



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:36 PM UTC

PDB ID : 8PW5 / pdb_00008pw5
EMDB ID : EMD-17989
Title : CS respirasome from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-07-19
Resolution : 3.60 Å(reported)
Based on initial models : 7o3c, 6g2j

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

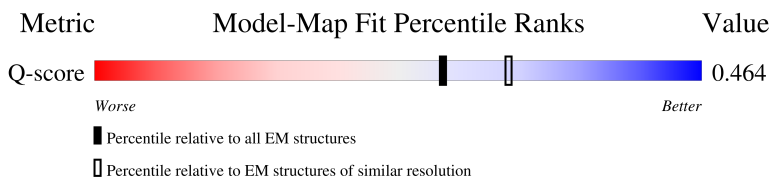
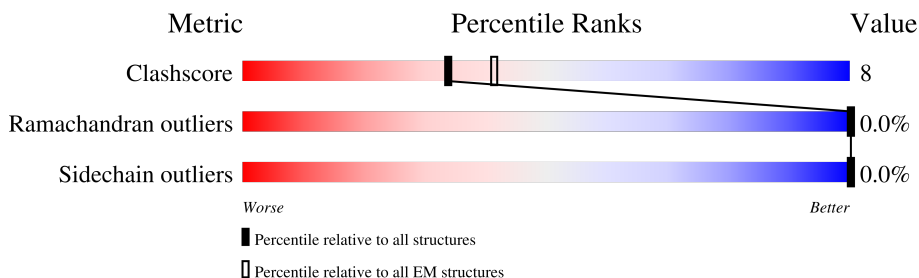
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



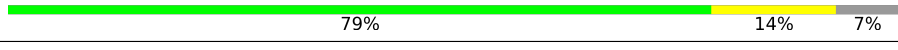
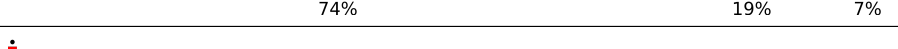
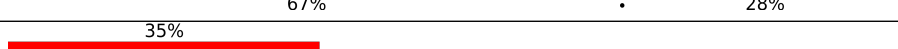
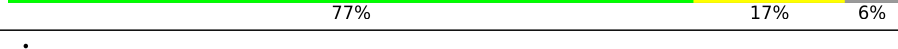
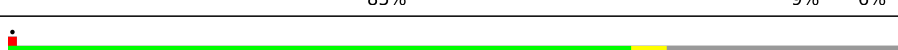
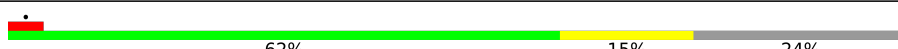
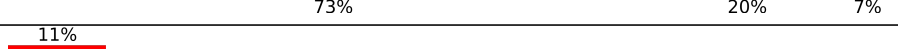
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	g	111	
1	t	111	
2	m	69	
2	z	69	

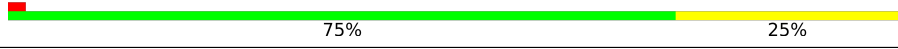
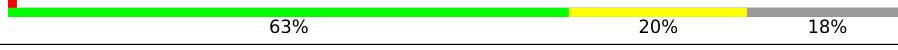
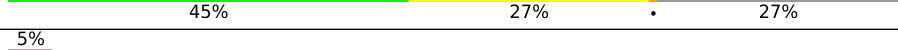
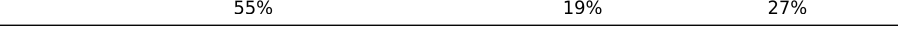
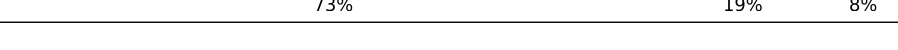
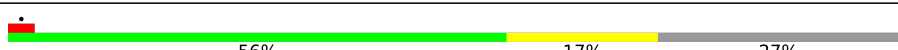
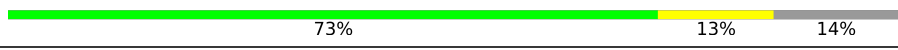
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Mol	Chain	Length	Quality of chain
3	A	480	
3	L	480	
4	B	453	
4	M	453	
5	C	381	
5	N	381	
6	D	325	
6	O	325	
7	E	274	
7	P	274	
7	T	274	
8	F	111	
8	Q	111	
9	G	82	
9	R	82	
10	H	89	
10	S	89	
11	J	64	
11	U	64	
12	K	56	
12	V	56	
13	I	113	
14	a	514	
14	n	514	
15	b	227	

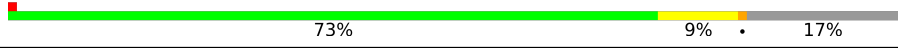
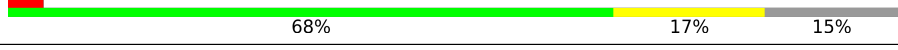
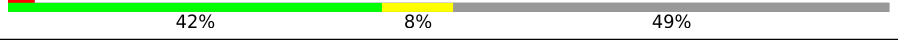
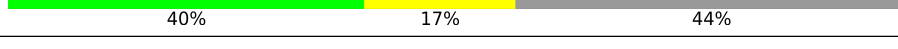
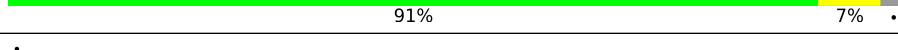
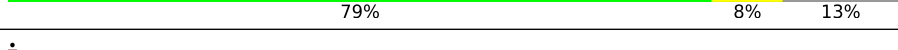
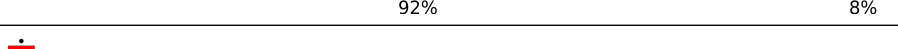
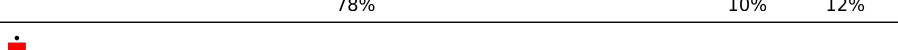
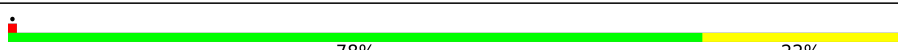
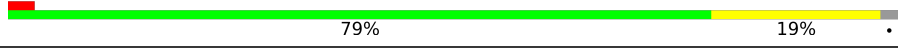
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Mol	Chain	Length	Quality of chain
15	o	227	
16	c	261	
16	p	261	
17	d	169	
17	q	169	
18	e	146	
18	r	146	
19	f	128	
19	s	128	
20	h	86	
20	u	86	
21	i	76	
21	v	76	
22	k	80	
22	x	80	
23	l	63	
23	y	63	
24	w	83	
25	6	224	
26	C1	263	
27	D1	463	
28	2	248	
29	1	464	
30	3	727	
31	9	212	

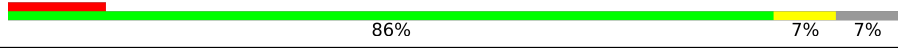
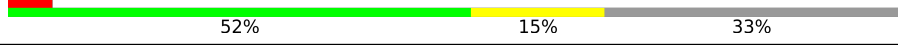
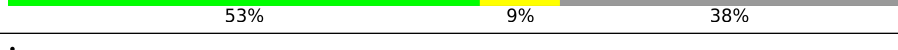
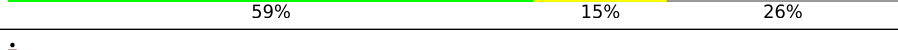
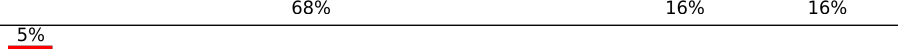
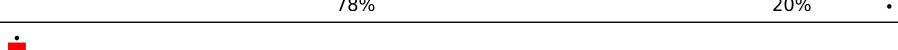
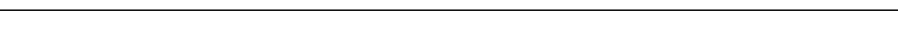
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Mol	Chain	Length	Quality of chain
32	P1	377	
33	Q1	175	
34	7	116	
35	S1	99	
36	T1	156	
36	U1	156	
37	V1	116	
38	W1	131	
39	q1	145	
40	r1	113	
41	s1	104	
42	A1	115	
43	H1	318	
44	J1	172	
45	K1	98	
46	L1	607	
47	M1	459	
48	N1	345	
49	O1	355	
50	X1	172	
51	Y1	141	
52	Z1	144	
53	a1	70	
54	b1	84	
55	c1	76	

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Mol	Chain	Length	Quality of chain
56	d1	120	
57	e1	106	
58	f1	57	
59	g1	151	
60	h1	189	
61	i1	128	
62	j1	105	
63	k1	104	
64	l1	186	
65	m1	129	
66	n1	179	
67	o1	137	
68	p1	176	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
74	FES	P	201	-	-	X	-

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 130610 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 Cytochrome c oxidase subunit 6A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	t	76	Total	C	N	O	S	0	0
			620	404	112	102	2		
1	g	76	Total	C	N	O	S	0	0
			620	404	112	102	2		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	44	Total	C	N	O	S	0	0
			343	220	59	61	3		
2	z	44	Total	C	N	O	S	0	0
			343	220	59	61	3		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
3	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
4	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 5 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
5	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 6 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		
6	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	196	Total	C	N	O	S	0	0
			1167	705	219	237	6		
7	P	196	Total	C	N	O	S	0	0
			1164	702	219	237	6		
7	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	98	Total	C	N	O	S	0	0
			865	552	154	156	3		
8	Q	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	77	Total	C	N	O	S	0	0
			654	424	120	109	1		
9	R	77	Total	C	N	O	S	0	0
			654	424	120	109	1		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
10	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	60	Total	C	N	O		0	0
			495	323	86	86			
11	U	60	Total	C	N	O		0	0
			495	323	86	86			

- Molecule 12 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	52	Total	C	N	O	S	0	0
			430	287	76	66	1		
12	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 13 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	111	Total	C	N	O	S	0	0
			807	520	138	144	5		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		
14	a	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		
15	b	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	260	Total	C	N	O	S	0	0
			2118	1418	339	351	10		
16	c	259	Total	C	N	O	S	0	0
			2111	1414	338	349	10		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	139	Total	C	N	O	S	0	0
			1156	745	192	212	7		
17	d	139	Total	C	N	O	S	0	0
			1156	745	192	212	7		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	104	Total	C	N	O	S	0	0
			842	538	141	161	2		
18	e	103	Total	C	N	O	S	0	0
			833	533	140	158	2		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	94	Total	C	N	O	S	0	0
			721	449	126	138	8		
19	f	93	Total	C	N	O	S	0	0
			717	447	125	137	8		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	79	Total	C	N	O	S	0	0
			654	416	116	117	5		
20	h	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		
21	i	72	Total	C	N	O	S	0	0
			572	372	103	94	3		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		
22	k	48	Total	C	N	O	S	0	0
			378	245	64	67	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		
23	l	46	Total	C	N	O	S	0	0
			380	253	64	61	2		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	57	Total	C	N	O	S	0	0
			435	283	71	78	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C1	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D1	430	Total	C	N	O	S	0	0
			3464	2215	595	630	24		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P1	342	Total	C	N	O	S	0	0
			2748	1777	483	481	7		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q1	126	Total	C	N	O	S	0	0
			1022	646	180	192	4		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	S1	84	Total	C	N	O	S	0	0
			671	421	127	120	3		

- Molecule 36 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T1	79	Total	C	N	O	S	0	0
			637	410	95	127	5		
36	U1	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	V1	113	Total	C	N	O	S	0	0
			923	602	153	165	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	W1	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q1	145	Total	C	N	O	S	0	0
			1209	777	215	212	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r1	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	s1	42	Total	C	N	O	0	0
			351	219	62	70		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	A1	115	Total	C	N	O	S	0	0
			932	633	132	160	7		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	H1	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	J1	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	K1	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L1	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M1	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N1	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O1	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	X1	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Y1	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Z1	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	a1	70	Total	C	N	O	S	0	0
			572	370	101	97	4		

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	b1	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	c1	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	d1	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	e1	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	f1	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	g1	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	h1	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	i1	106	Total	C	N	O	S	0	0
			897	584	157	152	4		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	j1	65	Total	C	N	O	S	0	0
			562	370	93	98	1		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	k1	77	Total	C	N	O	S	0	0
			626	414	106	104	2		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	l1	157	Total	C	N	O	S	0	0
			1323	855	220	237	11		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	m1	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	n1	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

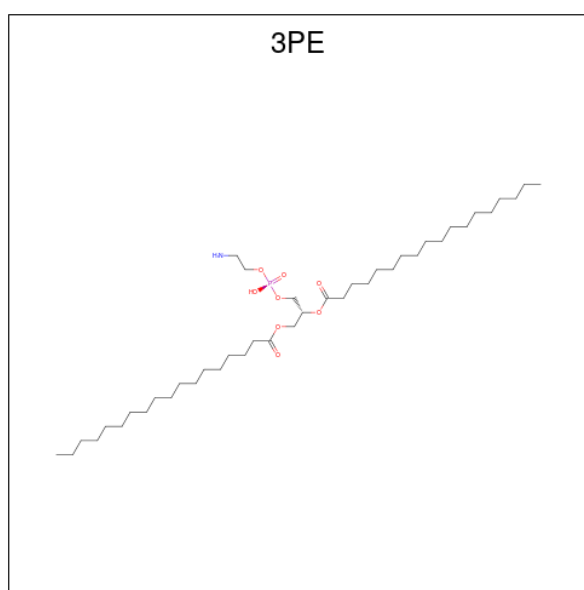
- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	o1	118	Total	C	N	O	S	0	0
			1014	639	190	177	8		

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	p1	170	Total	C	N	O	S	0	0
			1438	903	258	269	8		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



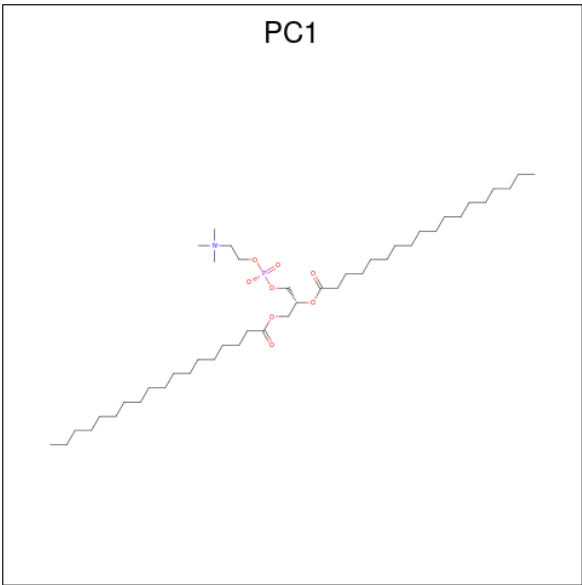
Mol	Chain	Residues	Atoms					AltConf
69	t	1	Total	C	N	O	P	0
			25	15	1	8	1	
69	z	1	Total	C	N	O	P	0
			26	16	1	8	1	
69	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
69	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	E	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
69	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
69	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	R	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	n	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	n	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	n	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	o	1	Total	C	N	O	P	0
			29	19	1	8	1	
69	p	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	v	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	r1	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	H1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	

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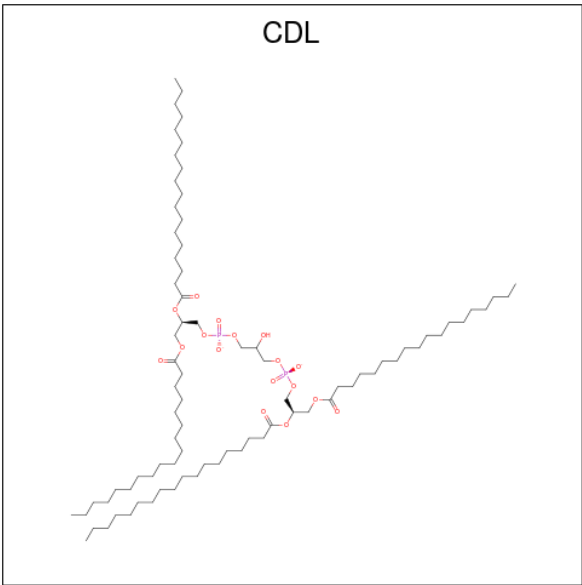
Mol	Chain	Residues	Atoms					AltConf
69	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
69	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	b1	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	m1	1	Total	C	N	O	P	0
			36	26	1	8	1	
69	a	1	Total	C	N	O	P	0
			28	18	1	8	1	
69	a	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
69	c	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	d	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	g	1	Total	C	N	O	P	0
			25	15	1	8	1	
69	i	1	Total	C	N	O	P	0
			28	18	1	8	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
70	z	1	Total	C	N	O	P	0
			28	18	1	8	1	
70	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	K	1	Total	C	N	O	P	0
			28	18	1	8	1	
70	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
70	V	1	Total	C	N	O	P	0
			28	18	1	8	1	
70	I	1	Total	C	N	O	P	0
			50	40	1	8	1	
70	p	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
70	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	P1	1	Total	C	N	O	P	0
			31	21	1	8	1	
70	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	g	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 71 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



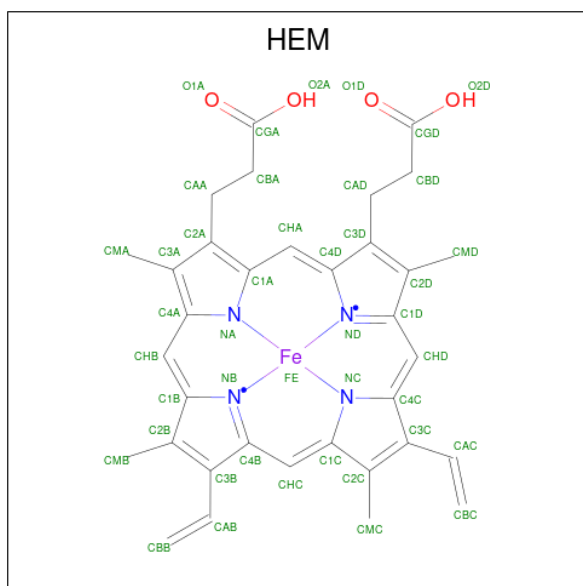
Mol	Chain	Residues	Atoms				AltConf
71	A	1	Total	C	O	P	0
			46	27	17	2	
71	D	1	Total	C	O	P	0
			56	37	17	2	
71	G	1	Total	C	O	P	0
			42	23	17	2	
71	L	1	Total	C	O	P	0
			46	27	17	2	
71	O	1	Total	C	O	P	0
			57	38	17	2	
71	R	1	Total	C	O	P	0
			41	22	17	2	
71	R	1	Total	C	O	P	0
			57	38	17	2	
71	R	1	Total	C	O	P	0
			72	53	17	2	
71	V	1	Total	C	O	P	0
			46	27	17	2	
71	r1	1	Total	C	O	P	0
			57	38	17	2	
71	H1	1	Total	C	O	P	0
			51	33	16	2	
71	L1	1	Total	C	O	P	0
			78	59	17	2	
71	L1	1	Total	C	O	P	0
			46	27	17	2	
71	N1	1	Total	C	O	P	0
			90	71	17	2	

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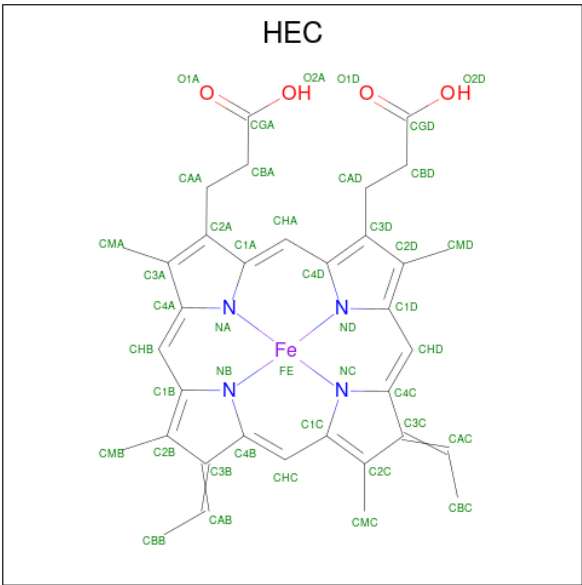
Mol	Chain	Residues	Atoms				AltConf
71	Y1	1	Total	C	O	P	0
			94	75	17	2	
71	d1	1	Total	C	O	P	0
			67	48	17	2	
71	h1	1	Total	C	O	P	0
			70	51	17	2	
71	g	1	Total	C	O	P	0
			38	20	16	2	

- Molecule 72 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



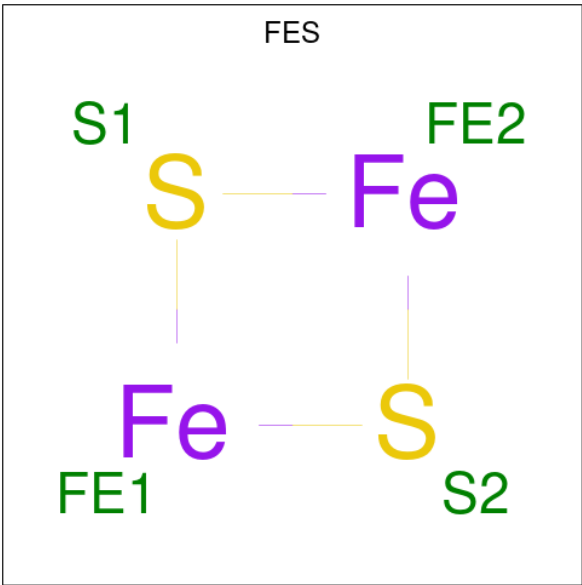
Mol	Chain	Residues	Atoms					AltConf
72	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 73 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 74 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
74	E	1	Total	Fe	S	0
			4	2	2	
74	P	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
74	2	1	Total	Fe	S	0
			4	2	2	
74	3	1	Total	Fe	S	0
			4	2	2	

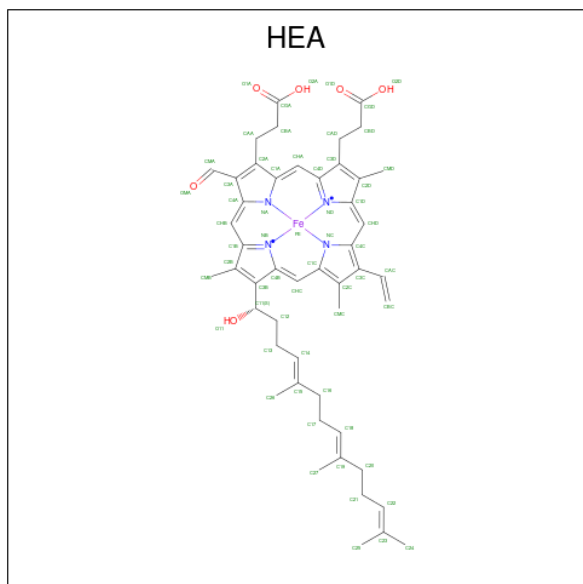
- Molecule 75 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
75	n	1	Total	Cu	0
			1	1	
75	a	1	Total	Cu	0
			1	1	

- Molecule 76 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
76	n	1	Total	Na	0
			1	1	
76	a	1	Total	Na	0
			1	1	

- Molecule 77 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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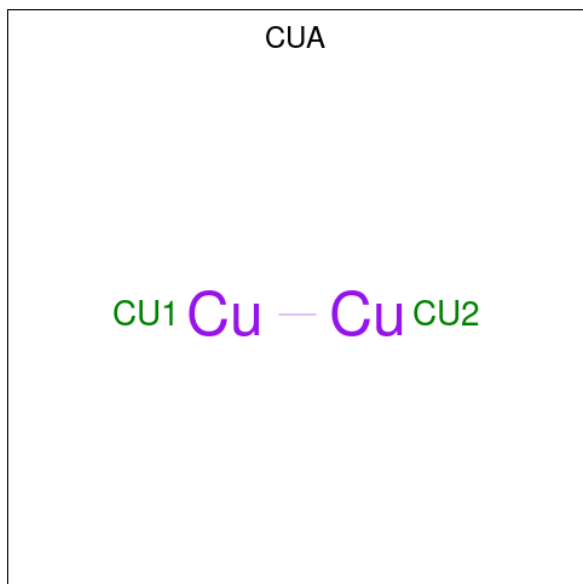
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Mol	Chain	Residues	Atoms					AltConf
77	n	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
77	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 78 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
78	o	1	Total	Mg	0
			1	1	
78	O1	1	Total	Mg	0
			1	1	
78	a	1	Total	Mg	0
			1	1	

- Molecule 79 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

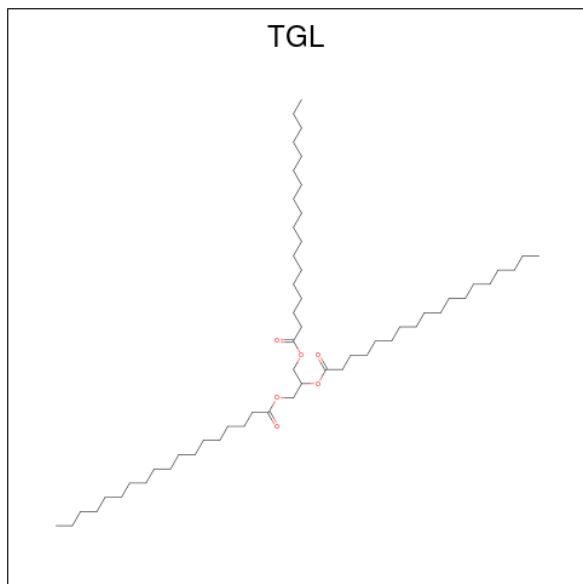


Mol	Chain	Residues	Atoms		AltConf
79	o	1	Total	Cu	0
			2	2	
79	b	1	Total	Cu	0
			2	2	

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

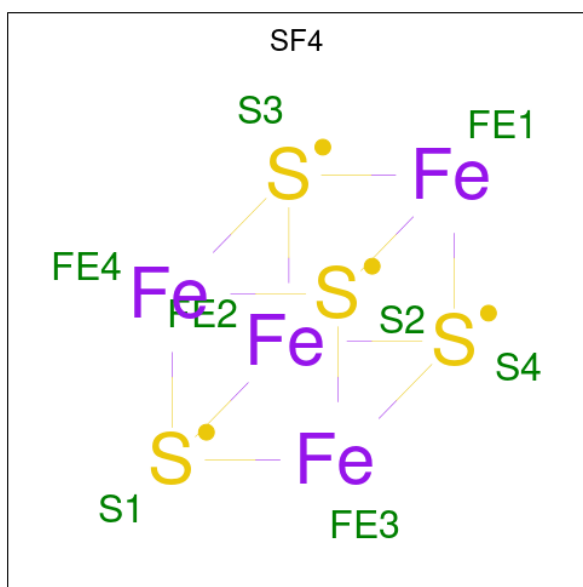
Mol	Chain	Residues	Atoms		AltConf
80	s	1	Total	Zn	0
			1	1	
80	7	1	Total	Zn	0
			1	1	
80	f	1	Total	Zn	0
			1	1	

- Molecule 81 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



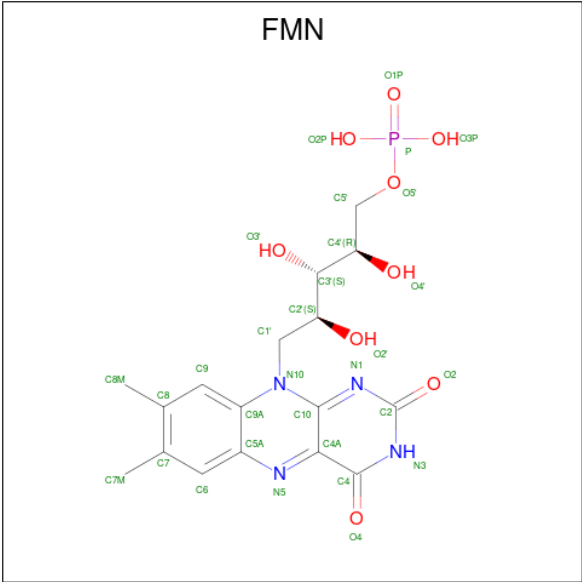
Mol	Chain	Residues	Atoms			AltConf
81	y	1	Total	C	O	0
			37	31	6	
81	l	1	Total	C	O	0
			37	31	6	

- Molecule 82 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
82	6	1	Total	Fe	S	0
			8	4	4	
82	1	1	Total	Fe	S	0
			8	4	4	
82	3	1	Total	Fe	S	0
			8	4	4	
82	3	1	Total	Fe	S	0
			8	4	4	
82	9	1	Total	Fe	S	0
			8	4	4	
82	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 83 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

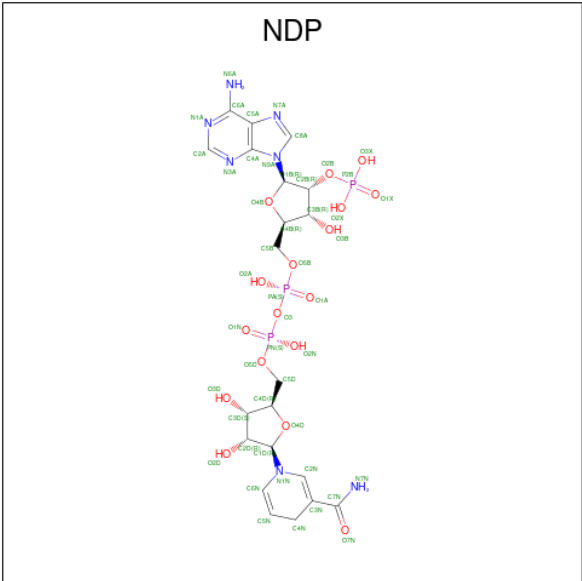


Mol	Chain	Residues	Atoms					AltConf
83	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

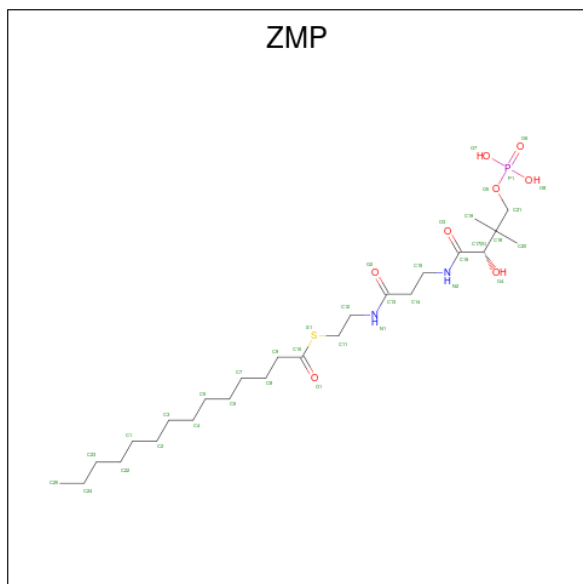
Mol	Chain	Residues	Atoms		AltConf
84	3	1	Total	K	0
			1	1	

- Molecule 85 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



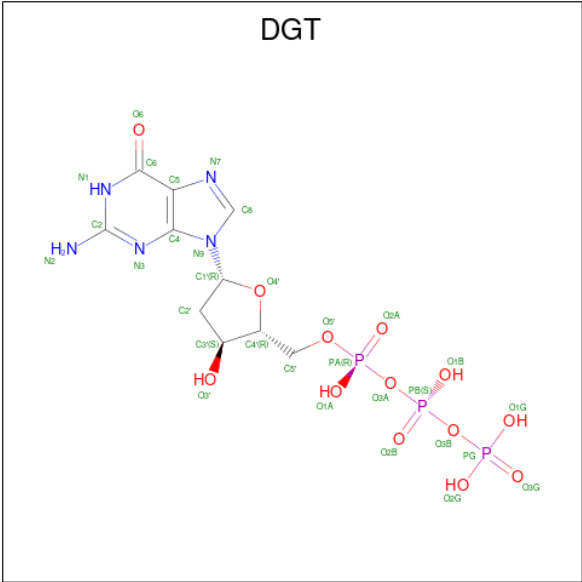
Mol	Chain	Residues	Atoms					AltConf
85	P1	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 86 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
86	W1	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
86	n1	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

- Molecule 87 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).

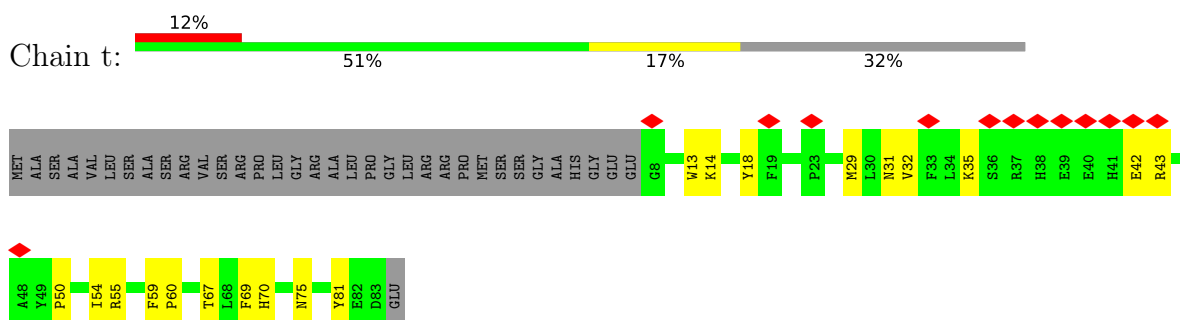


Mol	Chain	Residues	Atoms					AltConf
87	O1	1	Total	C	N	O	P	0
			31	10	5	13	3	

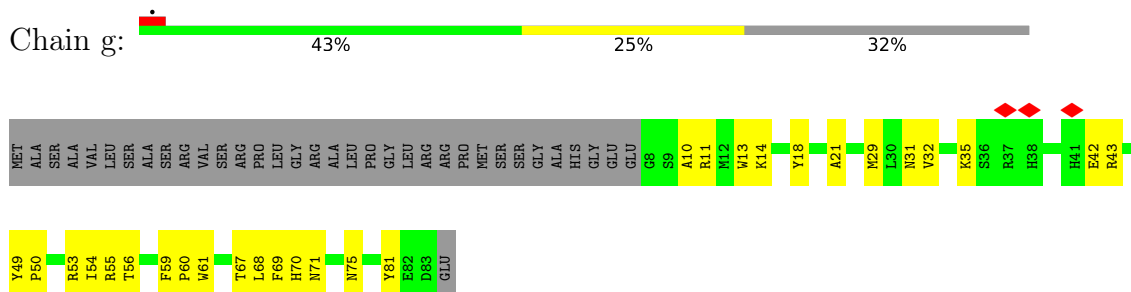
3 Residue-property plots [i](#)

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

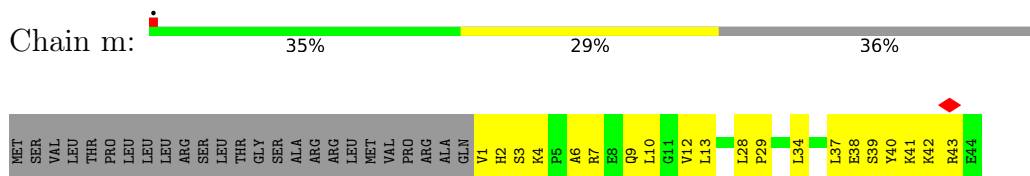
- Molecule 1: Cytochrome c oxidase subunit 6A1, mitochondrial



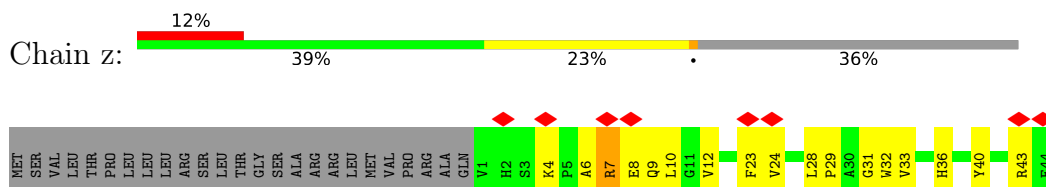
- Molecule 1: Cytochrome c oxidase subunit 6A1, mitochondrial



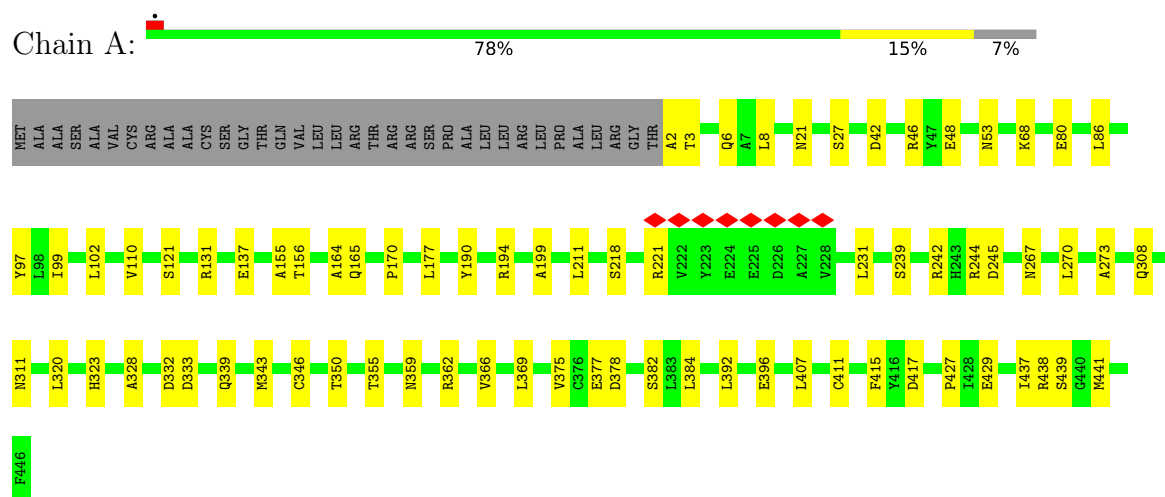
- Molecule 2: Cytochrome c oxidase subunit 8A, mitochondrial



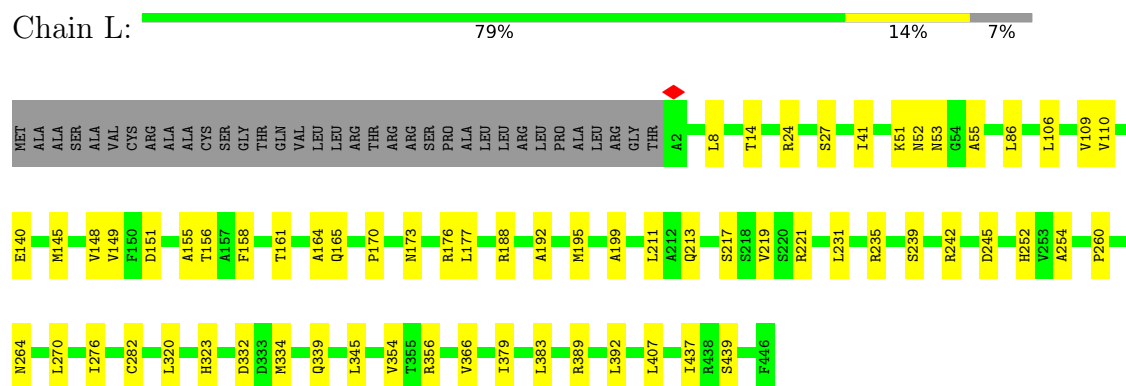
- Molecule 2: Cytochrome c oxidase subunit 8A, mitochondrial



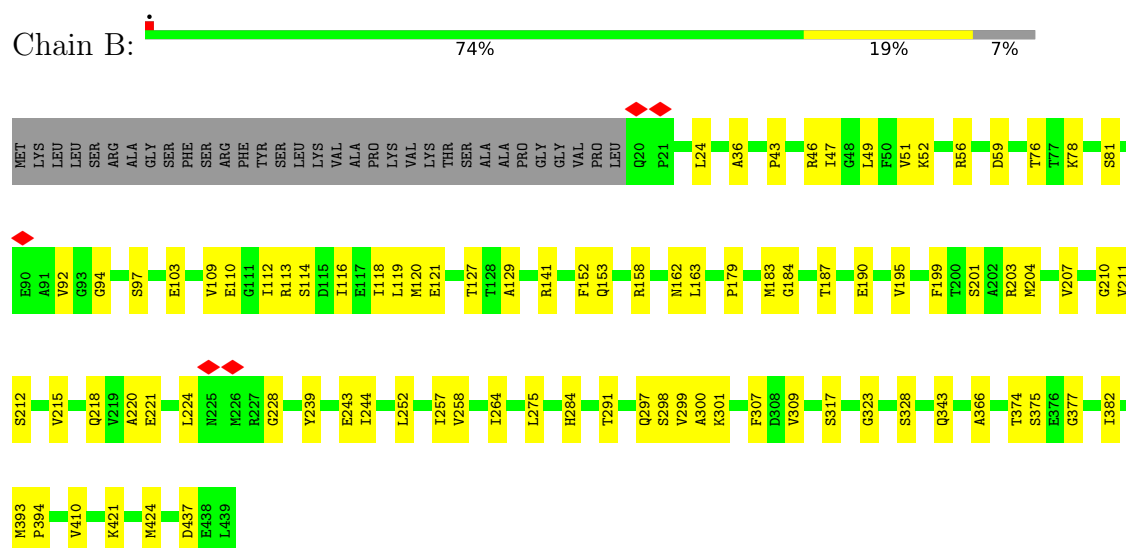
- Molecule 3: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 3: Cytochrome b-c1 complex subunit 1, mitochondrial

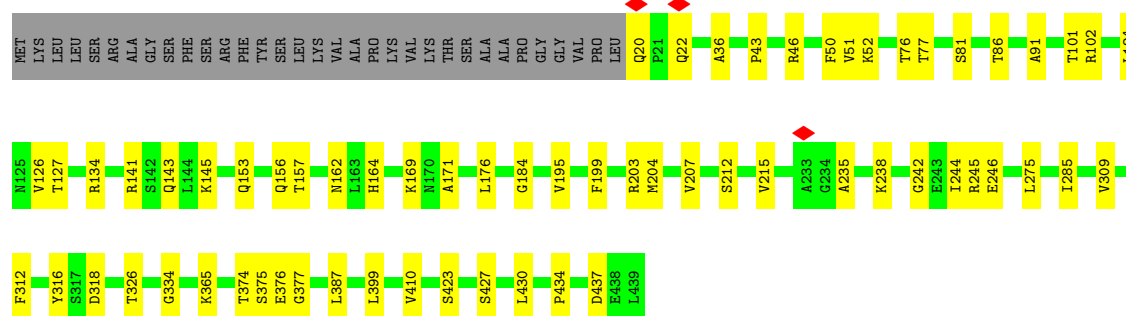


- Molecule 4: Cytochrome b-c1 complex subunit 2, mitochondrial



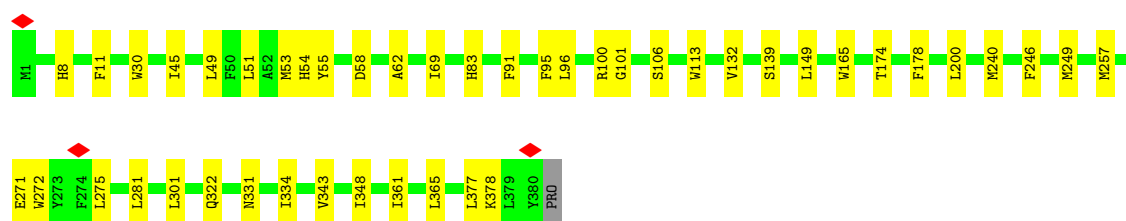
- Molecule 4: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 



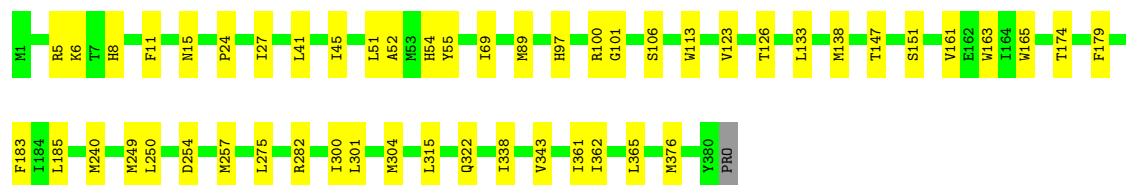
• Molecule 5: Cytochrome b

Chain C: 



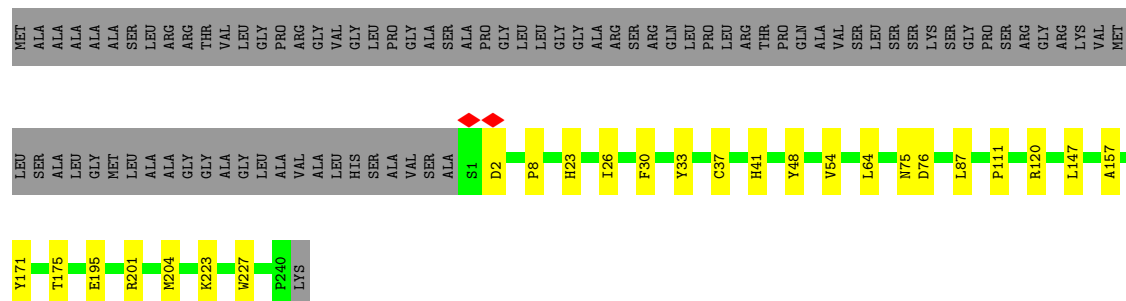
• Molecule 5: Cytochrome b

Chain N: 



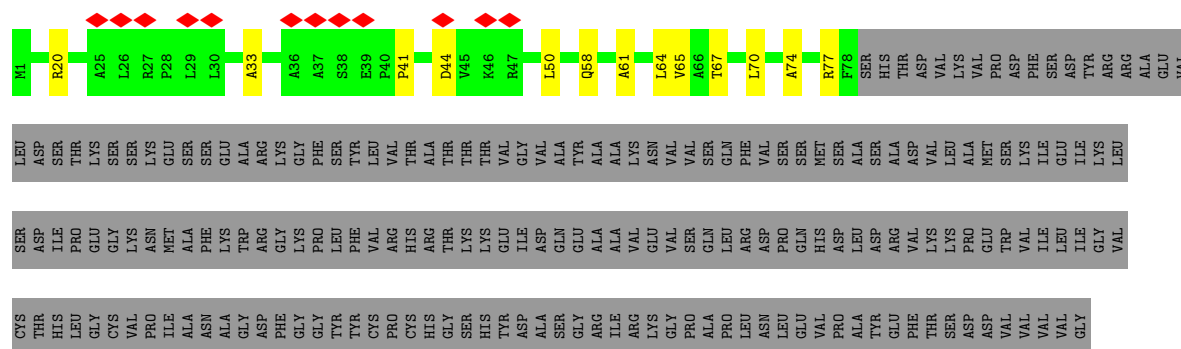
• Molecule 6: Cytochrome c1, heme protein, mitochondrial

Chain D: 

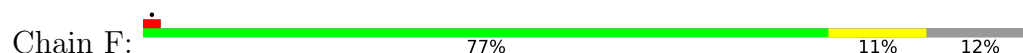


• Molecule 6: Cytochrome c1, heme protein, mitochondrial

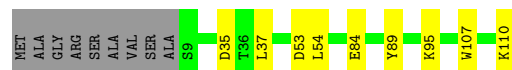
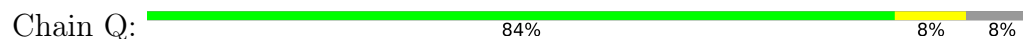
Chain O: 



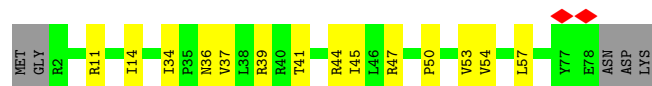
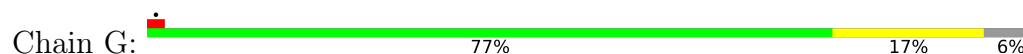
- Molecule 8: Cytochrome b-c1 complex subunit 7



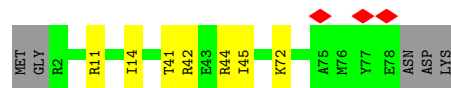
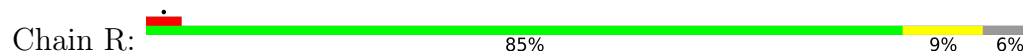
- Molecule 8: Cytochrome b-c1 complex subunit 7



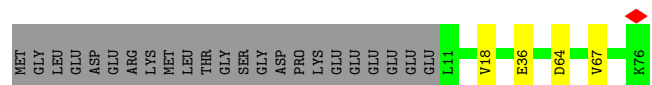
- Molecule 9: Cytochrome b-c1 complex subunit 8



- Molecule 9: Cytochrome b-c1 complex subunit 8

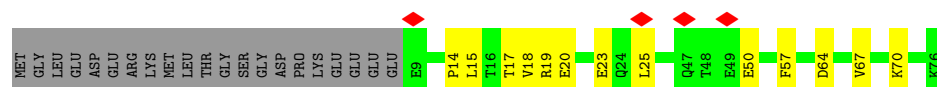


- Molecule 10: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 10: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain S: 



- Molecule 11: Cytochrome b-c1 complex subunit 9

Chain J: 



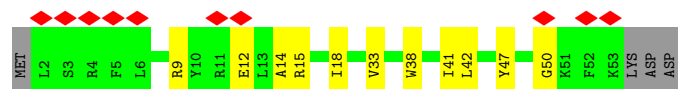
- Molecule 11: Cytochrome b-c1 complex subunit 9

Chain U: 



- Molecule 12: Cytochrome b-c1 complex subunit 10

Chain K: 



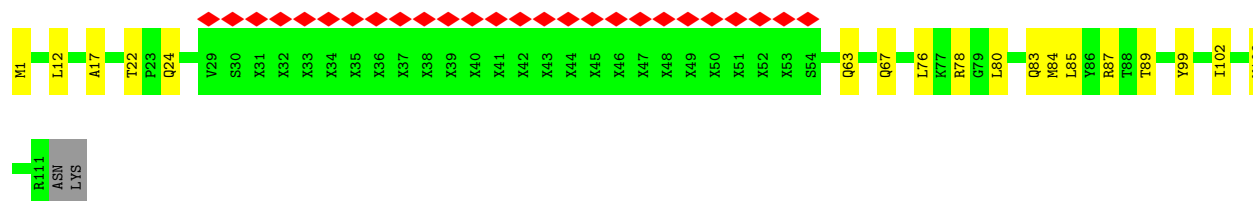
- Molecule 12: Cytochrome b-c1 complex subunit 10

Chain V: 



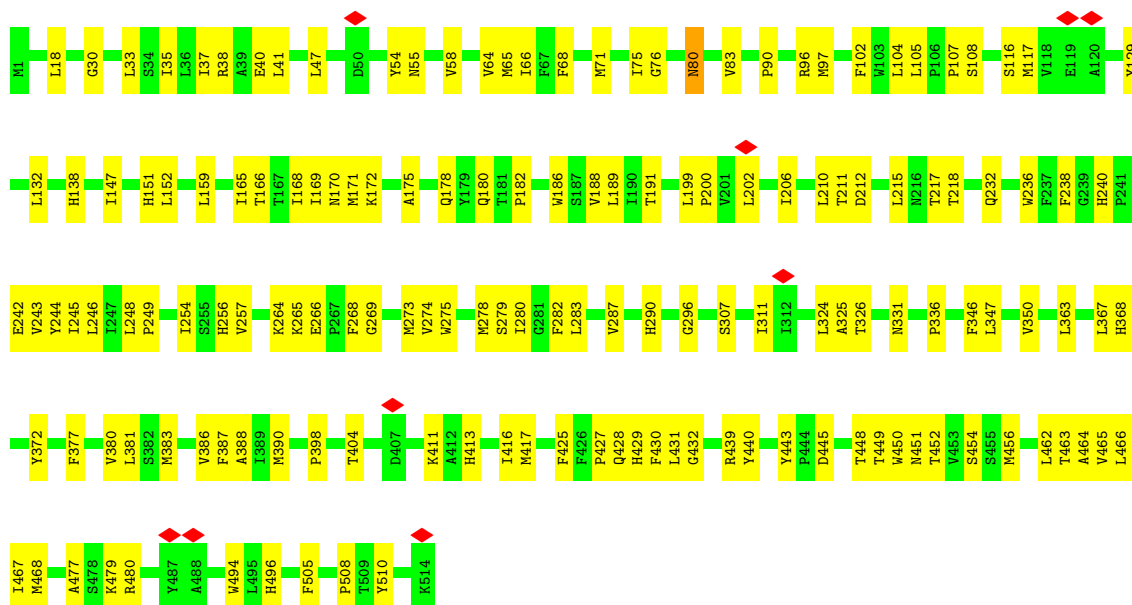
- Molecule 13: Cox7a2l protein

Chain I: 



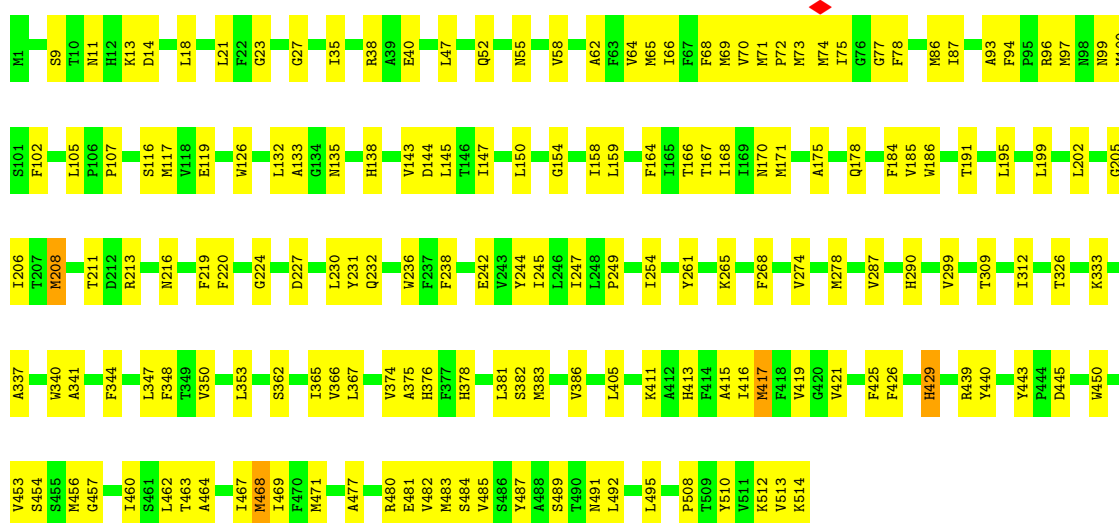
- Molecule 14: Cytochrome c oxidase subunit 1

Chain n: 



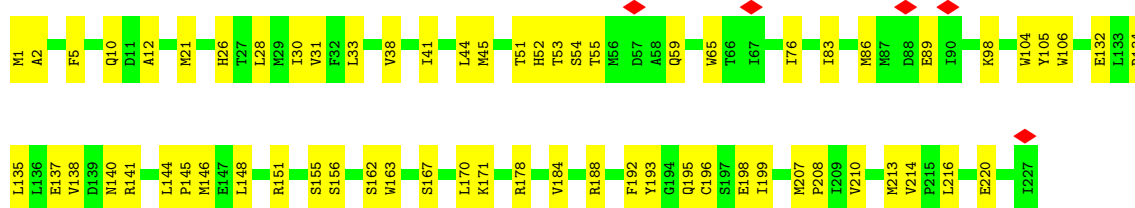
• Molecule 14: Cytochrome c oxidase subunit 1

Chain a: 67% 32%



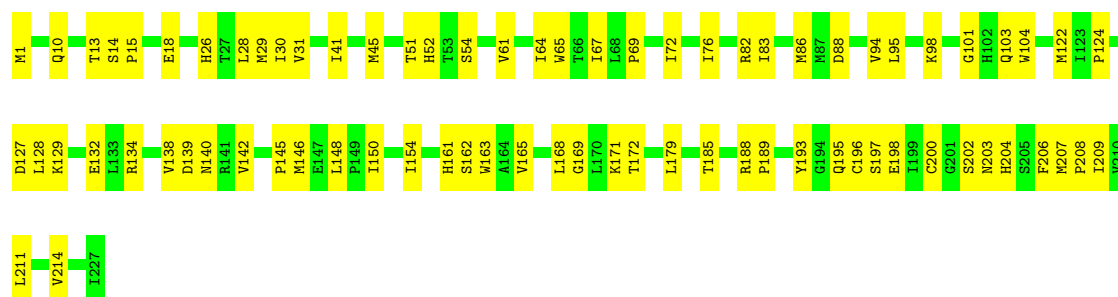
• Molecule 15: Cytochrome c oxidase subunit 2

Chain o: 71% 29%



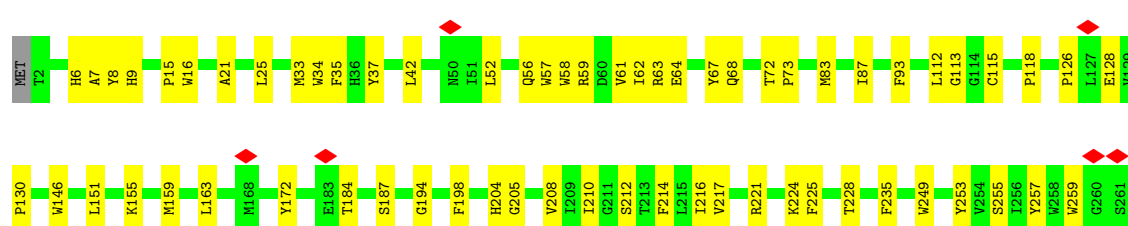
• Molecule 15: Cytochrome c oxidase subunit 2

Chain b:  67% 33%



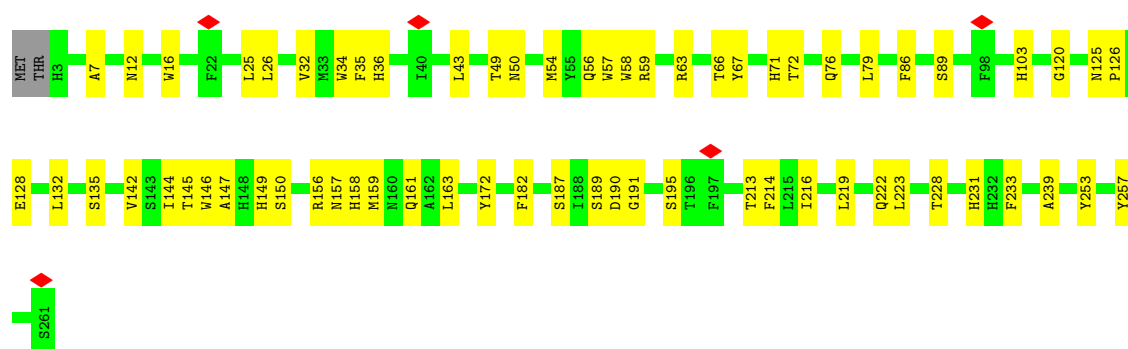
• Molecule 16: Cytochrome c oxidase subunit 3

Chain p:  75% 25%



• Molecule 16: Cytochrome c oxidase subunit 3

Chain c:  74% 25%



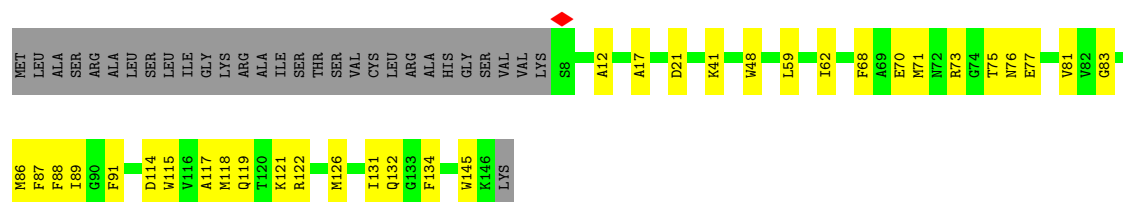
• Molecule 17: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain q:  64% 18% 18%



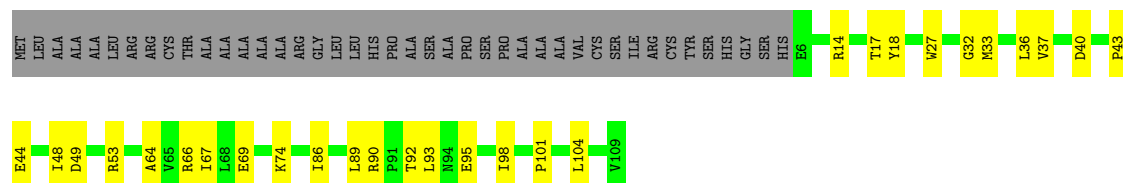
• Molecule 17: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain d:  63% 20% 18%



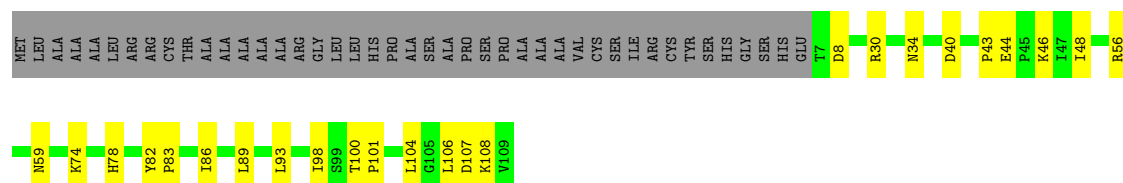
- Molecule 18: Cytochrome c oxidase subunit 5A, mitochondrial

Chain r:  52% 19% 29%



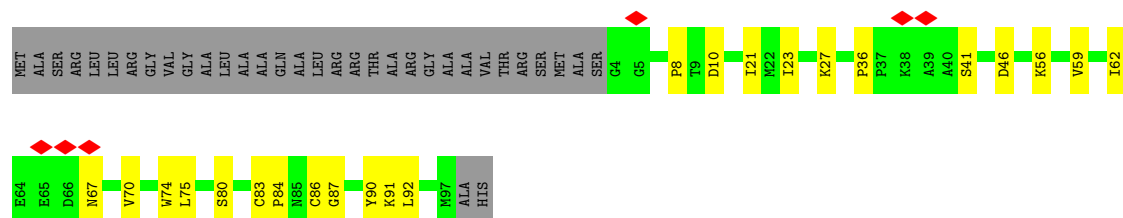
- Molecule 18: Cytochrome c oxidase subunit 5A, mitochondrial

Chain e:  54% 16% 29%

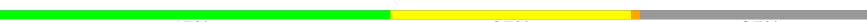


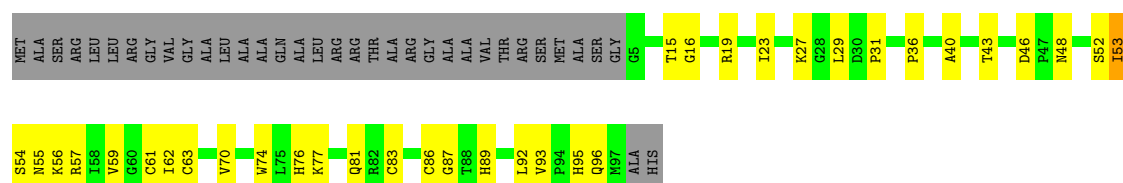
- Molecule 19: Cytochrome c oxidase subunit 5B, mitochondrial

Chain s:  5% 55% 19% 27%



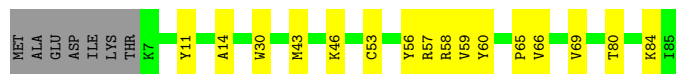
- Molecule 19: Cytochrome c oxidase subunit 5B, mitochondrial

Chain f:  45% 27% 27%



- Molecule 20: Cytochrome c oxidase subunit 6B1

Chain u:  73% 19% 8%



- Molecule 20: Cytochrome c oxidase subunit 6B1

Chain h:  73% 19% 8%



- Molecule 21: Cytochrome c oxidase subunit 6C

Chain v:  5% 71% 22% 7%



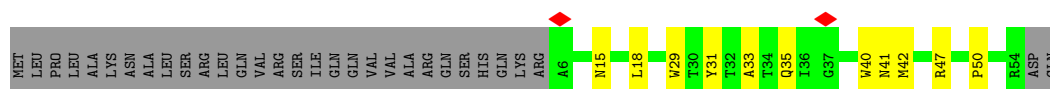
- Molecule 21: Cytochrome c oxidase subunit 6C

Chain i:  68% 24% 5%



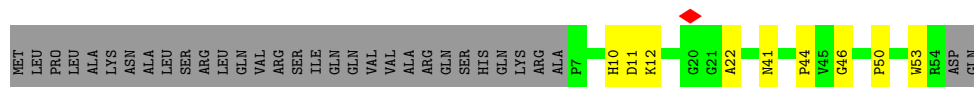
- Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

Chain x:  48% 14% 39%



- Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial

Chain k:  49% 11% 40%

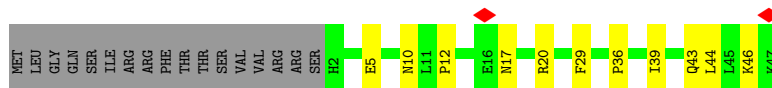


- Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial

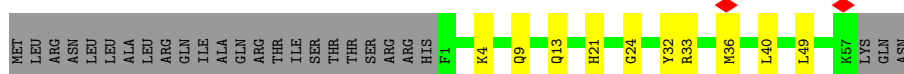
Chain y:  54% 21% 25%



- Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial



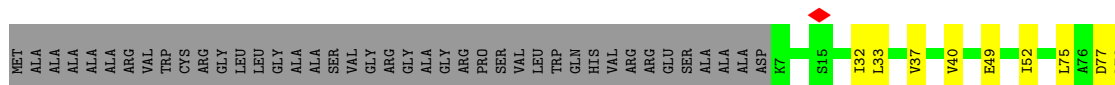
- Molecule 24: Cytochrome c oxidase subunit 7A2, mitochondrial



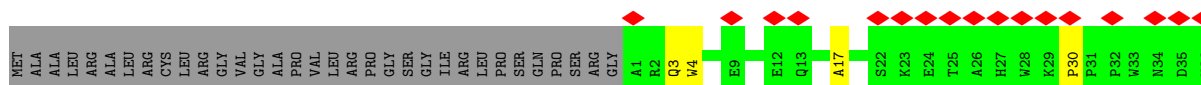
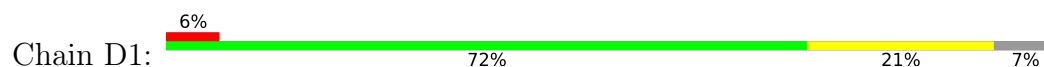
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

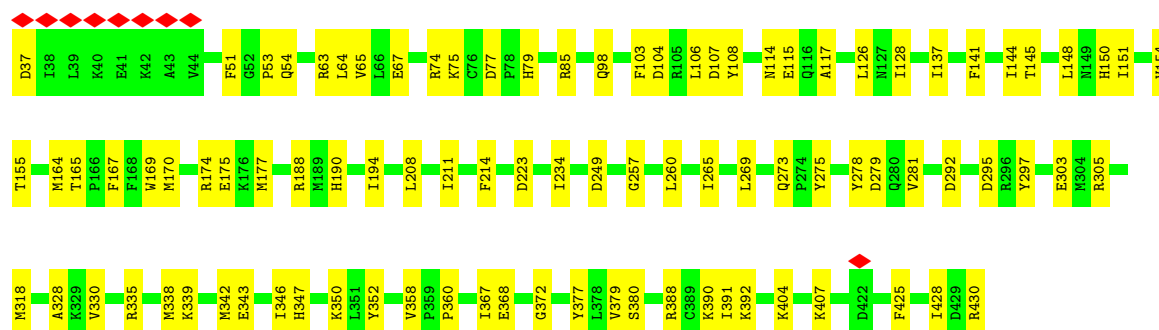


- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



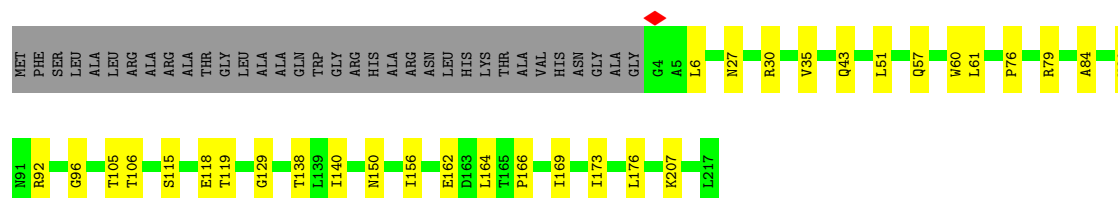
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial





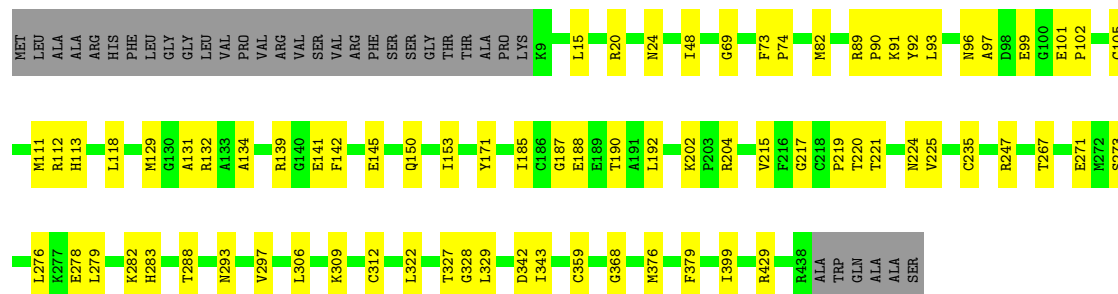
- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2: 73% 13% 14%



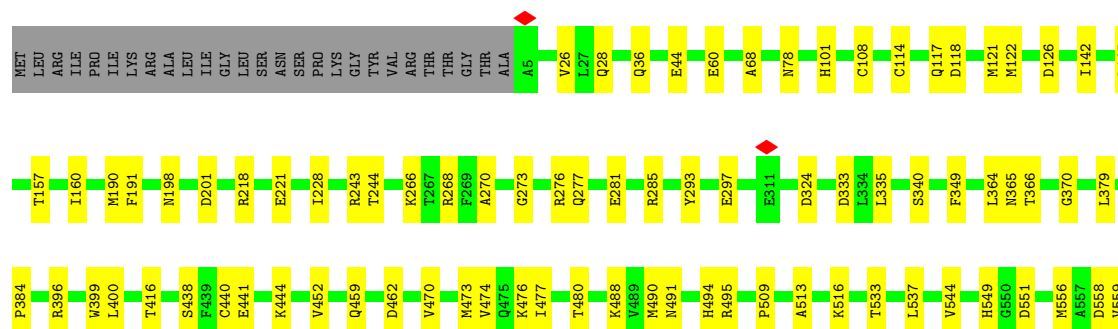
- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 76% 16% 7%



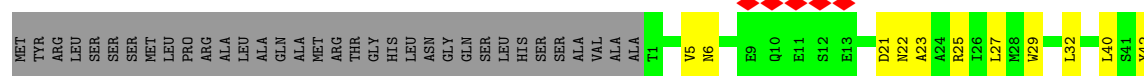
- Molecule 30: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3: 81% 14% 5%

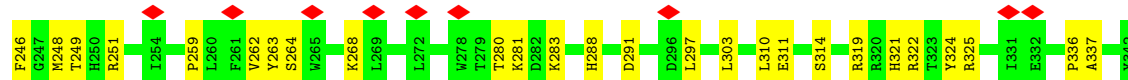
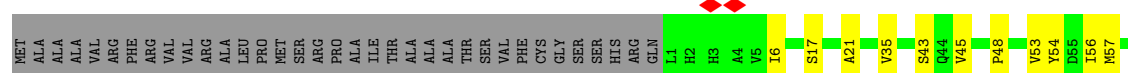




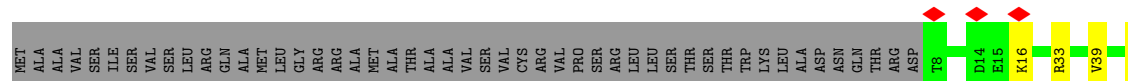
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

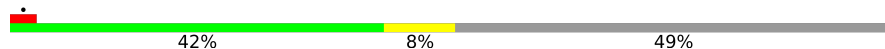


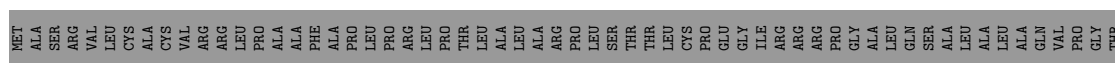
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S1: 

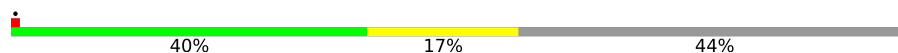


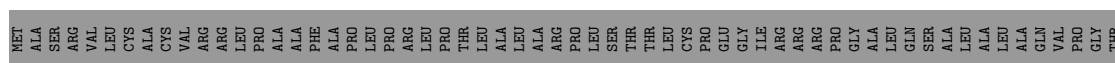
- Molecule 36: Acyl carrier protein, mitochondrial

Chain T1: 

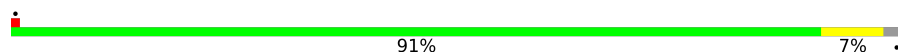


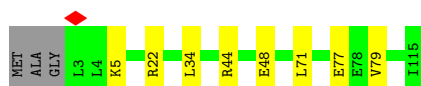
- Molecule 36: Acyl carrier protein, mitochondrial

Chain U1: 



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1: 

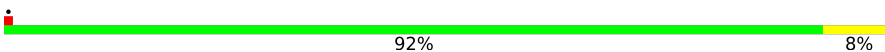


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1: 

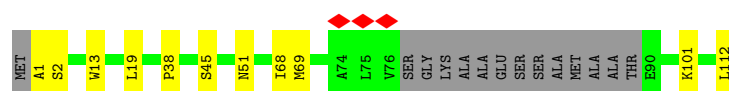
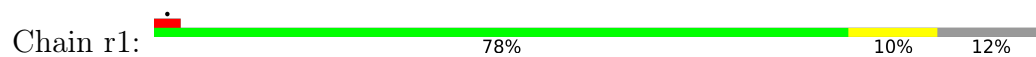


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

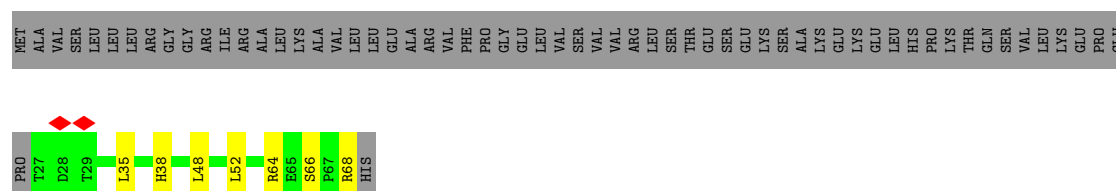
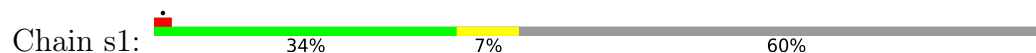
Chain q1: 



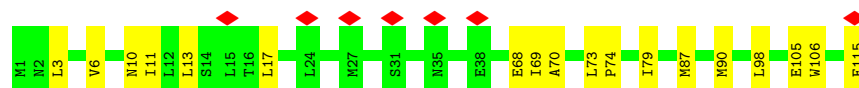
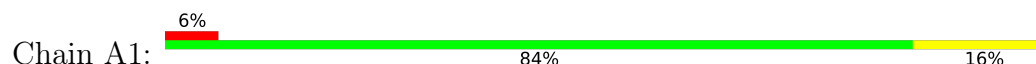
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



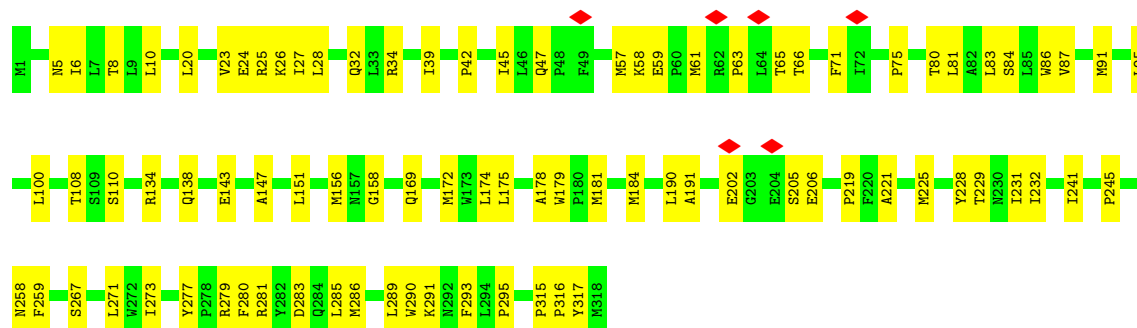
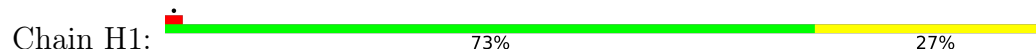
- Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



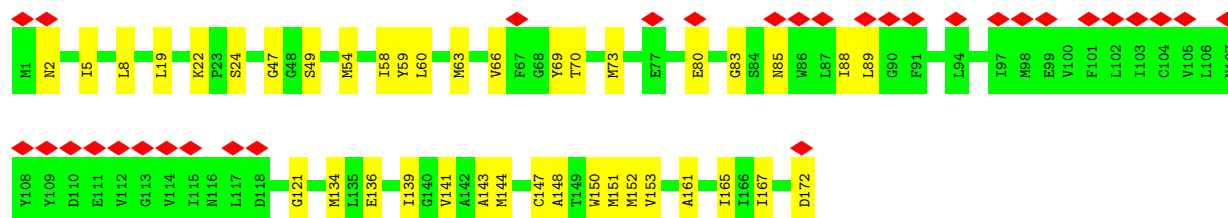
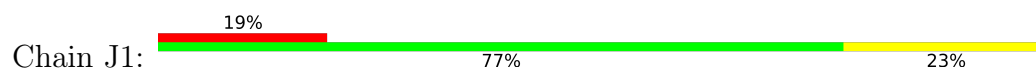
- Molecule 42: NADH-ubiquinone oxidoreductase chain 3



- Molecule 43: NADH-ubiquinone oxidoreductase chain 1

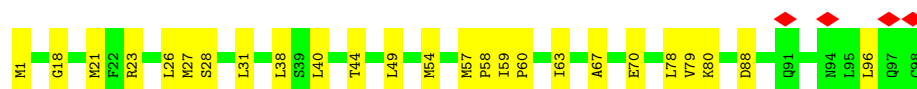


- Molecule 44: NADH-ubiquinone oxidoreductase chain 6



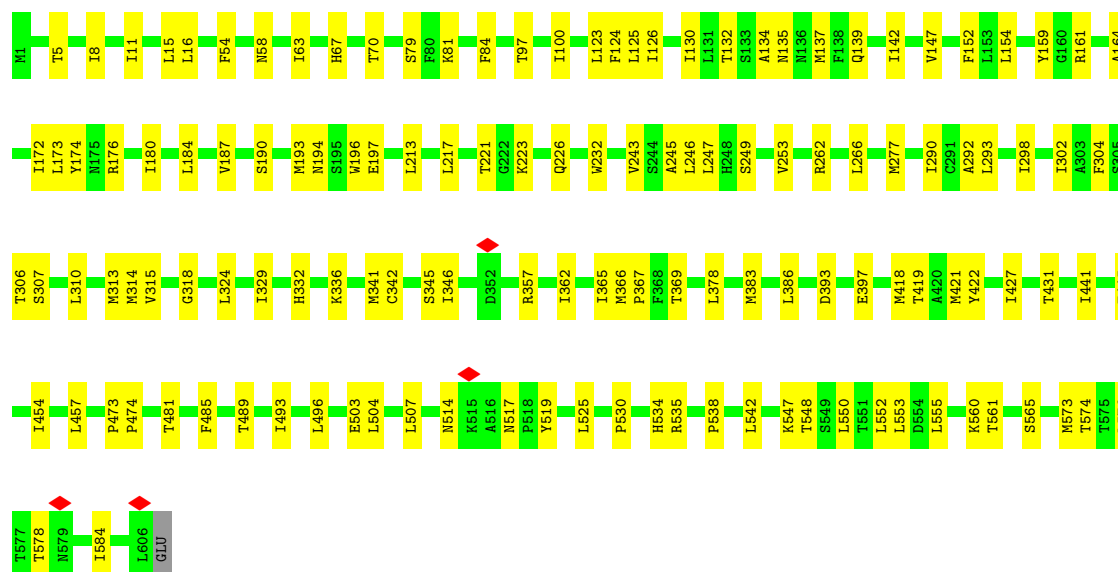
- Molecule 45: NADH-ubiquinone oxidoreductase chain 4L

Chain K1:  74% 26%



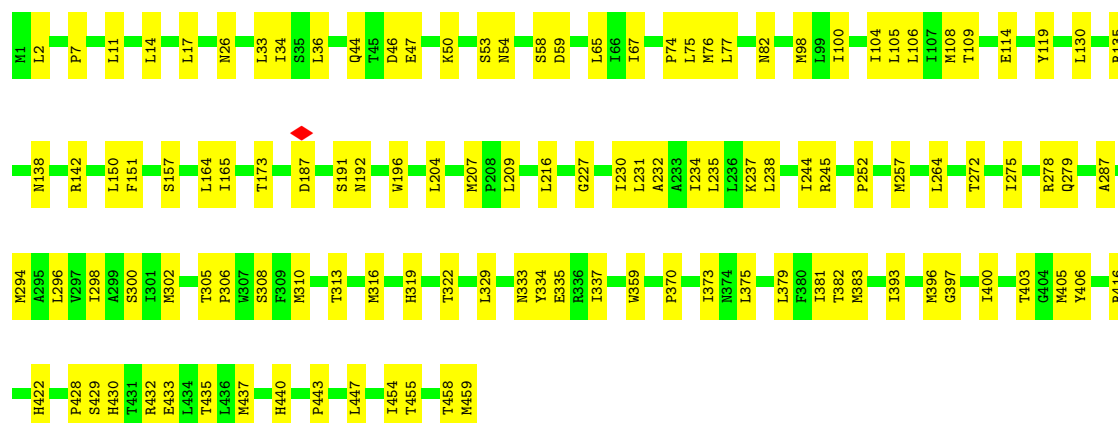
• Molecule 46: NADH-ubiquinone oxidoreductase chain 5

Chain L1:  78% 22%



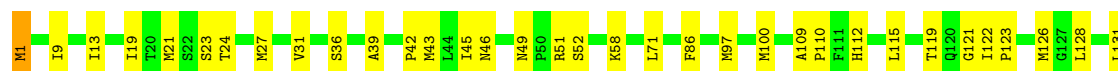
• Molecule 47: NADH-ubiquinone oxidoreductase chain 4

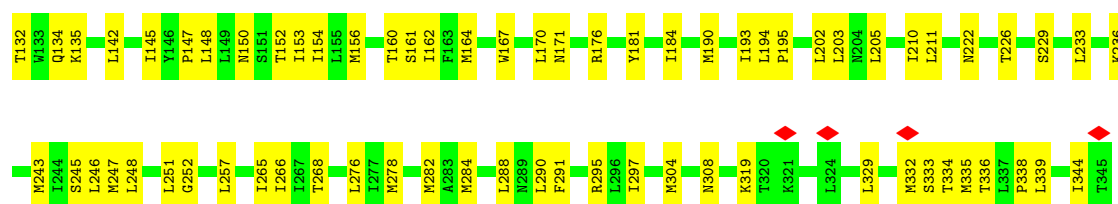
Chain M1:  74% 26%



• Molecule 48: NADH-ubiquinone oxidoreductase chain 2

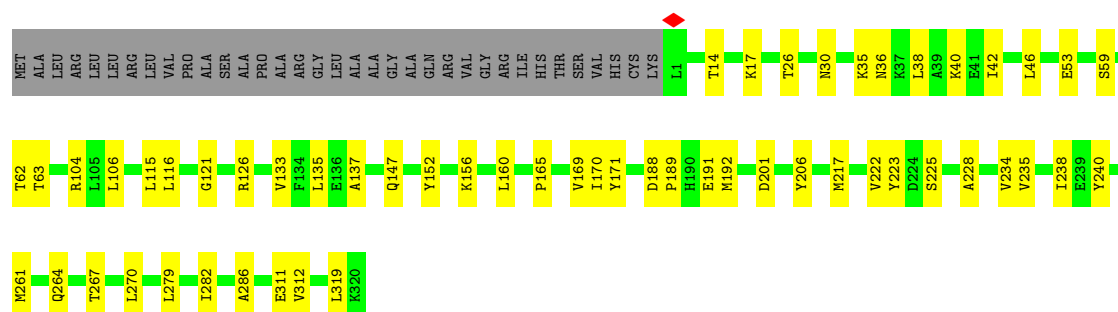
Chain N1:  70% 29%





- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1: 74% 16% 10%



- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1: 83% 17%



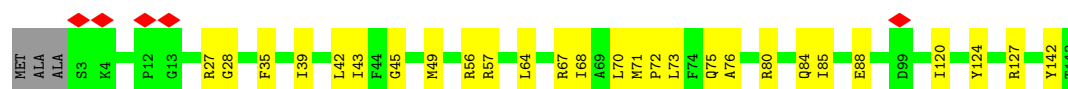
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y1: 86% 13%



- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z1: 79% 19%

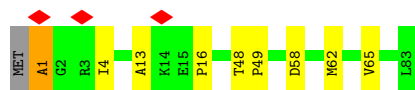
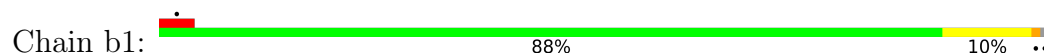


- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

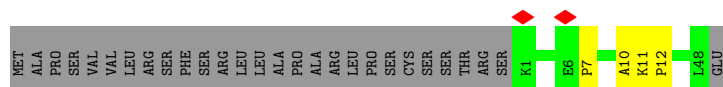
Chain a1: 84% 16%



- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



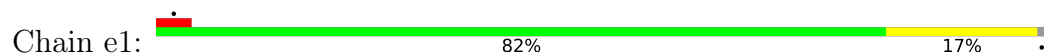
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



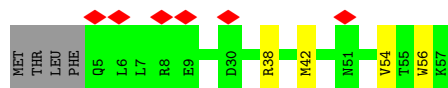
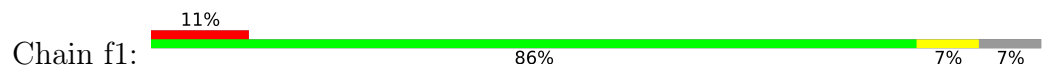
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 subunit C2



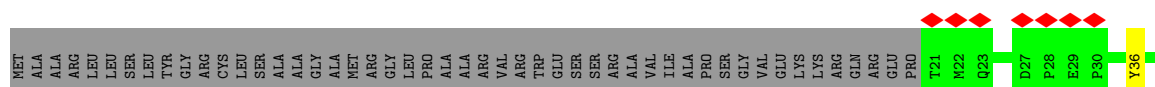
- Molecule 57: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



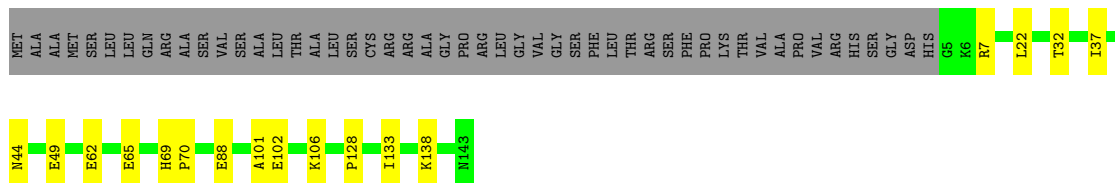
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial





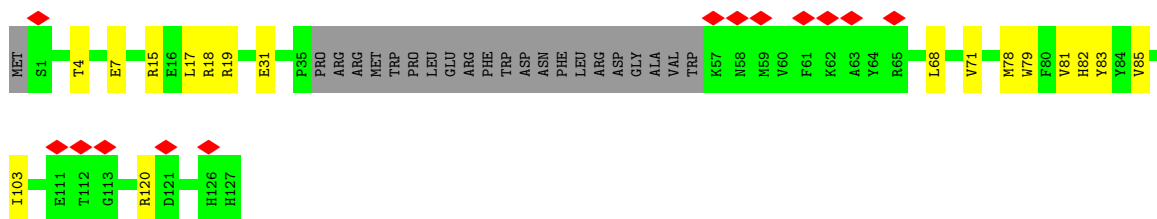
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h1: 65% 9% 26%



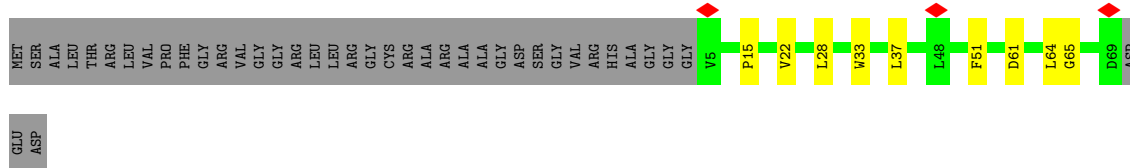
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i1: 10% 70% 13% 17%



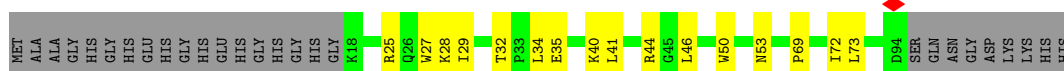
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j1: 53% 9% 38%



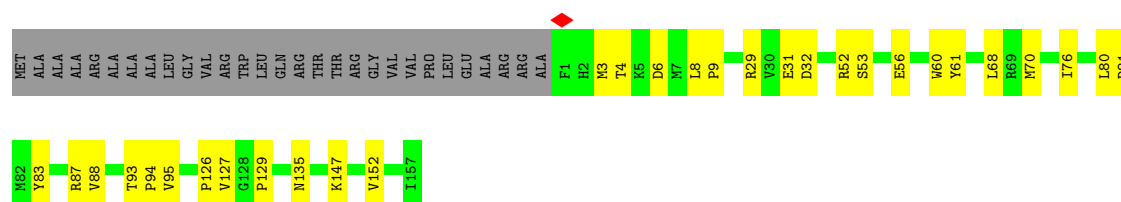
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k1: 59% 15% 26%

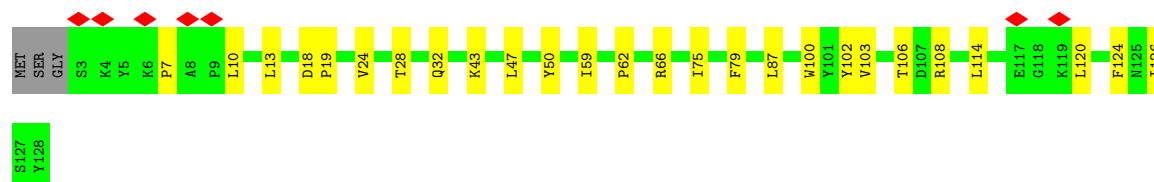
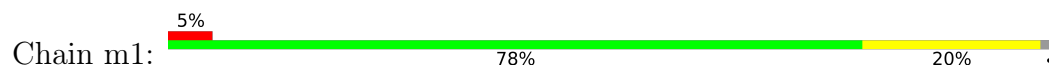


- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

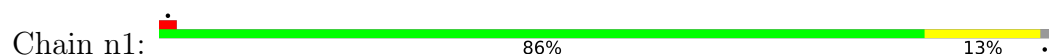
Chain l1: 68% 16% 16%



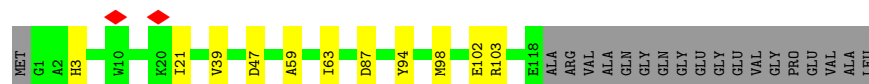
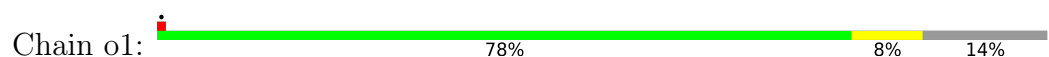
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



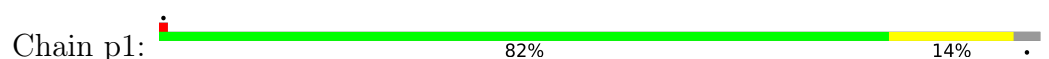
- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 67: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 68: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	299.97998, 218.35999, 262.87997	wwPDB
Map dimensions	283, 206, 248	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, ZMP, FMN, HEA, SF4, ZN, K, CUA, NA, 2MR, NDP, AYA, TGL, DGT, HEM, FME, PC1, SAC, CDL, HEC, MG, FES, 3PE

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	g	0.83	0/646	1.20	1/882 (0.1%)
1	t	0.83	0/646	1.20	1/882 (0.1%)
2	m	0.98	0/350	1.11	0/472
2	z	0.99	0/350	1.11	0/472
3	A	0.17	0/3529	0.43	0/4793
3	L	0.17	0/3530	0.40	1/4793 (0.0%)
4	B	0.16	0/3205	0.36	0/4332
4	M	0.15	0/3205	0.35	0/4332
5	C	0.21	0/3147	0.48	0/4297
5	N	0.21	0/3147	0.47	0/4297
6	D	0.17	0/1968	0.42	0/2674
6	O	0.17	0/1968	0.39	0/2674
7	E	0.14	0/1176	0.36	0/1609
7	P	0.16	0/1173	0.37	0/1605
7	T	0.15	0/565	0.44	0/772
8	F	0.18	0/885	0.46	0/1184
8	Q	0.17	0/922	0.40	0/1234
9	G	0.22	0/673	0.51	0/909
9	R	0.22	0/673	0.50	0/909
10	H	0.25	0/552	0.70	1/739 (0.1%)
10	S	0.25	0/570	0.61	0/763
11	J	0.19	0/509	0.45	0/687
11	U	0.21	0/509	0.49	0/687
12	K	0.19	0/446	0.49	0/609
12	V	0.20	0/454	0.52	0/619
13	I	0.21	0/709	0.60	0/955
14	a	0.27	0/4162	0.66	4/5686 (0.1%)
14	n	0.26	0/4162	0.56	0/5686
15	b	0.25	0/1863	0.67	0/2542
15	o	0.23	0/1863	0.56	1/2542 (0.0%)
16	c	0.21	0/2195	0.54	0/3000

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	p	0.22	0/2202	0.54	0/3010
17	d	0.19	0/1190	0.59	0/1609
17	q	0.23	0/1190	0.57	0/1609
18	e	0.25	0/851	0.64	0/1155
18	r	0.21	0/860	0.55	0/1167
19	f	0.22	0/734	0.61	1/996 (0.1%)
19	s	0.20	0/738	0.52	0/1001
20	h	0.26	0/674	0.81	0/910
20	u	0.23	0/674	0.63	0/910
21	i	0.28	0/584	0.86	3/778 (0.4%)
21	v	0.25	0/579	0.64	0/771
22	k	0.18	0/391	0.43	0/533
22	x	0.22	0/396	0.55	0/541
23	l	0.22	0/393	0.57	0/527
23	y	0.25	0/399	0.55	0/535
24	w	0.17	0/444	0.45	0/598
25	6	0.24	0/1289	0.57	0/1744
26	C1	0.16	0/1780	0.37	0/2424
27	D1	0.22	0/3540	0.45	0/4795
28	2	0.18	0/1700	0.42	0/2316
29	1	0.19	0/3396	0.46	0/4586
30	3	0.18	0/5392	0.40	0/7305
31	9	0.22	0/1461	0.41	0/1974
32	P1	0.18	0/2823	0.45	0/3828
33	Q1	0.16	0/1045	0.34	0/1411
34	7	0.16	0/773	0.35	0/1041
35	S1	0.20	0/682	0.51	0/920
36	T1	0.19	0/646	0.51	0/869
36	U1	0.21	0/718	0.51	0/970
37	V1	0.16	0/945	0.31	0/1281
38	W1	0.19	0/993	0.42	0/1335
39	q1	0.17	0/1251	0.38	0/1702
40	r1	0.17	0/806	0.34	0/1090
41	s1	0.15	0/360	0.50	0/489
42	A1	0.25	0/948	0.53	0/1295
43	H1	0.28	0/2607	0.59	0/3564
44	J1	0.22	0/1330	0.52	0/1810
45	K1	0.25	0/738	0.51	0/1002
46	L1	0.23	0/4913	0.51	0/6686
47	M1	0.24	0/3709	0.52	0/5052
48	N1	0.23	0/2755	0.53	0/3751
49	O1	0.16	0/2674	0.39	0/3626
50	X1	0.17	0/1434	0.44	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
51	Y1	0.17	0/1061	0.43	0/1439
52	Z1	0.17	0/1198	0.37	0/1616
53	a1	0.22	0/585	0.45	0/788
54	b1	0.15	0/666	0.39	0/914
55	c1	0.14	0/409	0.37	0/555
56	d1	0.17	0/1028	0.42	0/1387
57	e1	0.18	0/900	0.41	0/1199
58	f1	0.17	0/468	0.45	0/630
59	g1	0.15	0/878	0.41	0/1196
60	h1	0.18	0/1201	0.45	0/1626
61	i1	0.15	0/917	0.35	0/1243
62	j1	0.19	0/587	0.49	0/804
63	k1	0.19	0/646	0.47	0/873
64	l1	0.16	0/1379	0.43	0/1882
65	m1	0.22	0/1079	0.52	0/1463
66	n1	0.18	0/1596	0.38	0/2162
67	o1	0.18	0/1039	0.44	0/1394
68	p1	0.16	0/1471	0.36	0/1988
All	All	0.23	0/129867	0.50	13/176249 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	m	0	2
2	z	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	468	MET	CG-SD-CE	6.78	115.81	100.90
21	i	64	GLU	CA-C-N	-6.31	112.56	122.65
21	i	64	GLU	C-N-CA	-6.31	112.56	122.65
14	a	417	MET	CB-CG-SD	-6.22	94.05	112.70
19	f	53	ILE	N-CA-C	-5.62	108.37	113.71
14	a	429	HIS	N-CA-C	-5.57	105.11	111.07
1	g	70	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	t	70	HIS	CB-CG-CD2	-5.53	124.01	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	36	GLU	N-CA-CB	5.35	119.27	110.39
3	L	219	VAL	N-CA-C	-5.20	108.43	113.53
21	i	63	GLU	N-CA-CB	5.14	117.77	110.16
15	o	220	GLU	N-CA-CB	5.09	118.83	110.39
14	a	208	MET	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	m	43	ARG	Sidechain
2	m	7	ARG	Sidechain
2	z	7	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	g	620	0	597	121	0
1	t	620	0	597	27	0
2	m	343	0	356	26	0
2	z	343	0	356	42	0
3	A	3459	0	3367	47	0
3	L	3460	0	3367	43	0
4	B	3154	0	3158	54	0
4	M	3154	0	3158	41	0
5	C	3046	0	3112	41	0
5	N	3046	0	3112	40	0
6	D	1909	0	1854	16	0
6	O	1909	0	1854	18	0
7	E	1167	0	842	14	0
7	P	1164	0	833	13	0
7	T	554	0	590	12	0
8	F	865	0	854	11	0
8	Q	900	0	887	6	0
9	G	654	0	656	12	0
9	R	654	0	656	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	545	0	531	2	0
10	S	563	0	541	14	0
11	J	495	0	489	8	0
11	U	495	0	489	7	0
12	K	430	0	431	9	0
12	V	438	0	443	11	0
13	I	807	0	736	21	0
14	a	4021	0	3997	149	0
14	n	4021	0	3997	131	0
15	b	1817	0	1822	58	0
15	o	1817	0	1822	50	0
16	c	2111	0	2047	104	0
16	p	2118	0	2054	61	0
17	d	1156	0	1112	27	0
17	q	1156	0	1112	23	0
18	e	833	0	832	19	0
18	r	842	0	838	19	0
19	f	717	0	695	24	0
19	s	721	0	698	19	0
20	h	654	0	622	27	0
20	u	654	0	622	11	0
21	i	572	0	596	15	0
21	v	567	0	591	13	0
22	k	378	0	363	11	0
22	x	383	0	367	9	0
23	l	380	0	378	10	0
23	y	386	0	386	14	0
24	w	435	0	446	11	0
25	6	1258	0	1268	28	0
26	C1	1730	0	1686	22	0
27	D1	3464	0	3416	69	0
28	2	1660	0	1653	18	0
29	1	3321	0	3278	55	0
30	3	5305	0	5330	70	0
31	9	1431	0	1383	31	0
32	P1	2748	0	2768	43	0
33	Q1	1022	0	1023	13	0
34	7	758	0	731	7	0
35	S1	671	0	688	11	0
36	T1	637	0	640	10	0
36	U1	706	0	699	20	0
37	V1	923	0	965	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	W1	970	0	991	6	0
39	q1	1209	0	1170	9	0
40	r1	796	0	831	9	0
41	s1	351	0	331	5	0
42	A1	932	0	967	19	0
43	H1	2540	0	2626	69	0
44	J1	1308	0	1319	36	0
45	K1	737	0	768	24	0
46	L1	4800	0	4985	105	0
47	M1	3632	0	3853	87	0
48	N1	2703	0	2902	77	0
49	O1	2607	0	2566	35	0
50	X1	1396	0	1385	22	0
51	Y1	1037	0	1025	13	0
52	Z1	1167	0	1166	24	0
53	a1	572	0	583	7	0
54	b1	651	0	653	8	0
55	c1	398	0	401	2	0
56	d1	996	0	1001	13	0
57	e1	877	0	871	15	0
58	f1	456	0	452	3	0
59	g1	850	0	783	20	0
60	h1	1166	0	1166	14	0
61	i1	897	0	902	15	0
62	j1	562	0	515	8	0
63	k1	626	0	620	11	0
64	l1	1323	0	1216	23	0
65	m1	1050	0	1061	21	0
66	n1	1541	0	1473	20	0
67	o1	1014	0	1002	10	0
68	p1	1438	0	1404	26	0
69	6	32	0	38	1	0
69	A	23	0	20	2	0
69	C	66	0	80	3	0
69	E	66	0	80	2	0
69	G	51	0	82	1	0
69	H1	51	0	82	2	0
69	K1	41	0	59	0	0
69	L	23	0	20	1	0
69	L1	102	0	164	6	0
69	M1	102	0	164	6	0
69	N	37	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	N1	38	0	50	1	0
69	O	33	0	40	1	0
69	R	30	0	34	2	0
69	Y1	70	0	88	2	0
69	a	55	0	58	3	0
69	b	29	0	32	1	0
69	b1	43	0	60	1	0
69	c	45	0	67	5	0
69	d	34	0	42	2	0
69	d1	63	0	74	1	0
69	g	25	0	24	11	0
69	i	28	0	30	0	0
69	i1	42	0	61	1	0
69	m1	36	0	46	0	0
69	n	89	0	100	3	0
69	o	29	0	32	2	0
69	p	45	0	67	6	0
69	r1	46	0	66	1	0
69	t	25	0	24	11	0
69	v	28	0	30	1	0
69	z	26	0	26	2	0
70	6	43	0	63	2	0
70	9	101	0	159	4	0
70	I	50	0	77	0	0
70	J	35	0	44	0	0
70	K	28	0	30	1	0
70	L	24	0	22	0	0
70	M1	54	0	88	4	0
70	P1	31	0	36	1	0
70	V	28	0	30	0	0
70	g	50	0	77	3	0
70	p	35	0	44	1	0
70	z	28	0	30	20	0
71	A	46	0	36	0	0
71	D	56	0	56	1	0
71	G	42	0	28	1	0
71	H1	51	0	52	1	0
71	L	46	0	36	1	0
71	L1	124	0	136	5	0
71	N1	90	0	133	5	0
71	O	57	0	58	0	0
71	R	170	0	175	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	V	46	0	36	2	0
71	Y1	94	0	141	2	0
71	d1	67	0	81	1	0
71	g	38	0	22	7	0
71	h1	70	0	87	4	0
71	r1	57	0	58	3	0
72	C	86	0	60	6	0
72	N	86	0	60	4	0
73	D	43	0	29	1	0
73	O	43	0	30	0	0
74	2	4	0	0	0	0
74	3	4	0	0	0	0
74	E	4	0	0	0	0
74	P	4	0	0	2	0
75	a	1	0	0	0	0
75	n	1	0	0	0	0
76	a	1	0	0	0	0
76	n	1	0	0	0	0
77	a	120	0	108	8	0
77	n	120	0	108	9	0
78	O1	1	0	0	0	0
78	a	1	0	0	0	0
78	o	1	0	0	0	0
79	b	2	0	0	0	0
79	o	2	0	0	0	0
80	7	1	0	0	0	0
80	f	1	0	0	0	0
80	s	1	0	0	0	0
81	l	37	0	49	1	0
81	y	37	0	49	1	0
82	1	8	0	0	0	0
82	3	16	0	0	0	0
82	6	8	0	0	0	0
82	9	16	0	0	1	0
83	1	31	0	19	2	0
84	3	1	0	0	0	0
85	P1	48	0	26	1	0
86	W1	34	0	40	0	0
86	n1	32	0	36	2	0
87	O1	31	0	12	1	0
All	All	130610	0	130128	2135	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 8.

All (2135) 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)
14:n:240:HIS:NE2	14:n:244:TYR:CE2	1.69	1.60
1:g:50:PRO:CG	20:h:75:ARG:CZ	1.80	1.59
1:g:50:PRO:HG2	20:h:75:ARG:NH1	1.13	1.42
5:C:91:PHE:HB3	5:C:272:TRP:CH2	1.54	1.41
1:g:11:ARG:HH21	71:g:301:CDL:CA6	1.28	1.41
2:z:32:TRP:CH2	70:z:101:PC1:O22	1.73	1.39
1:g:50:PRO:CG	20:h:75:ARG:NH1	1.76	1.34
14:n:240:HIS:NE2	14:n:244:TYR:HE2	0.99	1.31
14:n:240:HIS:CD2	14:n:244:TYR:CE2	2.18	1.31
1:g:11:ARG:NH2	71:g:301:CDL:HA62	1.46	1.29
1:g:50:PRO:HD2	20:h:75:ARG:NH2	1.49	1.25
1:g:50:PRO:HG2	20:h:75:ARG:CZ	1.50	1.25
14:n:240:HIS:CD2	14:n:244:TYR:HE2	1.51	1.24
2:z:32:TRP:CZ3	70:z:101:PC1:O22	1.90	1.23
14:a:216:ASN:ND2	1:g:55:ARG:HA	1.56	1.20
2:z:32:TRP:CZ2	70:z:101:PC1:O22	1.98	1.17
1:g:50:PRO:CD	20:h:75:ARG:NH2	2.09	1.15
1:g:50:PRO:HG3	20:h:75:ARG:CZ	1.56	1.13
29:1:99:GLU:OE1	29:1:105:CYS:HA	1.49	1.12
5:C:91:PHE:CB	5:C:272:TRP:CH2	2.33	1.10
16:c:172:TYR:CE2	1:g:29:MET:HE3	1.85	1.10
1:g:11:ARG:NH2	71:g:301:CDL:CA6	2.05	1.08
1:g:50:PRO:CG	20:h:75:ARG:NH2	2.14	1.08
14:a:426:PHE:HA	14:a:429:HIS:HD2	1.16	1.08
14:a:216:ASN:HD21	1:g:55:ARG:HA	1.04	1.07
2:z:43:ARG:HG2	23:y:47:LYS:O	1.52	1.06
12:V:7:GLY:O	12:V:11:ARG:HG3	1.56	1.06
14:a:426:PHE:HA	14:a:429:HIS:CD2	1.91	1.05
16:c:128:GLU:HB2	1:g:32:VAL:HG22	1.36	1.04
1:g:68:LEU:HD22	69:g:303:3PE:C32	1.88	1.03
2:z:32:TRP:CZ2	70:z:101:PC1:C21	2.42	1.02
1:g:68:LEU:CD2	69:g:303:3PE:H322	1.88	1.02
7:E:161:HIS:HD2	5:N:343:VAL:HG21	1.20	1.01
16:c:35:PHE:CE1	1:g:60:PRO:HG3	1.96	1.01
16:c:34:TRP:NE1	1:g:60:PRO:O	1.93	1.00
16:c:172:TYR:HE2	1:g:29:MET:HE3	1.26	1.00
16:c:35:PHE:CD1	1:g:60:PRO:HG3	1.98	0.97
7:E:161:HIS:CD2	5:N:343:VAL:HG21	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:68:LEU:HD22	69:g:303:3PE:H322	0.97	0.97
2:z:32:TRP:CH2	70:z:101:PC1:H2	2.00	0.96
14:n:383:MET:O	14:n:387:PHE:HB2	1.67	0.94
14:a:216:ASN:HD21	1:g:55:ARG:CA	1.80	0.94
16:c:158:HIS:NE2	1:g:14:LYS:NZ	2.15	0.93
21:v:52:PHE:O	21:v:56:TYR:HB2	1.68	0.92
16:c:172:TYR:HE2	1:g:29:MET:CE	1.84	0.91
2:m:12:VAL:HG13	69:a:606:3PE:H322	1.52	0.91
13:I:84:MET:SD	13:I:87:ARG:NH2	2.43	0.91
16:c:146:TRP:HB2	1:g:13:TRP:HB3	1.51	0.89
2:m:6:ALA:HA	14:a:480:ARG:HB3	1.54	0.89
19:f:61:CYS:SG	19:f:63:CYS:HB3	2.11	0.89
7:E:161:HIS:HD2	5:N:343:VAL:CG2	1.85	0.89
16:c:132:LEU:HD11	1:g:29:MET:HG2	1.54	0.88
1:g:50:PRO:HG2	20:h:75:ARG:NH2	1.84	0.88
2:z:32:TRP:HZ2	70:z:101:PC1:H11	1.39	0.88
2:z:32:TRP:CE3	70:z:101:PC1:O22	2.26	0.88
5:C:91:PHE:CB	5:C:272:TRP:HH2	1.80	0.88
15:b:41:ILE:O	15:b:45:MET:HB2	1.74	0.87
29:1:99:GLU:OE1	29:1:105:CYS:CA	2.21	0.86
16:c:146:TRP:NE1	1:g:14:LYS:HB2	1.91	0.85
2:z:32:TRP:CE2	70:z:101:PC1:O22	2.28	0.85
14:n:240:HIS:NE2	14:n:244:TYR:CZ	2.43	0.85
2:z:32:TRP:CE2	70:z:101:PC1:C21	2.60	0.85
14:n:240:HIS:CD2	14:n:244:TYR:CD2	2.64	0.85
16:c:34:TRP:CH2	1:g:61:TRP:HE3	1.94	0.85
13:I:84:MET:CE	13:I:87:ARG:HH21	1.89	0.85
13:I:84:MET:HE1	13:I:87:ARG:NH2	1.91	0.84
15:o:145:PRO:HA	15:o:214:VAL:O	1.78	0.84
16:c:157:ASN:O	16:c:161:GLN:HG3	1.76	0.84
46:L1:245:ALA:O	46:L1:249:SER:HB2	1.78	0.84
14:a:381:LEU:HD23	77:a:604:HEA:HAC	1.59	0.84
1:g:11:ARG:HH21	71:g:301:CDL:HA62	0.66	0.83
32:P1:310:LEU:O	32:P1:314:SER:HB3	1.78	0.83
2:z:33:VAL:HG21	23:y:37:PHE:HB3	1.58	0.83
14:n:377:PHE:O	14:n:381:LEU:HB3	1.78	0.83
16:c:172:TYR:CE2	1:g:29:MET:CE	2.60	0.82
15:b:61:VAL:O	15:b:65:TRP:HB2	1.78	0.82
5:C:91:PHE:HB3	5:C:272:TRP:HH2	1.07	0.81
60:h1:49:GLU:H	60:h1:70:PRO:HD3	1.44	0.81
2:z:32:TRP:CZ2	70:z:101:PC1:C2	2.64	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:84:MET:CE	13:I:87:ARG:NH2	2.44	0.80
1:t:75:ASN:HD21	69:t:101:3PE:HN1	1.29	0.80
8:F:13:LEU:N	16:c:161:GLN:OE1	2.15	0.80
21:i:52:PHE:O	21:i:56:TYR:HB2	1.81	0.80
71:V:101:CDL:HB61	71:V:101:CDL:H312	1.62	0.80
9:G:41:THR:O	9:G:45:ILE:HB	1.82	0.80
1:g:50:PRO:HG2	20:h:75:ARG:HH12	0.99	0.79
2:z:32:TRP:HZ2	70:z:101:PC1:C1	1.95	0.79
30:3:570:SER:HA	30:3:583:THR:O	1.81	0.79
1:g:69:PHE:O	69:g:303:3PE:N	2.16	0.79
44:J1:144:MET:HB2	45:K1:58:PRO:HG3	1.64	0.78
14:a:426:PHE:CA	14:a:429:HIS:HD2	1.97	0.78
43:H1:86:TRP:HE1	43:H1:229:THR:HG22	1.48	0.77
16:c:187:SER:HB2	1:g:67:THR:HG21	1.65	0.77
15:b:154:ILE:O	15:b:179:LEU:HA	1.85	0.77
2:m:2:HIS:CD2	14:a:484:SER:OG	2.38	0.76
1:g:11:ARG:NH2	71:g:301:CDL:HA61	1.97	0.76
16:c:172:TYR:CZ	1:g:29:MET:HE3	2.21	0.76
1:g:50:PRO:CD	20:h:75:ARG:CZ	2.56	0.76
5:C:91:PHE:CB	5:C:272:TRP:CZ2	2.68	0.76
14:a:191:THR:HG21	14:a:249:PRO:HD3	1.66	0.76
1:g:50:PRO:HG3	20:h:75:ARG:NE	2.00	0.76
16:c:34:TRP:CH2	1:g:61:TRP:CE3	2.74	0.76
5:C:91:PHE:HB2	5:C:272:TRP:CZ2	2.21	0.76
29:1:150:GLN:HB3	41:s1:48:LEU:HD22	1.68	0.75
2:m:40:TYR:HB3	23:l:44:LEU:HD13	1.69	0.75
1:t:69:PHE:O	69:t:101:3PE:H122	1.87	0.74
16:c:190:ASP:OD1	1:g:53:ARG:HG3	1.87	0.74
2:z:12:VAL:HG13	69:n:607:3PE:H322	1.68	0.74
48:N1:243:MET:HG2	56:d1:44:MET:HE2	1.68	0.74
16:c:34:TRP:CZ2	1:g:61:TRP:HE3	2.06	0.73
2:m:2:HIS:NE2	17:d:17:ALA:HA	2.03	0.73
2:z:32:TRP:CZ2	70:z:101:PC1:H11	2.23	0.73
5:C:95:PHE:CE2	5:C:272:TRP:HZ3	2.06	0.72
14:n:116:SER:O	23:y:43:GLN:NE2	2.21	0.72
14:n:35:ILE:HD12	14:n:462:LEU:HG	1.71	0.72
46:L1:243:VAL:O	46:L1:247:LEU:HB2	1.90	0.72
63:k1:32:THR:HG22	63:k1:34:LEU:H	1.53	0.72
1:g:50:PRO:HD2	20:h:75:ARG:HH22	1.52	0.72
2:z:32:TRP:CD2	70:z:101:PC1:O22	2.43	0.72
5:C:132:VAL:HA	5:C:139:SER:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:128:GLU:CB	1:g:32:VAL:HG22	2.18	0.72
1:t:69:PHE:HD2	69:t:101:3PE:H11	1.55	0.72
2:z:32:TRP:CZ2	70:z:101:PC1:C1	2.73	0.71
14:a:383:MET:HG3	14:a:421:VAL:HG21	1.71	0.71
14:a:216:ASN:ND2	1:g:54:ILE:O	2.23	0.71
43:H1:175:LEU:O	43:H1:179:TRP:HB3	1.91	0.71
17:d:115:TRP:CD1	17:d:119:GLN:HE22	2.08	0.71
8:F:13:LEU:HD12	16:c:161:GLN:HG2	1.73	0.71
29:1:93:LEU:O	29:1:134:ALA:HA	1.91	0.71
16:c:146:TRP:CB	1:g:13:TRP:HB3	2.19	0.71
2:m:2:HIS:HB2	14:a:484:SER:OG	1.90	0.71
16:p:73:PRO:HD2	19:s:21:ILE:HD11	1.70	0.70
43:H1:228:TYR:HA	43:H1:231:ILE:HD12	1.72	0.70
11:J:52:TRP:O	11:J:56:LYS:HB2	1.91	0.70
48:N1:211:LEU:HD23	48:N1:333:SER:HB2	1.71	0.70
11:J:33:ARG:NH1	12:K:47:TYR:O	2.23	0.70
1:g:50:PRO:HG3	20:h:75:ARG:NH1	1.74	0.70
2:m:40:TYR:HB3	23:l:44:LEU:CD1	2.20	0.70
14:a:425:PHE:O	14:a:429:HIS:CD2	2.45	0.70
43:H1:169:GLN:NE2	43:H1:241:ILE:O	2.25	0.70
57:e1:29:ALA:HB2	60:h1:138:LYS:HG2	1.74	0.70
16:c:12:ASN:C	16:c:12:ASN:HD22	1.97	0.69
27:D1:328:ALA:HB3	30:3:126:ASP:HB2	1.72	0.69
16:c:56:GLN:HB2	16:c:59:ARG:HH21	1.58	0.69
19:f:48:ASN:HB2	19:f:89:HIS:O	1.93	0.69
46:L1:15:LEU:HD11	46:L1:125:LEU:HD23	1.75	0.68
14:a:375:ALA:HB1	14:a:429:HIS:CE1	2.29	0.68
47:M1:98:MET:HE1	71:N1:401:CDL:H801	1.74	0.68
47:M1:207:MET:HG3	47:M1:294:MET:HB3	1.76	0.68
14:a:38:ARG:NH2	14:a:454:SER:OG	2.26	0.68
4:M:46:ARG:NH2	4:M:376:GLU:OE1	2.26	0.68
2:z:32:TRP:CZ2	70:z:101:PC1:H2	2.27	0.67
68:p1:39:VAL:HG13	68:p1:40:VAL:HG23	1.75	0.67
27:D1:103:PHE:HB3	27:D1:114:ASN:HB3	1.76	0.67
29:1:96:ASN:ND2	29:1:187:GLY:O	2.26	0.67
5:C:378:LYS:HE2	16:c:156:ARG:HH12	1.59	0.67
45:K1:59:ILE:HD12	48:N1:27:MET:HG2	1.76	0.67
15:o:21:MET:SD	21:v:45:ARG:NH2	2.67	0.66
14:n:66:ILE:HG23	14:n:246:LEU:HD21	1.77	0.66
16:c:145:THR:HG23	1:g:13:TRP:CE3	2.30	0.66
14:n:151:HIS:HE1	14:n:210:LEU:HD12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:82:ARG:HG2	15:b:86:MET:HE1	1.76	0.66
28:2:119:THR:HG21	28:2:166:PRO:HB3	1.76	0.66
16:p:115:CYS:SG	20:u:84:LYS:NZ	2.68	0.66
2:z:36:HIS:NE2	69:z:102:3PE:O12	2.29	0.66
16:c:146:TRP:HE1	1:g:14:LYS:HB2	1.59	0.66
4:B:51:VAL:HG12	4:B:204:MET:HG2	1.78	0.66
2:z:32:TRP:CH2	70:z:101:PC1:C2	2.78	0.65
16:c:149:HIS:C	1:g:10:ALA:HB2	2.21	0.65
1:t:69:PHE:CD2	69:t:101:3PE:H11	2.31	0.65
63:k1:69:PRO:O	63:k1:73:LEU:HB2	1.96	0.65
16:c:34:TRP:HB2	16:c:43:LEU:HD21	1.78	0.65
20:u:43:MET:HA	20:u:46:LYS:HG2	1.78	0.65
36:U1:20:LYS:HG2	36:U1:27:PRO:HB3	1.78	0.65
14:n:381:LEU:HD13	77:n:604:HEA:HBC2	1.77	0.65
14:a:93:ALA:HB2	14:a:171:MET:HE3	1.78	0.65
5:C:343:VAL:HG23	5:C:348:ILE:HD11	1.79	0.65
14:n:172:LYS:HE2	14:n:178:GLN:HA	1.78	0.65
9:R:41:THR:O	9:R:45:ILE:HB	1.97	0.64
25:6:119:GLU:O	32:P1:54:TYR:OH	2.15	0.64
16:c:182:PHE:O	1:g:71:ASN:ND2	2.23	0.64
5:C:361:ILE:HA	5:C:365:LEU:HB2	1.78	0.64
13:I:78:ARG:HB2	16:c:63:ARG:HH22	1.62	0.64
14:n:76:GLY:O	14:n:80:ASN:HB2	1.98	0.64
2:z:32:TRP:HH2	70:z:101:PC1:H2	1.63	0.64
46:L1:97:THR:HG21	46:L1:125:LEU:HD22	1.80	0.64
65:m1:7:PRO:HG3	65:m1:13:LEU:HD12	1.79	0.64
1:t:75:ASN:ND2	69:t:101:3PE:HN1	1.94	0.64
1:g:50:PRO:HD2	20:h:75:ARG:HH21	1.56	0.64
5:N:8:HIS:HB3	5:N:11:PHE:HB2	1.80	0.64
29:1:188:GLU:O	29:1:192:LEU:HB2	1.97	0.64
16:c:132:LEU:HD11	1:g:29:MET:CG	2.28	0.64
2:m:10:LEU:HD21	14:a:477:ALA:HB1	1.80	0.64
5:C:95:PHE:CD2	5:C:272:TRP:HZ3	2.16	0.63
9:R:72:LYS:NZ	10:S:50:GLU:OE2	2.32	0.63
43:H1:20:LEU:HD22	43:H1:232:ILE:HG12	1.79	0.63
3:A:417:ASP:OD1	3:A:438:ARG:NH2	2.31	0.63
15:b:162:SER:O	15:b:196:CYS:HA	1.97	0.63
22:x:42:MET:SD	22:x:47:ARG:NH1	2.70	0.63
30:3:366:THR:HG22	30:3:370:GLY:HA3	1.81	0.63
14:a:168:ILE:HD11	14:a:185:VAL:HA	1.80	0.63
14:a:116:SER:O	23:l:43:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:264:LYS:HD3	15:o:53:THR:HG22	1.81	0.62
47:M1:310:MET:HE3	47:M1:459:MET:HG3	1.81	0.62
48:N1:152:THR:HG22	48:N1:156:MET:HE2	1.82	0.62
44:J1:63:MET:HA	44:J1:66:VAL:HB	1.81	0.62
71:R:103:CDL:HB62	51:Y1:107:TYR:HB2	1.82	0.62
26:C1:165:ASP:HA	33:Q1:82:MET:HE1	1.82	0.62
27:D1:51:PHE:HB3	27:D1:64:LEU:HB3	1.80	0.62
16:p:63:ARG:HA	16:p:67:TYR:HD2	1.64	0.62
3:L:110:VAL:HG11	3:L:211:LEU:HB3	1.81	0.62
5:N:315:LEU:O	5:N:322:GLN:NE2	2.29	0.62
46:L1:197:GLU:HG3	68:p1:110:LYS:HD3	1.82	0.62
15:b:145:PRO:HA	15:b:214:VAL:O	2.00	0.62
43:H1:24:GLU:HG3	43:H1:271:LEU:HD22	1.82	0.61
60:h1:37:ILE:HD11	71:h1:201:CDL:H552	1.81	0.61
27:D1:269:LEU:HB2	27:D1:368:GLU:HB2	1.82	0.61
35:S1:17:GLU:OE1	35:S1:67:ARG:NH1	2.33	0.61
14:a:135:ASN:ND2	1:g:56:THR:CB	2.63	0.61
15:o:134:ARG:HG2	15:o:135:LEU:HG	1.81	0.61
31:9:171:ILE:O	31:9:175:TYR:HB3	2.01	0.61
36:T1:70:LEU:HD23	36:T1:76:ILE:HD13	1.82	0.61
47:M1:138:ASN:ND2	47:M1:334:TYR:OH	2.33	0.61
64:l1:127:VAL:HG12	67:o1:98:MET:HG2	1.82	0.61
4:B:298:SER:HA	4:B:301:LYS:HE3	1.83	0.61
43:H1:295:PRO:HB3	69:b1:101:3PE:H381	1.83	0.61
51:Y1:16:GLN:HB3	51:Y1:19:ARG:HB3	1.82	0.61
14:a:70:VAL:O	14:a:74:MET:HB3	2.01	0.61
14:n:428:GLN:HG3	14:n:431:LEU:HD12	1.82	0.61
15:o:30:ILE:HG21	15:o:76:ILE:HD11	1.83	0.61
26:C1:77:ASP:HB3	27:D1:392:LYS:HG3	1.83	0.61
16:c:149:HIS:CD2	1:g:13:TRP:CD1	2.88	0.61
23:l:5:GLU:OE1	23:l:10:ASN:ND2	2.34	0.61
64:l1:9:PRO:HD3	65:m1:66:ARG:HG2	1.82	0.61
16:c:146:TRP:HA	1:g:13:TRP:CB	2.30	0.61
12:V:33:VAL:HG23	12:V:38:TRP:HB3	1.83	0.60
14:n:117:MET:HE2	23:y:39:ILE:HG12	1.83	0.60
14:n:147:ILE:HG23	14:n:206:ILE:HB	1.83	0.60
18:r:33:MET:HE3	18:r:67:ILE:HG12	1.82	0.60
32:P1:35:VAL:HG23	32:P1:45:VAL:HG11	1.83	0.60
42:A1:13:LEU:HD22	43:H1:10:LEU:HD21	1.83	0.60
46:L1:97:THR:HG23	46:L1:246:LEU:HD11	1.82	0.60
53:a1:52:ARG:NH1	53:a1:58:ASN:OD1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:365:ASN:HB3	30:3:488:LYS:HD3	1.83	0.60
32:P1:244:TYR:HB2	32:P1:337:ALA:HB2	1.83	0.60
46:L1:362:ILE:HB	46:L1:431:THR:HA	1.83	0.60
7:E:161:HIS:CD2	5:N:343:VAL:CG2	2.71	0.60
4:M:77:THR:HG21	4:M:126:VAL:HA	1.83	0.60
32:P1:251:ARG:NH1	71:H1:402:CDL:OB3	2.34	0.60
17:d:48:TRP:HZ2	18:e:59:ASN:HA	1.67	0.60
2:m:3:SER:HA	14:a:482:VAL:HA	1.83	0.60
2:z:32:TRP:CH2	70:z:101:PC1:C21	2.68	0.60
18:r:93:LEU:HD13	18:r:98:ILE:HG23	1.83	0.60
43:H1:110:SER:HB2	44:J1:60:LEU:HD23	1.84	0.60
19:s:62:ILE:HD11	19:s:70:VAL:HG22	1.82	0.60
42:A1:79:ILE:HA	42:A1:87:MET:HE2	1.81	0.60
44:J1:59:TYR:HE2	45:K1:38:LEU:HB2	1.66	0.60
48:N1:122:ILE:O	48:N1:176:ARG:NH1	2.35	0.60
14:a:508:PRO:O	19:f:57:ARG:NH1	2.33	0.60
5:C:8:HIS:HB3	5:C:11:PHE:HB2	1.84	0.60
26:C1:205:ALA:HA	30:3:122:MET:HE1	1.84	0.60
46:L1:161:ARG:NH1	66:n1:90:PHE:O	2.34	0.60
52:Z1:88:GLU:OE2	52:Z1:127:ARG:NH2	2.34	0.60
1:t:69:PHE:O	69:t:101:3PE:C12	2.49	0.60
2:z:40:TYR:HE1	70:z:101:PC1:O14	1.84	0.60
13:I:76:LEU:HD22	13:I:83:GLN:CG	2.31	0.60
48:N1:150:ASN:HB3	48:N1:153:ILE:HG12	1.84	0.60
2:z:10:LEU:HD21	14:n:477:ALA:HB1	1.83	0.60
32:P1:216:ASN:O	32:P1:220:ASP:HB2	2.02	0.60
14:a:135:ASN:HD21	1:g:56:THR:HG21	1.65	0.60
3:A:245:ASP:HA	9:G:11:ARG:HA	1.84	0.60
27:D1:151:ILE:HG12	27:D1:170:MET:HE3	1.83	0.60
5:C:51:LEU:HD13	72:C:401:HEM:HBA1	1.84	0.60
12:V:6:LEU:HG	13:I:80:LEU:H	1.66	0.60
16:p:62:ILE:HD12	70:p:302:PC1:H222	1.82	0.60
46:L1:135:ASN:ND2	46:L1:197:GLU:OE2	2.34	0.60
16:p:33:MET:HG3	16:p:37:TYR:HD2	1.67	0.59
27:D1:67:GLU:HB3	27:D1:75:LYS:HB3	1.82	0.59
29:1:92:TYR:HB2	29:1:220:THR:HG22	1.84	0.59
47:M1:187:ASP:OD1	47:M1:192:ASN:ND2	2.36	0.59
16:c:191:GLY:O	16:c:195:SER:HB3	2.01	0.59
1:t:54:ILE:HD12	14:n:218:THR:HG21	1.84	0.59
31:9:97:GLU:HB2	31:9:110:ARG:HB3	1.84	0.59
46:L1:290:ILE:HG13	46:L1:418:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L1:584:ILE:HD12	48:N1:58:LYS:HG2	1.84	0.59
16:c:145:THR:HG21	1:g:13:TRP:CZ3	2.37	0.59
16:c:189:SER:OG	1:g:54:ILE:O	2.19	0.59
47:M1:209:LEU:HD21	47:M1:264:LEU:HD13	1.84	0.59
47:M1:232:ALA:O	47:M1:237:LYS:NZ	2.35	0.59
15:b:101:GLY:HA3	15:b:161:HIS:HD2	1.66	0.59
20:h:35:ASP:HA	20:h:38:ARG:HG2	1.85	0.59
14:n:274:VAL:HG12	14:n:278:MET:HE2	1.83	0.59
27:D1:74:ARG:O	27:D1:407:LYS:NZ	2.35	0.59
21:i:43:GLU:HG2	21:i:44:PRO:HD3	1.85	0.59
2:m:13:LEU:HD22	14:n:278:MET:SD	2.42	0.59
25:6:135:TYR:HE1	31:9:90:PRO:HB2	1.67	0.59
20:h:38:ARG:NH1	20:h:84:LYS:O	2.34	0.59
17:q:89:ILE:HG22	22:x:29:TRP:HE1	1.66	0.59
43:H1:42:PRO:HD2	43:H1:45:ILE:HG12	1.85	0.59
47:M1:50:LYS:HB2	47:M1:58:SER:HB3	1.83	0.59
14:a:413:HIS:CG	14:a:468:MET:HE3	2.37	0.59
16:c:158:HIS:NE2	1:g:14:LYS:CE	2.65	0.59
16:c:189:SER:OG	1:g:54:ILE:N	2.36	0.59
4:B:374:THR:HG23	4:B:377:GLY:H	1.67	0.59
16:p:221:ARG:NH2	69:p:301:3PE:O14	2.36	0.59
46:L1:100:ILE:HG21	46:L1:246:LEU:HB2	1.85	0.59
48:N1:24:THR:HG22	57:e1:1:PRO:HG3	1.85	0.59
16:c:146:TRP:CA	1:g:13:TRP:HB3	2.32	0.59
14:n:38:ARG:NH2	14:n:454:SER:OG	2.35	0.59
43:H1:20:LEU:HD13	43:H1:232:ILE:HD11	1.84	0.59
50:X1:29:HIS:HB3	50:X1:119:PRO:HD2	1.84	0.59
59:g1:98:ARG:NH1	59:g1:105:ILE:O	2.36	0.59
5:C:45:ILE:HG12	72:C:401:HEM:HBB1	1.84	0.59
14:a:195:LEU:HD23	14:a:245:ILE:HD13	1.84	0.59
5:C:91:PHE:C	5:C:272:TRP:HH2	2.10	0.58
14:n:331:ASN:HD22	17:q:20:ARG:HB2	1.68	0.58
16:c:156:ARG:NH2	16:c:223:LEU:O	2.36	0.58
3:A:339:GLN:NE2	3:A:437:ILE:O	2.35	0.58
32:P1:167:ARG:HH21	32:P1:297:LEU:HD11	1.68	0.58
46:L1:306:THR:HG23	46:L1:332:HIS:HE1	1.68	0.58
47:M1:272:THR:HA	47:M1:275:ILE:HD12	1.85	0.58
2:m:34:LEU:HA	2:m:37:LEU:HG	1.86	0.58
20:u:11:TYR:O	20:u:58:ARG:NH2	2.37	0.58
27:D1:74:ARG:HH22	42:A1:115:GLU:HB3	1.69	0.58
48:N1:43:MET:HA	48:N1:46:ASN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:16:TRP:HE1	16:c:56:GLN:HG2	1.66	0.58
5:C:257:MET:SD	6:D:120:ARG:NH2	2.75	0.58
30:3:601:ARG:NH1	30:3:605:GLU:OE1	2.32	0.58
32:P1:246:PHE:HA	32:P1:249:THR:HG22	1.85	0.58
18:r:89:LEU:HB3	18:r:93:LEU:HD23	1.83	0.58
27:D1:126:LEU:HD13	27:D1:358:VAL:HG22	1.86	0.58
27:D1:141:PHE:HA	27:D1:144:ILE:HD12	1.84	0.58
46:L1:362:ILE:HA	46:L1:365:ILE:HG22	1.83	0.58
4:M:374:THR:HG23	4:M:377:GLY:H	1.68	0.58
31:9:22:ASN:ND2	54:b1:13:ALA:O	2.37	0.58
61:i1:78:MET:HG2	68:p1:40:VAL:HG21	1.86	0.58
14:a:378:HIS:O	14:a:382:SER:OG	2.22	0.58
14:n:166:THR:O	14:n:170:ASN:HB2	2.04	0.58
16:p:126:PRO:HB3	16:p:257:TYR:HB3	1.85	0.58
17:q:23:PRO:O	18:r:66:ARG:NH2	2.37	0.58
25:6:118:PRO:HB2	43:H1:58:LYS:HD2	1.86	0.58
27:D1:257:GLY:HA3	27:D1:372:GLY:HA2	1.85	0.58
59:g1:83:MET:HB2	59:g1:86:TRP:HB3	1.86	0.58
14:a:62:ALA:HB2	77:a:603:HEA:HBD1	1.86	0.58
14:a:299:VAL:HG11	15:b:88:ASP:HB3	1.85	0.58
16:c:66:THR:HB	69:c:301:3PE:H111	1.85	0.58
1:t:75:ASN:ND2	69:t:101:3PE:N	2.50	0.58
29:1:99:GLU:O	29:1:139:ARG:NH2	2.37	0.58
2:z:43:ARG:CD	23:y:47:LYS:OXT	2.52	0.58
4:M:145:LYS:HE2	7:T:41:PRO:HD3	1.86	0.58
40:r1:45:SER:O	40:r1:51:ASN:ND2	2.37	0.58
3:L:188:ARG:NH2	65:m1:24:VAL:O	2.37	0.57
14:n:83:VAL:HG11	14:n:188:VAL:HG11	1.85	0.57
21:v:52:PHE:O	21:v:56:TYR:CB	2.49	0.57
43:H1:20:LEU:HA	43:H1:23:VAL:HG12	1.86	0.57
48:N1:246:LEU:HD21	71:N1:401:CDL:H792	1.86	0.57
15:b:165:VAL:O	15:b:169:GLY:N	2.37	0.57
3:A:131:ARG:NH2	3:A:177:LEU:O	2.37	0.57
46:L1:217:LEU:HD13	46:L1:277:MET:HG2	1.85	0.57
16:c:12:ASN:C	16:c:12:ASN:ND2	2.61	0.57
19:f:74:TRP:O	19:f:81:GLN:NE2	2.32	0.57
3:A:350:THR:HG21	12:K:9:ARG:HG3	1.86	0.57
10:S:64:ASP:HA	10:S:67:VAL:HG22	1.85	0.57
16:p:56:GLN:HA	16:p:59:ARG:HB3	1.85	0.57
26:C1:78:LEU:HB3	26:C1:130:TYR:HB3	1.84	0.57
27:D1:63:ARG:HB3	27:D1:79:HIS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:A1:70:ALA:HB2	44:J1:58:ILE:HD11	1.86	0.57
5:N:300:ILE:HD12	5:N:362:ILE:HG12	1.85	0.57
15:b:198:GLU:O	15:b:204:HIS:CE1	2.57	0.57
5:N:113:TRP:NE1	5:N:301:LEU:O	2.30	0.57
16:p:217:VAL:HG21	69:p:301:3PE:H271	1.86	0.57
27:D1:4:TRP:O	47:M1:142:ARG:NH2	2.38	0.57
46:L1:221:THR:HG23	46:L1:226:GLN:HB2	1.86	0.57
60:h1:102:GLU:OE1	60:h1:106:LYS:NZ	2.36	0.57
14:a:513:VAL:HB	19:f:40:ALA:HB2	1.86	0.57
15:b:165:VAL:HG12	15:b:168:LEU:H	1.70	0.57
16:p:9:HIS:NE2	16:p:64:GLU:OE1	2.37	0.57
28:2:27:ASN:OD1	28:2:30:ARG:NH1	2.37	0.57
47:M1:105:LEU:HD21	71:d1:201:CDL:H673	1.87	0.57
4:B:299:VAL:HG21	4:B:309:VAL:HG21	1.87	0.57
7:P:165:TYR:HA	7:P:171:ILE:HA	1.86	0.57
14:n:211:THR:HG22	14:n:215:LEU:HD12	1.86	0.57
14:n:368:HIS:HB3	15:o:171:LYS:HD2	1.87	0.57
46:L1:15:LEU:HB3	46:L1:126:ILE:HG12	1.85	0.57
48:N1:142:LEU:HB3	48:N1:194:LEU:HD21	1.85	0.57
5:N:282:ARG:NH2	5:N:338:ILE:O	2.36	0.57
50:X1:93:MET:HB2	50:X1:95:LEU:HG	1.86	0.57
14:a:97:MET:HB2	14:a:159:LEU:HB3	1.87	0.57
16:c:142:VAL:HG11	1:g:21:ALA:HB2	1.87	0.57
15:o:151:ARG:NH2	20:u:14:ALA:O	2.38	0.57
26:C1:102:ASN:OD1	27:D1:273:GLN:NE2	2.38	0.57
35:S1:17:GLU:HG3	35:S1:51:PRO:HG2	1.85	0.57
50:X1:5:GLU:O	50:X1:53:ARG:NH1	2.38	0.57
16:p:7:ALA:HB1	16:p:72:THR:HG21	1.86	0.56
4:B:92:VAL:HG11	4:B:118:ILE:HD11	1.87	0.56
5:C:149:LEU:HD21	5:C:281:LEU:HD22	1.87	0.56
25:6:37:GLU:HA	25:6:40:VAL:HG12	1.87	0.56
14:a:347:LEU:HB3	14:a:383:MET:HE1	1.86	0.56
1:t:60:PRO:O	16:p:34:TRP:NE1	2.38	0.56
1:t:67:THR:HG21	16:p:187:SER:CB	2.35	0.56
3:A:53:ASN:HD21	3:A:165:GLN:HB2	1.70	0.56
5:C:95:PHE:CE2	5:C:272:TRP:CZ3	2.90	0.56
5:N:101:GLY:HA2	5:N:106:SER:HB2	1.88	0.56
6:O:197:GLU:O	6:O:201:ARG:HB3	2.05	0.56
11:U:10:TYR:HA	11:U:14:PHE:HB2	1.86	0.56
25:6:101:THR:OG1	25:6:129:CYS:SG	2.64	0.56
43:H1:26:LYS:HB3	53:a1:5:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:K1:26:LEU:HD23	45:K1:78:LEU:HD13	1.88	0.56
46:L1:194:ASN:ND2	68:p1:106:GLN:OE1	2.36	0.56
46:L1:307:SER:HA	46:L1:310:LEU:HD12	1.86	0.56
47:M1:109:THR:HG21	47:M1:238:LEU:HD11	1.87	0.56
14:a:135:ASN:ND2	1:g:56:THR:HB	2.20	0.56
14:a:227:ASP:HB2	14:a:230:LEU:HD23	1.86	0.56
14:a:453:VAL:HA	14:a:456:MET:HE2	1.87	0.56
17:d:86:MET:HA	17:d:89:ILE:HB	1.86	0.56
4:M:334:GLY:HA2	4:M:434:PRO:HD3	1.86	0.56
15:o:132:GLU:HB3	15:o:137:GLU:HG3	1.86	0.56
26:C1:49:GLU:OE2	26:C1:106:ARG:NH1	2.38	0.56
29:1:215:VAL:HG22	29:1:220:THR:HG21	1.87	0.56
36:T1:25:ILE:HD11	36:T1:42:LEU:HD11	1.87	0.56
42:A1:73:LEU:HD23	43:H1:151:LEU:HD13	1.87	0.56
47:M1:370:PRO:HG3	47:M1:375:LEU:HD13	1.88	0.56
16:c:172:TYR:OH	1:g:29:MET:HE3	2.05	0.56
27:D1:117:ALA:HA	27:D1:367:ILE:HG13	1.87	0.56
14:a:425:PHE:O	14:a:429:HIS:HD2	1.89	0.56
16:c:132:LEU:CD1	1:g:29:MET:HG2	2.33	0.56
6:O:180:SER:HB3	10:S:15:LEU:HB2	1.87	0.56
12:V:18:ILE:HD12	71:V:101:CDL:H112	1.87	0.56
44:J1:66:VAL:HG11	45:K1:31:LEU:HD21	1.88	0.56
48:N1:42:PRO:HA	48:N1:45:ILE:HG22	1.86	0.56
14:a:150:LEU:HD21	14:a:202:LEU:HD11	1.87	0.56
7:P:84:GLY:N	7:P:100:HIS:O	2.39	0.56
14:n:445:ASP:O	22:x:41:ASN:ND2	2.39	0.56
46:L1:54:PHE:O	46:L1:58:ASN:ND2	2.37	0.56
46:L1:161:ARG:NH2	66:n1:87:GLY:O	2.39	0.56
16:c:34:TRP:HZ2	1:g:61:TRP:HB3	1.70	0.56
29:1:82:MET:SD	29:1:221:THR:OG1	2.62	0.56
30:3:533:THR:O	30:3:537:LEU:HB2	2.06	0.56
44:J1:2:ASN:HB3	44:J1:121:GLY:HA3	1.88	0.56
69:L1:704:3PE:H3E1	70:M1:501:PC1:H3H1	1.88	0.56
3:A:244:ARG:NH2	3:A:429:GLU:OE1	2.38	0.56
8:F:32:MET:H	8:F:35:ASP:HB2	1.71	0.56
4:M:50:PHE:HB3	4:M:387:LEU:HD11	1.88	0.56
29:1:185:ILE:HG12	29:1:359:CYS:HB3	1.88	0.56
32:P1:157:ARG:NH1	32:P1:163:ALA:O	2.38	0.56
43:H1:317:TYR:OH	44:J1:136:GLU:OE2	2.24	0.56
66:n1:12:GLN:NE2	86:n1:201:ZMP:O7	2.38	0.56
14:a:145:LEU:HD22	16:c:32:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:146:TRP:HA	1:g:13:TRP:HB3	1.87	0.56
2:z:10:LEU:HD11	14:n:477:ALA:HB3	1.88	0.56
29:1:224:ASN:ND2	83:1:501:FMN:O2	2.38	0.56
30:3:364:LEU:HD12	30:3:491:ASN:HB3	1.88	0.56
47:M1:382:THR:HG23	47:M1:396:MET:HG3	1.88	0.56
56:d1:106:LYS:HE2	68:p1:78:GLU:HG3	1.87	0.56
66:n1:134:ARG:NH1	66:n1:134:ARG:O	2.38	0.56
15:b:41:ILE:O	15:b:45:MET:CB	2.51	0.56
1:g:61:TRP:CH2	69:g:303:3PE:H321	2.41	0.56
71:D:302:CDL:OA3	9:G:36:ASN:ND2	2.40	0.55
72:N:402:HEM:HBB2	72:N:402:HEM:HHC	1.87	0.55
14:n:324:LEU:HD21	15:o:38:VAL:HG23	1.88	0.55
14:a:135:ASN:HD22	1:g:56:THR:CB	2.19	0.55
3:A:339:GLN:HE21	3:A:441:MET:HE2	1.71	0.55
14:a:445:ASP:O	22:k:41:ASN:ND2	2.37	0.55
16:c:34:TRP:CE2	1:g:60:PRO:O	2.58	0.55
1:t:69:PHE:O	69:t:101:3PE:N	2.40	0.55
30:3:36:GLN:NE2	33:Q1:47:SER:O	2.39	0.55
33:Q1:16:LYS:HE3	33:Q1:97:GLU:HB3	1.89	0.55
48:N1:170:LEU:HD22	48:N1:288:LEU:HD11	1.88	0.55
36:U1:82:ASP:OD1	66:n1:172:ARG:NH2	2.39	0.55
15:b:154:ILE:HD13	15:b:172:THR:HG23	1.88	0.55
4:B:187:THR:HG23	4:B:190:GLU:H	1.72	0.55
16:p:58:TRP:CD2	69:p:301:3PE:H251	2.42	0.55
19:s:83:CYS:HB3	19:s:86:CYS:SG	2.46	0.55
32:P1:53:VAL:HA	32:P1:56:ILE:HG12	1.88	0.55
5:C:322:GLN:OE1	9:G:47:ARG:NH1	2.40	0.55
4:M:157:THR:HG23	7:T:64:LEU:HD11	1.88	0.55
5:N:249:MET:HG3	5:N:250:LEU:HD12	1.89	0.55
16:p:228:THR:HG21	19:s:10:ASP:HB3	1.88	0.55
18:r:86:ILE:HG22	18:r:90:ARG:HH12	1.71	0.55
43:H1:138:GLN:NE2	43:H1:191:ALA:O	2.39	0.55
26:C1:151:ILE:HG23	26:C1:152:LEU:HG	1.87	0.55
30:3:440:CYS:SG	30:3:476:LYS:NZ	2.80	0.55
42:A1:69:ILE:HG21	43:H1:147:ALA:HB1	1.89	0.55
43:H1:6:ILE:HD13	43:H1:95:LEU:HD21	1.87	0.55
46:L1:578:THR:OG1	48:N1:171:ASN:ND2	2.40	0.55
48:N1:226:THR:H	48:N1:229:SER:HB2	1.72	0.55
48:N1:252:GLY:HA3	48:N1:290:LEU:HD13	1.89	0.55
16:c:149:HIS:CD2	1:g:13:TRP:NE1	2.75	0.55
2:m:4:LYS:HD2	14:a:481:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:245:ASP:HA	9:R:11:ARG:HA	1.88	0.55
46:L1:176:ARG:NH1	47:M1:400:ILE:O	2.40	0.55
50:X1:23:VAL:HG21	53:a1:65:GLY:HA2	1.88	0.55
15:b:1:MET:O	15:b:10:GLN:NE2	2.39	0.55
19:f:43:THR:HG23	19:f:46:ASP:H	1.71	0.55
3:A:21:ASN:HD22	3:A:218:SER:H	1.54	0.55
4:B:112:ILE:HG22	4:B:114:SER:H	1.72	0.55
11:U:4:THR:HG23	11:U:6:PRO:HD2	1.89	0.55
44:J1:165:ILE:HD12	48:N1:42:PRO:HG2	1.88	0.55
44:J1:165:ILE:HG23	48:N1:42:PRO:HG3	1.88	0.55
1:t:67:THR:HG21	16:p:187:SER:HB2	1.89	0.55
4:B:215:VAL:HA	4:B:218:GLN:HG2	1.88	0.55
3:L:332:ASP:OD2	5:N:6:LYS:NZ	2.38	0.55
27:D1:150:HIS:NE2	27:D1:303:GLU:OE2	2.40	0.55
30:3:544:VAL:HG12	30:3:559:VAL:HB	1.89	0.55
32:P1:251:ARG:NH2	32:P1:321:HIS:O	2.40	0.55
43:H1:138:GLN:HG3	43:H1:285:LEU:HD21	1.89	0.55
43:H1:245:PRO:HB3	43:H1:258:ASN:HB3	1.88	0.55
46:L1:79:SER:O	46:L1:139:GLN:NE2	2.37	0.55
46:L1:485:PHE:O	46:L1:489:THR:OG1	2.25	0.55
46:L1:548:THR:O	46:L1:552:LEU:HB3	2.05	0.55
14:a:144:ASP:OD2	16:c:36:HIS:NE2	2.35	0.55
2:z:43:ARG:HD3	23:y:47:LYS:OXT	2.07	0.55
7:E:74:ILE:HD11	7:E:91:TRP:HA	1.89	0.55
15:o:106:TRP:CE2	15:o:207:MET:HE2	2.42	0.55
2:z:43:ARG:HG2	23:y:47:LYS:C	2.31	0.54
15:o:12:ALA:O	15:o:188:ARG:NH2	2.40	0.54
25:6:119:GLU:H	43:H1:59:GLU:HG2	1.71	0.54
42:A1:6:VAL:HG11	43:H1:87:VAL:HG21	1.88	0.54
44:J1:22:LYS:NZ	45:K1:18:GLY:O	2.40	0.54
14:a:135:ASN:ND2	1:g:56:THR:HG21	2.22	0.54
14:a:216:ASN:ND2	1:g:55:ARG:HD3	2.21	0.54
15:b:161:HIS:CE1	15:b:200:CYS:SG	3.00	0.54
18:e:101:PRO:HB3	18:e:106:LEU:HB2	1.89	0.54
4:B:46:ARG:NH1	4:B:375:SER:OG	2.40	0.54
14:n:296:GLY:O	15:o:178:ARG:NH2	2.39	0.54
15:o:195:GLN:HA	15:o:208:PRO:HA	1.88	0.54
17:q:18:ASP:HB3	17:q:71:MET:HE1	1.89	0.54
47:M1:106:LEU:HD11	47:M1:230:ILE:HD11	1.89	0.54
56:d1:112:ILE:O	68:p1:159:LYS:NZ	2.40	0.54
56:d1:120:ARG:O	65:m1:108:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:e:56:ARG:NH1	18:e:56:ARG:O	2.40	0.54
16:p:67:TYR:HA	24:w:9:GLN:HG2	1.89	0.54
26:C1:119:SER:HB2	26:C1:142:PHE:HB3	1.89	0.54
27:D1:377:TYR:HB3	27:D1:390:LYS:HB3	1.90	0.54
28:2:150:ASN:HB3	28:2:162:GLU:HB3	1.89	0.54
29:1:24:ASN:ND2	29:1:113:HIS:O	2.41	0.54
32:P1:325:ARG:NH1	32:P1:325:ARG:O	2.41	0.54
43:H1:134:ARG:NH1	43:H1:206:GLU:OE2	2.40	0.54
53:a1:57:VAL:O	53:a1:59:ARG:NH1	2.40	0.54
16:c:253:TYR:HA	16:c:257:TYR:HD2	1.72	0.54
1:t:60:PRO:HG3	16:p:35:PHE:CD1	2.43	0.54
37:V1:71:LEU:HD13	37:V1:79:VAL:HG11	1.90	0.54
46:L1:365:ILE:HG23	46:L1:366:MET:HG3	1.89	0.54
14:n:377:PHE:HA	14:n:380:VAL:HG12	1.89	0.54
28:2:76:PRO:HB2	28:2:79:ARG:HG2	1.89	0.54
43:H1:81:LEU:HD22	43:H1:108:THR:HG23	1.89	0.54
70:M1:501:PC1:H2	48:N1:276:LEU:HD22	1.90	0.54
60:h1:7:ARG:NH2	61:i1:31:GLU:O	2.40	0.54
14:a:117:MET:O	23:l:46:LYS:NZ	2.41	0.54
27:D1:335:ARG:NH2	31:9:128:CYS:O	2.36	0.54
32:P1:311:GLU:HG2	32:P1:336:PRO:HB3	1.90	0.54
17:d:126:MET:HE1	21:i:70:ILE:HG21	1.88	0.54
2:z:36:HIS:CE1	69:z:102:3PE:O12	2.60	0.54
3:A:366:VAL:HG11	4:B:43:PRO:HB2	1.90	0.54
5:N:51:LEU:HD13	72:N:401:HEM:HBA1	1.89	0.54
6:D:8:PRO:HG3	10:H:64:ASP:HB3	1.89	0.54
9:G:54:VAL:HA	9:G:57:LEU:HD12	1.90	0.54
29:1:153:ILE:HG22	41:s1:52:LEU:HD11	1.89	0.54
43:H1:172:MET:HE1	52:Z1:45:GLY:HA2	1.88	0.54
44:J1:85:ASN:HB3	44:J1:88:ILE:HG12	1.90	0.54
47:M1:458:THR:O	68:p1:149:TYR:OH	2.26	0.54
17:q:61:ARG:HH12	17:q:66:GLU:HA	1.71	0.54
30:3:632:ARG:HH12	35:S1:57:CYS:HB3	1.71	0.54
46:L1:574:THR:OG1	48:N1:167:TRP:O	2.24	0.54
48:N1:248:LEU:HB2	48:N1:297:ILE:HD11	1.90	0.54
1:g:35:LYS:HE2	70:g:302:PC1:O14	2.08	0.54
6:D:23:HIS:ND1	6:D:54:VAL:O	2.41	0.54
15:o:51:THR:O	18:r:74:LYS:NZ	2.40	0.54
32:P1:17:SER:HG	32:P1:43:SER:HG	1.56	0.54
14:a:337:ALA:HA	14:a:340:TRP:HD1	1.73	0.54
16:c:163:LEU:HB3	16:c:219:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:161:HIS:NE2	5:N:282:ARG:HD3	2.23	0.53
3:L:8:LEU:HD22	3:L:392:LEU:HB3	1.90	0.53
3:L:276:ILE:HG21	3:L:345:LEU:HD21	1.89	0.53
14:n:129:TYR:OH	14:n:236:TRP:NE1	2.38	0.53
16:p:58:TRP:HA	16:p:61:VAL:HG12	1.90	0.53
30:3:335:LEU:HB3	30:3:340:SER:HB3	1.89	0.53
46:L1:525:LEU:HD11	64:l1:94:PRO:HG2	1.90	0.53
47:M1:173:THR:HB	60:h1:101:ALA:HB2	1.90	0.53
47:M1:204:LEU:HD13	47:M1:209:LEU:HD13	1.90	0.53
48:N1:36:SER:OG	48:N1:134:GLN:OE1	2.25	0.53
17:d:76:ASN:HB2	22:k:10:HIS:HB3	1.90	0.53
18:e:107:ASP:OD1	18:e:108:LYS:NZ	2.35	0.53
9:G:36:ASN:OD1	9:G:39:ARG:NH2	2.41	0.53
14:n:254:ILE:HA	14:n:257:VAL:HG22	1.91	0.53
28:2:27:ASN:ND2	28:2:57:GLN:OE1	2.39	0.53
30:3:551:ASP:OD2	30:3:679:ARG:NE	2.41	0.53
31:9:55:GLU:OE2	39:q1:34:ARG:NH2	2.41	0.53
47:M1:275:ILE:O	47:M1:279:GLN:HB2	2.07	0.53
3:A:355:THR:O	3:A:359:ASN:ND2	2.41	0.53
69:N:403:3PE:O14	9:R:44:ARG:NH1	2.41	0.53
14:n:96:ARG:HE	16:p:57:TRP:HE1	1.56	0.53
27:D1:295:ASP:OD1	31:9:6:ASN:ND2	2.42	0.53
4:B:437:ASP:OD1	4:B:437:ASP:N	2.42	0.53
6:O:32:VAL:O	6:O:36:VAL:HB	2.09	0.53
42:A1:74:PRO:HG3	44:J1:141:VAL:HG12	1.90	0.53
47:M1:296:LEU:HD21	47:M1:396:MET:HE1	1.91	0.53
16:c:35:PHE:HD1	1:g:60:PRO:HG3	1.66	0.53
16:c:149:HIS:O	1:g:10:ALA:HB2	2.09	0.53
4:M:246:GLU:O	4:M:427:SER:HA	2.08	0.53
13:I:76:LEU:HD22	13:I:83:GLN:HG2	1.89	0.53
15:o:54:SER:OG	15:o:55:THR:N	2.40	0.53
50:X1:95:LEU:HD12	50:X1:98:HIS:HE1	1.74	0.53
62:j1:51:PHE:HZ	67:o1:87:ASP:HB3	1.72	0.53
19:f:77:LYS:HZ2	19:f:92:LEU:HD13	1.72	0.53
1:g:11:ARG:HH21	71:g:301:CDL:CA4	2.14	0.53
20:h:66:VAL:HA	20:h:69:VAL:HG22	1.90	0.53
3:L:158:PHE:O	3:L:161:THR:OG1	2.27	0.53
29:1:99:GLU:O	29:1:99:GLU:HG2	2.08	0.53
43:H1:83:LEU:HA	43:H1:86:TRP:HD1	1.74	0.53
48:N1:304:MET:HE2	49:O1:286:ALA:HB1	1.90	0.53
57:e1:96:HIS:HA	57:e1:101:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:101:GLY:HA3	15:b:161:HIS:CD2	2.43	0.53
25:6:96:MET:HE1	25:6:113:VAL:HG23	1.90	0.53
47:M1:106:LEU:HD13	47:M1:234:ILE:HG21	1.91	0.53
14:a:411:LYS:HD2	69:d:201:3PE:H321	1.90	0.53
15:b:138:VAL:HG12	15:b:140:ASN:H	1.73	0.53
11:U:52:TRP:O	11:U:56:LYS:HB3	2.09	0.53
69:L1:704:3PE:H3A1	70:M1:501:PC1:H3I3	1.90	0.53
47:M1:74:PRO:HA	47:M1:77:LEU:HD12	1.90	0.53
14:a:443:TYR:O	15:b:134:ARG:NH2	2.41	0.53
16:c:35:PHE:HE1	1:g:60:PRO:HG3	1.63	0.53
16:c:145:THR:CG2	1:g:13:TRP:CZ3	2.91	0.53
2:m:2:HIS:CG	14:a:484:SER:OG	2.61	0.53
7:E:62:MET:HG2	5:N:163:TRP:CE2	2.44	0.53
6:O:238:ARG:NH2	7:P:1:SER:O	2.41	0.53
7:P:139:CYS:HB3	74:P:201:FES:S2	2.48	0.53
14:n:108:SER:HB3	14:n:152:LEU:HB2	1.90	0.53
31:9:77:GLU:O	31:9:107:ARG:NH1	2.42	0.53
51:Y1:94:CYS:HA	51:Y1:114:CYS:HA	1.90	0.53
14:a:72:PRO:O	14:a:77:GLY:N	2.39	0.53
15:b:51:THR:OG1	18:e:74:LYS:NZ	2.38	0.53
16:c:7:ALA:HB1	16:c:72:THR:HG21	1.91	0.53
16:c:142:VAL:HG23	1:g:13:TRP:CZ3	2.43	0.53
19:f:15:THR:HA	19:f:19:ARG:HG2	1.90	0.53
4:B:24:LEU:HD11	4:B:382:ILE:HD13	1.91	0.53
14:n:248:LEU:HD21	14:n:280:ILE:HD11	1.91	0.53
16:p:62:ILE:HG13	69:p:301:3PE:H221	1.91	0.53
27:D1:223:ASP:OD1	27:D1:305:ARG:NH2	2.37	0.53
42:A1:11:ILE:HD13	43:H1:80:THR:HG21	1.90	0.53
14:a:254:ILE:HD11	14:a:341:ALA:HA	1.89	0.53
17:d:68:PHE:HA	17:d:71:MET:HG3	1.91	0.53
1:g:68:LEU:CB	69:g:303:3PE:O32	2.56	0.53
21:i:28:ILE:HD12	21:i:31:LEU:HD21	1.90	0.53
5:N:5:ARG:NH1	5:N:15:ASN:OD1	2.42	0.52
27:D1:352:TYR:HD1	31:9:88:ILE:HG12	1.75	0.52
42:A1:10:ASN:HD21	43:H1:83:LEU:HB2	1.73	0.52
46:L1:5:THR:HG22	46:L1:63:ILE:HG12	1.91	0.52
47:M1:44:GLN:NE2	47:M1:46:ASP:O	2.41	0.52
48:N1:332:MET:HE3	48:N1:336:THR:HG21	1.90	0.52
4:B:220:ALA:O	4:B:224:LEU:HB2	2.09	0.52
12:K:33:VAL:HG11	12:K:41:ILE:HD12	1.90	0.52
3:L:41:ILE:HG13	3:L:195:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:6:62:LEU:HB2	25:6:100:GLY:HA3	1.91	0.52
28:2:129:GLY:HA2	28:2:140:ILE:HG22	1.89	0.52
60:h1:69:HIS:NE2	71:h1:201:CDL:OA3	2.41	0.52
2:z:6:ALA:HA	14:n:480:ARG:HB3	1.90	0.52
3:L:156:THR:O	3:L:239:SER:OG	2.27	0.52
8:Q:35:ASP:OD1	8:Q:89:TYR:OH	2.28	0.52
14:n:64:VAL:HA	14:n:68:PHE:HD2	1.74	0.52
14:n:151:HIS:HE1	14:n:210:LEU:CD1	2.21	0.52
28:2:6:LEU:O	28:2:92:ARG:NH2	2.42	0.52
46:L1:367:PRO:HG2	62:j1:22:VAL:HG12	1.91	0.52
36:U1:35:HIS:HB3	36:U1:38:LYS:HB2	1.90	0.52
3:L:53:ASN:HD22	3:L:170:PRO:HD3	1.74	0.52
24:w:33:ARG:HG3	46:L1:503:GLU:HG2	1.92	0.52
30:3:349:PHE:H	30:3:509:PRO:HB2	1.74	0.52
32:P1:166:ILE:HG22	32:P1:168:PRO:HD3	1.91	0.52
44:J1:73:MET:HE1	45:K1:79:VAL:HG22	1.91	0.52
49:O1:106:LEU:HD13	49:O1:270:LEU:HD11	1.90	0.52
64:l1:61:TYR:OH	65:m1:43:LYS:NZ	2.41	0.52
15:b:94:VAL:HG11	15:b:148:LEU:HD22	1.92	0.52
18:e:8:ASP:N	18:e:8:ASP:OD1	2.43	0.52
3:A:42:ASP:HB2	3:A:194:ARG:HB2	1.91	0.52
3:A:270:LEU:HD13	3:A:320:LEU:HD22	1.91	0.52
4:M:51:VAL:HG22	4:M:204:MET:HG2	1.92	0.52
14:n:427:PRO:HB3	14:n:450:TRP:HB3	1.91	0.52
14:n:508:PRO:HG3	16:p:6:HIS:HB3	1.92	0.52
26:C1:204:GLU:OE1	26:C1:210:ARG:NH1	2.43	0.52
46:L1:441:ILE:HG21	62:j1:15:PRO:HB3	1.91	0.52
69:L1:701:3PE:H222	64:l1:87:ARG:HA	1.91	0.52
3:A:267:ASN:OD1	3:A:311:ASN:ND2	2.41	0.52
46:L1:561:THR:O	46:L1:565:SER:OG	2.23	0.52
49:O1:14:THR:HG21	49:O1:116:LEU:HD22	1.90	0.52
36:U1:66:ASP:OD2	66:n1:1:ALA:N	2.43	0.52
2:m:12:VAL:HA	69:a:606:3PE:H321	1.90	0.52
4:B:212:SER:HB2	4:B:215:VAL:HG12	1.89	0.52
3:L:366:VAL:HG11	4:M:43:PRO:HB2	1.92	0.52
4:M:101:THR:HG22	7:T:65:VAL:HG22	1.92	0.52
14:n:254:ILE:HD11	14:n:388:ALA:HA	1.90	0.52
14:n:282:PHE:HD2	14:n:283:LEU:HD12	1.73	0.52
26:C1:133:GLU:OE1	27:D1:430:ARG:NH1	2.41	0.52
30:3:228:ILE:HB	30:3:583:THR:HG22	1.89	0.52
30:3:595:GLU:OE1	30:3:597:TRP:NE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:7:32:GLN:NE2	39:q1:122:GLU:O	2.35	0.52
36:T1:47:GLN:NE2	36:T1:70:LEU:O	2.43	0.52
46:L1:277:MET:HB3	46:L1:314:MET:HE3	1.91	0.52
48:N1:97:MET:HA	48:N1:100:MET:HG2	1.91	0.52
2:m:12:VAL:HG11	14:n:275:TRP:NE1	2.25	0.52
14:n:440:TYR:OH	15:o:196:CYS:O	2.23	0.52
30:3:60:GLU:OE1	30:3:78:ASN:ND2	2.42	0.52
30:3:396:ARG:NH1	30:3:416:THR:O	2.43	0.52
32:P1:280:THR:H	32:P1:283:LYS:HB3	1.75	0.52
43:H1:172:MET:HE2	52:Z1:49:MET:HE3	1.92	0.52
43:H1:281:ARG:NH1	43:H1:283:ASP:OD2	2.43	0.52
43:H1:316:PRO:HG3	52:Z1:56:ARG:HB3	1.92	0.52
36:U1:39:ASP:N	36:U1:39:ASP:OD1	2.43	0.52
3:A:438:ARG:HH22	7:E:33:LYS:HD2	1.74	0.52
4:M:20:GLN:OE1	4:M:22:GLN:NE2	2.42	0.52
18:r:92:THR:HA	18:r:95:GLU:HG2	1.90	0.52
27:D1:3:GLN:NE2	47:M1:135:ARG:O	2.38	0.52
30:3:569:LYS:HG3	30:3:571:ALA:HB2	1.90	0.52
47:M1:455:THR:OG1	59:g1:82:ARG:NH1	2.43	0.52
48:N1:109:ALA:HB3	48:N1:161:SER:HA	1.91	0.52
14:a:383:MET:HA	14:a:386:VAL:HG22	1.91	0.52
15:b:95:LEU:HB3	15:b:150:ILE:HG12	1.92	0.52
4:M:153:GLN:NE2	7:T:44:ASP:O	2.43	0.52
14:n:325:ALA:HB2	15:o:65:TRP:HH2	1.75	0.52
14:n:413:HIS:CE1	14:n:468:MET:HB2	2.45	0.52
16:p:151:LEU:HD11	16:p:159:MET:HE3	1.92	0.52
25:6:58:MET:SD	25:6:60:PHE:HB2	2.49	0.52
27:D1:249:ASP:OD2	27:D1:404:LYS:NZ	2.43	0.52
30:3:221:GLU:HB3	30:3:243:ARG:HG3	1.92	0.52
43:H1:32:GLN:HB2	43:H1:34:ARG:HG2	1.92	0.52
47:M1:435:THR:HG23	59:g1:64:PHE:HE1	1.75	0.52
48:N1:147:PRO:HG2	48:N1:148:LEU:HD12	1.92	0.52
49:O1:30:ASN:O	49:O1:126:ARG:NH2	2.43	0.52
14:a:87:ILE:HD11	14:a:168:ILE:HD12	1.91	0.52
1:t:54:ILE:CD1	14:n:218:THR:HG21	2.39	0.51
4:B:47:ILE:HD11	4:B:211:VAL:HG11	1.92	0.51
4:B:76:THR:HG23	4:B:81:SER:HA	1.92	0.51
4:B:153:GLN:NE2	7:T:33:ALA:O	2.43	0.51
4:M:36:ALA:HB3	4:M:207:VAL:HG12	1.91	0.51
69:L1:704:3PE:H2C2	48:N1:284:MET:HB3	1.92	0.51
49:O1:147:GLN:HB3	49:O1:279:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:a1:49:GLU:OE1	53:a1:52:ARG:NE	2.43	0.51
14:a:374:VAL:O	14:a:378:HIS:HB2	2.09	0.51
4:B:152:PHE:O	4:B:158:ARG:NH1	2.42	0.51
15:o:2:ALA:HB2	15:o:10:GLN:HE21	1.75	0.51
26:C1:96:LEU:HB2	26:C1:105:ILE:HG22	1.92	0.51
30:3:474:VAL:HG11	30:3:490:MET:HB2	1.92	0.51
32:P1:76:ARG:NH2	32:P1:103:ASN:O	2.44	0.51
32:P1:319:ARG:HA	32:P1:322:ARG:HE	1.76	0.51
47:M1:36:LEU:HB2	59:g1:67:VAL:HG22	1.91	0.51
36:U1:21:LEU:HD13	63:k1:53:ASN:HA	1.91	0.51
57:e1:40:ILE:HD12	60:h1:128:PRO:HB2	1.92	0.51
58:f1:56:TRP:NE1	60:h1:88:GLU:OE1	2.32	0.51
59:g1:109:ASN:OD1	68:p1:161:ARG:NH1	2.42	0.51
16:c:128:GLU:C	1:g:32:VAL:HG22	2.35	0.51
18:e:86:ILE:O	18:e:89:LEU:N	2.42	0.51
15:o:138:VAL:HG12	15:o:140:ASN:H	1.74	0.51
18:r:27:TRP:HZ2	19:s:84:PRO:HA	1.76	0.51
29:1:202:LYS:O	33:Q1:133:LYS:NZ	2.41	0.51
32:P1:248:MET:O	32:P1:322:ARG:NH2	2.43	0.51
47:M1:428:PRO:HD3	66:n1:105:TYR:HD2	1.75	0.51
66:n1:138:GLN:NE2	66:n1:155:PRO:O	2.43	0.51
16:c:63:ARG:HA	16:c:67:TYR:HD2	1.75	0.51
69:t:101:3PE:H111	16:p:187:SER:HA	1.92	0.51
14:n:41:LEU:HD22	14:n:451:ASN:HD21	1.75	0.51
14:n:97:MET:HE1	69:n:606:3PE:H261	1.92	0.51
30:3:44:GLU:OE2	33:Q1:114:LYS:NZ	2.43	0.51
44:J1:143:ALA:O	44:J1:147:CYS:N	2.36	0.51
59:g1:65:SER:HA	60:h1:32:THR:HG21	1.91	0.51
14:a:510:TYR:HB3	19:f:59:VAL:HG23	1.92	0.51
18:e:30:ARG:O	18:e:34:ASN:ND2	2.43	0.51
18:e:101:PRO:HA	18:e:104:LEU:HG	1.91	0.51
3:L:151:ASP:OD2	7:P:2:HIS:NE2	2.43	0.51
14:n:105:LEU:O	14:n:108:SER:OG	2.25	0.51
29:1:190:THR:HB	29:1:204:ARG:HG2	1.92	0.51
46:L1:159:TYR:HB3	47:M1:416:ARG:HH11	1.75	0.51
36:U1:17:TYR:OH	63:k1:27:TRP:NE1	2.37	0.51
17:d:86:MET:HE1	22:k:22:ALA:HA	1.92	0.51
17:d:121:LYS:HE3	22:k:50:PRO:HB2	1.91	0.51
12:V:7:GLY:O	12:V:11:ARG:CG	2.44	0.51
14:n:168:ILE:O	14:n:172:LYS:NZ	2.38	0.51
30:3:190:MET:HE3	30:3:690:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:29:TRP:HB3	31:9:32:LEU:HD12	1.92	0.51
48:N1:222:ASN:OD1	48:N1:319:LYS:NZ	2.43	0.51
1:g:50:PRO:CD	20:h:75:ARG:HH22	2.11	0.51
5:C:240:MET:HG3	69:E:202:3PE:H342	1.93	0.51
6:D:30:PHE:HE2	6:D:64:LEU:HD21	1.75	0.51
15:o:104:TRP:HA	15:o:207:MET:SD	2.50	0.51
27:D1:165:THR:HB	27:D1:169:TRP:CZ2	2.46	0.51
30:3:108:CYS:O	30:3:218:ARG:NH1	2.36	0.51
42:A1:105:GLU:HG3	44:J1:167:ILE:HD11	1.92	0.51
14:a:413:HIS:CD2	14:a:468:MET:HE3	2.46	0.51
15:b:163:TRP:O	15:b:171:LYS:HA	2.11	0.51
1:g:55:ARG:NH1	1:g:59:PHE:CE2	2.79	0.51
4:B:162:ASN:HB3	4:B:244:ILE:HD11	1.92	0.51
8:F:33:ARG:NH1	8:F:34:ASP:OD1	2.43	0.51
5:N:361:ILE:HA	5:N:365:LEU:HB2	1.92	0.51
14:n:38:ARG:NH2	14:n:451:ASN:O	2.44	0.51
16:p:184:THR:HG21	16:p:198:PHE:HZ	1.76	0.51
14:a:64:VAL:HA	14:a:68:PHE:HD2	1.76	0.51
44:J1:70:THR:HG22	45:K1:27:MET:HG2	1.92	0.51
46:L1:535:ARG:HB3	65:m1:10:LEU:HD13	1.93	0.51
48:N1:334:THR:HG22	48:N1:335:MET:HG3	1.92	0.51
49:O1:38:LEU:HD11	49:O1:234:VAL:HG21	1.93	0.51
50:X1:100:ARG:NH1	50:X1:103:GLN:OE1	2.41	0.51
64:l1:29:ARG:NH1	64:l1:32:ASP:OD2	2.40	0.51
14:a:405:LEU:HD11	14:a:471:MET:HE3	1.92	0.51
1:t:42:GLU:O	1:t:43:ARG:C	2.53	0.51
1:t:55:ARG:NH1	1:t:59:PHE:CE2	2.79	0.51
6:D:33:TYR:HA	6:D:37:CYS:HB2	1.93	0.51
6:D:120:ARG:NH1	73:D:301:HEC:O1A	2.44	0.51
17:q:13:PHE:HD1	17:q:14:PRO:HD2	1.76	0.51
26:C1:32:ILE:HG22	26:C1:33:LEU:HG	1.92	0.51
46:L1:184:LEU:HD13	47:M1:393:ILE:HG12	1.92	0.51
52:Z1:57:ARG:NH2	54:b1:48:THR:OG1	2.44	0.51
14:a:216:ASN:HD22	1:g:55:ARG:HD3	1.76	0.51
3:A:156:THR:O	3:A:239:SER:OG	2.25	0.50
13:I:83:GLN:O	13:I:87:ARG:HG2	2.11	0.50
25:6:87:ARG:NH2	43:H1:202:GLU:OE2	2.44	0.50
29:1:105:CYS:SG	29:1:267:THR:OG1	2.65	0.50
32:P1:169:SER:OG	32:P1:170:ASP:N	2.43	0.50
37:V1:5:LYS:NZ	37:V1:77:GLU:OE1	2.43	0.50
50:X1:43:MET:HE3	50:X1:47:TRP:HZ3	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:269:GLY:O	14:n:273:MET:N	2.41	0.50
29:1:93:LEU:HD13	29:1:129:MET:HE1	1.93	0.50
45:K1:78:LEU:HD11	45:K1:88:ASP:HB2	1.94	0.50
49:O1:170:ILE:HD11	49:O1:238:ILE:HD11	1.93	0.50
1:g:42:GLU:O	1:g:43:ARG:C	2.53	0.50
12:K:12:GLU:HA	12:K:15:ARG:HG2	1.91	0.50
5:N:138:MET:HE2	5:N:254:ASP:HB2	1.93	0.50
30:3:494:HIS:HB2	30:3:576:THR:HG22	1.93	0.50
35:S1:16:ARG:HH21	35:S1:69:ALA:HB2	1.76	0.50
48:N1:123:PRO:HG2	48:N1:126:MET:HG2	1.93	0.50
48:N1:248:LEU:HD23	48:N1:251:LEU:HD12	1.93	0.50
52:Z1:84:GLN:OE1	57:e1:104:ARG:NH1	2.44	0.50
64:l1:70:MET:HE1	64:l1:76:ILE:HG12	1.94	0.50
14:a:9:SER:O	14:a:99:ASN:ND2	2.44	0.50
16:c:144:ILE:HD12	16:c:239:ALA:HA	1.92	0.50
21:i:52:PHE:O	21:i:56:TYR:CB	2.56	0.50
4:M:169:LYS:HB2	4:M:238:LYS:HG3	1.94	0.50
9:R:42:ARG:NH2	71:R:103:CDL:OA3	2.45	0.50
30:3:477:ILE:HA	30:3:480:THR:HG22	1.93	0.50
47:M1:429:SER:O	59:g1:36:TYR:OH	2.28	0.50
66:n1:156:ALA:HB1	66:n1:161:ASP:HB3	1.93	0.50
14:a:150:LEU:HD23	14:a:206:ILE:HG21	1.94	0.50
16:c:132:LEU:CD1	1:g:29:MET:CG	2.89	0.50
69:t:101:3PE:H242	69:t:101:3PE:H332	1.94	0.50
3:L:254:ALA:HB2	3:L:323:HIS:HD2	1.76	0.50
69:R:104:3PE:H332	65:m1:87:LEU:HB2	1.93	0.50
27:D1:350:LYS:HG3	30:3:121:MET:HG3	1.94	0.50
46:L1:293:LEU:HD21	46:L1:418:MET:HB3	1.94	0.50
61:i1:18:ARG:NH1	66:n1:170:VAL:O	2.38	0.50
14:a:178:GLN:O	14:a:186:TRP:NE1	2.44	0.50
14:a:512:LYS:HG3	14:a:514:LYS:H	1.76	0.50
15:b:69:PRO:HA	15:b:72:ILE:HG22	1.93	0.50
20:h:37:HIS:ND1	20:h:40:GLU:OE2	2.45	0.50
4:B:78:LYS:HB2	4:B:129:ALA:HB1	1.94	0.50
4:M:52:LYS:HB2	4:M:203:ARG:HB3	1.93	0.50
14:n:377:PHE:O	14:n:381:LEU:CB	2.55	0.50
29:1:142:PHE:HB3	29:1:145:GLU:HB2	1.94	0.50
29:1:306:LEU:HD22	29:1:343:ILE:HD11	1.92	0.50
31:9:164:GLU:HB3	39:q1:109:ILE:HG12	1.94	0.50
32:P1:324:TYR:HB2	43:H1:65:THR:HA	1.93	0.50
35:S1:78:LEU:HD12	35:S1:86:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:S1:82:SER:N	35:S1:85:GLU:OE2	2.43	0.50
14:a:86:MET:HE3	14:a:184:PHE:HB2	1.93	0.50
5:C:30:TRP:HZ3	5:C:96:LEU:HD22	1.76	0.50
14:n:191:THR:HG23	14:n:245:ILE:HA	1.93	0.50
15:o:162:SER:HB2	15:o:198:GLU:HB2	1.93	0.50
20:u:56:TYR:HA	20:u:59:VAL:HG12	1.94	0.50
43:H1:61:MET:HG3	43:H1:63:PRO:HD3	1.94	0.50
14:a:208:MET:HA	14:a:211:THR:HG22	1.93	0.50
14:a:366:VAL:HG13	14:a:367:LEU:HG	1.94	0.50
18:e:82:TYR:OH	18:e:100:THR:OG1	2.29	0.50
3:A:86:LEU:HD13	3:A:99:ILE:HG12	1.92	0.50
3:L:354:VAL:HG22	3:L:407:LEU:HD13	1.94	0.50
14:n:331:ASN:HD21	17:q:21:ASP:HB2	1.74	0.50
29:1:279:LEU:HD12	29:1:283:HIS:HD2	1.76	0.50
46:L1:190:SER:HB3	46:L1:196:TRP:NE1	2.27	0.50
14:a:244:TYR:HA	14:a:247:ILE:HG22	1.93	0.50
14:a:261:TYR:HD1	14:a:333:LYS:HE2	1.76	0.50
71:L:502:CDL:OA4	5:N:5:ARG:NE	2.42	0.50
21:v:57:ASP:HB3	21:v:60:LYS:HB3	1.93	0.50
29:1:327:THR:HG22	29:1:328:GLY:H	1.76	0.50
46:L1:369:THR:OG1	46:L1:445:GLU:OE1	2.27	0.50
55:c1:11:LYS:HE3	55:c1:12:PRO:HD2	1.93	0.50
1:g:75:ASN:HD21	69:g:303:3PE:HN1	1.60	0.50
3:A:137:GLU:HB2	13:I:24:GLN:HB3	1.93	0.49
5:N:97:HIS:CE1	5:N:100:ARG:HH21	2.30	0.49
33:Q1:33:ARG:NH2	33:Q1:60:ASP:O	2.45	0.49
36:T1:37:MET:HA	36:T1:42:LEU:H	1.77	0.49
46:L1:253:VAL:HB	46:L1:310:LEU:HD11	1.93	0.49
14:a:457:GLY:HA2	14:a:460:ILE:HD12	1.93	0.49
15:b:195:GLN:HA	15:b:208:PRO:HA	1.92	0.49
31:9:145:THR:OG1	31:9:148:GLU:OE2	2.30	0.49
46:L1:16:LEU:HD23	46:L1:126:ILE:HD13	1.94	0.49
14:a:147:ILE:HG23	14:a:206:ILE:HB	1.94	0.49
14:a:242:GLU:HA	14:a:245:ILE:HD12	1.94	0.49
16:c:158:HIS:CE1	1:g:14:LYS:NZ	2.80	0.49
3:A:242:ARG:O	9:G:14:ILE:HA	2.12	0.49
4:M:46:ARG:NH1	4:M:375:SER:OG	2.43	0.49
14:n:76:GLY:O	14:n:80:ASN:CB	2.60	0.49
16:p:15:PRO:HG3	24:w:32:TYR:HE1	1.76	0.49
19:s:80:SER:HA	19:s:90:TYR:O	2.12	0.49
42:A1:6:VAL:O	42:A1:10:ASN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L1:139:GLN:HA	46:L1:142:ILE:HD12	1.93	0.49
48:N1:339:LEU:HD13	56:d1:34:MET:HE2	1.94	0.49
14:a:413:HIS:NE2	14:a:417:MET:HE2	2.27	0.49
15:b:52:HIS:CG	18:e:40:ASP:HB2	2.47	0.49
1:t:32:VAL:HG22	16:p:128:GLU:HB3	1.95	0.49
8:F:49:ARG:O	4:M:134:ARG:NH2	2.43	0.49
3:L:439:SER:O	69:L:501:3PE:N	2.39	0.49
4:M:275:LEU:HB2	4:M:410:VAL:HG13	1.95	0.49
10:S:14:PRO:HA	10:S:17:THR:HG22	1.94	0.49
14:n:199:LEU:HD22	14:n:238:PHE:HE1	1.76	0.49
14:n:439:ARG:HD2	15:o:199:ILE:HD12	1.95	0.49
32:P1:264:SER:HB2	32:P1:281:LYS:HG3	1.93	0.49
45:K1:67:ALA:HA	45:K1:70:GLU:HG2	1.94	0.49
47:M1:191:SER:HB3	70:M1:501:PC1:H12	1.94	0.49
61:i1:4:THR:HG23	61:i1:7:GLU:H	1.77	0.49
64:l1:4:THR:OG1	64:l1:6:ASP:OD1	2.29	0.49
14:a:175:ALA:HB2	19:f:36:PRO:HB3	1.95	0.49
14:n:416:ILE:HD11	17:q:85:ALA:HA	1.94	0.49
70:P1:502:PC1:H11	70:P1:502:PC1:H152	1.94	0.49
24:w:36:MET:HE3	24:w:40:LEU:HD11	1.94	0.49
27:D1:260:LEU:HB3	27:D1:265:ILE:HB	1.95	0.49
39:q1:117:VAL:O	39:q1:120:THR:OG1	2.26	0.49
43:H1:205:SER:OG	43:H1:279:ARG:NH1	2.40	0.49
47:M1:53:SER:OG	47:M1:54:ASN:N	2.45	0.49
47:M1:231:LEU:HD23	47:M1:235:LEU:HD12	1.95	0.49
49:O1:225:SER:O	49:O1:228:ALA:C	2.55	0.49
36:U1:48:VAL:O	36:U1:52:MET:HG3	2.12	0.49
14:a:309:THR:HA	14:a:312:ILE:HG22	1.94	0.49
16:c:71:HIS:O	16:c:76:GLN:NE2	2.46	0.49
3:A:3:THR:HG22	3:A:6:GLN:HG2	1.94	0.49
5:C:165:TRP:O	5:C:174:THR:OG1	2.30	0.49
7:T:67:THR:O	7:T:74:ALA:HA	2.12	0.49
14:n:240:HIS:HD2	14:n:244:TYR:CD2	2.25	0.49
29:1:69:GLY:HA2	29:1:224:ASN:ND2	2.27	0.49
44:J1:134:MET:HB3	44:J1:139:ILE:HG12	1.94	0.49
47:M1:244:ILE:O	68:p1:148:TYR:OH	2.28	0.49
50:X1:39:ASN:HB3	52:Z1:72:PRO:HG2	1.94	0.49
14:a:469:ILE:HG23	23:l:29:PHE:HD2	1.77	0.49
16:c:145:THR:CG2	1:g:13:TRP:CE3	2.95	0.49
3:L:270:LEU:HB3	3:L:320:LEU:HD11	1.93	0.49
27:D1:106:LEU:HD11	27:D1:391:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:L1:703:CDL:H311	71:L1:703:CDL:H132	1.93	0.49
63:k1:25:ARG:O	63:k1:28:LYS:NZ	2.44	0.49
64:l1:29:ARG:NH2	64:l1:31:GLU:OE2	2.46	0.49
1:t:13:TRP:HB3	16:p:146:TRP:HB2	1.95	0.49
2:z:28:LEU:HB2	2:z:29:PRO:HD3	1.95	0.49
25:6:77:TYR:HB3	25:6:167:LEU:HD22	1.94	0.49
25:6:101:THR:HA	25:6:129:CYS:HB3	1.95	0.49
32:P1:191:VAL:HG11	32:P1:242:VAL:HG11	1.95	0.49
48:N1:202:LEU:HD21	57:e1:2:PHE:HZ	1.78	0.49
14:a:71:MET:HG3	14:a:75:ILE:HD13	1.94	0.49
14:a:440:TYR:OH	15:b:196:CYS:O	2.29	0.49
17:d:131:ILE:HG22	17:d:132:GLN:HG2	1.95	0.49
20:h:57:ARG:HA	20:h:60:TYR:CE2	2.48	0.49
3:L:339:GLN:NE2	3:L:437:ILE:O	2.46	0.49
30:3:118:ASP:O	30:3:122:MET:HG2	2.13	0.49
31:9:22:ASN:OD1	31:9:25:ARG:NH2	2.45	0.49
45:K1:54:MET:HA	45:K1:57:MET:HG3	1.94	0.49
45:K1:96:LEU:HD23	48:N1:51:ARG:HH11	1.77	0.49
47:M1:430:HIS:HD2	47:M1:432:ARG:HH21	1.61	0.49
17:d:70:GLU:HA	17:d:73:ARG:HD2	1.94	0.49
5:C:100:ARG:NH1	72:C:402:HEM:O2A	2.40	0.48
11:J:10:TYR:HA	11:J:14:PHE:HB2	1.94	0.48
14:n:18:LEU:HB3	14:n:102:PHE:CZ	2.48	0.48
43:H1:75:PRO:HG2	43:H1:219:PRO:HB3	1.94	0.48
51:Y1:19:ARG:O	51:Y1:23:ILE:HG13	2.13	0.48
71:h1:201:CDL:H751	68:p1:47:VAL:HG21	1.95	0.48
14:a:96:ARG:HD2	16:c:57:TRP:HE1	1.78	0.48
19:f:31:PRO:O	19:f:96:GLN:NE2	2.46	0.48
4:B:113:ARG:NH1	4:B:210:GLY:O	2.46	0.48
8:F:35:ASP:OD2	8:F:61:ARG:NE	2.43	0.48
5:N:165:TRP:O	5:N:174:THR:OG1	2.31	0.48
13:I:63:GLN:NE2	19:f:15:THR:OG1	2.46	0.48
16:p:214:PHE:HE1	69:p:301:3PE:H242	1.78	0.48
27:D1:103:PHE:HA	27:D1:106:LEU:HB2	1.93	0.48
43:H1:28:LEU:O	43:H1:32:GLN:HG2	2.13	0.48
44:J1:83:GLY:HA2	44:J1:89:LEU:HD21	1.95	0.48
47:M1:59:ASP:OD2	47:M1:245:ARG:NH2	2.46	0.48
36:U1:47:GLN:NE2	36:U1:67:ALA:O	2.44	0.48
15:o:98:LYS:HZ2	20:u:65:PRO:HA	1.77	0.48
44:J1:19:LEU:HD11	45:K1:31:LEU:HB3	1.94	0.48
61:i1:82:HIS:ND1	68:p1:36:TYR:OH	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:l1:52:ARG:HB3	64:l1:56:GLU:HG3	1.94	0.48
14:a:93:ALA:H	14:a:167:THR:HG22	1.78	0.48
3:L:53:ASN:HD21	3:L:165:GLN:HB2	1.78	0.48
3:L:356:ARG:HG3	4:M:91:ALA:HA	1.95	0.48
14:n:107:PRO:HB3	16:p:25:LEU:HD13	1.96	0.48
46:L1:315:VAL:O	46:L1:318:GLY:N	2.46	0.48
47:M1:207:MET:HG2	47:M1:298:ILE:HG13	1.96	0.48
47:M1:443:PRO:HB3	69:M1:502:3PE:H3C1	1.95	0.48
60:h1:44:ASN:ND2	71:h1:201:CDL:O1	2.46	0.48
64:l1:53:SER:HA	64:l1:83:TYR:HB3	1.94	0.48
66:n1:169:ILE:O	66:n1:172:ARG:NH1	2.45	0.48
69:C:404:3PE:H272	12:V:35:ALA:HB1	1.96	0.48
25:6:102:LEU:HD22	25:6:110:LEU:HD13	1.96	0.48
27:D1:292:ASP:OD1	27:D1:292:ASP:N	2.47	0.48
32:P1:178:PHE:HZ	32:P1:241:LEU:HD21	1.77	0.48
34:7:1:GLY:N	34:7:42:ASP:OD2	2.46	0.48
50:X1:79:GLU:HG2	50:X1:80:PRO:HD3	1.96	0.48
50:X1:82:THR:HA	50:X1:85:TRP:CD1	2.48	0.48
17:d:59:LEU:HA	17:d:62:ILE:HG22	1.96	0.48
5:C:51:LEU:O	5:C:55:TYR:HB3	2.13	0.48
6:D:204:MET:HG3	69:E:202:3PE:H12	1.94	0.48
11:U:5:ILE:HG13	11:U:6:PRO:HD3	1.96	0.48
30:3:588:THR:HG21	33:Q1:63:GLU:HA	1.95	0.48
51:Y1:42:LEU:HG	71:Y1:401:CDL:H122	1.95	0.48
68:p1:98:ASP:OD2	68:p1:141:ARG:NH1	2.45	0.48
14:a:230:LEU:HD11	16:c:103:HIS:HB3	1.96	0.48
14:n:129:TYR:CE1	14:n:232:GLN:HG3	2.49	0.48
20:u:57:ARG:HA	20:u:60:TYR:CE1	2.49	0.48
27:D1:279:ASP:OD1	27:D1:279:ASP:N	2.46	0.48
40:r1:2:SER:O	71:r1:202:CDL:O1	2.31	0.48
16:c:86:PHE:O	16:c:89:SER:OG	2.25	0.48
16:c:135:SER:HA	70:g:302:PC1:H2D2	1.95	0.48
4:B:109:VAL:HG22	4:B:119:LEU:HD13	1.94	0.48
9:G:54:VAL:HG11	69:G:102:3PE:H2A1	1.95	0.48
27:D1:379:VAL:HB	27:D1:388:ARG:HB3	1.95	0.48
32:P1:217:ALA:HB2	32:P1:303:LEU:HD21	1.95	0.48
43:H1:86:TRP:HH2	43:H1:232:ILE:HG22	1.79	0.48
44:J1:24:SER:N	44:J1:80:GLU:O	2.45	0.48
48:N1:170:LEU:O	48:N1:295:ARG:NH2	2.46	0.48
48:N1:329:LEU:HD11	69:N1:402:3PE:H261	1.96	0.48
36:U1:73:PRO:HA	36:U1:76:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:50:PRO:HG2	20:h:75:ARG:HH22	1.76	0.48
4:B:118:ILE:HA	4:B:121:GLU:HG3	1.96	0.48
8:Q:53:ASP:OD1	8:Q:54:LEU:N	2.47	0.48
29:1:376:MET:HE3	29:1:376:MET:HB3	1.80	0.48
5:C:113:TRP:NE1	5:C:301:LEU:O	2.35	0.48
4:M:76:THR:HG23	4:M:81:SER:HA	1.95	0.48
4:M:309:VAL:HG23	4:M:326:THR:HG22	1.96	0.48
25:6:52:ARG:NH1	69:6:202:3PE:O12	2.44	0.48
25:6:186:TRP:HB2	70:6:203:PC1:H11	1.95	0.48
27:D1:155:THR:HB	27:D1:167:PHE:HA	1.96	0.48
47:M1:82:ASN:ND2	47:M1:335:GLU:OE1	2.39	0.48
49:O1:115:LEU:HD12	49:O1:121:GLY:HA2	1.96	0.48
14:a:426:PHE:O	14:a:429:HIS:HB2	2.14	0.48
2:m:2:HIS:CB	14:a:484:SER:OG	2.60	0.47
5:C:95:PHE:HE2	5:C:272:TRP:CZ3	2.31	0.47
15:o:52:HIS:CG	18:r:40:ASP:HB2	2.48	0.47
17:q:61:ARG:NH1	17:q:65:ASN:O	2.47	0.47
18:r:101:PRO:HA	18:r:104:LEU:HG	1.96	0.47
29:1:96:ASN:O	29:1:225:VAL:HG23	2.13	0.47
35:S1:64:LEU:HB3	35:S1:76:VAL:HB	1.96	0.47
43:H1:24:GLU:HA	43:H1:271:LEU:HD13	1.96	0.47
36:U1:44:SER:HB2	66:n1:16:LEU:HD11	1.96	0.47
14:a:97:MET:HE1	69:a:605:3PE:H2	1.95	0.47
15:b:95:LEU:O	15:b:150:ILE:HA	2.14	0.47
4:B:52:LYS:HB2	4:B:203:ARG:HB3	1.96	0.47
3:L:173:ASN:HA	3:L:176:ARG:HG2	1.96	0.47
11:U:21:ALA:HA	11:U:24:ILE:HD12	1.95	0.47
31:9:27:LEU:HD22	70:9:203:PC1:H251	1.96	0.47
34:7:18:TYR:OH	34:7:27:ARG:NH1	2.47	0.47
61:i1:83:TYR:OH	68:p1:48:ARG:NH1	2.47	0.47
66:n1:108:PRO:HA	66:n1:111:LYS:HB2	1.94	0.47
19:f:83:CYS:HB2	19:f:87:GLY:H	1.79	0.47
1:g:68:LEU:HB3	69:g:303:3PE:O32	2.13	0.47
1:t:35:LYS:HG3	16:p:128:GLU:CD	2.39	0.47
2:m:28:LEU:HB2	2:m:29:PRO:HD3	1.95	0.47
4:M:245:ARG:HB3	4:M:430:LEU:HD13	1.96	0.47
16:p:194:GLY:O	16:p:198:PHE:HB2	2.14	0.47
23:y:41:ARG:HH21	23:y:45:LEU:HD11	1.79	0.47
26:C1:175:ARG:NH2	26:C1:177:ASP:OD2	2.47	0.47
69:H1:401:3PE:N	52:Z1:142:TYR:O	2.45	0.47
69:M1:502:3PE:H351	59:g1:75:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:208:MET:HB2	14:a:219:PHE:CD2	2.49	0.47
15:b:98:LYS:HZ2	20:h:65:PRO:HA	1.80	0.47
16:c:58:TRP:CE3	69:c:301:3PE:H251	2.49	0.47
1:g:68:LEU:HB2	69:g:303:3PE:O32	2.14	0.47
21:i:17:LYS:HA	21:i:20:ARG:HG3	1.96	0.47
14:n:510:TYR:HB3	19:s:59:VAL:HG23	1.95	0.47
16:p:113:GLY:HA2	20:u:30:TRP:HZ2	1.78	0.47
27:D1:144:ILE:HG23	27:D1:177:MET:HG2	1.96	0.47
29:1:131:ALA:H	29:1:171:TYR:HH	1.62	0.47
61:i1:120:ARG:HH11	67:o1:39:VAL:HA	1.79	0.47
14:a:268:PHE:H	14:a:326:THR:HG22	1.80	0.47
2:z:32:TRP:CZ2	70:z:101:PC1:O14	2.68	0.47
3:A:53:ASN:HD22	3:A:170:PRO:HD3	1.80	0.47
3:L:24:ARG:NH1	3:L:383:LEU:O	2.47	0.47
13:I:1:MET:HA	13:I:17:ALA:HA	1.96	0.47
21:v:17:LYS:HA	21:v:20:ARG:HG2	1.95	0.47
42:A1:106:TRP:CE2	43:H1:291:LYS:HD2	2.48	0.47
47:M1:403:THR:HA	47:M1:406:TYR:CE2	2.49	0.47
36:U1:75:GLU:HA	36:U1:78:ASP:HB2	1.96	0.47
64:l1:68:LEU:HD13	64:l1:80:LEU:HD21	1.95	0.47
14:a:132:LEU:HD13	15:b:200:CYS:HA	1.96	0.47
14:a:481:GLU:N	14:a:481:GLU:OE1	2.47	0.47
1:g:69:PHE:O	69:g:303:3PE:C12	2.61	0.47
21:i:14:LEU:HA	21:i:17:LYS:HZ3	1.79	0.47
4:B:141:ARG:HD3	4:B:184:GLY:HA2	1.96	0.47
5:C:377:LEU:HG	8:F:20:TYR:HE2	1.80	0.47
3:L:51:LYS:O	3:L:176:ARG:NH2	2.48	0.47
27:D1:37:ASP:OD2	48:N1:51:ARG:NE	2.48	0.47
27:D1:148:LEU:HD23	27:D1:174:ARG:HG2	1.96	0.47
44:J1:59:TYR:HB3	44:J1:63:MET:HE1	1.96	0.47
46:L1:530:PRO:O	46:L1:534:HIS:HB2	2.14	0.47
48:N1:181:TYR:HA	48:N1:184:ILE:HD12	1.95	0.47
64:l1:93:THR:OG1	64:l1:95:VAL:O	2.30	0.47
1:g:31:ASN:O	1:g:35:LYS:HG2	2.15	0.47
3:L:242:ARG:O	9:R:14:ILE:HA	2.15	0.47
4:M:162:ASN:HB3	4:M:244:ILE:HD11	1.95	0.47
6:O:18:LEU:HD22	6:O:206:LEU:HB2	1.97	0.47
6:O:49:ARG:NH2	7:P:67:ASP:OD1	2.47	0.47
14:n:265:LYS:HD2	14:n:266:GLU:HG2	1.96	0.47
14:n:346:PHE:HD2	14:n:347:LEU:HD22	1.79	0.47
15:o:170:LEU:HD11	15:o:184:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:48:TRP:HZ3	18:r:98:ILE:HD12	1.78	0.47
25:6:71:HIS:CE1	27:D1:174:ARG:HE	2.33	0.47
29:1:139:ARG:HD2	29:1:141:GLU:HB2	1.97	0.47
43:H1:110:SER:OG	43:H1:143:GLU:OE2	2.24	0.47
44:J1:22:LYS:HD3	45:K1:28:SER:HB3	1.96	0.47
46:L1:418:MET:HA	46:L1:421:MET:HB2	1.97	0.47
47:M1:196:TRP:CH2	47:M1:302:MET:HE1	2.50	0.47
50:X1:129:LYS:HB2	54:b1:65:VAL:HG23	1.97	0.47
63:k1:29:ILE:HG13	63:k1:35:GLU:HG3	1.96	0.47
14:a:166:THR:O	14:a:170:ASN:HB3	2.14	0.47
14:a:439:ARG:N	77:a:603:HEA:O1A	2.47	0.47
77:a:604:HEA:H261	77:a:604:HEA:H172	1.65	0.47
15:b:196:CYS:SG	15:b:207:MET:HG3	2.54	0.47
16:c:145:THR:HG21	1:g:13:TRP:CH2	2.50	0.47
4:M:195:VAL:O	4:M:199:PHE:HB2	2.15	0.47
17:q:23:PRO:HG2	18:r:37:VAL:HG21	1.96	0.47
27:D1:425:PHE:HA	27:D1:428:ILE:HG12	1.97	0.47
29:1:288:THR:O	29:1:293:ASN:ND2	2.40	0.47
46:L1:187:VAL:HG22	47:M1:383:MET:HG2	1.96	0.47
16:c:128:GLU:HB2	1:g:32:VAL:CG2	2.26	0.47
23:l:36:PRO:HA	23:l:39:ILE:HD12	1.97	0.47
25:6:189:ARG:NH1	85:P1:501:NDP:O2X	2.48	0.47
31:9:134:VAL:HG21	31:9:167:ILE:HG21	1.97	0.47
54:b1:58:ASP:HA	54:b1:62:MET:HE2	1.96	0.47
56:d1:114:GLU:OE1	68:p1:152:ARG:NH2	2.48	0.47
15:b:146:MET:HE1	15:b:189:PRO:HB3	1.96	0.47
4:B:257:ILE:HG13	4:B:424:MET:HG3	1.97	0.47
6:D:171:TYR:HD2	6:D:175:THR:HB	1.80	0.47
14:n:200:PRO:HB3	16:p:93:PHE:HB2	1.97	0.47
15:o:83:ILE:HA	15:o:86:MET:HG2	1.97	0.47
15:o:86:MET:HA	15:o:89:GLU:HG2	1.97	0.47
23:y:36:PRO:HA	23:y:39:ILE:HD12	1.96	0.47
25:6:82:PHE:HA	43:H1:39:ILE:HD12	1.96	0.47
30:3:631:VAL:HG23	30:3:632:ARG:HD2	1.97	0.47
31:9:119:ILE:HG12	82:9:201:SF4:S3	2.55	0.47
44:J1:172:ASP:OD1	45:K1:80:LYS:NZ	2.47	0.47
51:Y1:101:GLY:HA3	51:Y1:110:ALA:HB2	1.96	0.47
61:i1:82:HIS:HA	61:i1:85:VAL:HG22	1.97	0.47
61:i1:103:ILE:HB	67:o1:47:ASP:HB3	1.95	0.47
1:t:31:ASN:O	1:t:35:LYS:HG2	2.15	0.46
3:A:48:GLU:O	3:A:165:GLN:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:46:ARG:NH2	4:B:110:GLU:OE2	2.46	0.46
5:C:53:MET:HE1	7:E:62:MET:SD	2.55	0.46
14:n:398:PRO:HB3	14:n:404:THR:HG22	1.95	0.46
16:p:63:ARG:HH22	24:w:24:GLY:HA3	1.80	0.46
20:u:53:CYS:HB2	20:u:56:TYR:HB2	1.96	0.46
23:y:24:MET:HA	23:y:27:VAL:HG12	1.97	0.46
31:9:76:GLU:OE2	31:9:101:ARG:NH1	2.45	0.46
43:H1:27:ILE:HD12	43:H1:271:LEU:HD12	1.96	0.46
46:L1:393:ASP:O	46:L1:397:GLU:HG2	2.15	0.46
50:X1:165:ARG:NH1	56:d1:87:ASP:OD2	2.39	0.46
14:a:11:ASN:OD1	14:a:14:ASP:HB2	2.15	0.46
12:K:15:ARG:HA	12:K:18:ILE:HG12	1.97	0.46
3:L:86:LEU:HB3	4:M:285:ILE:HG12	1.97	0.46
10:S:18:VAL:HG12	10:S:67:VAL:HG12	1.96	0.46
14:n:75:ILE:HG13	14:n:249:PRO:HG2	1.96	0.46
21:v:38:LYS:NZ	69:v:101:3PE:O22	2.47	0.46
22:x:33:ALA:HA	22:x:40:TRP:HE1	1.79	0.46
26:C1:192:GLN:HG3	33:Q1:72:TRP:HB3	1.97	0.46
27:D1:115:GLU:HB3	27:D1:194:ILE:HB	1.96	0.46
27:D1:339:LYS:NZ	31:9:131:ASP:OD1	2.47	0.46
30:3:201:ASP:OD2	30:3:268:ARG:NH2	2.43	0.46
36:T1:48:VAL:HG22	36:T1:52:MET:HE2	1.96	0.46
46:L1:378:LEU:HD11	63:k1:72:ILE:HG23	1.97	0.46
47:M1:196:TRP:HH2	47:M1:302:MET:HE1	1.80	0.46
48:N1:162:ILE:HD12	48:N1:282:MET:HG2	1.98	0.46
52:Z1:120:ILE:O	52:Z1:124:TYR:HB2	2.15	0.46
65:m1:126:ILE:HG22	68:p1:139:GLN:HG3	1.97	0.46
21:i:61:ASP:HA	21:i:64:GLU:OE1	2.15	0.46
29:1:91:LYS:HG2	29:1:219:PRO:HG2	1.97	0.46
30:3:114:CYS:HB3	30:3:117:GLN:HB2	1.97	0.46
30:3:266:LYS:O	30:3:270:ALA:CB	2.64	0.46
46:L1:341:MET:HE3	46:L1:454:ILE:HG12	1.97	0.46
49:O1:26:THR:HG23	49:O1:169:VAL:HG23	1.97	0.46
54:b1:1:AYA:H	54:b1:4:ILE:HD11	1.80	0.46
14:a:411:LYS:HG3	17:d:81:VAL:HG11	1.96	0.46
69:d:201:3PE:H351	69:d:201:3PE:H251	1.96	0.46
23:l:17:ASN:HD22	23:l:20:ARG:HD3	1.79	0.46
5:N:52:ALA:HA	5:N:55:TYR:HB3	1.96	0.46
77:n:604:HEA:H162	77:n:604:HEA:H132	1.74	0.46
15:o:144:LEU:O	15:o:213:MET:HA	2.15	0.46
19:s:91:LYS:NZ	19:s:92:LEU:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D1:343:GLU:O	27:D1:347:HIS:ND1	2.48	0.46
30:3:324:ASP:HB3	30:3:571:ALA:HB1	1.98	0.46
32:P1:108:ASP:OD1	32:P1:112:ASN:ND2	2.49	0.46
32:P1:215:VAL:O	32:P1:218:THR:OG1	2.25	0.46
47:M1:227:GLY:HA2	47:M1:230:ILE:HG22	1.98	0.46
48:N1:265:ILE:HG12	48:N1:344:ILE:HG12	1.96	0.46
52:Z1:68:ILE:HD11	54:b1:49:PRO:HB2	1.95	0.46
61:i1:79:TRP:HD1	68:p1:40:VAL:HG13	1.81	0.46
16:c:50:ASN:HB3	16:c:54:MET:HE1	1.97	0.46
2:m:2:HIS:HD2	14:a:484:SER:OG	1.97	0.46
4:B:97:SER:HA	7:T:20:ARG:HA	1.97	0.46
4:B:195:VAL:O	4:B:199:PHE:HB2	2.15	0.46
3:L:213:GLN:O	3:L:217:SER:OG	2.33	0.46
5:N:304:MET:HE1	5:N:362:ILE:HD11	1.98	0.46
14:n:132:LEU:O	14:n:138:HIS:ND1	2.36	0.46
14:n:268:PHE:H	14:n:326:THR:HB	1.79	0.46
27:D1:175:GLU:OE2	27:D1:188:ARG:NH1	2.48	0.46
47:M1:47:GLU:HG2	68:p1:92:ARG:HG2	1.98	0.46
36:U1:37:MET:N	36:U1:37:MET:SD	2.88	0.46
59:g1:97:TYR:O	59:g1:101:ASN:ND2	2.48	0.46
14:a:205:GLY:HA2	14:a:208:MET:SD	2.56	0.46
13:I:76:LEU:CD2	13:I:83:GLN:HG2	2.45	0.46
18:r:64:ALA:HA	18:r:67:ILE:HD12	1.96	0.46
31:9:42:TYR:HA	31:9:45:ARG:HG3	1.97	0.46
46:L1:152:PHE:HB2	46:L1:172:ILE:HD11	1.96	0.46
46:L1:154:LEU:HD13	46:L1:247:LEU:HD21	1.97	0.46
47:M1:67:ILE:HG22	69:M1:502:3PE:H3D1	1.97	0.46
48:N1:319:LYS:HE2	49:O1:267:THR:HG21	1.97	0.46
57:e1:98:SER:OG	57:e1:100:ARG:NH2	2.49	0.46
14:a:40:GLU:HG2	14:a:47:LEU:HB2	1.97	0.46
1:t:60:PRO:HG3	16:p:35:PHE:HD1	1.80	0.46
3:A:8:LEU:HD22	3:A:392:LEU:HB3	1.98	0.46
4:M:365:LYS:HG2	4:M:399:LEU:HD22	1.98	0.46
14:n:180:GLN:NE2	19:s:67:ASN:O	2.48	0.46
37:V1:34:LEU:HD22	37:V1:44:ARG:HA	1.98	0.46
47:M1:119:TYR:HE1	47:M1:157:SER:HB2	1.81	0.46
50:X1:120:ASP:OD1	50:X1:121:LEU:N	2.44	0.46
16:c:146:TRP:NE1	1:g:14:LYS:CB	2.70	0.46
17:q:79:LYS:HA	17:q:82:VAL:HG22	1.97	0.46
17:q:121:LYS:HD3	22:x:50:PRO:HB2	1.98	0.46
29:1:97:ALA:HB1	29:1:111:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:276:ARG:HG3	30:3:277:GLN:HG2	1.98	0.46
36:T1:51:ILE:O	36:T1:55:GLU:HG3	2.16	0.46
48:N1:190:MET:HE2	48:N1:205:LEU:HA	1.98	0.46
14:a:18:LEU:HD23	14:a:21:LEU:HD21	1.98	0.46
16:c:146:TRP:CZ2	1:g:14:LYS:HG3	2.50	0.46
18:e:44:GLU:HG3	18:e:46:LYS:H	1.80	0.46
33:Q1:60:ASP:N	33:Q1:60:ASP:OD1	2.49	0.46
43:H1:156:MET:HE1	43:H1:178:ALA:HB2	1.98	0.46
14:a:18:LEU:HB3	14:a:102:PHE:CZ	2.50	0.46
14:a:274:VAL:O	14:a:278:MET:HG2	2.16	0.46
2:z:7:ARG:HG2	14:n:479:LYS:O	2.15	0.46
4:B:36:ALA:HB3	4:B:207:VAL:HG13	1.98	0.46
14:n:240:HIS:O	14:n:243:VAL:HB	2.16	0.46
14:n:287:VAL:O	14:n:290:HIS:ND1	2.35	0.46
15:o:28:LEU:HD11	69:o:302:3PE:H322	1.98	0.46
29:1:89:ARG:NH1	29:1:217:GLY:O	2.49	0.46
30:3:273:GLY:O	30:3:549:HIS:NE2	2.43	0.46
32:P1:133:SER:OG	32:P1:134:HIS:N	2.48	0.46
42:A1:90:MET:HE2	42:A1:90:MET:HB2	1.64	0.46
60:h1:62:GLU:O	60:h1:65:GLU:HB2	2.16	0.46
62:j1:64:LEU:HD11	67:o1:102:GLU:HG3	1.96	0.46
14:a:468:MET:SD	14:a:471:MET:HE2	2.55	0.46
15:b:103:GLN:NE2	15:b:104:TRP:CE3	2.84	0.46
4:B:201:SER:HB2	4:B:228:GLY:HA2	1.98	0.45
11:J:44:GLU:HB3	11:J:54:HIS:HE2	1.81	0.45
16:p:112:LEU:HD13	16:p:118:PRO:HG3	1.97	0.45
26:C1:75:LEU:HA	26:C1:96:LEU:HD23	1.97	0.45
30:3:513:ALA:HA	30:3:516:LYS:HG2	1.98	0.45
37:V1:44:ARG:O	37:V1:48:GLU:HB2	2.16	0.45
38:W1:64:LYS:O	38:W1:68:MET:HG2	2.16	0.45
47:M1:11:LEU:HB3	47:M1:100:ILE:HD13	1.97	0.45
52:Z1:39:ILE:O	52:Z1:43:ILE:HG12	2.16	0.45
67:o1:59:ALA:O	67:o1:63:ILE:HG12	2.16	0.45
2:z:36:HIS:HB2	2:z:40:TYR:CZ	2.52	0.45
20:u:66:VAL:HA	20:u:69:VAL:HG22	1.97	0.45
22:x:15:ASN:HA	22:x:18:LEU:HB2	1.98	0.45
29:1:69:GLY:HA2	29:1:224:ASN:HD22	1.81	0.45
30:3:281:GLU:HB2	30:3:293:TYR:HD1	1.80	0.45
46:L1:293:LEU:HD11	46:L1:421:MET:HB3	1.98	0.45
48:N1:19:ILE:O	48:N1:23:SER:CB	2.64	0.45
53:a1:55:SER:HB2	53:a1:62:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:d1:29:PRO:HA	56:d1:32:VAL:HG22	1.99	0.45
14:a:413:HIS:HA	14:a:416:ILE:HG22	1.98	0.45
16:c:132:LEU:HD13	1:g:29:MET:HA	1.98	0.45
21:i:62:PHE:O	21:i:66:ARG:HB2	2.16	0.45
2:z:24:VAL:O	2:z:28:LEU:HG	2.16	0.45
8:F:13:LEU:CD1	16:c:161:GLN:HG2	2.45	0.45
4:M:242:GLY:O	4:M:423:SER:HA	2.16	0.45
4:M:437:ASP:OD1	4:M:437:ASP:N	2.47	0.45
11:U:33:ARG:HD3	12:V:51:LYS:HB2	1.97	0.45
13:I:1:MET:HG3	13:I:17:ALA:HB2	1.98	0.45
15:o:41:ILE:O	15:o:45:MET:HG2	2.16	0.45
16:p:205:GLY:HA2	16:p:208:VAL:HG12	1.99	0.45
30:3:470:VAL:HA	30:3:473:MET:HG2	1.97	0.45
36:T1:37:MET:N	36:T1:37:MET:SD	2.89	0.45
40:r1:13:TRP:O	52:Z1:27:ARG:NH1	2.49	0.45
43:H1:5:ASN:HA	43:H1:8:THR:HG22	1.99	0.45
47:M1:17:LEU:HD11	71:N1:401:CDL:H141	1.98	0.45
48:N1:246:LEU:HD12	48:N1:257:LEU:HD11	1.98	0.45
71:N1:401:CDL:H251	56:d1:35:GLY:HA3	1.98	0.45
14:a:344:PHE:O	14:a:348:PHE:HB3	2.17	0.45
14:n:465:VAL:HG22	77:n:603:HEA:H273	1.99	0.45
16:p:126:PRO:HA	16:p:130:PRO:HG2	1.98	0.45
42:A1:3:LEU:HD23	69:H1:401:3PE:H221	1.98	0.45
47:M1:75:LEU:HD23	47:M1:440:HIS:CE1	2.50	0.45
59:g1:95:VAL:HG11	68:p1:108:ARG:HH22	1.80	0.45
14:a:224:GLY:HA3	1:g:54:ILE:HD11	1.98	0.45
3:A:21:ASN:O	3:A:221:ARG:NH1	2.49	0.45
12:K:14:ALA:O	12:K:18:ILE:HG12	2.16	0.45
71:R:102:CDL:O1	69:Y1:402:3PE:N	2.39	0.45
14:n:168:ILE:HD13	14:n:189:LEU:HB2	1.99	0.45
17:q:25:PRO:HD2	17:q:64:PHE:HE1	1.81	0.45
27:D1:98:GLN:HE21	31:9:90:PRO:HA	1.81	0.45
44:J1:161:ALA:O	44:J1:165:ILE:HG12	2.17	0.45
46:L1:132:THR:O	46:L1:262:ARG:NH2	2.49	0.45
47:M1:257:MET:HE2	47:M1:257:MET:HB2	1.72	0.45
48:N1:210:ILE:HG22	48:N1:333:SER:HB3	1.99	0.45
49:O1:135:LEU:HD22	49:O1:152:TYR:CD1	2.51	0.45
12:V:51:LYS:HD2	12:V:53:LYS:HB2	1.98	0.45
69:n:606:3PE:N	16:p:64:GLU:OE1	2.46	0.45
18:r:49:ASP:OD1	18:r:53:ARG:NH2	2.49	0.45
25:6:135:TYR:CD1	31:9:119:ILE:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D1:360:PRO:HA	27:D1:380:SER:O	2.16	0.45
30:3:438:SER:O	30:3:441:GLU:HG3	2.17	0.45
32:P1:136:ASN:HD22	32:P1:291:ASP:HA	1.82	0.45
32:P1:263:TYR:HE2	32:P1:288:HIS:HE1	1.63	0.45
33:Q1:39:VAL:HG21	33:Q1:108:LYS:HG3	1.98	0.45
46:L1:180:ILE:HD12	47:M1:397:GLY:HA2	1.98	0.45
49:O1:36:ASN:OD1	49:O1:40:LYS:NZ	2.49	0.45
49:O1:46:LEU:HG	49:O1:235:VAL:HG13	1.99	0.45
14:a:35:ILE:HG13	14:a:462:LEU:HD21	1.97	0.45
22:k:11:ASP:OD1	22:k:11:ASP:N	2.50	0.45
3:A:328:ALA:HB2	3:A:427:PRO:HB2	1.99	0.45
4:B:264:ILE:HG22	4:B:317:SER:HA	1.99	0.45
8:F:109:LYS:HE3	12:V:6:LEU:HB2	1.98	0.45
16:p:255:SER:O	16:p:259:TRP:HB3	2.17	0.45
17:q:120:THR:HA	17:q:123:MET:HG2	1.99	0.45
29:1:309:LYS:HA	29:1:312:CYS:HB2	1.99	0.45
46:L1:336:LYS:HA	46:L1:336:LYS:HD3	1.79	0.45
46:L1:538:PRO:HB2	64:l1:88:VAL:HG22	1.98	0.45
14:a:514:LYS:HE2	19:f:62:ILE:HB	1.98	0.45
15:b:13:THR:HG23	15:b:188:ARG:HE	1.81	0.45
3:A:2:ALA:O	4:B:113:ARG:NE	2.43	0.45
4:B:243:GLU:HA	4:B:424:MET:O	2.17	0.45
5:C:132:VAL:HG11	5:C:178:PHE:HD2	1.82	0.45
8:F:74:ILE:HG12	9:G:39:ARG:NH1	2.32	0.45
3:L:155:ALA:HA	3:L:164:ALA:HB1	1.97	0.45
17:q:93:ALA:O	17:q:97:ILE:HG12	2.17	0.45
28:2:207:LYS:HD3	28:2:207:LYS:HA	1.80	0.45
39:q1:9:ARG:HH21	71:r1:202:CDL:HA22	1.82	0.45
46:L1:313:MET:HE2	46:L1:329:ILE:HA	1.98	0.45
2:m:6:ALA:HB3	2:m:9:GLN:HG2	1.98	0.45
2:m:10:LEU:HD11	14:a:477:ALA:HB3	1.98	0.45
4:M:212:SER:HB3	4:M:215:VAL:HG23	1.99	0.45
18:r:14:ARG:HA	18:r:17:THR:HG22	1.99	0.45
27:D1:65:VAL:HB	27:D1:77:ASP:HB3	1.97	0.45
29:1:15:LEU:HD13	29:1:271:GLU:HB2	1.99	0.45
30:3:462:ASP:OD1	30:3:462:ASP:N	2.44	0.45
47:M1:7:PRO:HB2	47:M1:34:ILE:HD11	1.98	0.45
51:Y1:128:LYS:HD3	51:Y1:128:LYS:HA	1.67	0.45
52:Z1:76:ALA:HB1	52:Z1:80:ARG:HH22	1.82	0.45
58:f1:38:ARG:HD3	58:f1:54:VAL:HB	1.98	0.45
14:a:487:TYR:OH	17:d:21:ASP:OD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:a:603:HEA:H172	77:a:603:HEA:H261	1.66	0.45
16:c:128:GLU:C	1:g:32:VAL:CG2	2.90	0.45
3:L:161:THR:HG21	3:L:235:ARG:H	1.82	0.45
6:O:158:ILE:HG13	6:O:160:MET:H	1.82	0.45
12:V:1:MET:HG3	12:V:2:LEU:HG	1.99	0.45
13:I:99:TYR:HA	13:I:102:ILE:HG22	1.99	0.45
14:n:372:TYR:HB2	14:n:432:GLY:HA3	1.99	0.45
23:y:15:VAL:HA	23:y:21:LEU:HD12	1.99	0.45
36:U1:26:ASP:OD1	36:U1:26:ASP:N	2.49	0.45
57:e1:37:LYS:HG3	60:h1:133:ILE:HG21	1.99	0.45
64:l1:129:PRO:HD3	67:o1:21:ILE:HB	1.99	0.45
77:a:604:HEA:H241	15:b:72:ILE:HG21	1.99	0.45
15:b:139:ASP:OD1	15:b:139:ASP:N	2.50	0.45
16:c:146:TRP:CD1	1:g:14:LYS:N	2.85	0.45
18:e:43:PRO:HB2	18:e:48:ILE:HD11	1.99	0.45
2:z:23:PHE:HE2	14:n:463:THR:HG23	1.82	0.44
3:A:27:SER:HA	3:A:199:ALA:O	2.17	0.44
4:B:239:TYR:HE2	4:B:421:LYS:HG3	1.82	0.44
6:O:124:GLU:OE1	6:O:191:ARG:NH2	2.50	0.44
7:P:141:HIS:HB2	7:P:176:ALA:HA	1.99	0.44
15:o:21:MET:HB3	21:v:45:ARG:HH21	1.81	0.44
70:9:204:PC1:H112	52:Z1:28:GLY:HA3	1.97	0.44
42:A1:70:ALA:HA	44:J1:54:MET:HE2	1.99	0.44
43:H1:20:LEU:HD23	43:H1:228:TYR:HB3	1.99	0.44
43:H1:181:MET:HA	43:H1:184:MET:HB2	1.98	0.44
46:L1:573:MET:HE2	46:L1:573:MET:HB2	1.83	0.44
47:M1:300:SER:HB3	47:M1:381:ILE:HG12	1.99	0.44
51:Y1:24:THR:HG21	51:Y1:69:PHE:HD2	1.82	0.44
52:Z1:67:ARG:O	52:Z1:71:MET:HG2	2.17	0.44
56:d1:11:LEU:HD23	69:d1:202:3PE:H11	1.99	0.44
63:k1:40:LYS:HD2	63:k1:40:LYS:HA	1.78	0.44
14:a:13:LYS:HE2	14:a:13:LYS:HB2	1.78	0.44
14:a:132:LEU:O	14:a:138:HIS:ND1	2.48	0.44
14:a:133:ALA:O	14:a:213:ARG:NH1	2.46	0.44
15:b:161:HIS:ND1	15:b:200:CYS:SG	2.90	0.44
16:c:213:THR:HA	16:c:216:ILE:HG12	1.99	0.44
3:L:192:ALA:HB3	3:L:221:ARG:HB3	2.00	0.44
4:M:312:PHE:HA	7:T:61:ALA:HA	1.99	0.44
5:N:126:THR:HG22	5:N:185:LEU:HB3	1.98	0.44
14:n:30:GLY:HA2	14:n:33:LEU:HD12	1.99	0.44
46:L1:137:MET:HE2	46:L1:137:MET:HB3	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:M1:313:THR:HA	47:M1:316:MET:SD	2.57	0.44
64:l1:3:MET:HE1	65:m1:62:PRO:HB3	1.99	0.44
14:a:23:GLY:HA3	14:a:73:MET:SD	2.57	0.44
14:a:119:GLU:HG3	23:l:46:LYS:HD2	1.99	0.44
14:a:265:LYS:NZ	14:a:489:SER:OG	2.51	0.44
15:b:124:PRO:HD2	15:b:127:ASP:HB2	1.99	0.44
16:c:26:LEU:HD23	16:c:49:THR:HG21	1.99	0.44
16:c:145:THR:HG23	1:g:13:TRP:CD2	2.50	0.44
17:d:75:THR:OG1	17:d:77:GLU:OE1	2.31	0.44
5:C:331:ASN:HA	5:C:334:ILE:HB	1.99	0.44
6:O:8:PRO:HG3	10:S:64:ASP:HB3	1.99	0.44
21:v:19:LEU:O	21:v:23:ILE:HG12	2.18	0.44
30:3:28:GLN:NE2	33:Q1:114:LYS:O	2.49	0.44
30:3:198:ASN:HA	30:3:201:ASP:HB2	1.99	0.44
38:W1:37:LEU:HD21	38:W1:88:GLY:HA3	2.00	0.44
43:H1:100:LEU:HD12	44:J1:49:SER:HB2	1.99	0.44
46:L1:67:HIS:NE2	46:L1:70:THR:OG1	2.40	0.44
53:a1:13:GLY:O	53:a1:17:VAL:HG23	2.17	0.44
61:i1:81:VAL:HG22	69:i1:201:3PE:H2A1	1.98	0.44
14:a:27:GLY:HA2	14:a:69:MET:HE2	1.99	0.44
14:a:135:ASN:ND2	1:g:56:THR:CG2	2.80	0.44
15:b:26:HIS:HA	15:b:29:MET:SD	2.57	0.44
19:f:55:ASN:O	19:f:76:HIS:HA	2.17	0.44
21:i:63:GLU:C	21:i:67:LYS:HZ3	2.25	0.44
1:t:43:ARG:HD2	1:t:81:TYR:CE1	2.53	0.44
12:K:38:TRP:O	12:K:42:LEU:HB2	2.17	0.44
14:n:212:ASP:OD1	14:n:217:THR:OG1	2.27	0.44
16:p:253:TYR:HA	16:p:257:TYR:HD2	1.82	0.44
25:6:126:MET:HE3	25:6:161:PRO:HG2	1.99	0.44
29:1:97:ALA:HB1	29:1:111:MET:HE1	1.99	0.44
31:9:21:ASP:HB3	70:9:204:PC1:H141	1.99	0.44
69:L1:701:3PE:H231	64:l1:87:ARG:HG2	1.99	0.44
47:M1:165:ILE:HG21	48:N1:268:THR:HA	1.98	0.44
48:N1:154:ILE:HD13	48:N1:195:PRO:HG3	1.99	0.44
36:U1:37:MET:HE2	36:U1:37:MET:HB2	1.84	0.44
52:Z1:127:ARG:NH1	57:e1:96:HIS:O	2.50	0.44
14:a:417:MET:O	14:a:421:VAL:HG12	2.18	0.44
15:b:142:VAL:O	15:b:211:LEU:HA	2.18	0.44
2:m:38:GLU:HG3	2:m:42:LYS:HE3	2.00	0.44
3:A:362:ARG:NH1	3:A:396:GLU:OE2	2.51	0.44
7:E:63:SER:OG	7:E:64:ALA:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:443:TYR:HE2	14:n:448:THR:HA	1.82	0.44
15:o:141:ARG:HA	15:o:210:VAL:HG13	1.99	0.44
25:6:160:PRO:HD3	27:D1:190:HIS:CD2	2.52	0.44
70:6:203:PC1:H351	43:H1:57:MET:HE3	1.98	0.44
28:2:164:LEU:HD13	28:2:169:ILE:HD13	2.00	0.44
30:3:571:ALA:O	30:3:582:GLN:HA	2.18	0.44
39:q1:6:VAL:HG11	71:r1:202:CDL:HB62	1.99	0.44
43:H1:221:ALA:O	43:H1:225:MET:HG3	2.18	0.44
47:M1:207:MET:HB2	47:M1:207:MET:HE2	1.77	0.44
47:M1:422:HIS:HB2	65:m1:59:ILE:HD12	1.98	0.44
48:N1:154:ILE:HD11	48:N1:194:LEU:HD23	1.99	0.44
48:N1:193:ILE:HG12	48:N1:266:ILE:HG12	1.99	0.44
14:a:287:VAL:O	14:a:290:HIS:ND1	2.42	0.44
4:B:275:LEU:HB2	4:B:410:VAL:HG13	2.00	0.44
5:C:200:LEU:HD13	72:C:402:HEM:HAD2	1.99	0.44
19:s:10:ASP:N	19:s:10:ASP:OD1	2.49	0.44
29:1:278:GLU:O	29:1:282:LYS:CB	2.66	0.44
43:H1:225:MET:O	43:H1:229:THR:OG1	2.19	0.44
44:J1:69:TYR:HB3	45:K1:27:MET:HE1	1.99	0.44
47:M1:130:LEU:HD12	47:M1:150:LEU:HB2	1.99	0.44
49:O1:189:PRO:HA	49:O1:192:MET:HG2	2.00	0.44
11:J:33:ARG:HH12	12:K:50:GLY:N	2.16	0.44
14:n:104:LEU:HD12	16:p:21:ALA:HA	2.00	0.44
18:r:36:LEU:HD21	18:r:43:PRO:HB3	2.00	0.44
26:C1:165:ASP:N	26:C1:165:ASP:OD1	2.47	0.44
27:D1:104:ASP:O	27:D1:108:TYR:HA	2.18	0.44
27:D1:128:ILE:HD13	27:D1:330:VAL:HG11	1.98	0.44
28:2:61:LEU:HD12	28:2:90:TYR:HB3	2.00	0.44
29:1:92:TYR:O	29:1:220:THR:HA	2.17	0.44
45:K1:44:THR:HG23	45:K1:60:PRO:HG3	1.99	0.44
46:L1:419:THR:HA	46:L1:422:TYR:CE2	2.52	0.44
47:M1:104:ILE:O	47:M1:108:MET:HG3	2.18	0.44
47:M1:319:HIS:HA	47:M1:322:THR:HG22	2.00	0.44
47:M1:379:LEU:HG	47:M1:383:MET:HE2	1.98	0.44
49:O1:156:LYS:O	49:O1:160:LEU:HB2	2.18	0.44
20:h:17:ASP:OD1	20:h:19:ARG:NH2	2.50	0.44
2:z:8:GLU:HB3	14:n:477:ALA:O	2.17	0.44
4:B:258:VAL:HA	4:B:323:GLY:HA3	1.99	0.44
6:D:75:ASN:OD1	6:D:76:ASP:N	2.47	0.44
14:n:398:PRO:HG2	14:n:494:TRP:HH2	1.83	0.44
15:o:145:PRO:HB2	15:o:216:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:204:HIS:NE2	16:p:249:TRP:HB2	2.33	0.44
19:s:23:ILE:HG22	19:s:27:LYS:HZ2	1.83	0.44
19:s:41:SER:OG	19:s:46:ASP:OD2	2.30	0.44
30:3:157:THR:HA	30:3:160:ILE:HD12	1.99	0.44
32:P1:259:PRO:HB2	32:P1:262:VAL:HG12	2.00	0.44
41:s1:35:LEU:HD13	41:s1:38:HIS:CE1	2.53	0.44
46:L1:357:ARG:HG2	66:n1:31:ILE:HG12	1.99	0.44
46:L1:560:LYS:HD3	65:m1:79:PHE:HE2	1.83	0.44
48:N1:86:PHE:HD2	48:N1:145:ILE:HG21	1.83	0.44
49:O1:165:PRO:HB3	49:O1:217:MET:HE3	2.00	0.44
36:U1:51:ILE:HG21	36:U1:67:ALA:HB1	1.98	0.44
51:Y1:3:ARG:NH1	51:Y1:4:PHE:HB2	2.33	0.44
14:a:164:PHE:O	14:a:168:ILE:HB	2.18	0.44
14:a:492:LEU:HD12	14:a:495:LEU:HD12	1.99	0.44
17:d:117:ALA:HB1	22:k:50:PRO:HA	1.99	0.44
8:F:53:ASP:OD1	8:F:54:LEU:N	2.50	0.44
11:J:44:GLU:HG2	11:J:53:LYS:HD3	2.00	0.44
10:S:17:THR:HA	10:S:20:GLU:HG3	2.00	0.44
14:n:386:VAL:O	14:n:390:MET:HG2	2.18	0.44
15:o:28:LEU:HA	15:o:31:VAL:HG12	1.98	0.44
27:D1:234:ILE:HG12	43:H1:280:PHE:HE1	1.82	0.44
29:1:118:LEU:HD13	29:1:225:VAL:HG13	2.00	0.44
46:L1:519:TYR:HB3	71:L1:703:CDL:H322	2.00	0.44
46:L1:542:LEU:HB3	47:M1:278:ARG:HD3	2.00	0.44
14:a:463:THR:O	14:a:467:ILE:HG12	2.17	0.44
15:b:15:PRO:O	15:b:18:GLU:HG2	2.18	0.44
16:c:150:SER:HA	1:g:10:ALA:CB	2.48	0.44
17:d:88:PHE:HA	17:d:91:PHE:HD2	1.83	0.44
2:m:37:LEU:HD23	2:m:40:TYR:HD2	1.82	0.43
5:C:58:ASP:O	5:C:62:ALA:N	2.52	0.43
14:n:413:HIS:CE1	14:n:417:MET:HE2	2.53	0.43
16:p:42:LEU:HD12	24:w:49:LEU:HD12	2.00	0.43
27:D1:154:VAL:HG13	27:D1:297:TYR:HE1	1.83	0.43
27:D1:339:LYS:NZ	34:7:65:ALA:O	2.48	0.43
27:D1:342:MET:HE2	30:3:101:HIS:HD2	1.82	0.43
29:1:276:LEU:HD21	29:1:297:VAL:HG11	2.00	0.43
56:d1:75:TYR:O	56:d1:79:GLN:HG2	2.17	0.43
59:g1:64:PHE:HA	59:g1:68:LEU:HB2	1.99	0.43
14:a:168:ILE:HG13	14:a:185:VAL:HG13	1.99	0.43
5:C:272:TRP:O	5:C:275:LEU:HB2	2.18	0.43
7:P:63:SER:OG	7:P:64:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:71:MET:HA	14:n:75:ILE:HD13	2.00	0.43
14:n:165:ILE:O	14:n:169:ILE:HG12	2.18	0.43
27:D1:107:ASP:HB3	27:D1:114:ASN:OD1	2.18	0.43
28:2:35:VAL:HG13	28:2:43:GLN:HB2	2.00	0.43
39:q1:43:LYS:NZ	39:q1:111:THR:O	2.47	0.43
47:M1:114:GLU:HG2	50:X1:168:PHE:HB3	1.99	0.43
49:O1:14:THR:HA	49:O1:17:LYS:HG2	2.00	0.43
52:Z1:64:LEU:O	52:Z1:68:ILE:HG13	2.18	0.43
59:g1:99:GLU:OE2	68:p1:108:ARG:NH1	2.48	0.43
61:i1:17:LEU:HD11	66:n1:162:LEU:HD22	1.99	0.43
14:a:107:PRO:HB3	16:c:25:LEU:HD13	1.99	0.43
14:a:199:LEU:HD22	14:a:238:PHE:HE1	1.83	0.43
15:b:128:LEU:HD22	15:b:132:GLU:HB2	1.99	0.43
16:c:172:TYR:HE2	1:g:29:MET:SD	2.41	0.43
1:g:43:ARG:HD2	1:g:81:TYR:CE1	2.53	0.43
2:m:1:VAL:HG22	14:a:485:VAL:HG23	2.01	0.43
3:A:343:MET:HA	3:A:346:CYS:HB2	2.01	0.43
4:B:49:LEU:HD22	4:B:127:THR:HG21	2.00	0.43
3:L:149:VAL:HG21	3:L:252:HIS:HB2	1.99	0.43
5:N:123:VAL:HG21	72:N:402:HEM:HBB1	2.01	0.43
6:O:33:TYR:HD1	6:O:37:CYS:HB2	1.84	0.43
6:O:160:MET:HE1	6:O:163:PRO:HG3	2.00	0.43
6:O:199:ASP:N	6:O:199:ASP:OD1	2.52	0.43
14:n:33:LEU:O	14:n:37:ILE:HG12	2.19	0.43
14:n:307:SER:O	14:n:311:ILE:HG12	2.18	0.43
14:n:425:PHE:HA	14:n:428:GLN:OE1	2.18	0.43
28:2:115:SER:HA	28:2:118:GLU:HG2	2.00	0.43
28:2:156:ILE:HG21	28:2:176:LEU:HD11	1.99	0.43
42:A1:68:GLU:OE1	42:A1:98:LEU:HG	2.18	0.43
62:j1:65:GLY:O	67:o1:103:ARG:NH1	2.51	0.43
16:c:142:VAL:HG23	1:g:13:TRP:HZ3	1.83	0.43
4:B:298:SER:HB2	4:B:343:GLN:HE21	1.84	0.43
7:E:146:PRO:HA	7:E:158:CYS:HA	2.00	0.43
4:M:318:ASP:OD1	4:M:318:ASP:N	2.51	0.43
15:o:146:MET:HE2	15:o:146:MET:HB2	1.82	0.43
16:p:52:LEU:HD23	16:p:56:GLN:HE22	1.83	0.43
18:r:18:TYR:HE2	18:r:32:GLY:HA3	1.83	0.43
25:6:79:MET:HE3	25:6:84:VAL:HG12	2.00	0.43
35:S1:41:VAL:O	35:S1:45:LYS:HG2	2.17	0.43
43:H1:179:TRP:HE1	52:Z1:42:LEU:HG	1.83	0.43
47:M1:333:ASN:O	47:M1:337:ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N1:115:LEU:O	48:N1:119:THR:OG1	2.28	0.43
57:e1:68:ARG:HB3	57:e1:71:THR:HB	2.00	0.43
57:e1:85:LEU:O	57:e1:89:GLY:N	2.52	0.43
61:i1:68:LEU:HA	61:i1:71:VAL:HG22	2.00	0.43
68:p1:105:ILE:HG21	68:p1:134:VAL:HG11	2.00	0.43
14:a:220:PHE:CZ	14:a:231:TYR:HB2	2.53	0.43
18:e:78:HIS:CE1	21:i:14:LEU:HD11	2.53	0.43
6:O:27:ARG:NH2	6:O:172:ASP:OD2	2.52	0.43
6:O:152:TYR:OH	10:S:64:ASP:OD2	2.24	0.43
13:I:22:THR:OG1	13:I:24:GLN:NE2	2.51	0.43
14:n:275:TRP:O	14:n:279:SER:OG	2.35	0.43
29:1:368:GLY:HA3	29:1:399:ILE:HD11	2.00	0.43
43:H1:169:GLN:HE21	43:H1:174:LEU:HD12	1.82	0.43
46:L1:383:MET:HB3	46:L1:386:LEU:HD12	2.00	0.43
48:N1:110:PRO:HD3	48:N1:160:THR:HG21	2.00	0.43
58:f1:42:MET:HE3	68:p1:71:PRO:HD2	2.00	0.43
65:m1:28:THR:O	65:m1:32:GLN:HG3	2.18	0.43
14:a:86:MET:HE1	14:a:185:VAL:HG23	2.00	0.43
14:a:94:PHE:HB3	14:a:97:MET:HG2	2.01	0.43
24:w:33:ARG:NE	46:L1:503:GLU:CD	2.77	0.43
30:3:366:THR:OG1	30:3:488:LYS:O	2.29	0.43
30:3:595:GLU:O	30:3:599:ILE:HG12	2.18	0.43
31:9:23:ALA:HA	54:b1:16:PRO:HG3	2.00	0.43
59:g1:86:TRP:NE1	68:p1:65:ARG:O	2.42	0.43
14:a:97:MET:HA	14:a:100:MET:HG2	2.00	0.43
15:b:104:TRP:NE1	15:b:203:ASN:H	2.16	0.43
19:f:52:SER:OG	19:f:53:ILE:N	2.51	0.43
23:l:12:PRO:HB2	81:l:601:TGL:HG32	2.01	0.43
3:A:46:ARG:HD3	3:A:231:LEU:HD22	2.01	0.43
3:A:273:ALA:HB2	3:A:407:LEU:HD11	1.99	0.43
7:P:72:SER:HB2	7:P:92:ARG:HA	2.01	0.43
8:Q:107:TRP:HA	8:Q:110:LYS:HE2	2.01	0.43
16:p:16:TRP:CH2	24:w:21:HIS:HB2	2.53	0.43
25:6:99:ALA:HA	25:6:126:MET:HB3	2.01	0.43
26:C1:81:VAL:HG22	27:D1:388:ARG:HG2	2.01	0.43
30:3:243:ARG:HG2	30:3:244:THR:HG23	2.01	0.43
31:9:108:THR:O	31:9:153:LYS:NZ	2.48	0.43
39:q1:11:VAL:HA	39:q1:14:VAL:HG22	2.01	0.43
44:J1:47:GLY:HA3	45:K1:49:LEU:HD22	2.01	0.43
47:M1:252:PRO:HB3	56:d1:117:HIS:CG	2.54	0.43
48:N1:131:LEU:HA	48:N1:135:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Z1:85:ILE:HG12	52:Z1:127:ARG:HH21	1.82	0.43
17:d:41:LYS:HA	17:d:41:LYS:HD2	1.84	0.43
17:d:114:ASP:O	17:d:118:MET:HG2	2.18	0.43
19:f:54:SER:O	19:f:77:LYS:NZ	2.43	0.43
3:A:68:LYS:HD2	3:A:121:SER:HB3	2.01	0.43
8:Q:95:LYS:HE3	8:Q:95:LYS:HB2	1.86	0.43
25:6:88:ALA:O	27:D1:54:GLN:NE2	2.47	0.43
36:T1:26:ASP:OD1	36:T1:26:ASP:N	2.52	0.43
38:W1:92:LEU:O	38:W1:96:ILE:HG12	2.19	0.43
42:A1:10:ASN:HD21	43:H1:83:LEU:CB	2.32	0.43
48:N1:233:LEU:HA	48:N1:236:LYS:HB2	1.99	0.43
63:k1:41:LEU:HD22	63:k1:46:LEU:HB2	2.01	0.43
63:k1:44:ARG:NH1	66:n1:38:TYR:OH	2.52	0.43
65:m1:124:PHE:HD1	68:p1:135:THR:HG21	1.84	0.43
16:c:79:LEU:HB3	16:c:233:PHE:CZ	2.54	0.43
17:d:121:LYS:HB2	22:k:50:PRO:HB2	2.01	0.43
18:e:93:LEU:HG	18:e:98:ILE:HG23	2.00	0.43
1:t:14:LYS:HB2	16:p:146:TRP:NE1	2.34	0.43
6:D:223:LYS:O	6:D:227:TRP:HB2	2.19	0.43
13:I:67:GLN:NE2	16:c:67:TYR:O	2.38	0.43
14:n:97:MET:HB2	14:n:159:LEU:HD13	2.01	0.43
14:n:427:PRO:HA	14:n:430:PHE:HD2	1.83	0.43
14:n:429:HIS:CD2	69:o:302:3PE:H331	2.54	0.43
15:o:144:LEU:HD13	15:o:184:VAL:HG21	2.01	0.43
17:q:67:SER:OG	18:r:69:GLU:OE1	2.31	0.43
26:C1:83:VAL:HG12	26:C1:85:THR:HG22	2.00	0.43
27:D1:318:MET:HE2	27:D1:318:MET:HB2	1.81	0.43
29:1:90:PRO:HB3	29:1:132:ARG:HD2	2.00	0.43
83:1:501:FMN:N1	83:1:501:FMN:O3'	2.43	0.43
31:9:40:LEU:HD12	31:9:43:LEU:HD23	2.01	0.43
32:P1:199:LYS:HE2	32:P1:199:LYS:HB3	1.86	0.43
46:L1:547:LYS:HB3	46:L1:547:LYS:HE2	1.77	0.43
49:O1:59:SER:HA	49:O1:62:THR:HG22	2.00	0.43
49:O1:223:TYR:CE2	49:O1:234:VAL:HG12	2.53	0.43
49:O1:319:LEU:HD23	49:O1:319:LEU:HA	1.89	0.43
15:b:52:HIS:CE1	15:b:54:SER:HB3	2.53	0.43
3:A:439:SER:HB3	69:A:501:3PE:H111	2.01	0.43
3:L:260:PRO:HB2	3:L:264:ASN:HB3	1.99	0.43
6:O:75:ASN:OD1	6:O:79:GLU:N	2.49	0.43
7:P:84:GLY:CA	7:P:100:HIS:O	2.67	0.43
17:q:131:ILE:HG21	21:v:49:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:379:LEU:HD13	30:3:384:PRO:HG2	2.00	0.43
30:3:399:TRP:HE3	30:3:400:LEU:HD12	1.84	0.43
45:K1:54:MET:HB2	57:e1:25:PRO:HD2	2.01	0.43
46:L1:193:MET:HE3	46:L1:193:MET:HB3	1.83	0.43
46:L1:298:ILE:O	46:L1:302:ILE:HG12	2.18	0.43
48:N1:112:HIS:HE1	48:N1:164:MET:HE3	1.83	0.43
14:a:55:ASN:HA	14:a:58:VAL:HG12	2.00	0.43
14:a:65:MET:HA	14:a:69:MET:SD	2.59	0.43
14:a:216:ASN:HD21	1:g:54:ILE:C	2.27	0.43
15:b:64:ILE:HA	15:b:67:ILE:HG22	2.00	0.43
3:A:155:ALA:HA	3:A:164:ALA:HB1	2.01	0.42
3:A:369:LEU:HD12	3:A:375:VAL:HG23	2.01	0.42
71:G:101:CDL:H512	71:G:101:CDL:HA32	2.00	0.42
3:L:106:LEU:HA	3:L:109:VAL:HG12	2.01	0.42
3:L:282:CYS:O	4:M:143:GLN:NE2	2.52	0.42
4:M:124:LEU:HA	4:M:127:THR:HG22	2.01	0.42
5:N:89:MET:HE3	5:N:89:MET:HB3	1.87	0.42
14:n:55:ASN:HA	14:n:58:VAL:HG22	2.01	0.42
15:o:105:TYR:O	15:o:207:MET:CE	2.66	0.42
19:s:23:ILE:HG22	19:s:27:LYS:NZ	2.34	0.42
25:6:106:MET:HE1	27:D1:53:PRO:HB2	2.01	0.42
27:D1:338:MET:HE3	27:D1:338:MET:HB3	1.91	0.42
28:2:60:TRP:CD1	28:2:60:TRP:H	2.37	0.42
31:9:52:TYR:HE1	31:9:56:LYS:HE3	1.84	0.42
32:P1:57:MET:HE3	32:P1:57:MET:HB3	1.84	0.42
49:O1:42:ILE:O	49:O1:46:LEU:HB2	2.18	0.42
14:a:74:MET:HA	14:a:78:PHE:HD2	1.83	0.42
19:f:86:CYS:SG	19:f:87:GLY:N	2.91	0.42
1:g:11:ARG:CZ	71:g:301:CDL:HA62	2.32	0.42
21:i:60:LYS:NZ	21:i:60:LYS:O	2.52	0.42
3:A:332:ASP:OD1	3:A:333:ASP:N	2.52	0.42
14:n:171:MET:HG3	16:p:8:TYR:CZ	2.53	0.42
29:1:215:VAL:H	29:1:220:THR:HG21	1.84	0.42
31:9:119:ILE:HG13	31:9:121:CYS:HB3	2.01	0.42
47:M1:433:GLU:O	47:M1:437:MET:HG2	2.19	0.42
48:N1:19:ILE:O	48:N1:23:SER:OG	2.31	0.42
64:l1:135:ASN:HA	64:l1:152:VAL:HB	2.01	0.42
16:c:147:ALA:O	16:c:159:MET:HE1	2.20	0.42
17:d:12:ALA:HA	19:f:56:LYS:HZ3	1.84	0.42
17:d:134:PHE:HZ	22:k:44:PRO:HG2	1.84	0.42
21:i:25:GLY:HA2	21:i:28:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:6:ALA:HB3	2:z:9:GLN:HG2	2.01	0.42
3:A:384:LEU:HD23	3:A:384:LEU:HA	1.90	0.42
4:B:393:MET:HA	4:B:394:PRO:HD3	1.92	0.42
5:C:83:HIS:HE1	72:C:401:HEM:NB	2.17	0.42
9:G:50:PRO:HA	9:G:53:VAL:HG12	2.00	0.42
5:N:24:PRO:HB2	5:N:27:ILE:HG23	2.01	0.42
5:N:275:LEU:HD23	5:N:275:LEU:HA	1.88	0.42
14:n:182:PRO:HB3	14:n:256:HIS:HE1	1.84	0.42
34:7:68:HIS:ND1	34:7:69:PRO:O	2.51	0.42
45:K1:40:LEU:HD13	48:N1:71:LEU:HD23	2.01	0.42
65:m1:50:TYR:HE2	66:n1:168:HIS:HB3	1.84	0.42
66:n1:97:LYS:HB3	66:n1:173:PRO:HB2	2.00	0.42
15:b:197:SER:O	15:b:197:SER:OG	2.28	0.42
1:t:29:MET:HE3	16:p:172:TYR:CE2	2.54	0.42
2:z:23:PHE:HA	14:n:466:LEU:HD13	2.00	0.42
5:C:51:LEU:O	5:C:55:TYR:CB	2.67	0.42
4:M:141:ARG:HD2	4:M:184:GLY:H	1.84	0.42
4:M:171:ALA:HB2	4:M:235:ALA:HB3	2.02	0.42
5:N:151:SER:HB3	5:N:161:VAL:HG21	2.00	0.42
17:q:114:ASP:OD1	17:q:115:TRP:N	2.53	0.42
25:6:48:ASN:ND2	25:6:180:GLU:O	2.51	0.42
30:3:601:ARG:HA	30:3:611:LEU:HD12	2.02	0.42
35:S1:63:LYS:HA	35:S1:63:LYS:HD2	1.83	0.42
49:O1:234:VAL:O	49:O1:238:ILE:HG12	2.19	0.42
50:X1:46:ARG:NH1	52:Z1:75:GLN:OE1	2.52	0.42
55:c1:7:PRO:HD2	55:c1:10:ALA:HB2	2.00	0.42
14:a:105:LEU:HD23	14:a:105:LEU:HA	1.92	0.42
16:c:214:PHE:HE1	69:c:301:3PE:H242	1.84	0.42
21:i:20:ARG:HA	21:i:23:ILE:HG12	2.01	0.42
2:z:29:PRO:HB3	23:y:34:ALA:HB2	2.00	0.42
3:A:378:ASP:O	3:A:382:SER:OG	2.28	0.42
6:D:147:LEU:HD12	6:D:157:ALA:HB1	2.01	0.42
5:N:257:MET:SD	6:O:120:ARG:NH1	2.90	0.42
14:n:107:PRO:HB3	16:p:25:LEU:HB2	2.02	0.42
27:D1:275:TYR:CZ	27:D1:367:ILE:HG23	2.55	0.42
32:P1:48:PRO:HA	32:P1:71:LEU:O	2.20	0.42
44:J1:22:LYS:HD2	45:K1:23:ARG:HG3	2.01	0.42
44:J1:150:TRP:HZ2	48:N1:19:ILE:HG12	1.84	0.42
46:L1:386:LEU:HD23	46:L1:386:LEU:HA	1.90	0.42
50:X1:43:MET:HE3	50:X1:47:TRP:CZ3	2.53	0.42
14:a:362:SER:HA	14:a:365:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:a:487:TYR:O	14:a:491:ASN:ND2	2.52	0.42
16:c:58:TRP:CD2	69:c:301:3PE:H251	2.54	0.42
16:c:125:ASN:HA	16:c:126:PRO:HD3	1.88	0.42
1:g:69:PHE:O	69:g:303:3PE:H122	2.19	0.42
3:A:411:CYS:O	3:A:415:PHE:HB2	2.20	0.42
3:L:170:PRO:HG2	3:L:173:ASN:HB2	2.01	0.42
6:O:156:GLN:HE21	10:S:57:PHE:HZ	1.67	0.42
6:O:195:GLU:OE2	6:O:201:ARG:NE	2.53	0.42
14:n:416:ILE:HG22	14:n:464:ALA:HB2	2.01	0.42
14:n:449:THR:HG21	15:o:5:PHE:HE1	1.84	0.42
27:D1:177:MET:HE2	27:D1:214:PHE:CZ	2.55	0.42
27:D1:208:LEU:HA	27:D1:211:ILE:HG22	2.01	0.42
30:3:121:MET:HE3	30:3:121:MET:HB3	1.85	0.42
35:S1:21:HIS:HA	35:S1:55:ARG:O	2.19	0.42
44:J1:150:TRP:HA	44:J1:153:VAL:HG22	2.01	0.42
44:J1:152:MET:HE2	44:J1:152:MET:HB2	1.85	0.42
45:K1:21:MET:HE2	45:K1:21:MET:HB2	1.89	0.42
46:L1:173:LEU:HD13	47:M1:405:MET:HE3	2.01	0.42
46:L1:473:PRO:HA	46:L1:474:PRO:HD3	1.90	0.42
46:L1:550:LEU:HB2	47:M1:275:ILE:HG12	2.01	0.42
48:N1:338:PRO:HA	50:X1:169:TRP:HZ2	1.83	0.42
71:N1:401:CDL:H781	71:N1:401:CDL:H812	1.91	0.42
49:O1:188:ASP:HB3	49:O1:191:GLU:HB3	2.01	0.42
50:X1:40:LYS:HD3	50:X1:40:LYS:HA	1.78	0.42
51:Y1:133:GLU:OE2	51:Y1:139:LYS:NZ	2.52	0.42
59:g1:61:PHE:O	59:g1:65:SER:HB2	2.19	0.42
62:j1:33:TRP:O	62:j1:37:LEU:HG	2.20	0.42
62:j1:61:ASP:OD1	62:j1:61:ASP:N	2.53	0.42
19:f:23:ILE:HG22	19:f:27:LYS:NZ	2.34	0.42
2:m:39:SER:HA	2:m:42:LYS:HD2	2.02	0.42
2:m:40:TYR:O	2:m:41:LYS:C	2.63	0.42
3:A:439:SER:O	69:A:501:3PE:N	2.45	0.42
4:B:116:ILE:O	4:B:120:MET:HG3	2.19	0.42
4:B:252:LEU:HA	4:B:328:SER:O	2.19	0.42
3:L:140:GLU:OE2	7:T:50:LEU:N	2.49	0.42
4:M:102:ARG:HG3	4:M:176:LEU:HD13	2.02	0.42
14:n:363:LEU:O	14:n:367:LEU:HB2	2.19	0.42
16:p:15:PRO:HG3	24:w:32:TYR:CE1	2.53	0.42
30:3:142:ILE:O	30:3:191:PHE:N	2.44	0.42
46:L1:130:ILE:O	46:L1:134:ALA:HB2	2.19	0.42
46:L1:457:LEU:HD23	46:L1:457:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:M1:216:LEU:HD23	47:M1:287:ALA:HB1	2.02	0.42
51:Y1:113:GLY:HA2	69:Y1:403:3PE:H371	2.01	0.42
54:b1:1:AYA:HB2	54:b1:4:ILE:HG12	2.01	0.42
18:e:107:ASP:OD1	18:e:107:ASP:N	2.51	0.42
20:h:37:HIS:HA	20:h:40:GLU:HG2	2.02	0.42
1:t:69:PHE:C	69:t:101:3PE:H122	2.44	0.42
3:L:145:MET:HE2	3:L:252:HIS:HD2	1.84	0.42
13:I:76:LEU:HD22	13:I:83:GLN:HG3	2.00	0.42
15:o:33:LEU:HD12	21:v:30:ALA:HB1	2.01	0.42
29:1:48:ILE:HD12	29:1:235:CYS:HB3	2.01	0.42
29:1:278:GLU:O	29:1:282:LYS:HB2	2.20	0.42
32:P1:35:VAL:HG13	32:P1:62:MET:HG3	2.02	0.42
36:T1:35:HIS:HB2	36:T1:38:LYS:HG2	2.02	0.42
46:L1:504:LEU:HD23	46:L1:507:LEU:HD12	2.02	0.42
14:a:52:GLN:HB2	15:b:202:SER:HB2	2.01	0.42
14:a:74:MET:HE2	14:a:249:PRO:HG2	2.00	0.42
17:d:114:ASP:OD1	17:d:115:TRP:N	2.52	0.42
19:f:27:LYS:HG3	19:f:29:LEU:HD23	2.02	0.42
5:N:183:PHE:CD1	72:N:401:HEM:HMB3	2.55	0.42
17:q:96:LEU:HA	17:q:99:GLU:HB3	2.02	0.42
27:D1:17:ALA:HB2	27:D1:30:PRO:HA	2.01	0.42
30:3:26:VAL:HB	30:3:68:ALA:HA	2.02	0.42
30:3:533:THR:HA	30:3:556:MET:HE1	2.01	0.42
70:9:204:PC1:H2E2	43:H1:175:LEU:HD21	2.02	0.42
41:s1:66:SER:OG	41:s1:68:ARG:NH1	2.51	0.42
43:H1:286:MET:O	43:H1:290:TRP:HB2	2.20	0.42
43:H1:289:LEU:HD13	43:H1:293:PHE:HD2	1.85	0.42
69:M1:503:3PE:H292	69:M1:503:3PE:H2C2	1.89	0.42
36:U1:66:ASP:O	36:U1:70:LEU:HG	2.20	0.42
14:a:232:GLN:OE1	14:a:236:TRP:NE1	2.46	0.42
16:c:120:GLY:HA2	1:g:49:TYR:CE2	2.55	0.42
1:g:14:LYS:HG3	1:g:18:TYR:HE2	1.85	0.42
4:B:218:GLN:HA	4:B:221:GLU:HG3	2.02	0.42
69:C:403:3PE:O12	9:G:44:ARG:NE	2.50	0.42
6:D:41:HIS:HE1	6:D:111:PRO:HD2	1.85	0.42
14:n:202:LEU:HD22	14:n:238:PHE:CE2	2.54	0.42
15:o:44:LEU:HD11	21:v:22:HIS:ND1	2.35	0.42
18:r:44:GLU:O	18:r:48:ILE:HG12	2.20	0.42
19:s:56:LYS:HA	19:s:75:LEU:O	2.19	0.42
25:6:111:ARG:HA	25:6:111:ARG:HD2	1.92	0.42
29:1:15:LEU:O	29:1:20:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:297:GLU:HG3	38:W1:125:TYR:CZ	2.55	0.42
31:9:177:TYR:CZ	40:r1:38:PRO:HG3	2.55	0.42
32:P1:79:ASP:OD1	32:P1:79:ASP:N	2.52	0.42
46:L1:161:ARG:HG2	46:L1:164:ALA:H	1.85	0.42
46:L1:223:LYS:HA	46:L1:223:LYS:HD3	1.83	0.42
46:L1:493:ILE:HA	46:L1:496:LEU:HG	2.01	0.42
48:N1:119:THR:HG22	48:N1:176:ARG:HB3	2.02	0.42
36:U1:63:PRO:HB3	64:l1:60:TRP:CG	2.55	0.42
57:e1:85:LEU:HB3	57:e1:91:TYR:HB3	2.01	0.42
15:b:14:SER:OG	15:b:185:THR:O	2.26	0.42
18:e:74:LYS:HA	18:e:74:LYS:HD3	1.83	0.42
19:f:62:ILE:HD11	19:f:70:VAL:HG22	2.01	0.42
3:L:14:THR:HG21	3:L:389:ARG:HB3	2.02	0.41
5:N:41:LEU:O	5:N:45:ILE:HG12	2.20	0.41
5:N:147:THR:HG21	5:N:165:TRP:NE1	2.34	0.41
8:Q:84:GLU:OE2	8:Q:84:GLU:N	2.52	0.41
14:n:54:TYR:OH	77:n:603:HEA:O1A	2.29	0.41
22:x:31:TYR:HA	22:x:35:GLN:HE21	1.85	0.41
30:3:266:LYS:O	30:3:270:ALA:HB2	2.20	0.41
36:T1:52:MET:SD	38:W1:39:ARG:HG3	2.59	0.41
46:L1:553:LEU:HD23	46:L1:553:LEU:HA	1.79	0.41
46:L1:555:LEU:HD13	65:m1:75:ILE:HD13	2.01	0.41
47:M1:11:LEU:HD23	47:M1:14:LEU:HD23	2.01	0.41
61:i1:15:ARG:O	61:i1:19:ARG:HG2	2.20	0.41
14:a:450:TRP:HA	14:a:453:VAL:HG12	2.02	0.41
3:A:377:GLU:HG3	13:I:12:LEU:HG	2.02	0.41
4:B:94:GLY:CA	4:B:110:GLU:O	2.68	0.41
5:C:51:LEU:HD23	5:C:51:LEU:HA	1.94	0.41
5:N:54:HIS:HB3	5:N:69:ILE:HG12	2.02	0.41
14:n:175:ALA:HB2	19:s:36:PRO:HB3	2.02	0.41
14:n:380:VAL:HG13	77:n:604:HEA:HBC1	2.01	0.41
14:n:448:THR:HB	22:x:41:ASN:HD22	1.85	0.41
16:p:155:LYS:HE3	16:p:155:LYS:HA	2.01	0.41
16:p:210:ILE:HG23	69:p:301:3PE:H2A2	2.02	0.41
29:1:97:ALA:HB1	29:1:111:MET:SD	2.60	0.41
30:3:145:LEU:HD23	30:3:145:LEU:HA	1.91	0.41
30:3:333:ASP:OD2	30:3:622:ARG:NE	2.52	0.41
30:3:591:GLY:HA2	32:P1:6:ILE:HG21	2.02	0.41
32:P1:80:SER:HA	32:P1:83:LYS:HE2	2.02	0.41
47:M1:373:ILE:HG21	47:M1:454:ILE:HD11	2.02	0.41
48:N1:203:LEU:HD22	48:N1:344:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N1:245:SER:HA	48:N1:297:ILE:HD12	2.03	0.41
49:O1:171:TYR:HD2	49:O1:222:VAL:HG23	1.84	0.41
50:X1:17:VAL:HG21	52:Z1:73:LEU:HD21	2.02	0.41
59:g1:96:LYS:NZ	68:p1:7:ASP:OD2	2.53	0.41
4:B:59:ASP:OD1	4:B:59:ASP:N	2.54	0.41
4:B:224:LEU:HD23	4:B:224:LEU:HA	1.88	0.41
4:B:291:THR:O	4:B:297:GLN:NE2	2.52	0.41
6:D:195:GLU:OE2	6:D:201:ARG:NE	2.53	0.41
3:L:231:LEU:HD23	3:L:231:LEU:HA	1.93	0.41
7:P:161:HIS:HB2	74:P:201:FES:S1	2.59	0.41
14:n:452:THR:O	14:n:456:MET:HG3	2.20	0.41
28:2:51:LEU:HD21	28:2:84:ALA:HB2	2.02	0.41
43:H1:190:LEU:HD11	43:H1:273:ILE:HD13	2.03	0.41
45:K1:40:LEU:HA	45:K1:40:LEU:HD23	1.87	0.41
46:L1:8:ILE:HA	46:L1:11:ILE:HD12	2.03	0.41
46:L1:213:LEU:HD21	46:L1:266:LEU:HB3	2.02	0.41
46:L1:306:THR:HG23	46:L1:332:HIS:CE1	2.52	0.41
46:L1:427:ILE:O	46:L1:431:THR:OG1	2.34	0.41
46:L1:514:ASN:ND2	71:L1:703:CDL:OB5	2.52	0.41
47:M1:447:LEU:HD21	69:M1:502:3PE:H3G2	2.01	0.41
52:Z1:35:PHE:O	52:Z1:39:ILE:HG12	2.20	0.41
59:g1:68:LEU:HD23	59:g1:68:LEU:HA	1.91	0.41
59:g1:106:MET:HE2	59:g1:106:MET:HB2	1.97	0.41
14:a:154:GLY:O	14:a:158:ILE:HG12	2.19	0.41
5:N:133:LEU:HA	5:N:133:LEU:HD23	1.80	0.41
5:N:133:LEU:HD21	5:N:179:PHE:HA	2.03	0.41
14:n:178:GLN:HG3	14:n:186:TRP:CZ2	2.55	0.41
15:o:148:LEU:HD11	15:o:216:LEU:HD11	2.01	0.41
26:C1:196:LYS:HB3	26:C1:196:LYS:HE3	1.79	0.41
27:D1:137:ILE:HD13	27:D1:137:ILE:HA	1.93	0.41
30:3:459:GLN:HG3	30:3:495:ARG:HH22	1.85	0.41
40:r1:101:LYS:HD3	40:r1:101:LYS:HA	1.93	0.41
47:M1:306:PRO:HA	47:M1:458:THR:HG21	2.02	0.41
14:a:347:LEU:HA	14:a:350:VAL:HG22	2.03	0.41
16:c:58:TRP:HB3	69:c:301:3PE:H232	2.01	0.41
17:d:118:MET:SD	22:k:53:TRP:HB3	2.61	0.41
5:C:49:LEU:O	5:C:53:MET:HG3	2.21	0.41
14:n:347:LEU:HA	14:n:350:VAL:HG22	2.02	0.41
77:n:604:HEA:HMC3	77:n:604:HEA:HHC	1.86	0.41
19:s:86:CYS:SG	19:s:87:GLY:N	2.93	0.41
27:D1:346:ILE:HG12	30:3:117:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:322:LEU:HD12	29:1:329:LEU:HB2	2.02	0.41
32:P1:172:PHE:HB2	32:P1:179:LEU:HG	2.01	0.41
46:L1:324:LEU:HD23	46:L1:324:LEU:HA	1.90	0.41
65:m1:114:LEU:HB3	65:m1:120:LEU:HB2	2.01	0.41
14:a:353:LEU:HD13	15:b:31:VAL:HG23	2.02	0.41
18:e:83:PRO:HA	18:e:86:ILE:HG22	2.03	0.41
4:B:163:LEU:HD11	4:B:258:VAL:HG22	2.03	0.41
10:H:18:VAL:HG12	10:H:67:VAL:HG22	2.02	0.41
3:L:148:VAL:HG22	7:P:2:HIS:CG	2.55	0.41
3:L:334:MET:HE3	3:L:334:MET:HB3	1.97	0.41
77:n:603:HEA:HMC1	77:n:603:HEA:HHC	1.89	0.41
15:o:134:ARG:HD3	17:q:110:THR:HG21	2.01	0.41
16:p:33:MET:HG3	16:p:37:TYR:CD2	2.51	0.41
16:p:83:MET:O	16:p:87:ILE:HG12	2.20	0.41
27:D1:164:MET:O	27:D1:167:PHE:HB3	2.19	0.41
44:J1:148:ALA:HB1	44:J1:151:MET:HB2	2.03	0.41
45:K1:60:PRO:HA	45:K1:63:ILE:HG12	2.02	0.41
46:L1:54:PHE:CZ	46:L1:84:PHE:HB2	2.56	0.41
46:L1:534:HIS:HB3	69:L1:701:3PE:H2	2.03	0.41
47:M1:65:LEU:HD11	47:M1:237:LYS:HB3	2.02	0.41
48:N1:1:FME:HE1	48:N1:9:ILE:HD12	2.02	0.41
61:i1:79:TRP:HE1	68:p1:40:VAL:HA	1.85	0.41
66:n1:66:ALA:HB1	86:n1:201:ZMP:H7	2.03	0.41
14:a:254:ILE:HA	14:a:254:ILE:HD12	1.85	0.41
15:b:162:SER:HB2	15:b:198:GLU:OE2	2.21	0.41
18:e:104:LEU:HD12	18:e:106:LEU:HD23	2.01	0.41
1:g:35:LYS:CE	70:g:302:PC1:O14	2.67	0.41
20:h:43:MET:HA	20:h:46:LYS:HG2	2.02	0.41
3:A:80:GLU:OE2	4:B:284:HIS:ND1	2.54	0.41
3:A:97:TYR:OH	3:A:190:TYR:OH	2.34	0.41
5:N:51:LEU:O	5:N:55:TYR:HB2	2.20	0.41
14:n:443:TYR:CE2	14:n:448:THR:HA	2.55	0.41
23:y:25:MET:HE2	81:y:601:TGL:HB71	2.02	0.41
27:D1:278:TYR:HA	27:D1:281:VAL:HG22	2.03	0.41
29:1:101:GLU:HA	29:1:102:PRO:HD3	1.90	0.41
29:1:376:MET:HA	29:1:379:PHE:HB2	2.03	0.41
43:H1:91:MET:HG2	43:H1:259:PHE:CE2	2.56	0.41
48:N1:13:ILE:HG13	48:N1:39:ALA:HB1	2.02	0.41
48:N1:49:ASN:OD1	48:N1:52:SER:N	2.41	0.41
48:N1:243:MET:HB3	48:N1:247:MET:HE2	2.03	0.41
51:Y1:94:CYS:O	51:Y1:98:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:l1:126:PRO:HD3	67:o1:3:HIS:CE1	2.56	0.41
15:b:28:LEU:HA	15:b:31:VAL:HG12	2.02	0.41
15:b:83:ILE:HD12	15:b:83:ILE:HA	1.94	0.41
2:m:2:HIS:HB3	14:a:483:MET:CG	2.51	0.41
7:E:65:SER:OG	7:E:67:ASP:OD1	2.38	0.41
7:E:73:LYS:NZ	7:E:74:ILE:O	2.51	0.41
9:R:42:ARG:HH22	71:R:103:CDL:HA61	1.85	0.41
7:T:65:VAL:HG11	7:T:77:ARG:HH21	1.85	0.41
15:o:26:HIS:O	15:o:30:ILE:HG12	2.21	0.41
28:2:96:GLY:H	28:2:138:THR:HG1	1.68	0.41
28:2:105:THR:HG22	28:2:106:THR:H	1.84	0.41
31:9:150:LEU:HD23	33:Q1:70:MET:HE3	2.03	0.41
43:H1:66:THR:HG23	43:H1:71:PHE:CD2	2.56	0.41
44:J1:151:MET:HB2	44:J1:151:MET:HE2	1.96	0.41
46:L1:124:PHE:HE1	46:L1:147:VAL:HG13	1.85	0.41
46:L1:124:PHE:CE1	46:L1:147:VAL:HG13	2.56	0.41
46:L1:292:ALA:HB2	46:L1:304:PHE:HB3	2.03	0.41
47:M1:14:LEU:HD11	47:M1:26:ASN:HB3	2.02	0.41
50:X1:75:SER:OG	50:X1:76:HIS:ND1	2.49	0.41
52:Z1:124:TYR:HD1	52:Z1:127:ARG:HD2	1.85	0.41
64:l1:8:LEU:HD12	64:l1:9:PRO:HD2	2.02	0.41
64:l1:147:LYS:HA	64:l1:147:LYS:HD3	1.86	0.41
65:m1:47:LEU:HB3	66:n1:165:LEU:HD13	2.02	0.41
65:m1:114:LEU:HD23	65:m1:120:LEU:HB2	2.03	0.41
14:a:415:ALA:O	14:a:419:VAL:HG22	2.21	0.41
77:a:604:HEA:HHA	77:a:604:HEA:HAA2	1.89	0.41
15:b:129:LYS:HB3	15:b:132:GLU:HG2	2.03	0.41
15:b:163:TRP:CD1	15:b:209:ILE:HD13	2.55	0.41
69:b:301:3PE:O12	21:i:45:ARG:NH2	2.54	0.41
1:t:14:LYS:HG3	1:t:18:TYR:HE2	1.85	0.41
3:A:110:VAL:HG11	3:A:211:LEU:HB3	2.03	0.41
3:A:177:LEU:HD23	3:A:177:LEU:HA	1.93	0.41
5:C:101:GLY:HA2	5:C:106:SER:HB2	2.03	0.41
69:C:404:3PE:H282	7:P:55:VAL:HB	2.03	0.41
11:J:33:ARG:HH12	12:K:50:GLY:H	1.69	0.41
5:N:240:MET:HE2	69:O:302:3PE:H232	2.03	0.41
5:N:376:MET:HB2	5:N:376:MET:HE2	1.80	0.41
71:R:103:CDL:H771	69:R:104:3PE:H391	2.03	0.41
10:S:18:VAL:HG22	10:S:70:LYS:HE3	2.03	0.41
10:S:20:GLU:HA	10:S:23:GLU:HG2	2.03	0.41
13:I:85:LEU:O	13:I:89:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:38:ARG:NH2	14:n:451:ASN:OD1	2.42	0.41
14:n:65:MET:SD	77:n:603:HEA:HMC2	2.60	0.41
14:n:238:PHE:O	14:n:242:GLU:HG3	2.21	0.41
15:o:1:MET:H1	15:o:193:TYR:H	1.69	0.41
15:o:167:SER:HB2	15:o:192:PHE:HB3	2.03	0.41
25:6:42:LYS:HA	25:6:42:LYS:HD3	1.66	0.41
26:C1:37:VAL:HG12	40:r1:69:MET:HE1	2.03	0.41
26:C1:37:VAL:HA	26:C1:52:ILE:HG22	2.03	0.41
29:1:99:GLU:OE1	29:1:105:CYS:C	2.63	0.41
30:3:324:ASP:OD1	30:3:324:ASP:N	2.45	0.41
31:9:5:VAL:HG23	40:r1:112:LEU:HD22	2.02	0.41
31:9:45:ARG:HE	40:r1:19:LEU:HD23	1.86	0.41
32:P1:137:ALA:HB2	32:P1:146:LEU:HD22	2.01	0.41
43:H1:25:ARG:HH22	43:H1:47:GLN:HE21	1.69	0.41
43:H1:267:SER:O	43:H1:271:LEU:HG	2.21	0.41
46:L1:342:CYS:O	46:L1:345:SER:OG	2.31	0.41
47:M1:76:MET:HE1	47:M1:230:ILE:HD13	2.02	0.41
47:M1:164:LEU:HD23	47:M1:164:LEU:HA	1.93	0.41
47:M1:278:ARG:HD2	47:M1:278:ARG:HA	1.90	0.41
47:M1:329:LEU:HB3	47:M1:359:TRP:CE2	2.56	0.41
48:N1:121:GLY:H	48:N1:176:ARG:CZ	2.34	0.41
48:N1:128:LEU:O	48:N1:132:THR:OG1	2.30	0.41
48:N1:202:LEU:HD23	48:N1:202:LEU:HA	1.90	0.41
49:O1:104:ARG:NH2	87:O1:401:DGT:N7	2.68	0.41
49:O1:137:ALA:HA	49:O1:201:ASP:HB3	2.03	0.41
50:X1:46:ARG:HD2	50:X1:46:ARG:HA	1.88	0.41
56:d1:43:LEU:HG	56:d1:53:VAL:HG12	2.03	0.41
59:g1:111:PHE:O	68:p1:158:GLN:NE2	2.51	0.41
62:j1:28:LEU:HD23	62:j1:28:LEU:HA	1.86	0.41
64:l1:81:ASP:N	64:l1:81:ASP:OD1	2.54	0.41
65:m1:102:TYR:O	65:m1:106:THR:HG23	2.21	0.41
14:a:247:ILE:HD13	77:a:604:HEA:HBC1	2.02	0.41
14:a:366:VAL:O	15:b:171:LYS:NZ	2.54	0.41
15:b:193:TYR:OH	17:d:122:ARG:NH1	2.51	0.41
16:c:128:GLU:O	1:g:32:VAL:CG2	2.69	0.41
16:c:189:SER:HG	1:g:54:ILE:C	2.24	0.41
17:d:145:TRP:CG	22:k:46:GLY:H	2.38	0.41
1:g:50:PRO:CG	20:h:75:ARG:HH22	2.23	0.41
4:B:56:ARG:HD2	4:B:103:GLU:HG2	2.03	0.41
4:B:300:ALA:HB2	4:B:307:PHE:HZ	1.86	0.41
6:D:48:TYR:HB2	6:D:87:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:52:ASN:HB2	3:L:55:ALA:HB2	2.03	0.41
3:L:173:ASN:O	3:L:177:LEU:HG	2.21	0.41
15:o:59:GLN:HB2	22:k:12:LYS:HD2	2.03	0.41
15:o:144:LEU:HB2	15:o:213:MET:SD	2.61	0.41
17:q:67:SER:O	17:q:71:MET:HG2	2.20	0.41
19:s:63:CYS:SG	19:s:86:CYS:HB3	2.61	0.41
28:2:173:ILE:HD13	28:2:173:ILE:HA	1.94	0.41
29:1:247:ARG:HB2	29:1:273:SER:OG	2.21	0.41
30:3:441:GLU:HA	30:3:444:LYS:HG3	2.02	0.41
32:P1:21:ALA:HA	32:P1:90:VAL:O	2.21	0.41
43:H1:273:ILE:HG12	43:H1:277:TYR:HE2	1.85	0.41
46:L1:81:LYS:N	46:L1:135:ASN:HB2	2.35	0.41
46:L1:123:LEU:HD21	71:L1:702:CDL:H532	2.03	0.41
46:L1:565:SER:HB2	51:Y1:112:MET:HE1	2.03	0.41
71:L1:702:CDL:HA32	60:h1:22:LEU:HD13	2.02	0.41
49:O1:156:LYS:HE2	49:O1:160:LEU:HD22	2.02	0.41
57:e1:70:LYS:HA	57:e1:73:ARG:HB3	2.02	0.41
65:m1:100:TRP:HA	65:m1:103:VAL:HG12	2.02	0.41
2:z:4:LYS:O	14:n:480:ARG:HB2	2.21	0.40
2:z:31:GLY:HA2	17:q:98:TRP:CH2	2.55	0.40
6:D:2:ASP:OD1	6:D:2:ASP:N	2.53	0.40
8:Q:37:LEU:HD23	8:Q:37:LEU:HA	1.96	0.40
10:S:18:VAL:HG13	10:S:70:LYS:HD3	2.03	0.40
10:S:19:ARG:O	10:S:23:GLU:HG2	2.22	0.40
12:V:10:TYR:HA	12:V:13:LEU:HB2	2.02	0.40
14:n:479:LYS:HD2	23:y:15:VAL:HG12	2.02	0.40
15:o:163:TRP:O	15:o:171:LYS:HA	2.21	0.40
22:x:15:ASN:HA	22:x:18:LEU:HD12	2.03	0.40
29:1:112:ARG:HB2	29:1:145:GLU:HG3	2.03	0.40
30:3:285:ARG:HG2	30:3:558:ASP:HA	2.03	0.40
47:M1:151:PHE:HZ	48:N1:291:PHE:HA	1.86	0.40
48:N1:27:MET:O	48:N1:31:VAL:HG13	2.21	0.40
48:N1:112:HIS:CE1	48:N1:164:MET:HE3	2.56	0.40
48:N1:308:ASN:HB2	49:O1:282:ILE:HG22	2.03	0.40
49:O1:62:THR:HG23	49:O1:63:THR:HG23	2.03	0.40
59:g1:66:ILE:HA	59:g1:70:PHE:HD2	1.87	0.40
15:b:30:ILE:HG21	15:b:76:ILE:HD11	2.02	0.40
16:c:228:THR:HG23	16:c:231:HIS:H	1.86	0.40
17:d:83:GLY:O	17:d:87:PHE:HB2	2.20	0.40
19:f:16:GLY:O	19:f:19:ARG:N	2.54	0.40
3:A:102:LEU:HD21	4:B:366:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:179:PRO:O	4:B:183:MET:HG3	2.21	0.40
4:B:183:MET:HE2	4:B:183:MET:HB3	1.80	0.40
72:C:402:HEM:HMC2	72:C:402:HEM:HBC2	2.03	0.40
9:G:34:ILE:HA	9:G:37:VAL:HG12	2.02	0.40
3:L:379:ILE:HG12	3:L:389:ARG:HD3	2.03	0.40
4:M:86:THR:HA	7:T:70:LEU:HD21	2.03	0.40
4:M:164:HIS:NE2	4:M:316:TYR:OH	2.37	0.40
14:n:80:ASN:C	14:n:80:ASN:HD22	2.29	0.40
14:n:90:PRO:HA	14:n:505:PHE:HB2	2.03	0.40
21:v:71:PHE:HB3	21:v:74:ALA:H	1.85	0.40
27:D1:145:THR:HA	27:D1:148:LEU:HD12	2.04	0.40
34:7:36:ASN:HD22	34:7:36:ASN:HA	1.58	0.40
38:W1:24:SER:OG	38:W1:33:ARG:NH1	2.55	0.40
46:L1:573:MET:HG2	48:N1:167:TRP:CZ2	2.56	0.40
47:M1:2:LEU:HD23	47:M1:2:LEU:HA	1.94	0.40
47:M1:296:LEU:HA	47:M1:296:LEU:HD23	1.83	0.40
49:O1:35:LYS:NZ	49:O1:53:GLU:OE1	2.44	0.40
50:X1:24:LEU:HD22	52:Z1:70:LEU:HD11	2.03	0.40
14:a:464:ALA:O	14:a:468:MET:HG2	2.21	0.40
16:c:222:GLN:HE21	16:c:222:GLN:HB3	1.73	0.40
19:f:93:VAL:HG13	19:f:95:HIS:CE1	2.56	0.40
3:A:308:GLN:HE21	3:A:323:HIS:HB3	1.86	0.40
5:C:246:PHE:HB3	5:C:249:MET:HB2	2.03	0.40
4:M:52:LYS:O	4:M:203:ARG:NH2	2.54	0.40
4:M:156:GLN:NE2	7:T:58:GLN:O	2.43	0.40
14:n:40:GLU:HG2	14:n:47:LEU:HB3	2.02	0.40
15:o:105:TYR:O	15:o:207:MET:HE3	2.22	0.40
15:o:155:SER:OG	15:o:156:SER:N	2.54	0.40
16:p:68:GLN:HA	24:w:13:GLN:HE21	1.85	0.40
16:p:163:LEU:HD21	16:p:235:PHE:HE1	1.86	0.40
21:v:43:GLU:HG2	21:v:44:PRO:HD3	2.04	0.40
29:1:73:PHE:HA	29:1:74:PRO:HD3	1.99	0.40
30:3:651:LEU:HD22	35:S1:45:LYS:HE3	2.03	0.40
32:P1:264:SER:O	32:P1:268:LYS:HG3	2.21	0.40
33:Q1:125:ASN:O	41:s1:64:ARG:NE	2.54	0.40
34:7:92:LYS:NZ	34:7:93:GLN:O	2.53	0.40
37:V1:22:ARG:HD3	49:O1:240:TYR:CZ	2.56	0.40
43:H1:84:SER:O	43:H1:87:VAL:HG12	2.21	0.40
43:H1:158:GLY:HA3	43:H1:315:PRO:HB2	2.03	0.40
47:M1:33:LEU:HB3	69:M1:503:3PE:H2C1	2.02	0.40
49:O1:133:VAL:HG21	49:O1:206:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:O1:261:MET:HA	49:O1:264:GLN:HG2	2.04	0.40
36:U1:8:LEU:HD22	36:U1:86:VAL:HG12	2.03	0.40
36:U1:49:GLU:HB3	63:k1:50:TRP:HE1	1.86	0.40
65:m1:18:ASP:HA	65:m1:19:PRO:HD3	1.97	0.40
14:a:143:VAL:HG11	14:a:213:ARG:NH1	2.36	0.40
15:b:122:MET:HE2	15:b:206:PHE:HD1	1.85	0.40
1:t:50:PRO:HD3	20:u:80:THR:OG1	2.22	0.40
5:C:54:HIS:HB3	5:C:69:ILE:HG12	2.02	0.40
13:I:102:ILE:O	13:I:106:MET:HG2	2.21	0.40
14:n:336:PRO:HG3	14:n:411:LYS:HG3	2.03	0.40
14:n:463:THR:O	14:n:467:ILE:HG12	2.22	0.40
16:p:212:SER:O	16:p:216:ILE:HG12	2.22	0.40
27:D1:234:ILE:HG23	43:H1:280:PHE:CD1	2.56	0.40
29:1:342:ASP:OD1	29:1:429:ARG:NH2	2.40	0.40
30:3:616:LEU:O	30:3:620:ARG:HG2	2.21	0.40
32:P1:244:TYR:CE1	32:P1:248:MET:HE3	2.56	0.40
39:q1:8:LYS:HA	39:q1:11:VAL:HG22	2.03	0.40
69:r1:201:3PE:H361	69:r1:201:3PE:H332	1.91	0.40
42:A1:17:LEU:HD23	42:A1:17:LEU:HA	1.93	0.40
46:L1:342:CYS:O	46:L1:346:ILE:HG12	2.22	0.40
46:L1:481:THR:HB	67:o1:94:TYR:HD2	1.85	0.40
46:L1:517:ASN:OD1	46:L1:517:ASN:N	2.53	0.40
48:N1:278:MET:O	48:N1:282:MET:HE3	2.20	0.40
14:a:66:ILE:HG21	14:a:126:TRP:HE1	1.86	0.40
6:D:23:HIS:HA	6:D:26:ILE:HD12	2.03	0.40
7:E:161:HIS:NE2	5:N:282:ARG:CD	2.84	0.40
11:J:13:LEU:O	11:J:19:THR:OG1	2.34	0.40
70:K:101:PC1:H133	70:K:101:PC1:H112	1.86	0.40
3:L:27:SER:HA	3:L:199:ALA:O	2.21	0.40
10:S:25:LEU:HD12	10:S:25:LEU:HA	1.91	0.40
11:U:33:ARG:HA	11:U:33:ARG:HD2	1.97	0.40
14:n:30:GLY:C	14:n:65:MET:HE3	2.47	0.40
14:n:243:VAL:HG13	77:n:604:HEA:C3C	2.52	0.40
14:n:496:HIS:HA	19:s:74:TRP:HZ2	1.86	0.40
16:p:224:LYS:HE2	24:w:4:LYS:HE2	2.03	0.40
16:p:225:PHE:HB3	19:s:8:PRO:HG3	2.04	0.40
26:C1:40:VAL:HG12	40:r1:68:ILE:HD12	2.02	0.40
30:3:379:LEU:HD23	30:3:452:VAL:HB	2.03	0.40
44:J1:5:ILE:HA	44:J1:8:LEU:HB2	2.02	0.40
46:L1:174:TYR:CD2	46:L1:232:TRP:HB3	2.56	0.40
46:L1:576:LEU:HD11	71:Y1:401:CDL:H521	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:M1:305:THR:HB	47:M1:308:SER:HB3	2.04	0.40
48:N1:21:MET:HB3	57:e1:2:PHE:HD2	1.87	0.40
49:O1:311:GLU:HG3	49:O1:312:VAL:HG13	2.04	0.40
15:b:13:THR:OG1	15:b:188:ARG:NH2	2.51	0.40
16:c:34:TRP:HH2	1:g:61:TRP:CE3	2.32	0.40
16:c:142:VAL:HG23	1:g:13:TRP:CE3	2.56	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	g	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
1	t	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
2	m	42/69 (61%)	41 (98%)	1 (2%)	0	100	100
2	z	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
3	A	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
3	L	443/480 (92%)	429 (97%)	14 (3%)	0	100	100
4	B	418/453 (92%)	409 (98%)	9 (2%)	0	100	100
4	M	418/453 (92%)	403 (96%)	15 (4%)	0	100	100
5	C	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
5	N	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
6	D	238/325 (73%)	233 (98%)	5 (2%)	0	100	100
6	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
7	E	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
7	P	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
7	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	F	96/111 (86%)	96 (100%)	0	0	100	100
8	Q	100/111 (90%)	100 (100%)	0	0	100	100
9	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
9	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
10	H	64/89 (72%)	64 (100%)	0	0	100	100
10	S	66/89 (74%)	63 (96%)	3 (4%)	0	100	100
11	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
11	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
12	K	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
12	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
13	I	86/113 (76%)	82 (95%)	4 (5%)	0	100	100
14	a	512/514 (100%)	491 (96%)	20 (4%)	1 (0%)	43	72
14	n	512/514 (100%)	489 (96%)	23 (4%)	0	100	100
15	b	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
15	o	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
16	c	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
16	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
17	d	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
17	q	137/169 (81%)	127 (93%)	10 (7%)	0	100	100
18	e	101/146 (69%)	100 (99%)	1 (1%)	0	100	100
18	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
19	f	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
19	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
20	h	77/86 (90%)	73 (95%)	3 (4%)	1 (1%)	9	39
20	u	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
21	i	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
21	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
22	k	46/80 (58%)	44 (96%)	2 (4%)	0	100	100
22	x	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
23	l	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
23	y	45/63 (71%)	45 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	w	55/83 (66%)	55 (100%)	0	0	100	100
25	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
26	C1	206/263 (78%)	200 (97%)	6 (3%)	0	100	100
27	D1	427/463 (92%)	412 (96%)	15 (4%)	0	100	100
28	2	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
29	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
30	3	688/727 (95%)	666 (97%)	22 (3%)	0	100	100
31	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
32	P1	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
33	Q1	124/175 (71%)	120 (97%)	4 (3%)	0	100	100
34	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
35	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
36	T1	77/156 (49%)	76 (99%)	1 (1%)	0	100	100
36	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
37	V1	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
38	W1	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
39	q1	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
40	r1	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
41	s1	40/104 (38%)	38 (95%)	2 (5%)	0	100	100
42	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
43	H1	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
44	J1	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
45	K1	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
46	L1	604/607 (100%)	567 (94%)	37 (6%)	0	100	100
47	M1	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
48	N1	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
49	O1	318/355 (90%)	300 (94%)	18 (6%)	0	100	100
50	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
51	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
52	Z1	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
53	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
55	c1	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
56	d1	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
57	e1	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
58	f1	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
59	g1	99/151 (66%)	95 (96%)	4 (4%)	0	100	100
60	h1	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
61	i1	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
62	j1	63/105 (60%)	61 (97%)	2 (3%)	0	100	100
63	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
64	l1	155/186 (83%)	152 (98%)	3 (2%)	0	100	100
65	m1	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
66	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
67	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
68	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	15749/18172 (87%)	15149 (96%)	598 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	h	8	ILE
14	a	376	HIS

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	g	66/92 (72%)	66 (100%)	0	100	100
1	t	66/92 (72%)	66 (100%)	0	100	100
2	m	39/61 (64%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	z	39/61 (64%)	39 (100%)	0	100	100
3	A	372/398 (94%)	372 (100%)	0	100	100
3	L	372/398 (94%)	372 (100%)	0	100	100
4	B	330/356 (93%)	330 (100%)	0	100	100
4	M	330/356 (93%)	330 (100%)	0	100	100
5	C	332/333 (100%)	331 (100%)	1 (0%)	86	83
5	N	332/333 (100%)	332 (100%)	0	100	100
6	D	205/260 (79%)	205 (100%)	0	100	100
6	O	205/260 (79%)	205 (100%)	0	100	100
7	E	69/224 (31%)	69 (100%)	0	100	100
7	P	68/224 (30%)	67 (98%)	1 (2%)	57	70
7	T	58/224 (26%)	58 (100%)	0	100	100
8	F	90/99 (91%)	90 (100%)	0	100	100
8	Q	94/99 (95%)	94 (100%)	0	100	100
9	G	70/74 (95%)	70 (100%)	0	100	100
9	R	70/74 (95%)	70 (100%)	0	100	100
10	H	63/83 (76%)	63 (100%)	0	100	100
10	S	65/83 (78%)	65 (100%)	0	100	100
11	J	51/55 (93%)	51 (100%)	0	100	100
11	U	51/55 (93%)	51 (100%)	0	100	100
12	K	42/46 (91%)	42 (100%)	0	100	100
12	V	43/46 (94%)	43 (100%)	0	100	100
13	I	73/75 (97%)	73 (100%)	0	100	100
14	a	425/425 (100%)	425 (100%)	0	100	100
14	n	425/425 (100%)	424 (100%)	1 (0%)	87	85
15	b	210/210 (100%)	210 (100%)	0	100	100
15	o	210/210 (100%)	210 (100%)	0	100	100
16	c	225/227 (99%)	225 (100%)	0	100	100
16	p	226/227 (100%)	226 (100%)	0	100	100
17	d	122/146 (84%)	122 (100%)	0	100	100
17	q	122/146 (84%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	e	90/118 (76%)	90 (100%)	0	100	100
18	r	91/118 (77%)	91 (100%)	0	100	100
19	f	80/101 (79%)	80 (100%)	0	100	100
19	s	80/101 (79%)	80 (100%)	0	100	100
20	h	70/76 (92%)	70 (100%)	0	100	100
20	u	70/76 (92%)	70 (100%)	0	100	100
21	i	54/57 (95%)	54 (100%)	0	100	100
21	v	54/57 (95%)	54 (100%)	0	100	100
22	k	39/67 (58%)	39 (100%)	0	100	100
22	x	39/67 (58%)	39 (100%)	0	100	100
23	l	39/55 (71%)	39 (100%)	0	100	100
23	y	40/55 (73%)	40 (100%)	0	100	100
24	w	43/67 (64%)	43 (100%)	0	100	100
25	6	133/185 (72%)	133 (100%)	0	100	100
26	C1	190/227 (84%)	190 (100%)	0	100	100
27	D1	370/394 (94%)	370 (100%)	0	100	100
28	2	184/206 (89%)	184 (100%)	0	100	100
29	1	345/370 (93%)	345 (100%)	0	100	100
30	3	580/610 (95%)	580 (100%)	0	100	100
31	9	152/178 (85%)	152 (100%)	0	100	100
32	P1	299/325 (92%)	299 (100%)	0	100	100
33	Q1	113/153 (74%)	113 (100%)	0	100	100
34	7	81/96 (84%)	80 (99%)	1 (1%)	63	73
35	S1	74/80 (92%)	74 (100%)	0	100	100
36	T1	73/135 (54%)	73 (100%)	0	100	100
36	U1	81/135 (60%)	81 (100%)	0	100	100
37	V1	101/102 (99%)	101 (100%)	0	100	100
38	W1	108/114 (95%)	108 (100%)	0	100	100
39	q1	131/131 (100%)	131 (100%)	0	100	100
40	r1	88/96 (92%)	88 (100%)	0	100	100
41	s1	41/95 (43%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	A1	103/103 (100%)	103 (100%)	0	100	100
43	H1	279/279 (100%)	279 (100%)	0	100	100
44	J1	137/137 (100%)	137 (100%)	0	100	100
45	K1	87/87 (100%)	87 (100%)	0	100	100
46	L1	548/549 (100%)	548 (100%)	0	100	100
47	M1	414/414 (100%)	414 (100%)	0	100	100
48	N1	307/307 (100%)	307 (100%)	0	100	100
49	O1	284/309 (92%)	284 (100%)	0	100	100
50	X1	153/154 (99%)	153 (100%)	0	100	100
51	Y1	105/106 (99%)	105 (100%)	0	100	100
52	Z1	122/123 (99%)	122 (100%)	0	100	100
53	a1	60/60 (100%)	60 (100%)	0	100	100
54	b1	72/73 (99%)	72 (100%)	0	100	100
55	c1	42/67 (63%)	42 (100%)	0	100	100
56	d1	107/107 (100%)	107 (100%)	0	100	100
57	e1	93/94 (99%)	93 (100%)	0	100	100
58	f1	49/53 (92%)	49 (100%)	0	100	100
59	g1	92/129 (71%)	92 (100%)	0	100	100
60	h1	123/162 (76%)	123 (100%)	0	100	100
61	i1	99/119 (83%)	99 (100%)	0	100	100
62	j1	61/87 (70%)	61 (100%)	0	100	100
63	k1	60/78 (77%)	60 (100%)	0	100	100
64	l1	142/161 (88%)	142 (100%)	0	100	100
65	m1	112/114 (98%)	112 (100%)	0	100	100
66	n1	163/164 (99%)	163 (100%)	0	100	100
67	o1	109/121 (90%)	109 (100%)	0	100	100
68	p1	155/158 (98%)	155 (100%)	0	100	100
All	All	13571/15439 (88%)	13567 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	271	GLU

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Mol	Chain	Res	Type
7	P	53	ASN
14	n	80	ASN
34	7	36	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	t	75	ASN
2	m	2	HIS
3	A	6	GLN
3	A	53	ASN
3	A	94	HIS
3	A	139	GLN
3	A	206	GLN
3	A	213	GLN
3	A	289	HIS
3	A	339	GLN
4	B	342	ASN
4	B	343	GLN
5	C	3	ASN
5	C	16	HIS
5	C	54	HIS
5	C	267	HIS
6	D	156	GLN
7	E	161	HIS
9	G	12	HIS
3	L	53	ASN
3	L	69	ASN
3	L	73	ASN
3	L	323	HIS
3	L	363	ASN
4	M	196	GLN
4	M	222	GLN
4	M	247	GLN
4	M	329	GLN
4	M	342	ASN
5	N	44	GLN
5	N	54	HIS
5	N	148	ASN
5	N	312	GLN
5	N	345	HIS
6	O	35	GLN

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Mol	Chain	Res	Type
7	P	141	HIS
11	U	61	ASN
12	V	49	ASN
14	n	151	HIS
14	n	328	HIS
14	n	331	ASN
15	o	26	HIS
16	p	12	ASN
16	p	70	HIS
16	p	161	GLN
19	s	48	ASN
24	w	13	GLN
26	C1	124	HIS
27	D1	50	ASN
27	D1	55	HIS
27	D1	59	HIS
27	D1	157	HIS
28	2	37	ASN
29	1	373	ASN
30	3	43	HIS
30	3	155	GLN
30	3	182	GLN
30	3	286	ASN
30	3	313	ASN
30	3	402	ASN
32	P1	36	ASN
32	P1	216	ASN
32	P1	341	ASN
33	Q1	50	ASN
34	7	3	GLN
35	S1	61	GLN
35	S1	79	ASN
37	V1	36	HIS
37	V1	40	HIS
37	V1	72	GLN
38	W1	93	GLN
39	q1	101	ASN
39	q1	113	HIS
43	H1	93	HIS
43	H1	230	ASN
43	H1	258	ASN
43	H1	304	HIS

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Mol	Chain	Res	Type
46	L1	29	HIS
46	L1	58	ASN
46	L1	72	ASN
46	L1	170	GLN
46	L1	332	HIS
46	L1	506	ASN
46	L1	543	ASN
47	M1	83	HIS
47	M1	138	ASN
47	M1	366	ASN
48	N1	88	GLN
48	N1	223	ASN
48	N1	309	ASN
49	O1	89	ASN
49	O1	120	GLN
50	X1	123	GLN
51	Y1	9	HIS
52	Z1	111	HIS
52	Z1	136	ASN
53	a1	31	ASN
54	b1	82	ASN
56	d1	88	HIS
57	e1	24	GLN
57	e1	44	HIS
59	g1	23	GLN
61	i1	12	GLN
64	l1	54	GLN
65	m1	51	ASN
66	n1	13	GLN
68	p1	130	GLN
14	a	98	ASN
14	a	216	ASN
14	a	233	HIS
14	a	429	HIS
15	b	26	HIS
15	b	52	HIS
15	b	102	HIS
15	b	103	GLN
15	b	161	HIS
16	c	68	GLN
16	c	149	HIS
16	c	157	ASN

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Mol	Chain	Res	Type
16	c	160	ASN
16	c	161	GLN
16	c	222	GLN
16	c	231	HIS
17	d	119	GLN
18	e	20	ASN
1	g	31	ASN
1	g	75	ASN
20	h	25	GLN
20	h	32	ASN
23	l	10	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	FME	A1	1	42	8,9,10	0.98	0	8,9,11	0.82	0
48	FME	N1	1	48	8,9,10	0.99	0	8,9,11	1.05	1 (12%)
40	AYA	r1	1	40	6,7,8	1.27	1 (16%)	6,8,10	1.14	1 (16%)
27	2MR	D1	85	27	10,12,13	2.66	2 (20%)	5,13,15	2.84	2 (40%)
43	FME	H1	1	43	8,9,10	1.00	0	8,9,11	0.88	0
54	AYA	b1	1	54	6,7,8	1.25	1 (16%)	6,8,10	1.17	1 (16%)
47	FME	M1	1	47	8,9,10	1.00	0	8,9,11	0.78	0
45	FME	K1	1	45	8,9,10	0.96	0	8,9,11	1.54	2 (25%)
61	SAC	i1	1	61	7,8,9	1.03	0	7,9,11	0.94	0
44	FME	J1	1	44	8,9,10	0.99	0	8,9,11	0.85	0
46	FME	L1	1	46	8,9,10	0.96	0	8,9,11	0.91	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
42	FME	A1	1	42	-	1/7/9/11	-
48	FME	N1	1	48	-	2/7/9/11	-
40	AYA	r1	1	40	-	0/5/6/8	-
27	2MR	D1	85	27	-	4/10/13/15	-
43	FME	H1	1	43	-	3/7/9/11	-
54	AYA	b1	1	54	-	0/5/6/8	-
47	FME	M1	1	47	-	2/7/9/11	-
45	FME	K1	1	45	-	3/7/9/11	-
61	SAC	i1	1	61	-	2/7/8/10	-
44	FME	J1	1	44	-	4/7/9/11	-
46	FME	L1	1	46	-	4/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D1	85	2MR	CZ-NE	5.93	1.46	1.34
27	D1	85	2MR	CZ-NH2	5.41	1.44	1.33
40	r1	1	AYA	CA-N	-2.42	1.43	1.46
54	b1	1	AYA	CA-N	-2.23	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D1	85	2MR	CD-NE-CZ	4.87	132.50	123.36
27	D1	85	2MR	NE-CZ-NH2	-3.72	116.07	119.48
45	K1	1	FME	C-CA-N	3.40	116.06	109.50
40	r1	1	AYA	CB-CA-N	2.60	112.61	109.68
54	b1	1	AYA	CB-CA-N	2.48	112.47	109.68
45	K1	1	FME	O-C-CA	-2.17	119.18	124.77
48	N1	1	FME	C-CA-N	2.11	113.56	109.50

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D1	85	2MR	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
43	H1	1	FME	N-CA-CB-CG
44	J1	1	FME	C-CA-CB-CG
44	J1	1	FME	O-C-CA-CB
45	K1	1	FME	O1-CN-N-CA
46	L1	1	FME	N-CA-CB-CG
48	N1	1	FME	C-CA-CB-CG
27	D1	85	2MR	NE-CD-CG-CB
47	M1	1	FME	N-CA-CB-CG
27	D1	85	2MR	CA-CB-CG-CD
45	K1	1	FME	CA-CB-CG-SD
44	J1	1	FME	CB-CG-SD-CE
48	N1	1	FME	CA-CB-CG-SD
43	H1	1	FME	C-CA-CB-CG
46	L1	1	FME	C-CA-CB-CG
43	H1	1	FME	CB-CA-N-CN
46	L1	1	FME	CB-CA-N-CN
42	A1	1	FME	N-CA-CB-CG
44	J1	1	FME	N-CA-CB-CG
45	K1	1	FME	N-CA-CB-CG
46	L1	1	FME	CB-CG-SD-CE
27	D1	85	2MR	CG-CD-NE-CZ
47	M1	1	FME	CB-CA-N-CN
61	i1	1	SAC	C-CA-CB-OG
61	i1	1	SAC	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	N1	1	FME	1	0
54	b1	1	AYA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 11 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	$\# Z > 2$
79	CUA	o	303	15	0,1,1	-	-	-		
69	3PE	c	301	-	44,44,50	0.31	0	47,49,55	0.33	0
72	HEM	N	401	5	50,50,50	1.38	5 (10%)	67,82,82	1.32	5 (7%)
69	3PE	C	404	-	30,30,50	0.38	0	33,35,55	0.35	0
70	PC1	I	201	-	49,49,53	0.32	0	55,57,61	0.54	1 (1%)
69	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.35	0
69	3PE	m1	601	-	35,35,50	0.35	0	38,40,55	0.31	0
69	3PE	t	101	-	24,24,50	0.44	0	27,29,55	0.61	1 (3%)
73	HEC	D	301	6	46,50,50	1.82	7 (15%)	58,82,82	1.95	6 (10%)
70	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.63	0
69	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
70	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.37	0
69	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.39	0
82	SF4	3	801	30	0,12,12	-	-	-		
71	CDL	g	301	-	34,37,99	0.37	0	37,47,111	0.54	1 (2%)
70	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.60	0
69	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.32	0
71	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
69	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.30	0
69	3PE	M1	503	-	50,50,50	0.30	0	53,55,55	0.27	0
69	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.32	0
74	FES	3	803	30	0,4,4	-	-	-		
69	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.30	0
72	HEM	C	402	5	50,50,50	1.36	8 (16%)	67,82,82	1.14	3 (4%)
69	3PE	Y1	402	-	27,27,50	0.39	0	30,32,55	0.37	0
82	SF4	3	802	30	0,12,12	-	-	-		
79	CUA	b	302	15	0,1,1	-	-	-		
70	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.34	0
71	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
81	TGL	y	601	-	36,36,62	0.23	0	39,39,65	0.18	0
72	HEM	C	401	5	50,50,50	1.33	5 (10%)	67,82,82	1.24	4 (5%)
69	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.34	0
82	SF4	1	502	29	0,12,12	-	-	-		
70	PC1	g	302	-	49,49,53	0.30	0	55,57,61	0.30	0
82	SF4	6	201	25	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	HEM	N	402	5	50,50,50	1.40	7 (14%)	67,82,82	1.26	6 (8%)
77	HEA	a	604	14	67,67,67	1.35	6 (8%)	81,103,103	2.25	29 (35%)
69	3PE	b	301	-	28,28,50	0.39	0	31,33,55	0.37	0
74	FES	E	201	7	0,4,4	-	-	-		
69	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.34	0
74	FES	2	301	28	0,4,4	-	-	-		
71	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.52	1 (1%)
70	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.36	0
71	CDL	V	101	-	45,45,99	0.34	0	51,57,111	0.46	0
71	CDL	N1	401	-	89,89,99	0.31	0	95,101,111	0.39	1 (1%)
71	CDL	R	103	-	71,71,99	0.35	0	77,83,111	0.43	1 (1%)
71	CDL	L1	703	-	45,45,99	0.42	0	51,57,111	0.35	0
71	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
71	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.48	1 (1%)
70	PC1	z	101	-	27,27,53	0.40	0	33,35,61	0.37	0
69	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.38	0
69	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.48	1 (1%)
69	3PE	a	605	-	27,27,50	0.40	0	30,32,55	0.47	0
69	3PE	z	102	-	25,25,50	0.41	0	28,30,55	0.39	0
69	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.34	0
69	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.31	0
69	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.34	0
71	CDL	G	101	-	41,41,99	0.44	0	47,53,111	0.36	0
69	3PE	a	606	-	26,26,50	0.40	0	29,31,55	0.37	0
69	3PE	d	201	-	33,33,50	0.37	0	36,38,55	0.55	1 (2%)
69	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.30	0
82	SF4	9	201	31	0,12,12	-	-	-		
86	ZMP	n1	201	-	26,31,36	0.72	1 (3%)	30,38,45	0.94	1 (3%)
69	3PE	G	102	-	50,50,50	0.30	0	53,55,55	0.28	0
69	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.42	0
69	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.34	0
85	NDP	P1	501	-	51,52,52	0.33	0	71,80,80	0.42	0
69	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.33	0
71	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.29	0
69	3PE	i	101	-	27,27,50	0.39	0	30,32,55	0.34	0
70	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.49	0
69	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.30	0
69	3PE	L1	704	-	50,50,50	0.31	0	53,55,55	0.29	0
69	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.68	0
69	3PE	E	203	-	33,33,50	0.36	0	36,38,55	0.33	0
87	DGT	O1	401	78	32,33,33	0.29	0	48,52,52	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
70	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.48	0
71	CDL	Y1	401	-	93,93,99	0.30	0	99,105,111	0.28	0
74	FES	P	201	7	0,4,4	-	-	-		
81	TGL	l	601	-	36,36,62	0.23	0	39,39,65	0.16	0
71	CDL	r1	202	-	56,56,99	0.39	0	62,68,111	0.48	1 (1%)
69	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
69	3PE	g	303	-	24,24,50	0.43	0	27,29,55	0.65	1 (3%)
77	HEA	n	604	14	67,67,67	1.37	6 (8%)	81,103,103	2.36	30 (37%)
71	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.33	0
71	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.43	0
71	CDL	R	101	-	40,40,99	0.45	0	46,52,111	0.54	0
70	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.46	0
77	HEA	n	603	14	67,67,67	1.35	7 (10%)	81,103,103	2.31	25 (30%)
71	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
69	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.36	0
69	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.57	1 (2%)
70	PC1	V	102	-	27,27,53	0.40	0	33,35,61	0.37	0
86	ZMP	W1	201	-	28,33,36	0.67	1 (3%)	32,40,45	0.93	1 (3%)
77	HEA	a	603	14	67,67,67	1.41	6 (8%)	81,103,103	2.31	28 (34%)
69	3PE	b1	101	-	42,42,50	0.33	0	45,47,55	0.36	0
73	HEC	O	303	6	46,50,50	1.84	5 (10%)	58,82,82	1.93	4 (6%)
69	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.37	0
83	FMN	1	501	-	33,33,33	0.27	0	48,50,50	0.36	0
82	SF4	9	202	31	0,12,12	-	-	-		
70	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.31	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
69	3PE	c	301	-	-	10/48/48/54	-
72	HEM	N	401	5	-	2/14/54/54	-
69	3PE	C	404	-	-	4/34/34/54	-
70	PC1	I	201	-	-	9/53/53/57	-
69	3PE	R	104	-	-	5/33/33/54	-
69	3PE	m1	601	-	-	12/39/39/54	-
69	3PE	t	101	-	-	6/28/28/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	HEC	D	301	6	-	6/14/54/54	-
70	PC1	L	503	-	-	9/27/27/57	-
69	3PE	C	403	-	-	9/38/38/54	-
70	PC1	M1	501	-	-	8/57/57/57	-
69	3PE	L	501	-	-	6/26/26/54	-
82	SF4	3	801	30	-	-	0/6/5/5
71	CDL	g	301	-	-	8/41/45/110	-
70	PC1	P1	502	-	-	15/34/34/57	-
69	3PE	Y1	403	-	-	5/45/45/54	-
71	CDL	A	502	-	-	12/56/56/110	-
69	3PE	M1	502	-	-	17/54/54/54	-
69	3PE	M1	503	-	-	13/54/54/54	-
69	3PE	N	403	-	-	7/40/40/54	-
74	FES	3	803	30	-	-	0/1/1/1
69	3PE	r1	201	-	-	9/49/49/54	-
72	HEM	C	402	5	-	1/14/54/54	-
69	3PE	Y1	402	-	-	4/31/31/54	-
82	SF4	3	802	30	-	-	0/6/5/5
70	PC1	p	302	-	-	10/38/38/57	-
71	CDL	d1	201	-	-	15/77/77/110	-
81	TGL	y	601	-	-	3/39/39/65	-
72	HEM	C	401	5	-	1/14/54/54	-
69	3PE	6	202	-	-	4/35/35/54	-
82	SF4	1	502	29	-	-	0/6/5/5
70	PC1	g	302	-	-	6/53/53/57	-
82	SF4	6	201	25	-	-	0/6/5/5
72	HEM	N	402	5	-	4/14/54/54	-
77	HEA	a	604	14	-	14/36/76/76	-
69	3PE	b	301	-	-	8/32/32/54	-
74	FES	E	201	7	-	-	0/1/1/1
69	3PE	N1	402	-	-	5/41/41/54	-
74	FES	2	301	28	-	-	0/1/1/1
71	CDL	L	502	-	-	7/56/56/110	-
70	PC1	J	101	-	-	7/38/38/57	-
71	CDL	V	101	-	-	15/55/55/110	-
71	CDL	N1	401	-	-	20/100/100/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	CDL	R	103	-	-	19/82/82/110	-
71	CDL	L1	703	-	-	14/56/56/110	-
71	CDL	O	301	-	-	14/67/67/110	-
71	CDL	R	102	-	-	16/67/67/110	-
70	PC1	z	101	-	-	4/31/31/57	-
69	3PE	o	302	-	-	10/32/32/54	-
69	3PE	H1	401	-	-	9/54/54/54	-
69	3PE	a	605	-	-	3/31/31/54	-
69	3PE	z	102	-	-	1/29/29/54	-
69	3PE	v	101	-	-	7/31/31/54	-
69	3PE	i1	201	-	-	6/45/45/54	-
69	3PE	O	302	-	-	9/36/36/54	-
71	CDL	G	101	-	-	13/52/52/110	-
69	3PE	a	606	-	-	8/30/30/54	-
69	3PE	d	201	-	-	5/37/37/54	-
69	3PE	p	301	-	-	12/48/48/54	-
82	SF4	9	201	31	-	-	0/6/5/5
86	ZMP	n1	201	-	-	19/36/38/43	-
69	3PE	G	102	-	-	8/54/54/54	-
69	3PE	n	606	-	-	8/31/31/54	-
69	3PE	d1	202	-	-	8/34/34/54	-
85	NDP	P1	501	-	-	4/34/77/77	0/5/5/5
69	3PE	E	202	-	-	8/35/35/54	-
71	CDL	L1	702	-	-	15/88/88/110	-
69	3PE	i	101	-	-	8/31/31/54	-
70	PC1	6	203	-	-	12/46/46/57	-
69	3PE	K1	201	-	-	11/44/44/54	-
69	3PE	L1	704	-	-	7/54/54/54	-
69	3PE	A	501	-	-	9/26/26/54	-
69	3PE	E	203	-	-	9/37/37/54	-
87	DGT	O1	401	78	-	2/22/34/34	0/3/3/3
70	PC1	K	101	-	-	5/31/31/57	-
71	CDL	Y1	401	-	-	11/104/104/110	-
81	TGL	l	601	-	-	0/39/39/65	-
74	FES	P	201	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	CDL	r1	202	-	-	12/67/67/110	-
69	3PE	L1	701	-	-	8/54/54/54	-
69	3PE	g	303	-	-	9/28/28/54	-
77	HEA	n	604	14	-	9/36/76/76	-
71	CDL	D	302	-	-	19/66/66/110	-
71	CDL	h1	201	-	-	21/80/80/110	-
71	CDL	R	101	-	-	13/51/51/110	-
70	PC1	9	203	-	-	10/57/57/57	-
77	HEA	n	603	14	-	12/36/76/76	-
71	CDL	H1	402	-	-	10/59/59/110	-
69	3PE	n	607	-	-	7/30/30/54	-
69	3PE	n	605	-	-	9/37/37/54	-
70	PC1	V	102	-	-	4/31/31/57	-
86	ZMP	W1	201	-	-	6/38/40/43	-
77	HEA	a	603	14	-	15/36/76/76	-
69	3PE	b1	101	-	-	10/46/46/54	-
73	HEC	O	303	6	-	8/14/54/54	-
69	3PE	d1	203	-	-	6/35/35/54	-
83	FMN	1	501	-	-	5/18/18/18	0/3/3/3
82	SF4	9	202	31	-	-	0/6/5/5
70	PC1	9	204	-	-	10/50/50/57	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	O	303	HEC	CAC-C3C	6.27	1.55	1.35
73	D	301	HEC	CAC-C3C	6.17	1.55	1.35
73	O	303	HEC	CAB-C3B	6.04	1.54	1.35
73	D	301	HEC	CAB-C3B	5.84	1.54	1.35
73	D	301	HEC	C3D-C2D	5.72	1.53	1.38
73	O	303	HEC	C3D-C2D	5.61	1.53	1.38
77	a	603	HEA	C3B-C2B	4.53	1.45	1.34
77	n	604	HEA	C3D-C2D	4.37	1.46	1.36
72	N	402	HEM	FE-NB	4.29	2.08	1.94
77	n	604	HEA	C3B-C2B	4.28	1.44	1.34
77	n	603	HEA	C3B-C2B	4.13	1.44	1.34
77	a	604	HEA	C3B-C2B	4.10	1.44	1.34
77	a	603	HEA	C3D-C2D	4.02	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	C	402	HEM	FE-NB	3.98	2.07	1.94
77	a	603	HEA	C3A-C2A	3.87	1.46	1.37
77	n	603	HEA	C3D-C2D	3.76	1.44	1.36
77	a	604	HEA	C3A-C2A	3.65	1.45	1.37
77	a	604	HEA	C3D-C2D	3.62	1.44	1.36
72	N	401	HEM	FE-NC	3.59	2.07	1.95
77	n	603	HEA	C3A-C2A	3.43	1.45	1.37
72	C	401	HEM	FE-NC	3.37	2.06	1.95
77	n	604	HEA	C3A-C2A	3.35	1.44	1.37
72	N	401	HEM	FE-ND	3.35	2.05	1.94
72	C	401	HEM	CAB-C3B	3.23	1.56	1.47
72	C	402	HEM	CAB-C3B	3.19	1.55	1.47
72	C	402	HEM	CAC-C3C	3.19	1.55	1.47
72	N	401	HEM	CAC-C3C	3.18	1.55	1.47
72	N	402	HEM	CAC-C3C	3.13	1.55	1.47
72	C	401	HEM	CAC-C3C	3.12	1.55	1.47
72	N	401	HEM	CAB-C3B	3.12	1.55	1.47
72	N	402	HEM	CAB-C3B	3.02	1.55	1.47
77	a	603	HEA	C4B-C3B	2.86	1.49	1.44
77	n	604	HEA	C4B-C3B	2.81	1.49	1.44
77	n	603	HEA	C4B-C3B	2.76	1.49	1.44
72	C	402	HEM	FE-NA	2.66	2.03	1.95
72	N	402	HEM	FE-NC	2.65	2.03	1.95
77	a	604	HEA	C4B-C3B	2.65	1.49	1.44
72	C	402	HEM	FE-NC	2.58	2.03	1.95
72	N	402	HEM	FE-NA	2.52	2.03	1.95
86	n1	201	ZMP	C9-C10	2.46	1.53	1.50
86	W1	201	ZMP	C9-C10	2.43	1.53	1.50
72	C	401	HEM	FE-ND	2.42	2.02	1.94
77	n	604	HEA	C1D-ND	-2.41	1.36	1.40
77	n	603	HEA	C1D-ND	-2.36	1.36	1.40
77	a	603	HEA	C1D-ND	-2.35	1.36	1.40
77	n	603	HEA	C11-C3B	-2.24	1.48	1.51
77	a	604	HEA	C1D-C2D	2.23	1.49	1.44
73	D	301	HEC	C3B-C2B	-2.20	1.33	1.41
72	C	402	HEM	CMB-C2B	2.15	1.55	1.50
72	C	401	HEM	CMC-C2C	2.12	1.55	1.50
72	N	401	HEM	CMC-C2C	2.11	1.55	1.50
72	N	402	HEM	CMC-C2C	2.11	1.55	1.50
72	C	402	HEM	C2A-C3A	-2.10	1.33	1.38
73	D	301	HEC	C3C-C2C	-2.10	1.34	1.41
77	a	604	HEA	C1D-ND	-2.10	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	N	402	HEM	C2A-C3A	-2.08	1.33	1.38
73	O	303	HEC	C3B-C2B	-2.08	1.34	1.41
77	a	603	HEA	C1C-C2C	2.07	1.48	1.43
77	n	604	HEA	C4D-C3D	2.06	1.48	1.45
77	n	603	HEA	C1C-C2C	2.04	1.47	1.43
73	D	301	HEC	CMC-C2C	2.04	1.55	1.50
72	C	402	HEM	CMC-C2C	2.03	1.54	1.50
73	D	301	HEC	CMB-C2B	2.01	1.54	1.50
73	O	303	HEC	C3C-C2C	-2.00	1.34	1.41

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	D	301	HEC	CBC-CAC-C3C	-8.99	109.47	127.43
73	O	303	HEC	CBB-CAB-C3B	-8.60	110.24	127.43
73	O	303	HEC	CBC-CAC-C3C	-8.49	110.47	127.43
73	D	301	HEC	CBB-CAB-C3B	-8.16	111.11	127.43
77	a	603	HEA	C3A-C2A-C1A	-7.03	100.39	107.05
77	a	604	HEA	C3A-C2A-C1A	-6.71	100.70	107.05
77	n	604	HEA	C3A-C2A-C1A	-6.64	100.76	107.05
77	n	603	HEA	C3A-C2A-C1A	-6.12	101.25	107.05
77	a	604	HEA	C2A-C1A-NA	5.52	115.65	110.32
77	a	603	HEA	C2A-C1A-NA	5.52	115.65	110.32
77	n	603	HEA	C13-C12-C11	-5.48	105.64	114.39
77	a	604	HEA	CMC-C2C-C3C	5.47	139.42	126.55
77	a	603	HEA	CMC-C2C-C3C	5.39	139.22	126.55
77	n	604	HEA	CMC-C2C-C3C	5.24	138.87	126.55
77	n	604	HEA	C3D-C4D-ND	5.15	115.33	110.35
77	n	603	HEA	C2A-C1A-NA	5.15	115.29	110.32
77	n	604	HEA	CMD-C2D-C1D	-5.11	117.05	125.03
77	n	603	HEA	CMC-C2C-C3C	5.11	138.56	126.55
77	n	603	HEA	C3D-C4D-ND	4.98	115.17	110.35
77	a	604	HEA	C3D-C4D-ND	4.98	115.16	110.35
77	a	604	HEA	CMC-C2C-C1C	-4.93	117.91	125.42
72	N	401	HEM	C3B-C2B-C1B	4.93	110.11	106.41
77	n	604	HEA	CMC-C2C-C1C	-4.81	118.09	125.42
77	n	603	HEA	CMC-C2C-C1C	-4.80	118.11	125.42
77	a	603	HEA	CMC-C2C-C1C	-4.74	118.20	125.42
72	C	401	HEM	C3B-C2B-C1B	4.60	109.87	106.41
77	a	603	HEA	C3D-C4D-ND	4.60	114.80	110.35
77	n	604	HEA	C2A-C1A-NA	4.57	114.74	110.32
77	a	603	HEA	CMD-C2D-C1D	-4.47	118.05	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	604	HEA	CHA-C1A-C2A	-4.36	117.98	124.86
77	a	603	HEA	CMB-C2B-C1B	-4.24	118.41	125.03
77	n	603	HEA	CHA-C4D-C3D	-4.23	118.60	124.77
77	n	603	HEA	CHA-C1A-C2A	-4.09	118.41	124.86
77	n	604	HEA	C13-C12-C11	-4.06	107.91	114.39
77	n	604	HEA	CMD-C2D-C3D	4.04	137.08	126.15
77	n	603	HEA	C4D-C3D-C2D	-4.00	101.07	106.89
77	a	604	HEA	CHA-C4D-C3D	-3.97	118.99	124.77
77	n	604	HEA	CHA-C4D-C3D	-3.94	119.03	124.77
77	a	603	HEA	C3C-C2C-C1C	-3.90	102.58	107.17
77	a	603	HEA	CHA-C1A-C2A	-3.85	118.78	124.86
77	a	603	HEA	C13-C12-C11	-3.84	108.27	114.39
77	a	603	HEA	C4D-C3D-C2D	-3.84	101.31	106.89
77	a	604	HEA	C3C-C2C-C1C	-3.83	102.65	107.17
77	n	604	HEA	C4D-C3D-C2D	-3.80	101.36	106.89
77	n	604	HEA	CMB-C2B-C1B	-3.76	119.16	125.03
77	n	603	HEA	CAA-CBA-CGA	-3.76	103.70	113.67
77	n	603	HEA	CMB-C2B-C1B	-3.75	119.17	125.03
77	n	603	HEA	C13-C14-C15	-3.74	119.07	127.62
77	n	604	HEA	CHA-C1A-C2A	-3.73	118.97	124.86
72	N	401	HEM	CHB-C1B-NB	3.73	128.98	124.37
77	a	604	HEA	C4D-C3D-C2D	-3.64	101.59	106.89
77	n	603	HEA	CMD-C2D-C1D	-3.61	119.39	125.03
73	D	301	HEC	C4D-ND-C1D	3.60	111.69	105.82
77	n	604	HEA	C3C-C2C-C1C	-3.58	102.94	107.17
77	a	603	HEA	CHA-C4D-C3D	-3.57	119.58	124.77
73	O	303	HEC	C4D-ND-C1D	3.36	111.30	105.82
77	a	603	HEA	CMD-C2D-C3D	3.33	135.15	126.15
77	a	604	HEA	C13-C12-C11	-3.31	109.11	114.39
77	n	603	HEA	C3C-C2C-C1C	-3.26	103.32	107.17
77	a	604	HEA	CAA-CBA-CGA	-3.26	105.02	113.67
77	a	604	HEA	CMB-C2B-C1B	-3.17	120.09	125.03
77	a	604	HEA	CAD-C3D-C4D	3.16	130.20	124.70
77	a	604	HEA	C26-C15-C16	3.16	120.70	115.23
77	a	603	HEA	CMB-C2B-C3B	3.14	136.34	130.28
72	N	402	HEM	C3B-C2B-C1B	3.13	108.76	106.41
77	n	604	HEA	OMA-CMA-C3A	-3.11	118.60	125.62
72	N	401	HEM	CMB-C2B-C1B	-3.07	120.23	125.03
77	n	603	HEA	CHB-C1B-C2B	-3.07	120.18	125.03
77	a	604	HEA	CAD-CBD-CGD	-3.05	105.57	113.67
77	n	604	HEA	C26-C15-C16	3.04	120.50	115.23
77	a	604	HEA	C13-C14-C15	-2.99	120.77	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	603	HEA	C26-C15-C16	2.97	120.38	115.23
77	n	604	HEA	CAA-CBA-CGA	-2.91	105.94	113.67
77	n	603	HEA	CMB-C2B-C3B	2.86	135.80	130.28
77	n	604	HEA	C17-C18-C19	-2.79	121.24	127.62
72	C	402	HEM	C4D-ND-C1D	2.78	108.50	105.21
73	O	303	HEC	CAA-CBA-CGA	-2.77	106.31	113.67
77	a	603	HEA	C13-C14-C15	-2.76	121.30	127.62
77	n	604	HEA	C12-C11-C3B	2.76	116.43	112.12
77	n	604	HEA	C13-C14-C15	-2.73	121.38	127.62
77	a	604	HEA	C27-C19-C20	2.71	119.93	115.23
77	a	604	HEA	C17-C18-C19	-2.69	121.47	127.62
77	n	603	HEA	CMD-C2D-C3D	2.68	133.40	126.15
77	a	603	HEA	C17-C18-C19	-2.67	121.50	127.62
77	a	603	HEA	CHB-C1B-C2B	-2.67	120.82	125.03
86	W1	201	ZMP	O1-C10-C9	-2.66	120.91	123.98
77	a	603	HEA	CAA-CBA-CGA	-2.65	106.64	113.67
86	n1	201	ZMP	O1-C10-C9	-2.62	120.95	123.98
77	n	604	HEA	C25-C23-C24	2.60	120.58	114.59
77	n	604	HEA	CAD-C3D-C2D	2.60	132.73	127.87
77	n	603	HEA	CHB-C1B-NB	2.60	127.22	124.42
77	n	604	HEA	C4B-C3B-C2B	-2.58	103.10	107.44
72	C	402	HEM	C3D-C4D-ND	-2.57	107.35	110.17
72	N	402	HEM	C4D-ND-C1D	2.56	108.24	105.21
77	a	604	HEA	CHC-C1C-C2C	-2.56	120.00	127.43
77	n	603	HEA	C26-C15-C16	2.55	119.65	115.23
77	n	603	HEA	C17-C18-C19	-2.53	121.83	127.62
77	n	603	HEA	CAD-C3D-C4D	2.53	129.10	124.70
77	a	603	HEA	C3B-C4B-NB	2.51	112.73	109.84
77	a	603	HEA	CHC-C1C-C2C	-2.48	120.23	127.43
77	a	604	HEA	C25-C23-C24	2.47	120.27	114.59
77	n	604	HEA	C3B-C4B-NB	2.46	112.66	109.84
77	a	604	HEA	C4B-C3B-C2B	-2.45	103.33	107.44
77	a	604	HEA	C3B-C4B-NB	2.44	112.65	109.84
77	a	603	HEA	C2B-C1B-NB	2.41	112.69	109.90
77	a	603	HEA	C4B-C3B-C2B	-2.41	103.39	107.44
72	N	402	HEM	C3B-C4B-NB	-2.39	107.75	109.47
77	n	604	HEA	CMB-C2B-C3B	2.38	134.89	130.28
77	a	603	HEA	CAD-C3D-C4D	2.38	128.85	124.70
77	a	603	HEA	C27-C19-C20	2.38	119.35	115.23
77	n	603	HEA	C27-C19-C20	2.38	119.35	115.23
73	D	301	HEC	C2A-C1A-NA	-2.38	108.03	110.32
77	n	604	HEA	CHC-C1C-C2C	-2.36	120.57	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	N	402	HEM	C3D-C4D-ND	-2.35	107.59	110.17
77	n	603	HEA	C2B-C1B-NB	2.33	112.60	109.90
72	N	402	HEM	C1B-NB-C4B	2.32	107.96	105.21
77	n	604	HEA	C2D-C1D-ND	2.32	112.50	109.84
77	n	604	HEA	CHB-C1B-C2B	-2.32	121.37	125.03
72	C	401	HEM	C4D-ND-C1D	2.32	107.95	105.21
77	n	603	HEA	C25-C23-C24	2.27	119.81	114.59
77	a	604	HEA	CMD-C2D-C1D	-2.25	121.52	125.03
72	C	402	HEM	C2A-C1A-NA	-2.25	107.66	110.15
77	n	603	HEA	CHC-C1C-C2C	-2.24	120.92	127.43
77	n	604	HEA	C27-C19-C20	2.24	119.11	115.23
72	C	401	HEM	C2B-C1B-NB	-2.23	107.27	109.84
70	I	201	PC1	C2-O21-C21	2.22	123.11	117.80
77	a	603	HEA	C12-C11-C3B	2.21	115.57	112.12
77	a	603	HEA	C25-C23-C24	2.20	119.66	114.59
72	N	401	HEM	C4D-ND-C1D	2.19	107.80	105.21
77	a	604	HEA	OMA-CMA-C3A	-2.18	120.71	125.62
72	N	402	HEM	C2A-C1A-NA	-2.15	107.76	110.15
72	C	401	HEM	C3D-C4D-ND	-2.14	107.82	110.17
77	a	604	HEA	CHB-C1B-C2B	-2.13	121.67	125.03
77	a	604	HEA	C2C-C1C-NC	2.13	113.55	110.14
71	R	103	CDL	CA4-OA6-CA5	2.10	122.83	117.80
77	a	604	HEA	CMD-C2D-C3D	2.10	131.82	126.15
71	r1	202	CDL	CA4-OA6-CA5	2.09	122.79	117.80
69	H1	401	3PE	C2-O21-C21	2.08	122.78	117.80
73	D	301	HEC	CHC-C4B-NB	2.08	126.72	124.45
71	R	102	CDL	CA4-OA6-CA5	2.07	122.76	117.80
69	n	605	3PE	C2-O21-C21	2.07	122.75	117.80
72	N	401	HEM	CHD-C1D-ND	2.06	126.64	124.42
69	t	101	3PE	C2-O21-C21	2.06	122.73	117.80
73	D	301	HEC	CAA-CBA-CGA	-2.06	108.20	113.67
77	a	603	HEA	C2C-C1C-NC	2.06	113.44	110.14
77	a	604	HEA	CHB-C1B-NB	2.04	126.62	124.42
71	N1	401	CDL	CB4-OB6-CB5	2.03	122.65	117.80
69	g	303	3PE	C2-O21-C21	2.02	122.63	117.80
77	n	604	HEA	CAA-C2A-C1A	2.02	128.96	124.85
77	a	604	HEA	C21-C22-C23	-2.01	120.92	127.64
77	n	604	HEA	CHD-C4C-NC	2.01	127.51	123.86
69	d	201	3PE	C2-O21-C21	2.01	122.61	117.80
71	L	502	CDL	CB4-OB6-CB5	2.01	122.61	117.80
71	g	301	CDL	CB4-OB6-CB5	2.00	122.58	117.80

There are no chirality outliers.

All (793) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	t	101	3PE	C11-O13-P-O11
69	t	101	3PE	C11-O13-P-O12
69	t	101	3PE	C11-O13-P-O14
69	t	101	3PE	O13-C11-C12-N
69	z	102	3PE	O13-C11-C12-N
69	A	501	3PE	C1-O11-P-O12
69	A	501	3PE	C1-O11-P-O13
69	A	501	3PE	C1-O11-P-O14
69	A	501	3PE	C11-O13-P-O11
69	A	501	3PE	C11-O13-P-O12
69	A	501	3PE	C11-O13-P-O14
69	A	501	3PE	O13-C11-C12-N
69	C	403	3PE	C1-O11-P-O12
69	C	403	3PE	C1-O11-P-O13
69	C	403	3PE	C1-O11-P-O14
69	C	403	3PE	C11-O13-P-O12
69	C	403	3PE	C11-O13-P-O14
69	E	202	3PE	C11-O13-P-O14
69	E	202	3PE	O13-C11-C12-N
69	E	203	3PE	C1-O11-P-O12
69	E	203	3PE	C1-O11-P-O13
69	E	203	3PE	C11-O13-P-O12
69	E	203	3PE	O13-C11-C12-N
69	G	102	3PE	C1-O11-P-O13
69	G	102	3PE	C1-O11-P-O14
69	G	102	3PE	C11-O13-P-O14
69	L	501	3PE	C11-O13-P-O11
69	L	501	3PE	C11-O13-P-O12
69	L	501	3PE	O13-C11-C12-N
69	N	403	3PE	C11-O13-P-O11
69	N	403	3PE	C11-O13-P-O12
69	N	403	3PE	C11-O13-P-O14
69	N	403	3PE	O13-C11-C12-N
69	O	302	3PE	C1-O11-P-O14
69	O	302	3PE	C11-O13-P-O14
69	O	302	3PE	O13-C11-C12-N
69	R	104	3PE	C11-O13-P-O11
69	R	104	3PE	O13-C11-C12-N
69	n	605	3PE	C1-O11-P-O12
69	n	605	3PE	C1-O11-P-O14
69	n	605	3PE	C11-O13-P-O11
69	n	605	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	n	605	3PE	C11-O13-P-O14
69	n	605	3PE	O13-C11-C12-N
69	n	606	3PE	C1-O11-P-O12
69	n	606	3PE	C1-O11-P-O13
69	n	606	3PE	C1-O11-P-O14
69	n	606	3PE	O11-C1-C2-O21
69	n	607	3PE	C1-O11-P-O13
69	n	607	3PE	C11-O13-P-O14
69	n	607	3PE	C2-C1-O11-P
69	n	607	3PE	O13-C11-C12-N
69	o	302	3PE	C1-O11-P-O13
69	o	302	3PE	C11-O13-P-O11
69	o	302	3PE	C12-C11-O13-P
69	p	301	3PE	C1-O11-P-O12
69	p	301	3PE	C1-O11-P-O13
69	p	301	3PE	C1-O11-P-O14
69	p	301	3PE	C11-O13-P-O11
69	p	301	3PE	C11-O13-P-O14
69	p	301	3PE	O13-C11-C12-N
69	v	101	3PE	C1-O11-P-O12
69	v	101	3PE	C1-O11-P-O13
69	v	101	3PE	O13-C11-C12-N
69	6	202	3PE	C11-O13-P-O14
69	6	202	3PE	O13-C11-C12-N
69	r1	201	3PE	C1-O11-P-O12
69	r1	201	3PE	C1-O11-P-O14
69	r1	201	3PE	C11-O13-P-O11
69	r1	201	3PE	C11-O13-P-O12
69	r1	201	3PE	C11-O13-P-O14
69	r1	201	3PE	O13-C11-C12-N
69	K1	201	3PE	C1-O11-P-O12
69	K1	201	3PE	C1-O11-P-O13
69	K1	201	3PE	C1-O11-P-O14
69	K1	201	3PE	C11-O13-P-O11
69	L1	701	3PE	C1-O11-P-O13
69	L1	701	3PE	C1-O11-P-O14
69	L1	701	3PE	C11-O13-P-O14
69	L1	704	3PE	C1-O11-P-O12
69	L1	704	3PE	C1-O11-P-O13
69	L1	704	3PE	O13-C11-C12-N
69	M1	502	3PE	C1-O11-P-O12
69	M1	502	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
69	M1	502	3PE	C11-O13-P-O11
69	M1	502	3PE	C11-O13-P-O12
69	M1	502	3PE	C11-O13-P-O14
69	M1	502	3PE	O13-C11-C12-N
69	M1	503	3PE	C11-O13-P-O11
69	M1	503	3PE	C11-O13-P-O12
69	M1	503	3PE	C11-O13-P-O14
69	M1	503	3PE	O13-C11-C12-N
69	N1	402	3PE	O13-C11-C12-N
69	Y1	402	3PE	C1-O11-P-O12
69	Y1	402	3PE	C1-O11-P-O13
69	Y1	402	3PE	C1-O11-P-O14
69	Y1	402	3PE	O13-C11-C12-N
69	Y1	403	3PE	C11-O13-P-O11
69	Y1	403	3PE	C11-O13-P-O14
69	b1	101	3PE	C11-O13-P-O11
69	d1	202	3PE	C11-O13-P-O11
69	d1	202	3PE	C11-O13-P-O12
69	d1	202	3PE	C11-O13-P-O14
69	d1	202	3PE	O13-C11-C12-N
69	d1	203	3PE	C1-O11-P-O12
69	d1	203	3PE	C1-O11-P-O13
69	d1	203	3PE	C1-O11-P-O14
69	i1	201	3PE	C11-O13-P-O11
69	i1	201	3PE	C11-O13-P-O12
69	m1	601	3PE	C1-O11-P-O13
69	m1	601	3PE	C1-O11-P-O14
69	m1	601	3PE	C11-O13-P-O11
69	m1	601	3PE	C11-O13-P-O12
69	m1	601	3PE	C11-O13-P-O14
69	a	605	3PE	C1-O11-P-O12
69	a	606	3PE	C11-O13-P-O11
69	a	606	3PE	C11-O13-P-O14
69	a	606	3PE	O13-C11-C12-N
69	b	301	3PE	C11-O13-P-O11
69	c	301	3PE	C11-O13-P-O11
69	c	301	3PE	C11-O13-P-O12
69	c	301	3PE	O13-C11-C12-N
69	d	201	3PE	C11-O13-P-O14
69	d	201	3PE	O13-C11-C12-N
69	g	303	3PE	C11-O13-P-O11
69	g	303	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	g	303	3PE	C11-O13-P-O14
69	g	303	3PE	O13-C11-C12-N
69	i	101	3PE	C1-O11-P-O13
69	i	101	3PE	C11-O13-P-O12
69	i	101	3PE	O13-C11-C12-N
70	J	101	PC1	C11-O13-P-O11
70	J	101	PC1	C1-O11-P-O12
70	J	101	PC1	C1-O11-P-O14
70	J	101	PC1	C1-O11-P-O13
70	K	101	PC1	C11-O13-P-O14
70	L	503	PC1	C11-O13-P-O12
70	L	503	PC1	C11-O13-P-O14
70	L	503	PC1	C11-O13-P-O11
70	L	503	PC1	C1-O11-P-O12
70	L	503	PC1	C1-O11-P-O13
70	I	201	PC1	C11-O13-P-O12
70	I	201	PC1	C11-O13-P-O11
70	I	201	PC1	C1-O11-P-O12
70	I	201	PC1	C1-O11-P-O13
70	p	302	PC1	C11-O13-P-O12
70	p	302	PC1	C11-O13-P-O14
70	p	302	PC1	C1-O11-P-O14
70	p	302	PC1	C1-O11-P-O13
70	6	203	PC1	C11-O13-P-O12
70	6	203	PC1	C1-O11-P-O12
70	6	203	PC1	C1-O11-P-O14
70	6	203	PC1	C1-O11-P-O13
70	9	203	PC1	C11-O13-P-O12
70	9	203	PC1	C11-O13-P-O11
70	9	203	PC1	C1-O11-P-O12
70	9	203	PC1	C1-O11-P-O14
70	9	203	PC1	C1-O11-P-O13
70	9	204	PC1	C1-O11-P-O14
70	P1	502	PC1	C11-O13-P-O12
70	P1	502	PC1	C11-O13-P-O14
70	P1	502	PC1	C11-O13-P-O11
70	P1	502	PC1	C1-O11-P-O12
70	P1	502	PC1	C1-O11-P-O14
70	M1	501	PC1	C11-O13-P-O12
70	M1	501	PC1	C11-O13-P-O11
70	g	302	PC1	C1-O11-P-O14
71	A	502	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
71	A	502	CDL	CB2-OB2-PB2-OB4
71	A	502	CDL	CB2-OB2-PB2-OB5
71	A	502	CDL	CB3-OB5-PB2-OB2
71	A	502	CDL	CB3-OB5-PB2-OB4
71	D	302	CDL	CA2-OA2-PA1-OA5
71	D	302	CDL	CA3-OA5-PA1-OA3
71	D	302	CDL	CA3-OA5-PA1-OA4
71	D	302	CDL	CB2-OB2-PB2-OB4
71	D	302	CDL	CB2-OB2-PB2-OB5
71	D	302	CDL	CB3-OB5-PB2-OB2
71	D	302	CDL	CB3-OB5-PB2-OB4
71	G	101	CDL	CA2-OA2-PA1-OA4
71	G	101	CDL	CB2-OB2-PB2-OB3
71	G	101	CDL	CB2-OB2-PB2-OB4
71	G	101	CDL	CB3-OB5-PB2-OB3
71	L	502	CDL	CA3-OA5-PA1-OA3
71	O	301	CDL	CA2-OA2-PA1-OA4
71	O	301	CDL	CB2-OB2-PB2-OB3
71	O	301	CDL	CB3-OB5-PB2-OB2
71	O	301	CDL	CB3-OB5-PB2-OB4
71	R	101	CDL	CA2-OA2-PA1-OA3
71	R	101	CDL	CA2-OA2-PA1-OA4
71	R	101	CDL	CA2-OA2-PA1-OA5
71	R	101	CDL	CB2-OB2-PB2-OB3
71	R	102	CDL	CA3-OA5-PA1-OA2
71	R	102	CDL	CA3-OA5-PA1-OA3
71	R	102	CDL	CA3-OA5-PA1-OA4
71	R	102	CDL	CB2-OB2-PB2-OB5
71	R	102	CDL	CB3-OB5-PB2-OB2
71	R	102	CDL	CB3-OB5-PB2-OB4
71	R	103	CDL	CA3-OA5-PA1-OA2
71	R	103	CDL	CA3-OA5-PA1-OA3
71	R	103	CDL	CA3-OA5-PA1-OA4
71	R	103	CDL	CB2-OB2-PB2-OB3
71	R	103	CDL	CB2-OB2-PB2-OB4
71	R	103	CDL	CB2-OB2-PB2-OB5
71	R	103	CDL	CB3-OB5-PB2-OB2
71	R	103	CDL	CB3-OB5-PB2-OB3
71	R	103	CDL	CB3-OB5-PB2-OB4
71	V	101	CDL	CA3-OA5-PA1-OA2
71	V	101	CDL	CA3-OA5-PA1-OA3
71	V	101	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
71	V	101	CDL	CB2-OB2-PB2-OB3
71	r1	202	CDL	CA2-OA2-PA1-OA3
71	r1	202	CDL	CA2-OA2-PA1-OA4
71	r1	202	CDL	CA2-OA2-PA1-OA5
71	r1	202	CDL	CA3-OA5-PA1-OA4
71	r1	202	CDL	CB2-OB2-PB2-OB5
71	H1	402	CDL	CA2-OA2-PA1-OA3
71	H1	402	CDL	CA2-OA2-PA1-OA4
71	H1	402	CDL	CA2-OA2-PA1-OA5
71	H1	402	CDL	CB2-OB2-PB2-OB3
71	H1	402	CDL	CB2-OB2-PB2-OB4
71	H1	402	CDL	CB2-OB2-PB2-OB5
71	L1	702	CDL	CA2-OA2-PA1-OA5
71	L1	702	CDL	CB2-OB2-PB2-OB3
71	L1	702	CDL	CB2-OB2-PB2-OB4
71	L1	702	CDL	CB2-OB2-PB2-OB5
71	L1	702	CDL	CB3-OB5-PB2-OB2
71	L1	702	CDL	CB3-OB5-PB2-OB4
71	L1	703	CDL	CA2-OA2-PA1-OA3
71	L1	703	CDL	CA2-OA2-PA1-OA4
71	L1	703	CDL	CA2-OA2-PA1-OA5
71	L1	703	CDL	CA3-OA5-PA1-OA2
71	L1	703	CDL	CA3-OA5-PA1-OA3
71	L1	703	CDL	CB2-OB2-PB2-OB5
71	N1	401	CDL	CA2-OA2-PA1-OA4
71	N1	401	CDL	OA6-CA4-CA6-OA8
71	N1	401	CDL	CB2-OB2-PB2-OB3
71	N1	401	CDL	CB2-OB2-PB2-OB4
71	N1	401	CDL	CB2-OB2-PB2-OB5
71	Y1	401	CDL	CA2-OA2-PA1-OA3
71	Y1	401	CDL	CA2-OA2-PA1-OA4
71	Y1	401	CDL	CA2-OA2-PA1-OA5
71	Y1	401	CDL	CB3-OB5-PB2-OB2
71	d1	201	CDL	CA2-OA2-PA1-OA3
71	d1	201	CDL	CA2-OA2-PA1-OA4
71	d1	201	CDL	CA3-OA5-PA1-OA2
71	d1	201	CDL	OB5-CB3-CB4-OB6
71	h1	201	CDL	CA2-OA2-PA1-OA3
71	h1	201	CDL	CA2-OA2-PA1-OA5
71	h1	201	CDL	CB2-OB2-PB2-OB4
71	h1	201	CDL	CB2-OB2-PB2-OB5
71	h1	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
71	h1	201	CDL	CB3-OB5-PB2-OB3
71	g	301	CDL	CA2-OA2-PA1-OA3
71	g	301	CDL	CA2-OA2-PA1-OA4
71	g	301	CDL	CA2-OA2-PA1-OA5
73	D	301	HEC	C2C-C3C-CAC-CBC
73	O	303	HEC	C2B-C3B-CAB-CBB
73	O	303	HEC	C2C-C3C-CAC-CBC
77	n	603	HEA	C2A-C3A-CMA-OMA
77	n	603	HEA	C4A-C3A-CMA-OMA
77	n	603	HEA	C11-C12-C13-C14
77	n	604	HEA	C2A-C3A-CMA-OMA
77	n	604	HEA	C4A-C3A-CMA-OMA
77	n	604	HEA	C2D-C3D-CAD-CBD
77	n	604	HEA	C4D-C3D-CAD-CBD
77	a	603	HEA	C1A-C2A-CAA-CBA
77	a	603	HEA	C3A-C2A-CAA-CBA
77	a	603	HEA	C2A-C3A-CMA-OMA
77	a	603	HEA	C4A-C3A-CMA-OMA
77	a	603	HEA	C11-C12-C13-C14
77	a	604	HEA	C2A-C3A-CMA-OMA
77	a	604	HEA	C4A-C3A-CMA-OMA
83	1	501	FMN	N10-C1'-C2'-O2'
83	1	501	FMN	N10-C1'-C2'-C3'
83	1	501	FMN	C5'-O5'-P-O1P
83	1	501	FMN	C5'-O5'-P-O2P
86	W1	201	ZMP	C19-C18-C21-O5
86	W1	201	ZMP	C20-C18-C21-O5
86	W1	201	ZMP	S1-C11-C12-N1
86	n1	201	ZMP	C17-C18-C21-O5
86	n1	201	ZMP	O4-C17-C18-C21
86	n1	201	ZMP	C16-C17-C18-C21
86	n1	201	ZMP	O4-C17-C18-C19
86	n1	201	ZMP	C16-C17-C18-C20
86	n1	201	ZMP	O3-C16-C17-O4
86	n1	201	ZMP	C17-C16-N2-C15
86	n1	201	ZMP	C13-C14-C15-N2
86	n1	201	ZMP	O1-C10-S1-C11
86	n1	201	ZMP	C9-C10-S1-C11
86	n1	201	ZMP	C7-C8-C9-C10
71	V	101	CDL	OA9-CA7-OA8-CA6
71	V	101	CDL	C31-CA7-OA8-CA6
77	a	603	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
77	a	604	HEA	C26-C15-C16-C17
77	a	603	HEA	C14-C15-C16-C17
77	a	604	HEA	C14-C15-C16-C17
86	n1	201	ZMP	O3-C16-N2-C15
77	n	603	HEA	C15-C16-C17-C18
77	n	603	HEA	C19-C20-C21-C22
77	n	604	HEA	C15-C16-C17-C18
77	a	604	HEA	C15-C16-C17-C18
72	N	402	HEM	C2A-CAA-CBA-CGA
69	M1	502	3PE	C31-C32-C33-C34
71	O	301	CDL	OB5-CB3-CB4-OB6
71	R	103	CDL	OB5-CB3-CB4-OB6
70	p	302	PC1	C11-C12-N-C13
72	C	401	HEM	C2A-CAA-CBA-CGA
72	N	401	HEM	C2A-CAA-CBA-CGA
70	M1	501	PC1	C21-C22-C23-C24
77	a	604	HEA	C1A-C2A-CAA-CBA
70	V	102	PC1	C11-C12-N-C13
70	6	203	PC1	C11-C12-N-C14
70	9	204	PC1	C11-C12-N-C15
70	P1	502	PC1	C11-C12-N-C15
71	V	101	CDL	C11-CA5-OA6-CA4
71	V	101	CDL	OA7-CA5-OA6-CA4
77	a	603	HEA	O11-C11-C12-C13
71	N1	401	CDL	C81-C82-C83-C84
71	H1	402	CDL	C13-C14-C15-C16
69	M1	503	3PE	C28-C29-C2A-C2B
69	L1	704	3PE	C38-C39-C3A-C3B
69	G	102	3PE	C37-C38-C39-C3A
69	b1	101	3PE	C3A-C3B-C3C-C3D
69	H1	401	3PE	C31-C32-C33-C34
69	N1	402	3PE	C1-C2-C3-O31
77	a	603	HEA	C15-C16-C17-C18
71	Y1	401	CDL	C82-C83-C84-C85
70	z	101	PC1	C11-C12-N-C13
70	V	102	PC1	C11-C12-N-C14
70	p	302	PC1	C11-C12-N-C14
70	p	302	PC1	C11-C12-N-C15
70	6	203	PC1	C11-C12-N-C15
70	9	204	PC1	C11-C12-N-C14
69	L1	701	3PE	C21-C22-C23-C24
69	N1	402	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
70	9	204	PC1	C2A-C2B-C2C-C2D
70	M1	501	PC1	C37-C38-C39-C3A
86	n1	201	ZMP	C6-C7-C8-C9
69	M1	502	3PE	C23-C24-C25-C26
69	M1	502	3PE	C36-C37-C38-C39
71	d1	201	CDL	C55-C56-C57-C58
71	R	103	CDL	CA5-C11-C12-C13
69	c	301	3PE	C23-C24-C25-C26
77	n	604	HEA	C26-C15-C16-C17
70	z	101	PC1	C11-C12-N-C15
70	V	102	PC1	C11-C12-N-C15
70	6	203	PC1	C11-C12-N-C13
70	9	204	PC1	C11-C12-N-C13
70	P1	502	PC1	C11-C12-N-C13
70	P1	502	PC1	C11-C12-N-C14
69	p	301	3PE	C23-C24-C25-C26
70	I	201	PC1	C25-C26-C27-C28
69	n	607	3PE	O21-C2-C3-O31
71	D	302	CDL	C74-C75-C76-C77
71	Y1	401	CDL	C73-C74-C75-C76
69	L1	704	3PE	C32-C33-C34-C35
70	9	204	PC1	C34-C35-C36-C37
69	C	404	3PE	C1-C2-C3-O31
71	d1	201	CDL	C63-C64-C65-C66
70	z	101	PC1	C11-C12-N-C14
71	V	101	CDL	C12-C11-CA5-OA6
71	D	302	CDL	C1-CB2-OB2-PB2
77	a	604	HEA	C3A-C2A-CAA-CBA
69	G	102	3PE	C32-C33-C34-C35
69	o	302	3PE	O21-C2-C3-O31
69	N1	402	3PE	O21-C2-C3-O31
77	a	603	HEA	C3B-C11-C12-C13
86	n1	201	ZMP	O4-C17-C18-C20
77	n	603	HEA	C1A-C2A-CAA-CBA
86	n1	201	ZMP	C5-C6-C7-C8
69	p	301	3PE	C2-C1-O11-P
69	a	606	3PE	C2-C1-O11-P
69	g	303	3PE	C2-C1-O11-P
70	J	101	PC1	C2-C1-O11-P
72	C	402	HEM	C2A-CAA-CBA-CGA
69	n	606	3PE	O11-C1-C2-C3
71	O	301	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
71	R	103	CDL	OB5-CB3-CB4-CB6
71	L1	703	CDL	OB5-CB3-CB4-CB6
71	d1	201	CDL	OB5-CB3-CB4-CB6
71	R	103	CDL	CB3-CB4-CB6-OB8
70	P1	502	PC1	O11-C1-C2-O21
71	L1	702	CDL	OB5-CB3-CB4-OB6
69	m1	601	3PE	C2-C1-O11-P
71	O	301	CDL	CB4-CB3-OB5-PB2
71	H1	402	CDL	C1-CB2-OB2-PB2
86	W1	201	ZMP	O1-C10-S1-C11
69	g	303	3PE	O31-C31-C32-C33
69	C	404	3PE	O21-C2-C3-O31
69	n	606	3PE	O21-C2-C3-O31
71	R	103	CDL	OB6-CB4-CB6-OB8
71	Y1	401	CDL	OB6-CB4-CB6-OB8
69	L	501	3PE	C31-C32-C33-C34
69	d1	203	3PE	C21-C22-C23-C24
71	R	101	CDL	OB5-CB3-CB4-CB6
70	P1	502	PC1	O21-C21-C22-C23
77	n	604	HEA	C14-C15-C16-C17
69	b	301	3PE	O11-C1-C2-O21
71	R	101	CDL	OB5-CB3-CB4-OB6
69	n	607	3PE	C1-C2-C3-O31
71	N1	401	CDL	CA3-CA4-CA6-OA8
71	Y1	401	CDL	CB3-CB4-CB6-OB8
72	N	402	HEM	C4B-C3B-CAB-CBB
71	D	302	CDL	C52-C51-CB5-OB6
69	M1	502	3PE	C12-C11-O13-P
69	b	301	3PE	C12-C11-O13-P
69	c	301	3PE	C12-C11-O13-P
69	g	303	3PE	C12-C11-O13-P
69	i	101	3PE	C12-C11-O13-P
86	n1	201	ZMP	C16-C17-C18-C19
69	N	403	3PE	C25-C26-C27-C28
71	G	101	CDL	C72-C71-CB7-OB8
70	J	101	PC1	O13-C11-C12-N
70	L	503	PC1	O13-C11-C12-N
70	I	201	PC1	O13-C11-C12-N
70	9	203	PC1	O13-C11-C12-N
70	M1	501	PC1	O13-C11-C12-N
70	g	302	PC1	O13-C11-C12-N
71	L1	702	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
69	b1	101	3PE	C23-C24-C25-C26
69	b1	101	3PE	C21-C22-C23-C24
69	c	301	3PE	C32-C33-C34-C35
71	L1	702	CDL	OB5-CB3-CB4-CB6
71	h1	201	CDL	OB5-CB3-CB4-CB6
86	n1	201	ZMP	C19-C18-C21-O5
86	n1	201	ZMP	C20-C18-C21-O5
71	L	502	CDL	C31-C32-C33-C34
71	N1	401	CDL	C78-C79-C80-C81
69	K1	201	3PE	C2-C1-O11-P
71	H1	402	CDL	C1-CA2-OA2-PA1
71	h1	201	CDL	CA4-CA3-OA5-PA1
71	g	301	CDL	CA4-CA3-OA5-PA1
73	D	301	HEC	C4B-C3B-CAB-CBB
73	D	301	HEC	C4C-C3C-CAC-CBC
73	O	303	HEC	C4B-C3B-CAB-CBB
73	O	303	HEC	C4C-C3C-CAC-CBC
70	K	101	PC1	O11-C1-C2-O21
71	L1	703	CDL	OB5-CB3-CB4-OB6
71	N1	401	CDL	OB5-CB3-CB4-OB6
71	h1	201	CDL	OB5-CB3-CB4-OB6
69	E	202	3PE	C1-C2-C3-O31
69	n	606	3PE	C1-C2-C3-O31
69	o	302	3PE	C1-C2-C3-O31
69	c	301	3PE	C25-C26-C27-C28
69	C	403	3PE	C11-O13-P-O11
69	E	203	3PE	C11-O13-P-O11
69	E	203	3PE	C11-O13-P-O14
69	G	102	3PE	C1-O11-P-O12
69	L	501	3PE	C11-O13-P-O14
69	O	302	3PE	C1-O11-P-O12
69	O	302	3PE	C1-O11-P-O13
69	O	302	3PE	C11-O13-P-O11
69	R	104	3PE	C11-O13-P-O14
69	n	605	3PE	C1-O11-P-O13
69	n	607	3PE	C1-O11-P-O14
69	o	302	3PE	C1-O11-P-O14
69	o	302	3PE	C11-O13-P-O14
69	p	301	3PE	C11-O13-P-O12
69	v	101	3PE	C1-O11-P-O14
69	v	101	3PE	C11-O13-P-O11
69	v	101	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	v	101	3PE	C11-O13-P-O14
69	6	202	3PE	C11-O13-P-O11
69	r1	201	3PE	C1-O11-P-O13
69	H1	401	3PE	C1-O11-P-O14
69	K1	201	3PE	C11-O13-P-O14
69	L1	701	3PE	C1-O11-P-O12
69	L1	701	3PE	C11-O13-P-O11
69	L1	701	3PE	O13-C11-C12-N
69	M1	502	3PE	C1-O11-P-O14
69	b1	101	3PE	C11-O13-P-O14
69	b1	101	3PE	O13-C11-C12-N
69	d1	202	3PE	C1-O11-P-O12
69	d1	202	3PE	C1-O11-P-O13
69	d1	202	3PE	C1-O11-P-O14
69	m1	601	3PE	C1-O11-P-O12
69	m1	601	3PE	O13-C11-C12-N
69	a	605	3PE	C11-O13-P-O14
69	a	606	3PE	C1-O11-P-O14
69	a	606	3PE	C11-O13-P-O12
69	b	301	3PE	C1-O11-P-O14
69	b	301	3PE	C11-O13-P-O14
69	b	301	3PE	O13-C11-C12-N
69	i	101	3PE	C1-O11-P-O14
69	i	101	3PE	C11-O13-P-O11
69	i	101	3PE	C11-O13-P-O14
70	z	101	PC1	C1-O11-P-O14
70	J	101	PC1	C11-O13-P-O14
70	L	503	PC1	C1-O11-P-O14
70	p	302	PC1	C11-O13-P-O11
70	p	302	PC1	C1-O11-P-O12
70	6	203	PC1	C11-O13-P-O14
70	6	203	PC1	C11-O13-P-O11
70	P1	502	PC1	C1-O11-P-O13
70	g	302	PC1	C11-O13-P-O14
70	g	302	PC1	C1-O11-P-O12
70	g	302	PC1	C1-O11-P-O13
71	A	502	CDL	CB3-OB5-PB2-OB3
71	D	302	CDL	CA2-OA2-PA1-OA3
71	D	302	CDL	CA3-OA5-PA1-OA2
71	G	101	CDL	CA2-OA2-PA1-OA3
71	G	101	CDL	CA2-OA2-PA1-OA5
71	G	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
71	G	101	CDL	CB3-OB5-PB2-OB2
71	G	101	CDL	CB3-OB5-PB2-OB4
71	L	502	CDL	CA3-OA5-PA1-OA2
71	O	301	CDL	CA2-OA2-PA1-OA3
71	O	301	CDL	CA2-OA2-PA1-OA5
71	O	301	CDL	CB2-OB2-PB2-OB4
71	O	301	CDL	CB2-OB2-PB2-OB5
71	R	102	CDL	CB2-OB2-PB2-OB3
71	V	101	CDL	CB3-OB5-PB2-OB3
71	r1	202	CDL	CA3-OA5-PA1-OA2
71	r1	202	CDL	CA3-OA5-PA1-OA3
71	r1	202	CDL	CB2-OB2-PB2-OB3
71	L1	702	CDL	CA2-OA2-PA1-OA3
71	L1	702	CDL	CB3-OB5-PB2-OB3
71	L1	703	CDL	CA3-OA5-PA1-OA4
71	L1	703	CDL	CB2-OB2-PB2-OB3
71	L1	703	CDL	CB3-OB5-PB2-OB3
71	N1	401	CDL	CA2-OA2-PA1-OA3
71	N1	401	CDL	CA2-OA2-PA1-OA5
71	N1	401	CDL	CA3-OA5-PA1-OA3
71	N1	401	CDL	CB3-OB5-PB2-OB2
71	N1	401	CDL	CB3-OB5-PB2-OB3
71	N1	401	CDL	CB3-OB5-PB2-OB4
71	Y1	401	CDL	CB3-OB5-PB2-OB3
71	d1	201	CDL	CA2-OA2-PA1-OA5
71	d1	201	CDL	CA3-OA5-PA1-OA3
71	d1	201	CDL	CB2-OB2-PB2-OB3
71	h1	201	CDL	CA2-OA2-PA1-OA4
71	h1	201	CDL	CB3-OB5-PB2-OB4
73	D	301	HEC	C2B-C3B-CAB-CBB
71	N1	401	CDL	C80-C81-C82-C83
71	L	502	CDL	C52-C51-CB5-OB6
69	t	101	3PE	C2-C1-O11-P
69	a	605	3PE	C2-C1-O11-P
69	c	301	3PE	C2-C1-O11-P
71	D	302	CDL	C1-CA2-OA2-PA1
71	D	302	CDL	CB4-CB3-OB5-PB2
71	G	101	CDL	C1-CA2-OA2-PA1
71	L	502	CDL	CB4-CB3-OB5-PB2
71	O	301	CDL	C1-CA2-OA2-PA1
71	R	101	CDL	CA4-CA3-OA5-PA1
71	R	103	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
71	h1	201	CDL	C1-CA2-OA2-PA1
71	D	302	CDL	C72-C73-C74-C75
69	M1	502	3PE	C3D-C3E-C3F-C3G
70	p	302	PC1	C21-C22-C23-C24
69	b1	101	3PE	C38-C39-C3A-C3B
69	t	101	3PE	C3-C2-O21-C21
70	9	203	PC1	C3-C2-O21-C21
71	V	101	CDL	CA3-CA4-OA6-CA5
71	G	101	CDL	C72-C71-CB7-OB9
71	R	102	CDL	C31-C32-C33-C34
69	6	202	3PE	C32-C33-C34-C35
77	a	604	HEA	O11-C11-C12-C13
71	d1	201	CDL	C1-CB2-OB2-PB2
69	E	202	3PE	O21-C2-C3-O31
69	H1	401	3PE	O31-C31-C32-C33
85	P1	501	NDP	PN-O3-PA-O2A
69	r1	201	3PE	O31-C31-C32-C33
77	n	603	HEA	C3A-C2A-CAA-CBA
71	L1	702	CDL	C12-C11-CA5-OA6
69	M1	502	3PE	C37-C38-C39-C3A
69	M1	503	3PE	O11-C1-C2-O21
71	D	302	CDL	OB5-CB3-CB4-OB6
71	g	301	CDL	CB4-CB3-OB5-PB2
69	L1	704	3PE	O21-C21-C22-C23
69	H1	401	3PE	C2A-C2B-C2C-C2D
70	I	201	PC1	C36-C37-C38-C39
69	O	302	3PE	C34-C35-C36-C37
69	H1	401	3PE	C2-C1-O11-P
69	i1	201	3PE	C2-C1-O11-P
77	a	603	HEA	C2A-CAA-CBA-CGA
86	n1	201	ZMP	N2-C16-C17-O4
77	a	604	HEA	CAA-CBA-CGA-O1A
77	a	604	HEA	CAA-CBA-CGA-O2A
69	H1	401	3PE	C21-C22-C23-C24
77	n	604	HEA	CAA-CBA-CGA-O2A
69	d1	203	3PE	O21-C21-C22-C23
69	H1	401	3PE	C3-C2-O21-C21
69	d	201	3PE	C3-C2-O21-C21
69	g	303	3PE	C3-C2-O21-C21
71	h1	201	CDL	CB6-CB4-OB6-CB5
77	a	603	HEA	CAD-CBD-CGD-O1D
71	V	101	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
69	p	301	3PE	C22-C23-C24-C25
69	N1	402	3PE	C2-C1-O11-P
77	n	603	HEA	O11-C11-C12-C13
77	a	603	HEA	CAD-CBD-CGD-O2D
77	a	604	HEA	CAD-CBD-CGD-O1D
69	H1	401	3PE	O11-C1-C2-C3
70	6	203	PC1	O11-C1-C2-C3
71	D	302	CDL	OB5-CB3-CB4-CB6
69	c	301	3PE	C28-C29-C2A-C2B
70	M1	501	PC1	O21-C2-C3-O31
85	P1	501	NDP	O4D-C1D-N1N-C6N
70	9	204	PC1	C35-C36-C37-C38
71	r1	202	CDL	C52-C51-CB5-OB6
77	n	604	HEA	CAA-CBA-CGA-O1A
69	M1	503	3PE	C27-C28-C29-C2A
77	n	603	HEA	C27-C19-C20-C21
69	n	606	3PE	C2-C1-O11-P
71	O	301	CDL	C1-CB2-OB2-PB2
71	N1	401	CDL	C1-CA2-OA2-PA1
70	I	201	PC1	O21-C21-C22-C23
71	g	301	CDL	CA3-CA4-CA6-OA8
77	a	604	HEA	C19-C20-C21-C22
69	M1	502	3PE	C33-C34-C35-C36
71	r1	202	CDL	OB5-CB3-CB4-OB6
71	N1	401	CDL	C79-C80-C81-C82
86	W1	201	ZMP	C9-C10-S1-C11
73	O	303	HEC	CAD-CBD-CGD-O2D
77	a	604	HEA	CAD-CBD-CGD-O2D
71	R	103	CDL	C75-C76-C77-C78
72	N	402	HEM	CAD-CBD-CGD-O2D
71	h1	201	CDL	C12-C11-CA5-OA6
69	M1	503	3PE	O11-C1-C2-C3
69	c	301	3PE	O11-C1-C2-C3
71	V	101	CDL	OB5-CB3-CB4-CB6
71	r1	202	CDL	OB5-CB3-CB4-CB6
70	V	102	PC1	C2-C1-O11-P
71	D	302	CDL	CA4-CA3-OA5-PA1
70	9	203	PC1	C37-C38-C39-C3A
85	P1	501	NDP	C2D-C1D-N1N-C6N
83	1	501	FMN	C5'-O5'-P-O3P
69	g	303	3PE	O32-C31-C32-C33
69	G	102	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
71	G	101	CDL	C32-C31-CA7-OA8
69	L1	701	3PE	C3-C2-O21-C21
70	I	201	PC1	C1-C2-O21-C21
70	6	203	PC1	C3-C2-O21-C21
69	b1	101	3PE	C34-C35-C36-C37
73	O	303	HEC	CAD-CBD-CGD-O1D
71	N1	401	CDL	C51-C52-C53-C54
72	N	402	HEM	CAD-CBD-CGD-O1D
69	Y1	403	3PE	C1-C2-C3-O31
69	b	301	3PE	C1-C2-C3-O31
71	d1	201	CDL	CA3-CA4-CA6-OA8
77	n	603	HEA	CAD-CBD-CGD-O1D
69	M1	503	3PE	O21-C2-C3-O31
69	K1	201	3PE	O21-C21-C22-C23
69	d	201	3PE	O21-C21-C22-C23
70	9	203	PC1	C29-C2A-C2B-C2C
69	L	501	3PE	O11-C1-C2-C3
71	A	502	CDL	OB5-CB3-CB4-CB6
69	E	202	3PE	O31-C31-C32-C33
71	A	502	CDL	C52-C51-CB5-OB6
77	a	604	HEA	C2C-C3C-CAC-CBC
69	C	403	3PE	O31-C31-C32-C33
69	N	403	3PE	O31-C31-C32-C33
70	K	101	PC1	O21-C21-C22-C23
70	P1	502	PC1	O31-C31-C32-C33
71	A	502	CDL	C12-C11-CA5-OA6
69	o	302	3PE	C22-C23-C24-C25
70	K	101	PC1	O13-C11-C12-N
85	P1	501	NDP	PN-O3-PA-O1A
87	O1	401	DGT	PB-O3A-PA-O1A
69	C	404	3PE	O21-C21-C22-C23
70	9	204	PC1	O31-C31-C32-C33
71	V	101	CDL	C75-C76-C77-C78
69	i1	201	3PE	O31-C31-C32-C33
71	A	502	CDL	C32-C31-CA7-OA8
71	R	102	CDL	C32-C31-CA7-OA8
69	C	403	3PE	C2A-C2B-C2C-C2D
69	K1	201	3PE	C25-C26-C27-C28
69	Y1	403	3PE	C23-C24-C25-C26
69	E	203	3PE	O31-C31-C32-C33
71	d1	201	CDL	C72-C71-CB7-OB8
71	h1	201	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
71	g	301	CDL	C12-C11-CA5-OA6
71	R	102	CDL	OA5-CA3-CA4-OA6
71	R	101	CDL	C32-C31-CA7-OA8
70	9	204	PC1	C21-C22-C23-C24
81	y	601	TGL	CC1-CC2-CC3-CC4
73	O	303	HEC	CAA-CBA-CGA-O2A
69	M1	503	3PE	C2-C1-O11-P
69	O	302	3PE	O21-C21-C22-C23
69	K1	201	3PE	O31-C31-C32-C33
69	M1	502	3PE	O21-C21-C22-C23
69	b1	101	3PE	O31-C31-C32-C33
69	a	606	3PE	O31-C31-C32-C33
71	R	102	CDL	C52-C51-CB5-OB6
71	L1	703	CDL	C32-C31-CA7-OA8
71	O	301	CDL	O1-C1-CA2-OA2
71	r1	202	CDL	C17-C18-C19-C20
71	R	102	CDL	C72-C71-CB7-OB8
71	h1	201	CDL	C72-C71-CB7-OB8
69	p	301	3PE	C25-C26-C27-C28
69	E	203	3PE	O21-C2-C3-O31
69	m1	601	3PE	O21-C2-C3-O31
70	P1	502	PC1	O22-C21-C22-C23
69	o	302	3PE	O21-C21-C22-C23
71	L1	702	CDL	C72-C71-CB7-OB8
71	h1	201	CDL	C32-C31-CA7-OA8
77	n	603	HEA	CAD-CBD-CGD-O2D
69	b	301	3PE	O11-C1-C2-C3
70	M1	501	PC1	O11-C1-C2-C3
81	y	601	TGL	OG1-CA1-CA2-CA3
71	L1	702	CDL	C12-C13-C14-C15
69	R	104	3PE	O31-C31-C32-C33
69	M1	503	3PE	O31-C31-C32-C33
69	A	501	3PE	C1-C2-O21-C21
69	n	605	3PE	C1-C2-O21-C21
70	L	503	PC1	C1-C2-O21-C21
70	P1	502	PC1	C3-C2-O21-C21
71	R	101	CDL	CA6-CA4-OA6-CA5
71	R	102	CDL	CA3-CA4-OA6-CA5
71	R	103	CDL	CA6-CA4-OA6-CA5
71	N1	401	CDL	CB6-CB4-OB6-CB5
73	D	301	HEC	CAD-CBD-CGD-O2D
71	D	302	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
77	a	603	HEA	CAA-CBA-CGA-O1A
71	d1	201	CDL	C62-C63-C64-C65
69	i	101	3PE	O31-C31-C32-C33
70	L	503	PC1	O21-C21-C22-C23
71	R	101	CDL	C52-C51-CB5-OB6
71	R	101	CDL	C72-C71-CB7-OB8
69	E	202	3PE	O21-C21-C22-C23
69	G	102	3PE	O21-C21-C22-C23
69	m1	601	3PE	O21-C21-C22-C23
69	K1	201	3PE	O22-C21-C22-C23
69	m1	601	3PE	C32-C33-C34-C35
70	M1	501	PC1	C3B-C3C-C3D-C3E
69	C	403	3PE	O32-C31-C32-C33
69	C	404	3PE	O22-C21-C22-C23
71	R	102	CDL	C32-C31-CA7-OA9
71	g	301	CDL	C12-C11-CA5-OA7
71	V	101	CDL	C72-C73-C74-C75
69	A	501	3PE	O31-C31-C32-C33
69	Y1	403	3PE	O31-C31-C32-C33
69	N	403	3PE	O32-C31-C32-C33
69	K1	201	3PE	O32-C31-C32-C33
69	M1	503	3PE	C29-C2A-C2B-C2C
69	L1	704	3PE	C39-C3A-C3B-C3C
70	6	203	PC1	C3A-C3B-C3C-C3D
69	i1	201	3PE	O32-C31-C32-C33
70	K	101	PC1	O22-C21-C22-C23
69	d	201	3PE	O22-C21-C22-C23
71	h1	201	CDL	C52-C51-CB5-OB7
71	Y1	401	CDL	C32-C31-CA7-OA8
69	E	202	3PE	O32-C31-C32-C33
69	O	302	3PE	O22-C21-C22-C23
69	a	606	3PE	O32-C31-C32-C33
71	R	101	CDL	C32-C31-CA7-OA9
73	O	303	HEC	CAA-CBA-CGA-O1A
71	R	101	CDL	C12-C11-CA5-OA7
70	9	204	PC1	O32-C31-C32-C33
81	y	601	TGL	OA1-CA1-CA2-CA3
71	h1	201	CDL	OB6-CB4-CB6-OB8
77	n	603	HEA	CAA-CBA-CGA-O2A
69	E	203	3PE	O32-C31-C32-C33
69	o	302	3PE	O22-C21-C22-C23
70	P1	502	PC1	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
71	A	502	CDL	C12-C11-CA5-OA7
71	h1	201	CDL	C32-C31-CA7-OA9
69	M1	502	3PE	O22-C21-C22-C23
69	M1	503	3PE	O32-C31-C32-C33
71	A	502	CDL	C32-C31-CA7-OA9
69	d1	202	3PE	C32-C33-C34-C35
69	i1	201	3PE	C2B-C2C-C2D-C2E
73	D	301	HEC	CAD-CBD-CGD-O1D
71	d1	201	CDL	C72-C71-CB7-OB9
71	h1	201	CDL	C72-C71-CB7-OB9
86	W1	201	ZMP	C17-C18-C21-O5
71	L	502	CDL	C32-C33-C34-C35
69	p	301	3PE	O31-C31-C32-C33
71	R	102	CDL	C12-C11-CA5-OA6
69	H1	401	3PE	C23-C24-C25-C26
71	R	102	CDL	C52-C51-CB5-OB7
71	L1	703	CDL	C32-C31-CA7-OA9
71	L	502	CDL	C12-C11-CA5-OA6
71	R	103	CDL	C76-C77-C78-C79
69	b1	101	3PE	O32-C31-C32-C33
71	Y1	401	CDL	C32-C31-CA7-OA9
69	n	605	3PE	O21-C21-C22-C23
69	M1	502	3PE	O31-C31-C32-C33
70	g	302	PC1	O31-C31-C32-C33
71	L1	703	CDL	C52-C51-CB5-OB6
69	r1	201	3PE	C33-C34-C35-C36
71	R	103	CDL	C81-C82-C83-C84
72	N	401	HEM	CAA-CBA-CGA-O1A
77	a	603	HEA	CAA-CBA-CGA-O2A
87	O1	401	DGT	PB-O3A-PA-O2A
69	R	104	3PE	O32-C31-C32-C33
69	m1	601	3PE	O22-C21-C22-C23
69	d1	203	3PE	C31-C32-C33-C34
70	9	203	PC1	O21-C21-C22-C23
69	E	202	3PE	O22-C21-C22-C23
71	L1	702	CDL	C72-C71-CB7-OB9
71	H1	402	CDL	C17-C18-C19-C20

There are no ring outliers.

76 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	c	301	3PE	5	0
72	N	401	HEM	2	0
69	C	404	3PE	2	0
69	R	104	3PE	2	0
69	t	101	3PE	11	0
73	D	301	HEC	1	0
69	C	403	3PE	1	0
70	M1	501	PC1	4	0
69	L	501	3PE	1	0
71	g	301	CDL	7	0
70	P1	502	PC1	1	0
69	Y1	403	3PE	1	0
69	M1	502	3PE	4	0
69	M1	503	3PE	2	0
69	N	403	3PE	1	0
69	r1	201	3PE	1	0
72	C	402	HEM	3	0
69	Y1	402	3PE	1	0
70	p	302	PC1	1	0
71	d1	201	CDL	1	0
81	y	601	TGL	1	0
72	C	401	HEM	3	0
69	6	202	3PE	1	0
70	g	302	PC1	3	0
72	N	402	HEM	2	0
77	a	604	HEA	5	0
69	b	301	3PE	1	0
69	N1	402	3PE	1	0
71	L	502	CDL	1	0
71	V	101	CDL	2	0
71	N1	401	CDL	5	0
71	R	103	CDL	4	0
71	L1	703	CDL	3	0
71	R	102	CDL	1	0
70	z	101	PC1	20	0
69	o	302	3PE	2	0
69	H1	401	3PE	2	0
69	a	605	3PE	1	0
69	z	102	3PE	2	0
69	v	101	3PE	1	0
69	i1	201	3PE	1	0
69	O	302	3PE	1	0
71	G	101	CDL	1	0

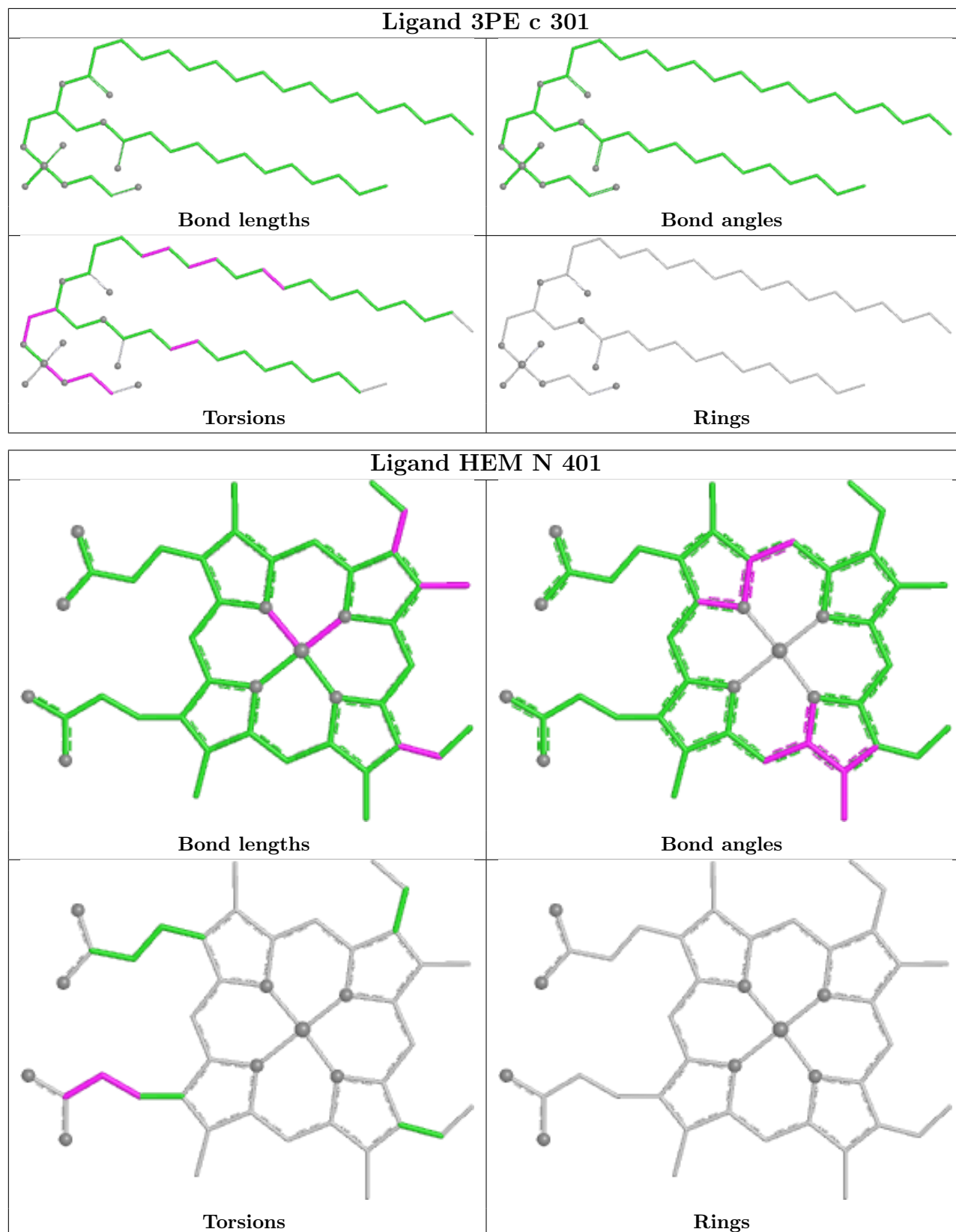
Continued on next page...

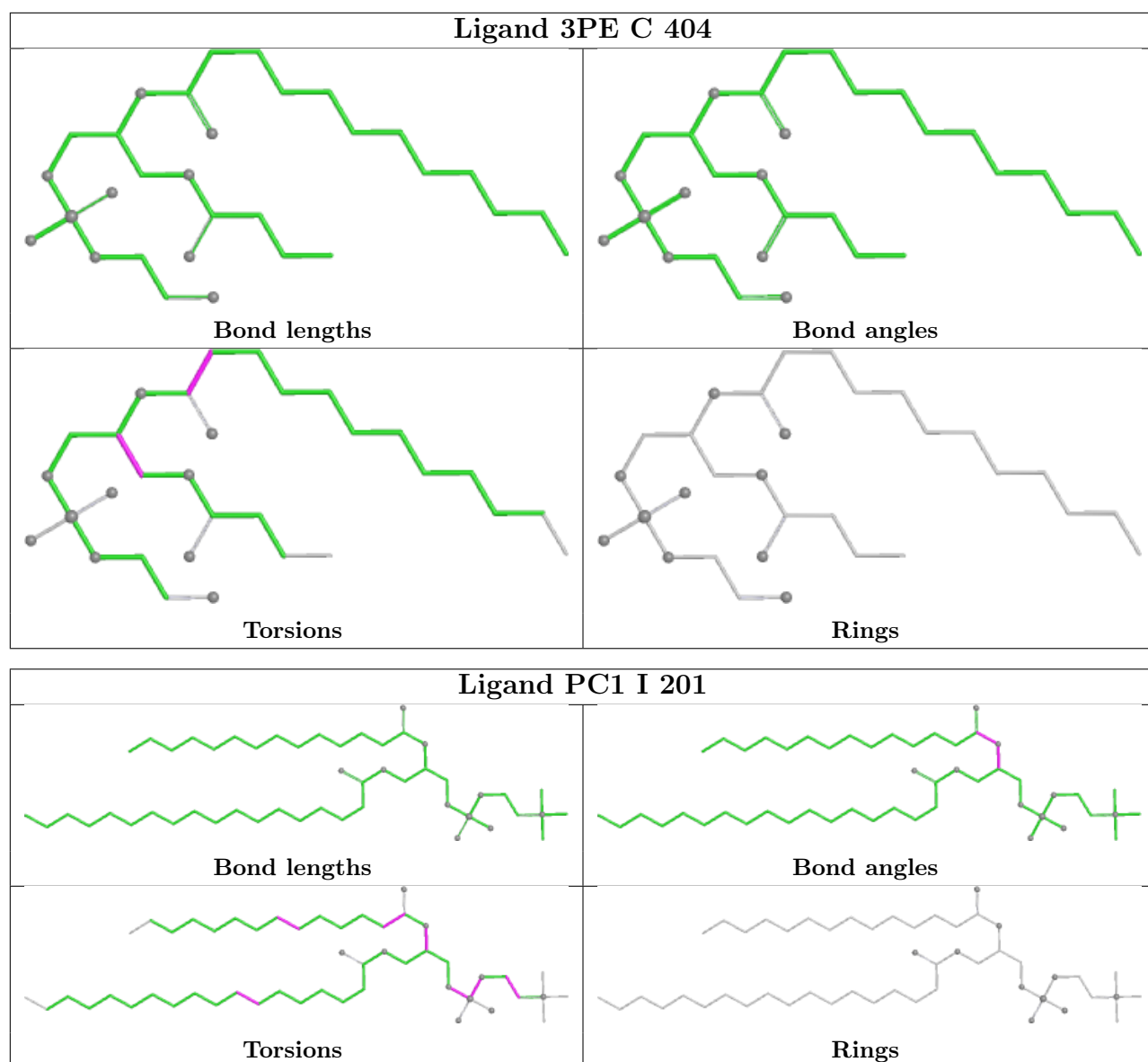
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	a	606	3PE	2	0
69	d	201	3PE	2	0
69	p	301	3PE	6	0
82	9	201	SF4	1	0
86	n1	201	ZMP	2	0
69	G	102	3PE	1	0
69	n	606	3PE	2	0
69	d1	202	3PE	1	0
85	P1	501	NDP	1	0
69	E	202	3PE	2	0
71	L1	702	CDL	2	0
70	6	203	PC1	2	0
69	L1	704	3PE	3	0
69	A	501	3PE	2	0
87	O1	401	DGT	1	0
70	K	101	PC1	1	0
71	Y1	401	CDL	2	0
74	P	201	FES	2	0
81	l	601	TGL	1	0
71	r1	202	CDL	3	0
69	L1	701	3PE	3	0
69	g	303	3PE	11	0
77	n	604	HEA	5	0
71	D	302	CDL	1	0
71	h1	201	CDL	4	0
70	9	203	PC1	1	0
77	n	603	HEA	4	0
71	H1	402	CDL	1	0
69	n	607	3PE	1	0
77	a	603	HEA	3	0
69	b1	101	3PE	1	0
83	1	501	FMN	2	0
70	9	204	PC1	3	0

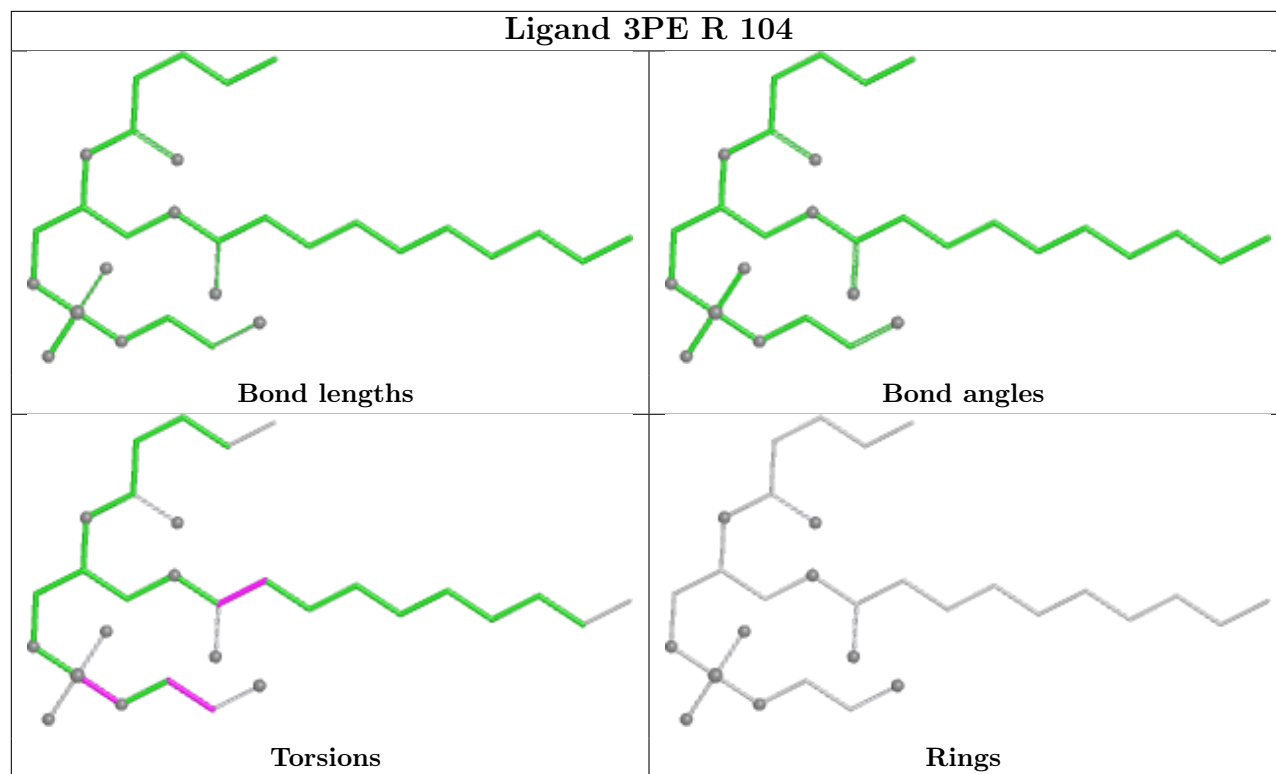
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

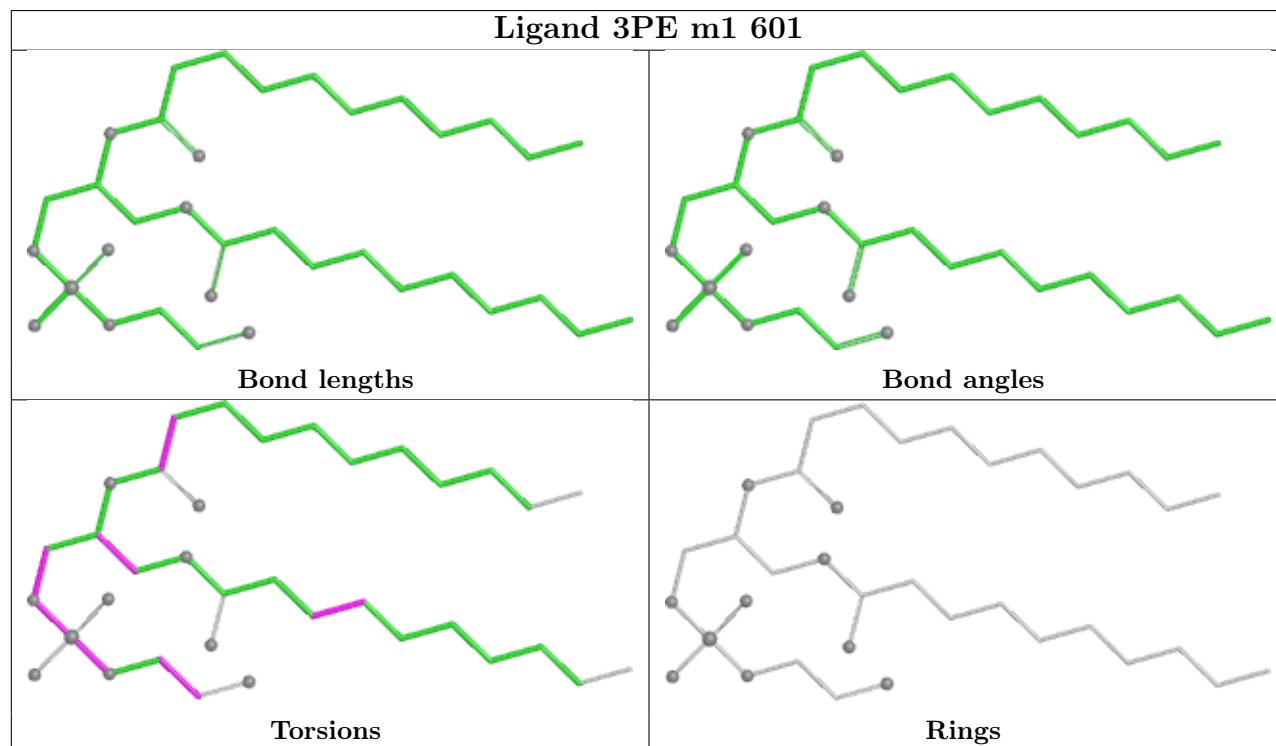


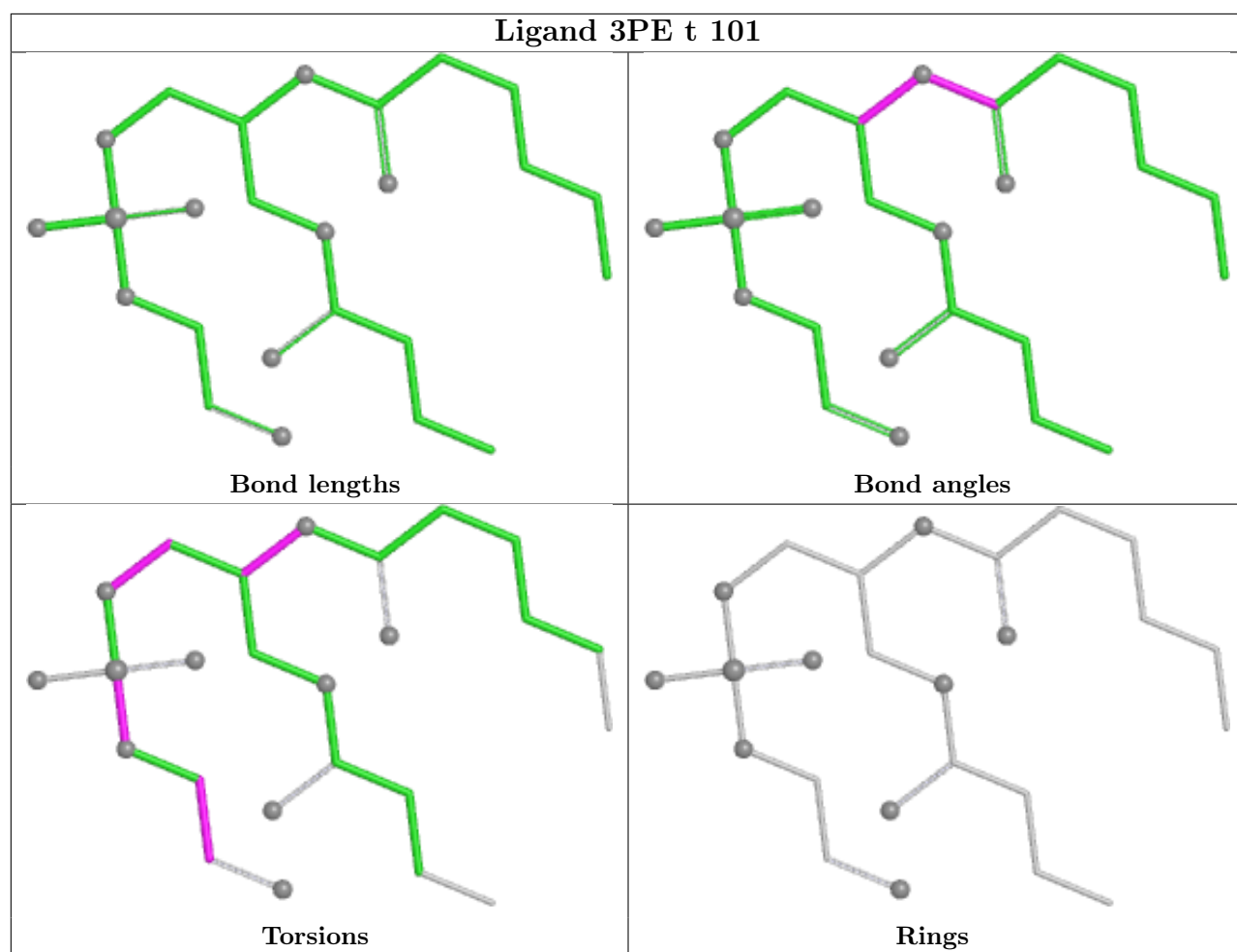


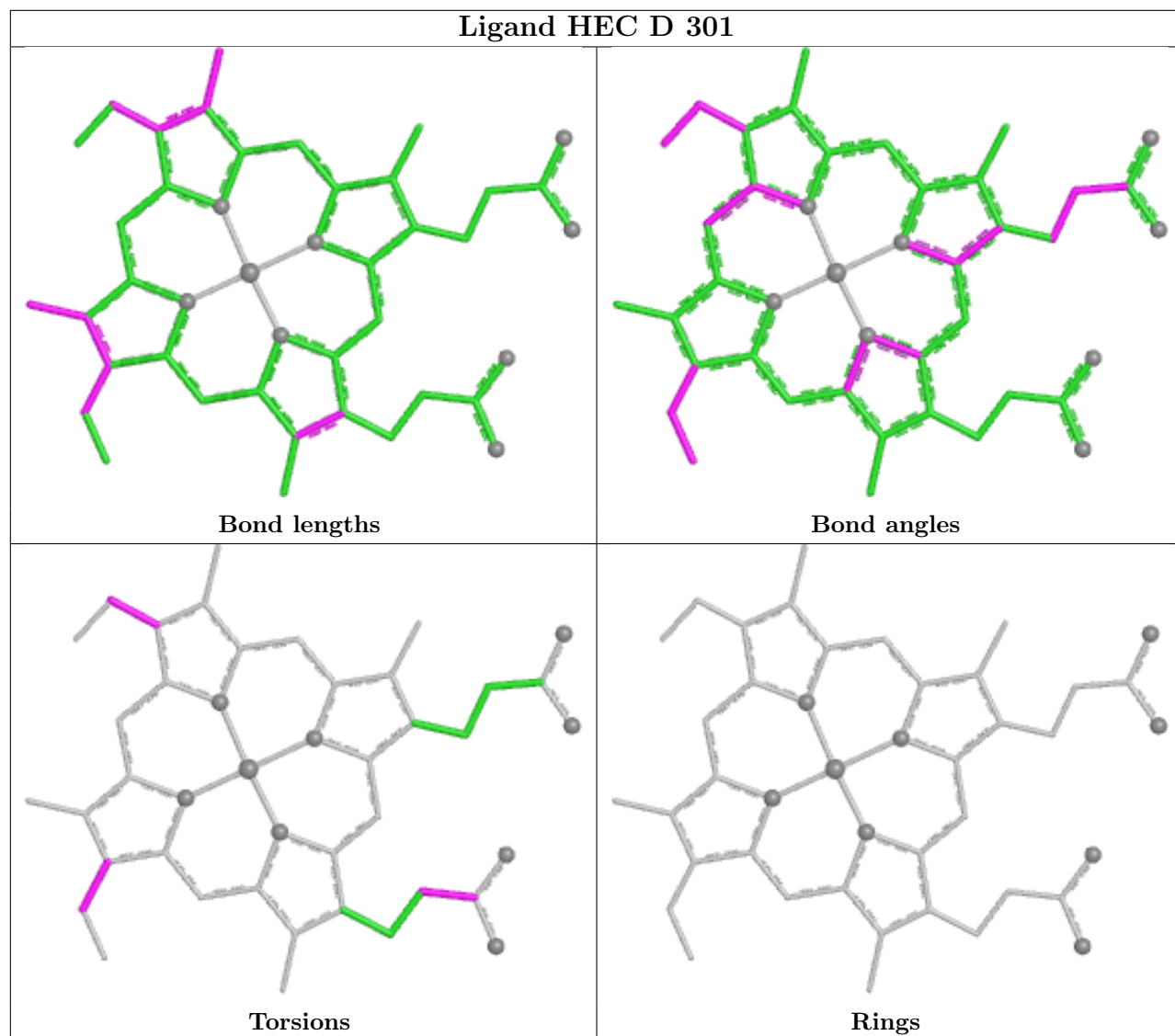
Ligand 3PE R 104

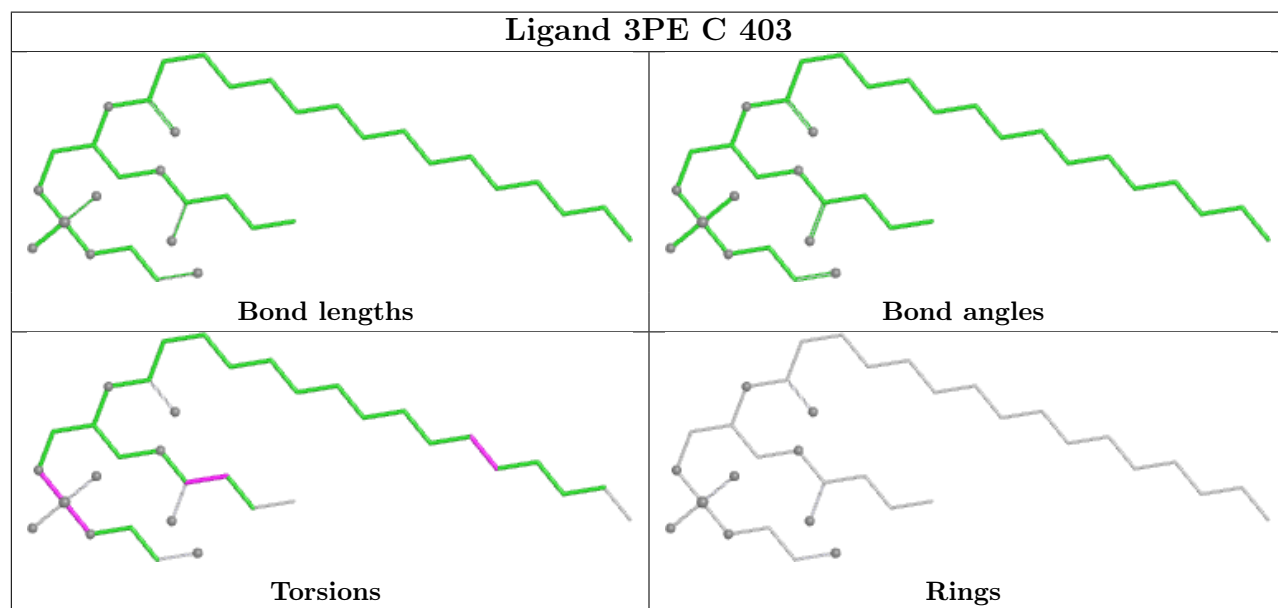
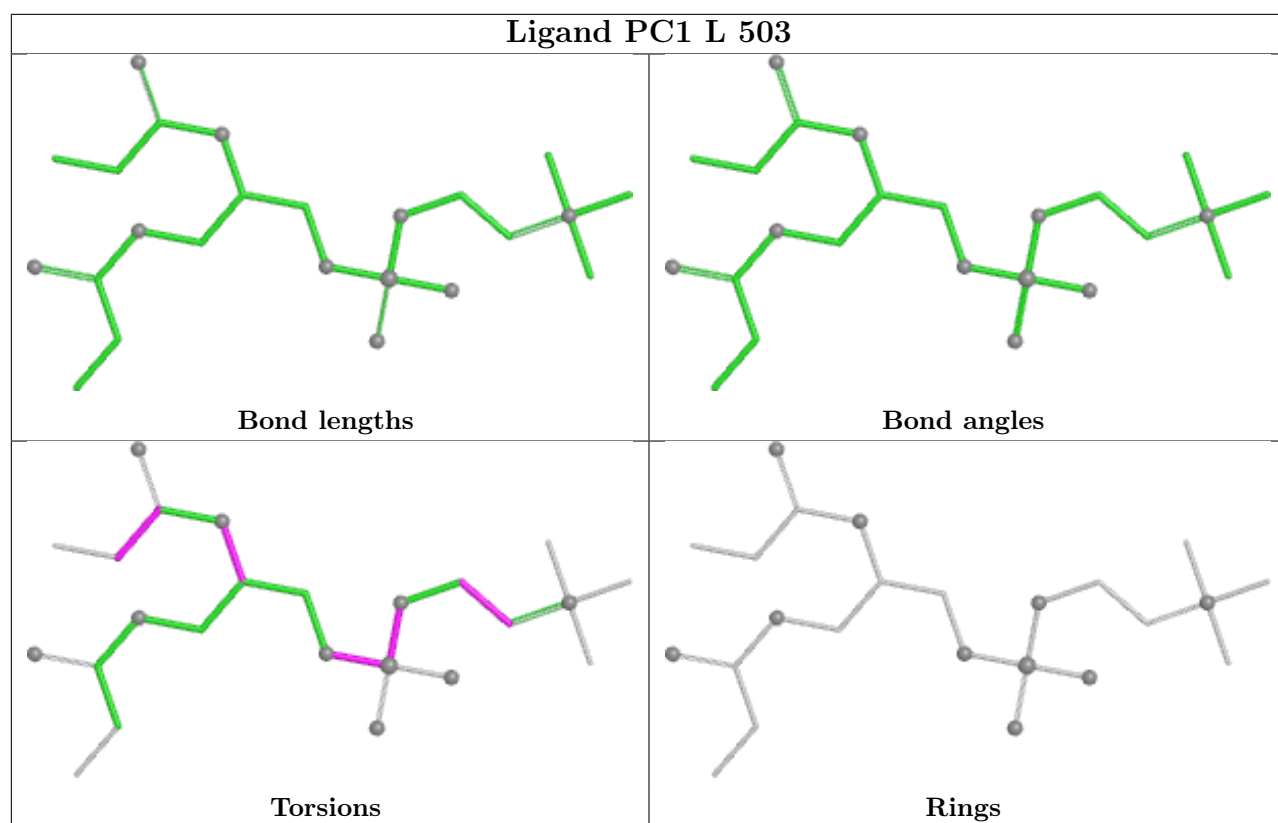


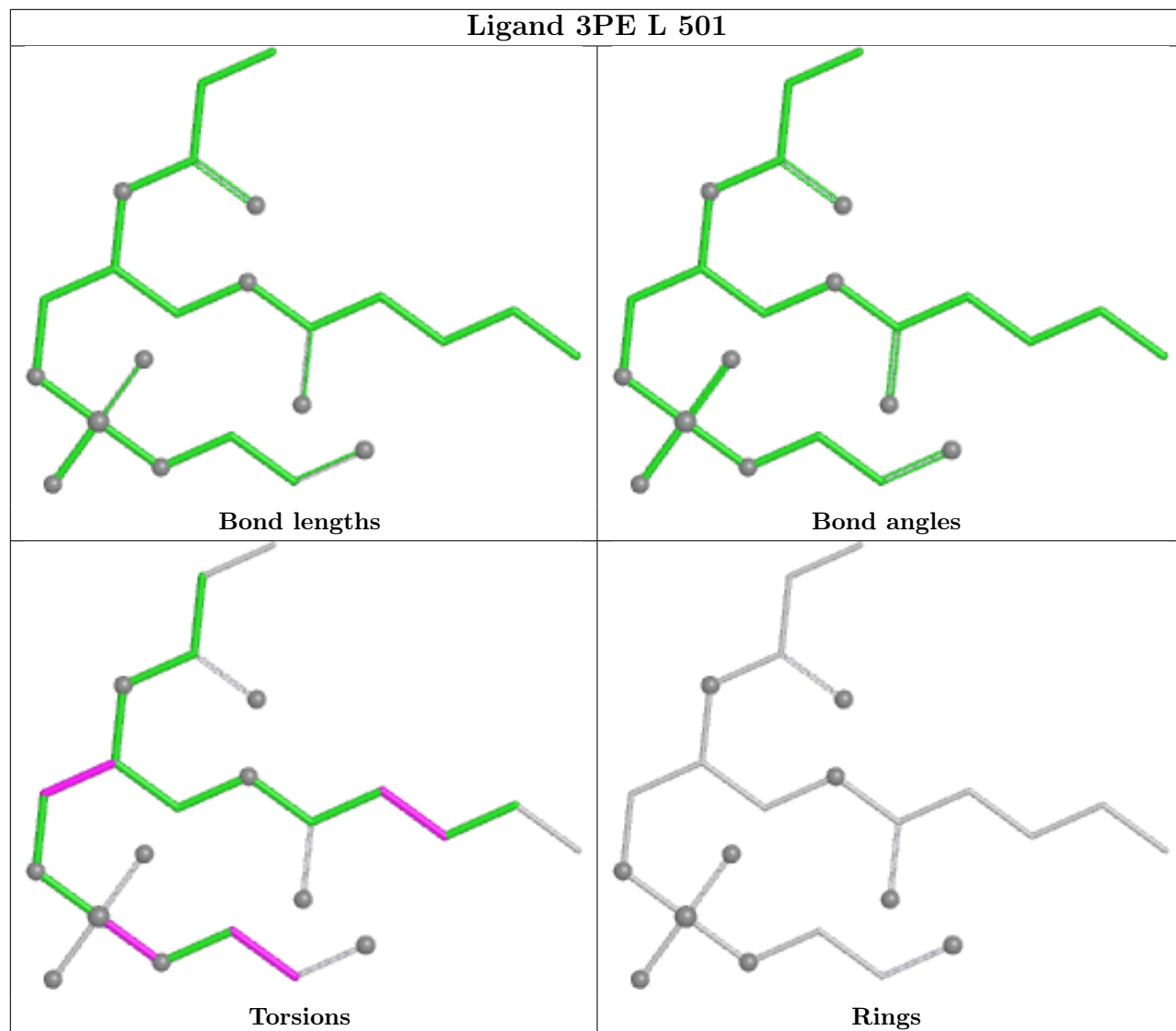
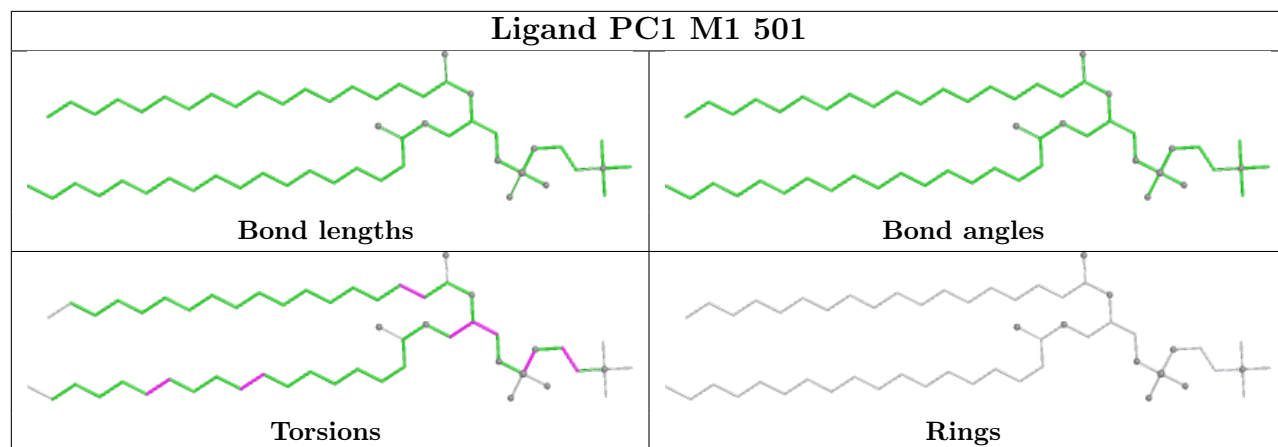
Ligand 3PE m1 601

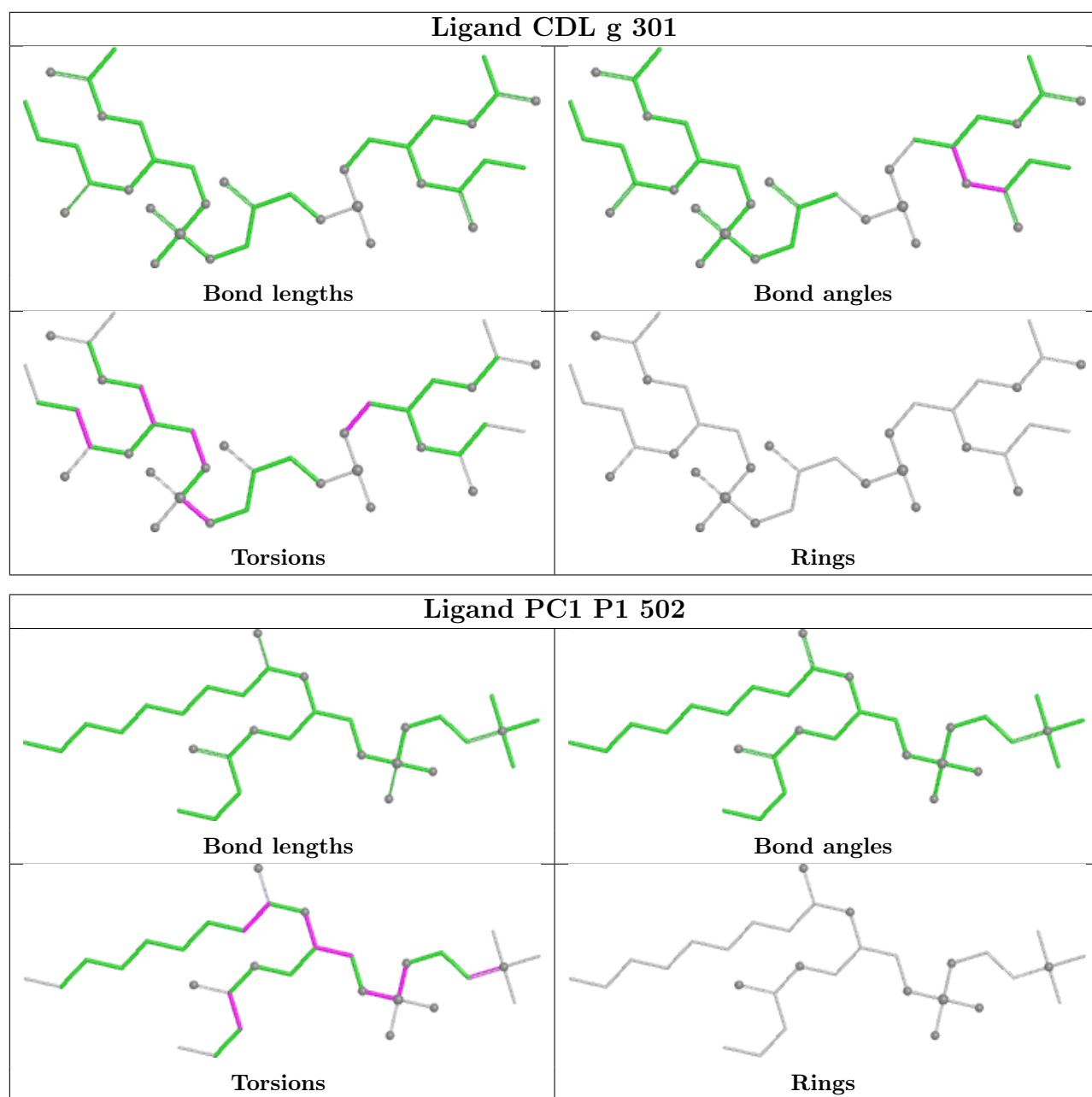


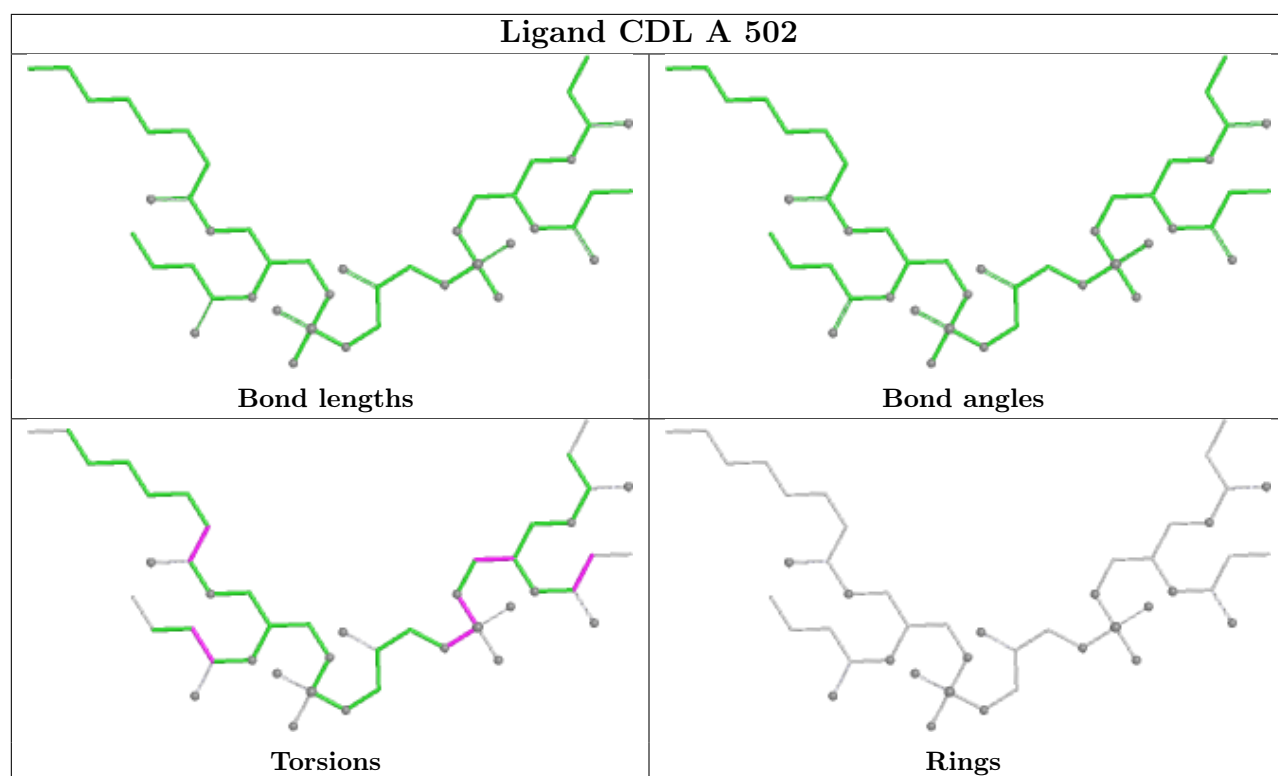
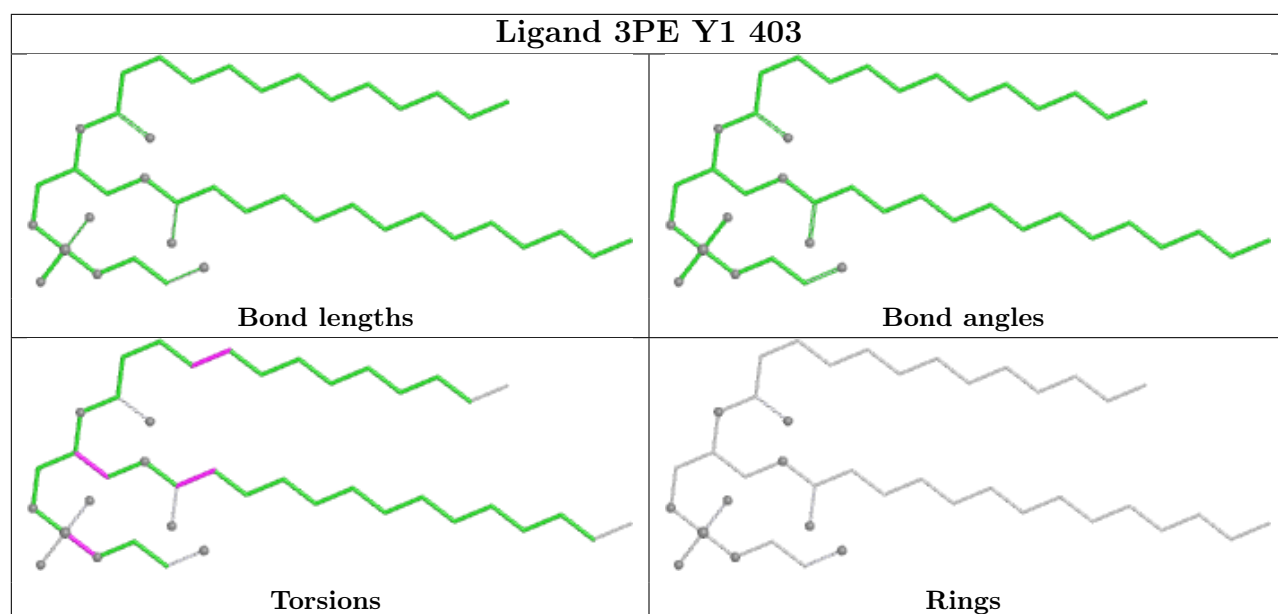


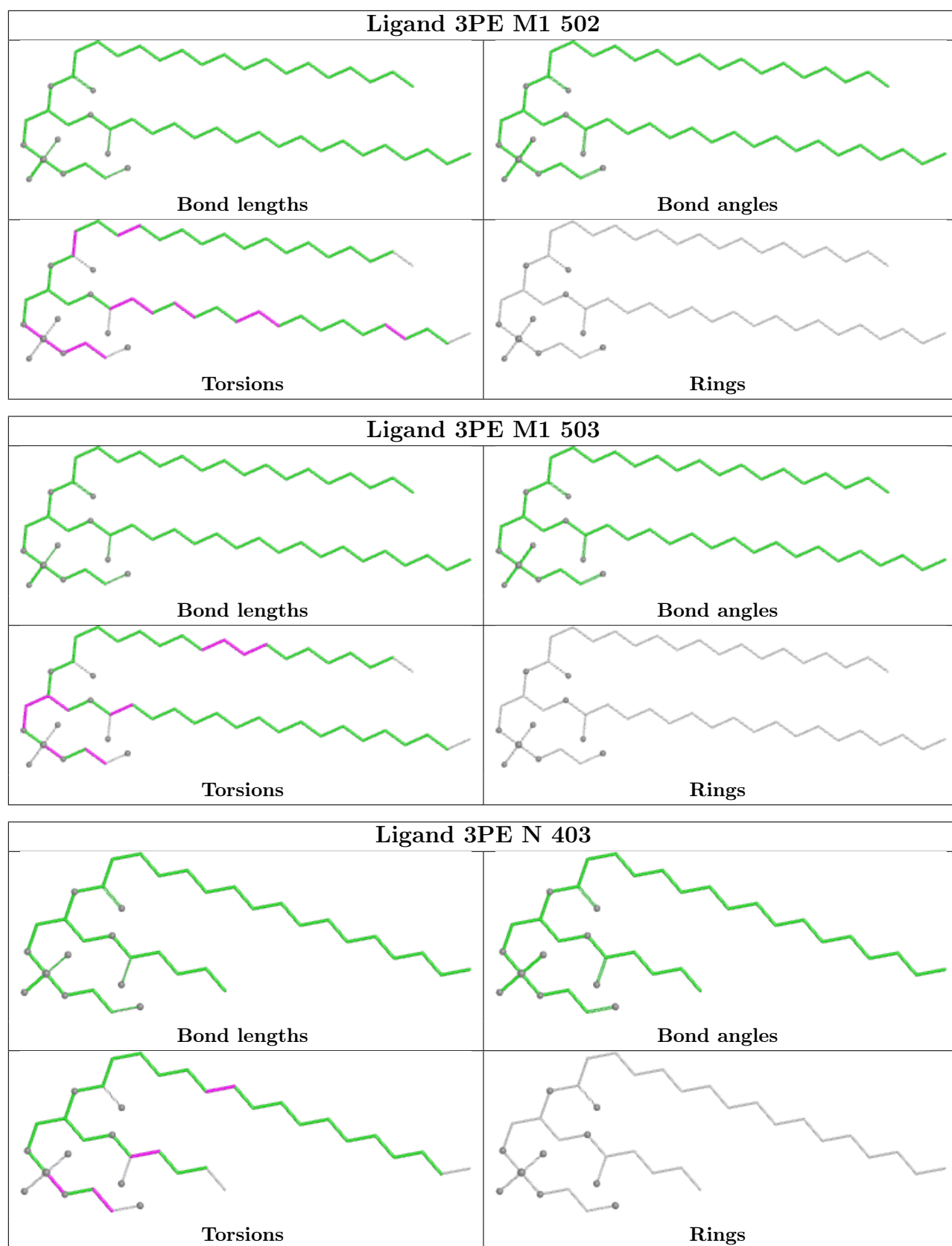




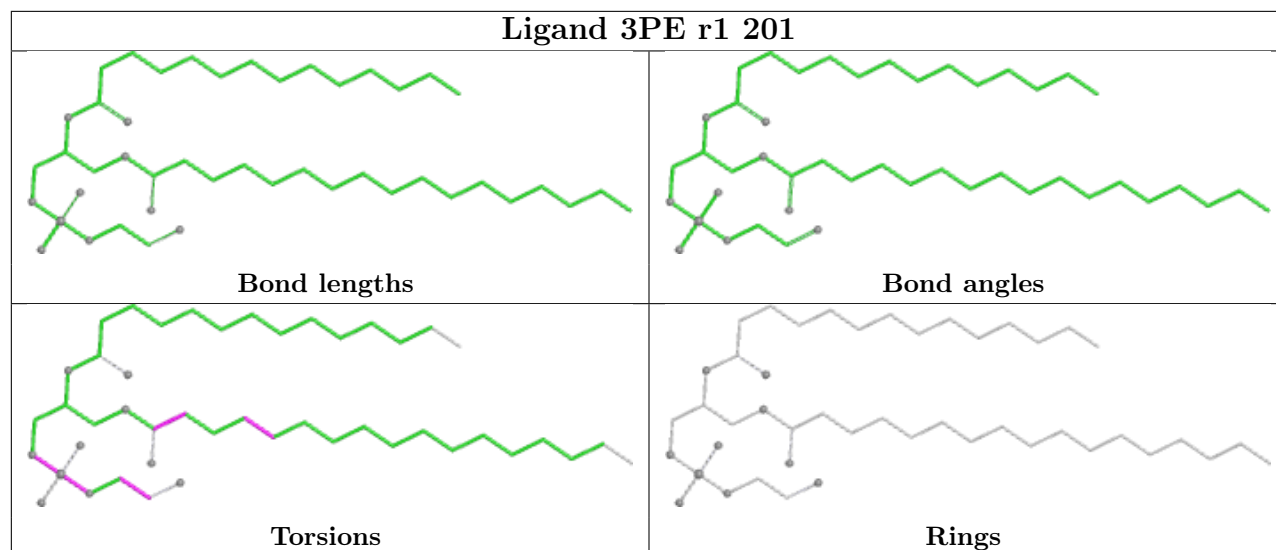




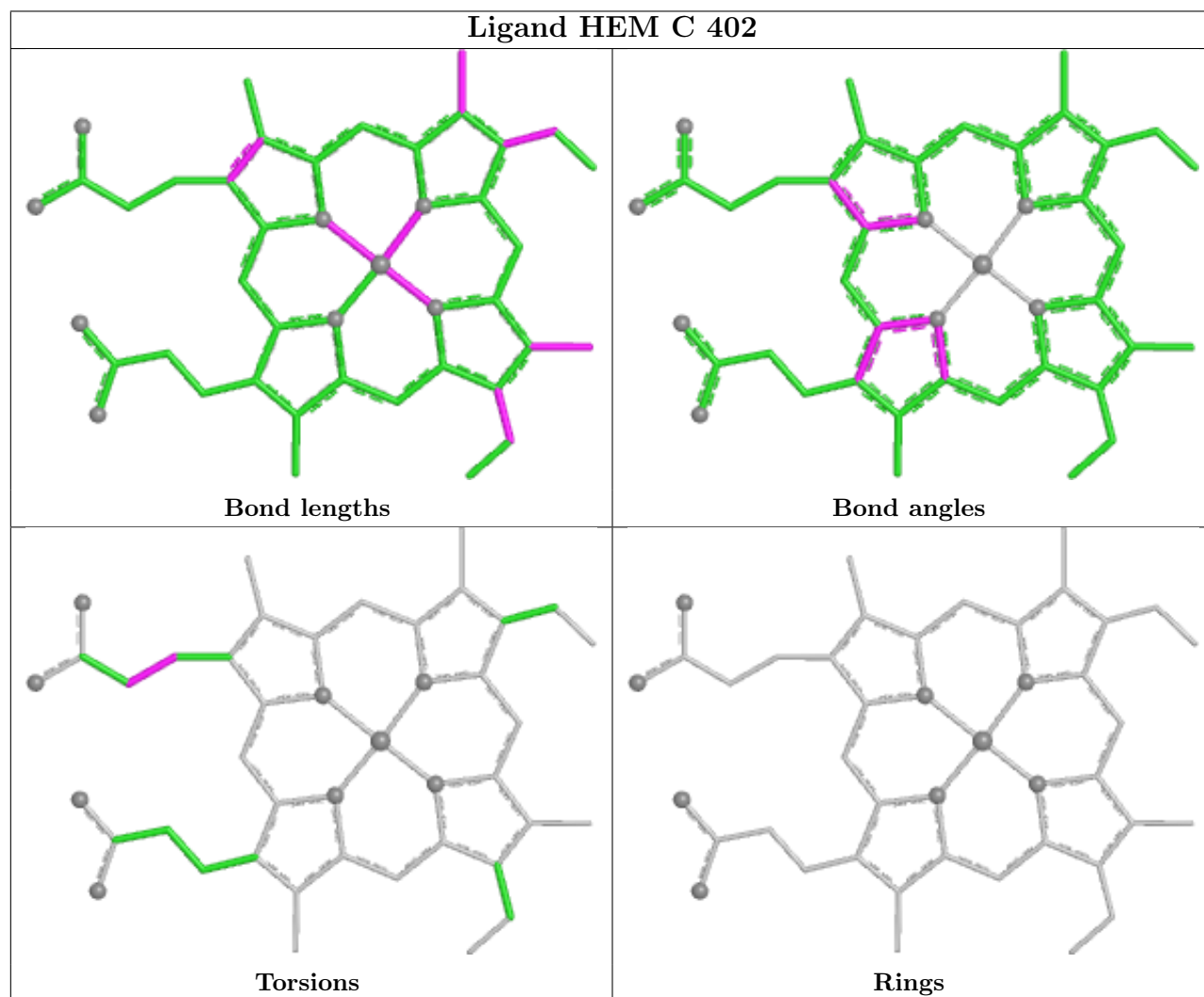


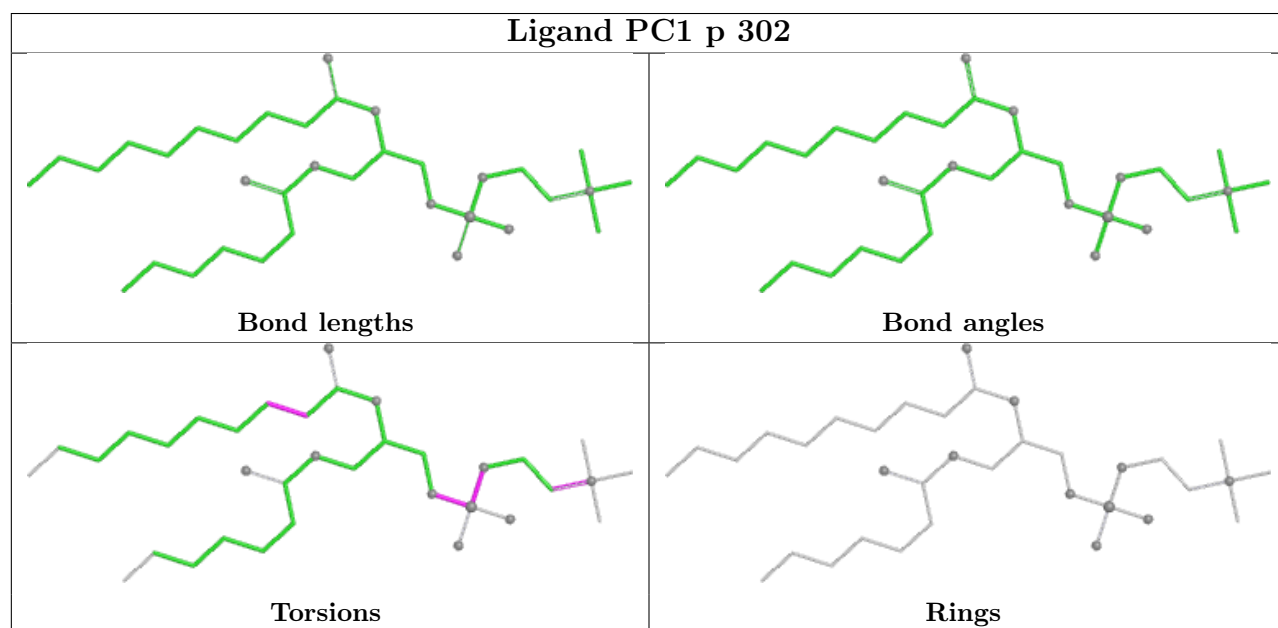
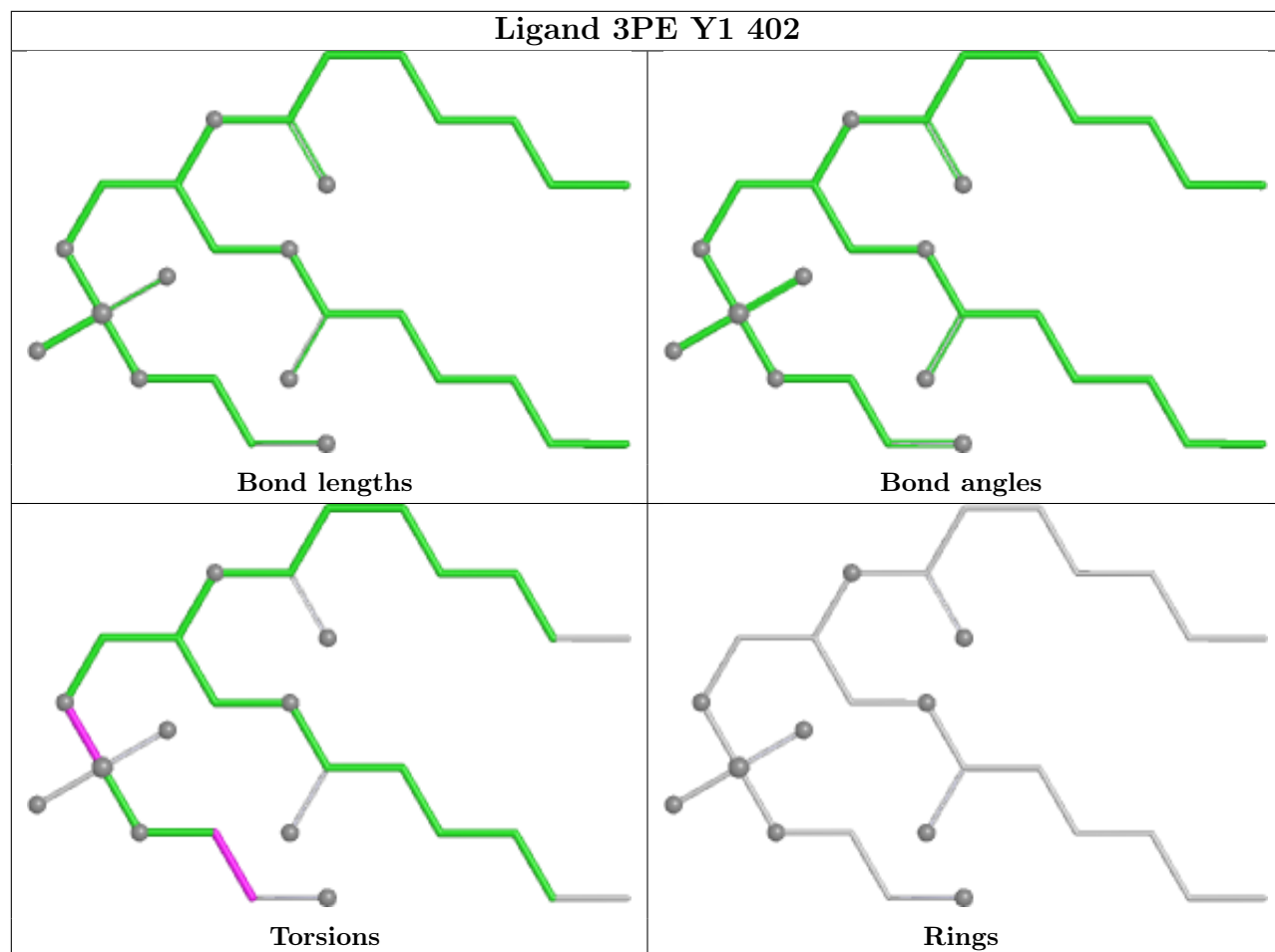


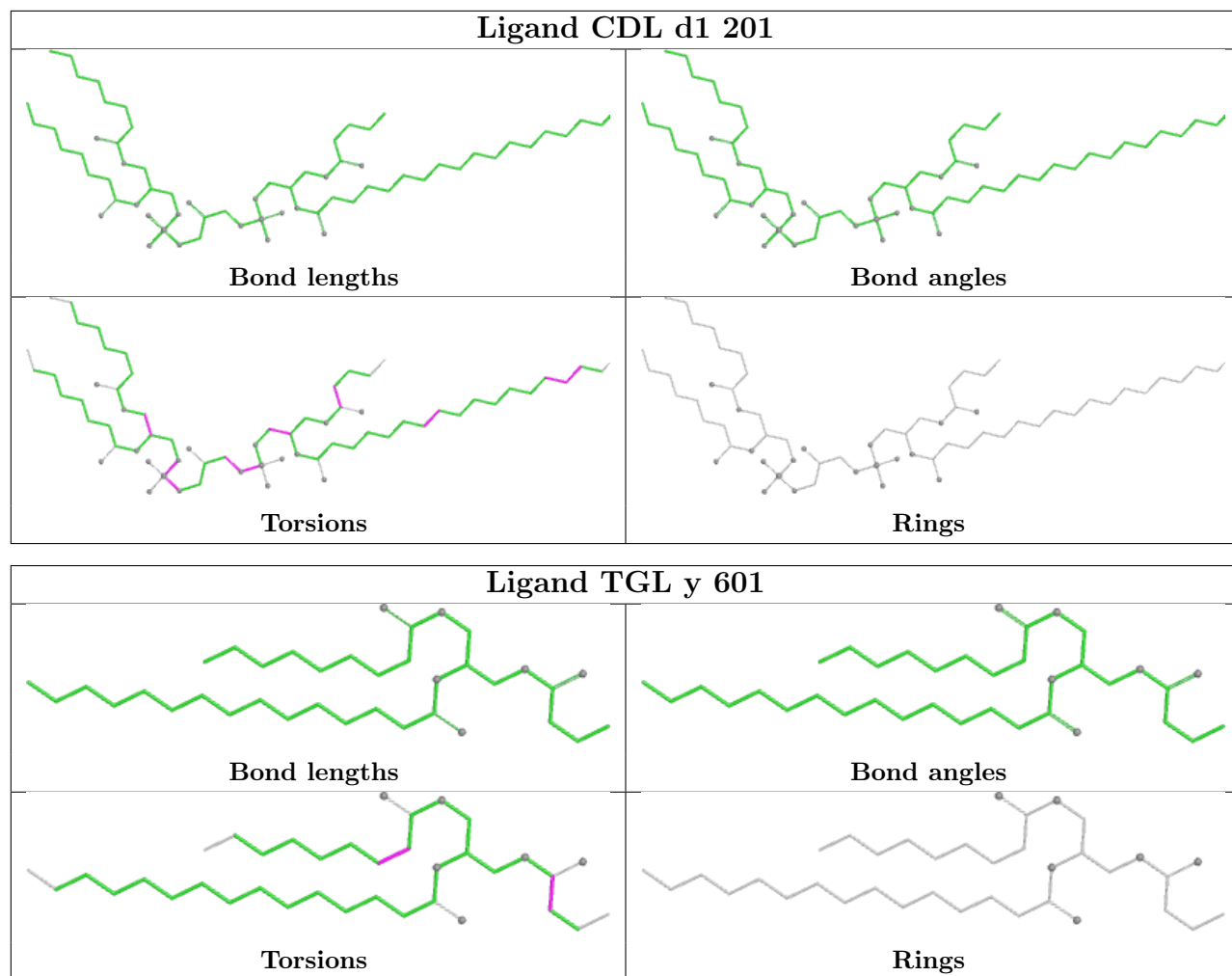
Ligand 3PE r1 201

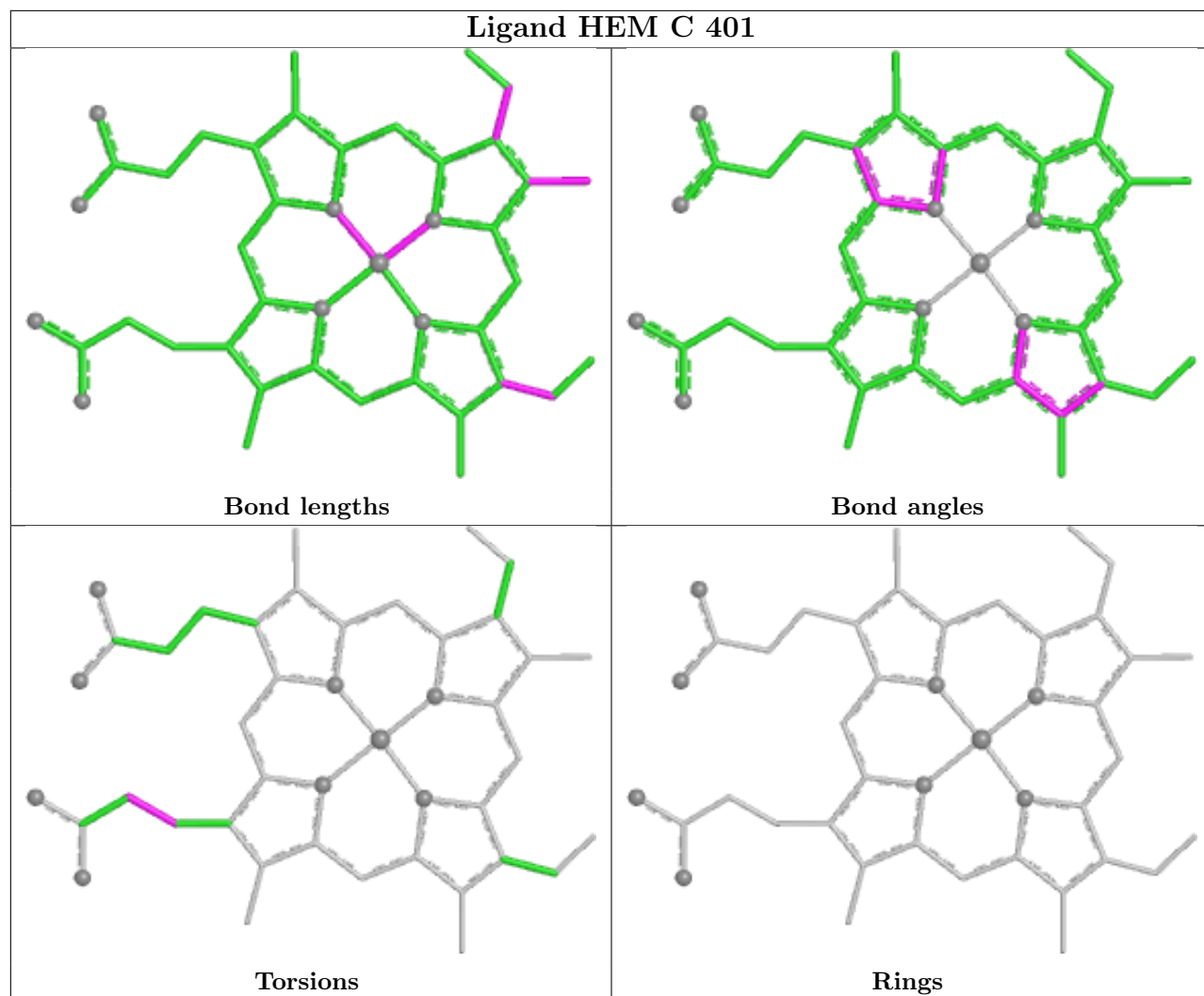


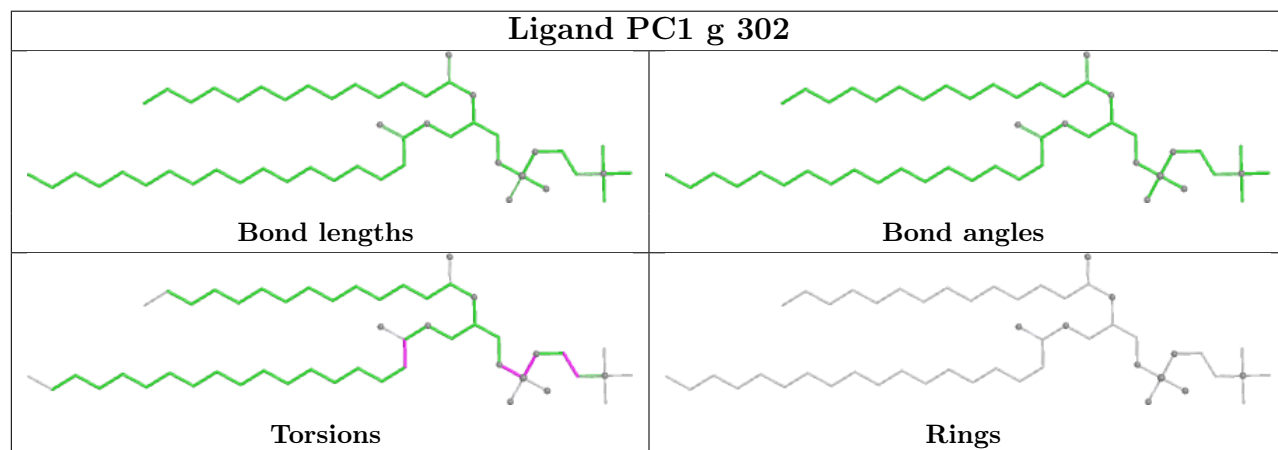
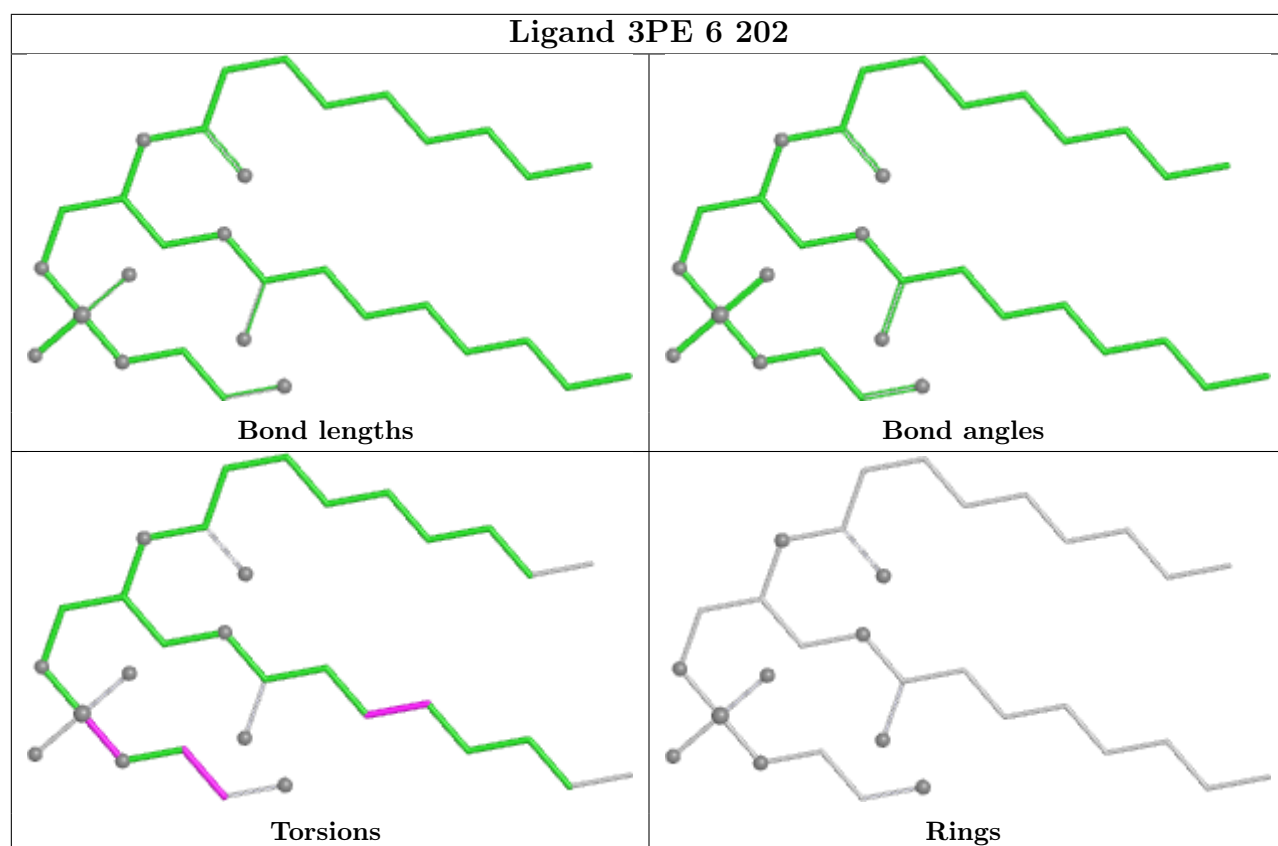
Ligand HEM C 402

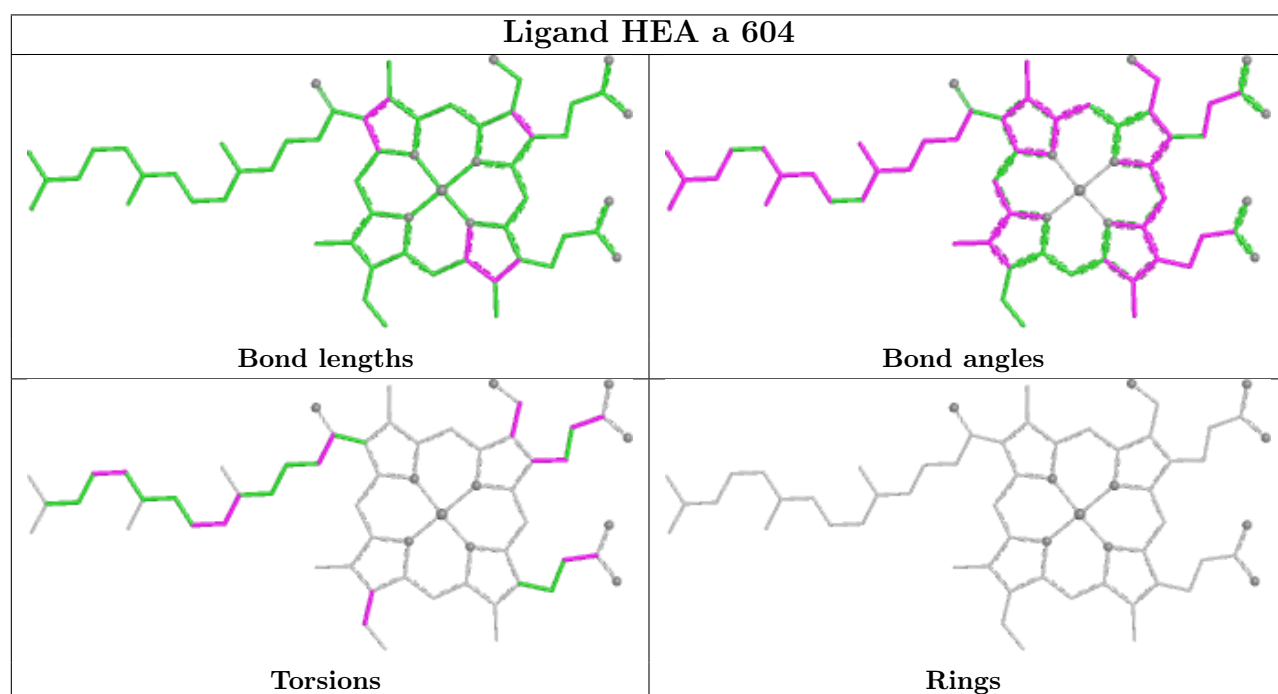
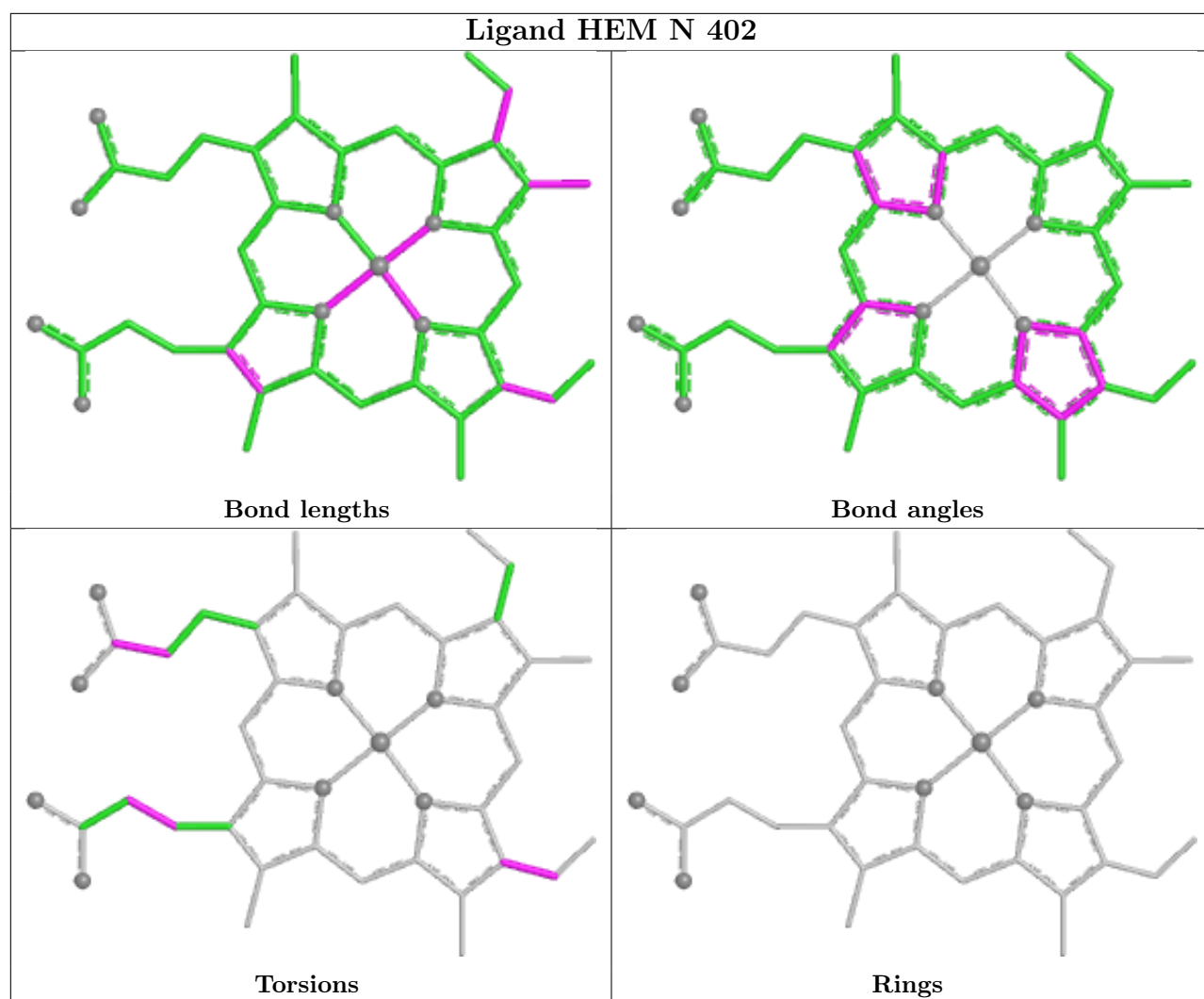




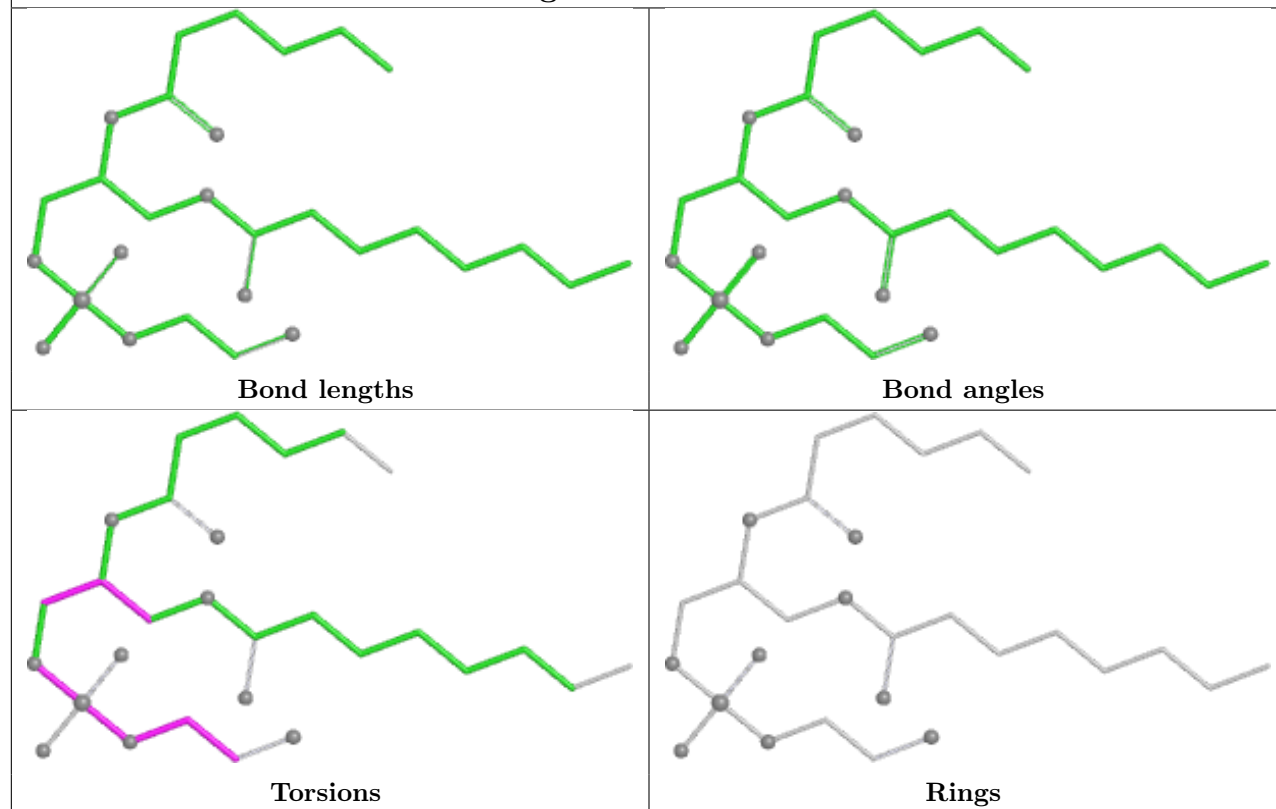




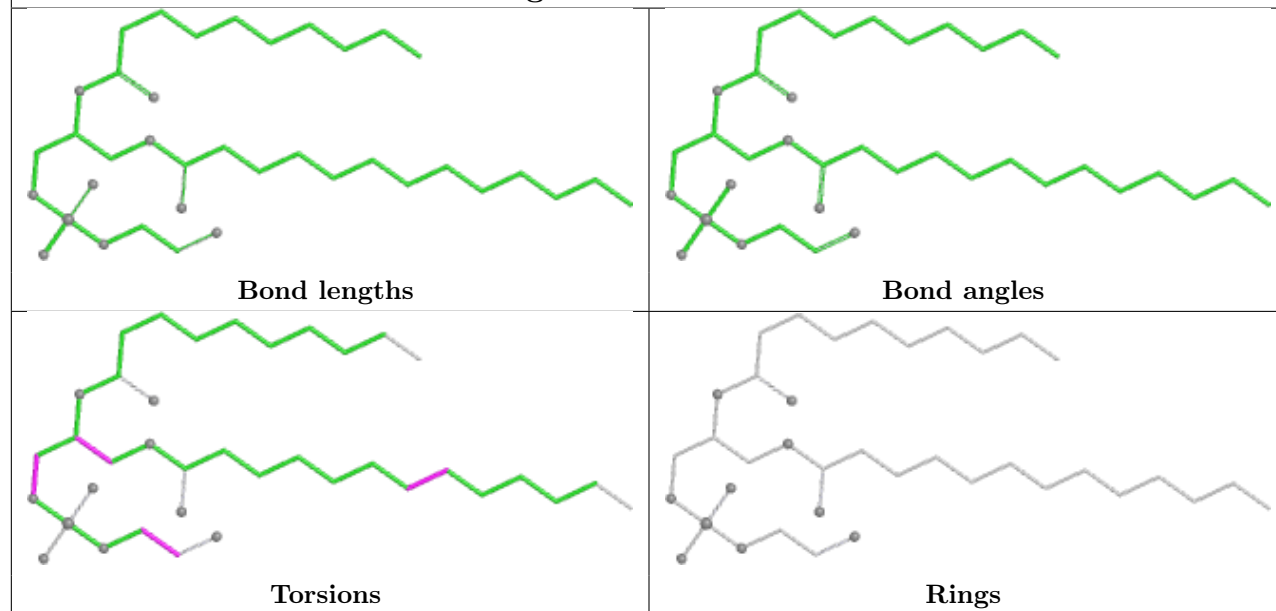


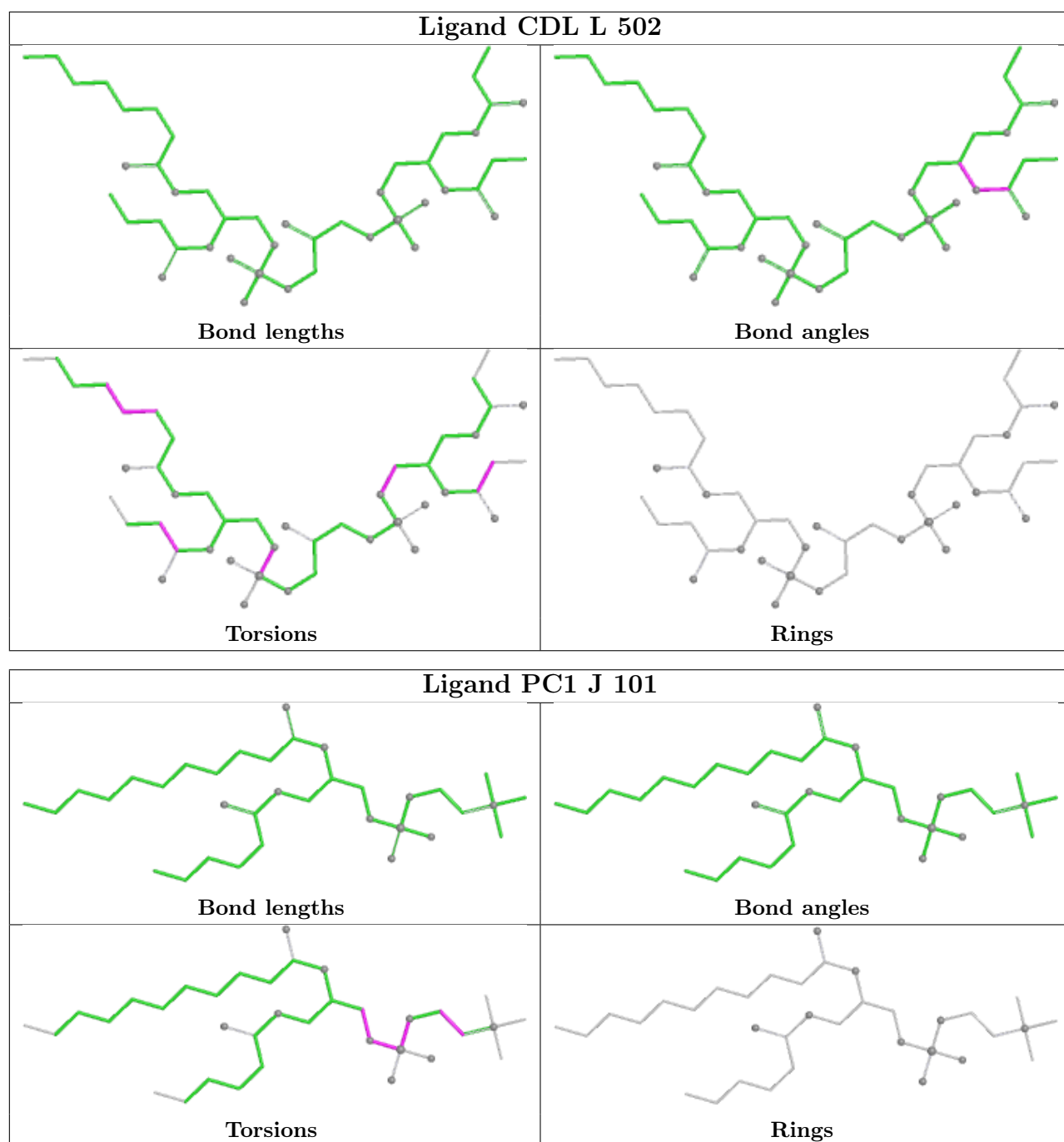


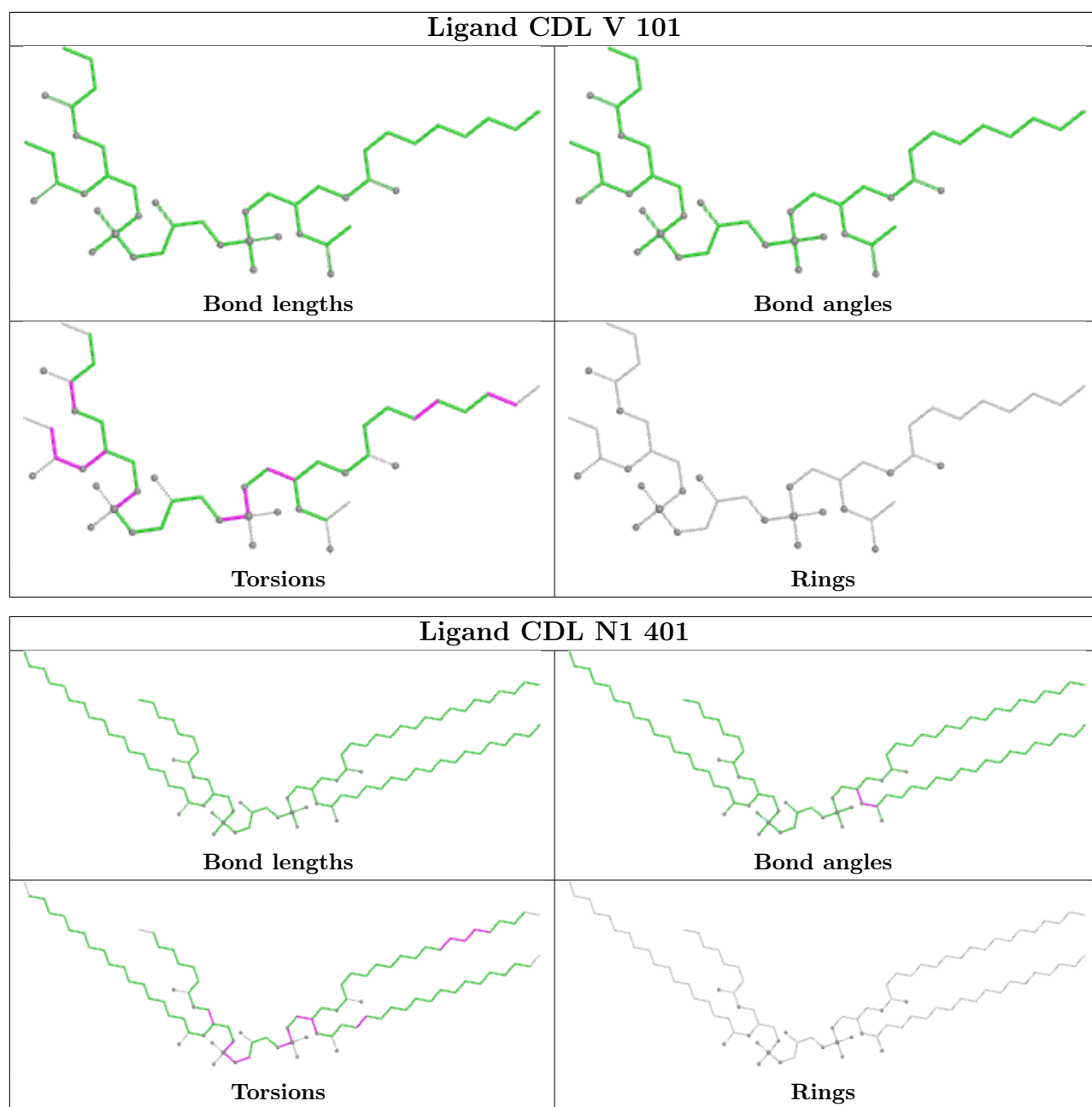
Ligand 3PE b 301

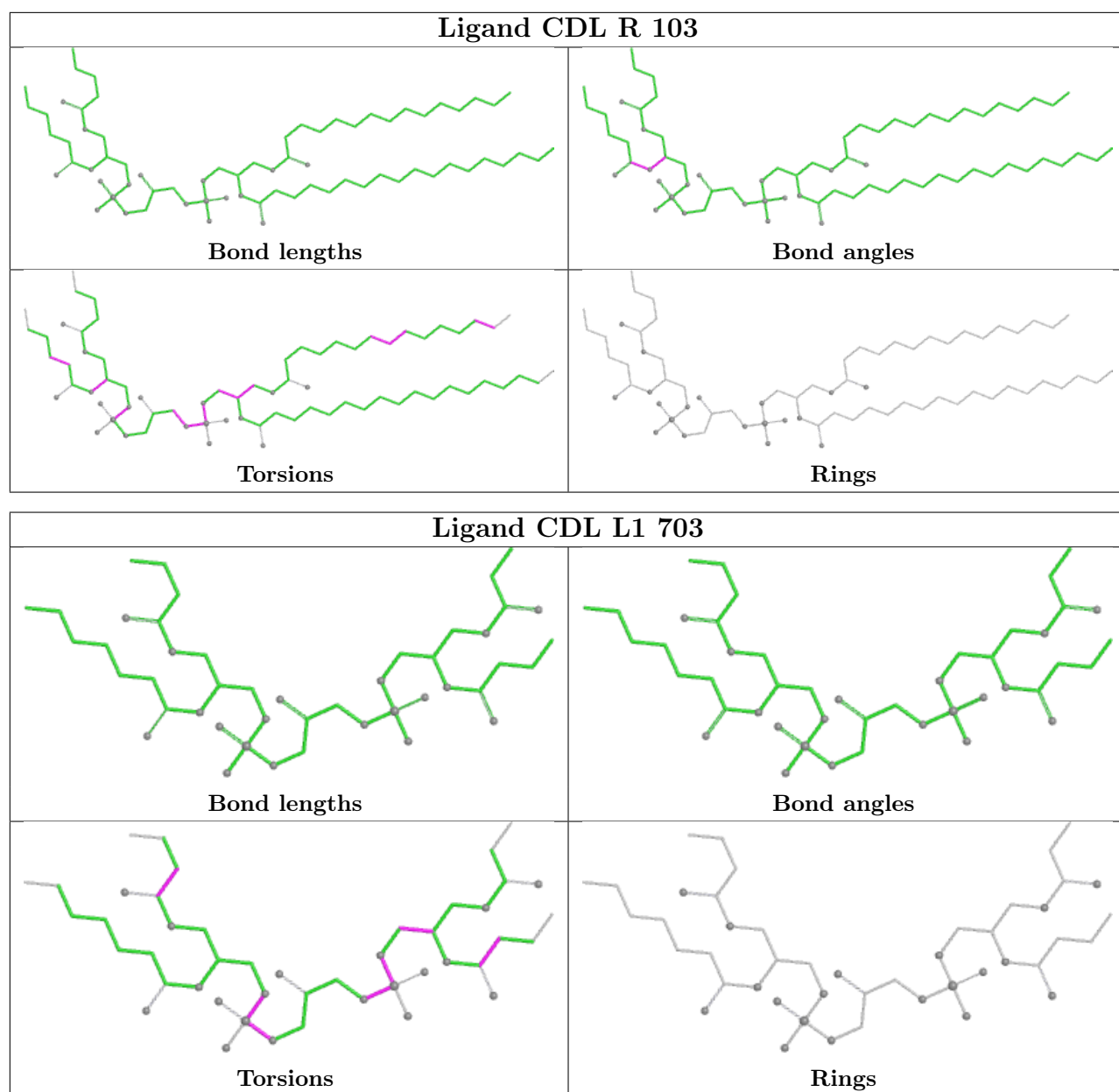


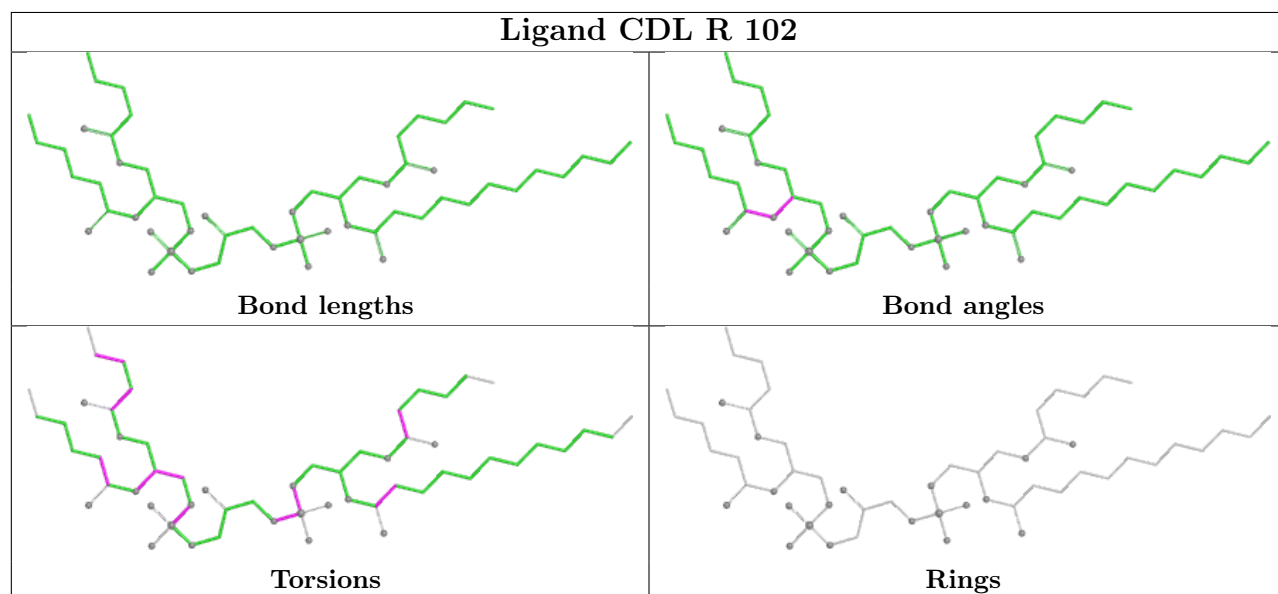
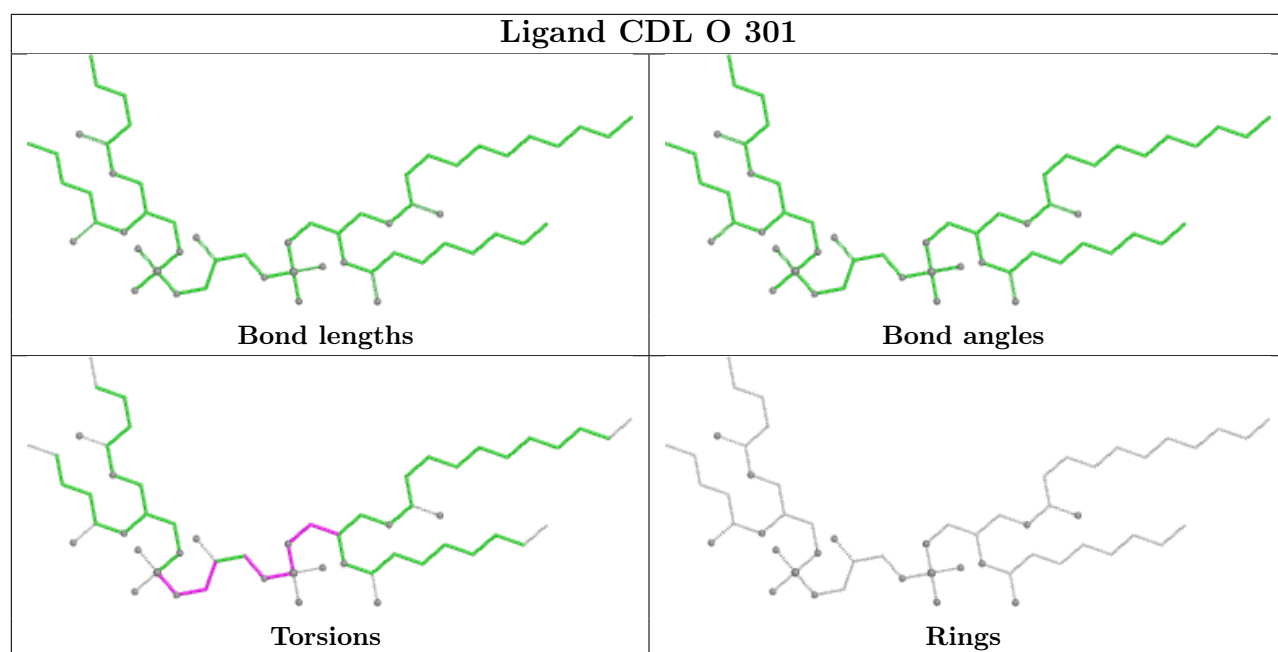
Ligand 3PE N1 402

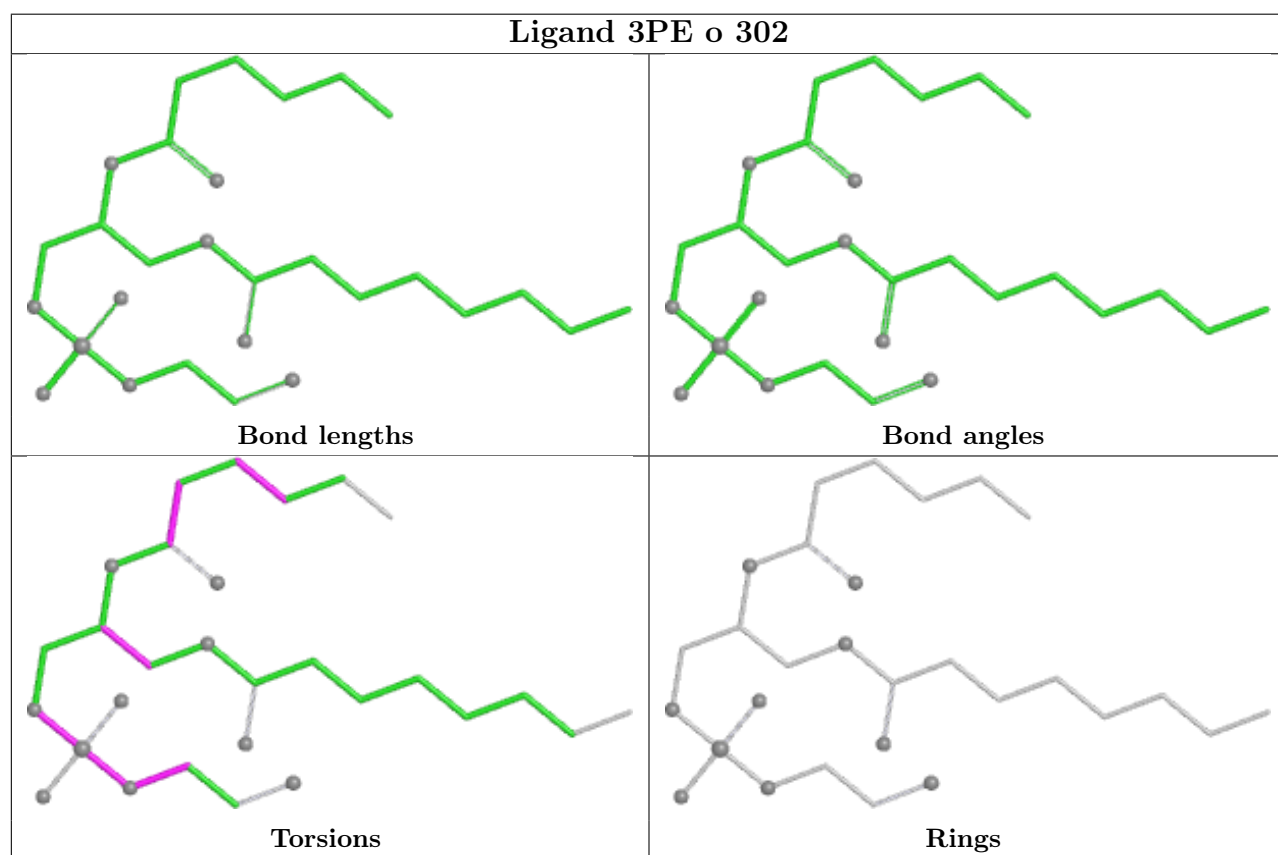
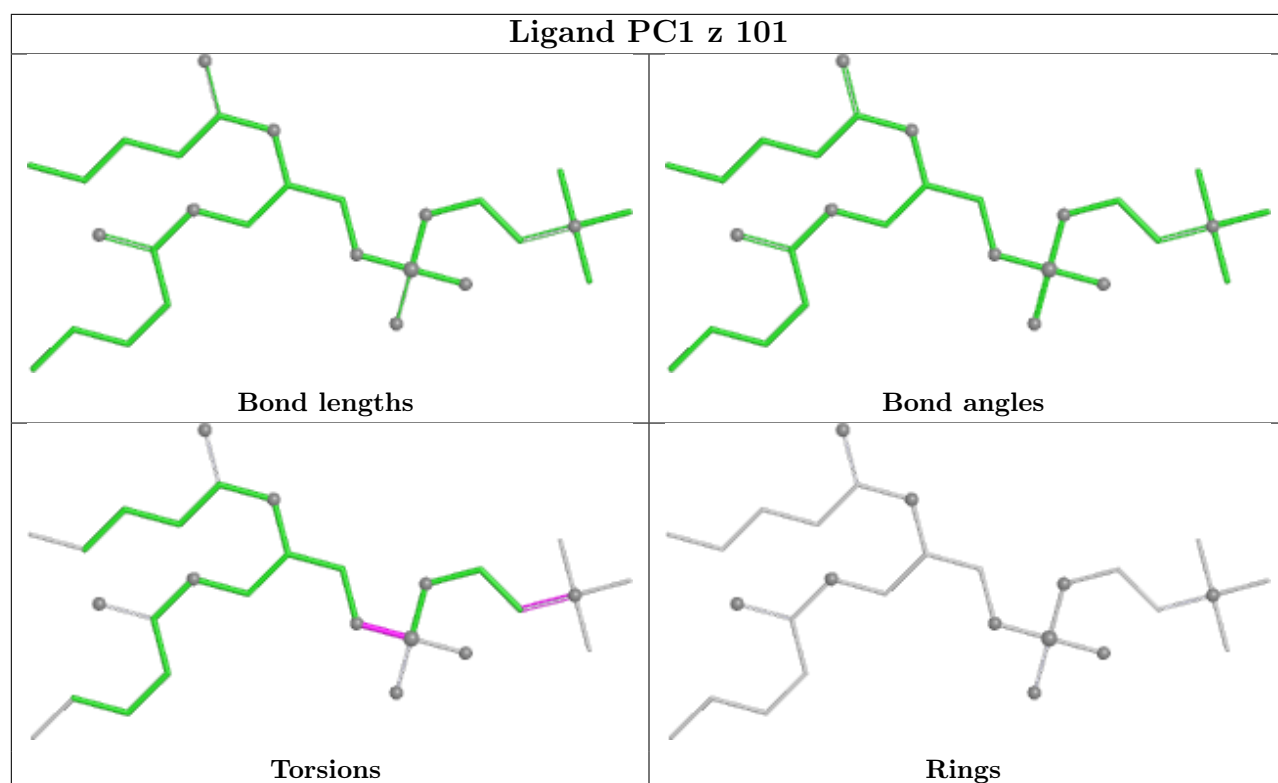


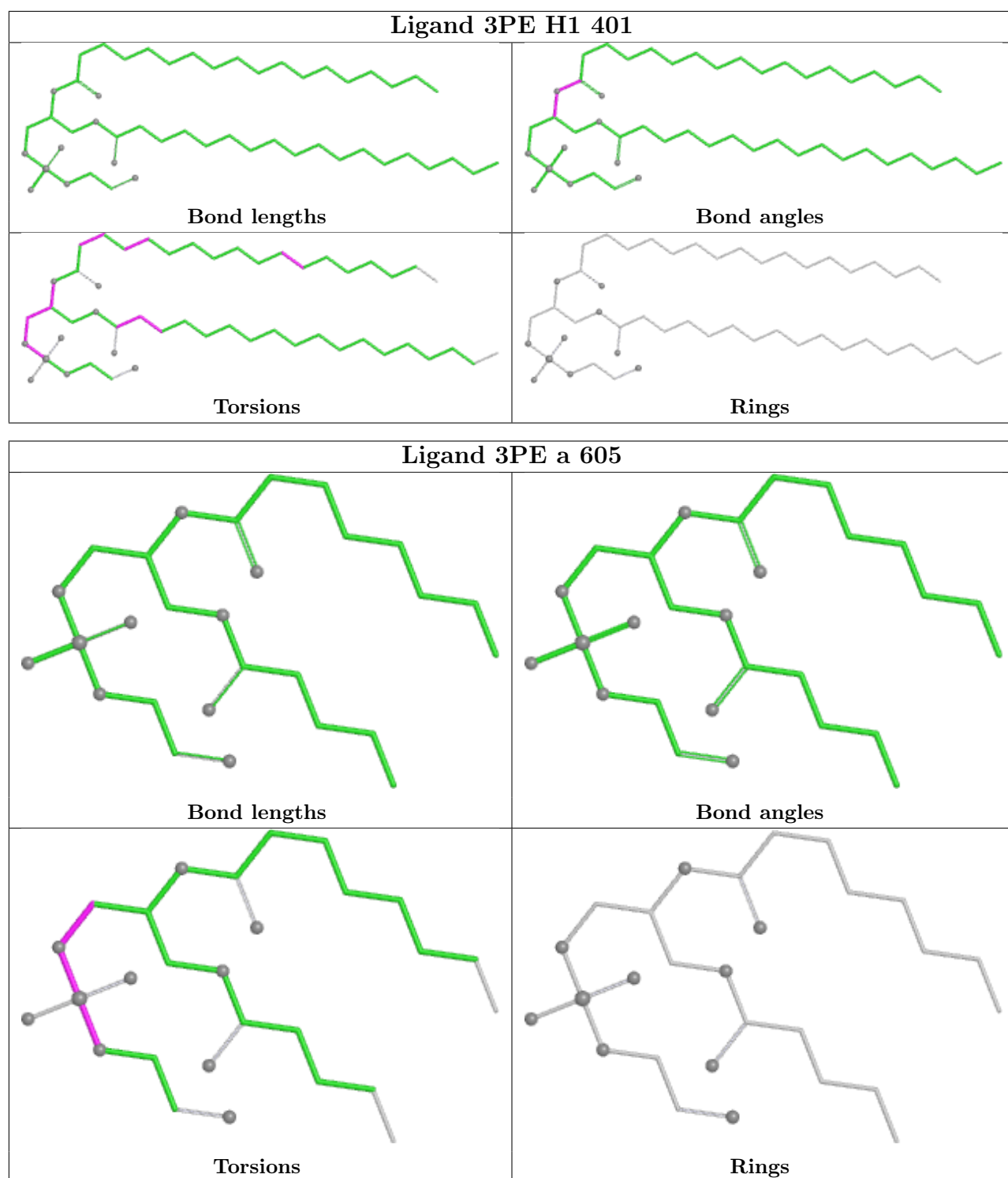


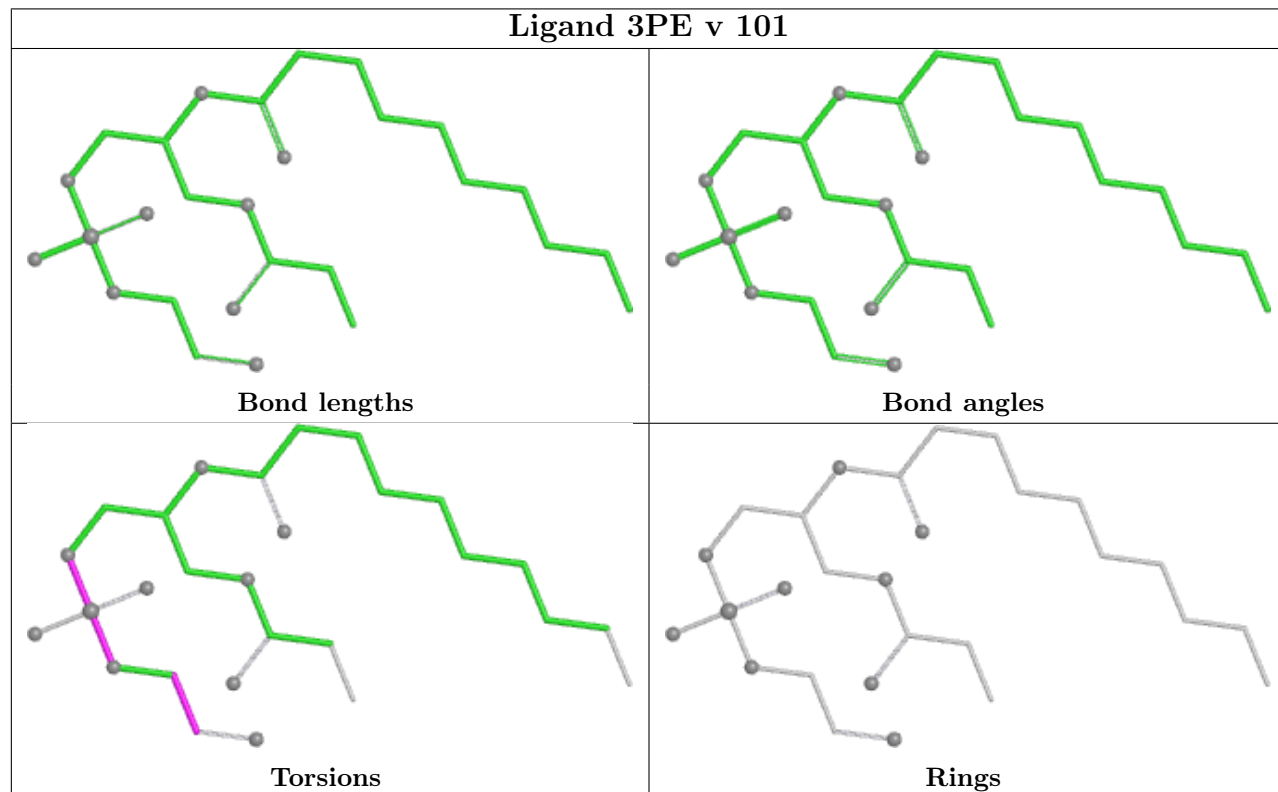
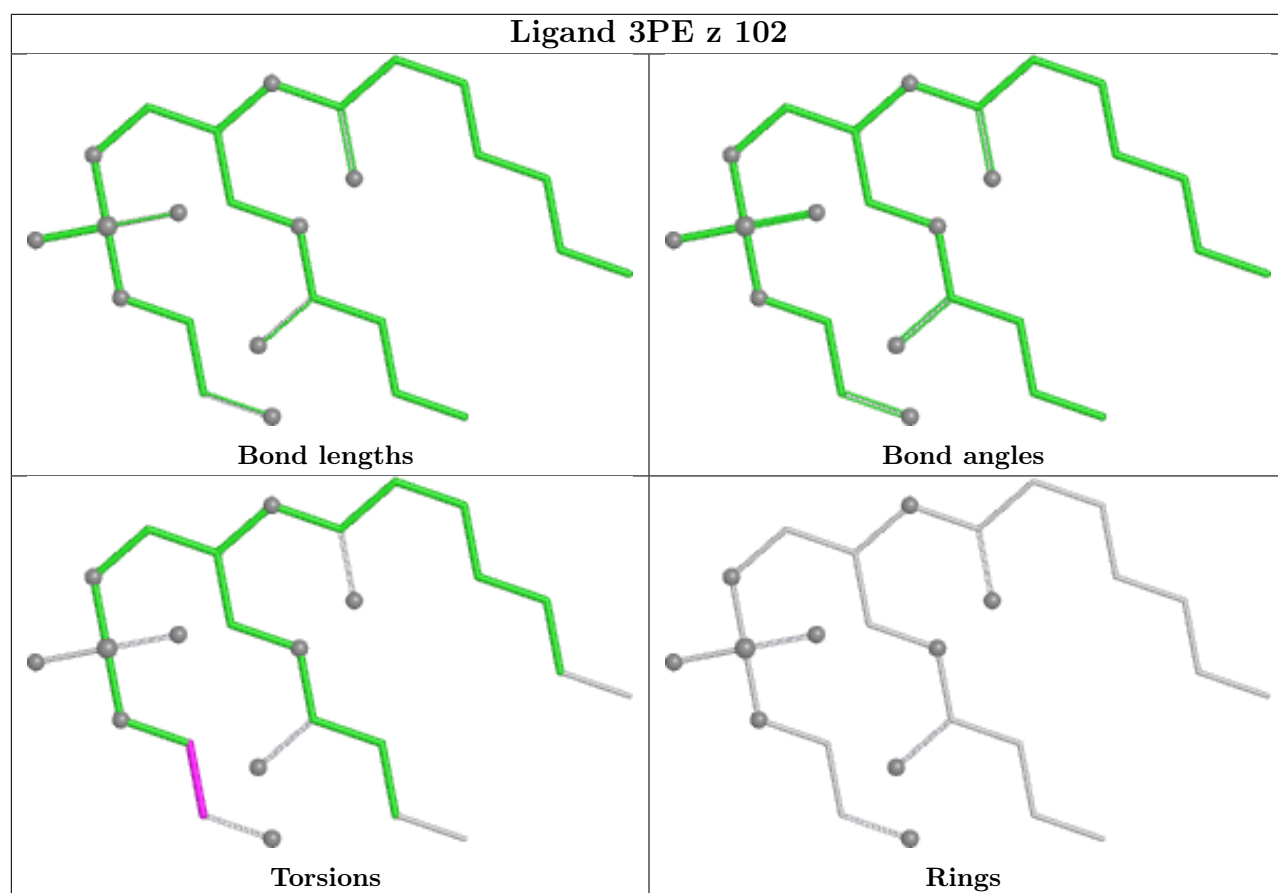


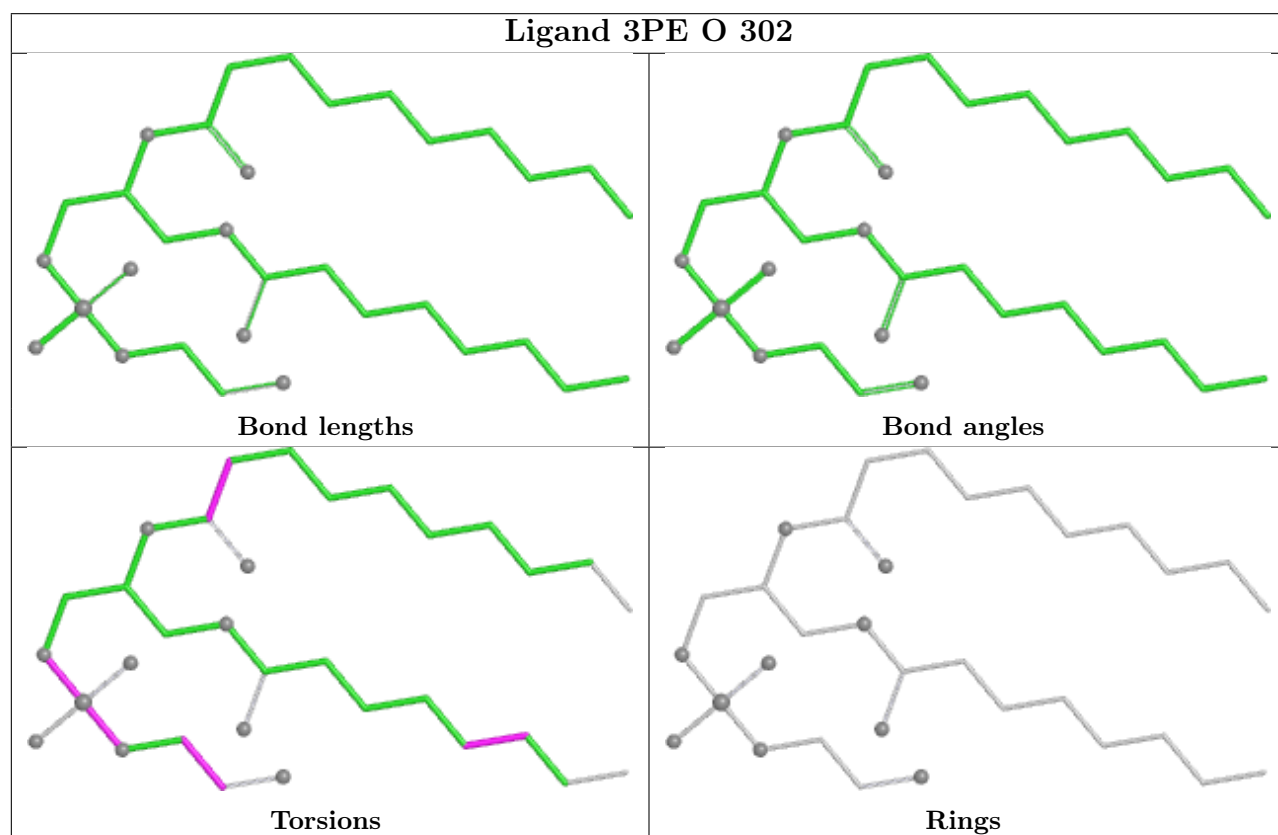
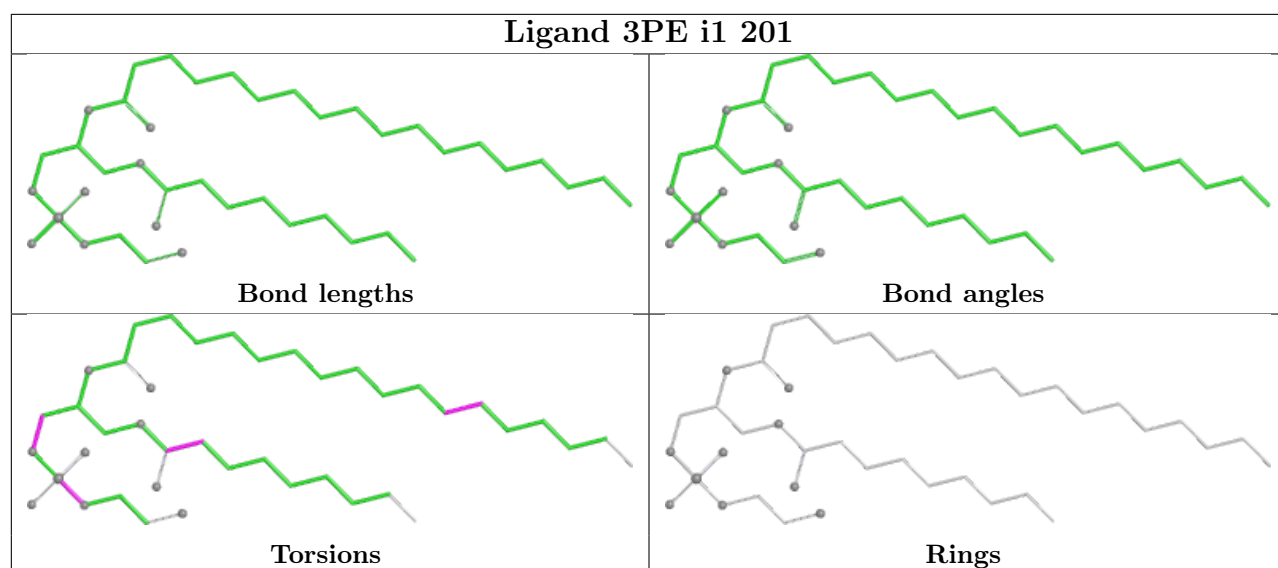


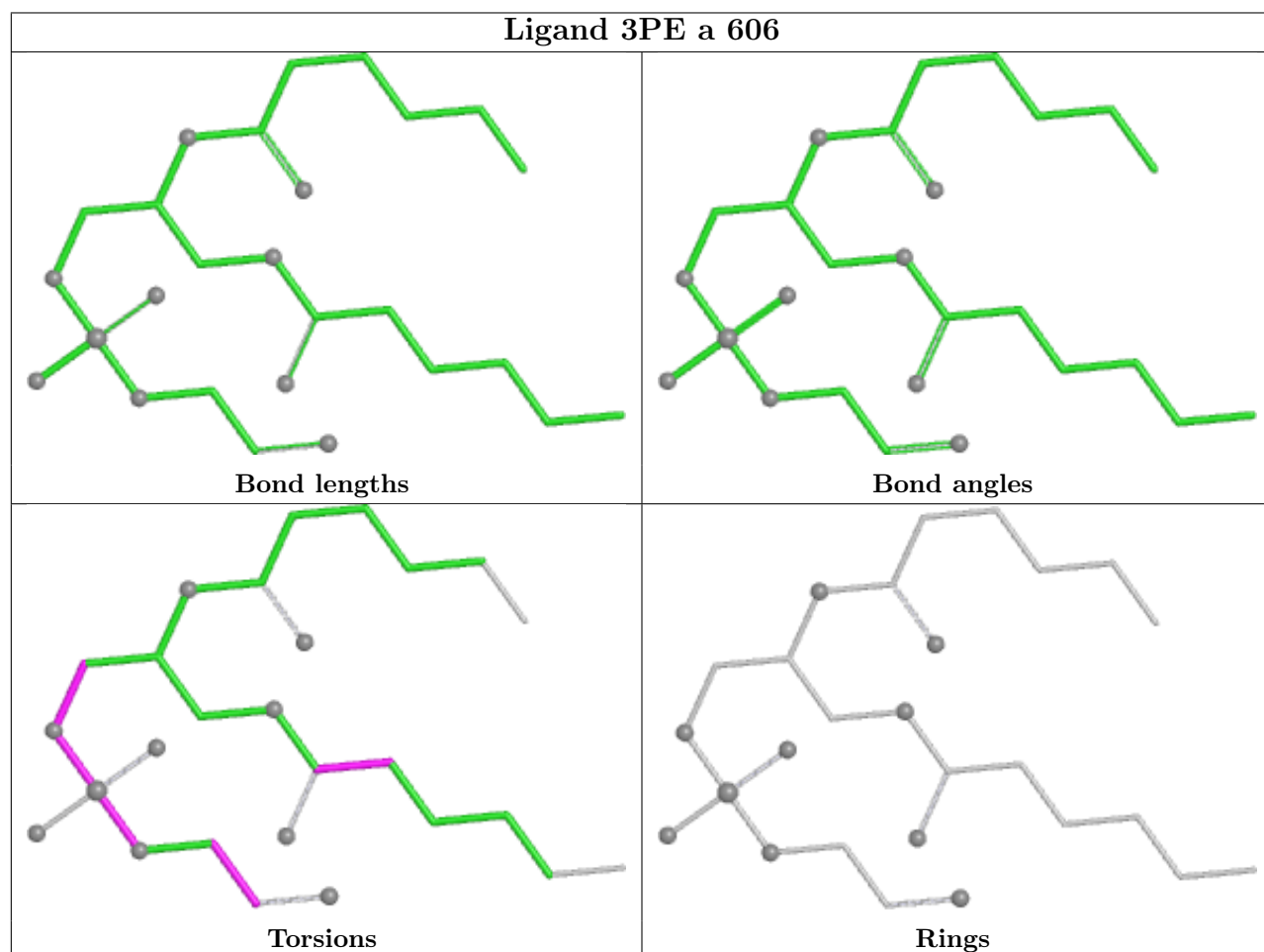
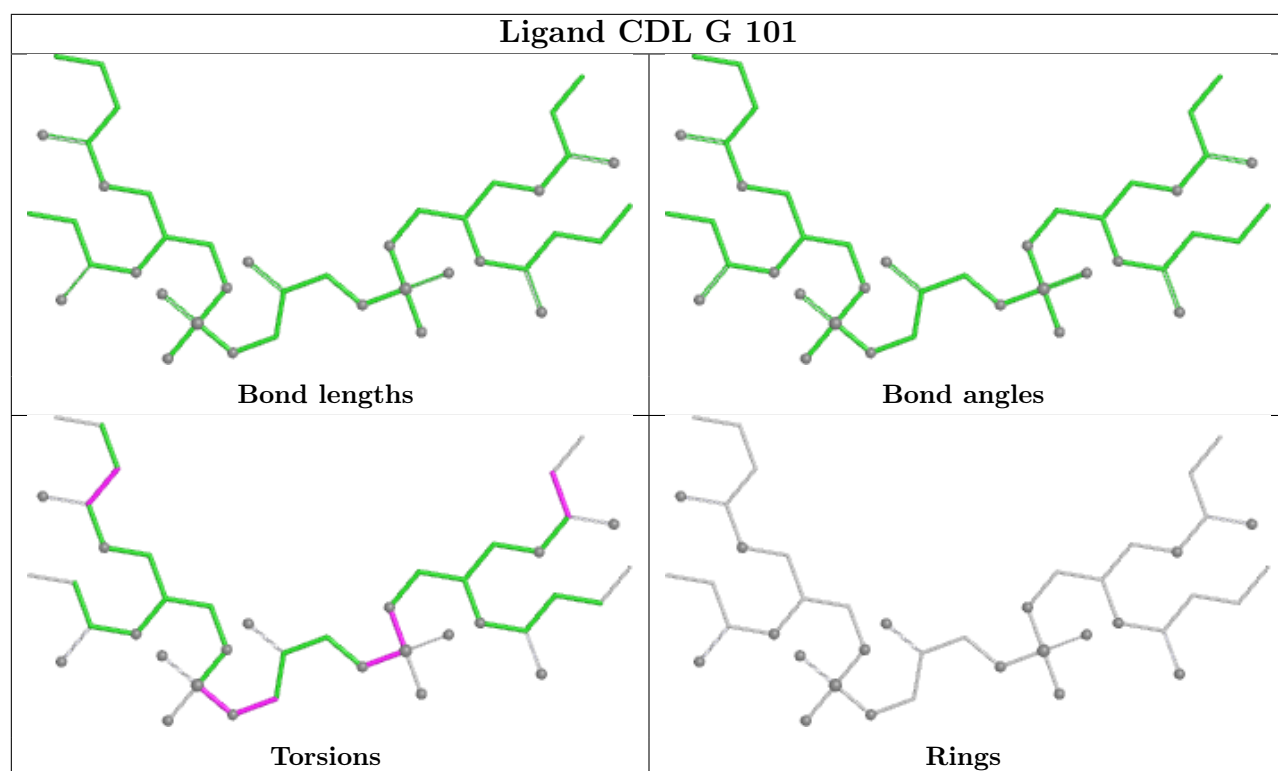


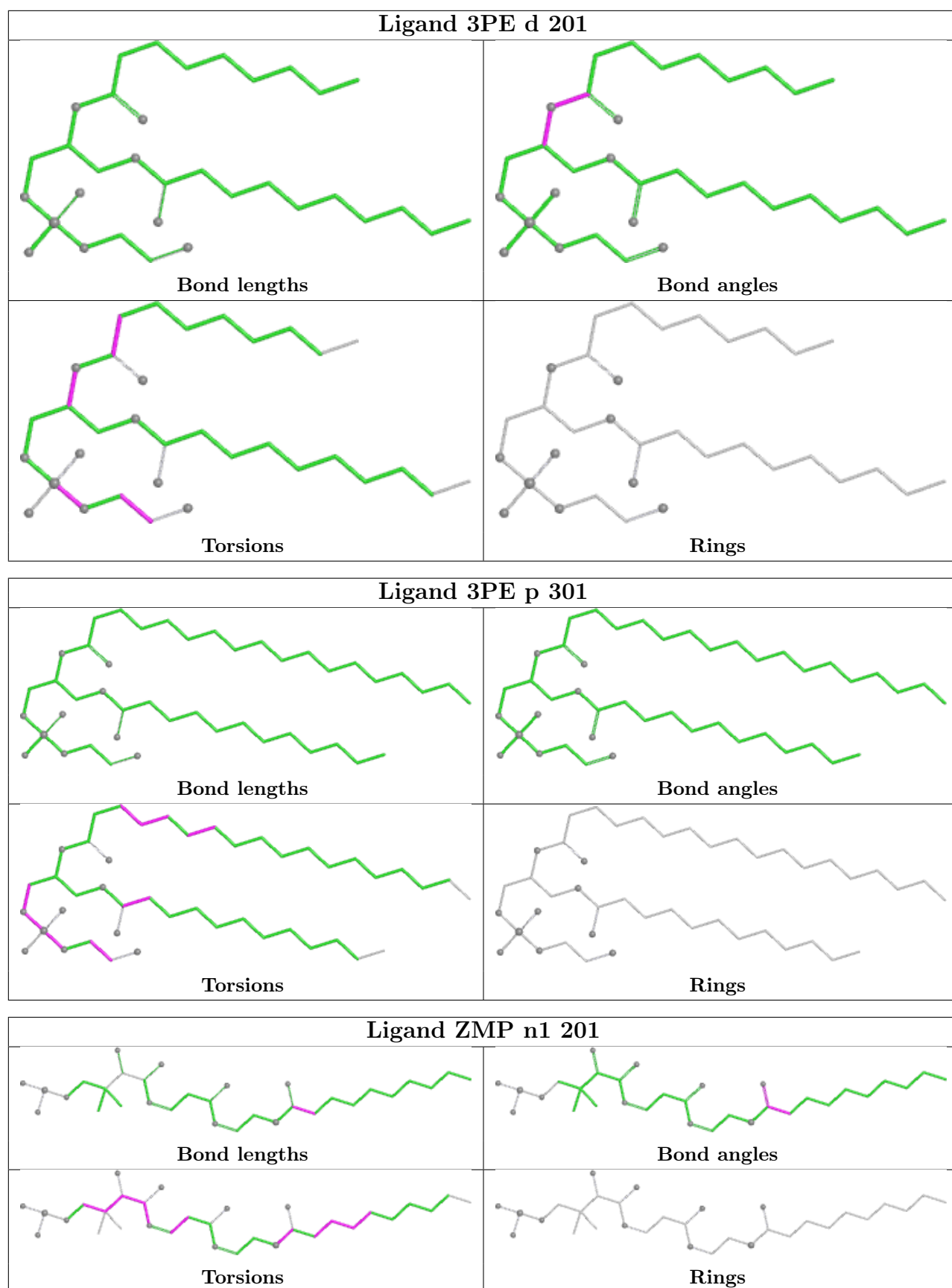


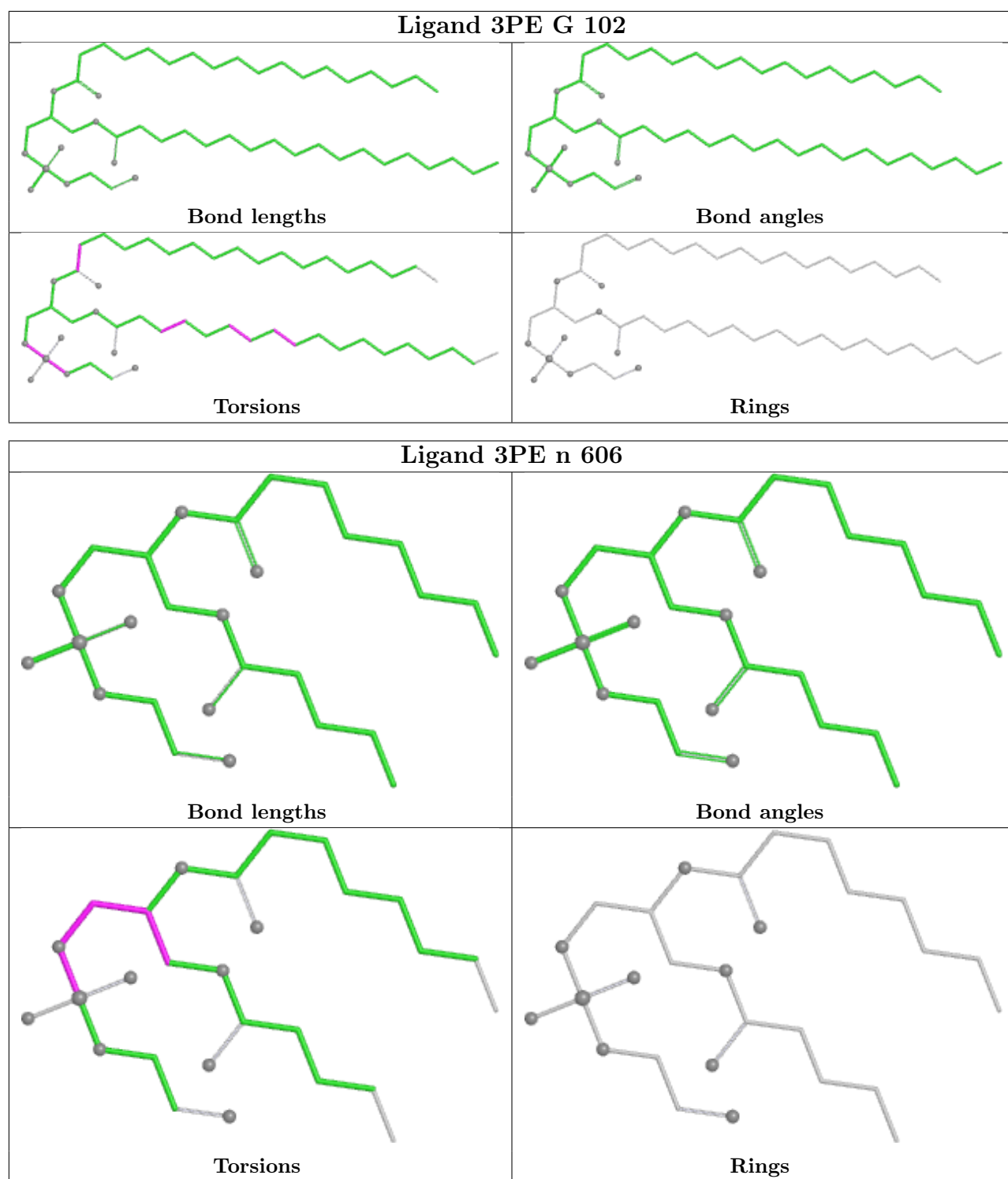


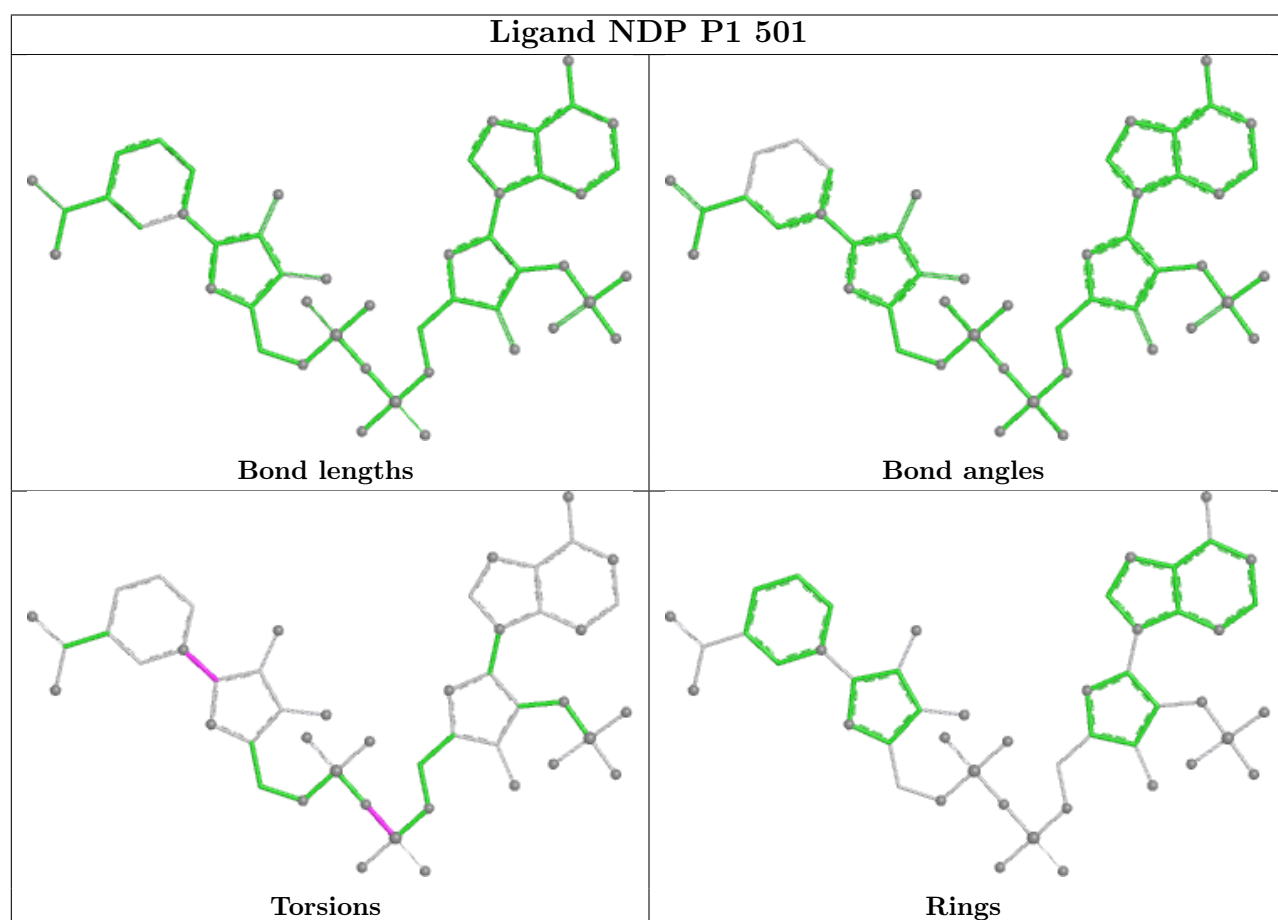
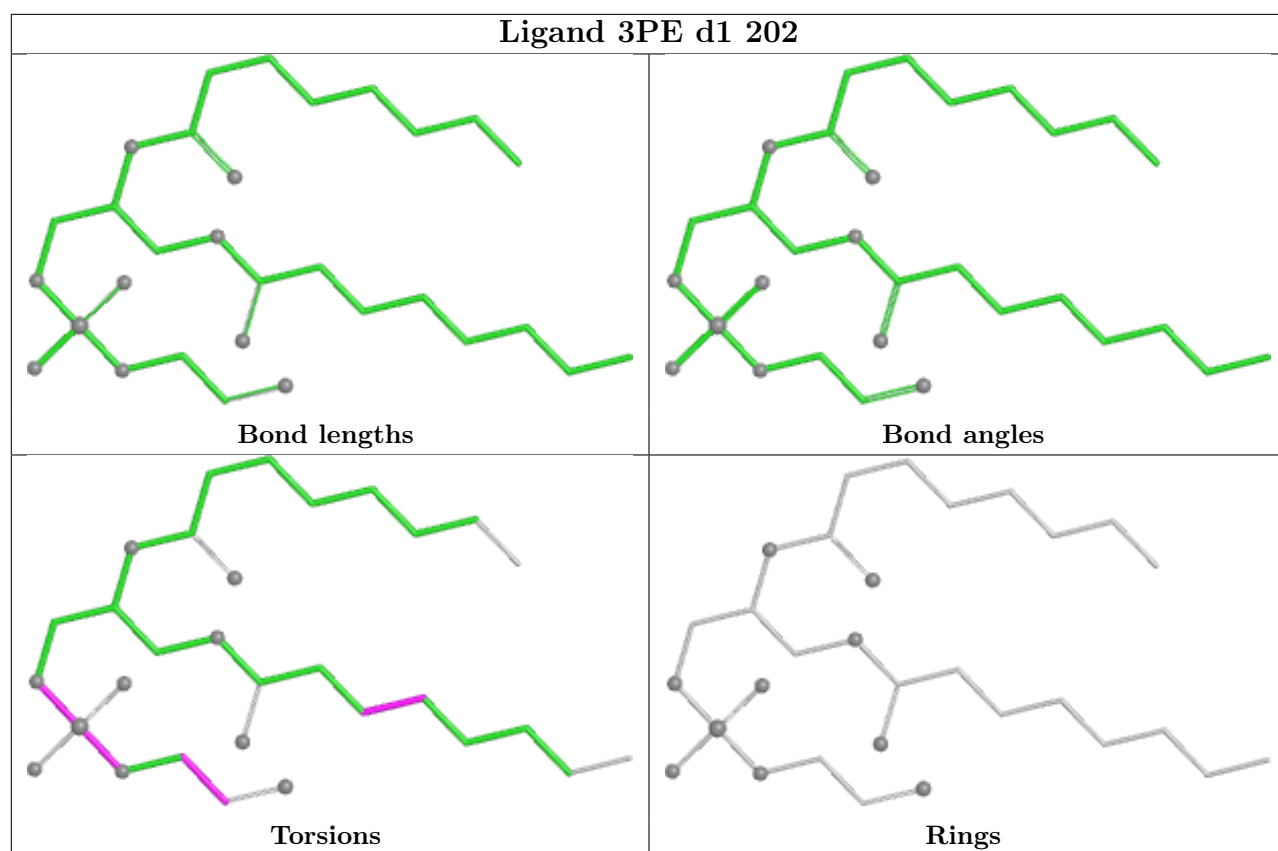


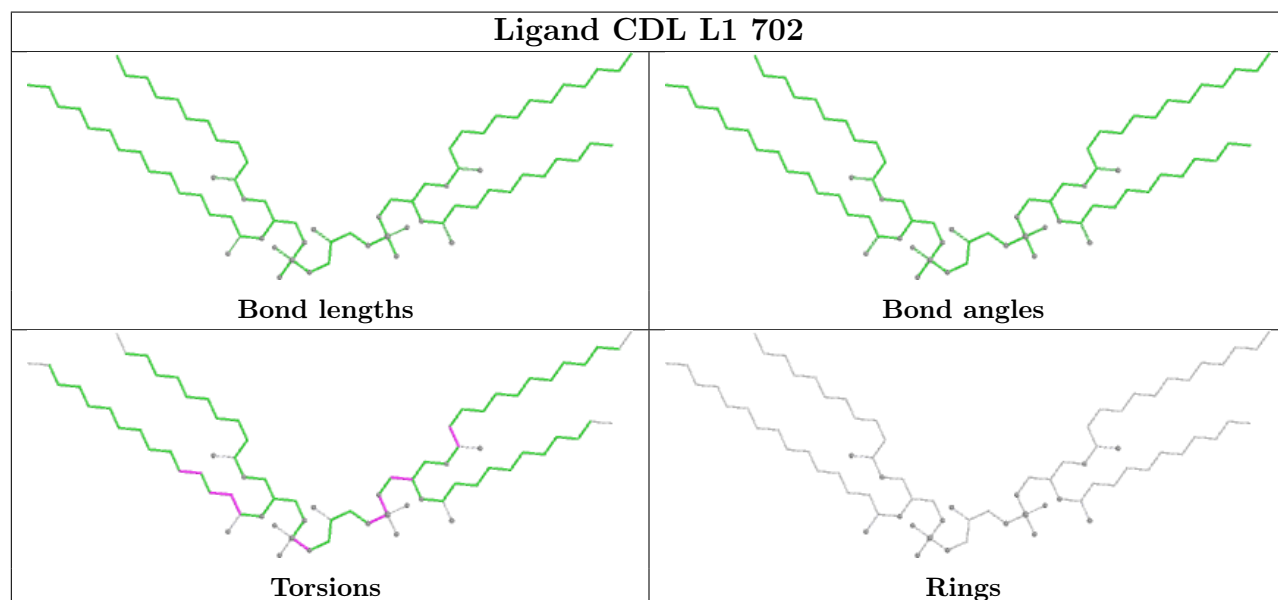
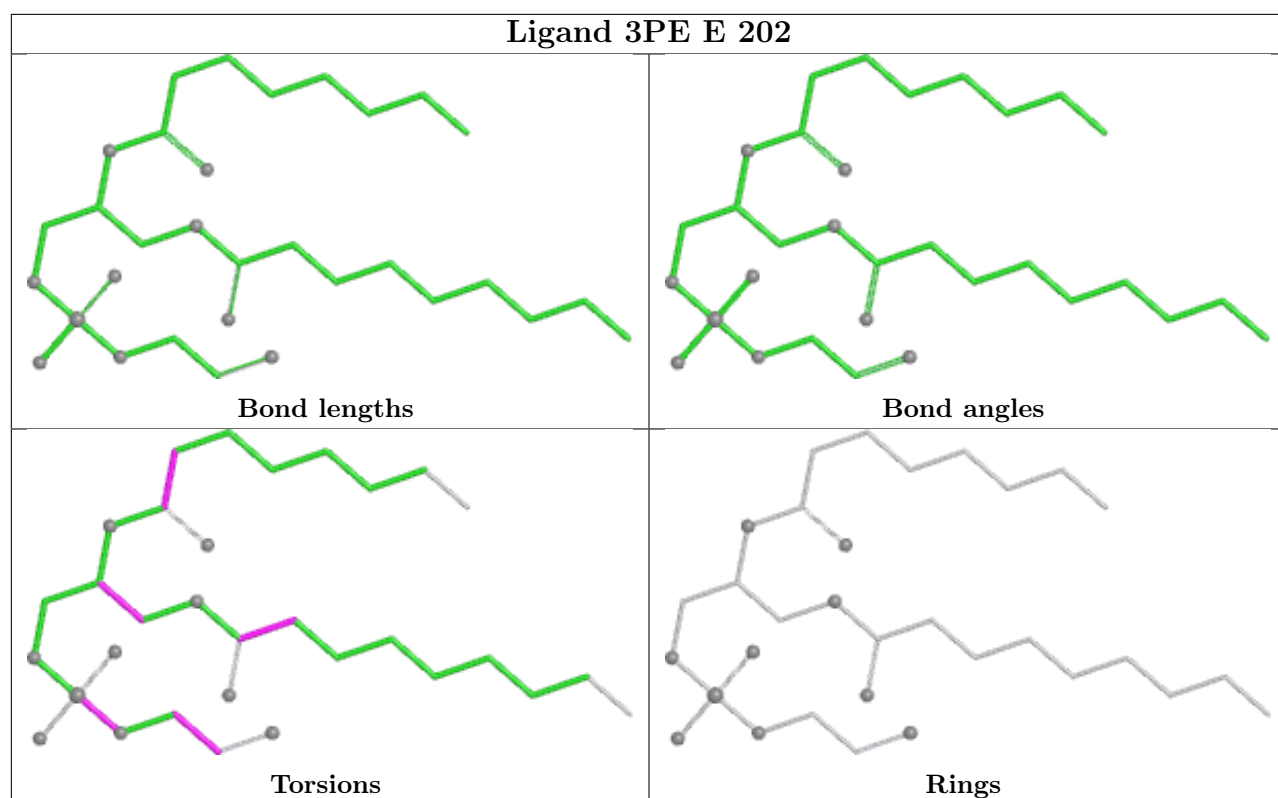


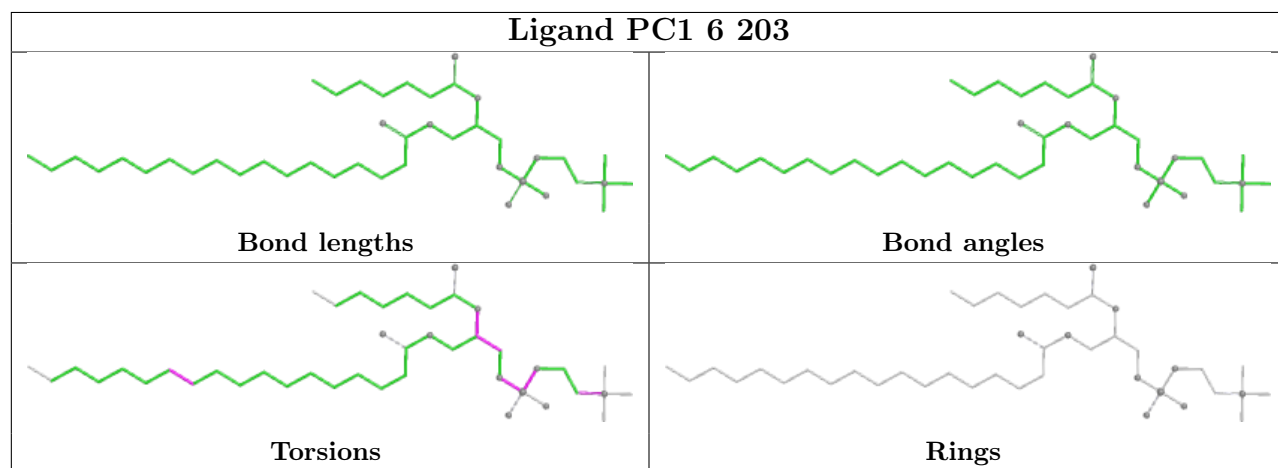
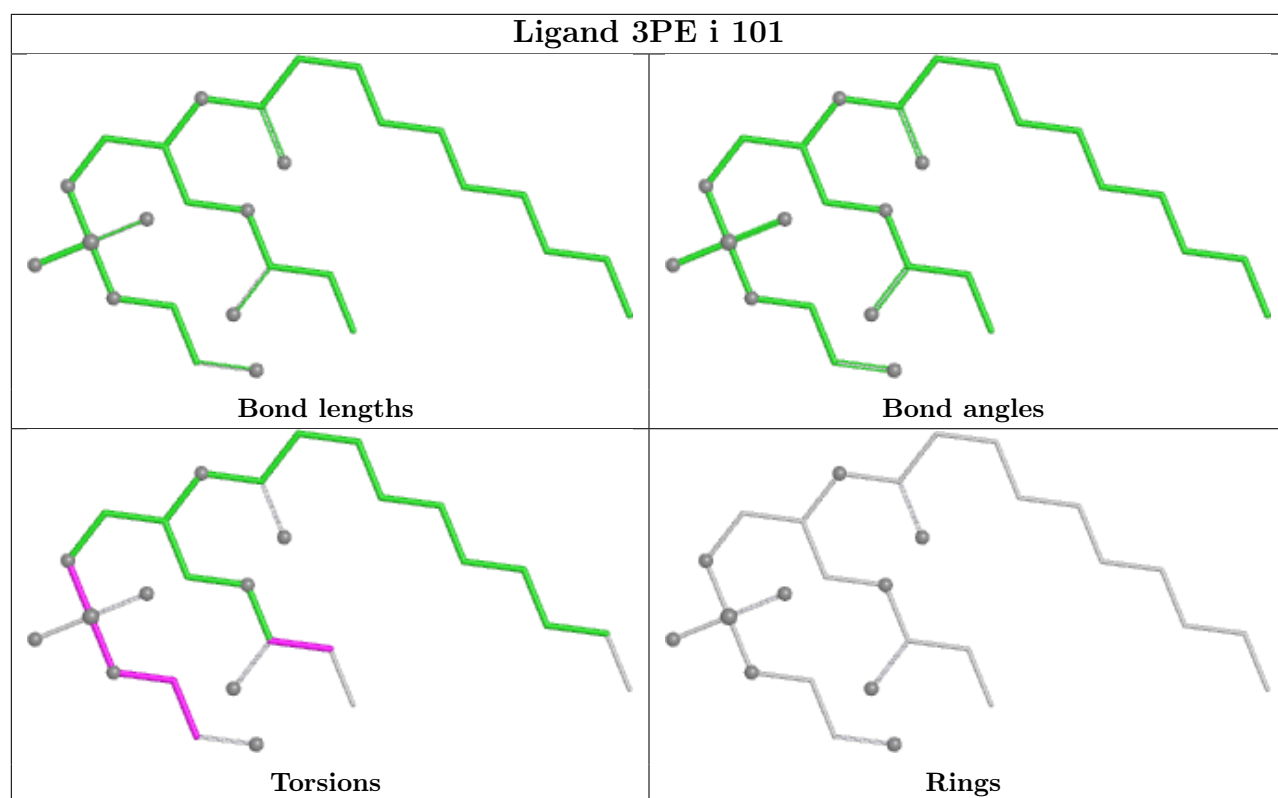


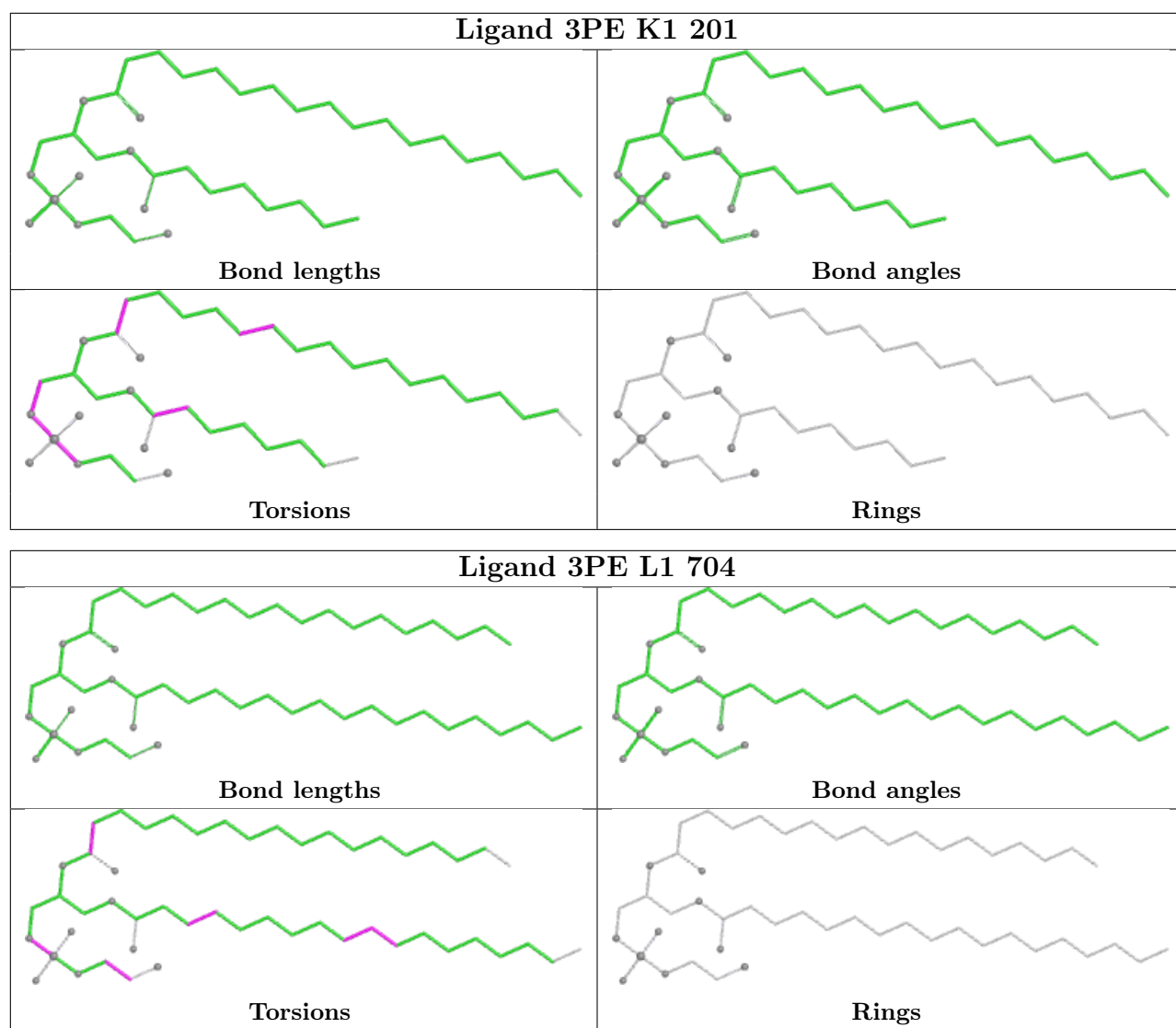


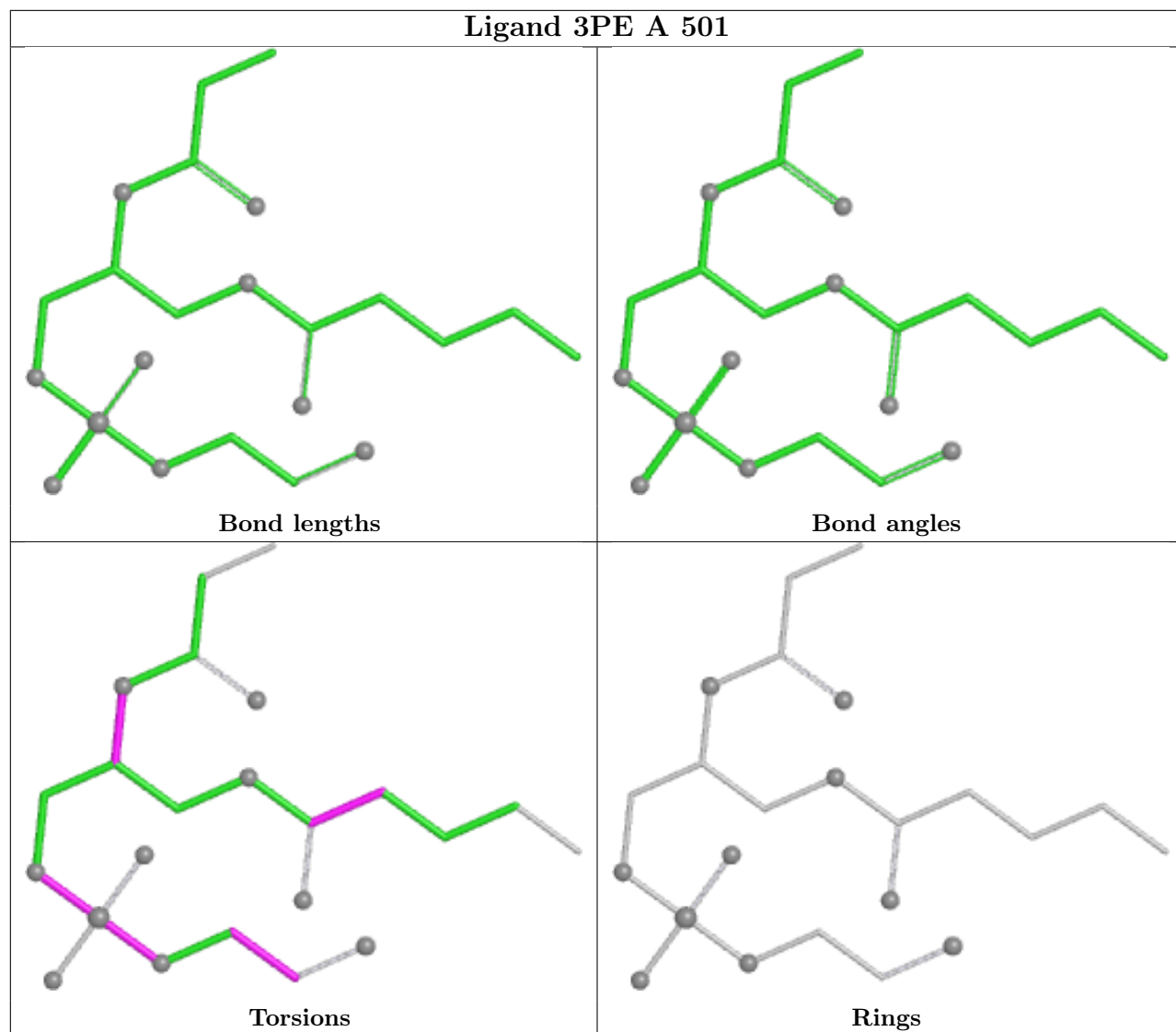




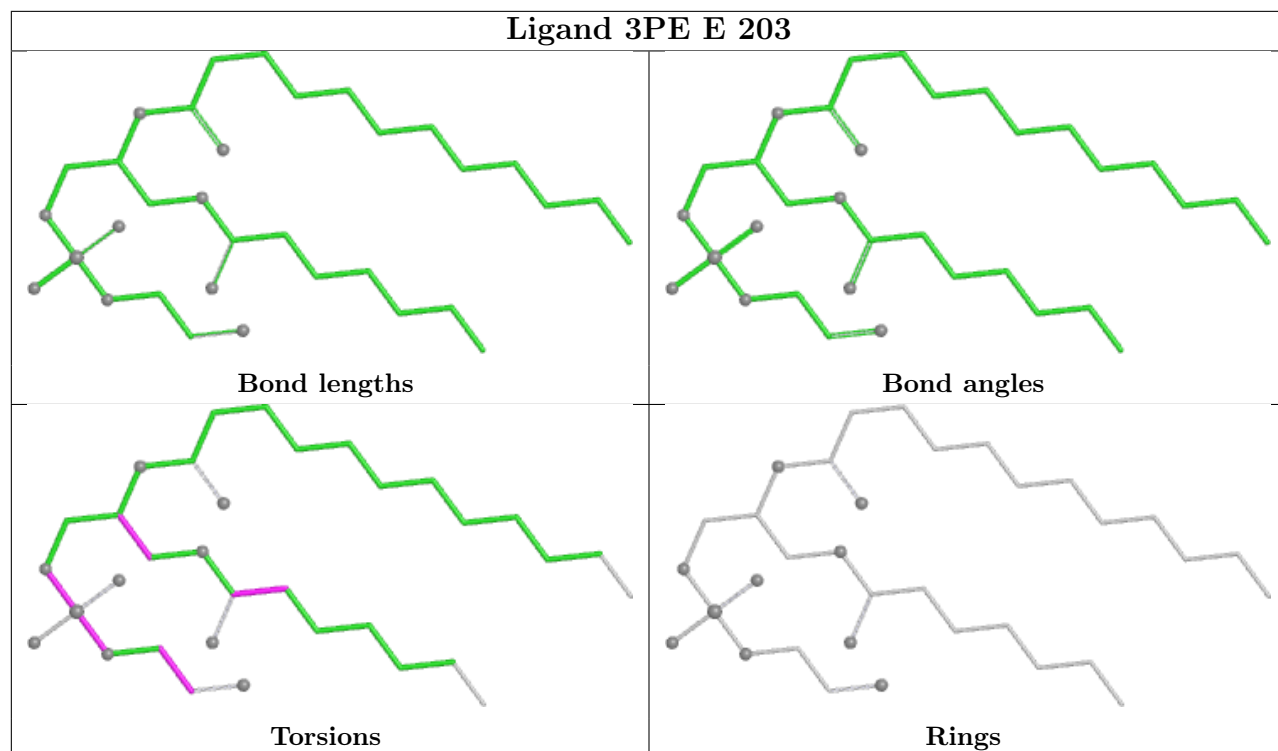




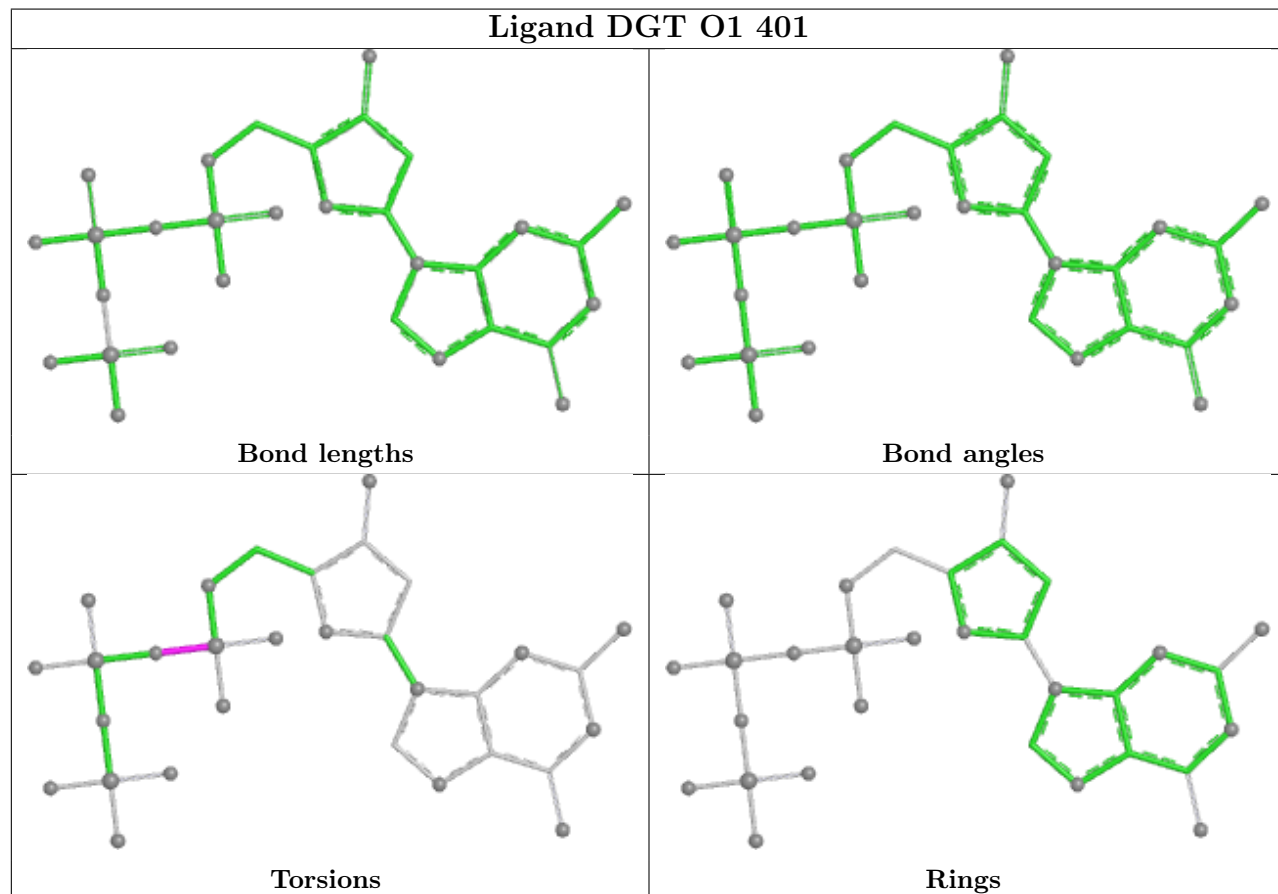


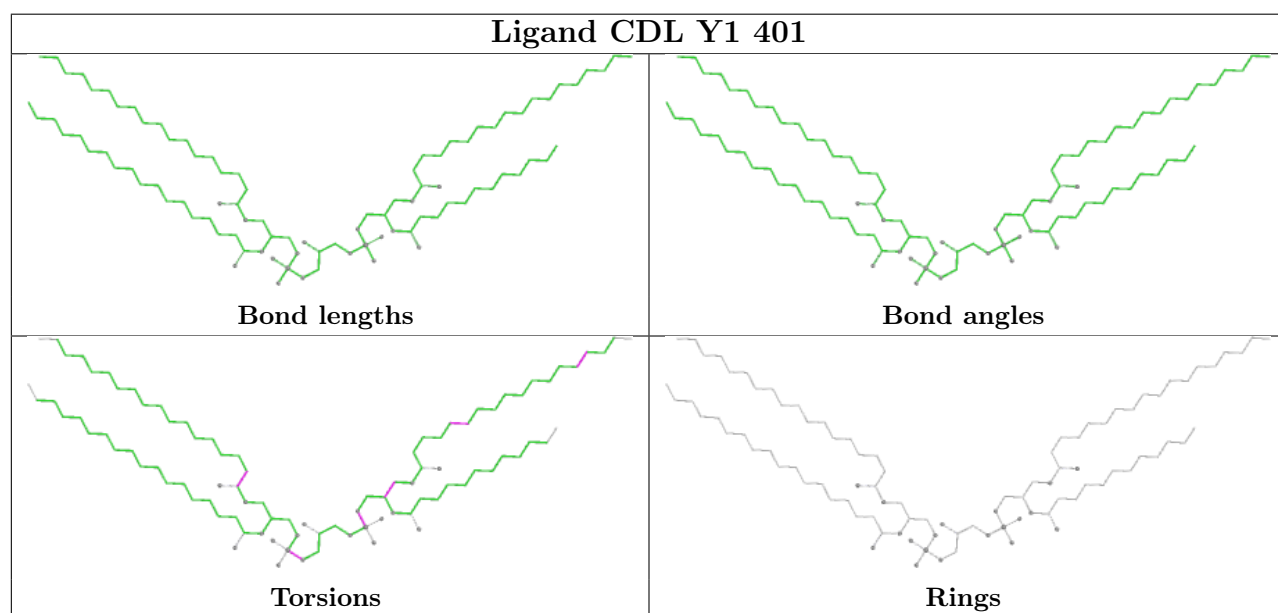
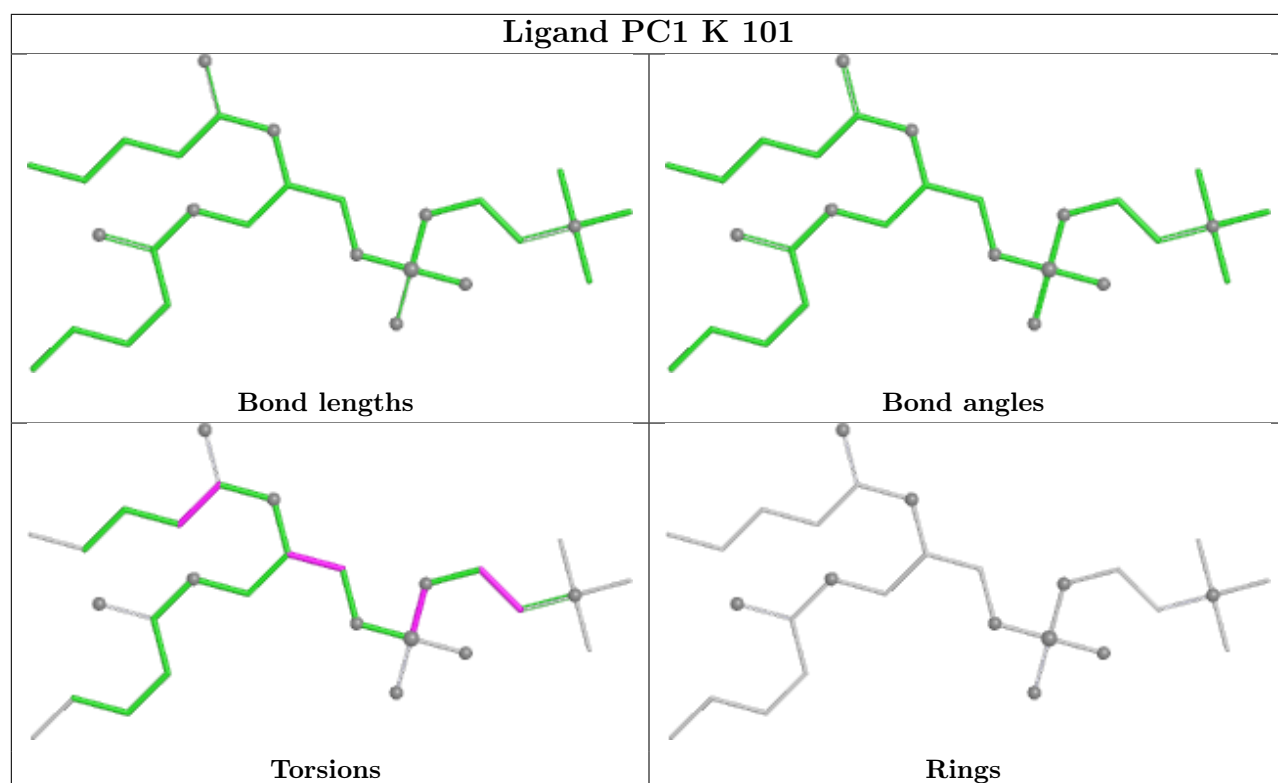


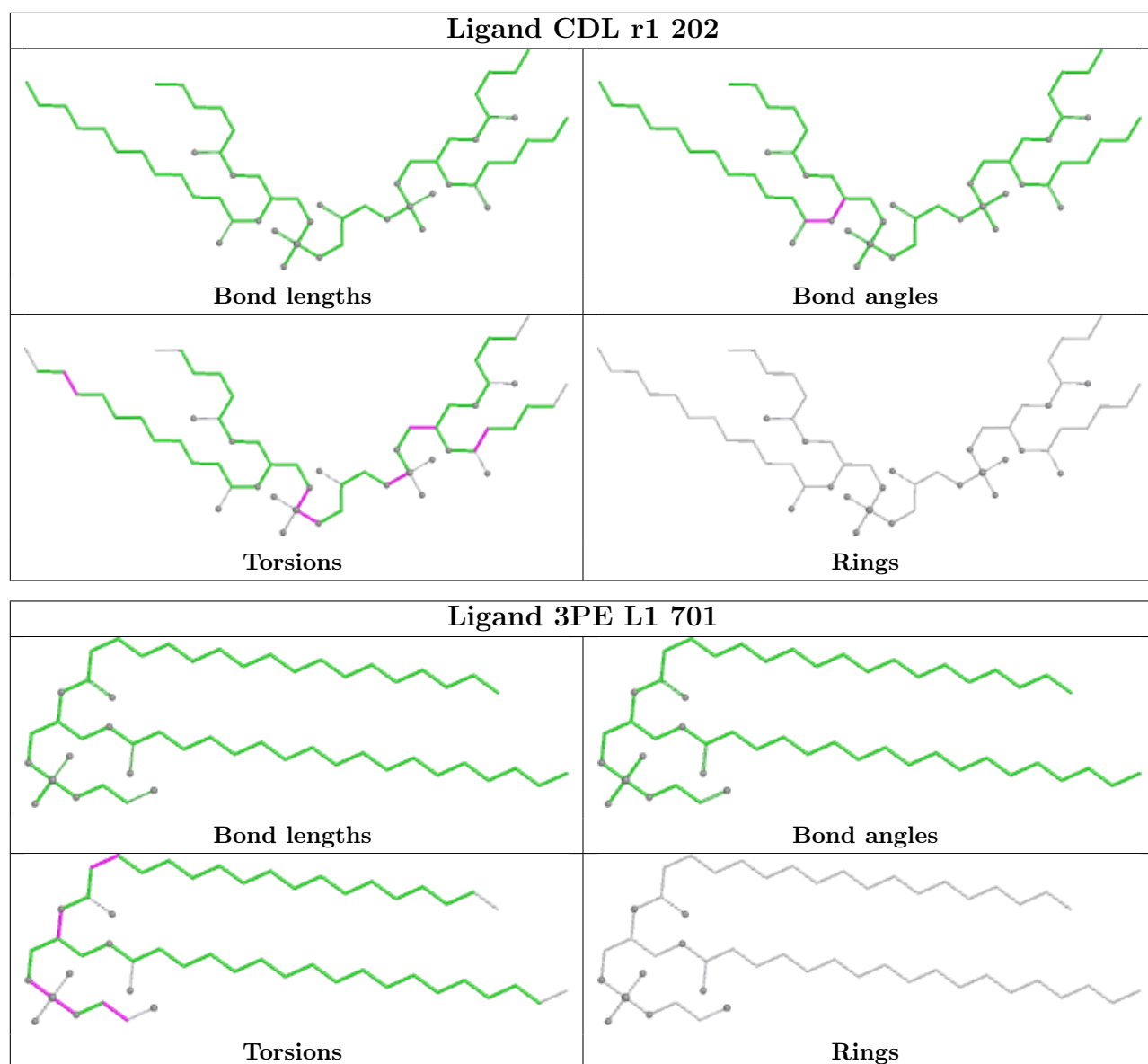
Ligand 3PE E 203

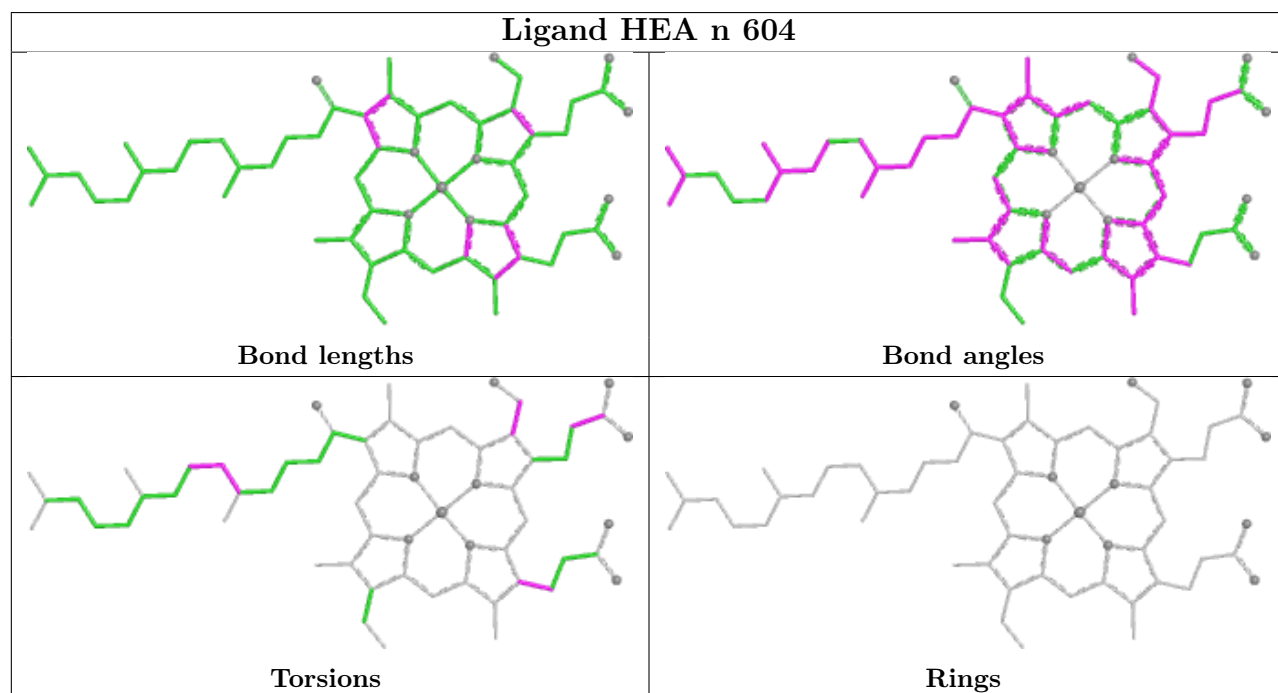
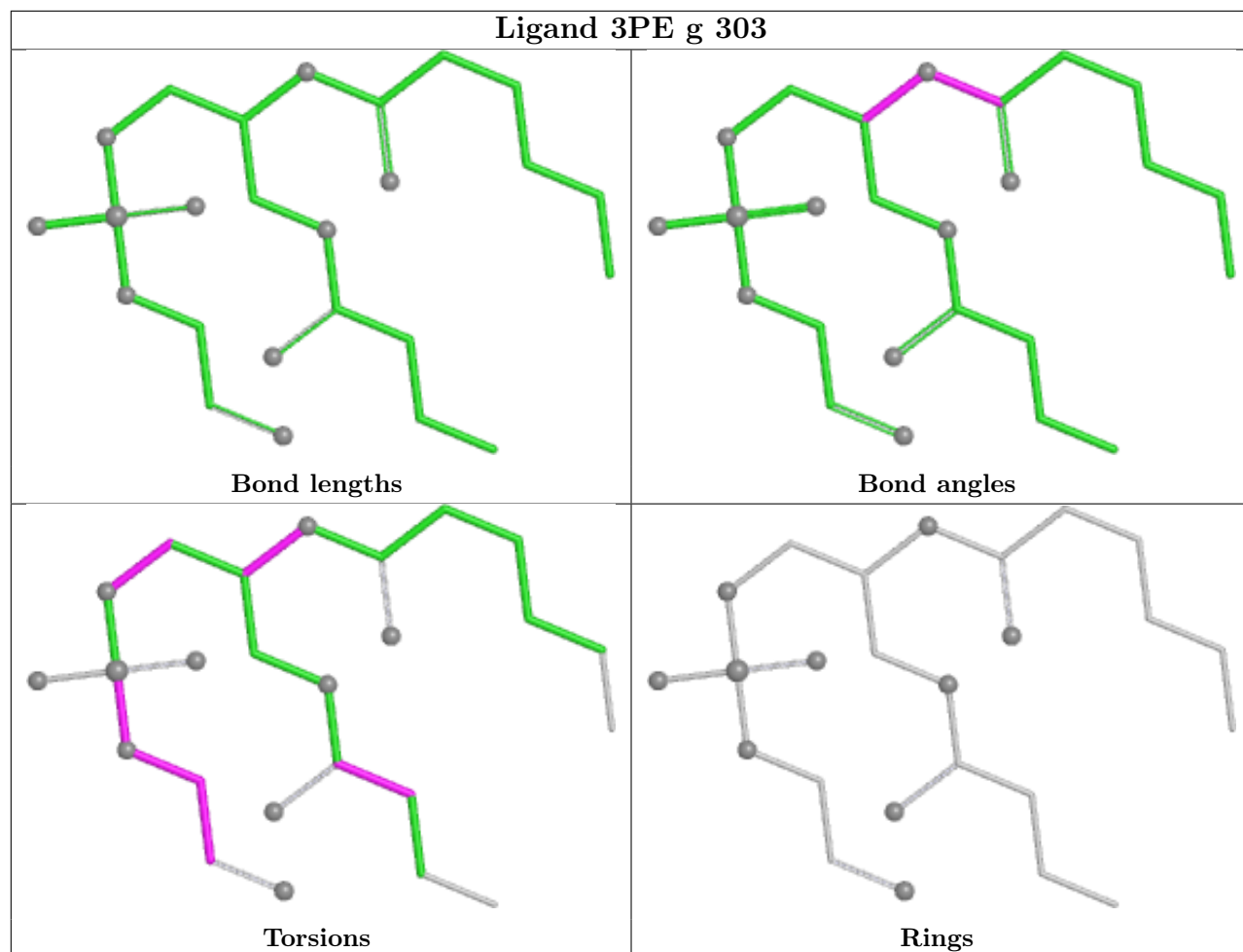


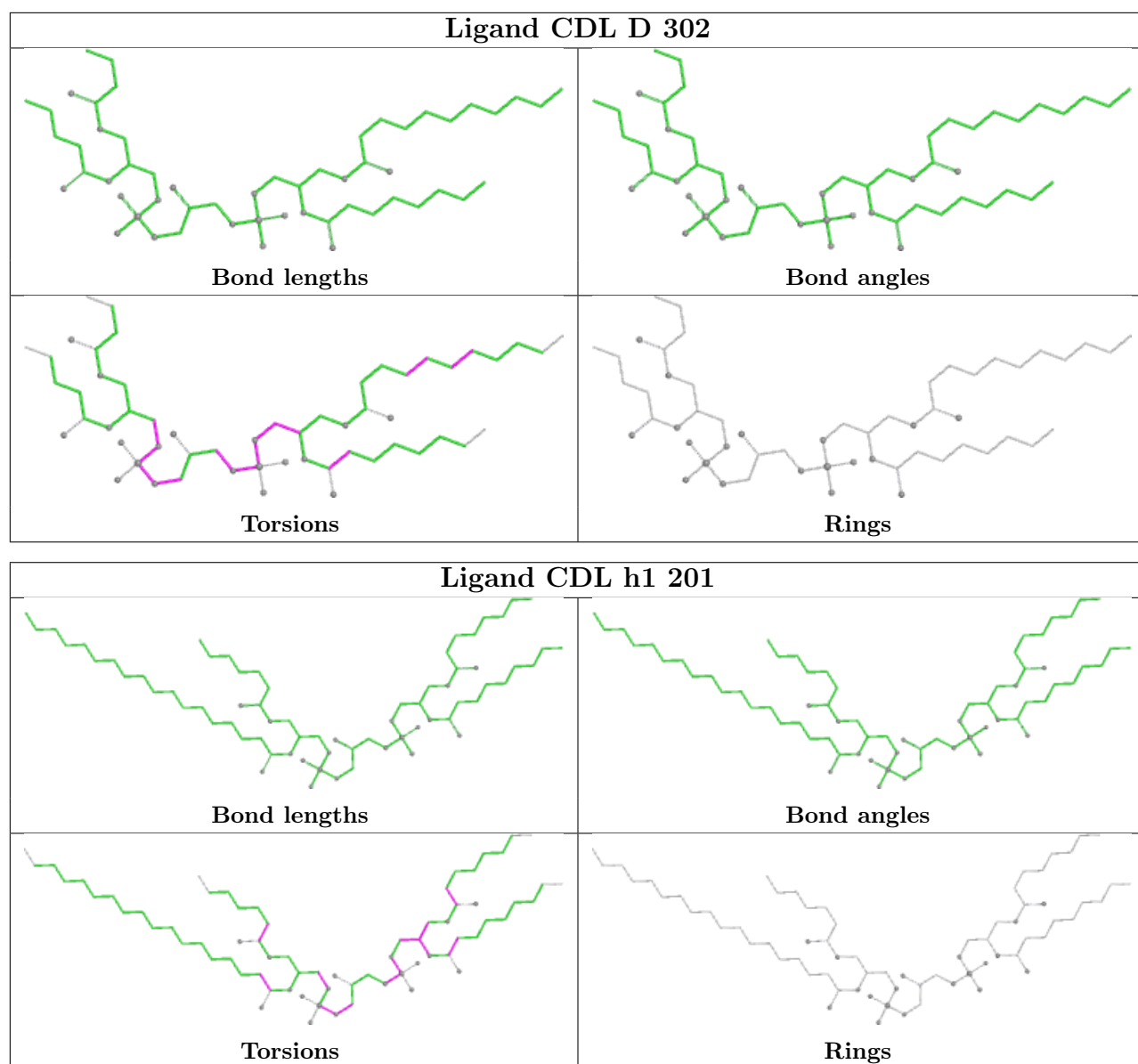
Ligand DGT O1 401

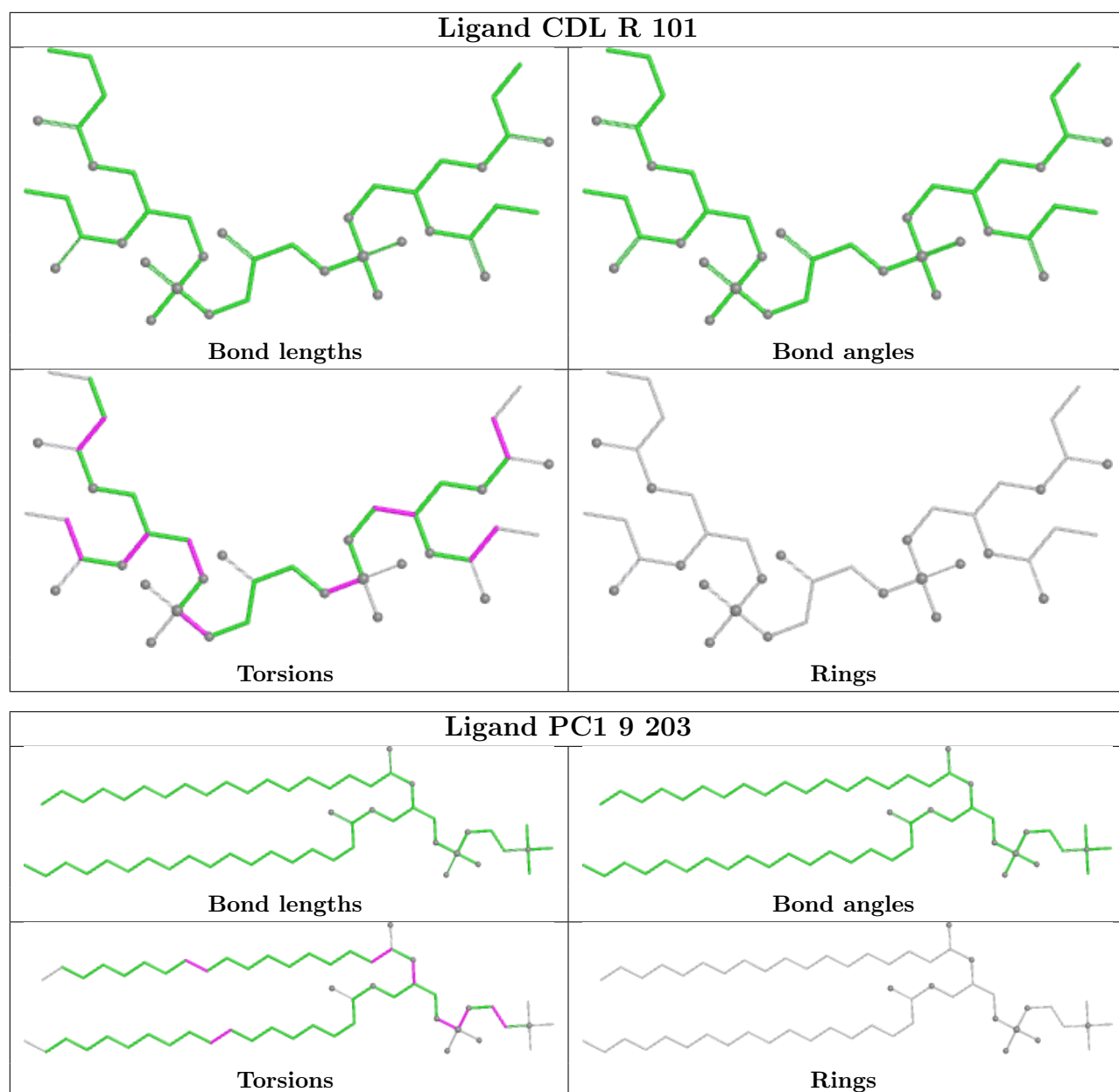


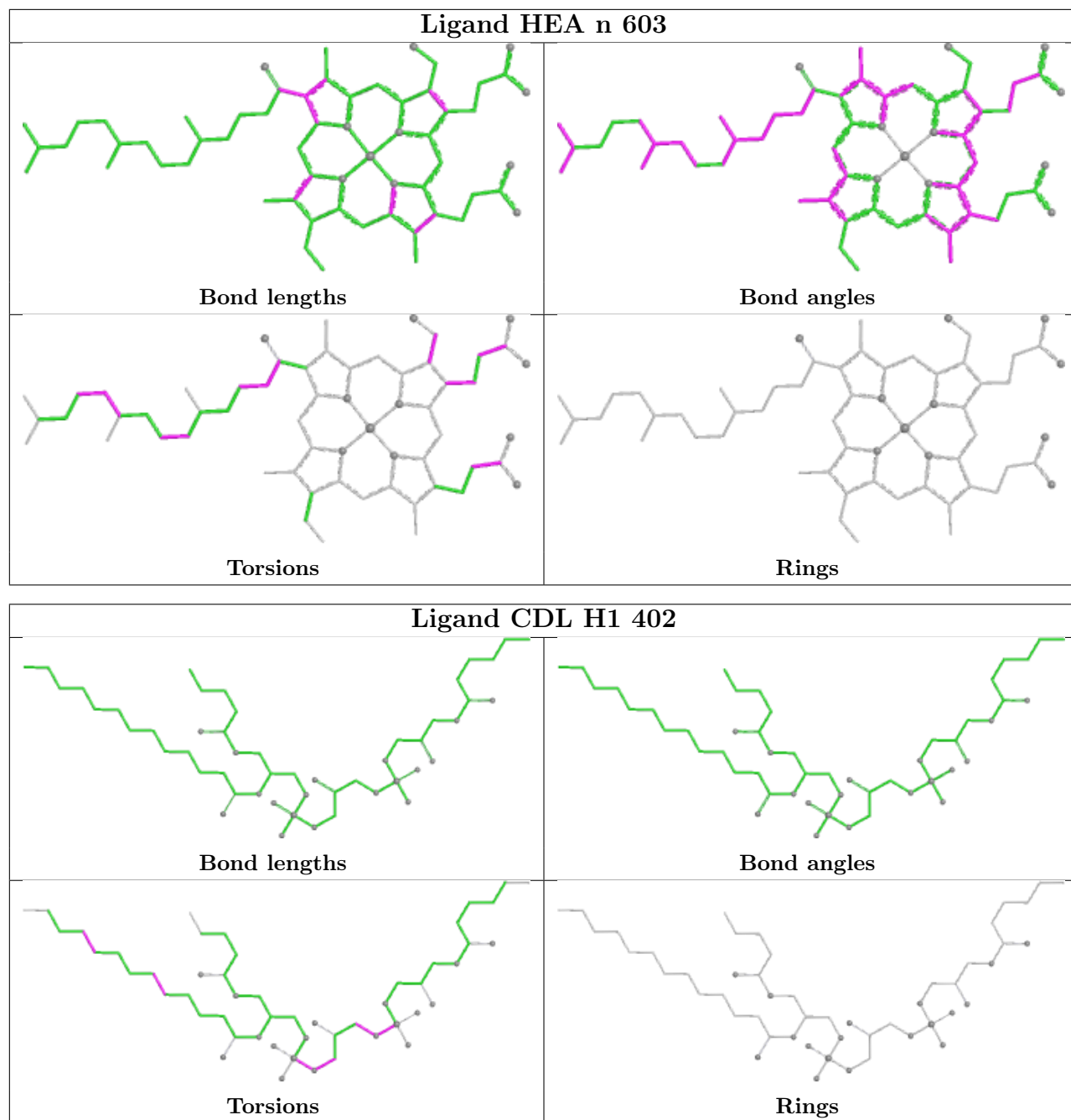


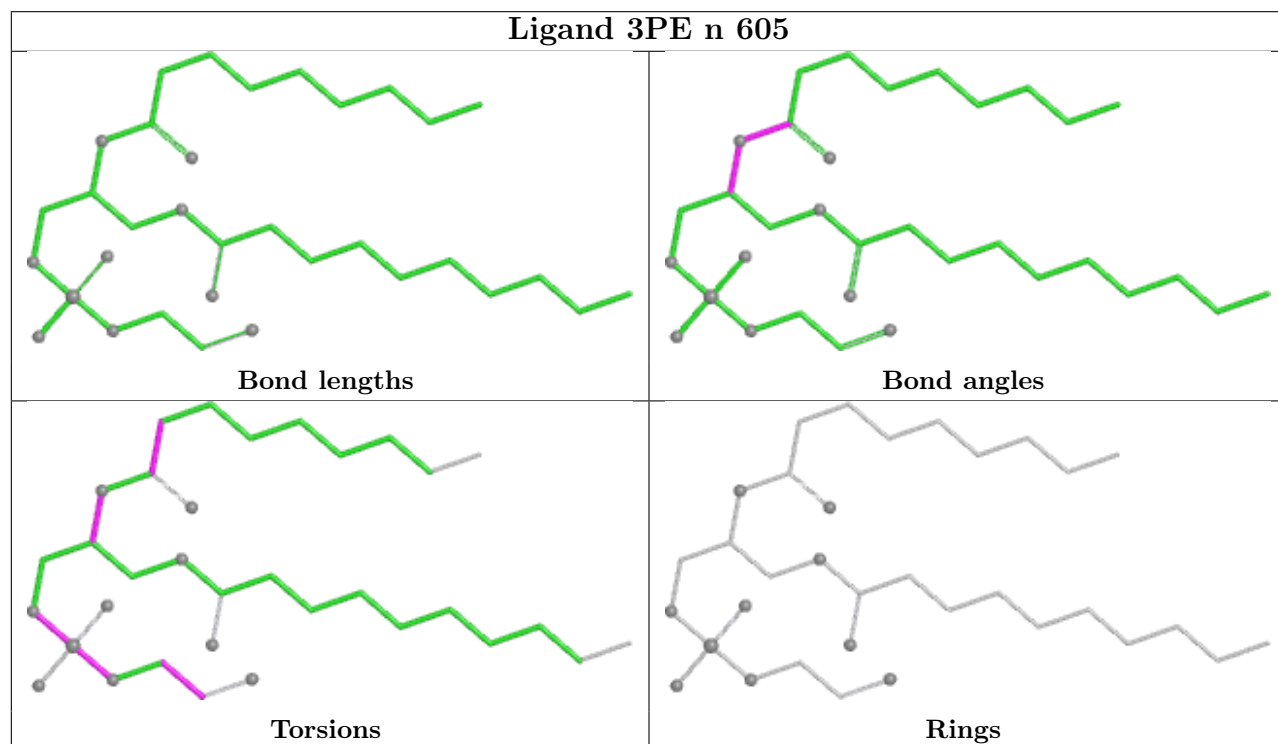
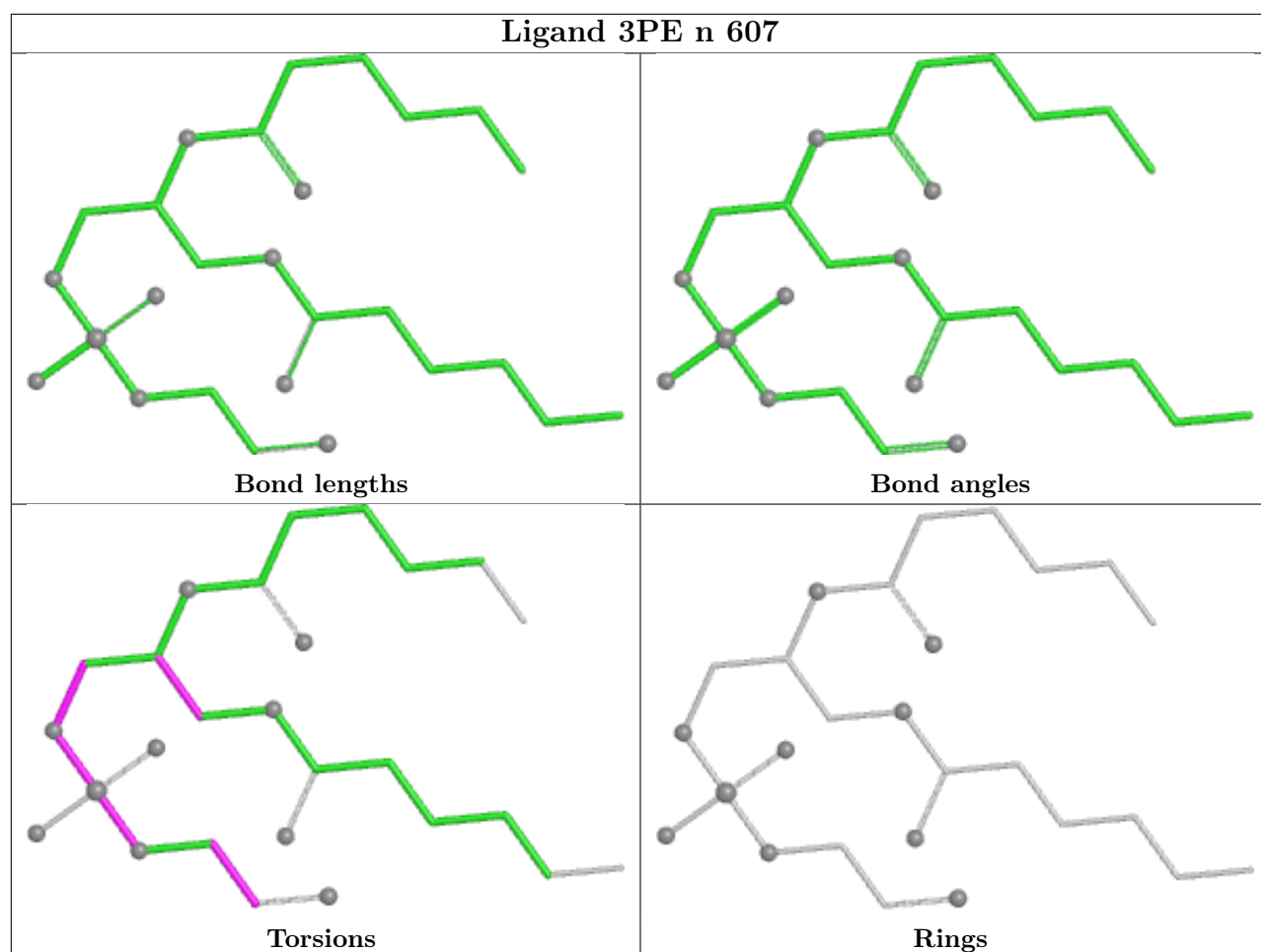


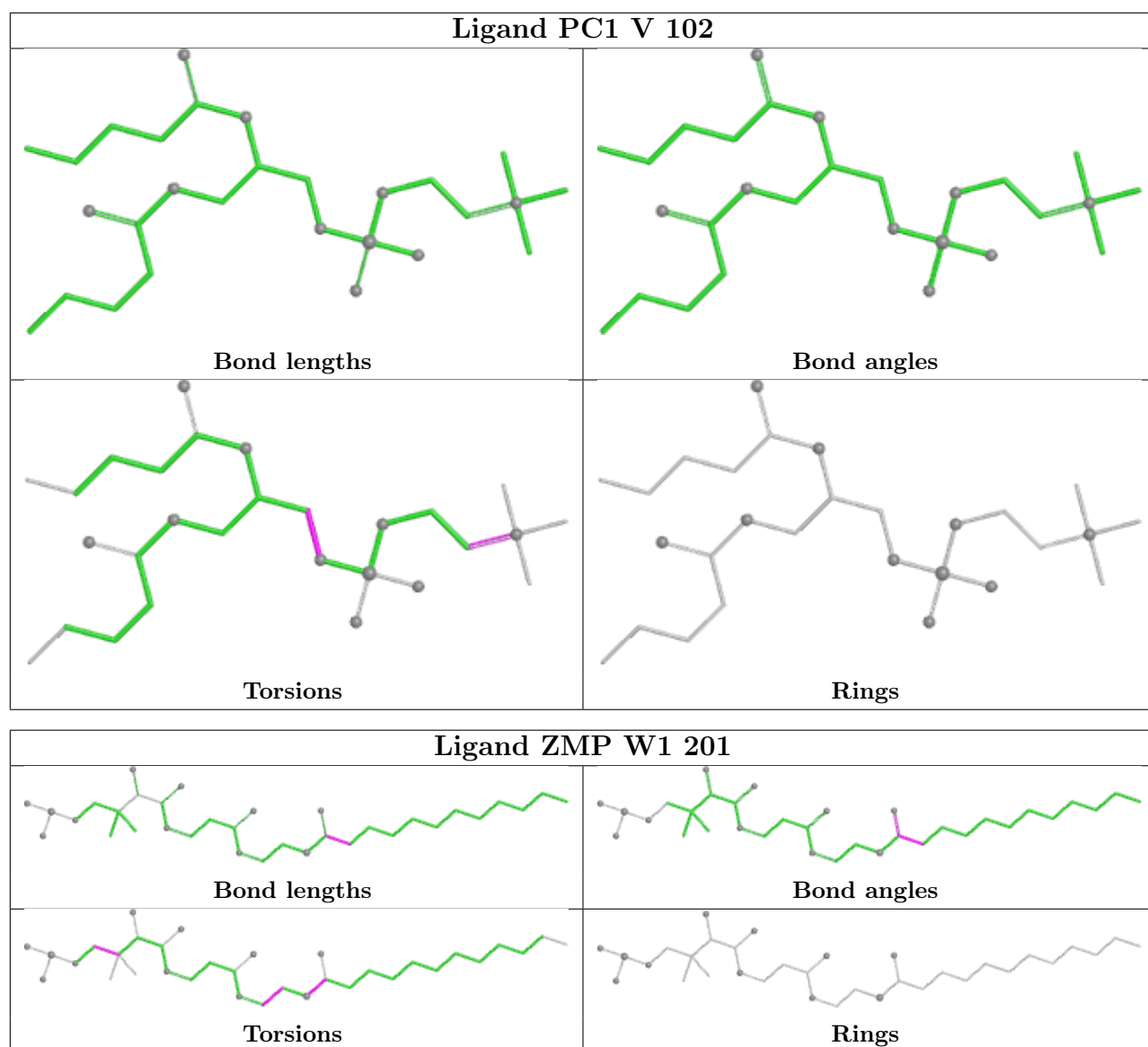


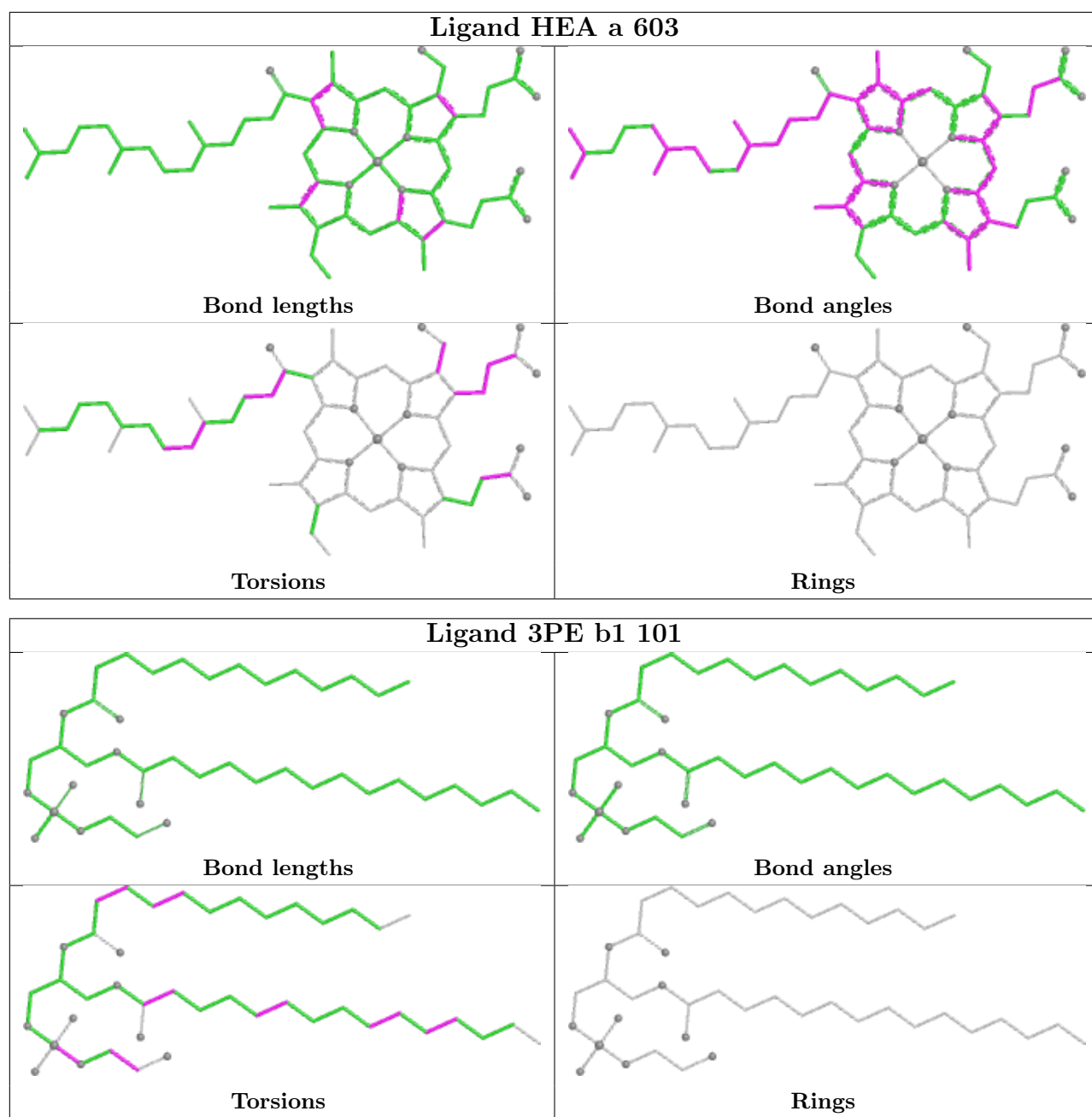


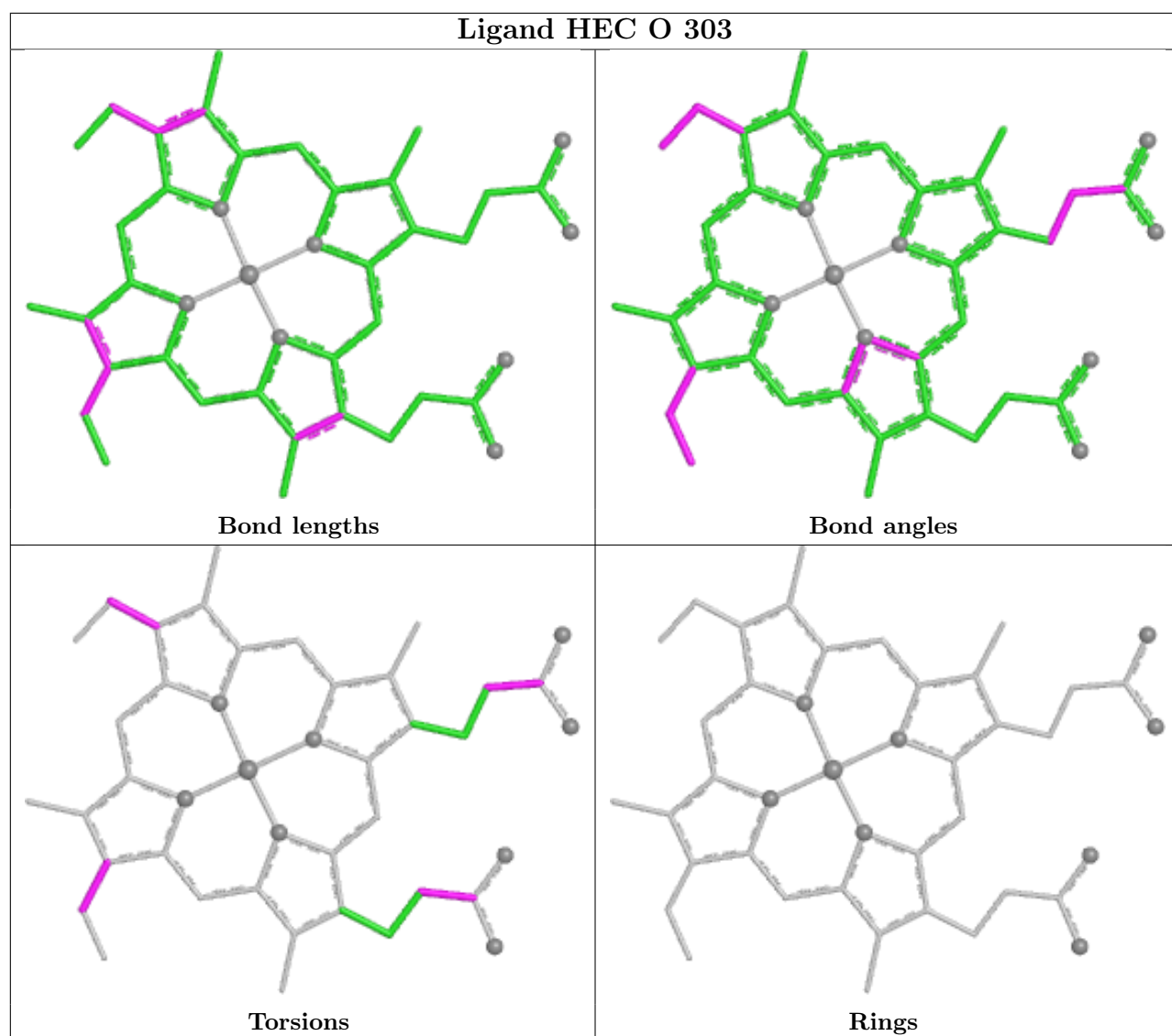


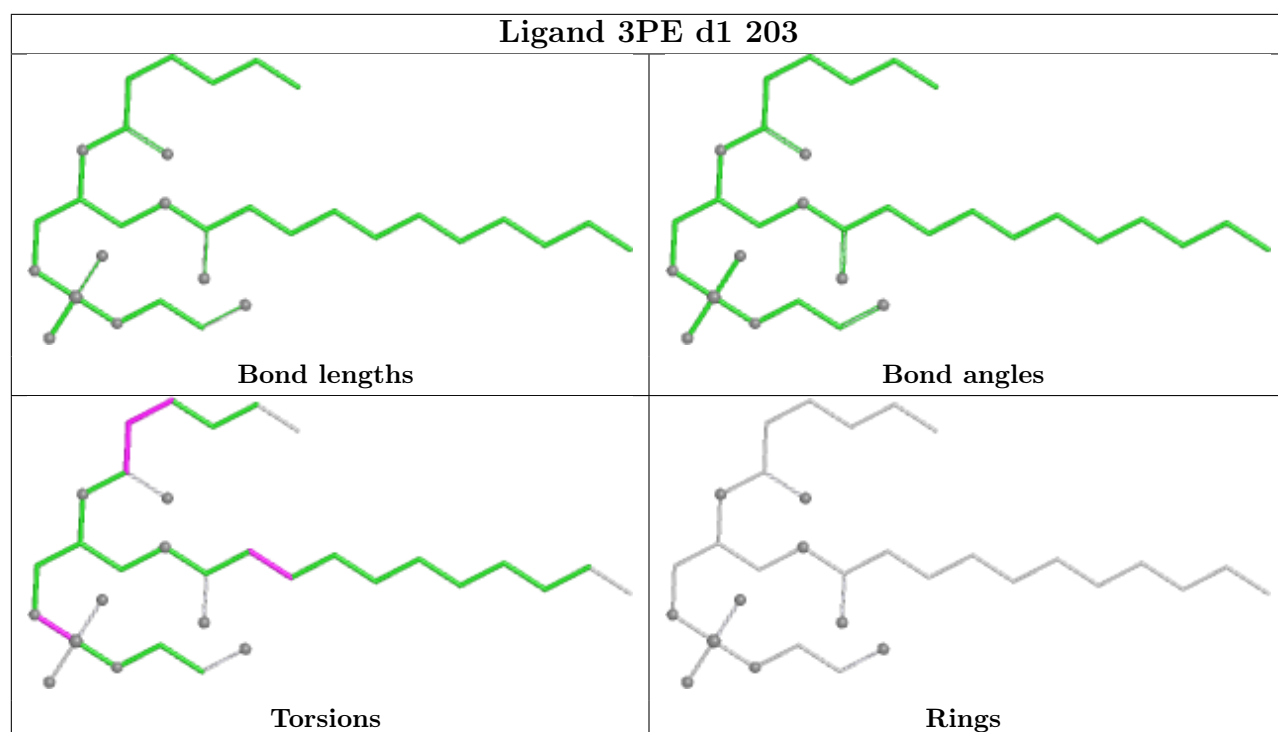


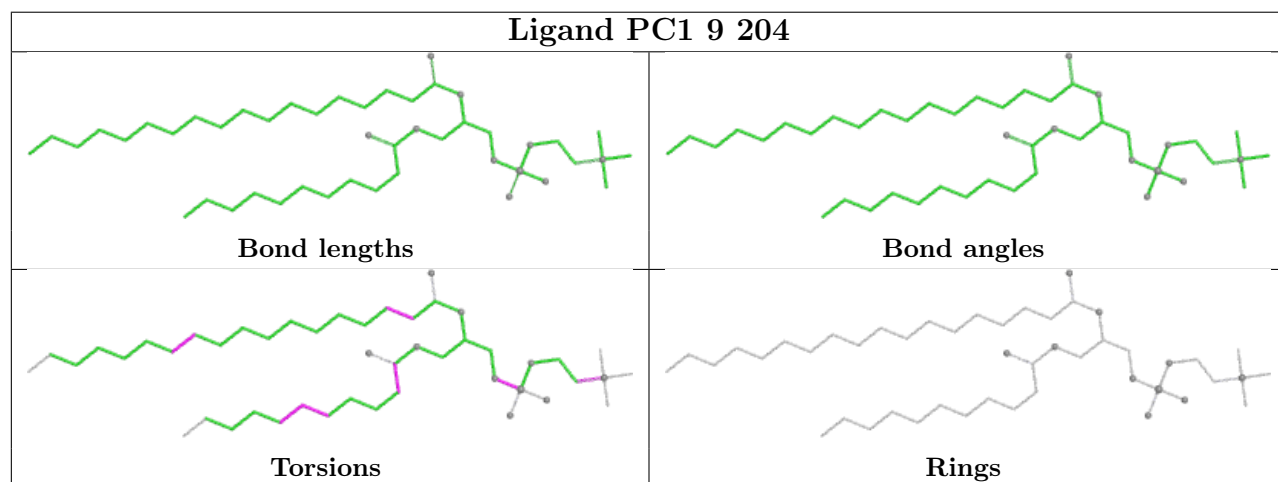
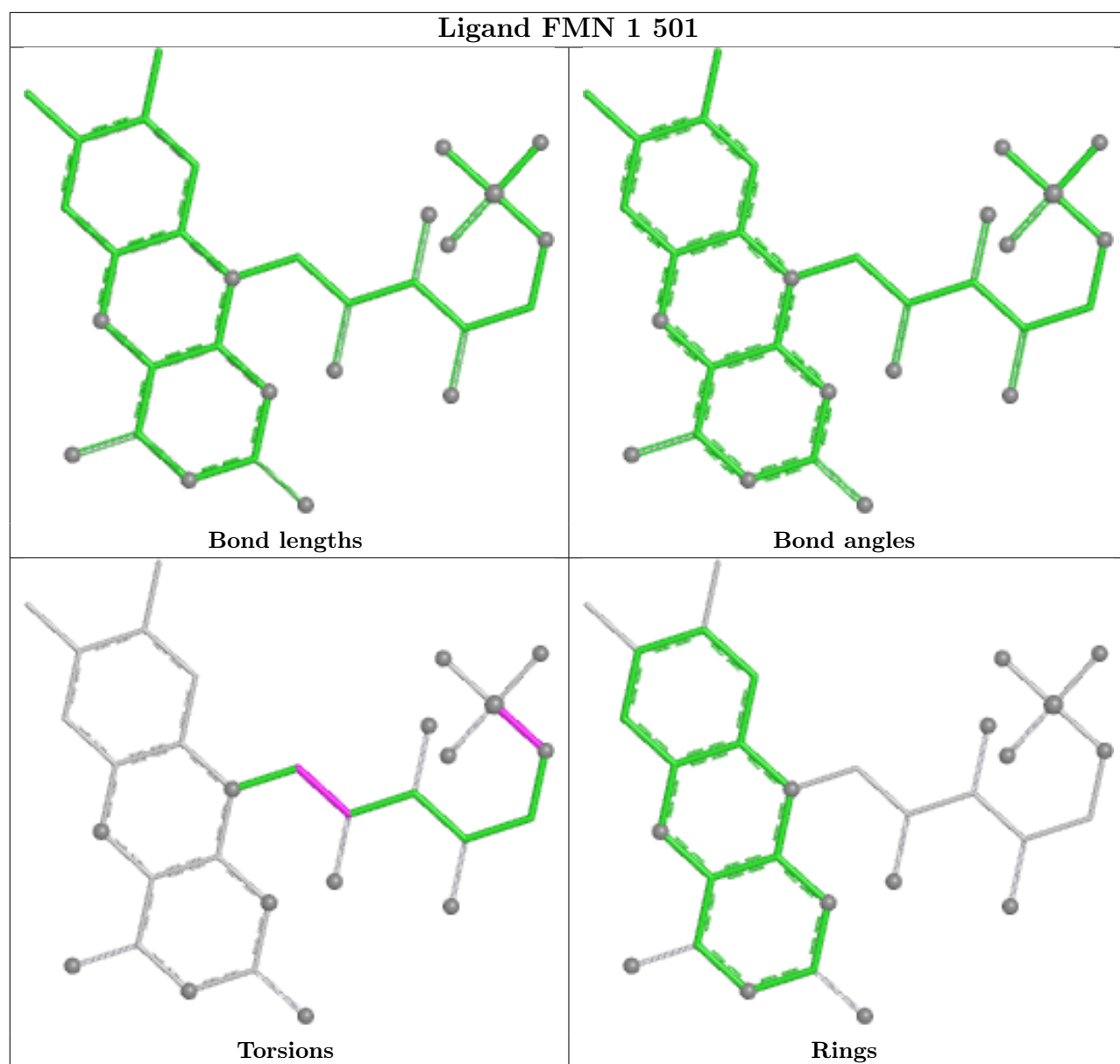












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

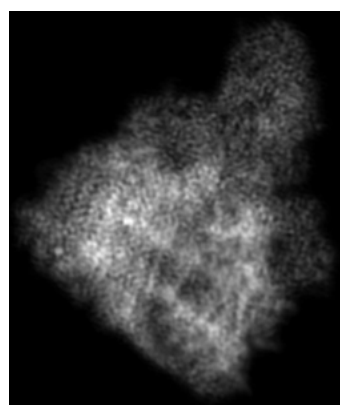
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17989. These allow visual inspection of the internal detail of the map and identification of artifacts.

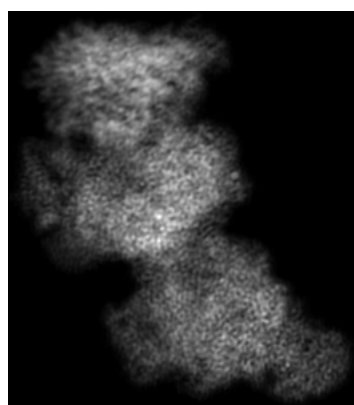
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

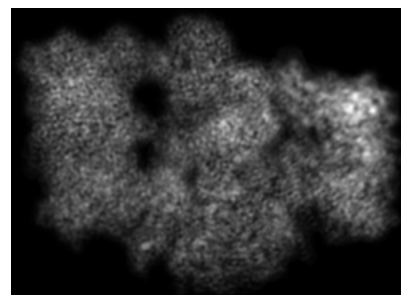
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

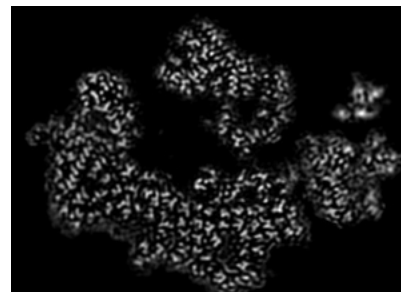
6.2.1 Primary map



X Index: 141



Y Index: 103

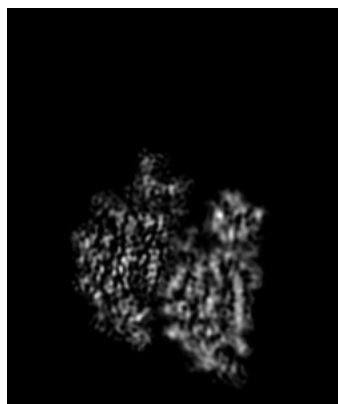


Z Index: 124

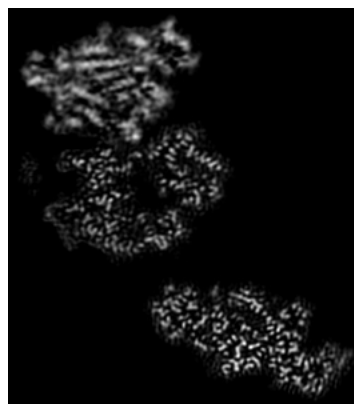
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

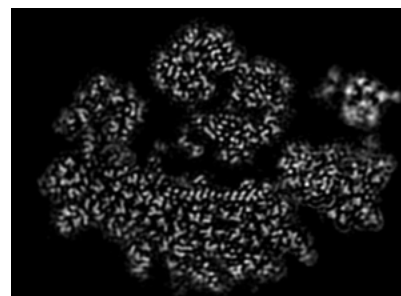
6.3.1 Primary map



X Index: 243



Y Index: 143

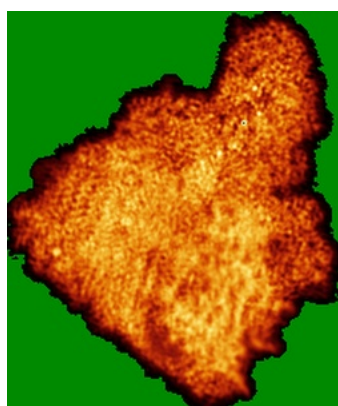


Z Index: 115

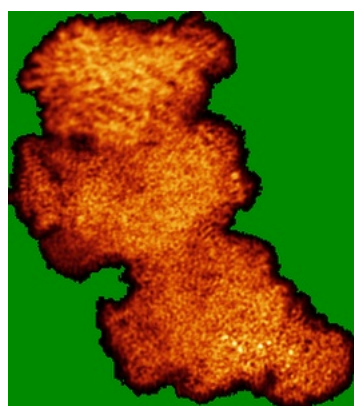
The images above show the largest variance slices of the map in three orthogonal directions.

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

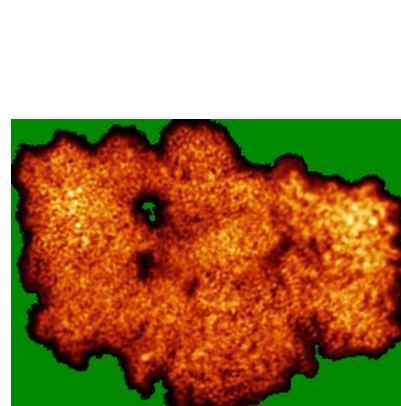
6.4.1 Primary map



X



Y

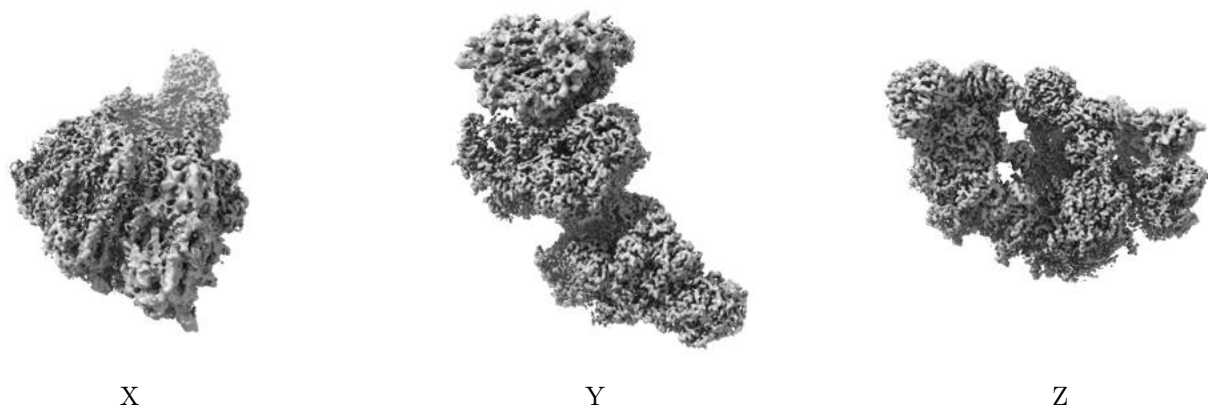


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

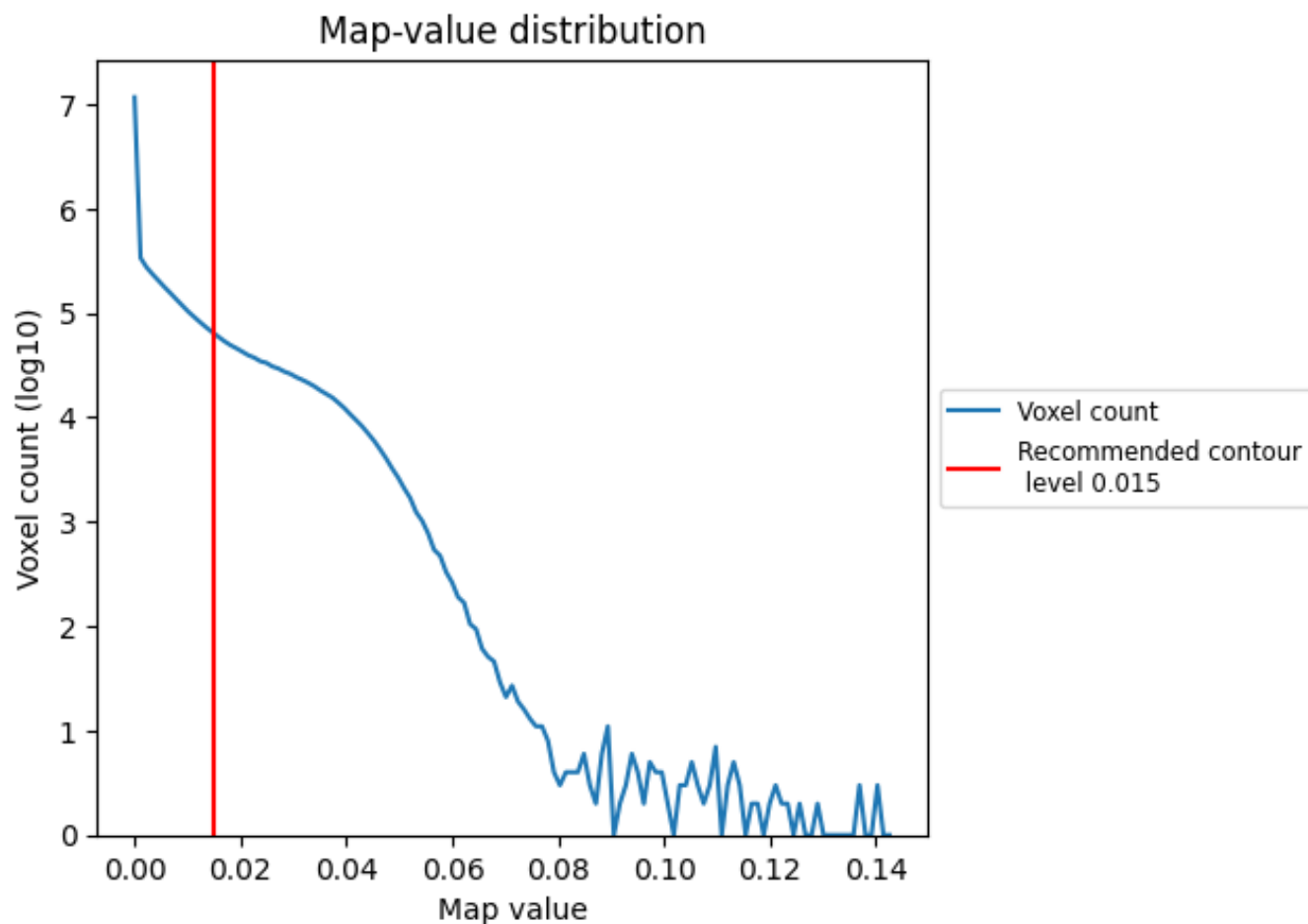
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

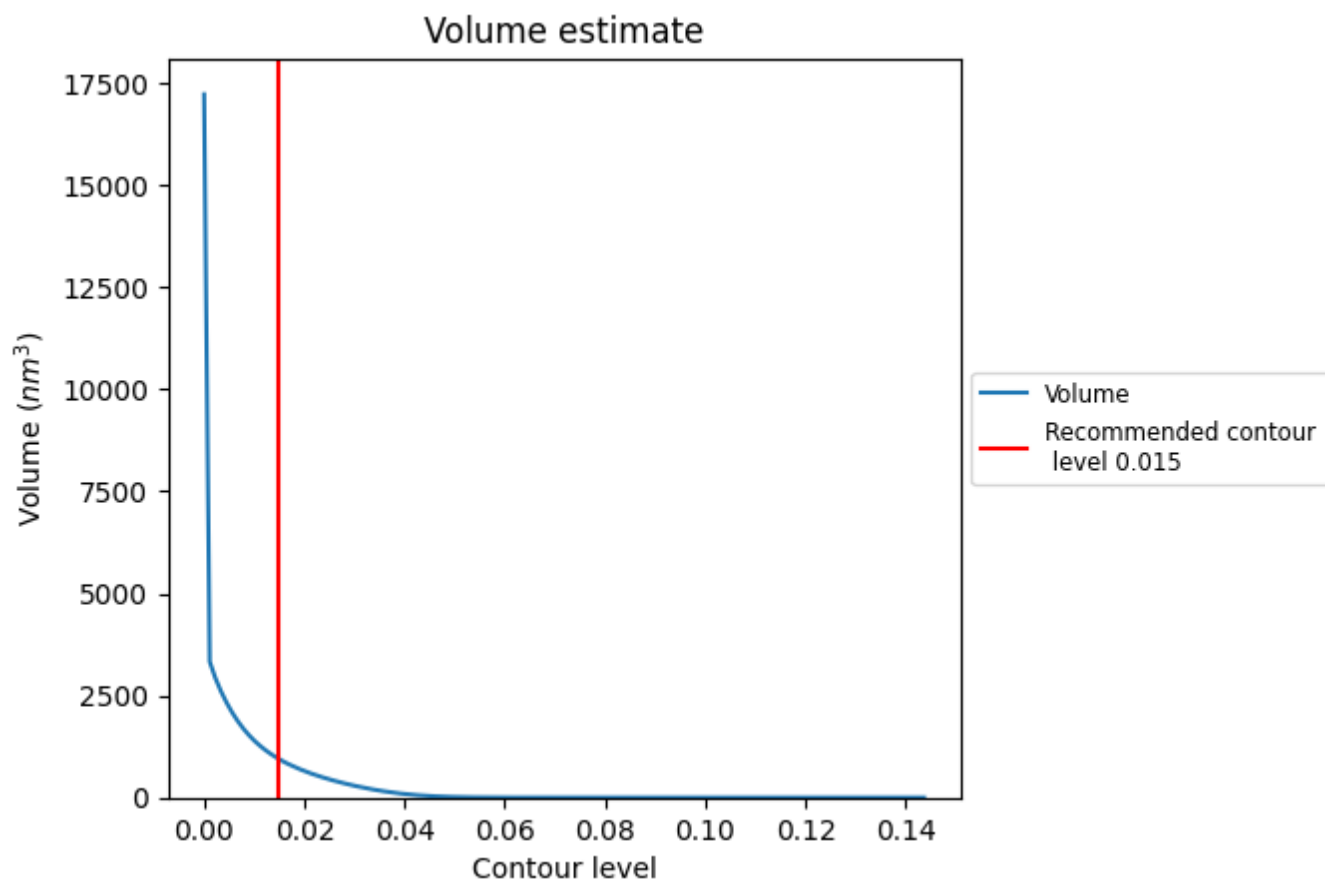
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 940 nm³; this corresponds to an approximate mass of 849 kDa.

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

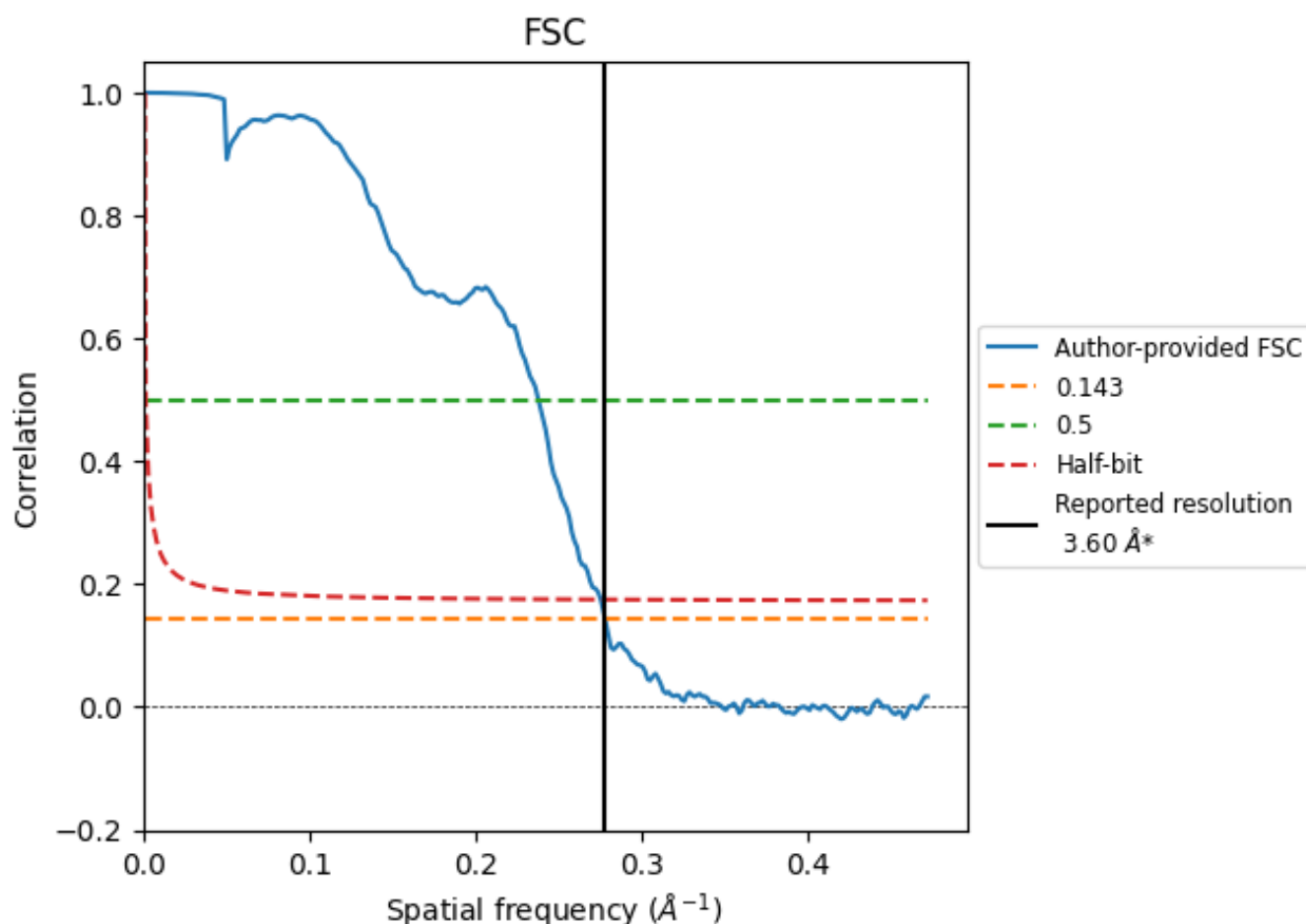
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.21	3.63
Unmasked-calculated*	-	-	-

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

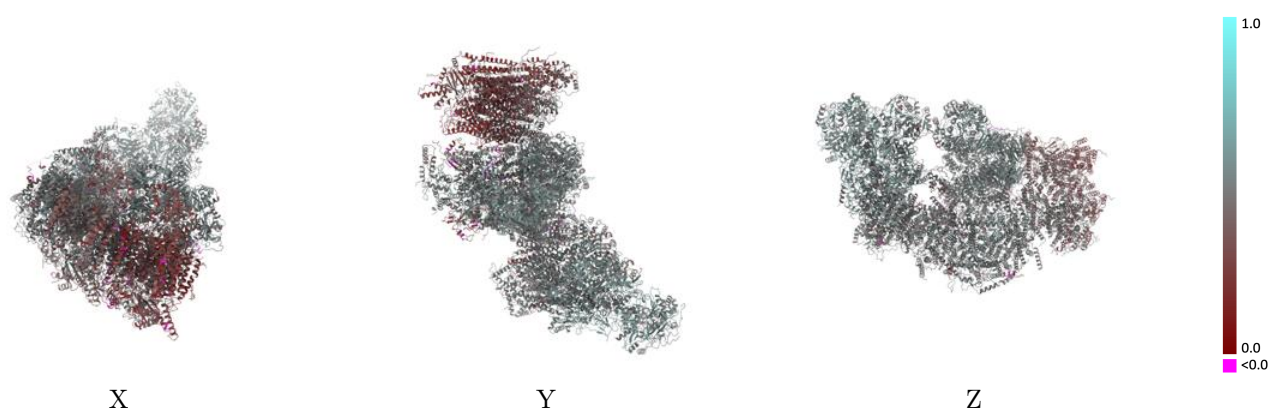
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17989 and PDB model 8PW5. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)

This section was not generated.

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

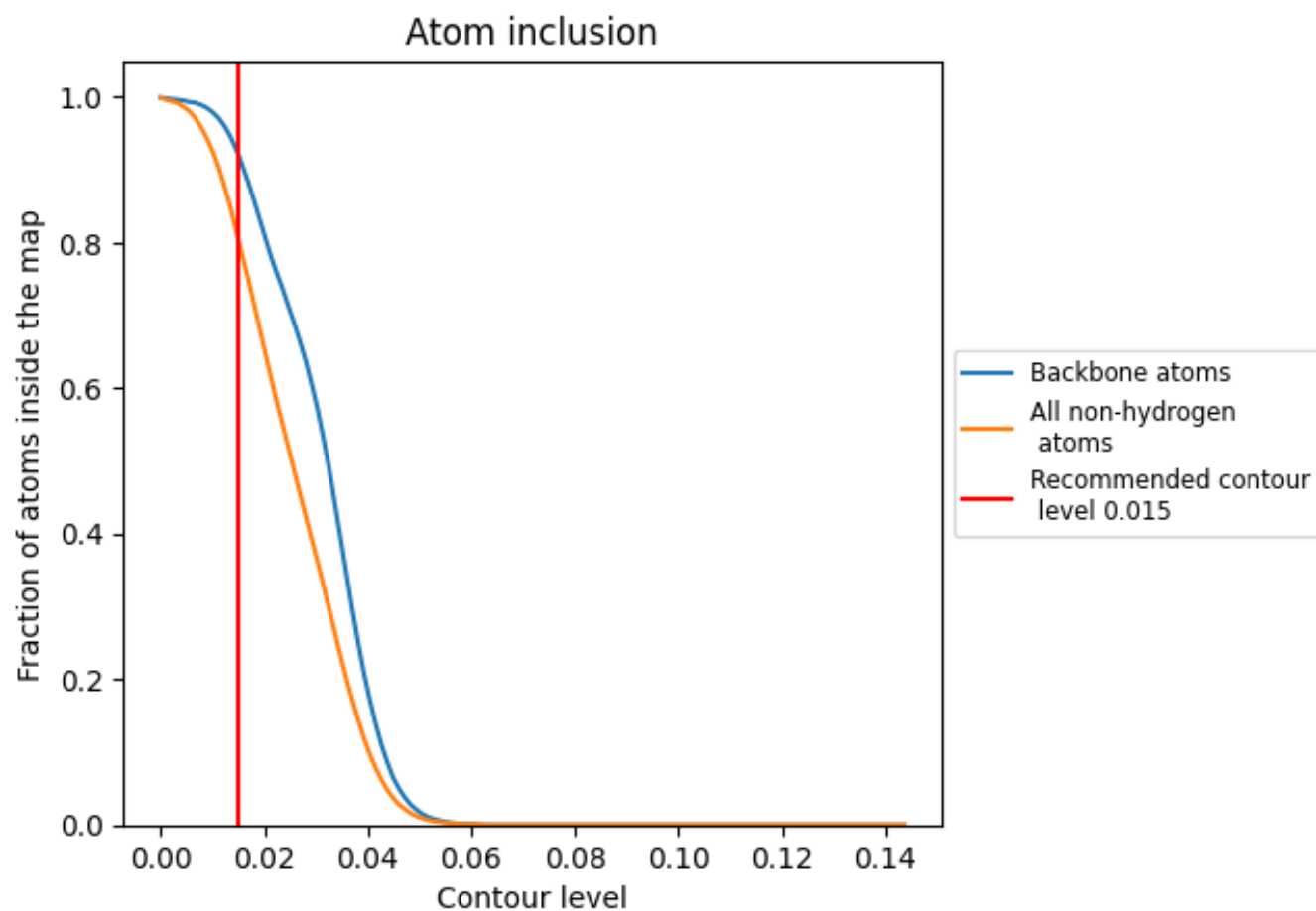


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.8060	 0.4640
1	 0.8980	 0.5360
2	 0.8890	 0.5310
3	 0.8580	 0.5280
6	 0.8540	 0.5200
7	 0.8730	 0.5440
9	 0.8630	 0.5330
A	 0.8270	 0.5110
A1	 0.7140	 0.4720
B	 0.8420	 0.5200
C	 0.7850	 0.4980
C1	 0.8800	 0.5470
D	 0.8520	 0.5090
D1	 0.8130	 0.5020
E	 0.5370	 0.3560
F	 0.8000	 0.5020
G	 0.7650	 0.4990
H	 0.7730	 0.4440
H1	 0.7390	 0.4660
I	 0.6610	 0.3060
J	 0.7720	 0.5000
J1	 0.6380	 0.4250
K	 0.6100	 0.4630
K1	 0.7170	 0.4750
L	 0.8180	 0.5060
L1	 0.7810	 0.4900
M	 0.8460	 0.5150
M1	 0.7950	 0.5010
N	 0.8000	 0.5010
N1	 0.7660	 0.4930
O	 0.8200	 0.5070
O1	 0.8260	 0.4900
P	 0.4970	 0.3440
P1	 0.7980	 0.5010
Q	 0.7900	 0.5140



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Chain	Atom inclusion	Q-score
Q1	 0.8470	 0.5420
R	 0.6750	 0.4690
S	 0.7460	 0.4470
S1	 0.8470	 0.4820
T	 0.7060	 0.4930
T1	 0.7500	 0.4280
U	 0.7500	 0.5020
U1	 0.8090	 0.4890
V	 0.6460	 0.4590
V1	 0.8620	 0.5210
W1	 0.8470	 0.5290
X1	 0.8360	 0.4840
Y1	 0.6780	 0.4530
Z1	 0.8260	 0.4950
a	 0.8350	 0.3120
a1	 0.8170	 0.4920
b	 0.9150	 0.3000
b1	 0.7670	 0.4650
c	 0.8060	 0.2880
c1	 0.7670	 0.4680
d	 0.9240	 0.3070
d1	 0.7590	 0.4940
e	 0.9290	 0.3000
e1	 0.7840	 0.4850
f	 0.8860	 0.3030
f1	 0.7310	 0.4540
g	 0.7920	 0.2650
g1	 0.7600	 0.4690
h	 0.9070	 0.2810
h1	 0.8220	 0.4900
i	 0.8940	 0.2620
i1	 0.7470	 0.4570
j1	 0.7900	 0.4620
k	 0.9290	 0.2960
k1	 0.7960	 0.4800
l	 0.7370	 0.2750
l1	 0.8240	 0.5090
m	 0.7180	 0.2200
m1	 0.7540	 0.4750
n	 0.8060	 0.4290
n1	 0.8350	 0.5020
o	 0.8340	 0.4160

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Chain	Atom inclusion	Q-score
o1	 0.7940	 0.4630
p	 0.7830	 0.4190
p1	 0.8270	 0.4910
q	 0.8680	 0.4120
q1	 0.8950	 0.5450
r	 0.8580	 0.3740
r1	 0.8280	 0.5340
s	 0.8090	 0.4010
s1	 0.8040	 0.4860
t	 0.6790	 0.3260
u	 0.8840	 0.3990
v	 0.7940	 0.3500
w	 0.7670	 0.4310
x	 0.8420	 0.3890
y	 0.8030	 0.4430
z	 0.6440	 0.2910