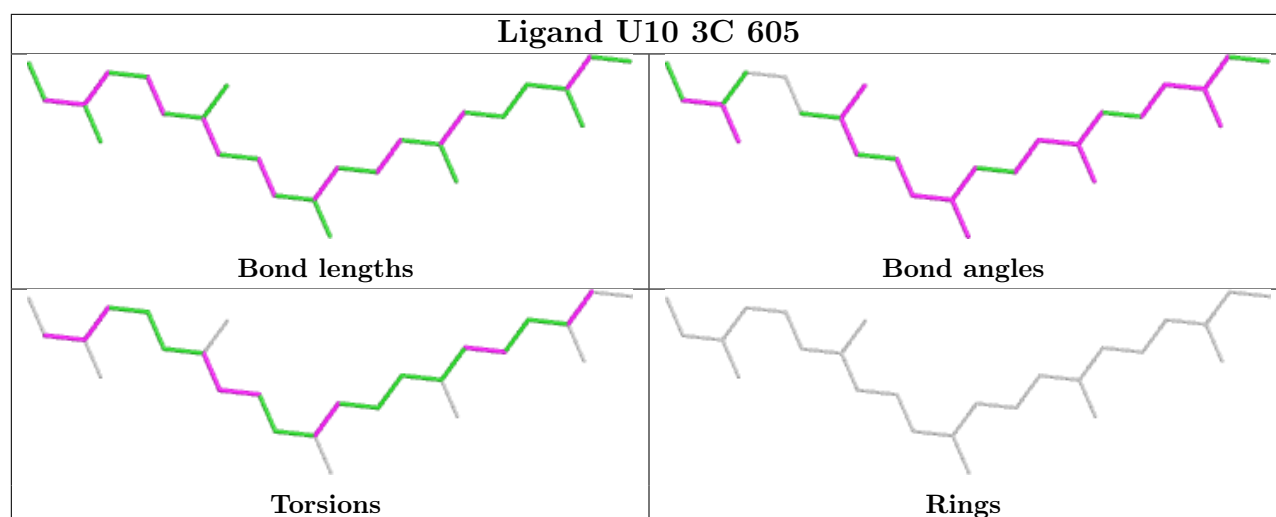


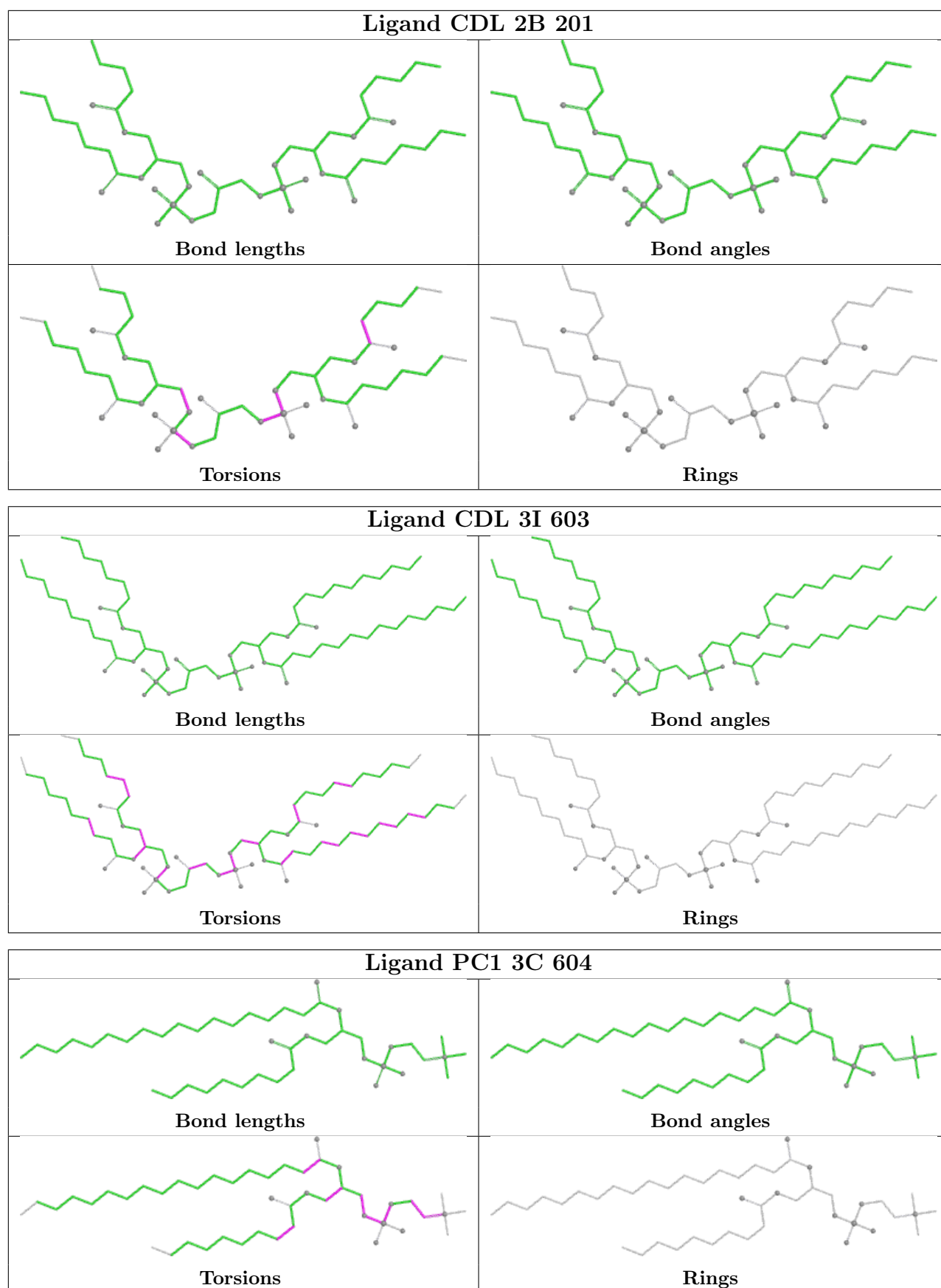
Ligand HEM 3C 602

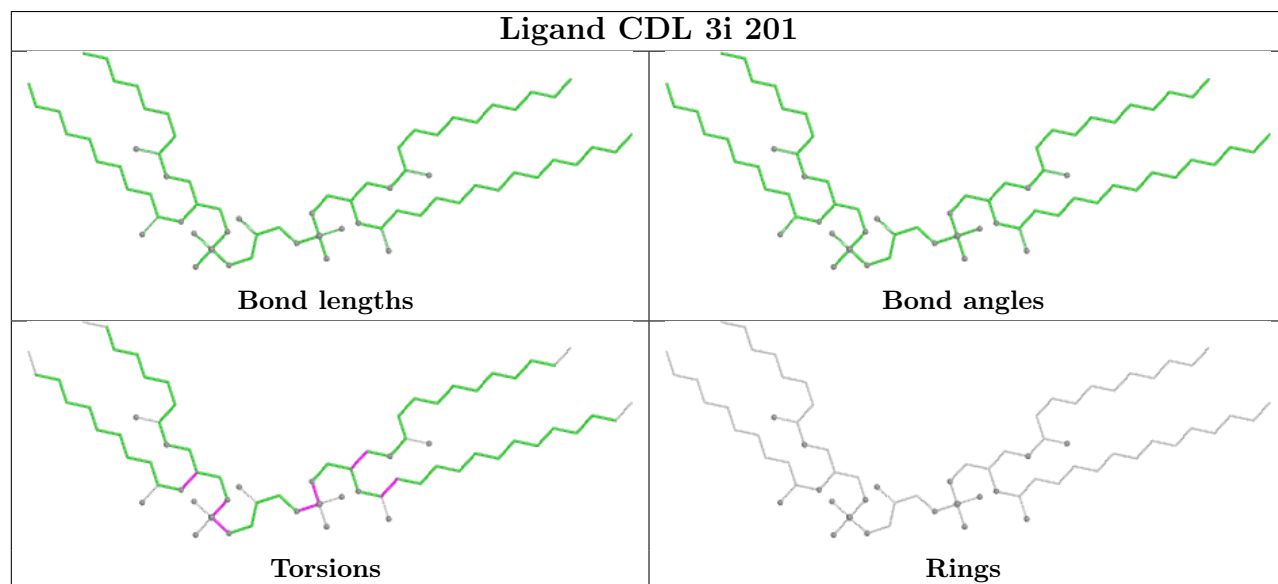
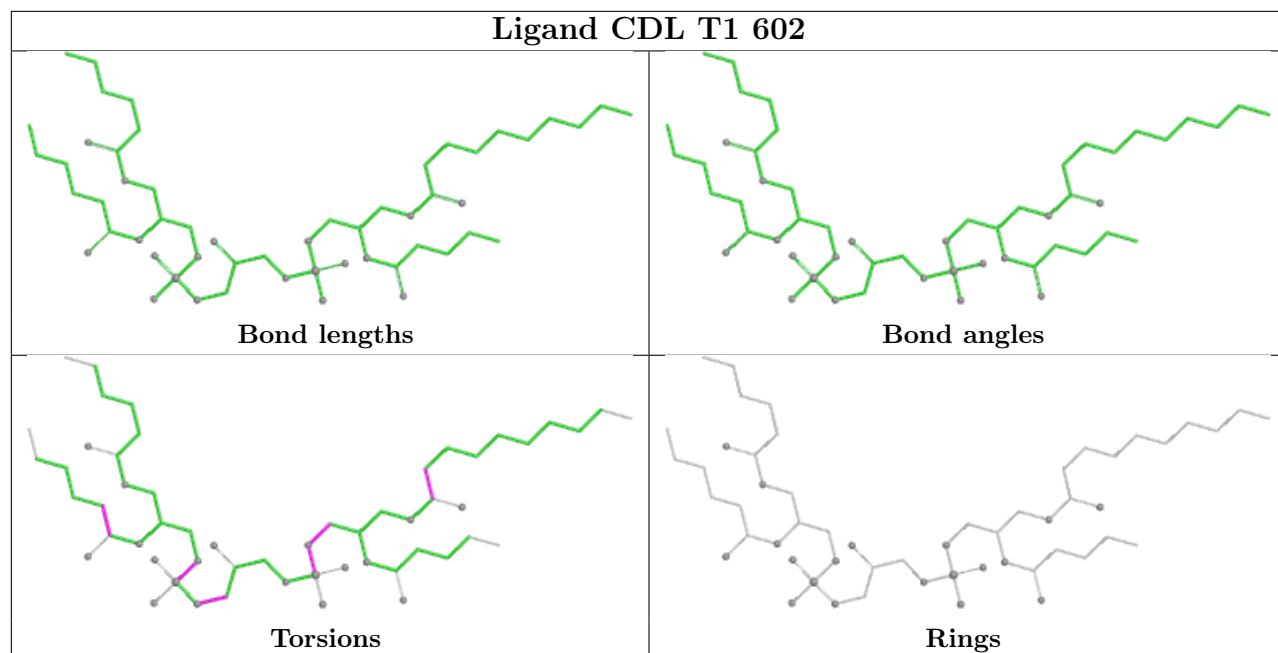


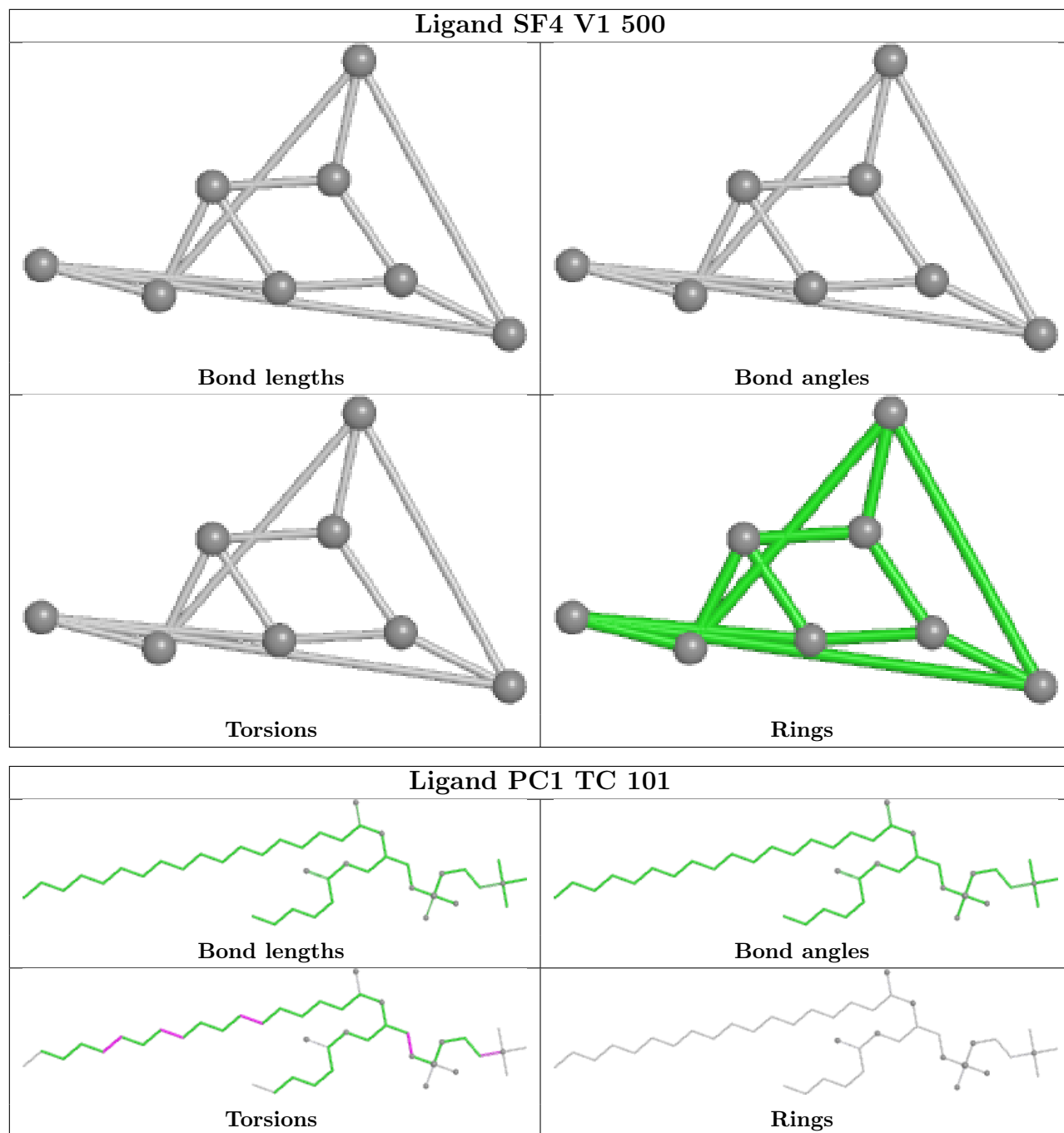
Ligand 3PE T8 201

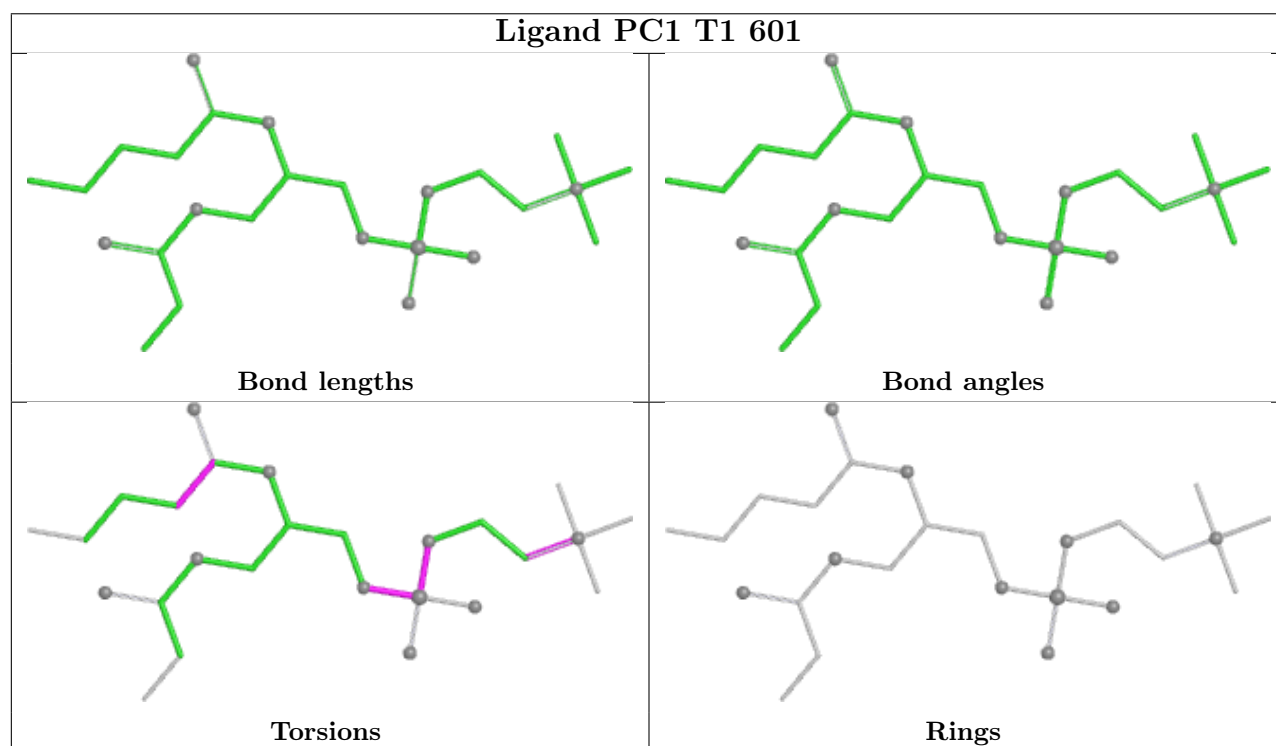
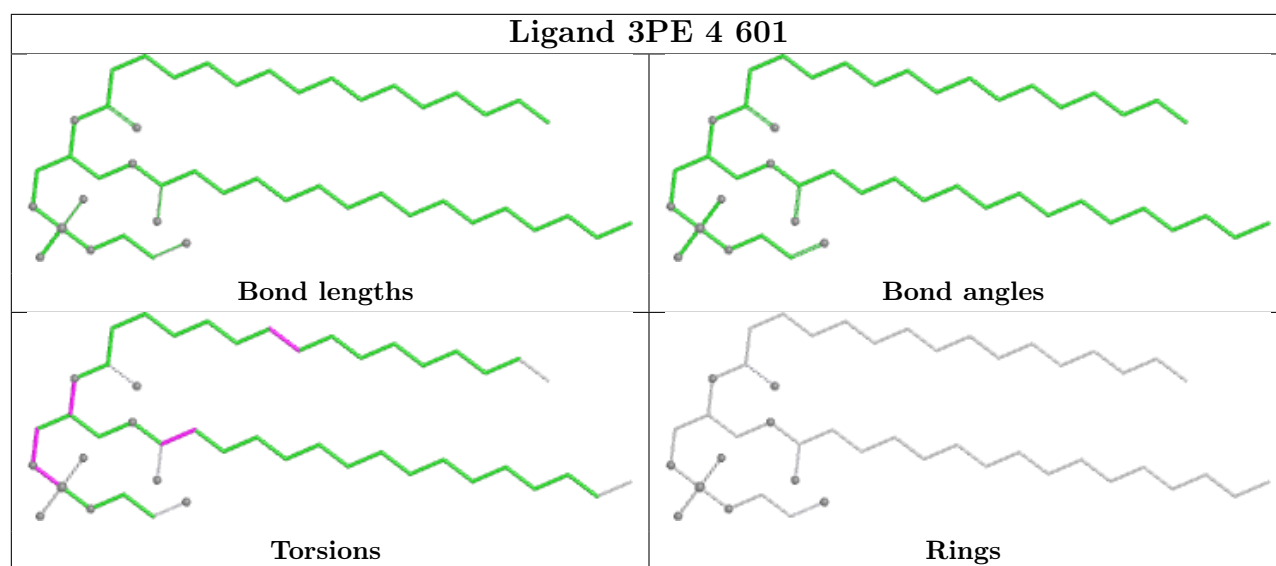


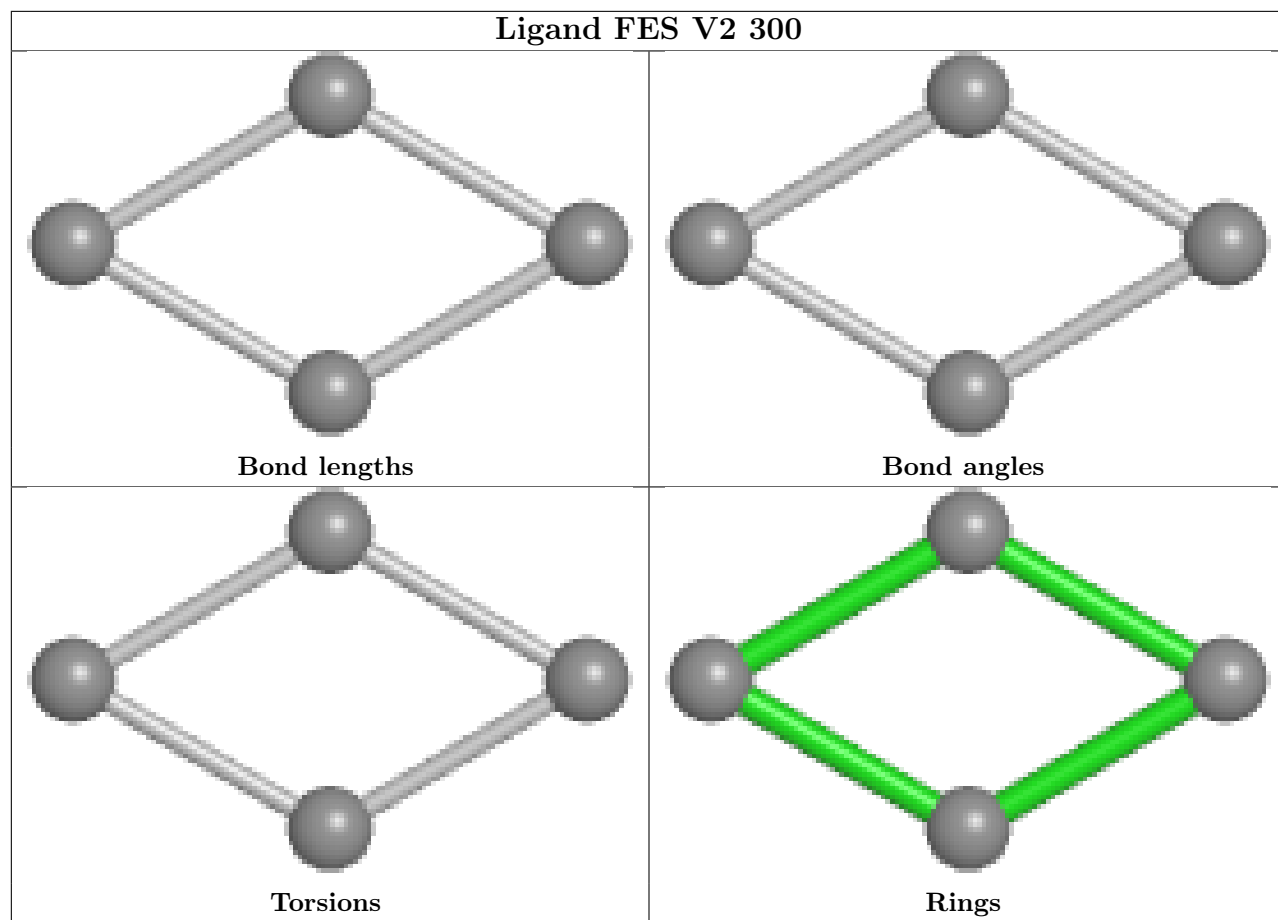


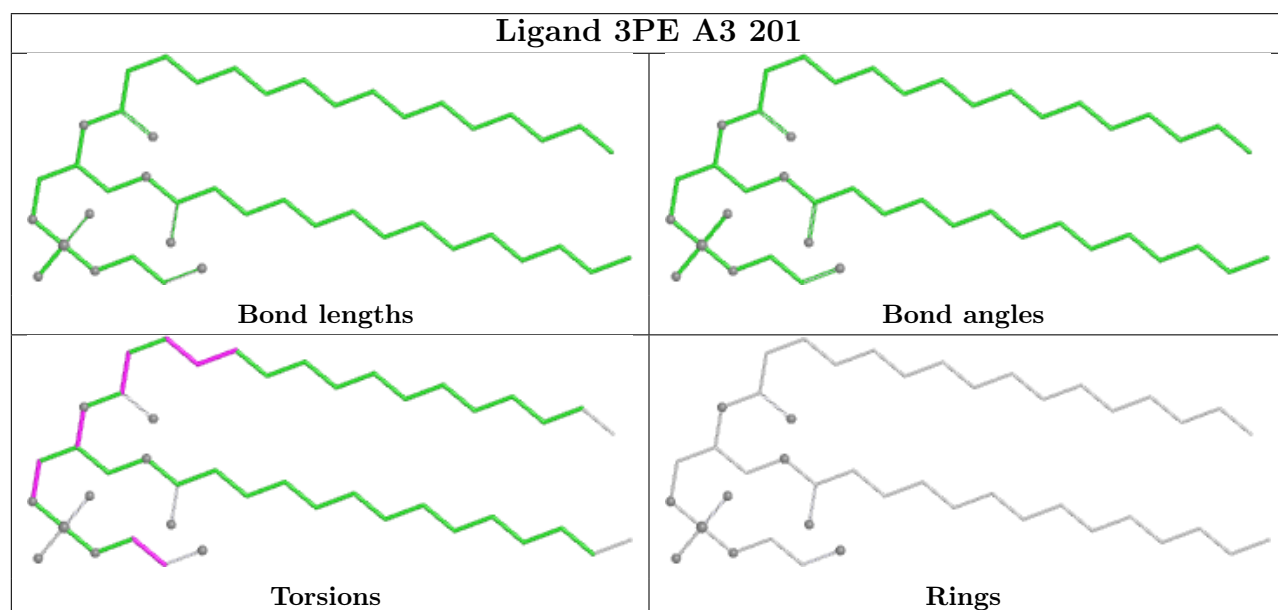
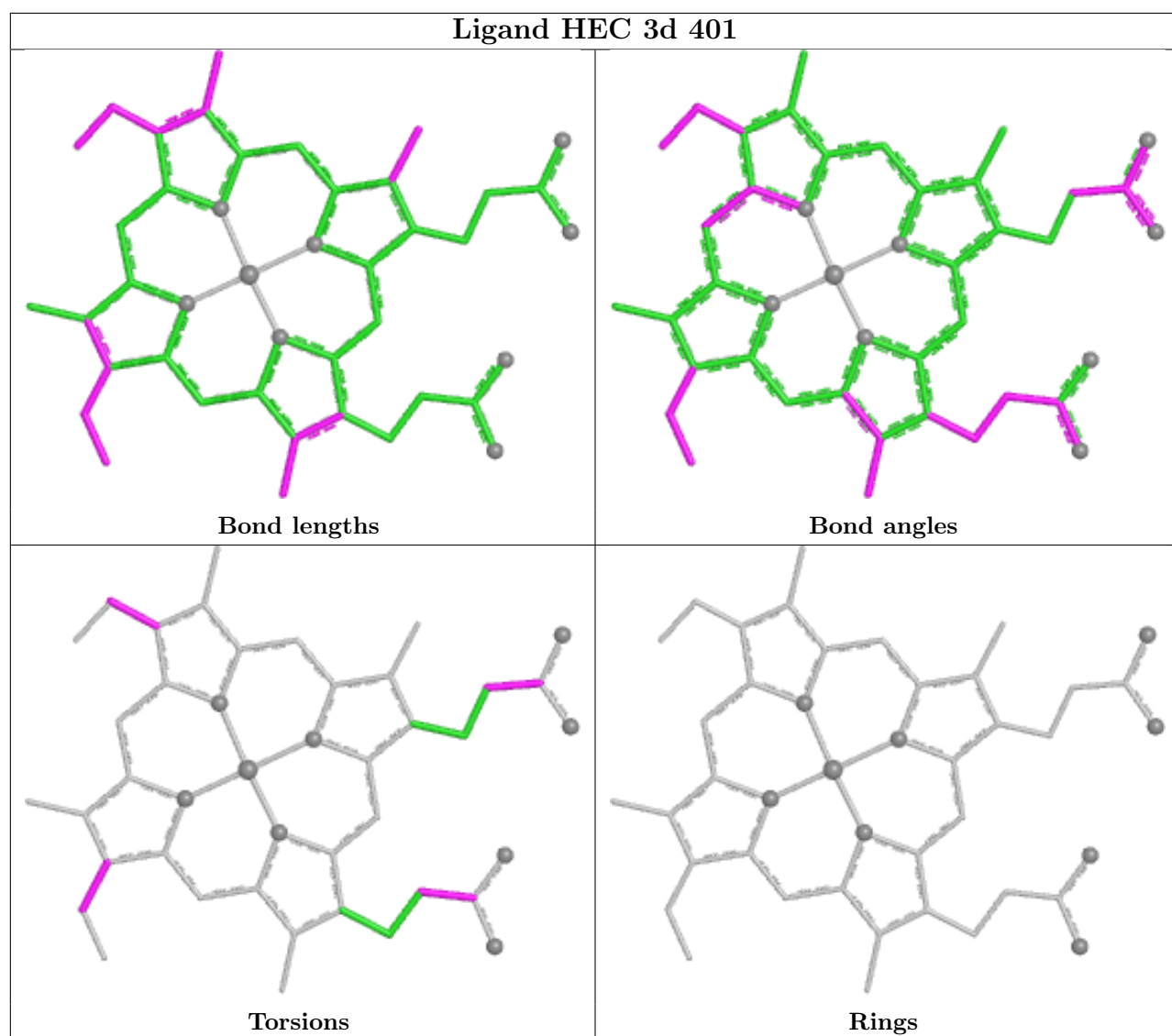


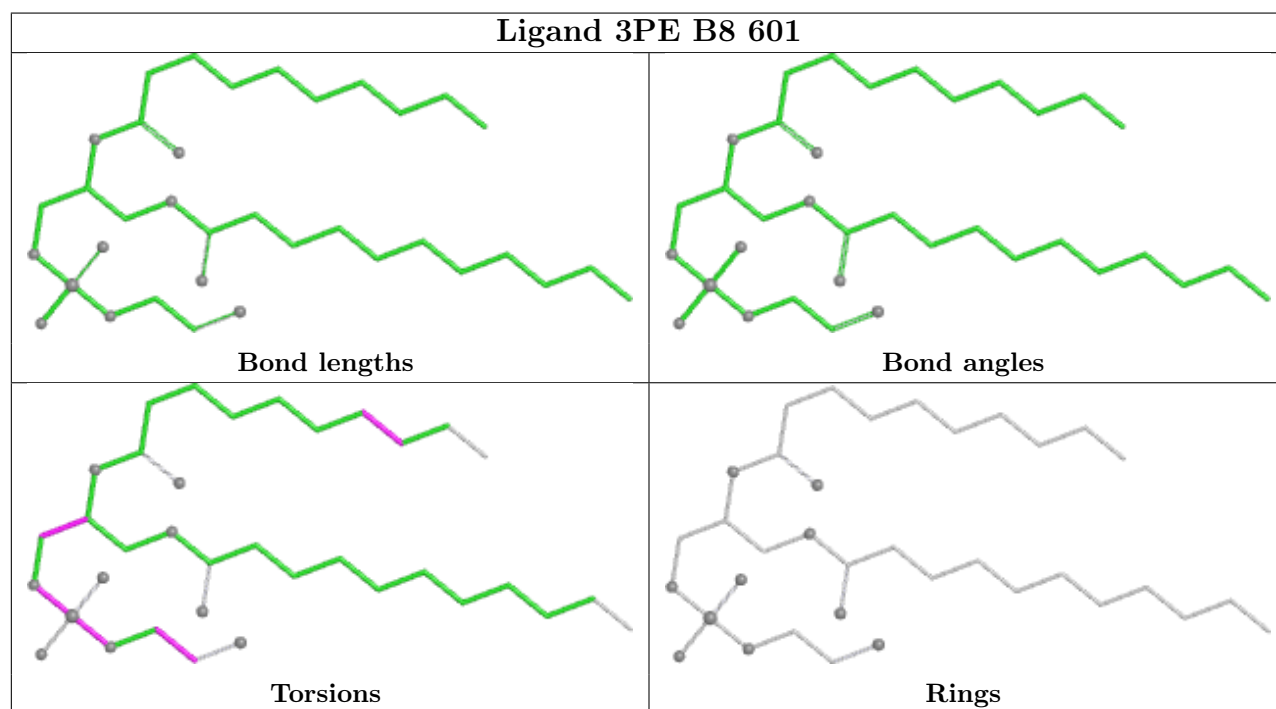
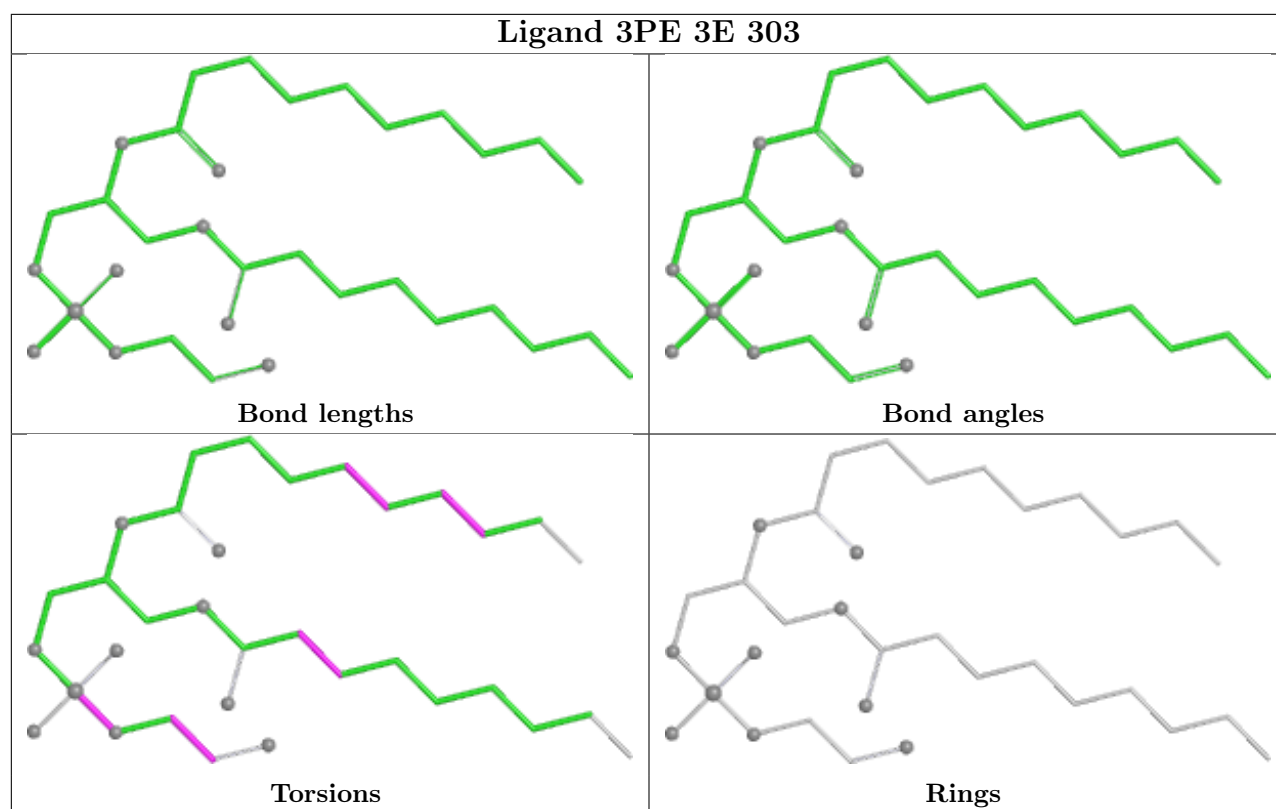


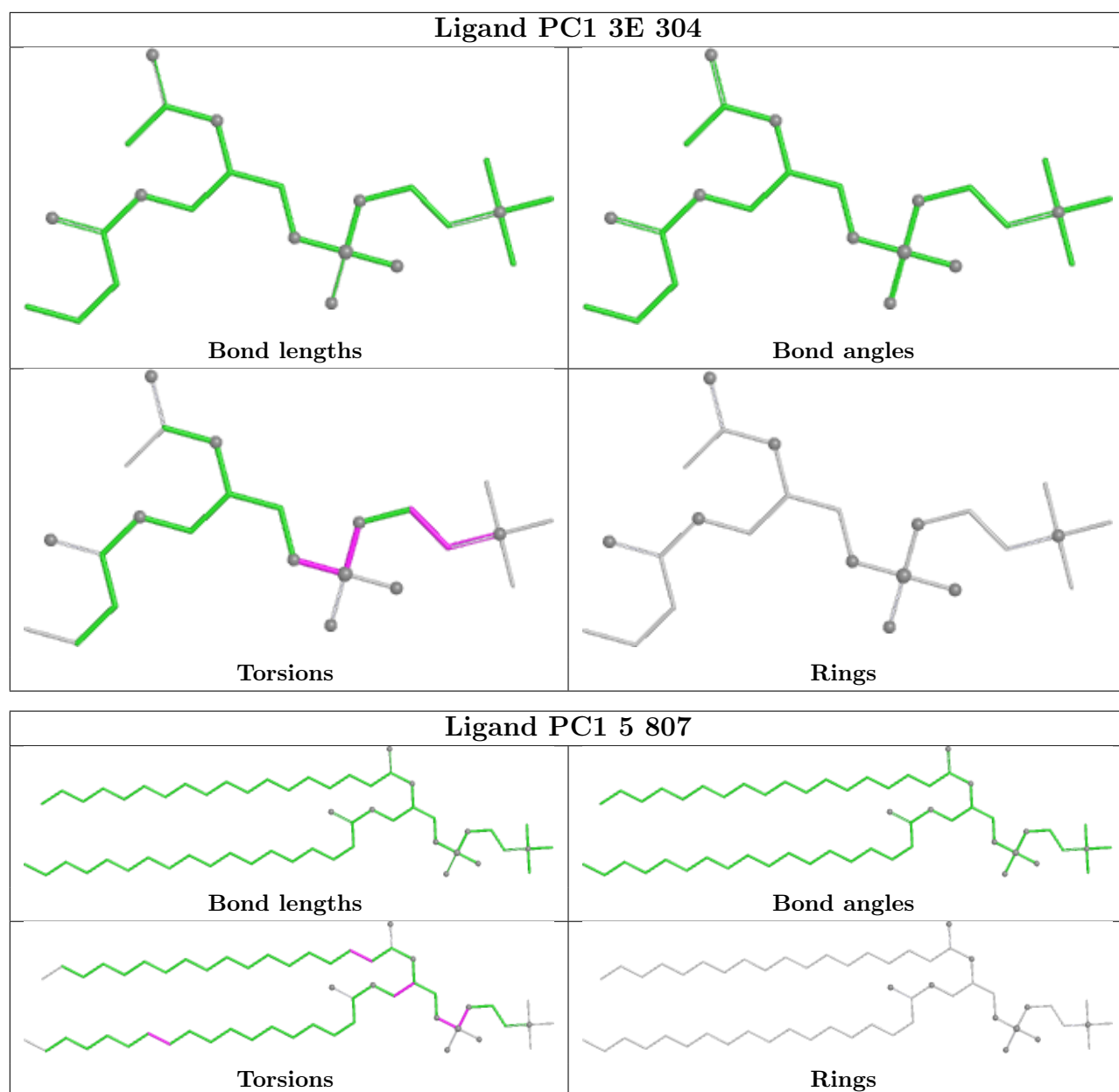


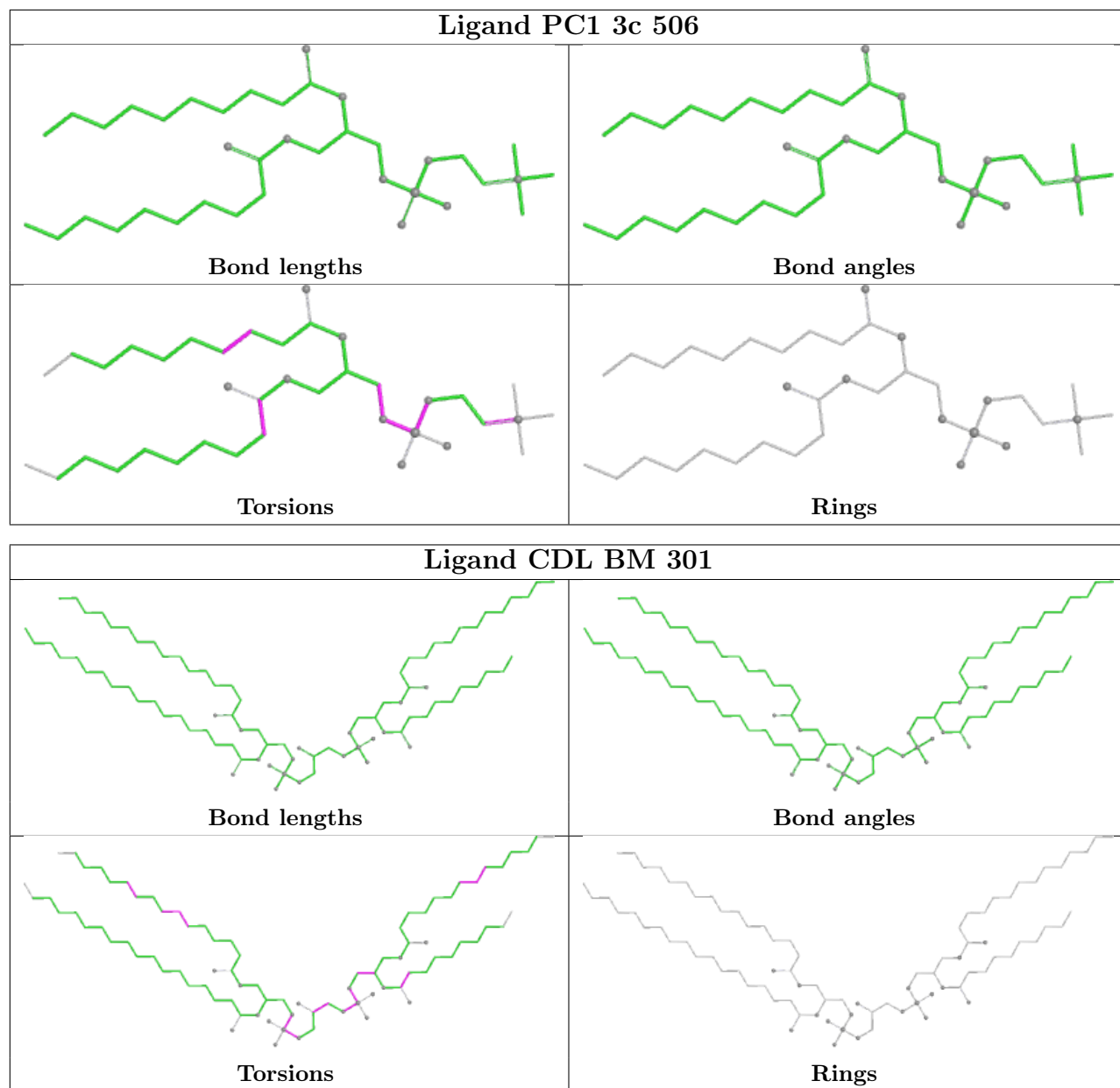


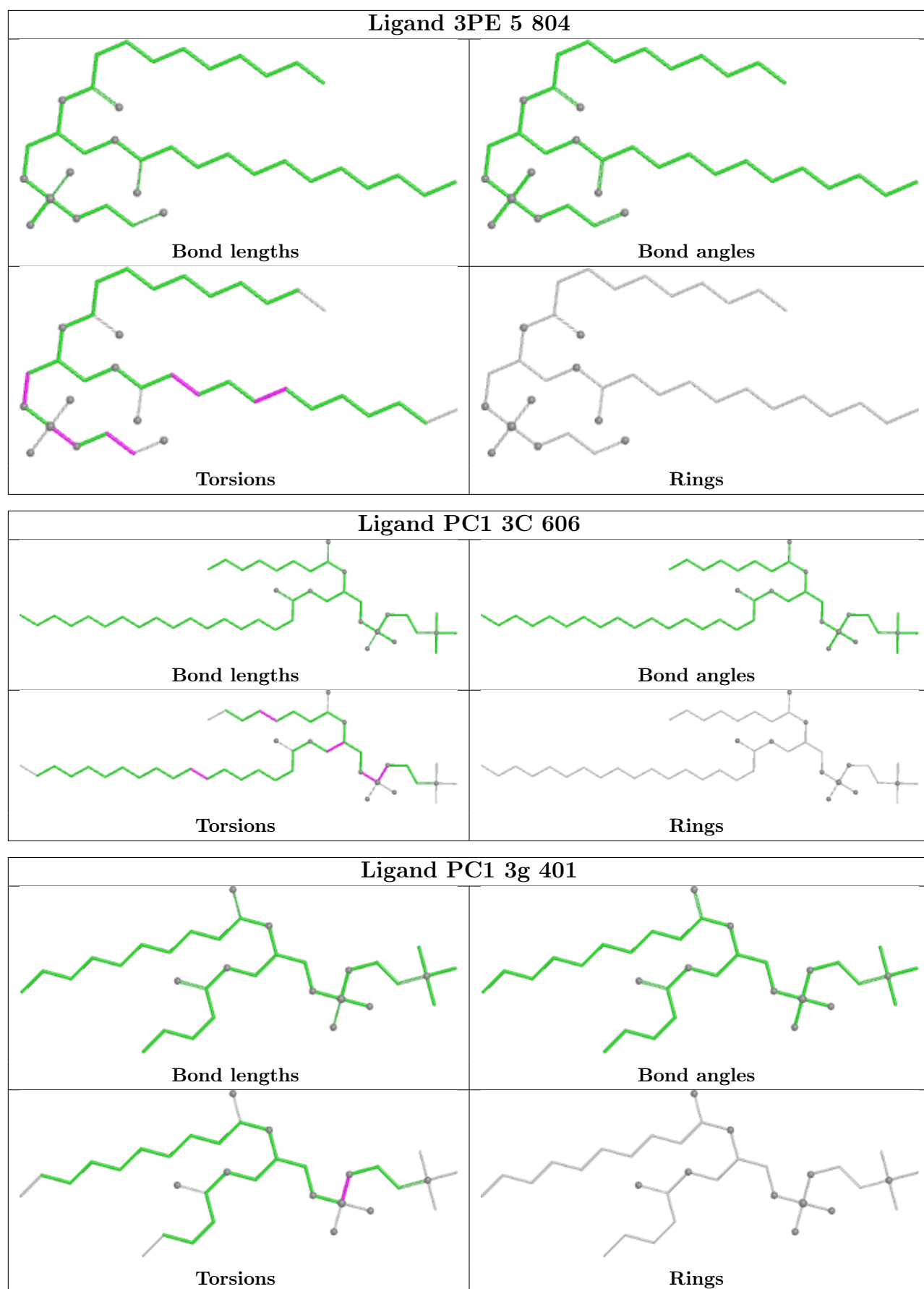


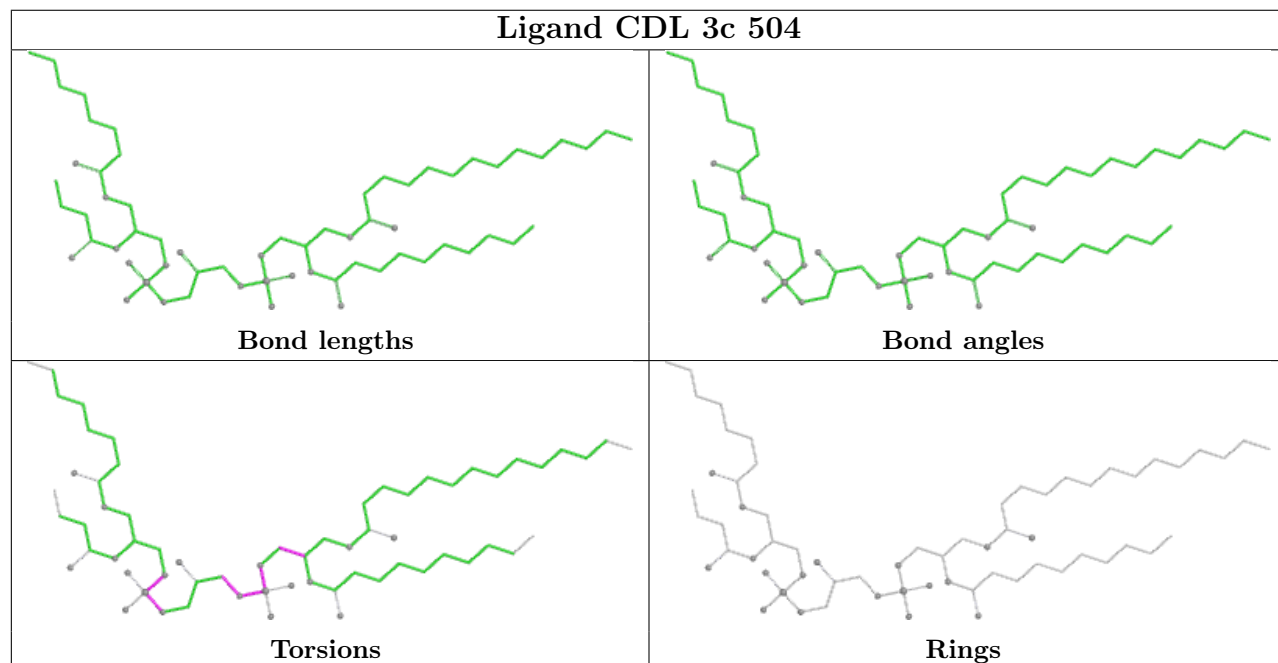
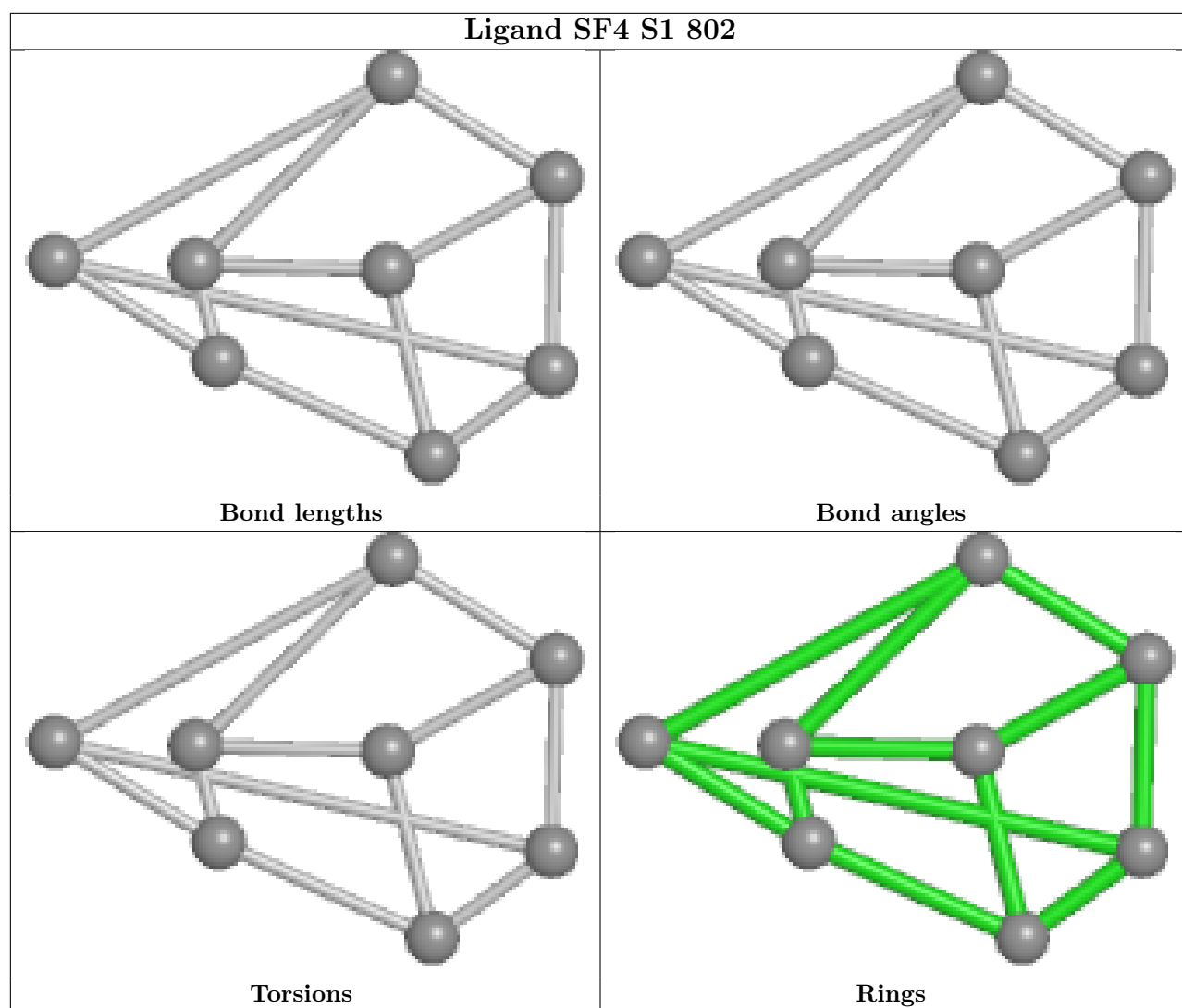


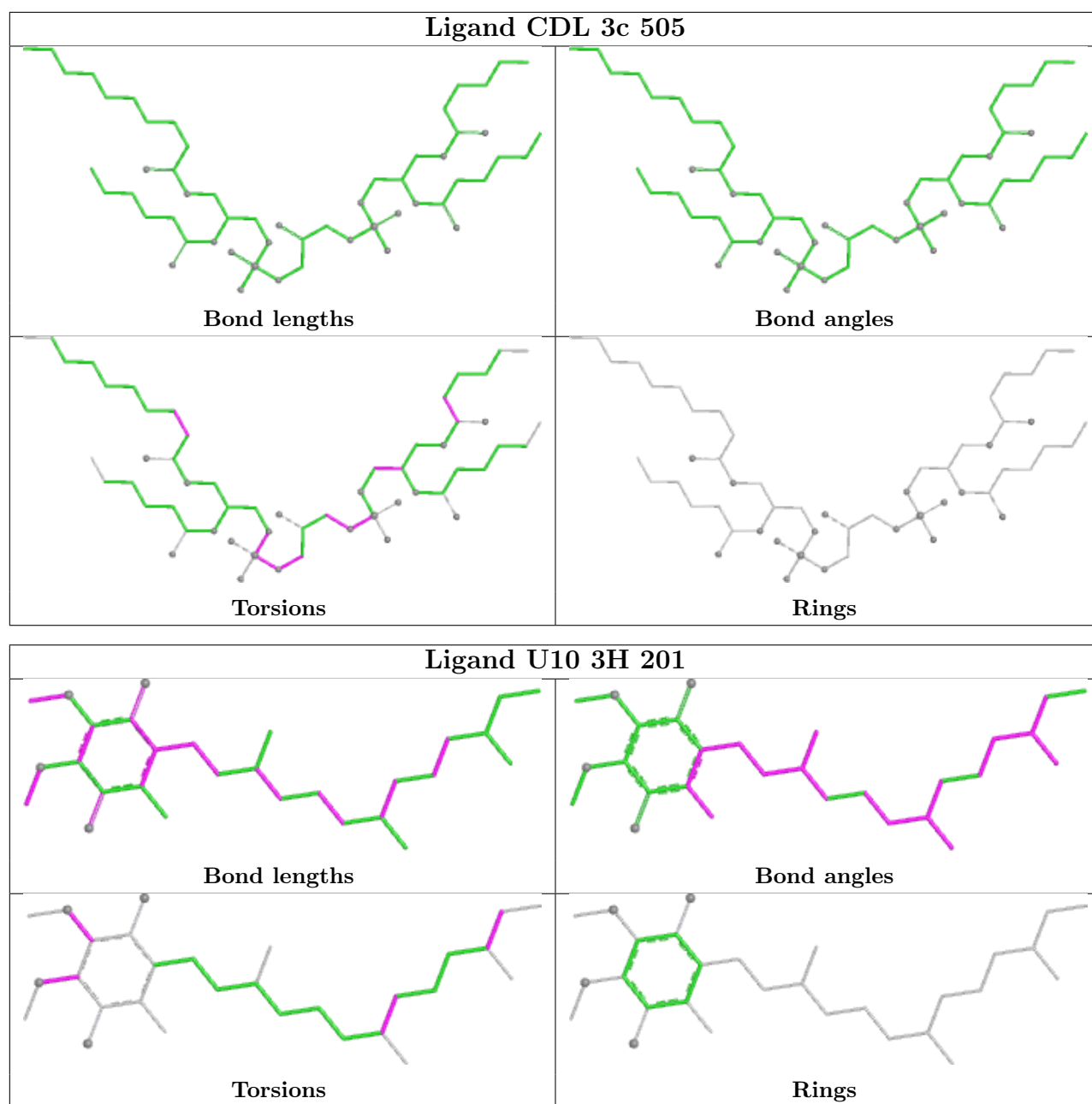


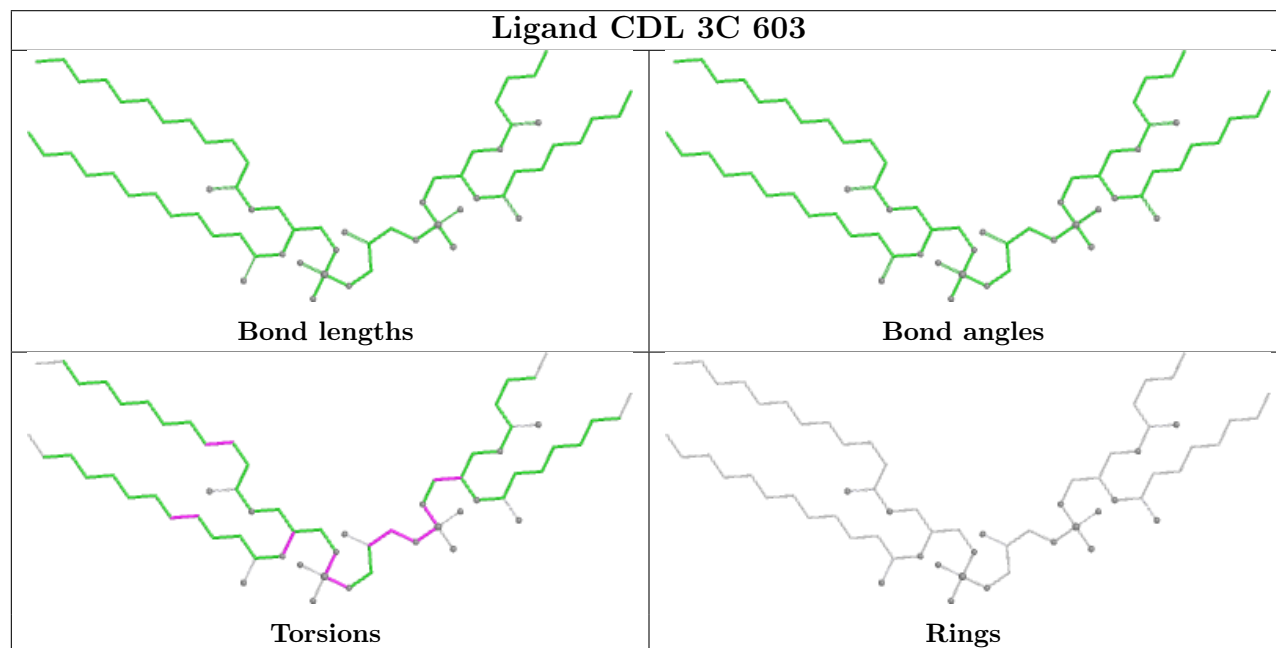
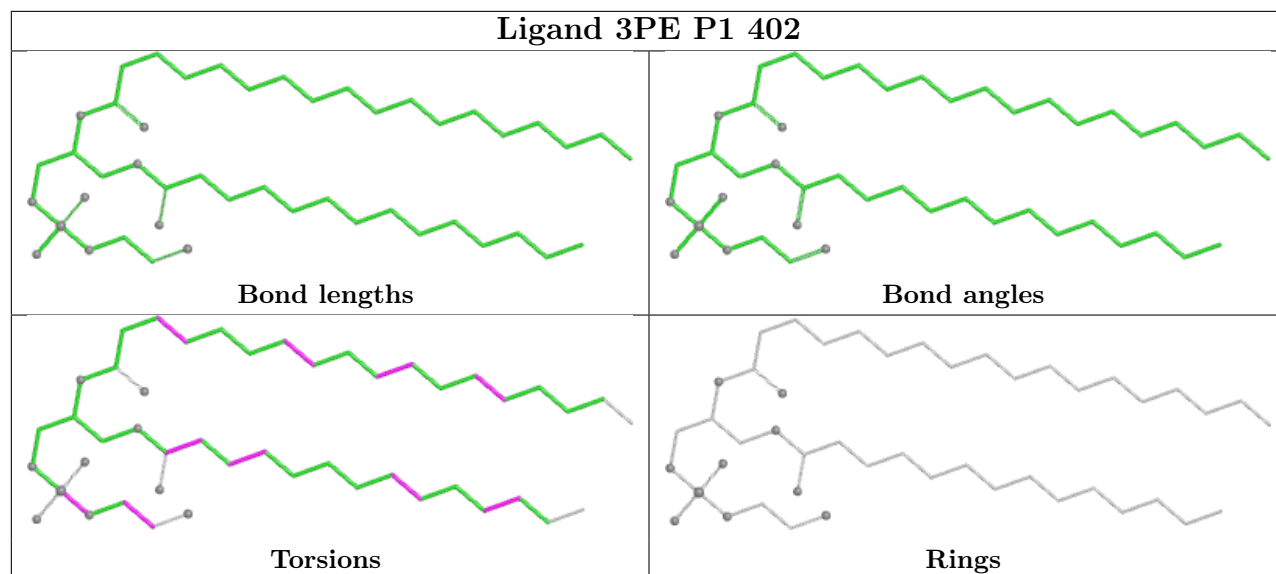


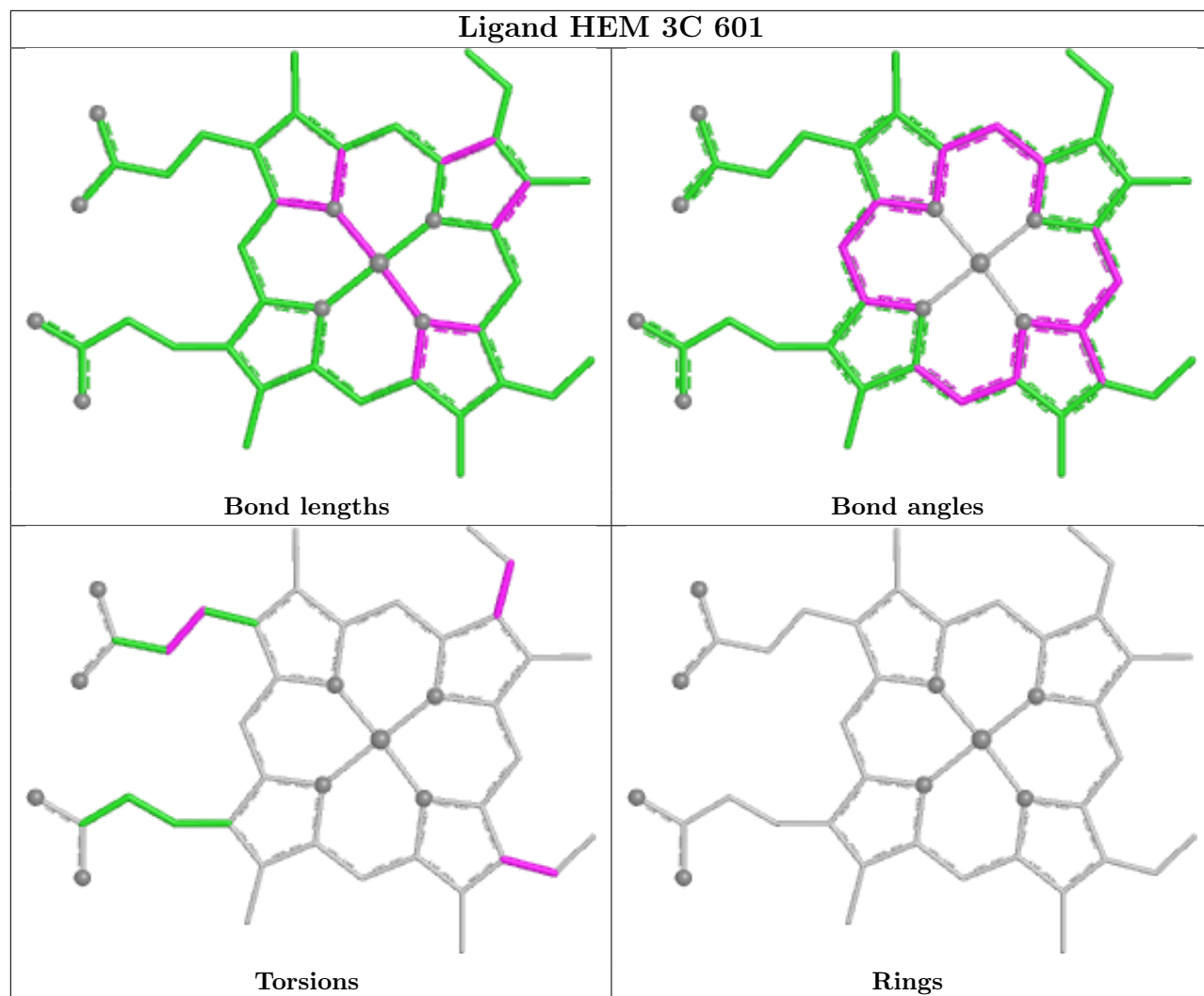


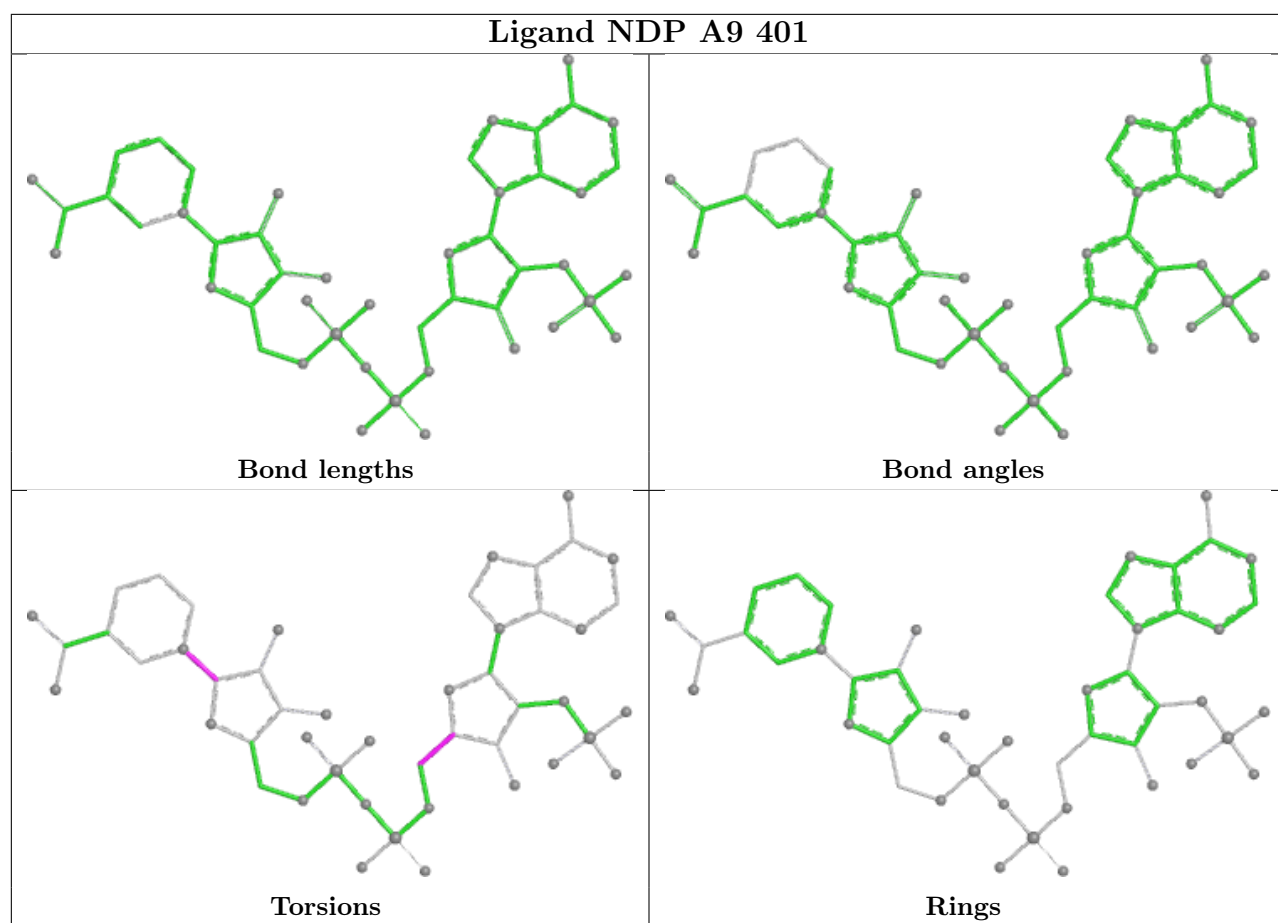


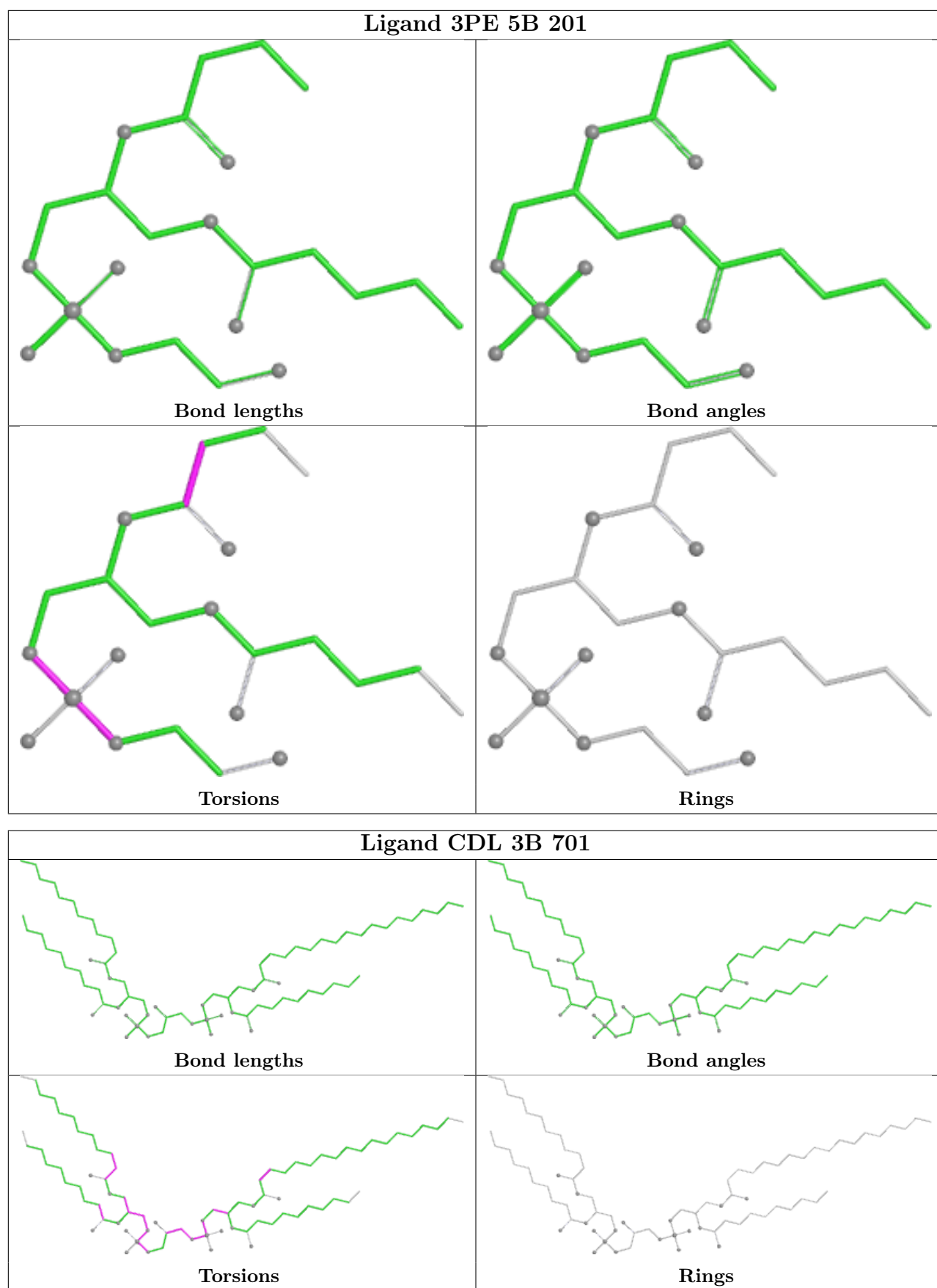




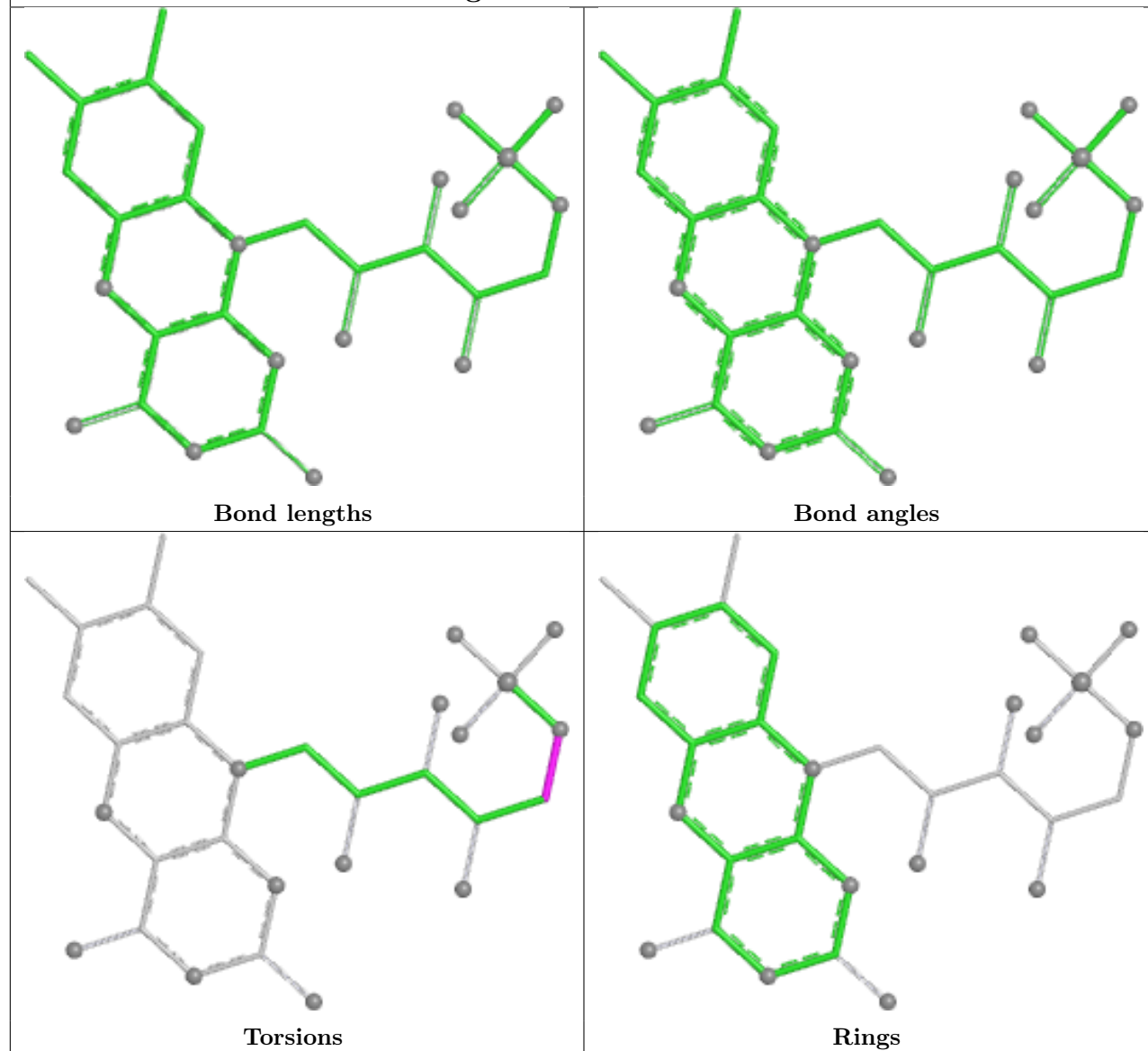




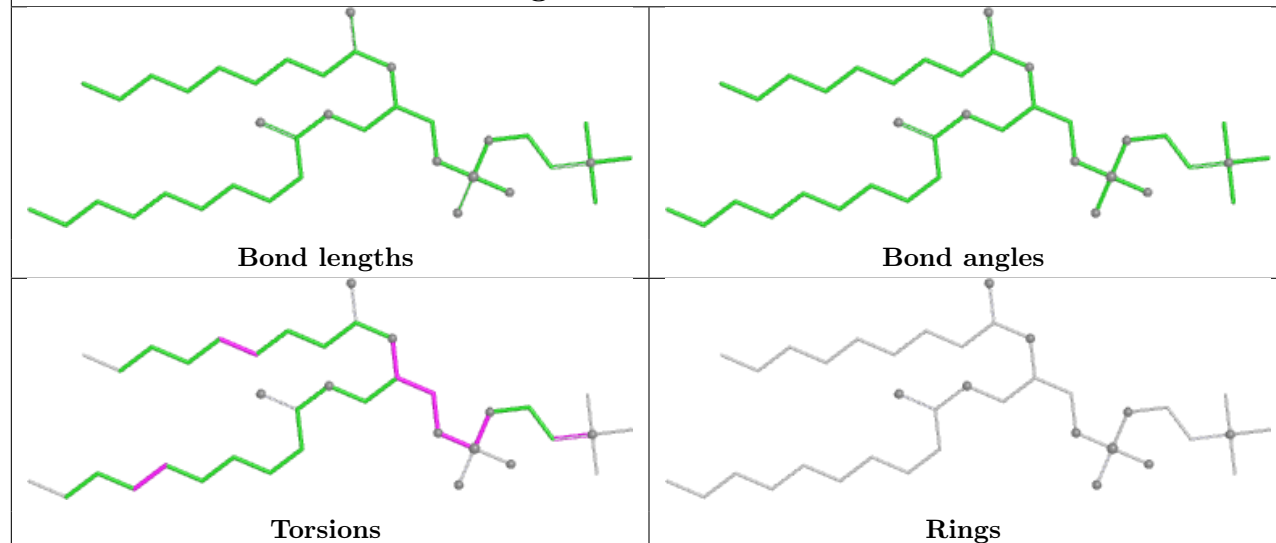


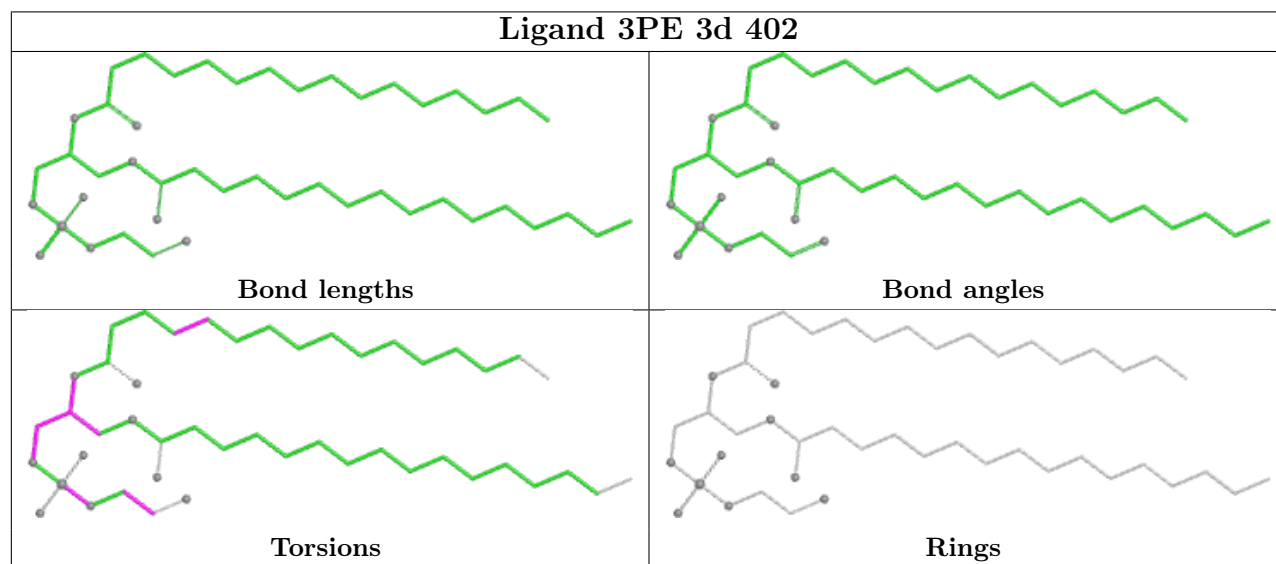
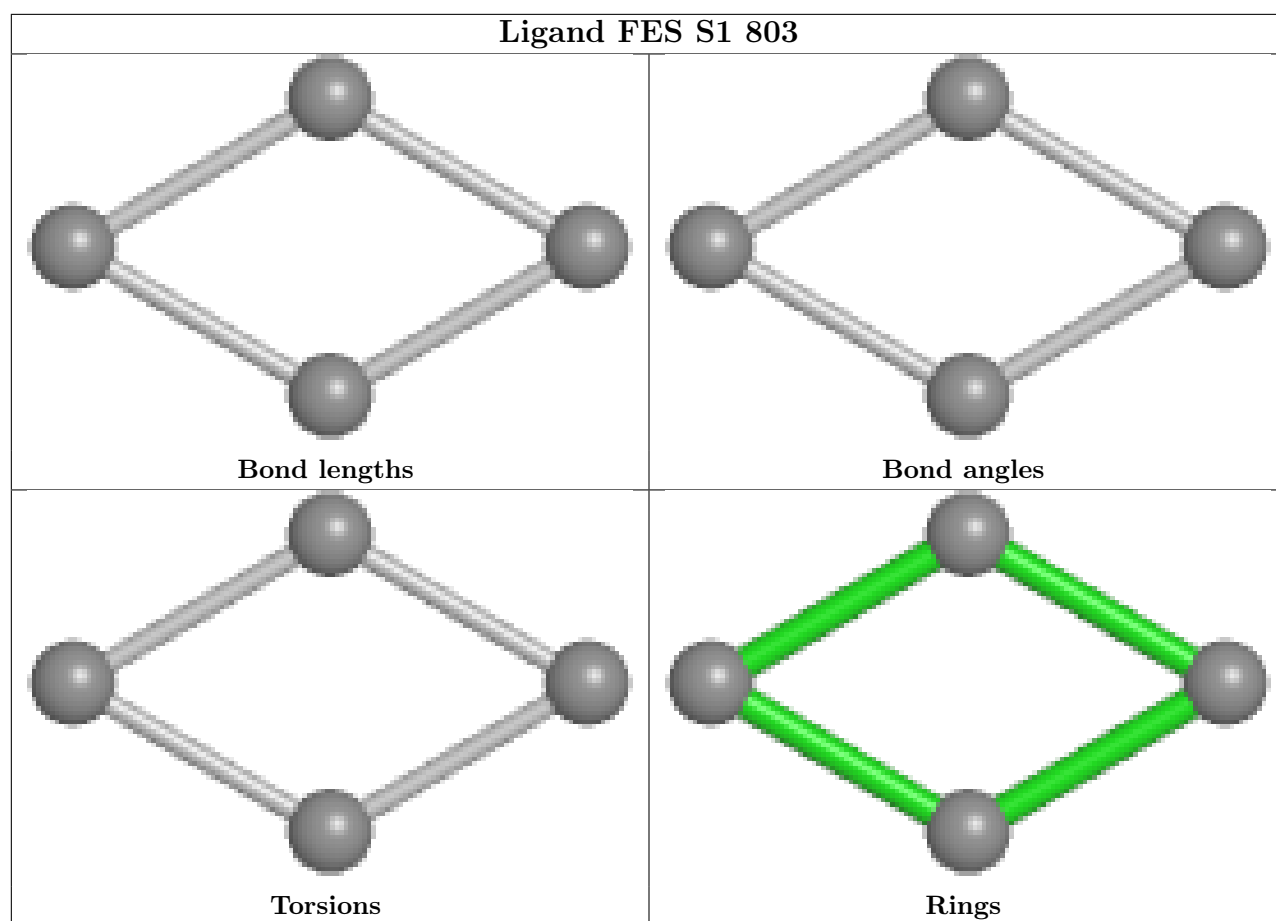


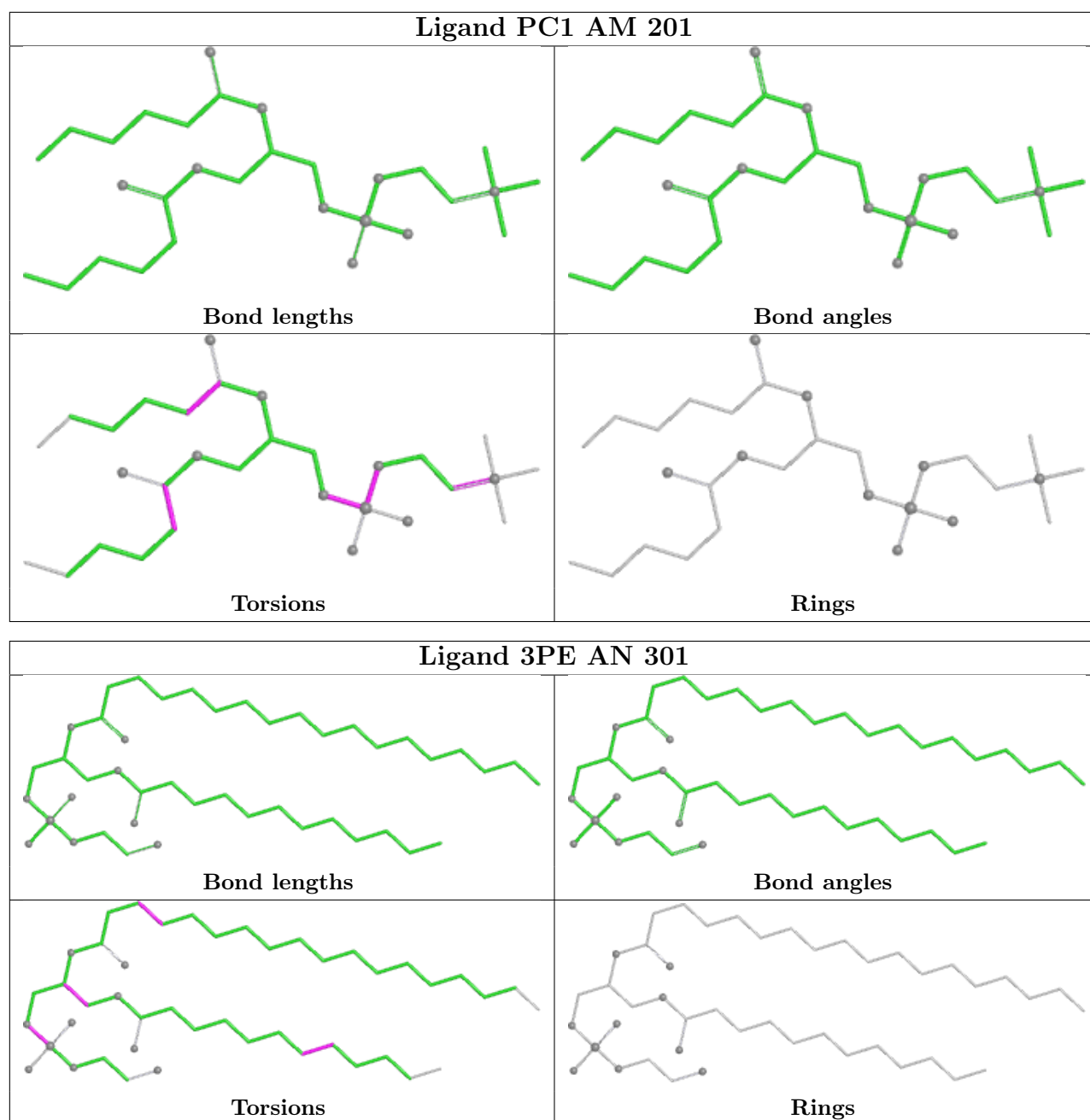
Ligand FMN V1 501

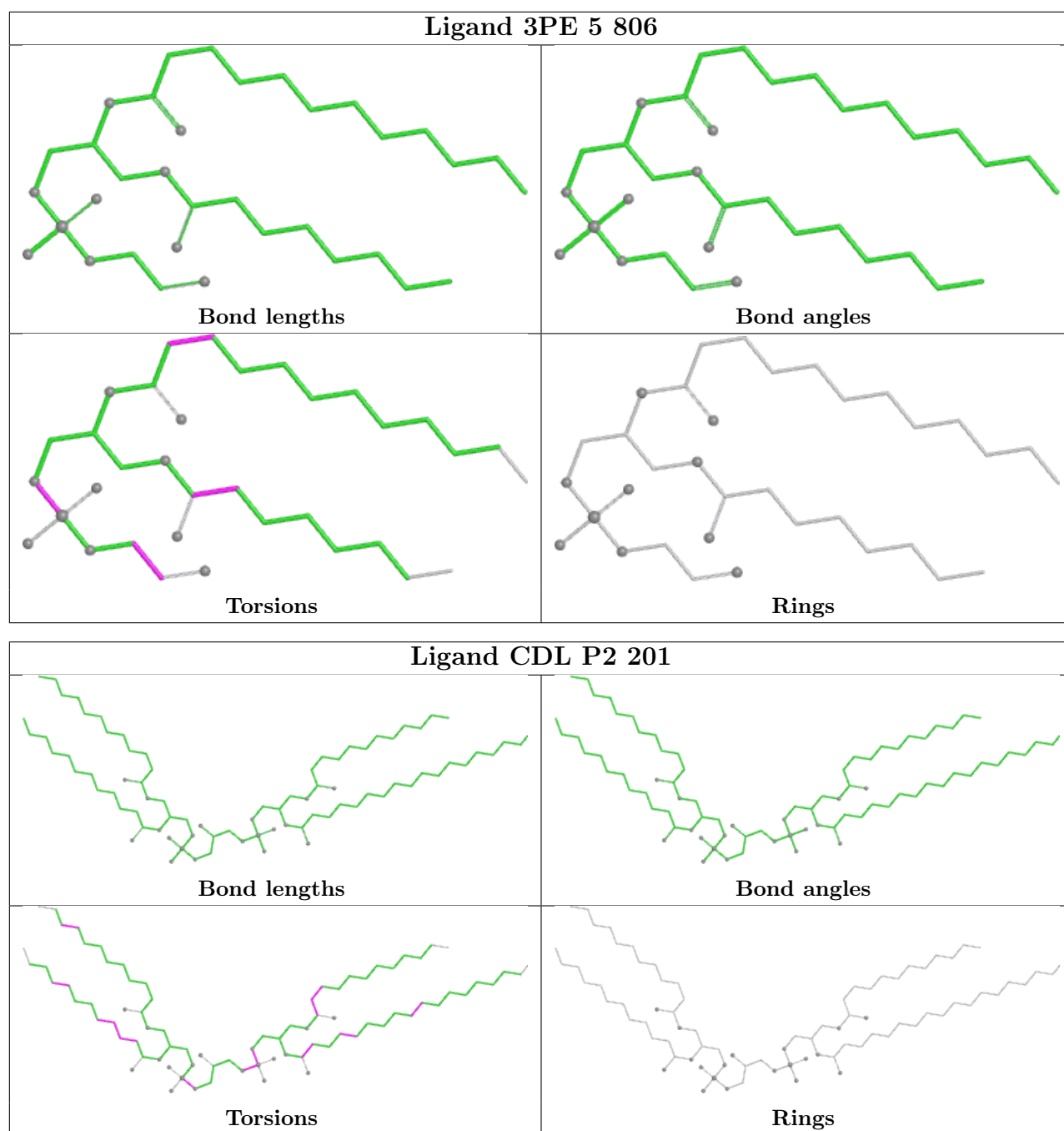


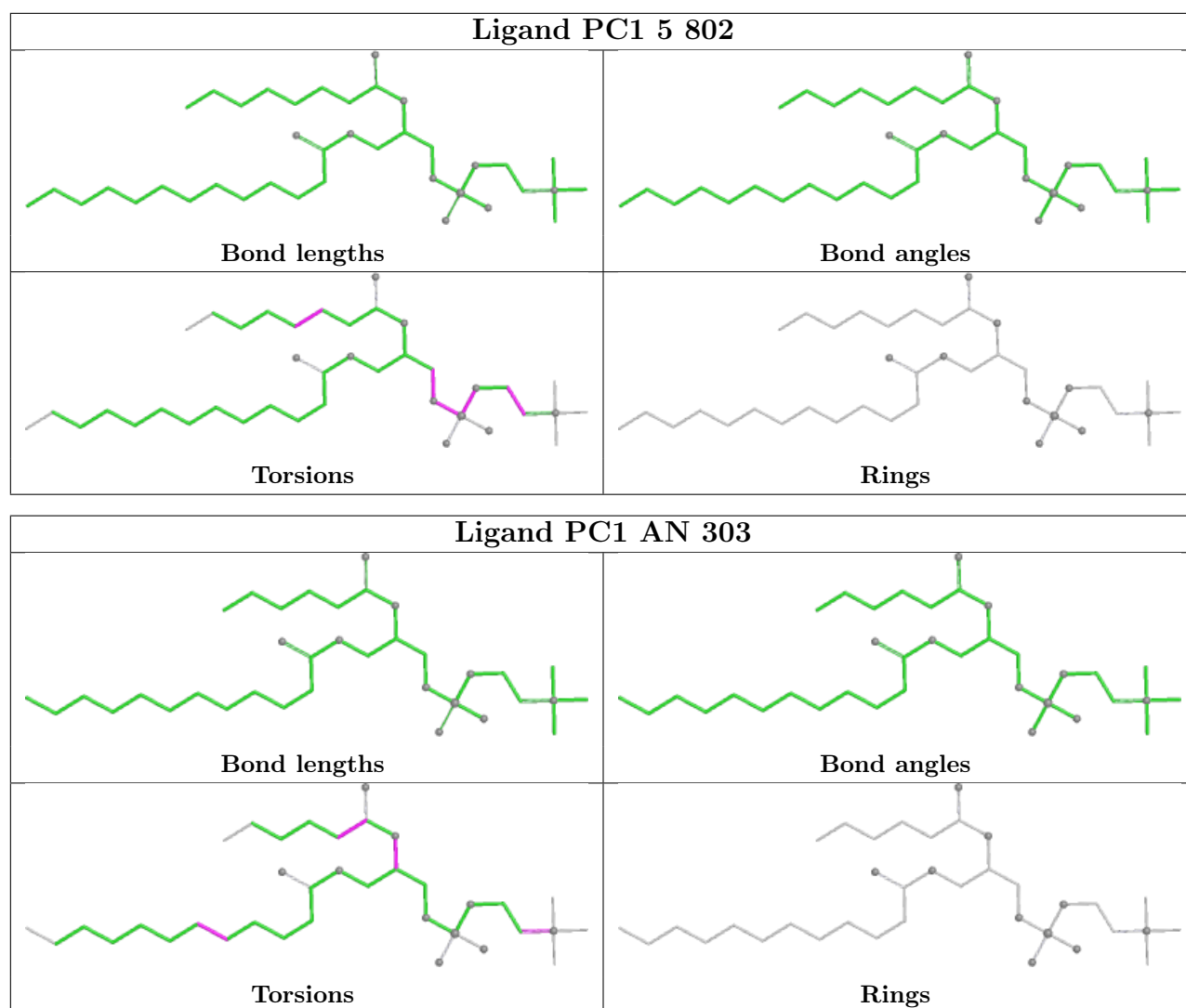
Ligand PC1 3J 101

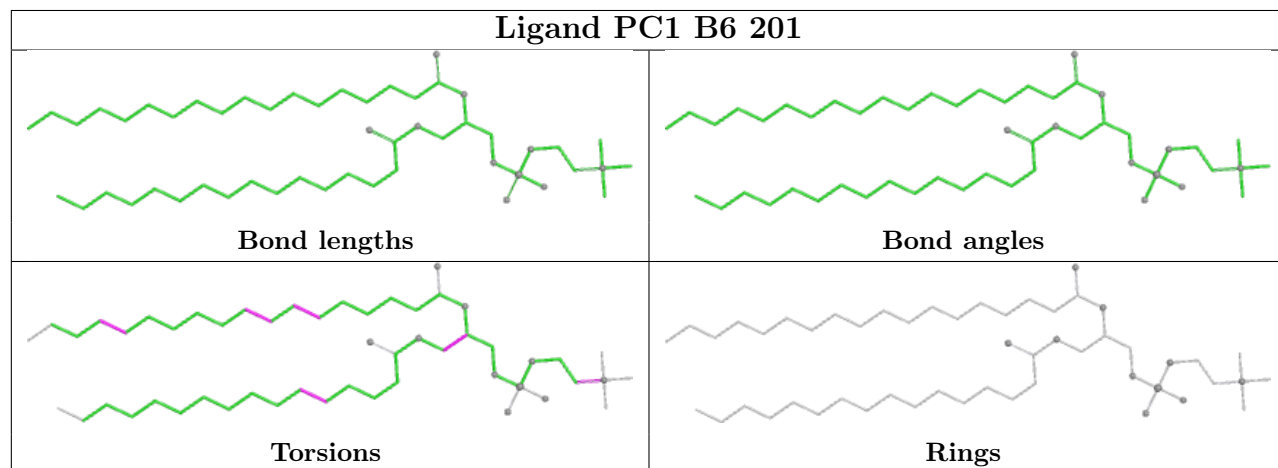
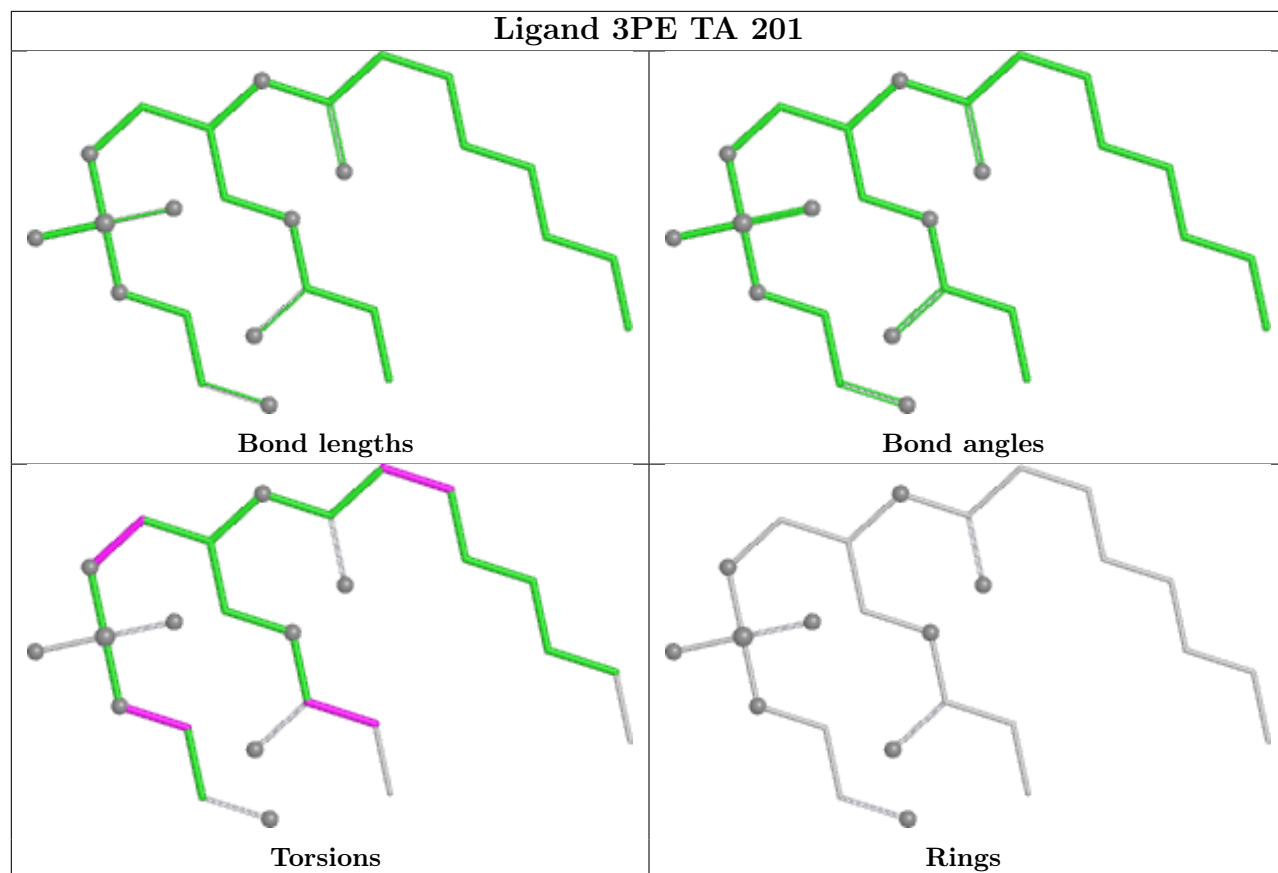


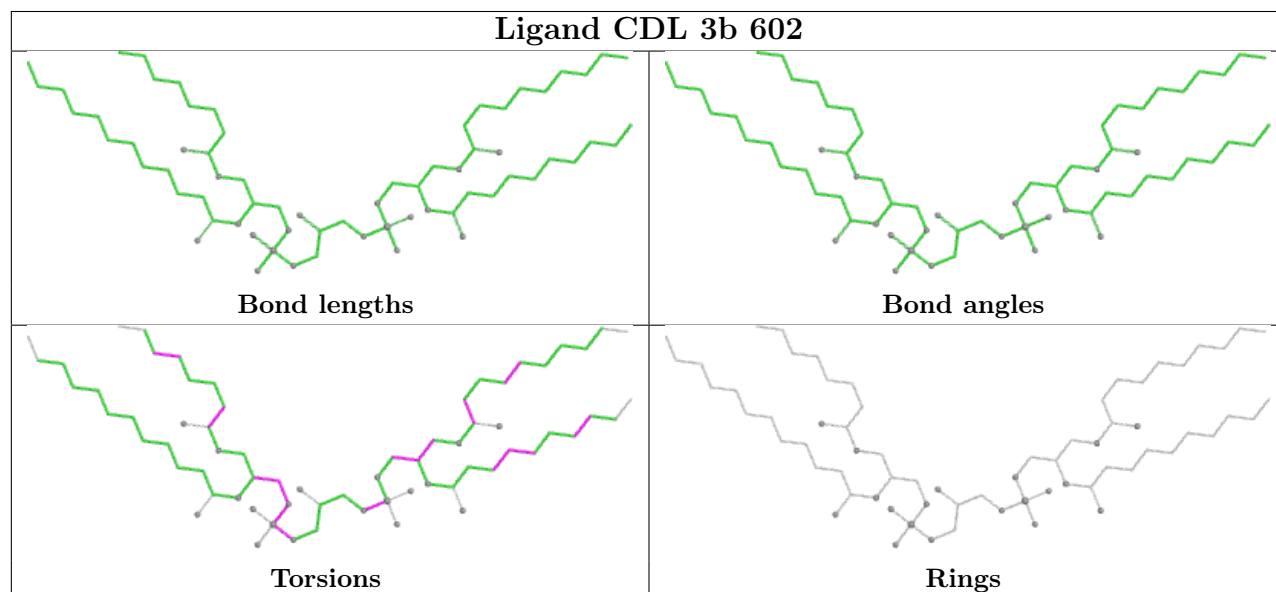
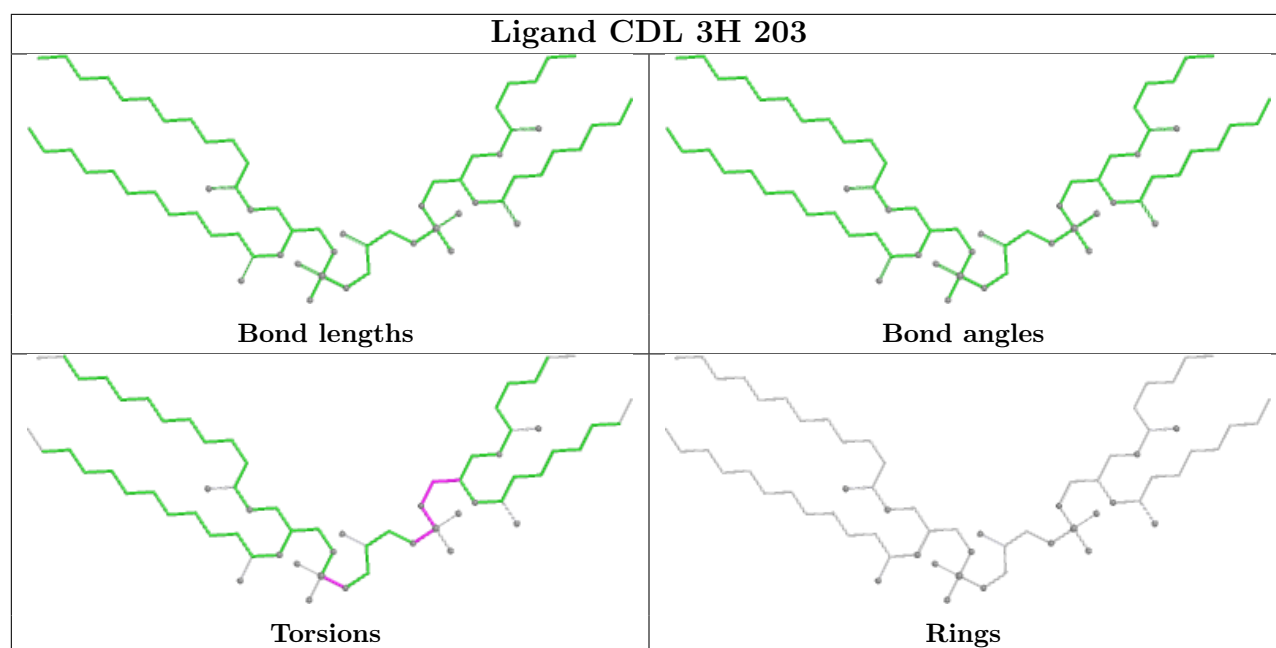




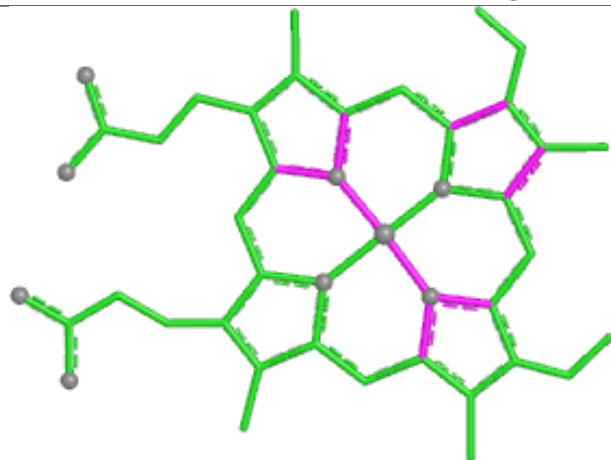




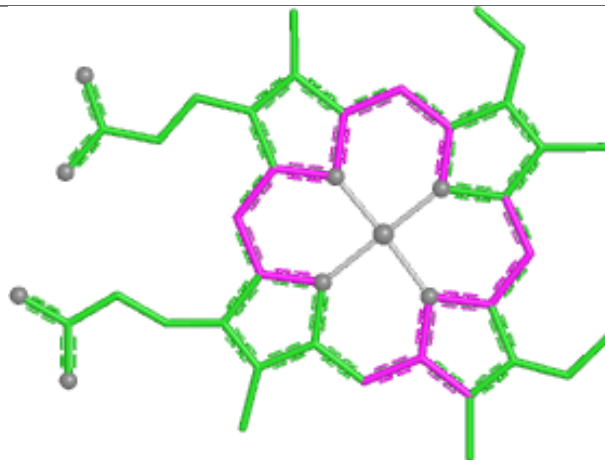




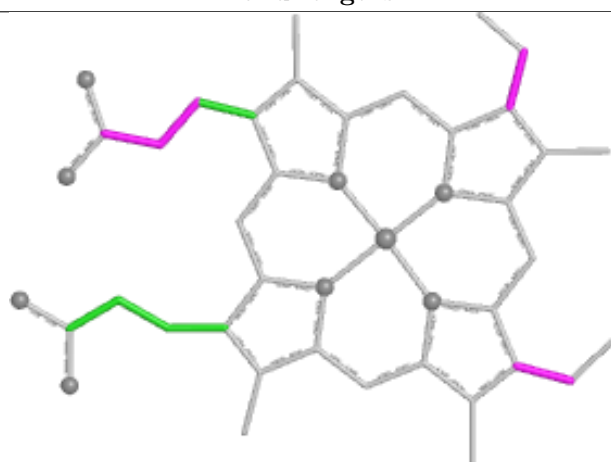
Ligand HEM 3c 502



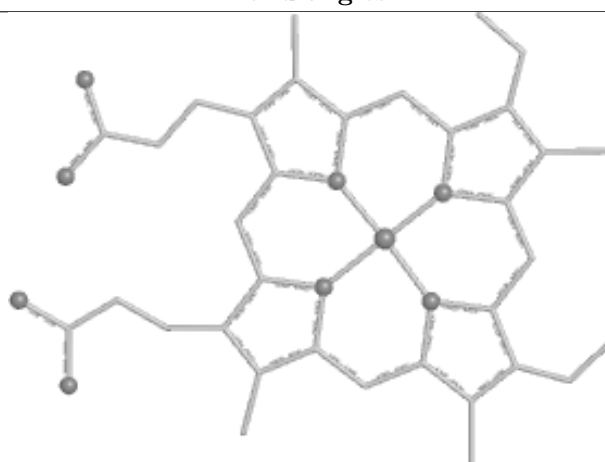
Bond lengths



Bond angles

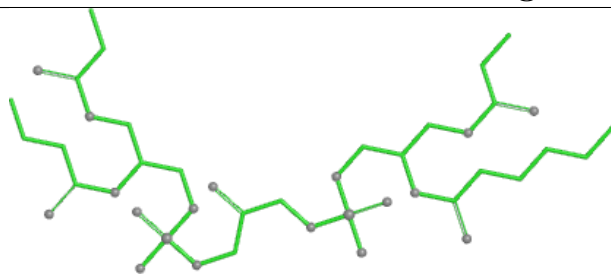


Torsions

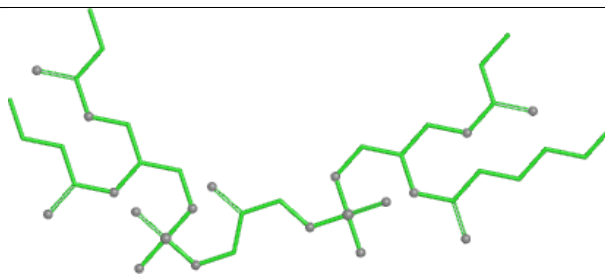


Rings

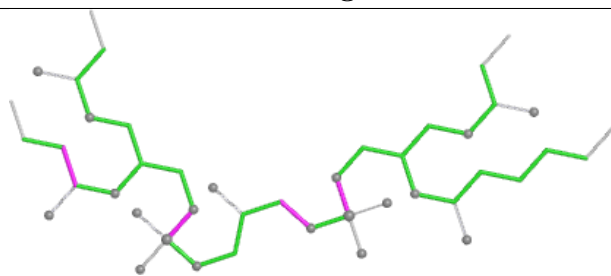
Ligand CDL 3 202



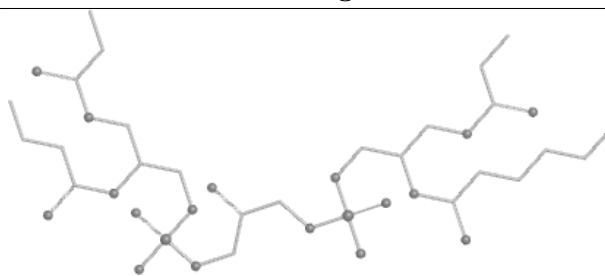
Bond lengths



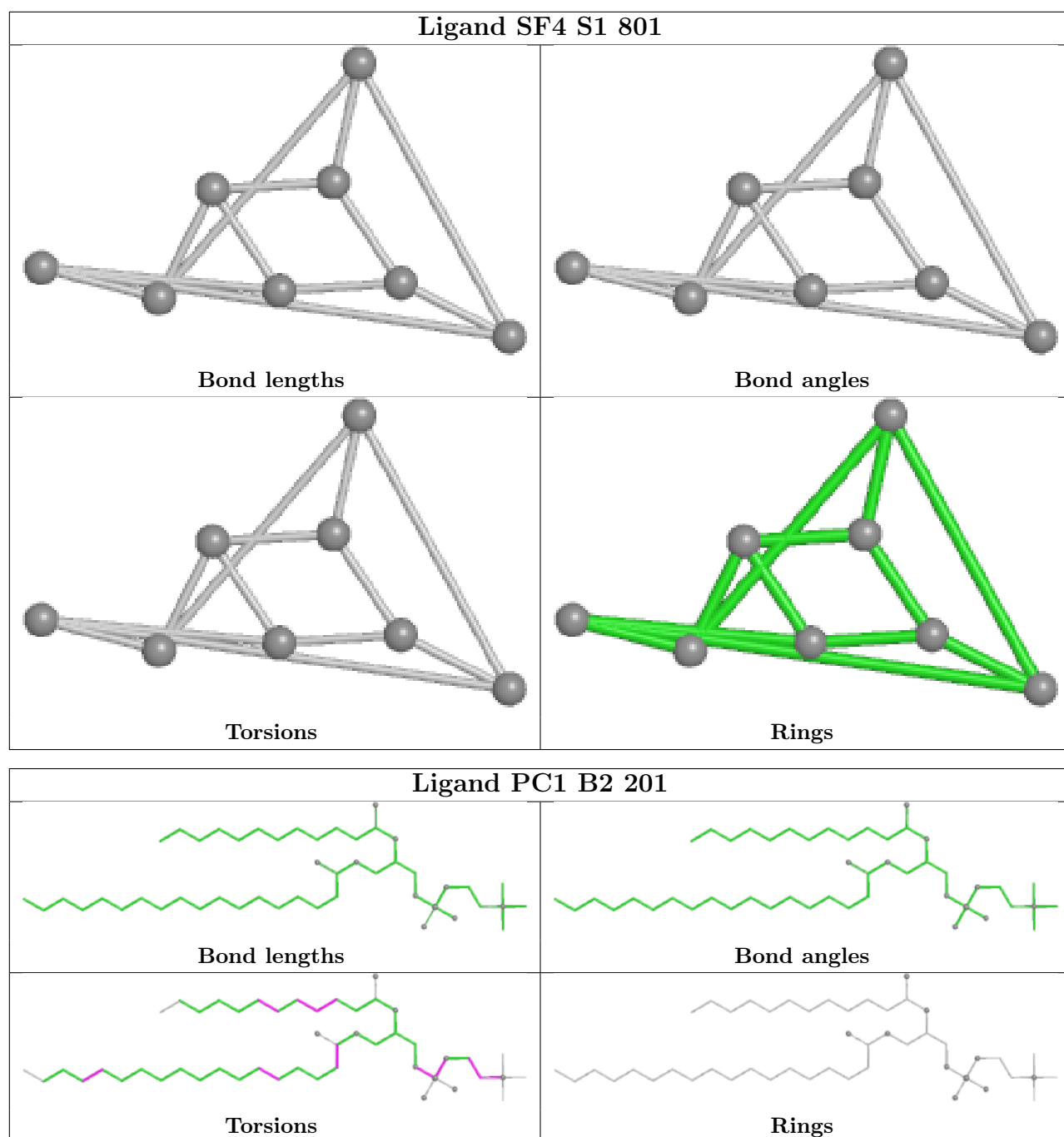
Bond angles

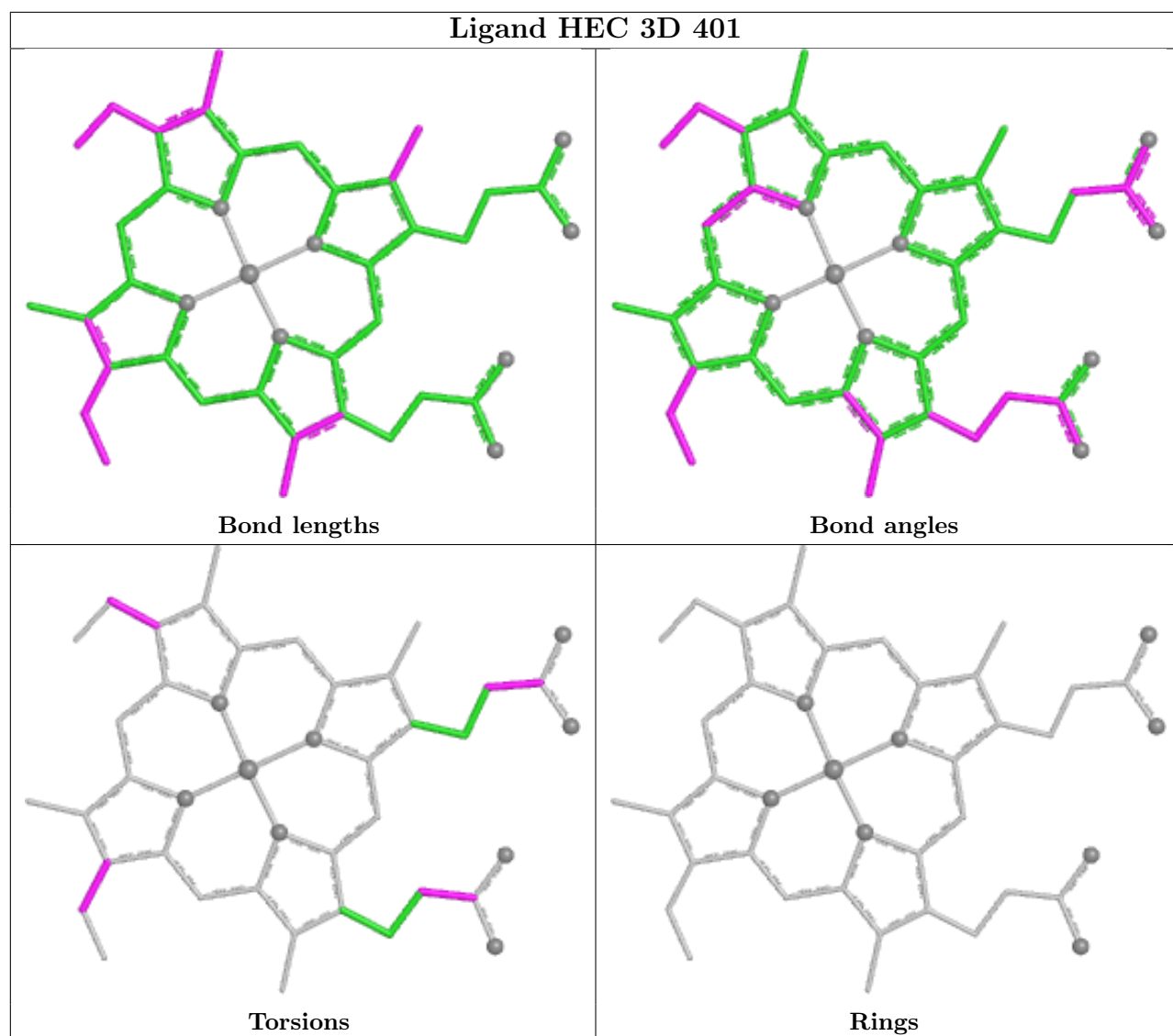
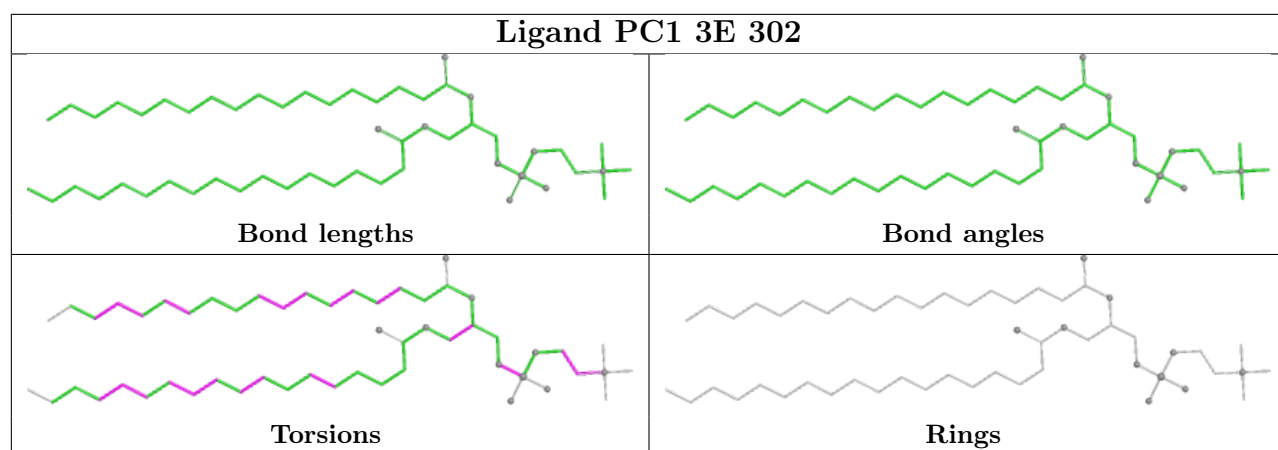


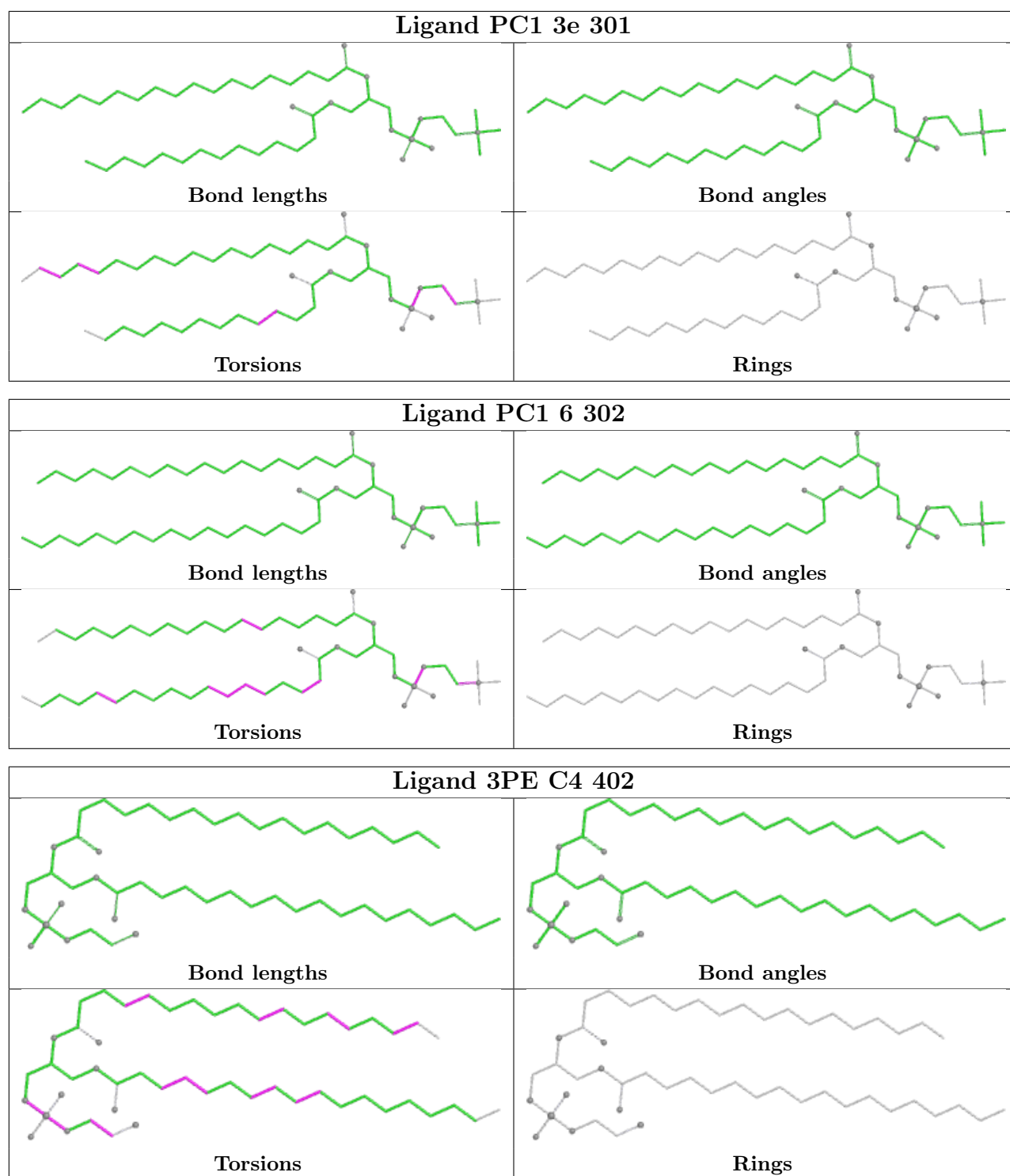
Torsions

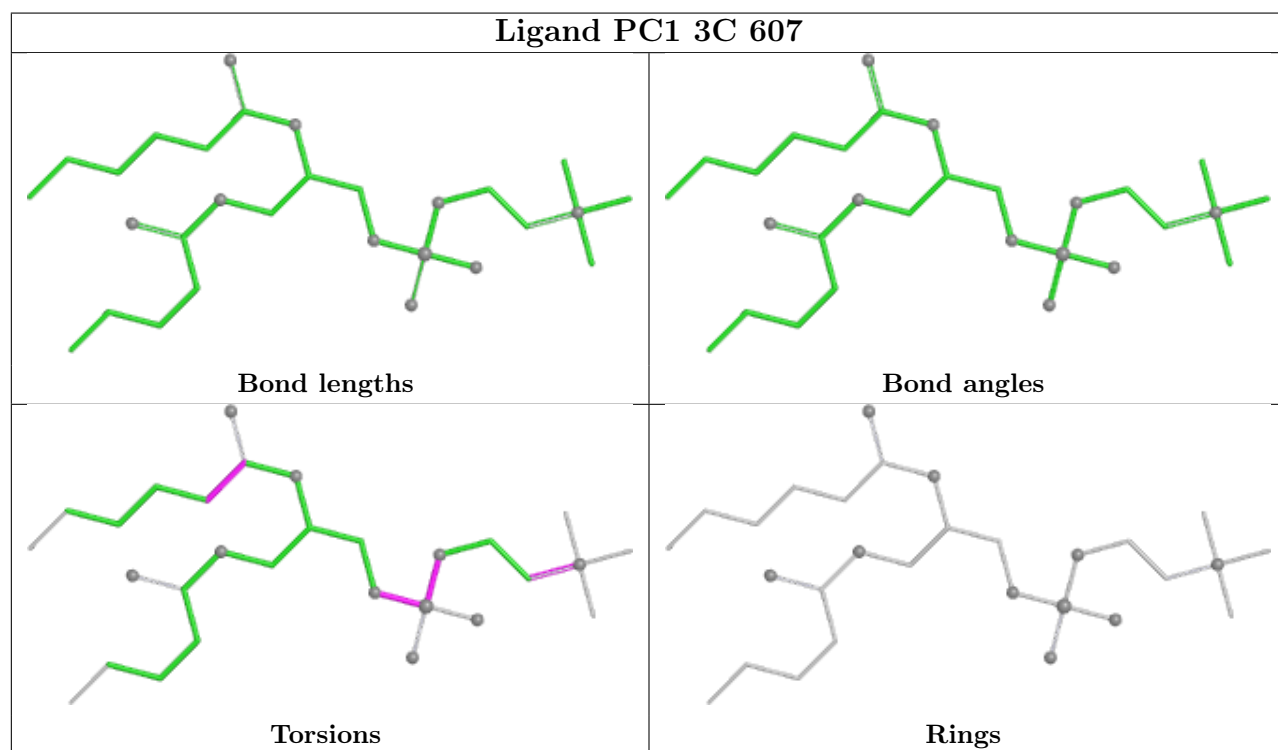
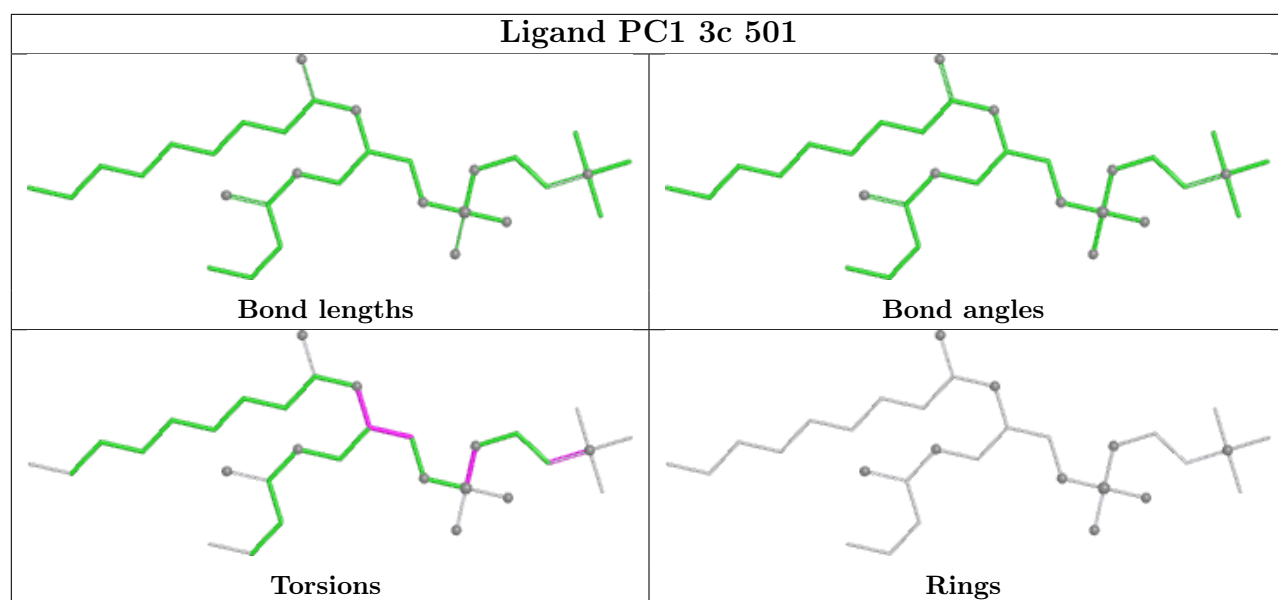


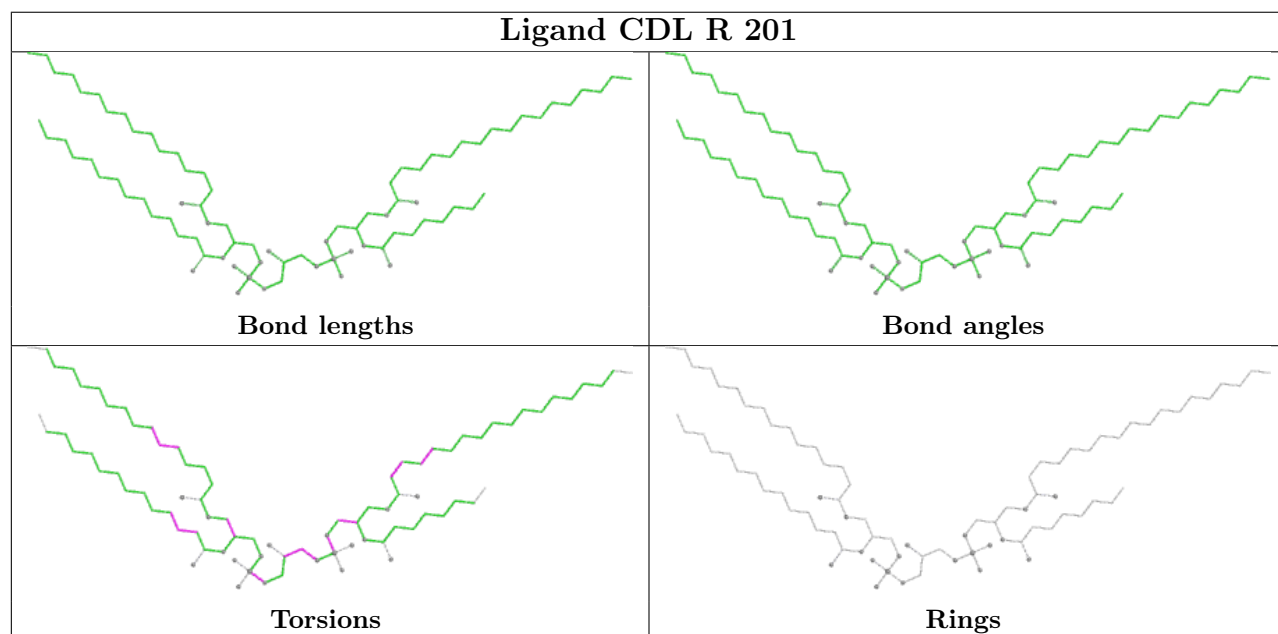
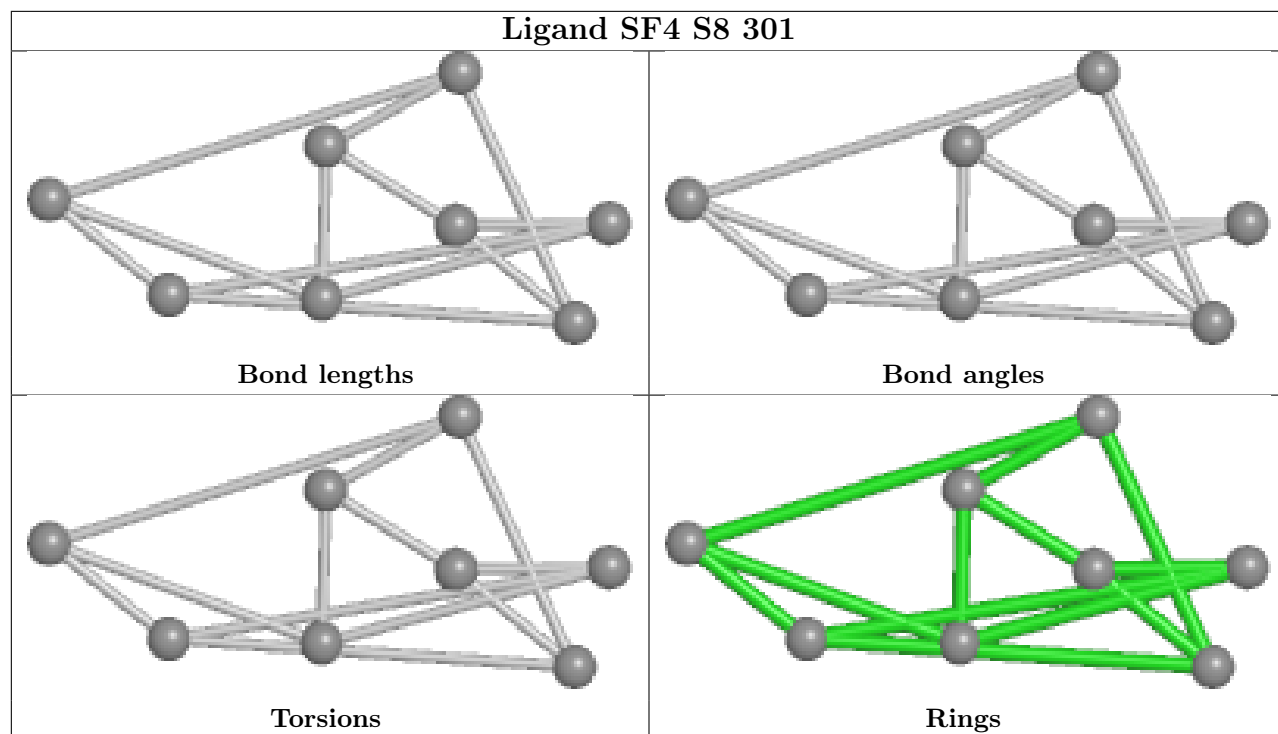
Rings



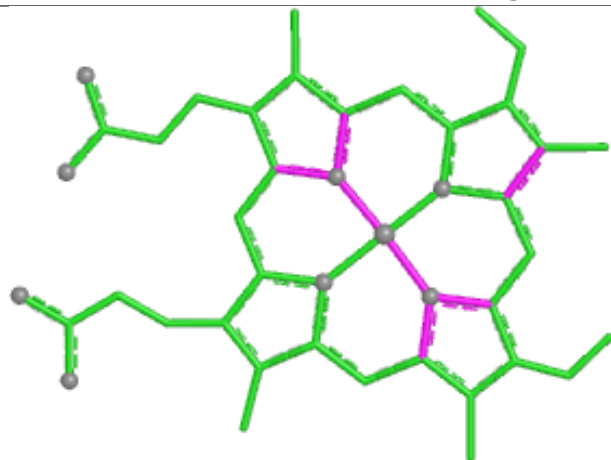




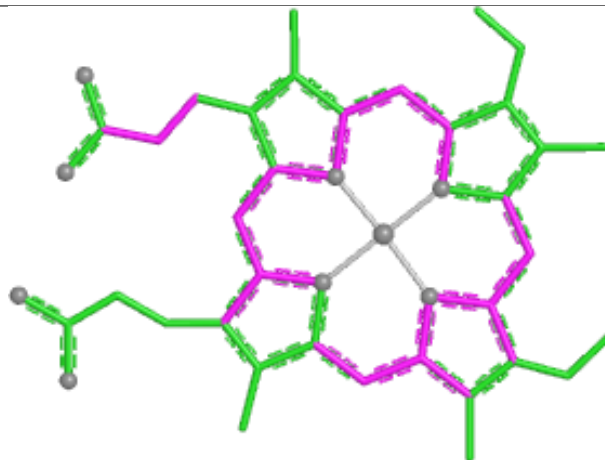




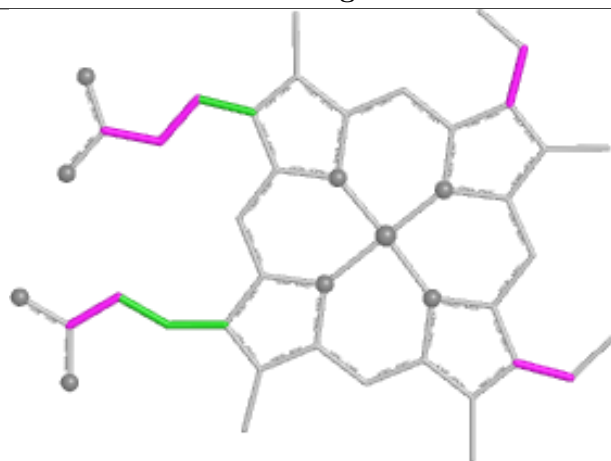
Ligand HEM 3c 503



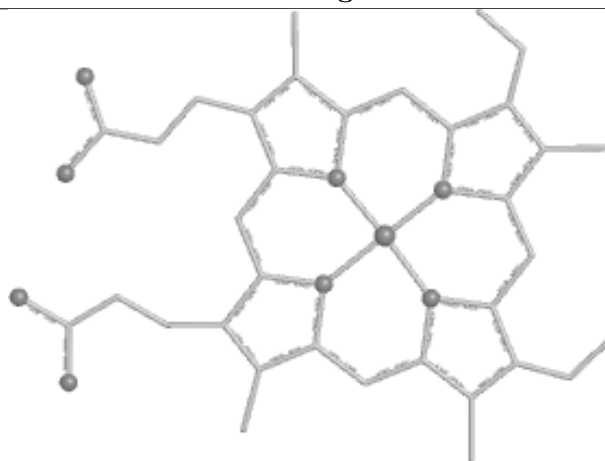
Bond lengths



Bond angles

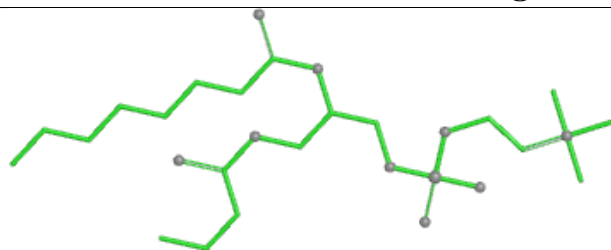


Torsions

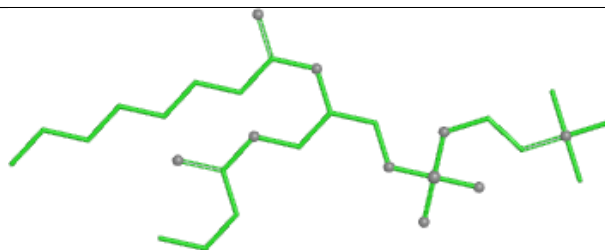


Rings

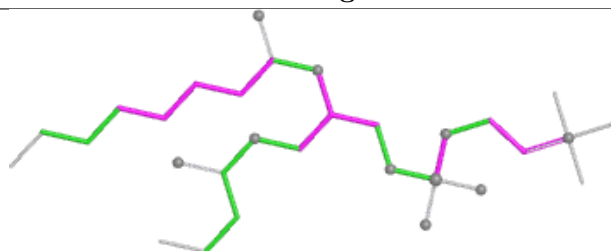
Ligand PC1 3b 601



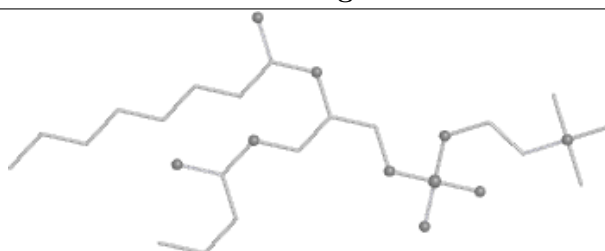
Bond lengths



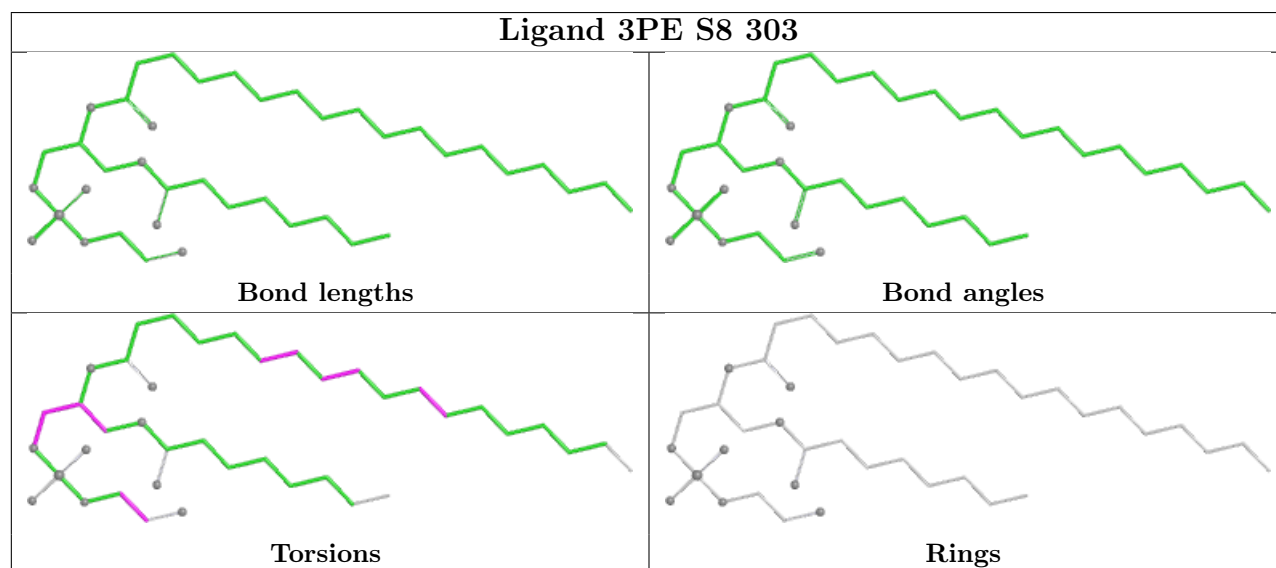
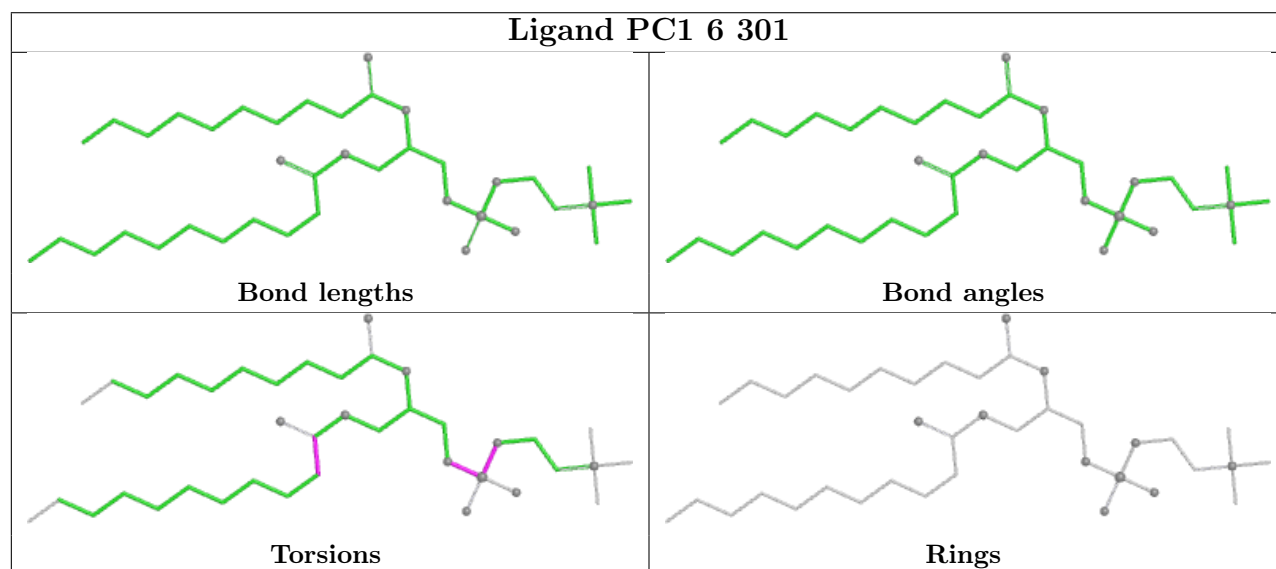
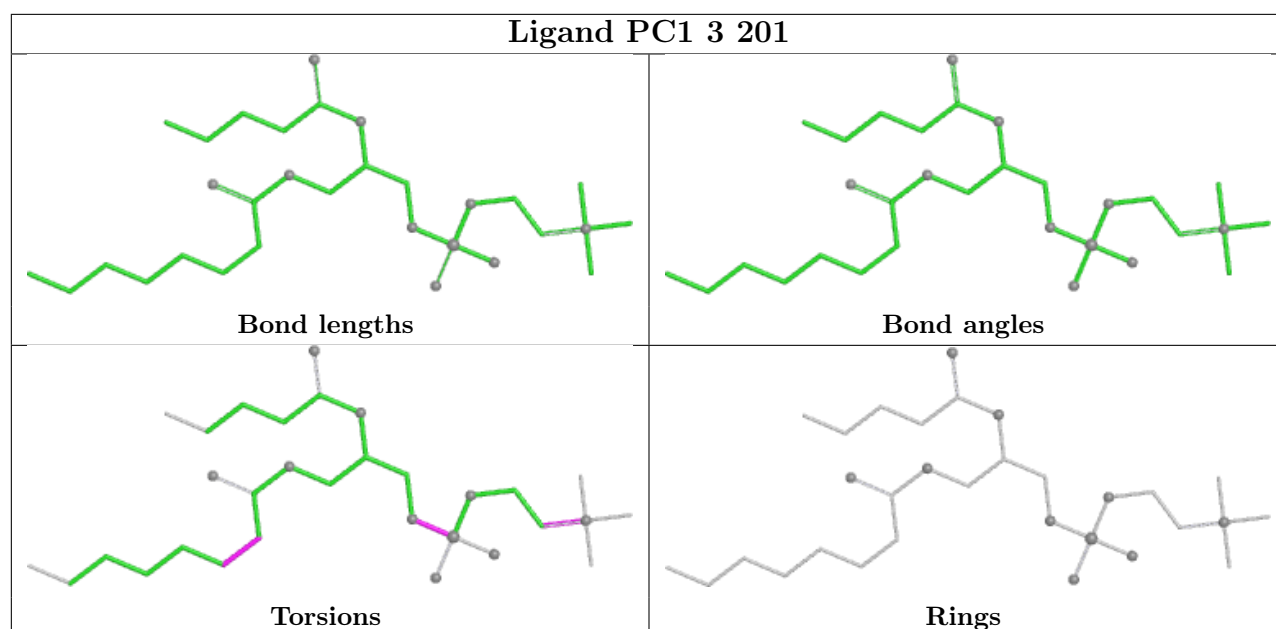
Bond angles

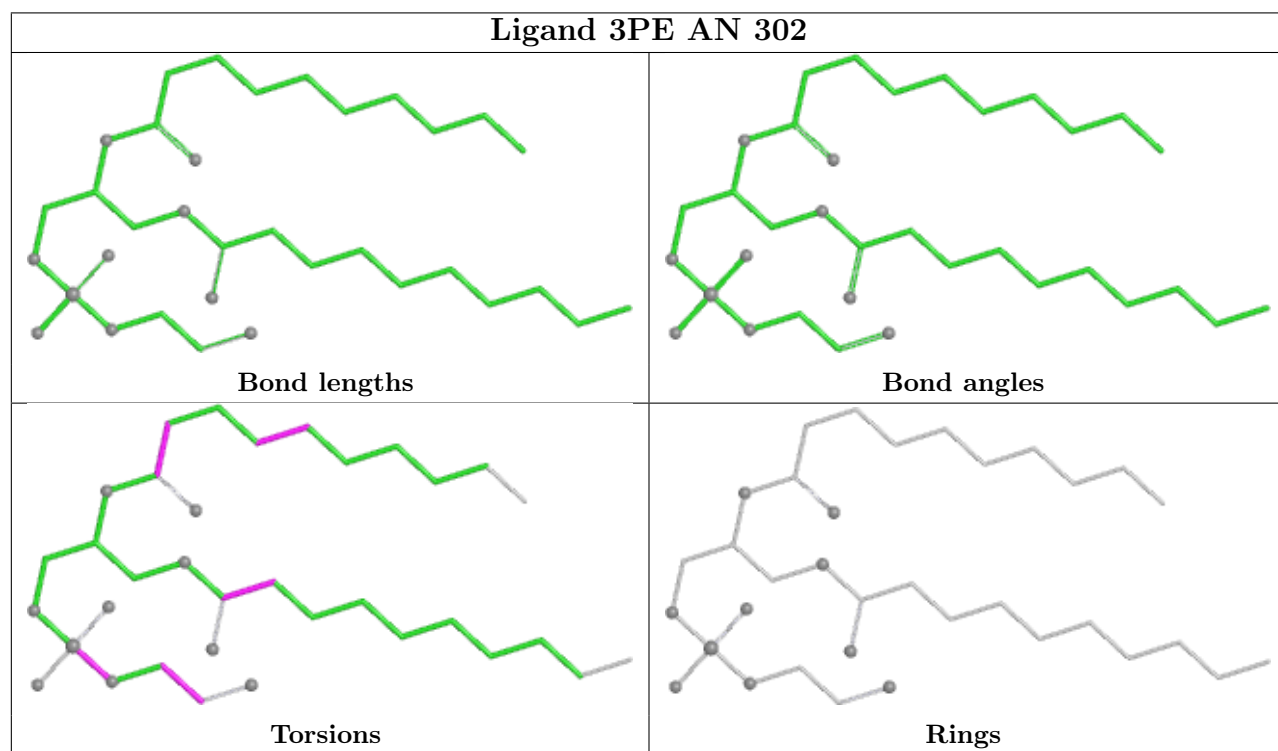
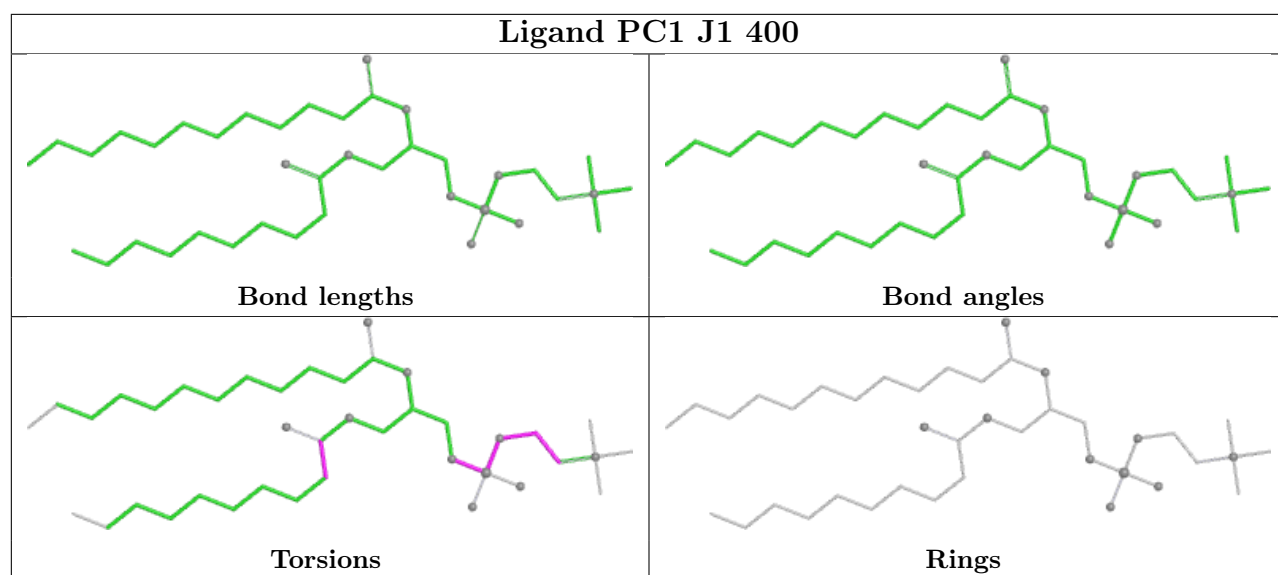


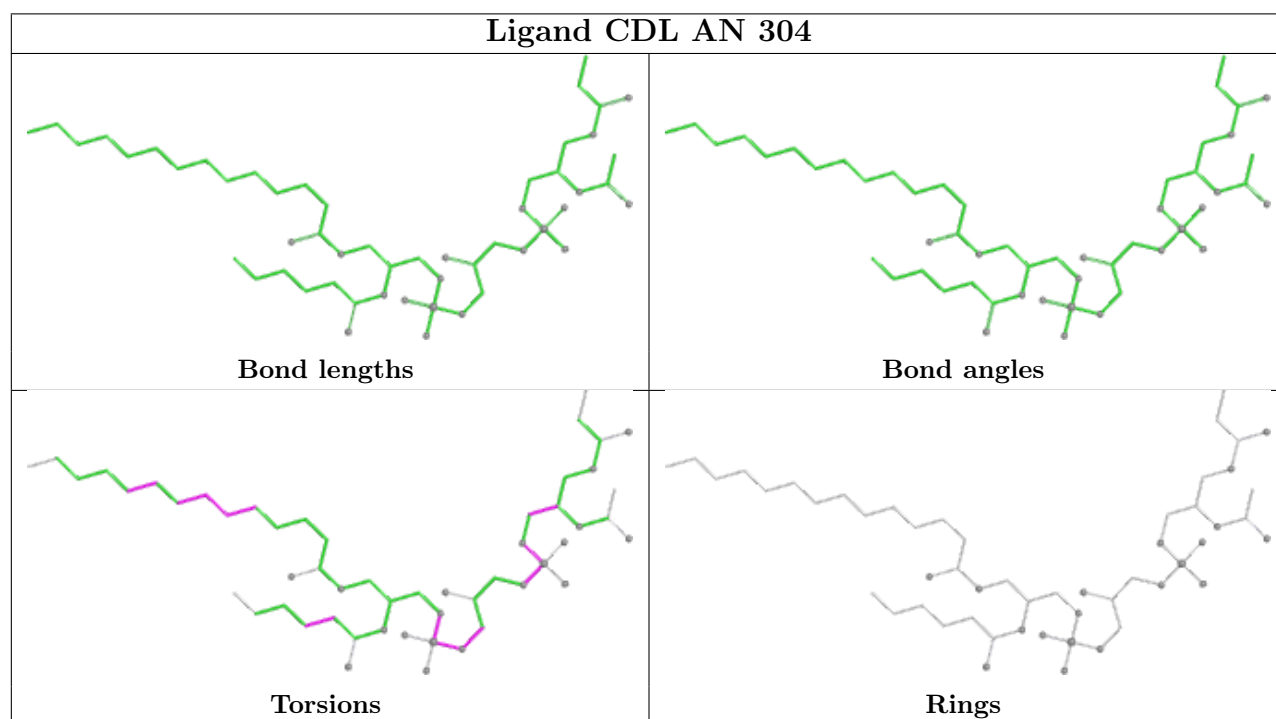
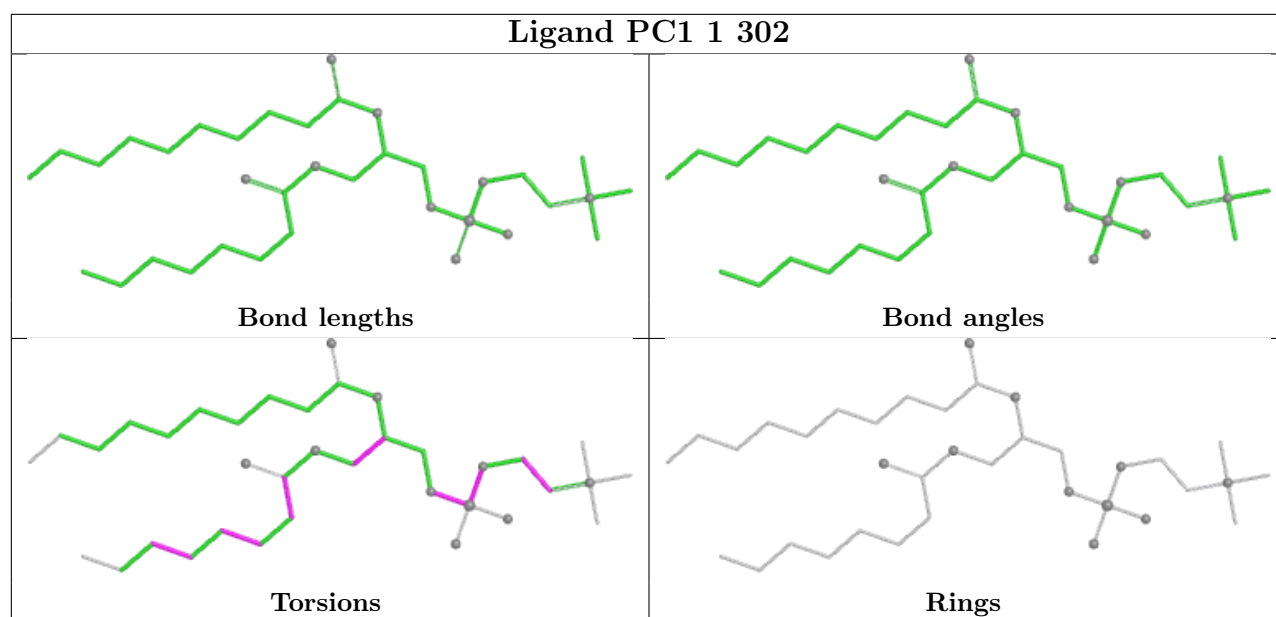
Torsions

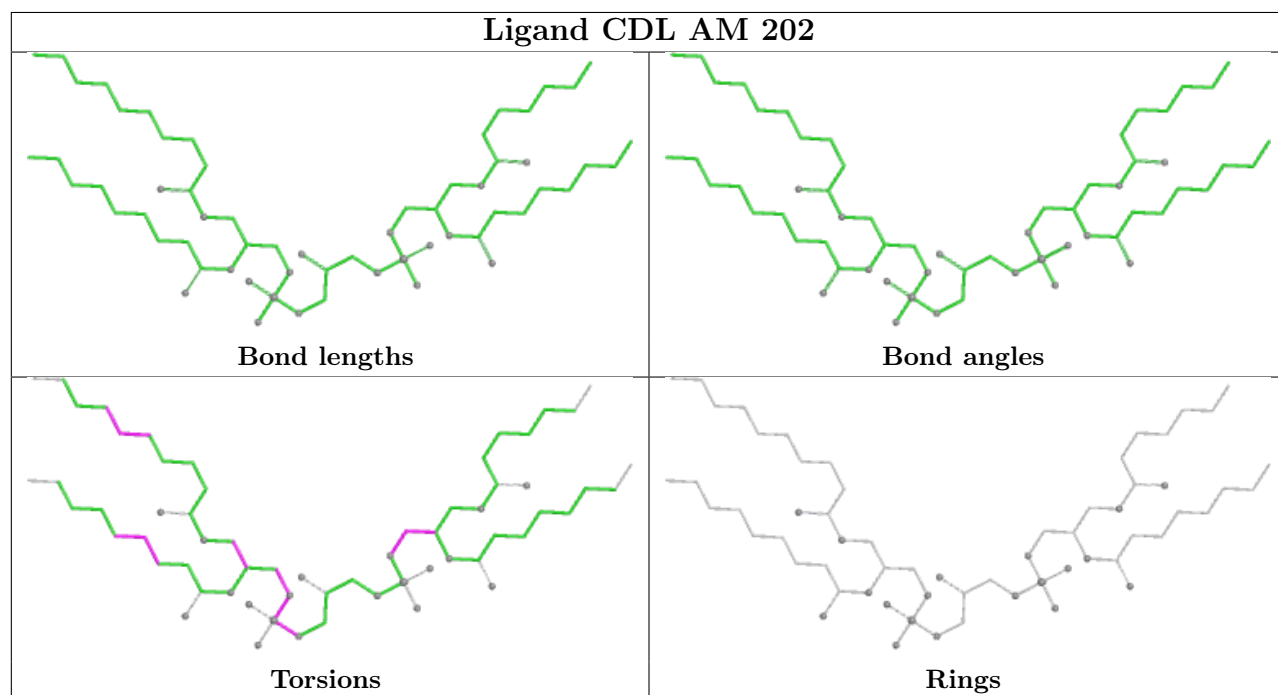
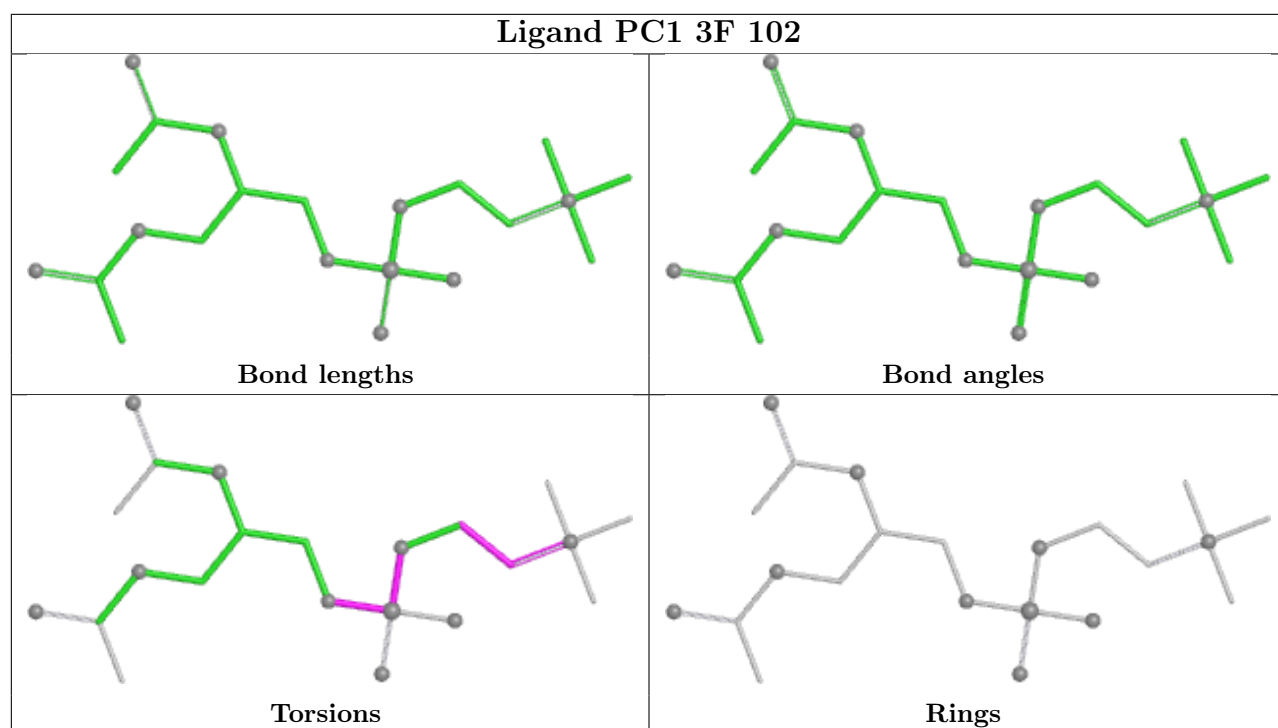


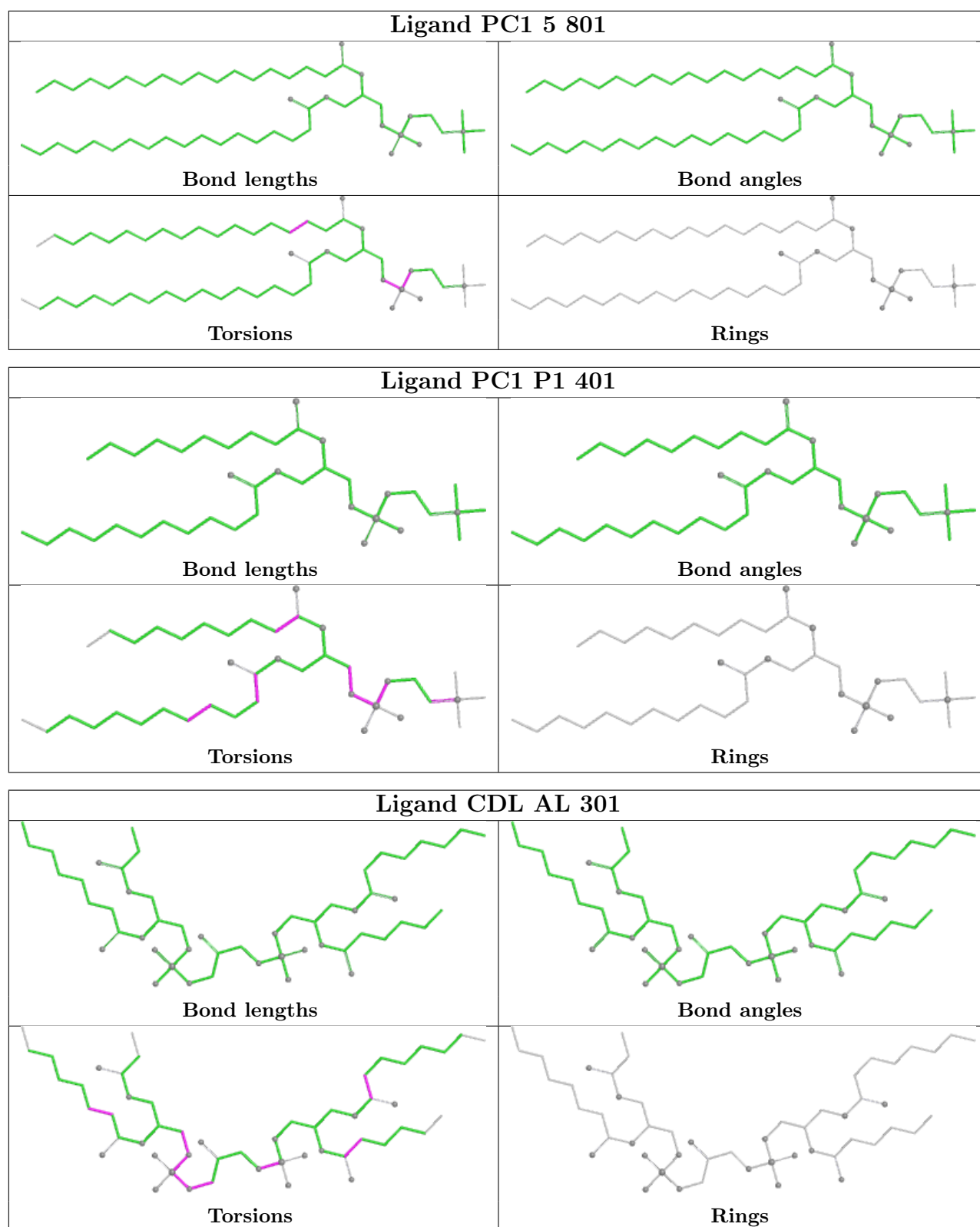
Rings











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

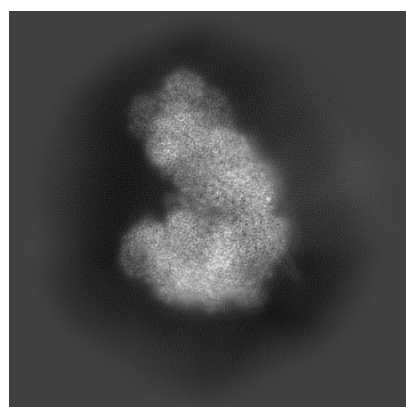
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25882. These allow visual inspection of the internal detail of the map and identification of artifacts.

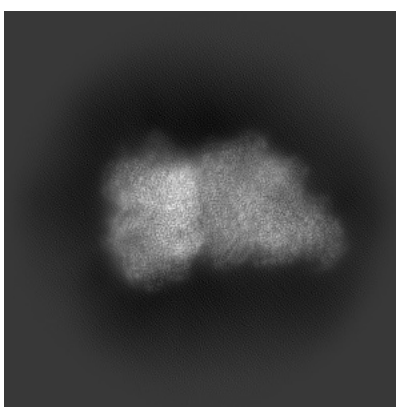
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

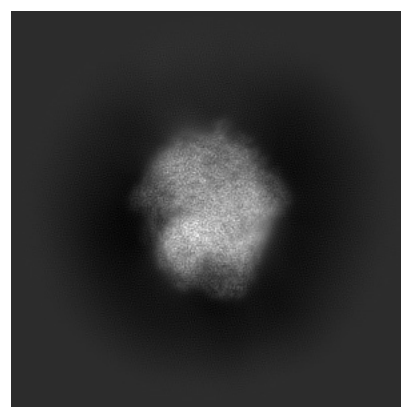
6.1.1 Primary map



X



Y

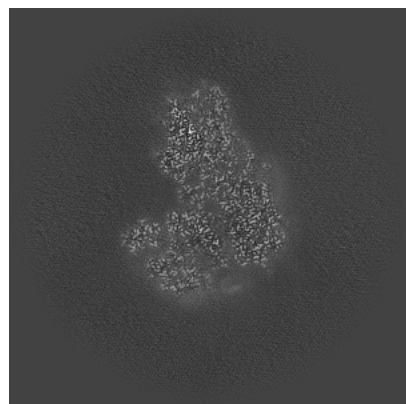


Z

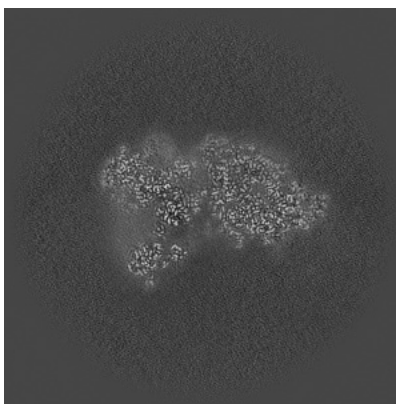
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

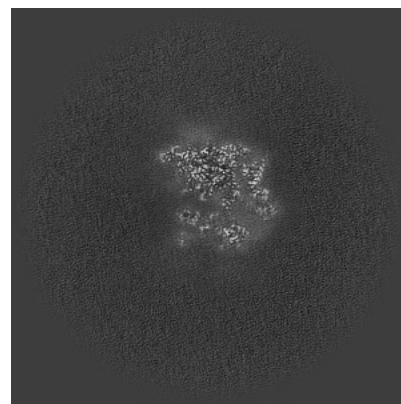
6.2.1 Primary map



X Index: 300



Y Index: 300

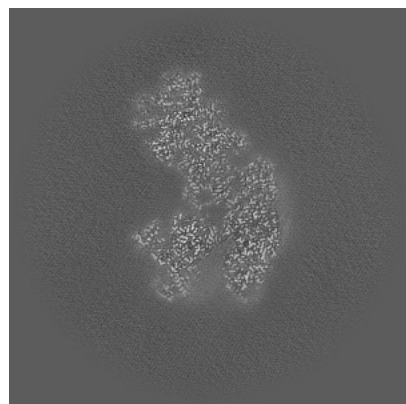


Z Index: 300

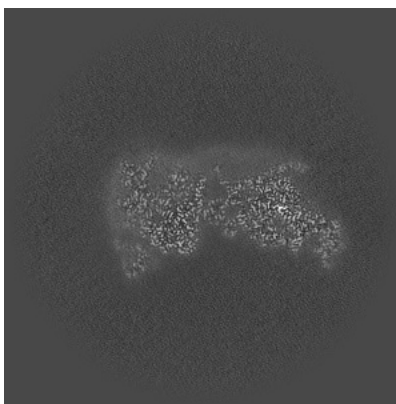
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

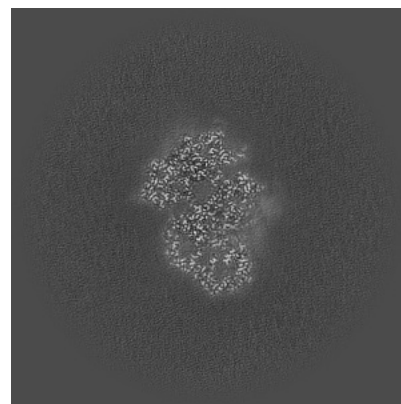
6.3.1 Primary map



X Index: 276



Y Index: 271

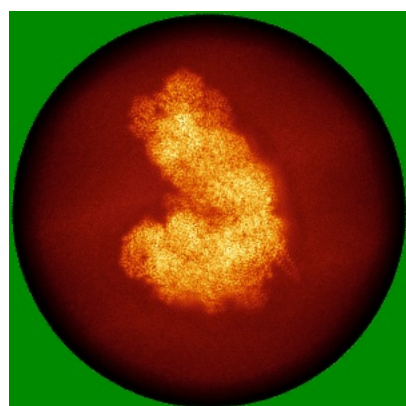


Z Index: 248

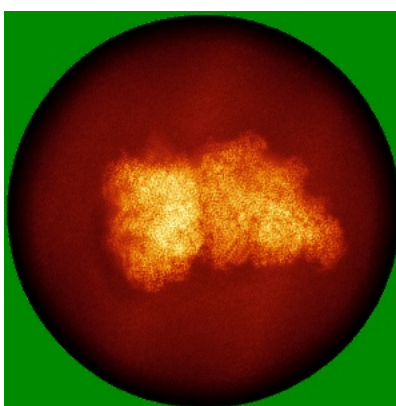
The images above show the largest variance slices of the map in three orthogonal directions.

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

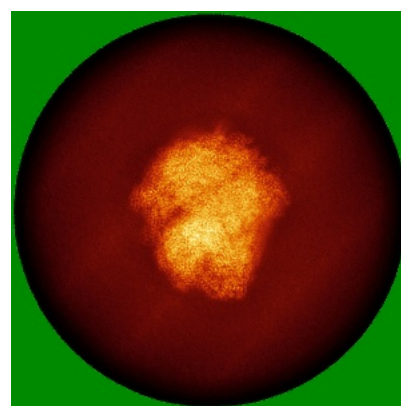
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

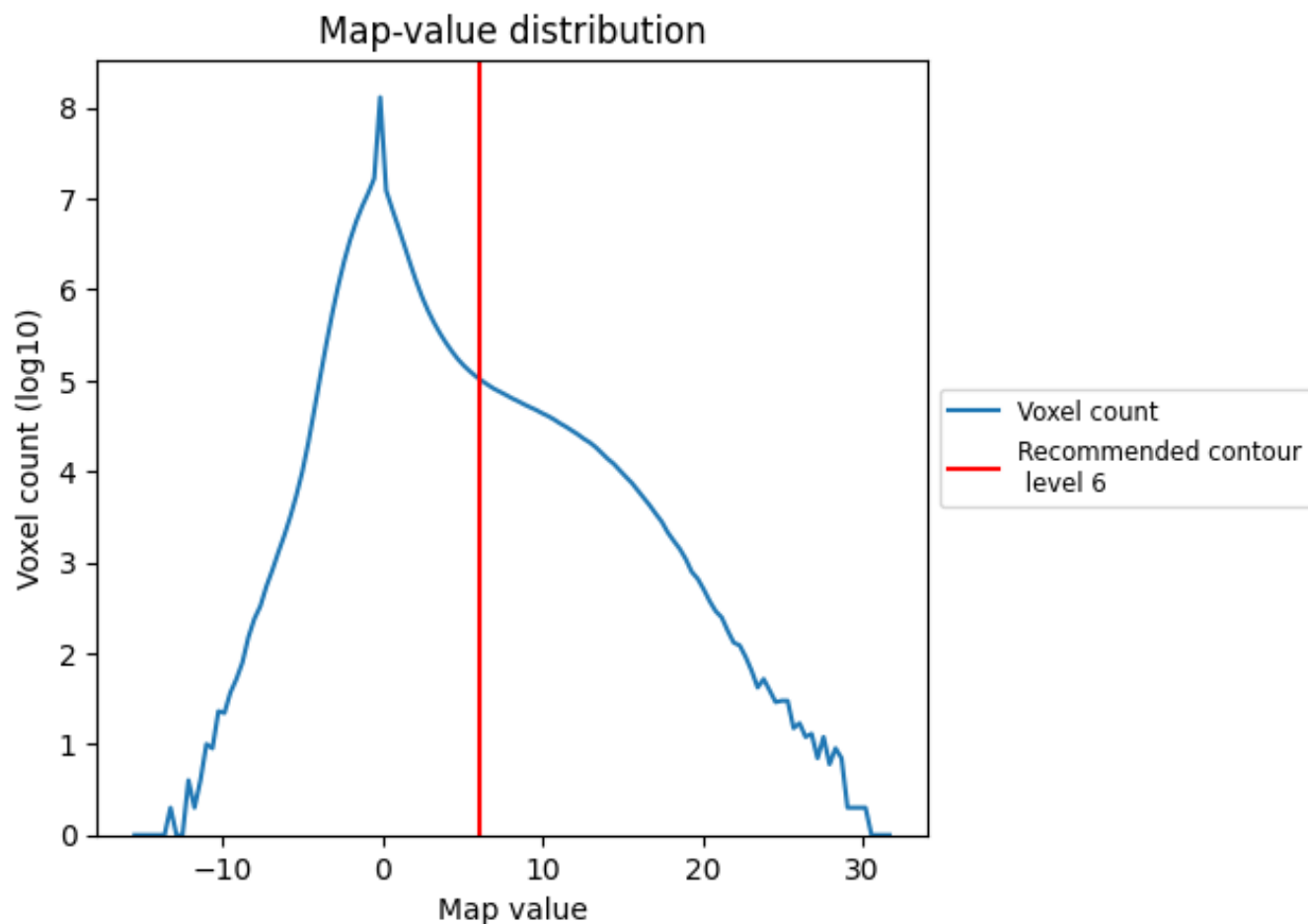
6.6 Mask visualisation

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

7 Map analysis [i](#)

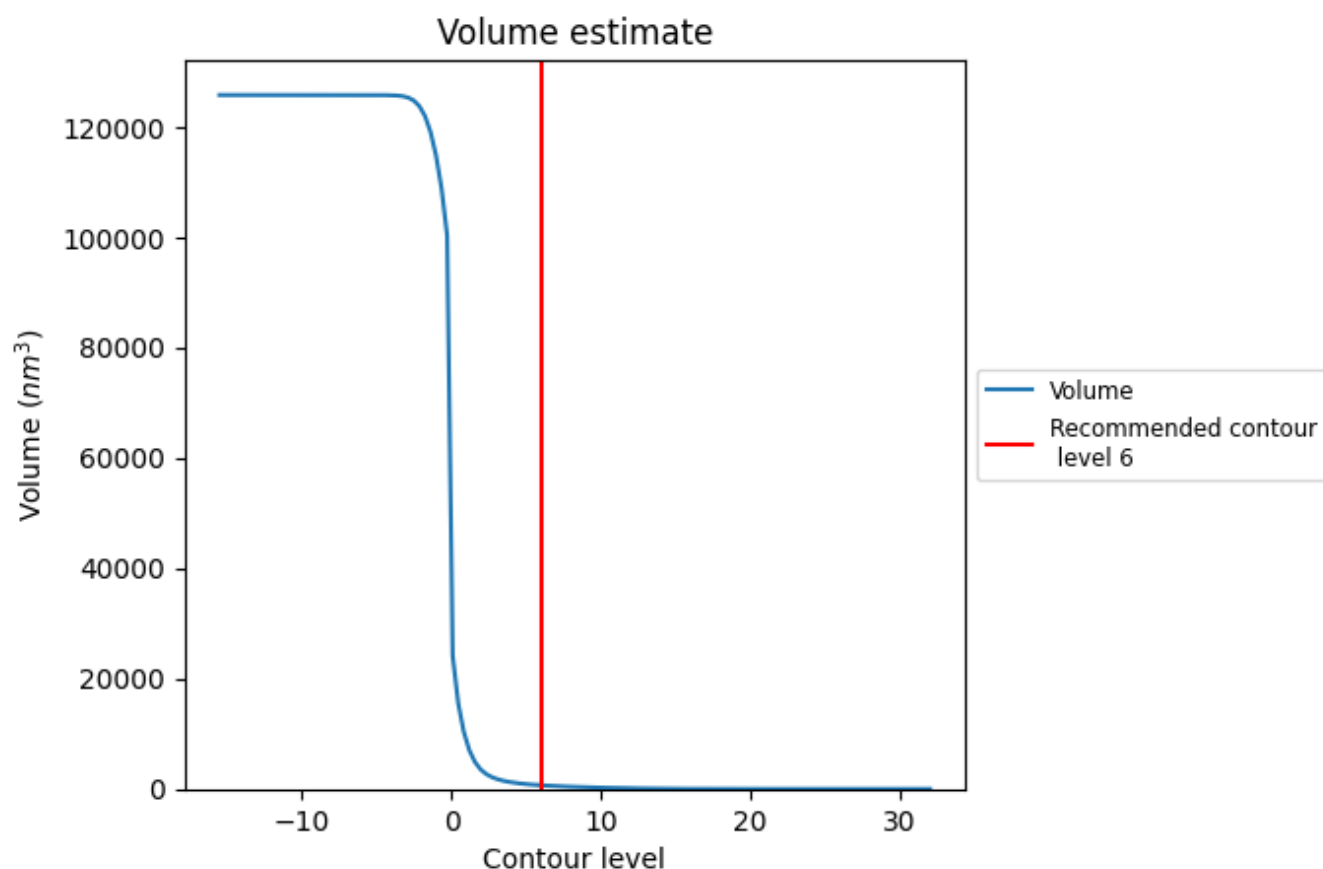
This section contains the results of statistical analysis of the map.

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.

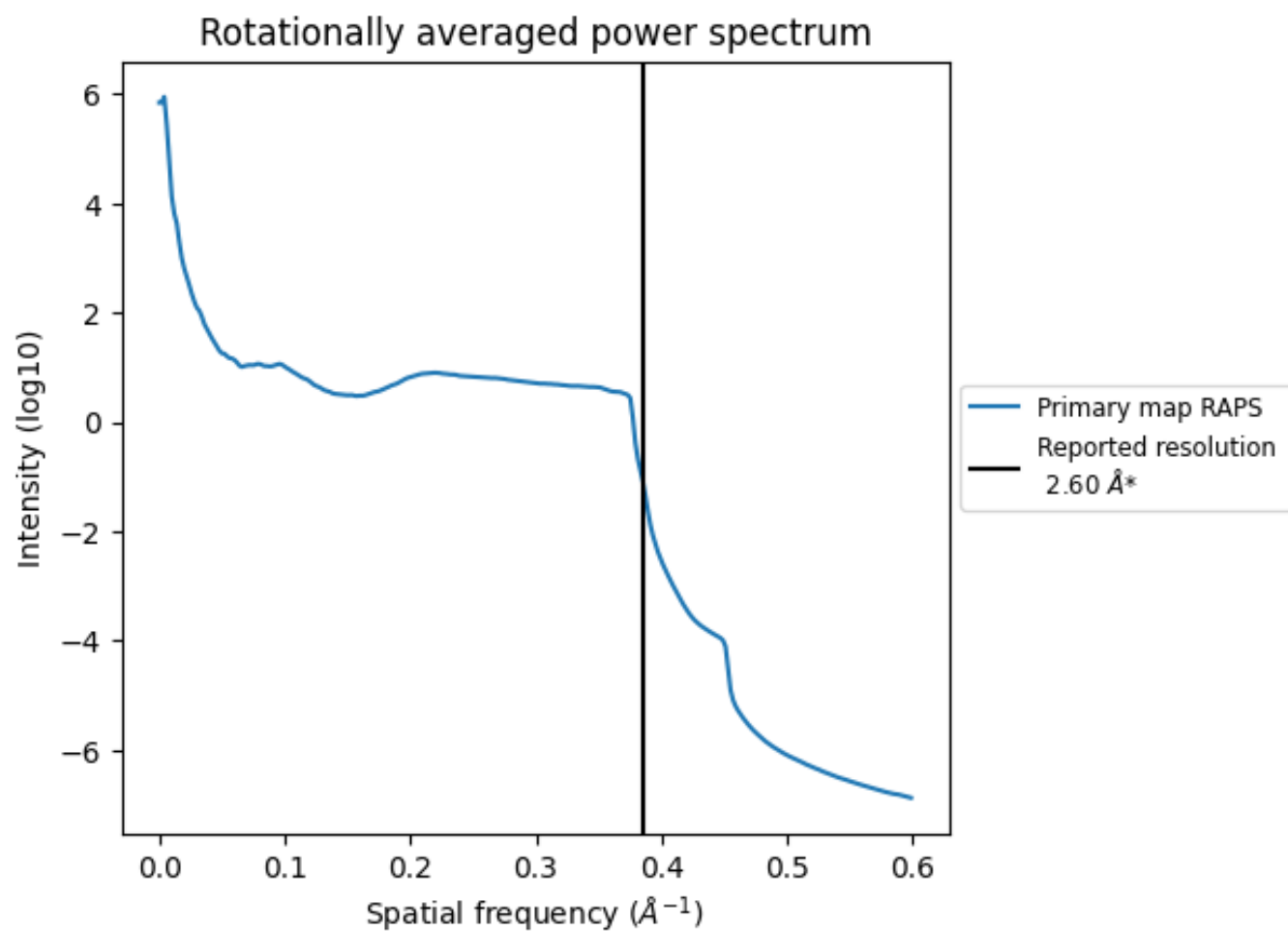
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 673 nm³; this corresponds to an approximate mass of 608 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 ⓘ

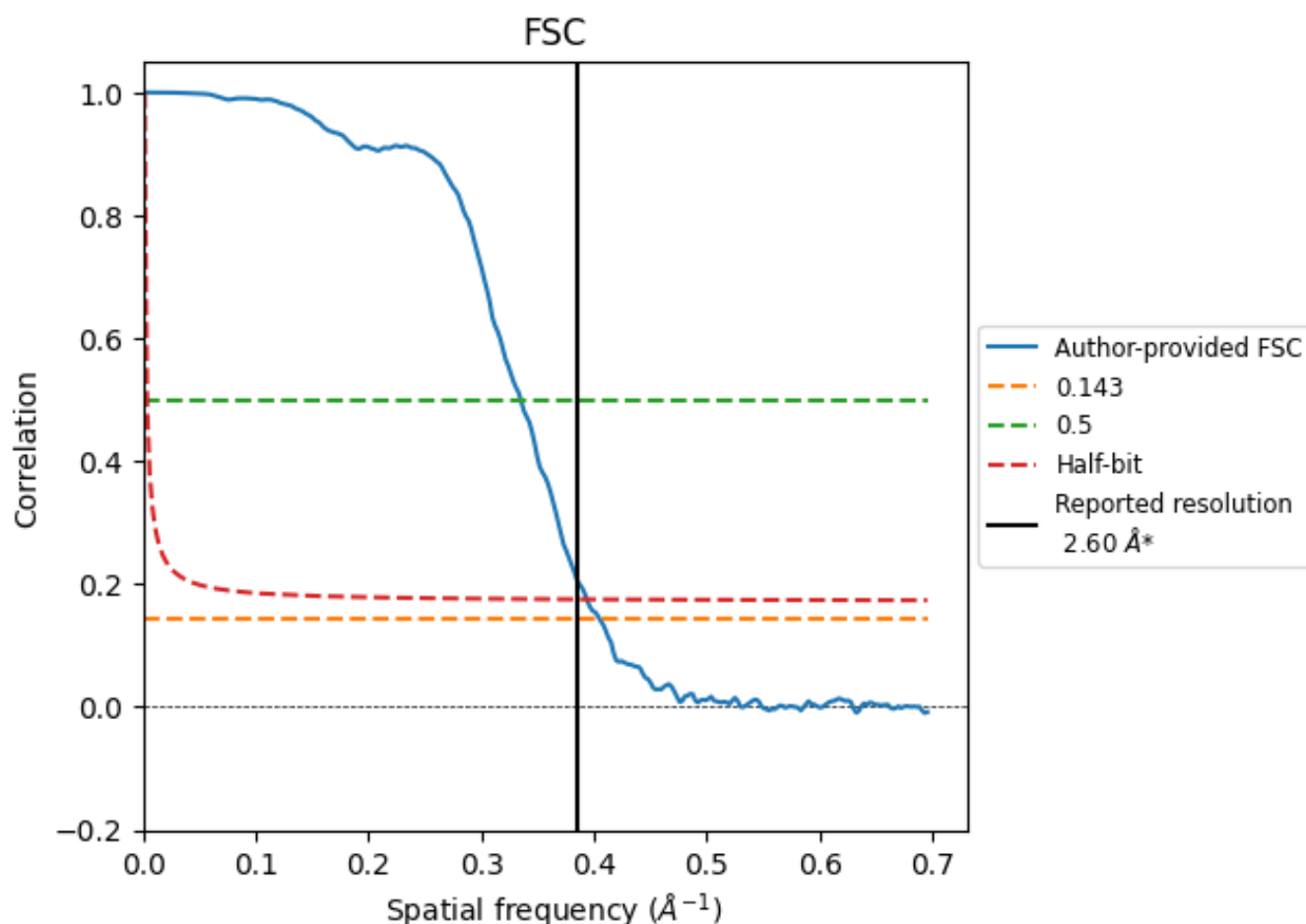


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.47	2.99	2.54
Unmasked-calculated*	-	-	-

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

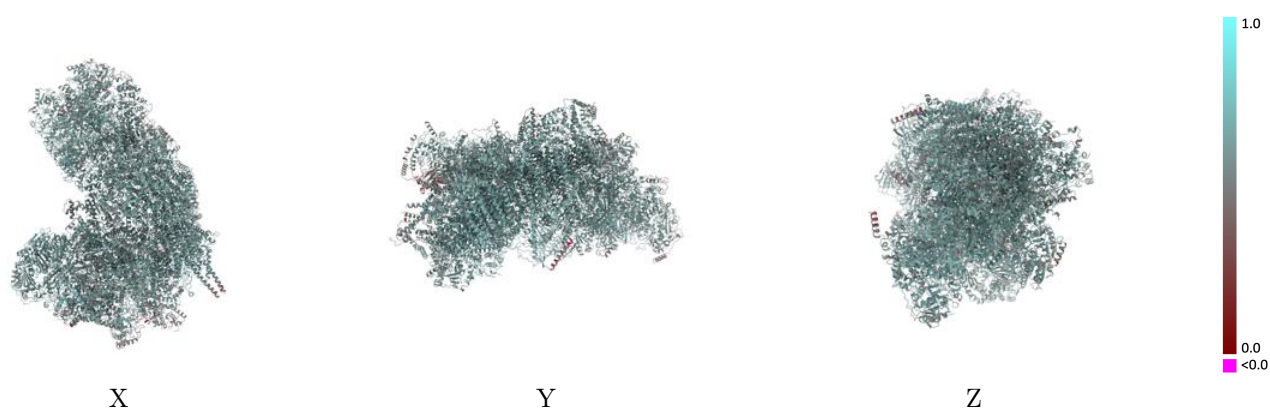
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-25882 and PDB model 7TGH. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)

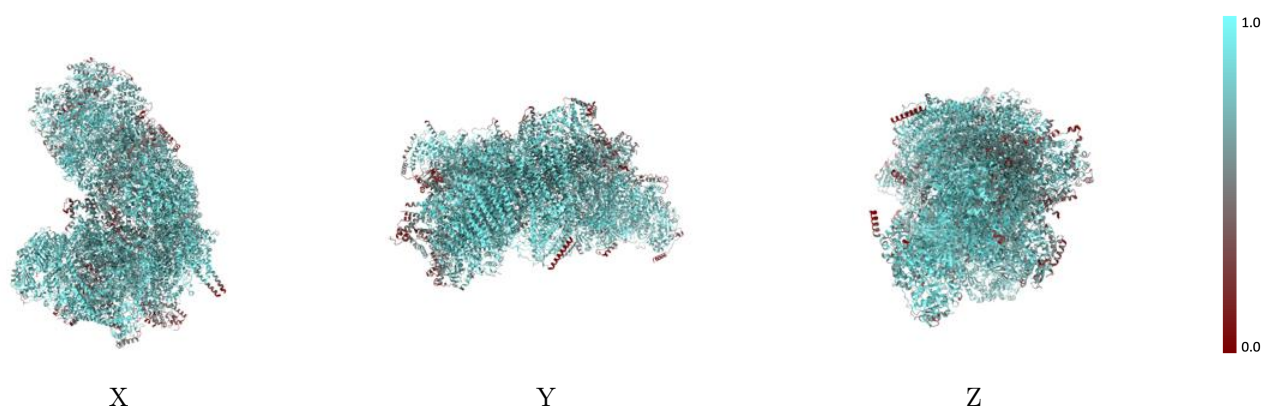
This section was not generated.

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



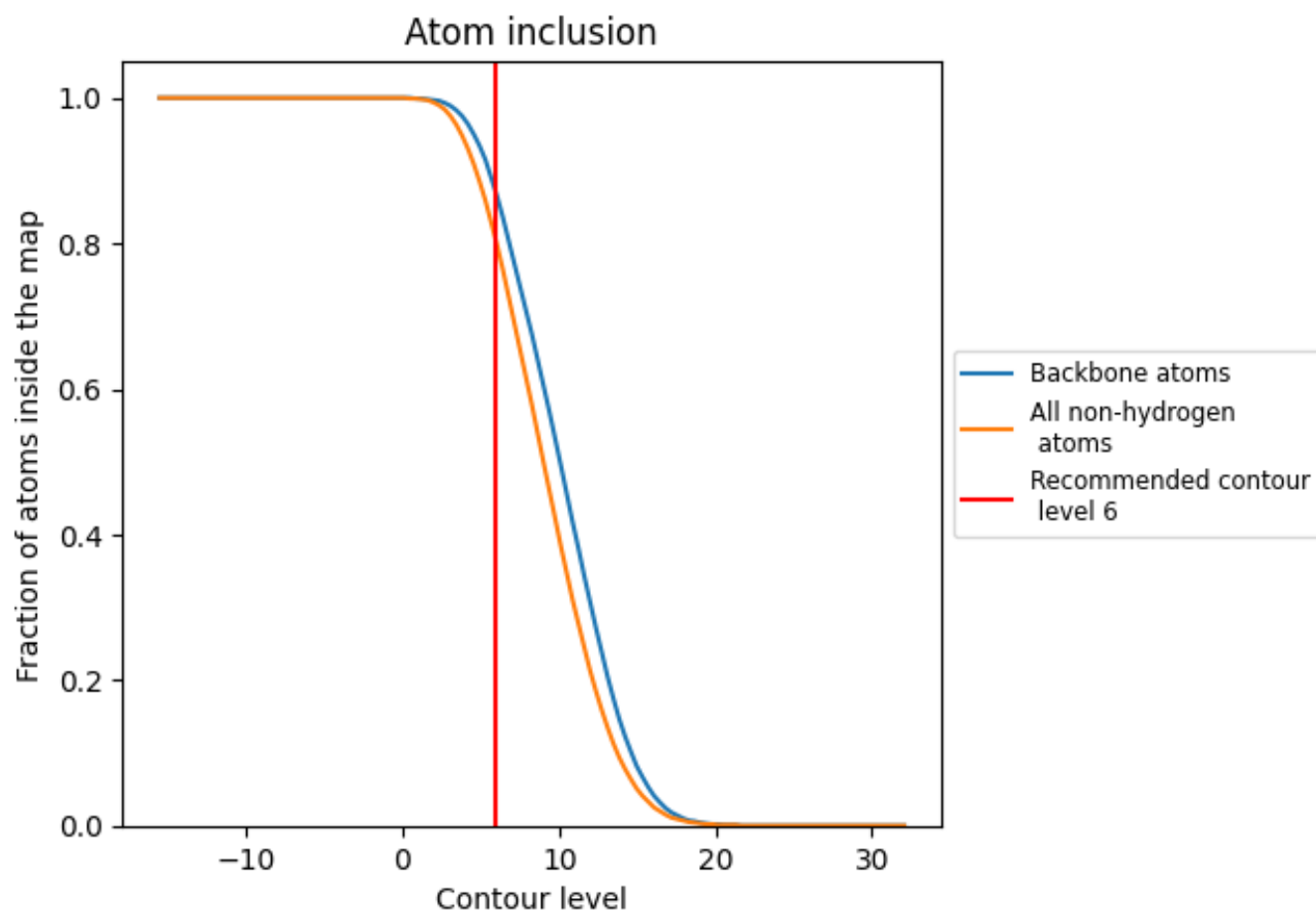
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8020	 0.6050
1	 0.7560	 0.6000
1B	 0.8320	 0.6230
2	 0.9050	 0.6450
2B	 0.9020	 0.6420
3	 0.8080	 0.6230
3A	 0.8860	 0.6160
3B	 0.9010	 0.6320
3C	 0.7980	 0.5920
3D	 0.9260	 0.6340
3E	 0.6380	 0.5290
3F	 0.7560	 0.5760
3G	 0.7280	 0.5750
3H	 0.8030	 0.6080
3I	 0.8340	 0.6220
3J	 0.8060	 0.6210
3M	 0.7720	 0.5900
3a	 0.8340	 0.6060
3b	 0.8590	 0.6030
3c	 0.7600	 0.5770
3d	 0.8820	 0.6020
3e	 0.8320	 0.5980
3f	 0.5320	 0.4700
3g	 0.7150	 0.5560
3h	 0.7450	 0.5700
3i	 0.7890	 0.5870
3j	 0.7850	 0.5630
3l	 0.4350	 0.4300
3m	 0.8710	 0.6070
4	 0.9010	 0.6390
4L	 0.8760	 0.6250
5	 0.9060	 0.6420
5B	 0.8430	 0.6410
6	 0.8340	 0.6270
A1	 0.7800	 0.6080



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Chain	Atom inclusion	Q-score
A2	 0.7560	 0.5850
A3	 0.8090	 0.6140
A5	 0.7690	 0.5900
A6	 0.9140	 0.6430
A7	 0.6990	 0.5830
A8	 0.8040	 0.5990
A9	 0.9040	 0.6420
AB	 0.7690	 0.6210
AC	 0.8360	 0.6250
AL	 0.8330	 0.6240
AM	 0.7340	 0.5920
AN	 0.7350	 0.6020
B2	 0.7240	 0.5860
B3	 0.8300	 0.6310
B4	 0.8500	 0.6380
B6	 0.9310	 0.6580
B7	 0.8550	 0.6170
B8	 0.8420	 0.6290
B9	 0.8390	 0.6230
BL	 0.8960	 0.6330
BM	 0.7830	 0.6100
C	 0.7170	 0.5510
C1	 0.8850	 0.6350
C2	 0.8060	 0.5960
C3	 0.7680	 0.6020
C4	 0.8080	 0.6180
FX	 0.8640	 0.6390
J1	 0.6580	 0.5900
P1	 0.7600	 0.6040
P2	 0.6870	 0.5940
R	 0.8150	 0.5970
S1	 0.8850	 0.6300
S2	 0.8860	 0.6270
S3	 0.8910	 0.6330
S4	 0.8630	 0.6280
S5	 0.8470	 0.6230
S6	 0.8810	 0.6330
S7	 0.9160	 0.6390
S8	 0.7870	 0.6150
T1	 0.6840	 0.5720
T2	 0.7770	 0.5890
T3	 0.4530	 0.5160

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Chain	Atom inclusion	Q-score
T4	 0.4930	 0.5340
T5	 0.8230	 0.5990
T6	 0.8250	 0.6030
T7	 0.5040	 0.5310
T8	 0.7910	 0.6090
T9	 0.8080	 0.6010
TA	 0.6410	 0.5690
TB	 0.8380	 0.6220
TC	 0.7950	 0.6130
TD	 0.4560	 0.5450
TE	 0.6210	 0.5920
TX	 0.7130	 0.6110
V1	 0.7910	 0.5870
V2	 0.7040	 0.5690
X1	 0.8380	 0.6200