



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:13 AM UTC

PDB ID : 8PW6 / pdb_00008pw6
EMDB ID : EMD-17990
Title : C respirasome from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-07-19
Resolution : 3.30 Å (reported)
Based on initial models : 6g2j, 7o3c

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:

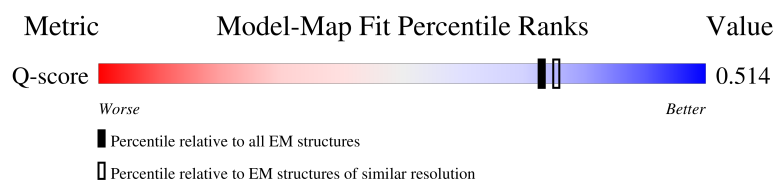
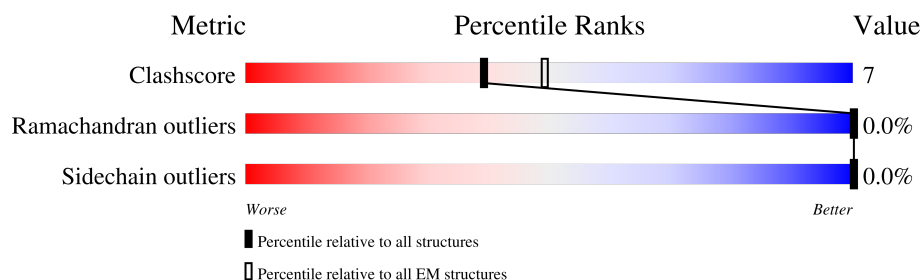
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

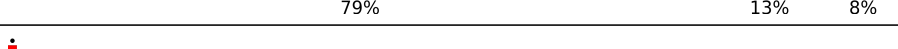
The reported resolution of this entry is 3.30 Å.

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	15087 (2.80 - 3.80)

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	A	480	
1	L	480	
2	B	453	
2	M	453	

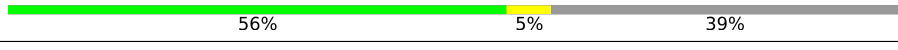
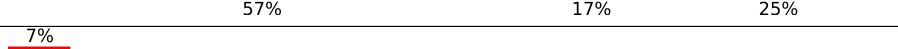
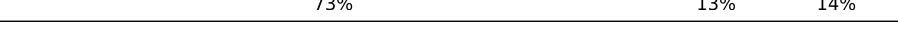
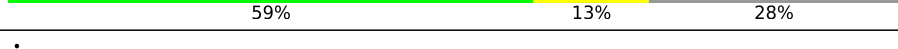
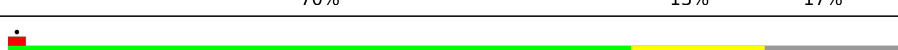
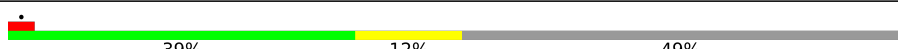
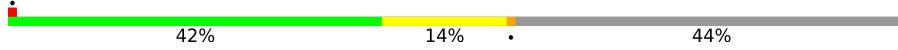
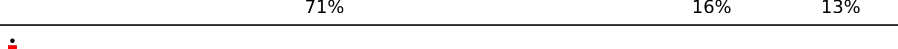
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Mol	Chain	Length	Quality of chain
3	C	381	
3	N	381	
4	D	325	
4	O	325	
5	E	274	
5	P	274	
5	T	274	
6	F	111	
6	Q	111	
7	G	82	
7	R	82	
8	H	89	
8	S	89	
9	J	64	
9	U	64	
10	K	56	
10	V	56	
11	n	514	
12	o	227	
13	p	261	
14	q	169	
15	r	146	
16	s	128	
17	t	111	
18	u	86	

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Mol	Chain	Length	Quality of chain
19	v	76	
20	x	80	
21	y	63	
22	z	69	
23	w	83	
24	6	224	
25	C1	263	
26	D1	463	
27	2	248	
28	1	464	
29	3	727	
30	9	212	
31	P1	377	
32	Q1	175	
33	7	116	
34	S1	99	
35	T1	156	
35	U1	156	
36	V1	116	
37	W1	131	
38	q1	145	
39	r1	113	
40	s1	104	
41	A1	115	
42	H1	318	

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Mol	Chain	Length	Quality of chain
43	J1	172	
44	K1	98	
45	L1	607	
46	M1	459	
47	N1	345	
48	O1	355	
49	X1	172	
50	Y1	141	
51	Z1	144	
52	a1	70	
53	b1	84	
54	c1	76	
55	d1	120	
56	e1	106	
57	f1	57	
58	g1	151	
59	h1	189	
60	i1	128	
61	j1	105	
62	k1	104	
63	l1	186	
64	m1	129	
65	n1	179	
66	o1	137	
67	p1	176	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 115652 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 b-c1 complex subunit 1, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	418	Total	C	N	O	S	0	0
			3138	1970	552	607	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			894	572	159	160	3		
6	Q	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

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

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

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	51	Total	C	N	O	S	0	0
			422	281	75	65	1		
10	V	52	Total	C	N	O	S	0	0
			430	287	76	66	1		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	260	Total	C	N	O	S	0	0
			2118	1418	339	351	10		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	93	Total	C	N	O	S	0	0
			717	447	125	137	8		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

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

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 35 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

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

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

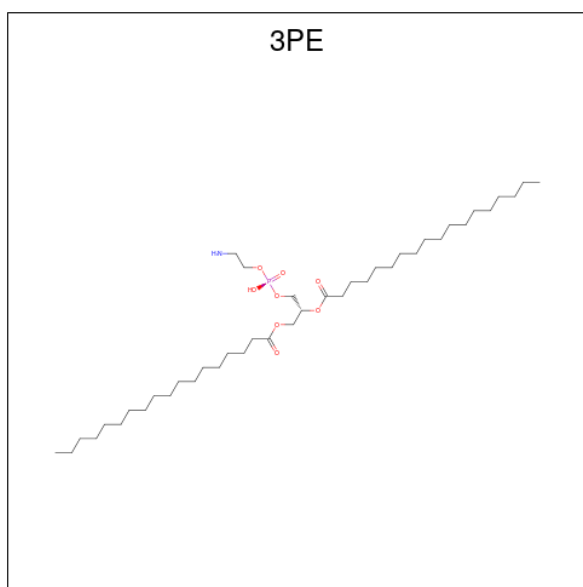
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 68 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



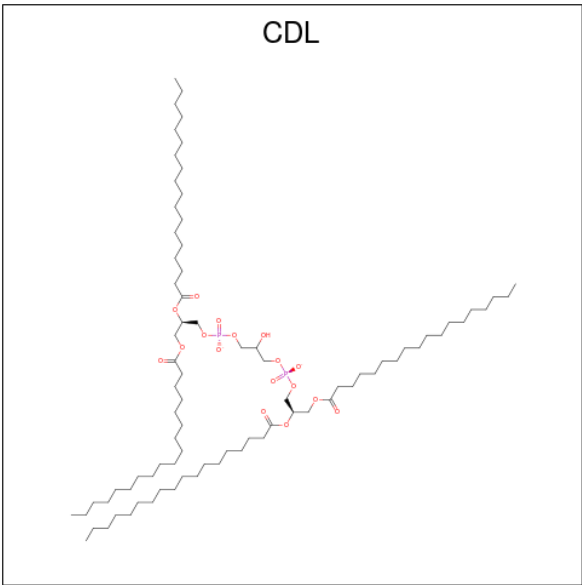
Mol	Chain	Residues	Atoms					AltConf
68	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
68	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
68	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
68	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
68	N	1	Total	C	N	O	P	0
			34	24	1	8	1	
68	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
68	P	1	Total	C	N	O	P	0
			33	23	1	8	1	
68	R	1	Total	C	N	O	P	0
			30	20	1	8	1	
68	n	1	Total	C	N	O	P	0
			34	24	1	8	1	
68	n	1	Total	C	N	O	P	0
			28	18	1	8	1	
68	o	1	Total	C	N	O	P	0
			29	19	1	8	1	
68	p	1	Total	C	N	O	P	0
			45	35	1	8	1	
68	t	1	Total	C	N	O	P	0
			25	15	1	8	1	

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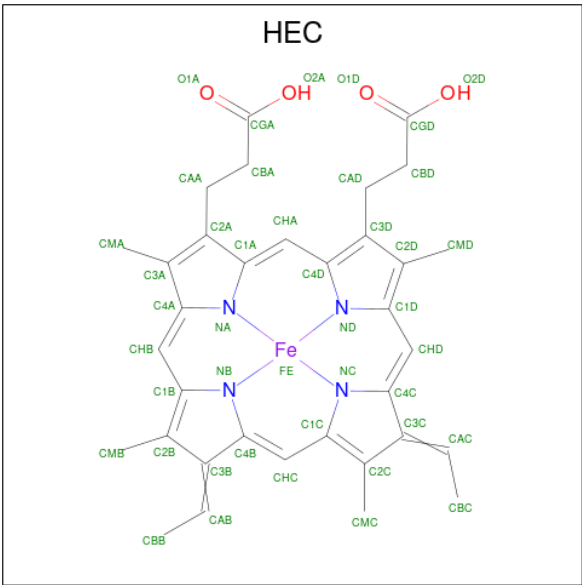
Mol	Chain	Residues	Atoms					AltConf
68	v	1	Total	C	N	O	P	0
			28	18	1	8	1	
68	x	1	Total	C	N	O	P	0
			27	17	1	8	1	
68	z	1	Total	C	N	O	P	0
			26	16	1	8	1	
68	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
68	D1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	A1	1	Total	C	N	O	P	0
			43	33	1	8	1	
68	H1	1	Total	C	N	O	P	0
			46	36	1	8	1	
68	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	
68	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	M1	1	Total	C	N	O	P	0
			36	26	1	8	1	
68	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
68	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
68	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
68	Z1	1	Total	C	N	O	P	0
			51	41	1	8	1	
68	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
68	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
68	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 69 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



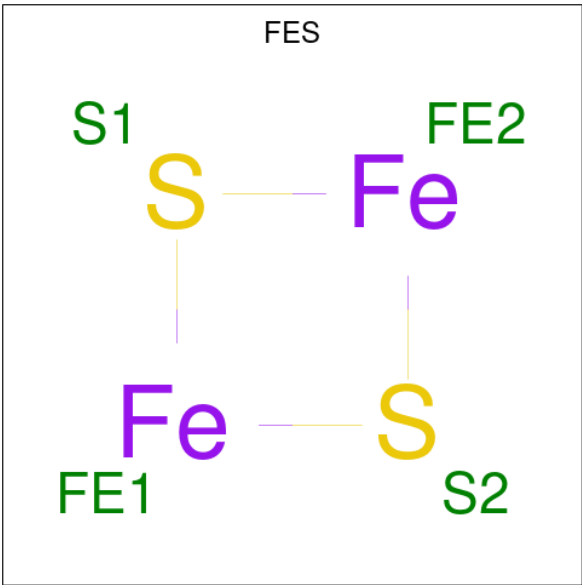
Mol	Chain	Residues	Atoms				AltConf
69	A	1	Total	C	O	P	0
			46	27	17	2	
69	C	1	Total	C	O	P	0
			42	23	17	2	
69	D	1	Total	C	O	P	0
			56	37	17	2	
69	L	1	Total	C	O	P	0
			46	27	17	2	
69	R	1	Total	C	O	P	0
			57	38	17	2	
69	R	1	Total	C	O	P	0
			41	22	17	2	
69	R	1	Total	C	O	P	0
			57	38	17	2	
69	H1	1	Total	C	O	P	0
			51	33	16	2	
69	L1	1	Total	C	O	P	0
			78	59	17	2	
69	L1	1	Total	C	O	P	0
			46	27	17	2	
69	N1	1	Total	C	O	P	0
			90	71	17	2	
69	Y1	1	Total	C	O	P	0
			94	75	17	2	
69	Y1	1	Total	C	O	P	0
			72	53	17	2	
69	a1	1	Total	C	O	P	0
			57	38	17	2	

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

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



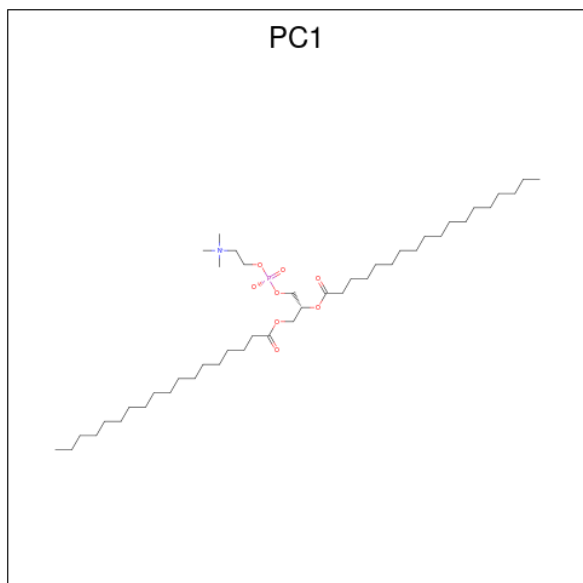
Mol	Chain	Residues	Atoms			AltConf
72	E	1	Total	Fe	S	0
			4	2	2	
72	P	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
72	2	1	Total	Fe	S	0
			4	2	2	
72	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 73 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
73	E	1	Total	C	N	O	P	0
			35	25	1	8	1	
73	K	1	Total	C	N	O	P	0
			28	18	1	8	1	
73	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
73	V	1	Total	C	N	O	P	0
			28	18	1	8	1	
73	p	1	Total	C	N	O	P	0
			35	25	1	8	1	
73	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
73	z	1	Total	C	N	O	P	0
			28	18	1	8	1	
73	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
73	9	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
73	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
73	A1	1	Total	C	N	O	P	0
			31	21	1	8	1	
73	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	

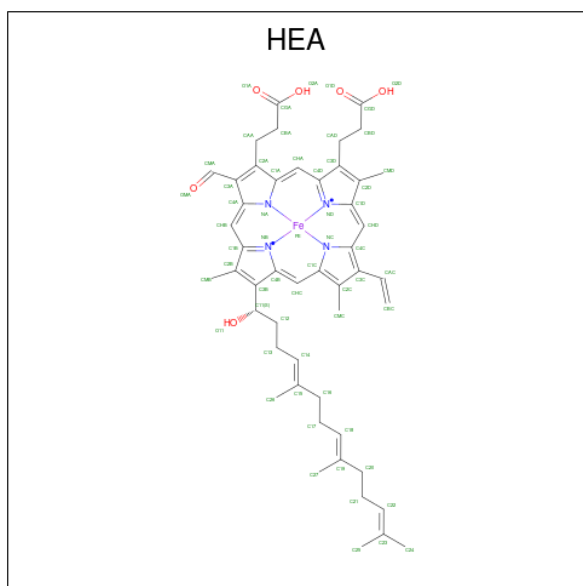
- Molecule 74 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
74	n	1	Total	Cu	0
			1	1	

- Molecule 75 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
75	n	1	Total	Na	0
			1	1	

- Molecule 76 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

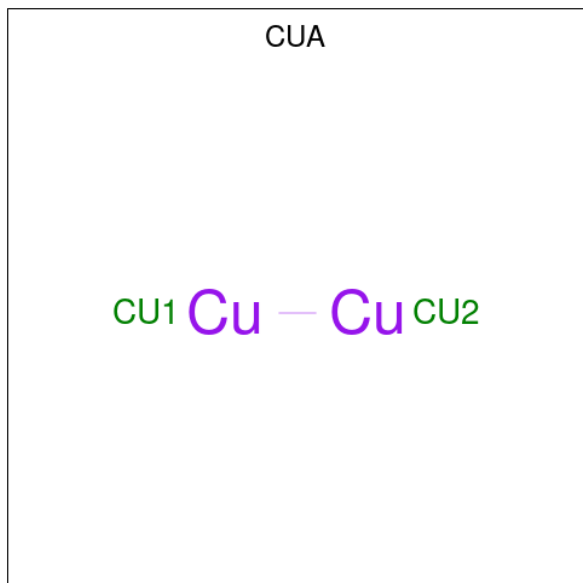


Mol	Chain	Residues	Atoms					AltConf
76	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
77	o	1	Total	Mg	0
			1	1	
77	O1	1	Total	Mg	0
			1	1	

- Molecule 78 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

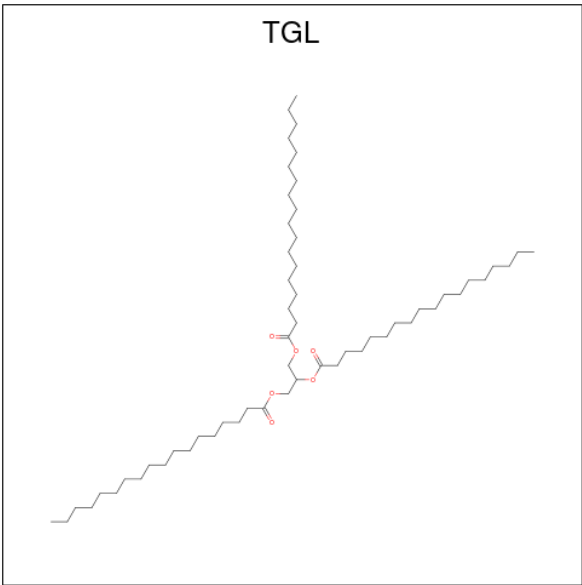


Mol	Chain	Residues	Atoms		AltConf
78	o	1	Total	Cu	0
			2	2	

- Molecule 79 is ZINC ION (CCD ID: ZN) (formula: Zn).

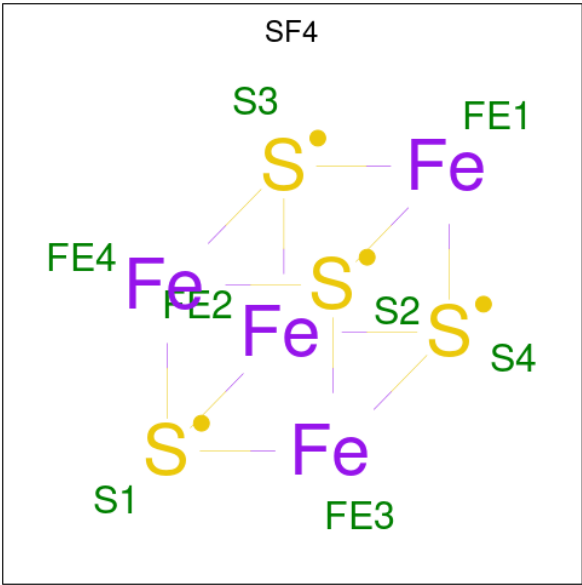
Mol	Chain	Residues	Atoms		AltConf
79	s	1	Total	Zn	0
			1	1	
79	7	1	Total	Zn	0
			1	1	

- Molecule 80 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



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

- Molecule 81 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



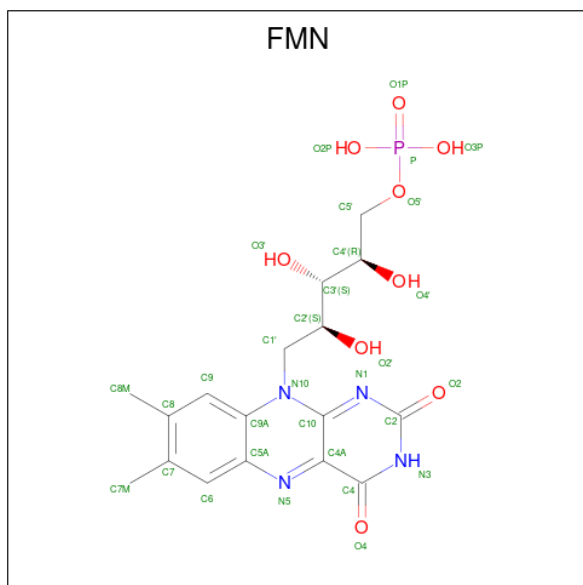
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
81	6	1	8	4	4	0
81	1	1	8	4	4	0
81	3	1	8	4	4	0

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Mol	Chain	Residues	Atoms			AltConf
81	3	1	Total	Fe	S	0
			8	4	4	
81	9	1	Total	Fe	S	0
			8	4	4	
81	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 82 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

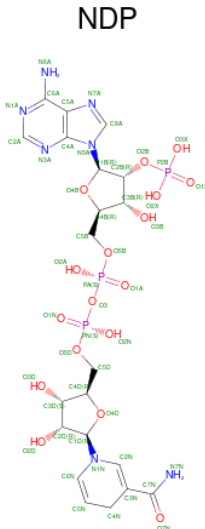


Mol	Chain	Residues	Atoms					AltConf
82	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

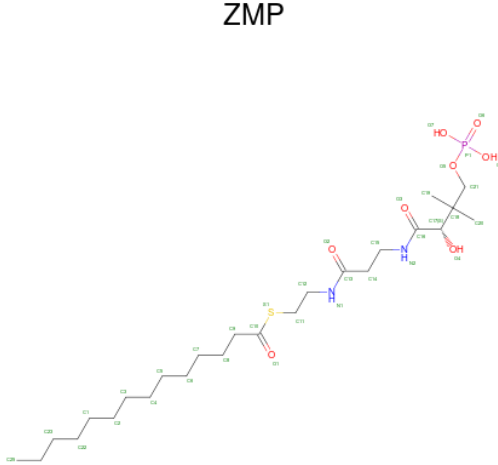
Mol	Chain	Residues	Atoms		AltConf
83	3	1	Total	K	0
			1	1	

- Molecule 84 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



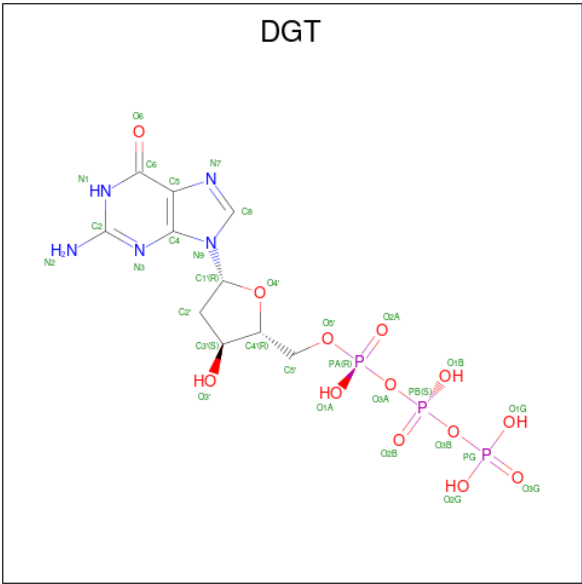
Mol	Chain	Residues	Atoms					AltConf
84	P1	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 85 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
85	W1	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
85	n1	1	Total 32	C 21	N 2	O 7	P 1	S 1	0

- Molecule 86 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).

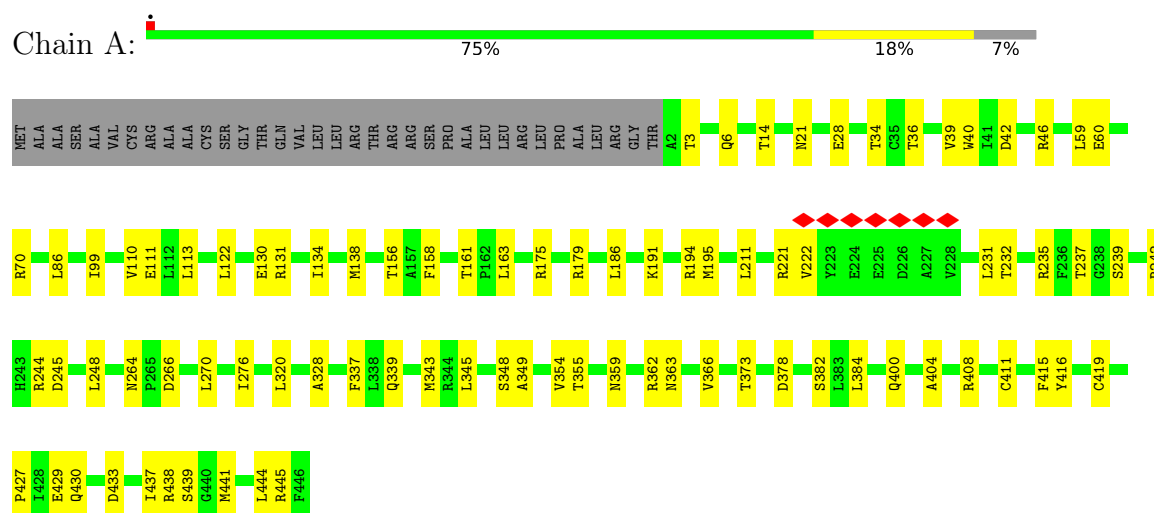


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	O1	1	31	10	5	13	3	0

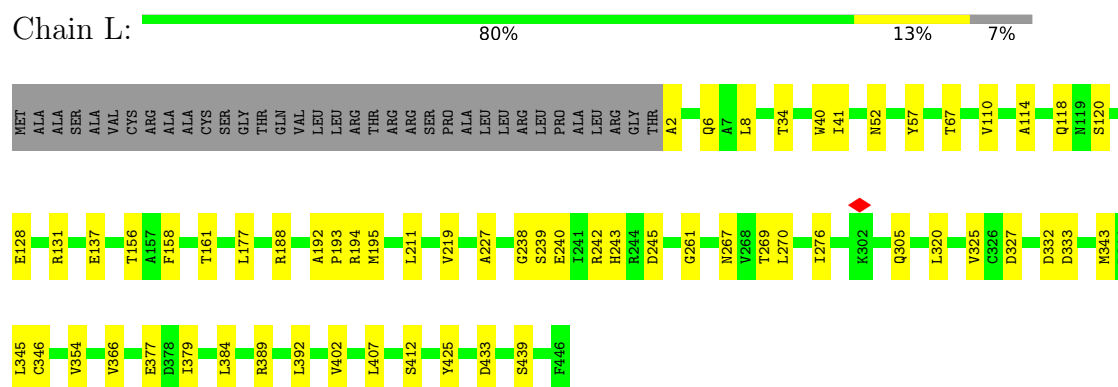
3 Residue-property plots [i](#)

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

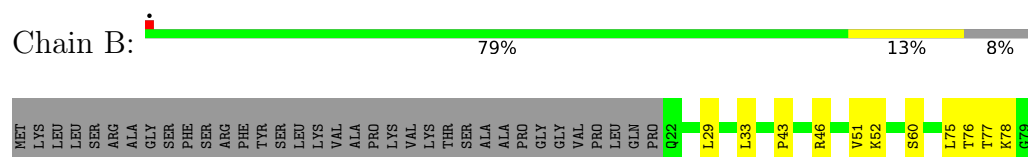
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

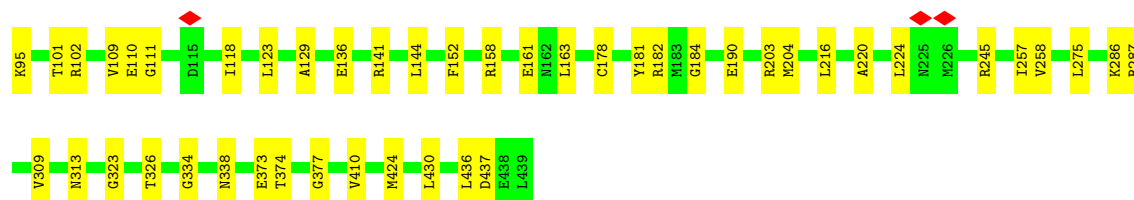


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



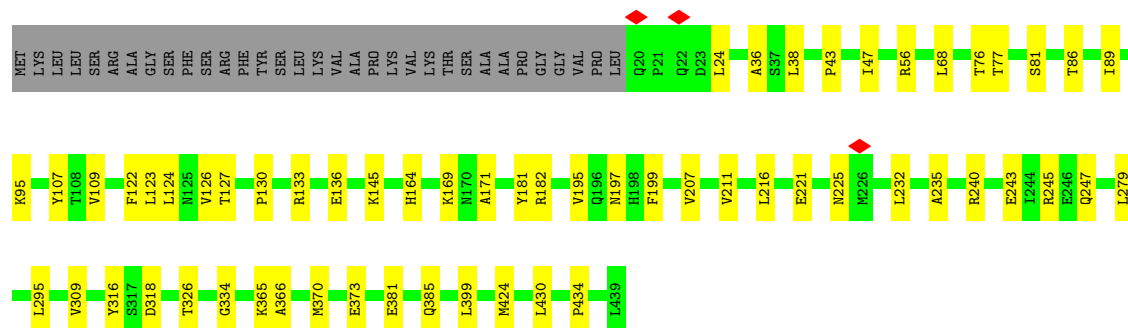
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





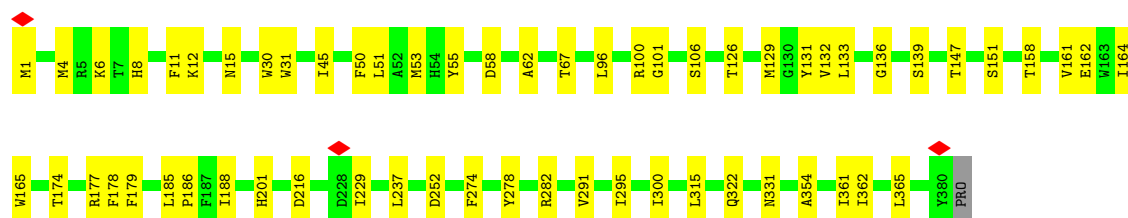
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 79% 13% 7%



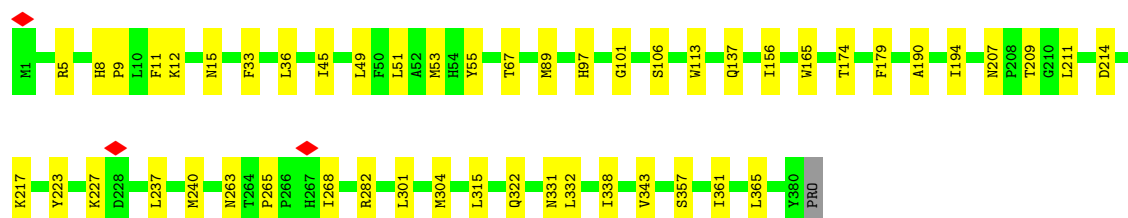
- Molecule 3: Cytochrome b

Chain C: 84% 16%



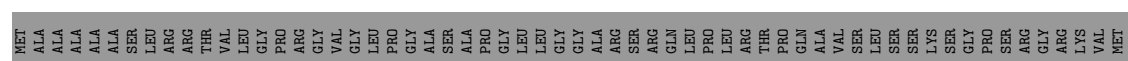
- Molecule 3: Cytochrome b

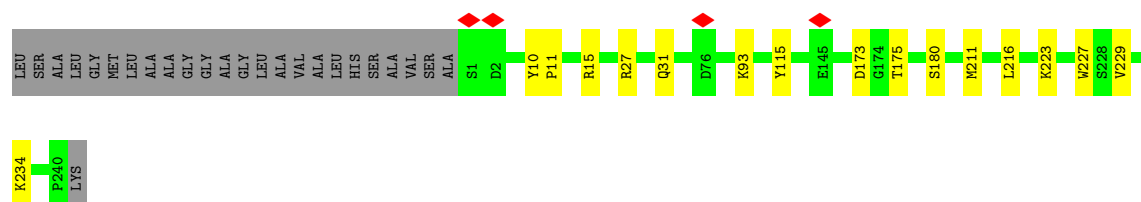
Chain N: 87% 13%



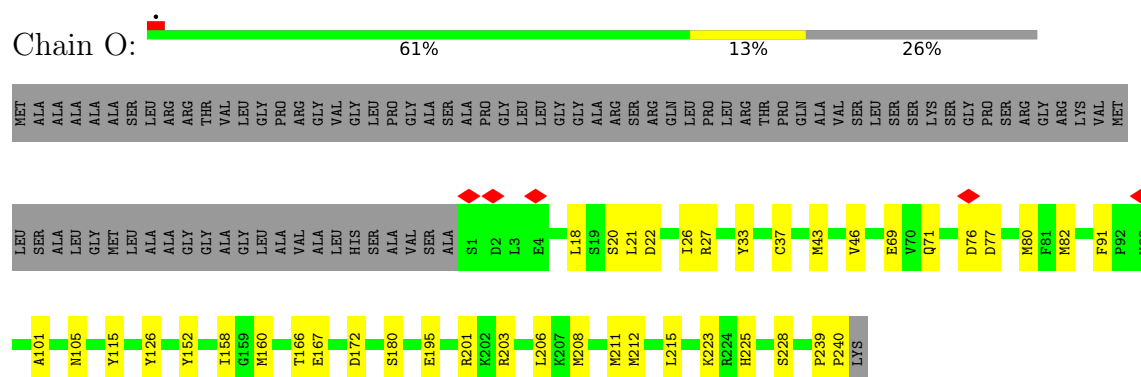
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 69% 5% 26%

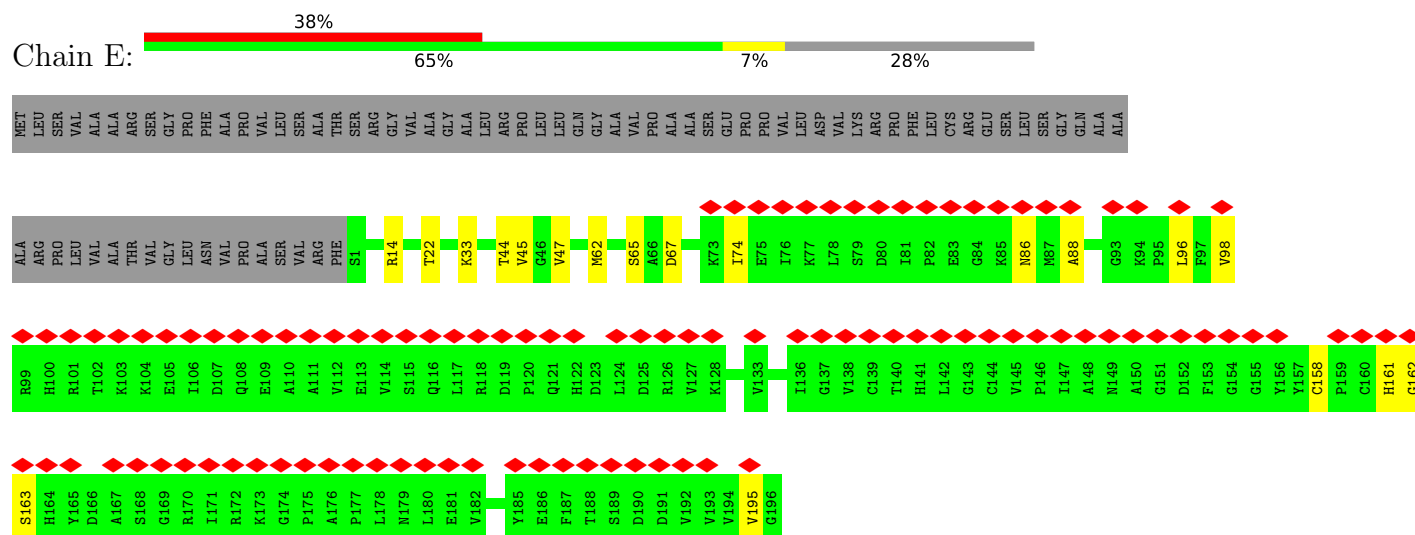




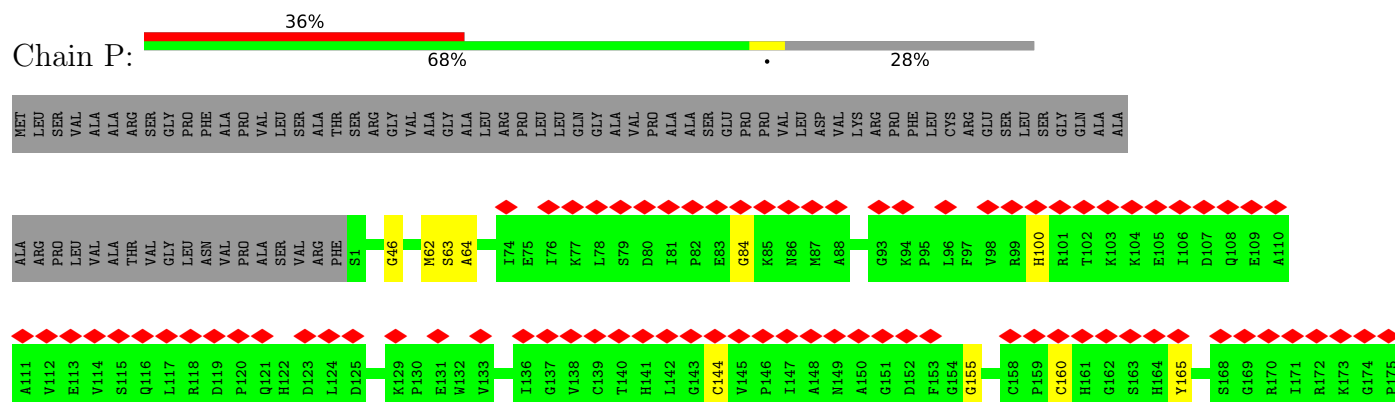
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

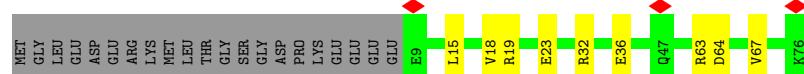


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

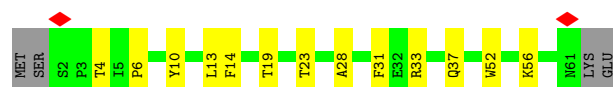




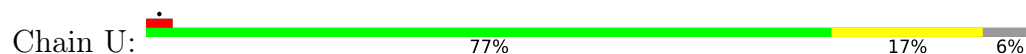
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



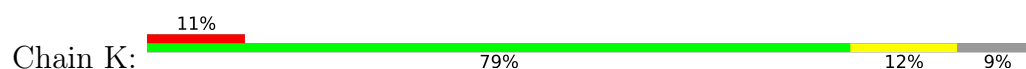
- Molecule 9: Cytochrome b-c1 complex subunit 9



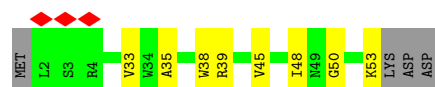
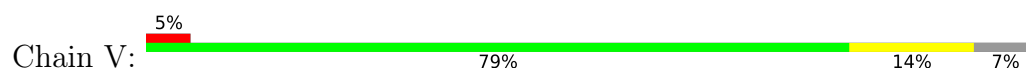
- Molecule 9: Cytochrome b-c1 complex subunit 9



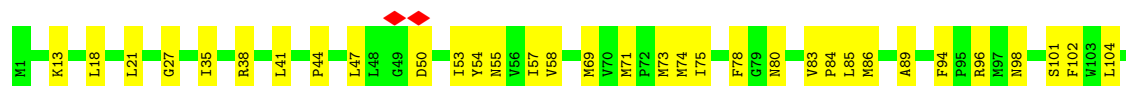
- Molecule 10: Cytochrome b-c1 complex subunit 10

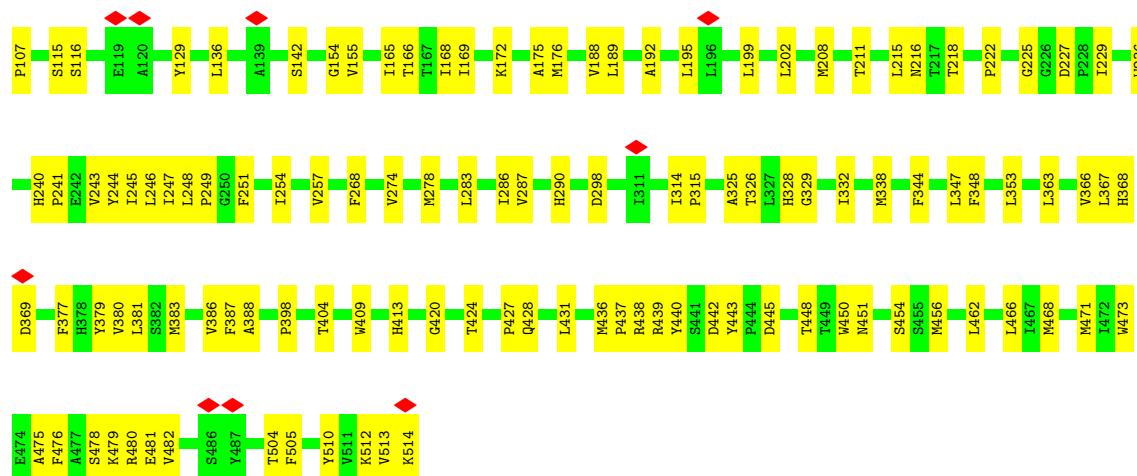


- Molecule 10: Cytochrome b-c1 complex subunit 10

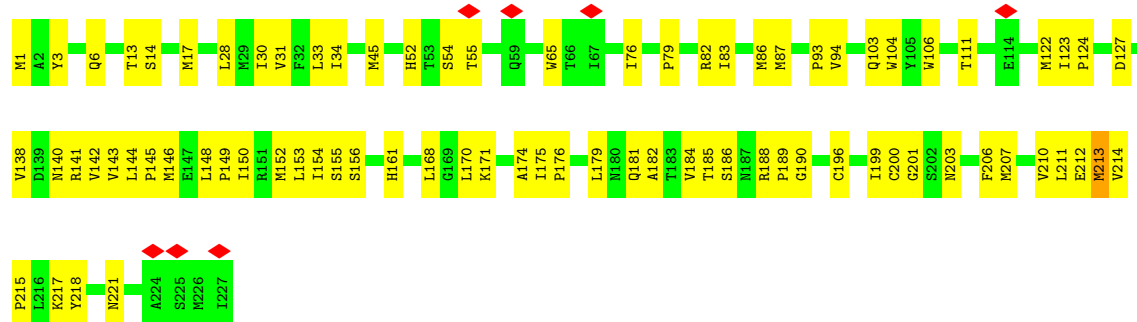


- Molecule 11: Cytochrome c oxidase subunit 1

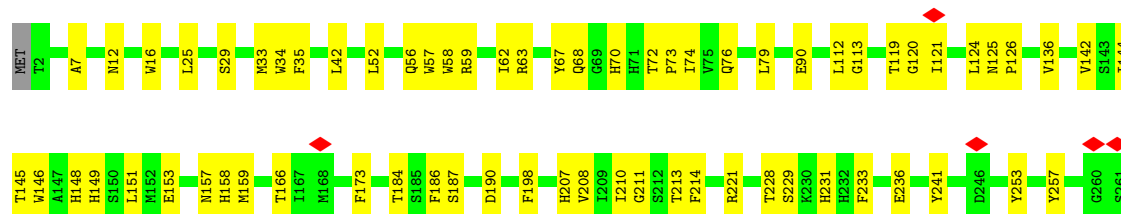




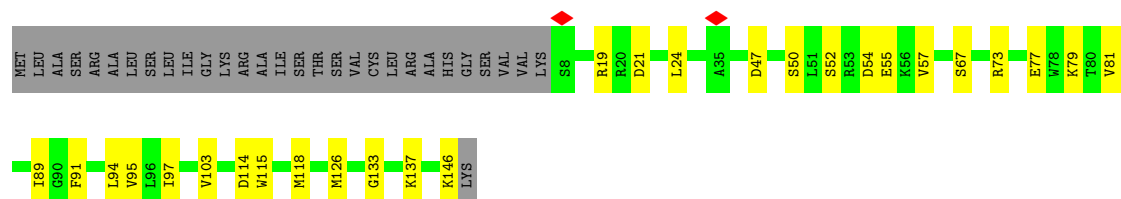
• Molecule 12: Cytochrome c oxidase subunit 2



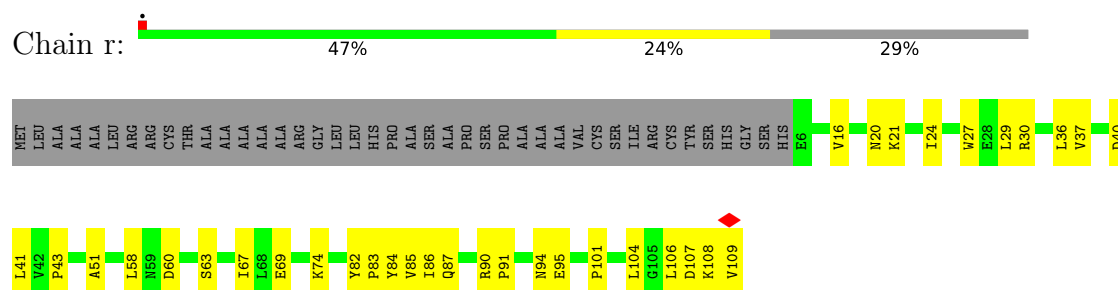
• Molecule 13: Cytochrome c oxidase subunit 3



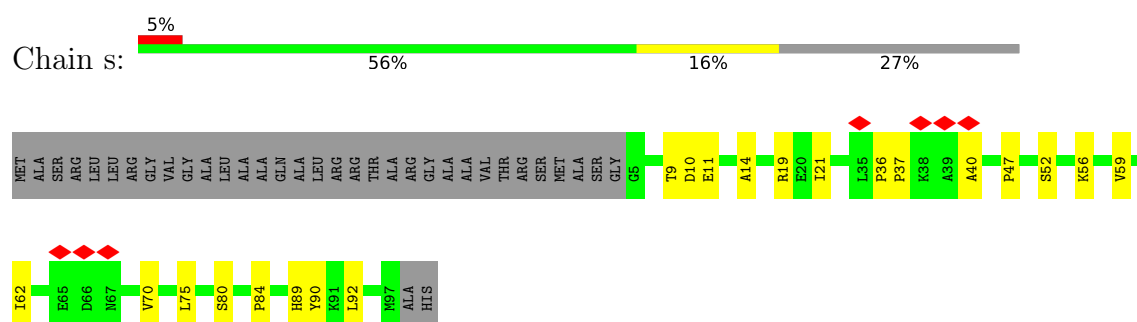
• Molecule 14: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



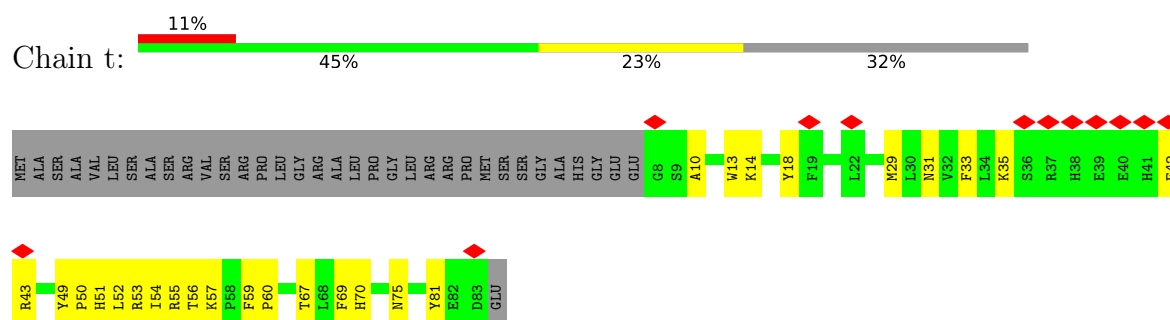
- Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial



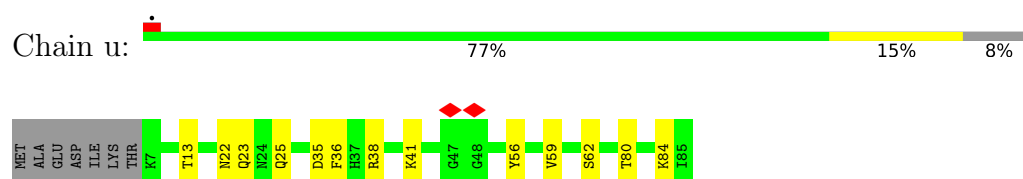
- Molecule 16: Cytochrome c oxidase subunit 5B, mitochondrial



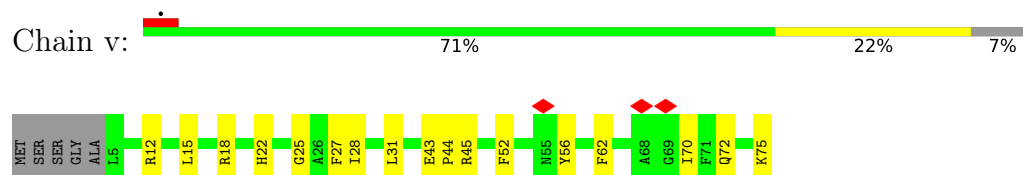
- Molecule 17: Cytochrome c oxidase subunit 6A1, mitochondrial



- Molecule 18: Cytochrome c oxidase subunit 6B1

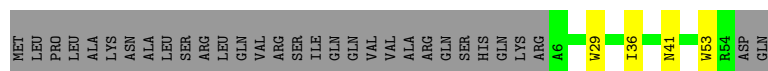


- Molecule 19: Cytochrome c oxidase subunit 6C



- Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial

Chain x: 



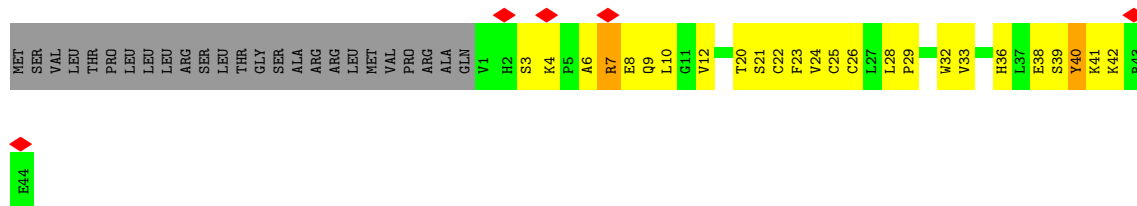
- Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial

Chain y: 



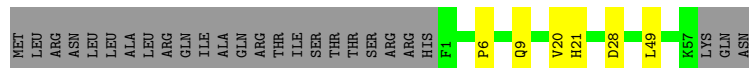
- Molecule 22: Cytochrome c oxidase subunit 8A, mitochondrial

Chain z: 



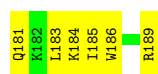
- Molecule 23: Cytochrome c oxidase subunit 7A2, mitochondrial

Chain w: 



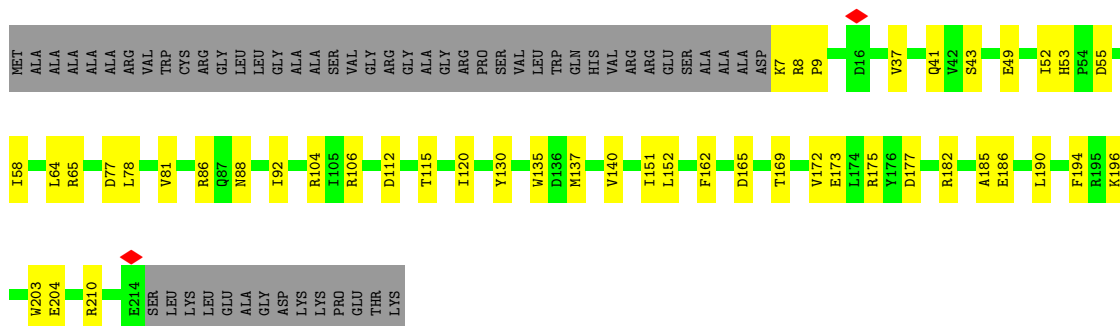
- Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6: 

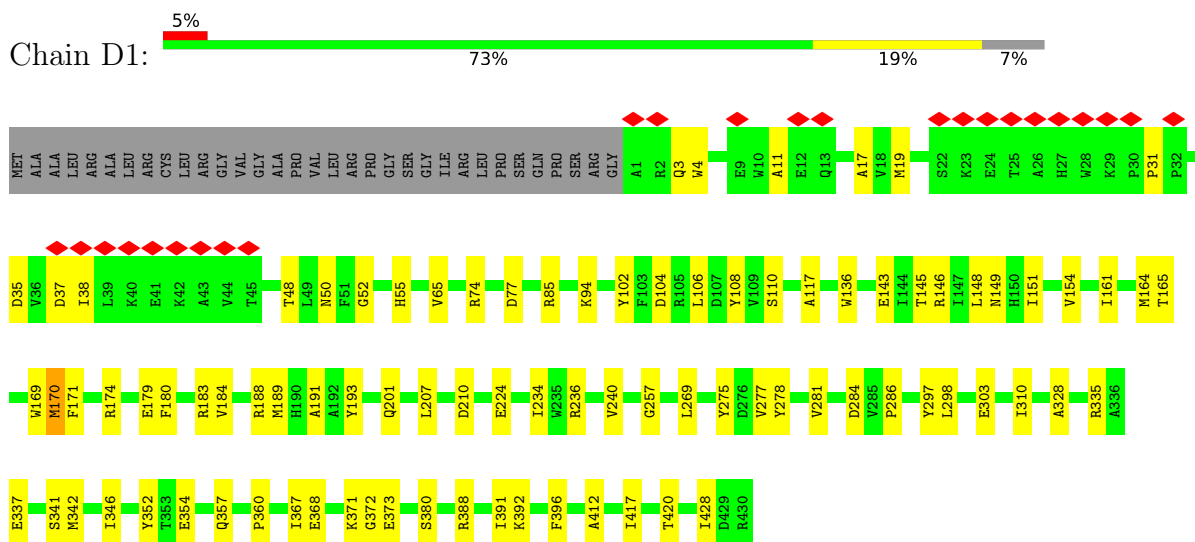


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C1: 

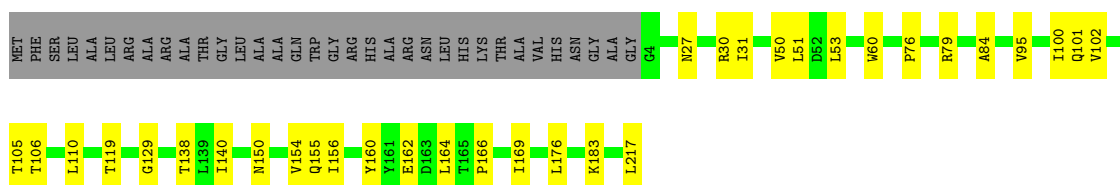


- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



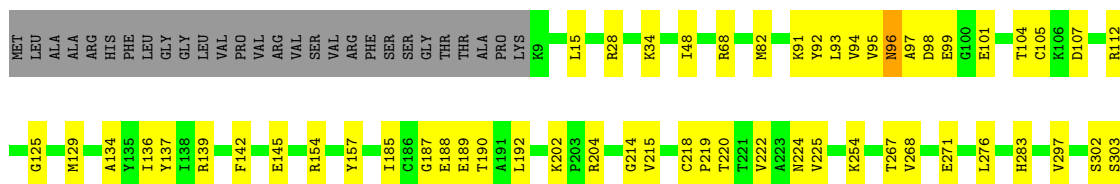
- Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

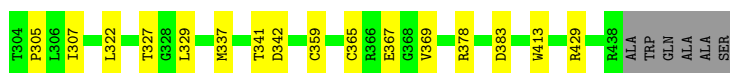
Chain 2: 73% 13% 14%



- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

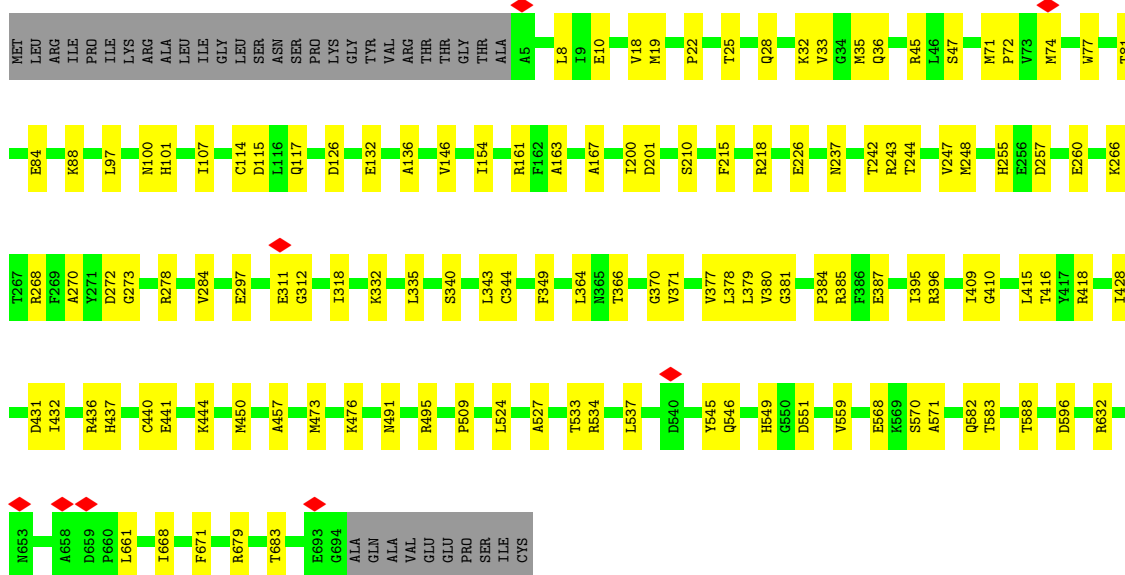
Chain 1: 77% 15% 7%





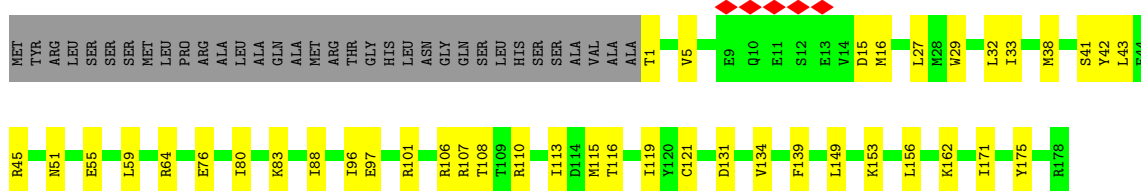
- Molecule 29: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3: 78% 17% 5%



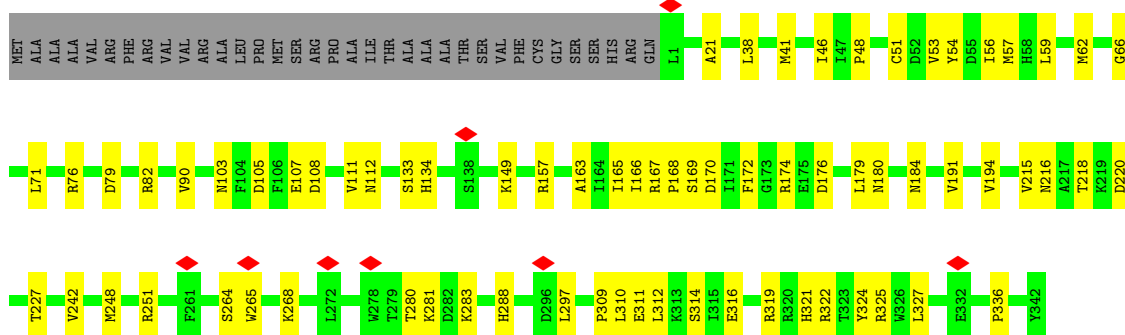
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9: 64% 20% 16%

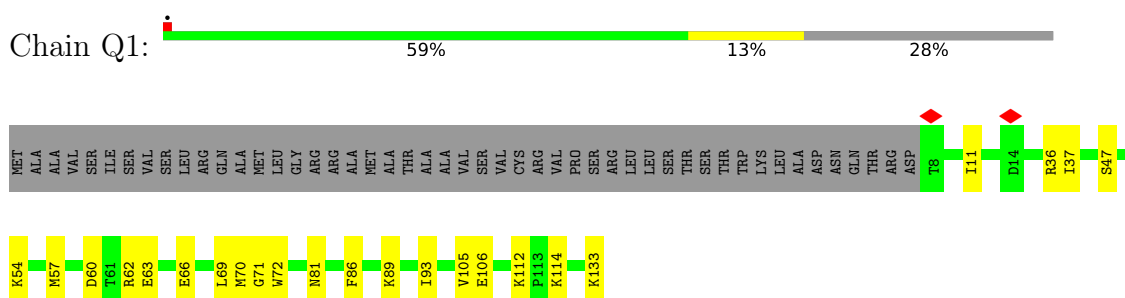


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

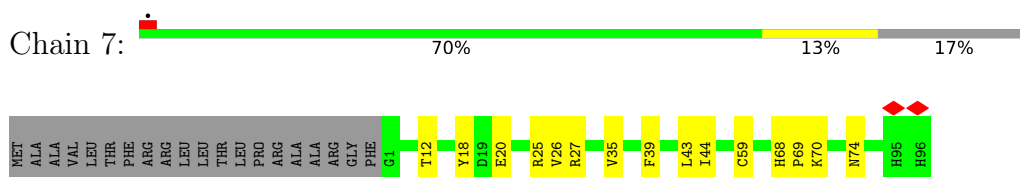
Chain P1: 72% 19% 9%



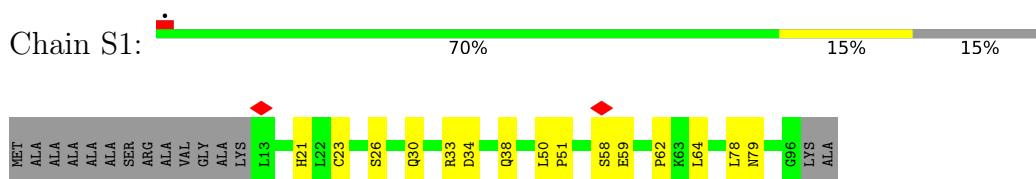
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



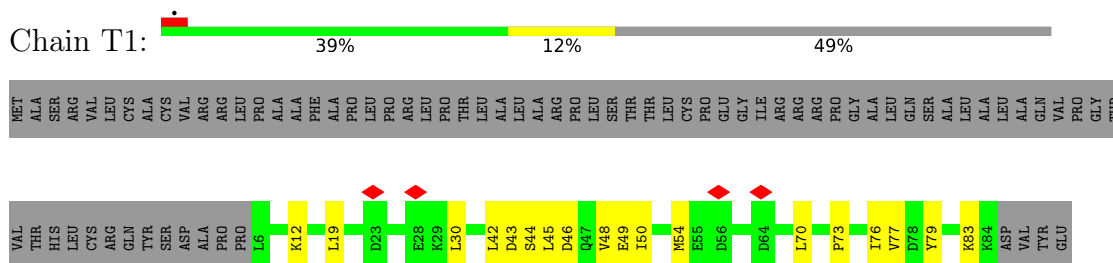
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



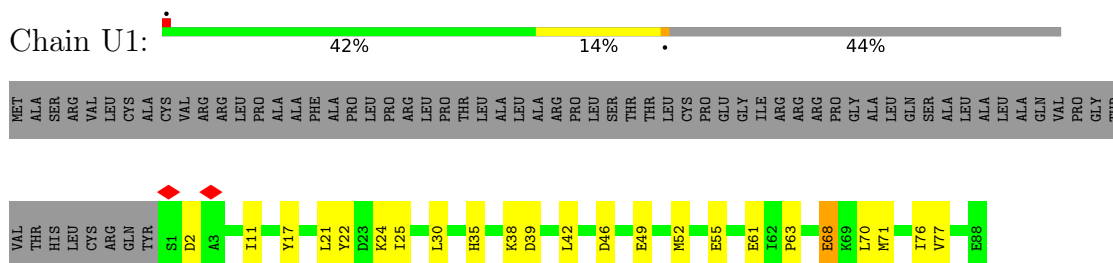
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 35: Acyl carrier protein, mitochondrial

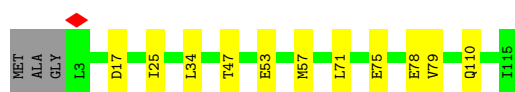


- Molecule 35: Acyl carrier protein, mitochondrial



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5





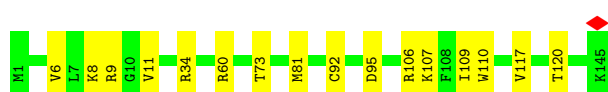
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1: 71% 16% 13%



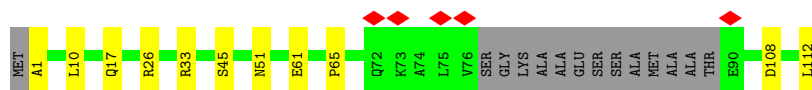
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q1: 89% 11%



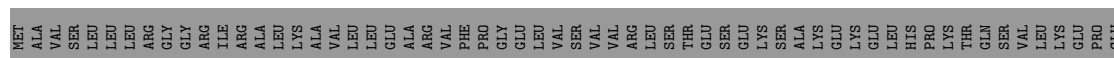
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1: 78% 10% 12%



- Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s1: 32% 9% 60%



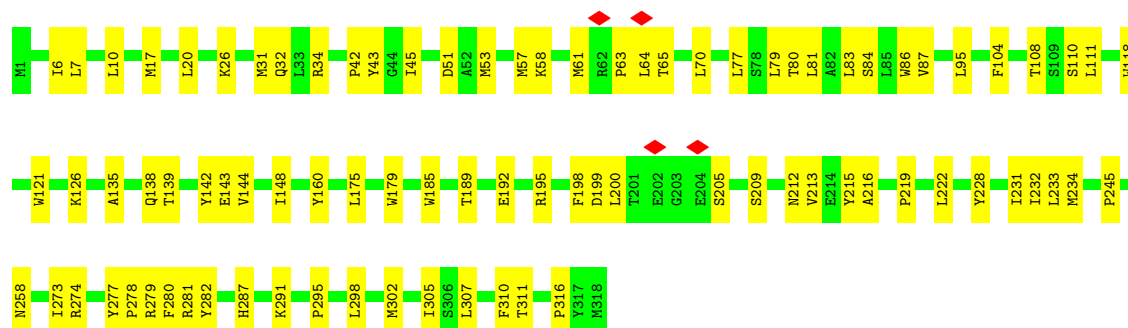
- Molecule 41: NADH-ubiquinone oxidoreductase chain 3

Chain A1: 79% 21%

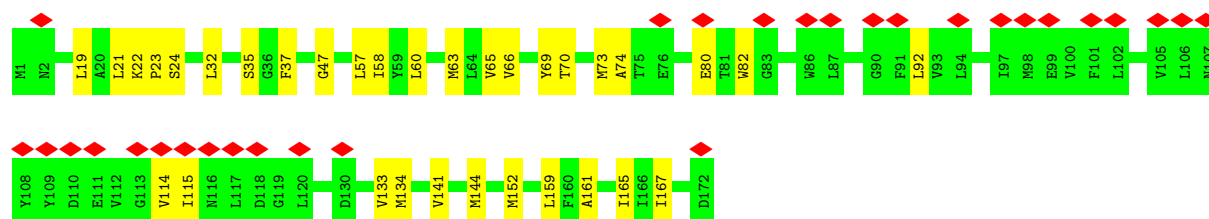
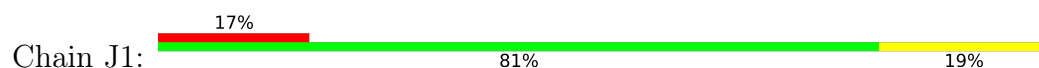


- Molecule 42: NADH-ubiquinone oxidoreductase chain 1

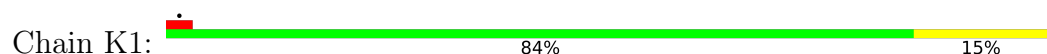
Chain H1: 73% 27%



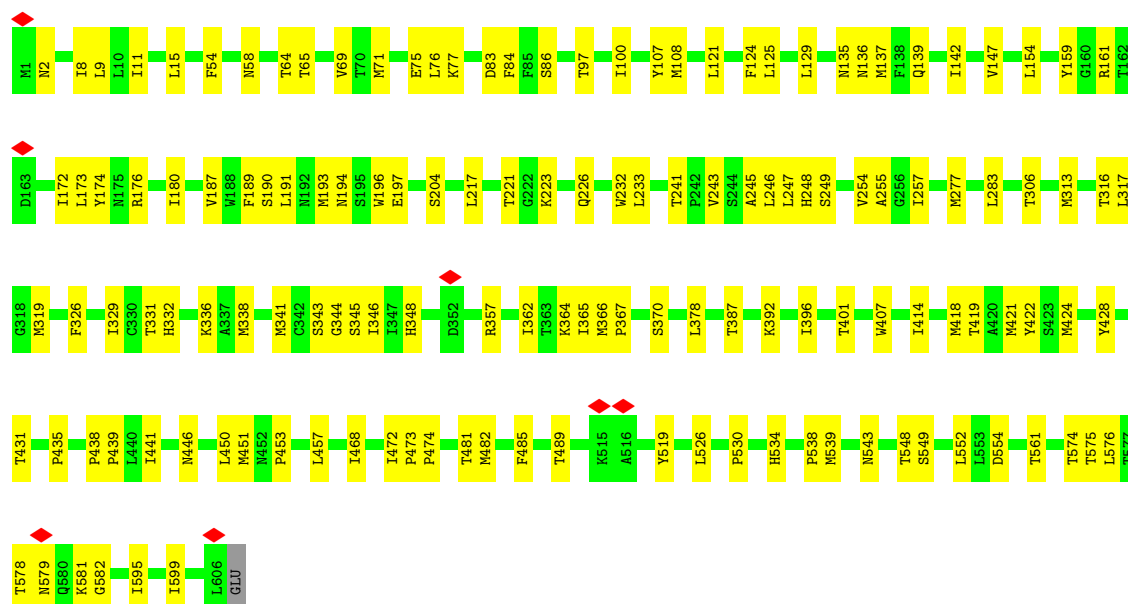
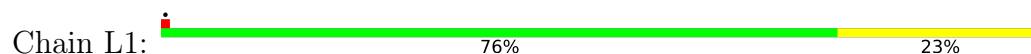
• Molecule 43: NADH-ubiquinone oxidoreductase chain 6



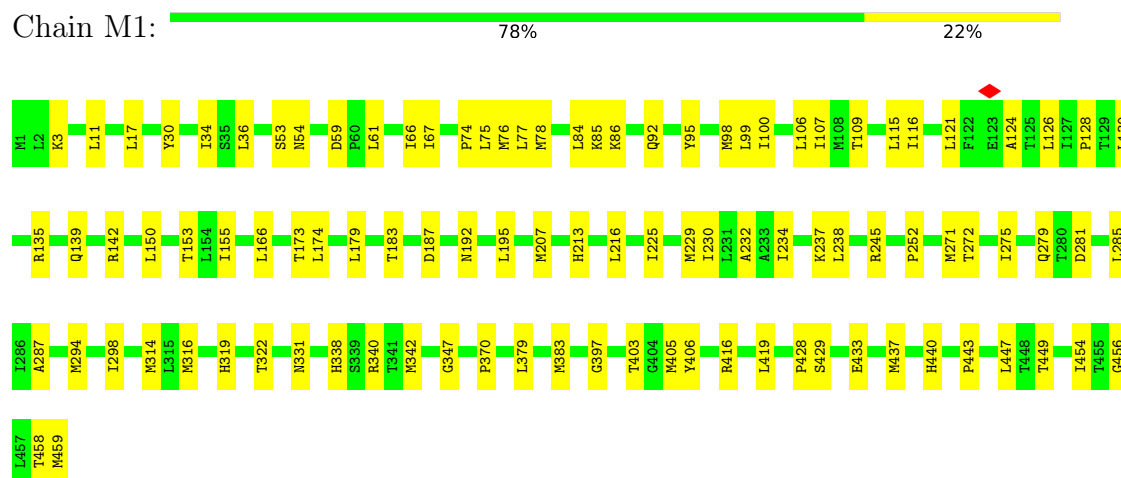
• Molecule 44: NADH-ubiquinone oxidoreductase chain 4L



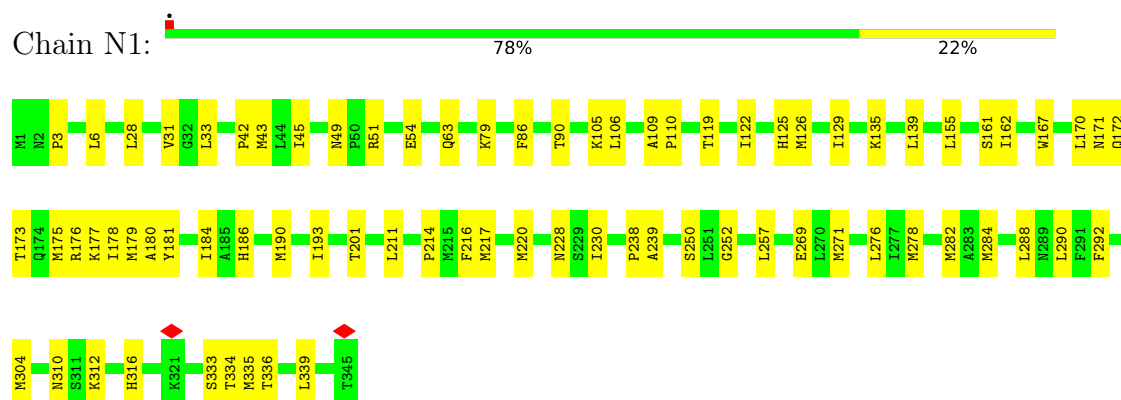
• Molecule 45: NADH-ubiquinone oxidoreductase chain 5



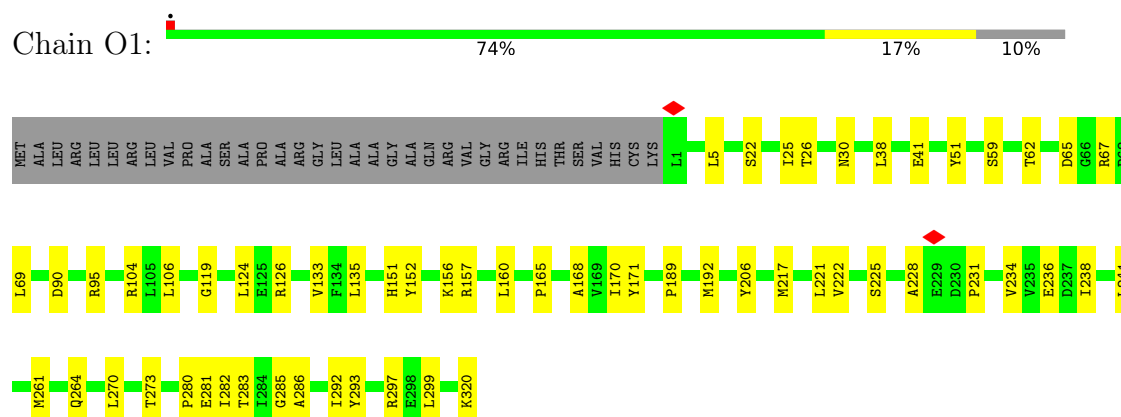
- Molecule 46: NADH-ubiquinone oxidoreductase chain 4



- Molecule 47: NADH-ubiquinone oxidoreductase chain 2

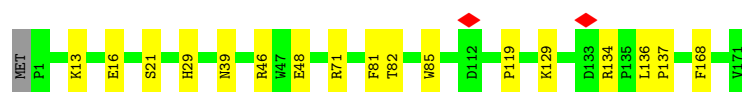


- Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

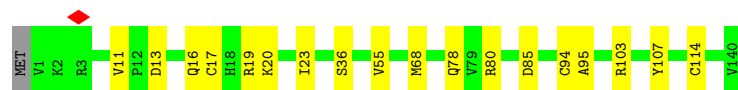


- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

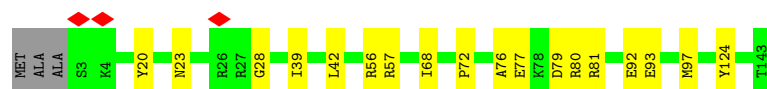
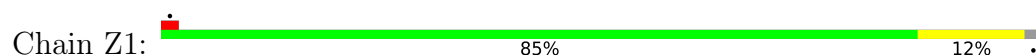




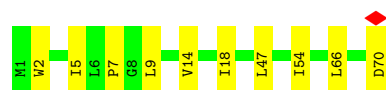
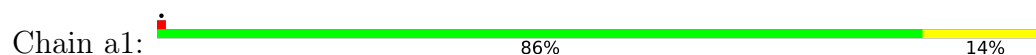
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



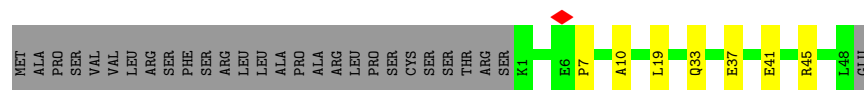
- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



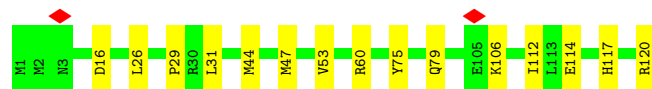
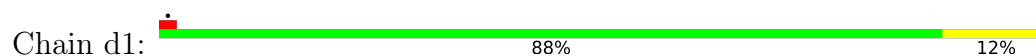
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C2



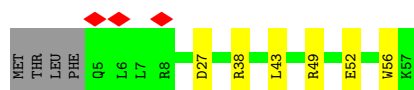
- Molecule 56: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e1: 



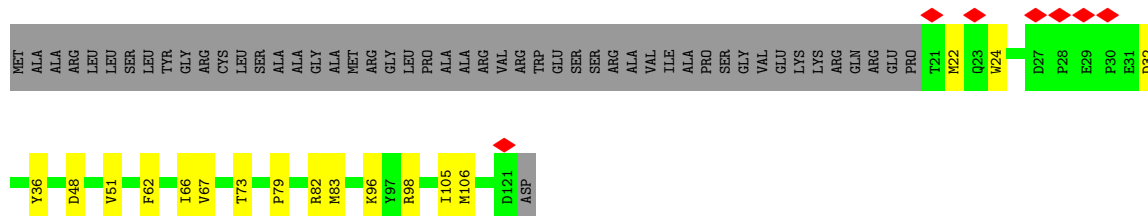
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f1: 



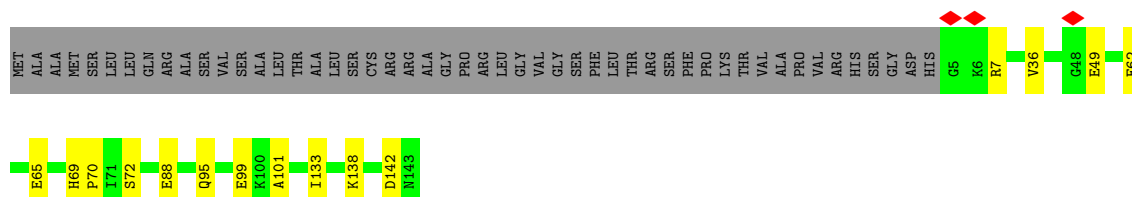
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g1: 



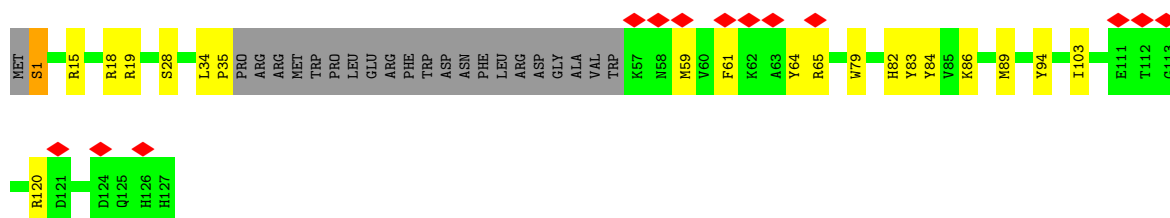
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h1: 

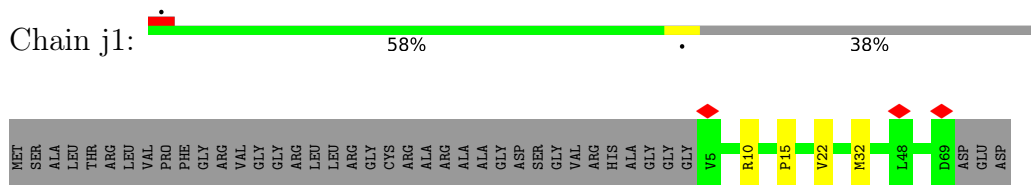


- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

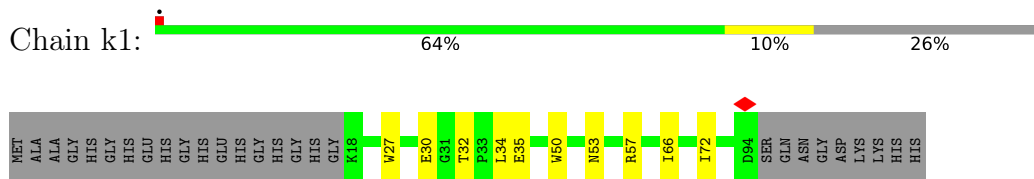
Chain i1: 



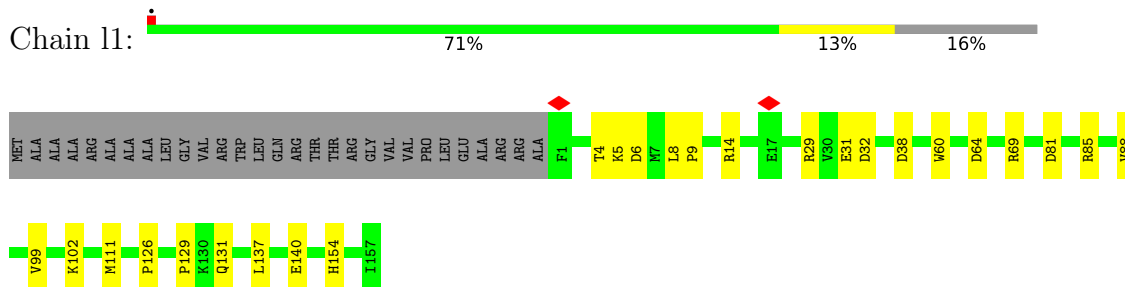
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



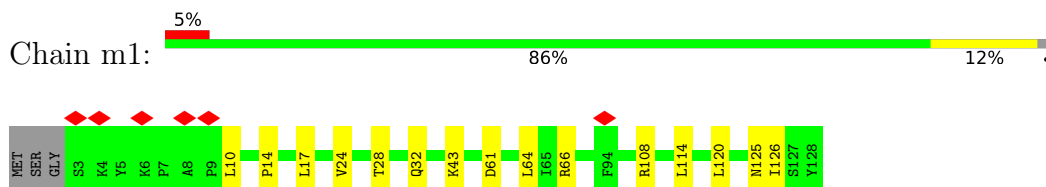
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



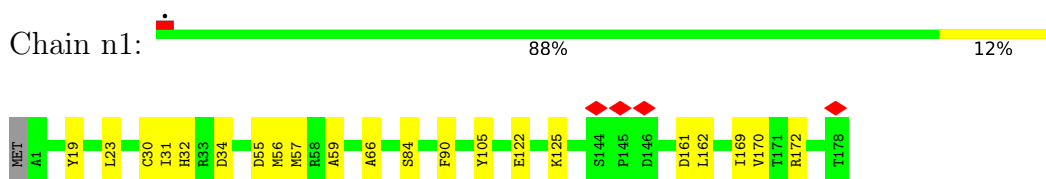
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



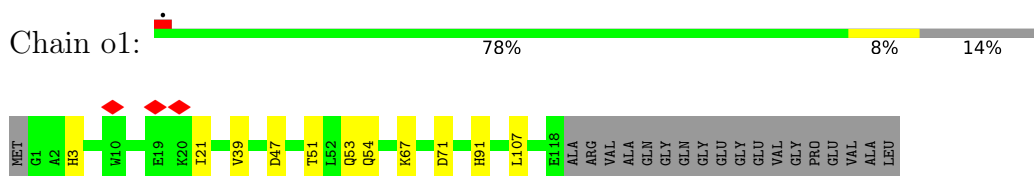
- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



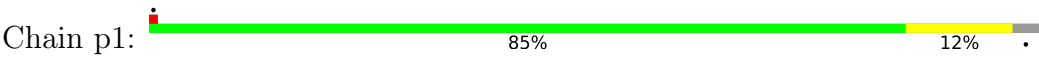
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 67: 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	103207	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	0.154	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	297.86, 218.35999, 261.81998	wwPDB
Map dimensions	281, 206, 247	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: SAC, FMN, CU, HEA, HEM, 2MR, HEC, 3PE, NDP, CUA, SF4, TGL, NA, FES, FME, K, PC1, MG, ZN, CDL, AYA, ZMP, DGT

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	A	0.19	0/3529	0.44	0/4793
1	L	0.19	0/3530	0.42	0/4793
2	B	0.16	0/3188	0.37	0/4308
2	M	0.17	0/3205	0.40	0/4332
3	C	0.21	0/3147	0.45	0/4297
3	N	0.21	0/3147	0.44	0/4297
4	D	0.17	0/1968	0.39	0/2674
4	O	0.16	0/1968	0.36	0/2674
5	E	0.16	0/1176	0.42	0/1609
5	P	0.17	0/1176	0.38	0/1609
5	T	0.18	0/565	0.43	0/772
6	F	0.17	0/916	0.37	0/1226
6	Q	0.18	0/922	0.38	0/1234
7	G	0.24	0/673	0.50	0/909
7	R	0.25	0/673	0.55	0/909
8	H	0.27	0/552	0.66	0/739
8	S	0.24	0/570	0.61	0/763
9	J	0.21	0/509	0.50	0/687
9	U	0.21	0/509	0.44	0/687
10	K	0.20	0/438	0.45	0/598
10	V	0.20	0/446	0.53	0/609
11	n	0.26	0/4162	0.56	0/5686
12	o	0.24	0/1863	0.59	0/2542
13	p	0.23	0/2202	0.53	0/3010
14	q	0.20	0/1190	0.49	0/1609
15	r	0.25	0/860	0.55	0/1167
16	s	0.20	0/734	0.45	0/996
17	t	0.83	0/646	1.20	1/882 (0.1%)
18	u	0.22	0/674	0.61	0/910
19	v	0.19	0/579	0.49	0/771
20	x	0.23	0/396	0.58	0/541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	y	0.19	0/399	0.44	0/535
22	z	0.95	0/350	1.18	0/472
23	w	0.18	0/444	0.49	0/598
24	6	0.26	0/1289	0.57	0/1744
25	C1	0.19	0/1780	0.41	0/2424
26	D1	0.23	0/3540	0.47	1/4795 (0.0%)
27	2	0.24	0/1700	0.54	0/2316
28	1	0.21	0/3396	0.51	1/4586 (0.0%)
29	3	0.20	0/5392	0.45	0/7305
30	9	0.21	0/1461	0.41	0/1974
31	P1	0.18	0/2823	0.44	0/3828
32	Q1	0.17	0/1045	0.36	0/1411
33	7	0.19	0/773	0.41	0/1041
34	S1	0.21	0/682	0.54	0/920
35	T1	0.24	0/646	0.58	0/869
35	U1	0.21	0/718	0.52	1/970 (0.1%)
36	V1	0.20	0/945	0.39	0/1281
37	W1	0.21	0/993	0.45	0/1335
38	q1	0.19	0/1251	0.43	0/1702
39	r1	0.19	0/806	0.41	0/1090
40	s1	0.28	0/360	0.70	2/489 (0.4%)
41	A1	0.24	0/948	0.48	0/1295
42	H1	0.29	0/2607	0.60	0/3564
43	J1	0.21	0/1330	0.45	0/1810
44	K1	0.24	0/738	0.48	0/1002
45	L1	0.24	0/4913	0.51	0/6686
46	M1	0.23	0/3709	0.47	0/5052
47	N1	0.24	0/2755	0.51	0/3751
48	O1	0.18	0/2674	0.40	0/3626
49	X1	0.16	0/1434	0.39	0/1937
50	Y1	0.17	0/1061	0.37	0/1439
51	Z1	0.18	0/1198	0.41	0/1616
52	a1	0.20	0/585	0.44	0/788
53	b1	0.14	0/666	0.38	0/914
54	c1	0.18	0/409	0.44	0/555
55	d1	0.18	0/1028	0.44	0/1387
56	e1	0.14	0/900	0.34	0/1199
57	f1	0.17	0/468	0.39	0/630
58	g1	0.16	0/878	0.39	0/1196
59	h1	0.18	0/1201	0.43	0/1626
60	i1	0.17	0/917	0.37	0/1243
61	j1	0.17	0/587	0.43	0/804
62	k1	0.18	0/646	0.43	0/873

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	l1	0.17	0/1379	0.42	0/1882
64	m1	0.19	0/1079	0.40	0/1463
65	n1	0.21	0/1596	0.47	0/2162
66	o1	0.20	0/1039	0.47	0/1394
67	p1	0.17	0/1471	0.35	0/1988
All	All	0.22	0/115122	0.47	6/156200 (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
22	z	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s1	67	PRO	CA-N-CD	-9.83	98.24	112.00
28	1	96	ASN	N-CA-C	-7.71	96.00	108.41
17	t	70	HIS	CB-CG-CD2	-5.51	124.04	131.20
35	U1	68	GLU	N-CA-CB	5.29	119.03	110.40
26	D1	170	MET	CB-CG-SD	5.29	128.58	112.70
40	s1	67	PRO	N-CD-CG	-5.24	95.34	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	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	A	3459	0	3367	56	0
1	L	3460	0	3367	43	0
2	B	3138	0	3143	39	0
2	M	3154	0	3158	36	0
3	C	3046	0	3112	46	0
3	N	3046	0	3112	35	0
4	D	1909	0	1854	13	0
4	O	1909	0	1854	30	0
5	E	1167	0	842	15	0
5	P	1167	0	842	8	0
5	T	554	0	590	8	0
6	F	894	0	882	9	0
6	Q	900	0	887	8	0
7	G	654	0	656	12	0
7	R	654	0	656	13	0
8	H	545	0	531	7	0
8	S	563	0	541	6	0
9	J	495	0	489	8	0
9	U	495	0	489	8	0
10	K	422	0	420	5	0
10	V	430	0	431	5	0
11	n	4021	0	3997	145	0
12	o	1817	0	1822	76	0
13	p	2118	0	2054	71	0
14	q	1156	0	1112	20	0
15	r	842	0	838	22	0
16	s	717	0	695	15	0
17	t	620	0	597	51	0
18	u	654	0	622	14	0
19	v	567	0	591	19	0
20	x	383	0	367	6	0
21	y	386	0	386	12	0
22	z	343	0	356	61	0
23	w	435	0	446	6	0
24	6	1258	0	1268	27	0
25	C1	1730	0	1686	34	0
26	D1	3464	0	3416	66	0
27	2	1660	0	1653	21	0
28	1	3321	0	3278	55	0
29	3	5305	0	5330	79	0
30	9	1431	0	1383	37	0
31	P1	2748	0	2768	47	0
32	Q1	1022	0	1023	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	7	758	0	731	10	0
34	S1	671	0	688	10	0
35	T1	637	0	640	12	0
35	U1	706	0	699	20	0
36	V1	923	0	965	7	0
37	W1	970	0	991	15	0
38	q1	1209	0	1170	11	0
39	r1	796	0	831	9	0
40	s1	351	0	331	8	0
41	A1	932	0	967	23	0
42	H1	2540	0	2626	75	0
43	J1	1308	0	1319	31	0
44	K1	737	0	768	15	0
45	L1	4800	0	4985	100	0
46	M1	3632	0	3853	70	0
47	N1	2703	0	2902	55	0
48	O1	2607	0	2566	38	0
49	X1	1396	0	1385	14	0
50	Y1	1037	0	1025	10	0
51	Z1	1167	0	1166	17	0
52	a1	572	0	583	10	0
53	b1	651	0	653	5	0
54	c1	398	0	401	5	0
55	d1	996	0	1001	13	0
56	e1	877	0	871	9	0
57	f1	456	0	452	5	0
58	g1	850	0	783	16	0
59	h1	1166	0	1166	13	0
60	i1	897	0	902	18	0
61	j1	562	0	515	4	0
62	k1	626	0	620	8	0
63	l1	1323	0	1216	18	0
64	m1	1050	0	1061	14	0
65	n1	1541	0	1473	16	0
66	o1	1014	0	1002	10	0
67	p1	1438	0	1404	20	0
68	6	32	0	38	1	0
68	A	23	0	20	2	0
68	A1	43	0	60	1	0
68	C	117	0	162	2	0
68	D1	51	0	82	3	0
68	H1	46	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	K1	41	0	59	1	0
68	L	23	0	20	2	0
68	L1	102	0	164	5	0
68	M1	87	0	128	0	0
68	N	71	0	90	2	0
68	N1	38	0	50	1	0
68	P	33	0	40	4	0
68	R	30	0	34	0	0
68	Y1	70	0	88	2	0
68	Z1	51	0	82	4	0
68	d1	63	0	74	1	0
68	i1	42	0	61	2	0
68	n	62	0	72	0	0
68	o	29	0	32	2	0
68	p	45	0	67	6	0
68	t	25	0	24	8	0
68	v	28	0	30	1	0
68	x	27	0	28	1	0
68	z	26	0	26	4	0
69	A	46	0	36	2	0
69	C	42	0	28	1	0
69	D	56	0	56	1	0
69	H1	51	0	52	2	0
69	L	46	0	36	0	0
69	L1	124	0	136	2	0
69	N1	90	0	133	5	0
69	R	155	0	142	1	0
69	Y1	166	0	232	4	0
69	a1	57	0	58	4	0
69	d1	67	0	81	3	0
69	h1	70	0	87	4	0
70	C	86	0	60	5	0
70	N	86	0	60	3	0
71	D	43	0	30	0	0
71	O	43	0	30	1	0
72	2	4	0	0	0	0
72	3	4	0	0	0	0
72	E	4	0	0	0	0
72	P	4	0	0	0	0
73	6	43	0	63	1	0
73	9	101	0	159	5	0
73	A1	31	0	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	E	35	0	44	2	0
73	K	28	0	30	1	0
73	L	24	0	22	0	0
73	M1	54	0	88	6	0
73	V	28	0	30	0	0
73	p	85	0	121	2	0
73	z	28	0	30	0	0
74	n	1	0	0	0	0
75	n	1	0	0	0	0
76	n	120	0	108	6	0
77	O1	1	0	0	0	0
77	o	1	0	0	0	0
78	o	2	0	0	0	0
79	7	1	0	0	0	0
79	s	1	0	0	0	0
80	y	37	0	49	1	0
81	1	8	0	0	0	0
81	3	16	0	0	0	0
81	6	8	0	0	0	0
81	9	16	0	0	1	0
82	1	31	0	19	4	0
83	3	1	0	0	0	0
84	P1	48	0	26	2	0
85	W1	34	0	40	2	0
85	n1	32	0	36	2	0
86	O1	31	0	12	1	0
All	All	115652	0	115389	1658	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 7.

All (1658) 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)
22:z:24:VAL:O	22:z:28:LEU:HG	1.35	1.26
11:n:480:ARG:HB2	22:z:4:LYS:O	1.47	1.11
11:n:404:THR:HG21	22:z:3:SER:HB3	1.31	1.09
11:n:481:GLU:O	22:z:4:LYS:N	1.94	1.01
22:z:24:VAL:HG12	22:z:28:LEU:HD11	1.43	1.00
12:o:214:VAL:HG12	19:v:62:PHE:CE1	1.96	1.00
11:n:218:THR:HG21	17:t:54:ILE:HD12	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:t:50:PRO:HD3	18:u:80:THR:CG2	1.93	0.98
11:n:481:GLU:HB2	22:z:4:LYS:HB2	1.45	0.97
12:o:214:VAL:CG1	19:v:62:PHE:CE1	2.49	0.94
12:o:186:SER:OG	12:o:213:MET:CE	2.16	0.94
11:n:404:THR:HG21	22:z:3:SER:CB	1.99	0.91
28:1:68:ARG:HD2	28:1:254:LYS:HZ2	1.34	0.90
12:o:200:CYS:SG	12:o:207:MET:HE1	2.14	0.87
11:n:218:THR:HG21	17:t:54:ILE:CD1	2.03	0.87
12:o:186:SER:OG	12:o:213:MET:HE1	1.74	0.87
13:p:120:GLY:HA2	17:t:49:TYR:CE2	2.09	0.87
19:v:52:PHE:O	19:v:56:TYR:HB2	1.75	0.86
28:1:68:ARG:HD2	28:1:254:LYS:NZ	1.89	0.86
11:n:478:SER:OG	22:z:6:ALA:CB	2.23	0.86
21:y:18:LYS:NZ	22:z:8:GLU:OE1	2.08	0.85
13:p:187:SER:HB2	17:t:67:THR:HG21	1.57	0.85
22:z:24:VAL:CG1	22:z:28:LEU:HD11	2.07	0.84
11:n:478:SER:OG	22:z:6:ALA:HB2	1.77	0.84
13:p:121:ILE:HG13	17:t:52:LEU:CD1	2.08	0.84
17:t:50:PRO:HD3	18:u:80:THR:HG22	1.60	0.83
22:z:36:HIS:HB2	22:z:40:TYR:CZ	2.12	0.83
13:p:142:VAL:HG23	17:t:13:TRP:CZ3	2.13	0.83
13:p:121:ILE:HD12	17:t:52:LEU:HD22	1.62	0.81
22:z:24:VAL:O	22:z:28:LEU:CG	2.26	0.81
17:t:75:ASN:ND2	68:t:101:3PE:N	2.30	0.80
12:o:200:CYS:SG	12:o:207:MET:CE	2.70	0.80
11:n:404:THR:CG2	22:z:3:SER:HB3	2.11	0.79
7:G:41:THR:O	7:G:45:ILE:HB	1.83	0.78
30:9:171:ILE:O	30:9:175:TYR:HB3	1.84	0.78
13:p:121:ILE:HG13	17:t:52:LEU:HD13	1.65	0.78
42:H1:287:HIS:O	42:H1:291:LYS:HB2	1.84	0.78
17:t:75:ASN:HD21	68:t:101:3PE:HN3	1.28	0.77
11:n:481:GLU:C	22:z:4:LYS:H	1.92	0.77
13:p:121:ILE:CG1	17:t:52:LEU:HD13	2.16	0.76
12:o:186:SER:OG	12:o:213:MET:HE2	1.84	0.76
11:n:481:GLU:HB2	22:z:4:LYS:HD2	1.69	0.75
45:L1:187:VAL:HG22	46:M1:383:MET:HG2	1.70	0.74
59:h1:49:GLU:H	59:h1:70:PRO:HD3	1.52	0.74
12:o:214:VAL:CG1	19:v:62:PHE:HE1	1.98	0.74
12:o:142:VAL:HB	12:o:211:LEU:HD23	1.68	0.73
11:n:481:GLU:CB	22:z:4:LYS:HD2	2.19	0.73
31:P1:216:ASN:O	31:P1:220:ASP:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:154:ILE:O	12:o:179:LEU:HA	1.89	0.72
45:L1:245:ALA:O	45:L1:249:SER:HB2	1.90	0.72
3:C:132:VAL:HA	3:C:139:SER:HB2	1.71	0.72
28:1:93:LEU:O	28:1:134:ALA:HA	1.90	0.72
2:B:220:ALA:O	2:B:224:LEU:HB2	1.90	0.71
12:o:214:VAL:HG12	19:v:62:PHE:CD1	2.25	0.71
22:z:24:VAL:HG12	22:z:28:LEU:CD1	2.20	0.70
31:P1:310:LEU:O	31:P1:314:SER:HB2	1.92	0.70
11:n:218:THR:CG2	17:t:54:ILE:HD12	2.20	0.70
2:B:144:LEU:HD21	2:B:178:CYS:HB3	1.74	0.70
9:U:53:LYS:HA	9:U:56:LYS:HE3	1.72	0.69
9:J:52:TRP:O	9:J:56:LYS:HB2	1.92	0.69
13:p:121:ILE:CD1	17:t:52:LEU:HD13	2.22	0.69
11:n:437:PRO:HG2	11:n:440:TYR:CZ	2.28	0.69
69:D:302:CDL:H122	69:D:302:CDL:H512	1.75	0.69
45:L1:193:MET:HE1	45:L1:204:SER:HB2	1.73	0.69
12:o:146:MET:CE	12:o:215:PRO:HD3	2.22	0.68
13:p:121:ILE:CD1	17:t:52:LEU:HD22	2.23	0.68
12:o:214:VAL:HG11	19:v:62:PHE:CE1	2.29	0.68
58:g1:106:MET:HG3	67:p1:134:VAL:HG23	1.76	0.68
62:k1:32:THR:HG22	62:k1:34:LEU:H	1.57	0.68
45:L1:249:SER:HB3	45:L1:336:LYS:HB3	1.74	0.68
2:B:257:ILE:HG12	2:B:424:MET:HG3	1.76	0.68
27:2:119:THR:HG21	27:2:166:PRO:HB3	1.75	0.68
9:U:10:TYR:HA	9:U:14:PHE:HB2	1.76	0.68
11:n:481:GLU:HB2	22:z:4:LYS:CB	2.21	0.67
13:p:121:ILE:HG21	13:p:186:PHE:HB3	1.75	0.67
11:n:478:SER:OG	22:z:6:ALA:HB1	1.94	0.67
17:t:69:PHE:HD2	68:t:101:3PE:H11	1.57	0.67
29:3:533:THR:O	29:3:537:LEU:HB2	1.95	0.67
12:o:153:LEU:HB3	12:o:179:LEU:HD13	1.77	0.67
22:z:20:THR:O	22:z:24:VAL:HG23	1.95	0.67
21:y:38:PHE:HA	21:y:41:ARG:HG2	1.77	0.66
2:M:245:ARG:HB3	2:M:430:LEU:HD13	1.77	0.66
13:p:121:ILE:HG13	17:t:52:LEU:HD11	1.78	0.66
47:N1:42:PRO:HA	47:N1:45:ILE:HG22	1.78	0.66
13:p:142:VAL:HG23	17:t:13:TRP:HZ3	1.57	0.66
17:t:75:ASN:ND2	68:t:101:3PE:HN3	1.89	0.66
47:N1:252:GLY:HA3	47:N1:290:LEU:HD13	1.78	0.66
1:A:438:ARG:HH22	5:E:33:LYS:HD3	1.60	0.66
12:o:190:GLY:O	12:o:212:GLU:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:214:VAL:HG11	19:v:62:PHE:HE1	1.60	0.65
29:3:588:THR:HG21	32:Q1:63:GLU:HA	1.79	0.65
32:Q1:36:ARG:O	32:Q1:57:MET:HA	1.96	0.65
42:H1:81:LEU:HD11	42:H1:111:LEU:HB3	1.79	0.65
26:D1:146:ARG:NH2	26:D1:368:GLU:O	2.30	0.65
3:N:8:HIS:HB3	3:N:11:PHE:HB2	1.79	0.65
11:n:480:ARG:CB	22:z:4:LYS:O	2.37	0.65
13:p:146:TRP:HB2	17:t:13:TRP:HB3	1.77	0.65
26:D1:281:VAL:HG21	26:D1:310:ILE:HG23	1.78	0.65
48:O1:104:ARG:NH2	86:O1:401:DGT:N7	2.45	0.65
60:i1:82:HIS:HD1	67:p1:36:TYR:HH	1.45	0.64
28:1:224:ASN:ND2	82:1:501:FMN:O2	2.30	0.64
29:3:201:ASP:OD2	29:3:268:ARG:NH1	2.30	0.64
13:p:121:ILE:HD11	17:t:52:LEU:HD13	1.77	0.64
28:1:96:ASN:O	28:1:225:VAL:HG23	1.96	0.64
13:p:35:PHE:CD1	17:t:60:PRO:HG3	2.32	0.64
27:2:101:GLN:NE2	27:2:155:GLN:OE1	2.30	0.64
3:C:361:ILE:HG22	3:C:365:LEU:HD12	1.77	0.64
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.71	0.64
26:D1:148:LEU:HD23	26:D1:174:ARG:HG2	1.79	0.64
29:3:243:ARG:HH12	30:9:97:GLU:HG2	1.62	0.64
31:P1:176:ASP:OD1	31:P1:180:ASN:ND2	2.31	0.64
2:M:77:THR:HG21	2:M:126:VAL:HA	1.78	0.64
17:t:50:PRO:HD3	18:u:80:THR:HG23	1.78	0.64
46:M1:66:ILE:HG23	46:M1:107:ILE:HD12	1.80	0.64
42:H1:139:THR:O	42:H1:143:GLU:HB2	1.98	0.63
43:J1:144:MET:HG2	43:J1:152:MET:HG2	1.80	0.63
56:e1:29:ALA:HB2	59:h1:138:LYS:HD3	1.80	0.63
4:O:166:THR:HG22	4:O:167:GLU:HG2	1.80	0.63
12:o:1:MET:HE1	14:q:126:MET:HG3	1.80	0.63
11:n:75:ILE:HG12	11:n:249:PRO:HG2	1.81	0.63
27:2:100:ILE:HG12	27:2:156:ILE:HG12	1.80	0.63
41:A1:34:ALA:HB1	42:H1:63:PRO:HA	1.80	0.63
60:i1:120:ARG:HB2	66:o1:39:VAL:HG13	1.81	0.63
28:1:99:GLU:OE2	28:1:104:THR:HG22	1.98	0.63
29:3:570:SER:HA	29:3:583:THR:O	1.98	0.63
45:L1:180:ILE:HD12	46:M1:397:GLY:HA2	1.81	0.63
3:N:240:MET:HE2	68:P:201:3PE:H232	1.80	0.63
39:r1:45:SER:O	39:r1:51:ASN:ND2	2.32	0.63
45:L1:137:MET:HB2	45:L1:196:TRP:HB3	1.79	0.63
45:L1:221:THR:HG23	45:L1:226:GLN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D1:328:ALA:HB3	29:3:126:ASP:HB2	1.79	0.63
12:o:30:ILE:HG21	12:o:76:ILE:HD11	1.80	0.62
12:o:143:VAL:HG22	12:o:212:GLU:OE2	1.99	0.62
17:t:75:ASN:ND2	68:t:101:3PE:HN1	1.97	0.62
15:r:90:ARG:O	15:r:94:ASN:ND2	2.32	0.62
22:z:22:CYS:O	22:z:23:PHE:C	2.43	0.62
26:D1:269:LEU:HB2	26:D1:368:GLU:HB2	1.81	0.62
7:R:28:SER:OG	7:R:32:LYS:NZ	2.30	0.62
28:1:92:TYR:HB2	28:1:220:THR:HG22	1.81	0.62
1:A:242:ARG:O	7:G:14:ILE:HA	2.00	0.62
3:C:361:ILE:HA	3:C:365:LEU:HB2	1.80	0.62
22:z:28:LEU:HB2	22:z:29:PRO:HD3	1.82	0.62
26:D1:191:ALA:O	30:9:64:ARG:NH2	2.33	0.62
13:p:35:PHE:CE1	17:t:60:PRO:HG3	2.34	0.62
45:L1:578:THR:OG1	47:N1:171:ASN:ND2	2.32	0.62
3:N:51:LEU:HD13	70:N:402:HEM:HBA1	1.81	0.62
11:n:216:ASN:OD1	17:t:56:THR:N	2.33	0.62
28:1:68:ARG:CD	28:1:254:LYS:NZ	2.63	0.62
11:n:38:ARG:NH1	11:n:454:SER:OG	2.32	0.61
45:L1:243:VAL:O	45:L1:247:LEU:HB2	2.00	0.61
11:n:328:HIS:HA	12:o:45:MET:HG2	1.80	0.61
46:M1:232:ALA:O	46:M1:237:LYS:NZ	2.33	0.61
3:C:274:PHE:O	3:C:278:TYR:HB2	2.01	0.61
13:p:184:THR:HG21	13:p:198:PHE:HZ	1.65	0.61
73:9:203:PC1:H2D1	51:Z1:39:ILE:HD11	1.81	0.61
18:u:35:ASP:HA	18:u:38:ARG:HG3	1.83	0.61
45:L1:97:THR:HG21	45:L1:125:LEU:HD22	1.83	0.61
11:n:481:GLU:CB	22:z:4:LYS:HB2	2.25	0.61
37:W1:48:THR:HG23	37:W1:52:MET:HE3	1.83	0.61
47:N1:155:LEU:HB3	47:N1:278:MET:HE2	1.82	0.61
2:M:36:ALA:HB3	2:M:207:VAL:HG12	1.83	0.60
2:B:245:ARG:HB3	2:B:430:LEU:HD13	1.82	0.60
1:L:40:TRP:O	1:L:195:MET:HA	2.01	0.60
19:v:43:GLU:HG2	19:v:44:PRO:HD3	1.81	0.60
29:3:440:CYS:SG	29:3:476:LYS:NZ	2.74	0.60
31:P1:327:LEU:HD11	42:H1:64:LEU:HD23	1.82	0.60
42:H1:43:TYR:HD2	52:a1:7:PRO:HG2	1.65	0.60
3:C:177:ARG:NH1	5:P:62:MET:O	2.33	0.60
10:V:45:VAL:HG21	10:V:48:ILE:HB	1.81	0.60
11:n:274:VAL:HG12	11:n:278:MET:HE2	1.84	0.60
11:n:404:THR:CG2	22:z:3:SER:CB	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D1:4:TRP:O	46:M1:142:ARG:NH2	2.34	0.60
9:J:10:TYR:HA	9:J:14:PHE:HB2	1.82	0.60
1:L:67:THR:HG22	1:L:120:SER:HA	1.83	0.60
15:r:16:VAL:O	15:r:20:ASN:ND2	2.34	0.60
45:L1:257:ILE:HG23	45:L1:317:LEU:HD11	1.84	0.60
13:p:253:TYR:O	13:p:257:TYR:HB2	2.02	0.60
26:D1:110:SER:OG	26:D1:149:ASN:ND2	2.35	0.60
50:Y1:107:TYR:HB2	69:Y1:404:CDL:HB62	1.83	0.60
1:L:193:PRO:HG2	65:n1:55:ASP:HA	1.84	0.60
2:M:169:LYS:HG3	2:M:240:ARG:HB3	1.83	0.60
12:o:94:VAL:HG21	12:o:148:LEU:HD22	1.84	0.59
48:O1:26:THR:HG22	48:O1:124:LEU:HB2	1.84	0.59
11:n:172:LYS:NZ	11:n:176:MET:O	2.35	0.59
22:z:39:SER:O	22:z:42:LYS:N	2.33	0.59
1:L:131:ARG:NH2	1:L:177:LEU:O	2.34	0.59
60:i1:94:TYR:OH	67:p1:10:PRO:O	2.21	0.59
29:3:381:GLY:HA2	29:3:661:LEU:HD21	1.84	0.59
28:1:215:VAL:HG12	28:1:220:THR:HG21	1.84	0.59
68:A1:602:3PE:H381	42:H1:295:PRO:HB3	1.85	0.59
2:M:171:ALA:HB2	2:M:235:ALA:HB3	1.84	0.59
21:y:37:PHE:HB3	22:z:33:VAL:HG21	1.85	0.59
47:N1:162:ILE:HD12	47:N1:282:MET:HG2	1.83	0.59
11:n:377:PHE:O	11:n:381:LEU:HB3	2.02	0.59
48:O1:165:PRO:HB3	48:O1:217:MET:HE3	1.85	0.59
1:A:42:ASP:HB2	1:A:194:ARG:HB3	1.84	0.59
29:3:74:MET:SD	29:3:74:MET:N	2.76	0.59
50:Y1:17:CYS:SG	50:Y1:78:GLN:NE2	2.75	0.59
11:n:74:MET:HA	11:n:78:PHE:HD2	1.68	0.59
22:z:38:GLU:O	22:z:41:LYS:HB3	2.03	0.58
45:L1:161:ARG:NH1	65:n1:90:PHE:O	2.34	0.58
4:D:10:TYR:O	4:D:15:ARG:NH1	2.36	0.58
1:L:41:ILE:HG13	1:L:195:MET:HG2	1.84	0.58
5:P:84:GLY:N	5:P:100:HIS:O	2.36	0.58
12:o:28:LEU:HD11	68:o:302:3PE:H322	1.85	0.58
29:3:35:MET:HE1	29:3:81:THR:HG21	1.85	0.58
38:q1:8:LYS:HA	38:q1:11:VAL:HG12	1.85	0.58
46:M1:456:GLY:O	58:g1:82:ARG:NH1	2.36	0.58
3:N:207:ASN:ND2	3:N:209:THR:OG1	2.36	0.58
24:6:76:ARG:NH1	26:D1:179:GLU:OE2	2.34	0.58
26:D1:224:GLU:OE1	30:9:42:TYR:OH	2.20	0.58
31:P1:149:LYS:NZ	84:P1:501:NDP:O2D	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:NH2	1:A:111:GLU:OE1	2.37	0.58
2:M:221:GLU:O	2:M:225:ASN:ND2	2.36	0.58
11:n:129:TYR:OH	11:n:236:TRP:NE1	2.32	0.58
11:n:246:LEU:HD23	11:n:381:LEU:HD11	1.85	0.58
29:3:632:ARG:NH1	34:S1:58:SER:OG	2.37	0.58
35:T1:50:ILE:HG22	35:T1:54:MET:HE2	1.85	0.58
1:A:362:ARG:NH2	1:A:400:GLN:OE1	2.34	0.58
5:T:65:VAL:HB	5:T:77:ARG:HB3	1.85	0.58
11:n:244:TYR:HA	11:n:247:ILE:HG22	1.85	0.58
11:n:427:PRO:HB3	11:n:450:TRP:HB3	1.86	0.58
27:2:156:ILE:HD13	27:2:176:LEU:HD11	1.84	0.58
48:O1:189:PRO:HA	48:O1:192:MET:HG3	1.86	0.58
5:P:155:GLY:HA3	5:P:165:TYR:O	2.04	0.58
8:S:32:ARG:NH2	8:S:36:GLU:OE2	2.37	0.58
31:P1:248:MET:O	31:P1:322:ARG:NH2	2.36	0.58
46:M1:207:MET:HG3	46:M1:294:MET:HB3	1.86	0.58
31:P1:251:ARG:NH2	31:P1:321:HIS:O	2.37	0.58
43:J1:66:VAL:HG11	44:K1:31:LEU:HD21	1.86	0.58
46:M1:166:LEU:HD23	46:M1:195:LEU:HD13	1.86	0.58
48:O1:38:LEU:HD11	48:O1:234:VAL:HG21	1.85	0.58
11:n:175:ALA:HB2	16:s:36:PRO:HB3	1.86	0.58
43:J1:22:LYS:HG2	44:K1:28:SER:HB3	1.85	0.58
11:n:481:GLU:HB2	22:z:4:LYS:CD	2.33	0.58
2:B:51:VAL:HG22	2:B:204:MET:HG2	1.86	0.58
11:n:13:LYS:NZ	11:n:504:THR:OG1	2.37	0.58
25:C1:86:ARG:NH1	36:V1:110:GLN:O	2.36	0.58
11:n:283:LEU:HD23	11:n:286:ILE:HD11	1.86	0.57
26:D1:165:THR:HG22	42:H1:32:GLN:HG2	1.85	0.57
29:3:396:ARG:NH1	29:3:416:THR:O	2.37	0.57
29:3:668:ILE:HA	29:3:671:PHE:HB3	1.87	0.57
45:L1:362:ILE:HB	45:L1:431:THR:HA	1.85	0.57
55:d1:114:GLU:OE2	67:p1:152:ARG:NH2	2.37	0.57
58:g1:73:THR:HG22	69:h1:201:CDL:H331	1.85	0.57
3:C:31:TRP:NE1	70:C:402:HEM:O1D	2.37	0.57
3:N:101:GLY:HA2	3:N:106:SER:HB2	1.86	0.57
33:7:39:PHE:O	33:7:43:LEU:HB2	2.04	0.57
45:L1:446:ASN:HA	45:L1:451:MET:HE3	1.86	0.57
11:n:377:PHE:HA	11:n:380:VAL:HG12	1.85	0.57
12:o:200:CYS:SG	12:o:207:MET:HE2	2.44	0.57
13:p:221:ARG:NH2	68:p:301:3PE:O14	2.37	0.57
35:T1:42:LEU:HD23	35:T1:46:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:M1:115:LEU:HB2	46:M1:174:LEU:HD21	1.86	0.57
25:C1:175:ARG:NH2	25:C1:177:ASP:OD2	2.38	0.57
11:n:344:PHE:O	11:n:348:PHE:HB3	2.05	0.57
24:6:181:GLN:HB2	24:6:184:LYS:HB3	1.86	0.57
2:M:145:LYS:HE3	5:T:41:PRO:HD3	1.86	0.57
33:7:59:CYS:O	33:7:70:LYS:HA	2.04	0.57
13:p:173:PHE:HE2	13:p:208:VAL:HG21	1.70	0.57
31:P1:157:ARG:NH1	31:P1:163:ALA:O	2.37	0.57
45:L1:485:PHE:O	45:L1:489:THR:OG1	2.22	0.57
4:D:11:PRO:HA	4:D:15:ARG:HH12	1.68	0.56
12:o:144:LEU:O	12:o:213:MET:HA	2.05	0.56
28:1:378:ARG:NE	29:3:132:GLU:OE2	2.37	0.56
1:A:245:ASP:HA	7:G:11:ARG:HA	1.86	0.56
3:N:113:TRP:NE1	3:N:301:LEU:O	2.33	0.56
35:U1:55:GLU:HG2	35:U1:61:GLU:HA	1.87	0.56
60:i1:82:HIS:ND1	67:p1:36:TYR:OH	2.37	0.56
3:N:282:ARG:NH2	3:N:338:ILE:O	2.38	0.56
13:p:142:VAL:HG23	17:t:13:TRP:CE3	2.39	0.56
28:1:188:GLU:O	28:1:192:LEU:HB2	2.05	0.56
29:3:364:LEU:HD12	29:3:491:ASN:HB3	1.87	0.56
38:q1:9:ARG:NH1	69:a1:101:CDL:OA4	2.38	0.56
45:L1:15:LEU:HD11	45:L1:129:LEU:HD12	1.87	0.56
45:L1:424:MET:HE3	45:L1:428:TYR:HB2	1.88	0.56
57:f1:43:LEU:HD11	67:p1:67:TYR:HB3	1.88	0.56
28:1:98:ASP:O	28:1:139:ARG:HD2	2.06	0.56
41:A1:70:ALA:HB2	43:J1:58:ILE:HD11	1.87	0.56
46:M1:272:THR:HA	46:M1:275:ILE:HD12	1.88	0.56
69:N1:401:CDL:HA4	55:d1:53:VAL:HG11	1.88	0.56
29:3:226:GLU:HG3	32:Q1:36:ARG:HH22	1.70	0.56
29:3:418:ARG:HG2	40:s1:68:ARG:HG2	1.88	0.56
30:9:55:GLU:OE2	38:q1:34:ARG:NH2	2.39	0.56
47:N1:119:THR:HG21	47:N1:180:ALA:HB2	1.87	0.56
1:A:339:GLN:NE2	1:A:437:ILE:O	2.38	0.56
2:B:141:ARG:HD3	2:B:184:GLY:HA2	1.87	0.56
11:n:481:GLU:O	22:z:3:SER:HA	2.05	0.56
13:p:190:ASP:OD1	17:t:53:ARG:N	2.36	0.56
29:3:431:ASP:OD1	29:3:436:ARG:NH1	2.38	0.56
31:P1:166:ILE:HG22	31:P1:168:PRO:HD3	1.86	0.56
11:n:216:ASN:CG	17:t:55:ARG:HA	2.31	0.56
13:p:7:ALA:HB1	13:p:72:THR:HG21	1.87	0.56
14:q:97:ILE:HG12	20:x:36:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L1:362:ILE:HG22	45:L1:370:SER:HB2	1.88	0.56
48:O1:25:ILE:HG12	48:O1:168:ALA:HB3	1.88	0.56
52:a1:54:ILE:HD11	56:e1:105:PRO:HB3	1.88	0.56
4:O:43:MET:HB3	4:O:91:PHE:HD2	1.71	0.56
24:6:157:PRO:HB3	30:9:149:LEU:HD21	1.86	0.56
30:9:43:LEU:HB2	42:H1:31:MET:HG2	1.88	0.56
42:H1:138:GLN:NE2	42:H1:198:PHE:O	2.37	0.56
48:O1:225:SER:O	48:O1:228:ALA:C	2.49	0.56
1:L:8:LEU:HD22	1:L:392:LEU:HB3	1.87	0.56
1:L:194:ARG:NH1	65:n1:57:MET:SD	2.79	0.56
11:n:94:PHE:HE1	11:n:166:THR:HG21	1.71	0.56
25:C1:81:VAL:HG22	26:D1:388:ARG:HG2	1.88	0.56
45:L1:190:SER:HB2	45:L1:196:TRP:HE1	1.71	0.56
55:d1:29:PRO:HB2	69:d1:201:CDL:H712	1.88	0.56
56:e1:37:LYS:HG3	59:h1:133:ILE:HG21	1.88	0.56
1:A:433:ASP:N	1:A:433:ASP:OD1	2.39	0.55
28:1:99:GLU:OE1	28:1:107:ASP:HB2	2.06	0.55
45:L1:194:ASN:HD22	64:m1:126:ILE:HD11	1.70	0.55
47:N1:106:LEU:O	47:N1:135:LYS:NZ	2.39	0.55
1:A:14:THR:HG22	1:A:28:GLU:HB2	1.88	0.55
2:B:374:THR:HG23	2:B:377:GLY:H	1.70	0.55
1:L:110:VAL:HG11	1:L:211:LEU:HB3	1.87	0.55
45:L1:526:LEU:HD12	45:L1:530:PRO:HG2	1.88	0.55
3:C:51:LEU:O	3:C:55:TYR:HB2	2.06	0.55
17:t:69:PHE:CD2	68:t:101:3PE:H11	2.39	0.55
27:2:129:GLY:HA2	27:2:140:ILE:HG22	1.88	0.55
42:H1:205:SER:OG	42:H1:279:ARG:NH1	2.38	0.55
43:J1:133:VAL:HG12	43:J1:134:MET:HG2	1.87	0.55
1:A:34:THR:OG1	2:B:373:GLU:OE1	2.24	0.55
1:A:339:GLN:HE21	1:A:441:MET:HE2	1.71	0.55
3:C:67:THR:HG22	4:D:115:TYR:HE2	1.71	0.55
13:p:211:GLY:HA2	13:p:214:PHE:HD2	1.72	0.55
28:1:101:GLU:OE1	28:1:302:SER:N	2.39	0.55
35:T1:19:LEU:HB3	35:T1:30:LEU:HD11	1.89	0.55
43:J1:73:MET:HE1	44:K1:79:VAL:HG23	1.88	0.55
5:T:8:SER:HB3	5:T:11:PHE:HB2	1.89	0.55
12:o:146:MET:HE1	12:o:215:PRO:HD3	1.88	0.55
16:s:14:ALA:O	16:s:19:ARG:NH1	2.39	0.55
11:n:240:HIS:ND1	11:n:290:HIS:HE1	2.03	0.55
11:n:438:ARG:HH21	11:n:439:ARG:HH22	1.54	0.55
11:n:445:ASP:O	20:x:41:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:95:VAL:HB	27:2:138:THR:HG21	1.88	0.55
47:N1:214:PRO:HA	47:N1:217:MET:HG3	1.88	0.55
31:P1:167:ARG:HH21	31:P1:297:LEU:HD11	1.71	0.55
41:A1:95:VAL:HG11	42:H1:302:MET:HB2	1.89	0.55
45:L1:65:THR:HA	60:i1:89:MET:HE2	1.89	0.55
68:N1:402:3PE:H251	68:N1:402:3PE:H351	1.89	0.55
63:l1:64:ASP:OD1	64:m1:43:LYS:NZ	2.38	0.55
8:S:18:VAL:HG12	8:S:67:VAL:HG22	1.88	0.55
11:n:439:ARG:HD3	12:o:199:ILE:HD12	1.88	0.55
25:C1:78:LEU:HB3	25:C1:130:TYR:HB3	1.88	0.55
29:3:278:ARG:NH1	29:3:568:GLU:OE2	2.34	0.55
32:Q1:62:ARG:NH1	37:W1:129:ASP:OD1	2.40	0.55
46:M1:98:MET:HE1	69:N1:401:CDL:H801	1.87	0.55
24:6:91:ARG:HB3	42:H1:216:ALA:HB2	1.88	0.55
37:W1:81:VAL:HG23	85:W1:201:ZMP:HN1	1.72	0.55
68:C:405:3PE:H2A1	7:G:54:VAL:HG21	1.89	0.54
43:J1:19:LEU:HD11	44:K1:31:LEU:HB3	1.89	0.54
47:N1:211:LEU:HD23	47:N1:333:SER:HB2	1.89	0.54
11:n:216:ASN:ND2	17:t:57:LYS:O	2.40	0.54
12:o:28:LEU:HA	12:o:31:VAL:HG12	1.90	0.54
17:t:29:MET:HB3	17:t:33:PHE:CE2	2.42	0.54
47:N1:190:MET:HB3	47:N1:201:THR:HG23	1.89	0.54
55:d1:120:ARG:O	64:m1:108:ARG:NH2	2.40	0.54
63:l1:9:PRO:HD3	64:m1:66:ARG:HG2	1.88	0.54
3:C:151:SER:HB2	3:C:161:VAL:HG21	1.89	0.54
12:o:93:PRO:O	18:u:13:THR:OG1	2.21	0.54
24:6:44:ASP:HB2	24:6:183:LEU:HB2	1.89	0.54
48:O1:90:ASP:O	48:O1:95:ARG:NH2	2.40	0.54
41:A1:10:ASN:ND2	42:H1:80:THR:O	2.41	0.54
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.89	0.54
2:M:76:THR:HG23	2:M:81:SER:HA	1.90	0.54
25:C1:49:GLU:OE2	25:C1:106:ARG:NH1	2.38	0.54
34:S1:26:SER:O	34:S1:33:ARG:NH2	2.39	0.54
4:O:203:ARG:NH1	9:U:40:ASP:OD1	2.40	0.54
11:n:363:LEU:O	11:n:367:LEU:CB	2.56	0.54
11:n:481:GLU:O	22:z:3:SER:CA	2.56	0.54
12:o:186:SER:CB	12:o:213:MET:HE1	2.36	0.54
30:9:76:GLU:HB2	33:7:44:ILE:HD11	1.89	0.54
30:9:96:ILE:HA	30:9:110:ARG:O	2.08	0.54
45:L1:539:MET:HG3	64:m1:10:LEU:HD21	1.89	0.54
1:L:269:THR:HG22	1:L:402:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:107:PRO:HB3	13:p:25:LEU:HB2	1.90	0.54
14:q:79:LYS:HA	14:q:82:VAL:HG12	1.89	0.54
31:P1:108:ASP:OD1	31:P1:112:ASN:ND2	2.40	0.54
36:V1:71:LEU:HD13	36:V1:79:VAL:HG11	1.90	0.54
1:A:21:ASN:O	1:A:221:ARG:NH1	2.41	0.54
2:B:101:THR:HG21	5:T:4:VAL:HG21	1.89	0.54
11:n:379:TYR:HA	11:n:383:MET:HE2	1.90	0.54
26:D1:354:GLU:OE2	26:D1:357:GLN:NE2	2.40	0.54
41:A1:3:LEU:HD23	68:Z1:401:3PE:H221	1.90	0.54
45:L1:54:PHE:O	45:L1:58:ASN:ND2	2.41	0.54
26:D1:117:ALA:HA	26:D1:367:ILE:HG13	1.90	0.54
1:L:2:ALA:N	1:L:6:GLN:OE1	2.41	0.53
2:M:133:ARG:HB2	2:M:136:GLU:HG3	1.90	0.53
11:n:248:LEU:HA	11:n:251:PHE:HD2	1.73	0.53
15:r:41:LEU:HD11	19:v:12:ARG:HH11	1.73	0.53
29:3:84:GLU:OE2	29:3:88:LYS:NZ	2.40	0.53
31:P1:191:VAL:HG11	31:P1:242:VAL:HG11	1.89	0.53
45:L1:348:HIS:NE2	35:U1:2:ASP:OD2	2.41	0.53
48:O1:65:ASP:OD2	48:O1:67:ARG:NH2	2.41	0.53
2:M:365:LYS:HG2	2:M:399:LEU:HD22	1.89	0.53
28:1:97:ALA:HB3	28:1:137:TYR:O	2.07	0.53
28:1:98:ASP:OD2	82:1:501:FMN:O4	2.26	0.53
42:H1:110:SER:HB2	43:J1:60:LEU:HD13	1.90	0.53
4:O:180:SER:HB3	8:S:15:LEU:HB2	1.90	0.53
26:D1:37:ASP:OD2	47:N1:51:ARG:NE	2.42	0.53
43:J1:24:SER:N	43:J1:80:GLU:O	2.35	0.53
60:i1:18:ARG:NH1	65:n1:170:VAL:O	2.41	0.53
63:l1:81:ASP:OD1	63:l1:81:ASP:N	2.41	0.53
67:p1:105:ILE:HG21	67:p1:134:VAL:HG11	1.90	0.53
2:B:95:LYS:HG2	2:B:110:GLU:HB2	1.91	0.53
13:p:187:SER:HA	68:t:101:3PE:H111	1.89	0.53
14:q:54:ASP:HA	14:q:57:VAL:HG12	1.89	0.53
68:x:101:3PE:H322	22:z:12:VAL:HG13	1.89	0.53
29:3:136:ALA:O	33:7:74:ASN:ND2	2.41	0.53
11:n:71:MET:HG2	11:n:75:ILE:HD12	1.90	0.53
25:C1:165:ASP:N	25:C1:165:ASP:OD1	2.42	0.53
26:D1:145:THR:HA	26:D1:148:LEU:HD12	1.89	0.53
29:3:381:GLY:HA3	29:3:457:ALA:HB2	1.89	0.53
40:s1:34:ASN:O	40:s1:37:HIS:ND1	2.33	0.53
45:L1:217:LEU:HD13	45:L1:277:MET:HG2	1.90	0.53
47:N1:109:ALA:HB3	47:N1:161:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:o1:51:THR:HG22	66:o1:53:GLN:H	1.72	0.53
1:A:191:LYS:NZ	1:A:222:VAL:O	2.41	0.53
1:A:270:LEU:HD13	1:A:320:LEU:HD22	1.90	0.53
5:E:161:HIS:CD2	3:N:343:VAL:HG12	2.43	0.53
5:T:51:CYS:SG	5:T:54:SER:OG	2.64	0.53
22:z:28:LEU:HD23	68:z:102:3PE:C27	2.39	0.53
46:M1:459:MET:O	58:g1:82:ARG:NH1	2.41	0.53
3:C:237:LEU:HD22	4:D:216:LEU:HD11	1.90	0.53
3:C:331:ASN:HD21	3:C:354:ALA:HB1	1.73	0.53
18:u:22:ASN:O	18:u:25:GLN:NE2	2.42	0.53
24:6:68:GLU:OE2	26:D1:188:ARG:NH2	2.39	0.53
68:D1:501:3PE:H2C2	47:N1:284:MET:HB3	1.91	0.53
28:1:91:LYS:HG2	28:1:219:PRO:HG2	1.91	0.53
47:N1:304:MET:HE3	48:O1:286:ALA:HB1	1.90	0.53
1:L:276:ILE:HG21	1:L:345:LEU:HD21	1.91	0.53
24:6:119:GLU:O	31:P1:54:TYR:OH	2.22	0.53
28:1:112:ARG:HB3	28:1:145:GLU:HG3	1.90	0.53
32:Q1:37:ILE:HB	32:Q1:105:VAL:HG22	1.90	0.53
45:L1:8:ILE:HA	45:L1:11:ILE:HD12	1.91	0.53
47:N1:86:PHE:HB3	47:N1:90:THR:HG21	1.91	0.53
58:g1:98:ARG:NH1	58:g1:105:ILE:O	2.42	0.53
2:B:92:VAL:HG11	2:B:118:ILE:HD11	1.90	0.53
3:C:8:HIS:O	3:C:12:LYS:N	2.39	0.53
12:o:181:GLN:H	18:u:23:GLN:HB3	1.74	0.53
14:q:19:ARG:HG3	14:q:21:ASP:HB3	1.90	0.53
22:z:28:LEU:HD23	68:z:102:3PE:C26	2.39	0.53
30:9:27:LEU:HD22	73:9:203:PC1:H251	1.91	0.53
31:P1:251:ARG:NH1	69:H1:402:CDL:OB3	2.42	0.53
42:H1:20:LEU:HD22	42:H1:232:ILE:HG13	1.89	0.53
46:M1:84:LEU:O	46:M1:92:GLN:NE2	2.42	0.53
49:X1:129:LYS:HD3	53:b1:65:VAL:HG13	1.91	0.53
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.91	0.53
12:o:124:PRO:HD2	12:o:127:ASP:HB2	1.91	0.53
12:o:215:PRO:HB2	12:o:218:TYR:HD2	1.74	0.53
31:P1:324:TYR:HB2	42:H1:65:THR:HA	1.91	0.53
45:L1:331:THR:HG23	45:L1:387:THR:HG22	1.89	0.53
1:L:412:SER:O	9:U:15:ARG:NH2	2.42	0.52
12:o:196:CYS:SG	12:o:207:MET:HE3	2.49	0.52
14:q:67:SER:OG	15:r:69:GLU:OE2	2.26	0.52
16:s:75:LEU:HD21	16:s:90:TYR:HB3	1.91	0.52
28:1:15:LEU:HD13	28:1:271:GLU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:P1:174:ARG:NH2	31:P1:316:GLU:OE2	2.42	0.52
46:M1:109:THR:HG21	46:M1:238:LEU:HD11	1.89	0.52
82:1:501:FMN:N1	82:1:501:FMN:O3'	2.42	0.52
65:n1:122:GLU:HA	65:n1:125:LYS:HD3	1.91	0.52
1:A:439:SER:HB3	68:A:501:3PE:H111	1.90	0.52
7:R:42:ARG:NH2	69:Y1:404:CDL:OA3	2.42	0.52
11:n:241:PRO:O	11:n:245:ILE:HG12	2.10	0.52
29:3:432:ILE:HG23	29:3:473:MET:HG3	1.90	0.52
45:L1:191:LEU:O	64:m1:125:ASN:ND2	2.42	0.52
45:L1:574:THR:OG1	47:N1:167:TRP:O	2.25	0.52
48:O1:170:ILE:HD11	48:O1:238:ILE:HD11	1.91	0.52
1:A:130:GLU:O	1:A:134:ILE:HD12	2.09	0.52
4:O:27:ARG:NH2	4:O:172:ASP:OD2	2.41	0.52
29:3:45:ARG:NH1	29:3:260:GLU:OE1	2.42	0.52
44:K1:93:LEU:HB3	47:N1:54:GLU:HG3	1.90	0.52
11:n:268:PHE:H	11:n:326:THR:HB	1.74	0.52
12:o:155:SER:HB2	12:o:179:LEU:HB3	1.91	0.52
12:o:217:LYS:O	12:o:221:ASN:ND2	2.33	0.52
60:i1:79:TRP:HD1	67:p1:40:VAL:HG13	1.74	0.52
1:A:3:THR:HG22	1:A:6:GLN:HG3	1.91	0.52
1:L:243:HIS:HB3	1:L:425:TYR:HD1	1.75	0.52
46:M1:74:PRO:HA	46:M1:77:LEU:HD12	1.92	0.52
11:n:428:GLN:HA	11:n:431:LEU:HB2	1.91	0.52
31:P1:265:TRP:HD1	31:P1:268:LYS:HZ3	1.56	0.52
45:L1:190:SER:HB2	45:L1:196:TRP:NE1	2.24	0.52
46:M1:187:ASP:OD1	46:M1:192:ASN:ND2	2.43	0.52
46:M1:314:MET:HG2	46:M1:454:ILE:HG13	1.90	0.52
48:O1:171:TYR:HD2	48:O1:222:VAL:HG13	1.74	0.52
60:i1:83:TYR:OH	67:p1:48:ARG:NH1	2.40	0.52
3:N:315:LEU:O	3:N:322:GLN:NE2	2.38	0.52
29:3:18:VAL:HG11	29:3:33:VAL:HG22	1.92	0.52
8:S:19:ARG:HD2	8:S:63:ARG:HD3	1.91	0.52
24:6:54:SER:OG	42:H1:51:ASP:OD1	2.21	0.52
45:L1:316:THR:HA	45:L1:319:MET:HE3	1.92	0.52
51:Z1:57:ARG:NH2	53:b1:48:THR:OG1	2.43	0.52
3:C:165:TRP:O	3:C:174:THR:OG1	2.27	0.52
2:M:86:THR:HA	5:T:70:LEU:HD21	1.92	0.52
14:q:77:GLU:O	14:q:81:VAL:HG23	2.10	0.52
24:6:43:LEU:O	24:6:47:ILE:HG12	2.10	0.52
31:P1:325:ARG:O	31:P1:325:ARG:NH1	2.41	0.52
11:n:227:ASP:N	11:n:227:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:p:34:TRP:NE1	17:t:60:PRO:O	2.43	0.51
16:s:52:SER:HB3	16:s:92:LEU:HD11	1.92	0.51
17:t:42:GLU:O	17:t:43:ARG:C	2.54	0.51
26:D1:224:GLU:HA	30:9:38:MET:HE3	1.91	0.51
28:1:99:GLU:H	82:1:501:FMN:HN3	1.58	0.51
28:1:154:ARG:HA	40:s1:52:LEU:HD21	1.92	0.51
33:7:12:THR:HG22	33:7:35:VAL:HG22	1.92	0.51
42:H1:200:LEU:HD22	42:H1:282:TYR:HB3	1.92	0.51
49:X1:16:GLU:OE2	56:e1:104:ARG:NH2	2.43	0.51
1:A:36:THR:HG21	1:A:373:THR:HA	1.91	0.51
2:B:60:SER:HB3	2:M:247:GLN:HE22	1.75	0.51
13:p:113:GLY:O	18:u:84:LYS:NZ	2.42	0.51
30:9:5:VAL:HA	39:r1:112:LEU:HD13	1.92	0.51
41:A1:68:GLU:HG2	43:J1:159:LEU:HD13	1.92	0.51
45:L1:154:LEU:HD13	45:L1:247:LEU:HD21	1.91	0.51
46:M1:429:SER:O	58:g1:36:TYR:OH	2.28	0.51
55:d1:112:ILE:O	67:p1:159:LYS:NZ	2.43	0.51
63:l1:5:LYS:HD3	63:l1:8:LEU:HD12	1.93	0.51
7:R:18:LEU:HD23	7:R:23:GLN:HB3	1.92	0.51
7:R:41:THR:O	7:R:45:ILE:HB	2.10	0.51
11:n:41:LEU:HA	11:n:443:TYR:HE2	1.75	0.51
11:n:332:ILE:HG23	11:n:338:MET:HE3	1.93	0.51
27:2:31:ILE:HD12	27:2:50:VAL:HG22	1.92	0.51
29:3:28:GLN:NE2	32:Q1:114:LYS:O	2.41	0.51
45:L1:254:VAL:HG12	45:L1:313:MET:HE1	1.91	0.51
65:n1:66:ALA:HB1	85:n1:201:ZMP:H7	1.93	0.51
22:z:24:VAL:C	22:z:28:LEU:HG	2.25	0.51
29:3:410:GLY:HA2	29:3:661:LEU:HD22	1.93	0.51
30:9:29:TRP:HB3	30:9:32:LEU:HD12	1.92	0.51
42:H1:86:TRP:CD1	42:H1:233:LEU:HD12	2.46	0.51
43:J1:69:TYR:HB3	44:K1:27:MET:HE1	1.92	0.51
43:J1:70:THR:HA	43:J1:74:ALA:HB3	1.92	0.51
45:L1:124:PHE:HE1	45:L1:147:VAL:HG13	1.76	0.51
1:A:366:VAL:HG11	2:B:43:PRO:HB2	1.91	0.51
1:L:261:GLY:O	1:L:267:ASN:ND2	2.38	0.51
1:L:439:SER:HB3	68:L:501:3PE:H111	1.92	0.51
3:N:67:THR:HG22	4:O:115:TYR:HE2	1.76	0.51
4:O:215:LEU:HD21	5:P:46:GLY:HA3	1.92	0.51
13:p:148:HIS:NE2	13:p:236:GLU:OE2	2.43	0.51
26:D1:171:PHE:HA	26:D1:174:ARG:HB2	1.92	0.51
27:2:76:PRO:HB2	27:2:79:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:M1:59:ASP:OD2	46:M1:245:ARG:NH2	2.43	0.51
51:Z1:68:ILE:HD11	53:b1:49:PRO:HB2	1.93	0.51
2:M:381:GLU:OE2	2:M:385:GLN:NE2	2.41	0.51
19:v:72:GLN:HA	19:v:75:LYS:HE3	1.92	0.51
22:z:39:SER:O	22:z:40:TYR:C	2.53	0.51
26:D1:94:LYS:HD2	26:D1:102:TYR:HE2	1.75	0.51
26:D1:149:ASN:HD21	26:D1:371:LYS:HG3	1.76	0.51
29:3:243:ARG:HG2	29:3:244:THR:HG23	1.92	0.51
42:H1:302:MET:HE3	53:b1:28:ALA:HB3	1.92	0.51
45:L1:365:ILE:HG13	45:L1:366:MET:HG3	1.92	0.51
46:M1:155:ILE:HG22	73:M1:501:PC1:H3I3	1.91	0.51
24:6:52:ARG:NH2	68:6:202:3PE:O32	2.44	0.51
36:V1:34:LEU:HD11	36:V1:47:THR:HG23	1.92	0.51
43:J1:19:LEU:HD22	43:J1:32:LEU:HD13	1.93	0.51
43:J1:161:ALA:O	43:J1:165:ILE:HG12	2.11	0.51
54:c1:19:LEU:HB3	68:d1:203:3PE:H252	1.91	0.51
9:J:4:THR:HG23	9:J:6:PRO:HD2	1.93	0.51
3:N:5:ARG:NH1	3:N:15:ASN:OD1	2.43	0.51
13:p:144:ILE:HD11	13:p:166:THR:HG21	1.92	0.51
18:u:38:ARG:HA	18:u:41:LYS:HG2	1.93	0.51
21:y:26:THR:HG23	22:z:25:CYS:HB2	1.92	0.51
31:P1:319:ARG:NH1	37:W1:53:GLN:OE1	2.43	0.51
58:g1:48:ASP:HB3	58:g1:51:VAL:HG22	1.91	0.51
6:Q:43:VAL:O	6:Q:47:ILE:HG12	2.10	0.51
68:p:301:3PE:H321	68:p:301:3PE:H241	1.93	0.51
29:3:243:ARG:HB3	29:3:248:MET:HE3	1.91	0.51
29:3:546:GLN:HE22	29:3:596:ASP:HA	1.76	0.51
43:J1:165:ILE:HG23	47:N1:42:PRO:HG3	1.93	0.51
58:g1:96:LYS:NZ	67:p1:5:ASP:OD2	2.37	0.51
16:s:56:LYS:HA	16:s:75:LEU:O	2.10	0.51
25:C1:151:ILE:HG23	25:C1:152:LEU:HG	1.92	0.51
29:3:377:VAL:HG12	29:3:450:MET:HB3	1.92	0.51
29:3:571:ALA:O	29:3:582:GLN:HA	2.10	0.51
42:H1:79:LEU:HD22	42:H1:222:LEU:HD22	1.93	0.51
47:N1:3:PRO:HG3	48:O1:5:LEU:HD11	1.92	0.51
57:f1:56:TRP:NE1	59:h1:88:GLU:OE1	2.38	0.51
59:h1:69:HIS:NE2	69:h1:201:CDL:OA3	2.44	0.51
3:C:129:MET:HE1	3:C:185:LEU:HD12	1.94	0.50
3:N:49:LEU:HG	3:N:53:MET:HE3	1.93	0.50
3:N:361:ILE:HA	3:N:365:LEU:HB2	1.92	0.50
13:p:120:GLY:CA	17:t:49:TYR:CE2	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C1:41:GLN:NE2	25:C1:49:GLU:OE1	2.42	0.50
26:D1:35:ASP:O	47:N1:49:ASN:ND2	2.44	0.50
26:D1:154:VAL:HG13	26:D1:297:TYR:HE1	1.76	0.50
33:7:43:LEU:HD11	38:q1:107:LYS:HE2	1.92	0.50
45:L1:9:LEU:HD11	60:i1:89:MET:HE1	1.93	0.50
46:M1:458:THR:O	67:p1:149:TYR:OH	2.29	0.50
17:t:55:ARG:NH1	17:t:59:PHE:CE2	2.79	0.50
26:D1:19:MET:HE2	47:N1:173:THR:HG22	1.93	0.50
28:1:214:GLY:N	28:1:218:CYS:O	2.44	0.50
45:L1:173:LEU:HD13	46:M1:405:MET:HE3	1.93	0.50
46:M1:85:LYS:HE2	46:M1:86:LYS:HE3	1.93	0.50
49:X1:29:HIS:HB3	49:X1:119:PRO:HD2	1.93	0.50
2:B:78:LYS:HB2	2:B:129:ALA:HB1	1.93	0.50
1:L:156:THR:O	1:L:239:SER:OG	2.30	0.50
2:M:47:ILE:HD11	2:M:211:VAL:HG11	1.94	0.50
11:n:513:VAL:HB	16:s:40:ALA:HB2	1.93	0.50
13:p:12:ASN:HB2	23:w:20:VAL:HG12	1.93	0.50
2:B:78:LYS:HE2	2:B:129:ALA:HB1	1.94	0.50
3:C:132:VAL:HG11	3:C:178:PHE:HD2	1.74	0.50
6:F:75:LEU:O	6:F:80:TRP:NE1	2.44	0.50
7:G:73:ASN:HB3	7:G:76:MET:HE1	1.93	0.50
1:L:366:VAL:HG11	2:M:43:PRO:HB2	1.93	0.50
3:N:331:ASN:ND2	3:N:357:SER:OG	2.44	0.50
11:n:229:ILE:HD11	12:o:175:ILE:HG21	1.93	0.50
11:n:287:VAL:O	11:n:290:HIS:ND1	2.44	0.50
43:J1:57:LEU:HA	43:J1:60:LEU:HD12	1.94	0.50
63:l1:99:VAL:HA	63:l1:102:LYS:HE3	1.94	0.50
1:A:156:THR:O	1:A:239:SER:OG	2.25	0.50
43:J1:22:LYS:NZ	44:K1:18:GLY:O	2.41	0.50
63:l1:14:ARG:NH1	63:l1:38:ASP:OD2	2.43	0.50
10:K:14:ALA:O	10:K:18:ILE:HG12	2.12	0.50
2:M:24:LEU:HD12	2:M:38:LEU:HB2	1.92	0.50
4:O:228:SER:O	7:R:23:GLN:NE2	2.45	0.50
11:n:510:TYR:HB3	16:s:59:VAL:HG23	1.93	0.50
12:o:122:MET:HG2	12:o:206:PHE:HB3	1.94	0.50
12:o:186:SER:HG	12:o:213:MET:HE2	1.76	0.50
16:s:62:ILE:HG12	16:s:70:VAL:HG12	1.94	0.50
26:D1:184:VAL:HG22	26:D1:207:LEU:HD21	1.93	0.50
33:7:20:GLU:O	33:7:25:ARG:NH2	2.41	0.50
14:q:47:ASP:HB3	14:q:50:SER:HB2	1.93	0.50
31:P1:79:ASP:OD1	31:P1:82:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:T1:12:LYS:HD3	35:T1:77:VAL:HG11	1.94	0.50
42:H1:104:PHE:HD1	68:Z1:401:3PE:H322	1.77	0.50
42:H1:316:PRO:HG3	51:Z1:56:ARG:HB3	1.93	0.50
45:L1:136:ASN:HD21	69:h1:201:CDL:H261	1.77	0.50
26:D1:278:TYR:HA	26:D1:281:VAL:HG12	1.94	0.50
28:1:342:ASP:OD1	28:1:429:ARG:NH2	2.39	0.50
41:A1:48:ARG:NH2	42:H1:121:TRP:O	2.45	0.50
47:N1:216:PHE:O	47:N1:220:MET:HG3	2.11	0.50
65:n1:169:ILE:O	65:n1:172:ARG:NH1	2.44	0.50
68:N:404:3PE:O14	7:R:44:ARG:NH1	2.45	0.50
4:O:69:GLU:HG2	4:O:82:MET:HE2	1.93	0.50
13:p:29:SER:O	13:p:33:MET:HG2	2.12	0.50
15:r:91:PRO:O	15:r:95:GLU:HB2	2.12	0.50
26:D1:412:ALA:HB3	42:H1:281:ARG:HD3	1.92	0.50
29:3:215:PHE:CG	30:9:106:ARG:HB3	2.46	0.50
45:L1:530:PRO:O	45:L1:534:HIS:HB2	2.11	0.50
48:O1:106:LEU:HD13	48:O1:270:LEU:HD11	1.94	0.50
35:U1:17:TYR:OH	62:k1:27:TRP:NE1	2.38	0.50
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.93	0.49
5:E:74:ILE:HG21	5:E:195:VAL:H	1.75	0.49
48:O1:281:GLU:HG3	58:g1:22:MET:HE2	1.94	0.49
48:O1:320:LYS:O	55:d1:60:ARG:NH2	2.45	0.49
65:n1:161:ASP:OD1	65:n1:162:LEU:N	2.46	0.49
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.93	0.49
13:p:90:GLU:HG2	13:p:207:HIS:CE1	2.47	0.49
24:6:91:ARG:HD2	42:H1:61:MET:HG3	1.92	0.49
26:D1:352:TYR:HD1	30:9:88:ILE:HG12	1.77	0.49
45:L1:401:THR:HG21	45:L1:482:MET:HE2	1.94	0.49
69:L1:703:CDL:H311	69:L1:703:CDL:H152	1.92	0.49
46:M1:279:GLN:HG3	46:M1:281:ASP:H	1.77	0.49
3:C:185:LEU:HD23	3:C:188:ILE:HD12	1.94	0.49
25:C1:137:MET:HB3	25:C1:162:PHE:HB2	1.93	0.49
28:1:68:ARG:CD	28:1:254:LYS:HZ3	2.24	0.49
45:L1:343:SER:HA	45:L1:346:ILE:HD12	1.93	0.49
2:B:102:ARG:HH22	2:B:161:GLU:HG2	1.76	0.49
2:B:313:ASN:O	5:T:8:SER:OG	2.31	0.49
12:o:54:SER:OG	12:o:55:THR:N	2.45	0.49
25:C1:88:ASN:HA	25:C1:112:ASP:HB3	1.94	0.49
26:D1:48:THR:O	42:H1:126:LYS:NZ	2.45	0.49
29:3:432:ILE:HG13	29:3:440:CYS:HB2	1.95	0.49
45:L1:481:THR:OG1	66:o1:91:HIS:ND1	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:M1:30:TYR:O	46:M1:34:ILE:HG12	2.13	0.49
49:X1:46:ARG:NH1	51:Z1:79:ASP:OD2	2.45	0.49
1:A:59:LEU:HD13	1:A:186:LEU:HD13	1.95	0.49
3:C:8:HIS:HB3	3:C:11:PHE:HB2	1.94	0.49
1:L:188:ARG:NH2	64:m1:24:VAL:O	2.46	0.49
1:L:354:VAL:HG22	1:L:407:LEU:HD13	1.95	0.49
6:Q:41:GLU:N	6:Q:41:GLU:OE1	2.43	0.49
29:3:36:GLN:NE2	32:Q1:47:SER:O	2.43	0.49
29:3:242:THR:HG22	29:3:247:VAL:HA	1.94	0.49
42:H1:195:ARG:HH22	42:H1:274:ARG:HD2	1.78	0.49
46:M1:106:LEU:HD13	46:M1:234:ILE:HG21	1.94	0.49
1:A:244:ARG:NH2	1:A:429:GLU:OE2	2.42	0.49
2:B:46:ARG:NH1	2:B:110:GLU:OE1	2.43	0.49
2:B:76:THR:HG23	2:B:81:SER:HA	1.94	0.49
6:Q:101:ARG:NH1	6:Q:105:GLU:OE1	2.45	0.49
12:o:214:VAL:HB	12:o:215:PRO:HD2	1.94	0.49
13:p:16:TRP:CH2	23:w:21:HIS:HB2	2.47	0.49
18:u:56:TYR:HA	18:u:59:VAL:HG12	1.94	0.49
25:C1:92:ILE:HD11	25:C1:140:VAL:HG11	1.94	0.49
45:L1:364:LYS:HD2	62:k1:66:ILE:HD11	1.94	0.49
73:M1:501:PC1:H3F1	73:M1:501:PC1:H2B2	1.93	0.49
3:C:30:TRP:HZ3	3:C:96:LEU:HD22	1.77	0.49
4:D:234:LYS:HB2	7:G:16:TYR:HB2	1.95	0.49
11:n:512:LYS:HG3	11:n:514:LYS:H	1.77	0.49
17:t:69:PHE:O	68:t:101:3PE:H122	2.13	0.49
26:D1:106:LEU:HD13	26:D1:391:ILE:HG21	1.95	0.49
38:q1:106:ARG:HB2	38:q1:109:ILE:HG13	1.93	0.49
46:M1:11:LEU:HB3	46:M1:100:ILE:HD13	1.95	0.49
46:M1:116:ILE:HG12	46:M1:174:LEU:HD22	1.95	0.49
35:U1:42:LEU:HD23	35:U1:46:ASP:HB3	1.95	0.49
50:Y1:94:CYS:HA	50:Y1:114:CYS:HA	1.94	0.49
5:E:47:VAL:HG21	73:E:202:PC1:H352	1.95	0.49
11:n:85:LEU:HA	11:n:505:PHE:HE2	1.77	0.49
13:p:73:PRO:HD2	16:s:21:ILE:HD11	1.94	0.49
22:z:28:LEU:CD2	68:z:102:3PE:C27	2.91	0.49
26:D1:342:MET:HE2	29:3:101:HIS:HD2	1.77	0.49
45:L1:534:HIS:HB3	68:L1:701:3PE:H2	1.94	0.49
47:N1:239:ALA:HB1	55:d1:47:MET:HG2	1.95	0.49
48:O1:135:LEU:HD22	48:O1:152:TYR:CD1	2.47	0.49
11:n:54:TYR:HA	11:n:57:ILE:HD12	1.94	0.49
11:n:428:GLN:HG3	11:n:431:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D1:180:PHE:O	26:D1:184:VAL:HG23	2.13	0.49
29:3:237:ASN:HD21	29:3:255:HIS:HB2	1.77	0.49
73:M1:501:PC1:H2	47:N1:276:LEU:HD22	1.95	0.49
4:D:11:PRO:HG2	8:H:72:PHE:HB2	1.94	0.49
3:N:165:TRP:O	3:N:174:THR:OG1	2.28	0.49
7:R:51:PRO:O	7:R:55:VAL:HG23	2.12	0.49
11:n:329:GLY:HA2	19:v:15:LEU:HD21	1.95	0.49
22:z:36:HIS:HB2	22:z:40:TYR:CE2	2.46	0.49
25:C1:53:HIS:ND1	25:C1:55:ASP:OD1	2.46	0.49
31:P1:169:SER:OG	31:P1:170:ASP:N	2.46	0.49
42:H1:86:TRP:HZ2	42:H1:232:ILE:HG22	1.78	0.49
68:A:501:3PE:H342	3:C:229:ILE:HD11	1.95	0.48
73:K:101:PC1:H242	3:N:156:ILE:HD12	1.95	0.48
17:t:50:PRO:CD	18:u:80:THR:HG22	2.36	0.48
27:2:150:ASN:HB3	27:2:162:GLU:HB3	1.95	0.48
38:q1:117:VAL:O	38:q1:120:THR:OG1	2.25	0.48
45:L1:142:ILE:HA	46:M1:370:PRO:HB2	1.94	0.48
35:U1:21:LEU:HD13	62:k1:53:ASN:HA	1.95	0.48
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.46	0.48
1:L:128:GLU:OE2	1:L:131:ARG:NH1	2.46	0.48
13:p:59:ARG:HA	73:p:302:PC1:H221	1.96	0.48
64:m1:28:THR:O	64:m1:32:GLN:HG3	2.13	0.48
1:L:52:ASN:HA	1:L:177:LEU:HD21	1.95	0.48
11:n:383:MET:O	11:n:387:PHE:HB2	2.13	0.48
21:y:26:THR:CG2	22:z:25:CYS:HB2	2.42	0.48
24:6:189:ARG:NH1	84:P1:501:NDP:O2X	2.45	0.48
29:3:385:ARG:HB2	29:3:415:LEU:HD12	1.95	0.48
31:P1:322:ARG:HG3	31:P1:327:LEU:HD12	1.95	0.48
35:U1:49:GLU:HB3	62:k1:50:TRP:HE1	1.78	0.48
69:R:303:CDL:OA7	50:Y1:103:ARG:NH1	2.47	0.48
11:n:368:HIS:NE2	11:n:369:ASP:OD2	2.47	0.48
24:6:92:GLN:NE2	42:H1:215:TYR:O	2.46	0.48
42:H1:245:PRO:HB3	42:H1:258:ASN:HB3	1.94	0.48
45:L1:338:MET:HB2	45:L1:457:LEU:HB3	1.96	0.48
45:L1:341:MET:HE1	45:L1:453:PRO:HB2	1.95	0.48
45:L1:357:ARG:HG2	65:n1:31:ILE:HG12	1.96	0.48
45:L1:554:ASP:OD1	46:M1:213:HIS:NE2	2.46	0.48
2:M:77:THR:HG22	2:M:130:PRO:HA	1.95	0.48
11:n:478:SER:O	22:z:6:ALA:HB1	2.14	0.48
26:D1:337:GLU:O	26:D1:341:SER:HB3	2.14	0.48
29:3:114:CYS:HB3	29:3:117:GLN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:P1:264:SER:HB3	31:P1:281:LYS:HG3	1.95	0.48
36:V1:75:GLU:HB2	36:V1:78:GLU:HG3	1.95	0.48
42:H1:215:TYR:HD2	42:H1:219:PRO:HB2	1.78	0.48
2:B:152:PHE:O	2:B:158:ARG:NH1	2.47	0.48
1:L:305:GLN:HB3	1:L:325:VAL:HG13	1.95	0.48
11:n:192:ALA:HA	11:n:195:LEU:HD12	1.94	0.48
15:r:37:VAL:HA	15:r:74:LYS:HE3	1.95	0.48
24:6:62:LEU:HB2	24:6:100:GLY:HA3	1.95	0.48
28:1:82:MET:HB2	28:1:129:MET:HB3	1.95	0.48
1:A:349:ALA:O	1:A:408:ARG:NH2	2.46	0.48
12:o:83:ILE:HG22	12:o:87:MET:HE1	1.96	0.48
25:C1:204:GLU:OE1	25:C1:210:ARG:NH1	2.43	0.48
29:3:284:VAL:HG12	29:3:559:VAL:HG22	1.96	0.48
31:P1:180:ASN:O	31:P1:184:ASN:HB2	2.14	0.48
34:S1:23:CYS:O	34:S1:33:ARG:NH1	2.41	0.48
46:M1:36:LEU:HB2	58:g1:67:VAL:HG22	1.95	0.48
59:h1:62:GLU:O	59:h1:65:GLU:HB2	2.14	0.48
8:S:19:ARG:O	8:S:23:GLU:HG2	2.13	0.48
13:p:42:LEU:HD22	23:w:49:LEU:HD12	1.96	0.48
30:9:116:THR:HG22	30:9:149:LEU:HD23	1.95	0.48
32:Q1:36:ARG:NH1	32:Q1:106:GLU:OE2	2.42	0.48
44:K1:41:PHE:HA	44:K1:63:ILE:HD11	1.94	0.48
45:L1:135:ASN:ND2	45:L1:197:GLU:OE1	2.46	0.48
45:L1:172:ILE:O	45:L1:176:ARG:HG2	2.14	0.48
46:M1:76:MET:HE3	46:M1:230:ILE:HD13	1.95	0.48
66:o1:67:LYS:NZ	66:o1:71:ASP:OD2	2.44	0.48
3:C:30:TRP:NE1	69:C:404:CDL:O1	2.47	0.48
1:L:343:MET:HA	1:L:346:CYS:HB2	1.96	0.48
10:V:33:VAL:HG12	10:V:38:TRP:HE3	1.79	0.48
11:n:18:LEU:HB3	11:n:102:PHE:CZ	2.48	0.48
11:n:216:ASN:ND2	17:t:55:ARG:HD2	2.29	0.48
14:q:126:MET:HE1	19:v:70:ILE:HD13	1.95	0.48
21:y:18:LYS:HD3	22:z:8:GLU:CD	2.39	0.48
27:2:51:LEU:HD21	27:2:84:ALA:HB2	1.96	0.48
29:3:8:LEU:HA	29:3:22:PRO:HD3	1.96	0.48
29:3:632:ARG:HH22	34:S1:59:GLU:H	1.61	0.48
45:L1:233:LEU:HD11	45:L1:248:HIS:HB3	1.95	0.48
49:X1:82:THR:HA	49:X1:85:TRP:CD1	2.49	0.48
59:h1:7:ARG:NH2	60:i1:28:SER:O	2.47	0.48
1:L:158:PHE:O	1:L:161:THR:OG1	2.32	0.48
11:n:347:LEU:HD22	11:n:383:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:W1:94:GLU:HG2	37:W1:100:LYS:HG3	1.96	0.48
3:C:100:ARG:NH1	70:C:402:HEM:O2A	2.47	0.47
11:n:218:THR:CG2	17:t:54:ILE:CD1	2.82	0.47
13:p:157:ASN:OD1	13:p:158:HIS:N	2.46	0.47
14:q:94:LEU:HA	14:q:97:ILE:HD12	1.95	0.47
24:6:185:ILE:HG21	31:P1:51:CYS:HA	1.95	0.47
33:7:68:HIS:ND1	33:7:69:PRO:O	2.43	0.47
52:a1:14:VAL:O	52:a1:18:ILE:HG12	2.13	0.47
11:n:83:VAL:HA	11:n:86:MET:HB2	1.96	0.47
26:D1:3:GLN:NE2	46:M1:135:ARG:O	2.46	0.47
29:3:387:GLU:HG2	29:3:495:ARG:HD2	1.96	0.47
36:V1:53:GLU:HG2	36:V1:57:MET:HE2	1.96	0.47
44:K1:1:FME:HE1	47:N1:79:LYS:HE2	1.95	0.47
1:A:122:LEU:O	1:A:179:ARG:NE	2.39	0.47
2:B:52:LYS:O	2:B:203:ARG:NH2	2.41	0.47
3:C:129:MET:HA	3:C:132:VAL:HG12	1.96	0.47
6:Q:35:ASP:OD1	6:Q:89:TYR:OH	2.27	0.47
14:q:133:GLY:O	14:q:137:LYS:NZ	2.47	0.47
26:D1:286:PRO:HG2	26:D1:303:GLU:HB3	1.96	0.47
69:H1:402:CDL:H162	43:J1:92:LEU:HD21	1.97	0.47
45:L1:69:VAL:HG11	45:L1:71:MET:HE3	1.95	0.47
45:L1:139:GLN:HA	45:L1:142:ILE:HD12	1.95	0.47
46:M1:17:LEU:HD11	69:N1:401:CDL:H141	1.95	0.47
47:N1:122:ILE:O	47:N1:176:ARG:NH1	2.46	0.47
35:U1:22:TYR:CE2	35:U1:24:LYS:HB2	2.49	0.47
58:g1:83:MET:HE1	67:p1:93:ARG:HG2	1.97	0.47
1:L:245:ASP:HA	7:R:11:ARG:HA	1.96	0.47
11:n:69:MET:HE2	76:n:603:HEA:H18	1.97	0.47
11:n:154:GLY:HA2	11:n:199:LEU:HD12	1.97	0.47
14:q:24:LEU:HD23	15:r:30:ARG:HG2	1.95	0.47
42:H1:189:THR:HG22	42:H1:234:MET:HE2	1.95	0.47
44:K1:97:GLN:HB3	45:L1:582:GLY:HA3	1.95	0.47
45:L1:100:ILE:HG21	45:L1:246:LEU:HB2	1.96	0.47
46:M1:207:MET:HG2	46:M1:298:ILE:HG13	1.96	0.47
35:U1:35:HIS:HB3	35:U1:38:LYS:HB2	1.95	0.47
1:A:363:ASN:HD21	2:B:111:GLY:HA2	1.79	0.47
11:n:80:ASN:OD1	11:n:98:ASN:ND2	2.41	0.47
28:1:365:CYS:O	28:1:369:VAL:HB	2.14	0.47
29:3:163:ALA:HA	29:3:167:ALA:HB3	1.96	0.47
29:3:380:VAL:HG22	29:3:409:ILE:HD13	1.97	0.47
41:A1:98:LEU:HD22	42:H1:298:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:O1:30:ASN:O	48:O1:126:ARG:NH2	2.47	0.47
60:i1:84:TYR:HB2	68:i1:201:3PE:H272	1.96	0.47
7:G:26:PHE:HB3	7:G:29:TYR:HB2	1.95	0.47
8:H:19:ARG:HG2	8:H:63:ARG:HD3	1.96	0.47
2:M:366:ALA:O	2:M:370:MET:HG3	2.14	0.47
11:n:168:ILE:HD13	11:n:189:LEU:HB2	1.97	0.47
25:C1:112:ASP:OD1	25:C1:112:ASP:N	2.48	0.47
27:2:27:ASN:O	27:2:31:ILE:HG12	2.14	0.47
28:1:378:ARG:HG3	28:1:383:ASP:HB3	1.95	0.47
31:P1:311:GLU:HG2	31:P1:336:PRO:HB3	1.95	0.47
45:L1:549:SER:OG	46:M1:271:MET:SD	2.67	0.47
1:A:232:THR:HB	5:E:22:THR:HG23	1.96	0.47
3:C:315:LEU:O	3:C:322:GLN:NE2	2.41	0.47
68:C:406:3PE:H272	10:V:35:ALA:HB1	1.97	0.47
8:H:67:VAL:O	8:H:71:LEU:N	2.44	0.47
3:N:45:ILE:HG12	70:N:402:HEM:HBB1	1.95	0.47
11:n:199:LEU:HD13	11:n:202:LEU:HD21	1.96	0.47
12:o:170:LEU:HD22	12:o:182:ALA:HB1	1.96	0.47
15:r:101:PRO:HA	15:r:104:LEU:HG	1.97	0.47
17:t:31:ASN:O	17:t:35:LYS:HG2	2.15	0.47
24:6:101:THR:HA	24:6:129:CYS:HB3	1.96	0.47
29:3:441:GLU:HA	29:3:444:LYS:HG3	1.96	0.47
73:9:204:PC1:H112	51:Z1:28:GLY:HA3	1.96	0.47
31:P1:90:VAL:HG11	31:P1:218:THR:HG22	1.97	0.47
33:7:18:TYR:OH	33:7:27:ARG:NH1	2.47	0.47
35:T1:43:ASP:OD1	35:T1:44:SER:N	2.46	0.47
42:H1:185:TRP:O	42:H1:189:THR:HG23	2.15	0.47
43:J1:47:GLY:HA3	44:K1:49:LEU:HD22	1.95	0.47
3:C:50:PHE:HA	3:C:53:MET:HE3	1.96	0.47
11:n:211:THR:HG23	11:n:215:LEU:HD12	1.96	0.47
11:n:363:LEU:O	11:n:367:LEU:HB3	2.15	0.47
13:p:63:ARG:NH2	23:w:28:ASP:OD2	2.45	0.47
27:2:30:ARG:NH2	40:s1:47:ASP:OD1	2.47	0.47
28:1:215:VAL:H	28:1:220:THR:HG21	1.80	0.47
48:O1:41:GLU:HG2	48:O1:231:PRO:HG2	1.97	0.47
67:p1:107:GLU:HA	67:p1:110:LYS:HE2	1.96	0.47
3:C:201:HIS:O	7:G:2:ARG:NH1	2.48	0.47
8:H:35:LEU:O	8:H:38:CYS:HB3	2.14	0.47
2:M:279:LEU:HB3	2:M:295:LEU:HD13	1.97	0.47
11:n:96:ARG:HD2	13:p:57:TRP:NE1	2.29	0.47
11:n:431:LEU:HD21	11:n:450:TRP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:v:18:ARG:O	19:v:22:HIS:ND1	2.47	0.47
45:L1:419:THR:HA	45:L1:422:TYR:CE2	2.49	0.47
48:O1:156:LYS:O	48:O1:160:LEU:HB2	2.15	0.47
49:X1:71:ARG:NH1	52:a1:70:ASP:OD1	2.48	0.47
64:m1:14:PRO:HG2	64:m1:17:LEU:HD12	1.97	0.47
3:C:278:TYR:O	3:C:282:ARG:HG3	2.15	0.47
5:E:88:ALA:HA	5:E:96:LEU:O	2.15	0.47
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.24	0.47
2:M:95:LYS:O	2:M:109:VAL:HA	2.14	0.47
9:U:40:ASP:O	9:U:44:GLU:HG2	2.15	0.47
11:n:479:LYS:O	22:z:7:ARG:HG2	2.15	0.47
12:o:150:ILE:HB	12:o:184:VAL:HG13	1.97	0.47
13:p:67:TYR:HA	23:w:9:GLN:HG2	1.96	0.47
22:z:20:THR:O	22:z:21:SER:C	2.58	0.47
28:1:276:LEU:HD21	28:1:297:VAL:HG11	1.96	0.47
35:T1:12:LYS:HE2	35:T1:77:VAL:HG21	1.97	0.47
42:H1:42:PRO:HD2	42:H1:45:ILE:HG12	1.96	0.47
48:O1:51:TYR:HB2	48:O1:124:LEU:HD23	1.97	0.47
50:Y1:19:ARG:O	50:Y1:23:ILE:HG13	2.15	0.47
12:o:79:PRO:HA	12:o:82:ARG:HB2	1.97	0.46
13:p:68:GLN:HE21	13:p:70:HIS:CE1	2.32	0.46
15:r:29:LEU:HD13	15:r:58:LEU:HD22	1.96	0.46
34:S1:21:HIS:O	34:S1:62:PRO:HA	2.14	0.46
45:L1:107:TYR:HD2	45:L1:108:MET:HG2	1.80	0.46
2:B:181:TYR:CZ	2:B:182:ARG:HG2	2.51	0.46
12:o:13:THR:OG1	12:o:188:ARG:NH2	2.47	0.46
13:p:228:THR:OG1	13:p:229:SER:N	2.46	0.46
28:1:202:LYS:O	32:Q1:133:LYS:NZ	2.46	0.46
29:3:71:MET:HE2	29:3:77:TRP:HH2	1.81	0.46
31:P1:280:THR:H	31:P1:283:LYS:HB3	1.81	0.46
42:H1:199:ASP:OD1	42:H1:200:LEU:N	2.45	0.46
48:O1:133:VAL:HG21	48:O1:206:TYR:HE1	1.80	0.46
61:j1:10:ARG:HG3	61:j1:15:PRO:HA	1.98	0.46
3:C:51:LEU:O	3:C:55:TYR:CB	2.63	0.46
3:C:51:LEU:HD13	70:C:401:HEM:HBA1	1.97	0.46
2:M:318:ASP:N	2:M:318:ASP:OD1	2.47	0.46
31:P1:105:ASP:OD1	31:P1:105:ASP:N	2.44	0.46
41:A1:74:PRO:HG3	43:J1:141:VAL:HG12	1.97	0.46
46:M1:75:LEU:HD23	46:M1:440:HIS:CE1	2.50	0.46
46:M1:403:THR:HA	46:M1:406:TYR:CE2	2.50	0.46
49:X1:168:PHE:HE2	69:d1:201:CDL:H542	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:g1:73:THR:HG21	59:h1:36:VAL:HG11	1.96	0.46
9:J:33:ARG:CZ	9:J:37:GLN:HE21	2.29	0.46
2:M:164:HIS:NE2	2:M:316:TYR:OH	2.43	0.46
15:r:83:PRO:HA	15:r:86:ILE:HG22	1.97	0.46
23:w:6:PRO:HA	23:w:9:GLN:HB2	1.97	0.46
26:D1:151:ILE:HD12	26:D1:170:MET:HB3	1.96	0.46
68:D1:501:3PE:H3C2	73:M1:501:PC1:H3H1	1.97	0.46
44:K1:1:FME:HE2	44:K1:1:FME:HB2	1.69	0.46
1:A:39:VAL:HG23	1:A:113:LEU:HD13	1.98	0.46
6:F:53:ASP:OD1	6:F:54:LEU:N	2.48	0.46
2:M:107:TYR:HB3	2:M:123:LEU:HD11	1.97	0.46
11:n:116:SER:O	21:y:43:GLN:NE2	2.43	0.46
12:o:138:VAL:HG12	12:o:140:ASN:H	1.81	0.46
13:p:149:HIS:HD1	17:t:13:TRP:CD1	2.34	0.46
29:3:349:PHE:H	29:3:509:PRO:HB2	1.79	0.46
37:W1:92:LEU:O	37:W1:96:ILE:HG12	2.16	0.46
37:W1:103:THR:O	37:W1:107:ARG:HG3	2.16	0.46
45:L1:548:THR:O	45:L1:552:LEU:HB3	2.15	0.46
63:l1:29:ARG:NH1	63:l1:32:ASP:OD2	2.44	0.46
1:L:57:TYR:OH	1:L:137:GLU:OE2	2.20	0.46
11:n:381:LEU:HD13	76:n:604:HEA:HBC2	1.98	0.46
13:p:149:HIS:ND1	17:t:13:TRP:CD1	2.83	0.46
22:z:28:LEU:HD23	68:z:102:3PE:H261	1.98	0.46
25:C1:37:VAL:HA	25:C1:52:ILE:HG22	1.98	0.46
30:9:110:ARG:HH21	32:Q1:72:TRP:CD1	2.33	0.46
41:A1:10:ASN:HD21	42:H1:83:LEU:HB2	1.80	0.46
45:L1:367:PRO:HG2	61:j1:22:VAL:HG12	1.96	0.46
48:O1:151:HIS:CE1	48:O1:282:ILE:HD13	2.51	0.46
63:l1:131:GLN:OE1	63:l1:154:HIS:ND1	2.49	0.46
64:m1:114:LEU:HB3	64:m1:120:LEU:HB2	1.98	0.46
11:n:165:ILE:O	11:n:169:ILE:HG12	2.16	0.46
13:p:151:LEU:HD21	13:p:159:MET:HE2	1.96	0.46
31:P1:309:PRO:HG2	31:P1:312:LEU:HB2	1.98	0.46
42:H1:6:ILE:O	42:H1:10:LEU:HB2	2.15	0.46
45:L1:83:ASP:H	45:L1:86:SER:HB2	1.81	0.46
47:N1:170:LEU:HD22	47:N1:288:LEU:HD11	1.96	0.46
9:J:13:LEU:HB3	9:J:23:THR:HG21	1.98	0.46
12:o:52:HIS:CG	15:r:40:ASP:HB2	2.51	0.46
26:D1:17:ALA:HB2	26:D1:31:PRO:HD3	1.98	0.46
73:9:204:PC1:H2E2	42:H1:175:LEU:HD21	1.97	0.46
45:L1:418:MET:HA	45:L1:421:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:M1:225:ILE:O	46:M1:229:MET:HG2	2.16	0.46
47:N1:336:THR:HG23	47:N1:339:LEU:HD12	1.98	0.46
48:O1:221:LEU:HD11	48:O1:241:LEU:HD11	1.98	0.46
1:A:134:ILE:O	1:A:138:MET:HG3	2.16	0.46
6:F:22:ASN:O	6:F:28:LYS:NZ	2.49	0.46
11:n:225:GLY:HA3	13:p:112:LEU:HD21	1.98	0.46
68:o:302:3PE:O12	19:v:45:ARG:NH2	2.49	0.46
15:r:82:TYR:HA	15:r:85:VAL:HG22	1.98	0.46
26:D1:275:TYR:CZ	26:D1:367:ILE:HG23	2.51	0.46
27:2:60:TRP:CD1	27:2:60:TRP:H	2.34	0.46
38:q1:60:ARG:HH22	38:q1:95:ASP:HA	1.81	0.46
41:A1:65:PHE:HZ	41:A1:102:LEU:HB2	1.80	0.46
42:H1:179:TRP:HE1	51:Z1:42:LEU:HG	1.80	0.46
47:N1:250:SER:HB2	47:N1:257:LEU:HD12	1.96	0.46
54:c1:7:PRO:HD2	54:c1:10:ALA:HB2	1.98	0.46
1:A:237:THR:HG21	5:E:14:ARG:HH22	1.81	0.46
11:n:481:GLU:HB3	22:z:4:LYS:HD2	1.95	0.46
14:q:118:MET:HB3	20:x:53:TRP:HB3	1.97	0.46
15:r:60:ASP:HB3	15:r:63:SER:HB2	1.96	0.46
25:C1:8:ARG:NH1	39:r1:61:GLU:OE1	2.44	0.46
29:3:266:LYS:O	29:3:270:ALA:HB3	2.15	0.46
47:N1:28:LEU:HA	47:N1:31:VAL:HG22	1.98	0.46
1:A:276:ILE:HG21	1:A:345:LEU:HD21	1.96	0.45
1:L:439:SER:O	68:L:501:3PE:N	2.38	0.45
15:r:36:LEU:HD21	15:r:43:PRO:HB3	1.97	0.45
42:H1:77:LEU:O	42:H1:81:LEU:HB2	2.16	0.45
42:H1:175:LEU:O	42:H1:179:TRP:HB3	2.15	0.45
45:L1:468:ILE:O	45:L1:472:ILE:HG12	2.16	0.45
47:N1:33:LEU:HD13	47:N1:105:LYS:HE3	1.98	0.45
47:N1:125:HIS:O	47:N1:129:ILE:HG13	2.17	0.45
60:i1:103:ILE:HB	66:o1:47:ASP:HB3	1.98	0.45
3:N:190:ALA:O	3:N:194:ILE:HG12	2.16	0.45
3:N:332:LEU:HD13	68:N:404:3PE:H2C1	1.98	0.45
12:o:13:THR:HG22	12:o:186:SER:HB2	1.97	0.45
30:9:33:ILE:HD12	73:9:204:PC1:H3A2	1.98	0.45
41:A1:29:LEU:HD11	41:A1:34:ALA:HB2	1.97	0.45
42:H1:53:MET:HB3	42:H1:57:MET:HE3	1.98	0.45
42:H1:302:MET:HA	42:H1:305:ILE:HD12	1.99	0.45
2:B:334:GLY:O	2:B:338:ASN:ND2	2.50	0.45
2:B:437:ASP:OD1	2:B:437:ASP:N	2.49	0.45
6:F:18:LYS:HE2	6:F:18:LYS:HB3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:314:ILE:HG23	11:n:315:PRO:HD3	1.99	0.45
12:o:161:HIS:HB2	12:o:174:ALA:HB3	1.99	0.45
13:p:228:THR:HG23	13:p:231:HIS:H	1.81	0.45
14:q:89:ILE:HG22	20:x:29:TRP:HE1	1.81	0.45
22:z:22:CYS:O	22:z:26:CYS:N	2.50	0.45
29:3:32:LYS:HB2	29:3:32:LYS:HE2	1.77	0.45
32:Q1:66:GLU:HG3	32:Q1:71:GLY:HA2	1.98	0.45
35:T1:49:GLU:OE1	37:W1:38:TYR:OH	2.34	0.45
1:A:445:ARG:NE	69:A:502:CDL:OB3	2.50	0.45
2:M:309:VAL:HG23	2:M:326:THR:HG22	1.98	0.45
3:N:207:ASN:HD21	3:N:211:LEU:H	1.64	0.45
28:1:34:LYS:HE2	28:1:34:LYS:HB2	1.84	0.45
29:3:146:VAL:HG22	29:3:200:ILE:HD11	1.99	0.45
38:q1:73:THR:HG21	38:q1:81:MET:HE1	1.99	0.45
45:L1:326:PHE:HA	45:L1:329:ILE:HD12	1.97	0.45
35:U1:49:GLU:OE2	65:n1:19:TYR:OH	2.31	0.45
7:G:72:LYS:HB3	7:G:72:LYS:HE2	1.74	0.45
1:L:192:ALA:HB2	1:L:219:VAL:HB	1.98	0.45
3:N:51:LEU:O	3:N:55:TYR:HB2	2.16	0.45
26:D1:257:GLY:HA3	26:D1:372:GLY:HA2	1.98	0.45
31:P1:172:PHE:HB2	31:P1:179:LEU:HG	1.98	0.45
42:H1:70:LEU:HD11	42:H1:118:TRP:HB3	1.99	0.45
47:N1:186:HIS:O	47:N1:190:MET:HG3	2.17	0.45
48:O1:261:MET:SD	48:O1:264:GLN:NE2	2.89	0.45
49:X1:39:ASN:HB3	51:Z1:72:PRO:HG2	1.98	0.45
58:g1:79:PRO:HG3	59:h1:72:SER:HB3	1.98	0.45
3:C:158:THR:O	3:C:162:GLU:HG3	2.17	0.45
3:C:300:ILE:HD12	3:C:362:ILE:HG21	1.97	0.45
4:D:223:LYS:O	4:D:227:TRP:HB2	2.17	0.45
11:n:21:LEU:HD23	80:y:601:TGL:H111	1.97	0.45
11:n:83:VAL:HG11	11:n:188:VAL:HG11	1.98	0.45
11:n:104:LEU:HD13	11:n:155:VAL:HG23	1.97	0.45
13:p:214:PHE:HZ	68:p:301:3PE:H382	1.81	0.45
28:1:189:GLU:HG3	28:1:222:VAL:HB	1.97	0.45
30:9:59:LEU:HD11	30:9:139:PHE:HE2	1.82	0.45
32:Q1:60:ASP:OD1	32:Q1:60:ASP:N	2.50	0.45
41:A1:75:LEU:O	41:A1:79:ILE:HG12	2.16	0.45
47:N1:125:HIS:HA	47:N1:220:MET:HE2	1.99	0.45
35:U1:11:ILE:HG22	35:U1:77:VAL:HG22	1.98	0.45
4:O:20:SER:OG	4:O:21:LEU:N	2.50	0.45
4:O:195:GLU:OE2	4:O:201:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:398:PRO:HG3	11:n:404:THR:HA	1.99	0.45
11:n:473:TRP:CZ3	22:z:10:LEU:HD13	2.52	0.45
12:o:111:THR:HG23	18:u:62:SER:HA	1.99	0.45
25:C1:169:THR:HG21	25:C1:190:LEU:HD11	1.98	0.45
29:3:272:ASP:OD2	29:3:683:THR:OG1	2.26	0.45
34:S1:50:LEU:HD12	34:S1:51:PRO:HD2	1.98	0.45
41:A1:10:ASN:ND2	42:H1:83:LEU:HB2	2.32	0.45
43:J1:114:VAL:HG23	43:J1:115:ILE:HG13	1.99	0.45
45:L1:176:ARG:O	45:L1:180:ILE:HG12	2.17	0.45
46:M1:78:MET:HE2	46:M1:78:MET:HB3	1.68	0.45
46:M1:379:LEU:O	46:M1:383:MET:HG3	2.16	0.45
47:N1:139:LEU:HD23	47:N1:139:LEU:HA	1.85	0.45
47:N1:238:PRO:HG3	48:O1:293:TYR:HE2	1.82	0.45
5:P:84:GLY:CA	5:P:100:HIS:O	2.65	0.45
11:n:409:TRP:HB3	11:n:471:MET:HE3	1.98	0.45
11:n:456:MET:HE3	20:x:29:TRP:HZ3	1.82	0.45
11:n:473:TRP:CH2	22:z:10:LEU:HD13	2.52	0.45
15:r:104:LEU:HD12	15:r:106:LEU:HD23	1.99	0.45
24:6:68:GLU:HG2	24:6:161:PRO:O	2.17	0.45
24:6:117:MET:HE3	24:6:121:ARG:HB2	1.99	0.45
25:C1:196:LYS:HE2	25:C1:196:LYS:HB3	1.79	0.45
28:1:98:ASP:O	28:1:139:ARG:HG3	2.16	0.45
50:Y1:68:MET:HE3	50:Y1:95:ALA:HB1	1.99	0.45
62:k1:30:GLU:HA	62:k1:35:GLU:OE2	2.17	0.45
1:A:131:ARG:HD3	1:A:175:ARG:HA	1.98	0.45
1:A:328:ALA:HB2	1:A:427:PRO:HB2	1.99	0.45
2:B:309:VAL:HG23	2:B:326:THR:HG22	1.99	0.45
4:O:71:GLN:HE21	4:O:80:MET:HB3	1.81	0.45
28:1:322:LEU:HD12	28:1:329:LEU:HB2	1.99	0.45
29:3:366:THR:HG22	29:3:370:GLY:HA3	1.98	0.45
31:P1:59:LEU:HD23	31:P1:62:MET:HE3	1.99	0.45
35:T1:70:LEU:HD22	35:T1:76:ILE:HA	1.99	0.45
39:r1:17:GLN:NE2	51:Z1:23:ASN:O	2.48	0.45
45:L1:121:LEU:HD22	45:L1:246:LEU:HD23	1.99	0.45
46:M1:319:HIS:HA	46:M1:322:THR:HG22	1.98	0.45
1:A:158:PHE:O	1:A:161:THR:OG1	2.29	0.45
12:o:106:TRP:HE1	12:o:207:MET:HB3	1.82	0.45
24:6:186:TRP:HB2	73:6:203:PC1:H11	1.99	0.45
29:3:335:LEU:HB3	29:3:340:SER:HB3	1.98	0.45
42:H1:87:VAL:HG23	42:H1:95:LEU:HD23	2.00	0.45
45:L1:576:LEU:HD11	69:Y1:401:CDL:H521	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:MET:HB2	2:B:436:LEU:HD21	1.99	0.44
5:E:44:THR:OG1	73:E:202:PC1:O32	2.35	0.44
7:G:19:SER:HB2	7:G:22:GLU:HB2	1.99	0.44
10:K:53:LYS:HA	10:K:53:LYS:HD3	1.75	0.44
4:O:101:ALA:O	4:O:105:ASN:HB2	2.17	0.44
9:U:16:ARG:HB2	9:U:19:THR:HG22	1.99	0.44
21:y:36:PRO:HA	21:y:39:ILE:HD12	1.98	0.44
25:C1:137:MET:HE3	25:C1:152:LEU:HB2	1.98	0.44
46:M1:166:LEU:HD13	47:N1:276:LEU:HD21	1.98	0.44
54:c1:41:GLU:OE2	54:c1:45:ARG:HG3	2.18	0.44
1:L:227:ALA:HA	64:m1:24:VAL:HG13	1.98	0.44
1:L:240:GLU:HG2	7:R:17:SER:HB2	1.99	0.44
3:N:214:ASP:HA	3:N:217:LYS:HD2	1.99	0.44
5:P:144:CYS:HB3	5:P:160:CYS:HB2	1.96	0.44
6:Q:70:MET:HE3	6:Q:70:MET:HB3	1.89	0.44
7:R:36:ASN:OD1	7:R:39:ARG:NH2	2.49	0.44
12:o:145:PRO:HB2	12:o:148:LEU:HD12	2.00	0.44
26:D1:236:ARG:O	26:D1:240:VAL:HB	2.17	0.44
27:2:53:LEU:HD13	40:s1:46:LEU:HD12	2.00	0.44
28:1:98:ASP:OD2	28:1:187:GLY:HA3	2.18	0.44
31:P1:53:VAL:HA	31:P1:56:ILE:HG12	1.99	0.44
42:H1:26:LYS:HB3	52:a1:5:ILE:HG12	1.99	0.44
45:L1:193:MET:HB3	45:L1:193:MET:HE2	1.71	0.44
48:O1:156:LYS:HE2	48:O1:160:LEU:HD22	2.00	0.44
65:n1:34:ASP:N	65:n1:34:ASP:OD1	2.49	0.44
1:A:355:THR:O	1:A:359:ASN:ND2	2.51	0.44
1:A:411:CYS:O	1:A:415:PHE:HB2	2.17	0.44
3:C:291:VAL:O	3:C:295:ILE:HG12	2.18	0.44
5:P:62:MET:HE3	5:P:62:MET:HB2	1.83	0.44
11:n:476:PHE:HB3	21:y:21:LEU:HD21	1.99	0.44
16:s:47:PRO:HB3	16:s:89:HIS:HB3	2.00	0.44
28:1:268:VAL:HG21	28:1:283:HIS:CD2	2.52	0.44
37:W1:23:PHE:HE2	37:W1:86:ILE:HD11	1.82	0.44
45:L1:414:ILE:HG22	45:L1:418:MET:HE2	2.00	0.44
49:X1:81:PHE:HD2	52:a1:66:LEU:HD11	1.82	0.44
63:l1:69:ARG:HG3	63:l1:85:ARG:HD2	1.99	0.44
5:E:65:SER:OG	5:E:67:ASP:OD1	2.29	0.44
3:N:304:MET:HB2	3:N:304:MET:HE2	1.64	0.44
16:s:80:SER:HA	16:s:90:TYR:O	2.17	0.44
28:1:94:VAL:O	28:1:222:VAL:HA	2.17	0.44
68:L1:704:3PE:H3D1	46:M1:67:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:m1:61:ASP:OD2	64:m1:64:LEU:N	2.47	0.44
2:B:163:LEU:HD11	2:B:258:VAL:HG22	2.00	0.44
2:B:275:LEU:HB2	2:B:410:VAL:HG13	1.99	0.44
2:M:109:VAL:HG22	2:M:123:LEU:HD22	2.00	0.44
11:n:47:LEU:HD11	14:q:103:VAL:HG22	1.99	0.44
11:n:254:ILE:HD11	11:n:388:ALA:HA	2.00	0.44
11:n:366:VAL:HG21	12:o:17:MET:HE1	1.98	0.44
11:n:383:MET:HA	11:n:386:VAL:HB	2.00	0.44
11:n:482:VAL:HA	22:z:3:SER:HA	1.99	0.44
15:r:27:TRP:HZ2	16:s:84:PRO:HA	1.83	0.44
28:1:101:GLU:OE1	28:1:303:SER:N	2.51	0.44
28:1:125:GLY:O	28:1:129:MET:HG3	2.17	0.44
31:P1:38:LEU:HD23	31:P1:41:MET:HE2	1.99	0.44
41:A1:105:GLU:HG3	43:J1:167:ILE:HD11	1.99	0.44
43:J1:21:LEU:HD23	68:K1:201:3PE:H252	1.98	0.44
45:L1:538:PRO:HB2	63:l1:88:VAL:HG22	1.98	0.44
47:N1:312:LYS:HZ2	48:O1:292:ILE:HG21	1.83	0.44
63:l1:137:LEU:HB3	63:l1:140:GLU:HB2	1.99	0.44
1:L:270:LEU:HB3	1:L:320:LEU:HD11	1.99	0.44
2:M:124:LEU:HA	2:M:127:THR:HG22	1.99	0.44
2:M:195:VAL:O	2:M:199:PHE:HB2	2.18	0.44
4:O:126:TYR:OH	71:O:301:HEC:O2A	2.33	0.44
13:p:76:GLN:HA	13:p:79:LEU:HB2	2.00	0.44
25:C1:104:ARG:NH2	26:D1:373:GLU:OE1	2.38	0.44
26:D1:38:ILE:HD11	48:O1:157:ARG:HD2	1.99	0.44
29:3:200:ILE:HD13	29:3:210:SER:HB3	2.00	0.44
43:J1:37:PHE:HE1	68:Z1:401:3PE:H361	1.82	0.44
47:N1:172:GLN:HG3	47:N1:177:LYS:HB3	1.99	0.44
69:N1:401:CDL:H861	69:d1:201:CDL:H651	2.00	0.44
52:a1:2:TRP:NE1	69:a1:101:CDL:OB4	2.41	0.44
4:O:211:MET:HE1	9:U:31:PHE:HE2	1.83	0.44
14:q:52:SER:OG	14:q:55:GLU:OE1	2.22	0.44
19:v:18:ARG:HD2	19:v:18:ARG:HA	1.80	0.44
24:6:66:ALA:HA	24:6:69:MET:HG2	1.99	0.44
25:C1:173:GLU:O	25:C1:185:ALA:HA	2.18	0.44
26:D1:65:VAL:HG23	26:D1:77:ASP:HB3	1.99	0.44
31:P1:134:HIS:HB2	31:P1:149:LYS:HE2	1.99	0.44
42:H1:84:SER:O	42:H1:87:VAL:HG12	2.18	0.44
47:N1:181:TYR:HA	47:N1:184:ILE:HD12	1.99	0.44
48:O1:280:PRO:HA	48:O1:283:THR:HG22	2.00	0.44
35:U1:71:MET:HE2	35:U1:71:MET:HB2	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HB3	69:A:502:CDL:H711	2.00	0.44
5:E:158:CYS:O	5:E:162:GLY:HA2	2.17	0.44
1:L:240:GLU:OE1	1:L:242:ARG:NH1	2.50	0.44
6:Q:45:GLU:OE2	6:Q:48:ARG:NH1	2.50	0.44
16:s:9:THR:HG22	16:s:11:GLU:H	1.83	0.44
16:s:36:PRO:HA	16:s:37:PRO:HD3	1.89	0.44
24:6:78:ASP:OD2	42:H1:34:ARG:HB2	2.17	0.44
26:D1:179:GLU:OE1	39:r1:26:ARG:NH2	2.50	0.44
39:r1:108:ASP:OD2	51:Z1:20:TYR:OH	2.29	0.44
45:L1:519:TYR:HB3	69:L1:703:CDL:H322	1.99	0.44
35:U1:70:LEU:HD22	35:U1:76:ILE:HA	1.99	0.44
3:C:45:ILE:HG12	70:C:401:HEM:HBB1	2.00	0.44
4:O:158:ILE:HG23	4:O:160:MET:H	1.82	0.44
21:y:37:PHE:HA	21:y:40:VAL:HG12	1.99	0.44
25:C1:203:TRP:NE1	29:3:115:ASP:OD1	2.47	0.44
28:l:157:TYR:HD2	40:s1:52:LEU:HD22	1.82	0.44
29:3:47:SER:O	29:3:161:ARG:NH1	2.44	0.44
30:9:108:THR:O	30:9:153:LYS:NZ	2.34	0.44
31:P1:21:ALA:HA	31:P1:90:VAL:O	2.17	0.44
31:P1:194:VAL:H	31:P1:288:HIS:CE1	2.36	0.44
41:A1:67:LEU:HD22	43:J1:58:ILE:HD12	2.00	0.44
43:J1:21:LEU:HD23	43:J1:21:LEU:HA	1.87	0.44
45:L1:306:THR:HG23	45:L1:332:HIS:CE1	2.53	0.44
52:a1:7:PRO:HG3	69:a1:101:CDL:H192	2.00	0.44
11:n:298:ASP:OD2	18:u:22:ASN:ND2	2.51	0.43
11:n:353:LEU:HD13	12:o:31:VAL:HG23	1.99	0.43
12:o:104:TRP:CG	12:o:203:ASN:HB2	2.52	0.43
17:t:43:ARG:HD2	17:t:81:TYR:CE1	2.53	0.43
25:C1:194:PHE:O	32:Q1:81:ASN:ND2	2.47	0.43
26:D1:143:GLU:OE2	26:D1:146:ARG:NH1	2.51	0.43
45:L1:2:ASN:HD21	60:i1:86:LYS:HG3	1.82	0.43
49:X1:46:ARG:NH2	59:h1:142:ASP:OD1	2.51	0.43
51:Z1:92:GLU:OE1	56:e1:91:TYR:OH	2.35	0.43
3:C:179:PHE:HE2	3:N:179:PHE:HE2	1.66	0.43
6:Q:67:ASP:OD1	6:Q:71:ARG:NH2	2.51	0.43
12:o:104:TRP:HE1	12:o:201:GLY:HA3	1.83	0.43
42:H1:81:LEU:HD21	42:H1:108:THR:O	2.18	0.43
43:J1:63:MET:HA	43:J1:66:VAL:HB	2.01	0.43
51:Z1:81:ARG:NH2	51:Z1:124:TYR:OH	2.41	0.43
57:f1:49:ARG:HB2	57:f1:52:GLU:HG2	1.99	0.43
5:E:67:ASP:OD1	5:E:67:ASP:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:THR:OG1	2:M:373:GLU:OE1	2.30	0.43
15:r:84:TYR:O	15:r:87:GLN:HG3	2.18	0.43
25:C1:43:SER:HA	39:r1:65:PRO:HB3	1.99	0.43
27:2:27:ASN:OD1	27:2:30:ARG:NH1	2.52	0.43
36:V1:25:ILE:HD12	48:O1:236:GLU:HB3	2.00	0.43
37:W1:37:LEU:HD13	37:W1:89:LYS:HG3	1.99	0.43
46:M1:3:LYS:NZ	57:f1:27:ASP:OD2	2.50	0.43
58:g1:62:PHE:HA	58:g1:66:ILE:HG12	1.99	0.43
1:A:430:GLN:HA	7:G:4:PHE:HB3	2.01	0.43
1:L:433:ASP:OD2	3:N:223:TYR:OH	2.31	0.43
4:O:18:LEU:HD22	4:O:206:LEU:HB2	2.00	0.43
11:n:413:HIS:CD2	11:n:468:MET:HB2	2.53	0.43
13:p:124:LEU:HD21	13:p:257:TYR:HE1	1.83	0.43
26:D1:104:ASP:O	26:D1:108:TYR:HA	2.18	0.43
29:3:524:LEU:HD22	29:3:527:ALA:HB3	1.99	0.43
32:Q1:89:LYS:O	32:Q1:93:ILE:HG12	2.17	0.43
42:H1:144:VAL:O	42:H1:148:ILE:HG22	2.19	0.43
46:M1:53:SER:OG	46:M1:54:ASN:N	2.51	0.43
69:h1:201:CDL:OB4	67:p1:48:ARG:NH1	2.47	0.43
10:K:33:VAL:HG13	10:K:38:TRP:HB3	2.01	0.43
4:O:225:HIS:O	4:O:228:SER:OG	2.35	0.43
13:p:58:TRP:CD2	68:p:301:3PE:H251	2.54	0.43
14:q:114:ASP:OD1	14:q:115:TRP:N	2.51	0.43
15:r:107:ASP:OD1	15:r:108:LYS:N	2.50	0.43
25:C1:77:ASP:HB3	26:D1:392:LYS:HG3	2.00	0.43
26:D1:284:ASP:OD1	30:9:1:THR:OG1	2.30	0.43
45:L1:392:LYS:O	45:L1:396:ILE:HG12	2.19	0.43
45:L1:441:ILE:HG21	61:j1:15:PRO:HB3	2.01	0.43
45:L1:575:THR:O	45:L1:579:ASN:HB2	2.19	0.43
46:M1:338:HIS:NE2	58:g1:32:ASP:OD2	2.48	0.43
2:B:182:ARG:NH2	2:B:190:GLU:OE1	2.39	0.43
2:B:286:LYS:HG2	2:B:287:ARG:HG3	2.00	0.43
13:p:228:THR:HG21	16:s:10:ASP:HB3	2.01	0.43
22:z:6:ALA:HB3	22:z:9:GLN:HG2	2.01	0.43
26:D1:342:MET:HE3	26:D1:346:ILE:HG13	2.00	0.43
27:2:106:THR:O	27:2:110:LEU:HB2	2.18	0.43
44:K1:54:MET:HA	44:K1:57:MET:HG3	1.99	0.43
68:L1:704:3PE:H3G2	46:M1:447:LEU:HD21	2.01	0.43
46:M1:61:LEU:HD11	46:M1:316:MET:HE1	2.01	0.43
49:X1:48:GLU:OE1	49:X1:134:ARG:NH2	2.51	0.43
11:n:208:MET:HB2	11:n:208:MET:HE2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:33:LEU:HD22	68:v:101:3PE:H122	2.01	0.43
14:q:73:ARG:HH21	15:r:109:VAL:HG21	1.83	0.43
24:6:164:GLU:HB3	30:9:139:PHE:CE1	2.52	0.43
28:1:98:ASP:O	28:1:139:ARG:CD	2.66	0.43
29:3:25:THR:HA	29:3:72:PRO:HA	2.00	0.43
68:L1:704:3PE:H3C1	46:M1:443:PRO:HB3	2.00	0.43
46:M1:179:LEU:O	46:M1:183:THR:HB	2.19	0.43
46:M1:433:GLU:O	46:M1:437:MET:HG2	2.18	0.43
47:N1:6:LEU:HD23	47:N1:6:LEU:HA	1.91	0.43
2:B:29:LEU:HB2	2:B:33:LEU:HB3	2.00	0.43
3:C:53:MET:HE1	5:E:62:MET:HE2	2.00	0.43
11:n:438:ARG:HH22	76:n:604:HEA:CGD	2.31	0.43
11:n:466:LEU:CD1	22:z:23:PHE:HA	2.49	0.43
25:C1:58:ILE:HD13	25:C1:120:ILE:HG22	2.01	0.43
26:D1:161:ILE:HG22	42:H1:278:PRO:HB2	2.00	0.43
34:S1:64:LEU:HB2	34:S1:78:LEU:HD22	2.00	0.43
42:H1:17:MET:HE3	42:H1:17:MET:HB3	1.89	0.43
60:i1:59:MET:HB2	60:i1:64:TYR:HB2	2.01	0.43
1:A:138:MET:HE2	1:A:138:MET:HB3	1.86	0.43
2:B:216:LEU:HD12	2:B:216:LEU:HA	1.92	0.43
4:D:27:ARG:O	4:D:31:GLN:HG3	2.18	0.43
6:F:67:ASP:OD2	6:F:71:ARG:NH2	2.52	0.43
1:L:276:ILE:HB	1:L:345:LEU:HD11	2.01	0.43
11:n:420:GLY:O	11:n:424:THR:OG1	2.27	0.43
14:q:137:LYS:HA	14:q:146:LYS:HD2	2.00	0.43
30:9:162:LYS:HD3	38:q1:110:TRP:CZ3	2.53	0.43
48:O1:59:SER:HA	48:O1:62:THR:HG22	2.00	0.43
1:A:46:ARG:HG3	1:A:163:LEU:HG	2.01	0.43
1:L:114:ALA:O	1:L:118:GLN:HB2	2.19	0.43
11:n:115:SER:OG	11:n:142:SER:OG	2.26	0.43
11:n:363:LEU:O	11:n:367:LEU:HB2	2.18	0.43
12:o:103:GLN:NE2	12:o:200:CYS:O	2.52	0.43
12:o:189:PRO:HG3	19:v:62:PHE:HB2	2.01	0.43
13:p:7:ALA:HB3	13:p:74:ILE:HD11	2.01	0.43
13:p:52:LEU:HG	13:p:56:GLN:HE22	1.84	0.43
13:p:142:VAL:HA	13:p:145:THR:HG22	2.01	0.43
24:6:50:ALA:HB2	42:H1:53:MET:HE3	2.01	0.43
45:L1:283:LEU:HD13	63:l1:111:MET:HG3	2.00	0.43
60:i1:61:PHE:HA	60:i1:65:ARG:HB3	2.01	0.43
65:n1:30:CYS:O	65:n1:32:HIS:N	2.50	0.43
66:o1:107:LEU:HD23	66:o1:107:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:137:GLN:NE2	3:N:263:ASN:O	2.52	0.42
3:N:237:LEU:HD13	4:O:212:MET:HG2	2.02	0.42
5:T:69:GLY:HA3	5:T:72:VAL:HG12	2.02	0.42
26:D1:298:LEU:HB3	30:9:5:VAL:HB	2.00	0.42
28:1:307:ILE:HB	28:1:327:THR:HG21	2.00	0.42
29:3:332:LYS:HA	29:3:343:LEU:HD11	2.01	0.42
42:H1:307:LEU:O	42:H1:311:THR:OG1	2.28	0.42
45:L1:378:LEU:HD21	62:k1:72:ILE:HD12	2.00	0.42
45:L1:435:PRO:HG2	62:k1:57:ARG:HB3	2.01	0.42
51:Z1:93:GLU:OE2	56:e1:74:ARG:NH2	2.52	0.42
59:h1:49:GLU:OE2	67:p1:55:HIS:NE2	2.52	0.42
1:A:348:SER:HB2	10:K:13:LEU:HD22	1.99	0.42
5:E:45:VAL:HG13	9:J:28:ALA:HA	2.01	0.42
10:V:39:ARG:HD3	10:V:53:LYS:HA	2.01	0.42
11:n:445:ASP:HB3	20:x:41:ASN:HD21	1.84	0.42
13:p:173:PHE:HD2	13:p:208:VAL:HG11	1.84	0.42
26:D1:50:ASN:HB2	41:A1:38:GLU:HG3	2.01	0.42
30:9:110:ARG:NH2	32:Q1:70:MET:O	2.43	0.42
30:9:134:VAL:HG11	30:9:171:ILE:HD11	2.01	0.42
73:M1:501:PC1:H2C1	47:N1:284:MET:HE3	2.02	0.42
59:h1:95:GLN:O	59:h1:99:GLU:HG3	2.19	0.42
3:N:227:LYS:HD2	4:O:223:LYS:HE3	2.02	0.42
4:O:43:MET:HG2	4:O:46:VAL:HB	2.00	0.42
11:n:69:MET:O	11:n:73:MET:HB2	2.19	0.42
12:o:82:ARG:O	12:o:86:MET:HG3	2.20	0.42
13:p:142:VAL:CG2	17:t:13:TRP:CE3	3.03	0.42
13:p:153:GLU:CD	17:t:10:ALA:HB3	2.44	0.42
26:D1:52:GLY:HA2	26:D1:55:HIS:HB2	2.00	0.42
26:D1:164:MET:HG2	42:H1:32:GLN:OE1	2.19	0.42
26:D1:234:ILE:HG12	42:H1:280:PHE:CZ	2.54	0.42
31:P1:66:GLY:HA3	32:Q1:69:LEU:HD13	2.00	0.42
46:M1:230:ILE:HD12	46:M1:230:ILE:HA	1.89	0.42
47:N1:271:MET:HE3	47:N1:276:LEU:HG	2.02	0.42
55:d1:75:TYR:O	55:d1:79:GLN:HG2	2.19	0.42
63:l1:126:PRO:HD3	66:o1:3:HIS:CE1	2.55	0.42
6:F:74:ILE:HD12	6:F:80:TRP:HZ2	1.84	0.42
1:L:238:GLY:H	7:R:22:GLU:CD	2.27	0.42
2:M:243:GLU:HA	2:M:424:MET:O	2.19	0.42
3:N:9:PRO:HA	3:N:12:LYS:HG2	2.01	0.42
11:n:442:ASP:OD1	11:n:442:ASP:N	2.52	0.42
14:q:91:PHE:O	14:q:95:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C1:135:TRP:CZ2	37:W1:90:MET:HE1	2.55	0.42
28:1:337:MET:HG2	28:1:341:THR:HG21	2.00	0.42
29:3:378:LEU:HD11	29:3:409:ILE:HD12	2.01	0.42
31:P1:157:ARG:NH2	31:P1:227:THR:OG1	2.49	0.42
41:A1:73:LEU:O	42:H1:160:TYR:OH	2.34	0.42
42:H1:273:ILE:HG23	42:H1:277:TYR:HD2	1.83	0.42
43:J1:23:PRO:HG3	43:J1:82:TRP:CE2	2.55	0.42
35:U1:63:PRO:HB3	63:l1:60:TRP:CD2	2.55	0.42
49:X1:21:SER:HB2	52:a1:47:LEU:HD13	2.01	0.42
56:e1:98:SER:OG	56:e1:100:ARG:NH2	2.53	0.42
63:l1:4:THR:OG1	63:l1:6:ASP:OD1	2.28	0.42
64:m1:14:PRO:HB2	64:m1:17:LEU:HB2	2.02	0.42
1:L:40:TRP:CZ2	1:L:377:GLU:HA	2.55	0.42
1:L:379:ILE:HG12	1:L:389:ARG:HD3	2.02	0.42
3:N:51:LEU:O	3:N:55:TYR:CB	2.67	0.42
26:D1:11:ALA:O	47:N1:228:ASN:ND2	2.47	0.42
26:D1:74:ARG:HH22	41:A1:115:GLU:HB3	1.85	0.42
26:D1:165:THR:HB	26:D1:169:TRP:CZ2	2.55	0.42
26:D1:417:ILE:HA	26:D1:420:THR:HG22	2.00	0.42
28:1:305:PRO:HD3	28:1:413:TRP:HB3	2.02	0.42
30:9:15:ASP:OD1	30:9:16:MET:N	2.52	0.42
31:P1:53:VAL:O	31:P1:57:MET:HB2	2.20	0.42
31:P1:215:VAL:O	31:P1:218:THR:OG1	2.27	0.42
37:W1:34:VAL:HG22	85:W1:201:ZMP:H11	2.01	0.42
38:q1:6:VAL:HG11	69:a1:101:CDL:HB62	2.00	0.42
42:H1:212:ASN:HB2	42:H1:215:TYR:HB2	2.01	0.42
45:L1:159:TYR:HB2	46:M1:416:ARG:HB3	2.01	0.42
45:L1:362:ILE:HD13	45:L1:365:ILE:HD11	2.02	0.42
50:Y1:11:VAL:HG21	50:Y1:16:GLN:HG2	2.00	0.42
50:Y1:36:SER:HB2	50:Y1:55:VAL:HA	2.00	0.42
3:C:136:GLY:N	3:C:139:SER:OG	2.52	0.42
27:2:217:LEU:HD11	28:1:48:ILE:HG12	2.02	0.42
29:3:255:HIS:HD2	29:3:257:ASP:H	1.67	0.42
47:N1:310:ASN:ND2	48:O1:273:THR:O	2.37	0.42
63:l1:31:GLU:OE2	63:l1:31:GLU:N	2.51	0.42
3:C:126:THR:HG21	3:C:186:PRO:HG3	2.01	0.42
11:n:50:ASP:OD1	11:n:50:ASP:N	2.53	0.42
11:n:436:MET:HE1	11:n:451:ASN:HD21	1.82	0.42
12:o:30:ILE:O	12:o:34:ILE:HG13	2.20	0.42
18:u:36:PHE:HB2	18:u:56:TYR:HB3	2.01	0.42
68:D1:501:3PE:H3E1	73:M1:501:PC1:H3H1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:551:ASP:OD2	29:3:679:ARG:NE	2.45	0.42
35:T1:45:LEU:HA	35:T1:48:VAL:HG12	2.01	0.42
42:H1:77:LEU:HD13	68:Z1:401:3PE:H3G1	2.02	0.42
45:L1:407:TRP:HE1	63:l1:111:MET:HE3	1.85	0.42
46:M1:130:LEU:HD12	46:M1:150:LEU:HB2	2.00	0.42
46:M1:225:ILE:HD13	46:M1:331:ASN:HB2	2.01	0.42
48:O1:293:TYR:O	48:O1:297:ARG:HG2	2.19	0.42
35:U1:2:ASP:OD1	35:U1:2:ASP:N	2.51	0.42
49:X1:13:LYS:HB2	49:X1:13:LYS:HE3	1.78	0.42
68:i1:201:3PE:H2C2	68:i1:201:3PE:H352	2.01	0.42
67:p1:72:ASP:N	67:p1:75:GLU:OE2	2.48	0.42
4:D:173:ASP:OD1	4:D:175:THR:OG1	2.34	0.42
11:n:84:PRO:HA	11:n:89:ALA:HB3	2.02	0.42
12:o:149:PRO:HA	12:o:185:THR:HG22	2.01	0.42
26:D1:189:MET:HE2	26:D1:189:MET:HB2	1.92	0.42
26:D1:193:TYR:OH	26:D1:201:GLN:O	2.31	0.42
30:9:101:ARG:NH1	30:9:107:ARG:HG3	2.35	0.42
31:P1:107:GLU:O	31:P1:111:VAL:HB	2.20	0.42
34:S1:62:PRO:HD2	34:S1:79:ASN:HB2	2.01	0.42
45:L1:69:VAL:HG12	45:L1:76:LEU:HB2	2.01	0.42
48:O1:38:LEU:HD12	48:O1:231:PRO:HB3	2.02	0.42
57:f1:38:ARG:NH1	57:f1:56:TRP:O	2.53	0.42
3:C:101:GLY:HA2	3:C:106:SER:HB2	2.02	0.42
2:M:181:TYR:CZ	2:M:182:ARG:HG2	2.54	0.42
11:n:480:ARG:HB3	22:z:6:ALA:CA	2.50	0.42
12:o:168:LEU:HD21	12:o:184:VAL:HG23	2.02	0.42
13:p:119:THR:O	17:t:51:HIS:NE2	2.47	0.42
19:v:27:PHE:O	19:v:31:LEU:HG	2.20	0.42
31:P1:48:PRO:HA	31:P1:71:LEU:O	2.20	0.42
32:Q1:54:LYS:HD3	32:Q1:54:LYS:HA	1.84	0.42
36:V1:17:ASP:N	36:V1:17:ASP:OD1	2.52	0.42
40:s1:52:LEU:HA	40:s1:52:LEU:HD23	1.83	0.42
41:A1:6:VAL:HG11	42:H1:87:VAL:HG21	2.02	0.42
42:H1:135:ALA:O	42:H1:139:THR:HG23	2.20	0.42
43:J1:22:LYS:HD3	44:K1:23:ARG:HB2	2.00	0.42
47:N1:175:MET:O	47:N1:179:MET:HG2	2.20	0.42
1:A:110:VAL:HG11	1:A:211:LEU:HB3	2.02	0.42
1:A:343:MET:HE1	1:A:416:TYR:HA	2.02	0.42
1:A:378:ASP:O	1:A:382:SER:OG	2.26	0.42
4:D:180:SER:HB3	8:H:15:LEU:HB2	2.01	0.42
3:N:89:MET:HE2	3:N:89:MET:HB2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:27:GLY:HA3	76:n:603:HEA:H202	2.01	0.42
11:n:229:ILE:HD12	11:n:229:ILE:H	1.84	0.42
12:o:156:SER:HB2	12:o:161:HIS:HD2	1.85	0.42
26:D1:360:PRO:HA	26:D1:380:SER:O	2.20	0.42
28:1:185:ILE:HG12	28:1:359:CYS:HB3	2.02	0.42
30:9:119:ILE:HG13	30:9:121:CYS:HB3	2.02	0.42
46:M1:121:LEU:HA	46:M1:124:ALA:HB3	2.02	0.42
47:N1:178:ILE:HG23	47:N1:292:PHE:HE1	1.84	0.42
35:U1:25:ILE:HG21	35:U1:30:LEU:HD13	2.02	0.42
9:J:19:THR:O	9:J:23:THR:HG23	2.20	0.41
11:n:475:ALA:HA	11:n:480:ARG:NH1	2.35	0.41
15:r:40:ASP:OD2	19:v:15:LEU:HB3	2.20	0.41
24:6:118:PRO:HG2	42:H1:58:LYS:HD3	2.02	0.41
25:C1:172:VAL:HA	25:C1:186:GLU:O	2.19	0.41
26:D1:183:ARG:NH1	26:D1:210:ASP:OD2	2.31	0.41
28:1:95:VAL:HB	28:1:136:ILE:HG23	2.02	0.41
31:P1:76:ARG:NH2	31:P1:103:ASN:O	2.53	0.41
41:A1:7:ILE:O	41:A1:11:ILE:HG12	2.20	0.41
45:L1:64:THR:HG21	45:L1:77:LYS:HD3	2.02	0.41
45:L1:75:GLU:HG2	45:L1:77:LYS:HE2	2.01	0.41
46:M1:84:LEU:HD11	46:M1:95:TYR:CD2	2.55	0.41
47:N1:334:THR:HG22	47:N1:335:MET:HG3	2.01	0.41
48:O1:69:LEU:HD22	48:O1:299:LEU:HD21	2.02	0.41
51:Z1:77:GLU:OE2	56:e1:105:PRO:HB2	2.20	0.41
8:H:51:ASP:OD1	8:H:52:CYS:N	2.53	0.41
11:n:243:VAL:HB	76:n:604:HEA:HAC	2.01	0.41
12:o:3:TYR:CE1	12:o:6:GLN:HG3	2.55	0.41
13:p:121:ILE:HD12	17:t:52:LEU:CD2	2.42	0.41
13:p:136:VAL:HG11	13:p:173:PHE:HB2	2.01	0.41
15:r:21:LYS:HE3	15:r:24:ILE:HA	2.02	0.41
19:v:25:GLY:HA2	19:v:28:ILE:HG12	2.02	0.41
27:2:164:LEU:HD13	27:2:169:ILE:HD13	2.01	0.41
28:1:105:CYS:SG	28:1:267:THR:OG1	2.78	0.41
28:1:142:PHE:HB3	28:1:145:GLU:HB2	2.02	0.41
29:3:107:ILE:HG23	30:9:80:ILE:HD12	2.02	0.41
29:3:218:ARG:HG2	30:9:83:LYS:HE2	2.02	0.41
42:H1:7:LEU:HD23	42:H1:7:LEU:HA	1.90	0.41
46:M1:124:ALA:O	46:M1:128:PRO:HD3	2.20	0.41
46:M1:139:GLN:HG3	46:M1:340:ARG:HH22	1.85	0.41
46:M1:173:THR:HB	59:h1:101:ALA:HB2	2.02	0.41
35:U1:61:GLU:HB3	65:n1:84:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:j1:32:MET:HE2	61:j1:32:MET:HB3	1.89	0.41
3:C:58:ASP:O	3:C:62:ALA:N	2.54	0.41
5:E:158:CYS:HB3	5:E:163:SER:H	1.85	0.41
1:L:384:LEU:HD23	1:L:384:LEU:HA	1.88	0.41
12:o:152:MET:HB3	12:o:182:ALA:HB3	2.03	0.41
13:p:210:ILE:HG23	68:p:301:3PE:H2A2	2.03	0.41
28:1:96:ASN:O	28:1:225:VAL:CG2	2.68	0.41
28:1:157:TYR:HB3	40:s1:55:PHE:HD2	1.85	0.41
29:3:311:GLU:HG3	29:3:312:GLY:H	1.85	0.41
32:Q1:57:MET:HG2	32:Q1:86:PHE:HE1	1.84	0.41
32:Q1:112:LYS:HE2	32:Q1:112:LYS:HB3	1.82	0.41
41:A1:59:ALA:HB1	43:J1:65:VAL:HG13	2.02	0.41
42:H1:316:PRO:HA	51:Z1:57:ARG:HH11	1.84	0.41
47:N1:43:MET:HB3	47:N1:126:MET:SD	2.60	0.41
47:N1:211:LEU:HD23	47:N1:211:LEU:HA	1.93	0.41
55:d1:106:LYS:H	55:d1:106:LYS:HG2	1.72	0.41
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.95	0.41
2:M:334:GLY:HA2	2:M:434:PRO:HD3	2.01	0.41
3:N:237:LEU:HA	4:O:212:MET:HE3	2.02	0.41
68:P:201:3PE:H231	68:P:201:3PE:H332	2.03	0.41
11:n:325:ALA:HB2	12:o:65:TRP:HH2	1.86	0.41
11:n:329:GLY:O	12:o:52:HIS:N	2.45	0.41
25:C1:182:ARG:NH2	37:W1:111:GLU:OE2	2.36	0.41
26:D1:335:ARG:NH2	30:9:131:ASP:OD1	2.54	0.41
29:3:10:GLU:HB2	29:3:19:MET:HE1	2.02	0.41
44:K1:24:SER:HB3	44:K1:89:TYR:CE2	2.54	0.41
46:M1:285:LEU:HD13	46:M1:342:MET:HE2	2.01	0.41
46:M1:347:GLY:HA3	46:M1:419:LEU:HA	2.02	0.41
85:n1:201:ZMP:H17	85:n1:201:ZMP:H15	1.65	0.41
2:B:109:VAL:HG22	2:B:123:LEU:HD22	2.02	0.41
3:C:161:VAL:HA	3:C:164:ILE:HG22	2.01	0.41
11:n:35:ILE:HG13	11:n:462:LEU:HD22	2.02	0.41
11:n:101:SER:HA	11:n:104:LEU:HD12	2.02	0.41
11:n:347:LEU:HB3	11:n:383:MET:HE3	2.01	0.41
13:p:253:TYR:HA	13:p:257:TYR:HD2	1.85	0.41
31:P1:133:SER:O	31:P1:168:PRO:HD2	2.20	0.41
35:T1:45:LEU:O	35:T1:49:GLU:HG3	2.20	0.41
68:L1:704:3PE:H232	46:M1:449:THR:HG21	2.02	0.41
52:a1:5:ILE:HG22	52:a1:9:LEU:HG	2.02	0.41
60:i1:34:LEU:HA	60:i1:35:PRO:HD3	1.93	0.41
65:n1:56:MET:HA	65:n1:59:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:29:ALA:O	10:K:33:VAL:HG23	2.20	0.41
2:M:216:LEU:HD12	2:M:216:LEU:HA	1.93	0.41
4:O:76:ASP:OD1	4:O:77:ASP:N	2.54	0.41
7:R:42:ARG:HD3	68:Y1:402:3PE:H112	2.03	0.41
11:n:44:PRO:HG3	11:n:448:THR:HG22	2.02	0.41
11:n:443:TYR:CE1	11:n:448:THR:HA	2.55	0.41
11:n:481:GLU:O	22:z:3:SER:C	2.58	0.41
12:o:171:LYS:HB2	12:o:171:LYS:HE3	1.93	0.41
17:t:14:LYS:HZ1	17:t:18:TYR:HE2	1.69	0.41
21:y:21:LEU:HA	21:y:24:MET:HG2	2.02	0.41
22:z:33:VAL:HA	22:z:40:TYR:HE2	1.85	0.41
25:C1:7:LYS:HA	25:C1:7:LYS:HD2	1.87	0.41
25:C1:112:ASP:OD1	25:C1:115:THR:OG1	2.26	0.41
42:H1:209:SER:HB3	42:H1:213:VAL:HA	2.01	0.41
45:L1:345:SER:HB3	45:L1:450:LEU:HD11	2.02	0.41
47:N1:312:LYS:O	47:N1:316:HIS:ND1	2.39	0.41
60:i1:15:ARG:O	60:i1:19:ARG:HG2	2.21	0.41
4:D:229:VAL:HG13	7:G:17:SER:HB3	2.02	0.41
3:N:265:PRO:HD2	3:N:268:ILE:HD11	2.03	0.41
9:U:33:ARG:HH21	10:V:50:GLY:HA3	1.86	0.41
11:n:55:ASN:HA	11:n:58:VAL:HG22	2.02	0.41
11:n:413:HIS:NE2	11:n:468:MET:HB2	2.36	0.41
11:n:471:MET:HE2	11:n:471:MET:HA	2.03	0.41
13:p:35:PHE:HA	17:t:60:PRO:HB3	2.01	0.41
13:p:62:ILE:HG13	73:p:302:PC1:H222	2.02	0.41
27:2:155:GLN:HG3	27:2:160:TYR:CD1	2.56	0.41
30:9:119:ILE:HG12	81:9:201:SF4:S3	2.61	0.41
43:J1:32:LEU:HD12	43:J1:35:SER:HB2	2.02	0.41
45:L1:539:MET:O	45:L1:543:ASN:HB2	2.20	0.41
46:M1:76:MET:HB3	46:M1:99:LEU:HD13	2.03	0.41
35:U1:39:ASP:OD1	35:U1:39:ASP:N	2.52	0.41
35:U1:68:GLU:HG3	60:i1:1:SAC:H2A2	2.02	0.41
50:Y1:80:ARG:NH2	50:Y1:85:ASP:OD2	2.49	0.41
51:Z1:97:MET:HE3	56:e1:78:ILE:HA	2.01	0.41
66:o1:51:THR:HA	67:p1:118:GLU:HG2	2.03	0.41
2:B:258:VAL:HA	2:B:323:GLY:HA3	2.02	0.41
3:C:133:LEU:HD21	3:C:179:PHE:HB2	2.03	0.41
4:O:22:ASP:O	4:O:26:ILE:HG13	2.21	0.41
4:O:208:MET:HE3	4:O:208:MET:HB3	1.95	0.41
11:n:481:GLU:HB2	22:z:4:LYS:CG	2.51	0.41
27:2:102:VAL:HG13	27:2:154:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:297:GLU:HG3	37:W1:125:TYR:CZ	2.56	0.41
29:3:318:ILE:HA	29:3:344:CYS:O	2.20	0.41
30:9:156:LEU:HD23	30:9:156:LEU:HA	1.86	0.41
41:A1:33:LYS:HG2	42:H1:61:MET:HE1	2.02	0.41
42:H1:142:TYR:CZ	42:H1:192:GLU:HA	2.55	0.41
46:M1:252:PRO:HB3	55:d1:117:HIS:CG	2.55	0.41
51:Z1:76:ALA:HB1	51:Z1:80:ARG:HH22	1.86	0.41
1:A:40:TRP:O	1:A:195:MET:HA	2.21	0.41
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.90	0.41
2:B:109:VAL:HG13	2:B:123:LEU:HD13	2.03	0.41
3:C:131:TYR:OH	3:C:252:ASP:OD2	2.34	0.41
1:L:332:ASP:OD1	1:L:333:ASP:N	2.54	0.41
3:N:33:PHE:HA	3:N:36:LEU:HB2	2.01	0.41
4:O:33:TYR:HD1	4:O:37:CYS:HB2	1.86	0.41
4:O:152:TYR:OH	8:S:64:ASP:OD2	2.27	0.41
11:n:404:THR:CB	22:z:3:SER:HB3	2.50	0.41
12:o:146:MET:HA	12:o:213:MET:HE3	2.03	0.41
13:p:207:HIS:ND1	13:p:241:TYR:OH	2.52	0.41
22:z:41:LYS:HB3	22:z:41:LYS:HE2	1.98	0.41
24:6:48:ASN:ND2	24:6:180:GLU:O	2.53	0.41
25:C1:64:LEU:HD23	25:C1:64:LEU:HA	1.95	0.41
28:1:190:THR:HB	28:1:204:ARG:HG2	2.02	0.41
28:1:367:GLU:OE1	29:3:100:ASN:ND2	2.47	0.41
29:3:379:LEU:HD13	29:3:384:PRO:HG2	2.01	0.41
32:Q1:11:ILE:HD13	37:W1:21:PRO:HB3	2.03	0.41
35:T1:73:PRO:HA	35:T1:76:ILE:HD12	2.02	0.41
38:q1:92:CYS:SG	39:r1:33:ARG:HG3	2.61	0.41
45:L1:54:PHE:CZ	45:L1:84:PHE:HB2	2.56	0.41
45:L1:174:TYR:CD2	45:L1:232:TRP:HB3	2.56	0.41
45:L1:223:LYS:HG2	45:L1:255:ALA:HB3	2.03	0.41
47:N1:63:GLN:OE1	47:N1:105:LYS:HG2	2.21	0.41
1:A:337:PHE:HE1	3:C:1:MET:HG3	1.84	0.41
2:M:68:LEU:HD12	2:M:68:LEU:HA	1.91	0.41
4:O:211:MET:HG2	68:P:201:3PE:H322	2.02	0.41
11:n:431:LEU:HD22	11:n:436:MET:HE2	2.02	0.41
76:n:603:HEA:HMB3	76:n:603:HEA:HHB	1.86	0.41
24:6:72:MET:HE3	24:6:79:MET:HB3	2.03	0.41
26:D1:136:TRP:CD2	26:D1:277:VAL:HG21	2.56	0.41
29:3:97:LEU:HD22	29:3:154:ILE:HD12	2.02	0.41
29:3:534:ARG:HA	29:3:537:LEU:HB3	2.03	0.41
30:9:41:SER:O	30:9:45:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L1:362:ILE:HA	45:L1:365:ILE:HG12	2.02	0.41
45:L1:438:PRO:HA	45:L1:439:PRO:HD3	1.97	0.41
46:M1:126:LEU:HD13	46:M1:153:THR:HG21	2.02	0.41
69:N1:401:CDL:H311	55:d1:44:MET:HE1	2.03	0.41
48:O1:22:SER:OG	48:O1:119:GLY:O	2.28	0.41
55:d1:26:LEU:HA	55:d1:31:LEU:HD12	2.02	0.41
64:m1:126:ILE:HG22	67:p1:139:GLN:HG3	2.01	0.41
2:B:77:THR:OG1	2:B:80:ALA:O	2.35	0.40
4:O:208:MET:HG2	68:P:201:3PE:H342	2.02	0.40
5:P:63:SER:OG	5:P:64:ALA:N	2.54	0.40
6:Q:21:TYR:OH	6:Q:86:ASP:OD2	2.37	0.40
11:n:254:ILE:HA	11:n:257:VAL:HG22	2.02	0.40
11:n:481:GLU:H	22:z:4:LYS:HB2	1.86	0.40
12:o:123:ILE:HA	12:o:124:PRO:HD3	1.93	0.40
12:o:141:ARG:HA	12:o:210:VAL:HG13	2.02	0.40
13:p:210:ILE:O	13:p:213:THR:OG1	2.29	0.40
27:2:105:THR:HG22	27:2:106:THR:H	1.85	0.40
29:3:428:ILE:HD11	29:3:437:HIS:HE2	1.85	0.40
30:9:51:ASN:O	30:9:55:GLU:N	2.46	0.40
31:P1:46:ILE:HG12	33:7:26:VAL:HG21	2.03	0.40
32:Q1:93:ILE:HD11	32:Q1:105:VAL:HG21	2.03	0.40
34:S1:30:GLN:HG2	34:S1:33:ARG:HH21	1.86	0.40
47:N1:193:ILE:HD11	47:N1:269:GLU:HB3	2.02	0.40
1:L:327:ASP:OD1	1:L:327:ASP:N	2.44	0.40
3:N:97:HIS:HD2	70:N:403:HEM:C1C	2.39	0.40
12:o:14:SER:OG	12:o:185:THR:O	2.35	0.40
13:p:233:PHE:HD2	68:p:301:3PE:H32	1.86	0.40
22:z:32:TRP:O	22:z:36:HIS:ND1	2.45	0.40
24:6:102:LEU:HD13	24:6:110:LEU:HD22	2.04	0.40
31:P1:165:ILE:O	31:P1:227:THR:HA	2.21	0.40
32:Q1:57:MET:HE3	32:Q1:86:PHE:CZ	2.57	0.40
42:H1:215:TYR:CD2	42:H1:219:PRO:HB2	2.56	0.40
42:H1:228:TYR:HA	42:H1:231:ILE:HD12	2.02	0.40
45:L1:581:LYS:HE2	45:L1:581:LYS:HB3	1.83	0.40
35:U1:52:MET:HE1	65:n1:23:LEU:HB3	2.03	0.40
63:l1:129:PRO:HD3	66:o1:21:ILE:HB	2.03	0.40
66:o1:51:THR:HB	66:o1:54:GLN:HG2	2.03	0.40
1:A:46:ARG:HD3	1:A:231:LEU:HD11	2.03	0.40
1:A:161:THR:HG21	1:A:235:ARG:H	1.87	0.40
3:C:6:LYS:HG2	3:C:15:ASN:ND2	2.36	0.40
4:D:211:MET:HE1	9:J:31:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:GLU:HA	8:H:29:VAL:HG12	2.02	0.40
2:M:89:ILE:HG13	2:M:122:PHE:HD2	1.87	0.40
11:n:53:ILE:HD11	21:y:40:VAL:HG23	2.02	0.40
29:3:273:GLY:O	29:3:549:HIS:NE2	2.48	0.40
29:3:533:THR:OG1	29:3:534:ARG:N	2.54	0.40
46:M1:275:ILE:O	46:M1:279:GLN:HB2	2.21	0.40
46:M1:428:PRO:HD3	65:n1:105:TYR:HD2	1.86	0.40
47:N1:230:ILE:HD12	47:N1:230:ILE:HA	1.93	0.40
54:c1:33:GLN:O	54:c1:37:GLU:HG3	2.20	0.40
54:c1:45:ARG:NH2	55:d1:16:ASP:O	2.53	0.40
67:p1:8:VAL:O	67:p1:108:ARG:NH2	2.54	0.40
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.87	0.40
70:C:402:HEM:HBC2	70:C:402:HEM:HMC2	2.04	0.40
4:D:93:LYS:HD3	4:D:93:LYS:HA	1.76	0.40
1:L:242:ARG:O	7:R:14:ILE:HA	2.22	0.40
2:M:56:ARG:HB2	2:M:171:ALA:O	2.21	0.40
11:n:136:LEU:HD23	11:n:136:LEU:HA	1.96	0.40
11:n:222:PRO:HG3	12:o:176:PRO:HB2	2.02	0.40
12:o:94:VAL:HG11	12:o:148:LEU:HD13	2.04	0.40
13:p:125:ASN:HA	13:p:126:PRO:HD3	1.95	0.40
15:r:51:ALA:HB1	15:r:67:ILE:HD13	2.03	0.40
25:C1:8:ARG:HA	25:C1:9:PRO:HD3	1.97	0.40
26:D1:396:PHE:HD1	26:D1:428:ILE:HG23	1.85	0.40
28:1:28:ARG:HD3	28:1:28:ARG:HA	1.87	0.40
30:9:113:ILE:HG22	30:9:115:MET:HG2	2.03	0.40
34:S1:34:ASP:O	34:S1:38:GLN:HG3	2.22	0.40
35:T1:79:TYR:OH	35:T1:83:LYS:NZ	2.55	0.40
45:L1:137:MET:HE1	45:L1:189:PHE:HD2	1.86	0.40
45:L1:241:THR:HG21	45:L1:344:GLY:HA3	2.03	0.40
45:L1:561:THR:HG23	68:Y1:403:3PE:H271	2.03	0.40
45:L1:595:ILE:O	45:L1:599:ILE:HG12	2.22	0.40
47:N1:110:PRO:HB3	69:Y1:401:CDL:H162	2.04	0.40
48:O1:285:GLY:HA3	58:g1:24:TRP:HZ3	1.86	0.40
35:U1:22:TYR:HD2	35:U1:25:ILE:HG13	1.86	0.40
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.49	0.40
1:A:264:ASN:ND2	1:A:266:ASP:OD2	2.54	0.40
3:C:4:MET:HE2	3:C:11:PHE:HE2	1.87	0.40
3:C:216:ASP:HB2	6:F:63:LYS:HG3	2.03	0.40
5:E:86:ASN:HA	5:E:98:VAL:O	2.22	0.40
2:M:197:ASN:HB3	2:M:232:LEU:HD13	2.03	0.40
4:O:239:PRO:HA	4:O:240:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:212:GLU:HG3	12:o:212:GLU:O	2.22	0.40
25:C1:65:ARG:HE	25:C1:65:ARG:HB3	1.75	0.40
28:1:92:TYR:O	28:1:220:THR:HA	2.21	0.40
29:3:371:VAL:HG13	29:3:395:ILE:HD13	2.03	0.40
29:3:524:LEU:HB3	29:3:545:TYR:HD1	1.85	0.40
39:r1:10:LEU:HD22	68:H1:401:3PE:H352	2.04	0.40
42:H1:310:PHE:HB3	53:b1:32:PRO:HA	2.04	0.40
45:L1:473:PRO:HA	45:L1:474:PRO:HD3	1.91	0.40
46:M1:216:LEU:HD23	46:M1:287:ALA:HB1	2.04	0.40
49:X1:136:LEU:HD12	49:X1:137:PRO:HD2	2.03	0.40
50:Y1:13:ASP:HA	50:Y1:20:LYS:HE3	2.03	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	A	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
1	L	443/480 (92%)	427 (96%)	16 (4%)	0	100	100
2	B	416/453 (92%)	410 (99%)	6 (1%)	0	100	100
2	M	418/453 (92%)	400 (96%)	18 (4%)	0	100	100
3	C	378/381 (99%)	368 (97%)	10 (3%)	0	100	100
3	N	378/381 (99%)	364 (96%)	14 (4%)	0	100	100
4	D	238/325 (73%)	228 (96%)	10 (4%)	0	100	100
4	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
5	E	194/274 (71%)	188 (97%)	6 (3%)	0	100	100
5	P	194/274 (71%)	187 (96%)	7 (4%)	0	100	100
5	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/111 (89%)	99 (100%)	0	0	100	100
6	Q	100/111 (90%)	99 (99%)	1 (1%)	0	100	100
7	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
7	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
8	H	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
8	S	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
9	J	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
9	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
10	K	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
10	V	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
11	n	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
12	o	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
13	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
14	q	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
15	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
16	s	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
17	t	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
18	u	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
19	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
20	x	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
21	y	45/63 (71%)	45 (100%)	0	0	100	100
22	z	42/69 (61%)	36 (86%)	5 (12%)	1 (2%)	4	24
23	w	55/83 (66%)	55 (100%)	0	0	100	100
24	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
25	C1	206/263 (78%)	198 (96%)	8 (4%)	0	100	100
26	D1	427/463 (92%)	410 (96%)	17 (4%)	0	100	100
27	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	24	55
28	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
29	3	688/727 (95%)	658 (96%)	30 (4%)	0	100	100
30	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
31	P1	340/377 (90%)	324 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Q1	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
33	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
34	S1	82/99 (83%)	77 (94%)	5 (6%)	0	100	100
35	T1	77/156 (49%)	74 (96%)	3 (4%)	0	100	100
35	U1	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
36	V1	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
37	W1	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
38	q1	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
39	r1	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
40	s1	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
41	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
42	H1	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
43	J1	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
44	K1	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
45	L1	604/607 (100%)	575 (95%)	29 (5%)	0	100	100
46	M1	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
47	N1	343/345 (99%)	333 (97%)	10 (3%)	0	100	100
48	O1	318/355 (90%)	297 (93%)	21 (7%)	0	100	100
49	X1	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
50	Y1	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
51	Z1	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
52	a1	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
53	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
54	c1	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
55	d1	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
56	e1	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
57	f1	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
58	g1	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
59	h1	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
60	i1	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
61	j1	63/105 (60%)	58 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	k1	75/104 (72%)	74 (99%)	1 (1%)	0	100	100
63	l1	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
64	m1	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
65	n1	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
66	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
67	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	13985/16129 (87%)	13467 (96%)	516 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	z	40	TYR
27	2	183	LYS

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	A	372/398 (94%)	372 (100%)	0	100	100
1	L	372/398 (94%)	372 (100%)	0	100	100
2	B	328/356 (92%)	328 (100%)	0	100	100
2	M	330/356 (93%)	330 (100%)	0	100	100
3	C	332/333 (100%)	332 (100%)	0	100	100
3	N	332/333 (100%)	332 (100%)	0	100	100
4	D	205/260 (79%)	205 (100%)	0	100	100
4	O	205/260 (79%)	205 (100%)	0	100	100
5	E	69/224 (31%)	69 (100%)	0	100	100
5	P	69/224 (31%)	69 (100%)	0	100	100
5	T	58/224 (26%)	58 (100%)	0	100	100
6	F	93/99 (94%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Q	94/99 (95%)	94 (100%)	0	100	100
7	G	70/74 (95%)	70 (100%)	0	100	100
7	R	70/74 (95%)	70 (100%)	0	100	100
8	H	63/83 (76%)	63 (100%)	0	100	100
8	S	65/83 (78%)	65 (100%)	0	100	100
9	J	51/55 (93%)	51 (100%)	0	100	100
9	U	51/55 (93%)	51 (100%)	0	100	100
10	K	41/46 (89%)	41 (100%)	0	100	100
10	V	42/46 (91%)	42 (100%)	0	100	100
11	n	425/425 (100%)	425 (100%)	0	100	100
12	o	210/210 (100%)	209 (100%)	1 (0%)	81	83
13	p	226/227 (100%)	226 (100%)	0	100	100
14	q	122/146 (84%)	122 (100%)	0	100	100
15	r	91/118 (77%)	91 (100%)	0	100	100
16	s	80/101 (79%)	80 (100%)	0	100	100
17	t	66/92 (72%)	66 (100%)	0	100	100
18	u	70/76 (92%)	70 (100%)	0	100	100
19	v	54/57 (95%)	54 (100%)	0	100	100
20	x	39/67 (58%)	39 (100%)	0	100	100
21	y	40/55 (73%)	40 (100%)	0	100	100
22	z	39/61 (64%)	39 (100%)	0	100	100
23	w	43/67 (64%)	43 (100%)	0	100	100
24	6	133/185 (72%)	133 (100%)	0	100	100
25	C1	190/227 (84%)	190 (100%)	0	100	100
26	D1	370/394 (94%)	370 (100%)	0	100	100
27	2	184/206 (89%)	184 (100%)	0	100	100
28	1	345/370 (93%)	345 (100%)	0	100	100
29	3	580/610 (95%)	580 (100%)	0	100	100
30	9	152/178 (85%)	152 (100%)	0	100	100
31	P1	299/325 (92%)	299 (100%)	0	100	100
32	Q1	113/153 (74%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	7	81/96 (84%)	81 (100%)	0	100	100
34	S1	74/80 (92%)	74 (100%)	0	100	100
35	T1	73/135 (54%)	73 (100%)	0	100	100
35	U1	81/135 (60%)	81 (100%)	0	100	100
36	V1	101/102 (99%)	101 (100%)	0	100	100
37	W1	108/114 (95%)	108 (100%)	0	100	100
38	q1	131/131 (100%)	131 (100%)	0	100	100
39	r1	88/96 (92%)	88 (100%)	0	100	100
40	s1	41/95 (43%)	40 (98%)	1 (2%)	43	65
41	A1	103/103 (100%)	103 (100%)	0	100	100
42	H1	279/279 (100%)	279 (100%)	0	100	100
43	J1	137/137 (100%)	137 (100%)	0	100	100
44	K1	87/87 (100%)	87 (100%)	0	100	100
45	L1	548/549 (100%)	548 (100%)	0	100	100
46	M1	414/414 (100%)	414 (100%)	0	100	100
47	N1	307/307 (100%)	307 (100%)	0	100	100
48	O1	284/309 (92%)	284 (100%)	0	100	100
49	X1	153/154 (99%)	153 (100%)	0	100	100
50	Y1	105/106 (99%)	105 (100%)	0	100	100
51	Z1	122/123 (99%)	122 (100%)	0	100	100
52	a1	60/60 (100%)	60 (100%)	0	100	100
53	b1	72/73 (99%)	72 (100%)	0	100	100
54	c1	42/67 (63%)	42 (100%)	0	100	100
55	d1	107/107 (100%)	107 (100%)	0	100	100
56	e1	93/94 (99%)	93 (100%)	0	100	100
57	f1	49/53 (92%)	49 (100%)	0	100	100
58	g1	92/129 (71%)	92 (100%)	0	100	100
59	h1	123/162 (76%)	123 (100%)	0	100	100
60	i1	99/119 (83%)	99 (100%)	0	100	100
61	j1	61/87 (70%)	61 (100%)	0	100	100
62	k1	60/78 (77%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	l1	142/161 (88%)	142 (100%)	0	100	100
64	m1	112/114 (98%)	112 (100%)	0	100	100
65	n1	163/164 (99%)	163 (100%)	0	100	100
66	o1	109/121 (90%)	109 (100%)	0	100	100
67	p1	155/158 (98%)	155 (100%)	0	100	100
All	All	12039/13729 (88%)	12037 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
12	o	213	MET
40	s1	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	363	ASN
1	A	368	HIS
2	B	290	ASN
2	B	297	GLN
2	B	400	GLN
2	B	429	ASN
2	B	432	HIS
3	C	8	HIS
3	C	74	ASN
4	D	71	GLN
4	D	105	ASN
4	D	181	GLN
8	H	65	HIS
8	H	69	HIS
1	L	85	HIS
1	L	173	ASN
1	L	279	HIS
1	L	430	GLN
2	M	170	ASN
2	M	174	ASN
2	M	213	HIS
2	M	284	HIS

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Mol	Chain	Res	Type
3	N	207	ASN
3	N	212	ASN
4	O	198	HIS
5	T	31	GLN
11	n	256	HIS
12	o	103	GLN
12	o	180	ASN
12	o	187	ASN
13	p	70	HIS
13	p	76	GLN
13	p	158	HIS
13	p	204	HIS
14	q	63	GLN
15	r	94	ASN
17	t	75	ASN
18	u	10	ASN
18	u	37	HIS
20	x	41	ASN
23	w	3	ASN
26	D1	200	HIS
27	2	58	ASN
27	2	214	GLN
28	1	96	ASN
28	1	224	ASN
29	3	237	ASN
29	3	255	HIS
29	3	342	ASN
29	3	517	ASN
29	3	629	ASN
29	3	640	ASN
30	9	67	HIS
31	P1	44	GLN
31	P1	234	ASN
31	P1	306	GLN
33	7	95	HIS
33	7	96	HIS
35	T1	74	GLN
38	q1	31	ASN
38	q1	112	ASN
39	r1	51	ASN
41	A1	80	GLN
42	H1	169	GLN

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Mol	Chain	Res	Type
42	H1	194	ASN
43	J1	107	ASN
45	L1	2	ASN
45	L1	209	ASN
45	L1	320	ASN
45	L1	506	ASN
46	M1	279	GLN
46	M1	366	ASN
47	N1	46	ASN
47	N1	112	HIS
47	N1	144	GLN
47	N1	171	ASN
47	N1	222	ASN
47	N1	223	ASN
48	O1	97	GLN
48	O1	271	ASN
48	O1	288	GLN
35	U1	74	GLN
50	Y1	78	GLN
51	Z1	75	GLN
52	a1	31	ASN
54	c1	46	ASN
58	g1	101	ASN
60	i1	25	GLN
61	j1	6	HIS
61	j1	21	GLN
61	j1	50	HIS
62	k1	26	GLN
63	l1	51	ASN
64	m1	78	ASN
66	o1	84	HIS
67	p1	90	GLN
67	p1	123	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
39	AYA	r1	1	39	6,7,8	1.29	1 (16%)	6,8,10	1.15	1 (16%)
60	SAC	i1	1	60	7,8,9	1.02	0	7,9,11	1.10	1 (14%)
44	FME	K1	1	44	8,9,10	0.93	0	8,9,11	1.68	2 (25%)
46	FME	M1	1	46	8,9,10	1.01	0	8,9,11	0.82	0
43	FME	J1	1	43	8,9,10	0.98	0	8,9,11	0.87	0
47	FME	N1	1	47	8,9,10	0.96	0	8,9,11	0.93	0
41	FME	A1	1	41	8,9,10	0.98	0	8,9,11	0.85	0
53	AYA	b1	1	53	6,7,8	1.26	1 (16%)	6,8,10	1.17	1 (16%)
26	2MR	D1	85	26	10,12,13	2.66	2 (20%)	5,13,15	2.80	2 (40%)
42	FME	H1	1	42	8,9,10	1.01	0	8,9,11	0.77	0
45	FME	L1	1	45	8,9,10	0.95	0	8,9,11	0.94	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
39	AYA	r1	1	39	-	0/5/6/8	-
60	SAC	i1	1	60	-	0/7/8/10	-
44	FME	K1	1	44	-	5/7/9/11	-
46	FME	M1	1	46	-	2/7/9/11	-
43	FME	J1	1	43	-	3/7/9/11	-
47	FME	N1	1	47	-	4/7/9/11	-
41	FME	A1	1	41	-	1/7/9/11	-
53	AYA	b1	1	53	-	0/5/6/8	-
26	2MR	D1	85	26	-	3/10/13/15	-
42	FME	H1	1	42	-	3/7/9/11	-
45	FME	L1	1	45	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D1	85	2MR	CZ-NE	5.93	1.46	1.34
26	D1	85	2MR	CZ-NH2	5.31	1.44	1.33
39	r1	1	AYA	CA-N	-2.48	1.43	1.46
53	b1	1	AYA	CA-N	-2.28	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D1	85	2MR	CD-NE-CZ	5.27	133.27	123.36
44	K1	1	FME	C-CA-N	3.91	117.05	109.50
26	D1	85	2MR	NE-CZ-NH2	-3.00	116.73	119.48
39	r1	1	AYA	CB-CA-N	2.61	112.63	109.68
53	b1	1	AYA	CB-CA-N	2.51	112.51	109.68
44	K1	1	FME	O-C-CA	-2.24	119.02	124.77
60	i1	1	SAC	OG-CB-CA	-2.23	104.98	111.13

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
26	D1	85	2MR	CG-CD-NE-CZ
42	H1	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	i1	1	SAC	1	0
44	K1	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 7 are monoatomic - leaving 86 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	$\# Z > 2$
68	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.39	0
71	HEC	D	301	4	46,50,50	1.83	7 (15%)	58,82,82	1.93	5 (8%)
80	TGL	y	601	-	36,36,62	0.22	0	39,39,65	0.17	0
72	FES	3	803	29	0,4,4	-	-	-		
81	SF4	1	502	28	0,12,12	-	-	-		
81	SF4	9	201	30	0,12,12	-	-	-		
73	PC1	p	303	-	49,49,53	0.32	0	55,57,61	0.59	1 (1%)
68	3PE	z	102	-	25,25,50	0.41	0	28,30,55	0.41	0
68	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.67	1 (4%)
68	3PE	D1	501	-	50,50,50	0.30	0	53,55,55	0.29	0
69	CDL	R	303	-	56,56,99	0.39	0	62,68,111	0.48	1 (1%)
69	CDL	Y1	401	-	93,93,99	0.30	0	99,105,111	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	HEC	O	301	4	46,50,50	1.83	6 (13%)	58,82,82	1.93	4 (6%)
69	CDL	Y1	404	-	71,71,99	0.35	0	77,83,111	0.44	1 (1%)
73	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
73	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.35	0
76	HEA	n	604	11	67,67,67	1.39	6 (8%)	81,103,103	2.25	27 (33%)
73	PC1	A1	601	-	30,30,53	0.40	0	36,38,61	0.58	0
69	CDL	R	302	-	40,40,99	0.45	0	46,52,111	0.55	0
73	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.37	0
70	HEM	N	402	3	50,50,50	1.37	7 (14%)	67,82,82	1.18	5 (7%)
68	3PE	N	401	-	33,33,50	0.36	0	36,38,55	0.34	0
81	SF4	3	801	29	0,12,12	-	-	-	-	-
68	3PE	C	405	-	50,50,50	0.31	0	53,55,55	0.29	0
81	SF4	6	201	24	0,12,12	-	-	-	-	-
68	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.62	1 (3%)
68	3PE	Y1	402	-	27,27,50	0.40	0	30,32,55	0.37	0
72	FES	2	301	27	0,4,4	-	-	-	-	-
86	DGT	O1	401	77	32,33,33	0.30	0	48,52,52	0.31	0
68	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.48	0
85	ZMP	n1	201	-	26,31,36	0.74	1 (3%)	30,38,45	0.90	1 (3%)
68	3PE	Z1	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
73	PC1	z	101	-	27,27,53	0.38	0	33,35,61	0.38	0
72	FES	P	202	5	0,4,4	-	-	-	-	-
70	HEM	C	402	3	50,50,50	1.38	8 (16%)	67,82,82	1.17	5 (7%)
68	3PE	H1	401	-	45,45,50	0.31	0	48,50,55	0.30	0
68	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.33	0
72	FES	E	201	5	0,4,4	-	-	-	-	-
73	PC1	6	203	-	42,42,53	0.33	0	48,50,61	0.51	0
76	HEA	n	603	11	67,67,67	1.38	8 (11%)	81,103,103	2.31	29 (35%)
68	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.32	0
68	3PE	d1	202	-	30,30,50	0.38	0	33,35,55	0.33	0
73	PC1	V	101	-	27,27,53	0.39	0	33,35,61	0.36	0
73	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.38	0
73	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.64	1 (3%)
68	3PE	v	101	-	27,27,50	0.39	0	30,32,55	0.35	0
69	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.36	0
69	CDL	h1	201	-	69,69,99	0.35	0	75,81,111	0.43	1 (1%)
68	3PE	R	304	-	29,29,50	0.38	0	32,34,55	0.34	0
68	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.36	0
68	3PE	N	404	-	36,36,50	0.35	0	39,41,55	0.33	0
69	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.35	0
68	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
85	ZMP	W1	201	-	28,33,36	0.65	1 (3%)	32,40,45	0.98	1 (3%)
68	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
70	HEM	N	403	3	50,50,50	1.34	7 (14%)	67,82,82	1.11	4 (5%)
69	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.34	0
68	3PE	P	201	-	32,32,50	0.37	0	35,37,55	0.35	0
69	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.30	0
84	NDP	P1	501	-	51,52,52	0.34	0	71,80,80	0.43	0
69	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.40	1 (1%)
68	3PE	A1	602	-	42,42,50	0.33	0	45,47,55	0.32	0
73	PC1	9	203	-	53,53,53	0.29	0	59,61,61	0.47	0
68	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.31	0
73	PC1	E	202	-	34,34,53	0.35	0	40,42,61	0.38	0
68	3PE	n	606	-	27,27,50	0.41	0	30,32,55	0.39	0
70	HEM	C	401	3	50,50,50	1.34	7 (14%)	67,82,82	1.15	3 (4%)
68	3PE	M1	503	-	35,35,50	0.35	0	38,40,55	0.31	0
68	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.27	0
81	SF4	9	202	30	0,12,12	-	-	-	-	-
68	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.57	1 (2%)
69	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.51	0
81	SF4	3	802	29	0,12,12	-	-	-	-	-
78	CUA	o	303	12	0,1,1	-	-	-	-	-
68	3PE	i1	201	-	41,41,50	0.33	0	44,46,55	0.31	0
68	3PE	L1	704	-	50,50,50	0.30	0	53,55,55	0.31	0
82	FMN	1	501	-	33,33,33	0.27	0	48,50,50	0.35	0
69	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
69	CDL	a1	101	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
69	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
68	3PE	C	406	-	30,30,50	0.39	0	33,35,55	0.35	0
69	CDL	R	301	-	56,56,99	0.38	0	62,68,111	0.33	0
69	CDL	L1	703	-	45,45,99	0.42	0	51,57,111	0.37	0
68	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.31	0
68	3PE	x	101	-	26,26,50	0.40	0	29,31,55	0.36	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
68	3PE	L	501	-	-	6/26/26/54	-
71	HEC	D	301	4	-	4/14/54/54	-
80	TGL	y	601	-	-	1/39/39/65	-
72	FES	3	803	29	-	-	0/1/1/1
81	SF4	1	502	28	-	-	0/6/5/5
81	SF4	9	201	30	-	-	0/6/5/5
73	PC1	p	303	-	-	11/53/53/57	-
68	3PE	z	102	-	-	10/29/29/54	-
68	3PE	A	501	-	-	10/26/26/54	-
68	3PE	D1	501	-	-	8/54/54/54	-
69	CDL	R	303	-	-	14/67/67/110	-
69	CDL	Y1	401	-	-	13/104/104/110	-
71	HEC	O	301	4	-	4/14/54/54	-
69	CDL	Y1	404	-	-	19/82/82/110	-
73	PC1	9	204	-	-	13/50/50/57	-
73	PC1	p	302	-	-	8/38/38/57	-
76	HEA	n	604	11	-	11/36/76/76	-
73	PC1	A1	601	-	-	14/34/34/57	-
69	CDL	R	302	-	-	10/51/51/110	-
73	PC1	M1	501	-	-	12/57/57/57	-
70	HEM	N	402	3	-	2/14/54/54	-
68	3PE	N	401	-	-	4/37/37/54	-
81	SF4	3	801	29	-	-	0/6/5/5
68	3PE	C	405	-	-	7/54/54/54	-
81	SF4	6	201	24	-	-	0/6/5/5
68	3PE	t	101	-	-	9/28/28/54	-
68	3PE	Y1	402	-	-	7/31/31/54	-
72	FES	2	301	27	-	-	0/1/1/1
86	DGT	O1	401	77	-	3/22/34/34	0/3/3/3
68	3PE	L1	701	-	-	7/54/54/54	-
85	ZMP	n1	201	-	-	18/36/38/43	-
68	3PE	Z1	401	-	-	9/54/54/54	-
73	PC1	z	101	-	-	3/31/31/57	-
72	FES	P	202	5	-	-	0/1/1/1
70	HEM	C	402	3	-	1/14/54/54	-
68	3PE	H1	401	-	-	11/49/49/54	-
68	3PE	K1	201	-	-	11/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	FES	E	201	5	-	-	0/1/1/1
73	PC1	6	203	-	-	6/46/46/57	-
76	HEA	n	603	11	-	11/36/76/76	-
68	3PE	6	202	-	-	3/35/35/54	-
68	3PE	d1	202	-	-	9/34/34/54	-
73	PC1	V	101	-	-	5/31/31/57	-
73	PC1	K	101	-	-	9/31/31/57	-
73	PC1	L	503	-	-	8/27/27/57	-
68	3PE	v	101	-	-	4/31/31/54	-
69	CDL	C	404	-	-	12/52/52/110	-
69	CDL	h1	201	-	-	20/80/80/110	-
68	3PE	R	304	-	-	6/33/33/54	-
68	3PE	C	403	-	-	10/38/38/54	-
68	3PE	N	404	-	-	7/40/40/54	-
69	CDL	A	502	-	-	13/56/56/110	-
68	3PE	d1	203	-	-	6/35/35/54	-
68	3PE	o	302	-	-	8/32/32/54	-
85	ZMP	W1	201	-	-	6/38/40/43	-
68	3PE	N1	402	-	-	10/41/41/54	-
70	HEM	N	403	3	-	4/14/54/54	-
69	CDL	D	302	-	-	17/66/66/110	-
68	3PE	P	201	-	-	5/36/36/54	-
69	CDL	L1	702	-	-	19/88/88/110	-
84	NDP	P1	501	-	-	6/34/77/77	0/5/5/5
69	CDL	N1	401	-	-	14/100/100/110	-
68	3PE	A1	602	-	-	9/46/46/54	-
73	PC1	9	203	-	-	9/57/57/57	-
68	3PE	Y1	403	-	-	10/45/45/54	-
73	PC1	E	202	-	-	7/38/38/57	-
68	3PE	n	606	-	-	13/31/31/54	-
70	HEM	C	401	3	-	1/14/54/54	-
68	3PE	M1	503	-	-	8/39/39/54	-
68	3PE	M1	502	-	-	12/54/54/54	-
81	SF4	9	202	30	-	-	0/6/5/5
68	3PE	n	605	-	-	9/37/37/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	CDL	L	502	-	-	8/56/56/110	-
81	SF4	3	802	29	-	-	0/6/5/5
68	3PE	i1	201	-	-	5/45/45/54	-
68	3PE	L1	704	-	-	14/54/54/54	-
82	FMN	1	501	-	-	5/18/18/18	0/3/3/3
69	CDL	H1	402	-	-	13/59/59/110	-
69	CDL	a1	101	-	-	13/67/67/110	-
69	CDL	d1	201	-	-	14/77/77/110	-
68	3PE	C	406	-	-	5/34/34/54	-
69	CDL	R	301	-	-	17/67/67/110	-
69	CDL	L1	703	-	-	11/56/56/110	-
68	3PE	p	301	-	-	9/48/48/54	-
68	3PE	x	101	-	-	9/30/30/54	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	O	301	HEC	CAC-C3C	6.13	1.54	1.35
71	D	301	HEC	CAC-C3C	6.11	1.54	1.35
71	D	301	HEC	CAB-C3B	6.07	1.54	1.35
71	O	301	HEC	CAB-C3B	6.05	1.54	1.35
71	O	301	HEC	C3D-C2D	5.64	1.53	1.38
71	D	301	HEC	C3D-C2D	5.57	1.53	1.38
76	n	603	HEA	C3B-C2B	4.37	1.44	1.34
76	n	604	HEA	C3D-C2D	4.35	1.46	1.36
70	C	402	HEM	FE-NB	4.27	2.08	1.94
76	n	604	HEA	C3B-C2B	4.20	1.44	1.34
76	n	603	HEA	C3D-C2D	4.08	1.45	1.36
76	n	604	HEA	C3A-C2A	3.73	1.45	1.37
70	N	403	HEM	FE-NB	3.56	2.05	1.94
70	N	402	HEM	FE-NC	3.56	2.06	1.95
76	n	603	HEA	C3A-C2A	3.47	1.45	1.37
70	N	403	HEM	CAB-C3B	3.21	1.56	1.47
70	N	402	HEM	CAC-C3C	3.20	1.55	1.47
70	N	402	HEM	FE-ND	3.20	2.04	1.94
70	N	402	HEM	CAB-C3B	3.19	1.55	1.47
70	C	401	HEM	CAC-C3C	3.19	1.55	1.47
70	C	402	HEM	CAB-C3B	3.16	1.55	1.47
70	C	402	HEM	CAC-C3C	3.16	1.55	1.47
70	C	401	HEM	CAB-C3B	3.12	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	N	403	HEM	CAC-C3C	3.08	1.55	1.47
70	C	401	HEM	FE-NC	3.03	2.05	1.95
76	n	603	HEA	C4B-C3B	2.90	1.49	1.44
70	C	401	HEM	FE-NB	2.76	2.03	1.94
70	N	403	HEM	FE-NC	2.76	2.04	1.95
70	C	402	HEM	FE-NA	2.76	2.04	1.95
76	n	604	HEA	C4B-C3B	2.75	1.49	1.44
70	C	402	HEM	FE-NC	2.64	2.03	1.95
85	n1	201	ZMP	C9-C10	2.60	1.53	1.50
70	C	401	HEM	FE-ND	2.53	2.02	1.94
70	N	402	HEM	FE-NB	2.52	2.02	1.94
76	n	603	HEA	C1D-ND	-2.44	1.36	1.40
70	N	403	HEM	FE-NA	2.36	2.02	1.95
70	C	401	HEM	FE-NA	2.32	2.02	1.95
76	n	603	HEA	C1C-C2C	2.31	1.48	1.43
85	W1	201	ZMP	C9-C10	2.30	1.53	1.50
76	n	604	HEA	C1D-ND	-2.22	1.36	1.40
70	C	401	HEM	CMC-C2C	2.13	1.55	1.50
70	N	403	HEM	CMB-C2B	2.13	1.55	1.50
71	O	301	HEC	C3B-C2B	-2.13	1.34	1.41
70	N	402	HEM	CMC-C2C	2.12	1.55	1.50
71	D	301	HEC	C3C-C2C	-2.12	1.34	1.41
70	C	402	HEM	C2A-C3A	-2.10	1.33	1.38
71	O	301	HEC	C3C-C2C	-2.10	1.34	1.41
70	N	403	HEM	CMC-C2C	2.09	1.55	1.50
70	C	402	HEM	CMC-C2C	2.08	1.55	1.50
70	C	402	HEM	CMB-C2B	2.08	1.55	1.50
71	D	301	HEC	C3B-C2B	-2.07	1.34	1.41
70	N	402	HEM	C2A-C3A	-2.06	1.33	1.38
71	D	301	HEC	CMB-C2B	2.06	1.55	1.50
71	D	301	HEC	CMC-C2C	2.04	1.55	1.50
76	n	604	HEA	C1A-C2A	2.03	1.48	1.45
71	O	301	HEC	CMC-C2C	2.03	1.54	1.50
76	n	603	HEA	C4D-C3D	2.01	1.48	1.45
76	n	603	HEA	C11-C3B	-2.01	1.48	1.51

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	D	301	HEC	CBC-CAC-C3C	-8.79	109.87	127.43
71	O	301	HEC	CBC-CAC-C3C	-8.69	110.06	127.43
71	D	301	HEC	CBB-CAB-C3B	-8.36	110.73	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	O	301	HEC	CBB-CAB-C3B	-8.32	110.80	127.43
76	n	604	HEA	C3A-C2A-C1A	-6.77	100.64	107.05
76	n	603	HEA	C3A-C2A-C1A	-6.34	101.05	107.05
76	n	604	HEA	C2A-C1A-NA	5.12	115.26	110.32
76	n	603	HEA	CMC-C2C-C3C	4.85	137.95	126.55
76	n	604	HEA	CMC-C2C-C3C	4.82	137.89	126.55
76	n	604	HEA	CMD-C2D-C1D	-4.82	117.51	125.03
76	n	603	HEA	C2A-C1A-NA	4.79	114.94	110.32
76	n	604	HEA	C3D-C4D-ND	4.79	114.98	110.35
76	n	603	HEA	CMD-C2D-C1D	-4.67	117.74	125.03
76	n	603	HEA	C3D-C4D-ND	4.43	114.63	110.35
76	n	603	HEA	CMB-C2B-C1B	-4.43	118.12	125.03
76	n	604	HEA	CMC-C2C-C1C	-4.38	118.76	125.42
76	n	603	HEA	CMC-C2C-C1C	-4.32	118.83	125.42
76	n	603	HEA	C13-C12-C11	-4.23	107.64	114.39
76	n	604	HEA	CMB-C2B-C1B	-4.19	118.49	125.03
76	n	604	HEA	CHA-C4D-C3D	-3.97	118.99	124.77
76	n	604	HEA	CMD-C2D-C3D	3.82	136.49	126.15
76	n	603	HEA	C26-C15-C16	3.82	121.86	115.23
76	n	603	HEA	C4D-C3D-C2D	-3.74	101.44	106.89
76	n	603	HEA	CHA-C4D-C3D	-3.68	119.41	124.77
76	n	604	HEA	C4D-C3D-C2D	-3.60	101.65	106.89
76	n	604	HEA	C13-C12-C11	-3.57	108.69	114.39
76	n	604	HEA	CHA-C1A-C2A	-3.54	119.28	124.86
76	n	603	HEA	CMD-C2D-C3D	3.53	135.69	126.15
71	O	301	HEC	C4D-ND-C1D	3.53	111.57	105.82
76	n	604	HEA	C26-C15-C16	3.49	121.29	115.23
76	n	603	HEA	CHA-C1A-C2A	-3.42	119.46	124.86
71	D	301	HEC	C4D-ND-C1D	3.41	111.37	105.82
76	n	603	HEA	C3C-C2C-C1C	-3.35	103.22	107.17
76	n	603	HEA	CMB-C2B-C3B	3.27	136.61	130.28
76	n	604	HEA	C3C-C2C-C1C	-3.25	103.34	107.17
76	n	603	HEA	C17-C18-C19	-3.24	120.20	127.62
76	n	603	HEA	CAA-CBA-CGA	-3.21	105.16	113.67
76	n	603	HEA	C13-C14-C15	-3.05	120.63	127.62
76	n	603	HEA	CHB-C1B-C2B	-3.00	120.28	125.03
70	C	402	HEM	C4D-ND-C1D	2.85	108.58	105.21
70	C	401	HEM	C3B-C2B-C1B	2.71	108.44	106.41
76	n	604	HEA	CMB-C2B-C3B	2.70	135.50	130.28
70	N	402	HEM	C3B-C2B-C1B	2.69	108.43	106.41
76	n	604	HEA	C17-C18-C19	-2.68	121.49	127.62
85	W1	201	ZMP	O1-C10-C9	-2.67	120.89	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	n	603	HEA	C12-C11-C3B	2.65	116.27	112.12
76	n	604	HEA	CHB-C1B-C2B	-2.64	120.86	125.03
70	N	403	HEM	C4D-ND-C1D	2.63	108.32	105.21
76	n	604	HEA	C4B-C3B-C2B	-2.58	103.10	107.44
70	C	402	HEM	C3D-C4D-ND	-2.56	107.36	110.17
85	n1	201	ZMP	O1-C10-C9	-2.56	121.03	123.98
76	n	603	HEA	CHB-C1B-NB	2.52	127.14	124.42
76	n	604	HEA	CHC-C1C-C2C	-2.46	120.27	127.43
76	n	603	HEA	C27-C19-C20	2.43	119.44	115.23
70	C	401	HEM	C4D-ND-C1D	2.43	108.08	105.21
76	n	604	HEA	CHB-C1B-NB	2.41	127.01	124.42
76	n	604	HEA	C3B-C4B-NB	2.38	112.58	109.84
76	n	604	HEA	C13-C14-C15	-2.38	122.17	127.62
70	N	403	HEM	C3D-C4D-ND	-2.37	107.57	110.17
70	N	402	HEM	C4D-ND-C1D	2.35	107.99	105.21
76	n	604	HEA	CAA-CBA-CGA	-2.34	107.45	113.67
76	n	604	HEA	CAD-C3D-C2D	2.34	132.25	127.87
71	O	301	HEC	C2A-C1A-NA	-2.33	108.07	110.32
76	n	604	HEA	C25-C23-C24	2.32	119.93	114.59
76	n	603	HEA	C2B-C1B-NB	2.31	112.58	109.90
70	N	402	HEM	C2A-C1A-NA	-2.31	107.59	110.15
76	n	603	HEA	C25-C23-C24	2.28	119.83	114.59
76	n	603	HEA	C3C-C4C-NC	2.27	111.71	109.80
73	p	303	PC1	C2-O21-C21	2.26	123.20	117.80
70	C	402	HEM	CMB-C2B-C1B	-2.17	121.64	125.03
70	N	402	HEM	C3D-C4D-ND	-2.17	107.79	110.17
76	n	603	HEA	CAD-C3D-C4D	2.16	128.47	124.70
68	t	101	3PE	C2-O21-C21	2.15	122.95	117.80
70	C	402	HEM	C2A-C1A-NA	-2.15	107.77	110.15
76	n	603	HEA	C4B-C3B-C2B	-2.14	103.84	107.44
71	D	301	HEC	C2A-C1A-NA	-2.14	108.26	110.32
71	D	301	HEC	CAA-CBA-CGA	-2.14	108.00	113.67
69	Y1	404	CDL	CA4-OA6-CA5	2.14	122.91	117.80
76	n	604	HEA	CAD-CBD-CGD	-2.13	108.01	113.67
68	n	605	3PE	C2-O21-C21	2.13	122.89	117.80
70	C	402	HEM	C2D-C1D-ND	-2.13	107.44	109.90
70	C	401	HEM	C3D-C4D-ND	-2.13	107.84	110.17
76	n	603	HEA	CHC-C1C-C2C	-2.12	121.28	127.43
69	a1	101	CDL	CA4-OA6-CA5	2.10	122.81	117.80
69	R	303	CDL	CA4-OA6-CA5	2.09	122.80	117.80
68	Z1	401	3PE	C2-O21-C21	2.09	122.79	117.80
69	N1	401	CDL	CB4-OB6-CB5	2.08	122.77	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	N	403	HEM	CMB-C2B-C1B	-2.06	121.81	125.03
73	L	503	PC1	C2-O21-C21	2.05	122.71	117.80
76	n	604	HEA	C27-C19-C20	2.04	118.77	115.23
68	A	501	3PE	C2-O21-C21	2.04	122.68	117.80
69	h1	201	CDL	CB4-OB6-CB5	2.04	122.67	117.80
76	n	603	HEA	C26-C15-C14	-2.03	118.42	123.63
70	N	403	HEM	C2A-C1A-NA	-2.02	107.91	110.15
70	N	402	HEM	CAA-CBA-CGA	-2.01	108.34	113.67

There are no chirality outliers.

All (679) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	A	501	3PE	C11-O13-P-O11
68	A	501	3PE	C11-O13-P-O12
68	A	501	3PE	C11-O13-P-O14
68	C	403	3PE	C1-O11-P-O12
68	C	403	3PE	C1-O11-P-O13
68	C	403	3PE	C1-O11-P-O14
68	C	403	3PE	C11-O13-P-O11
68	C	403	3PE	C11-O13-P-O12
68	C	403	3PE	C11-O13-P-O14
68	C	403	3PE	O13-C11-C12-N
68	C	405	3PE	C11-O13-P-O11
68	C	405	3PE	O13-C11-C12-N
68	C	406	3PE	O13-C11-C12-N
68	L	501	3PE	C11-O13-P-O11
68	L	501	3PE	C11-O13-P-O12
68	L	501	3PE	C11-O13-P-O14
68	L	501	3PE	O13-C11-C12-N
68	N	404	3PE	C11-O13-P-O11
68	N	404	3PE	C11-O13-P-O12
68	N	404	3PE	C11-O13-P-O14
68	N	404	3PE	O13-C11-C12-N
68	P	201	3PE	C1-O11-P-O14
68	P	201	3PE	C11-O13-P-O11
68	P	201	3PE	O13-C11-C12-N
68	R	304	3PE	C11-O13-P-O11
68	R	304	3PE	C11-O13-P-O12
68	n	605	3PE	C1-O11-P-O12
68	n	605	3PE	C11-O13-P-O11
68	n	605	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
68	n	605	3PE	C11-O13-P-O14
68	n	605	3PE	O13-C11-C12-N
68	n	606	3PE	C1-O11-P-O12
68	n	606	3PE	C1-O11-P-O13
68	n	606	3PE	C1-O11-P-O14
68	n	606	3PE	C11-O13-P-O11
68	o	302	3PE	C1-O11-P-O13
68	o	302	3PE	C11-O13-P-O11
68	p	301	3PE	C11-O13-P-O11
68	p	301	3PE	C11-O13-P-O12
68	p	301	3PE	O13-C11-C12-N
68	t	101	3PE	C11-O13-P-O11
68	t	101	3PE	C11-O13-P-O12
68	t	101	3PE	C11-O13-P-O14
68	t	101	3PE	O13-C11-C12-N
68	v	101	3PE	C1-O11-P-O12
68	v	101	3PE	C1-O11-P-O13
68	v	101	3PE	C1-O11-P-O14
68	x	101	3PE	C1-O11-P-O13
68	x	101	3PE	C11-O13-P-O11
68	x	101	3PE	C11-O13-P-O12
68	x	101	3PE	C11-O13-P-O14
68	x	101	3PE	O13-C11-C12-N
68	z	102	3PE	C1-O11-P-O12
68	z	102	3PE	C1-O11-P-O13
68	z	102	3PE	C1-O11-P-O14
68	z	102	3PE	C11-O13-P-O11
68	z	102	3PE	C11-O13-P-O12
68	z	102	3PE	C11-O13-P-O14
68	D1	501	3PE	C1-O11-P-O12
68	D1	501	3PE	C1-O11-P-O13
68	D1	501	3PE	O13-C11-C12-N
68	A1	602	3PE	C11-O13-P-O11
68	A1	602	3PE	C11-O13-P-O12
68	A1	602	3PE	C11-O13-P-O14
68	H1	401	3PE	C1-O11-P-O12
68	H1	401	3PE	C1-O11-P-O13
68	H1	401	3PE	C1-O11-P-O14
68	H1	401	3PE	C11-O13-P-O11
68	K1	201	3PE	C1-O11-P-O12
68	K1	201	3PE	C1-O11-P-O13
68	K1	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
68	K1	201	3PE	C11-O13-P-O14
68	K1	201	3PE	O13-C11-C12-N
68	L1	701	3PE	C1-O11-P-O12
68	L1	701	3PE	C1-O11-P-O13
68	L1	701	3PE	C1-O11-P-O14
68	L1	701	3PE	O13-C11-C12-N
68	L1	704	3PE	C1-O11-P-O12
68	L1	704	3PE	C1-O11-P-O13
68	L1	704	3PE	C11-O13-P-O11
68	L1	704	3PE	C11-O13-P-O12
68	L1	704	3PE	O13-C11-C12-N
68	M1	502	3PE	C11-O13-P-O11
68	M1	502	3PE	C11-O13-P-O12
68	M1	502	3PE	C11-O13-P-O14
68	M1	502	3PE	O13-C11-C12-N
68	M1	503	3PE	C1-O11-P-O14
68	M1	503	3PE	C11-O13-P-O11
68	M1	503	3PE	C11-O13-P-O12
68	M1	503	3PE	C11-O13-P-O14
68	N1	402	3PE	C1-O11-P-O12
68	N1	402	3PE	C1-O11-P-O13
68	N1	402	3PE	C11-O13-P-O11
68	N1	402	3PE	C11-O13-P-O12
68	N1	402	3PE	C11-O13-P-O14
68	N1	402	3PE	O13-C11-C12-N
68	Y1	402	3PE	C1-O11-P-O12
68	Y1	402	3PE	C1-O11-P-O13
68	Y1	402	3PE	C1-O11-P-O14
68	Y1	402	3PE	C11-O13-P-O11
68	Y1	402	3PE	C11-O13-P-O12
68	Y1	402	3PE	C11-O13-P-O14
68	Y1	403	3PE	C1-O11-P-O12
68	Y1	403	3PE	C1-O11-P-O13
68	Y1	403	3PE	C11-O13-P-O11
68	Y1	403	3PE	C11-O13-P-O12
68	Y1	403	3PE	C11-O13-P-O14
68	d1	202	3PE	C1-O11-P-O12
68	d1	202	3PE	C11-O13-P-O11
68	d1	202	3PE	C11-O13-P-O12
68	d1	202	3PE	C11-O13-P-O14
68	d1	202	3PE	O13-C11-C12-N
68	d1	203	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
68	d1	203	3PE	C1-O11-P-O13
68	d1	203	3PE	C1-O11-P-O14
68	d1	203	3PE	O13-C11-C12-N
69	A	502	CDL	CB2-OB2-PB2-OB4
69	A	502	CDL	CB2-OB2-PB2-OB5
69	A	502	CDL	CB3-OB5-PB2-OB3
69	A	502	CDL	CB3-OB5-PB2-OB4
69	C	404	CDL	CA2-OA2-PA1-OA3
69	C	404	CDL	CA2-OA2-PA1-OA4
69	C	404	CDL	CA2-OA2-PA1-OA5
69	C	404	CDL	CB3-OB5-PB2-OB2
69	C	404	CDL	CB3-OB5-PB2-OB3
69	C	404	CDL	CB3-OB5-PB2-OB4
69	D	302	CDL	CA2-OA2-PA1-OA3
69	D	302	CDL	CA2-OA2-PA1-OA4
69	D	302	CDL	CA2-OA2-PA1-OA5
69	D	302	CDL	CA3-OA5-PA1-OA3
69	D	302	CDL	CA3-OA5-PA1-OA4
69	D	302	CDL	CB2-OB2-PB2-OB4
69	D	302	CDL	CB2-OB2-PB2-OB5
69	D	302	CDL	CB3-OB5-PB2-OB2
69	D	302	CDL	CB3-OB5-PB2-OB4
69	L	502	CDL	CA3-OA5-PA1-OA3
69	R	301	CDL	CA2-OA2-PA1-OA4
69	R	301	CDL	CB2-OB2-PB2-OB3
69	R	301	CDL	CB2-OB2-PB2-OB5
69	R	301	CDL	CB3-OB5-PB2-OB2
69	R	301	CDL	CB3-OB5-PB2-OB4
69	R	302	CDL	CA2-OA2-PA1-OA3
69	R	302	CDL	CA2-OA2-PA1-OA4
69	R	302	CDL	CA2-OA2-PA1-OA5
69	R	302	CDL	CB2-OB2-PB2-OB5
69	R	303	CDL	CA2-OA2-PA1-OA4
69	R	303	CDL	CA3-OA5-PA1-OA2
69	R	303	CDL	CB2-OB2-PB2-OB3
69	H1	402	CDL	CA2-OA2-PA1-OA3
69	H1	402	CDL	CA2-OA2-PA1-OA5
69	H1	402	CDL	CB2-OB2-PB2-OB4
69	H1	402	CDL	CB2-OB2-PB2-OB5
69	L1	702	CDL	CA2-OA2-PA1-OA3
69	L1	702	CDL	CA2-OA2-PA1-OA4
69	L1	702	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
69	L1	702	CDL	CA3-OA5-PA1-OA2
69	L1	702	CDL	CA3-OA5-PA1-OA3
69	L1	702	CDL	CB2-OB2-PB2-OB3
69	L1	702	CDL	CB2-OB2-PB2-OB4
69	L1	702	CDL	CB2-OB2-PB2-OB5
69	L1	702	CDL	CB3-OB5-PB2-OB2
69	L1	702	CDL	CB3-OB5-PB2-OB3
69	L1	702	CDL	CB3-OB5-PB2-OB4
69	L1	703	CDL	CA2-OA2-PA1-OA3
69	L1	703	CDL	CA2-OA2-PA1-OA4
69	L1	703	CDL	CA2-OA2-PA1-OA5
69	L1	703	CDL	CA3-OA5-PA1-OA3
69	L1	703	CDL	CB2-OB2-PB2-OB3
69	L1	703	CDL	CB2-OB2-PB2-OB5
69	N1	401	CDL	CB2-OB2-PB2-OB3
69	N1	401	CDL	CB2-OB2-PB2-OB4
69	N1	401	CDL	CB2-OB2-PB2-OB5
69	Y1	401	CDL	CA2-OA2-PA1-OA3
69	Y1	401	CDL	CA2-OA2-PA1-OA4
69	Y1	401	CDL	CA2-OA2-PA1-OA5
69	Y1	401	CDL	CA3-OA5-PA1-OA3
69	Y1	401	CDL	CB3-OB5-PB2-OB2
69	Y1	404	CDL	CA2-OA2-PA1-OA3
69	Y1	404	CDL	CA3-OA5-PA1-OA2
69	Y1	404	CDL	CB2-OB2-PB2-OB3
69	Y1	404	CDL	CB2-OB2-PB2-OB4
69	Y1	404	CDL	CB2-OB2-PB2-OB5
69	Y1	404	CDL	CB3-OB5-PB2-OB2
69	Y1	404	CDL	CB3-OB5-PB2-OB3
69	Y1	404	CDL	CB3-OB5-PB2-OB4
69	a1	101	CDL	CA2-OA2-PA1-OA3
69	a1	101	CDL	CA2-OA2-PA1-OA4
69	a1	101	CDL	CA2-OA2-PA1-OA5
69	a1	101	CDL	CA3-OA5-PA1-OA4
69	a1	101	CDL	CB2-OB2-PB2-OB4
69	a1	101	CDL	CB2-OB2-PB2-OB5
69	d1	201	CDL	CA3-OA5-PA1-OA2
69	d1	201	CDL	CA3-OA5-PA1-OA3
69	d1	201	CDL	CB2-OB2-PB2-OB5
69	d1	201	CDL	OB5-CB3-CB4-OB6
69	h1	201	CDL	CA2-OA2-PA1-OA3
69	h1	201	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
69	h1	201	CDL	CB2-OB2-PB2-OB3
69	h1	201	CDL	CB2-OB2-PB2-OB4
69	h1	201	CDL	CB2-OB2-PB2-OB5
69	h1	201	CDL	CB3-OB5-PB2-OB2
69	h1	201	CDL	CB3-OB5-PB2-OB4
71	D	301	HEC	C2B-C3B-CAB-CBB
71	D	301	HEC	C2C-C3C-CAC-CBC
71	O	301	HEC	C2B-C3B-CAB-CBB
71	O	301	HEC	C2C-C3C-CAC-CBC
73	E	202	PC1	C11-O13-P-O11
73	E	202	PC1	C1-O11-P-O12
73	K	101	PC1	C1-O11-P-O12
73	K	101	PC1	C1-O11-P-O14
73	K	101	PC1	C1-O11-P-O13
73	L	503	PC1	C11-O13-P-O12
73	L	503	PC1	C11-O13-P-O14
73	L	503	PC1	C11-O13-P-O11
73	L	503	PC1	C1-O11-P-O12
73	L	503	PC1	C1-O11-P-O13
73	V	101	PC1	C11-O13-P-O12
73	p	302	PC1	C1-O11-P-O12
73	p	302	PC1	C1-O11-P-O13
73	p	303	PC1	C1-O11-P-O12
73	p	303	PC1	C1-O11-P-O14
73	p	303	PC1	C1-O11-P-O13
73	6	203	PC1	C1-O11-P-O12
73	6	203	PC1	C1-O11-P-O14
73	6	203	PC1	C1-O11-P-O13
73	9	203	PC1	C1-O11-P-O12
73	9	203	PC1	C1-O11-P-O14
73	9	203	PC1	C1-O11-P-O13
73	9	203	PC1	O13-C11-C12-N
73	A1	601	PC1	C11-O13-P-O12
73	A1	601	PC1	C11-O13-P-O14
73	A1	601	PC1	C11-O13-P-O11
73	A1	601	PC1	C1-O11-P-O13
73	M1	501	PC1	C11-O13-P-O12
73	M1	501	PC1	C11-O13-P-O14
73	M1	501	PC1	C11-O13-P-O11
76	n	603	HEA	C2A-C3A-CMA-OMA
76	n	603	HEA	C4A-C3A-CMA-OMA
76	n	604	HEA	C2A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
76	n	604	HEA	C4A-C3A-CMA-OMA
82	1	501	FMN	N10-C1'-C2'-O2'
82	1	501	FMN	N10-C1'-C2'-C3'
82	1	501	FMN	C5'-O5'-P-O1P
82	1	501	FMN	C5'-O5'-P-O2P
84	P1	501	NDP	C5B-O5B-PA-O3
85	W1	201	ZMP	S1-C11-C12-N1
85	W1	201	ZMP	O1-C10-S1-C11
85	W1	201	ZMP	C9-C10-S1-C11
85	n1	201	ZMP	C19-C18-C21-O5
85	n1	201	ZMP	C20-C18-C21-O5
85	n1	201	ZMP	C17-C18-C21-O5
85	n1	201	ZMP	O4-C17-C18-C21
85	n1	201	ZMP	C16-C17-C18-C21
85	n1	201	ZMP	O4-C17-C18-C19
85	n1	201	ZMP	C16-C17-C18-C20
85	n1	201	ZMP	O3-C16-C17-O4
85	n1	201	ZMP	C17-C16-N2-C15
86	O1	401	DGT	PB-O3B-PG-O1G
76	n	604	HEA	C26-C15-C16-C17
76	n	604	HEA	C14-C15-C16-C17
76	n	604	HEA	C4D-C3D-CAD-CBD
85	n1	201	ZMP	O3-C16-N2-C15
76	n	603	HEA	C19-C20-C21-C22
76	n	604	HEA	C15-C16-C17-C18
69	D	302	CDL	C1-CB2-OB2-PB2
76	n	604	HEA	C2D-C3D-CAD-CBD
70	C	401	HEM	C2A-CAA-CBA-CGA
76	n	604	HEA	C1A-C2A-CAA-CBA
73	9	204	PC1	C11-C12-N-C15
73	p	303	PC1	C31-C32-C33-C34
69	N1	401	CDL	OA6-CA4-CA6-OA8
69	L1	702	CDL	CA5-C11-C12-C13
68	M1	503	3PE	C2-C1-O11-P
69	H1	402	CDL	C1-CB2-OB2-PB2
68	L1	701	3PE	C21-C22-C23-C24
68	L1	704	3PE	C31-C32-C33-C34
73	9	204	PC1	C11-C12-N-C13
76	n	603	HEA	C15-C16-C17-C18
68	M1	502	3PE	C27-C28-C29-C2A
70	N	402	HEM	C2A-CAA-CBA-CGA
68	C	405	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
73	V	101	PC1	C11-C12-N-C13
68	D1	501	3PE	C38-C39-C3A-C3B
85	n1	201	ZMP	C6-C7-C8-C9
68	M1	502	3PE	C28-C29-C2A-C2B
73	9	204	PC1	C2A-C2B-C2C-C2D
68	C	405	3PE	C37-C38-C39-C3A
68	N1	402	3PE	C36-C37-C38-C39
68	L1	704	3PE	C23-C24-C25-C26
73	K	101	PC1	C11-C12-N-C13
73	9	204	PC1	C2B-C2C-C2D-C2E
68	A1	602	3PE	C3A-C3B-C3C-C3D
68	L1	704	3PE	C36-C37-C38-C39
69	N1	401	CDL	C81-C82-C83-C84
73	p	303	PC1	C25-C26-C27-C28
73	K	101	PC1	C11-C12-N-C15
73	V	101	PC1	C11-C12-N-C15
73	p	302	PC1	C11-C12-N-C13
73	9	204	PC1	C11-C12-N-C14
68	Z1	401	3PE	C31-C32-C33-C34
69	D	302	CDL	OB5-CB3-CB4-OB6
69	R	301	CDL	OB5-CB3-CB4-OB6
69	Y1	404	CDL	OB5-CB3-CB4-OB6
69	d1	201	CDL	C63-C64-C65-C66
68	n	606	3PE	O21-C2-C3-O31
68	A1	602	3PE	C38-C39-C3A-C3B
76	n	604	HEA	C3A-C2A-CAA-CBA
68	D1	501	3PE	C32-C33-C34-C35
69	d1	201	CDL	C55-C56-C57-C58
69	Y1	401	CDL	C82-C83-C84-C85
73	K	101	PC1	C11-C12-N-C14
73	V	101	PC1	C11-C12-N-C14
68	n	606	3PE	C23-C24-C25-C26
69	A	502	CDL	OB5-CB3-CB4-CB6
69	R	301	CDL	OB5-CB3-CB4-CB6
69	d1	201	CDL	OB5-CB3-CB4-CB6
68	H1	401	3PE	C31-C32-C33-C34
69	N1	401	CDL	CA3-CA4-CA6-OA8
69	Y1	401	CDL	CB3-CB4-CB6-OB8
69	Y1	404	CDL	CB3-CB4-CB6-OB8
73	M1	501	PC1	C37-C38-C39-C3A
68	D1	501	3PE	C31-C32-C33-C34
69	D	302	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
85	n1	201	ZMP	C5-C6-C7-C8
68	n	606	3PE	O11-C1-C2-O21
68	M1	502	3PE	O11-C1-C2-O21
68	N	404	3PE	C25-C26-C27-C28
73	p	302	PC1	C11-C12-N-C14
69	H1	402	CDL	C72-C71-CB7-OB8
84	P1	501	NDP	C2D-C1D-N1N-C6N
85	n1	201	ZMP	O4-C17-C18-C20
73	A1	601	PC1	C21-C22-C23-C24
68	x	101	3PE	C2-C1-O11-P
69	R	301	CDL	C1-CA2-OA2-PA1
70	C	402	HEM	C2A-CAA-CBA-CGA
73	9	204	PC1	C21-C22-C23-C24
68	M1	502	3PE	O11-C1-C2-C3
68	Z1	401	3PE	O11-C1-C2-C3
69	D	302	CDL	OB5-CB3-CB4-CB6
69	Y1	404	CDL	OB5-CB3-CB4-CB6
69	a1	101	CDL	OB5-CB3-CB4-CB6
68	Z1	401	3PE	O31-C31-C32-C33
69	H1	402	CDL	C13-C14-C15-C16
73	9	204	PC1	C34-C35-C36-C37
68	N1	402	3PE	C1-C2-C3-O31
69	h1	201	CDL	CB3-CB4-CB6-OB8
69	A	502	CDL	OB5-CB3-CB4-OB6
69	R	301	CDL	CB4-CB3-OB5-PB2
73	E	202	PC1	C2-C1-O11-P
85	n1	201	ZMP	O1-C10-S1-C11
68	x	101	3PE	O21-C2-C3-O31
68	N1	402	3PE	O21-C2-C3-O31
69	Y1	401	CDL	OB6-CB4-CB6-OB8
69	Y1	404	CDL	OB6-CB4-CB6-OB8
73	A1	601	PC1	C11-C12-N-C15
85	n1	201	ZMP	C13-C14-C15-N2
68	d1	203	3PE	C21-C22-C23-C24
73	M1	501	PC1	C21-C22-C23-C24
84	P1	501	NDP	C2D-C1D-N1N-C2N
73	p	302	PC1	C11-C12-N-C15
69	R	301	CDL	O1-C1-CA2-OA2
68	z	102	3PE	O11-C1-C2-O21
69	L1	702	CDL	OB5-CB3-CB4-OB6
68	N	401	3PE	C12-C11-O13-P
68	P	201	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
68	n	606	3PE	C12-C11-O13-P
68	p	301	3PE	C12-C11-O13-P
68	L1	704	3PE	C12-C11-O13-P
85	n1	201	ZMP	C16-C17-C18-C19
73	M1	501	PC1	C3B-C3C-C3D-C3E
73	6	203	PC1	C35-C36-C37-C38
68	p	301	3PE	C34-C35-C36-C37
73	A1	601	PC1	C11-C12-N-C14
73	E	202	PC1	O13-C11-C12-N
73	L	503	PC1	O13-C11-C12-N
73	p	303	PC1	O13-C11-C12-N
73	z	101	PC1	O13-C11-C12-N
73	M1	501	PC1	O13-C11-C12-N
84	P1	501	NDP	PN-O3-PA-O2A
86	O1	401	DGT	PB-O3A-PA-O1A
73	9	204	PC1	C35-C36-C37-C38
68	z	102	3PE	O11-C1-C2-C3
69	L1	702	CDL	OB5-CB3-CB4-CB6
69	h1	201	CDL	OB5-CB3-CB4-CB6
69	L	502	CDL	CB4-CB3-OB5-PB2
69	R	303	CDL	C1-CB2-OB2-PB2
69	H1	402	CDL	C1-CA2-OA2-PA1
69	Y1	404	CDL	C1-CB2-OB2-PB2
71	D	301	HEC	C4B-C3B-CAB-CBB
71	D	301	HEC	C4C-C3C-CAC-CBC
71	O	301	HEC	C4B-C3B-CAB-CBB
71	O	301	HEC	C4C-C3C-CAC-CBC
69	R	302	CDL	OB5-CB3-CB4-OB6
69	a1	101	CDL	OB5-CB3-CB4-OB6
69	h1	201	CDL	OB5-CB3-CB4-OB6
68	p	301	3PE	C32-C33-C34-C35
68	o	302	3PE	O21-C2-C3-O31
69	h1	201	CDL	OB6-CB4-CB6-OB8
68	o	302	3PE	C1-C2-C3-O31
68	d1	202	3PE	C1-C2-C3-O31
69	H1	402	CDL	C15-C16-C17-C18
68	A	501	3PE	C1-O11-P-O12
68	A	501	3PE	C1-O11-P-O13
68	A	501	3PE	C1-O11-P-O14
68	A	501	3PE	O13-C11-C12-N
68	C	405	3PE	C11-O13-P-O14
68	N	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
68	N	401	3PE	C11-O13-P-O12
68	N	401	3PE	C11-O13-P-O14
68	P	201	3PE	C11-O13-P-O14
68	R	304	3PE	C1-O11-P-O14
68	R	304	3PE	C11-O13-P-O14
68	n	605	3PE	C1-O11-P-O13
68	n	605	3PE	C1-O11-P-O14
68	n	606	3PE	C11-O13-P-O14
68	o	302	3PE	C1-O11-P-O14
68	o	302	3PE	C11-O13-P-O14
68	o	302	3PE	O13-C11-C12-N
68	x	101	3PE	C1-O11-P-O14
68	6	202	3PE	C11-O13-P-O14
68	H1	401	3PE	C11-O13-P-O14
68	L1	704	3PE	C1-O11-P-O14
68	M1	503	3PE	C1-O11-P-O12
68	M1	503	3PE	C1-O11-P-O13
68	N1	402	3PE	C1-O11-P-O14
68	Y1	403	3PE	C1-O11-P-O14
68	d1	202	3PE	C1-O11-P-O13
68	d1	202	3PE	C1-O11-P-O14
69	A	502	CDL	CA2-OA2-PA1-OA3
69	A	502	CDL	CB2-OB2-PB2-OB3
69	A	502	CDL	CB3-OB5-PB2-OB2
69	C	404	CDL	CB2-OB2-PB2-OB3
69	C	404	CDL	CB2-OB2-PB2-OB4
69	C	404	CDL	CB2-OB2-PB2-OB5
69	D	302	CDL	CA3-OA5-PA1-OA2
69	L	502	CDL	CA2-OA2-PA1-OA3
69	L	502	CDL	CA3-OA5-PA1-OA2
69	L	502	CDL	CA3-OA5-PA1-OA4
69	R	301	CDL	CA2-OA2-PA1-OA3
69	R	301	CDL	CA2-OA2-PA1-OA5
69	R	301	CDL	CB2-OB2-PB2-OB4
69	R	302	CDL	CB2-OB2-PB2-OB3
69	R	303	CDL	CA2-OA2-PA1-OA3
69	R	303	CDL	CA2-OA2-PA1-OA5
69	R	303	CDL	CA3-OA5-PA1-OA3
69	H1	402	CDL	CA2-OA2-PA1-OA4
69	H1	402	CDL	CB2-OB2-PB2-OB3
69	L1	702	CDL	CA3-OA5-PA1-OA4
69	L1	703	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
69	L1	703	CDL	CA3-OA5-PA1-OA4
69	L1	703	CDL	CB3-OB5-PB2-OB3
69	N1	401	CDL	CA2-OA2-PA1-OA3
69	N1	401	CDL	CA2-OA2-PA1-OA4
69	N1	401	CDL	CA2-OA2-PA1-OA5
69	N1	401	CDL	CB3-OB5-PB2-OB3
69	Y1	401	CDL	CB3-OB5-PB2-OB3
69	Y1	404	CDL	CA2-OA2-PA1-OA5
69	Y1	404	CDL	CA3-OA5-PA1-OA3
69	a1	101	CDL	CA3-OA5-PA1-OA2
69	a1	101	CDL	CA3-OA5-PA1-OA3
69	d1	201	CDL	CB2-OB2-PB2-OB3
69	h1	201	CDL	CA2-OA2-PA1-OA4
73	E	202	PC1	C11-O13-P-O14
73	E	202	PC1	C1-O11-P-O14
73	E	202	PC1	C1-O11-P-O13
73	K	101	PC1	C11-O13-P-O12
73	K	101	PC1	C11-O13-P-O14
73	K	101	PC1	C11-O13-P-O11
73	L	503	PC1	C1-O11-P-O14
73	9	203	PC1	C11-O13-P-O12
73	A1	601	PC1	C1-O11-P-O14
73	A1	601	PC1	C11-C12-N-C13
76	n	603	HEA	C11-C12-C13-C14
68	A	501	3PE	O21-C21-C22-C23
69	C	404	CDL	C72-C71-CB7-OB8
68	t	101	3PE	C2-C1-O11-P
68	K1	201	3PE	C2-C1-O11-P
68	Z1	401	3PE	C2-C1-O11-P
69	D	302	CDL	CB4-CB3-OB5-PB2
69	R	302	CDL	CA4-CA3-OA5-PA1
69	h1	201	CDL	CA4-CA3-OA5-PA1
73	V	101	PC1	C2-C1-O11-P
68	C	403	3PE	C2A-C2B-C2C-C2D
68	d1	203	3PE	O21-C21-C22-C23
68	p	301	3PE	C2C-C2D-C2E-C2F
69	a1	101	CDL	C52-C51-CB5-OB6
84	P1	501	NDP	O4D-C1D-N1N-C2N
84	P1	501	NDP	O4D-C1D-N1N-C6N
76	n	603	HEA	O11-C11-C12-C13
68	n	605	3PE	C2-C1-O11-P
69	a1	101	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
68	L1	704	3PE	C37-C38-C39-C3A
73	z	101	PC1	O31-C31-C32-C33
68	n	606	3PE	C1-C2-C3-O31
69	C	404	CDL	C72-C71-CB7-OB9
69	Y1	401	CDL	C73-C74-C75-C76
76	n	603	HEA	C27-C19-C20-C21
69	N1	401	CDL	C51-C52-C53-C54
68	Y1	403	3PE	C23-C24-C25-C26
69	Y1	404	CDL	C72-C73-C74-C75
68	Z1	401	3PE	O11-C1-C2-O21
68	n	606	3PE	O11-C1-C2-C3
68	H1	401	3PE	O31-C31-C32-C33
73	A1	601	PC1	O21-C21-C22-C23
73	M1	501	PC1	C28-C29-C2A-C2B
68	L1	704	3PE	C3D-C3E-C3F-C3G
73	6	203	PC1	C37-C38-C39-C3A
73	M1	501	PC1	O21-C2-C3-O31
68	L1	701	3PE	C2-C1-O11-P
68	il	201	3PE	C2-C1-O11-P
68	D1	501	3PE	O21-C21-C22-C23
68	A1	602	3PE	C35-C36-C37-C38
73	9	204	PC1	C23-C24-C25-C26
69	d1	201	CDL	CA3-CA4-CA6-OA8
85	n1	201	ZMP	N2-C16-C17-O4
69	H1	402	CDL	C72-C71-CB7-OB9
68	t	101	3PE	C3-C2-O21-C21
73	p	303	PC1	C1-C2-O21-C21
73	6	203	PC1	C3-C2-O21-C21
73	9	203	PC1	C3-C2-O21-C21
68	Z1	401	3PE	C21-C22-C23-C24
69	d1	201	CDL	C54-C55-C56-C57
76	n	603	HEA	CAD-CBD-CGD-O1D
68	A1	602	3PE	C2-C1-O11-P
68	M1	502	3PE	C2-C1-O11-P
69	D	302	CDL	C1-CA2-OA2-PA1
76	n	604	HEA	CAA-CBA-CGA-O1A
73	p	302	PC1	O11-C1-C2-C3
76	n	603	HEA	C18-C19-C20-C21
68	M1	502	3PE	O21-C2-C3-O31
69	N1	401	CDL	OB6-CB4-CB6-OB8
69	d1	201	CDL	OA6-CA4-CA6-OA8
69	d1	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
73	p	303	PC1	C23-C24-C25-C26
69	L1	702	CDL	O1-C1-CB2-OB2
69	d1	201	CDL	O1-C1-CB2-OB2
68	H1	401	3PE	C22-C23-C24-C25
73	9	204	PC1	C29-C2A-C2B-C2C
76	n	604	HEA	CAA-CBA-CGA-O2A
68	p	301	3PE	C2-C1-O11-P
69	R	301	CDL	C1-CB2-OB2-PB2
68	i1	201	3PE	C24-C25-C26-C27
68	Y1	403	3PE	C1-C2-C3-O31
69	L1	703	CDL	CB3-CB4-CB6-OB8
68	R	304	3PE	O11-C1-C2-O21
73	p	302	PC1	O11-C1-C2-O21
85	n1	201	ZMP	C9-C10-S1-C11
69	Y1	401	CDL	C72-C71-CB7-OB8
69	h1	201	CDL	C12-C11-CA5-OA6
70	N	403	HEM	CAD-CBD-CGD-O2D
69	L1	703	CDL	OB6-CB4-CB6-OB8
69	L	502	CDL	C72-C71-CB7-OB8
69	R	302	CDL	C72-C71-CB7-OB8
69	Y1	401	CDL	C17-C18-C19-C20
73	z	101	PC1	C2-C1-O11-P
73	9	203	PC1	C37-C38-C39-C3A
82	1	501	FMN	C5'-O5'-P-O3P
76	n	603	HEA	CAD-CBD-CGD-O2D
68	C	405	3PE	C35-C36-C37-C38
69	H1	402	CDL	C17-C18-C19-C20
73	p	303	PC1	C22-C23-C24-C25
68	Z1	401	3PE	O32-C31-C32-C33
69	Y1	401	CDL	C15-C16-C17-C18
68	A	501	3PE	O31-C31-C32-C33
69	C	404	CDL	C32-C31-CA7-OA8
68	D1	501	3PE	C39-C3A-C3B-C3C
68	Z1	401	3PE	C3-C2-O21-C21
73	A1	601	PC1	C3-C2-O21-C21
70	N	403	HEM	CAA-CBA-CGA-O2A
73	M1	501	PC1	C3A-C3B-C3C-C3D
68	p	301	3PE	C23-C24-C25-C26
69	R	303	CDL	C31-C32-C33-C34
73	A1	601	PC1	O11-C1-C2-O21
85	W1	201	ZMP	C2-C1-C22-C23
73	9	203	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
70	N	403	HEM	CAD-CBD-CGD-O1D
68	M1	502	3PE	C2C-C2D-C2E-C2F
70	N	403	HEM	CAA-CBA-CGA-O1A
69	R	301	CDL	C52-C51-CB5-OB6
68	t	101	3PE	O21-C2-C3-O31
68	d1	202	3PE	O21-C2-C3-O31
69	h1	201	CDL	C32-C31-CA7-OA8
73	A1	601	PC1	O31-C31-C32-C33
68	R	304	3PE	O11-C1-C2-C3
68	t	101	3PE	O11-C1-C2-C3
69	R	302	CDL	OB5-CB3-CB4-CB6
73	M1	501	PC1	O11-C1-C2-C3
69	Y1	404	CDL	CA5-C11-C12-C13
68	A1	602	3PE	O31-C31-C32-C33
68	H1	401	3PE	C3B-C3C-C3D-C3E
68	v	101	3PE	O31-C31-C32-C33
69	R	302	CDL	C12-C11-CA5-OA6
69	h1	201	CDL	C1-CA2-OA2-PA1
68	N	404	3PE	O31-C31-C32-C33
69	R	303	CDL	C72-C71-CB7-OB8
69	h1	201	CDL	C72-C71-CB7-OB8
69	L1	702	CDL	C72-C71-CB7-OB8
73	9	204	PC1	O31-C31-C32-C33
73	M1	501	PC1	C29-C2A-C2B-C2C
68	K1	201	3PE	C25-C26-C27-C28
68	L	501	3PE	O31-C31-C32-C33
69	A	502	CDL	C12-C11-CA5-OA6
68	i1	201	3PE	C2B-C2C-C2D-C2E
68	K1	201	3PE	O31-C31-C32-C33
73	9	204	PC1	C2F-C2G-C2H-C2I
73	9	203	PC1	C29-C2A-C2B-C2C
69	L1	702	CDL	C1-CB2-OB2-PB2
69	R	303	CDL	C52-C51-CB5-OB6
69	A	502	CDL	C32-C31-CA7-OA8
68	Z1	401	3PE	C2A-C2B-C2C-C2D
68	C	403	3PE	O31-C31-C32-C33
68	C	406	3PE	O31-C31-C32-C33
68	n	606	3PE	O21-C21-C22-C23
68	t	101	3PE	O31-C31-C32-C33
68	K1	201	3PE	O21-C21-C22-C23
68	o	302	3PE	C21-C22-C23-C24
86	O1	401	DGT	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
68	6	202	3PE	O21-C21-C22-C23
68	i1	201	3PE	O31-C31-C32-C33
68	L1	704	3PE	O21-C21-C22-C23
68	A	501	3PE	C3-C2-O21-C21
68	n	605	3PE	C1-C2-O21-C21
68	L1	701	3PE	C3-C2-O21-C21
69	L	502	CDL	CB6-CB4-OB6-CB5
69	N1	401	CDL	CB6-CB4-OB6-CB5
69	Y1	404	CDL	CA3-CA4-OA6-CA5
69	a1	101	CDL	CA3-CA4-OA6-CA5
69	h1	201	CDL	CB6-CB4-OB6-CB5
73	L	503	PC1	C1-C2-O21-C21
69	R	303	CDL	C12-C11-CA5-OA6
85	W1	201	ZMP	C22-C1-C2-C3
69	L	502	CDL	C52-C51-CB5-OB6
68	N	404	3PE	O32-C31-C32-C33
73	9	204	PC1	O32-C31-C32-C33
73	p	303	PC1	C2-C1-O11-P
76	n	603	HEA	CAA-CBA-CGA-O1A
69	A	502	CDL	C12-C11-CA5-OA7
69	A	502	CDL	C32-C31-CA7-OA9
68	z	102	3PE	O21-C21-C22-C23
69	D	302	CDL	C75-C76-C77-C78
69	d1	201	CDL	C57-C58-C59-C60
69	R	301	CDL	C52-C51-CB5-OB7
69	h1	201	CDL	C72-C71-CB7-OB9
68	K1	201	3PE	O32-C31-C32-C33
69	L1	702	CDL	C72-C71-CB7-OB9
68	M1	503	3PE	C21-C22-C23-C24
68	6	202	3PE	O22-C21-C22-C23
69	h1	201	CDL	C32-C31-CA7-OA9
68	A1	602	3PE	O32-C31-C32-C33
68	K1	201	3PE	O22-C21-C22-C23
69	R	303	CDL	C72-C71-CB7-OB9
68	Y1	403	3PE	O21-C2-C3-O31
68	H1	401	3PE	C33-C34-C35-C36
68	L1	704	3PE	O31-C31-C32-C33
69	N1	401	CDL	C52-C51-CB5-OB6
68	x	101	3PE	C1-C2-C3-O31
85	W1	201	ZMP	N2-C16-C17-O4
73	A1	601	PC1	O32-C31-C32-C33
69	R	303	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
68	L	501	3PE	O32-C31-C32-C33
69	R	303	CDL	C52-C51-CB5-OB7
68	C	406	3PE	O21-C21-C22-C23
80	y	601	TGL	OG2-CB1-CB2-CB3
68	C	406	3PE	O32-C31-C32-C33
68	n	606	3PE	O22-C21-C22-C23
70	N	402	HEM	CAD-CBD-CGD-O2D
68	C	403	3PE	O32-C31-C32-C33
68	Y1	402	3PE	O31-C31-C32-C33
73	p	302	PC1	O31-C31-C32-C33
69	Y1	404	CDL	C75-C76-C77-C78
68	C	405	3PE	O21-C21-C22-C23
73	p	303	PC1	O21-C21-C22-C23
68	C	406	3PE	O22-C21-C22-C23
68	Y1	403	3PE	O31-C31-C32-C33
69	R	301	CDL	C72-C71-CB7-OB8
68	z	102	3PE	O22-C21-C22-C23
68	i1	201	3PE	O32-C31-C32-C33
68	H1	401	3PE	C24-C25-C26-C27
68	M1	502	3PE	C26-C27-C28-C29

There are no ring outliers.

58 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	L	501	3PE	2	0
80	y	601	TGL	1	0
81	9	201	SF4	1	0
68	z	102	3PE	4	0
68	A	501	3PE	2	0
68	D1	501	3PE	3	0
69	R	303	CDL	1	0
69	Y1	401	CDL	2	0
71	O	301	HEC	1	0
69	Y1	404	CDL	2	0
73	9	204	PC1	3	0
73	p	302	PC1	2	0
76	n	604	HEA	3	0
73	M1	501	PC1	6	0
70	N	402	HEM	2	0
68	C	405	3PE	1	0
68	t	101	3PE	8	0

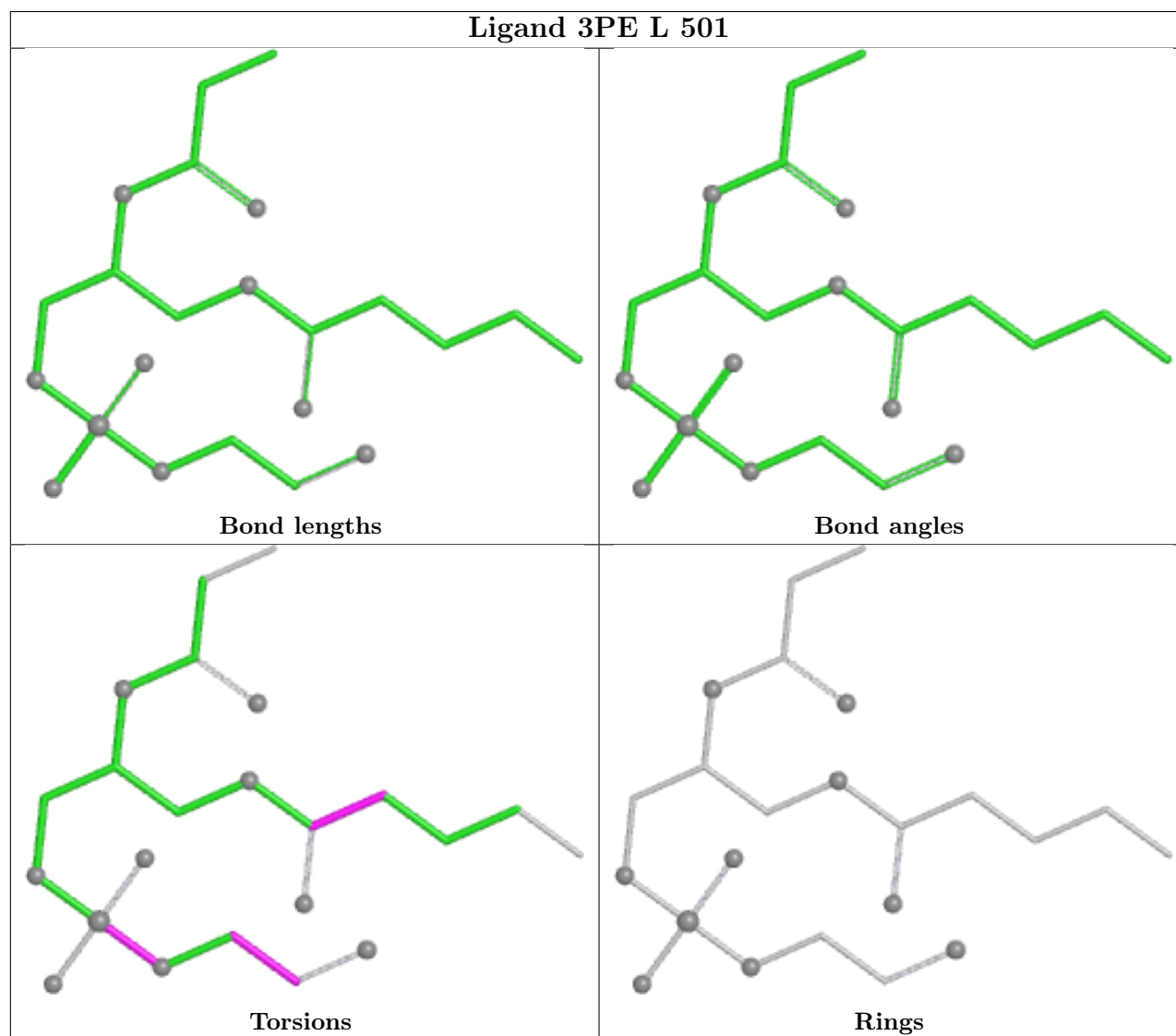
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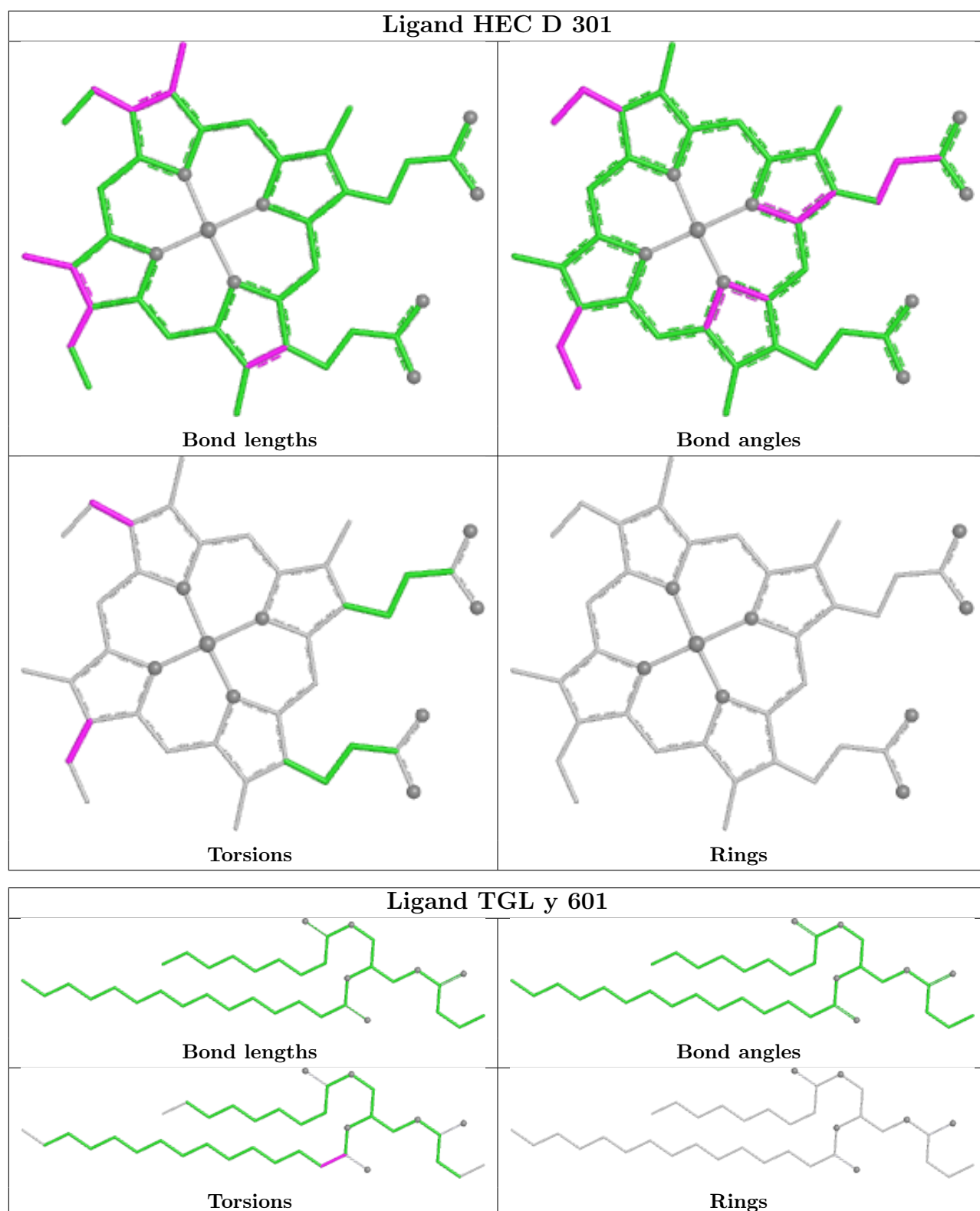
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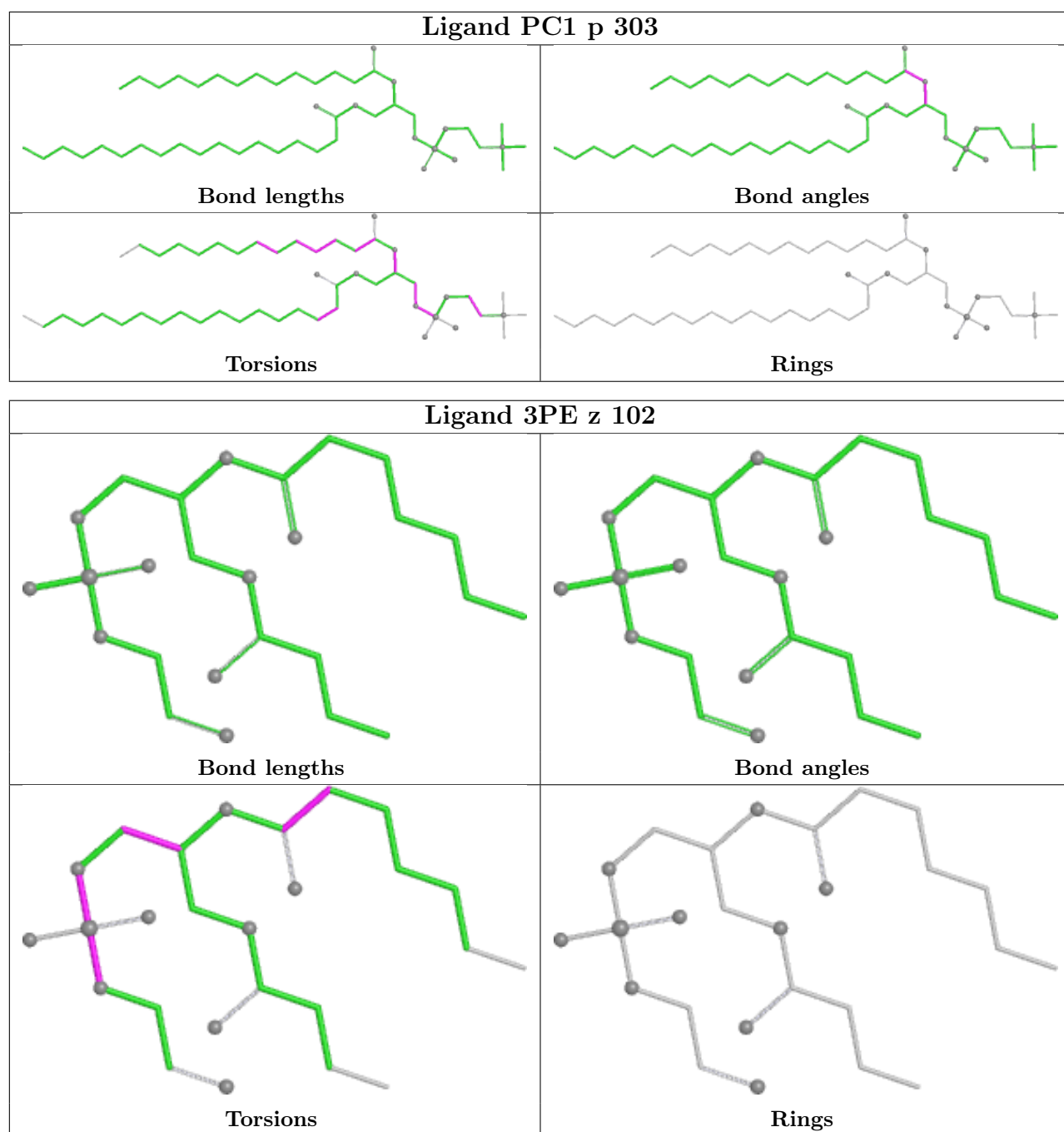
Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	Y1	402	3PE	1	0
86	O1	401	DGT	1	0
68	L1	701	3PE	1	0
85	n1	201	ZMP	2	0
68	Z1	401	3PE	4	0
70	C	402	HEM	3	0
68	H1	401	3PE	1	0
68	K1	201	3PE	1	0
73	6	203	PC1	1	0
76	n	603	HEA	3	0
68	6	202	3PE	1	0
73	K	101	PC1	1	0
68	v	101	3PE	1	0
69	C	404	CDL	1	0
69	h1	201	CDL	4	0
68	N	404	3PE	2	0
69	A	502	CDL	2	0
68	d1	203	3PE	1	0
68	o	302	3PE	2	0
85	W1	201	ZMP	2	0
68	N1	402	3PE	1	0
70	N	403	HEM	1	0
69	D	302	CDL	1	0
68	P	201	3PE	4	0
84	P1	501	NDP	2	0
69	N1	401	CDL	5	0
68	A1	602	3PE	1	0
73	9	203	PC1	2	0
68	Y1	403	3PE	1	0
73	E	202	PC1	2	0
70	C	401	HEM	2	0
68	i1	201	3PE	2	0
68	L1	704	3PE	4	0
82	1	501	FMN	4	0
69	H1	402	CDL	2	0
69	a1	101	CDL	4	0
69	d1	201	CDL	3	0
68	C	406	3PE	1	0
69	L1	703	CDL	2	0
68	p	301	3PE	6	0
68	x	101	3PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

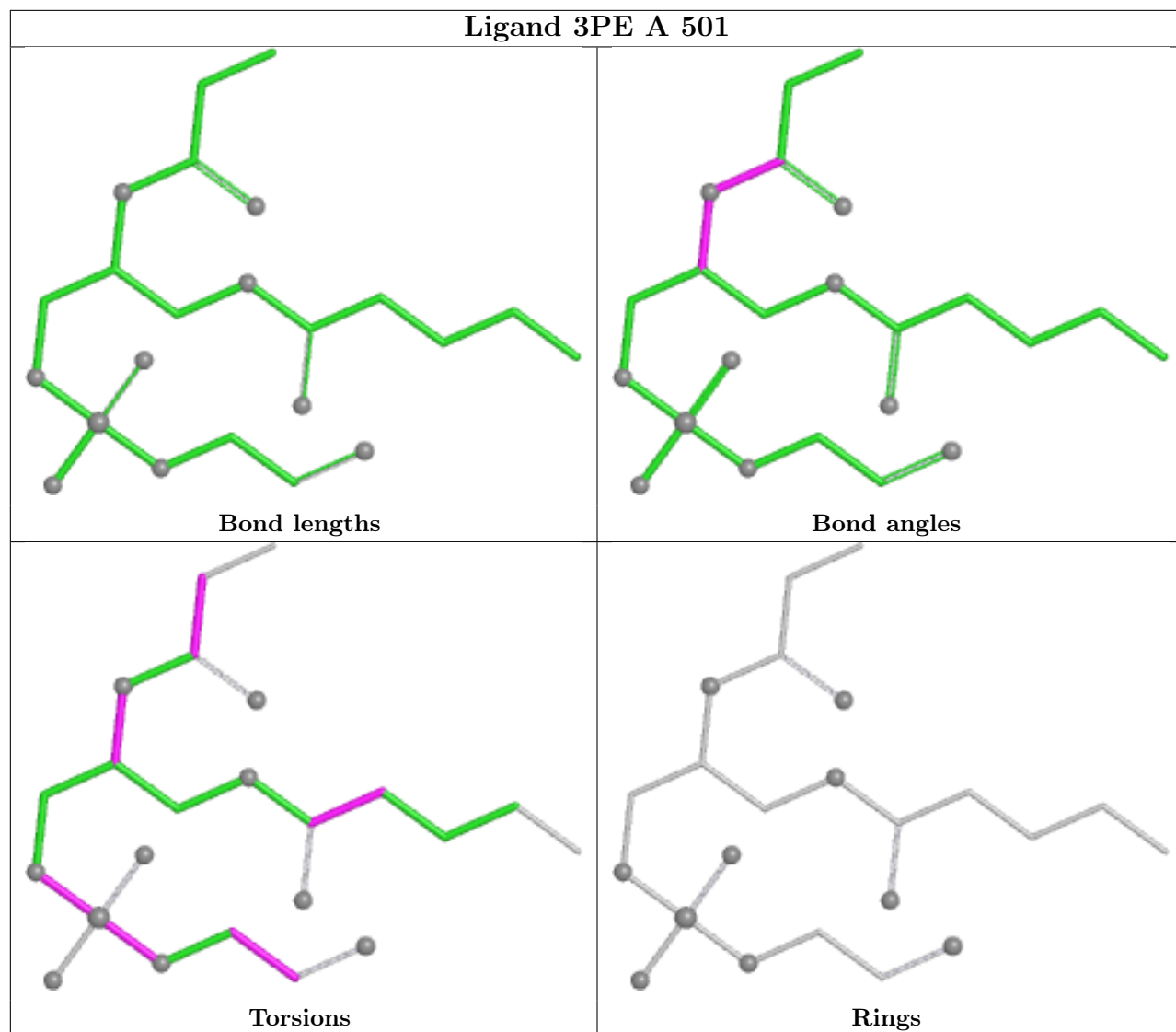
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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



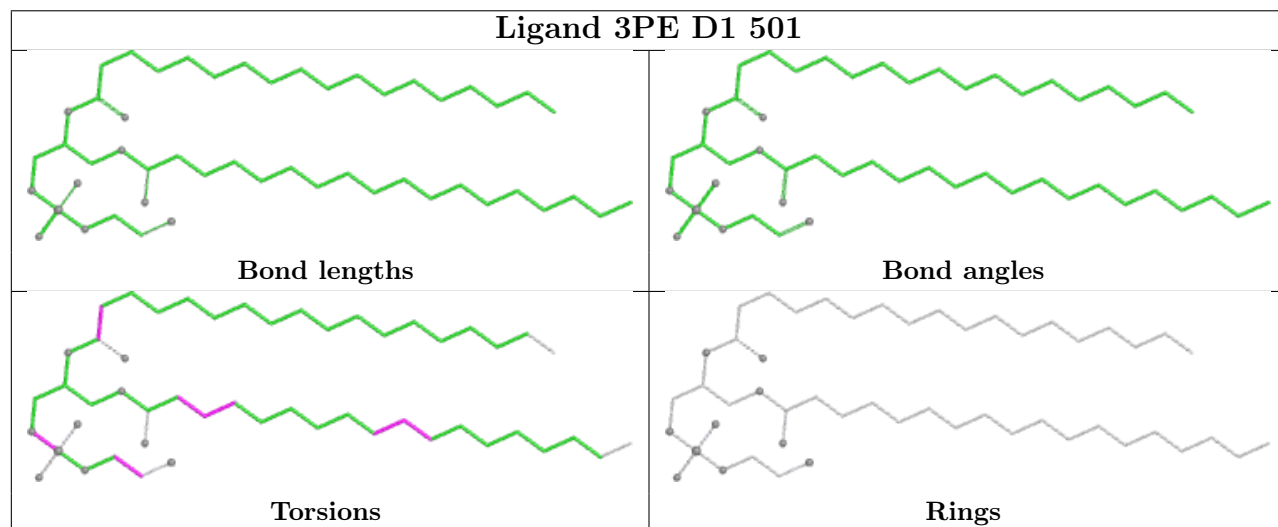


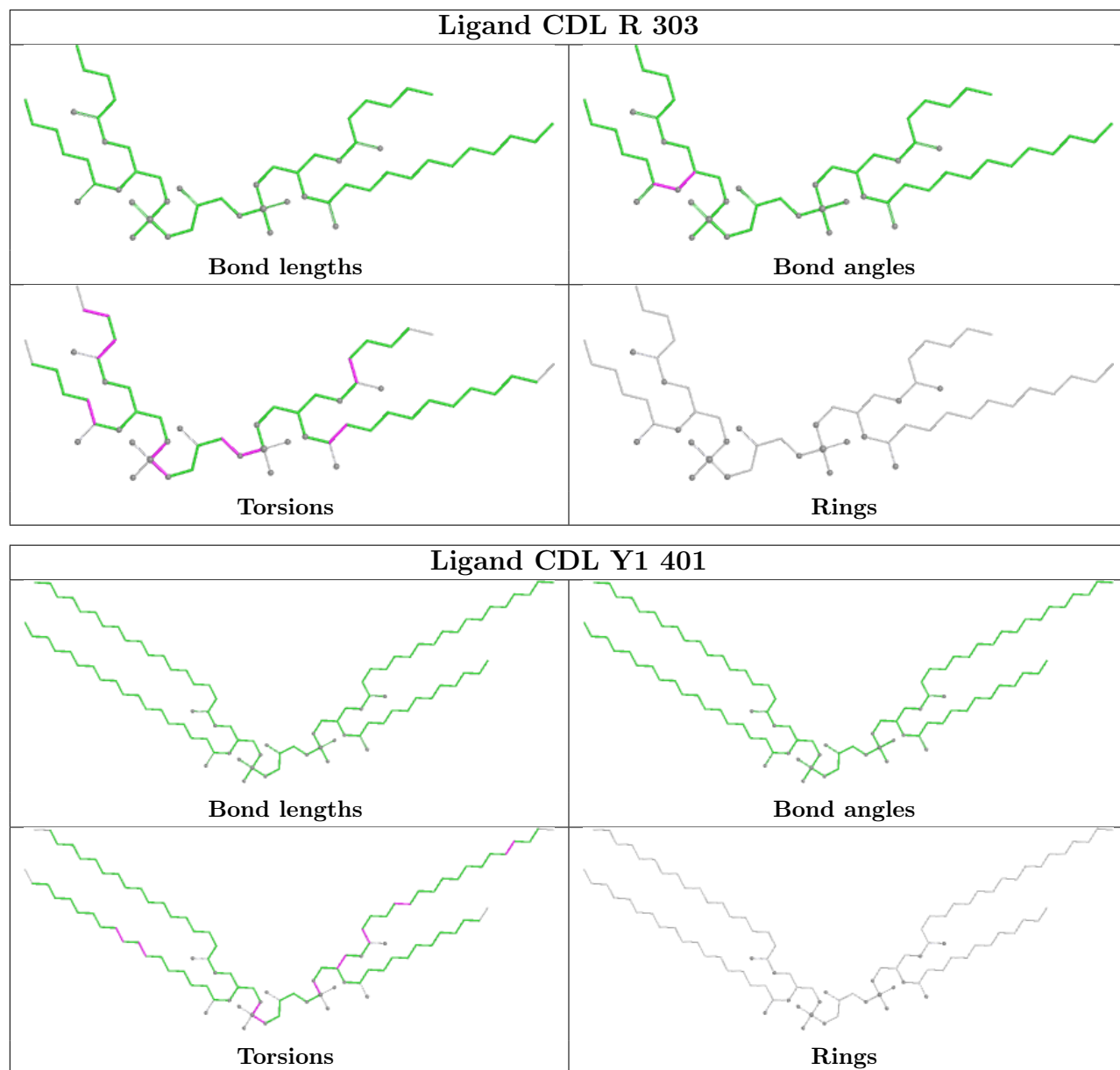


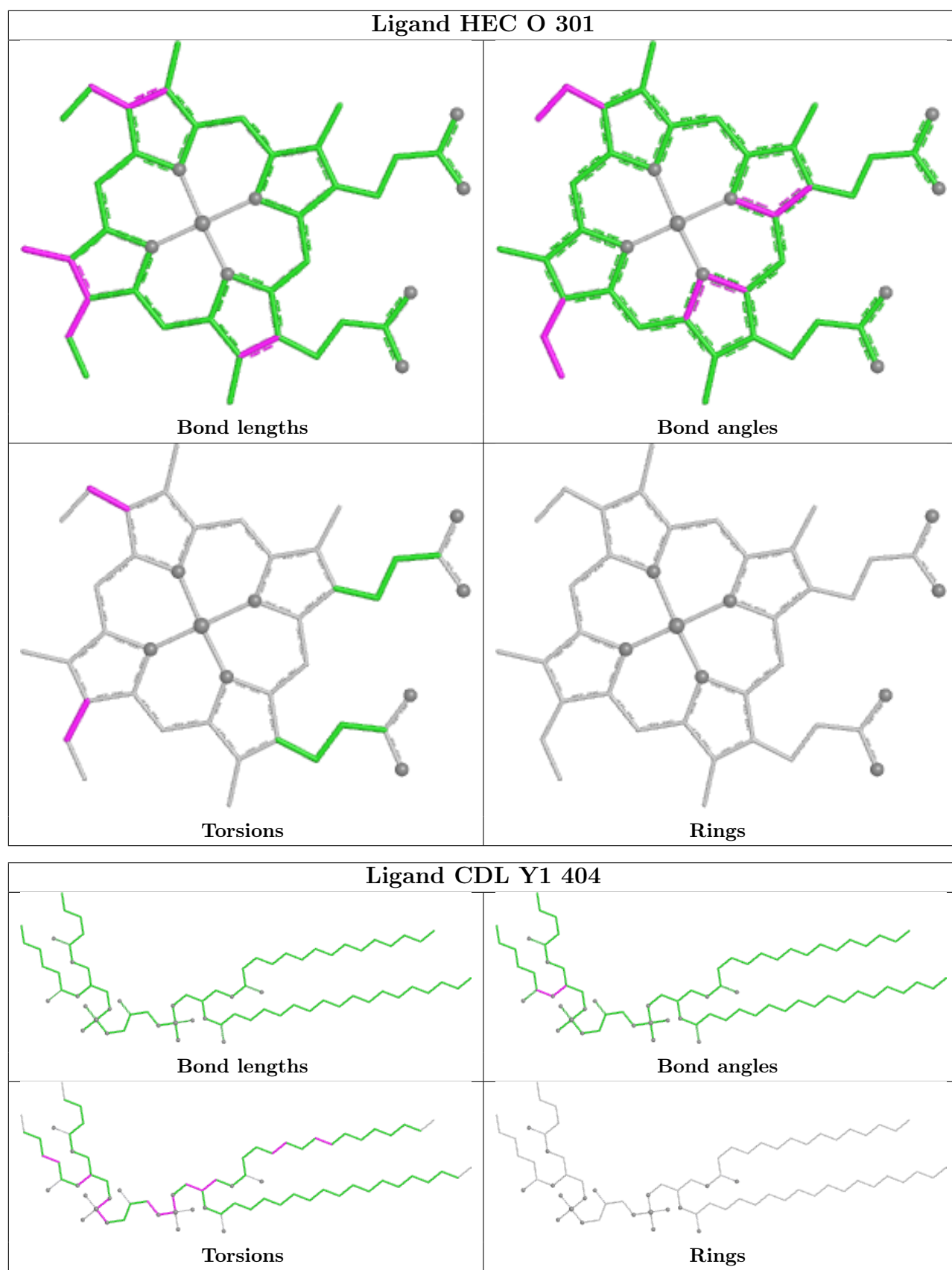
Ligand 3PE A 501

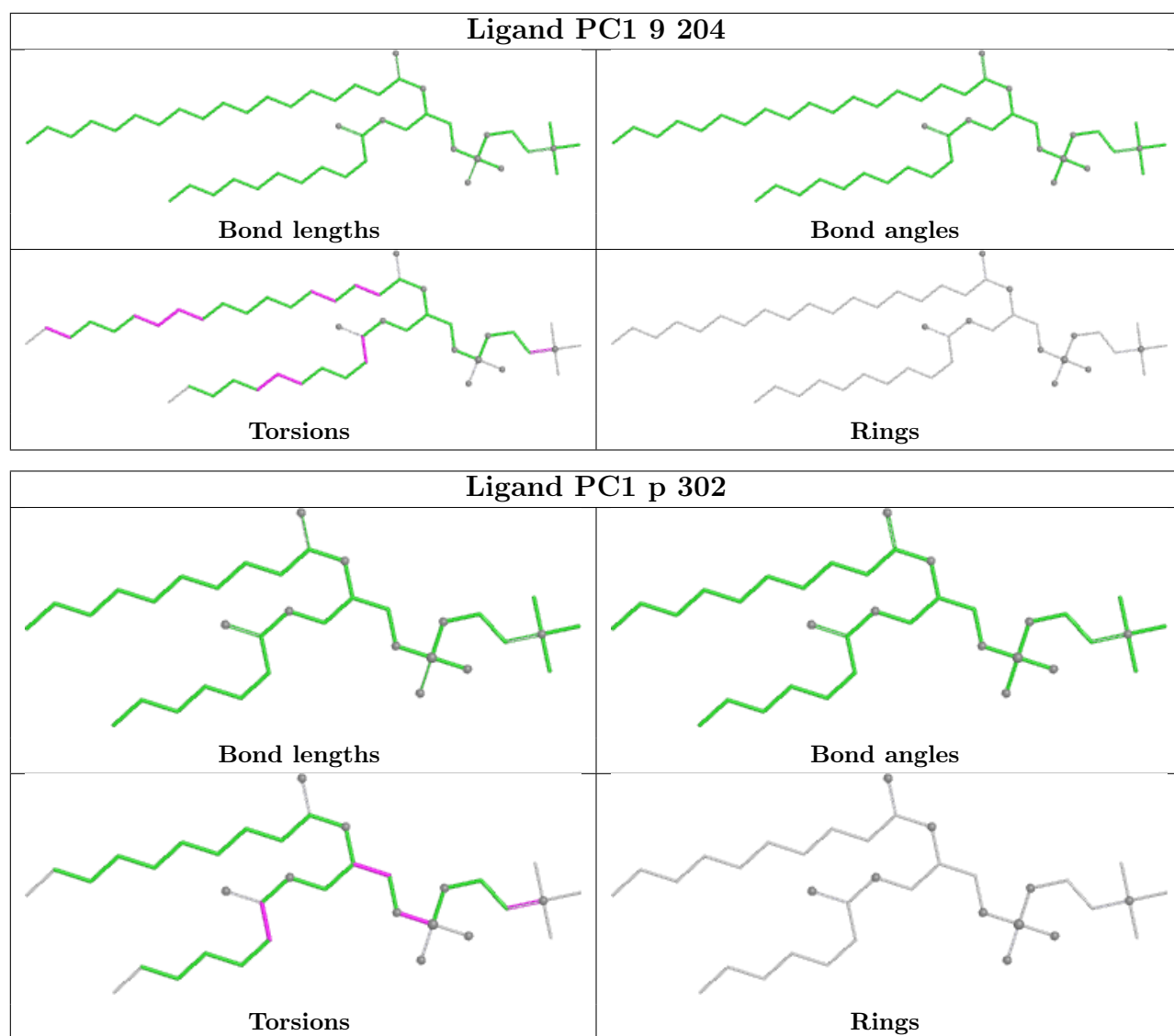


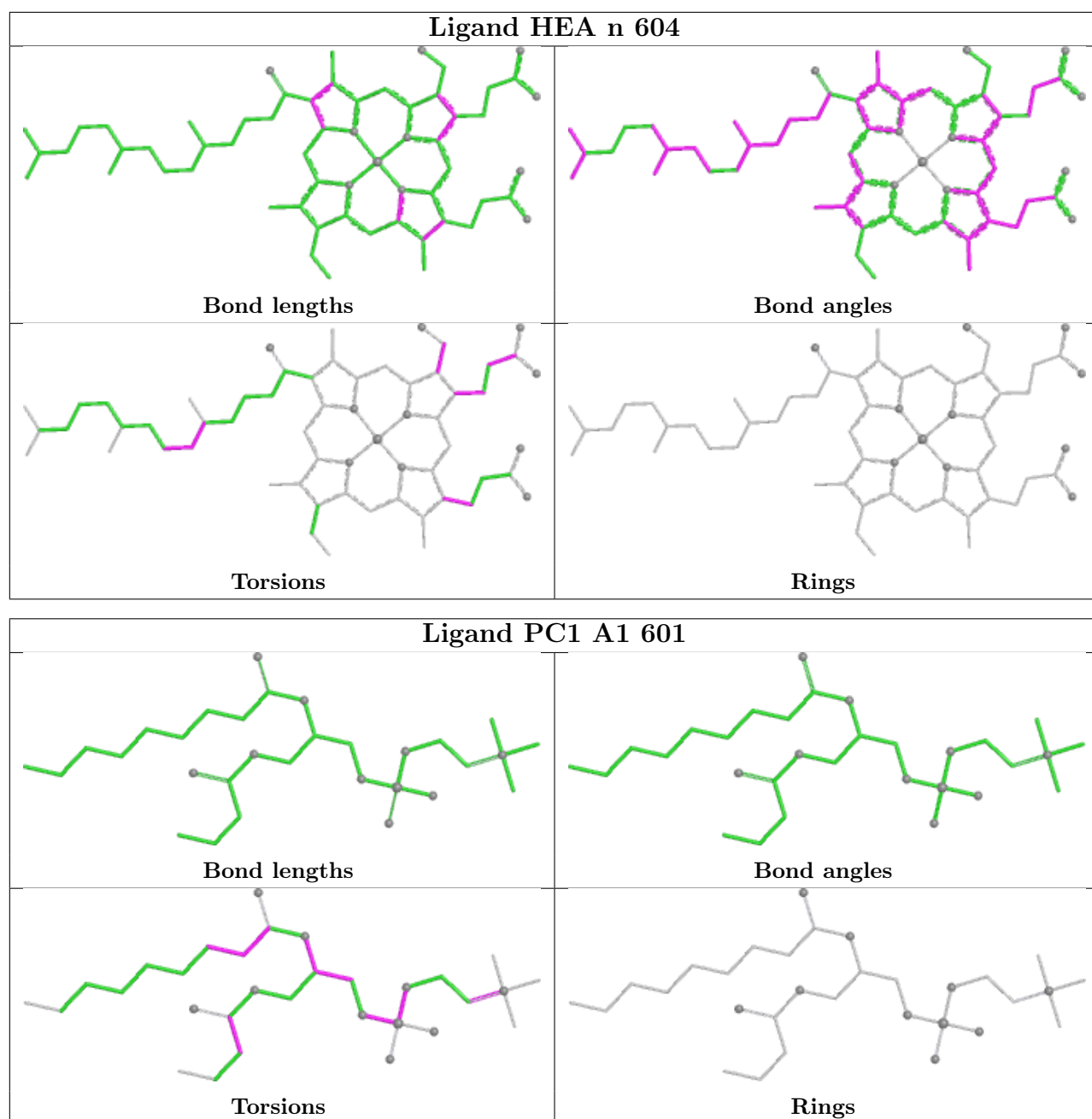
Ligand 3PE D1 501

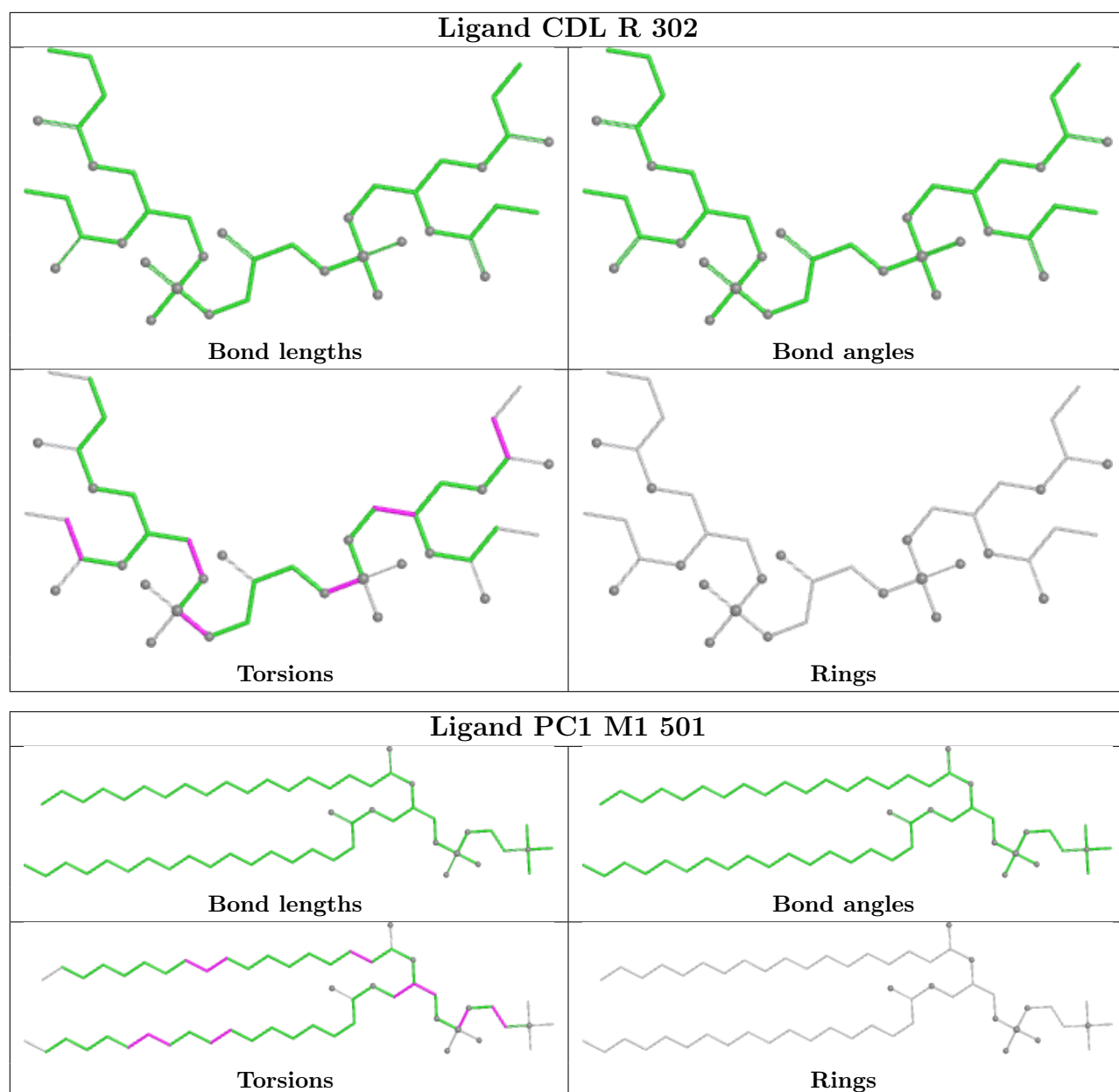


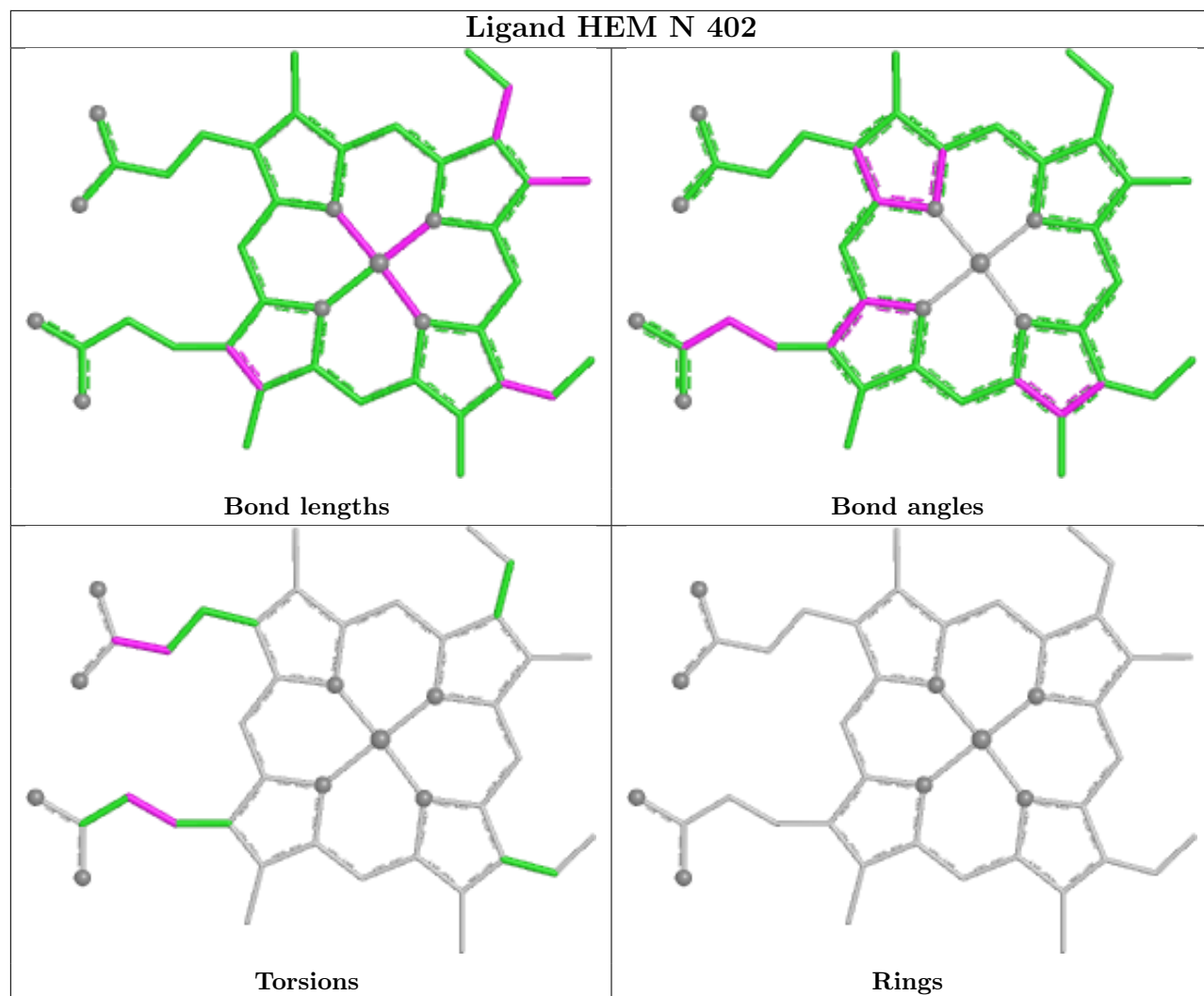


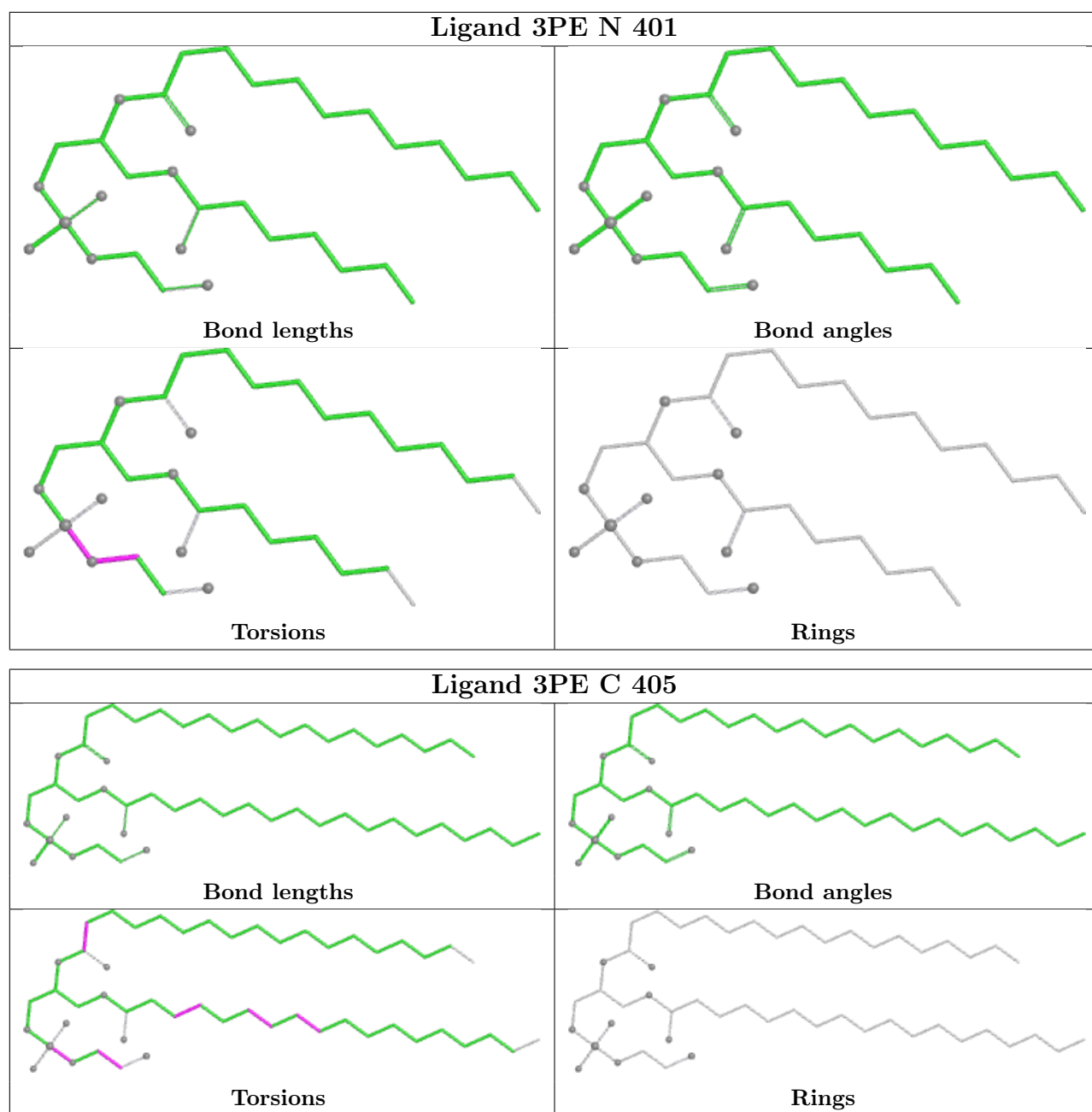


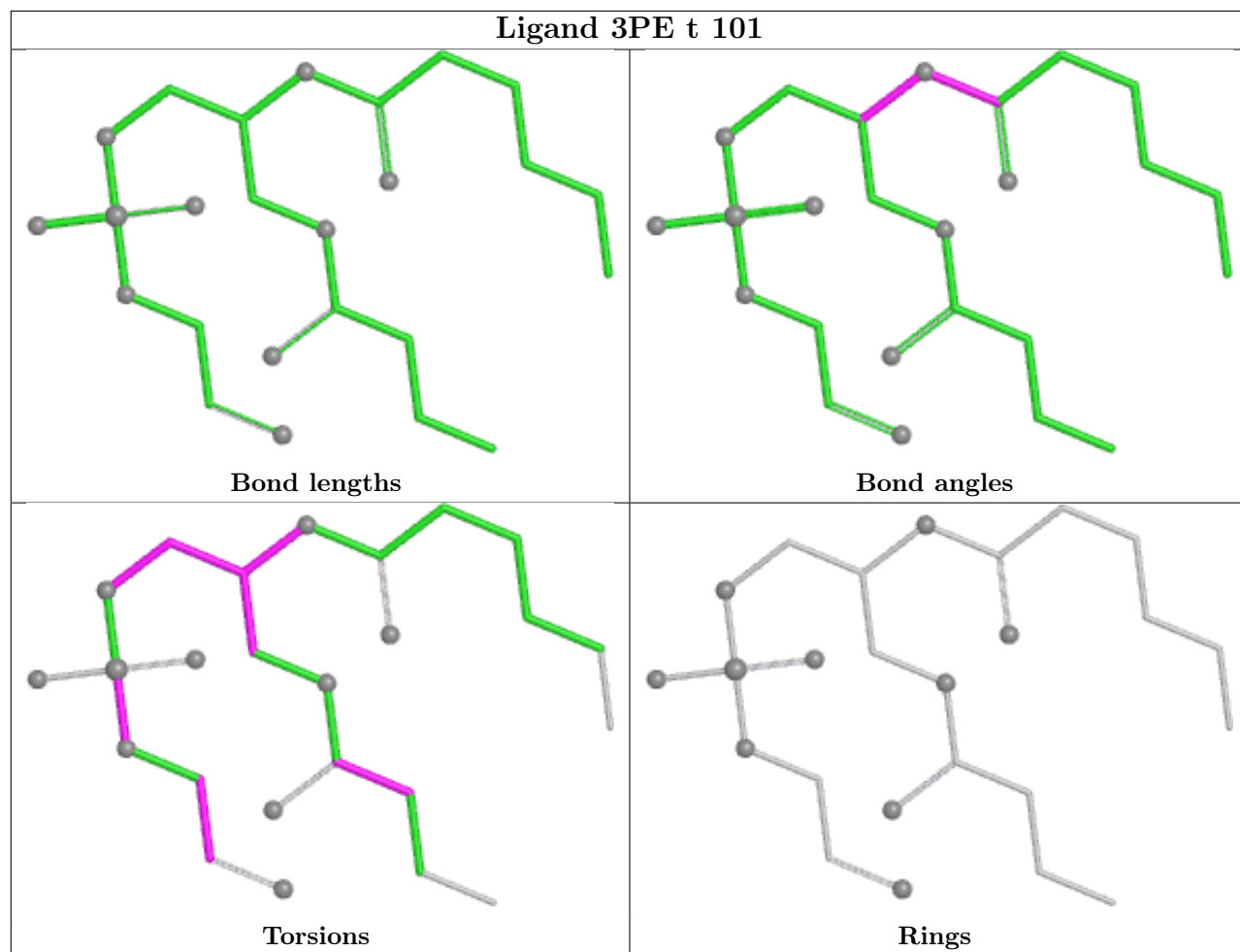


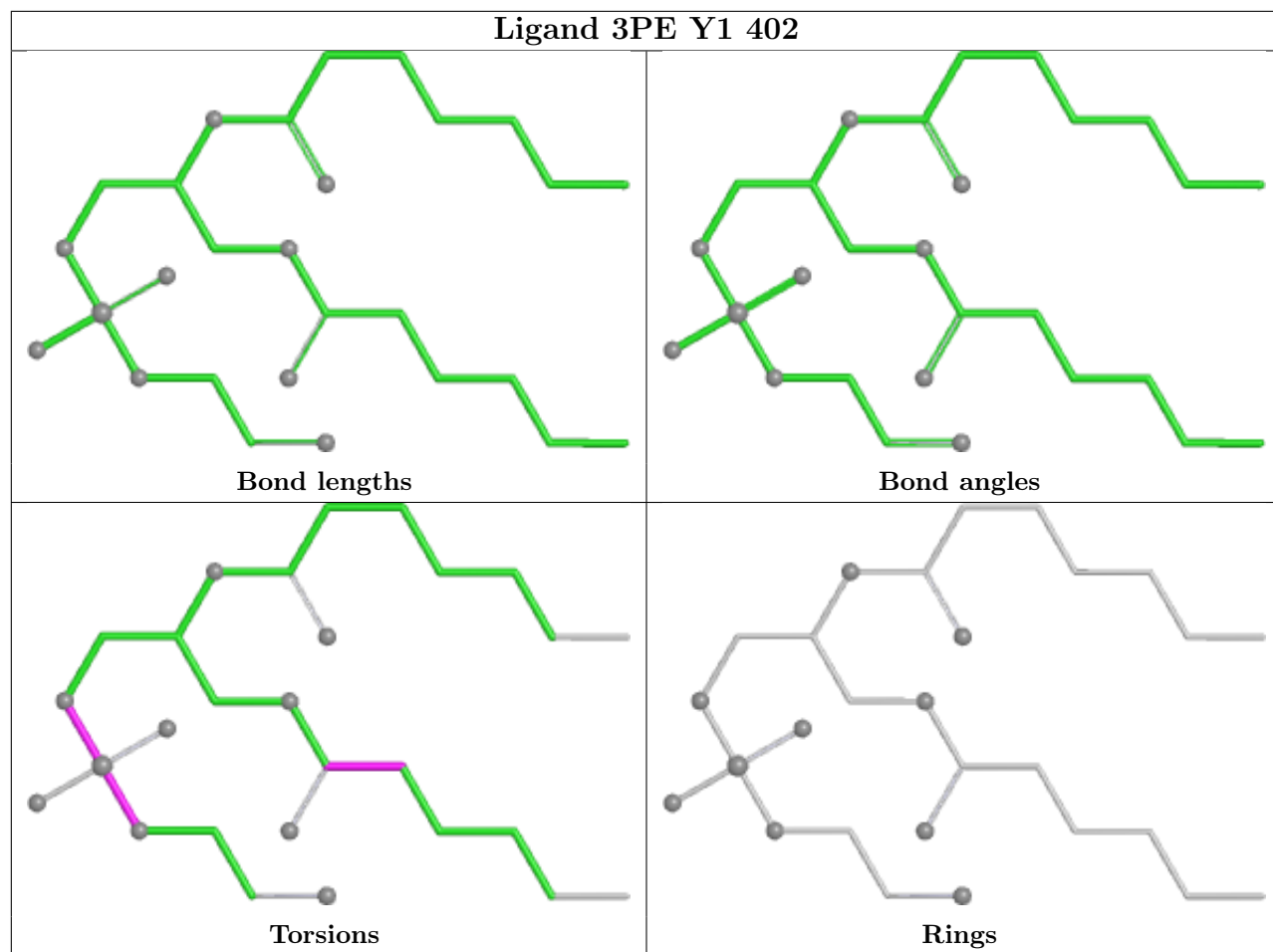


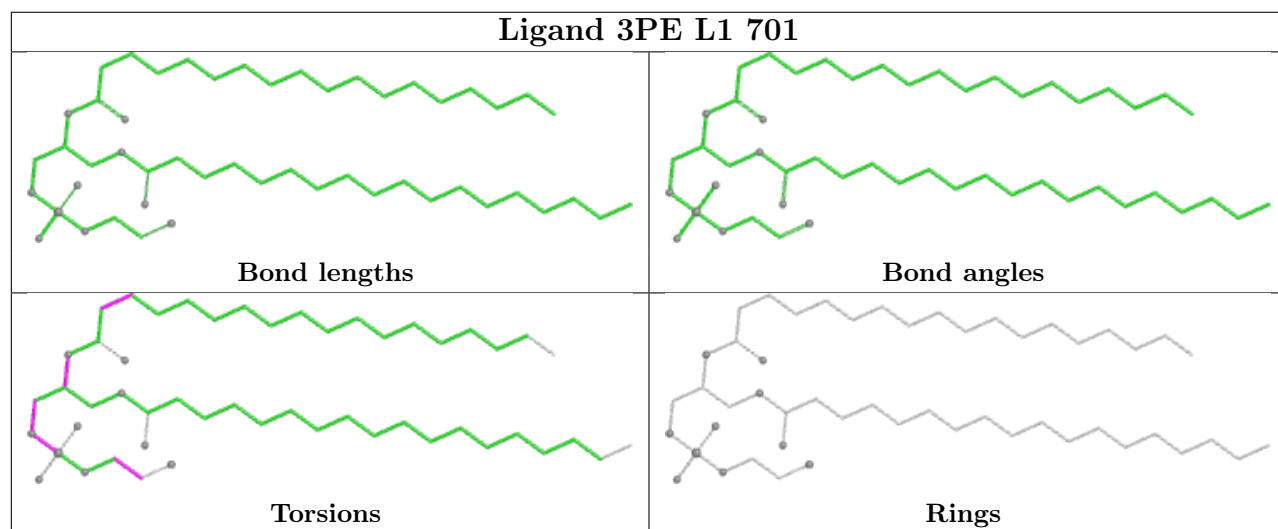
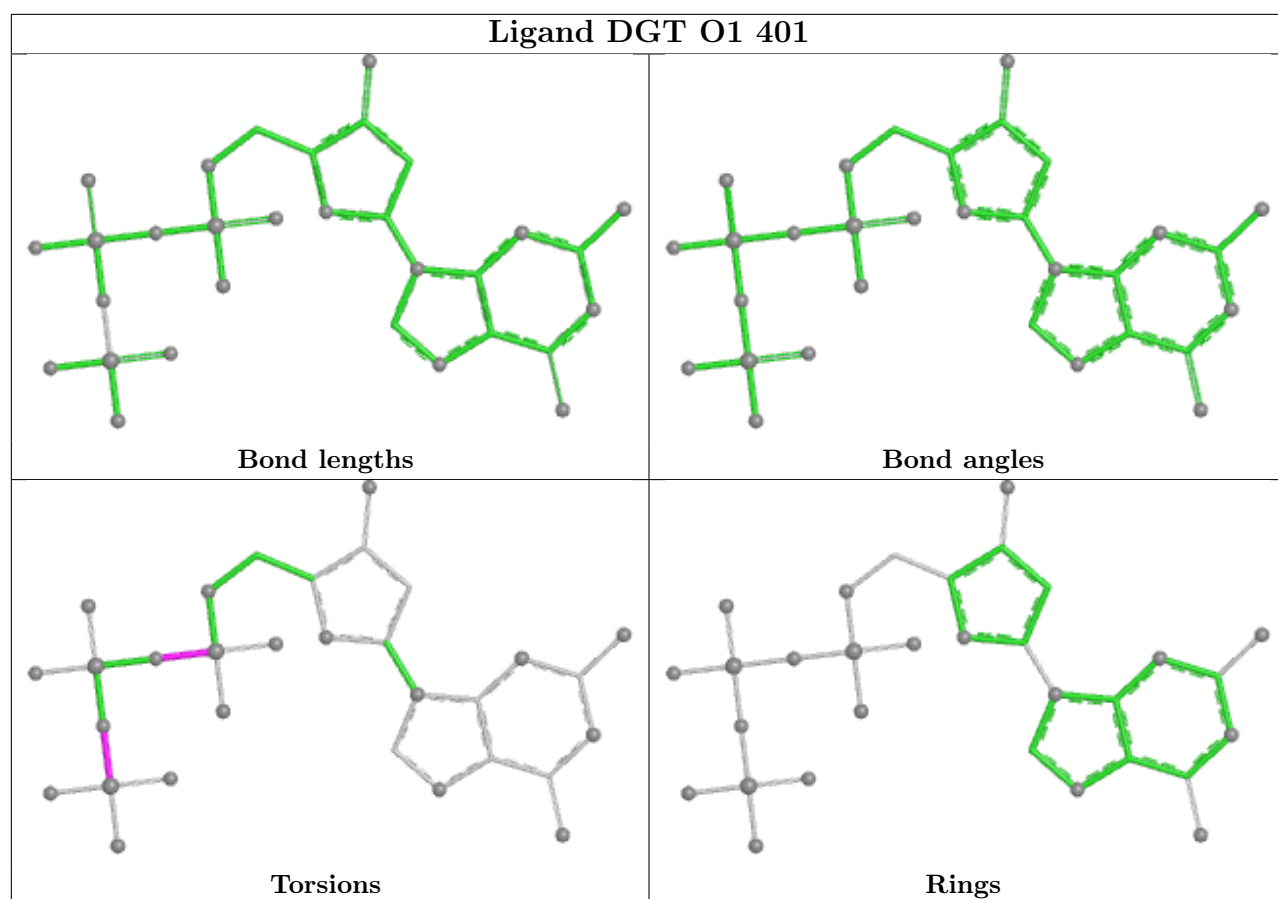


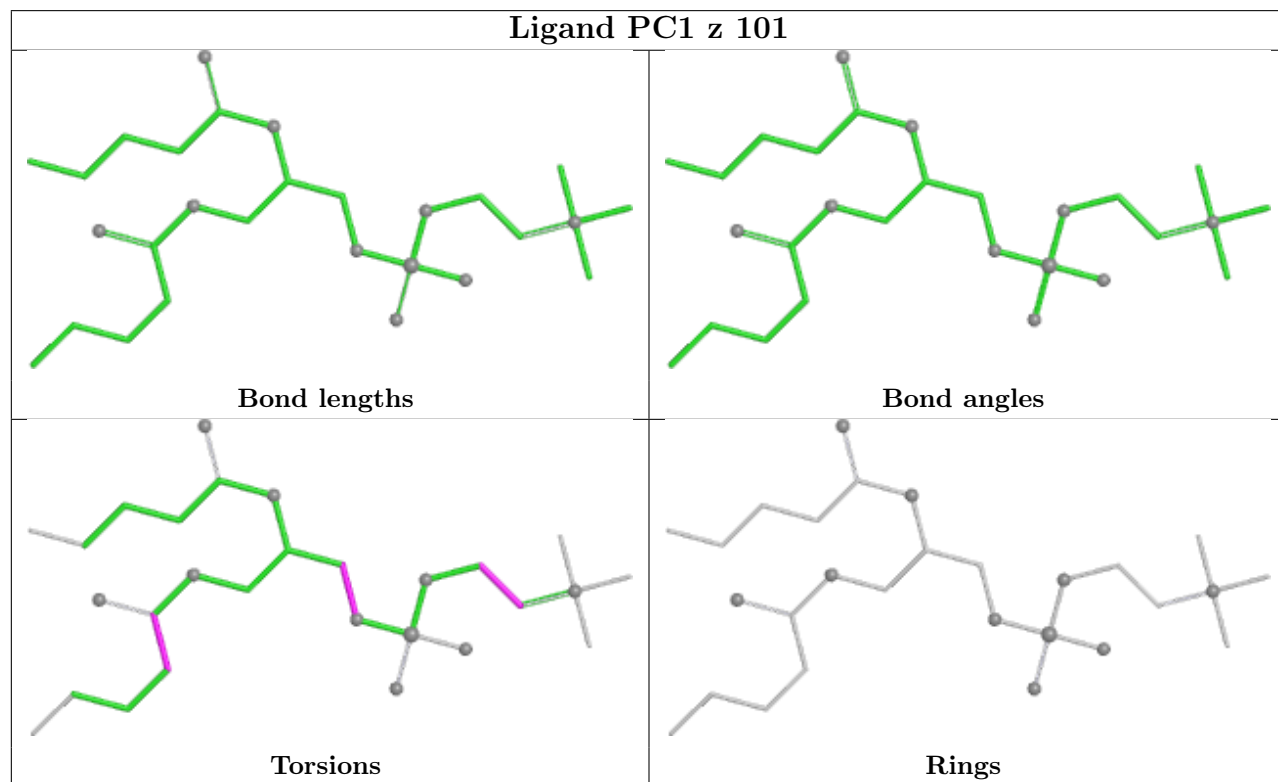
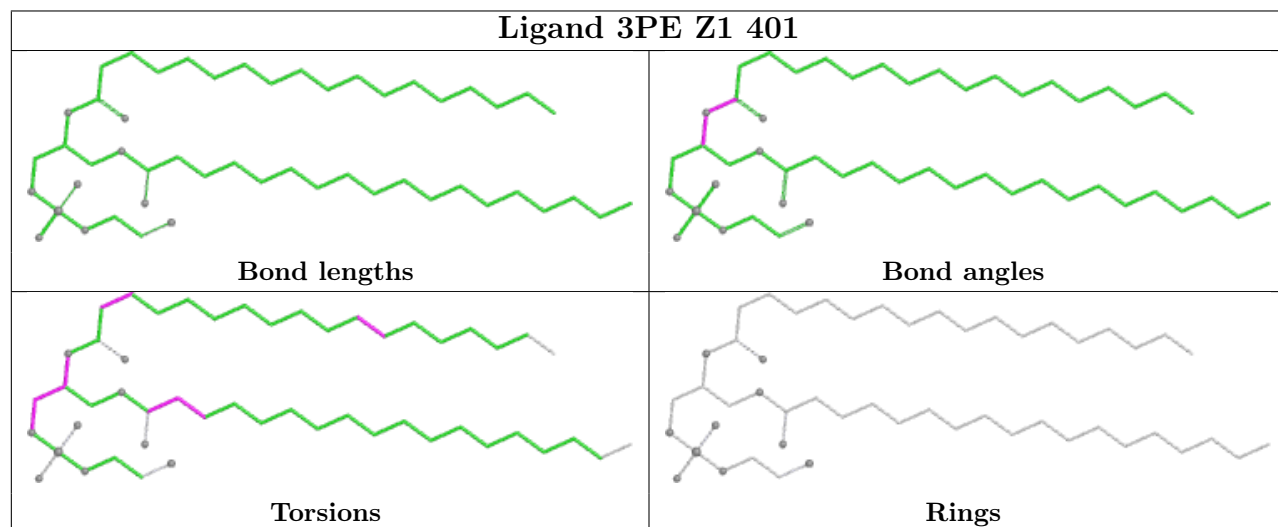
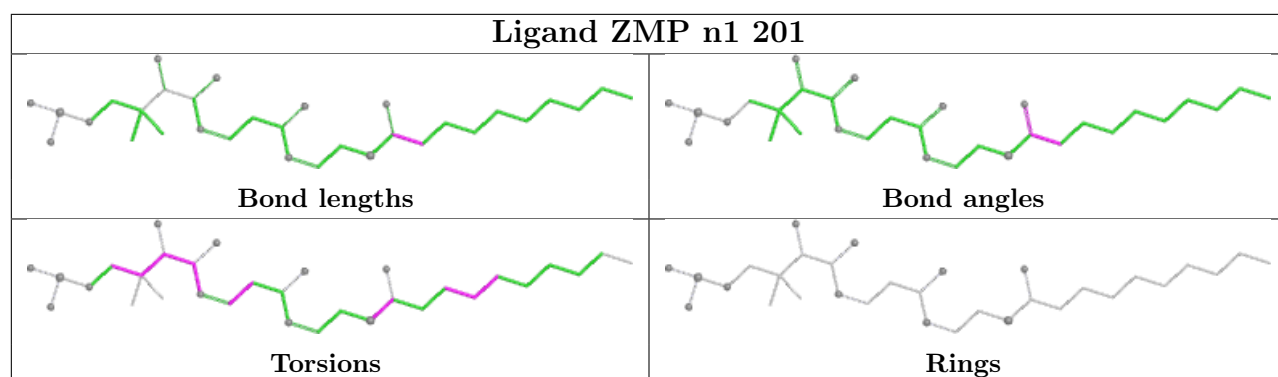


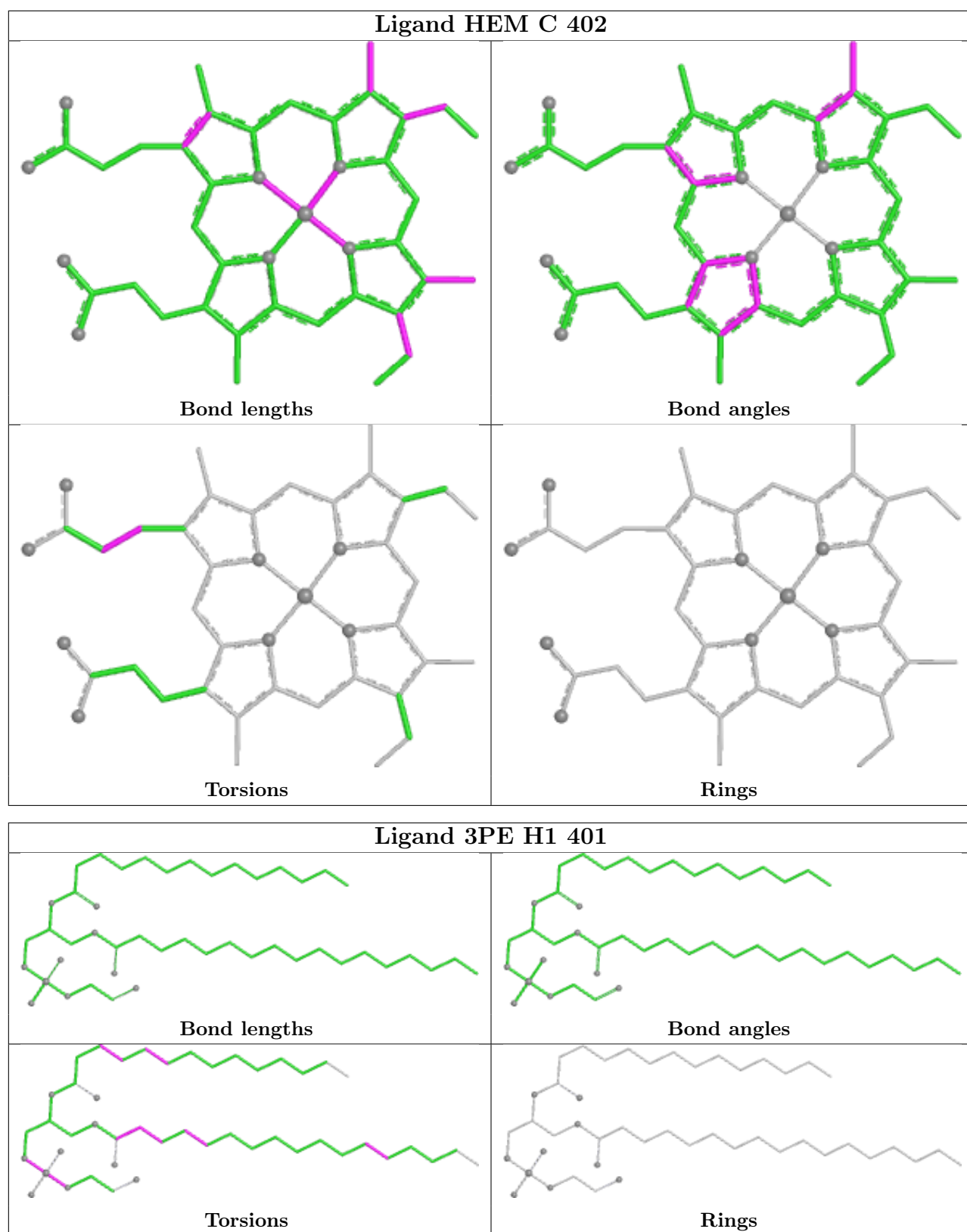


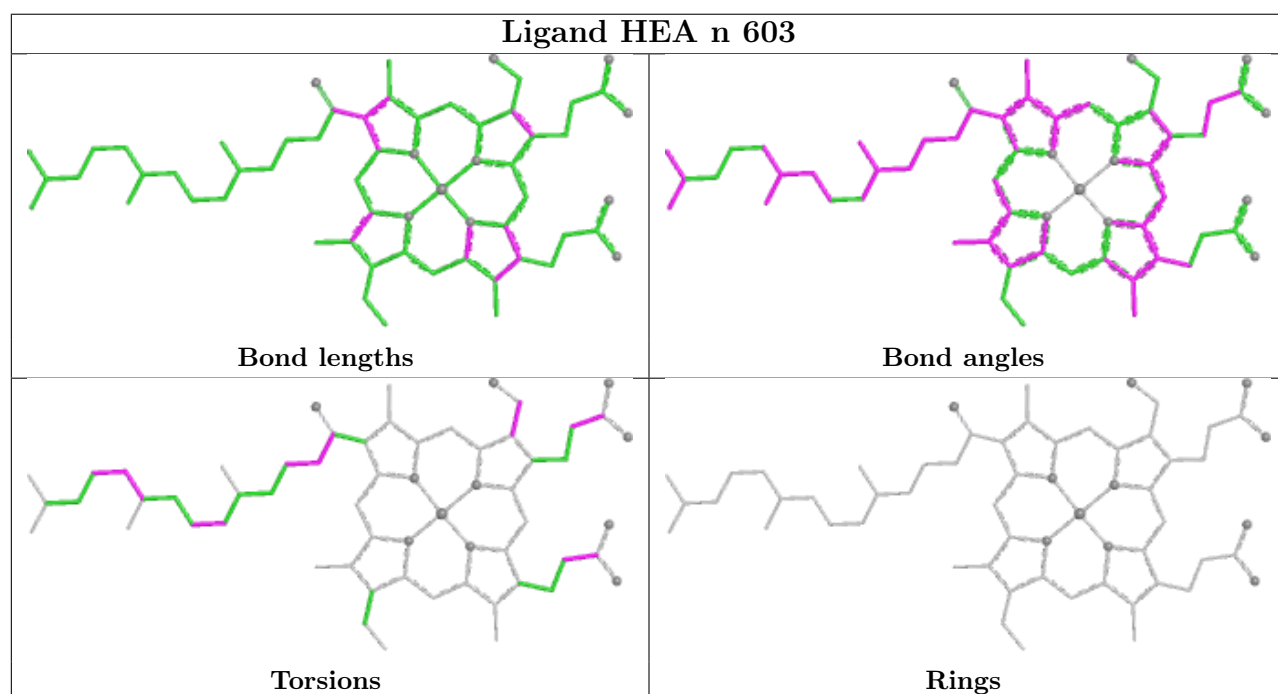
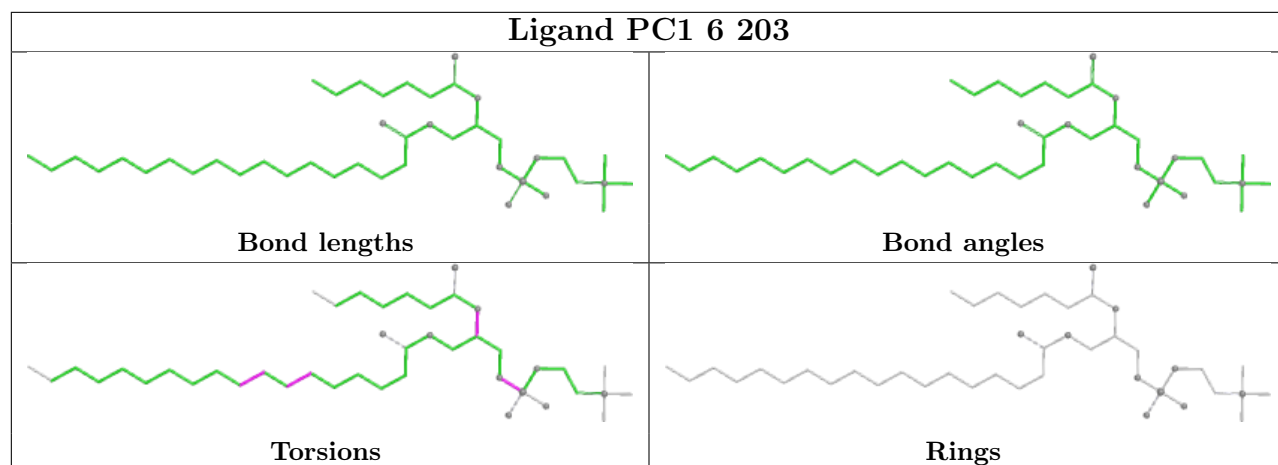
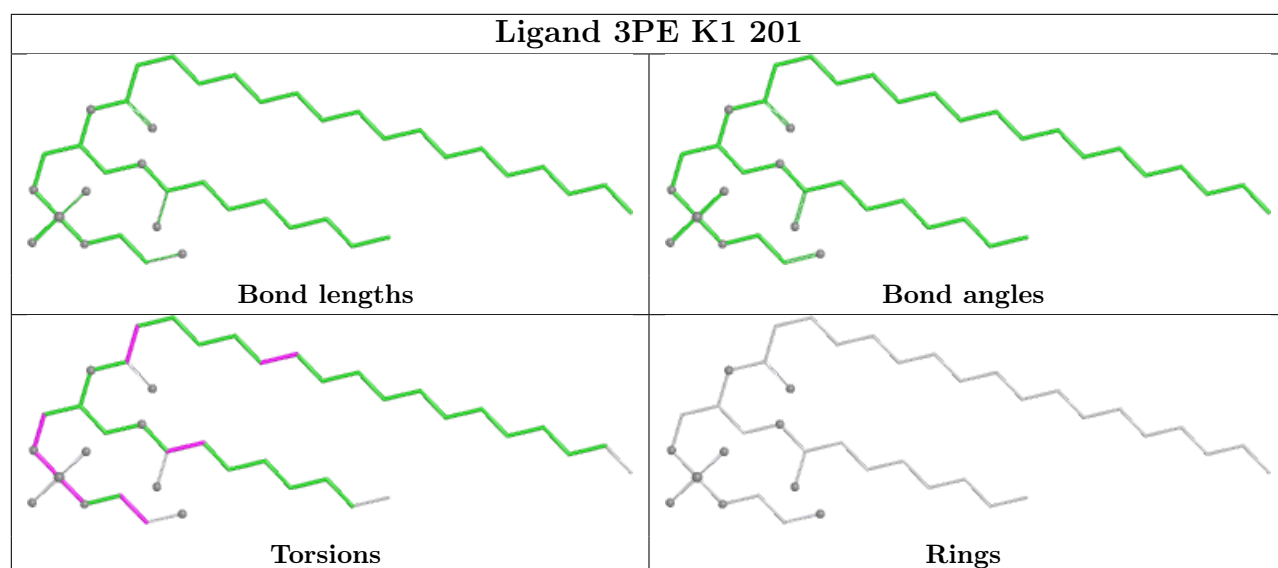


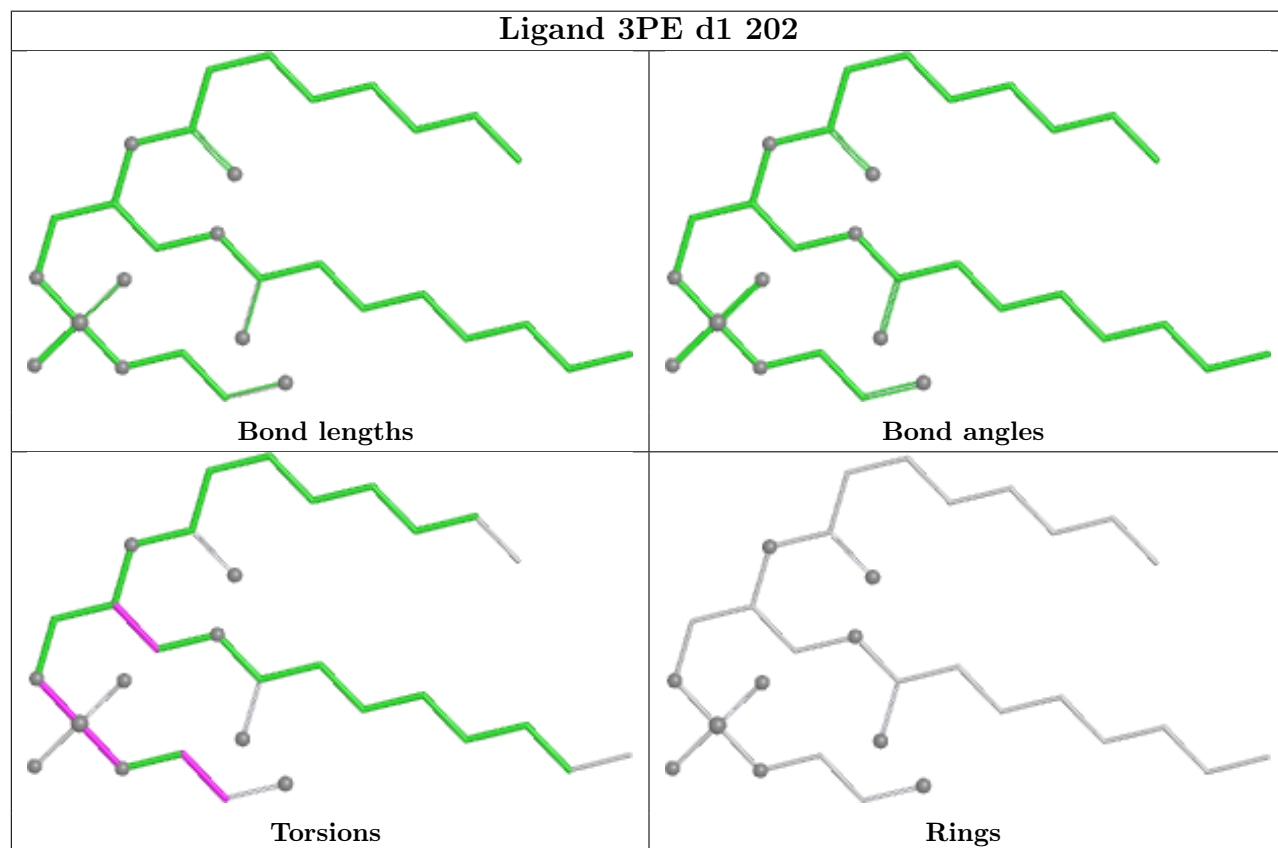
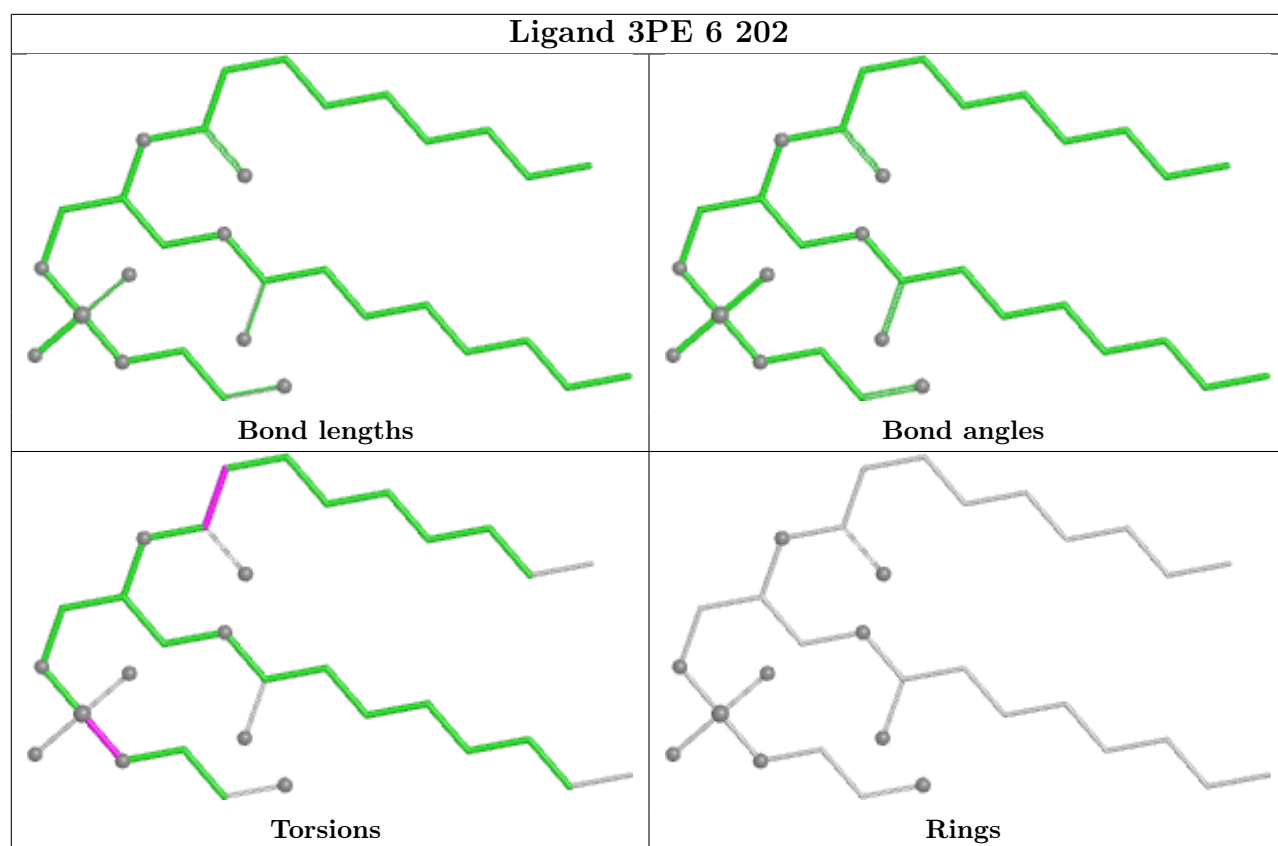


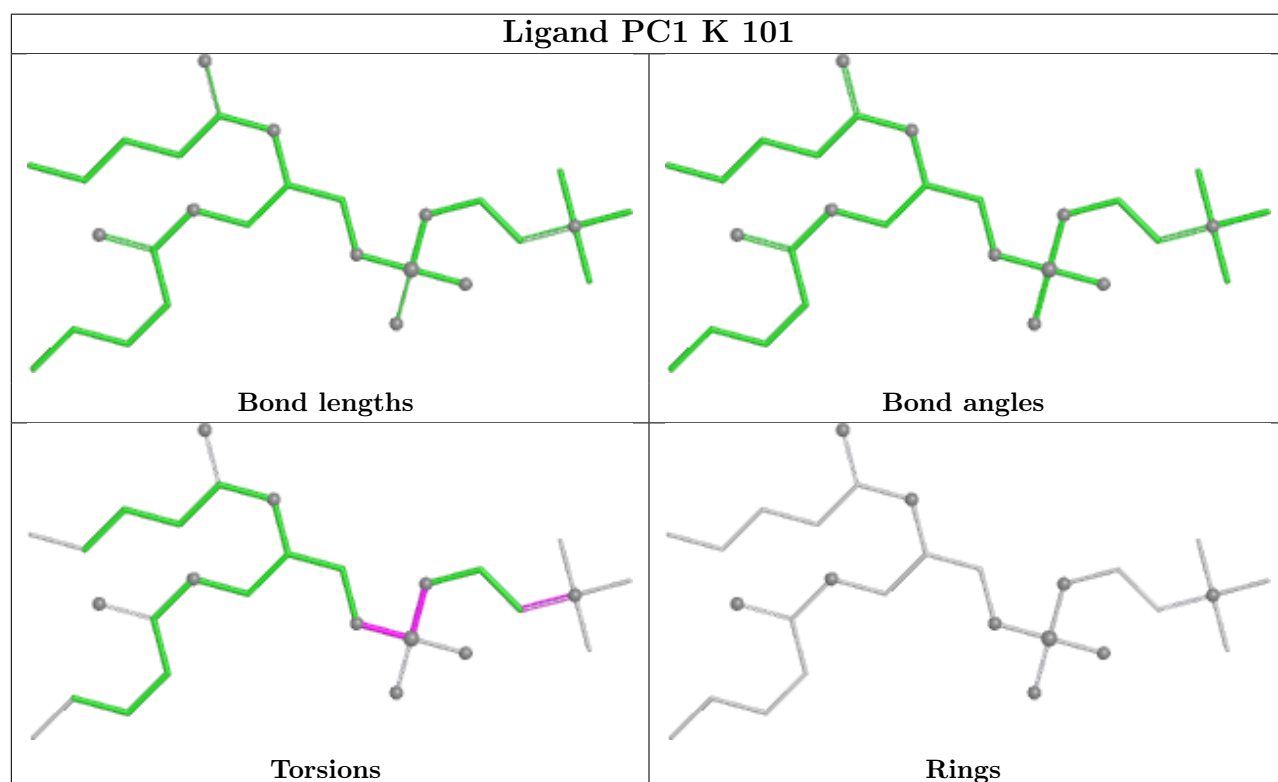
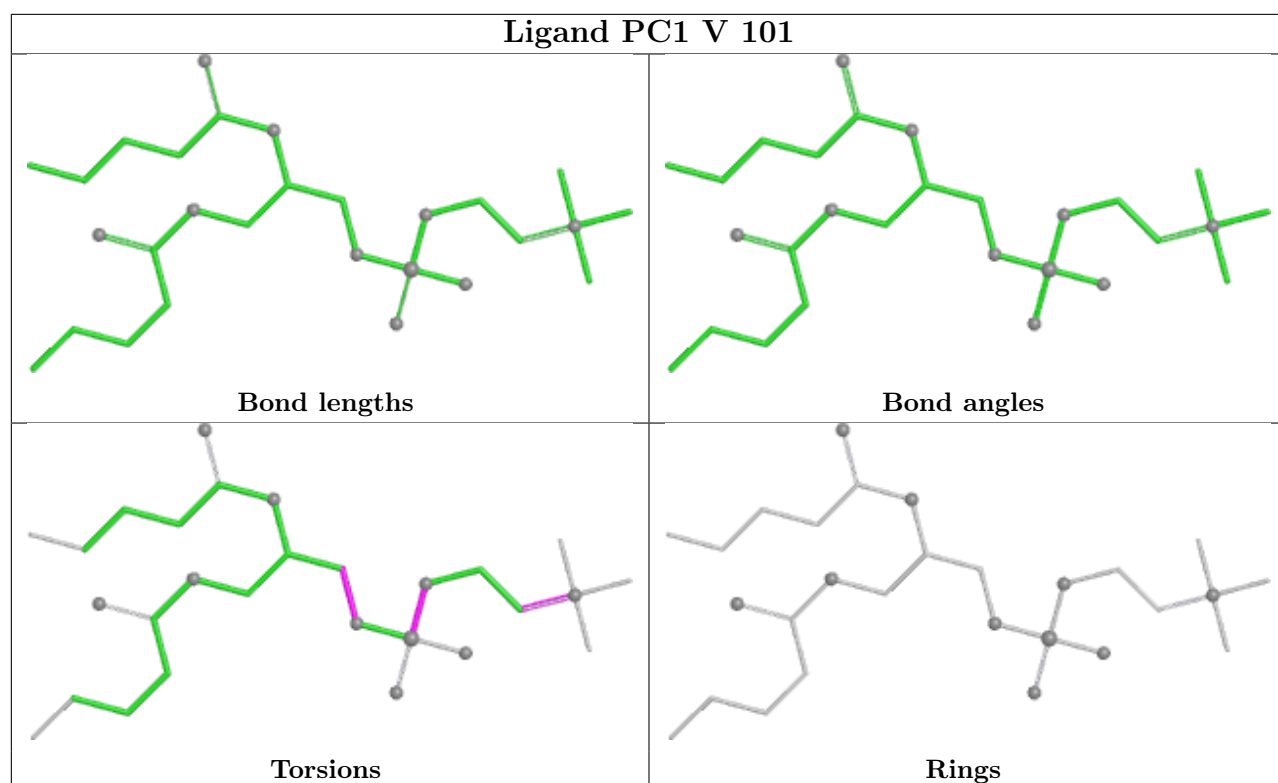


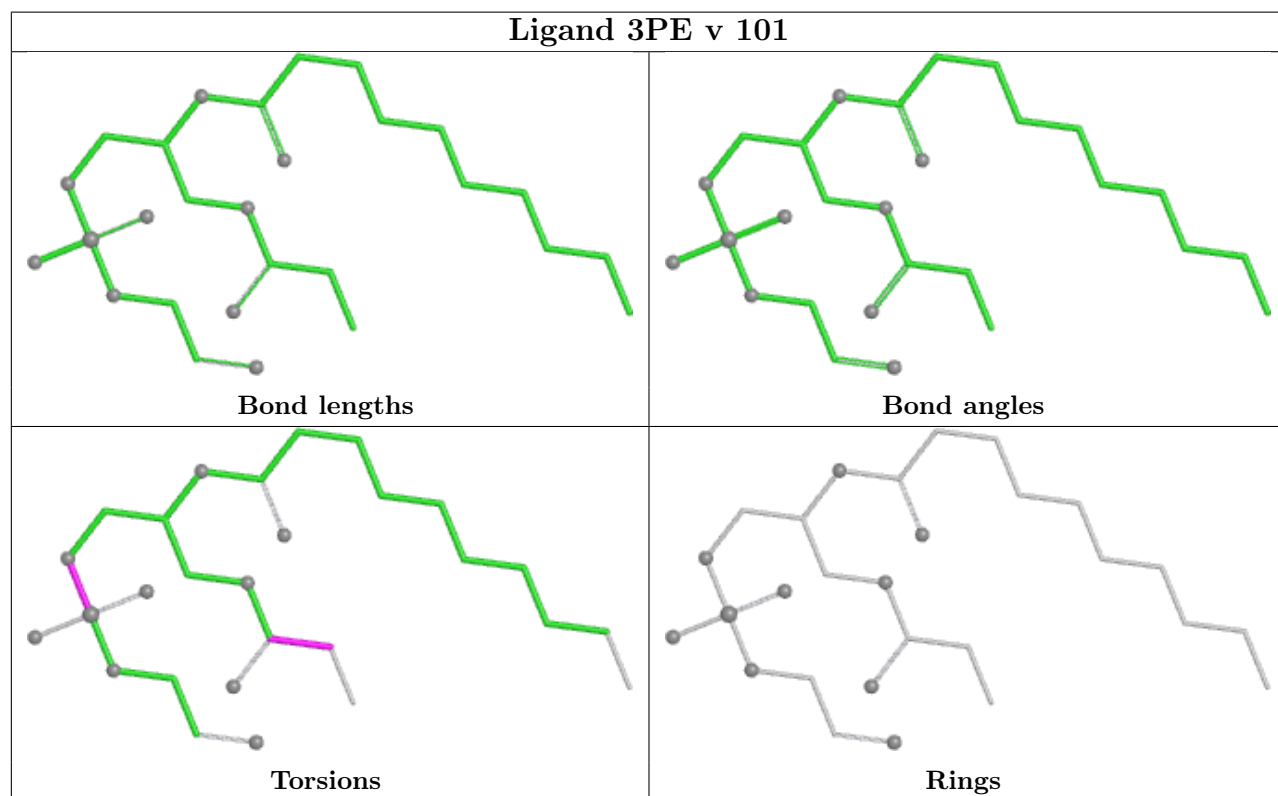
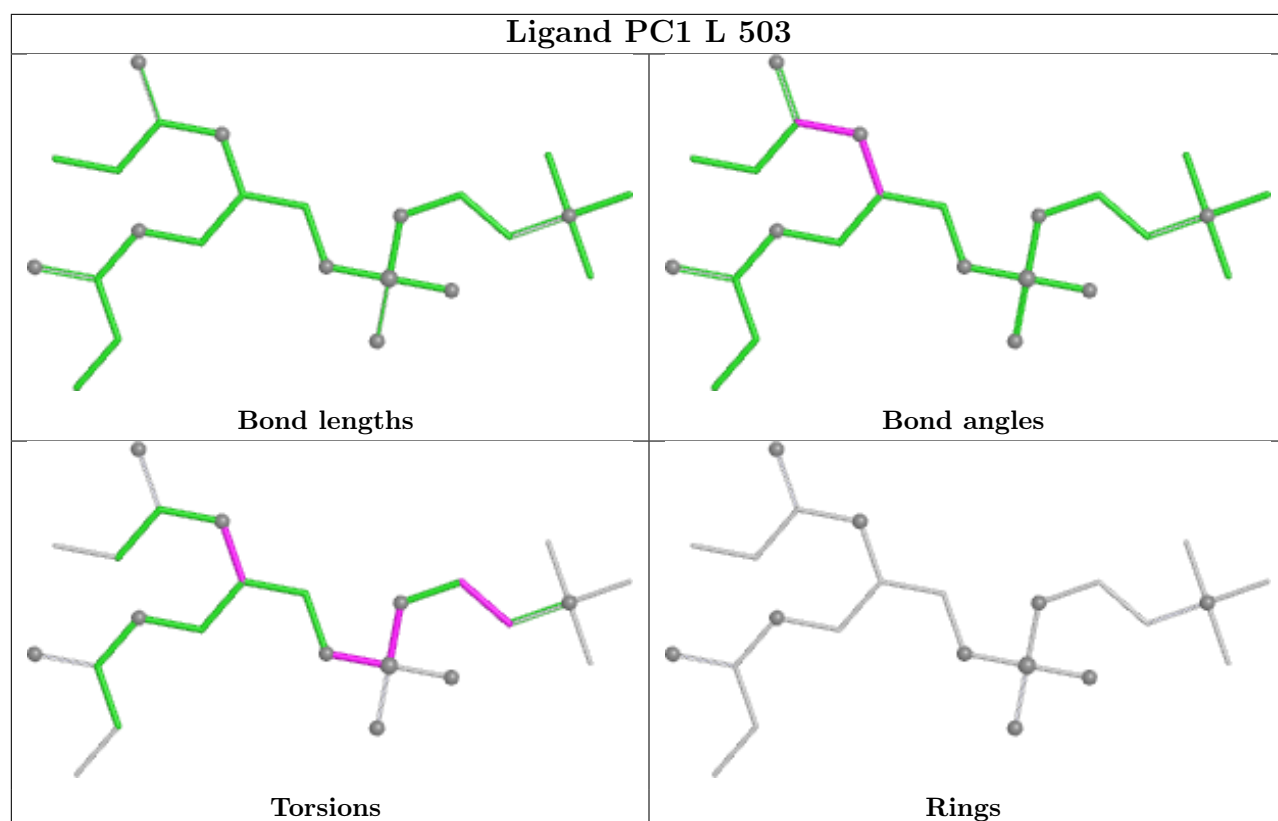


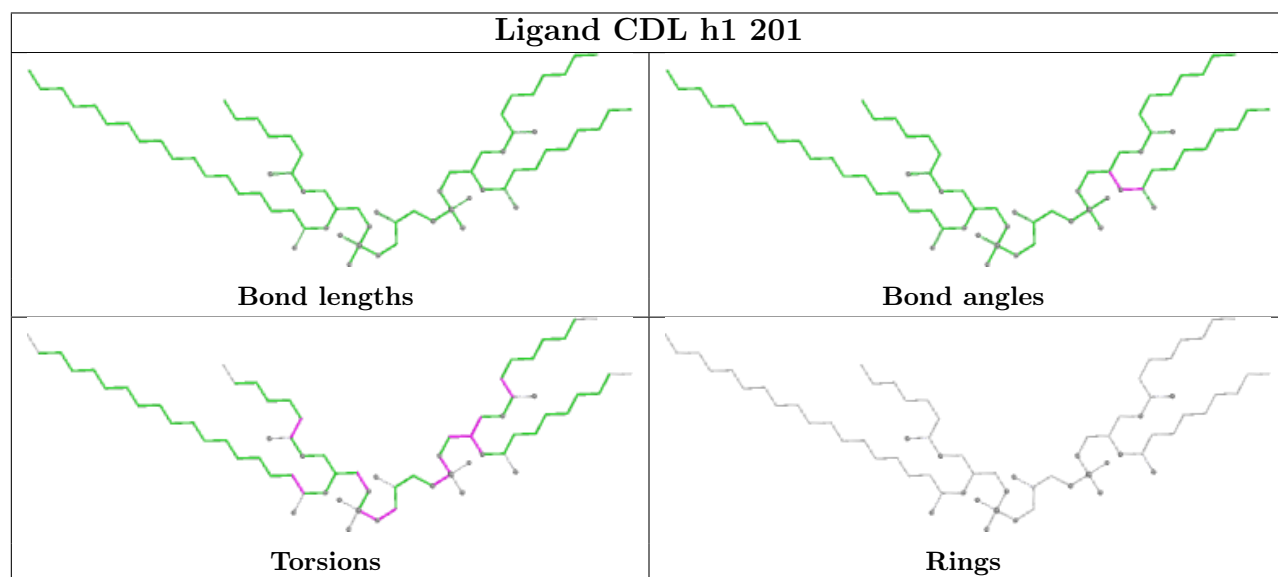
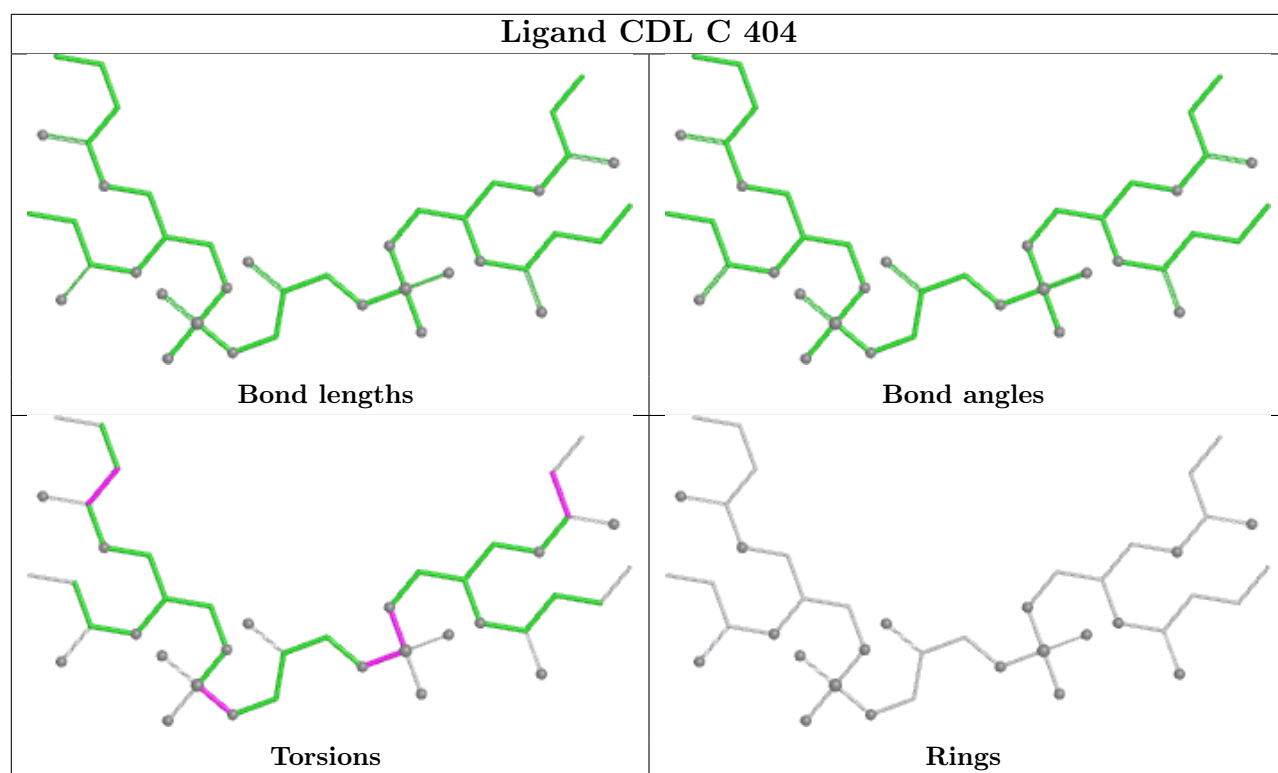


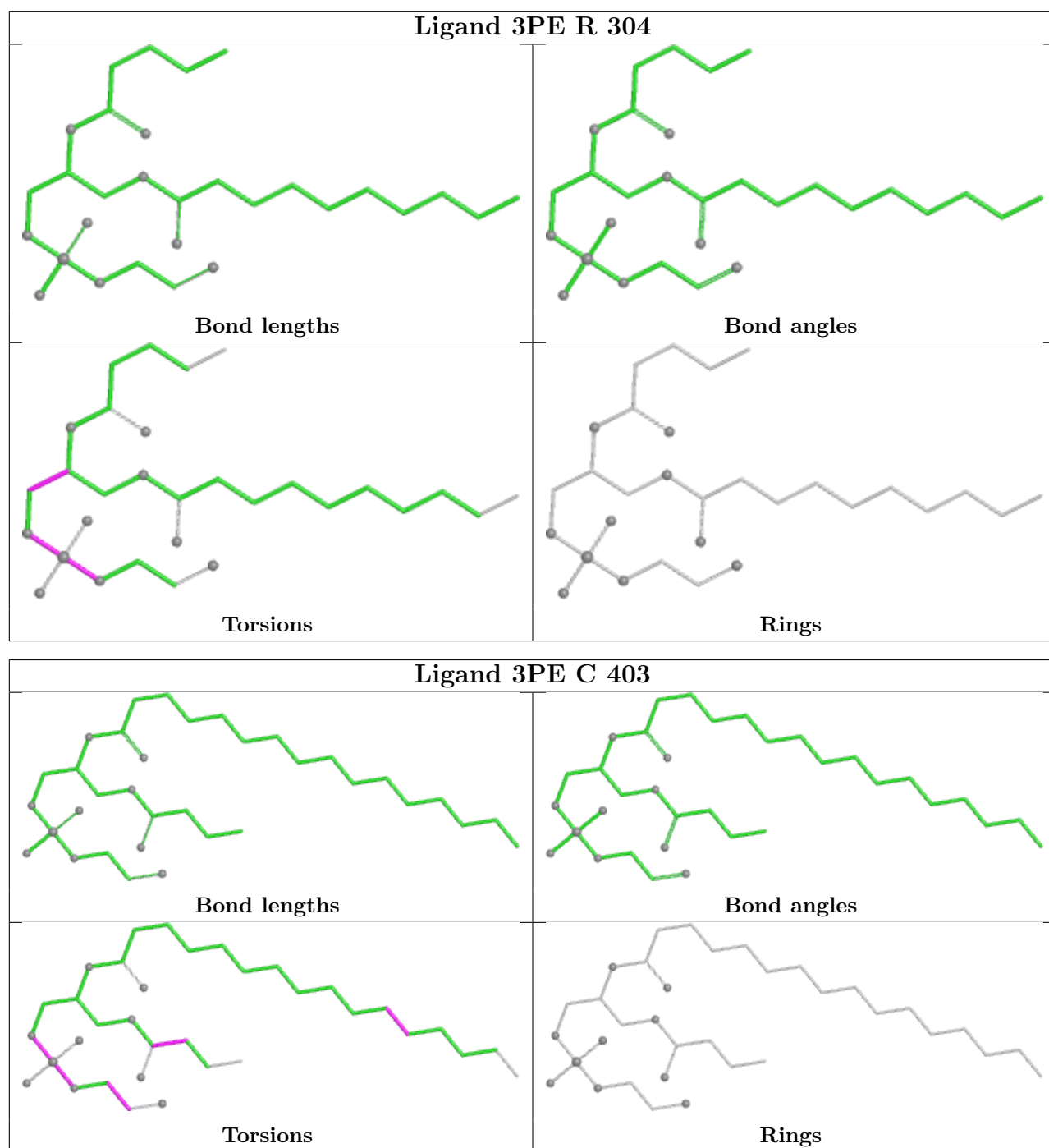


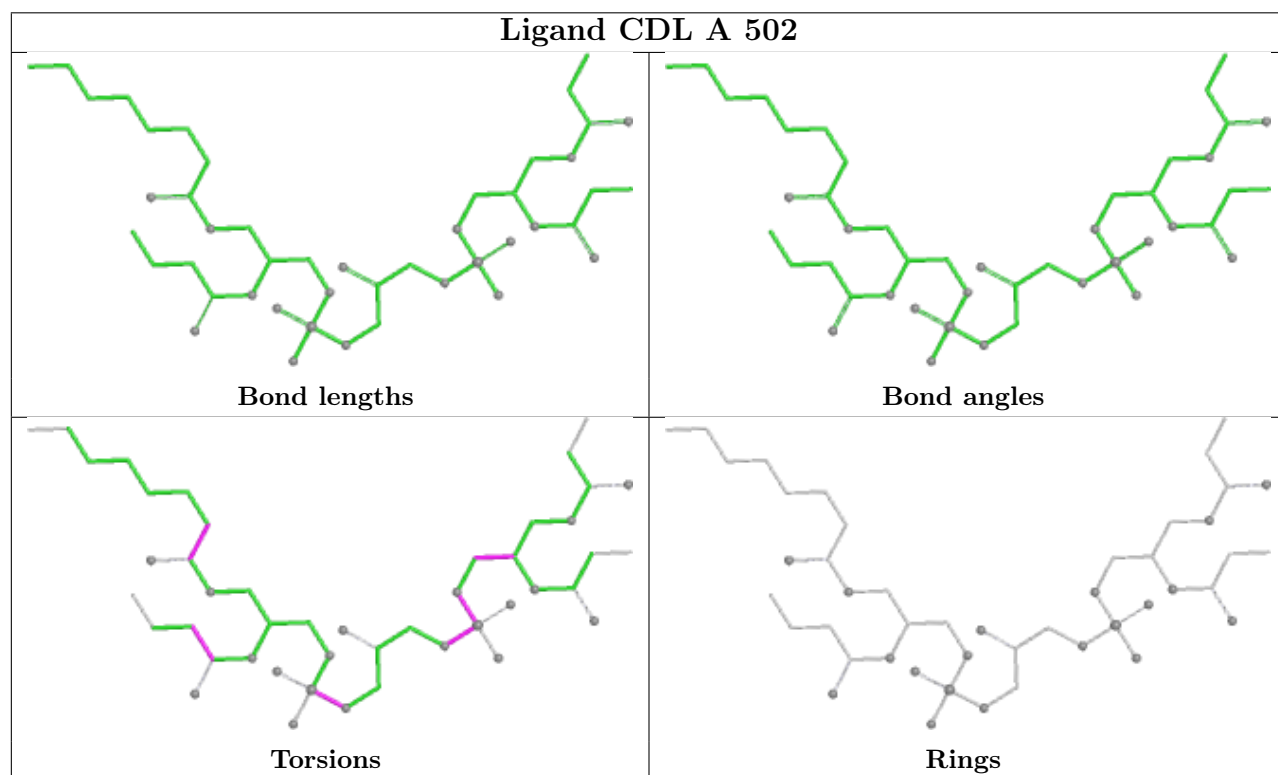
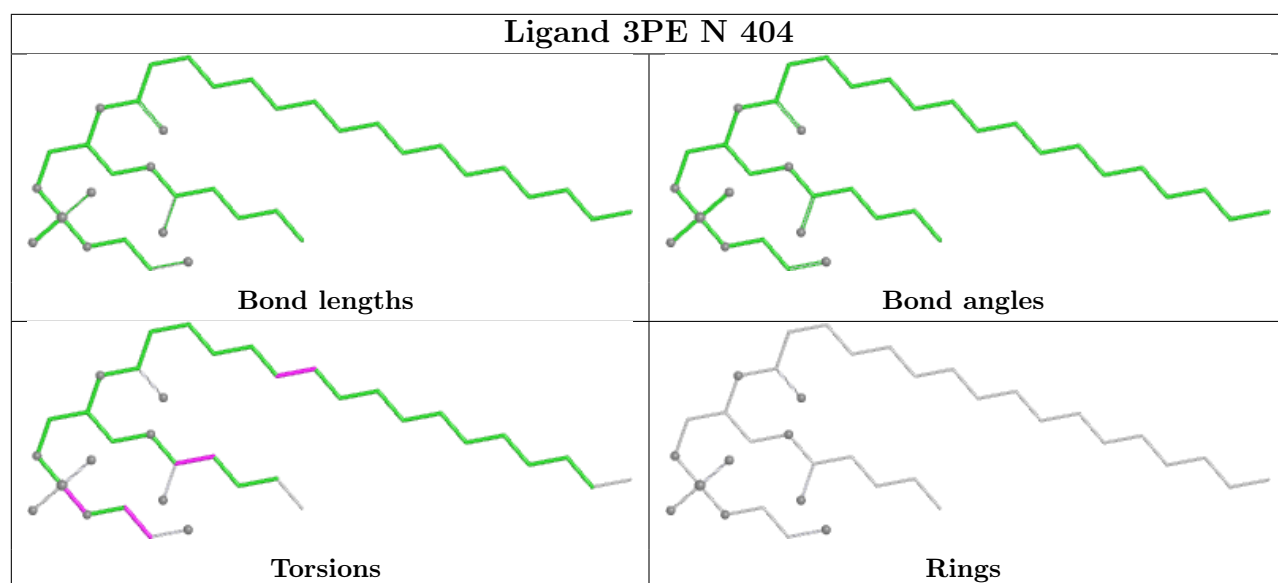


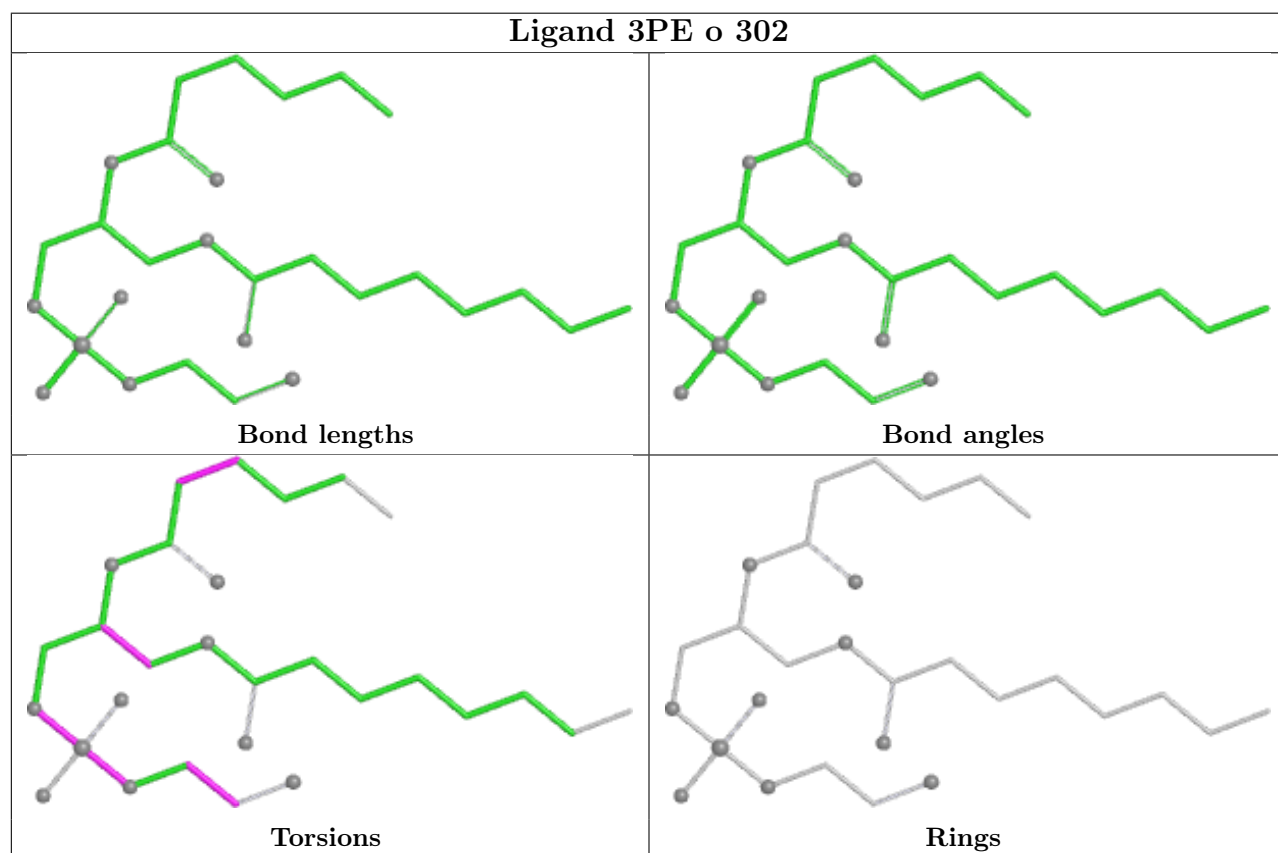
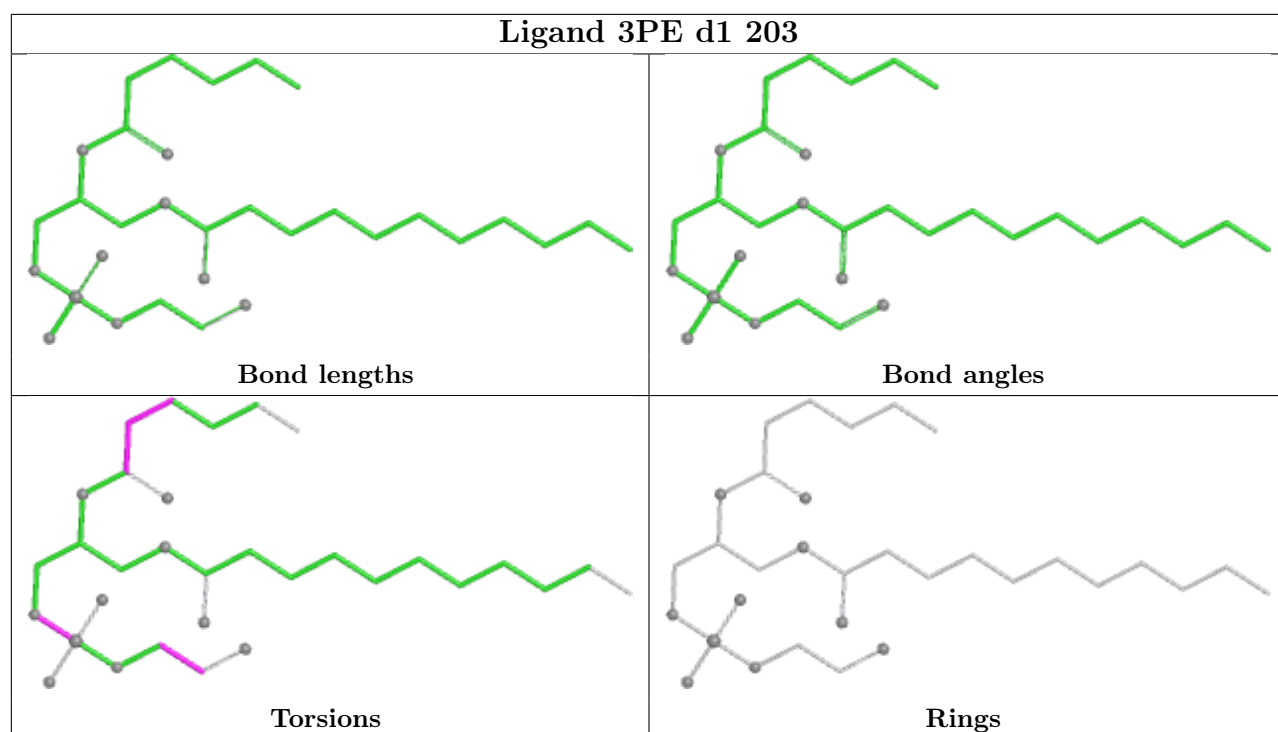


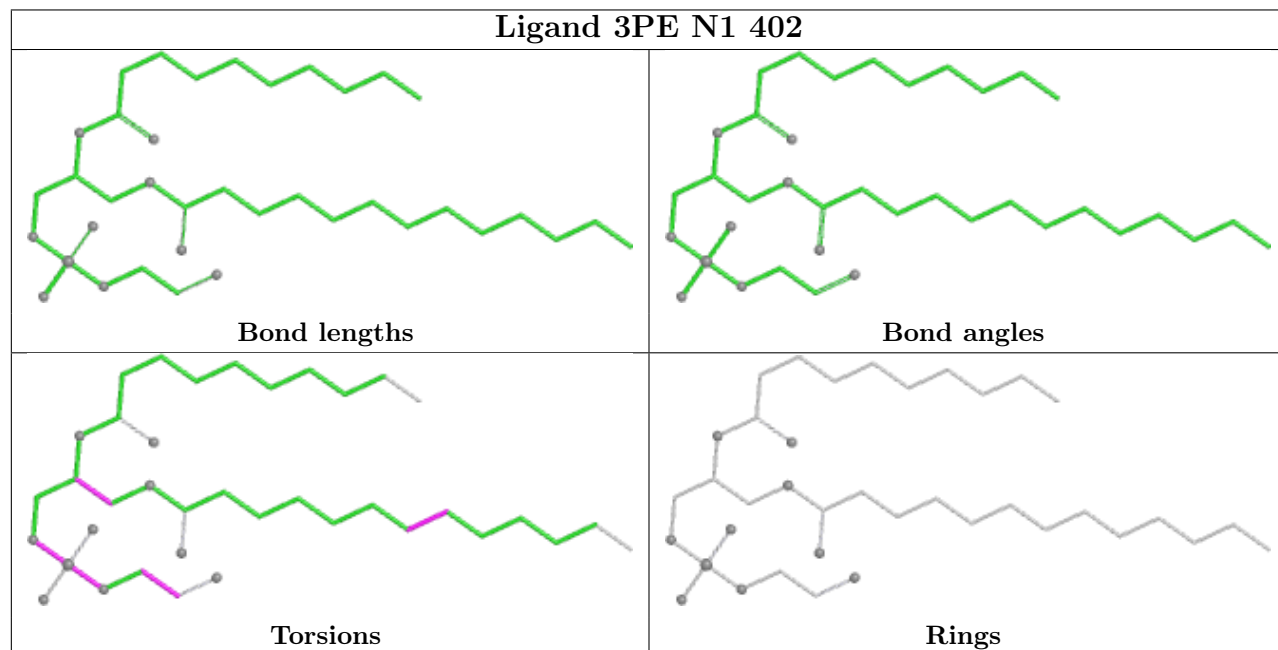
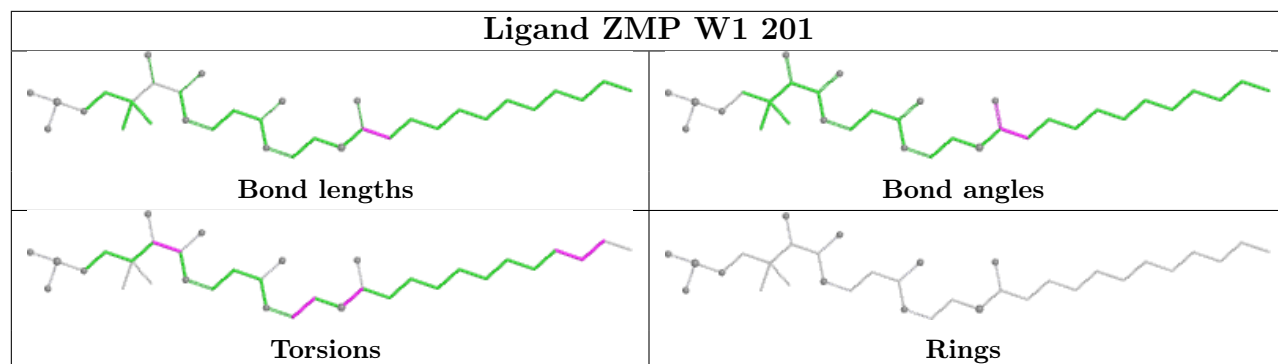


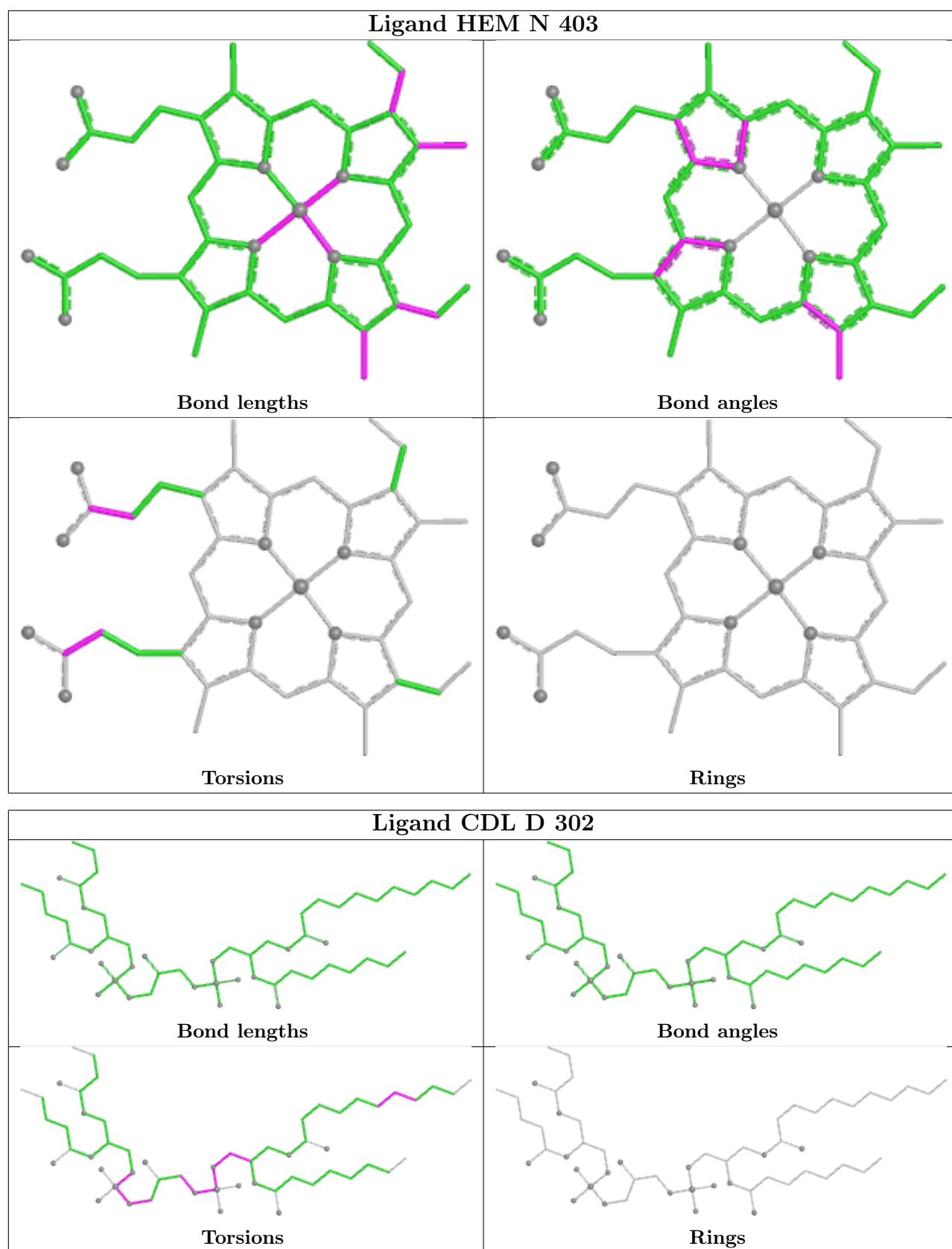


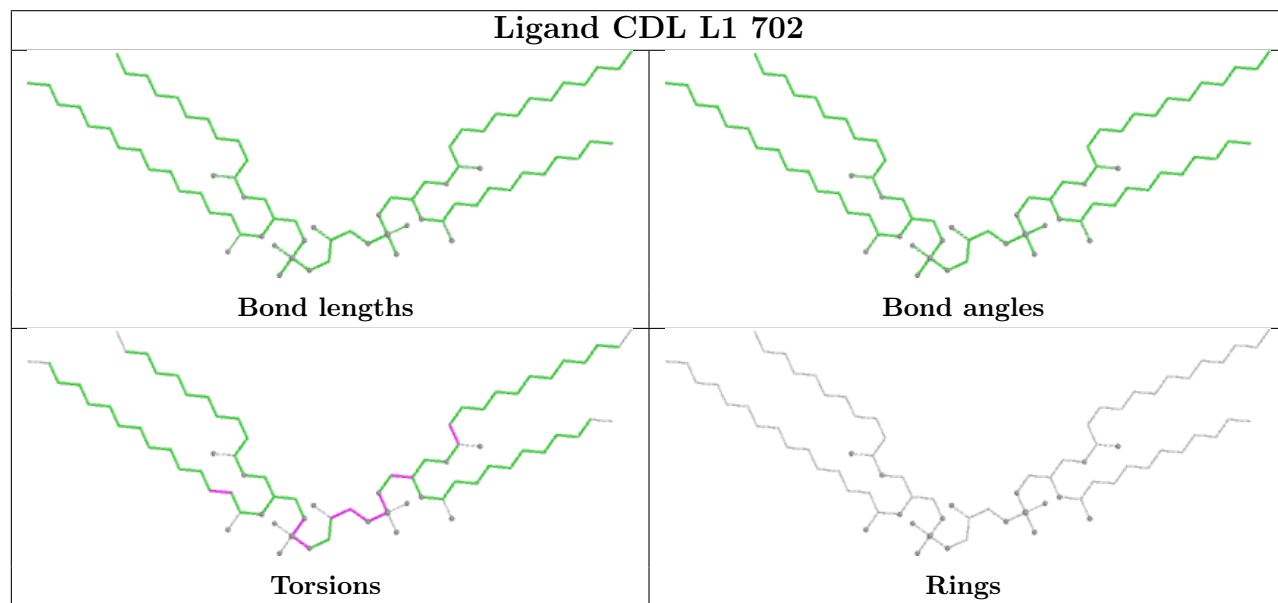
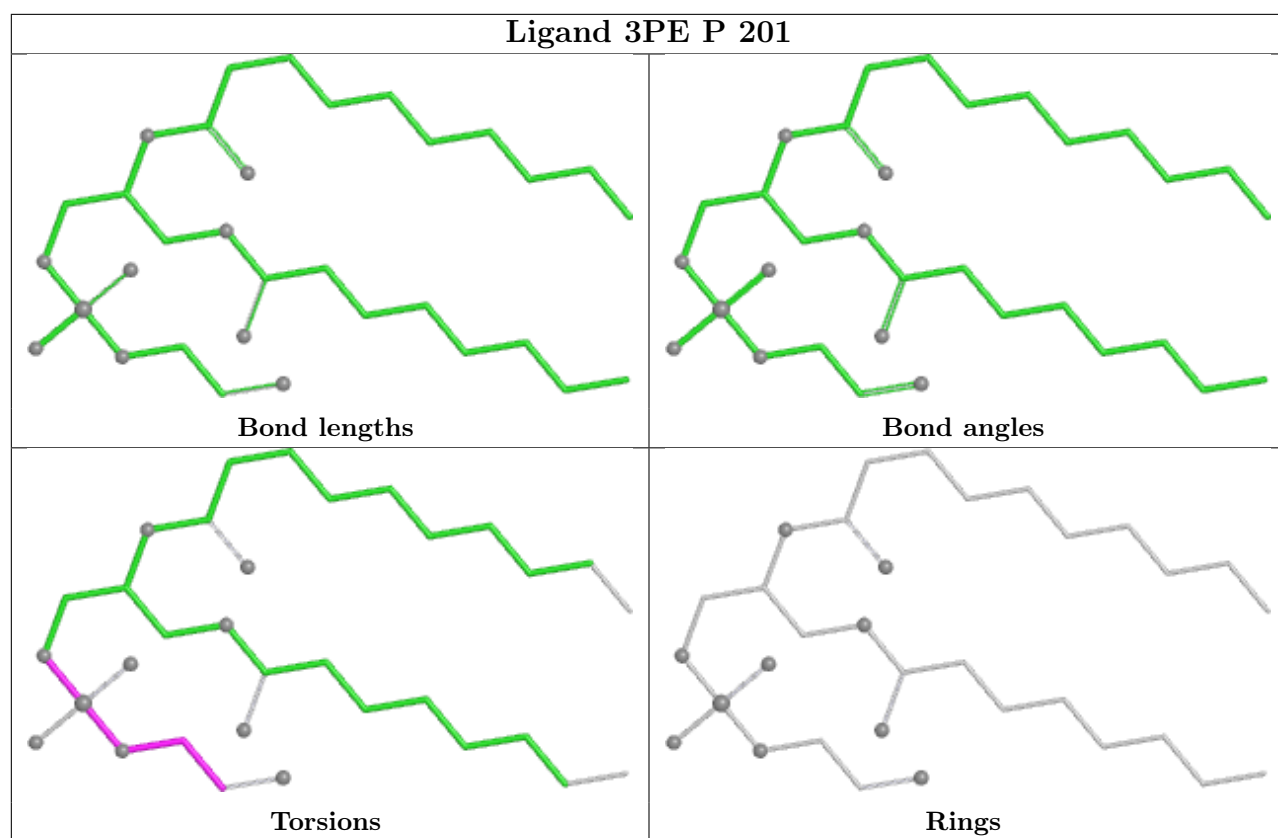


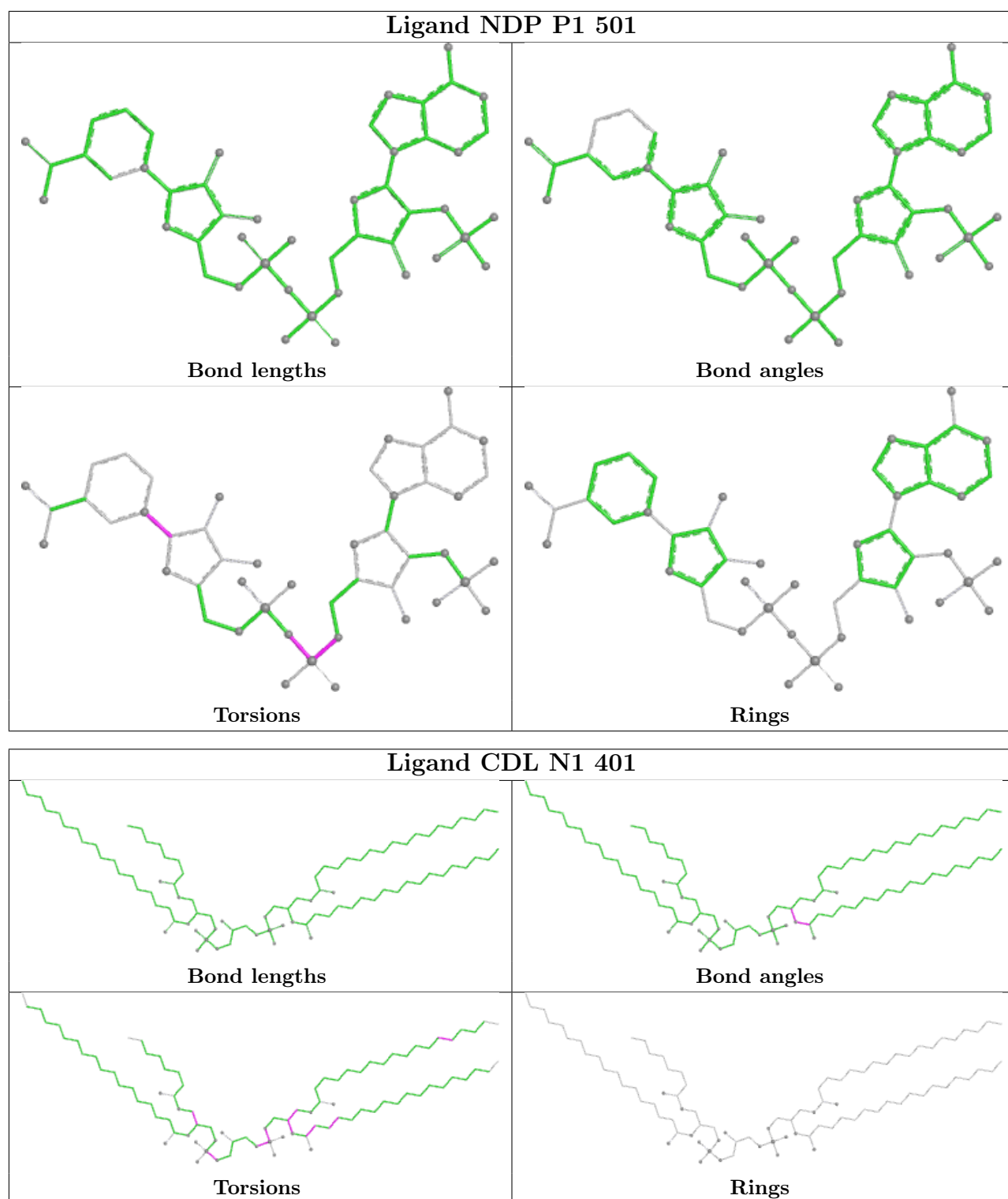


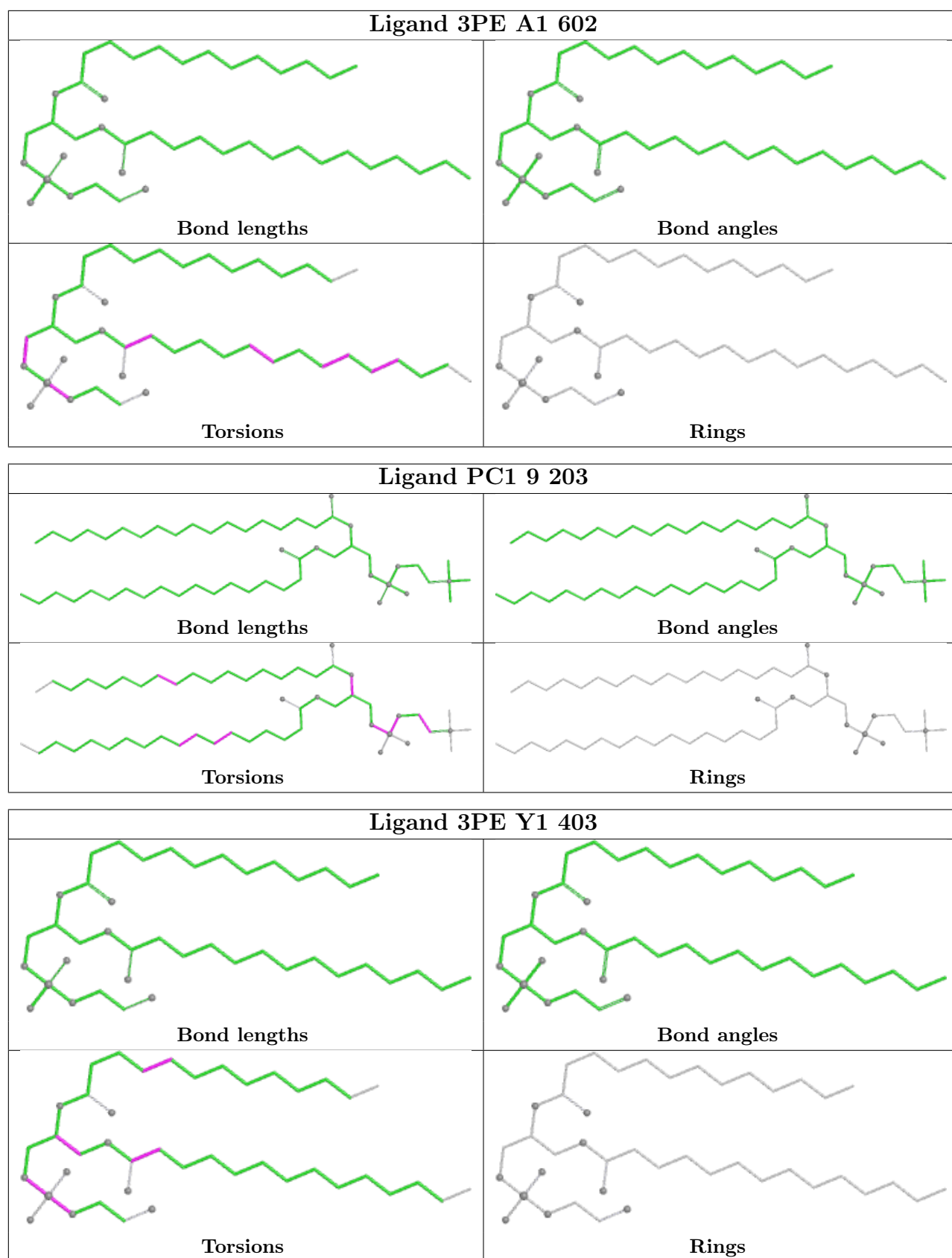


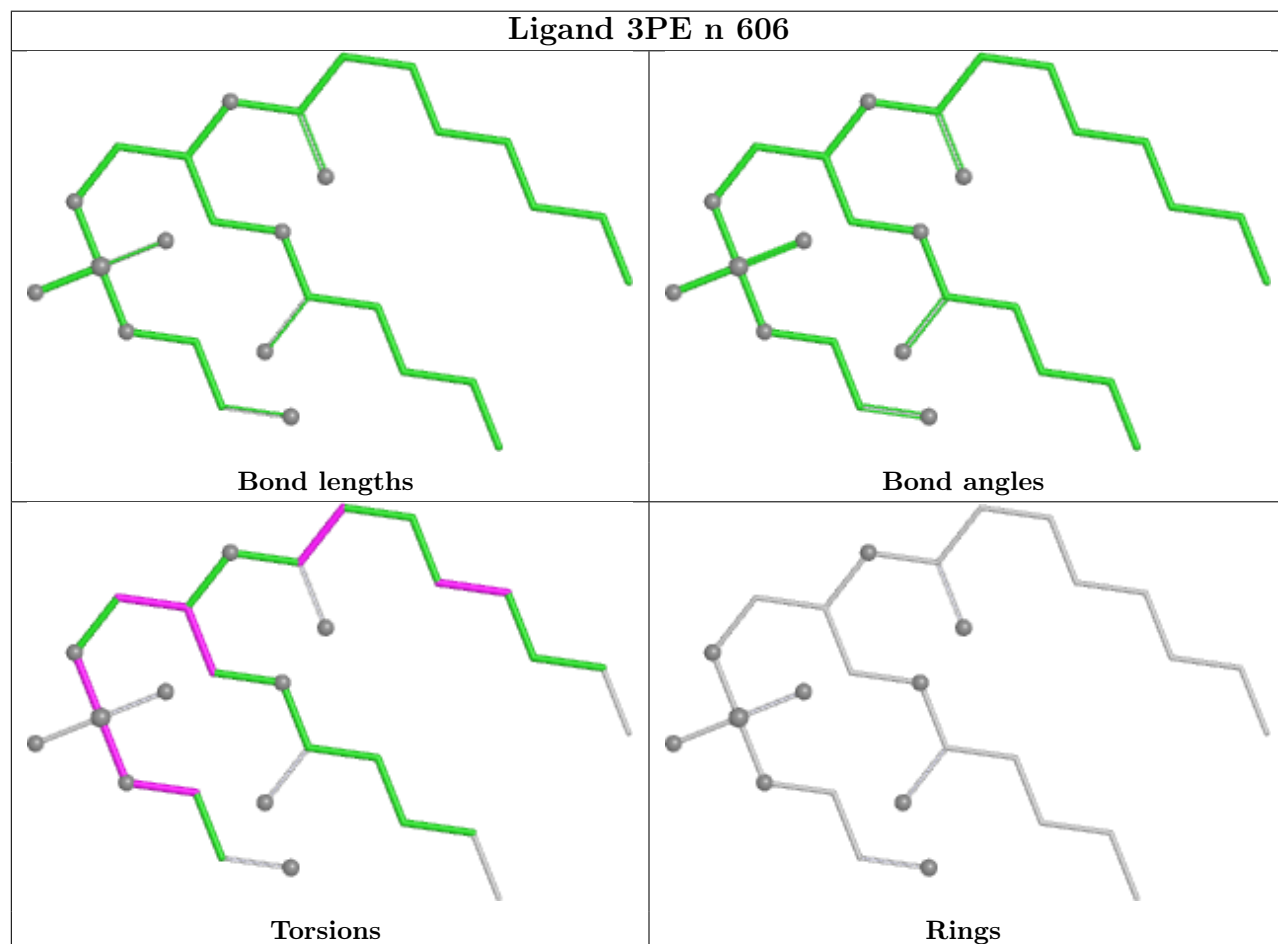
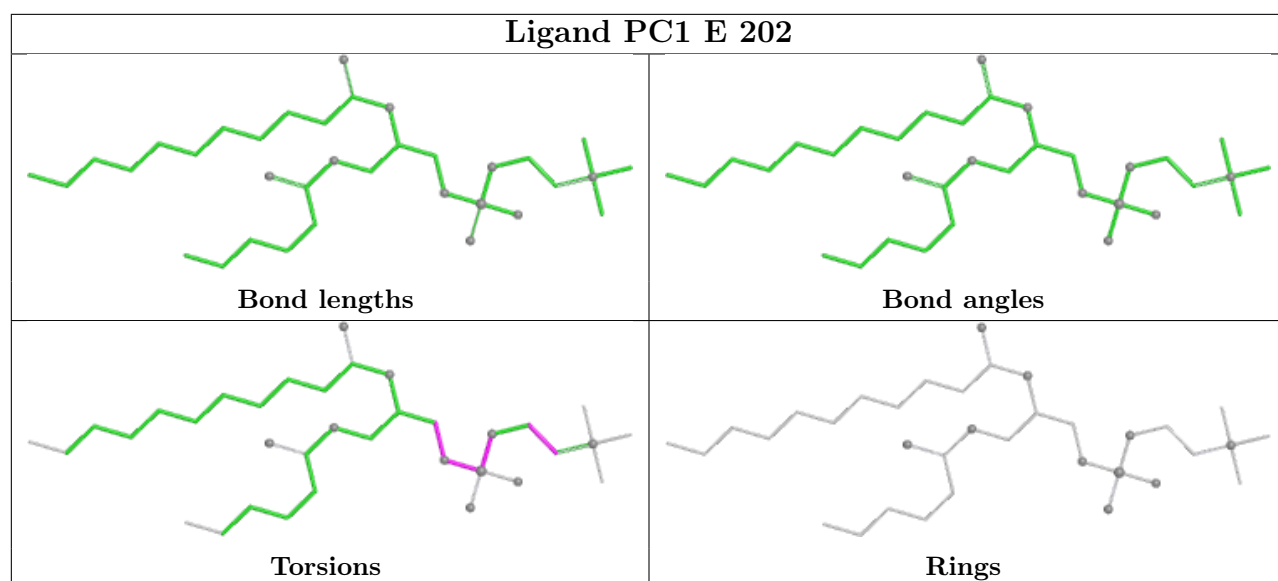


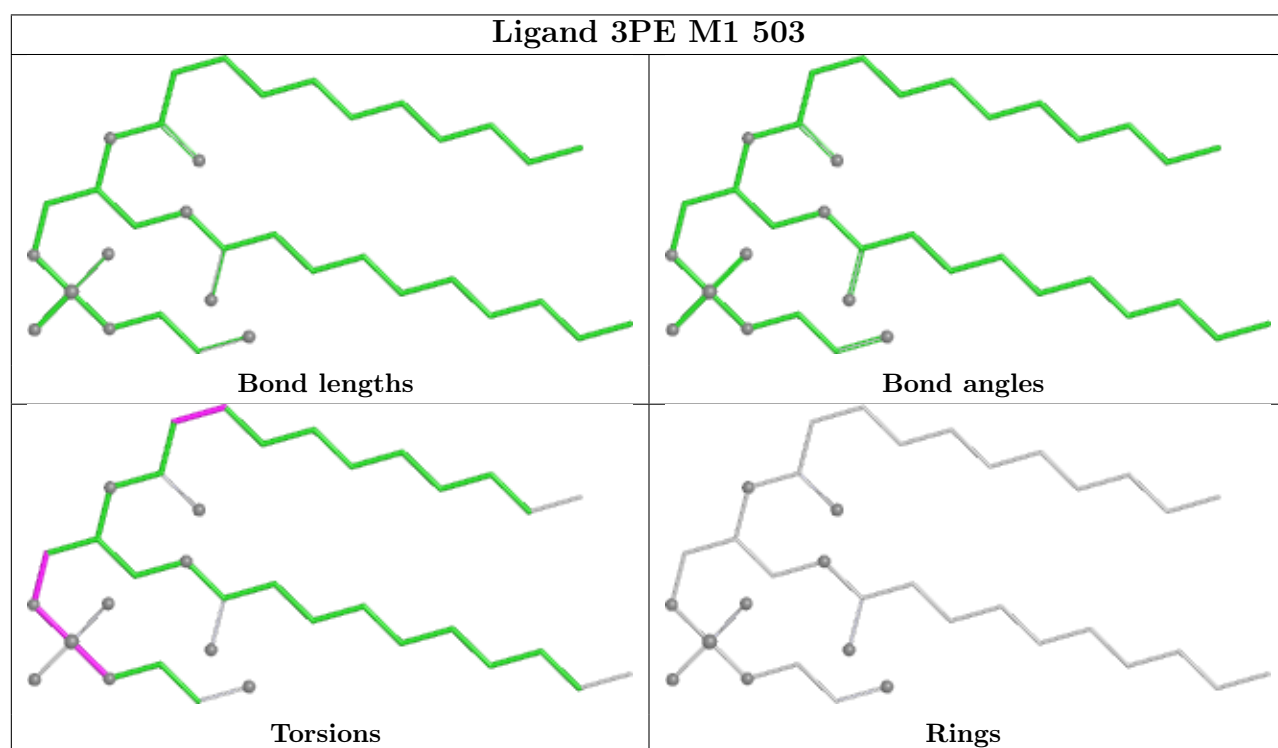
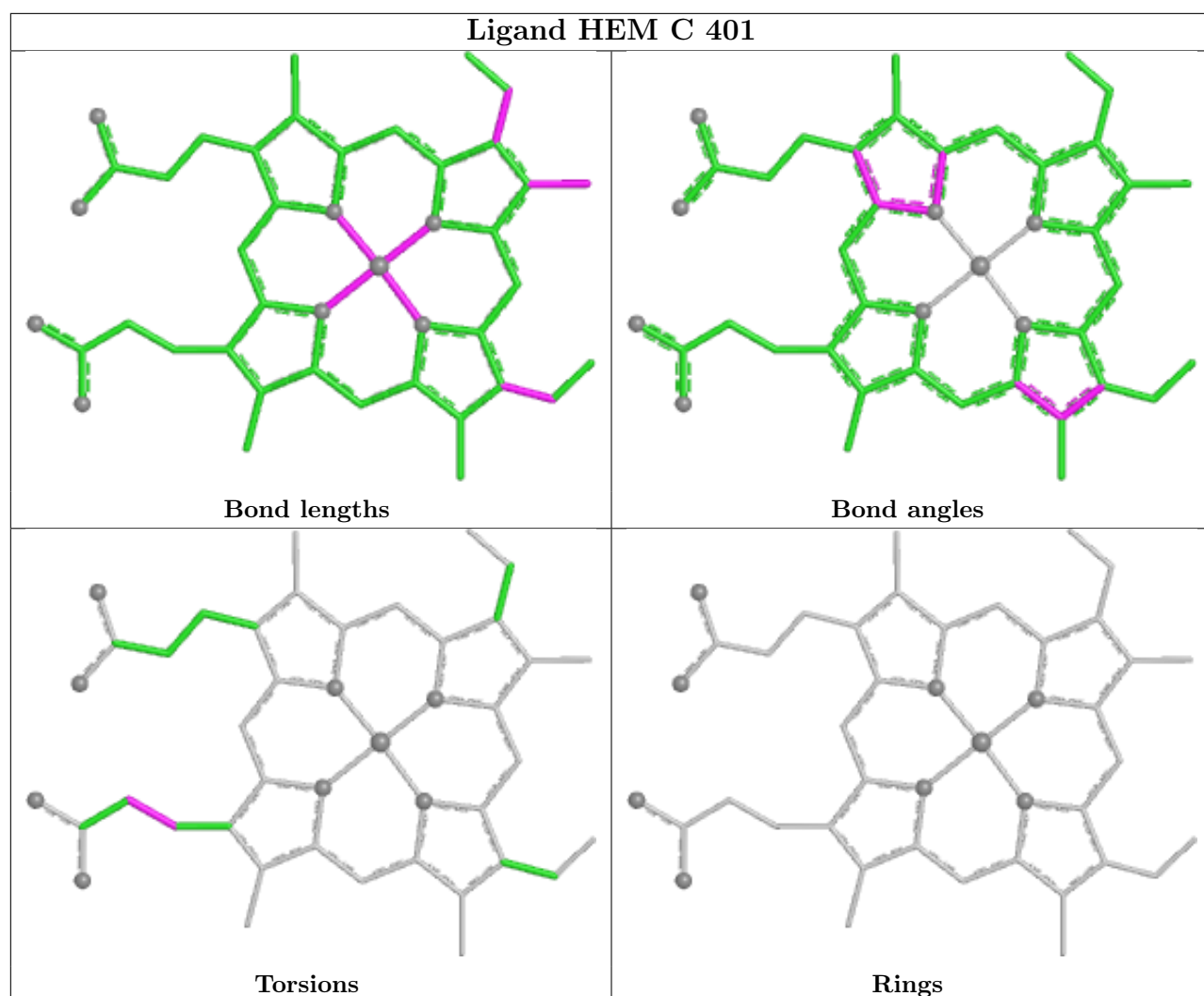


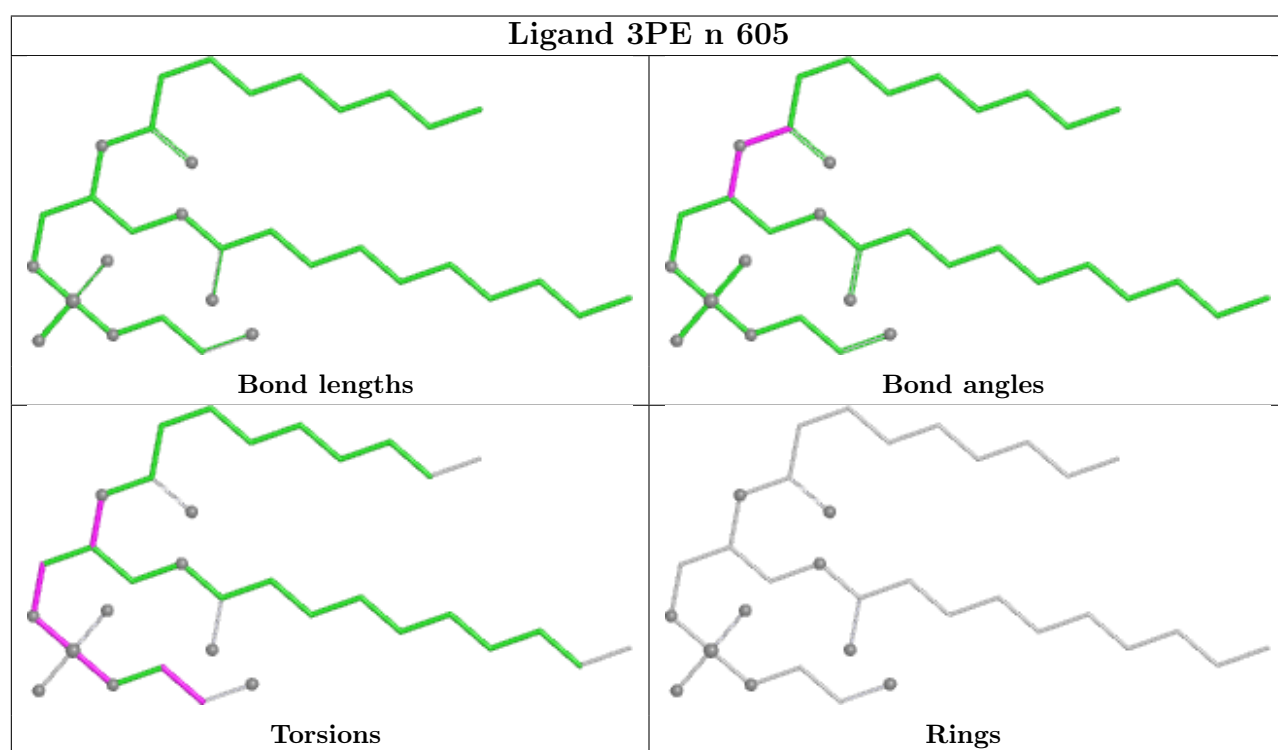
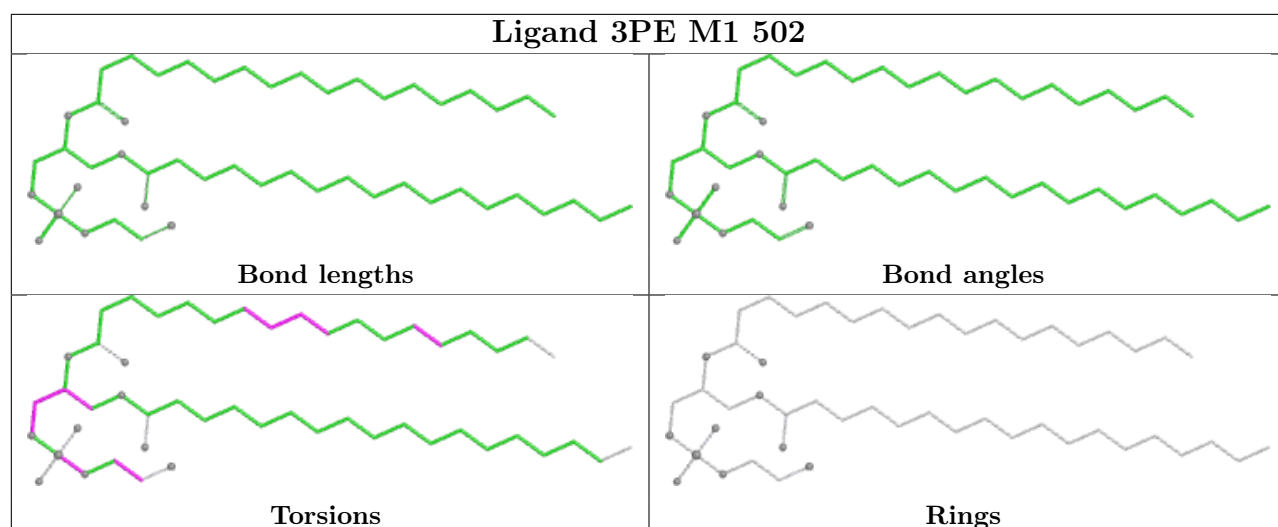


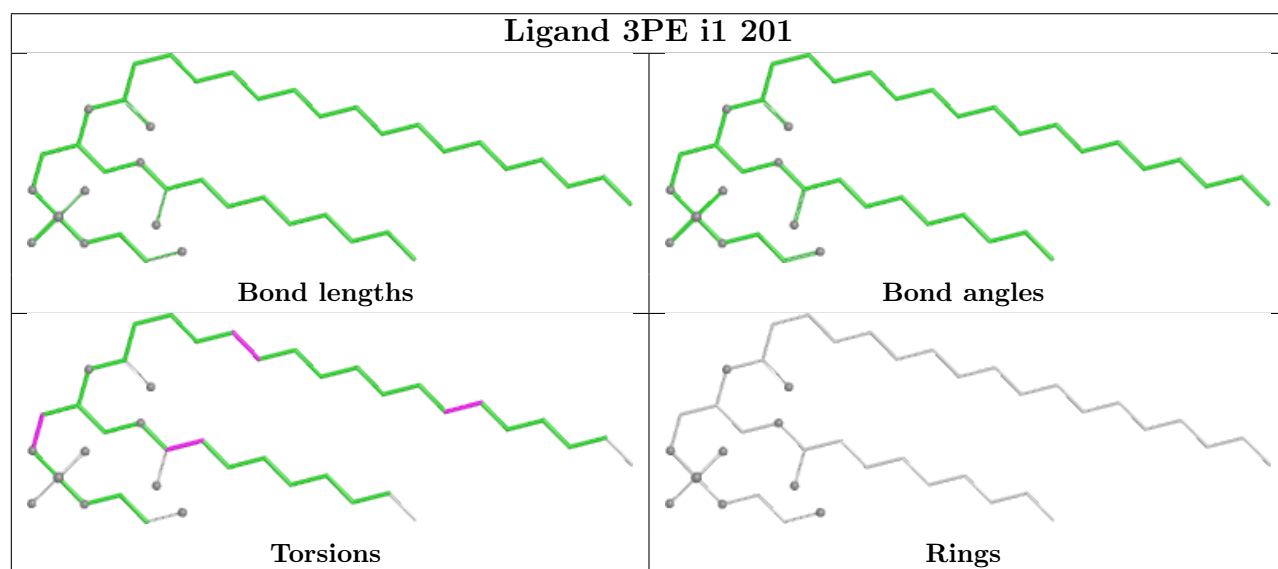
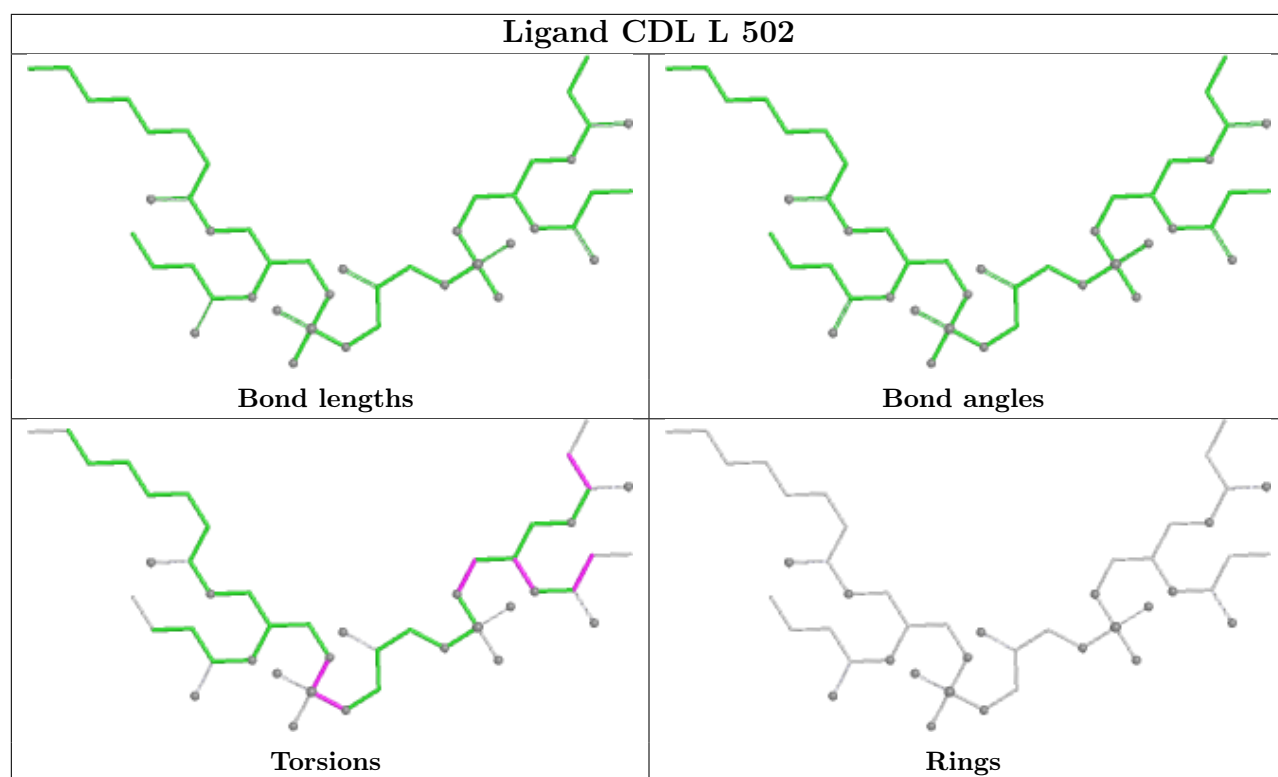


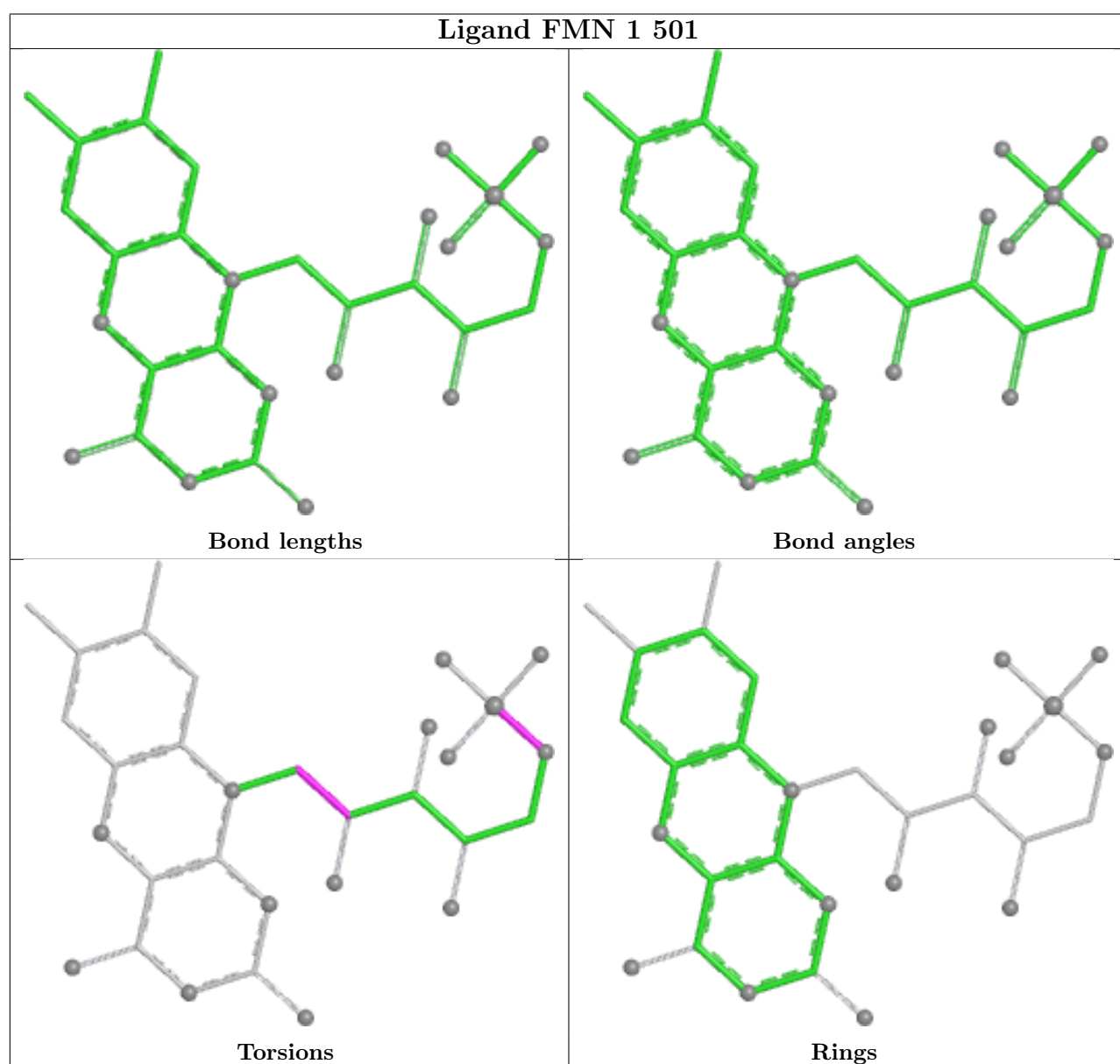
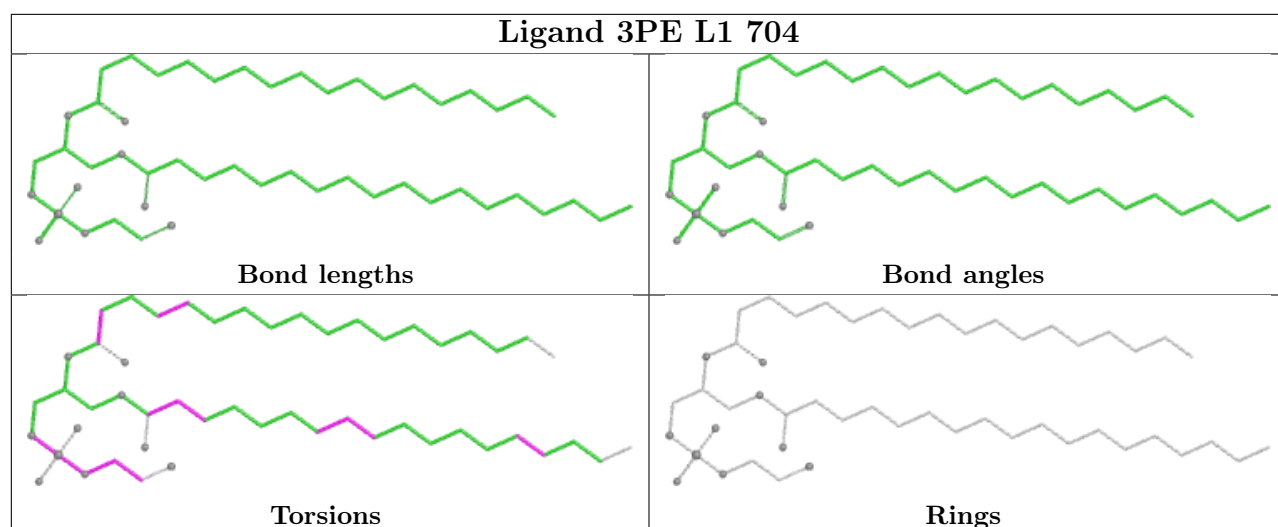


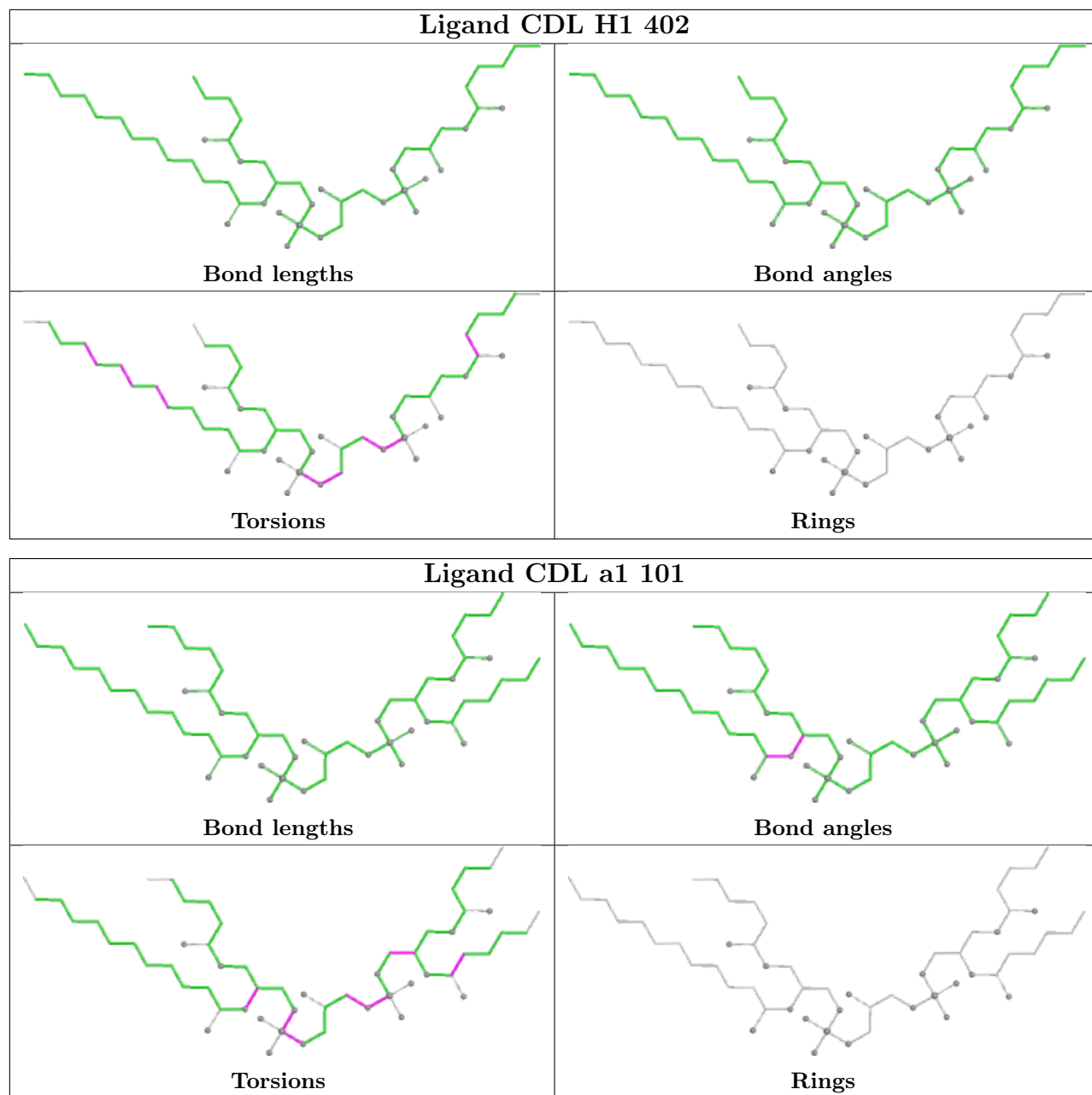


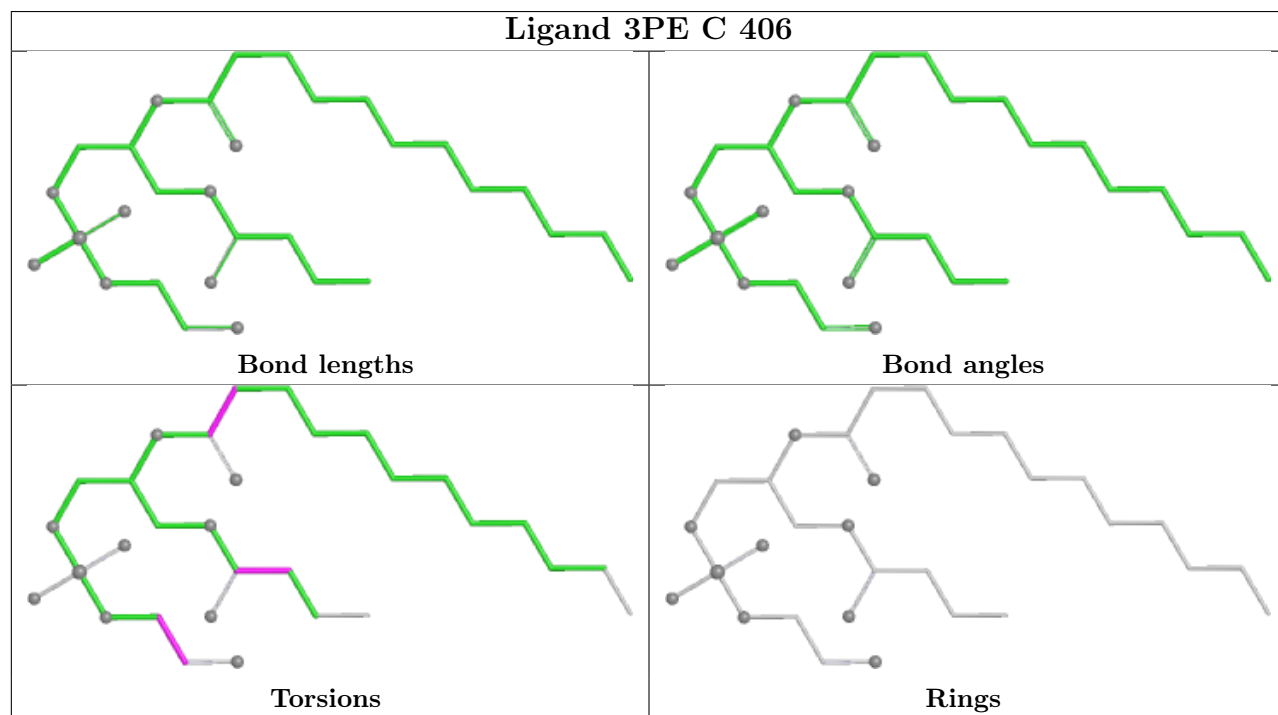
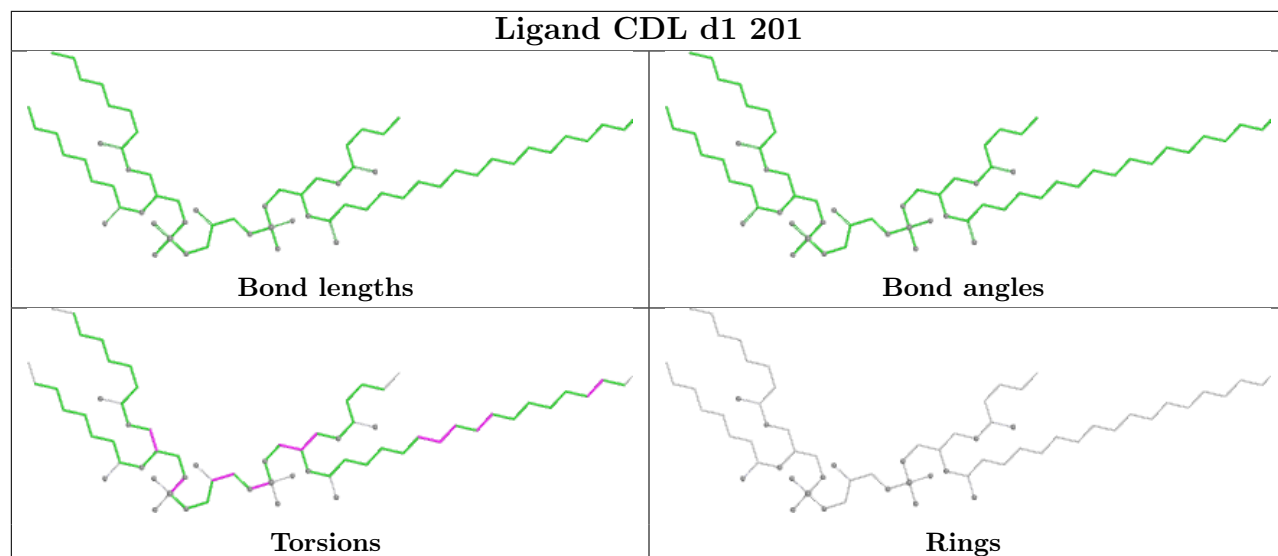


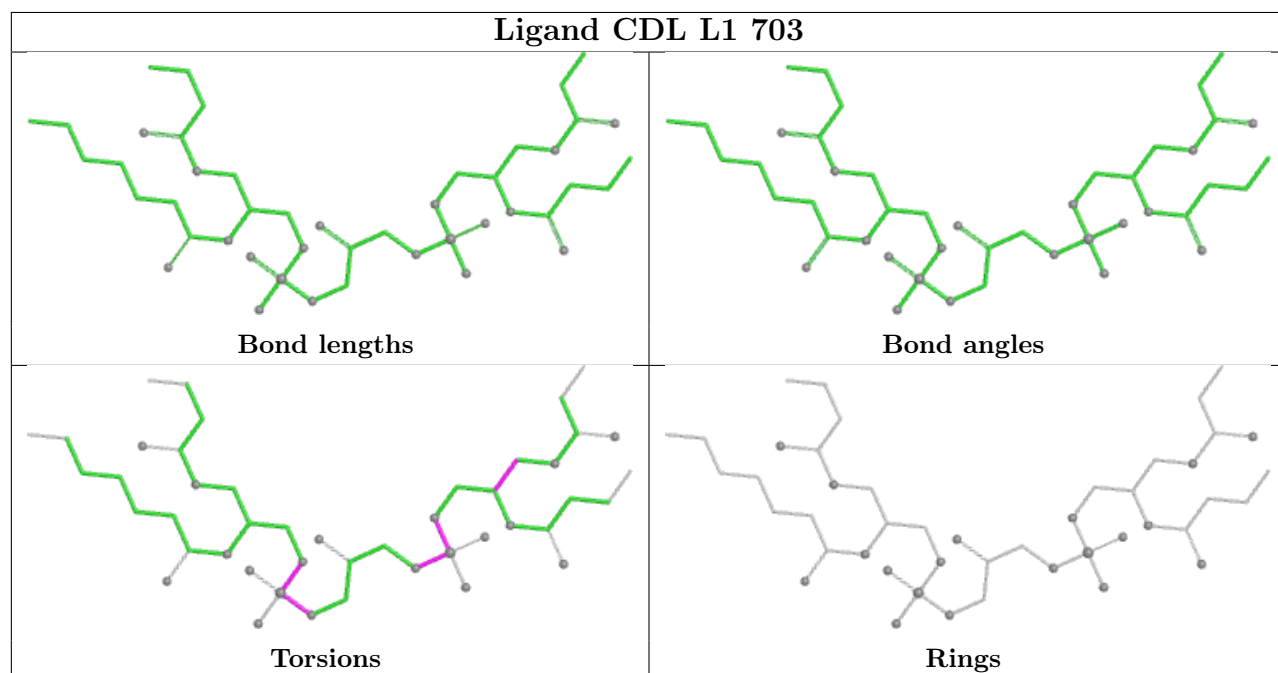
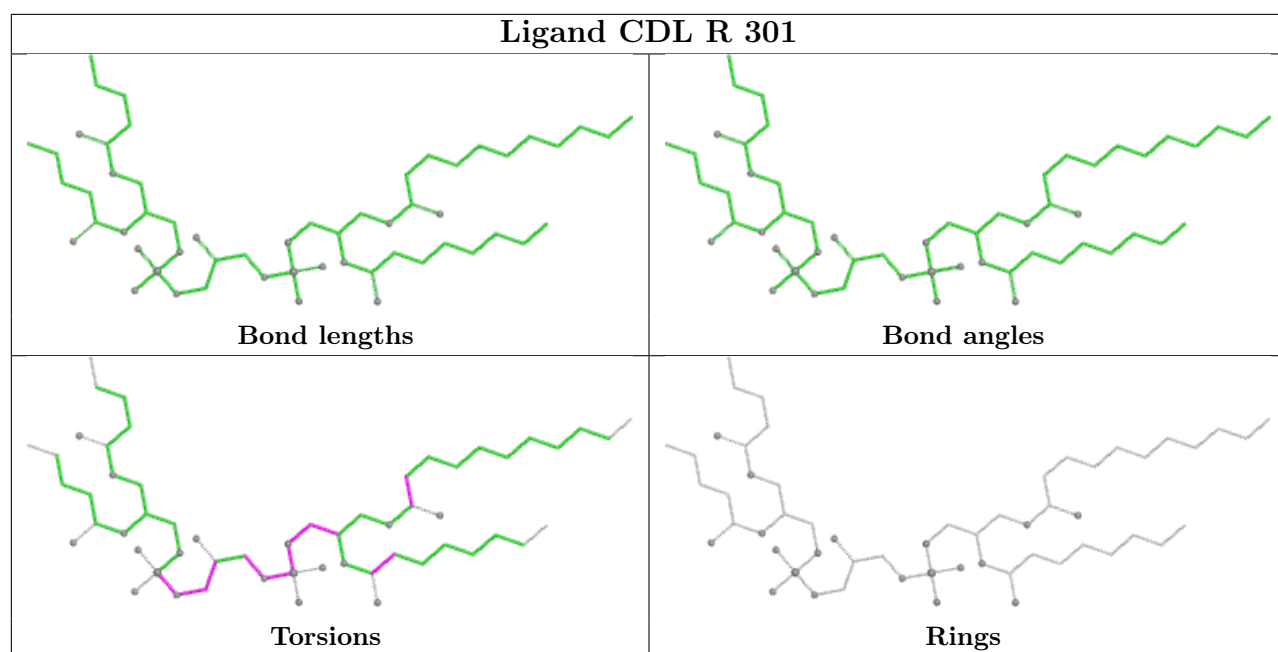


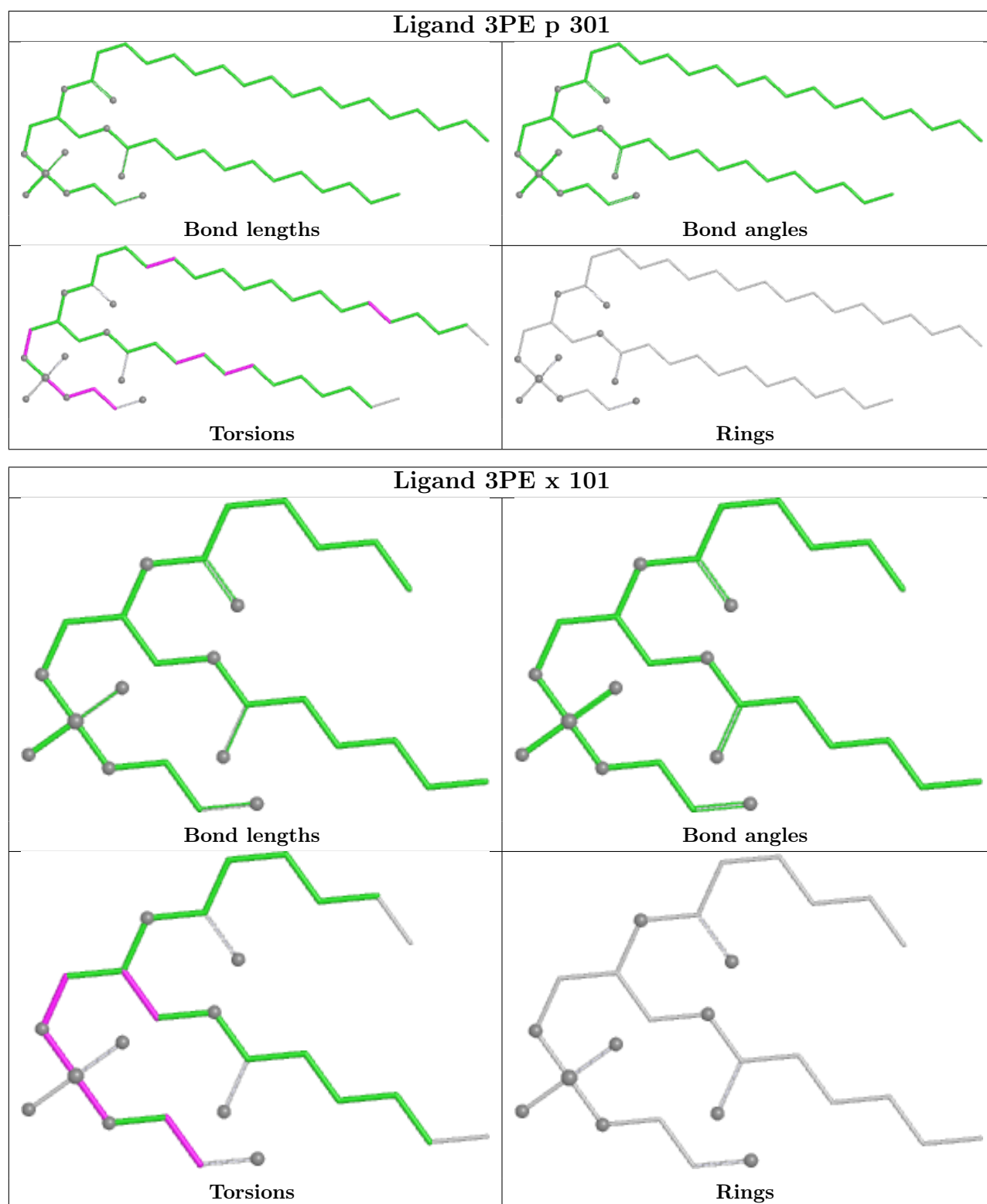












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

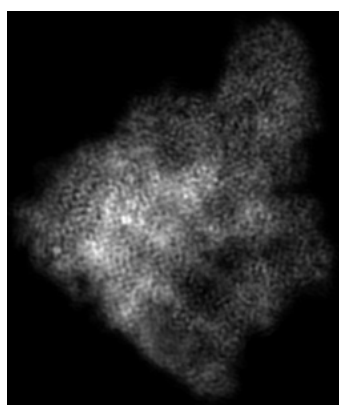
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17990. These allow visual inspection of the internal detail of the map and identification of artifacts.

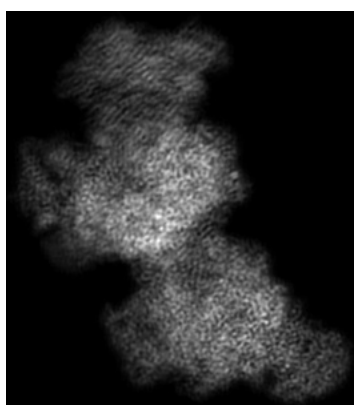
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

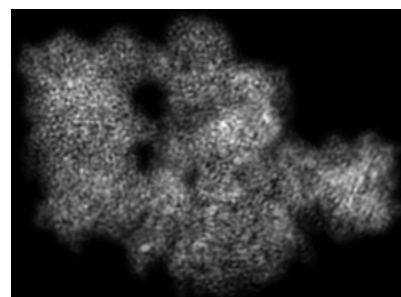
6.1.1 Primary map



X



Y



Z

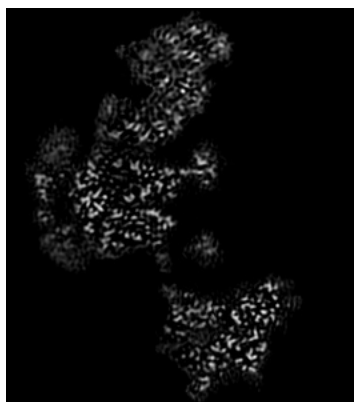
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

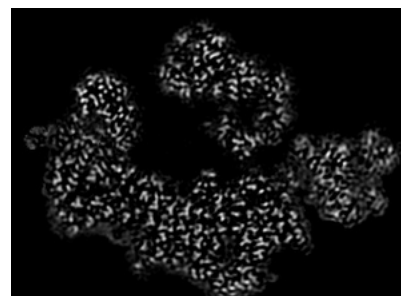
6.2.1 Primary map



X Index: 140



Y Index: 103



Z Index: 123

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: 140



Y Index: 75

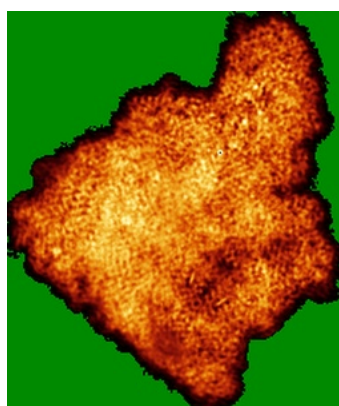


Z Index: 118

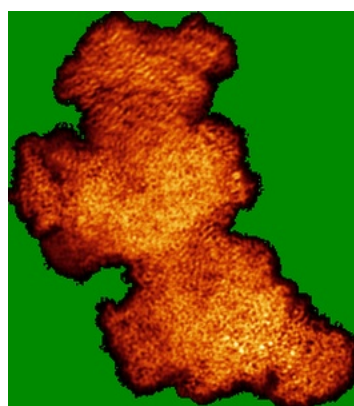
The images above show the largest variance slices of the map in three orthogonal directions.

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

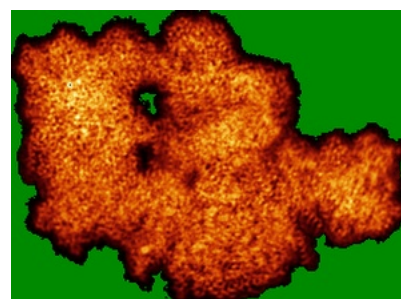
6.4.1 Primary map



X



Y

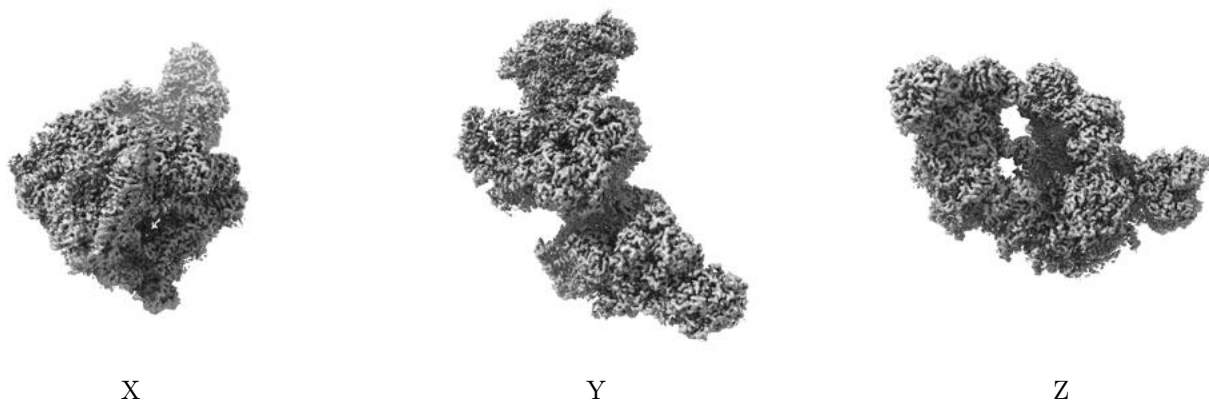


Z

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 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

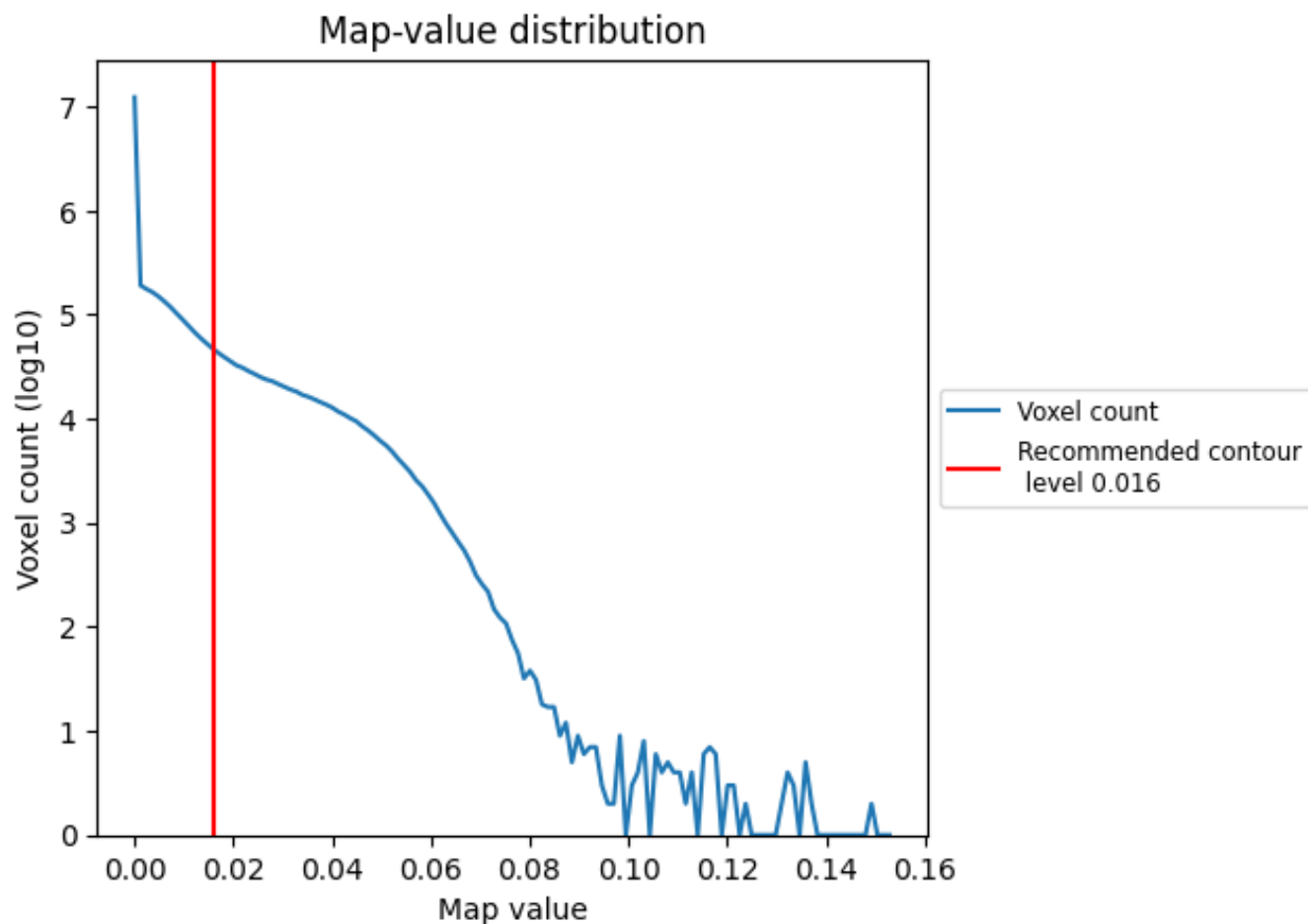
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

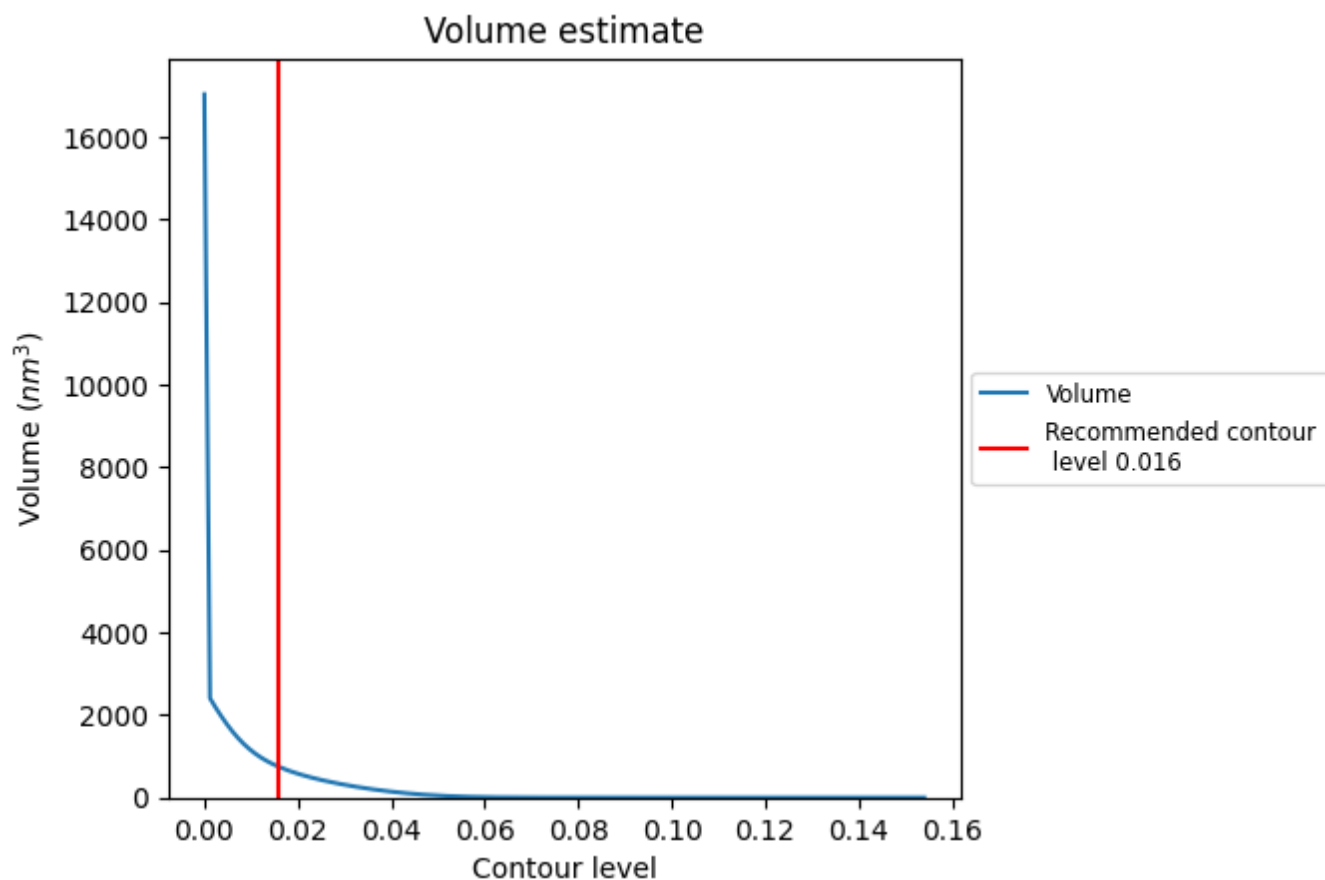
This section contains the results of statistical analysis of the map.

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 743 nm³; this corresponds to an approximate mass of 671 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.

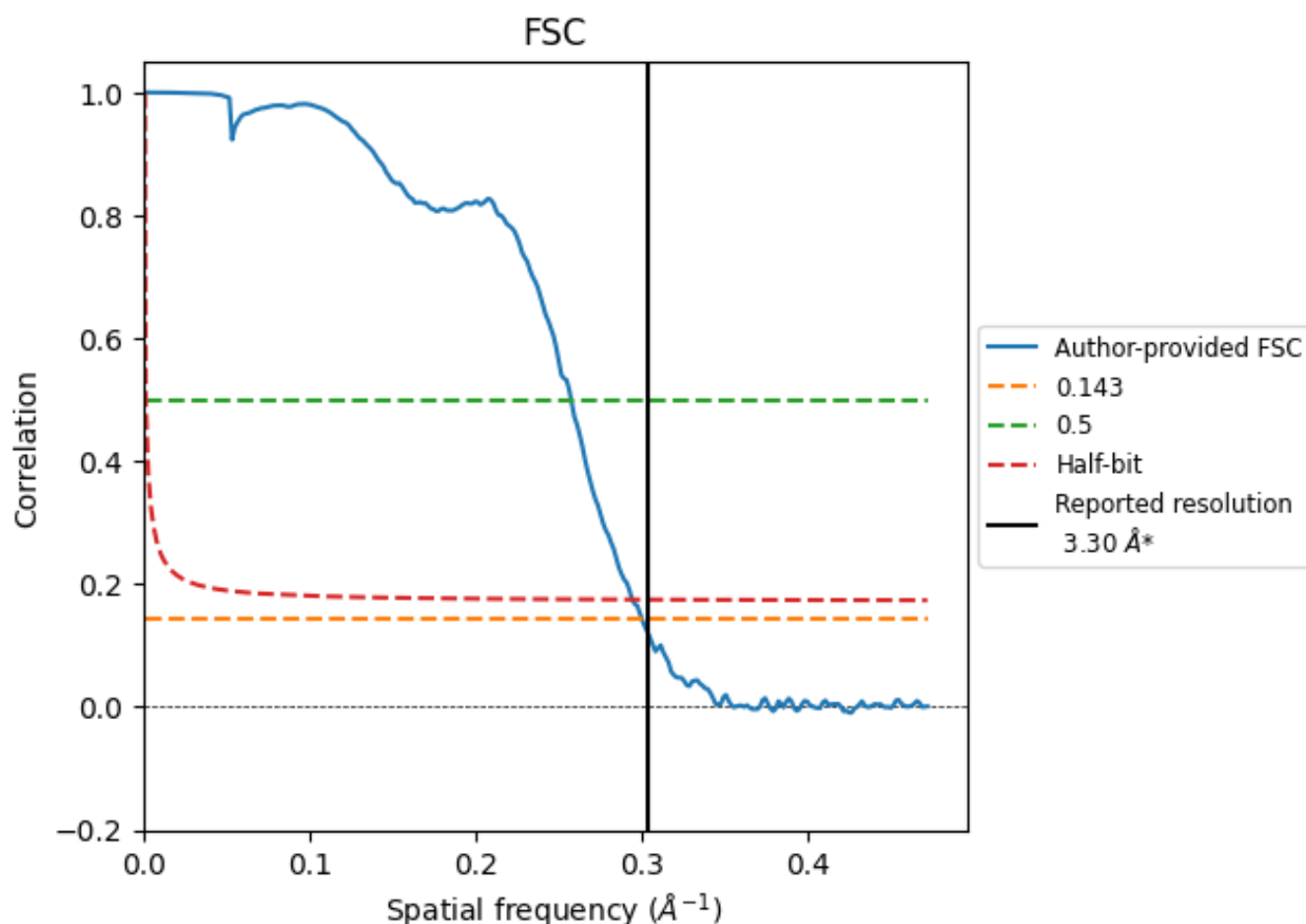
7.3 Rotationally averaged power spectrum [i](#)

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

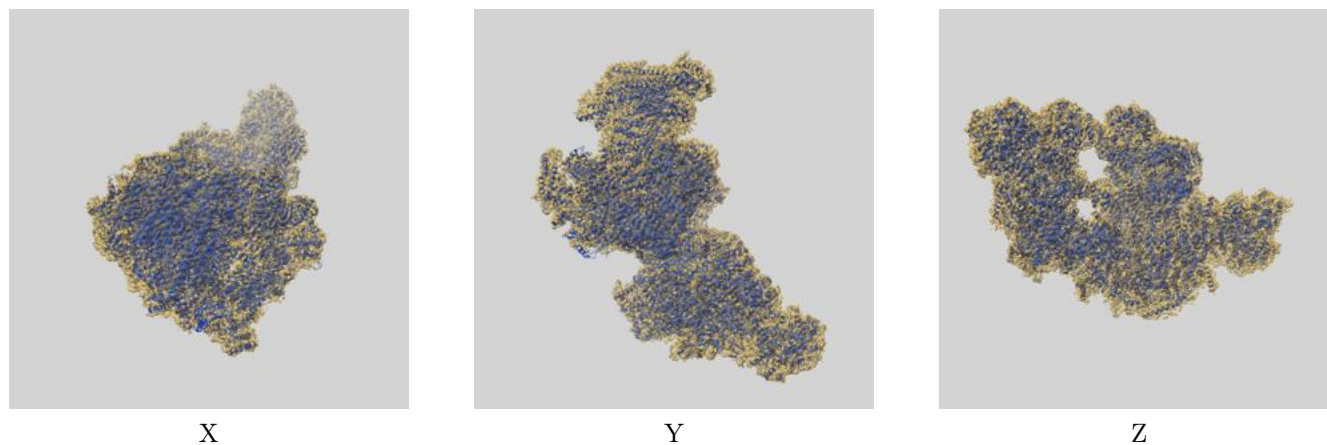
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.89	3.40
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

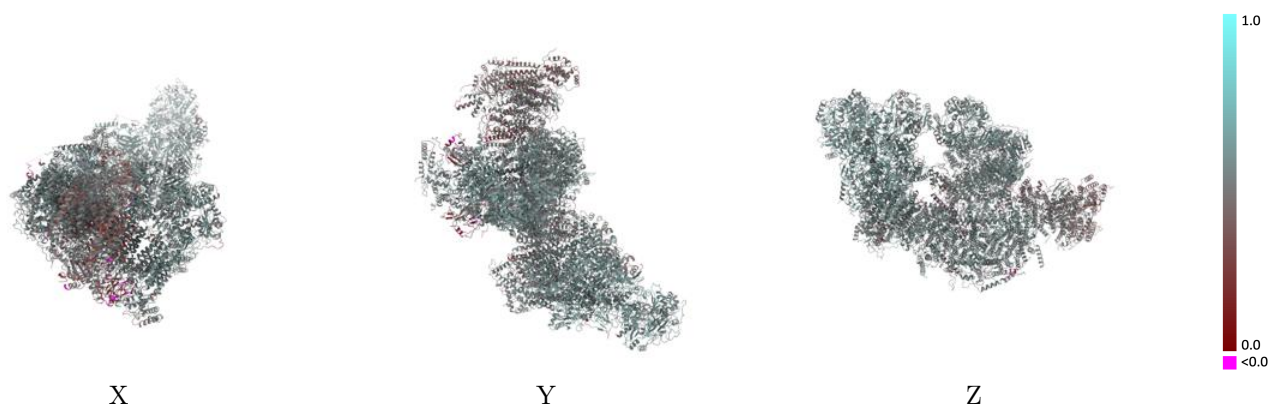
This section contains information regarding the fit between EMDB map EMD-17990 and PDB model 8PW6. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



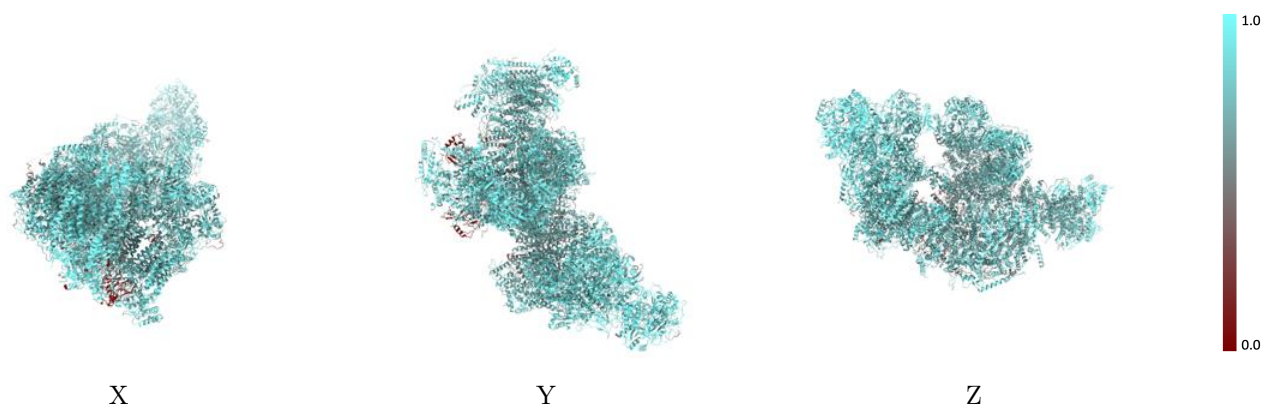
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



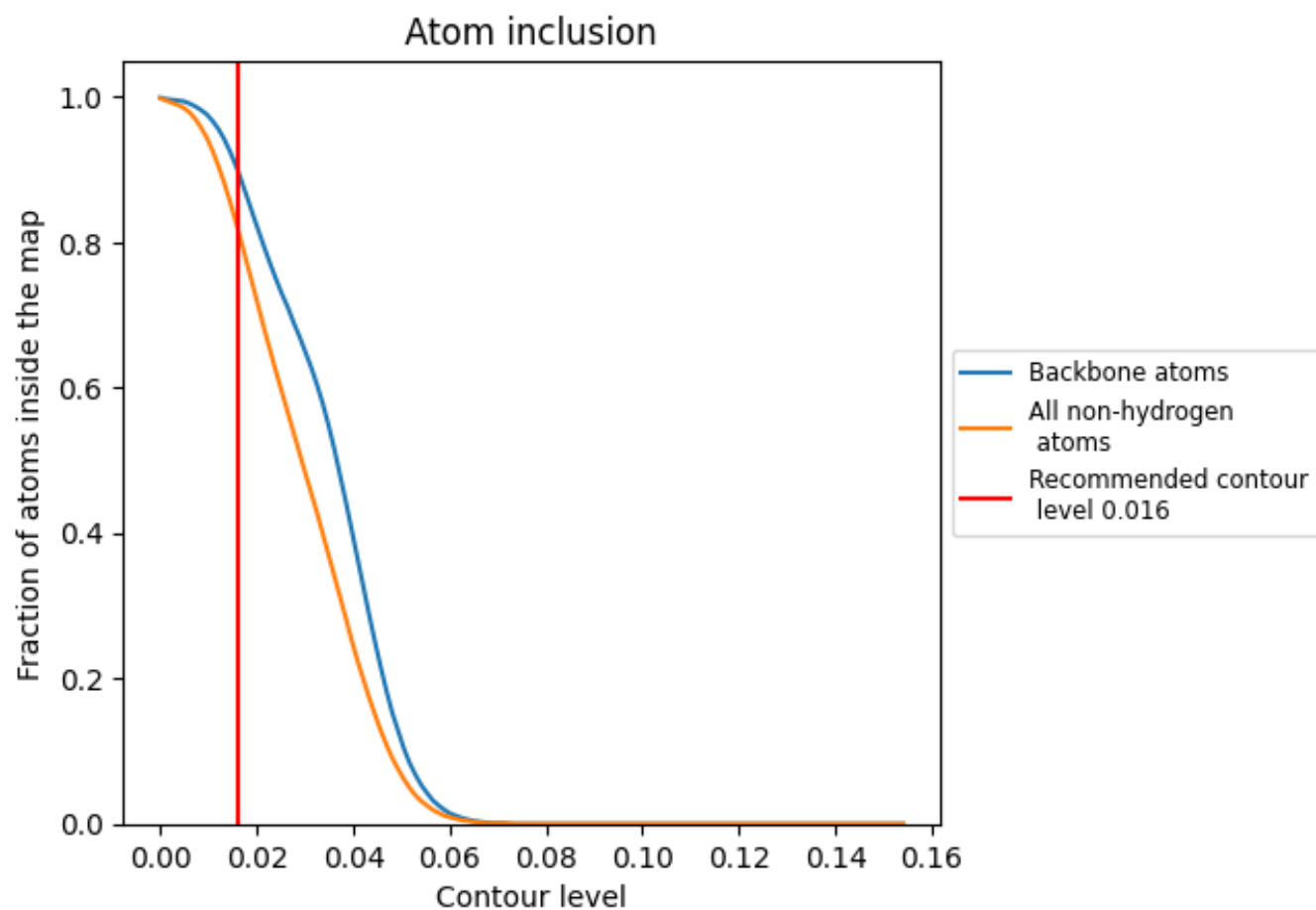
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5140
1	 0.8940	 0.5550
2	 0.8910	 0.5520
3	 0.8740	 0.5540
6	 0.8800	 0.5540
7	 0.8850	 0.5510
9	 0.8770	 0.5580
A	 0.8440	 0.5370
A1	 0.7500	 0.4950
B	 0.8410	 0.5430
C	 0.8390	 0.5430
C1	 0.9190	 0.5920
D	 0.8550	 0.5290
D1	 0.8470	 0.5410
E	 0.5030	 0.3560
F	 0.8360	 0.5430
G	 0.8380	 0.5250
H	 0.8120	 0.4680
H1	 0.7860	 0.5100
J	 0.8090	 0.5140
J1	 0.6690	 0.4550
K	 0.7000	 0.5130
K1	 0.7480	 0.5110
L	 0.8310	 0.5360
L1	 0.8060	 0.5290
M	 0.8470	 0.5380
M1	 0.8120	 0.5330
N	 0.8160	 0.5330
N1	 0.7890	 0.5270
O	 0.8390	 0.5300
O1	 0.8460	 0.5260
P	 0.5000	 0.3510
P1	 0.8440	 0.5460
Q	 0.7940	 0.5400
Q1	 0.8690	 0.5750



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Chain	Atom inclusion	Q-score
R	 0.7370	 0.5110
S	 0.7310	 0.4490
S1	 0.8740	 0.5240
T	 0.6040	 0.4810
T1	 0.7420	 0.4420
U	 0.7930	 0.5190
U1	 0.8370	 0.5320
V	 0.7210	 0.4870
V1	 0.8760	 0.5540
W1	 0.8700	 0.5590
X1	 0.8280	 0.5120
Y1	 0.6850	 0.4810
Z1	 0.8310	 0.5220
a1	 0.8150	 0.5240
b1	 0.8030	 0.5000
c1	 0.7850	 0.5030
d1	 0.7690	 0.5130
e1	 0.8050	 0.5210
f1	 0.7580	 0.5040
g1	 0.7910	 0.5040
h1	 0.8240	 0.5210
i1	 0.7470	 0.4790
j1	 0.7970	 0.4950
k1	 0.8290	 0.5200
l1	 0.8450	 0.5400
m1	 0.7990	 0.5160
n	 0.8410	 0.4480
n1	 0.8520	 0.5310
o	 0.8260	 0.4160
o1	 0.8130	 0.4980
p	 0.8070	 0.4360
p1	 0.8420	 0.5210
q	 0.8700	 0.4170
q1	 0.8950	 0.5660
r	 0.8690	 0.4010
r1	 0.8630	 0.5580
s	 0.8010	 0.4170
s1	 0.8040	 0.5260
t	 0.6650	 0.3130
u	 0.8570	 0.4230
v	 0.8050	 0.3780
w	 0.8160	 0.4630

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Chain	Atom inclusion	Q-score
x	 0.8680	 0.3990
y	 0.8440	 0.4680
z	 0.7320	 0.3760