



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:29 PM UTC

PDB ID : 8PW7 / pdb_00008pw7
EMDB ID : EMD-17991
Title : A respirasome from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-07-19
Resolution : 3.50 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:

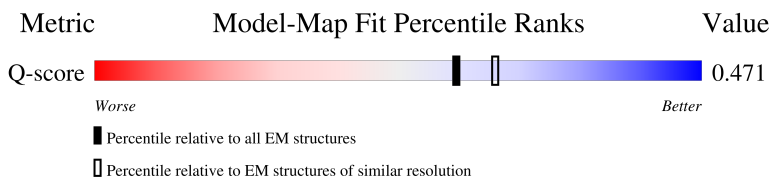
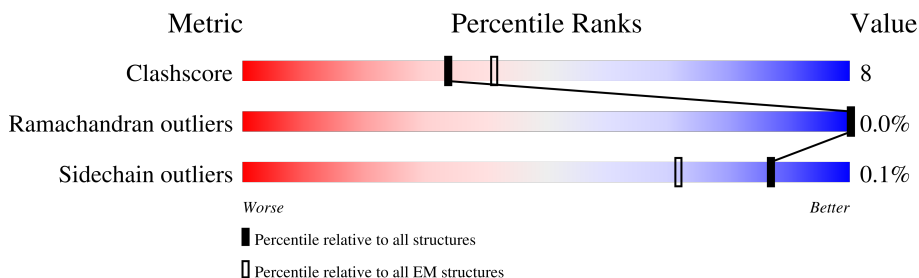
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



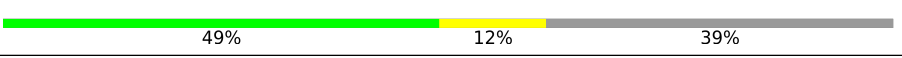
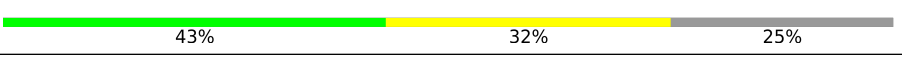
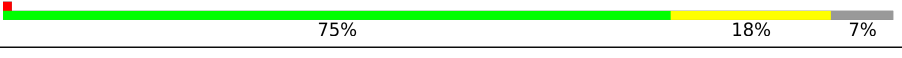
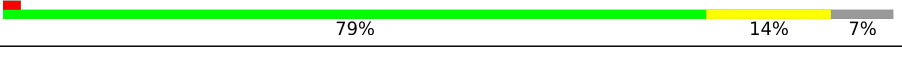
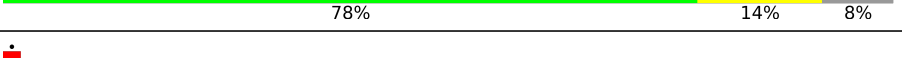
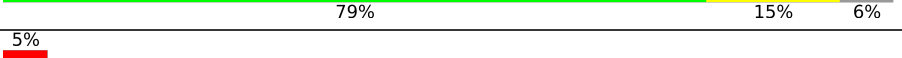
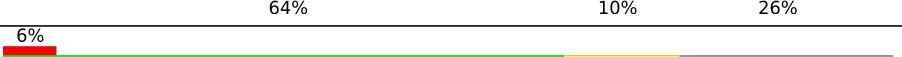
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	n	514	 71% 28%
2	o	227	 68% 32%
3	p	261	 71% 29% 5%
4	q	169	 59% 23% 18%

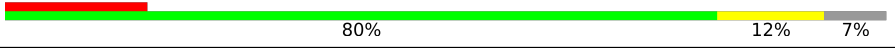
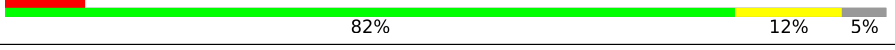
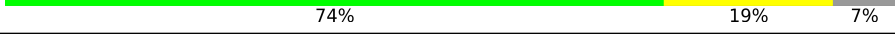
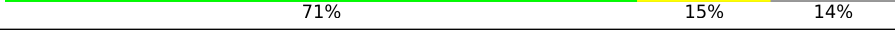
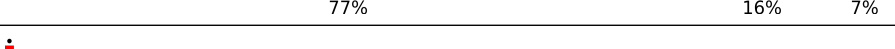
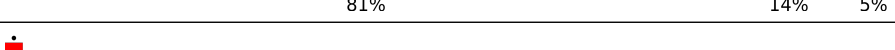
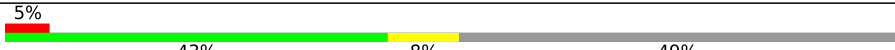
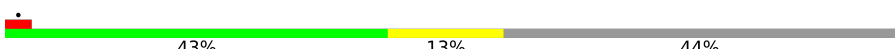
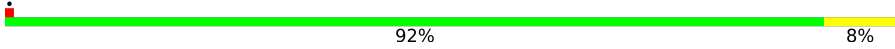
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Mol	Chain	Length	Quality of chain
5	r	146	
6	s	128	
7	t	111	
8	u	86	
9	v	76	
10	x	80	
11	y	63	
12	w	83	
13	A	480	
13	L	480	
14	B	453	
14	M	453	
15	C	381	
15	N	381	
16	D	325	
16	O	325	
17	E	274	
17	P	274	
17	T	274	
18	F	111	
18	Q	111	
19	G	82	
19	R	82	
20	H	89	
20	S	89	

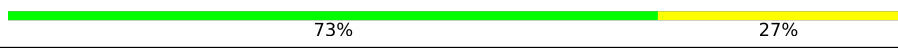
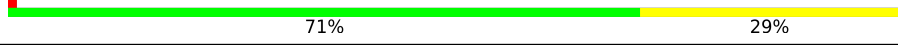
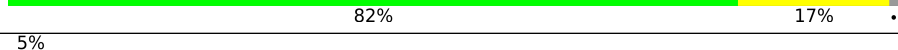
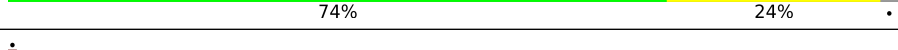
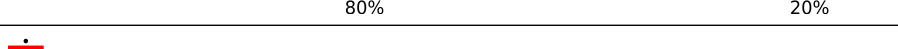
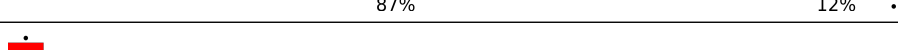
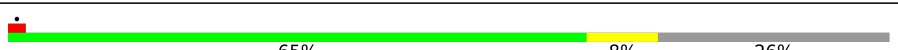
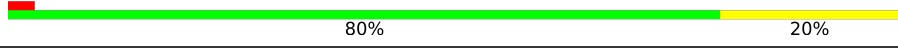
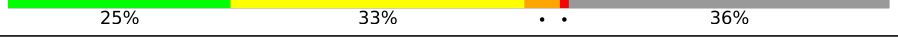
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Mol	Chain	Length	Quality of chain
21	J	64	
21	U	64	
22	K	56	
22	V	56	
23	6	224	
24	C1	263	
25	D1	463	
26	2	248	
27	1	464	
28	3	727	
29	9	212	
30	P1	377	
31	Q1	175	
32	7	116	
33	S1	99	
34	T1	156	
34	U1	156	
35	V1	116	
36	W1	131	
37	q1	145	
38	r1	113	
39	s1	104	
40	A1	115	
41	H1	318	
42	J1	172	

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Mol	Chain	Length	Quality of chain
43	K1	98	
44	L1	607	
45	M1	459	
46	N1	345	
47	O1	355	
48	X1	172	
49	Y1	141	
50	Z1	144	
51	a1	70	
52	b1	84	
53	c1	76	
54	d1	120	
55	e1	106	
56	f1	57	
57	g1	151	
58	h1	189	
59	i1	128	
60	j1	105	
61	k1	104	
62	l1	186	
63	m1	129	
64	n1	179	
65	o1	137	
66	p1	176	
67	z	69	

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 115575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	s	94	Total	C	N	O	S	0	0
			721	449	126	138	8		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

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

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

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

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

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

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

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

- Molecule 14 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

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

- Molecule 15 is a protein called Cytochrome b.

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

- Molecule 16 is a protein called Cytochrome c1, heme protein, mitochondrial.

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

- Molecule 17 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome b-c1 complex subunit 7.

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

- Molecule 19 is a protein called Cytochrome b-c1 complex subunit 8.

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

- Molecule 20 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

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

- Molecule 21 is a protein called Cytochrome b-c1 complex subunit 9.

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

- Molecule 22 is a protein called Cytochrome b-c1 complex subunit 10.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	214	Total	C	N	O	S	0	0
			1660	1056	279	314	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	430	Total	C	N	O	S	0	0
			3321	2092	596	611	22		

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	690	Total	C	N	O	S	0	0
			5305	3326	921	1017	41		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	96	Total	C	N	O	S	0	0
			758	470	141	144	3		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

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

- Molecule 34 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 12.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

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

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

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

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

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 67 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

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

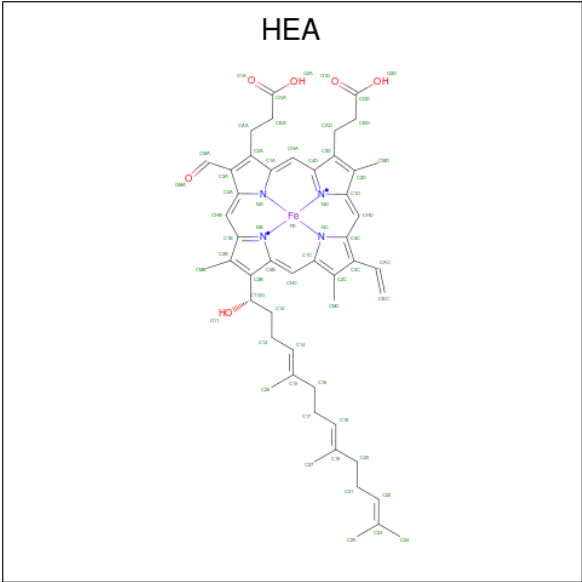
- Molecule 68 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 69 is SODIUM ION (CCD ID: NA) (formula: Na).

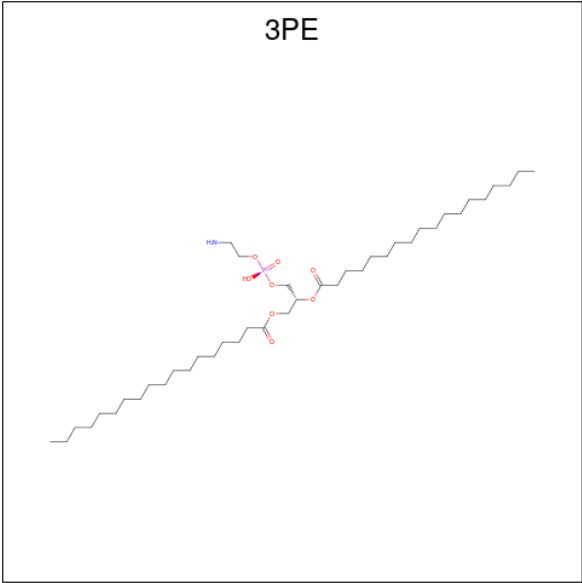
Mol	Chain	Residues	Atoms		AltConf
69	n	1	Total	Na	0
			1	1	

- Molecule 70 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 71 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
71	n	1	Total	C	N	O	P	0
			34	24	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	n	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	n	1	Total	C	N	O	P	0
			27	17	1	8	1	
71	o	1	Total	C	N	O	P	0
			29	19	1	8	1	
71	p	1	Total	C	N	O	P	0
			45	35	1	8	1	
71	t	1	Total	C	N	O	P	0
			25	15	1	8	1	
71	v	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
71	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	C	1	Total	C	N	O	P	0
			31	21	1	8	1	
71	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
71	N	1	Total	C	N	O	P	0
			34	24	1	8	1	
71	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
71	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	R	1	Total	C	N	O	P	0
			30	20	1	8	1	
71	6	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	D1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	r1	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	A1	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	H1	1	Total	C	N	O	P	0
			51	41	1	8	1	

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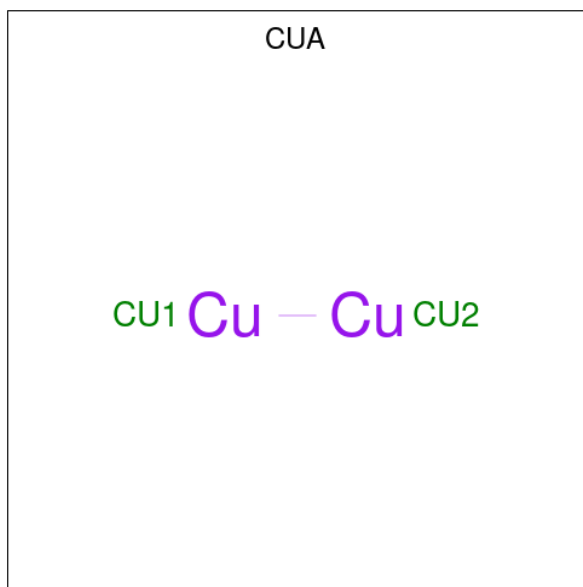
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Mol	Chain	Residues	Atoms					AltConf
71	K1	1	Total	C	N	O	P	0
			41	31	1	8	1	
71	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			51	41	1	8	1	
71	M1	1	Total	C	N	O	P	0
			36	26	1	8	1	
71	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
71	Y1	1	Total	C	N	O	P	0
			28	18	1	8	1	
71	Y1	1	Total	C	N	O	P	0
			42	32	1	8	1	
71	d1	1	Total	C	N	O	P	0
			31	21	1	8	1	
71	d1	1	Total	C	N	O	P	0
			32	22	1	8	1	
71	i1	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 72 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 73 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

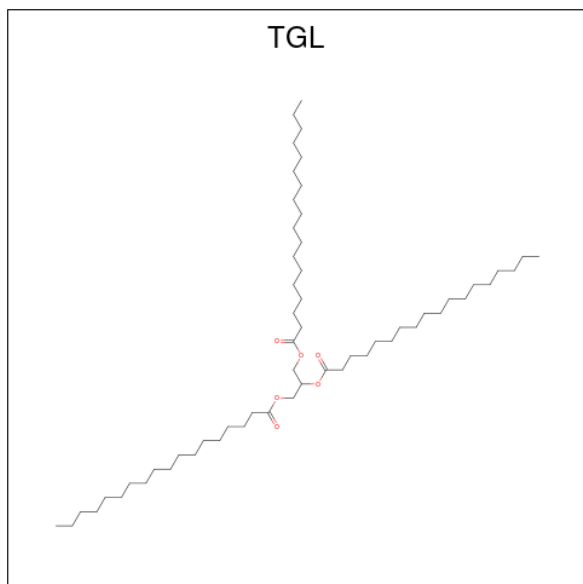


Mol	Chain	Residues	Atoms		AltConf
73	o	1	Total	Cu	0
			2	2	

- Molecule 74 is ZINC ION (CCD ID: ZN) (formula: Zn).

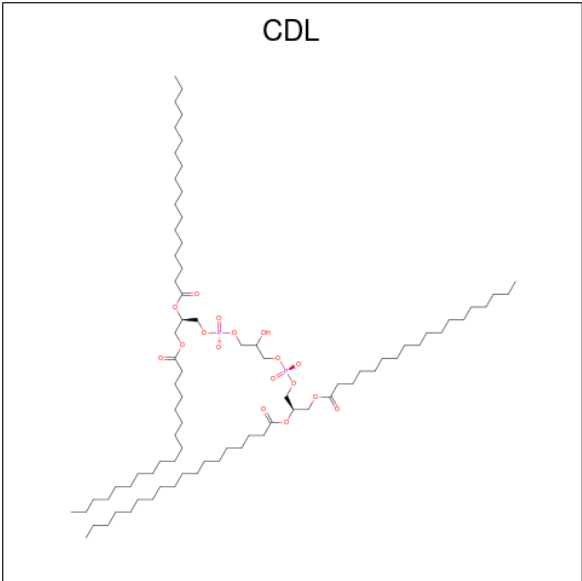
Mol	Chain	Residues	Atoms		AltConf
74	s	1	Total	Zn	0
			1	1	
74	7	1	Total	Zn	0
			1	1	

- Molecule 75 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



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

- Molecule 76 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



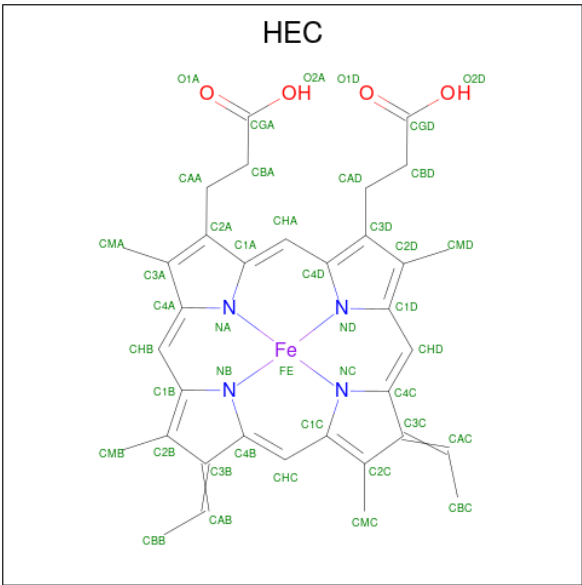
Mol	Chain	Residues	Atoms				AltConf
76	A	1	Total	C	O	P	0
			46	27	17	2	
76	C	1	Total	C	O	P	0
			42	23	17	2	
76	G	1	Total	C	O	P	0
			56	37	17	2	
76	N	1	Total	C	O	P	0
			46	27	17	2	
76	O	1	Total	C	O	P	0
			57	38	17	2	
76	R	1	Total	C	O	P	0
			41	22	17	2	
76	R	1	Total	C	O	P	0
			57	38	17	2	
76	R	1	Total	C	O	P	0
			72	53	17	2	
76	H1	1	Total	C	O	P	0
			51	33	16	2	
76	L1	1	Total	C	O	P	0
			78	59	17	2	
76	L1	1	Total	C	O	P	0
			46	27	17	2	

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Mol	Chain	Residues	Atoms				AltConf
76	N1	1	Total 90	C 71	O 17	P 2	0
76	Y1	1	Total 94	C 75	O 17	P 2	0
76	a1	1	Total 57	C 38	O 17	P 2	0
76	d1	1	Total 67	C 48	O 17	P 2	0
76	h1	1	Total 70	C 51	O 17	P 2	0

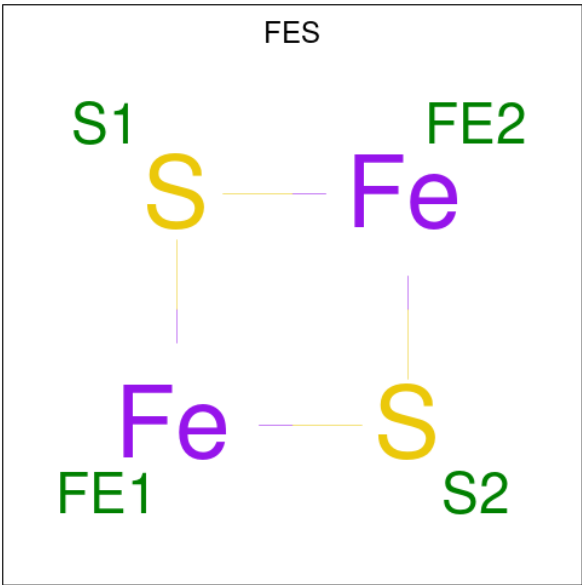
- # HEM

- Molecule 78 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 79 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



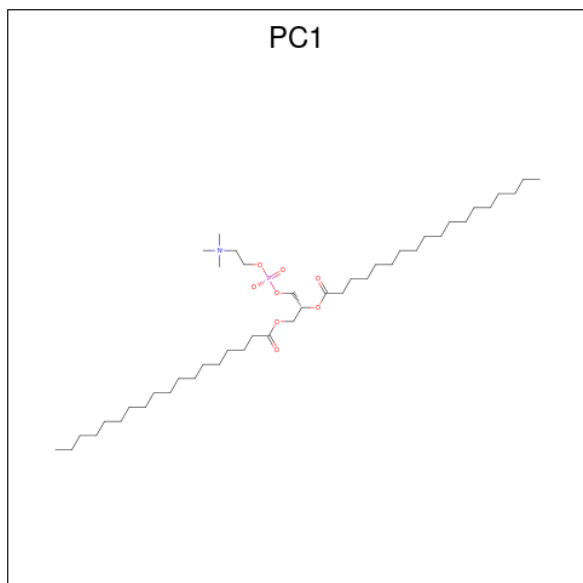
Mol	Chain	Residues	Atoms			AltConf
79	E	1	Total	Fe	S	0
			4	2	2	
79	P	1	Total	Fe	S	0
			4	2	2	

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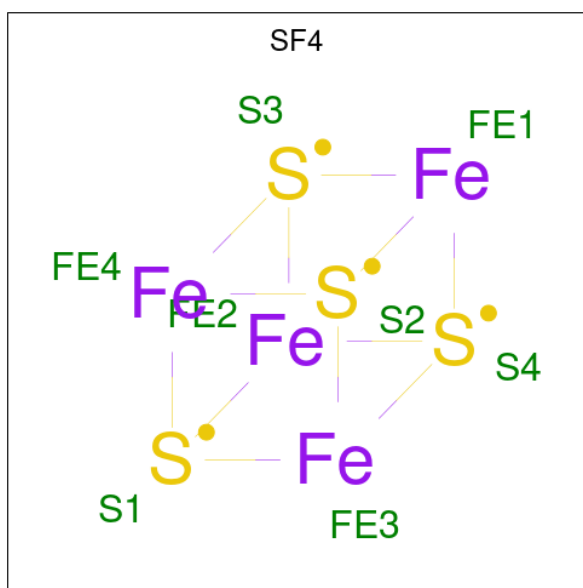
Mol	Chain	Residues	Atoms			AltConf
79	2	1	Total	Fe	S	0
			4	2	2	
79	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 80 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



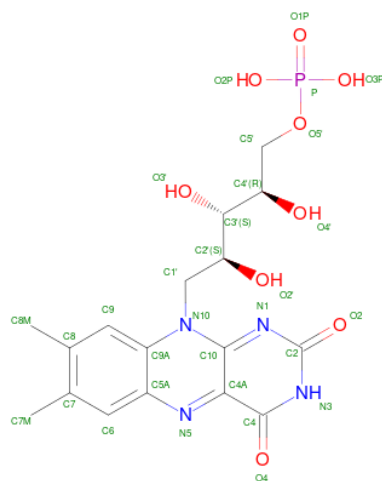
Mol	Chain	Residues	Atoms					AltConf
80	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
80	K	1	Total	C	N	O	P	0
			28	18	1	8	1	
80	L	1	Total	C	N	O	P	0
			24	14	1	8	1	
80	V	1	Total	C	N	O	P	0
			28	18	1	8	1	
80	6	1	Total	C	N	O	P	0
			43	33	1	8	1	
80	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
80	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
80	P1	1	Total	C	N	O	P	0
			31	21	1	8	1	
80	Y1	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 81 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
81	6	1	Total	Fe	S	0
			8	4	4	
81	1	1	Total	Fe	S	0
			8	4	4	
81	3	1	Total	Fe	S	0
			8	4	4	
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: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

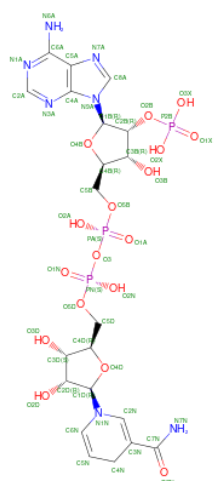


Mol	Chain	Residues	Atoms					AltConf
82	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

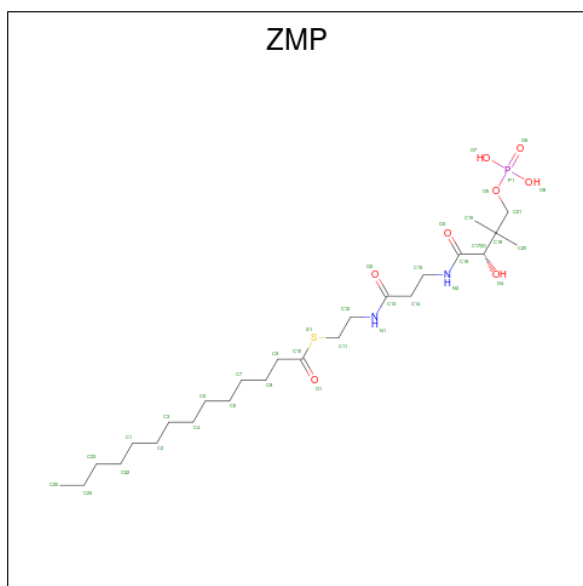
Mol	Chain	Residues	Atoms	AltConf
83	3	1	Total K 1 1	0

- Molecule 84 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



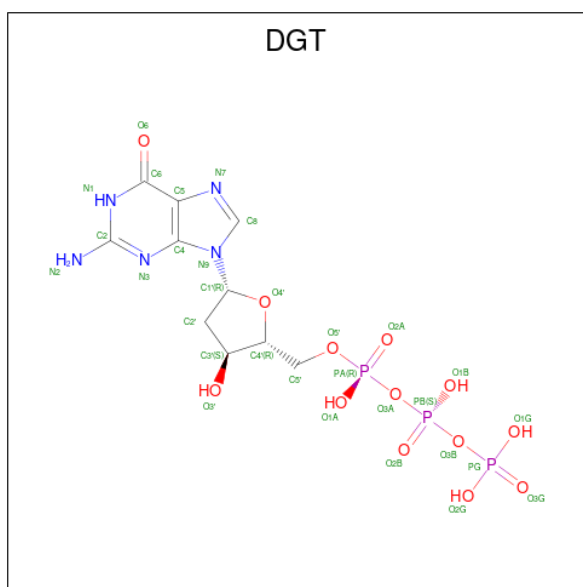
Mol	Chain	Residues	Atoms					AltConf
84	P1	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 85 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



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

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

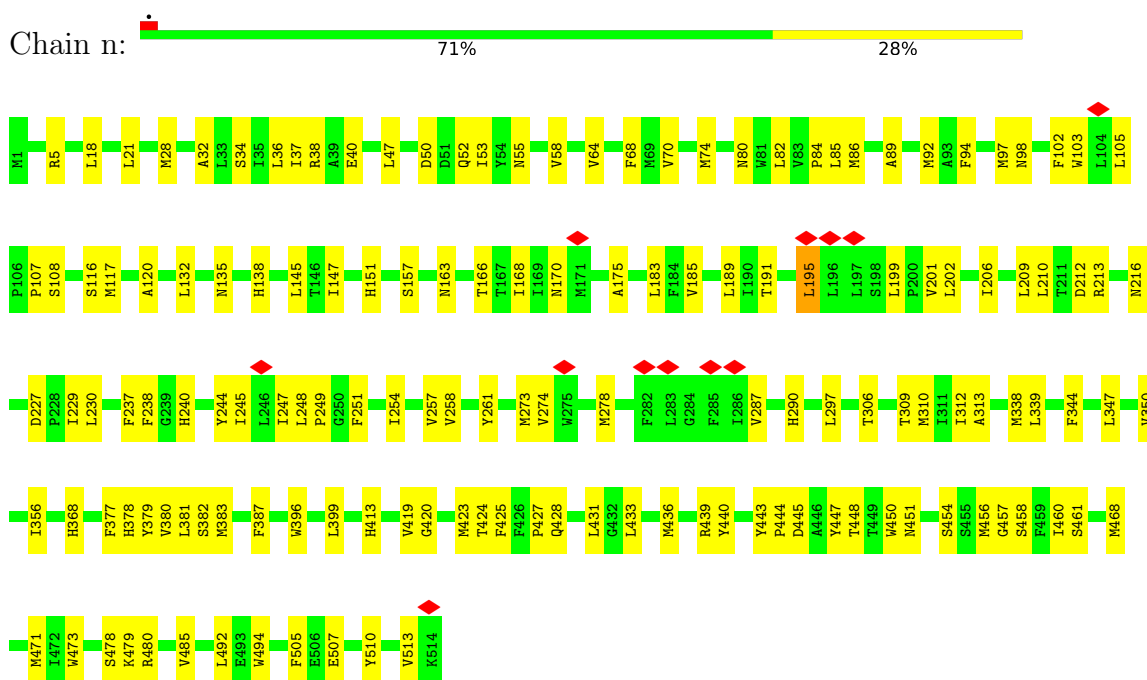


Mol	Chain	Residues	Atoms					AltConf
86	O1	1	Total 31	C 10	N 5	O 13	P 3	0

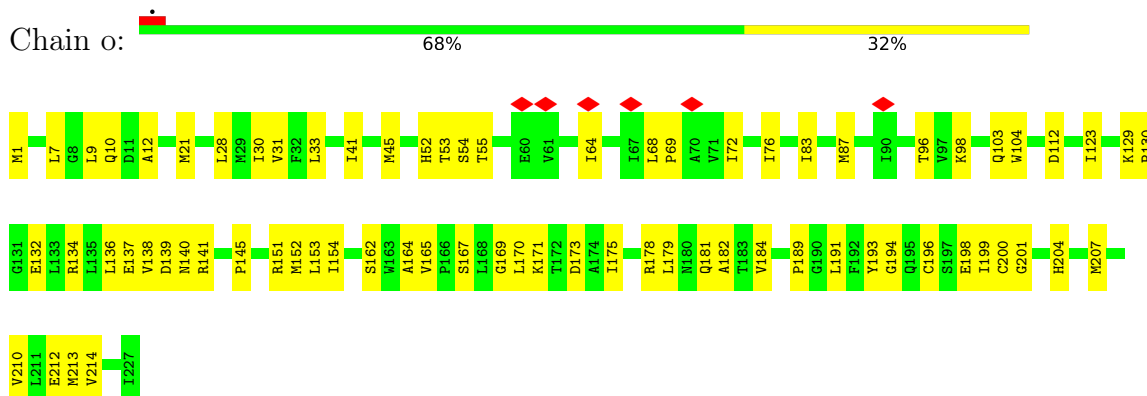
3 Residue-property plots

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

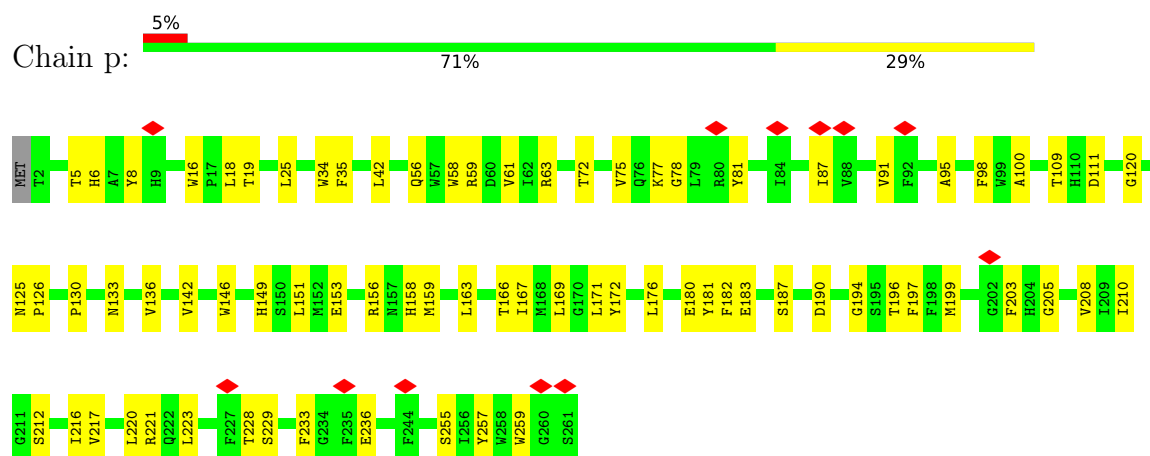
• Molecule 1: Cytochrome c oxidase subunit 1



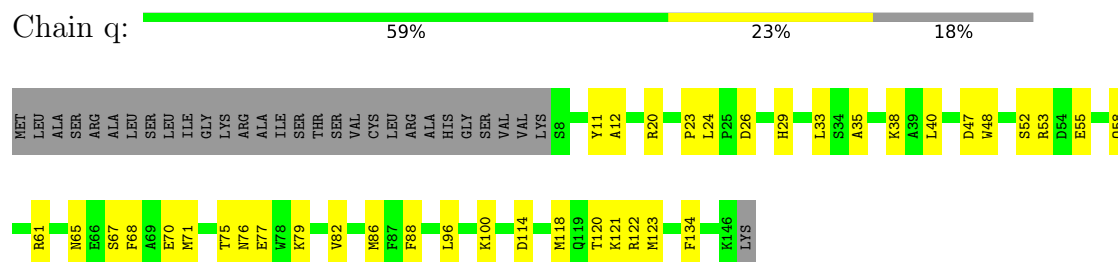
• Molecule 2: Cytochrome c oxidase subunit 2



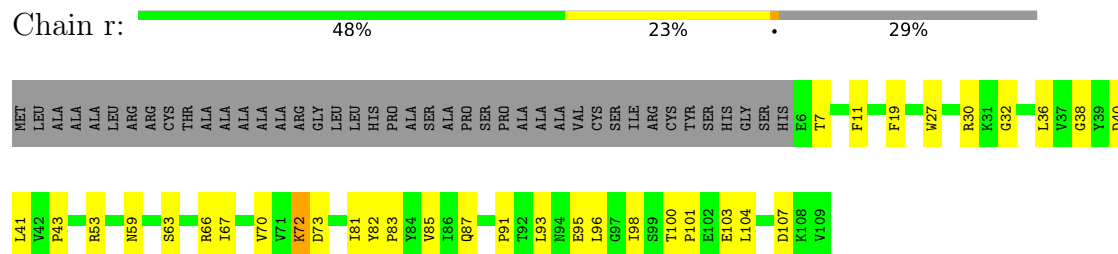
• Molecule 3: Cytochrome c oxidase subunit 3



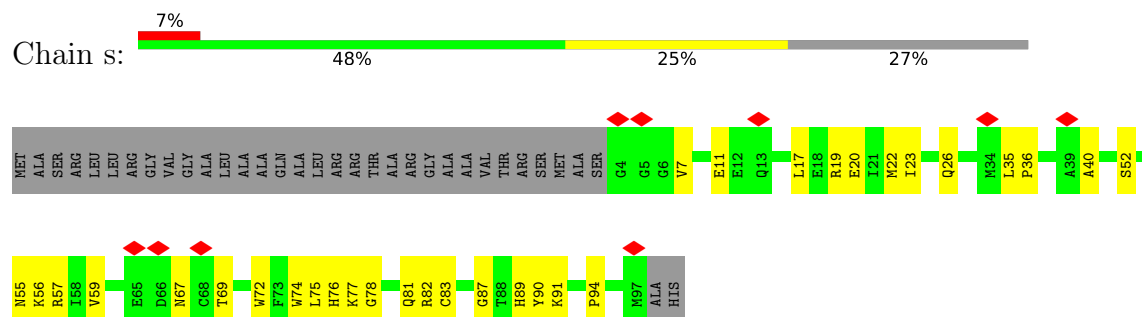
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



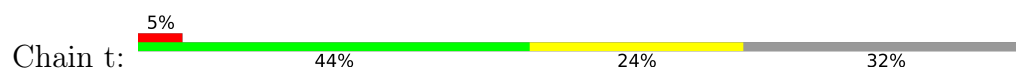
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

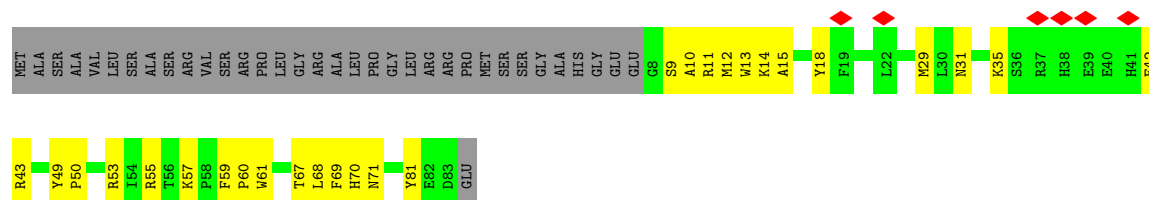


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



- Molecule 7: Cytochrome c oxidase subunit 6A1, mitochondrial





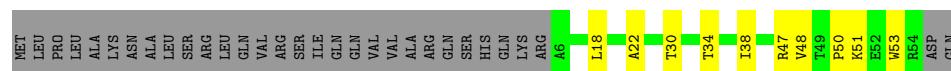
• Molecule 8: Cytochrome c oxidase subunit 6B1



• Molecule 9: Cytochrome c oxidase subunit 6C



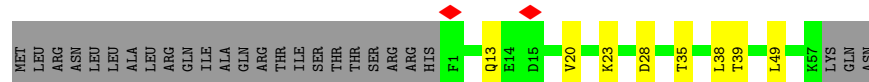
• Molecule 10: Cytochrome c oxidase subunit 7B, mitochondrial



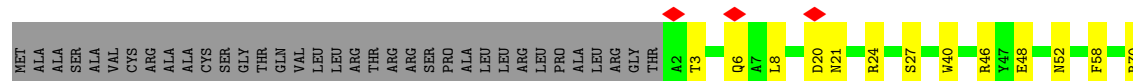
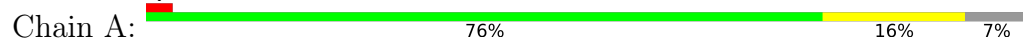
• Molecule 11: Cytochrome c oxidase subunit 7C, mitochondrial

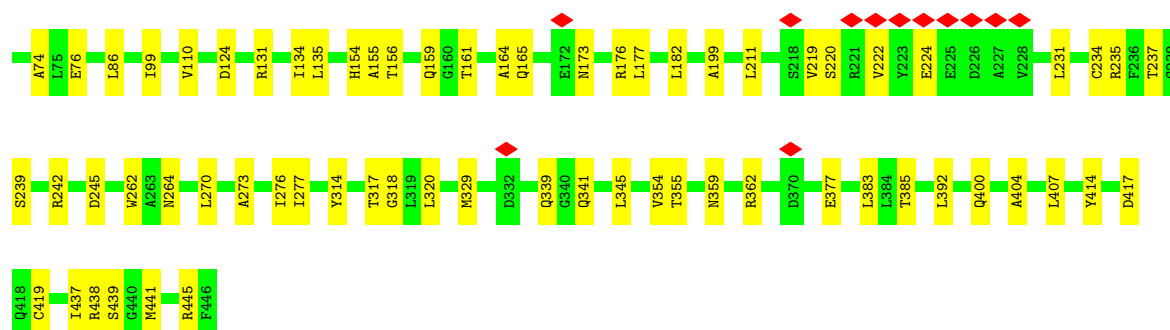


• Molecule 12: Cytochrome c oxidase subunit 7A2, mitochondrial



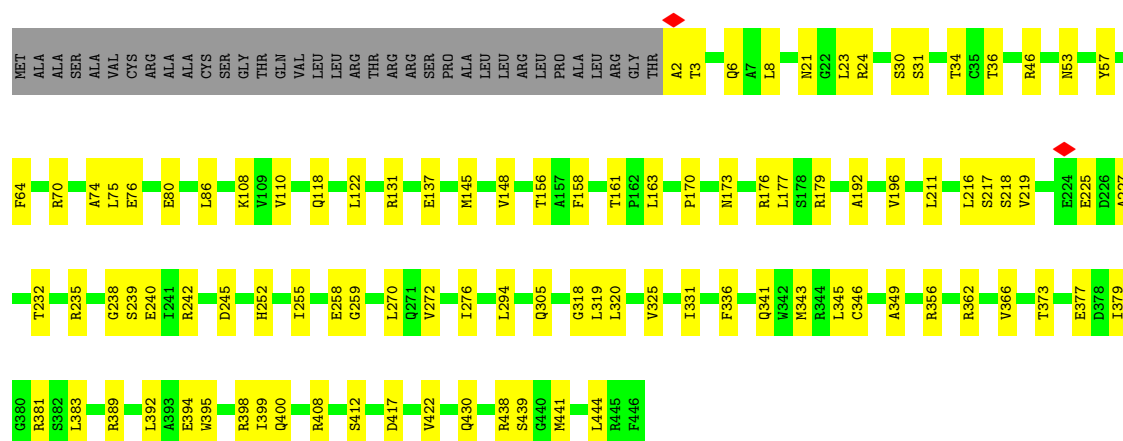
• Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial





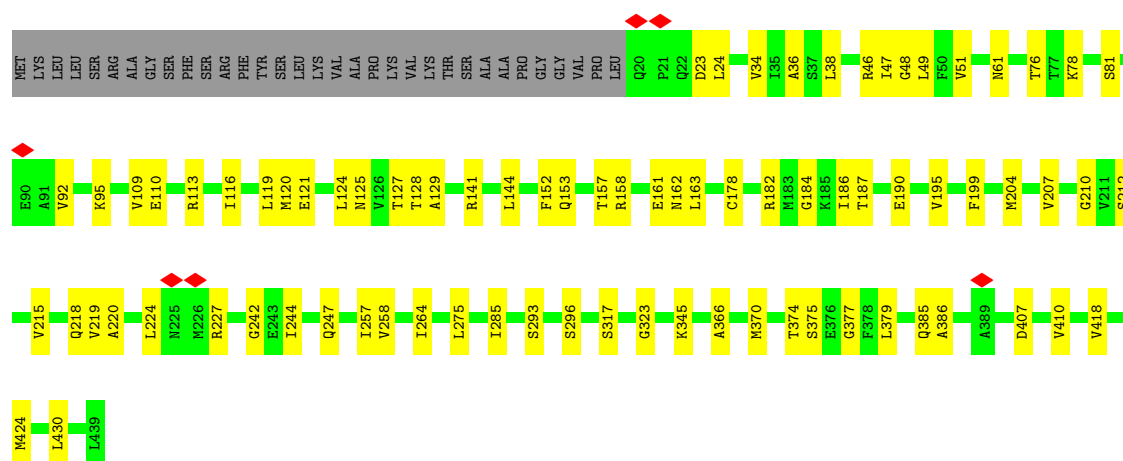
- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L: 72% 20% 7%



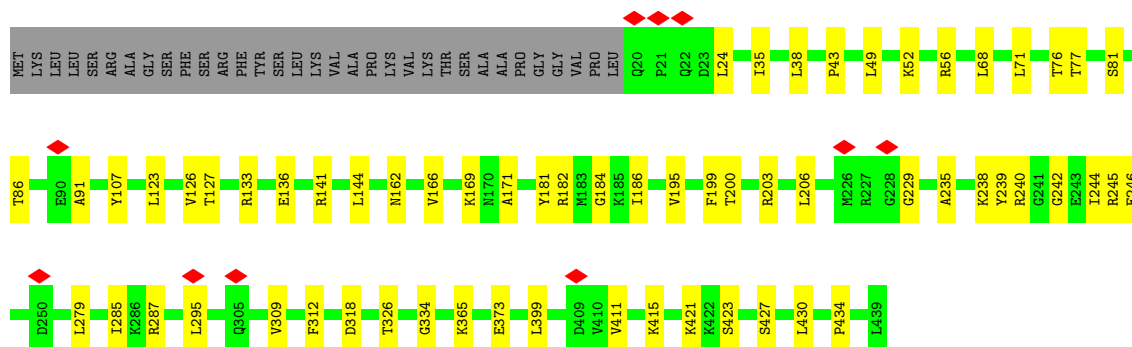
- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 75% 18% 7%



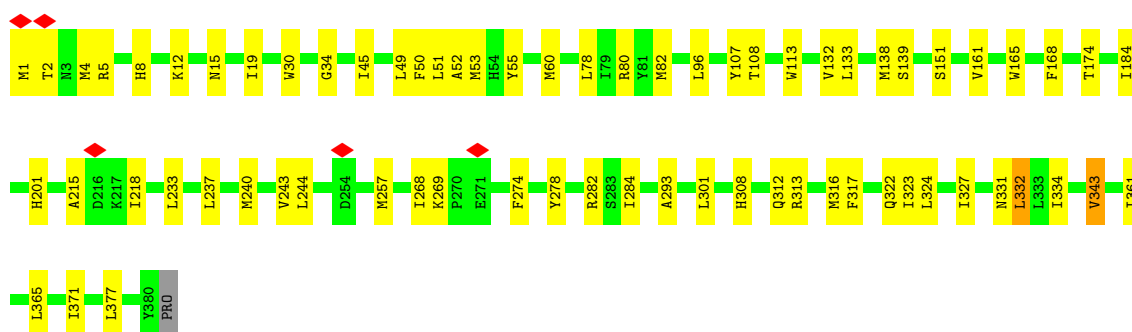
- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 79% 14% 7%



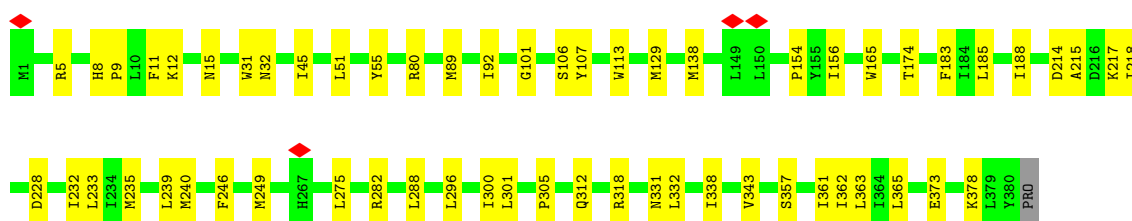
• Molecule 15: Cytochrome b

Chain C: 82% 18%



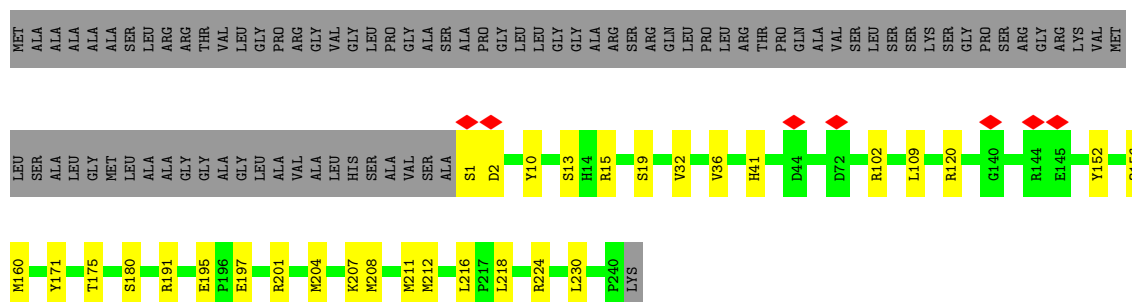
• Molecule 15: Cytochrome b

Chain N: 84% 15%

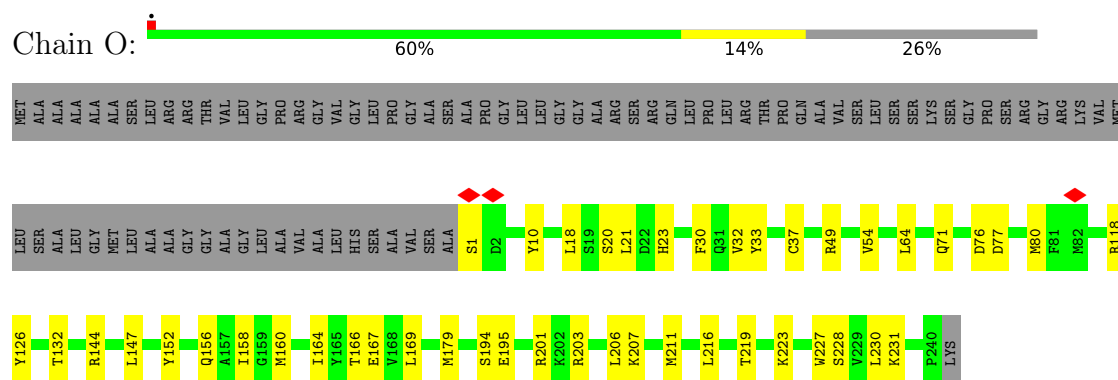


• Molecule 16: Cytochrome c1, heme protein, mitochondrial

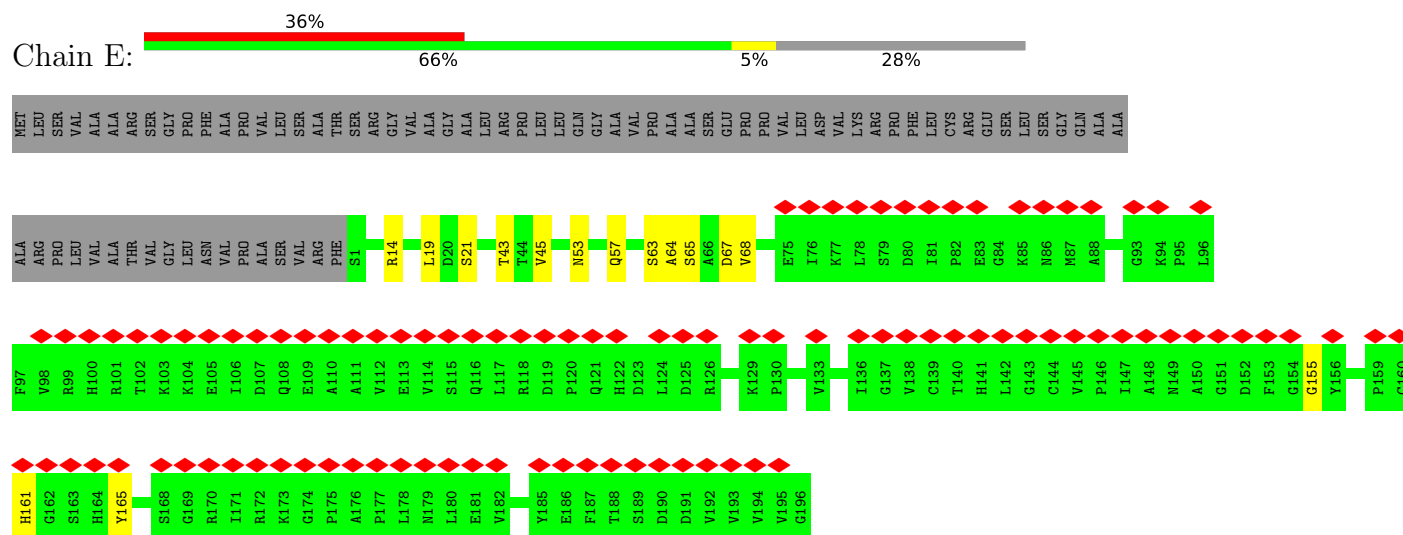
Chain D: 64% 10% 26%



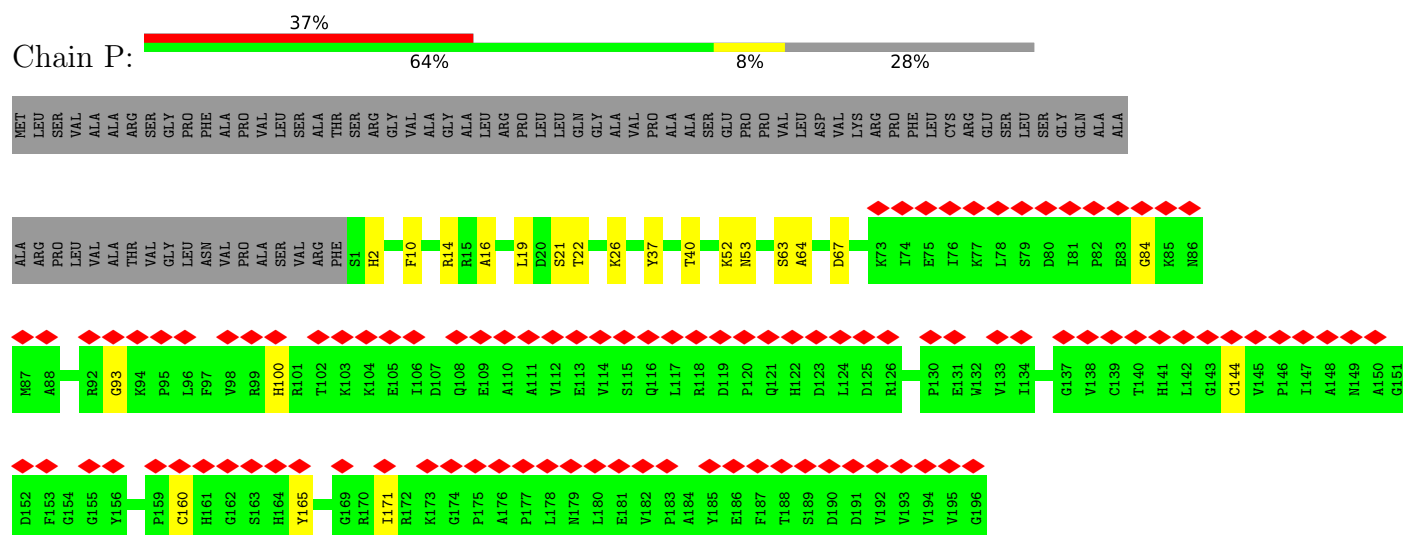
• Molecule 16: Cytochrome c1, heme protein, mitochondrial



• Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial

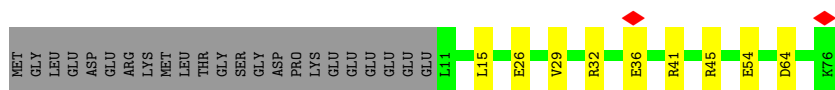


• Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial

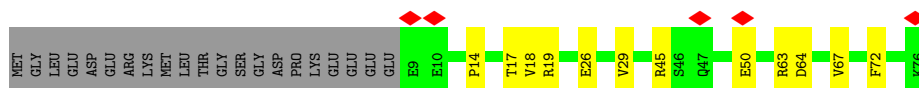


• Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial

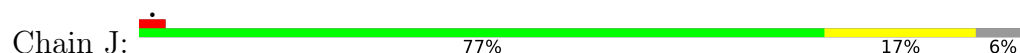




- Molecule 20: Cytochrome b-c1 complex subunit 6, mitochondrial



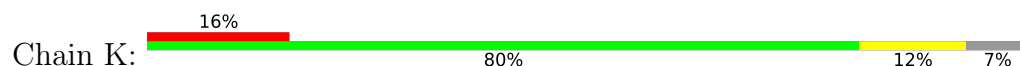
- Molecule 21: Cytochrome b-c1 complex subunit 9



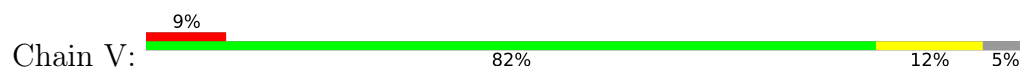
- Molecule 21: Cytochrome b-c1 complex subunit 9



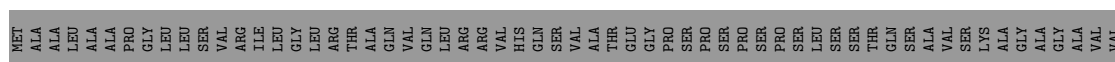
- Molecule 22: Cytochrome b-c1 complex subunit 10

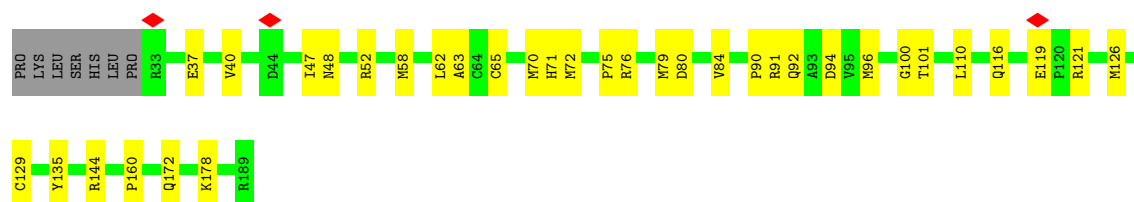


- Molecule 22: Cytochrome b-c1 complex subunit 10



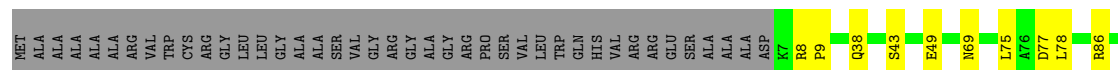
- Molecule 23: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





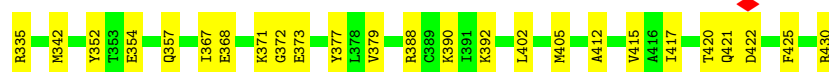
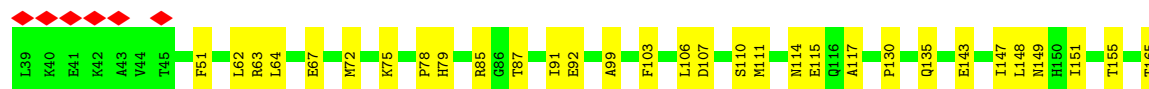
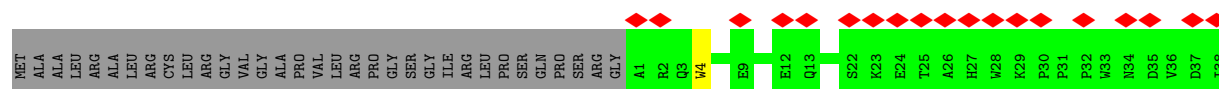
- Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C1: 67% 12% 21%



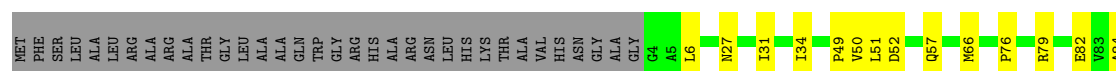
- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D1: 6% 74% 19% 7%



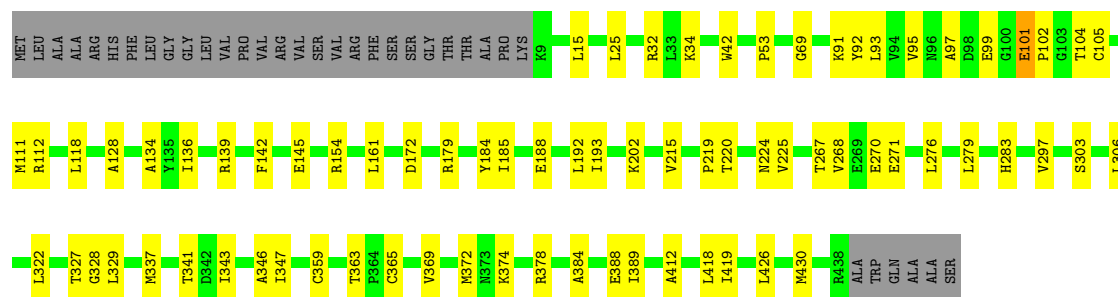
- Molecule 26: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2: 71% 15% 14%

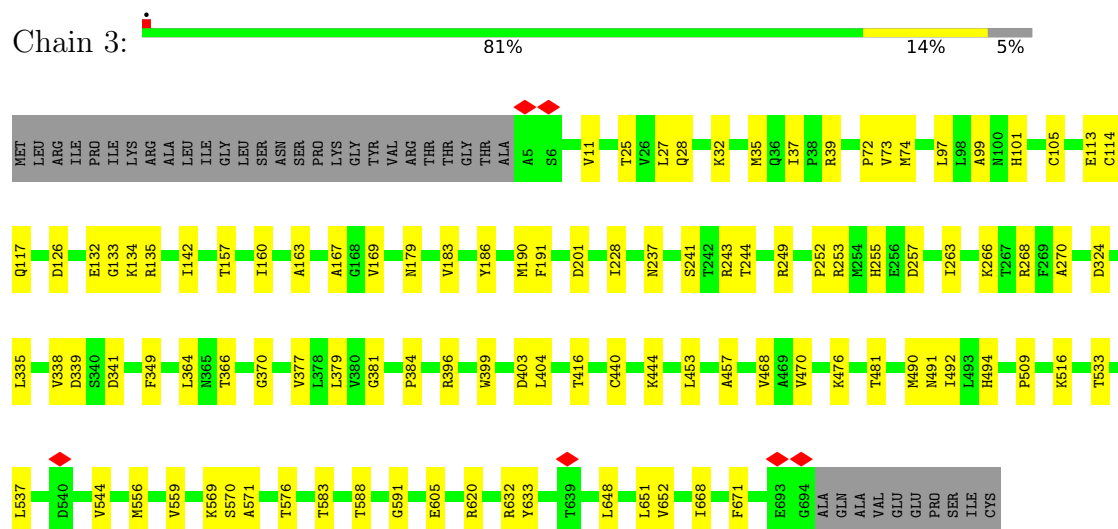


- Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

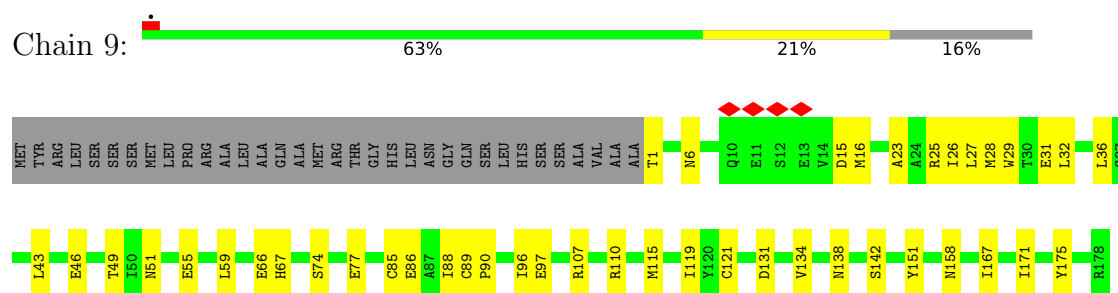
Chain 1: 77% 16% 7%



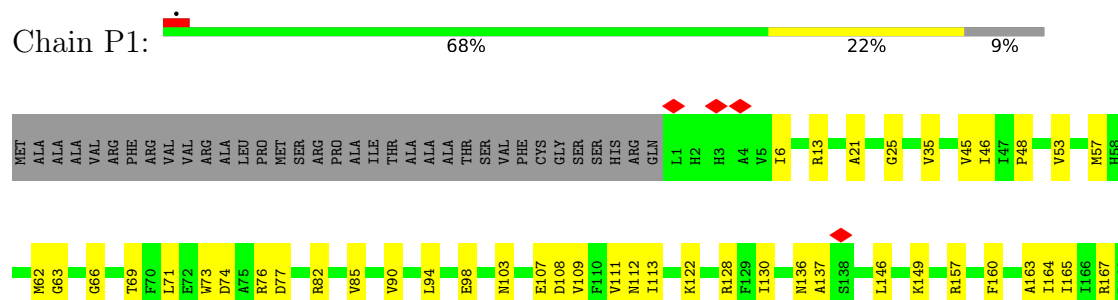
- Molecule 28: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

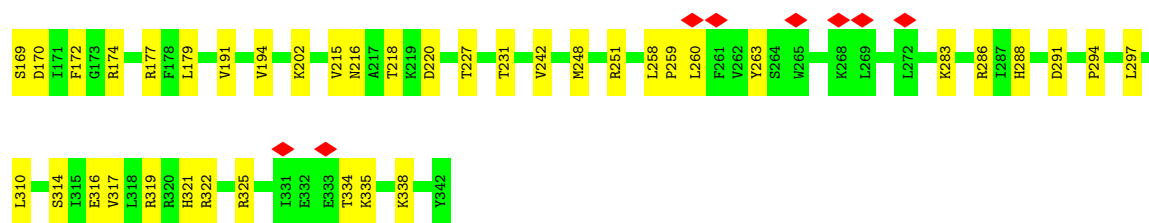


- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

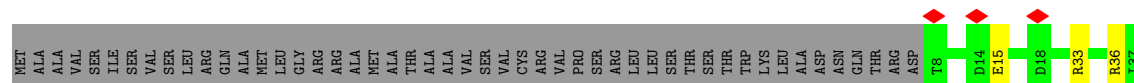


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial





- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



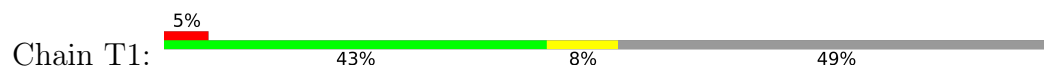
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

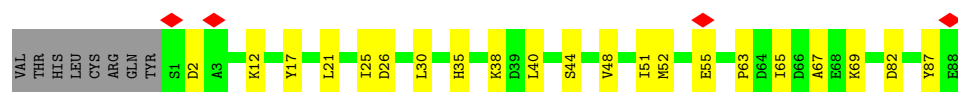


- Molecule 34: Acyl carrier protein, mitochondrial

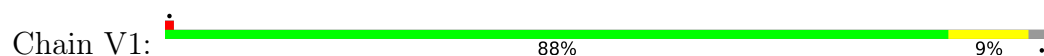


- Molecule 34: Acyl carrier protein, mitochondrial

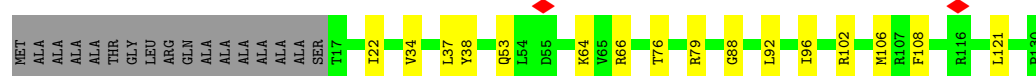
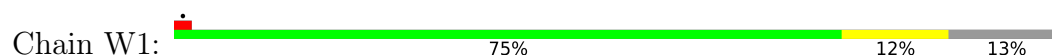




- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



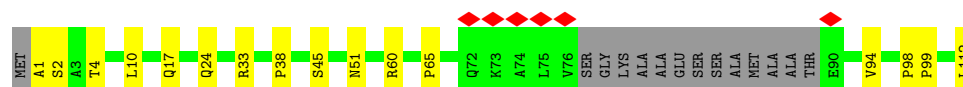
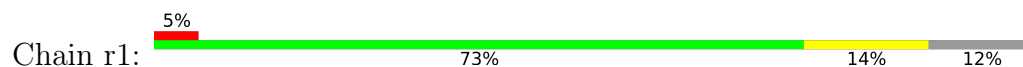
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



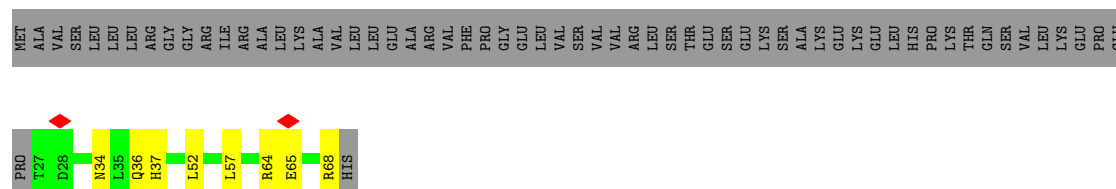
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



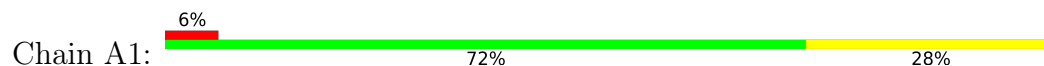
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

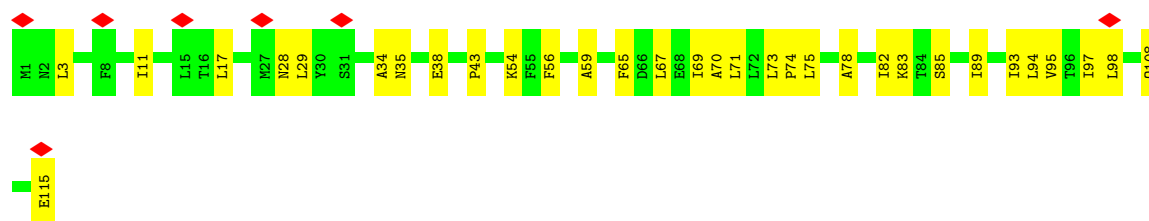


- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

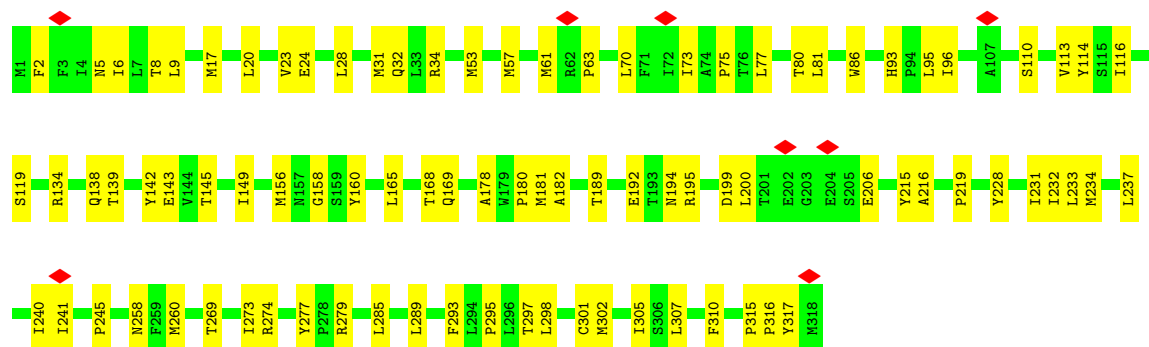
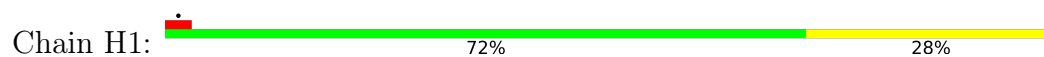


- Molecule 40: NADH-ubiquinone oxidoreductase chain 3

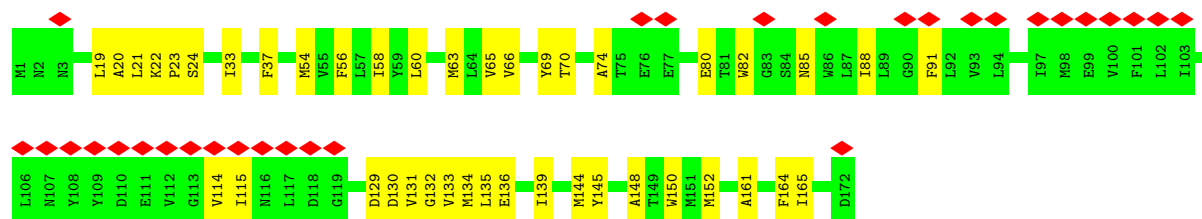
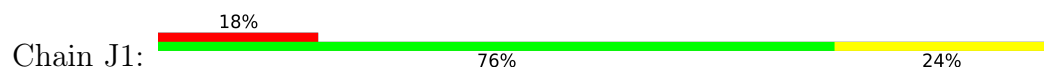




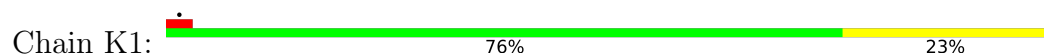
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



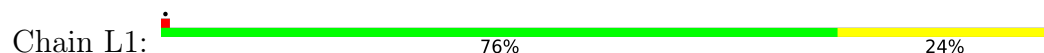
- Molecule 42: NADH-ubiquinone oxidoreductase chain 6

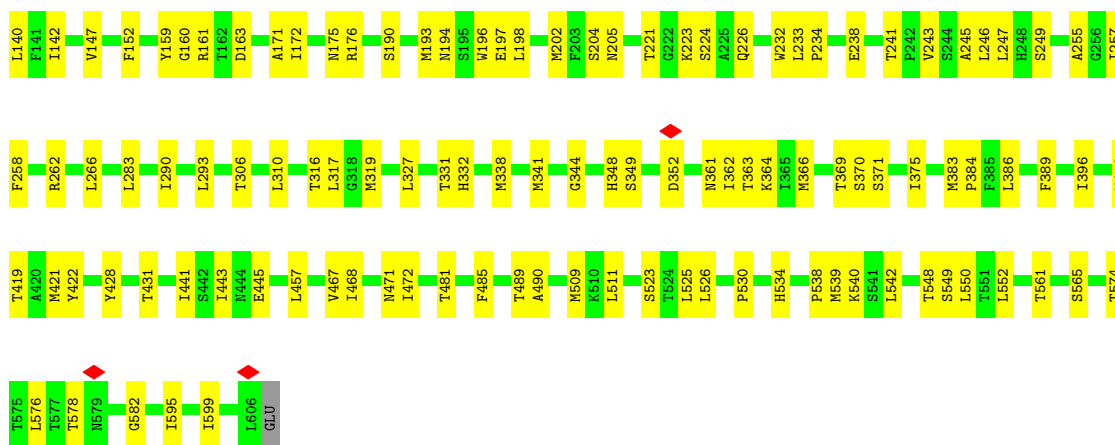


- Molecule 43: NADH-ubiquinone oxidoreductase chain 4L



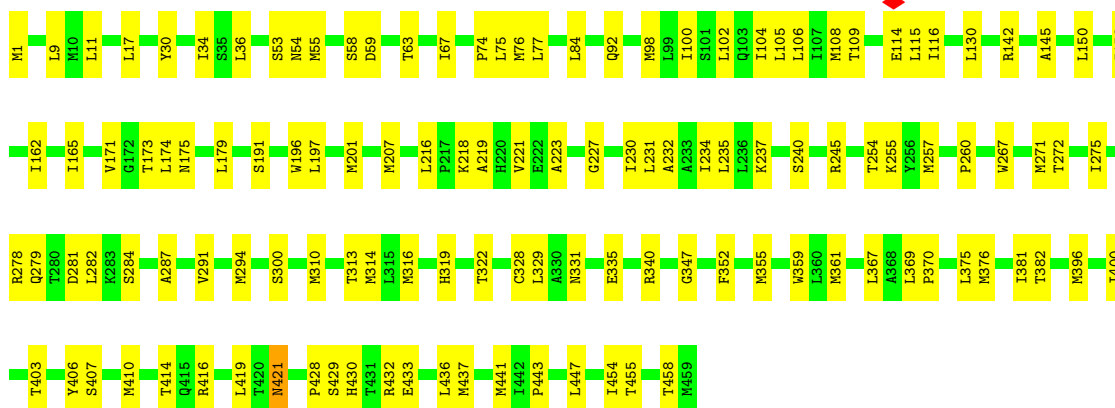
- Molecule 44: NADH-ubiquinone oxidoreductase chain 5





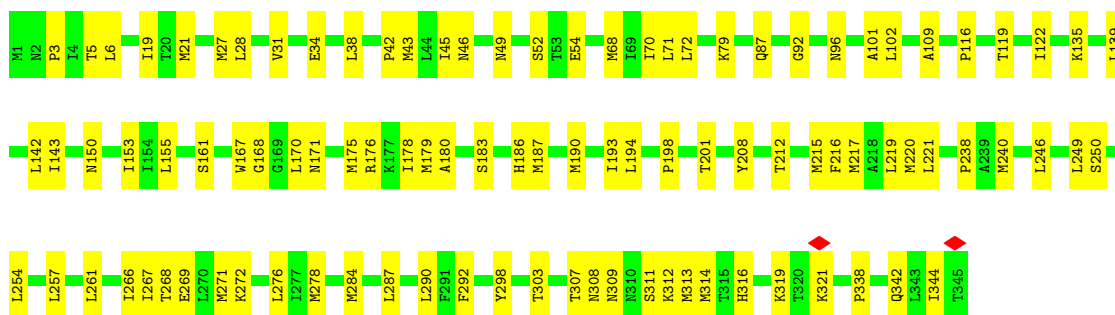
• Molecule 45: NADH-ubiquinone oxidoreductase chain 4

Chain M1: 73% 27%



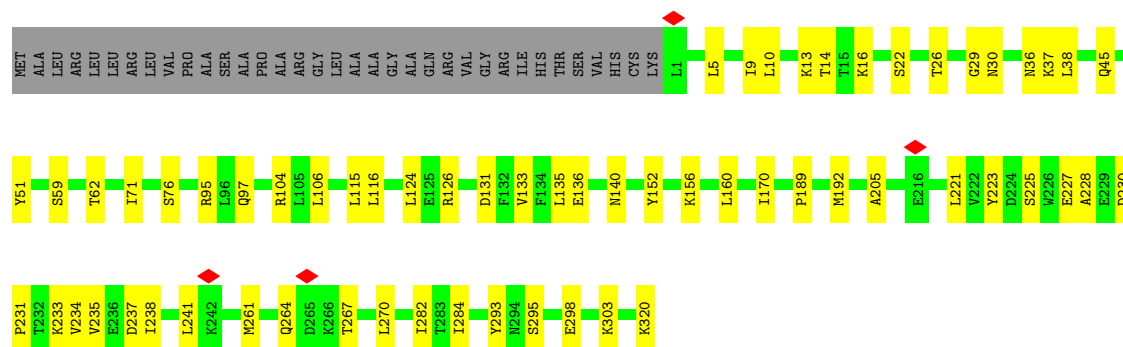
• Molecule 46: NADH-ubiquinone oxidoreductase chain 2

Chain N1: 71% 29%

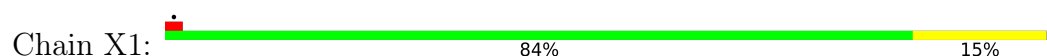


• Molecule 47: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

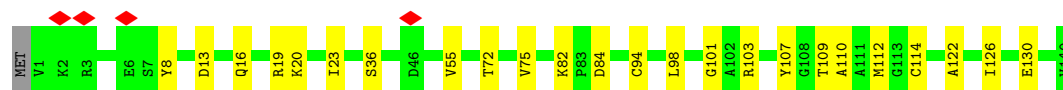
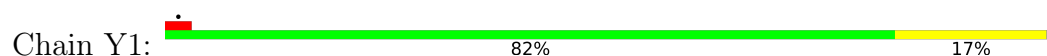
Chain O1: 72% 18% 10%



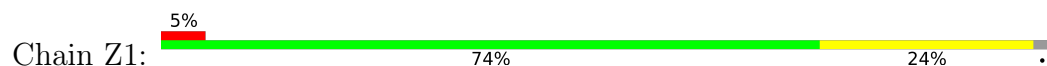
- Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

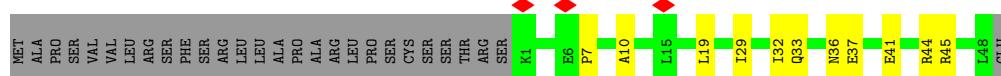


- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

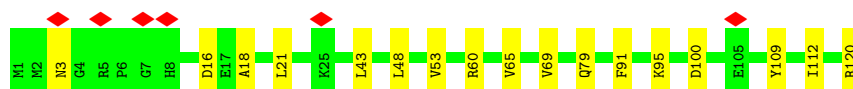
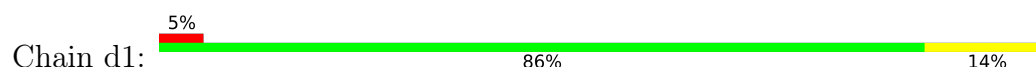




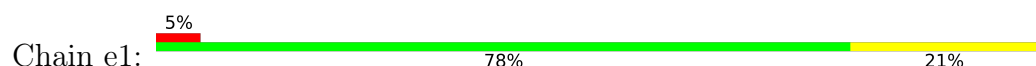
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



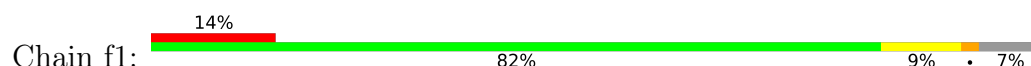
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C2



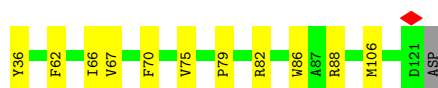
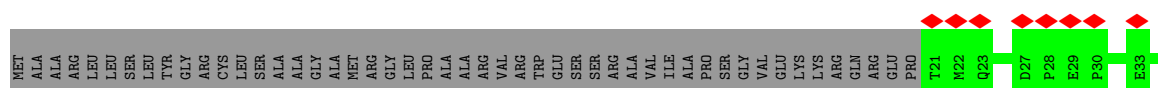
- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 56: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

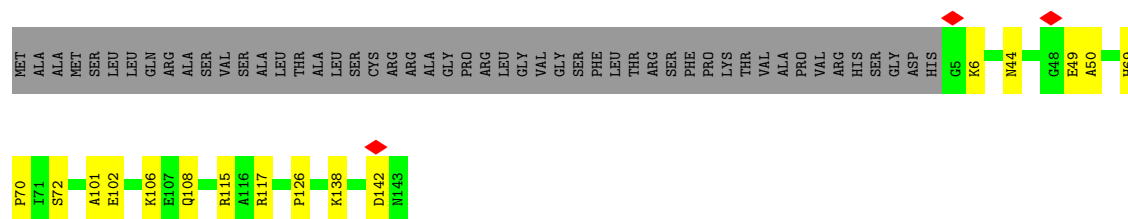


- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

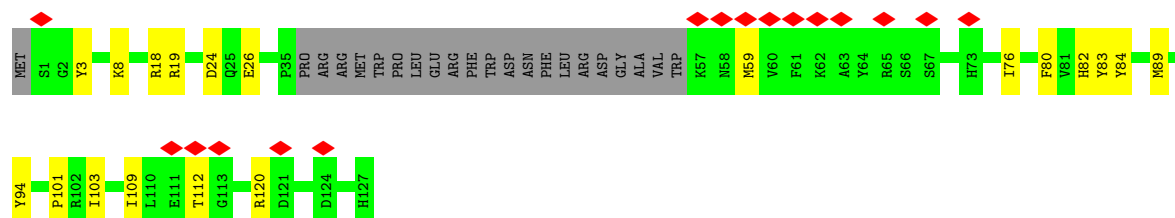


- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

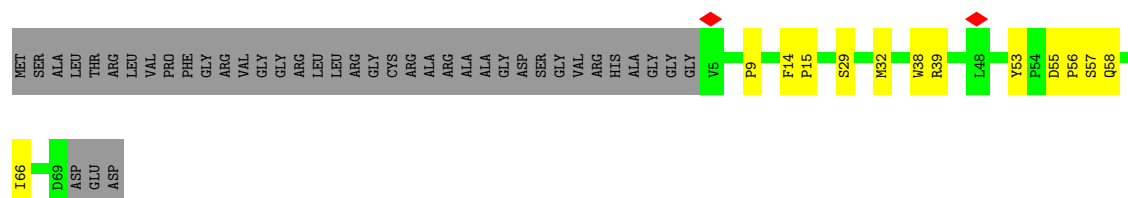




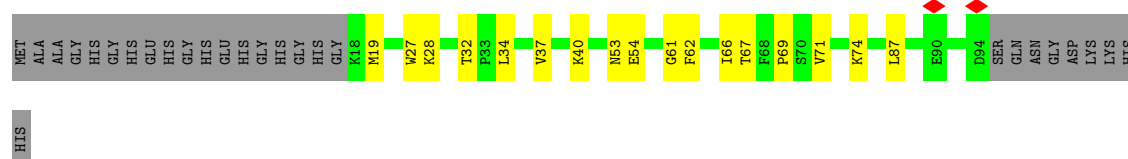
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



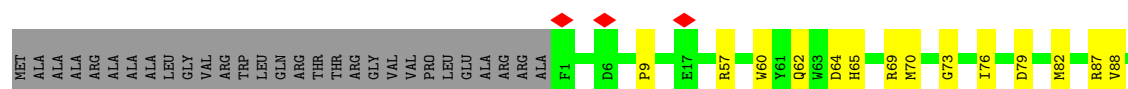
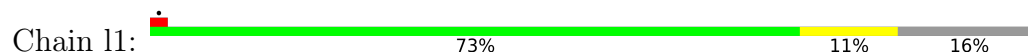
- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

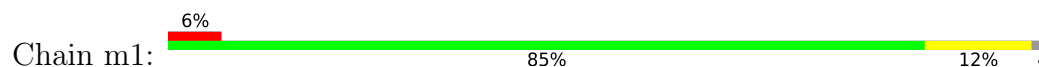


- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

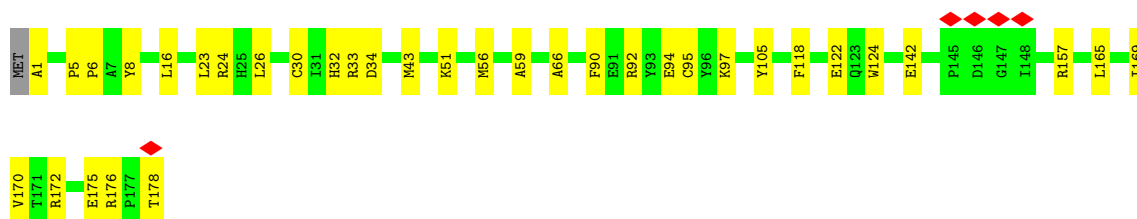
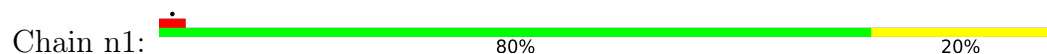




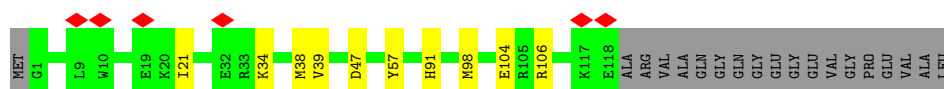
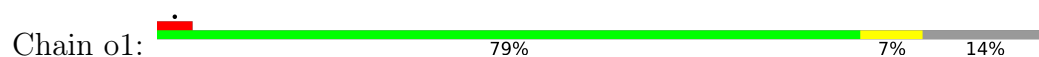
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



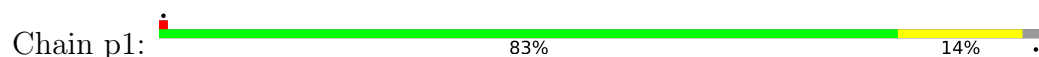
- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



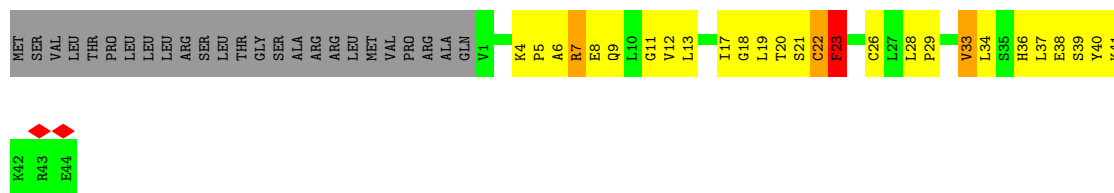
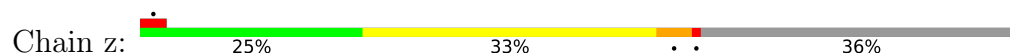
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 67: Cytochrome c oxidase subunit 8A, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57506	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	0.139	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	227.9, 263.93997, 262.87997	wwPDB
Map dimensions	215, 249, 248	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	n	0.26	0/4162	0.62	1/5686 (0.0%)
2	o	0.26	0/1863	0.69	1/2542 (0.0%)
3	p	0.26	0/2202	0.66	2/3010 (0.1%)
4	q	0.23	0/1190	0.65	2/1609 (0.1%)
5	r	0.24	0/860	0.66	1/1167 (0.1%)
6	s	0.23	0/738	0.59	0/1001
7	t	0.83	0/646	1.19	1/882 (0.1%)
8	u	0.23	0/674	0.63	0/910
9	v	0.23	0/579	0.75	0/771
10	x	0.21	0/396	0.51	0/541
11	y	0.24	0/399	0.61	0/535
12	w	0.19	0/444	0.54	0/598
13	A	0.17	0/3529	0.42	0/4793
13	L	0.18	0/3530	0.43	0/4793
14	B	0.17	0/3205	0.40	0/4332
14	M	0.15	0/3205	0.37	0/4332
15	C	0.21	0/3147	0.50	2/4297 (0.0%)
15	N	0.21	0/3147	0.50	1/4297 (0.0%)
16	D	0.19	0/1968	0.42	0/2674
16	O	0.16	0/1968	0.39	0/2674
17	E	0.16	0/1173	0.42	0/1605
17	P	0.16	0/1173	0.37	0/1605
17	T	0.18	0/565	0.41	0/772
18	F	0.16	0/916	0.40	0/1226
18	Q	0.16	0/922	0.36	0/1234
19	G	0.22	0/673	0.55	0/909
19	R	0.24	0/673	0.51	0/909
20	H	0.24	0/552	0.62	1/739 (0.1%)
20	S	0.24	0/570	0.59	0/763
21	J	0.19	0/509	0.47	0/687
21	U	0.18	0/509	0.36	0/687

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	K	0.19	0/446	0.48	0/609
22	V	0.17	0/454	0.47	0/619
23	6	0.26	0/1289	0.58	1/1744 (0.1%)
24	C1	0.17	0/1780	0.38	0/2424
25	D1	0.19	0/3540	0.42	0/4795
26	2	0.19	0/1700	0.43	0/2316
27	1	0.20	0/3396	0.50	2/4586 (0.0%)
28	3	0.17	0/5392	0.39	0/7305
29	9	0.19	0/1461	0.43	0/1974
30	P1	0.18	0/2823	0.45	0/3828
31	Q1	0.16	0/1045	0.34	0/1411
32	7	0.15	0/773	0.35	0/1041
33	S1	0.17	0/682	0.49	0/920
34	T1	0.21	0/646	0.58	0/869
34	U1	0.19	0/718	0.48	0/970
35	V1	0.16	0/945	0.34	0/1281
36	W1	0.20	0/993	0.46	0/1335
37	q1	0.17	0/1251	0.46	0/1702
38	r1	0.16	0/806	0.36	0/1090
39	s1	0.14	0/360	0.37	0/489
40	A1	0.26	0/948	0.59	1/1295 (0.1%)
41	H1	0.28	0/2607	0.64	0/3564
42	J1	0.23	0/1330	0.54	0/1810
43	K1	0.25	0/738	0.54	0/1002
44	L1	0.23	0/4913	0.54	0/6686
45	M1	0.24	0/3709	0.53	0/5052
46	N1	0.26	0/2755	0.56	0/3751
47	O1	0.17	0/2674	0.40	0/3626
48	X1	0.18	0/1434	0.43	0/1937
49	Y1	0.20	0/1061	0.46	0/1439
50	Z1	0.19	0/1198	0.46	0/1616
51	a1	0.20	0/585	0.49	0/788
52	b1	0.19	0/666	0.46	0/914
53	c1	0.19	0/409	0.48	0/555
54	d1	0.18	0/1028	0.46	0/1387
55	e1	0.15	0/900	0.39	0/1199
56	f1	0.19	0/468	0.58	2/630 (0.3%)
57	g1	0.15	0/878	0.39	0/1196
58	h1	0.19	0/1201	0.49	0/1626
59	i1	0.16	0/917	0.39	0/1243
60	j1	0.16	0/587	0.40	0/804
61	k1	0.15	0/646	0.35	0/873
62	l1	0.16	0/1379	0.41	0/1882

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	m1	0.19	0/1079	0.46	0/1463
64	n1	0.18	0/1596	0.42	0/2162
65	o1	0.22	0/1039	0.50	0/1394
66	p1	0.16	0/1471	0.36	0/1988
67	z	0.94	0/350	1.25	1/472 (0.2%)
All	All	0.22	0/115153	0.50	19/156242 (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
7	t	0	1
67	z	0	1
All	All	0	2

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	n	195	LEU	CA-CB-CG	6.96	140.66	116.30
15	N	156	ILE	N-CA-C	-6.94	107.12	113.71
5	r	72	LYS	N-CA-C	-6.61	104.15	111.36
27	1	101	GLU	CA-C-N	6.43	126.40	119.78
27	1	101	GLU	C-N-CA	6.43	126.40	119.78
56	f1	49	ARG	CA-C-N	6.19	125.89	119.82
56	f1	49	ARG	C-N-CA	6.19	125.89	119.82
67	z	22	CYS	CB-CA-C	-6.00	101.73	110.96
4	q	58	GLN	CA-CB-CG	5.77	125.64	114.10
4	q	58	GLN	N-CA-CB	5.75	119.19	110.28
7	t	70	HIS	CB-CG-CD2	-5.50	124.05	131.20
15	C	343	VAL	N-CA-C	5.31	111.89	106.21
2	o	201	GLY	N-CA-C	5.24	116.85	111.56
3	p	196	THR	CA-C-N	-5.19	111.86	120.68
3	p	196	THR	C-N-CA	-5.19	111.86	120.68
20	H	36	GLU	N-CA-CB	5.15	118.93	110.39
40	A1	98	LEU	CA-CB-CG	5.04	133.96	116.30
23	6	63	ALA	N-CA-C	5.04	114.69	108.19
15	C	332	LEU	CA-CB-CG	5.00	133.81	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	t	11	ARG	Sidechain
67	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	n	4021	0	3997	117	0
2	o	1817	0	1822	48	0
3	p	2118	0	2054	81	0
4	q	1156	0	1112	47	0
5	r	842	0	838	46	0
6	s	721	0	698	70	0
7	t	620	0	597	54	0
8	u	654	0	622	12	0
9	v	567	0	591	15	0
10	x	383	0	367	9	0
11	y	386	0	386	16	0
12	w	435	0	446	5	0
13	A	3459	0	3367	52	0
13	L	3460	0	3367	63	0
14	B	3154	0	3158	52	0
14	M	3154	0	3158	40	0
15	C	3046	0	3112	53	0
15	N	3046	0	3112	51	0
16	D	1909	0	1854	33	0
16	O	1909	0	1854	30	0
17	E	1164	0	833	17	0
17	P	1164	0	833	15	0
17	T	554	0	590	11	0
18	F	894	0	882	10	0
18	Q	900	0	887	10	0
19	G	654	0	656	9	0
19	R	654	0	656	17	0
20	H	545	0	531	6	0
20	S	563	0	541	8	0
21	J	495	0	489	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	495	0	489	12	0
22	K	430	0	431	5	0
22	V	438	0	443	4	0
23	6	1258	0	1268	29	0
24	C1	1730	0	1686	24	0
25	D1	3464	0	3416	66	0
26	2	1660	0	1653	22	0
27	1	3321	0	3278	53	0
28	3	5305	0	5330	70	0
29	9	1431	0	1383	36	0
30	P1	2748	0	2768	53	0
31	Q1	1022	0	1023	21	0
32	7	758	0	731	13	0
33	S1	671	0	688	10	0
34	T1	637	0	640	8	0
34	U1	706	0	699	21	0
35	V1	923	0	965	8	0
36	W1	970	0	991	12	0
37	q1	1209	0	1170	8	0
38	r1	796	0	831	13	0
39	s1	351	0	331	7	0
40	A1	932	0	967	26	0
41	H1	2540	0	2626	70	0
42	J1	1308	0	1319	38	0
43	K1	737	0	768	23	0
44	L1	4800	0	4985	109	0
45	M1	3632	0	3853	89	0
46	N1	2703	0	2902	76	0
47	O1	2607	0	2566	45	0
48	X1	1396	0	1385	21	0
49	Y1	1037	0	1025	15	0
50	Z1	1167	0	1166	30	0
51	a1	572	0	583	13	0
52	b1	651	0	653	8	0
53	c1	398	0	401	11	0
54	d1	996	0	1001	13	0
55	e1	877	0	871	17	0
56	f1	456	0	452	3	0
57	g1	850	0	783	11	0
58	h1	1166	0	1166	17	0
59	i1	897	0	902	17	0
60	j1	562	0	515	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	k1	626	0	620	16	0
62	l1	1323	0	1216	17	0
63	m1	1050	0	1061	15	0
64	n1	1541	0	1473	27	0
65	o1	1014	0	1002	9	0
66	p1	1438	0	1404	22	0
67	z	343	0	356	43	0
68	n	1	0	0	0	0
69	n	1	0	0	0	0
70	n	120	0	108	1	0
71	6	32	0	38	1	0
71	A	23	0	20	2	0
71	A1	43	0	60	1	0
71	C	66	0	80	3	0
71	D1	51	0	82	4	0
71	E	32	0	38	5	0
71	G	51	0	82	3	0
71	H1	51	0	82	1	0
71	K1	41	0	59	2	0
71	L	23	0	20	1	0
71	L1	51	0	82	3	0
71	M1	138	0	210	6	0
71	N	71	0	90	2	0
71	N1	38	0	50	3	0
71	O	33	0	40	2	0
71	R	30	0	34	1	0
71	Y1	70	0	88	4	0
71	d1	63	0	74	1	0
71	i1	42	0	61	5	0
71	n	89	0	100	2	0
71	o	29	0	32	3	0
71	p	45	0	67	3	0
71	r1	46	0	66	1	0
71	t	25	0	24	6	0
71	v	28	0	30	0	0
72	O1	1	0	0	0	0
72	o	1	0	0	0	0
73	o	2	0	0	0	0
74	7	1	0	0	0	0
74	s	1	0	0	0	0
75	y	37	0	49	1	0
76	A	46	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	C	42	0	28	0	0
76	G	56	0	56	2	0
76	H1	51	0	52	1	0
76	L1	124	0	136	1	0
76	N	46	0	36	3	0
76	N1	90	0	133	4	0
76	O	57	0	58	2	0
76	R	170	0	175	4	0
76	Y1	94	0	141	2	0
76	a1	57	0	58	2	0
76	d1	67	0	81	4	0
76	h1	70	0	87	5	0
77	C	86	0	60	5	0
77	N	86	0	60	6	0
78	D	43	0	30	3	0
78	O	43	0	30	1	0
79	2	4	0	0	0	0
79	3	4	0	0	0	0
79	E	4	0	0	0	0
79	P	4	0	0	0	0
80	6	43	0	63	3	0
80	9	101	0	159	4	0
80	J	35	0	44	0	0
80	K	28	0	30	0	0
80	L	24	0	22	0	0
80	P1	31	0	36	0	0
80	V	28	0	30	0	0
80	Y1	54	0	88	9	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	0	0
82	1	31	0	19	3	0
83	3	1	0	0	0	0
84	P1	48	0	26	1	0
85	W1	34	0	40	1	0
85	n1	32	0	36	4	0
86	O1	31	0	12	1	0
All	All	115575	0	115273	1882	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1882) 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)
6:s:75:LEU:HG	6:s:81:GLN:CG	1.43	1.46
6:s:75:LEU:CG	6:s:81:GLN:HG2	1.50	1.40
5:r:27:TRP:CG	6:s:82:ARG:HH21	1.50	1.28
5:r:27:TRP:CD1	6:s:82:ARG:HH21	1.51	1.26
67:z:4:LYS:CD	67:z:5:PRO:HD2	1.67	1.24
5:r:27:TRP:CG	6:s:82:ARG:NH2	2.04	1.23
6:s:75:LEU:CD2	6:s:81:GLN:HB2	1.68	1.23
17:E:161:HIS:HD2	15:N:343:VAL:CG2	1.55	1.18
17:E:161:HIS:HD2	15:N:343:VAL:HG21	1.06	1.15
4:q:12:ALA:HB2	6:s:56:LYS:NZ	1.63	1.12
6:s:75:LEU:HD23	6:s:81:GLN:OE1	1.53	1.09
6:s:75:LEU:HD21	6:s:81:GLN:HB2	1.14	1.08
3:p:158:HIS:CE1	7:t:14:LYS:NZ	2.21	1.08
3:p:187:SER:HB2	7:t:67:THR:HG21	1.28	1.07
17:E:161:HIS:CD2	15:N:343:VAL:HG21	1.90	1.06
4:q:12:ALA:HB2	6:s:56:LYS:CE	1.85	1.06
67:z:4:LYS:HD2	67:z:5:PRO:CD	1.86	1.05
5:r:27:TRP:CD2	6:s:82:ARG:NH2	2.24	1.05
6:s:75:LEU:CG	6:s:81:GLN:CG	2.18	1.05
2:o:145:PRO:HA	2:o:214:VAL:O	1.56	1.04
3:p:187:SER:CB	7:t:67:THR:HG21	1.89	1.03
3:p:158:HIS:NE2	7:t:14:LYS:NZ	2.07	1.01
5:r:27:TRP:CZ2	6:s:82:ARG:NE	2.28	1.01
7:t:12:MET:HG3	47:O1:10:LEU:CD1	1.90	1.01
7:t:12:MET:HG3	47:O1:10:LEU:HD13	1.38	1.01
6:s:75:LEU:HG	6:s:81:GLN:CB	1.89	1.01
5:r:27:TRP:CE2	6:s:82:ARG:NE	2.30	1.00
17:E:161:HIS:CD2	15:N:343:VAL:CG2	2.45	0.99
17:E:161:HIS:NE2	15:N:282:ARG:HD2	1.76	0.99
6:s:75:LEU:HD23	6:s:81:GLN:CD	1.86	0.99
3:p:158:HIS:CE1	7:t:14:LYS:HZ2	1.79	0.98
4:q:12:ALA:CB	6:s:56:LYS:HE3	1.92	0.98
1:n:216:ASN:ND2	7:t:57:LYS:O	1.96	0.98
6:s:75:LEU:CD2	6:s:81:GLN:CB	2.42	0.98
3:p:34:TRP:NE1	7:t:60:PRO:O	1.97	0.96
5:r:82:TYR:HB3	5:r:83:PRO:HD3	1.46	0.96
4:q:68:PHE:HA	4:q:71:MET:HG2	1.48	0.93
3:p:142:VAL:HG23	7:t:13:TRP:HZ3	1.32	0.91
4:q:68:PHE:HA	4:q:71:MET:CG	2.00	0.91
67:z:4:LYS:HD2	67:z:5:PRO:HD2	0.92	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:153:GLU:CD	7:t:10:ALA:HB3	1.96	0.91
19:G:41:THR:O	19:G:45:ILE:HB	1.70	0.90
3:p:182:PHE:O	7:t:71:ASN:ND2	2.04	0.90
4:q:68:PHE:HA	4:q:71:MET:SD	2.11	0.90
44:L1:245:ALA:O	44:L1:249:SER:HB2	1.71	0.90
5:r:27:TRP:CD1	6:s:82:ARG:NH2	2.30	0.89
4:q:12:ALA:HB2	6:s:56:LYS:HE3	1.52	0.88
6:s:75:LEU:CB	6:s:81:GLN:HG2	2.03	0.88
6:s:56:LYS:HE2	6:s:74:TRP:CD2	2.09	0.86
3:p:142:VAL:HG23	7:t:13:TRP:CZ3	2.09	0.86
16:D:32:VAL:O	16:D:36:VAL:HB	1.75	0.86
3:p:259:TRP:HZ3	53:c1:29:ILE:HG22	1.38	0.86
3:p:259:TRP:CZ3	53:c1:29:ILE:HG22	2.09	0.86
45:M1:421:ASN:H	45:M1:421:ASN:HD22	1.21	0.85
6:s:75:LEU:CD2	6:s:81:GLN:CG	2.55	0.85
4:q:12:ALA:HB2	6:s:56:LYS:HZ1	1.43	0.83
9:v:52:PHE:O	9:v:56:TYR:HB2	1.77	0.83
27:l:101:GLU:OE2	27:l:184:TYR:OH	1.95	0.83
30:P1:310:LEU:O	30:P1:314:SER:HB2	1.79	0.83
6:s:75:LEU:CG	6:s:81:GLN:CB	2.50	0.83
5:r:27:TRP:NE1	6:s:82:ARG:HH21	1.78	0.81
15:C:237:LEU:HB2	16:D:212:MET:HE2	1.61	0.80
3:p:259:TRP:CZ3	53:c1:29:ILE:CG2	2.64	0.80
4:q:12:ALA:HB1	6:s:56:LYS:HE3	1.64	0.78
14:B:220:ALA:O	14:B:224:LEU:HB2	1.82	0.78
2:o:154:ILE:O	2:o:179:LEU:HA	1.84	0.78
5:r:27:TRP:CH2	6:s:82:ARG:HD2	2.20	0.77
25:D1:103:PHE:HB3	25:D1:114:ASN:HB3	1.67	0.77
7:t:12:MET:CG	47:O1:10:LEU:HD13	2.15	0.76
5:r:27:TRP:CD2	6:s:82:ARG:CZ	2.68	0.76
3:p:255:SER:O	3:p:259:TRP:HB3	1.84	0.76
17:E:161:HIS:HD2	15:N:343:VAL:HG23	1.51	0.76
58:h1:49:GLU:H	58:h1:70:PRO:HD3	1.49	0.76
3:p:35:PHE:CE1	7:t:60:PRO:HG3	2.20	0.75
1:n:38:ARG:NH2	1:n:454:SER:OG	2.20	0.74
30:P1:216:ASN:O	30:P1:220:ASP:HB2	1.86	0.74
7:t:50:PRO:HG3	8:u:75:ARG:NE	2.03	0.74
6:s:75:LEU:HG	6:s:81:GLN:HG2	0.76	0.73
67:z:4:LYS:CG	67:z:5:PRO:HD2	2.17	0.73
2:o:41:ILE:HG22	2:o:45:MET:HE2	1.69	0.73
27:l:337:MET:HG2	27:l:341:THR:HG21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:188:GLU:O	27:1:192:LEU:HB2	1.88	0.73
1:n:480:ARG:HG2	67:z:6:ALA:HA	1.71	0.72
3:p:35:PHE:CD1	7:t:60:PRO:HG3	2.25	0.72
59:i1:120:ARG:HB2	65:o1:39:VAL:HG13	1.70	0.72
17:E:161:HIS:CD2	15:N:343:VAL:HG23	2.22	0.72
5:r:82:TYR:HB3	5:r:83:PRO:CD	2.19	0.72
1:n:473:TRP:CZ3	67:z:18:GLY:HA3	2.26	0.71
5:r:27:TRP:CH2	6:s:82:ARG:NE	2.58	0.71
7:t:69:PHE:O	71:t:101:3PE:N	2.20	0.71
58:h1:102:GLU:OE1	58:h1:106:LYS:NZ	2.24	0.71
5:r:27:TRP:CE2	6:s:82:ARG:NH2	2.56	0.70
14:B:51:VAL:HG12	14:B:204:MET:HG2	1.72	0.70
1:n:379:TYR:HA	1:n:383:MET:HE3	1.74	0.70
45:M1:361:MET:HE2	45:M1:441:MET:HE2	1.74	0.70
61:k1:67:THR:HG22	61:k1:69:PRO:HD2	1.74	0.70
27:1:99:GLU:OE2	27:1:105:CYS:HA	1.91	0.70
30:P1:59:LEU:HA	30:P1:62:MET:HE3	1.72	0.70
44:L1:221:THR:HG23	44:L1:226:GLN:HB2	1.74	0.69
15:N:312:GLN:HB2	15:N:318:ARG:HD3	1.74	0.69
3:p:158:HIS:CE1	7:t:14:LYS:HZ1	1.90	0.69
4:q:61:ARG:NH2	4:q:70:GLU:OE2	2.25	0.69
17:P:10:PHE:HB2	17:P:14:ARG:HH21	1.58	0.69
7:t:12:MET:HG3	47:O1:10:LEU:HD12	1.74	0.69
21:U:10:TYR:HA	21:U:14:PHE:HB2	1.75	0.69
67:z:4:LYS:CD	67:z:5:PRO:CD	2.60	0.68
1:n:92:MET:SD	1:n:98:ASN:ND2	2.66	0.68
4:q:68:PHE:CA	4:q:71:MET:HG2	2.23	0.68
71:L1:701:3PE:H222	62:l1:87:ARG:HA	1.75	0.68
71:D1:501:3PE:H3E1	80:Y1:201:PC1:H3H1	1.75	0.68
23:6:91:ARG:NH1	41:H1:61:MET:SD	2.67	0.68
28:3:588:THR:HG21	31:Q1:63:GLU:HA	1.76	0.68
28:3:632:ARG:HH22	33:S1:59:GLU:H	1.40	0.68
6:s:75:LEU:CG	6:s:81:GLN:HB2	2.20	0.67
23:6:144:ARG:NH2	24:C1:173:GLU:OE1	2.27	0.67
29:9:171:ILE:O	29:9:175:TYR:HB3	1.94	0.67
8:u:56:TYR:HA	8:u:59:VAL:HG12	1.77	0.67
21:J:10:TYR:HA	21:J:14:PHE:HB2	1.76	0.67
47:O1:104:ARG:NH2	86:O1:401:DGT:N7	2.42	0.67
1:n:116:SER:O	11:y:43:GLN:NE2	2.27	0.67
1:n:92:MET:SD	1:n:163:ASN:ND2	2.68	0.67
2:o:132:GLU:HB3	2:o:137:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:s:81:GLN:OE1	6:s:81:GLN:N	2.26	0.67
3:p:190:ASP:OD1	7:t:53:ARG:HA	1.96	0.66
1:n:28:MET:HE1	11:y:29:PHE:HB3	1.77	0.66
3:p:146:TRP:HB2	7:t:13:TRP:HB3	1.77	0.66
5:r:27:TRP:CE2	6:s:82:ARG:CZ	2.79	0.66
1:n:168:ILE:HD12	1:n:185:VAL:HG13	1.78	0.66
22:V:18:ILE:HG13	22:V:19:PRO:HD3	1.77	0.66
19:G:28:SER:OG	19:G:32:LYS:NZ	2.29	0.66
67:z:4:LYS:HG2	67:z:7:ARG:HH22	1.59	0.66
61:k1:32:THR:HG22	61:k1:34:LEU:H	1.60	0.66
27:1:92:TYR:HB2	27:1:220:THR:HG22	1.78	0.66
1:n:479:LYS:HG3	67:z:7:ARG:HB2	1.75	0.66
15:N:8:HIS:HB3	15:N:11:PHE:HB2	1.77	0.66
40:A1:67:LEU:HD21	43:K1:68:ALA:HB3	1.78	0.66
45:M1:114:GLU:HG2	48:X1:168:PHE:HB3	1.77	0.66
4:q:23:PRO:HB3	5:r:70:VAL:HG11	1.78	0.65
47:O1:133:VAL:HG23	47:O1:205:ALA:HB3	1.78	0.65
16:O:118:ARG:HG2	16:O:194:SER:HB3	1.78	0.65
44:L1:243:VAL:O	44:L1:247:LEU:HB2	1.97	0.65
67:z:4:LYS:HG3	67:z:7:ARG:NH1	2.12	0.65
46:N1:135:LYS:NZ	46:N1:183:SER:OG	2.30	0.65
16:D:41:HIS:CD2	78:D:301:HEC:NC	2.64	0.65
25:D1:328:ALA:HB3	28:3:126:ASP:HB2	1.79	0.65
19:R:41:THR:O	19:R:45:ILE:HB	1.96	0.65
50:Z1:132:MET:SD	50:Z1:136:ASN:ND2	2.69	0.65
26:2:150:ASN:HB3	26:2:162:GLU:HB3	1.79	0.64
2:o:152:MET:HB2	2:o:182:ALA:O	1.97	0.64
53:c1:32:ILE:O	53:c1:36:ASN:ND2	2.28	0.64
5:r:27:TRP:CH2	6:s:82:ARG:CD	2.80	0.64
27:1:15:LEU:HD13	27:1:271:GLU:HB2	1.79	0.64
2:o:198:GLU:O	2:o:204:HIS:CE1	2.51	0.64
44:L1:176:ARG:HH12	45:M1:400:ILE:HG22	1.62	0.64
51:a1:1:MET:HG3	76:a1:101:CDL:HB21	1.79	0.64
45:M1:98:MET:HE1	76:N1:401:CDL:H801	1.79	0.64
67:z:4:LYS:HG2	67:z:7:ARG:NH2	2.13	0.64
47:O1:170:ILE:HD11	47:O1:238:ILE:HD11	1.78	0.64
3:p:34:TRP:CZ2	7:t:61:TRP:HE3	2.15	0.64
5:r:7:THR:O	5:r:11:PHE:HB2	1.98	0.64
2:o:10:GLN:HG2	2:o:167:SER:HA	1.79	0.63
42:J1:144:MET:HB2	43:K1:58:PRO:HG3	1.80	0.63
67:z:36:HIS:HB2	67:z:40:TYR:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:J1:70:THR:HA	42:J1:74:ALA:HB3	1.79	0.63
46:N1:254:LEU:HG	46:N1:290:LEU:HD11	1.79	0.63
1:n:297:LEU:O	8:u:23:GLN:NE2	2.30	0.63
50:Z1:9:MET:HE3	50:Z1:10:PRO:HD2	1.79	0.63
6:s:75:LEU:CD2	6:s:81:GLN:CD	2.65	0.63
7:t:50:PRO:HG3	8:u:75:ARG:HE	1.64	0.62
67:z:4:LYS:CG	67:z:7:ARG:HH12	2.12	0.62
13:A:417:ASP:OD1	13:A:438:ARG:NH2	2.32	0.62
43:K1:1:FME:SD	43:K1:50:ASN:ND2	2.72	0.62
33:S1:78:LEU:HD12	33:S1:86:VAL:HG22	1.80	0.62
51:a1:52:ARG:NH1	51:a1:58:ASN:OD1	2.31	0.62
13:A:3:THR:HG22	13:A:6:GLN:HG2	1.81	0.62
25:D1:51:PHE:HB3	25:D1:64:LEU:HB3	1.80	0.62
26:2:144:CYS:O	27:1:139:ARG:NH2	2.31	0.62
46:N1:109:ALA:HB3	46:N1:161:SER:HA	1.81	0.62
67:z:22:CYS:O	67:z:23:PHE:C	2.42	0.62
27:1:224:ASN:ND2	82:1:501:FMN:O2	2.33	0.62
71:A1:201:3PE:H381	41:H1:295:PRO:HB3	1.81	0.62
5:r:27:TRP:CD2	6:s:82:ARG:NE	2.67	0.62
14:M:169:LYS:HG3	14:M:240:ARG:HB3	1.82	0.62
25:D1:4:TRP:O	45:M1:142:ARG:NH2	2.33	0.62
14:M:71:LEU:HD22	14:M:144:LEU:HD23	1.82	0.62
1:n:378:HIS:HD2	1:n:382:SER:HB3	1.65	0.61
14:B:141:ARG:HD3	14:B:184:GLY:HA2	1.82	0.61
80:9:204:PC1:H112	50:Z1:28:GLY:HA3	1.81	0.61
5:r:93:LEU:HD13	5:r:98:ILE:HG23	1.82	0.61
19:R:6:ASN:HD22	19:R:6:ASN:C	2.08	0.61
67:z:4:LYS:CG	67:z:7:ARG:NH1	2.63	0.61
26:2:119:THR:HG21	26:2:166:PRO:HB3	1.82	0.61
27:1:172:ASP:HB3	39:s1:57:LEU:HD11	1.81	0.61
42:J1:69:TYR:HD2	43:K1:75:LEU:HD22	1.65	0.61
41:H1:20:LEU:HD22	41:H1:232:ILE:HG12	1.81	0.61
42:J1:139:ILE:HB	43:K1:54:MET:HE1	1.81	0.61
44:L1:338:MET:HB2	44:L1:457:LEU:HB3	1.82	0.61
13:A:76:GLU:HG3	14:B:285:ILE:HD13	1.81	0.61
13:L:362:ARG:NH2	13:L:400:GLN:OE1	2.29	0.61
25:D1:149:ASN:HD21	25:D1:371:LYS:HG3	1.66	0.61
15:C:218:ILE:HG21	16:D:230:LEU:HD21	1.82	0.61
1:n:261:TYR:HB2	1:n:338:MET:HE3	1.83	0.61
2:o:112:ASP:O	8:u:58:ARG:NH1	2.34	0.61
20:S:45:ARG:NH2	20:S:50:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M1:272:THR:HA	45:M1:275:ILE:HD12	1.82	0.61
3:p:153:GLU:HG3	7:t:10:ALA:CB	2.31	0.61
24:C1:43:SER:HA	38:r1:65:PRO:HB3	1.82	0.61
25:D1:183:ARG:NH1	25:D1:210:ASP:OD2	2.33	0.61
2:o:162:SER:OG	2:o:173:ASP:OD1	2.19	0.61
13:L:86:LEU:HD22	14:M:285:ILE:HG23	1.82	0.61
14:M:77:THR:HG21	14:M:126:VAL:HA	1.83	0.61
25:D1:269:LEU:HB2	25:D1:368:GLU:HB2	1.81	0.61
45:M1:55:MET:HE1	76:d1:201:CDL:H532	1.81	0.61
46:N1:249:LEU:HD22	46:N1:254:LEU:HD12	1.81	0.61
49:Y1:8:TYR:HB2	49:Y1:23:ILE:HD13	1.82	0.61
3:p:180:GLU:HA	3:p:183:GLU:HB2	1.81	0.61
49:Y1:94:CYS:HA	49:Y1:114:CYS:HA	1.81	0.61
62:l1:133:PRO:HG3	65:o1:38:MET:HE1	1.82	0.60
71:o:302:3PE:H111	9:v:45:ARG:HH22	1.66	0.60
67:z:6:ALA:HB3	67:z:9:GLN:HG2	1.82	0.60
15:C:51:LEU:HD13	77:C:401:HEM:HBA1	1.82	0.60
27:1:99:GLU:OE2	27:1:105:CYS:CA	2.48	0.60
28:3:440:CYS:SG	28:3:476:LYS:NZ	2.73	0.60
2:o:28:LEU:HA	2:o:31:VAL:HG12	1.82	0.60
13:L:118:GLN:NE2	13:L:218:SER:O	2.33	0.60
62:l1:127:VAL:HG12	65:o1:98:MET:HG2	1.84	0.60
31:Q1:125:ASN:O	39:s1:64:ARG:NH1	2.33	0.60
40:A1:54:LYS:NZ	40:A1:115:GLU:OE1	2.34	0.60
41:H1:138:GLN:NE2	41:H1:194:ASN:OD1	2.35	0.60
42:J1:66:VAL:HG11	43:K1:31:LEU:HD21	1.84	0.60
47:O1:223:TYR:HD1	47:O1:227:GLU:HB3	1.66	0.60
50:Z1:127:ARG:NH1	55:e1:96:HIS:O	2.35	0.60
11:y:37:PHE:HB3	67:z:33:VAL:HG21	1.81	0.60
23:6:92:GLN:NE2	41:H1:215:TYR:O	2.35	0.60
45:M1:421:ASN:H	45:M1:421:ASN:ND2	1.95	0.60
49:Y1:82:LYS:NZ	49:Y1:84:ASP:OD1	2.31	0.60
13:A:86:LEU:HB3	14:B:285:ILE:HG13	1.84	0.60
14:B:153:GLN:NE2	17:T:33:ALA:O	2.35	0.60
11:y:15:VAL:HA	11:y:21:LEU:HD22	1.83	0.60
25:D1:281:VAL:HG21	25:D1:310:ILE:HG23	1.82	0.60
38:r1:112:LEU:HD23	50:Z1:22:ARG:HH11	1.66	0.60
46:N1:139:LEU:HD21	46:N1:187:MET:HE1	1.84	0.60
27:1:112:ARG:HB3	27:1:145:GLU:HG3	1.83	0.60
62:l1:9:PRO:HD3	63:m1:66:ARG:HG2	1.82	0.60
26:2:27:ASN:ND2	26:2:57:GLN:OE1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:O1:38:LEU:HD11	47:O1:234:VAL:HG21	1.84	0.59
34:U1:48:VAL:HG12	34:U1:52:MET:HE2	1.84	0.59
76:R:103:CDL:HB62	49:Y1:107:TYR:HB2	1.83	0.59
46:N1:342:GLN:O	54:d1:79:GLN:NE2	2.35	0.59
14:M:86:THR:HG23	17:T:70:LEU:HD11	1.83	0.59
15:N:233:LEU:HD23	16:O:219:THR:HG21	1.84	0.59
44:L1:578:THR:OG1	46:N1:171:ASN:ND2	2.33	0.59
17:P:84:GLY:N	17:P:100:HIS:O	2.36	0.59
27:1:142:PHE:HB3	27:1:145:GLU:HB2	1.85	0.59
1:n:457:GLY:HA2	1:n:460:ILE:HD12	1.85	0.59
25:D1:257:GLY:HA3	25:D1:372:GLY:HA2	1.84	0.59
35:V1:8:THR:HG23	35:V1:10:LEU:H	1.66	0.59
15:N:89:MET:HE1	15:N:235:MET:HG3	1.84	0.59
25:D1:72:MET:HB2	40:A1:54:LYS:HE3	1.84	0.59
15:N:318:ARG:NH1	15:N:373:GLU:OE1	2.35	0.59
37:q1:88:ARG:NH1	37:q1:94:THR:OG1	2.35	0.59
44:L1:363:THR:HG23	44:L1:431:THR:HB	1.84	0.59
47:O1:26:THR:HG22	47:O1:124:LEU:HB2	1.85	0.59
13:L:343:MET:HA	13:L:346:CYS:HB2	1.84	0.59
41:H1:113:VAL:HG11	41:H1:139:THR:HG21	1.84	0.59
29:9:55:GLU:OE2	37:q1:34:ARG:NH2	2.36	0.59
56:f1:31:ASP:O	56:f1:35:THR:OG1	2.20	0.59
48:X1:46:ARG:NH1	50:Z1:79:ASP:OD2	2.36	0.59
58:h1:50:ALA:HB2	66:p1:60:THR:HG23	1.84	0.59
9:v:43:GLU:HG2	9:v:44:PRO:HD3	1.85	0.58
35:V1:8:THR:HG21	35:V1:13:LEU:HB3	1.84	0.58
14:B:24:LEU:HD23	14:B:38:LEU:HB2	1.84	0.58
28:3:403:ASP:OD1	39:s1:64:ARG:NH2	2.34	0.58
1:n:117:MET:O	11:y:46:LYS:NZ	2.36	0.58
11:y:6:GLY:O	11:y:10:ASN:ND2	2.37	0.58
44:L1:75:GLU:OE1	57:g1:88:ARG:NH2	2.35	0.58
44:L1:362:ILE:HB	44:L1:431:THR:HA	1.86	0.58
13:A:245:ASP:HA	19:G:11:ARG:HA	1.84	0.58
60:j1:29:SER:OG	61:k1:74:LYS:O	2.21	0.58
1:n:377:PHE:HA	1:n:380:VAL:HG12	1.83	0.58
26:2:109:MET:HE1	27:1:346:ALA:HA	1.86	0.58
65:o1:38:MET:HE2	65:o1:57:TYR:HA	1.84	0.58
14:B:46:ARG:NH1	14:B:375:SER:OG	2.36	0.58
13:L:240:GLU:OE2	13:L:242:ARG:NH1	2.32	0.58
27:1:365:CYS:O	27:1:369:VAL:HB	2.04	0.58
44:L1:97:THR:HG21	44:L1:125:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N1:143:ILE:HG12	46:N1:198:PRO:HB3	1.84	0.58
1:n:70:VAL:HB	1:n:74:MET:HE2	1.86	0.58
1:n:439:ARG:HD2	2:o:199:ILE:HB	1.86	0.58
13:L:331:ILE:HD12	13:L:430:GLN:HB3	1.85	0.58
25:D1:110:SER:OG	25:D1:149:ASN:ND2	2.37	0.58
25:D1:233:ARG:NH2	29:9:25:ARG:O	2.37	0.58
45:M1:84:LEU:O	45:M1:92:GLN:NE2	2.36	0.58
38:r1:17:GLN:NE2	50:Z1:23:ASN:O	2.37	0.58
27:1:389:ILE:HG23	27:1:419:ILE:HD12	1.85	0.57
13:A:419:CYS:SG	13:A:438:ARG:NH1	2.77	0.57
40:A1:95:VAL:HG11	41:H1:302:MET:HB2	1.87	0.57
44:L1:539:MET:HG3	63:m1:10:LEU:HD21	1.86	0.57
46:N1:28:LEU:HA	46:N1:31:VAL:HG22	1.86	0.57
23:6:48:ASN:HB3	23:6:178:LYS:HA	1.86	0.57
29:9:77:GLU:O	29:9:107:ARG:NH1	2.37	0.57
48:X1:16:GLU:OE2	55:e1:104:ARG:NH2	2.37	0.57
1:n:151:HIS:HE1	1:n:210:LEU:HD13	1.69	0.57
38:r1:45:SER:O	38:r1:51:ASN:ND2	2.37	0.57
44:L1:290:ILE:HG13	44:L1:418:MET:HE1	1.85	0.57
47:O1:13:LYS:HB2	47:O1:16:LYS:HB2	1.85	0.57
59:i1:82:HIS:ND1	66:p1:36:TYR:OH	2.36	0.57
13:A:362:ARG:NH2	13:A:400:GLN:OE1	2.37	0.57
14:B:92:VAL:HG21	14:B:119:LEU:HD11	1.87	0.57
30:P1:316:GLU:HG3	30:P1:317:VAL:HG13	1.86	0.57
42:J1:33:ILE:HD11	42:J1:63:MET:HB2	1.87	0.57
2:o:54:SER:OG	2:o:55:THR:N	2.38	0.57
5:r:72:LYS:NZ	5:r:107:ASP:CG	2.62	0.57
30:P1:35:VAL:HG23	30:P1:45:VAL:HG11	1.86	0.57
45:M1:36:LEU:HB2	57:g1:67:VAL:HG22	1.87	0.57
45:M1:59:ASP:OD2	45:M1:245:ARG:NH2	2.37	0.57
3:p:259:TRP:CZ3	53:c1:33:GLN:CD	2.83	0.57
45:M1:430:HIS:HB2	45:M1:433:GLU:HG2	1.86	0.57
1:n:240:HIS:ND1	1:n:290:HIS:HE1	2.01	0.57
13:L:131:ARG:NH2	13:L:177:LEU:O	2.38	0.57
23:6:58:MET:HE2	23:6:90:PRO:HB3	1.86	0.57
27:1:91:LYS:HG2	27:1:219:PRO:HG2	1.87	0.57
40:A1:11:ILE:HD13	41:H1:80:THR:HG21	1.86	0.57
45:M1:191:SER:HB3	80:Y1:201:PC1:H12	1.86	0.57
46:N1:246:LEU:HD21	76:N1:401:CDL:H792	1.86	0.57
5:r:100:THR:HG23	5:r:103:GLU:H	1.69	0.57
14:B:153:GLN:HE22	17:T:33:ALA:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:228:SER:O	19:R:23:GLN:NE2	2.37	0.57
27:1:215:VAL:HG22	27:1:220:THR:HG21	1.86	0.57
31:Q1:36:ARG:O	31:Q1:57:MET:HA	2.05	0.57
41:H1:245:PRO:HB3	41:H1:258:ASN:HB3	1.86	0.57
42:J1:19:LEU:HD11	43:K1:31:LEU:HB3	1.86	0.57
51:a1:34:LYS:NZ	51:a1:61:TYR:O	2.33	0.57
15:N:51:LEU:HD13	77:N:402:HEM:HBA1	1.87	0.56
15:N:101:GLY:HA2	15:N:106:SER:HB2	1.87	0.56
25:D1:165:THR:HG22	41:H1:32:GLN:HG2	1.87	0.56
4:q:114:ASP:OD1	10:x:51:LYS:NZ	2.38	0.56
29:9:28:MET:HG3	50:Z1:34:MET:HE2	1.86	0.56
44:L1:197:GLU:HG3	66:p1:110:LYS:HD3	1.86	0.56
6:s:81:GLN:N	6:s:90:TYR:O	2.38	0.56
13:L:305:GLN:HB2	13:L:325:VAL:HG13	1.87	0.56
31:Q1:36:ARG:NH1	31:Q1:106:GLU:OE1	2.38	0.56
44:L1:139:GLN:HA	44:L1:142:ILE:HD12	1.87	0.56
34:U1:35:HIS:O	34:U1:40:LEU:HB2	2.06	0.56
1:n:183:LEU:HD21	1:n:273:MET:HB3	1.86	0.56
2:o:30:ILE:HG21	2:o:76:ILE:HD11	1.86	0.56
28:3:99:ALA:O	28:3:134:LYS:NZ	2.38	0.56
46:N1:87:GLN:NE2	58:h1:126:PRO:O	2.39	0.56
48:X1:39:ASN:HB3	50:Z1:72:PRO:HG2	1.88	0.56
14:M:141:ARG:HD2	14:M:184:GLY:H	1.70	0.56
25:D1:176:LYS:NZ	38:r1:24:GLN:O	2.38	0.56
41:H1:169:GLN:NE2	41:H1:241:ILE:O	2.39	0.56
42:J1:85:ASN:HB3	42:J1:88:ILE:HG12	1.87	0.56
1:n:216:ASN:OD1	7:t:55:ARG:HA	2.05	0.56
11:y:34:ALA:HB2	67:z:29:PRO:HB3	1.88	0.56
13:A:46:ARG:NH1	13:A:234:CYS:SG	2.79	0.56
34:T1:47:GLN:NE2	34:T1:70:LEU:O	2.38	0.56
55:e1:68:ARG:HB2	55:e1:72:MET:HE3	1.87	0.56
67:z:37:LEU:HA	67:z:40:TYR:CD2	2.40	0.56
1:n:191:THR:HG21	1:n:249:PRO:HD3	1.88	0.56
15:C:312:GLN:HE22	15:C:317:PHE:HB2	1.69	0.56
23:6:80:ASP:OD2	41:H1:34:ARG:NH2	2.38	0.56
67:z:38:GLU:O	67:z:41:LYS:HB3	2.05	0.56
2:o:141:ARG:HH11	2:o:210:VAL:HG21	1.71	0.56
16:D:207:LYS:HD2	71:E:202:3PE:H11	1.87	0.56
28:3:25:THR:HA	28:3:72:PRO:HA	1.87	0.56
29:9:134:VAL:HG21	29:9:167:ILE:HG21	1.88	0.56
18:F:35:ASP:OD1	18:F:89:TYR:OH	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:396:ARG:NH1	28:3:416:THR:O	2.39	0.56
28:3:570:SER:HA	28:3:583:THR:O	2.05	0.56
62:11:62:GLN:NE2	64:n1:1:ALA:O	2.38	0.56
2:o:69:PRO:HA	2:o:72:ILE:HG22	1.87	0.56
13:L:417:ASP:OD1	13:L:438:ARG:NH2	2.33	0.56
27:1:99:GLU:O	27:1:99:GLU:HG2	2.06	0.56
27:1:276:LEU:HD11	27:1:297:VAL:HG11	1.87	0.56
39:s1:65:GLU:HB3	39:s1:68:ARG:HH12	1.70	0.56
4:q:118:MET:SD	10:x:51:LYS:NZ	2.79	0.55
24:C1:78:LEU:HB3	24:C1:130:TYR:HB3	1.87	0.55
3:p:153:GLU:HG3	7:t:10:ALA:HB2	1.88	0.55
45:M1:9:LEU:HD23	45:M1:104:ILE:HD13	1.89	0.55
3:p:126:PRO:HA	3:p:130:PRO:HG2	1.87	0.55
6:s:56:LYS:HE2	6:s:74:TRP:CE3	2.40	0.55
13:A:8:LEU:HD22	13:A:392:LEU:HB3	1.88	0.55
23:6:79:MET:HB2	23:6:84:VAL:HB	1.87	0.55
28:3:470:VAL:HG12	28:3:490:MET:HE1	1.88	0.55
19:R:46:LEU:HD21	71:Y1:203:3PE:H251	1.89	0.55
28:3:364:LEU:HD12	28:3:491:ASN:HB3	1.88	0.55
41:H1:134:ARG:NH2	41:H1:206:GLU:OE2	2.39	0.55
1:n:287:VAL:O	1:n:290:HIS:ND1	2.38	0.55
13:A:445:ARG:NH1	76:A:502:CDL:OB3	2.39	0.55
25:D1:148:LEU:HD23	25:D1:174:ARG:HG2	1.88	0.55
31:Q1:112:LYS:O	31:Q1:114:LYS:NZ	2.37	0.55
46:N1:308:ASN:HB2	47:O1:282:ILE:HG22	1.87	0.55
48:X1:74:LYS:NZ	51:a1:69:ILE:O	2.40	0.55
50:Z1:92:GLU:HA	50:Z1:95:ILE:HG22	1.86	0.55
1:n:168:ILE:HG21	1:n:189:LEU:HD12	1.88	0.55
1:n:258:VAL:HA	1:n:338:MET:HE1	1.88	0.55
77:N:403:HEM:HBB2	77:N:403:HEM:HH1C	1.89	0.55
3:p:34:TRP:CZ2	7:t:60:PRO:HG2	2.42	0.55
13:A:339:GLN:NE2	13:A:437:ILE:O	2.40	0.55
25:D1:103:PHE:O	25:D1:114:ASN:ND2	2.39	0.55
27:1:384:ALA:HB1	27:1:388:GLU:HG3	1.89	0.55
15:C:1:MET:HE3	15:C:2:THR:H	1.71	0.55
27:1:105:CYS:SG	27:1:267:THR:OG1	2.65	0.55
14:B:113:ARG:NH1	14:B:210:GLY:O	2.40	0.55
13:L:156:THR:O	13:L:239:SER:OG	2.25	0.55
28:3:533:THR:O	28:3:537:LEU:HB2	2.07	0.55
30:P1:46:ILE:HG12	32:7:26:VAL:HG21	1.89	0.55
44:L1:467:VAL:O	44:L1:471:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:n1:142:GLU:OE2	64:n1:157:ARG:NH1	2.40	0.55
13:A:161:THR:HG22	17:E:21:SER:HB2	1.88	0.55
15:N:113:TRP:NE1	15:N:301:LEU:O	2.35	0.54
44:L1:428:TYR:OH	44:L1:509:MET:SD	2.65	0.54
1:n:510:TYR:HB3	6:s:59:VAL:HG23	1.90	0.54
18:F:53:ASP:OD1	18:F:54:LEU:N	2.40	0.54
15:N:89:MET:HA	15:N:92:ILE:HD12	1.88	0.54
30:P1:122:LYS:HD3	30:P1:160:PHE:HD1	1.72	0.54
30:P1:231:THR:HG21	30:P1:294:PRO:HG3	1.88	0.54
45:M1:370:PRO:HG3	45:M1:375:LEU:HD22	1.89	0.54
1:n:368:HIS:O	2:o:171:LYS:NZ	2.39	0.54
19:R:18:LEU:HD23	19:R:23:GLN:HB3	1.89	0.54
42:J1:130:ASP:OD2	50:Z1:78:LYS:NZ	2.41	0.54
44:L1:171:ALA:O	44:L1:175:ASN:ND2	2.41	0.54
14:B:109:VAL:HG22	14:B:119:LEU:HD23	1.90	0.54
24:C1:86:ARG:NH1	35:V1:110:GLN:O	2.40	0.54
44:L1:100:ILE:HG21	44:L1:246:LEU:HB2	1.87	0.54
55:e1:64:GLU:HG3	55:e1:70:LYS:HD3	1.89	0.54
67:z:36:HIS:HB2	67:z:40:TYR:CE1	2.43	0.54
44:L1:202:MET:O	44:L1:205:ASN:ND2	2.34	0.54
27:1:378:ARG:NH2	28:3:132:GLU:OE2	2.36	0.54
28:3:335:LEU:HA	28:3:338:VAL:HG12	1.89	0.54
67:z:4:LYS:HG3	67:z:7:ARG:HH12	1.70	0.54
14:B:374:THR:HG23	14:B:377:GLY:H	1.72	0.54
17:E:14:ARG:HB2	17:E:19:LEU:HD23	1.90	0.54
24:C1:49:GLU:OE2	24:C1:106:ARG:NH1	2.40	0.54
45:M1:191:SER:OG	49:Y1:130:GLU:OE1	2.25	0.54
67:z:18:GLY:O	67:z:21:SER:OG	2.12	0.54
1:n:244:TYR:HA	1:n:247:ILE:HG22	1.88	0.54
3:p:35:PHE:HE1	7:t:60:PRO:HG3	1.70	0.54
14:M:171:ALA:HB2	14:M:235:ALA:HB3	1.89	0.54
26:2:79:ARG:NH1	26:2:82:GLU:OE2	2.41	0.54
4:q:12:ALA:CB	6:s:56:LYS:CE	2.58	0.54
71:t:101:3PE:H242	71:t:101:3PE:H332	1.89	0.54
15:C:322:GLN:OE1	19:G:47:ARG:NH1	2.41	0.54
17:E:63:SER:OG	17:E:64:ALA:N	2.40	0.54
18:Q:67:ASP:OD1	18:Q:71:ARG:NH2	2.41	0.54
28:3:366:THR:HG22	28:3:370:GLY:HA3	1.89	0.54
4:q:35:ALA:HA	4:q:38:LYS:HE2	1.90	0.54
15:C:15:ASN:HA	15:C:19:ILE:HB	1.88	0.54
17:P:63:SER:OG	17:P:64:ALA:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:27:LEU:HA	28:3:37:ILE:HD12	1.90	0.54
28:3:114:CYS:HB3	28:3:117:GLN:HB2	1.89	0.54
44:L1:348:HIS:NE2	34:U1:2:ASP:OD2	2.41	0.54
59:i1:82:HIS:NE2	66:p1:41:ASP:OD1	2.39	0.54
3:p:205:GLY:HA2	3:p:208:VAL:HG12	1.88	0.53
15:C:50:PHE:HA	15:C:53:MET:HE3	1.91	0.53
77:C:402:HEM:HBB2	77:C:402:HEM:HHC	1.90	0.53
13:L:394:GLU:HG2	13:L:398:ARG:HE	1.73	0.53
18:Q:82:LYS:HB2	18:Q:85:GLU:HG2	1.90	0.53
28:3:591:GLY:HA2	30:P1:6:ILE:HG21	1.90	0.53
53:c1:45:ARG:NH2	54:d1:16:ASP:OD1	2.40	0.53
24:C1:151:ILE:HG23	24:C1:152:LEU:HG	1.90	0.53
45:M1:455:THR:OG1	57:g1:82:ARG:NH2	2.42	0.53
46:N1:217:MET:HE2	71:N1:402:3PE:H221	1.90	0.53
50:Z1:67:ARG:NH2	52:b1:50:TYR:O	2.42	0.53
1:n:377:PHE:O	1:n:381:LEU:HB2	2.08	0.53
25:D1:342:MET:HE2	28:3:101:HIS:HD2	1.72	0.53
29:9:86:GLU:OE2	29:9:96:ILE:N	2.41	0.53
41:H1:20:LEU:HD13	41:H1:232:ILE:HD11	1.90	0.53
44:L1:137:MET:HB2	44:L1:196:TRP:HB3	1.89	0.53
44:L1:190:SER:HB3	44:L1:196:TRP:NE1	2.23	0.53
46:N1:42:PRO:HA	46:N1:45:ILE:HG22	1.90	0.53
71:o:302:3PE:O12	9:v:45:ARG:NH2	2.41	0.53
3:p:6:HIS:HD2	3:p:8:TYR:HB2	1.73	0.53
8:u:43:MET:HA	8:u:46:LYS:HG2	1.89	0.53
15:N:215:ALA:HB2	18:Q:59:MET:HE3	1.89	0.53
28:3:648:LEU:HD23	28:3:651:LEU:HD12	1.90	0.53
36:W1:22:ILE:HG13	36:W1:79:ARG:HG2	1.90	0.53
5:r:87:GLN:NE2	9:v:6:LEU:O	2.41	0.53
28:3:341:ASP:OD1	33:S1:67:ARG:NH2	2.42	0.53
41:H1:75:PRO:HG2	41:H1:219:PRO:HB3	1.91	0.53
45:M1:458:THR:O	66:p1:149:TYR:OH	2.26	0.53
46:N1:272:LYS:HG2	58:h1:108:GLN:HE22	1.74	0.53
60:j1:9:PRO:HB2	61:k1:19:MET:HE1	1.90	0.53
13:L:245:ASP:HA	19:R:11:ARG:HA	1.89	0.53
30:P1:170:ASP:OD2	30:P1:202:LYS:NZ	2.41	0.53
30:P1:251:ARG:NH2	30:P1:321:HIS:O	2.41	0.53
44:L1:384:PRO:HA	44:L1:389:PHE:HD2	1.74	0.53
13:L:34:THR:OG1	14:M:373:GLU:OE1	2.26	0.53
25:D1:295:ASP:OD1	29:9:6:ASN:ND2	2.42	0.53
45:M1:421:ASN:HD22	45:M1:421:ASN:N	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N1:142:LEU:HB3	46:N1:194:LEU:HD21	1.90	0.53
50:Z1:84:GLN:OE1	55:e1:104:ARG:NH1	2.42	0.53
13:A:156:THR:O	13:A:239:SER:OG	2.25	0.53
15:C:78:LEU:O	15:C:82:MET:HB2	2.09	0.53
46:N1:150:ASN:HB3	46:N1:153:ILE:HG22	1.90	0.53
67:z:4:LYS:CG	67:z:5:PRO:CD	2.87	0.53
17:E:155:GLY:HA3	17:E:165:TYR:O	2.08	0.53
14:M:365:LYS:HG2	14:M:399:LEU:HD22	1.90	0.53
19:R:67:GLU:OE2	19:R:71:ARG:NH2	2.38	0.53
41:H1:149:ILE:HD11	41:H1:297:THR:HG22	1.91	0.53
44:L1:548:THR:O	44:L1:552:LEU:HB3	2.09	0.53
46:N1:261:LEU:HD11	46:N1:344:ILE:HD11	1.90	0.53
50:Z1:88:GLU:OE1	50:Z1:127:ARG:NH2	2.42	0.53
55:e1:29:ALA:HB2	58:h1:138:LYS:HD3	1.91	0.53
59:i1:94:TYR:OH	66:p1:10:PRO:O	2.27	0.53
66:p1:139:GLN:HG2	66:p1:143:LEU:HD22	1.90	0.53
4:q:11:TYR:CE2	6:s:56:LYS:NZ	2.77	0.52
14:B:36:ALA:HB3	14:B:207:VAL:HG12	1.91	0.52
28:3:339:ASP:OD1	33:S1:16:ARG:NH1	2.40	0.52
45:M1:447:LEU:HD21	71:M1:501:3PE:H3G2	1.90	0.52
63:m1:126:ILE:HG22	66:p1:139:GLN:HG3	1.91	0.52
3:p:149:HIS:CD2	7:t:13:TRP:CD1	2.97	0.52
4:q:12:ALA:HB2	6:s:56:LYS:HZ2	1.68	0.52
25:D1:67:GLU:HB3	25:D1:75:LYS:HB3	1.91	0.52
67:z:34:LEU:HA	67:z:37:LEU:HG	1.90	0.52
1:n:147:ILE:HG23	1:n:206:ILE:HB	1.91	0.52
28:3:27:LEU:HD21	28:3:39:ARG:HH21	1.73	0.52
41:H1:86:TRP:HZ2	41:H1:232:ILE:HG22	1.73	0.52
46:N1:92:GLY:O	46:N1:96:ASN:ND2	2.42	0.52
3:p:217:VAL:O	3:p:221:ARG:HG3	2.08	0.52
26:2:31:ILE:HG12	26:2:50:VAL:HG22	1.91	0.52
26:2:76:PRO:HB2	26:2:79:ARG:HG2	1.91	0.52
28:3:620:ARG:NH1	28:3:633:TYR:OH	2.42	0.52
44:L1:352:ASP:OD2	64:n1:92:ARG:NH1	2.42	0.52
45:M1:207:MET:HE1	45:M1:240:SER:HB3	1.91	0.52
48:X1:70:PHE:HA	48:X1:73:ILE:HG22	1.92	0.52
4:q:121:LYS:HE3	10:x:50:PRO:HB2	1.90	0.52
11:y:21:LEU:HG	11:y:25:MET:HE1	1.91	0.52
16:D:224:ARG:NH1	76:G:101:CDL:O1	2.42	0.52
14:M:68:LEU:HA	14:M:144:LEU:HD21	1.91	0.52
23:6:62:LEU:HB2	23:6:100:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C1:175:ARG:NH2	24:C1:177:ASP:OD2	2.42	0.52
34:T1:29:LYS:HE2	34:T1:40:LEU:HD23	1.91	0.52
44:L1:363:THR:HG21	61:k1:71:VAL:HG22	1.92	0.52
24:C1:133:GLU:OE2	25:D1:430:ARG:NH1	2.41	0.52
26:2:6:LEU:O	26:2:92:ARG:NH2	2.42	0.52
47:O1:261:MET:SD	47:O1:264:GLN:NE2	2.83	0.52
13:L:255:ILE:HG12	13:L:422:VAL:HG22	1.91	0.52
40:A1:38:GLU:HG2	40:A1:43:PRO:HA	1.92	0.52
44:L1:65:THR:HA	59:i1:89:MET:HE2	1.91	0.52
45:M1:232:ALA:O	45:M1:237:LYS:NZ	2.43	0.52
34:U1:87:TYR:HA	59:i1:19:ARG:HD3	1.90	0.52
1:n:413:HIS:NE2	1:n:468:MET:HB2	2.24	0.52
17:P:37:TYR:HA	17:P:40:THR:HG22	1.91	0.52
23:6:37:GLU:HA	23:6:40:VAL:HG12	1.91	0.52
48:X1:146:ARG:NH2	55:e1:38:GLU:OE1	2.40	0.52
17:T:67:THR:O	17:T:74:ALA:HA	2.10	0.52
47:O1:230:ASP:OD2	47:O1:233:LYS:NZ	2.42	0.52
2:o:103:GLN:HE21	2:o:104:TRP:CD1	2.28	0.52
15:N:80:ARG:NH1	77:N:402:HEM:O2D	2.39	0.52
40:A1:59:ALA:HB1	42:J1:65:VAL:HG13	1.91	0.52
43:K1:96:LEU:HD12	46:N1:54:GLU:HG2	1.92	0.52
45:M1:197:LEU:HB3	80:Y1:201:PC1:H3A2	1.92	0.52
46:N1:314:MET:HE1	47:O1:267:THR:HG23	1.91	0.52
2:o:164:ALA:O	2:o:194:GLY:HA3	2.09	0.51
71:p:301:3PE:H241	71:p:301:3PE:H331	1.92	0.51
14:M:141:ARG:NH1	14:M:186:ILE:O	2.43	0.51
27:1:270:GLU:OE1	27:1:283:HIS:NE2	2.37	0.51
27:1:372:MET:HE1	27:1:412:ALA:HA	1.92	0.51
30:P1:251:ARG:NH1	76:H1:402:CDL:OB3	2.43	0.51
42:J1:63:MET:HA	42:J1:66:VAL:HB	1.91	0.51
45:M1:430:HIS:HD2	45:M1:432:ARG:HH21	1.58	0.51
15:C:132:VAL:HA	15:C:139:SER:HB2	1.92	0.51
71:E:202:3PE:H342	71:E:202:3PE:H262	1.92	0.51
16:O:144:ARG:HH11	16:O:147:LEU:HD12	1.75	0.51
44:L1:161:ARG:NE	64:n1:90:PHE:O	2.42	0.51
45:M1:74:PRO:HA	45:M1:77:LEU:HD12	1.91	0.51
4:q:53:ARG:NH1	5:r:103:GLU:O	2.28	0.51
4:q:61:ARG:CZ	4:q:70:GLU:OE2	2.57	0.51
7:t:42:GLU:O	7:t:43:ARG:C	2.54	0.51
13:L:192:ALA:HB2	13:L:219:VAL:HB	1.92	0.51
25:D1:354:GLU:OE2	25:D1:357:GLN:NE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:135:ARG:NH1	28:3:179:ASN:O	2.40	0.51
34:U1:21:LEU:HD13	61:k1:53:ASN:HA	1.92	0.51
50:Z1:64:LEU:O	50:Z1:68:ILE:HG12	2.10	0.51
50:Z1:81:ARG:NH2	50:Z1:124:TYR:OH	2.44	0.51
3:p:109:THR:OG1	3:p:111:ASP:OD1	2.27	0.51
4:q:61:ARG:NH1	4:q:70:GLU:OE2	2.43	0.51
8:u:78:GLU:HG3	8:u:80:THR:HG22	1.92	0.51
15:C:215:ALA:HA	19:G:10:ILE:HD11	1.91	0.51
15:N:165:TRP:O	15:N:174:THR:OG1	2.29	0.51
28:3:494:HIS:HB2	28:3:576:THR:HG22	1.92	0.51
29:9:97:GLU:HB2	29:9:110:ARG:HB3	1.93	0.51
42:J1:161:ALA:O	42:J1:165:ILE:HG12	2.11	0.51
44:L1:161:ARG:NH1	44:L1:238:GLU:OE1	2.43	0.51
6:s:78:GLY:O	6:s:91:LYS:NZ	2.32	0.51
76:G:101:CDL:H122	76:G:101:CDL:H512	1.92	0.51
19:R:42:ARG:NH2	76:R:103:CDL:O1	2.43	0.51
76:R:102:CDL:OA7	49:Y1:103:ARG:NH1	2.43	0.51
29:9:85:CYS:O	29:9:89:CYS:HB2	2.10	0.51
58:h1:6:LYS:NZ	59:i1:26:GLU:OE1	2.36	0.51
64:n1:66:ALA:HB1	85:n1:201:ZMP:H7	1.93	0.51
14:B:182:ARG:HH21	14:B:186:ILE:HG12	1.75	0.51
48:X1:46:ARG:NH2	58:h1:142:ASP:OD1	2.43	0.51
54:d1:120:ARG:O	63:m1:108:ARG:NH2	2.43	0.51
1:n:105:LEU:O	1:n:108:SER:OG	2.21	0.51
1:n:216:ASN:CG	7:t:55:ARG:HA	2.35	0.51
7:t:55:ARG:NH1	7:t:59:PHE:CE2	2.79	0.51
15:C:45:ILE:HG12	77:C:401:HEM:HBB1	1.92	0.51
13:L:2:ALA:N	13:L:6:GLN:OE1	2.44	0.51
13:L:356:ARG:HG3	14:M:91:ALA:HA	1.92	0.51
15:N:331:ASN:ND2	15:N:357:SER:OG	2.43	0.51
25:D1:107:ASP:HB3	25:D1:114:ASN:HD21	1.75	0.51
25:D1:352:TYR:HD1	29:9:88:ILE:HG12	1.75	0.51
40:A1:34:ALA:HB1	41:H1:63:PRO:HA	1.91	0.51
42:J1:165:ILE:HG23	46:N1:42:PRO:HG3	1.93	0.51
44:L1:193:MET:HG3	44:L1:204:SER:HB2	1.93	0.51
46:N1:155:LEU:HB3	46:N1:278:MET:HE2	1.93	0.51
48:X1:5:GLU:O	48:X1:53:ARG:NH1	2.43	0.51
5:r:91:PRO:O	5:r:95:GLU:HB2	2.11	0.51
15:C:52:ALA:HA	15:C:55:TYR:HB3	1.93	0.51
16:O:231:LYS:NZ	76:O:301:CDL:O1	2.41	0.51
45:M1:443:PRO:HB3	71:M1:501:3PE:H3C1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:85:LEU:HA	1:n:505:PHE:HE2	1.75	0.51
4:q:79:LYS:HA	4:q:82:VAL:HG12	1.92	0.51
8:u:22:ASN:O	8:u:25:GLN:NE2	2.43	0.51
18:F:75:LEU:O	18:F:80:TRP:NE1	2.43	0.51
15:N:5:ARG:NH1	15:N:15:ASN:OD1	2.40	0.51
17:T:8:SER:HB3	17:T:11:PHE:HB2	1.92	0.51
40:A1:70:ALA:HB2	42:J1:58:ILE:HD11	1.91	0.51
46:N1:119:THR:HG21	46:N1:180:ALA:HB2	1.93	0.51
2:o:151:ARG:HB2	2:o:181:GLN:HE22	1.76	0.51
14:B:212:SER:HB3	14:B:215:VAL:HG12	1.92	0.51
41:H1:9:LEU:HD13	41:H1:95:LEU:HD22	1.92	0.51
45:M1:300:SER:HB3	45:M1:381:ILE:HG12	1.93	0.51
47:O1:320:LYS:O	54:d1:60:ARG:NH2	2.44	0.51
2:o:64:ILE:HG22	2:o:68:LEU:HD23	1.93	0.50
5:r:36:LEU:HD21	5:r:43:PRO:HB3	1.93	0.50
13:A:270:LEU:HD13	13:A:320:LEU:HD22	1.93	0.50
21:U:4:THR:HG22	21:U:6:PRO:HD2	1.93	0.50
25:D1:78:PRO:HG3	25:D1:402:LEU:HD23	1.93	0.50
41:H1:77:LEU:O	41:H1:81:LEU:HB2	2.11	0.50
47:O1:156:LYS:HE2	47:O1:160:LEU:HD22	1.93	0.50
59:i1:24:ASP:OD2	64:n1:124:TRP:NE1	2.44	0.50
2:o:139:ASP:OD1	2:o:139:ASP:N	2.43	0.50
13:A:264:ASN:ND2	13:A:414:TYR:OH	2.44	0.50
13:L:110:VAL:HG11	13:L:211:LEU:HB3	1.93	0.50
22:V:33:VAL:HG23	22:V:38:TRP:HB3	1.93	0.50
23:6:91:ARG:HB3	41:H1:216:ALA:HB2	1.92	0.50
26:2:147:ALA:HB3	26:2:153:MET:HE3	1.92	0.50
27:1:69:GLY:N	82:1:501:FMN:O1P	2.39	0.50
44:L1:441:ILE:HG21	60:j1:15:PRO:HB3	1.94	0.50
49:Y1:122:ALA:O	49:Y1:126:ILE:HG13	2.11	0.50
55:e1:33:HIS:CE1	58:h1:138:LYS:HE3	2.46	0.50
1:n:444:PRO:HD2	1:n:447:TYR:HD2	1.76	0.50
3:p:153:GLU:CG	7:t:10:ALA:HB3	2.41	0.50
6:s:35:LEU:HD12	6:s:36:PRO:HD2	1.92	0.50
16:D:197:GLU:O	16:D:201:ARG:HB3	2.12	0.50
29:9:59:LEU:O	38:r1:33:ARG:NH2	2.44	0.50
44:L1:112:PRO:HG3	64:n1:178:THR:HG21	1.93	0.50
45:M1:102:LEU:HD13	45:M1:230:ILE:HG12	1.93	0.50
48:X1:168:PHE:HE2	76:d1:201:CDL:H542	1.77	0.50
49:Y1:16:GLN:HB3	49:Y1:19:ARG:HB3	1.94	0.50
13:A:439:SER:O	71:A:501:3PE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:76:THR:HG23	14:B:81:SER:HA	1.94	0.50
14:B:120:MET:HE3	14:B:219:VAL:HG21	1.93	0.50
24:C1:77:ASP:HB3	25:D1:392:LYS:HG3	1.93	0.50
29:9:15:ASP:OD1	29:9:16:MET:N	2.44	0.50
32:7:43:LEU:HD22	37:q1:107:LYS:HE2	1.94	0.50
41:H1:20:LEU:HA	41:H1:23:VAL:HG12	1.93	0.50
44:L1:190:SER:HB3	44:L1:196:TRP:HE1	1.76	0.50
50:Z1:97:MET:HG2	55:e1:81:GLN:HG2	1.93	0.50
57:g1:106:MET:HE1	66:p1:138:TYR:HD2	1.75	0.50
4:q:88:PHE:HZ	67:z:19:LEU:HD21	1.76	0.50
14:B:121:GLU:OE2	14:B:125:ASN:ND2	2.43	0.50
14:B:144:LEU:HD21	14:B:178:CYS:HB3	1.94	0.50
16:D:1:SER:OG	16:D:2:ASP:N	2.43	0.50
16:D:19:SER:OG	21:J:50:LYS:NZ	2.44	0.50
27:1:32:ARG:HE	39:s1:36:GLN:HE21	1.59	0.50
32:7:32:GLN:HE22	32:7:34:GLU:HB2	1.77	0.50
40:A1:94:LEU:HD22	42:J1:152:MET:HE3	1.93	0.50
50:Z1:50:MET:SD	50:Z1:54:GLN:NE2	2.84	0.50
1:n:339:LEU:HD21	71:n:605:3PE:H332	1.93	0.50
1:n:433:LEU:HD22	2:o:9:LEU:HD11	1.92	0.50
3:p:233:PHE:HA	3:p:236:GLU:HG3	1.93	0.50
14:B:128:THR:O	14:B:227:ARG:NH2	2.45	0.50
44:L1:561:THR:HG23	71:Y1:204:3PE:H271	1.94	0.50
59:i1:18:ARG:NH1	64:n1:170:VAL:O	2.41	0.50
15:C:34:GLY:HA3	77:C:402:HEM:HBA2	1.94	0.50
16:D:211:MET:HE3	21:J:35:PHE:CD2	2.46	0.50
28:3:163:ALA:HA	28:3:167:ALA:HB3	1.93	0.50
28:3:544:VAL:HG12	28:3:559:VAL:HB	1.94	0.50
30:P1:319:ARG:NH1	36:W1:53:GLN:OE1	2.44	0.50
45:M1:115:LEU:HB2	45:M1:174:LEU:HD21	1.93	0.50
6:s:11:GLU:O	6:s:19:ARG:NH2	2.44	0.50
15:C:80:ARG:HH12	77:C:401:HEM:CGD	2.25	0.50
18:Q:35:ASP:OD1	18:Q:89:TYR:OH	2.27	0.50
27:1:202:LYS:O	31:Q1:133:LYS:NZ	2.39	0.50
27:1:279:LEU:HD12	27:1:283:HIS:HD2	1.77	0.50
28:3:113:GLU:HA	31:Q1:46:GLN:HE21	1.75	0.50
30:P1:66:GLY:HA3	31:Q1:69:LEU:HD13	1.94	0.50
30:P1:136:ASN:ND2	30:P1:291:ASP:OD1	2.45	0.50
44:L1:135:ASN:ND2	44:L1:197:GLU:OE2	2.45	0.50
44:L1:526:LEU:HD12	44:L1:530:PRO:HG2	1.93	0.50
44:L1:534:HIS:HB3	71:L1:701:3PE:H2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N1:3:PRO:HG3	47:O1:5:LEU:HD11	1.93	0.50
46:N1:276:LEU:HD22	80:Y1:201:PC1:H2	1.93	0.50
13:A:339:GLN:HE21	13:A:441:MET:HE2	1.77	0.50
17:E:45:VAL:HG13	21:J:28:ALA:HA	1.94	0.50
15:N:296:LEU:O	15:N:300:ILE:HG13	2.12	0.50
26:2:164:LEU:HD13	26:2:169:ILE:HD13	1.93	0.50
80:9:203:PC1:H281	41:H1:180:PRO:HG3	1.94	0.50
30:P1:48:PRO:HA	30:P1:71:LEU:O	2.12	0.50
30:P1:98:GLU:OE1	30:P1:286:ARG:NH2	2.45	0.50
30:P1:258:LEU:HD12	30:P1:259:PRO:HD2	1.94	0.50
30:P1:325:ARG:NH1	30:P1:325:ARG:O	2.44	0.50
45:M1:221:VAL:HG13	45:M1:340:ARG:HE	1.76	0.50
45:M1:313:THR:HA	45:M1:316:MET:SD	2.51	0.50
1:n:230:LEU:HD11	3:p:100:ALA:HA	1.94	0.49
4:q:48:TRP:HZ2	5:r:59:ASN:HA	1.77	0.49
5:r:81:ILE:HG23	9:v:11:MET:HE1	1.94	0.49
14:B:95:LYS:HG3	14:B:110:GLU:HB3	1.94	0.49
15:C:5:ARG:NH1	15:C:15:ASN:OD1	2.42	0.49
23:6:116:GLN:NE2	40:A1:35:ASN:O	2.45	0.49
25:D1:171:PHE:HA	25:D1:174:ARG:HB2	1.94	0.49
27:1:97:ALA:HB1	27:1:111:MET:SD	2.52	0.49
30:P1:157:ARG:NH1	30:P1:163:ALA:O	2.45	0.49
30:P1:169:SER:OG	30:P1:170:ASP:N	2.44	0.49
35:V1:33:ILE:HG12	35:V1:91:ARG:HD3	1.93	0.49
55:e1:94:PRO:HG2	55:e1:97:HIS:HB2	1.94	0.49
58:h1:44:ASN:ND2	76:h1:201:CDL:O1	2.45	0.49
18:F:67:ASP:OD1	18:F:71:ARG:NH2	2.45	0.49
13:L:57:TYR:OH	13:L:137:GLU:OE2	2.28	0.49
59:i1:103:ILE:HB	65:o1:47:ASP:HB3	1.94	0.49
1:n:447:TYR:O	1:n:451:ASN:ND2	2.46	0.49
25:D1:91:ILE:HG12	25:D1:99:ALA:HB1	1.95	0.49
25:D1:238:ARG:NH1	41:H1:279:ARG:O	2.42	0.49
42:J1:129:ASP:HB3	42:J1:135:LEU:HD21	1.94	0.49
34:U1:82:ASP:OD1	64:n1:172:ARG:NH2	2.45	0.49
48:X1:82:THR:HA	48:X1:85:TRP:CD1	2.46	0.49
62:l1:140:GLU:HA	66:p1:122:GLN:HB2	1.94	0.49
5:r:27:TRP:CZ2	6:s:82:ARG:CD	2.96	0.49
14:B:78:LYS:HB2	14:B:129:ALA:HB1	1.93	0.49
14:B:141:ARG:NH2	14:B:186:ILE:O	2.45	0.49
14:M:107:TYR:HB3	14:M:123:LEU:HD11	1.94	0.49
28:3:533:THR:HA	28:3:556:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A1:73:LEU:HD13	42:J1:54:MET:HE1	1.95	0.49
9:v:50:ALA:HB1	9:v:54:ARG:HH12	1.77	0.49
25:D1:117:ALA:HA	25:D1:367:ILE:HG13	1.94	0.49
26:2:52:ASP:OD2	27:1:179:ARG:NH1	2.44	0.49
28:3:377:VAL:HG23	28:3:404:LEU:HD11	1.95	0.49
29:9:23:ALA:HA	52:b1:16:PRO:HG3	1.94	0.49
33:S1:17:GLU:OE2	33:S1:67:ARG:NH1	2.45	0.49
45:M1:201:MET:HG2	80:Y1:201:PC1:H3H2	1.95	0.49
59:i1:84:TYR:HB2	71:i1:201:3PE:H272	1.95	0.49
1:n:5:ARG:HB2	11:y:3:TYR:HE2	1.78	0.49
2:o:200:CYS:SG	2:o:207:MET:HE3	2.52	0.49
9:v:25:GLY:HA2	9:v:28:ILE:HG12	1.94	0.49
15:N:129:MET:HE1	15:N:185:LEU:HD12	1.95	0.49
21:U:43:TYR:O	21:U:47:ASN:ND2	2.45	0.49
23:6:160:PRO:HG3	25:D1:189:MET:HE3	1.95	0.49
46:N1:208:TYR:O	46:N1:212:THR:OG1	2.24	0.49
71:N1:402:3PE:H351	71:N1:402:3PE:H251	1.95	0.49
47:O1:14:THR:HG21	47:O1:116:LEU:HD22	1.94	0.49
1:n:274:VAL:O	1:n:278:MET:HG3	2.12	0.49
3:p:146:TRP:NE1	7:t:14:LYS:HB2	2.28	0.49
13:A:131:ARG:NH2	13:A:177:LEU:O	2.45	0.49
21:U:10:TYR:OH	21:U:15:ARG:NH1	2.46	0.49
45:M1:105:LEU:O	45:M1:109:THR:OG1	2.25	0.49
49:Y1:98:LEU:HD22	71:Y1:203:3PE:H331	1.94	0.49
62:l1:70:MET:HE1	62:l1:76:ILE:HG12	1.94	0.49
5:r:53:ARG:HH22	5:r:96:LEU:HD21	1.78	0.49
15:C:151:SER:HB2	15:C:161:VAL:HG21	1.93	0.49
44:L1:283:LEU:HD13	62:l1:111:MET:HG3	1.93	0.49
45:M1:279:GLN:HG3	45:M1:281:ASP:H	1.77	0.49
1:n:132:LEU:O	1:n:138:HIS:ND1	2.43	0.49
3:p:58:TRP:HA	3:p:61:VAL:HG12	1.93	0.49
6:s:76:HIS:O	6:s:81:GLN:NE2	2.46	0.49
13:A:173:ASN:OD1	13:A:176:ARG:NH2	2.45	0.49
15:C:113:TRP:NE1	15:C:301:LEU:O	2.35	0.49
21:J:52:TRP:O	21:J:56:LYS:HB2	2.11	0.49
71:N:404:3PE:O14	19:R:44:ARG:NH1	2.45	0.49
1:n:425:PHE:HD1	1:n:428:GLN:HG3	1.78	0.49
3:p:194:GLY:HA2	3:p:197:PHE:CE1	2.48	0.49
4:q:68:PHE:O	4:q:71:MET:HG2	2.13	0.49
6:s:83:CYS:HB3	6:s:87:GLY:H	1.77	0.49
23:6:71:HIS:HE1	25:D1:174:ARG:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D1:286:PRO:HG2	25:D1:303:GLU:HG2	1.95	0.49
30:P1:319:ARG:HA	30:P1:322:ARG:HD2	1.95	0.49
44:L1:290:ILE:O	44:L1:523:SER:OG	2.30	0.49
46:N1:220:MET:HE1	71:N1:402:3PE:H11	1.95	0.49
53:c1:7:PRO:HD2	53:c1:10:ALA:HB2	1.95	0.49
60:j1:66:ILE:HD13	65:o1:106:ARG:HB3	1.93	0.49
16:D:1:SER:N	16:D:156:GLN:OE1	2.40	0.48
14:M:246:GLU:O	14:M:427:SER:HA	2.13	0.48
44:L1:485:PHE:O	44:L1:489:THR:OG1	2.28	0.48
47:O1:30:ASN:O	47:O1:126:ARG:NH2	2.46	0.48
34:U1:44:SER:HB3	64:n1:16:LEU:HD11	1.95	0.48
63:m1:47:LEU:HB3	64:n1:165:LEU:HD13	1.95	0.48
1:n:254:ILE:HA	1:n:257:VAL:HG12	1.95	0.48
15:C:184:ILE:HB	15:N:183:PHE:HZ	1.78	0.48
13:L:225:GLU:OE1	64:n1:8:TYR:OH	2.31	0.48
15:N:378:LYS:NZ	18:Q:83:TYR:OH	2.46	0.48
16:O:30:PHE:HE2	16:O:64:LEU:HD21	1.77	0.48
28:3:243:ARG:HD2	28:3:244:THR:HG23	1.96	0.48
40:A1:56:PHE:O	42:J1:69:TYR:OH	2.31	0.48
71:H1:401:3PE:H361	42:J1:37:PHE:HE1	1.78	0.48
44:L1:172:ILE:O	44:L1:176:ARG:HG3	2.12	0.48
44:L1:241:THR:HG21	44:L1:344:GLY:HA3	1.95	0.48
48:X1:7:PRO:HG3	48:X1:56:LEU:HD11	1.94	0.48
67:z:11:GLY:O	67:z:12:VAL:C	2.55	0.48
2:o:189:PRO:HA	2:o:213:MET:HB2	1.94	0.48
18:F:42:ASP:OD2	18:F:101:ARG:NE	2.46	0.48
15:N:5:ARG:NE	76:N:405:CDL:OA4	2.46	0.48
15:N:31:TRP:NE1	77:N:403:HEM:O1D	2.45	0.48
15:N:361:ILE:HA	15:N:365:LEU:HB2	1.94	0.48
27:1:327:THR:HG22	27:1:328:GLY:H	1.77	0.48
28:3:169:VAL:HG21	28:3:191:PHE:HE1	1.78	0.48
44:L1:205:ASN:HA	44:L1:266:LEU:HD23	1.94	0.48
44:L1:419:THR:HA	44:L1:422:TYR:CE2	2.48	0.48
45:M1:347:GLY:HA3	45:M1:419:LEU:HA	1.94	0.48
48:X1:93:MET:HB2	48:X1:95:LEU:HG	1.95	0.48
1:n:443:TYR:O	2:o:134:ARG:NH2	2.46	0.48
7:t:15:ALA:HB3	47:O1:10:LEU:HD22	1.96	0.48
14:B:34:VAL:HG11	14:B:386:ALA:HB1	1.95	0.48
30:P1:191:VAL:HG11	30:P1:242:VAL:HG11	1.95	0.48
34:T1:46:ASP:OD1	36:W1:66:ARG:NH2	2.46	0.48
41:H1:139:THR:O	41:H1:143:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:H1:199:ASP:OD1	41:H1:200:LEU:N	2.42	0.48
42:J1:144:MET:HG2	42:J1:148:ALA:HB3	1.95	0.48
43:K1:80:LYS:HD3	43:K1:80:LYS:HA	1.53	0.48
54:d1:100:ASP:OD2	58:h1:117:ARG:NH2	2.46	0.48
13:A:58:PHE:HD2	13:A:182:LEU:HD21	1.79	0.48
15:N:45:ILE:HG12	77:N:402:HEM:HBB1	1.95	0.48
19:R:39:ARG:NH1	19:R:43:GLU:OE2	2.47	0.48
23:6:47:ILE:HD12	41:H1:57:MET:HG3	1.95	0.48
27:1:154:ARG:HB2	39:s1:52:LEU:HD11	1.95	0.48
41:H1:228:TYR:HA	41:H1:231:ILE:HD12	1.94	0.48
44:L1:574:THR:HG21	46:N1:170:LEU:HD22	1.95	0.48
47:O1:189:PRO:HA	47:O1:192:MET:HE2	1.94	0.48
3:p:95:ALA:HA	3:p:98:PHE:HD2	1.79	0.48
3:p:120:GLY:HA3	7:t:49:TYR:CE2	2.49	0.48
4:q:122:ARG:HG3	10:x:53:TRP:CZ2	2.49	0.48
6:s:67:ASN:ND2	6:s:69:THR:OG1	2.45	0.48
15:C:257:MET:SD	16:D:120:ARG:NH2	2.86	0.48
16:D:41:HIS:CE1	78:D:301:HEC:NA	2.82	0.48
13:L:235:ARG:HH11	17:P:21:SER:HA	1.78	0.48
15:N:51:LEU:O	15:N:55:TYR:CB	2.61	0.48
41:H1:189:THR:HG22	41:H1:234:MET:HE2	1.94	0.48
45:M1:219:ALA:O	45:M1:223:ALA:HB2	2.14	0.48
34:U1:69:LYS:NZ	59:i1:3:TYR:HA	2.29	0.48
67:z:33:VAL:O	67:z:40:TYR:HE2	1.96	0.48
1:n:473:TRP:CH2	67:z:18:GLY:HA3	2.48	0.48
2:o:33:LEU:HD12	9:v:30:ALA:HB1	1.96	0.48
2:o:191:LEU:HD23	2:o:212:GLU:HB3	1.96	0.48
4:q:75:THR:OG1	4:q:77:GLU:OE1	2.29	0.48
13:A:242:ARG:O	19:G:14:ILE:HA	2.14	0.48
13:A:355:THR:O	13:A:359:ASN:ND2	2.47	0.48
71:E:202:3PE:H241	71:E:202:3PE:H321	1.96	0.48
20:S:18:VAL:HG12	20:S:67:VAL:HG22	1.95	0.48
24:C1:165:ASP:N	24:C1:165:ASP:OD1	2.45	0.48
25:D1:379:VAL:HB	25:D1:388:ARG:HB3	1.94	0.48
28:3:324:ASP:HB3	28:3:571:ALA:HB1	1.95	0.48
80:9:203:PC1:H3H2	41:H1:182:ALA:HB1	1.96	0.48
30:P1:21:ALA:HA	30:P1:90:VAL:O	2.13	0.48
41:H1:237:LEU:HA	41:H1:240:ILE:HG22	1.95	0.48
44:L1:371:SER:OG	61:k1:74:LYS:NZ	2.35	0.48
44:L1:574:THR:OG1	46:N1:167:TRP:O	2.29	0.48
56:f1:43:LEU:HD21	66:p1:67:TYR:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:n1:201:ZMP:H17	85:n1:201:ZMP:H15	1.62	0.48
5:r:72:LYS:HZ2	5:r:107:ASP:CG	2.22	0.48
10:x:30:THR:O	10:x:34:THR:OG1	2.32	0.48
31:Q1:60:ASP:N	31:Q1:60:ASP:OD1	2.47	0.48
45:M1:173:THR:HB	58:h1:101:ALA:HB2	1.95	0.48
45:M1:428:PRO:HD3	64:n1:105:TYR:HD2	1.79	0.48
51:a1:41:VAL:HG23	51:a1:44:GLN:H	1.78	0.48
1:n:34:SER:HA	1:n:37:ILE:HD12	1.96	0.48
2:o:123:ILE:HD12	2:o:137:GLU:HB3	1.95	0.48
9:v:52:PHE:O	9:v:56:TYR:CB	2.56	0.48
16:D:171:TYR:HD2	16:D:175:THR:HB	1.79	0.48
30:P1:53:VAL:O	30:P1:57:MET:HB2	2.14	0.48
45:M1:53:SER:OG	45:M1:54:ASN:N	2.47	0.48
46:N1:122:ILE:O	46:N1:176:ARG:NH1	2.45	0.48
48:X1:48:GLU:OE1	52:b1:57:ARG:NH2	2.41	0.48
2:o:83:ILE:HG13	2:o:87:MET:HE3	1.96	0.48
13:A:262:TRP:CG	13:A:385:THR:HG1	2.32	0.48
14:B:195:VAL:O	14:B:199:PHE:HB2	2.13	0.48
14:B:215:VAL:HA	14:B:218:GLN:HG2	1.95	0.48
15:C:237:LEU:HD22	16:D:216:LEU:HD11	1.94	0.48
14:M:287:ARG:HG2	17:T:53:GLU:HB3	1.95	0.48
15:N:185:LEU:HD23	15:N:188:ILE:HD12	1.95	0.48
33:S1:18:ILE:O	33:S1:52:ILE:HA	2.13	0.48
1:n:195:LEU:HD22	1:n:245:ILE:HG12	1.96	0.47
13:A:419:CYS:HA	13:A:438:ARG:HD3	1.95	0.47
25:D1:335:ARG:NH2	29:9:131:ASP:OD1	2.47	0.47
27:1:418:LEU:HD21	27:1:426:LEU:HD21	1.96	0.47
29:9:29:TRP:HB3	29:9:32:LEU:HD12	1.95	0.47
30:P1:177:ARG:O	30:P1:283:LYS:NZ	2.41	0.47
45:M1:403:THR:HA	45:M1:406:TYR:CE2	2.49	0.47
13:A:154:HIS:NE2	13:A:314:TYR:OH	2.36	0.47
16:D:102:ARG:HE	16:D:109:LEU:HB2	1.79	0.47
14:M:312:PHE:HA	17:T:61:ALA:HA	1.95	0.47
29:9:158:ASN:ND2	32:7:34:GLU:OE2	2.47	0.47
30:P1:69:THR:HG21	32:7:26:VAL:HG22	1.96	0.47
40:A1:67:LEU:HD23	43:K1:65:VAL:HA	1.96	0.47
40:A1:73:LEU:O	41:H1:160:TYR:OH	2.30	0.47
42:J1:23:PRO:HG3	42:J1:82:TRP:CE2	2.48	0.47
45:M1:231:LEU:HD23	45:M1:235:LEU:HD12	1.96	0.47
2:o:1:MET:HB2	2:o:193:TYR:HD2	1.79	0.47
6:s:52:SER:O	6:s:94:PRO:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:32:ASN:ND2	76:O:301:CDL:OB9	2.47	0.47
25:D1:151:ILE:O	25:D1:155:THR:OG1	2.28	0.47
30:P1:167:ARG:HH21	30:P1:297:LEU:HD11	1.79	0.47
42:J1:22:LYS:NZ	43:K1:18:GLY:O	2.41	0.47
43:K1:38:LEU:O	43:K1:42:ILE:HG12	2.15	0.47
64:n1:26:LEU:HD22	64:n1:43:MET:HE2	1.96	0.47
1:n:254:ILE:HD13	1:n:344:PHE:CD2	2.49	0.47
3:p:181:TYR:O	71:t:101:3PE:N	2.47	0.47
3:p:190:ASP:HA	7:t:53:ARG:H	1.79	0.47
13:L:122:LEU:O	13:L:179:ARG:NE	2.45	0.47
40:A1:82:ILE:HG23	40:A1:83:LYS:HG3	1.96	0.47
44:L1:257:ILE:HG23	44:L1:317:LEU:HD11	1.96	0.47
47:O1:225:SER:O	47:O1:228:ALA:C	2.57	0.47
64:n1:169:ILE:O	64:n1:172:ARG:NH1	2.48	0.47
5:r:72:LYS:HZ1	5:r:107:ASP:HB3	1.79	0.47
7:t:68:LEU:CD2	71:t:101:3PE:H331	2.45	0.47
11:y:38:PHE:HA	11:y:41:ARG:HG2	1.97	0.47
13:L:238:GLY:H	19:R:22:GLU:CD	2.22	0.47
31:Q1:15:GLU:OE2	36:W1:76:THR:OG1	2.26	0.47
38:r1:10:LEU:HD13	71:r1:201:3PE:H352	1.97	0.47
42:J1:66:VAL:O	42:J1:70:THR:HG23	2.15	0.47
44:L1:341:MET:HE2	44:L1:341:MET:HB3	1.72	0.47
44:L1:396:ILE:HG21	44:L1:490:ALA:HB2	1.96	0.47
14:B:242:GLY:O	14:B:423:SER:HA	2.14	0.47
17:E:53:ASN:O	17:E:57:GLN:HG2	2.14	0.47
13:L:24:ARG:NH1	13:L:383:LEU:O	2.48	0.47
13:L:30:SER:OG	13:L:31:SER:N	2.48	0.47
25:D1:143:GLU:OE2	25:D1:278:TYR:OH	2.27	0.47
54:d1:43:LEU:HG	54:d1:53:VAL:HG12	1.97	0.47
1:n:206:ILE:HA	1:n:209:LEU:HD23	1.96	0.47
2:o:12:ALA:HB2	2:o:21:MET:HE3	1.97	0.47
12:w:20:VAL:HA	12:w:23:LYS:HE3	1.96	0.47
13:L:349:ALA:O	13:L:408:ARG:NH2	2.48	0.47
15:N:9:PRO:HA	15:N:12:LYS:HG2	1.97	0.47
15:N:246:PHE:HB3	15:N:249:MET:HE3	1.96	0.47
19:R:51:PRO:O	19:R:55:VAL:HG23	2.14	0.47
24:C1:169:THR:HG21	24:C1:190:LEU:HD11	1.96	0.47
25:D1:278:TYR:HA	25:D1:281:VAL:HG12	1.97	0.47
27:1:99:GLU:OE2	27:1:104:THR:C	2.58	0.47
28:3:569:LYS:HG3	28:3:571:ALA:HB2	1.96	0.47
38:r1:2:SER:O	76:a1:101:CDL:O1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L1:15:LEU:HD11	44:L1:129:LEU:HD12	1.95	0.47
45:M1:369:LEU:HD12	45:M1:370:PRO:HD2	1.97	0.47
34:U1:17:TYR:OH	61:k1:27:TRP:NE1	2.39	0.47
55:e1:98:SER:OG	55:e1:100:ARG:NH2	2.47	0.47
67:z:4:LYS:HE3	67:z:5:PRO:HG2	1.97	0.47
1:n:40:GLU:HG2	1:n:47:LEU:HB3	1.96	0.47
1:n:419:VAL:O	1:n:423:MET:HG3	2.15	0.47
71:D1:501:3PE:H3A1	80:Y1:201:PC1:H3I3	1.96	0.47
58:h1:115:ARG:HA	58:h1:115:ARG:HD2	1.73	0.47
62:l1:57:ARG:HB2	62:l1:69:ARG:HG2	1.97	0.47
67:z:33:VAL:O	67:z:34:LEU:C	2.56	0.47
1:n:248:LEU:HA	1:n:251:PHE:CD1	2.50	0.47
3:p:255:SER:O	3:p:259:TRP:CB	2.58	0.47
4:q:100:LYS:HE3	10:x:38:ILE:HG22	1.96	0.47
13:L:276:ILE:HB	13:L:345:LEU:HD11	1.95	0.47
82:1:501:FMN:N1	82:1:501:FMN:O3'	2.44	0.47
41:H1:5:ASN:HA	41:H1:8:THR:HG22	1.97	0.47
41:H1:156:MET:HE1	41:H1:178:ALA:HB2	1.97	0.47
46:N1:175:MET:HE2	46:N1:219:LEU:HD21	1.97	0.47
46:N1:186:HIS:O	46:N1:190:MET:HG3	2.15	0.47
54:d1:112:ILE:O	66:p1:159:LYS:NZ	2.48	0.47
58:h1:69:HIS:NE2	76:h1:201:CDL:OA3	2.46	0.47
13:A:277:ILE:HD12	13:A:341:GLN:HB3	1.96	0.47
14:B:163:LEU:HD11	14:B:258:VAL:HG22	1.96	0.47
13:L:145:MET:HE3	13:L:252:HIS:CD2	2.49	0.47
15:N:217:LYS:HD2	19:R:7:LEU:HD13	1.97	0.47
16:O:132:THR:O	20:S:19:ARG:NH2	2.47	0.47
16:O:211:MET:HG3	71:O:302:3PE:H322	1.96	0.47
29:9:74:SER:HA	32:7:47:GLN:HE21	1.80	0.47
44:L1:54:PHE:O	44:L1:58:ASN:ND2	2.48	0.47
47:O1:71:ILE:HG13	47:O1:76:SER:HA	1.97	0.47
67:z:4:LYS:HG2	67:z:7:ARG:NH1	2.28	0.47
67:z:4:LYS:HG2	67:z:7:ARG:HH12	1.78	0.47
1:n:480:ARG:HG2	67:z:6:ALA:CA	2.41	0.46
3:p:72:THR:O	3:p:75:VAL:N	2.48	0.46
6:s:75:LEU:CG	6:s:81:GLN:CD	2.86	0.46
15:C:168:PHE:HB2	17:P:93:GLY:HA3	1.96	0.46
15:C:323:ILE:HD13	71:G:102:3PE:H232	1.98	0.46
14:M:76:THR:HG23	14:M:81:SER:HA	1.96	0.46
17:P:14:ARG:O	19:R:24:ARG:NH1	2.48	0.46
21:U:44:GLU:OE2	21:U:54:HIS:NE2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C1:96:LEU:HB2	24:C1:105:ILE:HG22	1.96	0.46
30:P1:76:ARG:NH2	30:P1:103:ASN:O	2.48	0.46
31:Q1:38:PHE:HE1	31:Q1:58:GLU:HG2	1.78	0.46
44:L1:369:THR:OG1	44:L1:445:GLU:OE1	2.29	0.46
45:M1:58:SER:OG	45:M1:63:THR:OG1	2.32	0.46
46:N1:307:THR:O	47:O1:284:ILE:N	2.48	0.46
3:p:87:ILE:O	3:p:91:VAL:HG23	2.15	0.46
6:s:56:LYS:HE2	6:s:74:TRP:CG	2.49	0.46
7:t:31:ASN:O	7:t:35:LYS:HG2	2.15	0.46
13:L:53:ASN:HB3	13:L:170:PRO:HD2	1.98	0.46
13:L:294:LEU:HB2	13:L:341:GLN:HG3	1.98	0.46
26:2:51:LEU:HD21	26:2:84:ALA:HB2	1.96	0.46
28:3:444:LYS:HA	28:3:481:THR:HG22	1.97	0.46
41:H1:70:LEU:HD23	41:H1:73:ILE:HD11	1.98	0.46
45:M1:382:THR:HG23	45:M1:396:MET:HG2	1.97	0.46
34:U1:35:HIS:CG	34:U1:38:LYS:HD2	2.50	0.46
59:i1:83:TYR:OH	66:p1:48:ARG:NH1	2.42	0.46
61:k1:54:GLU:OE2	64:n1:33:ARG:NE	2.46	0.46
4:q:86:MET:HE1	10:x:22:ALA:HA	1.96	0.46
6:s:23:ILE:HA	6:s:26:GLN:HG3	1.97	0.46
13:A:46:ARG:HG2	13:A:231:LEU:HD22	1.97	0.46
17:E:65:SER:OG	17:E:67:ASP:OD1	2.30	0.46
13:L:173:ASN:O	13:L:177:LEU:HB2	2.16	0.46
29:9:74:SER:HB2	32:7:47:GLN:HG3	1.97	0.46
1:n:309:THR:HA	1:n:312:ILE:HG22	1.97	0.46
14:B:157:THR:O	14:B:161:GLU:HG2	2.15	0.46
15:N:51:LEU:O	15:N:55:TYR:HB3	2.16	0.46
28:3:28:GLN:NE2	31:Q1:114:LYS:O	2.47	0.46
28:3:142:ILE:O	28:3:191:PHE:N	2.48	0.46
29:9:67:HIS:H	29:9:115:MET:HE1	1.79	0.46
41:H1:86:TRP:CD1	41:H1:233:LEU:HD12	2.50	0.46
42:J1:131:VAL:HG23	51:a1:43:TYR:HD1	1.80	0.46
44:L1:83:ASP:OD1	44:L1:84:PHE:N	2.48	0.46
44:L1:161:ARG:HH12	44:L1:163:ASP:HB2	1.81	0.46
44:L1:511:LEU:HD22	61:k1:40:LYS:HE2	1.97	0.46
46:N1:221:LEU:HD11	46:N1:240:MET:HE1	1.97	0.46
2:o:52:HIS:CG	5:r:40:ASP:HB2	2.51	0.46
3:p:42:LEU:HD22	12:w:49:LEU:HD12	1.97	0.46
13:A:159:GLN:O	13:A:235:ARG:NH2	2.39	0.46
13:A:354:VAL:HG21	13:A:404:ALA:HA	1.96	0.46
13:L:276:ILE:HG21	13:L:345:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L1:59:MET:HE1	59:i1:101:PRO:HA	1.96	0.46
59:i1:76:ILE:HG22	59:i1:80:PHE:HE1	1.81	0.46
1:n:431:LEU:HD13	1:n:436:MET:HE2	1.96	0.46
2:o:170:LEU:HD21	2:o:184:VAL:HG12	1.96	0.46
10:x:47:ARG:HG3	10:x:48:VAL:HG13	1.97	0.46
13:A:314:TYR:HB2	13:A:317:THR:HG23	1.98	0.46
14:B:293:SER:HB2	14:B:296:SER:HB2	1.97	0.46
20:H:29:VAL:HA	20:H:32:ARG:HB3	1.98	0.46
13:L:270:LEU:HB3	13:L:320:LEU:HD11	1.97	0.46
23:6:119:GLU:HG3	40:A1:28:ASN:HB3	1.97	0.46
27:1:42:TRP:CD2	27:1:161:LEU:HD13	2.50	0.46
27:1:118:LEU:HD13	27:1:225:VAL:HG13	1.97	0.46
28:3:255:HIS:HD2	28:3:257:ASP:H	1.64	0.46
31:Q1:33:ARG:NH1	31:Q1:60:ASP:OD1	2.47	0.46
32:7:19:ASP:N	32:7:22:ASP:OD2	2.39	0.46
40:A1:85:SER:O	40:A1:89:ILE:HG12	2.16	0.46
62:l1:73:GLY:HA3	63:m1:42:LEU:HD22	1.97	0.46
2:o:196:CYS:HB2	2:o:207:MET:HG3	1.98	0.46
3:p:159:MET:HE1	6:s:7:VAL:HB	1.98	0.46
5:r:82:TYR:O	5:r:85:VAL:HB	2.16	0.46
11:y:1:SER:OG	11:y:2:HIS:N	2.49	0.46
13:L:21:ASN:ND2	13:L:217:SER:O	2.49	0.46
23:6:72:MET:HE3	23:6:79:MET:HE2	1.96	0.46
23:6:94:ASP:O	23:6:121:ARG:HA	2.16	0.46
80:6:203:PC1:H3A1	41:H1:57:MET:HE1	1.97	0.46
25:D1:115:GLU:OE1	25:D1:194:ILE:N	2.47	0.46
27:1:25:LEU:HD21	27:1:267:THR:HG22	1.97	0.46
27:1:95:VAL:HB	27:1:136:ILE:HA	1.98	0.46
27:1:306:LEU:HD22	27:1:343:ILE:HD11	1.97	0.46
28:3:228:ILE:HB	28:3:583:THR:HG22	1.96	0.46
28:3:399:TRP:O	31:Q1:127:ARG:NH1	2.41	0.46
30:P1:130:ILE:HG12	30:P1:164:ILE:HB	1.98	0.46
41:H1:158:GLY:HA3	41:H1:315:PRO:HB2	1.98	0.46
46:N1:309:ASN:HD22	47:O1:95:ARG:HG2	1.81	0.46
3:p:156:ARG:HH22	3:p:223:LEU:HA	1.80	0.46
6:s:55:ASN:HA	6:s:77:LYS:HG3	1.98	0.46
14:B:275:LEU:HB2	14:B:410:VAL:HG13	1.98	0.46
15:N:362:ILE:HG23	15:N:363:LEU:HD12	1.97	0.46
30:P1:335:LYS:HA	30:P1:335:LYS:HD2	1.80	0.46
40:A1:65:PHE:O	40:A1:69:ILE:HG12	2.16	0.46
43:K1:27:MET:HE1	43:K1:75:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L1:131:LEU:HD12	44:L1:140:LEU:HD12	1.98	0.46
47:O1:51:TYR:HB2	47:O1:124:LEU:HD23	1.97	0.46
34:U1:65:ILE:O	34:U1:69:LYS:HB2	2.15	0.46
2:o:98:LYS:HG2	2:o:153:LEU:HB2	1.98	0.46
15:C:138:MET:HE2	15:C:269:LYS:H	1.80	0.46
16:D:2:ASP:N	16:D:2:ASP:OD1	2.46	0.46
16:D:10:TYR:O	16:D:15:ARG:NE	2.47	0.46
21:J:27:GLY:O	21:J:31:PHE:HB3	2.16	0.46
13:L:395:TRP:O	13:L:399:ILE:HG12	2.16	0.46
18:Q:42:ASP:OD2	18:Q:101:ARG:NH1	2.48	0.46
23:6:52:ARG:NH2	71:6:202:3PE:O32	2.49	0.46
25:D1:284:ASP:OD1	29:9:1:THR:OG1	2.29	0.46
26:2:108:CYS:HA	26:2:151:ALA:HB1	1.97	0.46
31:Q1:42:ARG:HG3	31:Q1:49:VAL:HG12	1.97	0.46
33:S1:62:PRO:HG2	33:S1:79:ASN:HA	1.96	0.46
44:L1:258:PHE:O	44:L1:262:ARG:HG2	2.14	0.46
34:U1:44:SER:OG	85:n1:201:ZMP:O7	2.31	0.46
64:n1:175:GLU:HG2	64:n1:176:ARG:HH11	1.81	0.46
1:n:209:LEU:HA	1:n:212:ASP:HB2	1.98	0.46
3:p:136:VAL:HG23	3:p:169:LEU:HG	1.98	0.46
4:q:33:LEU:O	4:q:38:LYS:NZ	2.38	0.46
21:J:33:ARG:HD3	22:K:51:LYS:HD3	1.98	0.46
14:M:242:GLY:O	14:M:423:SER:HA	2.16	0.46
16:O:23:HIS:ND1	16:O:54:VAL:O	2.44	0.46
23:6:96:MET:HE3	23:6:110:LEU:HD11	1.98	0.46
41:H1:317:TYR:OH	42:J1:136:GLU:OE2	2.29	0.46
65:o1:34:LYS:HD3	65:o1:34:LYS:HA	1.72	0.46
1:n:413:HIS:HB2	1:n:471:MET:HE1	1.96	0.45
1:n:485:VAL:HG11	1:n:494:TRP:HB3	1.97	0.45
71:n:605:3PE:H231	71:n:605:3PE:H331	1.98	0.45
12:w:28:ASP:OD1	12:w:28:ASP:N	2.49	0.45
13:A:70:ARG:HB3	13:A:74:ALA:HB3	1.98	0.45
13:A:329:MET:HE3	13:A:329:MET:HB3	1.86	0.45
14:M:133:ARG:HB2	14:M:136:GLU:HG3	1.98	0.45
23:6:76:ARG:NH1	25:D1:179:GLU:OE2	2.38	0.45
41:H1:316:PRO:HG3	50:Z1:56:ARG:HB3	1.98	0.45
44:L1:366:MET:HE2	44:L1:443:ILE:HG12	1.96	0.45
49:Y1:13:ASP:HA	49:Y1:20:LYS:HE3	1.97	0.45
66:p1:107:GLU:HA	66:p1:110:LYS:HE2	1.98	0.45
1:n:347:LEU:HA	1:n:350:VAL:HG12	1.97	0.45
1:n:443:TYR:HB2	1:n:447:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:478:SER:HA	67:z:8:GLU:O	2.16	0.45
1:n:510:TYR:N	6:s:57:ARG:HH12	2.13	0.45
20:H:26:GLU:HA	20:H:29:VAL:HG12	1.98	0.45
30:P1:25:GLY:HA3	30:P1:94:LEU:HB2	1.98	0.45
44:L1:124:PHE:HE1	44:L1:147:VAL:HG13	1.81	0.45
1:n:32:ALA:HB3	11:y:36:PRO:HG2	1.98	0.45
1:n:202:LEU:HB2	1:n:238:PHE:CG	2.52	0.45
2:o:178:ARG:HA	8:u:26:THR:HG21	1.99	0.45
13:A:439:SER:HB3	71:A:501:3PE:H111	1.97	0.45
16:D:208:MET:HA	71:E:202:3PE:H231	1.98	0.45
13:L:64:PHE:HA	13:L:75:LEU:HD11	1.98	0.45
16:O:71:GLN:HE21	16:O:80:MET:HG3	1.82	0.45
17:P:16:ALA:HA	17:P:19:LEU:HD12	1.99	0.45
28:3:324:ASP:OD1	28:3:324:ASP:N	2.46	0.45
47:O1:135:LEU:HD22	47:O1:152:TYR:CD1	2.51	0.45
4:q:68:PHE:C	4:q:71:MET:HG2	2.40	0.45
14:B:23:ASP:OD1	14:B:23:ASP:N	2.49	0.45
15:C:49:LEU:HG	15:C:53:MET:HE2	1.99	0.45
30:P1:82:ARG:HA	30:P1:85:VAL:HG22	1.98	0.45
30:P1:137:ALA:HB2	30:P1:146:LEU:HD22	1.98	0.45
36:W1:37:LEU:HD21	36:W1:88:GLY:HA3	1.96	0.45
41:H1:260:MET:SD	51:a1:13:GLY:HA2	2.56	0.45
45:M1:145:ALA:HA	45:M1:218:LYS:HD3	1.98	0.45
45:M1:257:MET:HE2	45:M1:257:MET:HB2	1.81	0.45
1:n:227:ASP:OD2	1:n:230:LEU:N	2.49	0.45
14:B:47:ILE:HG12	14:B:116:ILE:HD11	1.99	0.45
17:E:67:ASP:OD1	17:E:68:VAL:N	2.50	0.45
25:D1:111:MET:HB2	25:D1:111:MET:HE2	1.83	0.45
28:3:252:PRO:HB3	28:3:263:ILE:HG23	1.99	0.45
30:P1:108:ASP:OD1	30:P1:112:ASN:ND2	2.47	0.45
44:L1:67:HIS:NE2	44:L1:70:THR:OG1	2.45	0.45
44:L1:293:LEU:HD21	44:L1:418:MET:HB3	1.99	0.45
1:n:229:ILE:HD11	2:o:175:ILE:HD13	1.98	0.45
13:A:222:VAL:HG12	13:A:224:GLU:H	1.81	0.45
15:C:8:HIS:O	15:C:12:LYS:N	2.46	0.45
15:C:233:LEU:HG	16:D:212:MET:HE1	1.98	0.45
16:D:152:TYR:OH	20:H:64:ASP:OD2	2.35	0.45
21:J:18:SER:HB2	22:K:23:MET:HB3	1.99	0.45
14:M:162:ASN:HB3	14:M:244:ILE:HD11	1.99	0.45
14:M:411:VAL:HG12	14:M:415:LYS:HE3	1.99	0.45
16:O:18:LEU:HD13	16:O:206:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:R:104:3PE:H11	63:m1:84:LYS:HG3	1.99	0.45
37:q1:2:GLU:OE2	38:r1:4:THR:OG1	2.27	0.45
41:H1:53:MET:O	41:H1:57:MET:HG2	2.17	0.45
45:M1:104:ILE:O	45:M1:108:MET:HG3	2.16	0.45
45:M1:106:LEU:HD13	45:M1:234:ILE:HG21	1.98	0.45
45:M1:410:MET:O	45:M1:414:THR:OG1	2.25	0.45
47:O1:45:GLN:HG3	47:O1:235:VAL:HG11	1.98	0.45
47:O1:97:GLN:NE2	47:O1:131:ASP:OD2	2.48	0.45
34:U1:51:ILE:O	34:U1:55:GLU:HG3	2.16	0.45
49:Y1:72:THR:HA	49:Y1:75:VAL:HG12	1.98	0.45
54:d1:18:ALA:HA	54:d1:21:LEU:HD23	1.98	0.45
67:z:4:LYS:HG3	67:z:5:PRO:CD	2.47	0.45
4:q:79:LYS:HB2	10:x:18:LEU:HD11	1.98	0.45
13:L:148:VAL:HG22	17:P:2:HIS:CG	2.52	0.45
13:L:366:VAL:HG11	14:M:43:PRO:HB2	1.99	0.45
16:O:158:ILE:HG23	16:O:160:MET:H	1.82	0.45
16:O:166:THR:HG22	16:O:167:GLU:OE1	2.17	0.45
24:C1:147:ASP:OD1	24:C1:147:ASP:N	2.49	0.45
26:2:156:ILE:HB	26:2:161:TYR:HE2	1.81	0.45
45:M1:171:VAL:HG11	45:M1:179:LEU:HD21	1.98	0.45
55:e1:96:HIS:HA	55:e1:101:GLU:HB3	1.99	0.45
66:p1:105:ILE:HG21	66:p1:134:VAL:HG11	1.97	0.45
7:t:12:MET:CG	47:O1:10:LEU:CD1	2.79	0.45
16:O:152:TYR:OH	20:S:64:ASP:OD2	2.27	0.45
24:C1:69:ASN:ND2	38:r1:94:VAL:O	2.50	0.45
27:1:93:LEU:O	27:1:134:ALA:HA	2.17	0.45
28:3:632:ARG:HH21	33:S1:60:VAL:HG13	1.82	0.45
39:s1:34:ASN:O	39:s1:37:HIS:ND1	2.39	0.45
42:J1:24:SER:OG	42:J1:80:GLU:N	2.50	0.45
66:p1:74:THR:OG1	66:p1:75:GLU:OE1	2.34	0.45
1:n:92:MET:HE2	1:n:92:MET:HB3	1.77	0.45
3:p:149:HIS:CE1	7:t:9:SER:HB2	2.51	0.45
13:A:155:ALA:HA	13:A:164:ALA:HB1	1.99	0.45
14:B:366:ALA:O	14:B:370:MET:HG3	2.16	0.45
22:K:14:ALA:O	22:K:18:ILE:HG12	2.17	0.45
42:J1:21:LEU:HD22	71:K1:201:3PE:H252	1.98	0.45
44:L1:525:LEU:HD11	62:l1:94:PRO:HG2	1.98	0.45
44:L1:576:LEU:HD11	76:Y1:202:CDL:H521	1.99	0.45
45:M1:17:LEU:HD11	76:N1:401:CDL:H141	1.98	0.45
45:M1:329:LEU:HD22	45:M1:359:TRP:CD1	2.52	0.45
46:N1:246:LEU:HD12	46:N1:257:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N1:269:GLU:HA	46:N1:272:LYS:HB2	1.98	0.45
15:C:312:GLN:NE2	15:C:317:PHE:HB2	2.32	0.45
15:N:332:LEU:HD13	71:N:404:3PE:H2C1	1.98	0.45
28:3:157:THR:HA	28:3:160:ILE:HD12	1.99	0.45
28:3:201:ASP:OD2	28:3:268:ARG:NH2	2.45	0.45
33:S1:41:VAL:HG12	33:S1:45:LYS:HZ2	1.81	0.45
46:N1:193:ILE:HG12	46:N1:266:ILE:HG12	1.98	0.45
59:i1:3:TYR:HB3	59:i1:8:LYS:HB2	1.99	0.45
63:m1:124:PHE:HA	66:p1:135:THR:HG21	1.98	0.45
65:o1:21:ILE:HG23	65:o1:104:GLU:HG2	1.98	0.45
3:p:217:VAL:HA	3:p:220:LEU:HG	1.99	0.44
14:B:95:LYS:HB3	17:T:24:GLY:HA2	1.98	0.44
15:C:60:MET:HE3	15:C:60:MET:HB3	1.87	0.44
15:C:377:LEU:HG	18:F:20:TYR:HE2	1.81	0.44
13:L:438:ARG:HA	13:L:441:MET:HB2	1.99	0.44
24:C1:75:LEU:HD23	24:C1:126:ALA:HB3	2.00	0.44
29:9:66:GLU:OE1	29:9:138:ASN:ND2	2.38	0.44
34:T1:24:LYS:HE3	34:T1:24:LYS:HB2	1.79	0.44
44:L1:4:PHE:HE1	44:L1:82:THR:HG21	1.81	0.44
45:M1:429:SER:O	57:g1:36:TYR:OH	2.29	0.44
47:O1:38:LEU:HD12	47:O1:231:PRO:HB3	1.99	0.44
49:Y1:36:SER:HB2	49:Y1:55:VAL:HA	1.98	0.44
1:n:170:ASN:ND2	3:p:78:GLY:HA3	2.32	0.44
15:C:240:MET:HA	15:C:243:VAL:HB	2.00	0.44
13:L:86:LEU:HB3	14:M:285:ILE:HG12	1.99	0.44
25:D1:402:LEU:HA	25:D1:421:GLN:HE22	1.82	0.44
32:7:36:ASN:HD22	32:7:36:ASN:HA	1.64	0.44
41:H1:149:ILE:HG23	41:H1:181:MET:HG3	2.00	0.44
41:H1:301:CYS:O	41:H1:305:ILE:HD12	2.17	0.44
42:J1:56:PHE:O	42:J1:60:LEU:HD23	2.17	0.44
44:L1:152:PHE:HB2	44:L1:172:ILE:HD11	2.00	0.44
14:B:61:ASN:O	14:B:182:ARG:NH1	2.51	0.44
14:B:187:THR:HG22	14:B:190:GLU:HG3	2.00	0.44
15:C:316:MET:HG2	15:C:317:PHE:CE1	2.53	0.44
16:O:20:SER:OG	16:O:21:LEU:N	2.50	0.44
17:P:144:CYS:HB3	17:P:160:CYS:HB2	1.94	0.44
27:1:101:GLU:OE1	27:1:303:SER:N	2.49	0.44
29:9:119:ILE:HG13	29:9:121:CYS:HB3	1.99	0.44
43:K1:33:LEU:O	43:K1:37:VAL:HG23	2.18	0.44
43:K1:89:TYR:HD2	43:K1:91:GLN:HE22	1.65	0.44
44:L1:364:LYS:HE2	61:k1:66:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M1:281:ASP:HB3	45:M1:284:SER:HB2	1.99	0.44
47:O1:36:ASN:OD1	47:O1:37:LYS:N	2.50	0.44
55:e1:64:GLU:OE2	55:e1:71:THR:OG1	2.33	0.44
1:n:247:ILE:HG23	1:n:248:LEU:HD23	1.99	0.44
14:B:257:ILE:HG13	14:B:424:MET:HG3	1.99	0.44
16:O:195:GLU:OE2	16:O:201:ARG:NE	2.50	0.44
25:D1:175:GLU:OE1	25:D1:188:ARG:NH2	2.50	0.44
27:1:268:VAL:HG21	27:1:283:HIS:CG	2.52	0.44
28:3:453:LEU:HB3	28:3:492:ILE:HD13	1.99	0.44
30:P1:109:VAL:HA	30:P1:113:ILE:HD12	1.99	0.44
44:L1:540:LYS:HE3	44:L1:540:LYS:HB3	1.84	0.44
46:N1:49:ASN:O	46:N1:52:SER:OG	2.33	0.44
50:Z1:57:ARG:HH21	52:b1:48:THR:HG21	1.81	0.44
67:z:22:CYS:HB3	67:z:26:CYS:SG	2.57	0.44
1:n:445:ASP:O	1:n:448:THR:OG1	2.32	0.44
7:t:43:ARG:HD2	7:t:81:TYR:CE1	2.53	0.44
13:A:219:VAL:HG23	13:A:220:SER:H	1.81	0.44
13:L:227:ALA:HA	63:m1:24:VAL:HG13	1.99	0.44
13:L:379:ILE:HG12	13:L:389:ARG:HD3	2.00	0.44
25:D1:149:ASN:OD1	25:D1:371:LYS:NZ	2.37	0.44
26:2:34:ILE:HD13	26:2:49:PRO:HB2	1.99	0.44
28:3:349:PHE:H	28:3:509:PRO:HB2	1.82	0.44
29:9:27:LEU:HD22	80:9:203:PC1:H251	1.99	0.44
29:9:43:LEU:HB2	41:H1:31:MET:SD	2.58	0.44
30:P1:194:VAL:HG21	30:P1:260:LEU:HD13	2.00	0.44
36:W1:64:LYS:HA	36:W1:64:LYS:HD2	1.85	0.44
45:M1:165:ILE:HG21	46:N1:268:THR:HA	1.99	0.44
47:O1:59:SER:HA	47:O1:62:THR:HG22	1.99	0.44
80:Y1:201:PC1:H222	80:Y1:201:PC1:H332	1.98	0.44
67:z:4:LYS:HG2	67:z:7:ARG:CZ	2.47	0.44
3:p:167:ILE:HG23	3:p:171:LEU:HD23	1.98	0.44
4:q:67:SER:H	4:q:70:GLU:HG3	1.82	0.44
23:6:65:CYS:HB3	23:6:126:MET:SD	2.58	0.44
25:D1:405:MET:HE2	25:D1:405:MET:HB3	1.84	0.44
46:N1:3:PRO:HG2	47:O1:9:ILE:HD13	1.99	0.44
47:O1:295:SER:HA	47:O1:298:GLU:HG2	2.00	0.44
54:d1:91:PHE:O	54:d1:95:LYS:HG2	2.18	0.44
62:l1:64:ASP:OD1	63:m1:43:LYS:NZ	2.43	0.44
1:n:420:GLY:O	1:n:424:THR:OG1	2.30	0.44
1:n:507:GLU:HA	3:p:5:THR:HB	1.99	0.44
8:u:75:ARG:HG3	8:u:80:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:165:TRP:O	15:C:174:THR:OG1	2.32	0.44
28:3:160:ILE:HD11	28:3:183:VAL:HG13	1.99	0.44
28:3:468:VAL:HG11	28:3:652:VAL:HB	2.00	0.44
30:P1:172:PHE:HB2	30:P1:179:LEU:HG	1.98	0.44
32:7:5:SER:HB3	32:7:17:VAL:HG21	2.00	0.44
35:V1:91:ARG:NH1	47:O1:227:GLU:OE2	2.51	0.44
47:O1:136:GLU:O	47:O1:140:ASN:ND2	2.51	0.44
1:n:53:ILE:HD12	11:y:43:GLN:HB2	1.99	0.44
14:B:48:GLY:HA3	14:B:379:LEU:HD21	1.99	0.44
13:L:158:PHE:O	13:L:161:THR:OG1	2.26	0.44
13:L:232:THR:HB	17:P:22:THR:HG23	2.00	0.44
20:S:19:ARG:HG2	20:S:63:ARG:HD3	2.00	0.44
25:D1:417:ILE:HA	25:D1:420:THR:HG22	1.99	0.44
44:L1:538:PRO:HB2	62:l1:88:VAL:HG22	1.99	0.44
46:N1:21:MET:HB3	55:e1:3:LEU:HG	2.00	0.44
48:X1:23:VAL:HG22	48:X1:85:TRP:CD2	2.52	0.44
59:i1:109:ILE:HG22	59:i1:112:THR:H	1.82	0.44
1:n:55:ASN:HA	1:n:58:VAL:HG22	2.00	0.44
1:n:64:VAL:HA	1:n:68:PHE:HB2	1.99	0.44
1:n:175:ALA:HB2	6:s:36:PRO:HB3	2.00	0.44
3:p:34:TRP:HZ2	7:t:61:TRP:HE3	1.64	0.44
24:C1:207:PRO:HB3	24:C1:210:ARG:HH12	1.83	0.44
28:3:32:LYS:HE2	28:3:32:LYS:HB2	1.85	0.44
29:9:38:MET:HE2	29:9:38:MET:HB2	1.87	0.44
30:P1:149:LYS:NZ	84:P1:501:NDP:O2D	2.50	0.44
43:K1:1:FME:HE3	43:K1:1:FME:HB2	1.76	0.44
46:N1:102:LEU:HD13	46:N1:142:LEU:HG	1.99	0.44
46:N1:216:PHE:O	46:N1:220:MET:HG3	2.17	0.44
50:Z1:58:ARG:NH1	52:b1:80:LEU:O	2.51	0.44
51:a1:4:GLU:OE1	51:a1:4:GLU:N	2.50	0.44
1:n:52:GLN:NE2	1:n:120:ALA:O	2.51	0.43
2:o:129:LYS:HG2	2:o:130:PRO:HD2	2.00	0.43
3:p:151:LEU:HD23	3:p:159:MET:SD	2.58	0.43
3:p:259:TRP:CD2	53:c1:33:GLN:OE1	2.71	0.43
5:r:82:TYR:O	5:r:85:VAL:N	2.51	0.43
13:L:8:LEU:HD22	13:L:392:LEU:HB3	1.99	0.43
13:L:36:THR:HG21	13:L:373:THR:HA	2.00	0.43
14:M:68:LEU:HD13	14:M:144:LEU:HD11	2.00	0.43
15:N:232:ILE:O	15:N:235:MET:HB3	2.18	0.43
41:H1:2:PHE:O	41:H1:6:ILE:HG12	2.18	0.43
41:H1:70:LEU:HA	41:H1:73:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L1:78:MET:HE1	71:i1:201:3PE:H362	1.99	0.43
44:L1:327:LEU:O	44:L1:331:THR:HG23	2.18	0.43
44:L1:349:SER:HB2	44:L1:366:MET:HE1	2.00	0.43
45:M1:331:ASN:O	45:M1:335:GLU:HG3	2.17	0.43
46:N1:298:TYR:O	46:N1:303:THR:OG1	2.32	0.43
51:a1:55:SER:HB2	51:a1:62:VAL:HG23	2.00	0.43
57:g1:62:PHE:HA	57:g1:66:ILE:HG12	1.99	0.43
66:p1:98:ASP:OD2	66:p1:141:ARG:NH1	2.51	0.43
1:n:201:VAL:HG11	1:n:237:PHE:HD2	1.83	0.43
23:6:101:THR:HA	23:6:129:CYS:HB3	1.99	0.43
28:3:190:MET:HE3	28:3:190:MET:HB3	1.84	0.43
29:9:51:ASN:O	29:9:55:GLU:N	2.50	0.43
30:P1:13:ARG:NH2	30:P1:63:GLY:O	2.51	0.43
36:W1:64:LYS:HE2	36:W1:108:PHE:HB3	1.99	0.43
36:W1:92:LEU:O	36:W1:96:ILE:HG12	2.19	0.43
44:L1:54:PHE:CZ	44:L1:84:PHE:HB2	2.54	0.43
45:M1:30:TYR:O	45:M1:34:ILE:HG12	2.18	0.43
50:Z1:93:GLU:HG2	55:e1:78:ILE:HD11	2.00	0.43
1:n:50:ASP:OD1	11:y:47:LYS:NZ	2.47	0.43
3:p:77:LYS:HD2	3:p:77:LYS:HA	1.80	0.43
3:p:126:PRO:HB3	3:p:257:TYR:HB3	2.00	0.43
3:p:212:SER:O	3:p:216:ILE:HG12	2.19	0.43
13:A:48:GLU:O	13:A:165:GLN:NE2	2.50	0.43
16:D:191:ARG:NH1	16:D:195:GLU:OE1	2.52	0.43
13:L:377:GLU:OE2	13:L:381:ARG:NE	2.50	0.43
16:O:1:SER:OG	16:O:156:GLN:OE1	2.36	0.43
16:O:33:TYR:HD1	16:O:37:CYS:HB2	1.83	0.43
16:O:203:ARG:NH1	21:U:40:ASP:OD1	2.51	0.43
27:1:185:ILE:HG12	27:1:359:CYS:HB3	2.00	0.43
31:Q1:54:LYS:HA	31:Q1:54:LYS:HD3	1.83	0.43
31:Q1:93:ILE:HD11	31:Q1:105:VAL:HG21	2.00	0.43
34:T1:27:PRO:HA	34:T1:30:LEU:HB3	2.00	0.43
34:T1:49:GLU:OE2	36:W1:38:TYR:OH	2.32	0.43
40:A1:93:ILE:O	40:A1:97:ILE:HG12	2.17	0.43
41:H1:142:TYR:CZ	41:H1:192:GLU:HA	2.53	0.43
44:L1:383:MET:HB3	44:L1:386:LEU:HD12	2.00	0.43
44:L1:549:SER:OG	44:L1:550:LEU:N	2.51	0.43
76:Y1:202:CDL:H211	76:Y1:202:CDL:H382	2.00	0.43
60:j1:38:TRP:HD1	60:j1:39:ARG:HD2	1.82	0.43
64:n1:118:PHE:O	64:n1:122:GLU:HG2	2.18	0.43
7:t:69:PHE:HD2	71:t:101:3PE:H11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:245:ARG:HB3	14:M:430:LEU:HD22	2.01	0.43
15:N:365:LEU:HD23	15:N:365:LEU:HA	1.88	0.43
26:2:123:LYS:NZ	26:2:174:ASP:OD1	2.39	0.43
41:H1:138:GLN:HG2	41:H1:142:TYR:HE2	1.83	0.43
45:M1:275:ILE:O	45:M1:279:GLN:HB2	2.19	0.43
6:s:17:LEU:HA	6:s:20:GLU:HG3	2.00	0.43
9:v:16:ALA:O	9:v:20:ARG:HG2	2.18	0.43
13:A:27:SER:HA	13:A:199:ALA:O	2.18	0.43
14:B:49:LEU:HD23	14:B:127:THR:HG21	2.01	0.43
13:L:444:LEU:HA	21:U:17:THR:HG21	2.01	0.43
14:M:52:LYS:HE3	14:M:203:ARG:HD2	1.99	0.43
15:N:239:LEU:HG	15:N:240:MET:HE3	2.01	0.43
20:S:14:PRO:HA	20:S:17:THR:HG22	2.01	0.43
24:C1:164:LYS:NZ	25:D1:92:GLU:OE2	2.39	0.43
30:P1:57:MET:HB2	30:P1:57:MET:HE2	1.79	0.43
30:P1:215:VAL:O	30:P1:218:THR:OG1	2.27	0.43
44:L1:534:HIS:ND1	71:L1:701:3PE:O12	2.45	0.43
46:N1:183:SER:O	46:N1:187:MET:HG2	2.17	0.43
47:O1:223:TYR:OH	47:O1:237:ASP:OD2	2.37	0.43
80:Y1:201:PC1:H242	80:Y1:201:PC1:H352	2.00	0.43
50:Z1:67:ARG:HG3	51:a1:43:TYR:CZ	2.53	0.43
53:c1:41:GLU:HA	53:c1:44:ARG:HG2	1.99	0.43
1:n:347:LEU:HD13	1:n:383:MET:SD	2.59	0.43
4:q:68:PHE:HE1	5:r:66:ARG:HE	1.67	0.43
14:B:152:PHE:O	14:B:158:ARG:NH1	2.52	0.43
18:F:75:LEU:HD13	18:F:79:GLN:HG2	2.00	0.43
19:G:51:PRO:O	19:G:55:VAL:HG23	2.17	0.43
25:D1:194:ILE:HA	25:D1:199:VAL:HG12	1.99	0.43
25:D1:323:ILE:HG23	25:D1:324:LYS:HG3	1.99	0.43
37:q1:88:ARG:HA	37:q1:93:MET:HE2	2.00	0.43
45:M1:130:LEU:HD12	45:M1:150:LEU:HB2	2.01	0.43
46:N1:272:LYS:HG2	58:h1:108:GLN:NE2	2.33	0.43
4:q:123:MET:HE2	4:q:134:PHE:CD2	2.54	0.43
11:y:14:SER:OG	11:y:16:GLU:OE1	2.37	0.43
16:D:207:LYS:HD3	21:J:35:PHE:HE1	1.84	0.43
13:L:272:VAL:O	13:L:276:ILE:HG12	2.18	0.43
15:N:107:TYR:HB2	15:N:305:PRO:HG3	2.00	0.43
25:D1:130:PRO:HG2	25:D1:135:GLN:HG3	2.01	0.43
27:1:322:LEU:HD12	27:1:329:LEU:HB2	2.01	0.43
45:M1:287:ALA:O	45:M1:291:VAL:HG23	2.19	0.43
45:M1:376:MET:HE2	45:M1:376:MET:HB3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N1:240:MET:HE3	54:d1:48:LEU:HD22	2.01	0.43
48:X1:136:LEU:HD12	48:X1:137:PRO:HD2	2.00	0.43
53:c1:33:GLN:O	53:c1:37:GLU:OE1	2.36	0.43
67:z:28:LEU:O	67:z:29:PRO:C	2.62	0.43
1:n:183:LEU:HD11	1:n:273:MET:HG3	2.00	0.43
13:A:237:THR:HG22	13:A:239:SER:HB3	2.01	0.43
15:C:4:MET:HE2	15:C:4:MET:HB2	1.96	0.43
16:D:41:HIS:CE1	78:D:301:HEC:ND	2.86	0.43
80:6:203:PC1:H3D2	41:H1:57:MET:HE1	2.00	0.43
41:H1:293:PHE:O	41:H1:297:THR:HG23	2.18	0.43
44:L1:306:THR:HG23	44:L1:332:HIS:CE1	2.53	0.43
45:M1:196:TRP:HE1	45:M1:254:THR:HB	1.83	0.43
48:X1:43:MET:HG3	52:b1:52:TYR:CZ	2.54	0.43
54:d1:3:ASN:OD1	54:d1:3:ASN:N	2.51	0.43
62:l1:93:THR:OG1	62:l1:95:VAL:O	2.32	0.43
1:n:368:HIS:ND1	70:n:604:HEA:O1A	2.41	0.43
14:B:46:ARG:HB2	14:B:110:GLU:OE1	2.19	0.43
14:B:124:LEU:HD23	14:B:124:LEU:HA	1.85	0.43
13:L:412:SER:O	21:U:15:ARG:NH2	2.48	0.43
24:C1:49:GLU:HG2	24:C1:106:ARG:HD2	2.00	0.43
27:1:53:PRO:HA	27:1:128:ALA:HA	2.01	0.43
41:H1:24:GLU:OE2	41:H1:274:ARG:NH1	2.43	0.43
44:L1:595:ILE:O	44:L1:599:ILE:HG12	2.19	0.43
71:M1:501:3PE:H241	76:h1:201:CDL:H322	2.01	0.43
47:O1:221:LEU:HD21	47:O1:241:LEU:HD11	2.01	0.43
1:n:216:ASN:ND2	7:t:55:ARG:HA	2.34	0.43
2:o:96:THR:HA	2:o:151:ARG:HG3	2.00	0.43
3:p:210:ILE:HG23	71:p:301:3PE:H2B2	2.01	0.43
4:q:52:SER:OG	4:q:53:ARG:N	2.52	0.43
6:s:20:GLU:HA	6:s:23:ILE:HG12	1.99	0.43
6:s:75:LEU:HD23	6:s:81:GLN:CG	2.27	0.43
14:M:24:LEU:HD12	14:M:38:LEU:HB2	2.00	0.43
23:6:47:ILE:HD11	80:6:203:PC1:H382	2.01	0.43
28:3:244:THR:HB	31:Q1:73:ALA:HB2	2.00	0.43
28:3:379:LEU:HD13	28:3:384:PRO:HG2	2.00	0.43
42:J1:114:VAL:HG23	42:J1:115:ILE:HG13	2.01	0.43
44:L1:9:LEU:HD22	71:i1:201:3PE:H2E1	2.00	0.43
44:L1:530:PRO:O	44:L1:534:HIS:HB2	2.18	0.43
45:M1:162:ILE:HG23	46:N1:271:MET:HE3	2.01	0.43
46:N1:27:MET:HE1	46:N1:71:LEU:HD11	2.01	0.43
46:N1:178:ILE:HG23	46:N1:292:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:151:ARG:HD3	2:o:153:LEU:HD11	2.00	0.42
3:p:34:TRP:CE2	7:t:60:PRO:HB2	2.54	0.42
3:p:153:GLU:CG	7:t:10:ALA:CB	2.97	0.42
14:B:258:VAL:HA	14:B:323:GLY:HA3	2.00	0.42
14:B:385:GLN:HG2	17:T:2:LEU:HD12	2.00	0.42
22:K:53:LYS:HD3	22:K:53:LYS:HA	1.83	0.42
76:N:405:CDL:H112	76:N:405:CDL:HB31	2.00	0.42
28:3:266:LYS:O	28:3:270:ALA:CB	2.67	0.42
30:P1:174:ARG:NH1	30:P1:316:GLU:OE2	2.52	0.42
35:V1:55:LEU:HA	35:V1:58:VAL:HG12	2.01	0.42
41:H1:145:THR:HG23	41:H1:297:THR:HG21	2.02	0.42
44:L1:362:ILE:O	44:L1:370:SER:OG	2.35	0.42
44:L1:565:SER:HB2	49:Y1:112:MET:HE1	2.01	0.42
45:M1:227:GLY:HA2	45:M1:230:ILE:HG22	2.01	0.42
57:g1:79:PRO:HG3	58:h1:72:SER:HB3	2.00	0.42
63:m1:61:ASP:O	63:m1:65:ILE:HG12	2.19	0.42
1:n:440:TYR:OH	2:o:196:CYS:O	2.29	0.42
1:n:473:TRP:CD2	11:y:22:LEU:HD13	2.54	0.42
3:p:172:TYR:CZ	7:t:29:MET:HE3	2.54	0.42
5:r:63:SER:O	5:r:67:ILE:HG12	2.19	0.42
18:F:98:ILE:HG22	18:F:102:LYS:HE2	2.01	0.42
15:N:338:ILE:HD13	15:N:338:ILE:HA	1.89	0.42
17:T:1:MET:HE3	17:T:1:MET:HB3	1.91	0.42
26:2:128:VAL:HG11	26:2:141:GLU:HG3	2.00	0.42
30:P1:136:ASN:HD22	30:P1:291:ASP:HA	1.84	0.42
40:A1:3:LEU:HD13	41:H1:96:ILE:HG21	1.99	0.42
44:L1:542:LEU:HB3	45:M1:278:ARG:HD3	2.00	0.42
57:g1:86:TRP:NE1	66:p1:65:ARG:O	2.39	0.42
63:m1:14:PRO:HD2	63:m1:17:LEU:HB2	2.01	0.42
1:n:82:LEU:HB3	1:n:86:MET:HE3	2.01	0.42
3:p:16:TRP:NE1	3:p:56:GLN:HE21	2.16	0.42
3:p:133:ASN:ND2	3:p:176:LEU:HD11	2.35	0.42
15:C:30:TRP:NE1	71:C:403:3PE:O22	2.51	0.42
15:C:51:LEU:O	15:C:55:TYR:HB2	2.19	0.42
21:U:20:PHE:O	21:U:24:ILE:HG12	2.19	0.42
28:3:381:GLY:HA3	28:3:457:ALA:HB2	2.00	0.42
42:J1:20:ALA:HB1	71:K1:201:3PE:H261	2.01	0.42
43:K1:40:LEU:HD21	46:N1:72:LEU:HA	1.99	0.42
44:L1:2:ASN:O	44:L1:6:THR:OG1	2.30	0.42
45:M1:76:MET:HE1	45:M1:230:ILE:HD13	2.01	0.42
48:X1:142:HIS:HB2	50:Z1:114:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:z:20:THR:O	67:z:21:SER:C	2.62	0.42
2:o:151:ARG:HB2	2:o:181:GLN:NE2	2.34	0.42
14:M:35:ILE:HD13	14:M:206:LEU:HB3	2.02	0.42
14:M:49:LEU:HD23	14:M:127:THR:HG21	2.00	0.42
14:M:309:VAL:HG23	14:M:326:THR:HG22	2.01	0.42
22:V:45:VAL:HG23	22:V:48:ILE:HB	2.02	0.42
28:3:266:LYS:O	28:3:270:ALA:HB2	2.19	0.42
76:L1:703:CDL:H152	76:L1:703:CDL:H311	2.00	0.42
45:M1:275:ILE:O	45:M1:278:ARG:C	2.62	0.42
34:U1:26:ASP:OD1	34:U1:26:ASP:N	2.48	0.42
50:Z1:93:GLU:OE2	50:Z1:103:TRP:NE1	2.49	0.42
4:q:24:LEU:HB3	5:r:30:ARG:HG2	2.02	0.42
4:q:40:LEU:HD11	4:q:55:GLU:HB2	2.02	0.42
13:A:124:ASP:OD1	13:A:124:ASP:N	2.50	0.42
15:C:274:PHE:O	15:C:278:TYR:HB2	2.18	0.42
22:K:33:VAL:HG12	22:K:38:TRP:HE3	1.83	0.42
15:N:185:LEU:HD23	15:N:185:LEU:HA	1.89	0.42
29:9:66:GLU:OE2	29:9:151:TYR:OH	2.32	0.42
30:P1:48:PRO:HB2	30:P1:73:TRP:CD1	2.55	0.42
36:W1:34:VAL:HG21	85:W1:201:ZMP:HN1	1.84	0.42
41:H1:17:MET:HE3	41:H1:17:MET:HB3	1.88	0.42
41:H1:110:SER:OG	41:H1:143:GLU:OE1	2.37	0.42
42:J1:133:VAL:HG12	42:J1:134:MET:HG2	2.01	0.42
42:J1:164:PHE:HD2	46:N1:5:THR:HG22	1.84	0.42
44:L1:233:LEU:HB3	44:L1:234:PRO:HD3	2.02	0.42
45:M1:216:LEU:HD23	45:M1:287:ALA:HB1	2.02	0.42
1:n:84:PRO:HA	1:n:89:ALA:HB3	2.01	0.42
1:n:425:PHE:CD1	1:n:428:GLN:HG3	2.55	0.42
2:o:165:VAL:O	2:o:169:GLY:N	2.52	0.42
3:p:42:LEU:HD12	3:p:42:LEU:HA	1.90	0.42
4:q:76:ASN:HB3	4:q:79:LYS:HE3	2.02	0.42
15:N:138:MET:HE2	15:N:138:MET:HB2	1.85	0.42
26:2:66:MET:HE1	28:3:186:TYR:HE2	1.85	0.42
28:3:516:LYS:HB3	28:3:516:LYS:HE2	1.89	0.42
41:H1:28:LEU:O	41:H1:32:GLN:HG3	2.19	0.42
41:H1:269:THR:O	41:H1:273:ILE:HG12	2.20	0.42
42:J1:21:LEU:HD11	42:J1:91:PHE:HB2	2.01	0.42
44:L1:468:ILE:O	44:L1:472:ILE:HG12	2.20	0.42
44:L1:481:THR:HG22	60:j1:53:TYR:HD1	1.85	0.42
45:M1:314:MET:HG2	45:M1:454:ILE:HG13	2.00	0.42
46:N1:319:LYS:HG2	46:N1:321:LYS:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Y1:101:GLY:HA3	49:Y1:110:ALA:HB2	2.00	0.42
54:d1:65:VAL:O	54:d1:69:VAL:HG23	2.20	0.42
57:g1:88:ARG:HA	57:g1:88:ARG:HD3	1.88	0.42
1:n:135:ASN:CG	1:n:213:ARG:HE	2.28	0.42
1:n:383:MET:HB2	1:n:387:PHE:CE2	2.55	0.42
6:s:11:GLU:HA	6:s:22:MET:HE1	2.00	0.42
14:B:264:ILE:HG22	14:B:317:SER:HA	2.02	0.42
15:C:323:ILE:HD11	71:G:102:3PE:H12	2.02	0.42
15:C:331:ASN:HA	15:C:334:ILE:HB	2.02	0.42
21:U:40:ASP:O	21:U:44:GLU:HG3	2.20	0.42
23:6:75:PRO:O	29:9:49:THR:OG1	2.31	0.42
23:6:172:GLN:OE1	29:9:142:SER:OG	2.36	0.42
24:C1:210:ARG:NH1	28:3:35:MET:HG3	2.35	0.42
25:D1:211:ILE:HG22	25:D1:315:LEU:HD11	2.01	0.42
28:3:237:ASN:HD22	28:3:253:ARG:NH2	2.18	0.42
28:3:241:SER:HB2	28:3:249:ARG:HB3	2.01	0.42
32:7:4:VAL:HG12	32:7:10:LYS:HG2	2.02	0.42
41:H1:93:HIS:NE2	51:a1:35:GLU:OE2	2.45	0.42
41:H1:237:LEU:O	41:H1:241:ILE:HG12	2.20	0.42
44:L1:36:THR:O	44:L1:40:ILE:HG12	2.19	0.42
44:L1:198:LEU:O	44:L1:202:MET:HG2	2.19	0.42
44:L1:481:THR:OG1	65:o1:91:HIS:ND1	2.37	0.42
45:M1:158:ILE:HG13	46:N1:287:LEU:HD11	2.01	0.42
34:U1:63:PRO:HB3	62:l1:60:TRP:CD2	2.55	0.42
48:X1:120:ASP:N	48:X1:123:GLN:OE1	2.43	0.42
54:d1:109:TYR:HA	54:d1:112:ILE:HG12	2.00	0.42
63:m1:100:TRP:HA	63:m1:103:VAL:HG12	2.01	0.42
1:n:458:SER:O	1:n:461:SER:OG	2.30	0.42
2:o:136:LEU:HD23	2:o:193:TYR:CG	2.54	0.42
3:p:19:THR:HG22	12:w:39:THR:HG21	2.01	0.42
3:p:34:TRP:CE2	7:t:60:PRO:O	2.70	0.42
3:p:59:ARG:NE	3:p:63:ARG:HD2	2.35	0.42
14:B:345:LYS:HG2	14:B:418:VAL:HG21	2.01	0.42
18:F:25:GLY:HA2	18:F:28:LYS:HE2	2.02	0.42
13:L:319:LEU:HD23	13:L:319:LEU:HA	1.89	0.42
21:U:42:ILE:O	21:U:46:ILE:HG13	2.19	0.42
25:D1:87:THR:HG21	25:D1:106:LEU:HD21	2.02	0.42
25:D1:147:ILE:HD12	25:D1:218:PHE:HE2	1.84	0.42
25:D1:371:LYS:NZ	25:D1:422:ASP:OD1	2.34	0.42
27:1:34:LYS:HB2	27:1:34:LYS:HE2	1.78	0.42
34:T1:11:ILE:HB	34:T1:80:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:q1:44:TYR:OH	37:q1:113:HIS:N	2.49	0.42
45:M1:207:MET:HG3	45:M1:294:MET:HB3	2.02	0.42
47:O1:303:LYS:HE2	47:O1:303:LYS:HB2	1.86	0.42
34:U1:52:MET:HE1	64:n1:23:LEU:HD12	2.01	0.42
52:b1:37:TYR:HA	52:b1:40:TYR:HD2	1.85	0.42
1:n:513:VAL:HB	6:s:40:ALA:HB2	2.02	0.42
8:u:37:HIS:O	8:u:40:GLU:HG2	2.20	0.42
9:v:50:ALA:HB1	9:v:54:ARG:NH1	2.34	0.42
13:A:20:ASP:OD1	13:A:21:ASN:N	2.53	0.42
15:N:275:LEU:HD23	15:N:275:LEU:HA	1.90	0.42
16:O:77:ASP:OD1	16:O:77:ASP:N	2.48	0.42
16:O:207:LYS:NZ	71:O:302:3PE:O12	2.43	0.42
27:1:92:TYR:O	27:1:220:THR:HA	2.20	0.42
30:P1:165:ILE:O	30:P1:227:THR:HA	2.20	0.42
45:M1:319:HIS:HA	45:M1:322:THR:HG22	2.02	0.42
47:O1:106:LEU:HD13	47:O1:270:LEU:HD11	2.01	0.42
67:z:37:LEU:HA	67:z:40:TYR:HD2	1.83	0.42
1:n:313:ALA:HB2	1:n:356:ILE:HD11	2.02	0.42
2:o:7:LEU:HD23	71:o:302:3PE:H232	2.02	0.42
2:o:53:THR:N	5:r:38:GLY:O	2.53	0.42
4:q:120:THR:HA	4:q:123:MET:HG2	2.01	0.42
6:s:75:LEU:HD23	6:s:81:GLN:CB	2.43	0.42
13:A:110:VAL:HG11	13:A:211:LEU:HB3	2.01	0.42
13:A:317:THR:OG1	13:A:318:GLY:N	2.53	0.42
15:C:96:LEU:HD23	71:C:403:3PE:H271	2.02	0.42
15:C:107:TYR:HE1	15:C:308:HIS:HB2	1.85	0.42
15:C:108:THR:OG1	15:C:313:ARG:NH2	2.52	0.42
17:E:161:HIS:NE2	15:N:282:ARG:CD	2.66	0.42
13:L:23:LEU:HD11	13:L:216:LEU:HD13	2.02	0.42
14:M:334:GLY:HA2	14:M:434:PRO:HD3	2.01	0.42
16:O:164:ILE:HG13	16:O:179:MET:HG3	2.01	0.42
23:6:135:TYR:HE1	29:9:90:PRO:HB2	1.84	0.42
30:P1:107:GLU:O	30:P1:111:VAL:HB	2.20	0.42
30:P1:128:ARG:NH1	30:P1:220:ASP:O	2.37	0.42
32:7:12:THR:HG22	32:7:35:VAL:HG23	2.01	0.42
38:r1:98:PRO:HA	38:r1:99:PRO:HD3	1.95	0.42
40:A1:71:LEU:HD23	40:A1:71:LEU:HA	1.93	0.42
41:H1:114:TYR:CE2	42:J1:60:LEU:HD13	2.55	0.42
44:L1:224:SER:HB3	44:L1:310:LEU:HD23	2.01	0.42
46:N1:190:MET:HB3	46:N1:201:THR:HG23	2.02	0.42
46:N1:267:ILE:O	46:N1:271:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:p:163:LEU:HA	3:p:166:THR:HG22	2.01	0.41
16:D:180:SER:HB3	20:H:15:LEU:HB2	2.02	0.41
19:G:72:LYS:N	20:H:54:GLU:OE2	2.49	0.41
14:M:181:TYR:CZ	14:M:182:ARG:HG2	2.55	0.41
14:M:195:VAL:O	14:M:199:PHE:HB2	2.20	0.41
19:R:6:ASN:O	19:R:6:ASN:ND2	2.40	0.41
28:3:72:PRO:HG2	28:3:74:MET:HE1	2.01	0.41
29:9:46:GLU:HG3	51:a1:1:MET:SD	2.60	0.41
33:S1:26:SER:O	33:S1:33:ARG:NH2	2.45	0.41
48:X1:20:SER:HB3	48:X1:23:VAL:HG23	2.02	0.41
49:Y1:109:THR:OG1	71:Y1:204:3PE:O32	2.30	0.41
61:k1:28:LYS:HA	61:k1:28:LYS:HD2	1.88	0.41
1:n:103:TRP:CD2	3:p:18:LEU:HD13	2.55	0.41
1:n:199:LEU:HD22	1:n:238:PHE:HE1	1.85	0.41
1:n:492:LEU:HD13	6:s:72:TRP:CD2	2.56	0.41
2:o:138:VAL:HG12	2:o:140:ASN:H	1.84	0.41
3:p:133:ASN:HD21	3:p:176:LEU:HD11	1.85	0.41
4:q:29:HIS:CG	4:q:65:ASN:HB2	2.55	0.41
5:r:41:LEU:HD22	9:v:12:ARG:HG2	2.01	0.41
6:s:75:LEU:HB3	6:s:81:GLN:CD	2.45	0.41
14:B:124:LEU:O	14:B:128:THR:OG1	2.36	0.41
16:D:218:LEU:HB3	17:E:43:THR:HB	2.01	0.41
13:L:336:PHE:HE1	76:N:405:CDL:HA22	1.84	0.41
15:N:154:PRO:HD3	15:N:288:LEU:HD13	2.02	0.41
44:L1:361:ASN:HD22	61:k1:62:PHE:HD1	1.67	0.41
76:h1:201:CDL:H171	71:i1:201:3PE:H381	2.02	0.41
1:n:157:SER:HB2	1:n:195:LEU:HD12	2.01	0.41
1:n:166:THR:O	1:n:170:ASN:HB2	2.21	0.41
3:p:153:GLU:HG3	7:t:10:ALA:HB3	2.01	0.41
5:r:19:PHE:HE1	5:r:32:GLY:HA3	1.85	0.41
8:u:31:GLN:HA	8:u:34:LEU:HG	2.02	0.41
12:w:35:THR:HA	12:w:38:LEU:HG	2.02	0.41
15:C:138:MET:HE1	15:C:268:ILE:HA	2.02	0.41
16:D:197:GLU:O	16:D:201:ARG:CB	2.68	0.41
14:M:239:TYR:HE2	14:M:421:LYS:HB3	1.85	0.41
14:M:279:LEU:HD12	14:M:295:LEU:HG	2.02	0.41
16:O:76:ASP:OD1	16:O:76:ASP:N	2.52	0.41
17:P:52:LYS:HD3	22:V:34:TRP:CE2	2.56	0.41
30:P1:338:LYS:HE2	30:P1:338:LYS:HB2	1.91	0.41
43:K1:15:SER:OG	43:K1:32:CYS:O	2.38	0.41
44:L1:159:TYR:HB3	45:M1:416:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M1:67:ILE:HG22	71:M1:501:3PE:H3D1	2.02	0.41
45:M1:367:LEU:HD23	45:M1:407:SER:HB2	2.03	0.41
64:n1:56:MET:HA	64:n1:59:ALA:HB3	2.03	0.41
67:z:39:SER:O	67:z:40:TYR:C	2.62	0.41
1:n:80:ASN:ND2	1:n:98:ASN:HD21	2.18	0.41
1:n:166:THR:O	1:n:170:ASN:CB	2.69	0.41
1:n:306:THR:O	1:n:310:MET:HG2	2.21	0.41
3:p:217:VAL:HG11	71:p:301:3PE:H271	2.02	0.41
4:q:20:ARG:NH2	5:r:73:ASP:OD1	2.52	0.41
13:A:86:LEU:HD13	13:A:99:ILE:HG12	2.03	0.41
15:C:332:LEU:HG	71:C:403:3PE:H2C1	2.03	0.41
14:M:56:ARG:NH2	14:M:318:ASP:OD2	2.53	0.41
14:M:318:ASP:OD1	14:M:318:ASP:N	2.52	0.41
16:O:126:TYR:OH	78:O:303:HEC:O2A	2.32	0.41
19:R:38:LEU:HD13	76:R:103:CDL:HA62	2.01	0.41
25:D1:103:PHE:HA	25:D1:106:LEU:HD12	2.01	0.41
25:D1:220:LEU:O	25:D1:224:GLU:HG3	2.20	0.41
25:D1:233:ARG:NE	29:9:31:GLU:OE2	2.48	0.41
27:1:374:LYS:NZ	28:3:133:GLY:O	2.52	0.41
32:7:68:HIS:ND1	32:7:69:PRO:O	2.48	0.41
34:T1:37:MET:SD	34:T1:37:MET:N	2.93	0.41
37:q1:32:ASP:OD2	37:q1:58:ARG:NH2	2.53	0.41
40:A1:29:LEU:HD11	40:A1:34:ALA:HB2	2.02	0.41
44:L1:171:ALA:HA	44:L1:232:TRP:HB2	2.02	0.41
44:L1:204:SER:O	44:L1:204:SER:OG	2.34	0.41
71:M1:501:3PE:H351	57:g1:75:VAL:HG21	2.02	0.41
64:n1:24:ARG:HD3	64:n1:24:ARG:HA	1.94	0.41
9:v:63:GLU:HA	9:v:66:ARG:HG2	2.02	0.41
13:L:24:ARG:HB2	13:L:196:VAL:HG22	2.02	0.41
13:L:70:ARG:HB3	13:L:74:ALA:HB3	2.03	0.41
77:N:402:HEM:HBB2	77:N:402:HEM:HMB1	2.02	0.41
21:U:52:TRP:O	21:U:56:LYS:HB3	2.21	0.41
27:1:193:ILE:HG12	27:1:215:VAL:HG13	2.02	0.41
27:1:347:ILE:HD13	27:1:347:ILE:HA	1.92	0.41
30:P1:248:MET:HA	30:P1:334:THR:HG21	2.02	0.41
46:N1:116:PRO:HA	46:N1:119:THR:HG22	2.01	0.41
34:U1:51:ILE:HG21	34:U1:67:ALA:HB1	2.03	0.41
50:Z1:26:ARG:O	50:Z1:26:ARG:HD3	2.19	0.41
53:c1:19:LEU:HB3	71:d1:203:3PE:H252	2.01	0.41
55:e1:20:LEU:HD12	55:e1:36:GLU:HG2	2.02	0.41
1:n:456:MET:HE3	4:q:96:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:276:ILE:HG21	13:A:345:LEU:HD21	2.03	0.41
13:L:3:THR:HG23	13:L:6:GLN:H	1.84	0.41
15:N:228:ASP:O	15:N:232:ILE:HG12	2.20	0.41
23:6:72:MET:HG2	23:6:79:MET:HE2	2.02	0.41
25:D1:238:ARG:HA	25:D1:238:ARG:HD2	1.90	0.41
25:D1:412:ALA:HA	25:D1:415:VAL:HG22	2.03	0.41
40:A1:17:LEU:HD12	40:A1:17:LEU:HA	1.91	0.41
41:H1:165:LEU:HD11	41:H1:241:ILE:HD13	2.01	0.41
41:H1:168:THR:HG23	50:Z1:49:MET:HE1	2.03	0.41
44:L1:18:PRO:HG2	44:L1:122:THR:HG21	2.03	0.41
44:L1:75:GLU:HG3	66:p1:103:ASN:ND2	2.36	0.41
44:L1:386:LEU:HD21	60:j1:32:MET:HG3	2.02	0.41
46:N1:179:MET:HE1	46:N1:215:MET:HB3	2.02	0.41
46:N1:311:SER:HA	46:N1:314:MET:HB2	2.01	0.41
63:m1:126:ILE:HB	66:p1:138:TYR:CD1	2.55	0.41
64:n1:51:LYS:HG3	85:n1:201:ZMP:H19B	2.02	0.41
1:n:94:PHE:HB3	1:n:97:MET:HG2	2.03	0.41
1:n:396:TRP:HD1	1:n:399:LEU:HD12	1.86	0.41
3:p:77:LYS:HE3	3:p:81:TYR:CZ	2.56	0.41
4:q:47:ASP:N	4:q:47:ASP:OD1	2.53	0.41
5:r:72:LYS:HZ1	5:r:107:ASP:CB	2.34	0.41
5:r:101:PRO:HA	5:r:104:LEU:HG	2.01	0.41
13:A:40:TRP:CZ2	13:A:377:GLU:HA	2.56	0.41
14:B:247:GLN:HE22	14:B:430:LEU:H	1.68	0.41
15:C:324:LEU:HG	15:C:361:ILE:HD11	2.02	0.41
15:C:361:ILE:HA	15:C:365:LEU:HB2	2.01	0.41
16:O:216:LEU:HA	16:O:219:THR:HG22	2.02	0.41
24:C1:205:ALA:O	38:r1:60:ARG:NE	2.54	0.41
30:P1:248:MET:HE2	30:P1:248:MET:HB2	1.86	0.41
30:P1:263:TYR:CE2	30:P1:288:HIS:HE1	2.39	0.41
41:H1:273:ILE:HD12	41:H1:277:TYR:HE2	1.86	0.41
44:L1:578:THR:HG21	46:N1:168:GLY:HA2	2.02	0.41
45:M1:11:LEU:HB3	45:M1:100:ILE:HD13	2.03	0.41
45:M1:267:TRP:O	45:M1:271:MET:HG2	2.21	0.41
62:l1:79:ASP:HB3	62:l1:82:MET:HE2	2.02	0.41
64:n1:94:GLU:HA	64:n1:97:LYS:HD3	2.02	0.41
1:n:145:LEU:HD23	1:n:145:LEU:HA	1.93	0.41
3:p:199:MET:O	3:p:203:PHE:HB2	2.21	0.41
13:A:273:ALA:HB2	13:A:407:LEU:HD11	2.03	0.41
15:C:284:ILE:HD12	15:C:293:ALA:HB2	2.02	0.41
14:M:166:VAL:HG11	14:M:244:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C1:104:ARG:NH2	25:D1:373:GLU:OE1	2.45	0.41
25:D1:377:TYR:HB3	25:D1:390:LYS:HB3	2.03	0.41
28:3:105:CYS:SG	28:3:117:GLN:NE2	2.94	0.41
28:3:142:ILE:HB	28:3:191:PHE:HB3	2.01	0.41
30:P1:74:ASP:HB3	30:P1:77:ASP:HB2	2.03	0.41
41:H1:116:ILE:O	41:H1:119:SER:OG	2.37	0.41
44:L1:71:MET:SD	45:M1:310:MET:HE2	2.60	0.41
45:M1:114:GLU:HG3	45:M1:116:ILE:HG22	2.03	0.41
45:M1:255:LYS:HE3	45:M1:255:LYS:HB3	1.89	0.41
57:g1:66:ILE:HA	57:g1:70:PHE:HD2	1.86	0.41
60:j1:14:PHE:HB2	61:k1:61:GLY:HA3	2.02	0.41
1:n:18:LEU:HB3	1:n:102:PHE:CZ	2.56	0.41
1:n:427:PRO:HB3	1:n:450:TRP:HB3	2.02	0.41
2:o:189:PRO:HD2	9:v:56:TYR:OH	2.20	0.41
7:t:14:LYS:HG3	7:t:18:TYR:HE2	1.85	0.41
15:C:282:ARG:HH12	15:C:343:VAL:HB	1.86	0.41
16:D:13:SER:O	16:D:19:SER:OG	2.29	0.41
16:D:204:MET:HE2	16:D:204:MET:HB3	1.97	0.41
18:F:43:VAL:O	18:F:47:ILE:HG12	2.21	0.41
13:L:46:ARG:HG3	13:L:163:LEU:HD13	2.02	0.41
14:M:200:THR:OG1	14:M:229:GLY:O	2.33	0.41
15:N:218:ILE:HD13	16:O:230:LEU:HD11	2.03	0.41
18:Q:43:VAL:O	18:Q:47:ILE:HG12	2.20	0.41
23:6:75:PRO:HG3	25:D1:168:PHE:HD2	1.86	0.41
24:C1:8:ARG:HA	24:C1:9:PRO:HD3	1.98	0.41
71:D1:501:3PE:H2C2	46:N1:284:MET:HB3	2.03	0.41
26:2:105:THR:HG22	26:2:106:THR:H	1.85	0.41
26:2:183:LYS:HA	26:2:184:PRO:HD3	1.89	0.41
27:1:363:THR:HG21	28:3:97:LEU:HG	2.03	0.41
28:3:11:VAL:HG11	28:3:73:VAL:HB	2.02	0.41
28:3:668:ILE:HA	28:3:671:PHE:HB3	2.03	0.41
31:Q1:89:LYS:O	31:Q1:93:ILE:HG12	2.21	0.41
40:A1:74:PRO:HG2	42:J1:145:TYR:HE2	1.86	0.41
41:H1:195:ARG:NH2	41:H1:274:ARG:HD2	2.35	0.41
41:H1:298:LEU:HD23	41:H1:298:LEU:HA	1.89	0.41
41:H1:307:LEU:HA	41:H1:310:PHE:CE1	2.55	0.41
42:J1:150:TRP:HZ2	46:N1:19:ILE:HG12	1.86	0.41
43:K1:59:ILE:HD12	46:N1:27:MET:HG2	2.02	0.41
44:L1:15:LEU:HB3	44:L1:126:ILE:HG12	2.03	0.41
45:M1:1:FME:HE3	45:M1:1:FME:HB3	1.85	0.41
45:M1:173:THR:HG23	45:M1:175:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N1:43:MET:HA	46:N1:46:ASN:HB2	2.03	0.41
46:N1:338:PRO:HG3	76:d1:201:CDL:H612	2.02	0.41
76:N1:401:CDL:H842	76:d1:201:CDL:H671	2.03	0.41
34:U1:40:LEU:HD23	34:U1:40:LEU:HA	1.90	0.41
55:e1:6:GLN:NE2	55:e1:13:LEU:HB2	2.35	0.41
58:h1:44:ASN:HB3	76:h1:201:CDL:HB31	2.02	0.41
64:n1:30:CYS:O	64:n1:32:HIS:N	2.53	0.41
3:p:228:THR:OG1	3:p:229:SER:N	2.51	0.41
5:r:27:TRP:CZ3	6:s:82:ARG:NE	2.89	0.41
13:A:58:PHE:CD2	13:A:182:LEU:HD21	2.55	0.41
16:D:160:MET:HB3	16:D:160:MET:HE2	1.81	0.41
16:D:204:MET:HE3	71:E:202:3PE:H31	2.03	0.41
13:L:259:GLY:N	13:L:318:GLY:O	2.49	0.41
15:N:214:ASP:HB3	19:R:8:ALA:HB2	2.03	0.41
25:D1:228:MET:HB3	25:D1:228:MET:HE3	1.76	0.41
29:9:110:ARG:NH1	31:Q1:70:MET:O	2.40	0.41
36:W1:102:ARG:O	36:W1:106:MET:HB2	2.20	0.41
41:H1:285:LEU:HD12	41:H1:289:LEU:HD23	2.03	0.41
44:L1:316:THR:HA	44:L1:319:MET:HE3	2.02	0.41
45:M1:328:CYS:HB3	45:M1:437:MET:HE1	2.02	0.41
46:N1:34:GLU:O	46:N1:38:LEU:HG	2.20	0.41
46:N1:238:PRO:HG3	47:O1:293:TYR:HE2	1.86	0.41
71:i1:201:3PE:H352	71:i1:201:3PE:H2C2	2.03	0.41
64:n1:5:PRO:HA	64:n1:6:PRO:HD3	1.92	0.41
67:z:13:LEU:O	67:z:17:ILE:HG13	2.21	0.41
1:n:378:HIS:CD2	1:n:382:SER:HB3	2.50	0.40
4:q:26:ASP:N	4:q:26:ASP:OD1	2.52	0.40
4:q:68:PHE:CA	4:q:71:MET:SD	2.98	0.40
5:r:72:LYS:HA	5:r:82:TYR:CD2	2.56	0.40
6:s:81:GLN:CD	6:s:81:GLN:N	2.79	0.40
6:s:82:ARG:HD3	6:s:89:HIS:CE1	2.56	0.40
7:t:68:LEU:HD22	71:t:101:3PE:H331	2.02	0.40
13:A:135:LEU:HD23	13:A:135:LEU:HA	1.95	0.40
15:C:244:LEU:HD12	16:D:208:MET:HE2	2.03	0.40
13:L:76:GLU:O	13:L:80:GLU:HG2	2.20	0.40
13:L:173:ASN:HA	13:L:176:ARG:HG2	2.03	0.40
14:M:238:LYS:HE3	14:M:238:LYS:HB2	1.83	0.40
17:P:165:TYR:HA	17:P:171:ILE:HA	2.02	0.40
71:D1:501:3PE:H2D1	80:Y1:201:PC1:H2D2	2.02	0.40
27:1:101:GLU:HA	27:1:102:PRO:HD3	1.83	0.40
35:V1:34:LEU:HD22	35:V1:44:ARG:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:K1:37:VAL:HG22	46:N1:68:MET:HE2	2.03	0.40
44:L1:160:GLY:H	64:n1:95:CYS:HB3	1.87	0.40
45:M1:352:PHE:HB3	45:M1:355:MET:HB3	2.02	0.40
46:N1:70:ILE:HG13	46:N1:101:ALA:HB1	2.03	0.40
46:N1:313:MET:HA	46:N1:316:HIS:HB2	2.03	0.40
47:O1:22:SER:HB3	47:O1:115:LEU:HD11	2.03	0.40
48:X1:122:GLY:HA3	52:b1:77:LEU:HB2	2.02	0.40
60:j1:55:ASP:HA	60:j1:56:PRO:HD3	1.96	0.40
60:j1:57:SER:OG	60:j1:58:GLN:OE1	2.39	0.40
13:A:52:ASN:OD1	13:A:52:ASN:N	2.54	0.40
15:C:327:ILE:HG12	71:G:102:3PE:H2A2	2.03	0.40
15:C:371:ILE:HD12	15:C:371:ILE:HA	1.98	0.40
16:D:1:SER:HG	16:D:2:ASP:N	2.17	0.40
20:H:41:ARG:HG3	20:H:45:ARG:HH22	1.85	0.40
16:O:32:VAL:HG22	16:O:169:LEU:HD21	2.03	0.40
16:O:223:LYS:O	16:O:227:TRP:HB2	2.21	0.40
18:Q:95:LYS:HD3	18:Q:95:LYS:HA	1.79	0.40
25:D1:63:ARG:HB3	25:D1:79:HIS:HB2	2.02	0.40
38:r1:38:PRO:HA	50:Z1:6:LYS:HB3	2.03	0.40
40:A1:75:LEU:HA	40:A1:78:ALA:HB3	2.02	0.40
43:K1:1:FME:SD	46:N1:79:LYS:NZ	2.75	0.40
44:L1:194:ASN:HD21	63:m1:126:ILE:HG12	1.86	0.40
45:M1:75:LEU:HD22	45:M1:436:LEU:HD12	2.03	0.40
45:M1:282:LEU:HD21	45:M1:359:TRP:HH2	1.87	0.40
34:U1:63:PRO:HB3	62:l1:60:TRP:CG	2.56	0.40
66:p1:99:GLN:NE2	66:p1:138:TYR:OH	2.37	0.40
1:n:107:PRO:HB3	3:p:25:LEU:HB2	2.04	0.40
1:n:347:LEU:HA	1:n:347:LEU:HD23	1.84	0.40
3:p:35:PHE:HD1	7:t:60:PRO:HG3	1.79	0.40
14:B:162:ASN:HB3	14:B:244:ILE:HD11	2.04	0.40
15:C:133:LEU:HD23	15:C:133:LEU:HA	1.78	0.40
15:C:201:HIS:O	19:G:2:ARG:NH2	2.52	0.40
18:Q:70:MET:HE3	18:Q:70:MET:HB3	1.96	0.40
17:T:71:ASN:OD1	17:T:71:ASN:N	2.54	0.40
27:1:384:ALA:HB3	27:1:430:MET:HE3	2.03	0.40
42:J1:22:LYS:NZ	43:K1:21:MET:O	2.49	0.40
43:K1:97:GLN:HB3	44:L1:582:GLY:HA3	2.02	0.40
45:M1:260:PRO:HG2	71:M1:503:3PE:H271	2.03	0.40
46:N1:312:LYS:O	46:N1:316:HIS:ND1	2.47	0.40
47:O1:29:GLY:O	47:O1:126:ARG:NH2	2.52	0.40
50:Z1:24:LEU:HA	50:Z1:25:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:f1:49:ARG:HA	56:f1:50:PRO:HD3	1.85	0.40
61:k1:87:LEU:HD23	61:k1:87:LEU:HA	1.97	0.40
1:n:32:ALA:O	1:n:36:LEU:HG	2.22	0.40
13:A:24:ARG:NH1	13:A:383:LEU:O	2.54	0.40
13:A:131:ARG:HA	13:A:134:ILE:HG22	2.04	0.40
14:B:407:ASP:OD1	14:B:407:ASP:N	2.53	0.40
13:L:108:LYS:HB2	13:L:108:LYS:HE2	1.89	0.40
13:L:258:GLU:HG2	17:P:26:LYS:HD2	2.03	0.40
13:L:439:SER:HB3	71:L:501:3PE:H111	2.02	0.40
16:O:10:TYR:HB3	20:S:72:PHE:CE2	2.57	0.40
16:O:49:ARG:NH2	17:P:67:ASP:OD1	2.54	0.40
20:S:26:GLU:HA	20:S:29:VAL:HG12	2.02	0.40
23:6:70:MET:HE2	25:D1:171:PHE:CZ	2.56	0.40
25:D1:62:LEU:HB2	25:D1:425:PHE:CZ	2.56	0.40
26:2:173:ILE:HD13	26:2:173:ILE:HA	1.92	0.40
28:3:605:GLU:HG2	36:W1:121:LEU:HD11	2.02	0.40
29:9:36:LEU:HD21	41:H1:273:ILE:HD13	2.04	0.40
31:Q1:38:PHE:CE1	31:Q1:58:GLU:HG2	2.57	0.40
44:L1:223:LYS:HG2	44:L1:255:ALA:HB3	2.04	0.40
44:L1:375:ILE:HG12	60:j1:32:MET:SD	2.62	0.40
46:N1:6:LEU:HD23	46:N1:6:LEU:HA	1.98	0.40
34:U1:12:LYS:HE2	34:U1:12:LYS:HB3	1.95	0.40
34:U1:25:ILE:HG21	34:U1:30:LEU:HD13	2.02	0.40
51:a1:34:LYS:HE3	51:a1:34:LYS:HB2	1.86	0.40
61:k1:37:VAL:HG21	64:n1:34:ASP:HB2	2.03	0.40
1:n:21:LEU:HD11	75:y:601:TGL:HB61	2.04	0.40
1:n:38:ARG:HD2	1:n:38:ARG:HA	1.77	0.40
1:n:444:PRO:HD2	1:n:447:TYR:CD2	2.54	0.40
3:p:125:ASN:HA	3:p:126:PRO:HD3	1.95	0.40
18:Q:37:LEU:HD23	18:Q:37:LEU:HA	1.93	0.40
24:C1:38:GLN:HG2	35:V1:106:PRO:HD3	2.04	0.40
24:C1:180:VAL:HG23	24:C1:182:ARG:HB2	2.03	0.40
29:9:25:ARG:HH21	29:9:26:ILE:HD11	1.87	0.40
37:q1:60:ARG:HH22	37:q1:95:ASP:HA	1.86	0.40
42:J1:132:GLY:HA2	50:Z1:67:ARG:HH12	1.85	0.40
44:L1:293:LEU:HD11	44:L1:421:MET:HB3	2.04	0.40
45:M1:421:ASN:ND2	45:M1:421:ASN:N	2.62	0.40
46:N1:250:SER:HB2	46:N1:257:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	n	512/514 (100%)	490 (96%)	22 (4%)	0	100	100
2	o	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
3	p	258/261 (99%)	248 (96%)	10 (4%)	0	100	100
4	q	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
5	r	102/146 (70%)	98 (96%)	4 (4%)	0	100	100
6	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
7	t	74/111 (67%)	69 (93%)	5 (7%)	0	100	100
8	u	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
9	v	69/76 (91%)	65 (94%)	4 (6%)	0	100	100
10	x	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
11	y	45/63 (71%)	43 (96%)	2 (4%)	0	100	100
12	w	55/83 (66%)	54 (98%)	1 (2%)	0	100	100
13	A	443/480 (92%)	431 (97%)	12 (3%)	0	100	100
13	L	443/480 (92%)	431 (97%)	12 (3%)	0	100	100
14	B	418/453 (92%)	408 (98%)	10 (2%)	0	100	100
14	M	418/453 (92%)	399 (96%)	19 (4%)	0	100	100
15	C	378/381 (99%)	369 (98%)	9 (2%)	0	100	100
15	N	378/381 (99%)	369 (98%)	9 (2%)	0	100	100
16	D	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
16	O	238/325 (73%)	226 (95%)	12 (5%)	0	100	100
17	E	194/274 (71%)	184 (95%)	10 (5%)	0	100	100
17	P	194/274 (71%)	185 (95%)	9 (5%)	0	100	100
17	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
18	F	99/111 (89%)	97 (98%)	2 (2%)	0	100	100
18	Q	100/111 (90%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
19	R	75/82 (92%)	71 (95%)	4 (5%)	0	100	100
20	H	64/89 (72%)	64 (100%)	0	0	100	100
20	S	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
21	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
21	U	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
22	K	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
22	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
23	6	155/224 (69%)	149 (96%)	6 (4%)	0	100	100
24	C1	206/263 (78%)	197 (96%)	9 (4%)	0	100	100
25	D1	427/463 (92%)	413 (97%)	14 (3%)	0	100	100
26	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	24	57
27	1	428/464 (92%)	412 (96%)	16 (4%)	0	100	100
28	3	688/727 (95%)	659 (96%)	29 (4%)	0	100	100
29	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
30	P1	340/377 (90%)	327 (96%)	13 (4%)	0	100	100
31	Q1	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
32	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
33	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
34	T1	77/156 (49%)	77 (100%)	0	0	100	100
34	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
35	V1	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
36	W1	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
37	q1	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
38	r1	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
39	s1	40/104 (38%)	40 (100%)	0	0	100	100
40	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
41	H1	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
42	J1	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
43	K1	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
44	L1	604/607 (100%)	566 (94%)	38 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	M1	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
46	N1	343/345 (99%)	330 (96%)	13 (4%)	0	100	100
47	O1	318/355 (90%)	298 (94%)	20 (6%)	0	100	100
48	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
49	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
50	Z1	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
51	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
52	b1	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
53	c1	46/76 (60%)	46 (100%)	0	0	100	100
54	d1	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
55	e1	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
56	f1	51/57 (90%)	51 (100%)	0	0	100	100
57	g1	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
58	h1	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
59	i1	102/128 (80%)	98 (96%)	3 (3%)	1 (1%)	12	44
60	j1	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
61	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100
62	l1	155/186 (83%)	153 (99%)	2 (1%)	0	100	100
63	m1	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
64	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
65	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
66	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
67	z	42/69 (61%)	36 (86%)	4 (10%)	2 (5%)	2	16
All	All	13990/16129 (87%)	13464 (96%)	522 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	2	183	LYS
67	z	23	PHE
59	i1	59	MET
67	z	33	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	n	425/425 (100%)	425 (100%)	0	100	100
2	o	210/210 (100%)	210 (100%)	0	100	100
3	p	226/227 (100%)	226 (100%)	0	100	100
4	q	122/146 (84%)	122 (100%)	0	100	100
5	r	91/118 (77%)	91 (100%)	0	100	100
6	s	80/101 (79%)	80 (100%)	0	100	100
7	t	66/92 (72%)	66 (100%)	0	100	100
8	u	70/76 (92%)	70 (100%)	0	100	100
9	v	54/57 (95%)	54 (100%)	0	100	100
10	x	39/67 (58%)	39 (100%)	0	100	100
11	y	40/55 (73%)	40 (100%)	0	100	100
12	w	43/67 (64%)	42 (98%)	1 (2%)	44	64
13	A	372/398 (94%)	372 (100%)	0	100	100
13	L	372/398 (94%)	372 (100%)	0	100	100
14	B	330/356 (93%)	330 (100%)	0	100	100
14	M	330/356 (93%)	330 (100%)	0	100	100
15	C	332/333 (100%)	332 (100%)	0	100	100
15	N	332/333 (100%)	332 (100%)	0	100	100
16	D	205/260 (79%)	205 (100%)	0	100	100
16	O	205/260 (79%)	205 (100%)	0	100	100
17	E	68/224 (30%)	68 (100%)	0	100	100
17	P	68/224 (30%)	67 (98%)	1 (2%)	57	71
17	T	58/224 (26%)	58 (100%)	0	100	100
18	F	93/99 (94%)	93 (100%)	0	100	100
18	Q	94/99 (95%)	94 (100%)	0	100	100
19	G	70/74 (95%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	70/74 (95%)	69 (99%)	1 (1%)	59	71
20	H	63/83 (76%)	63 (100%)	0	100	100
20	S	65/83 (78%)	65 (100%)	0	100	100
21	J	51/55 (93%)	51 (100%)	0	100	100
21	U	51/55 (93%)	51 (100%)	0	100	100
22	K	42/46 (91%)	42 (100%)	0	100	100
22	V	43/46 (94%)	43 (100%)	0	100	100
23	6	133/185 (72%)	133 (100%)	0	100	100
24	C1	190/227 (84%)	190 (100%)	0	100	100
25	D1	370/394 (94%)	370 (100%)	0	100	100
26	2	184/206 (89%)	184 (100%)	0	100	100
27	1	345/370 (93%)	345 (100%)	0	100	100
28	3	580/610 (95%)	580 (100%)	0	100	100
29	9	152/178 (85%)	152 (100%)	0	100	100
30	P1	299/325 (92%)	299 (100%)	0	100	100
31	Q1	113/153 (74%)	113 (100%)	0	100	100
32	7	81/96 (84%)	80 (99%)	1 (1%)	63	73
33	S1	74/80 (92%)	74 (100%)	0	100	100
34	T1	73/135 (54%)	73 (100%)	0	100	100
34	U1	81/135 (60%)	81 (100%)	0	100	100
35	V1	101/102 (99%)	101 (100%)	0	100	100
36	W1	108/114 (95%)	108 (100%)	0	100	100
37	q1	131/131 (100%)	131 (100%)	0	100	100
38	r1	88/96 (92%)	88 (100%)	0	100	100
39	s1	41/95 (43%)	41 (100%)	0	100	100
40	A1	103/103 (100%)	102 (99%)	1 (1%)	68	75
41	H1	279/279 (100%)	279 (100%)	0	100	100
42	J1	137/137 (100%)	137 (100%)	0	100	100
43	K1	87/87 (100%)	87 (100%)	0	100	100
44	L1	548/549 (100%)	548 (100%)	0	100	100
45	M1	414/414 (100%)	413 (100%)	1 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	N1	307/307 (100%)	307 (100%)	0	100	100
47	O1	284/309 (92%)	284 (100%)	0	100	100
48	X1	153/154 (99%)	153 (100%)	0	100	100
49	Y1	105/106 (99%)	105 (100%)	0	100	100
50	Z1	122/123 (99%)	122 (100%)	0	100	100
51	a1	60/60 (100%)	60 (100%)	0	100	100
52	b1	72/73 (99%)	72 (100%)	0	100	100
53	c1	42/67 (63%)	42 (100%)	0	100	100
54	d1	107/107 (100%)	107 (100%)	0	100	100
55	e1	93/94 (99%)	93 (100%)	0	100	100
56	f1	49/53 (92%)	48 (98%)	1 (2%)	48	67
57	g1	92/129 (71%)	92 (100%)	0	100	100
58	h1	123/162 (76%)	123 (100%)	0	100	100
59	i1	99/119 (83%)	99 (100%)	0	100	100
60	j1	61/87 (70%)	61 (100%)	0	100	100
61	k1	60/78 (77%)	60 (100%)	0	100	100
62	l1	142/161 (88%)	141 (99%)	1 (1%)	76	78
63	m1	112/114 (98%)	112 (100%)	0	100	100
64	n1	163/164 (99%)	163 (100%)	0	100	100
65	o1	109/121 (90%)	109 (100%)	0	100	100
66	p1	155/158 (98%)	155 (100%)	0	100	100
67	z	39/61 (64%)	38 (97%)	1 (3%)	40	62
All	All	12041/13729 (88%)	12032 (100%)	9 (0%)	87	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	w	13	GLN
17	P	53	ASN
19	R	6	ASN
32	7	36	ASN
40	A1	108	GLN
45	M1	421	ASN
56	f1	10	HIS

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Mol	Chain	Res	Type
62	l1	65	HIS
67	z	23	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	n	80	ASN
1	n	151	HIS
1	n	422	ASN
1	n	491	ASN
2	o	187	ASN
3	p	133	ASN
3	p	160	ASN
4	q	65	ASN
6	s	67	ASN
7	t	75	ASN
8	u	24	ASN
8	u	32	ASN
13	A	69	ASN
13	A	85	HIS
13	A	141	ASN
13	A	339	GLN
13	A	359	ASN
14	B	22	GLN
14	B	61	ASN
14	B	153	GLN
14	B	313	ASN
14	B	338	ASN
14	B	351	ASN
14	B	362	ASN
14	B	400	GLN
14	B	429	ASN
17	E	53	ASN
17	E	161	HIS
13	L	53	ASN
13	L	73	ASN
13	L	94	HIS
13	L	126	GLN
13	L	139	GLN
13	L	289	HIS
13	L	323	HIS
13	L	430	GLN

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Mol	Chain	Res	Type
14	M	143	GLN
14	M	276	GLN
15	N	308	HIS
15	N	331	ASN
15	N	345	HIS
19	R	23	GLN
23	6	48	ASN
24	C1	124	HIS
24	C1	145	HIS
25	D1	114	ASN
25	D1	421	GLN
28	3	36	GLN
28	3	402	ASN
28	3	581	GLN
28	3	643	GLN
29	9	172	GLN
30	P1	86	GLN
30	P1	93	ASN
30	P1	136	ASN
30	P1	184	ASN
32	7	3	GLN
32	7	46	GLN
32	7	50	ASN
33	S1	30	GLN
33	S1	47	HIS
38	r1	8	GLN
39	s1	49	ASN
40	A1	108	GLN
41	H1	230	ASN
41	H1	235	ASN
44	L1	139	GLN
44	L1	194	ASN
44	L1	200	GLN
44	L1	506	ASN
45	M1	48	ASN
45	M1	51	ASN
45	M1	81	GLN
45	M1	144	ASN
45	M1	279	GLN
45	M1	366	ASN
45	M1	421	ASN
46	N1	289	ASN

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Mol	Chain	Res	Type
46	N1	342	GLN
47	O1	30	ASN
47	O1	57	GLN
47	O1	140	ASN
47	O1	147	GLN
47	O1	180	GLN
48	X1	72	GLN
48	X1	76	HIS
48	X1	150	ASN
48	X1	162	HIS
49	Y1	16	GLN
49	Y1	78	GLN
50	Z1	54	GLN
50	Z1	75	GLN
52	b1	51	ASN
54	d1	27	ASN
55	e1	97	HIS
57	g1	23	GLN
57	g1	25	GLN
57	g1	117	GLN
58	h1	108	GLN
59	i1	127	HIS
63	m1	51	ASN
64	n1	13	GLN
65	o1	83	GLN
66	p1	58	ASN
66	p1	99	GLN

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	$\# Z > 2$
25	2MR	D1	85	25	10,12,13	2.67	2 (20%)	5,13,15	2.78	2 (40%)
38	AYA	r1	1	38	6,7,8	1.27	1 (16%)	6,8,10	1.25	1 (16%)
52	AYA	b1	1	52	6,7,8	1.23	1 (16%)	6,8,10	1.17	1 (16%)
41	FME	H1	1	41	8,9,10	0.99	0	8,9,11	0.89	0
46	FME	N1	1	46	8,9,10	0.97	0	8,9,11	0.89	0
44	FME	L1	1	44	8,9,10	0.95	0	8,9,11	0.94	0
43	FME	K1	1	43	8,9,10	0.91	0	8,9,11	2.00	2 (25%)
40	FME	A1	1	40	8,9,10	0.98	0	8,9,11	0.84	0
45	FME	M1	1	45	8,9,10	0.99	0	8,9,11	0.77	0
42	FME	J1	1	42	8,9,10	0.95	0	8,9,11	0.88	0
59	SAC	i1	1	59	7,8,9	1.04	0	7,9,11	1.00	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
25	2MR	D1	85	25	-	2/10/13/15	-
38	AYA	r1	1	38	-	0/5/6/8	-
52	AYA	b1	1	52	-	0/5/6/8	-
41	FME	H1	1	41	-	2/7/9/11	-
46	FME	N1	1	46	-	4/7/9/11	-
44	FME	L1	1	44	-	4/7/9/11	-
43	FME	K1	1	43	-	4/7/9/11	-
40	FME	A1	1	40	-	1/7/9/11	-
45	FME	M1	1	45	-	1/7/9/11	-
42	FME	J1	1	42	-	4/7/9/11	-
59	SAC	i1	1	59	-	2/7/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D1	85	2MR	CZ-NE	5.97	1.47	1.34
25	D1	85	2MR	CZ-NH2	5.46	1.44	1.33
38	r1	1	AYA	CA-N	-2.36	1.44	1.46
52	b1	1	AYA	CA-N	-2.16	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D1	85	2MR	CD-NE-CZ	4.82	132.41	123.36
43	K1	1	FME	C-CA-N	4.76	118.69	109.50
25	D1	85	2MR	NE-CZ-NH2	-3.53	116.24	119.48
38	r1	1	AYA	CB-CA-N	2.85	112.90	109.68
52	b1	1	AYA	CB-CA-N	2.60	112.61	109.68
43	K1	1	FME	O-C-CA	-2.35	118.72	124.77

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	K1	1	FME	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	M1	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 7 are monoatomic - leaving 83 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
71	3PE	v	101	-	27,27,50	0.39	0	30,32,55	0.35	0
71	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.35	0
84	NDP	P1	501	-	51,52,52	0.33	0	71,80,80	0.41	0
76	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
71	3PE	L	501	-	22,22,50	0.44	0	25,27,55	0.37	0
71	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.33	0
71	3PE	Y1	204	-	41,41,50	0.33	0	44,46,55	0.33	0
81	SF4	3	802	28	0,12,12	-	-	-		
76	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.48	1 (1%)
85	ZMP	W1	201	-	28,33,36	0.66	1 (3%)	32,40,45	1.03	2 (6%)
80	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.58	0
81	SF4	9	202	29	0,12,12	-	-	-		
71	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.65	0
85	ZMP	n1	201	-	26,31,36	0.73	1 (3%)	30,38,45	0.97	1 (3%)
71	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.45	0
80	PC1	Y1	201	-	53,53,53	0.29	0	59,61,61	0.33	0
70	HEA	n	603	1	67,67,67	1.37	7 (10%)	81,103,103	2.22	27 (33%)
75	TGL	y	601	-	36,36,62	0.22	0	39,39,65	0.17	0
71	3PE	M1	501	-	50,50,50	0.29	0	53,55,55	0.31	0
76	CDL	L1	703	-	45,45,99	0.42	0	51,57,111	0.35	0
78	HEC	D	301	16	46,50,50	1.84	7 (15%)	58,82,82	1.96	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.34	0
71	3PE	r1	201	-	45,45,50	0.31	0	48,50,55	0.29	0
77	HEM	C	402	15	50,50,50	1.43	6 (12%)	67,82,82	1.28	8 (11%)
71	3PE	M1	503	-	35,35,50	0.35	0	38,40,55	0.31	0
78	HEC	O	303	16	46,50,50	1.84	7 (15%)	58,82,82	1.93	4 (6%)
79	FES	2	301	26	0,4,4	-	-	-	-	-
77	HEM	N	402	15	50,50,50	1.34	7 (14%)	67,82,82	1.23	5 (7%)
71	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.29	0
71	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.36	0
80	PC1	K	101	-	27,27,53	0.40	0	33,35,61	0.39	0
71	3PE	Y1	203	-	27,27,50	0.40	0	30,32,55	0.35	0
71	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.34	0
76	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
76	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.36	0
71	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.32	0
76	CDL	a1	101	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
76	CDL	h1	201	-	69,69,99	0.35	0	75,81,111	0.44	1 (1%)
71	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.67	0
79	FES	E	201	17	0,4,4	-	-	-	-	-
71	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.56	1 (2%)
76	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.29	0
76	CDL	G	101	-	55,55,99	0.39	0	61,67,111	0.32	0
76	CDL	Y1	202	-	93,93,99	0.30	0	99,105,111	0.27	0
80	PC1	L	502	-	23,23,53	0.44	0	29,31,61	0.64	0
71	3PE	D1	501	-	50,50,50	0.30	0	53,55,55	0.30	0
80	PC1	V	101	-	27,27,53	0.40	0	33,35,61	0.36	0
76	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.43	1 (1%)
71	3PE	p	301	-	44,44,50	0.33	0	47,49,55	0.30	0
81	SF4	1	502	27	0,12,12	-	-	-	-	-
71	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.48	1 (1%)
81	SF4	3	801	28	0,12,12	-	-	-	-	-
71	3PE	A1	201	-	42,42,50	0.32	0	45,47,55	0.33	0
81	SF4	6	201	23	0,12,12	-	-	-	-	-
71	3PE	G	102	-	50,50,50	0.29	0	53,55,55	0.28	0
80	PC1	9	203	-	53,53,53	0.29	0	59,61,61	0.46	0
82	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.36	0
71	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.35	0
80	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.35	0
81	SF4	9	201	29	0,12,12	-	-	-	-	-
71	3PE	N	401	-	33,33,50	0.36	0	36,38,55	0.35	0
71	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
79	FES	P	201	17	0,4,4	-	-	-		
80	PC1	9	204	-	46,46,53	0.31	0	52,54,61	0.30	0
71	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.39	0
73	CUA	o	303	2	0,1,1	-	-	-		
71	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.35	0
77	HEM	N	403	15	50,50,50	1.39	7 (14%)	67,82,82	1.26	6 (8%)
76	CDL	N	405	-	45,45,99	0.44	0	51,57,111	0.52	1 (1%)
71	3PE	N	404	-	36,36,50	0.35	0	39,41,55	0.31	0
71	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.35	0
71	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.31	0
76	CDL	R	101	-	40,40,99	0.46	0	46,52,111	0.54	0
79	FES	3	803	28	0,4,4	-	-	-		
86	DGT	O1	401	72	32,33,33	0.29	0	48,52,52	0.30	0
76	CDL	N1	401	-	89,89,99	0.31	0	95,101,111	0.40	1 (1%)
71	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.27	0
70	HEA	n	604	1	67,67,67	1.41	7 (10%)	81,103,103	2.35	28 (34%)
71	3PE	C	405	-	30,30,50	0.38	0	33,35,55	0.35	0
76	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
80	PC1	6	203	-	42,42,53	0.33	0	48,50,61	0.50	1 (2%)
77	HEM	C	401	15	50,50,50	1.34	7 (14%)	67,82,82	1.17	6 (8%)

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
71	3PE	v	101	-	-	9/31/31/54	-
71	3PE	O	302	-	-	6/36/36/54	-
84	NDP	P1	501	-	-	7/34/77/77	0/5/5/5
76	CDL	O	301	-	-	13/67/67/110	-
71	3PE	L	501	-	-	7/26/26/54	-
71	3PE	R	104	-	-	7/33/33/54	-
71	3PE	Y1	204	-	-	6/45/45/54	-
81	SF4	3	802	28	-	-	0/6/5/5
76	CDL	R	102	-	-	19/67/67/110	-
85	ZMP	W1	201	-	-	8/38/40/43	-
80	PC1	P1	502	-	-	15/34/34/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	SF4	9	202	29	-	-	0/6/5/5
71	3PE	t	101	-	-	6/28/28/54	-
85	ZMP	n1	201	-	-	16/36/38/43	-
71	3PE	n	606	-	-	11/31/31/54	-
80	PC1	Y1	201	-	-	15/57/57/57	-
70	HEA	n	603	1	-	11/36/76/76	-
75	TGL	y	601	-	-	1/39/39/65	-
71	3PE	M1	501	-	-	11/54/54/54	-
76	CDL	L1	703	-	-	8/56/56/110	-
78	HEC	D	301	16	-	6/14/54/54	-
71	3PE	C	403	-	-	11/38/38/54	-
71	3PE	r1	201	-	-	5/49/49/54	-
77	HEM	C	402	15	-	2/14/54/54	-
71	3PE	M1	503	-	-	9/39/39/54	-
78	HEC	O	303	16	-	4/14/54/54	-
79	FES	2	301	26	-	-	0/1/1/1
77	HEM	N	402	15	-	1/14/54/54	-
71	3PE	K1	201	-	-	10/44/44/54	-
71	3PE	E	202	-	-	6/35/35/54	-
80	PC1	K	101	-	-	9/31/31/57	-
71	3PE	Y1	203	-	-	6/31/31/54	-
71	3PE	d1	202	-	-	8/34/34/54	-
76	CDL	d1	201	-	-	12/77/77/110	-
76	CDL	C	404	-	-	13/52/52/110	-
71	3PE	6	202	-	-	3/35/35/54	-
76	CDL	a1	101	-	-	11/67/67/110	-
76	CDL	h1	201	-	-	20/80/80/110	-
71	3PE	A	501	-	-	9/26/26/54	-
79	FES	E	201	17	-	-	0/1/1/1
71	3PE	n	605	-	-	9/37/37/54	-
76	CDL	L1	702	-	-	20/88/88/110	-
76	CDL	G	101	-	-	14/66/66/110	-
76	CDL	Y1	202	-	-	16/104/104/110	-
80	PC1	L	502	-	-	7/27/27/57	-
71	3PE	D1	501	-	-	9/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	PC1	V	101	-	-	4/31/31/57	-
76	CDL	R	103	-	-	17/82/82/110	-
71	3PE	p	301	-	-	9/48/48/54	-
81	SF4	1	502	27	-	-	0/6/5/5
71	3PE	H1	401	-	-	11/54/54/54	-
81	SF4	3	801	28	-	-	0/6/5/5
71	3PE	A1	201	-	-	7/46/46/54	-
81	SF4	6	201	23	-	-	0/6/5/5
71	3PE	G	102	-	-	8/54/54/54	-
80	PC1	9	203	-	-	10/57/57/57	-
82	FMN	1	501	-	-	5/18/18/18	0/3/3/3
71	3PE	d1	203	-	-	6/35/35/54	-
80	PC1	J	101	-	-	7/38/38/57	-
81	SF4	9	201	29	-	-	0/6/5/5
71	3PE	N	401	-	-	4/37/37/54	-
71	3PE	L1	701	-	-	7/54/54/54	-
76	CDL	H1	402	-	-	10/59/59/110	-
79	FES	P	201	17	-	-	0/1/1/1
80	PC1	9	204	-	-	10/50/50/57	-
71	3PE	o	302	-	-	9/32/32/54	-
71	3PE	N1	402	-	-	6/41/41/54	-
77	HEM	N	403	15	-	4/14/54/54	-
76	CDL	N	405	-	-	8/56/56/110	-
71	3PE	N	404	-	-	5/40/40/54	-
71	3PE	n	607	-	-	5/30/30/54	-
71	3PE	i1	201	-	-	6/45/45/54	-
76	CDL	R	101	-	-	9/51/51/110	-
79	FES	3	803	28	-	-	0/1/1/1
86	DGT	O1	401	72	-	6/22/34/34	0/3/3/3
76	CDL	N1	401	-	-	17/100/100/110	-
71	3PE	M1	502	-	-	9/54/54/54	-
70	HEA	n	604	1	-	9/36/76/76	-
71	3PE	C	405	-	-	4/34/34/54	-
76	CDL	A	502	-	-	19/56/56/110	-
80	PC1	6	203	-	-	11/46/46/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	HEM	C	401	15	-	2/14/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	D	301	HEC	CAC-C3C	6.17	1.55	1.35
78	O	303	HEC	CAC-C3C	6.16	1.55	1.35
78	D	301	HEC	CAB-C3B	6.12	1.54	1.35
78	O	303	HEC	CAB-C3B	6.06	1.54	1.35
78	D	301	HEC	C3D-C2D	5.71	1.53	1.38
78	O	303	HEC	C3D-C2D	5.68	1.53	1.38
77	C	402	HEM	FE-NB	4.99	2.10	1.94
70	n	604	HEA	C3D-C2D	4.55	1.46	1.36
70	n	603	HEA	C3B-C2B	4.40	1.44	1.34
70	n	604	HEA	C3B-C2B	4.14	1.44	1.34
77	N	403	HEM	FE-NB	4.07	2.07	1.94
70	n	603	HEA	C3D-C2D	3.90	1.45	1.36
70	n	604	HEA	C3A-C2A	3.57	1.45	1.37
70	n	603	HEA	C3A-C2A	3.52	1.45	1.37
77	C	401	HEM	FE-NC	3.50	2.06	1.95
77	C	401	HEM	CAB-C3B	3.21	1.56	1.47
77	N	403	HEM	CAC-C3C	3.20	1.55	1.47
77	C	401	HEM	CAC-C3C	3.18	1.55	1.47
77	C	402	HEM	CAC-C3C	3.17	1.55	1.47
77	N	402	HEM	CAB-C3B	3.16	1.55	1.47
77	N	402	HEM	FE-NC	3.10	2.05	1.95
77	N	402	HEM	FE-ND	3.09	2.04	1.94
77	N	403	HEM	CAB-C3B	3.09	1.55	1.47
77	C	402	HEM	CAB-C3B	3.06	1.55	1.47
77	N	402	HEM	CAC-C3C	3.03	1.55	1.47
70	n	603	HEA	C4B-C3B	2.97	1.50	1.44
77	N	403	HEM	FE-NA	2.76	2.04	1.95
77	C	402	HEM	FE-NA	2.61	2.03	1.95
70	n	604	HEA	C4B-C3B	2.58	1.49	1.44
77	C	402	HEM	FE-NC	2.52	2.03	1.95
77	C	401	HEM	FE-NB	2.51	2.02	1.94
70	n	604	HEA	C1D-C2D	2.46	1.49	1.44
85	n1	201	ZMP	C9-C10	2.43	1.53	1.50
70	n	603	HEA	C1D-ND	-2.42	1.36	1.40
77	N	403	HEM	FE-NC	2.39	2.03	1.95
70	n	603	HEA	C1C-C2C	2.29	1.48	1.43
77	N	402	HEM	FE-NA	2.26	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	W1	201	ZMP	C9-C10	2.25	1.53	1.50
77	C	401	HEM	FE-NA	2.17	2.02	1.95
70	n	604	HEA	C3C-C4C	2.16	1.49	1.42
77	C	401	HEM	FE-ND	2.15	2.01	1.94
77	N	402	HEM	CMC-C2C	2.12	1.55	1.50
77	C	401	HEM	CMC-C2C	2.12	1.55	1.50
77	N	403	HEM	CMC-C2C	2.12	1.55	1.50
70	n	604	HEA	C1D-ND	-2.12	1.36	1.40
78	O	303	HEC	C3B-C2B	-2.10	1.34	1.41
78	O	303	HEC	C3C-C2C	-2.07	1.34	1.41
78	O	303	HEC	CMB-C2B	2.06	1.55	1.50
78	D	301	HEC	C3C-C2C	-2.06	1.34	1.41
77	C	402	HEM	C2A-C3A	-2.06	1.33	1.38
70	n	603	HEA	C4D-C3D	2.05	1.48	1.45
77	N	403	HEM	C2A-C3A	-2.04	1.33	1.38
77	N	402	HEM	C2A-C3A	-2.03	1.33	1.38
78	D	301	HEC	C3B-C2B	-2.02	1.34	1.41
78	D	301	HEC	CMC-C2C	2.02	1.54	1.50
78	D	301	HEC	CMD-C2D	2.01	1.54	1.50
78	O	303	HEC	CMC-C2C	2.00	1.54	1.50

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	D	301	HEC	CBC-CAC-C3C	-8.65	110.15	127.43
78	O	303	HEC	CBC-CAC-C3C	-8.60	110.24	127.43
78	D	301	HEC	CBB-CAB-C3B	-8.54	110.36	127.43
78	O	303	HEC	CBB-CAB-C3B	-8.47	110.50	127.43
70	n	604	HEA	C3A-C2A-C1A	-6.43	100.96	107.05
70	n	603	HEA	C3A-C2A-C1A	-6.25	101.13	107.05
70	n	604	HEA	CMC-C2C-C3C	5.45	139.38	126.55
70	n	604	HEA	C3D-C4D-ND	5.40	115.57	110.35
70	n	604	HEA	CMC-C2C-C1C	-5.20	117.50	125.42
70	n	604	HEA	C2A-C1A-NA	5.09	115.23	110.32
70	n	603	HEA	CMC-C2C-C3C	4.89	138.06	126.55
70	n	603	HEA	C2A-C1A-NA	4.82	114.97	110.32
70	n	603	HEA	C3D-C4D-ND	4.64	114.84	110.35
70	n	603	HEA	CMC-C2C-C1C	-4.62	118.39	125.42
70	n	604	HEA	C13-C12-C11	-4.48	107.23	114.39
70	n	603	HEA	CMD-C2D-C1D	-4.41	118.14	125.03
70	n	604	HEA	CHA-C4D-C3D	-4.40	118.36	124.77
70	n	604	HEA	CMD-C2D-C1D	-4.30	118.32	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	n	603	HEA	CMB-C2B-C1B	-4.16	118.53	125.03
70	n	604	HEA	CMB-C2B-C1B	-4.15	118.55	125.03
77	N	402	HEM	C3B-C2B-C1B	3.86	109.31	106.41
70	n	604	HEA	C4D-C3D-C2D	-3.85	101.28	106.89
70	n	603	HEA	C4D-C3D-C2D	-3.83	101.31	106.89
70	n	603	HEA	CHA-C1A-C2A	-3.71	119.01	124.86
70	n	603	HEA	CHA-C4D-C3D	-3.68	119.41	124.77
70	n	604	HEA	CHA-C1A-C2A	-3.53	119.30	124.86
78	O	303	HEC	C4D-ND-C1D	3.53	111.57	105.82
70	n	603	HEA	C13-C12-C11	-3.48	108.83	114.39
70	n	604	HEA	CMD-C2D-C3D	3.48	135.55	126.15
70	n	604	HEA	C3C-C2C-C1C	-3.45	103.11	107.17
77	C	401	HEM	C3B-C2B-C1B	3.41	108.97	106.41
70	n	604	HEA	CAD-C3D-C2D	3.32	134.08	127.87
70	n	603	HEA	CMD-C2D-C3D	3.30	135.09	126.15
70	n	603	HEA	C13-C14-C15	-3.24	120.20	127.62
77	N	403	HEM	C3B-C2B-C1B	3.20	108.81	106.41
78	D	301	HEC	C4D-ND-C1D	3.17	110.99	105.82
70	n	603	HEA	CAA-CBA-CGA	-3.14	105.34	113.67
77	C	402	HEM	C3B-C2B-C1B	3.10	108.74	106.41
70	n	603	HEA	CMB-C2B-C3B	3.10	136.26	130.28
70	n	603	HEA	C3C-C2C-C1C	-3.07	103.55	107.17
70	n	604	HEA	C26-C15-C16	3.04	120.51	115.23
70	n	603	HEA	CHB-C1B-C2B	-3.00	120.30	125.03
70	n	604	HEA	C13-C14-C15	-2.91	120.97	127.62
70	n	604	HEA	CAA-CBA-CGA	-2.88	106.02	113.67
77	C	402	HEM	C4D-ND-C1D	2.77	108.49	105.21
70	n	604	HEA	C3B-C4B-NB	2.76	113.02	109.84
85	W1	201	ZMP	O1-C10-C9	-2.74	120.81	123.98
70	n	604	HEA	CHC-C1C-C2C	-2.74	119.47	127.43
70	n	604	HEA	C4B-C3B-C2B	-2.71	102.88	107.44
70	n	603	HEA	C17-C18-C19	-2.71	121.43	127.62
77	N	402	HEM	CMB-C2B-C1B	-2.70	120.81	125.03
70	n	604	HEA	C27-C19-C20	2.69	119.90	115.23
70	n	604	HEA	C12-C11-C3B	2.66	116.28	112.12
70	n	604	HEA	CMB-C2B-C3B	2.63	135.35	130.28
70	n	604	HEA	CHB-C1B-C2B	-2.61	120.90	125.03
85	n1	201	ZMP	O1-C10-C9	-2.60	120.98	123.98
70	n	603	HEA	CAD-C3D-C4D	2.58	129.20	124.70
77	C	402	HEM	C3D-C4D-ND	-2.54	107.39	110.17
70	n	604	HEA	C25-C23-C24	2.53	120.42	114.59
77	N	403	HEM	C4D-ND-C1D	2.52	108.19	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	N	403	HEM	C1B-NB-C4B	2.49	108.15	105.21
77	N	403	HEM	C3B-C4B-NB	-2.48	107.69	109.47
70	n	603	HEA	C2B-C1B-NB	2.46	112.75	109.90
70	n	604	HEA	C17-C18-C19	-2.43	122.06	127.62
77	C	401	HEM	C4D-ND-C1D	2.37	108.02	105.21
70	n	603	HEA	CHB-C1B-NB	2.35	126.96	124.42
70	n	604	HEA	CHB-C1B-NB	2.35	126.95	124.42
77	N	402	HEM	CHB-C1B-NB	2.35	127.27	124.37
78	O	303	HEC	C2A-C1A-NA	-2.31	108.09	110.32
70	n	603	HEA	C26-C15-C16	2.31	119.23	115.23
77	N	402	HEM	C4D-ND-C1D	2.28	107.91	105.21
78	D	301	HEC	CHB-C4A-NA	2.26	126.91	124.45
78	D	301	HEC	C2A-C1A-NA	-2.26	108.15	110.32
77	N	403	HEM	C3D-C4D-ND	-2.24	107.72	110.17
77	C	402	HEM	C3B-C4B-NB	-2.23	107.87	109.47
85	W1	201	ZMP	C15-C14-C13	-2.22	108.69	112.39
70	n	603	HEA	C25-C23-C24	2.22	119.69	114.59
77	C	401	HEM	C3D-C4D-ND	-2.22	107.74	110.17
70	n	603	HEA	C3C-C4C-NC	2.20	111.65	109.80
77	N	402	HEM	C3D-C4D-ND	-2.18	107.78	110.17
77	C	402	HEM	C1B-NB-C4B	2.16	107.77	105.21
70	n	603	HEA	CHC-C1C-C2C	-2.16	121.16	127.43
70	n	603	HEA	C4B-C3B-C2B	-2.14	103.84	107.44
71	n	605	3PE	C2-O21-C21	2.14	122.92	117.80
77	C	402	HEM	C2A-C1A-NA	-2.13	107.79	110.15
70	n	604	HEA	C2C-C1C-NC	2.13	113.55	110.14
76	R	103	CDL	CA4-OA6-CA5	2.13	122.89	117.80
76	R	102	CDL	CA4-OA6-CA5	2.09	122.80	117.80
77	C	402	HEM	CAB-C3B-C2B	-2.06	121.73	128.43
76	N1	401	CDL	CB4-OB6-CB5	2.06	122.72	117.80
77	C	401	HEM	CAD-CBD-CGD	-2.05	108.24	113.67
77	C	401	HEM	CHD-C1D-ND	2.05	126.62	124.42
71	H1	401	3PE	C2-O21-C21	2.04	122.69	117.80
77	N	403	HEM	C2A-C1A-NA	-2.04	107.89	110.15
76	h1	201	CDL	CB4-OB6-CB5	2.04	122.68	117.80
76	a1	101	CDL	CA4-OA6-CA5	2.04	122.67	117.80
70	n	603	HEA	C27-C19-C20	2.04	118.76	115.23
77	C	401	HEM	C2A-C1A-NA	-2.04	107.89	110.15
76	N	405	CDL	CB4-OB6-CB5	2.02	122.63	117.80
77	C	402	HEM	C2D-C1D-ND	-2.01	107.58	109.90
80	6	203	PC1	O21-C2-C1	2.01	115.54	108.34

There are no chirality outliers.

All (640) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	n	603	HEA	C2A-C3A-CMA-OMA
70	n	603	HEA	C4A-C3A-CMA-OMA
70	n	603	HEA	C15-C16-C17-C18
70	n	604	HEA	C2A-C3A-CMA-OMA
70	n	604	HEA	C4A-C3A-CMA-OMA
70	n	604	HEA	C2D-C3D-CAD-CBD
70	n	604	HEA	C15-C16-C17-C18
71	n	605	3PE	C11-O13-P-O11
71	n	605	3PE	C11-O13-P-O12
71	n	605	3PE	C11-O13-P-O14
71	n	605	3PE	O13-C11-C12-N
71	n	606	3PE	C1-O11-P-O12
71	n	606	3PE	C1-O11-P-O13
71	n	606	3PE	C1-O11-P-O14
71	n	606	3PE	O13-C11-C12-N
71	n	606	3PE	O11-C1-C2-O21
71	n	607	3PE	C1-O11-P-O13
71	n	607	3PE	O13-C11-C12-N
71	o	302	3PE	C1-O11-P-O13
71	o	302	3PE	C1-O11-P-O14
71	o	302	3PE	C11-O13-P-O11
71	o	302	3PE	O13-C11-C12-N
71	p	301	3PE	C1-O11-P-O12
71	p	301	3PE	C1-O11-P-O13
71	p	301	3PE	C11-O13-P-O11
71	p	301	3PE	C11-O13-P-O14
71	p	301	3PE	O13-C11-C12-N
71	t	101	3PE	C11-O13-P-O11
71	t	101	3PE	C11-O13-P-O12
71	v	101	3PE	C1-O11-P-O12
71	v	101	3PE	C11-O13-P-O14
71	v	101	3PE	O13-C11-C12-N
71	A	501	3PE	C1-O11-P-O12
71	A	501	3PE	C1-O11-P-O13
71	A	501	3PE	C1-O11-P-O14
71	A	501	3PE	C11-O13-P-O11
71	A	501	3PE	C11-O13-P-O12
71	A	501	3PE	C11-O13-P-O14
71	A	501	3PE	O13-C11-C12-N
71	C	403	3PE	C1-O11-P-O12
71	C	403	3PE	C1-O11-P-O13
71	C	403	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
71	C	403	3PE	C11-O13-P-O11
71	C	403	3PE	C11-O13-P-O14
71	C	403	3PE	O13-C11-C12-N
71	E	202	3PE	O13-C11-C12-N
71	E	202	3PE	O21-C2-C3-O31
71	G	102	3PE	C1-O11-P-O13
71	G	102	3PE	C1-O11-P-O14
71	G	102	3PE	O13-C11-C12-N
71	L	501	3PE	C11-O13-P-O11
71	L	501	3PE	C11-O13-P-O12
71	L	501	3PE	C11-O13-P-O14
71	L	501	3PE	O13-C11-C12-N
71	N	404	3PE	C11-O13-P-O11
71	N	404	3PE	C11-O13-P-O12
71	N	404	3PE	C11-O13-P-O14
71	N	404	3PE	O13-C11-C12-N
71	O	302	3PE	C11-O13-P-O11
71	O	302	3PE	C11-O13-P-O12
71	O	302	3PE	C11-O13-P-O14
71	O	302	3PE	O13-C11-C12-N
71	R	104	3PE	C1-O11-P-O14
71	R	104	3PE	C11-O13-P-O11
71	R	104	3PE	C11-O13-P-O12
71	R	104	3PE	C11-O13-P-O14
71	R	104	3PE	O13-C11-C12-N
71	6	202	3PE	C1-O11-P-O14
71	D1	501	3PE	C1-O11-P-O12
71	D1	501	3PE	C1-O11-P-O13
71	D1	501	3PE	O13-C11-C12-N
71	r1	201	3PE	C1-O11-P-O12
71	r1	201	3PE	C1-O11-P-O13
71	r1	201	3PE	C1-O11-P-O14
71	A1	201	3PE	C1-O11-P-O14
71	A1	201	3PE	C11-O13-P-O14
71	H1	401	3PE	C11-O13-P-O11
71	H1	401	3PE	C11-O13-P-O12
71	H1	401	3PE	O13-C11-C12-N
71	K1	201	3PE	C1-O11-P-O12
71	K1	201	3PE	C1-O11-P-O13
71	K1	201	3PE	C1-O11-P-O14
71	K1	201	3PE	C11-O13-P-O11
71	K1	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
71	L1	701	3PE	C1-O11-P-O13
71	L1	701	3PE	C1-O11-P-O14
71	L1	701	3PE	O13-C11-C12-N
71	M1	501	3PE	C11-O13-P-O11
71	M1	501	3PE	C11-O13-P-O12
71	M1	501	3PE	C12-C11-O13-P
71	M1	501	3PE	O13-C11-C12-N
71	M1	502	3PE	C11-O13-P-O11
71	M1	502	3PE	C11-O13-P-O12
71	M1	503	3PE	C1-O11-P-O13
71	M1	503	3PE	C1-O11-P-O14
71	M1	503	3PE	C11-O13-P-O11
71	M1	503	3PE	C11-O13-P-O12
71	M1	503	3PE	C11-O13-P-O14
71	N1	402	3PE	C1-O11-P-O12
71	N1	402	3PE	C1-O11-P-O13
71	N1	402	3PE	C1-O11-P-O14
71	Y1	203	3PE	C1-O11-P-O13
71	Y1	203	3PE	C1-O11-P-O14
71	Y1	203	3PE	O13-C11-C12-N
71	Y1	204	3PE	C11-O13-P-O11
71	Y1	204	3PE	C11-O13-P-O12
71	Y1	204	3PE	C11-O13-P-O14
71	d1	202	3PE	C11-O13-P-O11
71	d1	202	3PE	C11-O13-P-O12
71	d1	202	3PE	O13-C11-C12-N
71	d1	203	3PE	C1-O11-P-O13
71	d1	203	3PE	C1-O11-P-O14
71	d1	203	3PE	O13-C11-C12-N
71	i1	201	3PE	C11-O13-P-O11
71	i1	201	3PE	C11-O13-P-O12
71	i1	201	3PE	C11-O13-P-O14
76	A	502	CDL	CA2-OA2-PA1-OA3
76	A	502	CDL	CA3-OA5-PA1-OA3
76	A	502	CDL	CB2-OB2-PB2-OB3
76	A	502	CDL	CB2-OB2-PB2-OB4
76	A	502	CDL	CB2-OB2-PB2-OB5
76	C	404	CDL	CA2-OA2-PA1-OA4
76	C	404	CDL	CB2-OB2-PB2-OB3
76	C	404	CDL	CB2-OB2-PB2-OB4
76	C	404	CDL	CB3-OB5-PB2-OB2
76	C	404	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
76	C	404	CDL	OB5-CB3-CB4-OB6
76	G	101	CDL	C1-CB2-OB2-PB2
76	G	101	CDL	CB2-OB2-PB2-OB4
76	G	101	CDL	CB2-OB2-PB2-OB5
76	G	101	CDL	CB3-OB5-PB2-OB2
76	G	101	CDL	CB3-OB5-PB2-OB4
76	N	405	CDL	CA3-OA5-PA1-OA2
76	N	405	CDL	CA3-OA5-PA1-OA3
76	O	301	CDL	CA2-OA2-PA1-OA3
76	O	301	CDL	CA2-OA2-PA1-OA4
76	O	301	CDL	CA2-OA2-PA1-OA5
76	O	301	CDL	CA3-OA5-PA1-OA2
76	O	301	CDL	CA3-OA5-PA1-OA3
76	O	301	CDL	CB2-OB2-PB2-OB3
76	O	301	CDL	CB3-OB5-PB2-OB2
76	O	301	CDL	CB3-OB5-PB2-OB3
76	O	301	CDL	CB3-OB5-PB2-OB4
76	O	301	CDL	OB5-CB3-CB4-OB6
76	R	101	CDL	CA2-OA2-PA1-OA3
76	R	101	CDL	CA2-OA2-PA1-OA4
76	R	101	CDL	CA2-OA2-PA1-OA5
76	R	101	CDL	CB2-OB2-PB2-OB3
76	R	102	CDL	CA2-OA2-PA1-OA4
76	R	102	CDL	CA2-OA2-PA1-OA5
76	R	102	CDL	CA3-OA5-PA1-OA2
76	R	102	CDL	CB2-OB2-PB2-OB5
76	R	102	CDL	CB3-OB5-PB2-OB2
76	R	102	CDL	CB3-OB5-PB2-OB4
76	R	103	CDL	CA2-OA2-PA1-OA3
76	R	103	CDL	CA2-OA2-PA1-OA5
76	R	103	CDL	CA3-OA5-PA1-OA2
76	R	103	CDL	CA3-OA5-PA1-OA3
76	R	103	CDL	CB2-OB2-PB2-OB3
76	R	103	CDL	CB2-OB2-PB2-OB4
76	R	103	CDL	CB2-OB2-PB2-OB5
76	R	103	CDL	CB3-OB5-PB2-OB2
76	R	103	CDL	CB3-OB5-PB2-OB3
76	R	103	CDL	CB3-OB5-PB2-OB4
76	H1	402	CDL	CA2-OA2-PA1-OA3
76	H1	402	CDL	CA2-OA2-PA1-OA4
76	H1	402	CDL	CA2-OA2-PA1-OA5
76	H1	402	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
76	H1	402	CDL	CB2-OB2-PB2-OB5
76	L1	702	CDL	CA2-OA2-PA1-OA3
76	L1	702	CDL	CA2-OA2-PA1-OA4
76	L1	702	CDL	CA2-OA2-PA1-OA5
76	L1	702	CDL	CA3-OA5-PA1-OA2
76	L1	702	CDL	CA3-OA5-PA1-OA3
76	L1	702	CDL	CB2-OB2-PB2-OB3
76	L1	702	CDL	CB2-OB2-PB2-OB4
76	L1	702	CDL	CB2-OB2-PB2-OB5
76	L1	702	CDL	CB3-OB5-PB2-OB2
76	L1	702	CDL	CB3-OB5-PB2-OB3
76	L1	702	CDL	CB3-OB5-PB2-OB4
76	L1	703	CDL	CA2-OA2-PA1-OA3
76	L1	703	CDL	CA2-OA2-PA1-OA4
76	L1	703	CDL	CA2-OA2-PA1-OA5
76	L1	703	CDL	CB2-OB2-PB2-OB5
76	N1	401	CDL	CA2-OA2-PA1-OA3
76	N1	401	CDL	CA3-OA5-PA1-OA3
76	N1	401	CDL	OA6-CA4-CA6-OA8
76	N1	401	CDL	CB2-OB2-PB2-OB3
76	N1	401	CDL	CB2-OB2-PB2-OB4
76	N1	401	CDL	CB2-OB2-PB2-OB5
76	Y1	202	CDL	CA2-OA2-PA1-OA3
76	Y1	202	CDL	CA2-OA2-PA1-OA4
76	Y1	202	CDL	CA2-OA2-PA1-OA5
76	Y1	202	CDL	CB3-OB5-PB2-OB2
76	Y1	202	CDL	CB3-OB5-PB2-OB3
76	Y1	202	CDL	CB3-OB5-PB2-OB4
76	a1	101	CDL	CA2-OA2-PA1-OA3
76	a1	101	CDL	CA2-OA2-PA1-OA4
76	a1	101	CDL	CA2-OA2-PA1-OA5
76	a1	101	CDL	CA3-OA5-PA1-OA2
76	d1	201	CDL	CA3-OA5-PA1-OA3
76	d1	201	CDL	CB2-OB2-PB2-OB5
76	h1	201	CDL	CA2-OA2-PA1-OA3
76	h1	201	CDL	CA2-OA2-PA1-OA5
76	h1	201	CDL	CB2-OB2-PB2-OB3
76	h1	201	CDL	CB2-OB2-PB2-OB4
76	h1	201	CDL	CB2-OB2-PB2-OB5
76	h1	201	CDL	CB3-OB5-PB2-OB2
76	h1	201	CDL	CB3-OB5-PB2-OB4
78	D	301	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
78	O	303	HEC	C2B-C3B-CAB-CBB
78	O	303	HEC	C2C-C3C-CAC-CBC
80	J	101	PC1	C11-O13-P-O11
80	J	101	PC1	C1-O11-P-O12
80	J	101	PC1	C1-O11-P-O14
80	J	101	PC1	C1-O11-P-O13
80	K	101	PC1	C1-O11-P-O14
80	K	101	PC1	C1-O11-P-O13
80	L	502	PC1	C11-O13-P-O12
80	L	502	PC1	C11-O13-P-O11
80	L	502	PC1	C1-O11-P-O12
80	L	502	PC1	C1-O11-P-O13
80	6	203	PC1	C1-O11-P-O12
80	6	203	PC1	C1-O11-P-O14
80	6	203	PC1	C1-O11-P-O13
80	9	203	PC1	C11-O13-P-O12
80	9	203	PC1	C11-O13-P-O11
80	9	203	PC1	C1-O11-P-O12
80	9	203	PC1	C1-O11-P-O14
80	9	203	PC1	C1-O11-P-O13
80	P1	502	PC1	C11-O13-P-O11
80	P1	502	PC1	C1-O11-P-O12
80	P1	502	PC1	C1-O11-P-O14
80	P1	502	PC1	C1-O11-P-O13
80	Y1	201	PC1	C11-O13-P-O12
80	Y1	201	PC1	C11-O13-P-O14
80	Y1	201	PC1	C11-O13-P-O11
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
82	1	501	FMN	C5'-O5'-P-O3P
84	P1	501	NDP	C5B-O5B-PA-O3
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

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Mol	Chain	Res	Type	Atoms
85	n1	201	ZMP	O3-C16-C17-O4
85	n1	201	ZMP	C17-C16-N2-C15
85	n1	201	ZMP	C13-C14-C15-N2
86	O1	401	DGT	PB-O3B-PG-O1G
86	O1	401	DGT	C5'-O5'-PA-O1A
70	n	604	HEA	C4D-C3D-CAD-CBD
85	n1	201	ZMP	O3-C16-N2-C15
77	C	401	HEM	C2A-CAA-CBA-CGA
76	L1	702	CDL	O1-C1-CB2-OB2
76	L1	702	CDL	CA5-C11-C12-C13
70	n	603	HEA	C19-C20-C21-C22
80	K	101	PC1	C11-C12-N-C13
71	p	301	3PE	C2-C1-O11-P
71	M1	501	3PE	C31-C32-C33-C34
80	K	101	PC1	C11-C12-N-C15
70	n	604	HEA	C26-C15-C16-C17
71	n	607	3PE	C2-C1-O11-P
71	M1	502	3PE	C27-C28-C29-C2A
76	R	103	CDL	OB5-CB3-CB4-OB6
71	G	102	3PE	C37-C38-C39-C3A
76	N1	401	CDL	C81-C82-C83-C84
80	Y1	201	PC1	C34-C35-C36-C37
85	n1	201	ZMP	C6-C7-C8-C9
71	D1	501	3PE	C38-C39-C3A-C3B
71	M1	502	3PE	C28-C29-C2A-C2B
80	Y1	201	PC1	C28-C29-C2A-C2B
85	W1	201	ZMP	S1-C11-C12-N1
80	9	204	PC1	C2A-C2B-C2C-C2D
71	G	102	3PE	C32-C33-C34-C35
80	Y1	201	PC1	C37-C38-C39-C3A
71	A1	201	3PE	C3A-C3B-C3C-C3D
71	M1	501	3PE	C36-C37-C38-C39
71	M1	501	3PE	C23-C24-C25-C26
76	d1	201	CDL	C63-C64-C65-C66
80	V	101	PC1	C11-C12-N-C13
80	6	203	PC1	C11-C12-N-C14
77	N	402	HEM	C2A-CAA-CBA-CGA
70	n	604	HEA	C14-C15-C16-C17
71	H1	401	3PE	C21-C22-C23-C24
71	N1	402	3PE	C36-C37-C38-C39
76	d1	201	CDL	C55-C56-C57-C58
71	n	606	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
80	K	101	PC1	C11-C12-N-C14
80	V	101	PC1	C11-C12-N-C15
80	6	203	PC1	C11-C12-N-C13
80	9	204	PC1	C11-C12-N-C15
80	P1	502	PC1	C11-C12-N-C15
76	G	101	CDL	OB5-CB3-CB4-OB6
76	d1	201	CDL	OB5-CB3-CB4-OB6
71	L1	701	3PE	C21-C22-C23-C24
85	n1	201	ZMP	C5-C6-C7-C8
76	H1	402	CDL	C1-CB2-OB2-PB2
76	Y1	202	CDL	C73-C74-C75-C76
71	D1	501	3PE	C32-C33-C34-C35
80	V	101	PC1	C11-C12-N-C14
80	6	203	PC1	C11-C12-N-C15
71	n	606	3PE	O11-C1-C2-C3
76	C	404	CDL	OB5-CB3-CB4-CB6
76	G	101	CDL	OB5-CB3-CB4-CB6
76	O	301	CDL	OB5-CB3-CB4-CB6
76	a1	101	CDL	OB5-CB3-CB4-CB6
76	d1	201	CDL	OB5-CB3-CB4-CB6
80	P1	502	PC1	C21-C22-C23-C24
71	E	202	3PE	C1-C2-C3-O31
76	R	103	CDL	CB3-CB4-CB6-OB8
76	a1	101	CDL	O1-C1-CA2-OA2
76	G	101	CDL	C74-C75-C76-C77
80	9	204	PC1	C11-C12-N-C14
80	P1	502	PC1	C11-C12-N-C14
80	Y1	201	PC1	O11-C1-C2-O21
71	N	404	3PE	C25-C26-C27-C28
76	Y1	202	CDL	C24-C25-C26-C27
80	9	204	PC1	C11-C12-N-C13
85	n1	201	ZMP	O4-C17-C18-C20
76	Y1	202	CDL	C82-C83-C84-C85
80	9	204	PC1	C34-C35-C36-C37
80	J	101	PC1	C2-C1-O11-P
77	C	402	HEM	C2A-CAA-CBA-CGA
77	N	403	HEM	C2A-CAA-CBA-CGA
76	A	502	CDL	OB5-CB3-CB4-CB6
76	R	103	CDL	OB5-CB3-CB4-CB6
70	n	603	HEA	C27-C19-C20-C21
70	n	603	HEA	C18-C19-C20-C21
71	n	606	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
76	N1	401	CDL	CA3-CA4-CA6-OA8
71	L	501	3PE	C32-C33-C34-C35
71	o	302	3PE	O11-C1-C2-O21
71	H1	401	3PE	O11-C1-C2-O21
76	R	101	CDL	OB5-CB3-CB4-OB6
76	L1	702	CDL	OB5-CB3-CB4-OB6
80	P1	502	PC1	O11-C1-C2-O21
71	M1	503	3PE	C2-C1-O11-P
76	R	103	CDL	OB6-CB4-CB6-OB8
76	h1	201	CDL	OB6-CB4-CB6-OB8
80	P1	502	PC1	C11-C12-N-C13
76	a1	101	CDL	CB2-C1-CA2-OA2
76	Y1	202	CDL	OB5-CB3-CB4-CB6
76	h1	201	CDL	OB5-CB3-CB4-CB6
76	R	102	CDL	C31-C32-C33-C34
71	D1	501	3PE	C31-C32-C33-C34
80	P1	502	PC1	O21-C21-C22-C23
76	N1	401	CDL	C51-C52-C53-C54
80	9	203	PC1	C29-C2A-C2B-C2C
71	L	501	3PE	O11-C1-C2-O21
76	A	502	CDL	OB5-CB3-CB4-OB6
76	h1	201	CDL	CB3-CB4-CB6-OB8
76	R	103	CDL	CA5-C11-C12-C13
77	C	402	HEM	C4B-C3B-CAB-CBB
77	N	403	HEM	C4B-C3B-CAB-CBB
71	N	401	3PE	C12-C11-O13-P
85	n1	201	ZMP	C16-C17-C18-C19
71	n	606	3PE	O21-C2-C3-O31
80	J	101	PC1	O13-C11-C12-N
80	L	502	PC1	O13-C11-C12-N
80	9	203	PC1	O13-C11-C12-N
80	Y1	201	PC1	O13-C11-C12-N
84	P1	501	NDP	PN-O3-PA-O2A
86	O1	401	DGT	PB-O3A-PA-O1A
80	Y1	201	PC1	C3A-C3B-C3C-C3D
71	H1	401	3PE	O11-C1-C2-C3
76	R	101	CDL	OB5-CB3-CB4-CB6
85	W1	201	ZMP	C19-C18-C21-O5
80	9	204	PC1	C35-C36-C37-C38
71	K1	201	3PE	C2-C1-O11-P
76	h1	201	CDL	CA4-CA3-OA5-PA1
78	D	301	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
78	D	301	HEC	C4C-C3C-CAC-CBC
78	O	303	HEC	C4B-C3B-CAB-CBB
78	O	303	HEC	C4C-C3C-CAC-CBC
76	Y1	202	CDL	OB5-CB3-CB4-OB6
76	a1	101	CDL	OB5-CB3-CB4-OB6
76	h1	201	CDL	OB5-CB3-CB4-OB6
80	Y1	201	PC1	C29-C2A-C2B-C2C
71	p	301	3PE	C23-C24-C25-C26
70	n	603	HEA	C11-C12-C13-C14
71	n	605	3PE	C1-O11-P-O12
71	n	605	3PE	C1-O11-P-O13
71	n	605	3PE	C1-O11-P-O14
71	n	606	3PE	C11-O13-P-O14
71	n	607	3PE	C1-O11-P-O14
71	o	302	3PE	C11-O13-P-O14
71	p	301	3PE	C11-O13-P-O12
71	t	101	3PE	C11-O13-P-O14
71	v	101	3PE	C1-O11-P-O13
71	v	101	3PE	C1-O11-P-O14
71	v	101	3PE	C11-O13-P-O11
71	v	101	3PE	C11-O13-P-O12
71	C	403	3PE	C11-O13-P-O12
71	G	102	3PE	C1-O11-P-O12
71	G	102	3PE	C11-O13-P-O14
71	N	401	3PE	C11-O13-P-O11
71	N	401	3PE	C11-O13-P-O12
71	N	401	3PE	C11-O13-P-O14
71	r1	201	3PE	C11-O13-P-O14
71	H1	401	3PE	C11-O13-P-O14
71	K1	201	3PE	C11-O13-P-O14
71	L1	701	3PE	C1-O11-P-O12
71	M1	502	3PE	C11-O13-P-O14
71	M1	503	3PE	C1-O11-P-O12
71	Y1	203	3PE	C1-O11-P-O12
71	d1	202	3PE	C1-O11-P-O12
71	d1	202	3PE	C1-O11-P-O13
71	d1	202	3PE	C1-O11-P-O14
71	d1	202	3PE	C11-O13-P-O14
71	d1	203	3PE	C1-O11-P-O12
76	A	502	CDL	CA3-OA5-PA1-OA2
76	A	502	CDL	CA3-OA5-PA1-OA4
76	A	502	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
76	A	502	CDL	CB3-OB5-PB2-OB3
76	A	502	CDL	CB3-OB5-PB2-OB4
76	C	404	CDL	CA2-OA2-PA1-OA3
76	C	404	CDL	CA2-OA2-PA1-OA5
76	C	404	CDL	CB2-OB2-PB2-OB5
76	N	405	CDL	CA3-OA5-PA1-OA4
76	O	301	CDL	CB2-OB2-PB2-OB4
76	R	102	CDL	CA2-OA2-PA1-OA3
76	R	102	CDL	CA3-OA5-PA1-OA3
76	R	102	CDL	CB2-OB2-PB2-OB3
76	H1	402	CDL	CB2-OB2-PB2-OB3
76	L1	702	CDL	CA3-OA5-PA1-OA4
76	L1	703	CDL	CB2-OB2-PB2-OB3
76	N1	401	CDL	CA2-OA2-PA1-OA4
76	N1	401	CDL	CA2-OA2-PA1-OA5
76	N1	401	CDL	CB3-OB5-PB2-OB3
76	a1	101	CDL	CB2-OB2-PB2-OB3
76	d1	201	CDL	CB2-OB2-PB2-OB3
76	h1	201	CDL	CA2-OA2-PA1-OA4
78	D	301	HEC	C2B-C3B-CAB-CBB
80	J	101	PC1	C11-O13-P-O14
80	K	101	PC1	C11-O13-P-O12
80	K	101	PC1	C11-O13-P-O14
80	K	101	PC1	C11-O13-P-O11
80	K	101	PC1	C1-O11-P-O12
80	L	502	PC1	C1-O11-P-O14
80	6	203	PC1	C11-O13-P-O12
80	6	203	PC1	C11-O13-P-O14
80	6	203	PC1	C11-O13-P-O11
80	P1	502	PC1	C11-O13-P-O14
86	O1	401	DGT	C5'-O5'-PA-O3A
76	d1	201	CDL	C59-C60-C61-C62
76	A	502	CDL	C52-C51-CB5-OB6
71	n	606	3PE	C2-C1-O11-P
71	t	101	3PE	C2-C1-O11-P
71	i1	201	3PE	C2-C1-O11-P
76	G	101	CDL	C1-CA2-OA2-PA1
76	O	301	CDL	CB4-CB3-OB5-PB2
76	H1	402	CDL	C1-CA2-OA2-PA1
76	N1	401	CDL	C1-CA2-OA2-PA1
76	a1	101	CDL	C52-C51-CB5-OB6
80	9	203	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
76	L1	702	CDL	OB5-CB3-CB4-CB6
80	Y1	201	PC1	O11-C1-C2-C3
71	M1	501	3PE	C3D-C3E-C3F-C3G
71	R	104	3PE	O11-C1-C2-O21
80	V	101	PC1	C2-C1-O11-P
75	y	601	TGL	CC1-CC2-CC3-CC4
71	r1	201	3PE	O31-C31-C32-C33
71	M1	501	3PE	C37-C38-C39-C3A
71	d1	203	3PE	O21-C21-C22-C23
71	Y1	203	3PE	C2-C1-O11-P
76	C	404	CDL	C1-CA2-OA2-PA1
76	R	101	CDL	CA4-CA3-OA5-PA1
76	L1	703	CDL	C1-CA2-OA2-PA1
71	d1	203	3PE	C21-C22-C23-C24
80	9	204	PC1	C2B-C2C-C2D-C2E
71	n	607	3PE	O21-C2-C3-O31
76	A	502	CDL	C52-C51-CB5-OB7
84	P1	501	NDP	C2D-C1D-N1N-C6N
84	P1	501	NDP	O4D-C1D-N1N-C6N
71	o	302	3PE	C2-C1-O11-P
76	G	101	CDL	CB4-CB3-OB5-PB2
76	N	405	CDL	CB4-CB3-OB5-PB2
70	n	604	HEA	CAA-CBA-CGA-O1A
71	d1	202	3PE	C1-C2-C3-O31
85	n1	201	ZMP	N2-C16-C17-O4
80	9	203	PC1	C3-C2-O21-C21
70	n	603	HEA	CAD-CBD-CGD-O1D
71	A1	201	3PE	C23-C24-C25-C26
76	Y1	202	CDL	C80-C81-C82-C83
71	E	202	3PE	C21-C22-C23-C24
70	n	604	HEA	CAA-CBA-CGA-O2A
76	A	502	CDL	C1-CA2-OA2-PA1
76	L1	702	CDL	C1-CB2-OB2-PB2
76	h1	201	CDL	C1-CA2-OA2-PA1
70	n	603	HEA	CAA-CBA-CGA-O1A
71	R	104	3PE	O11-C1-C2-C3
71	N1	402	3PE	O21-C2-C3-O31
76	Y1	202	CDL	OB6-CB4-CB6-OB8
76	d1	201	CDL	OA6-CA4-CA6-OA8
71	E	202	3PE	C32-C33-C34-C35
71	A1	201	3PE	C38-C39-C3A-C3B
76	A	502	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
76	C	404	CDL	C72-C71-CB7-OB9
71	Y1	204	3PE	C1-C2-C3-O31
76	Y1	202	CDL	CB3-CB4-CB6-OB8
76	d1	201	CDL	CA3-CA4-CA6-OA8
71	D1	501	3PE	O21-C21-C22-C23
70	n	603	HEA	CAA-CBA-CGA-O2A
76	G	101	CDL	CB2-C1-CA2-OA2
76	L1	702	CDL	CA2-C1-CB2-OB2
71	D1	501	3PE	C3D-C3E-C3F-C3G
70	n	603	HEA	CAD-CBD-CGD-O2D
77	N	403	HEM	CAD-CBD-CGD-O2D
80	9	204	PC1	C21-C22-C23-C24
76	N1	401	CDL	C80-C81-C82-C83
71	L	501	3PE	O11-C1-C2-C3
76	C	404	CDL	C72-C71-CB7-OB8
76	L1	703	CDL	C72-C71-CB7-OB8
71	M1	502	3PE	C2C-C2D-C2E-C2F
71	M1	502	3PE	C23-C24-C25-C26
76	R	102	CDL	C12-C11-CA5-OA6
71	t	101	3PE	C3-C2-O21-C21
76	a1	101	CDL	CA3-CA4-OA6-CA5
76	h1	201	CDL	CB6-CB4-OB6-CB5
80	6	203	PC1	C3-C2-O21-C21
86	O1	401	DGT	PB-O3B-PG-O2G
80	Y1	201	PC1	C35-C36-C37-C38
71	L1	701	3PE	C2-C1-O11-P
80	Y1	201	PC1	C33-C34-C35-C36
71	N1	402	3PE	C1-C2-C3-O31
77	N	403	HEM	CAD-CBD-CGD-O1D
71	H1	401	3PE	C2A-C2B-C2C-C2D
71	C	405	3PE	O31-C31-C32-C33
76	L1	703	CDL	C72-C71-CB7-OB9
80	P1	502	PC1	C12-C11-O13-P
71	D1	501	3PE	C39-C3A-C3B-C3C
71	Y1	204	3PE	O21-C2-C3-O31
76	h1	201	CDL	C12-C11-CA5-OA6
71	M1	502	3PE	O11-C1-C2-C3
78	D	301	HEC	CAD-CBD-CGD-O2D
71	i1	201	3PE	C2B-C2C-C2D-C2E
71	O	302	3PE	O21-C21-C22-C23
76	A	502	CDL	C72-C71-CB7-OB8
76	R	101	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
71	C	405	3PE	O21-C21-C22-C23
76	G	101	CDL	C52-C51-CB5-OB6
71	K1	201	3PE	O31-C31-C32-C33
76	R	102	CDL	C52-C51-CB5-OB6
84	P1	501	NDP	PN-O3-PA-O1A
76	Y1	202	CDL	CB7-C71-C72-C73
76	R	102	CDL	C32-C31-CA7-OA8
76	H1	402	CDL	C12-C13-C14-C15
76	R	102	CDL	OA5-CA3-CA4-OA6
76	d1	201	CDL	C57-C58-C59-C60
76	L1	702	CDL	C72-C71-CB7-OB8
71	Y1	204	3PE	C23-C24-C25-C26
71	M1	503	3PE	O21-C21-C22-C23
76	A	502	CDL	C32-C31-CA7-OA8
76	h1	201	CDL	C32-C31-CA7-OA8
71	o	302	3PE	C1-C2-C3-O31
76	d1	201	CDL	C14-C15-C16-C17
71	M1	501	3PE	O21-C21-C22-C23
76	h1	201	CDL	C72-C71-CB7-OB8
78	D	301	HEC	CAD-CBD-CGD-O1D
71	C	403	3PE	O21-C21-C22-C23
76	R	102	CDL	C72-C71-CB7-OB8
80	Y1	201	PC1	C3B-C3C-C3D-C3E
71	E	202	3PE	C33-C34-C35-C36
86	O1	401	DGT	PB-O3B-PG-O3G
71	o	302	3PE	O11-C1-C2-C3
85	W1	201	ZMP	C20-C18-C21-O5
71	v	101	3PE	O32-C31-C32-C33
80	9	204	PC1	O31-C31-C32-C33
71	n	605	3PE	C1-C2-O21-C21
71	A	501	3PE	C1-C2-O21-C21
71	H1	401	3PE	C3-C2-O21-C21
71	L1	701	3PE	C3-C2-O21-C21
76	N	405	CDL	CB6-CB4-OB6-CB5
76	R	102	CDL	CA6-CA4-OA6-CA5
76	R	103	CDL	CA3-CA4-OA6-CA5
76	N1	401	CDL	CB3-CB4-OB6-CB5
76	N1	401	CDL	CB6-CB4-OB6-CB5
80	L	502	PC1	C1-C2-O21-C21
80	P1	502	PC1	C3-C2-O21-C21
71	C	403	3PE	O31-C31-C32-C33
71	6	202	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
80	P1	502	PC1	O22-C21-C22-C23
71	v	101	3PE	O31-C31-C32-C33
76	N	405	CDL	C52-C51-CB5-OB6
71	H1	401	3PE	C2-C1-O11-P
84	P1	501	NDP	O4D-C1D-N1N-C2N
85	W1	201	ZMP	C12-C11-S1-C10
71	G	102	3PE	O21-C21-C22-C23
76	Y1	202	CDL	C13-C14-C15-C16
71	K1	201	3PE	O32-C31-C32-C33
76	R	102	CDL	C52-C51-CB5-OB7
71	K1	201	3PE	O21-C21-C22-C23
84	P1	501	NDP	C2D-C1D-N1N-C2N
85	W1	201	ZMP	C2-C1-C22-C23
76	G	101	CDL	C52-C51-CB5-OB7
76	R	103	CDL	C72-C73-C74-C75
76	A	502	CDL	C32-C31-CA7-OA9
76	R	102	CDL	C32-C31-CA7-OA9
71	i1	201	3PE	C24-C25-C26-C27
80	9	203	PC1	C2D-C2E-C2F-C2G
76	N	405	CDL	C52-C51-CB5-OB7
76	R	101	CDL	C72-C71-CB7-OB9
71	C	405	3PE	O22-C21-C22-C23
76	G	101	CDL	C72-C73-C74-C75
71	C	405	3PE	O32-C31-C32-C33
71	O	302	3PE	O22-C21-C22-C23
71	M1	503	3PE	O22-C21-C22-C23
80	9	204	PC1	O32-C31-C32-C33
71	A1	201	3PE	O31-C31-C32-C33
76	N1	401	CDL	C52-C51-CB5-OB6
85	W1	201	ZMP	N2-C16-C17-O4
77	C	401	HEM	CAA-CBA-CGA-O2A
80	6	203	PC1	C21-C22-C23-C24
71	C	403	3PE	O22-C21-C22-C23
76	h1	201	CDL	C72-C71-CB7-OB9
71	n	605	3PE	O21-C21-C22-C23
76	R	102	CDL	C72-C71-CB7-OB9
80	Y1	201	PC1	C2B-C2C-C2D-C2E
71	M1	501	3PE	O22-C21-C22-C23
76	L1	702	CDL	C72-C71-CB7-OB9
71	A	501	3PE	O31-C31-C32-C33
71	p	301	3PE	C25-C26-C27-C28
71	H1	401	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
71	M1	502	3PE	O31-C31-C32-C33
71	Y1	203	3PE	O31-C31-C32-C33
76	N	405	CDL	C12-C11-CA5-OA6
76	H1	402	CDL	C12-C11-CA5-OA6
76	h1	201	CDL	C52-C51-CB5-OB6
80	P1	502	PC1	O31-C31-C32-C33
71	C	403	3PE	O32-C31-C32-C33
71	t	101	3PE	O31-C31-C32-C33
71	A1	201	3PE	C35-C36-C37-C38
71	6	202	3PE	O22-C21-C22-C23

There are no ring outliers.

56 monomers are involved in 133 short contacts:

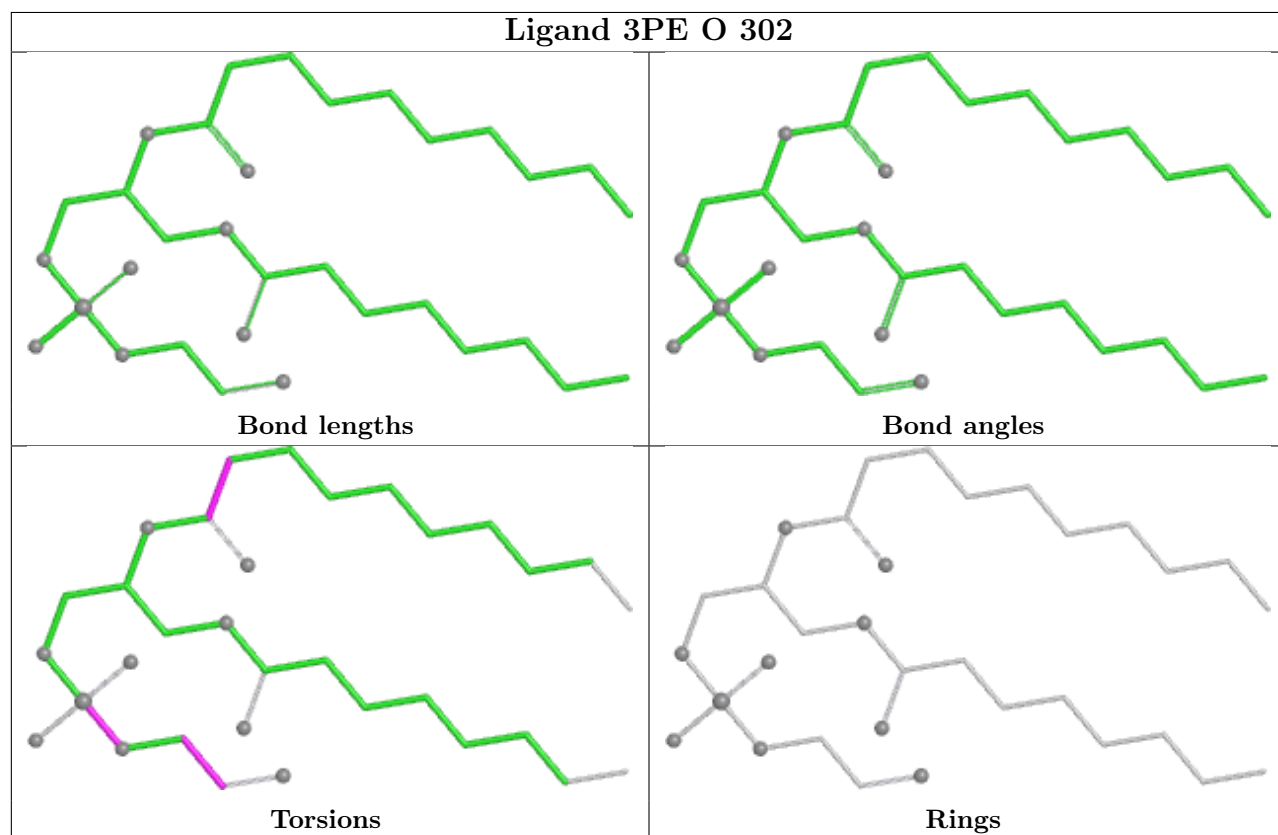
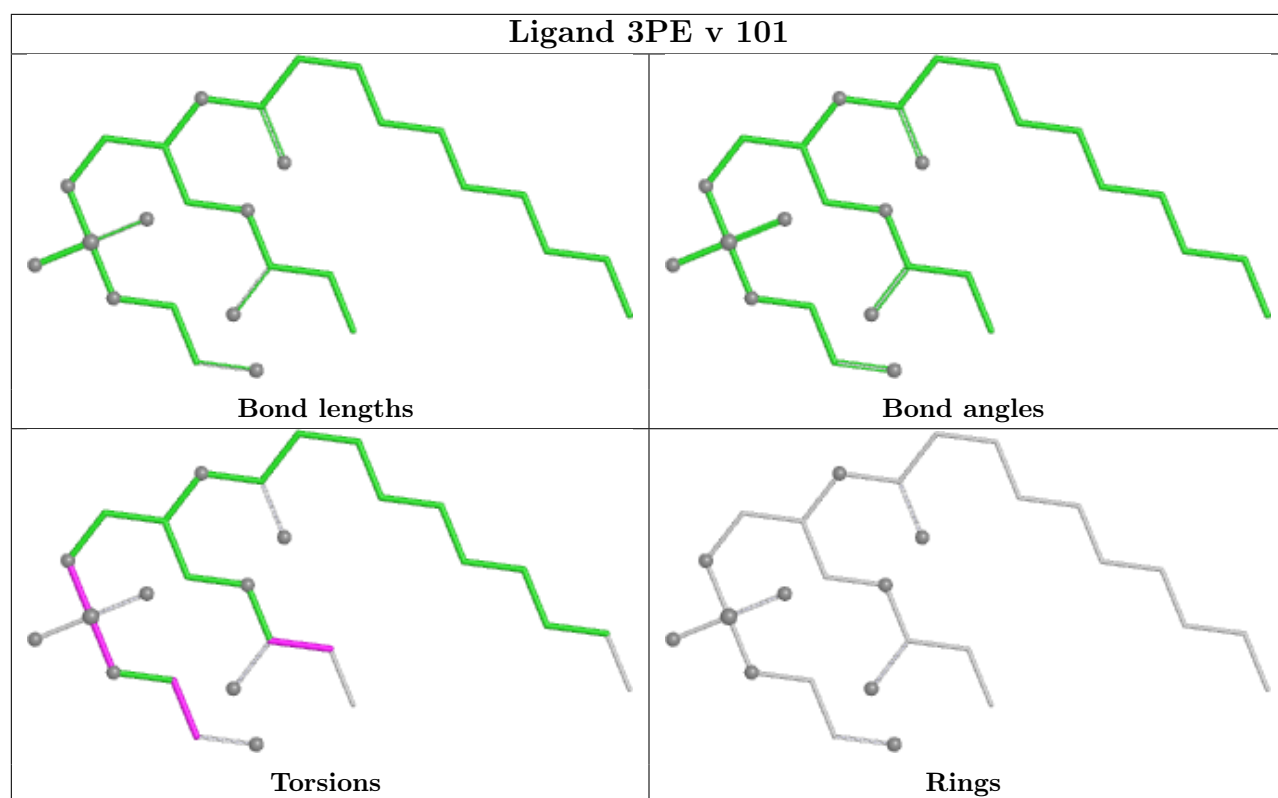
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	O	302	3PE	2	0
84	P1	501	NDP	1	0
76	O	301	CDL	2	0
71	L	501	3PE	1	0
71	R	104	3PE	1	0
71	Y1	204	3PE	2	0
76	R	102	CDL	1	0
85	W1	201	ZMP	1	0
71	t	101	3PE	6	0
85	n1	201	ZMP	4	0
80	Y1	201	PC1	9	0
75	y	601	TGL	1	0
71	M1	501	3PE	5	0
76	L1	703	CDL	1	0
78	D	301	HEC	3	0
71	C	403	3PE	3	0
71	r1	201	3PE	1	0
77	C	402	HEM	2	0
71	M1	503	3PE	1	0
78	O	303	HEC	1	0
77	N	402	HEM	4	0
71	K1	201	3PE	2	0
71	E	202	3PE	5	0
71	Y1	203	3PE	2	0
76	d1	201	CDL	4	0
71	6	202	3PE	1	0
76	a1	101	CDL	2	0

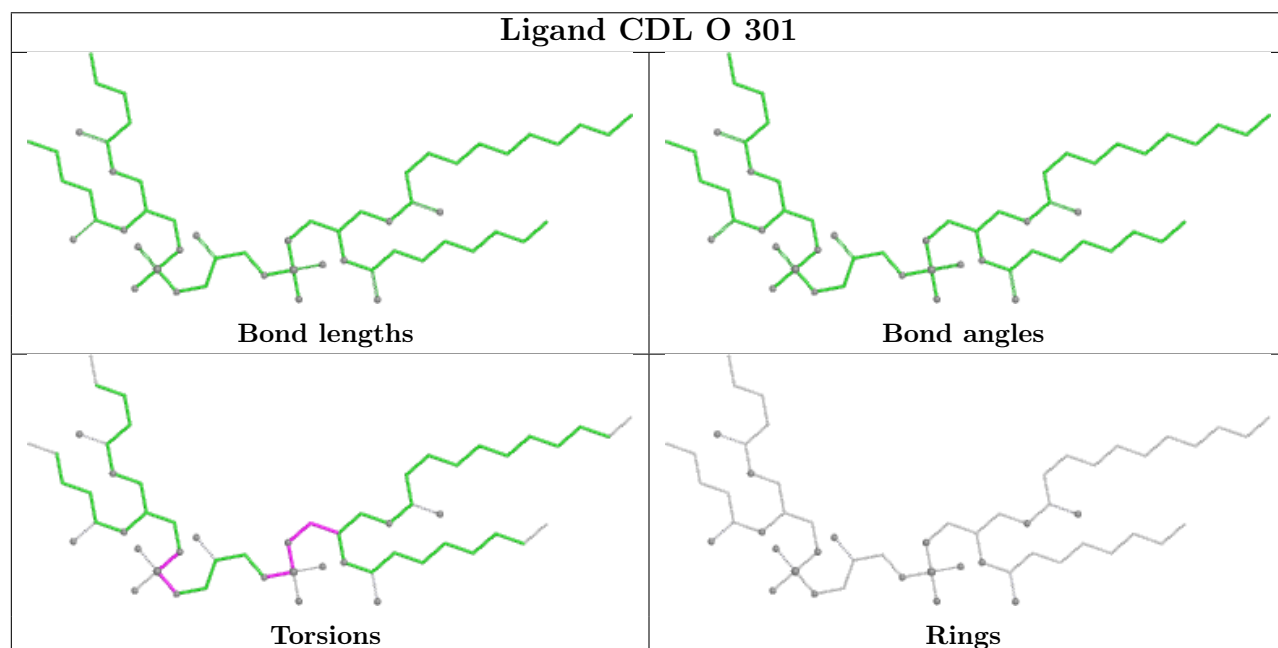
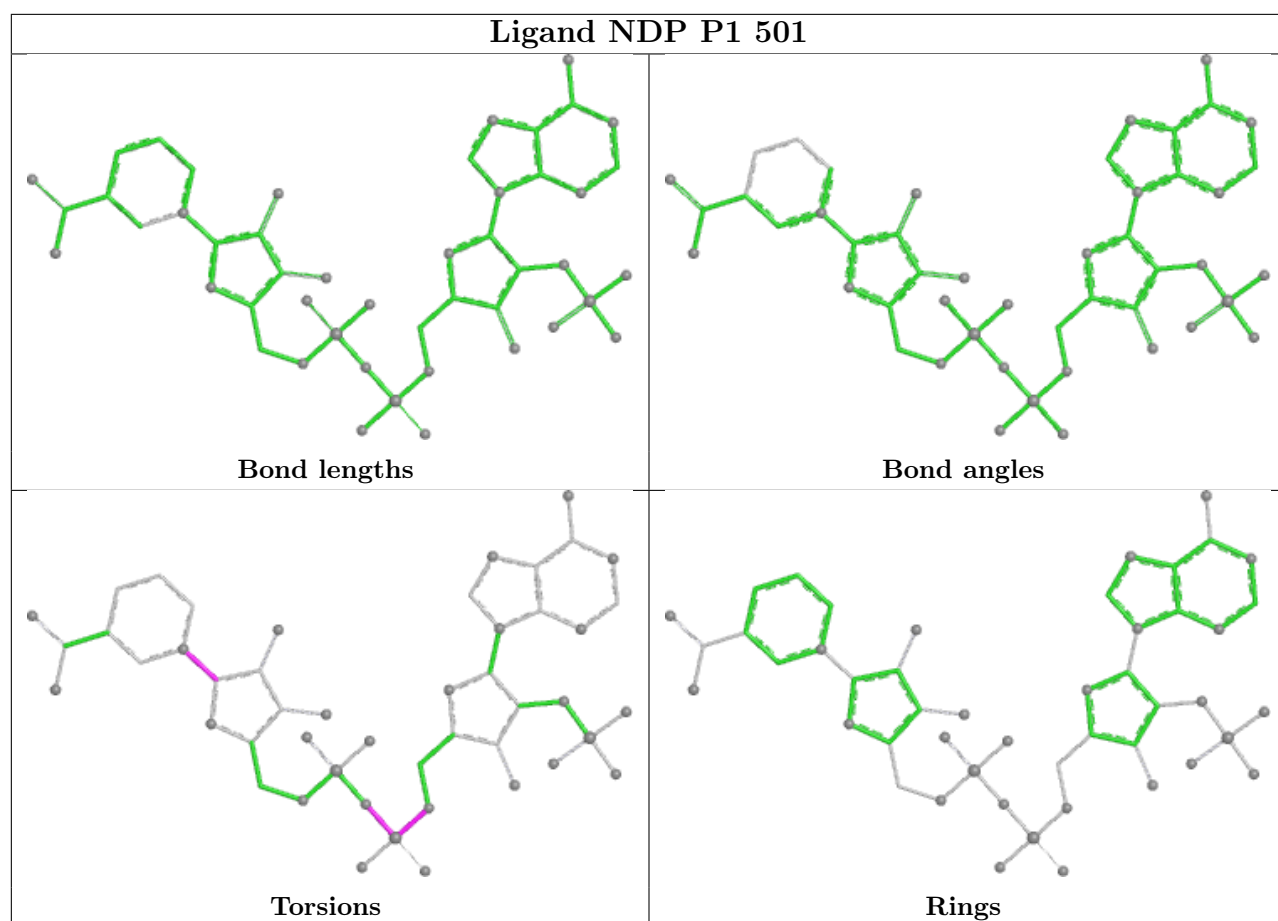
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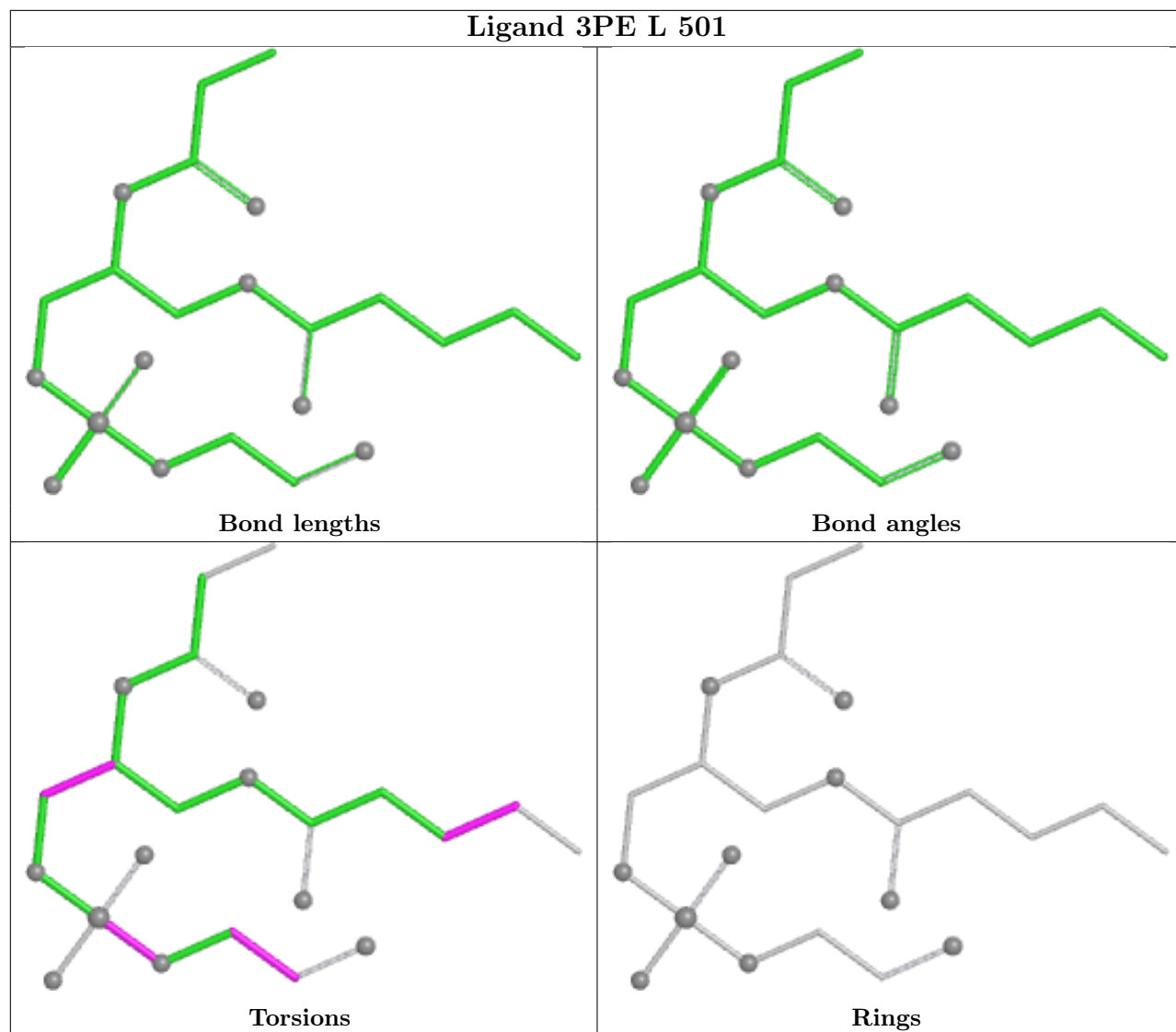
Mol	Chain	Res	Type	Clashes	Symm-Clashes
76	h1	201	CDL	5	0
71	A	501	3PE	2	0
71	n	605	3PE	2	0
76	G	101	CDL	2	0
76	Y1	202	CDL	2	0
71	D1	501	3PE	4	0
76	R	103	CDL	3	0
71	p	301	3PE	3	0
71	H1	401	3PE	1	0
71	A1	201	3PE	1	0
71	G	102	3PE	3	0
80	9	203	PC1	3	0
82	1	501	FMN	3	0
71	d1	203	3PE	1	0
71	L1	701	3PE	3	0
76	H1	402	CDL	1	0
80	9	204	PC1	1	0
71	o	302	3PE	3	0
71	N1	402	3PE	3	0
77	N	403	HEM	2	0
76	N	405	CDL	3	0
71	N	404	3PE	2	0
71	i1	201	3PE	5	0
86	O1	401	DGT	1	0
76	N1	401	CDL	4	0
70	n	604	HEA	1	0
76	A	502	CDL	1	0
80	6	203	PC1	3	0
77	C	401	HEM	3	0

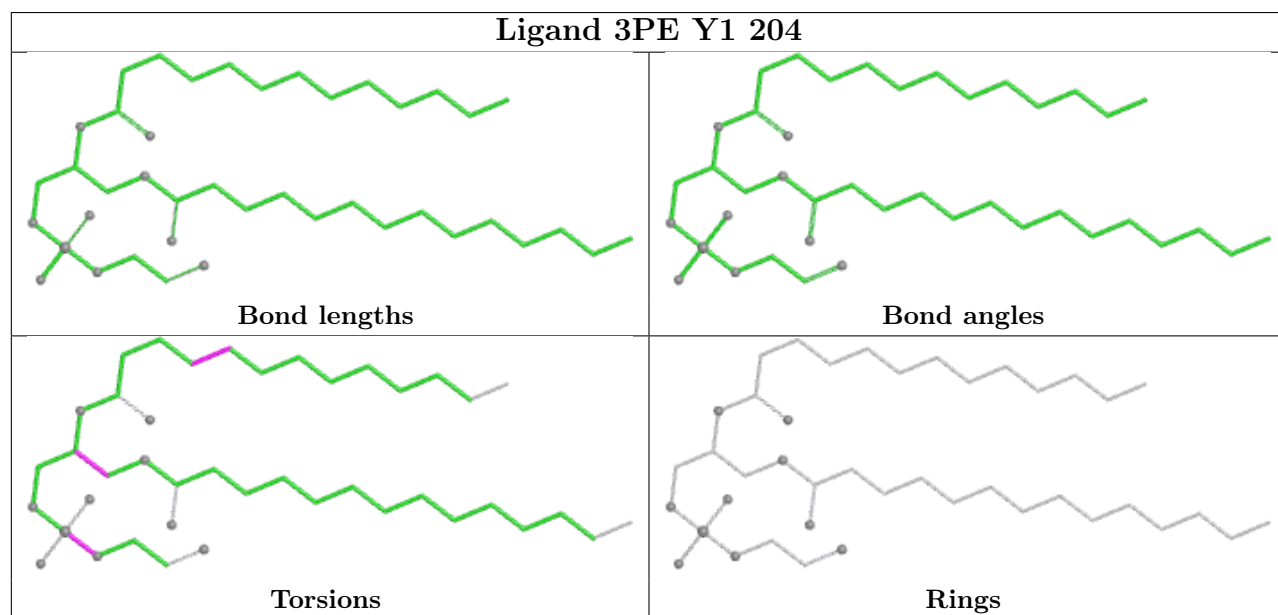
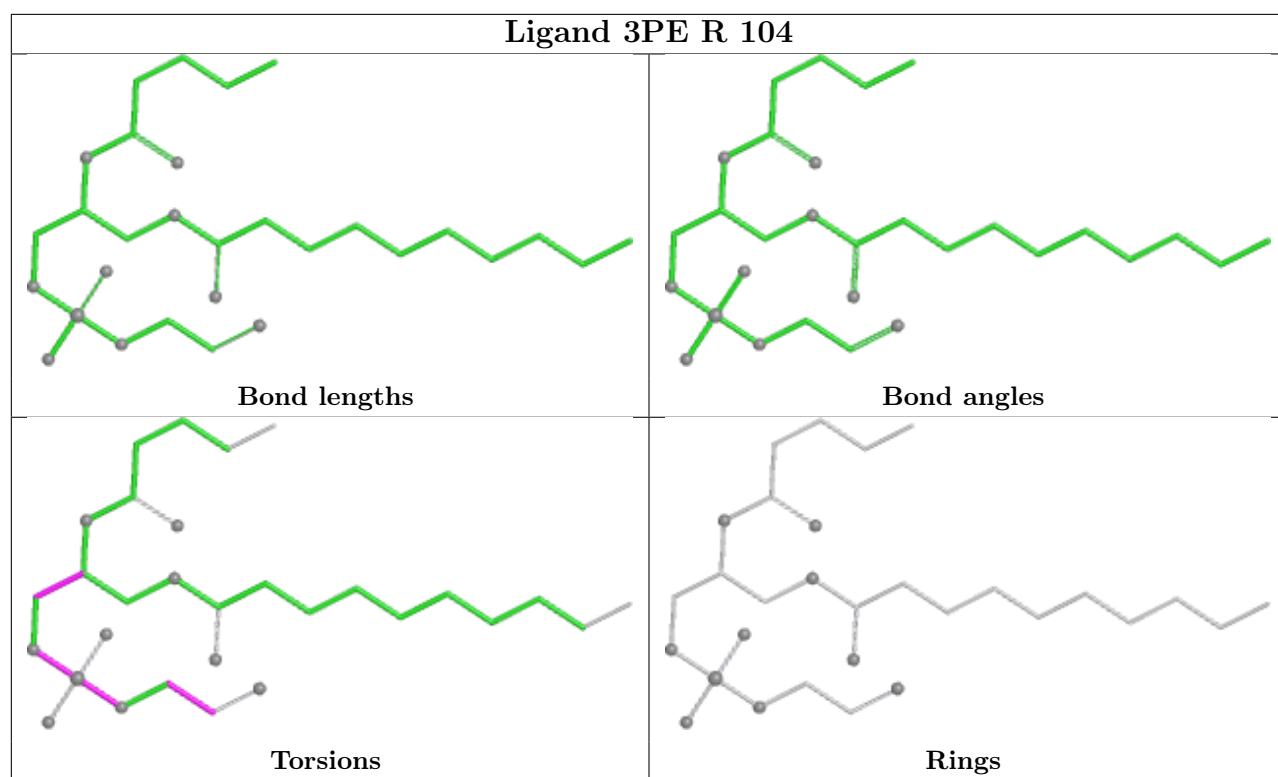
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

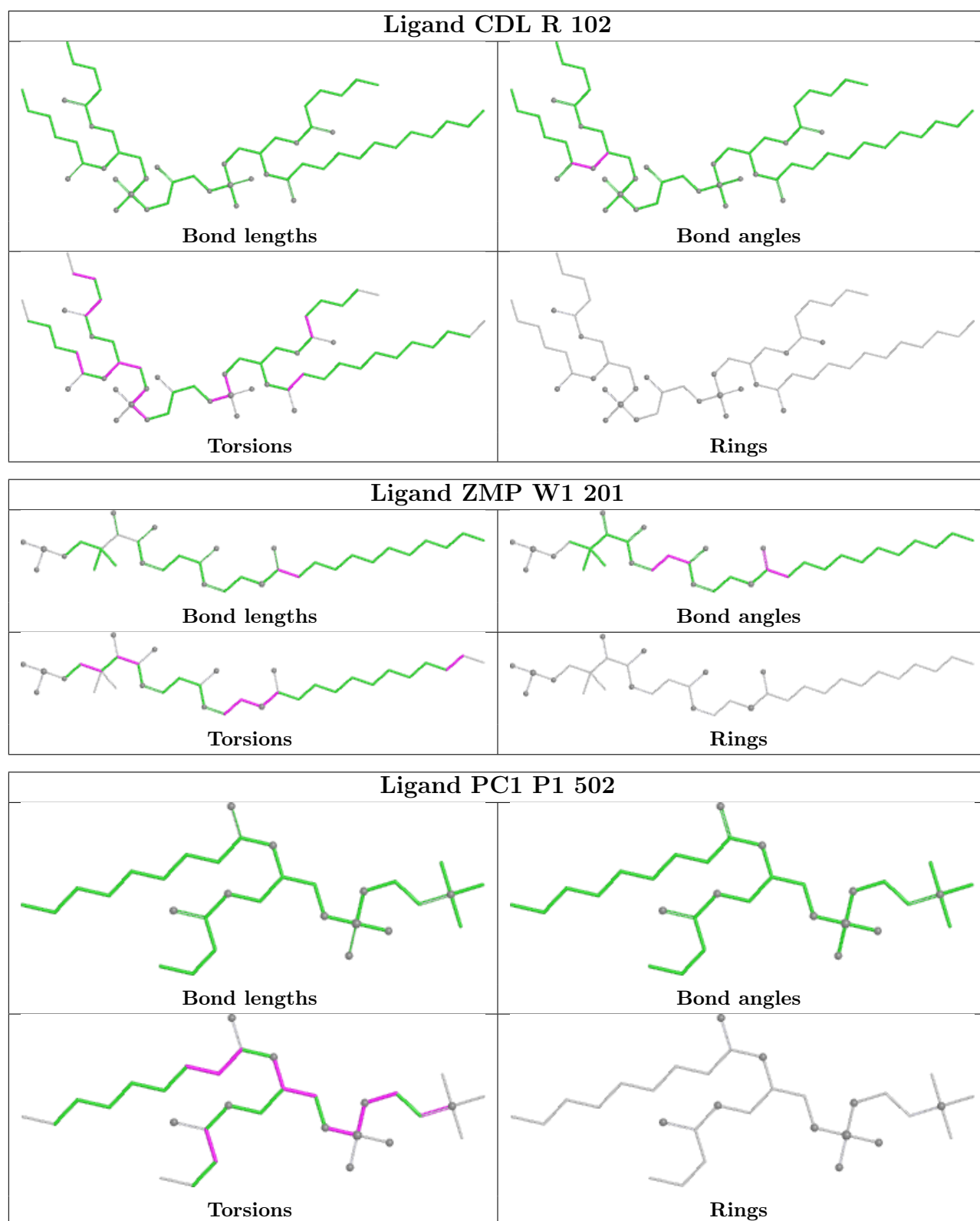


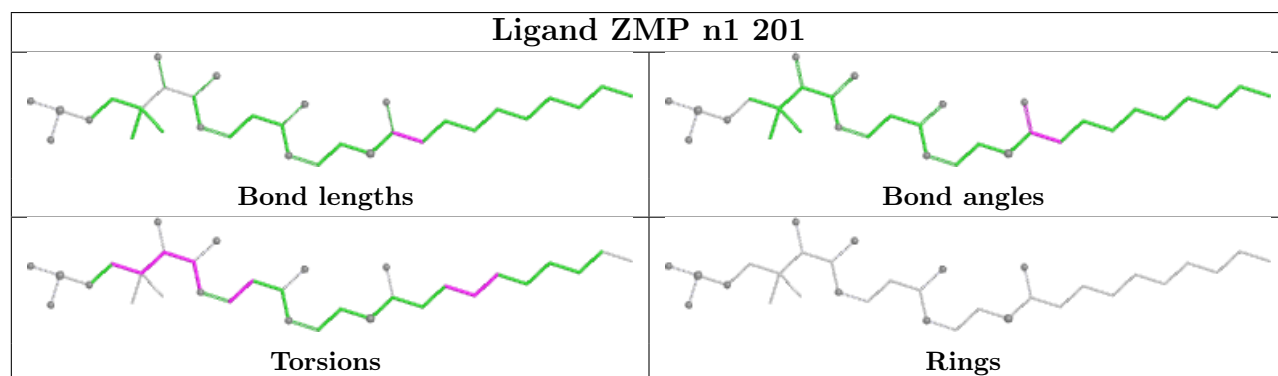
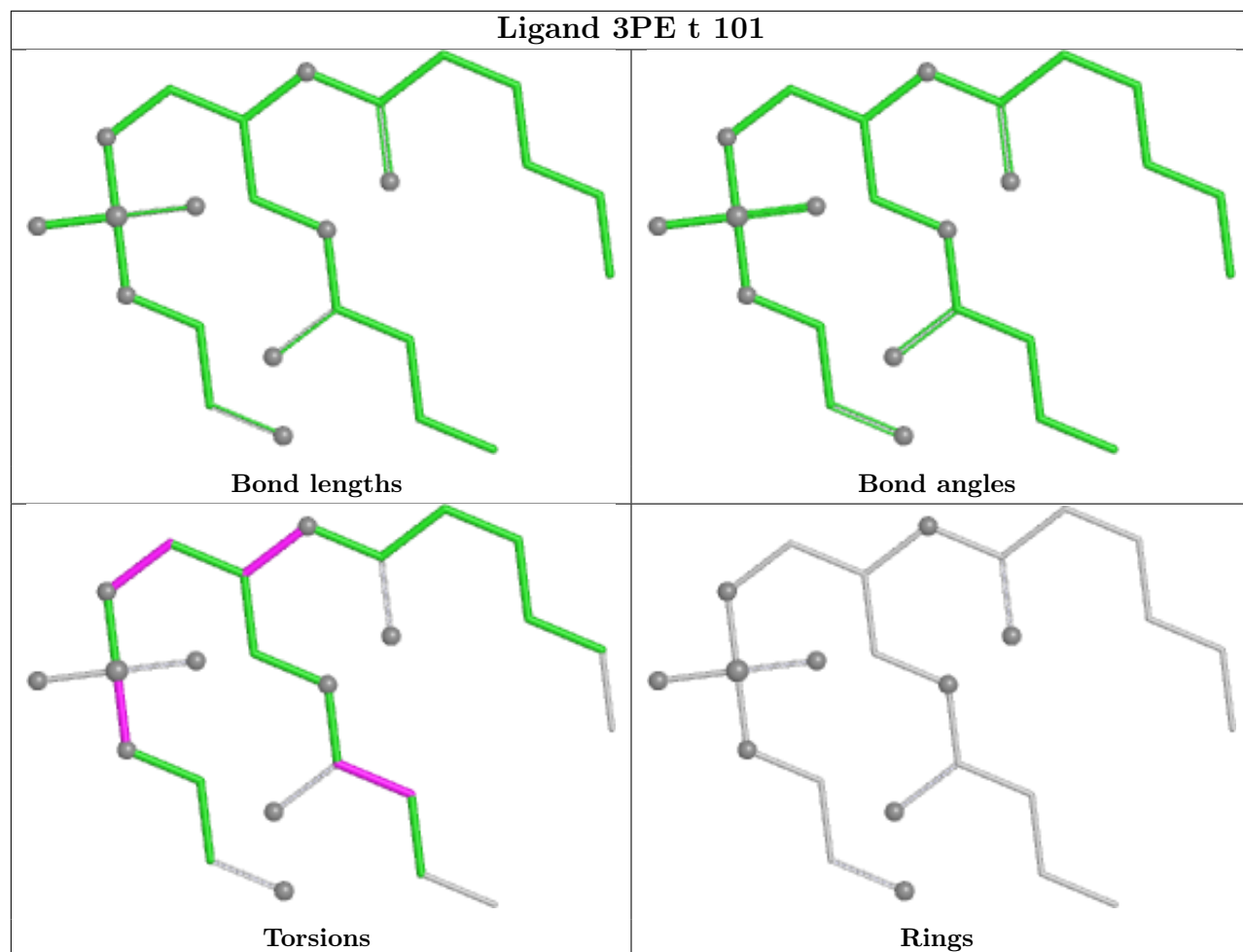


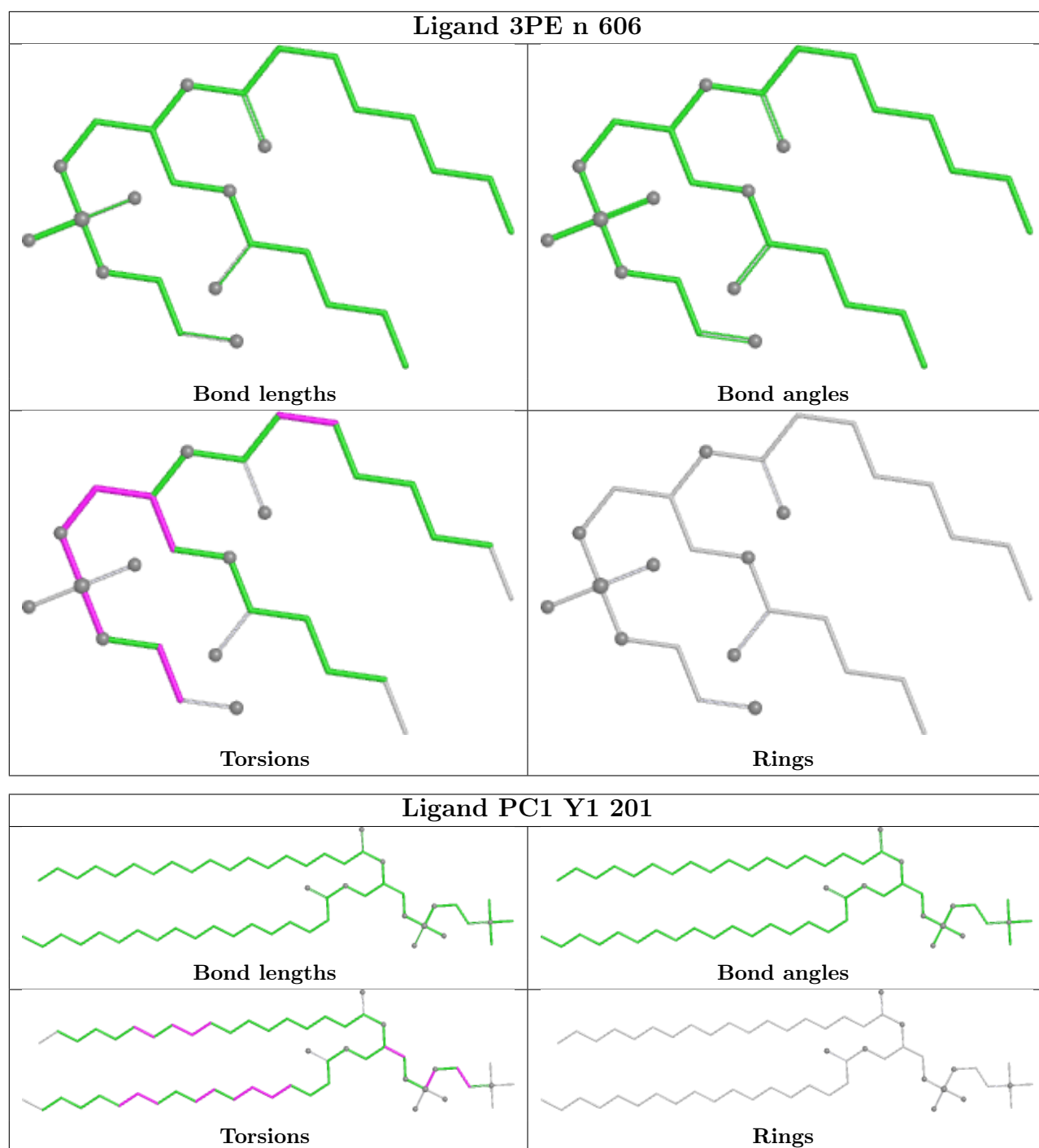
Ligand 3PE L 501

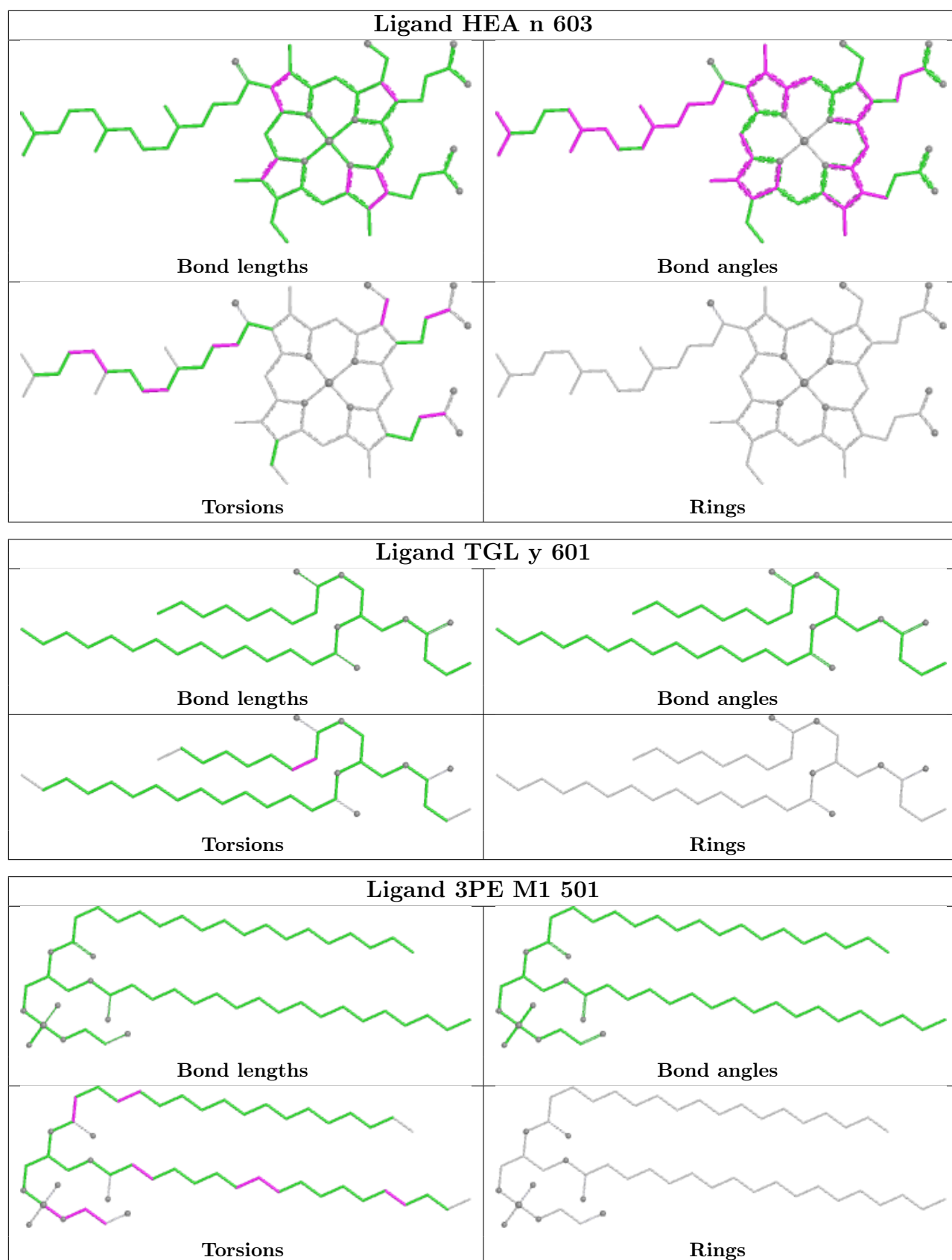


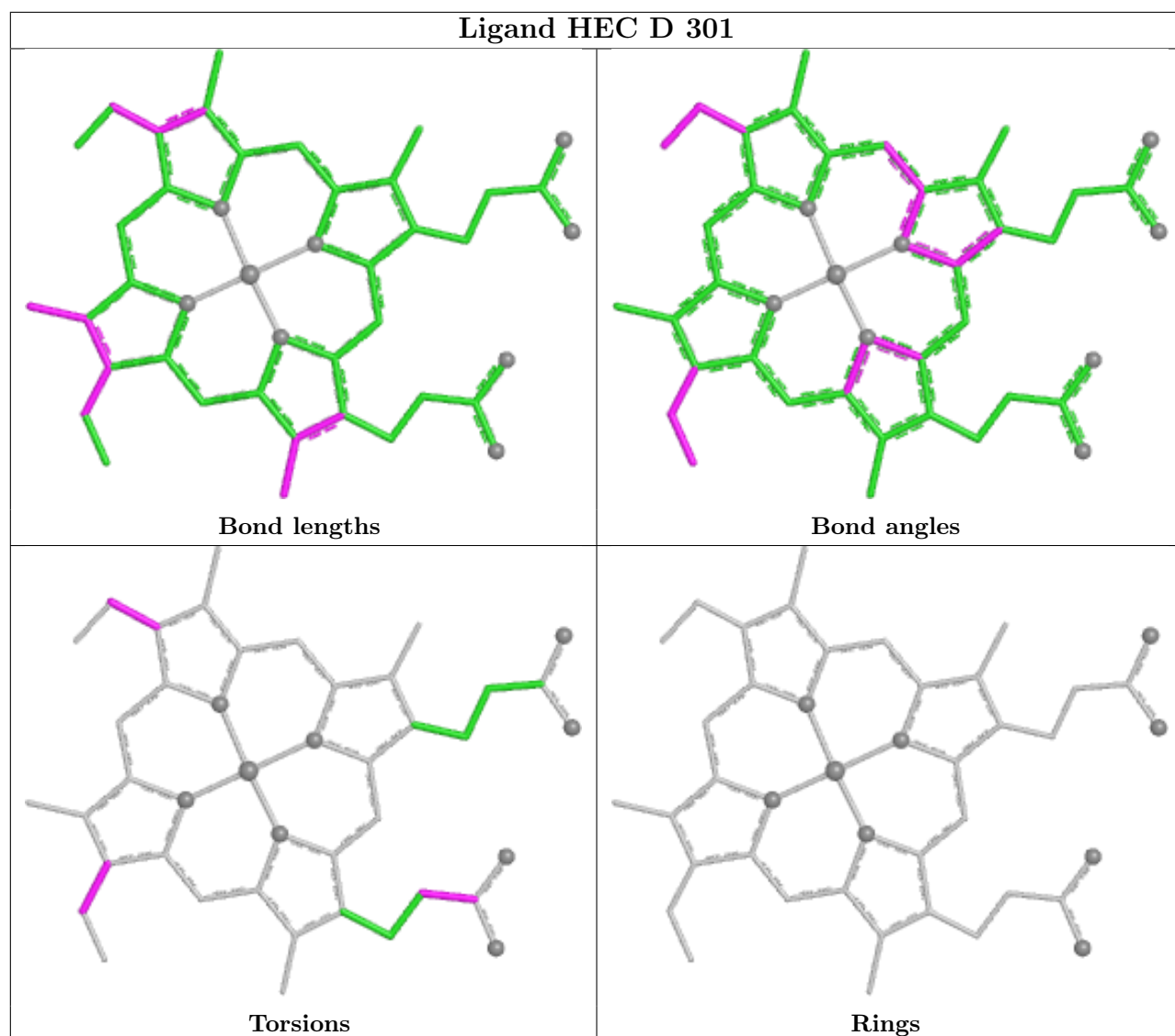
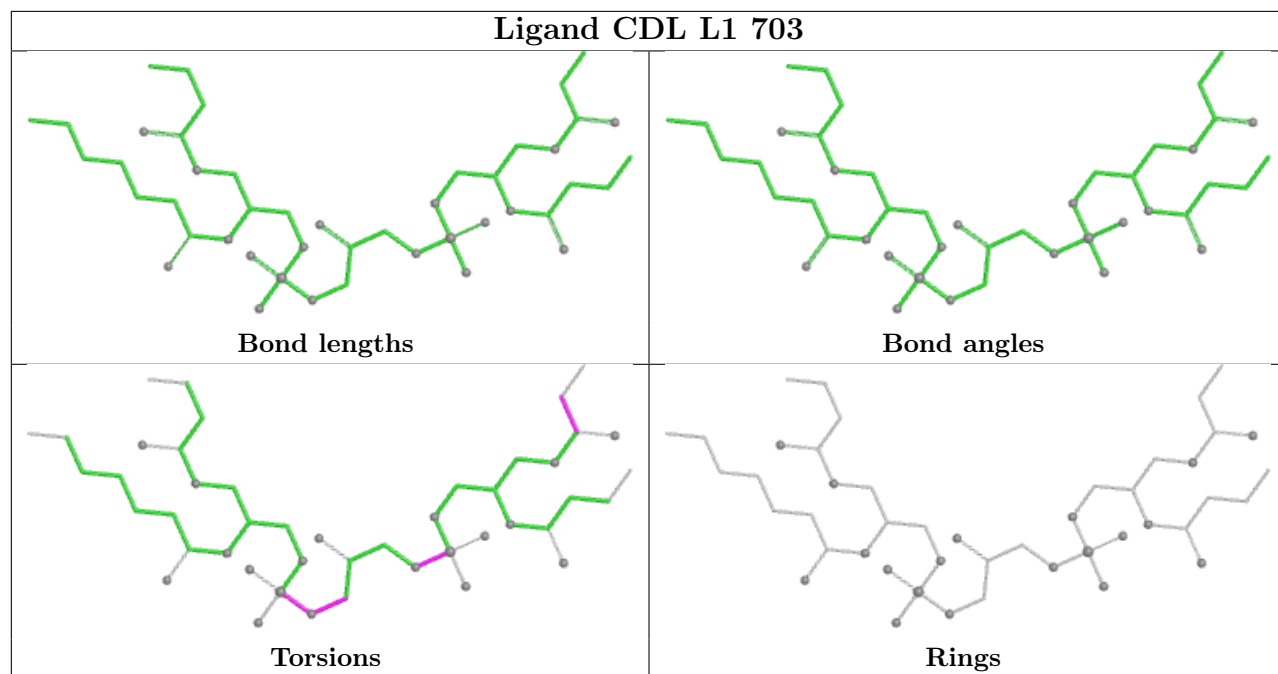


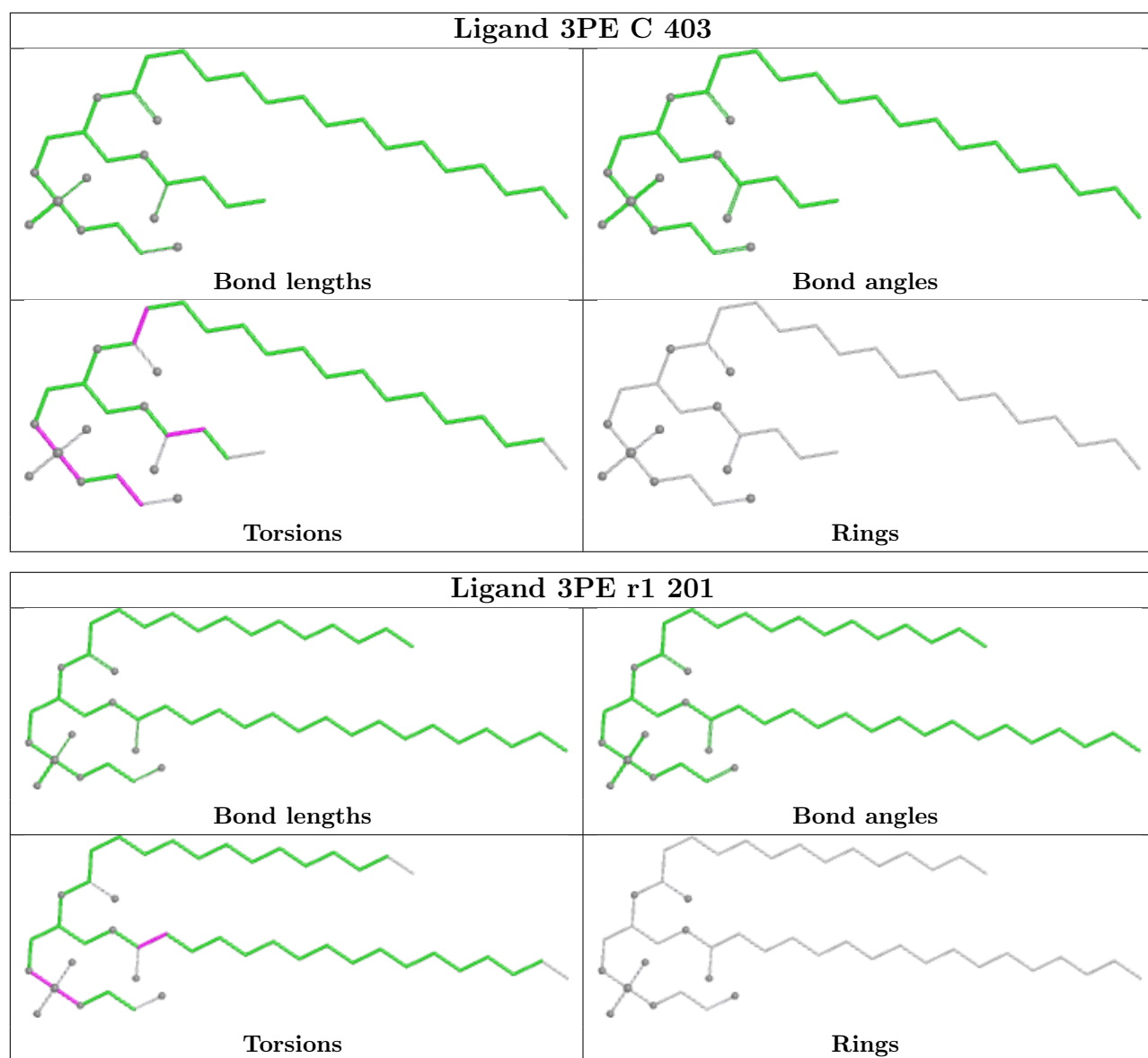


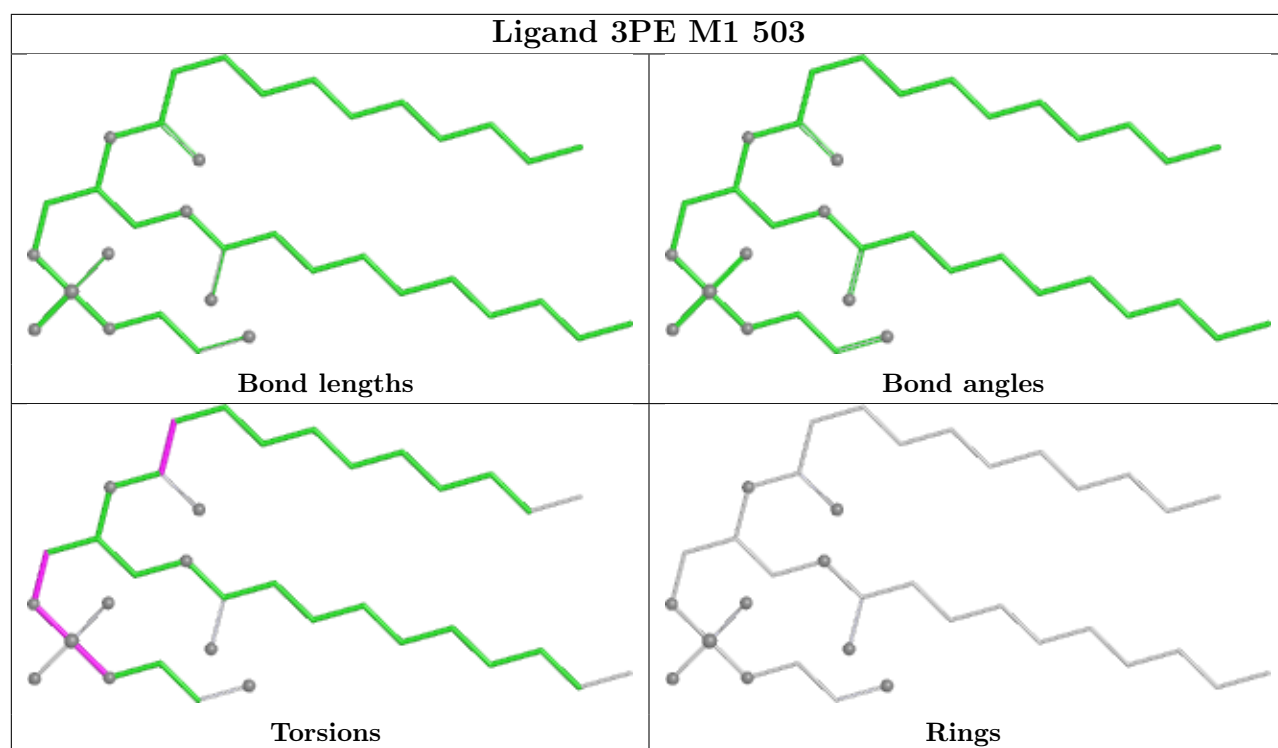
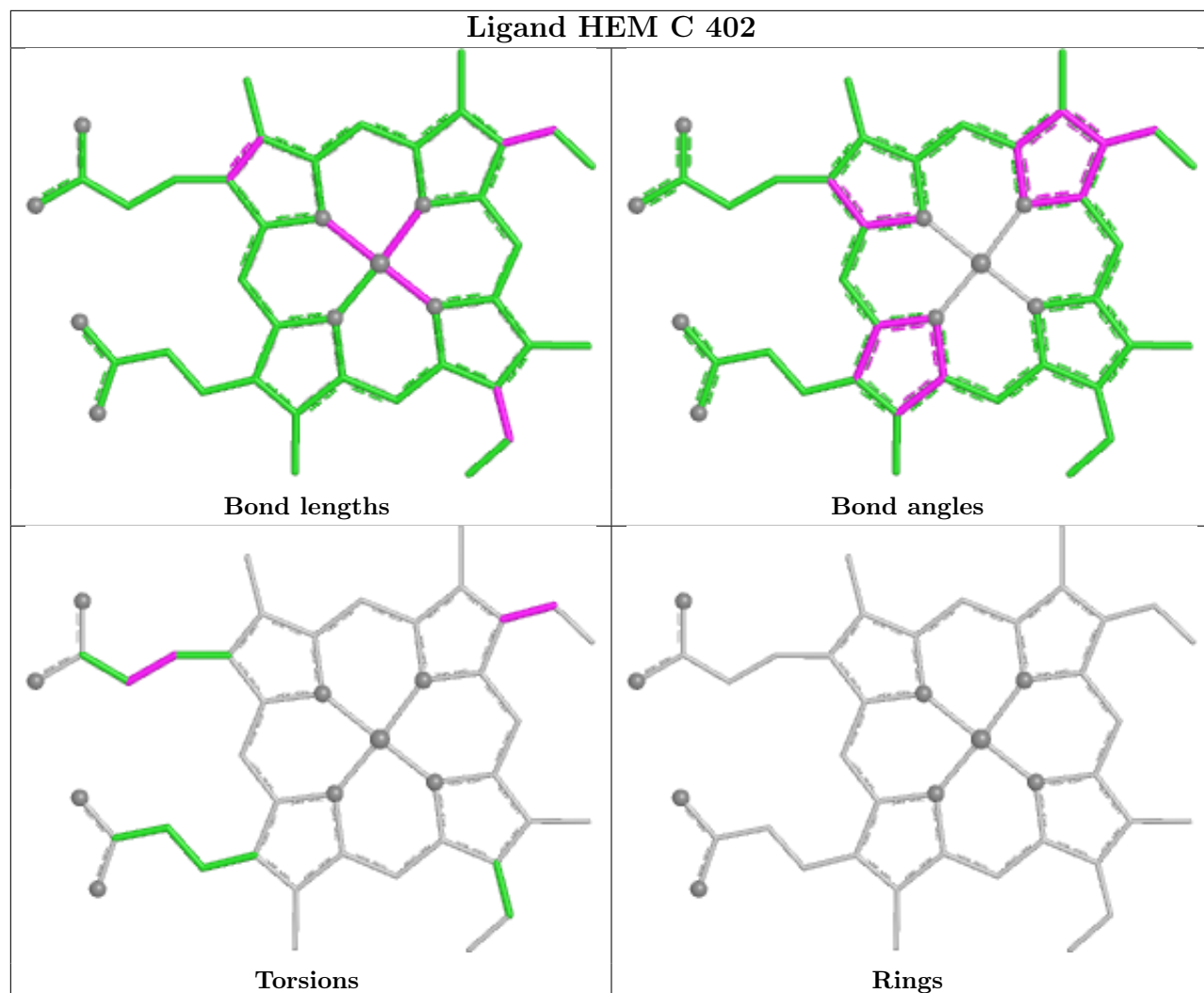


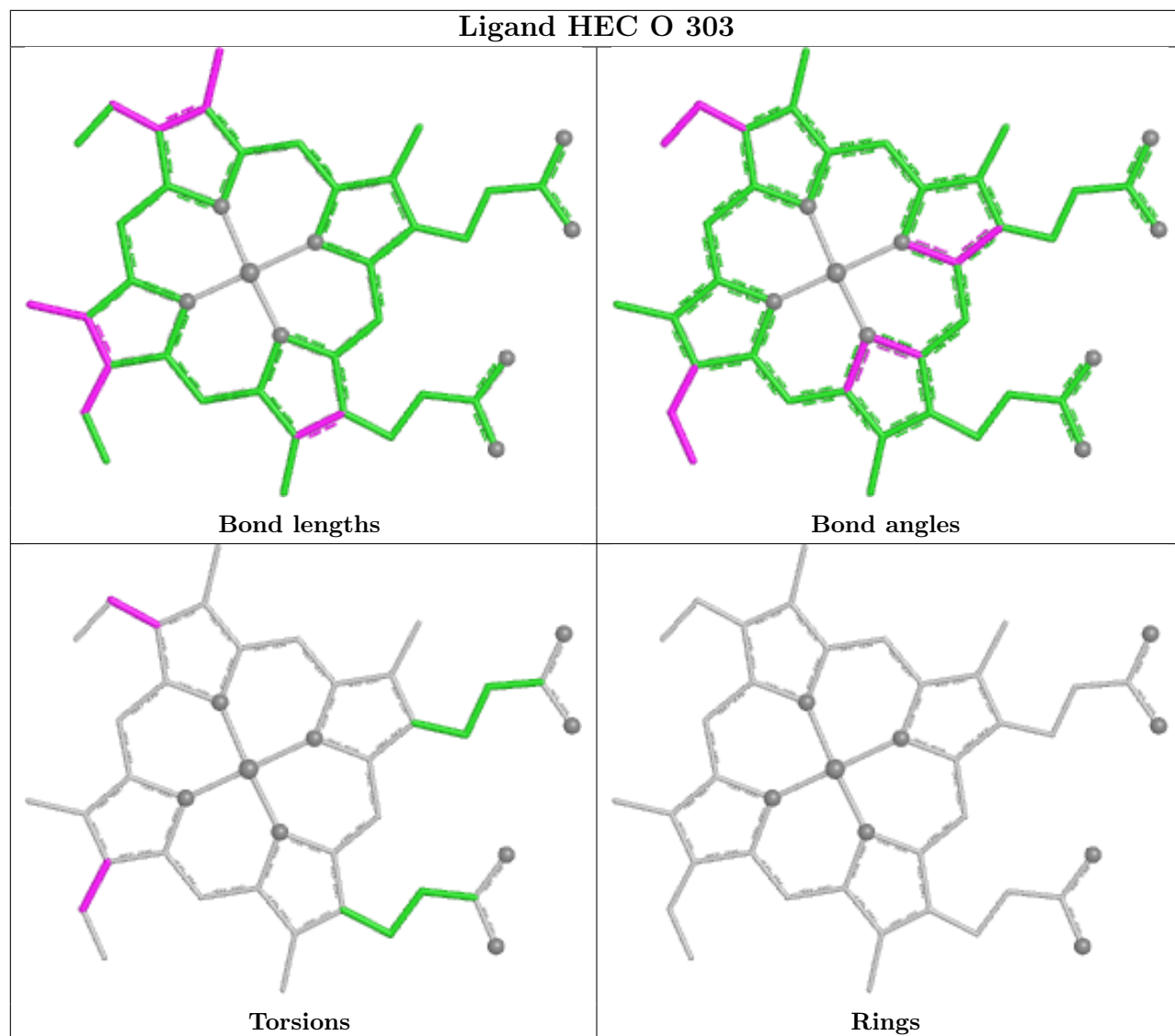


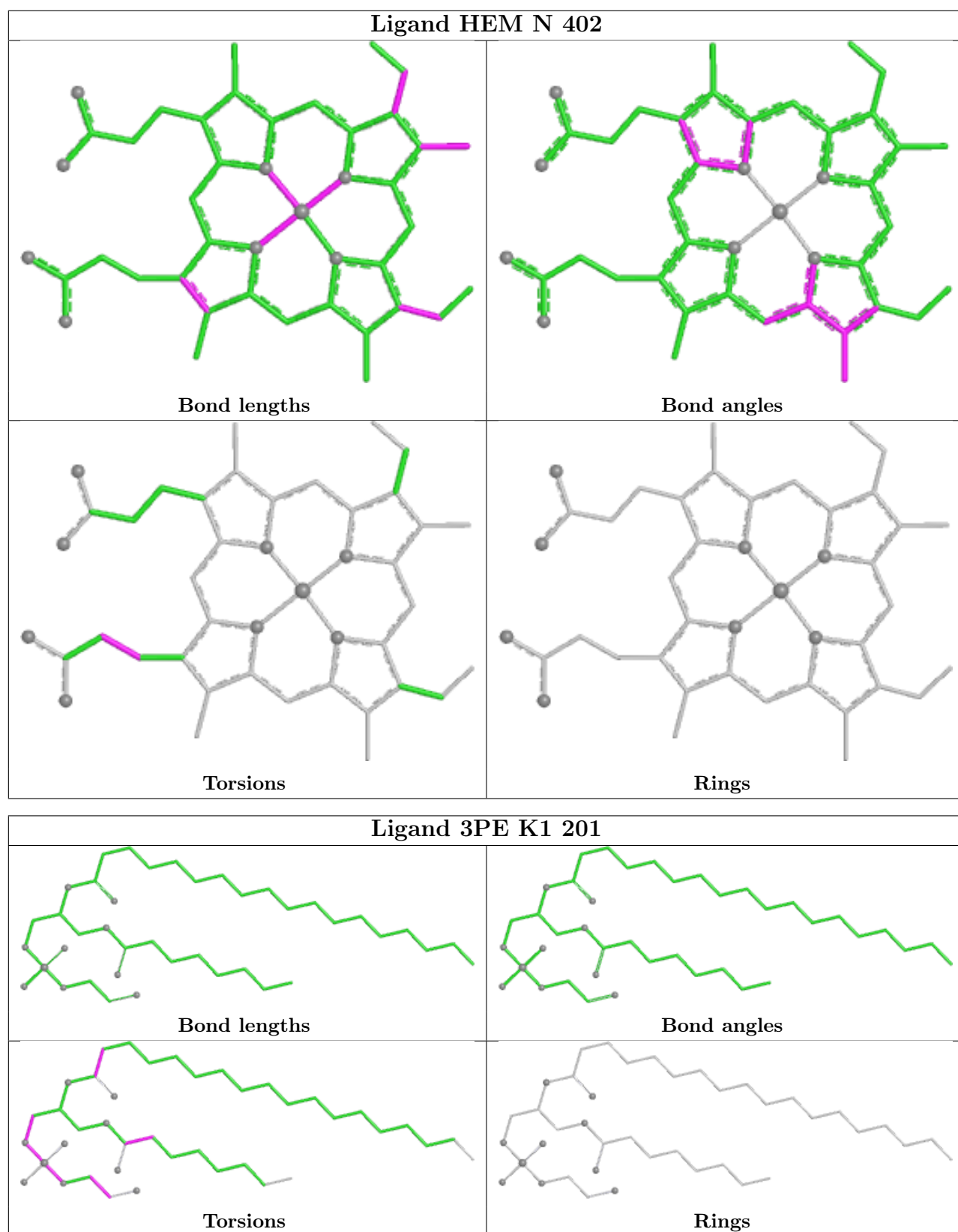


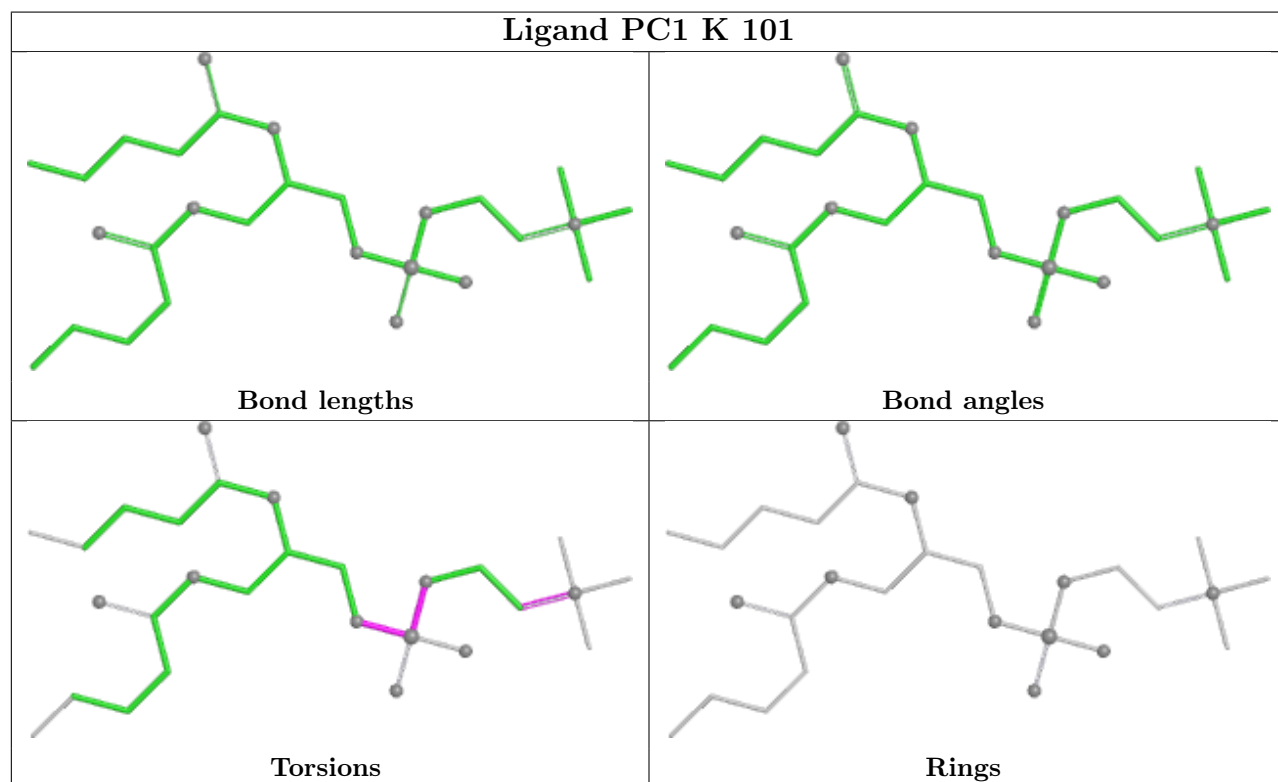
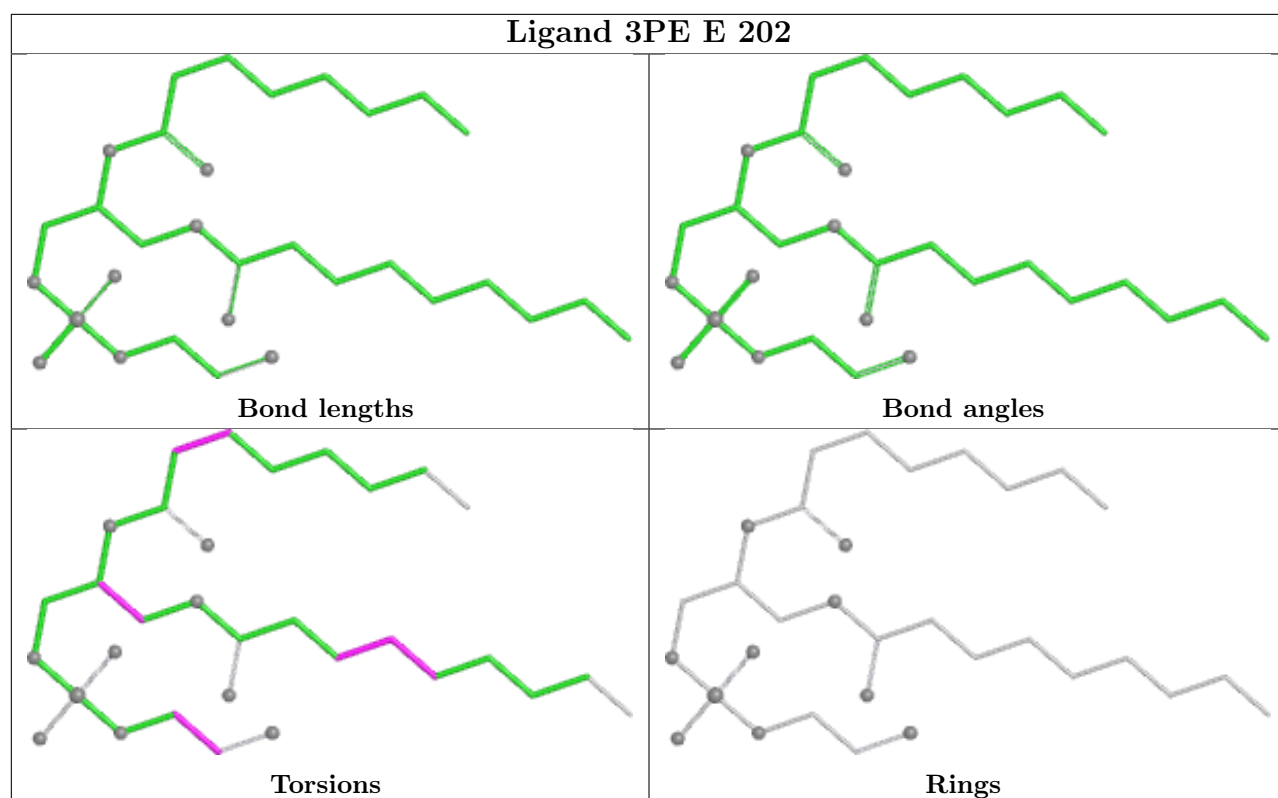


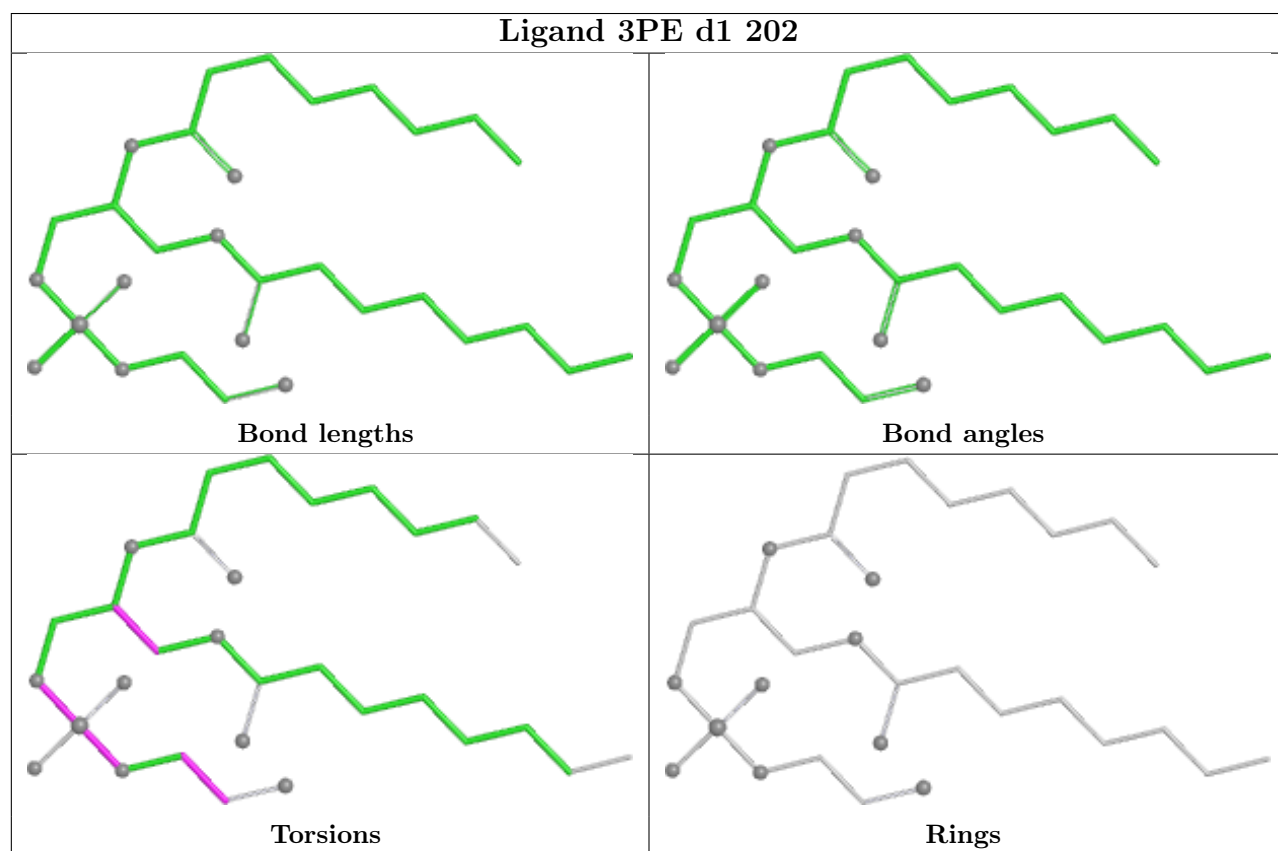
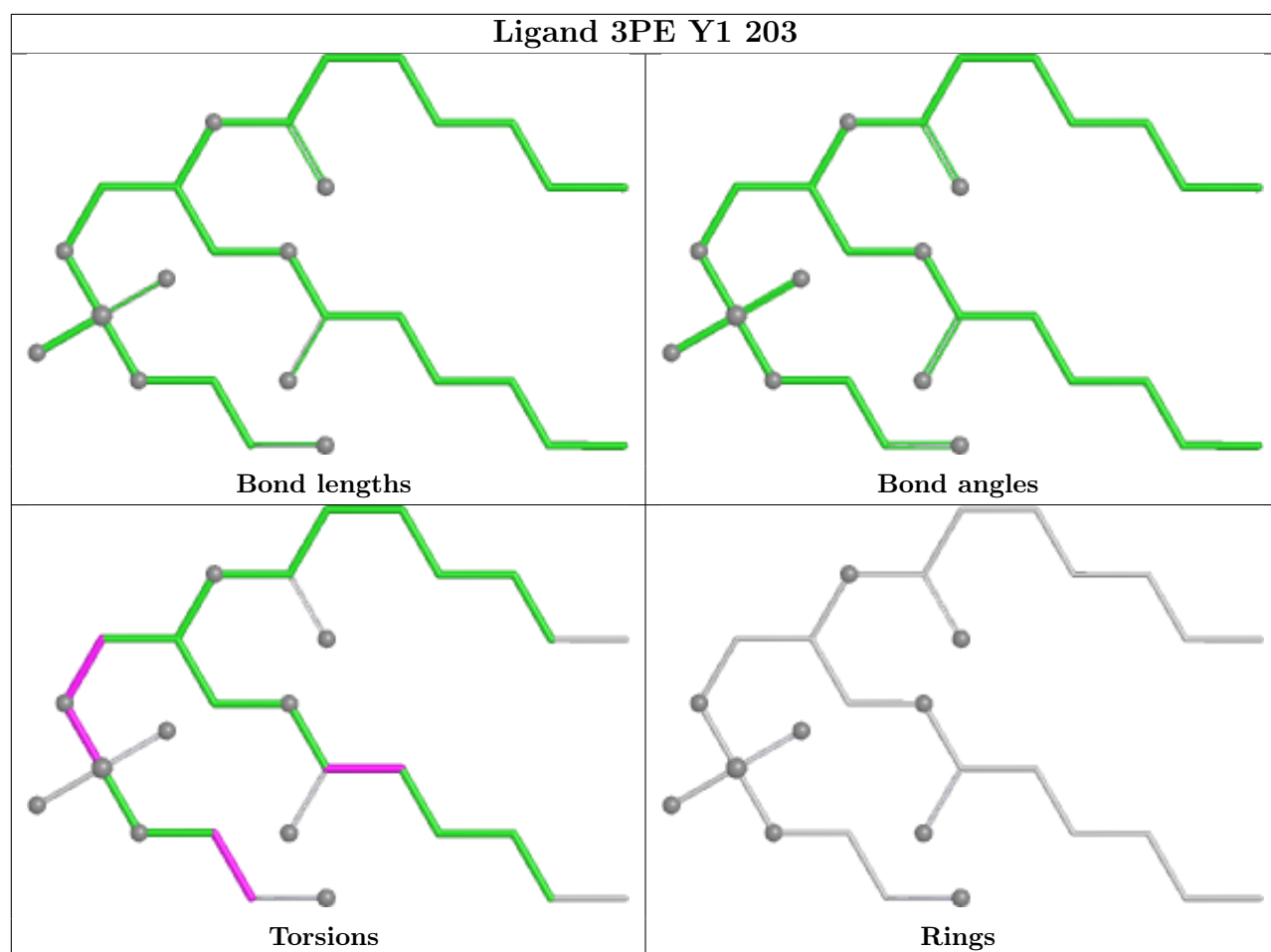


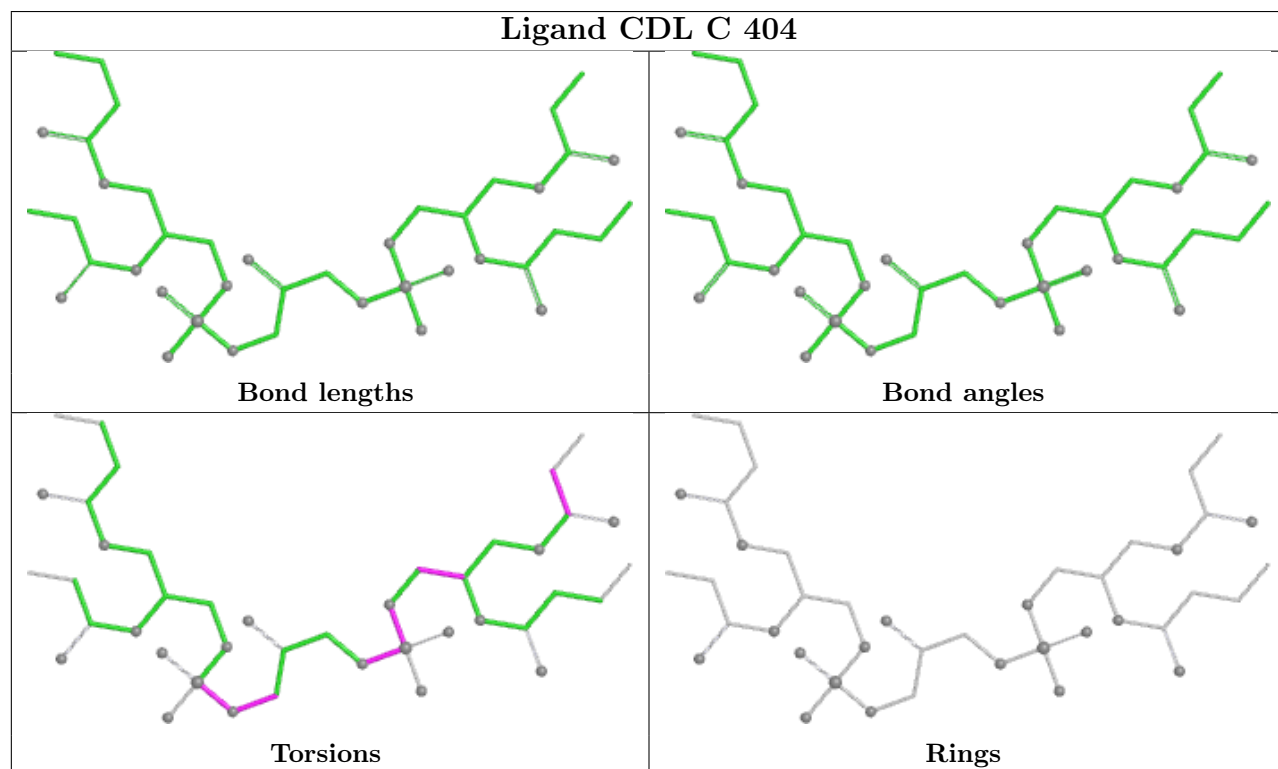
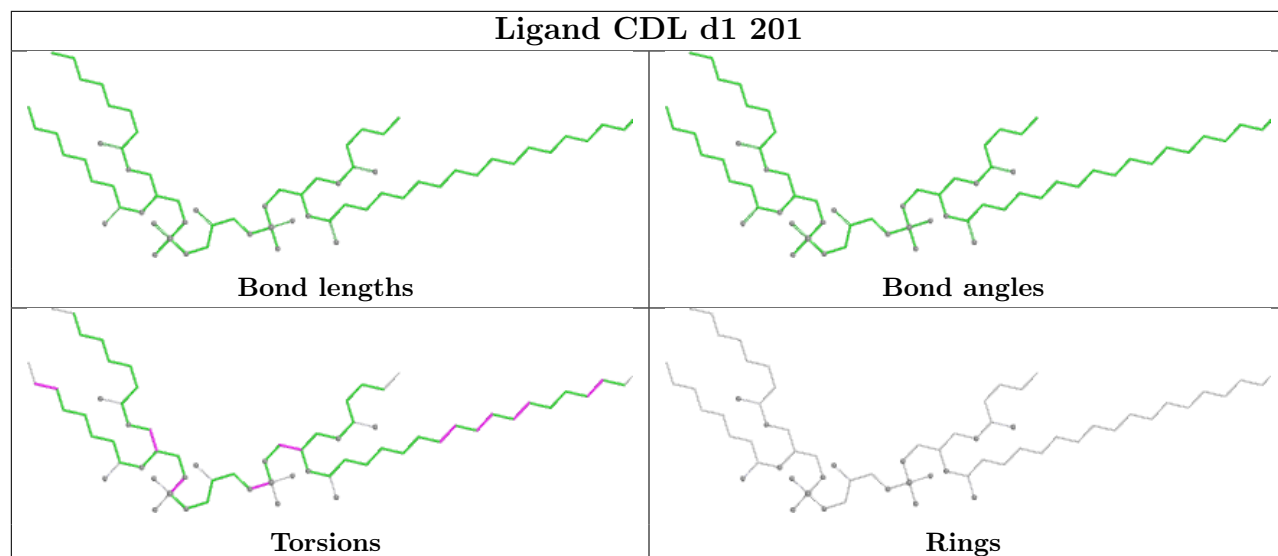


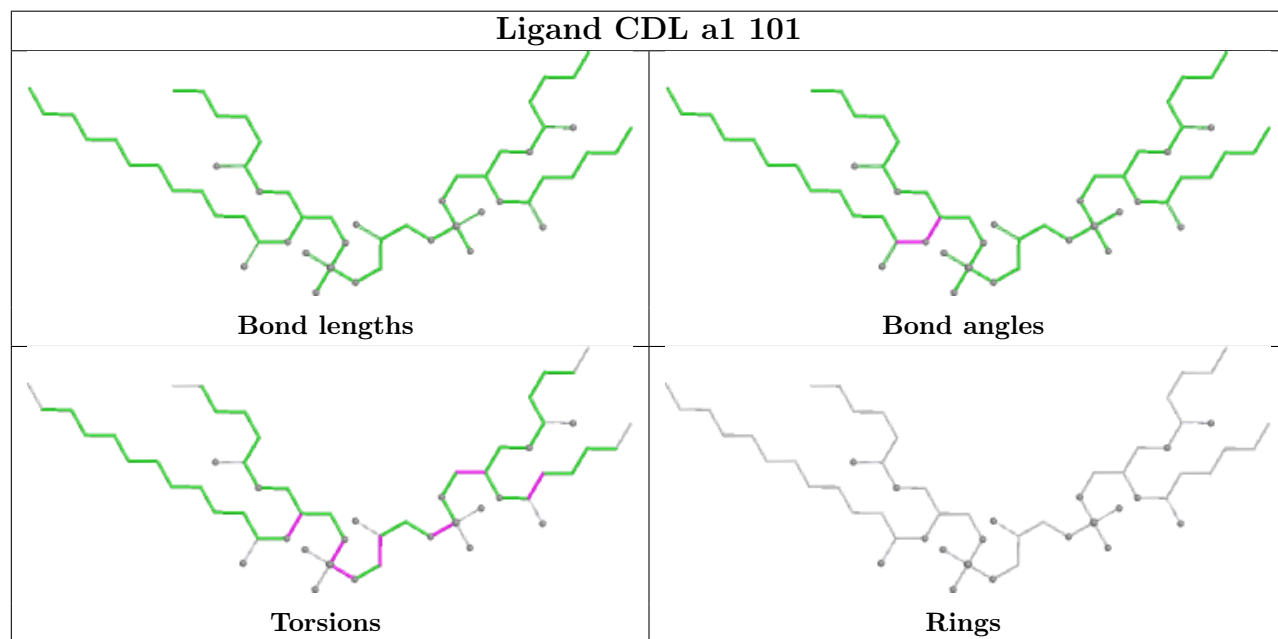
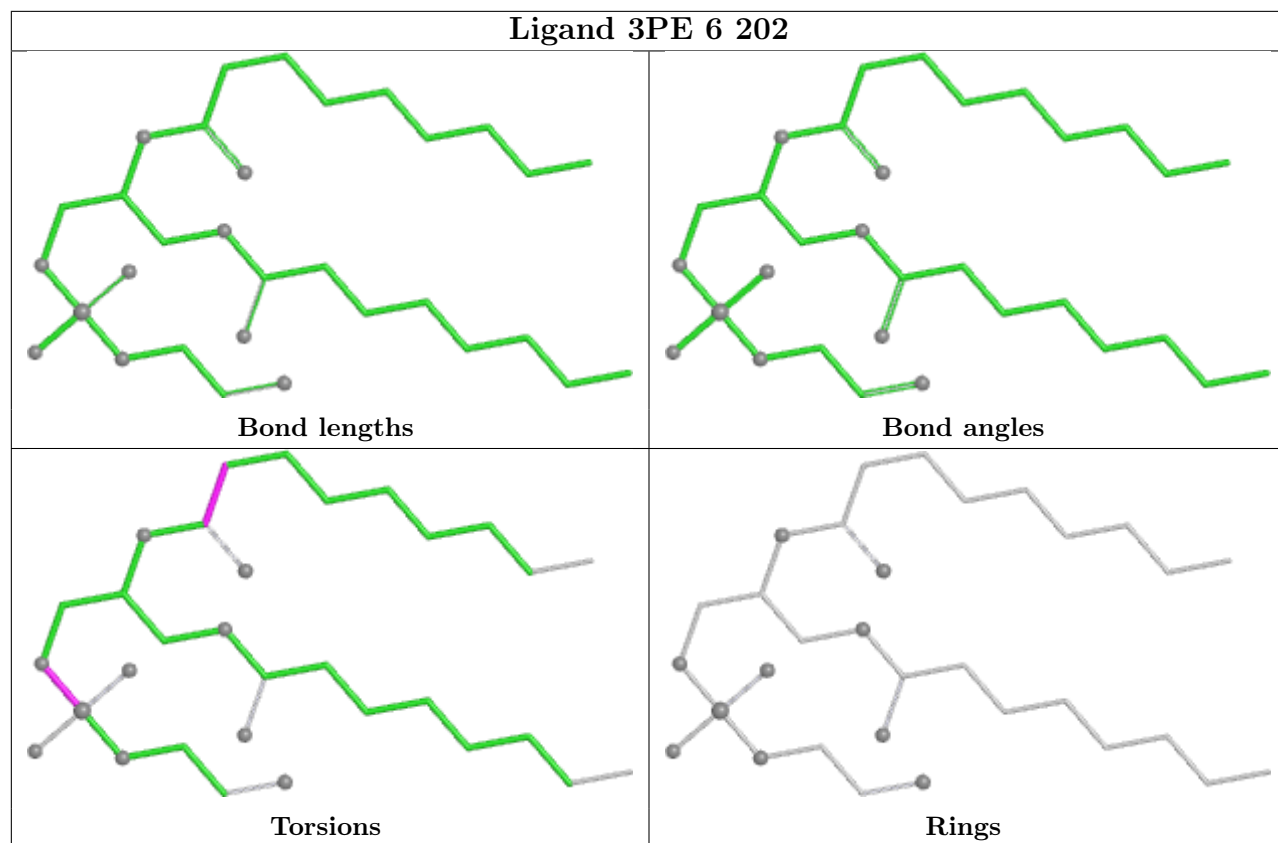


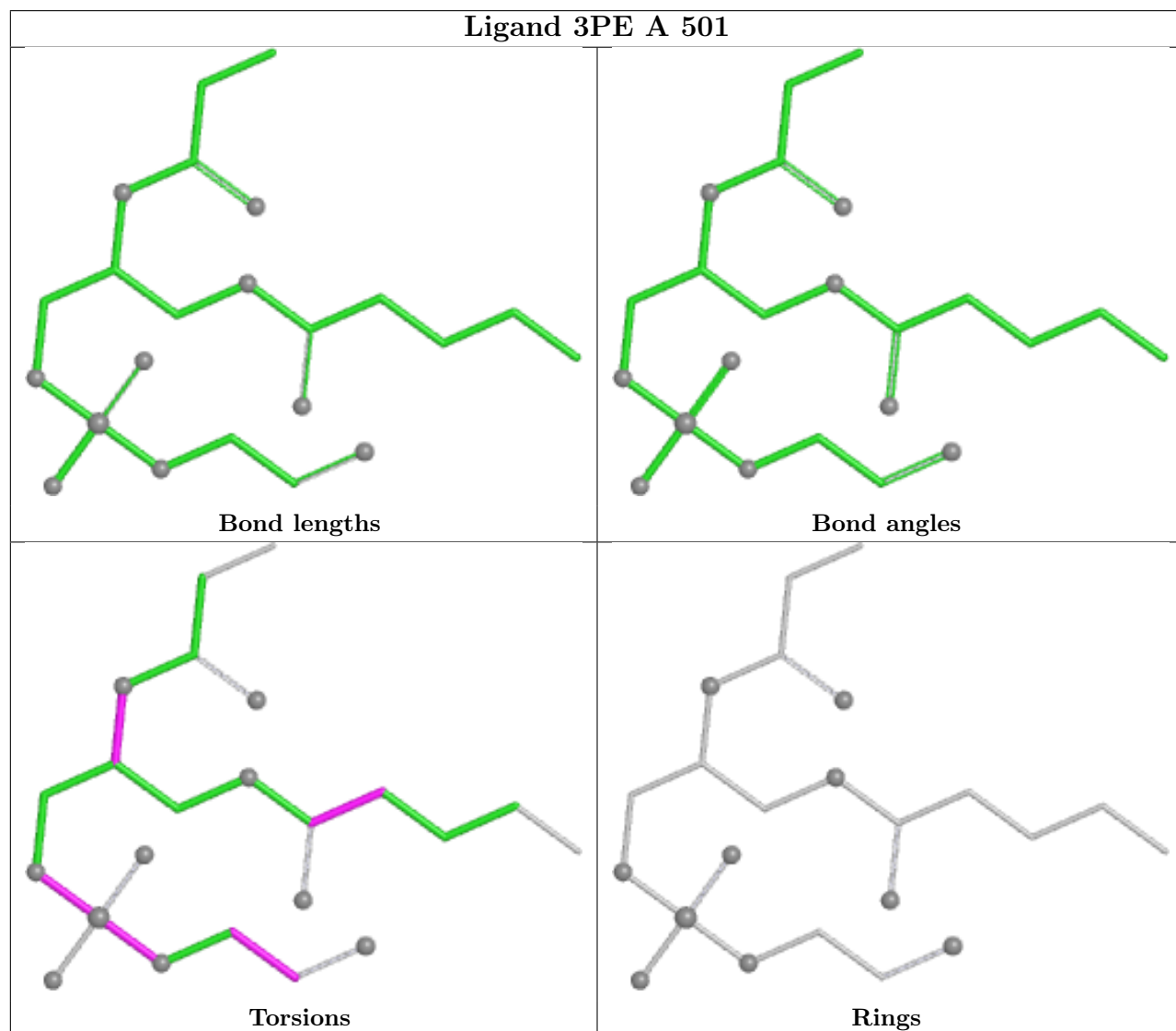
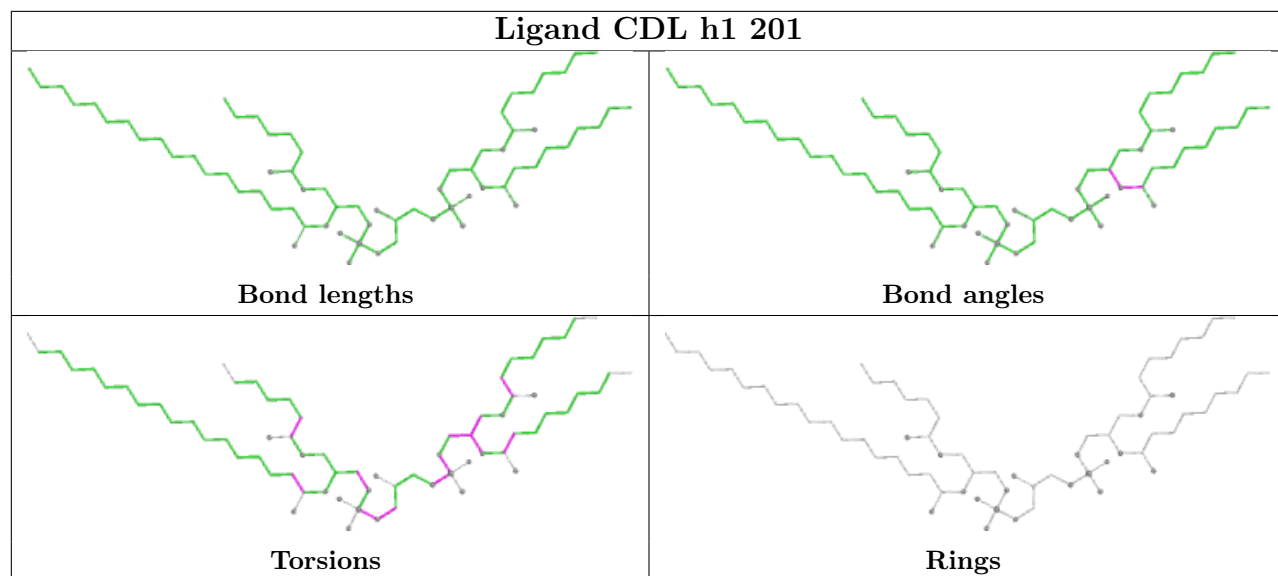


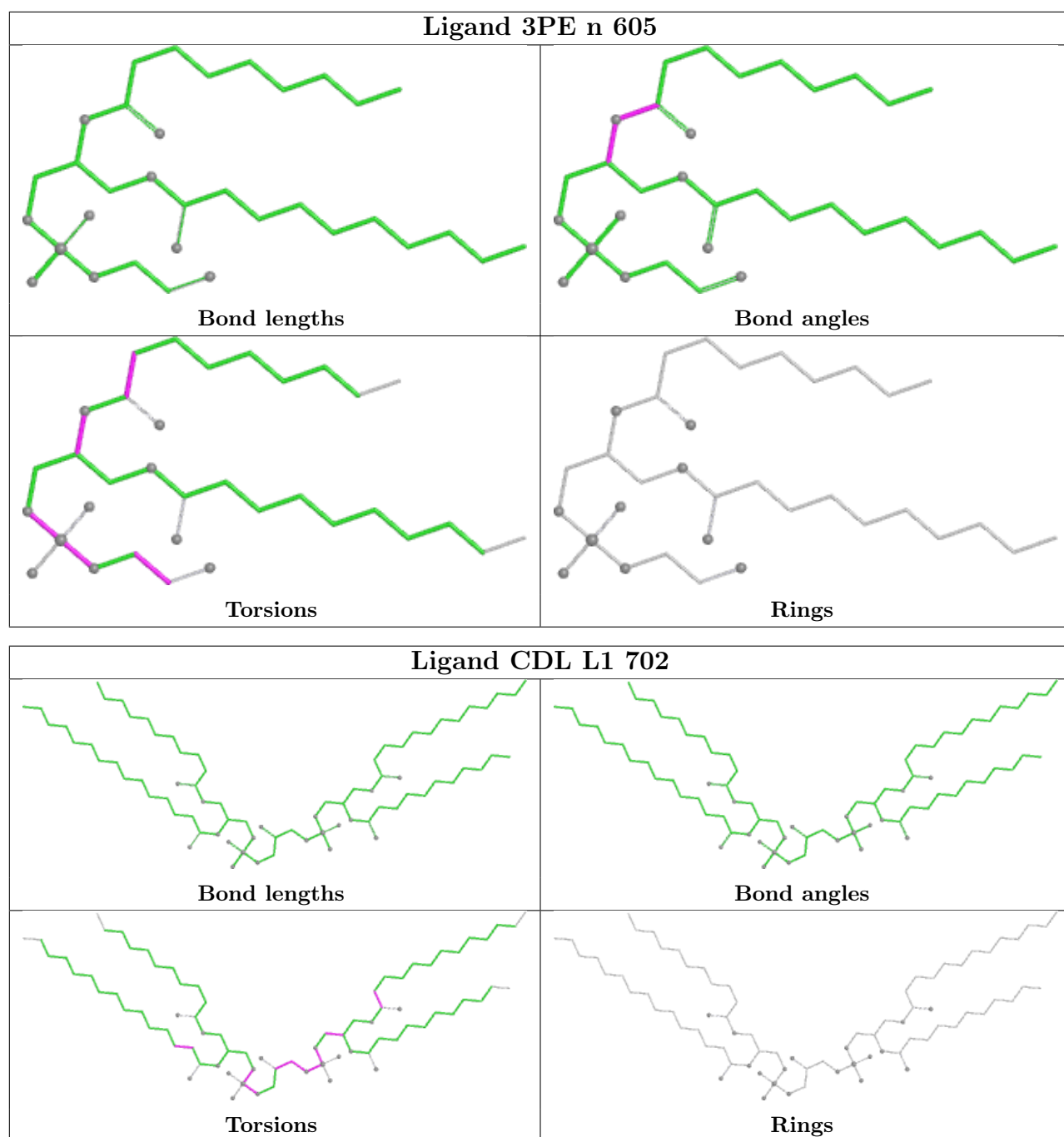


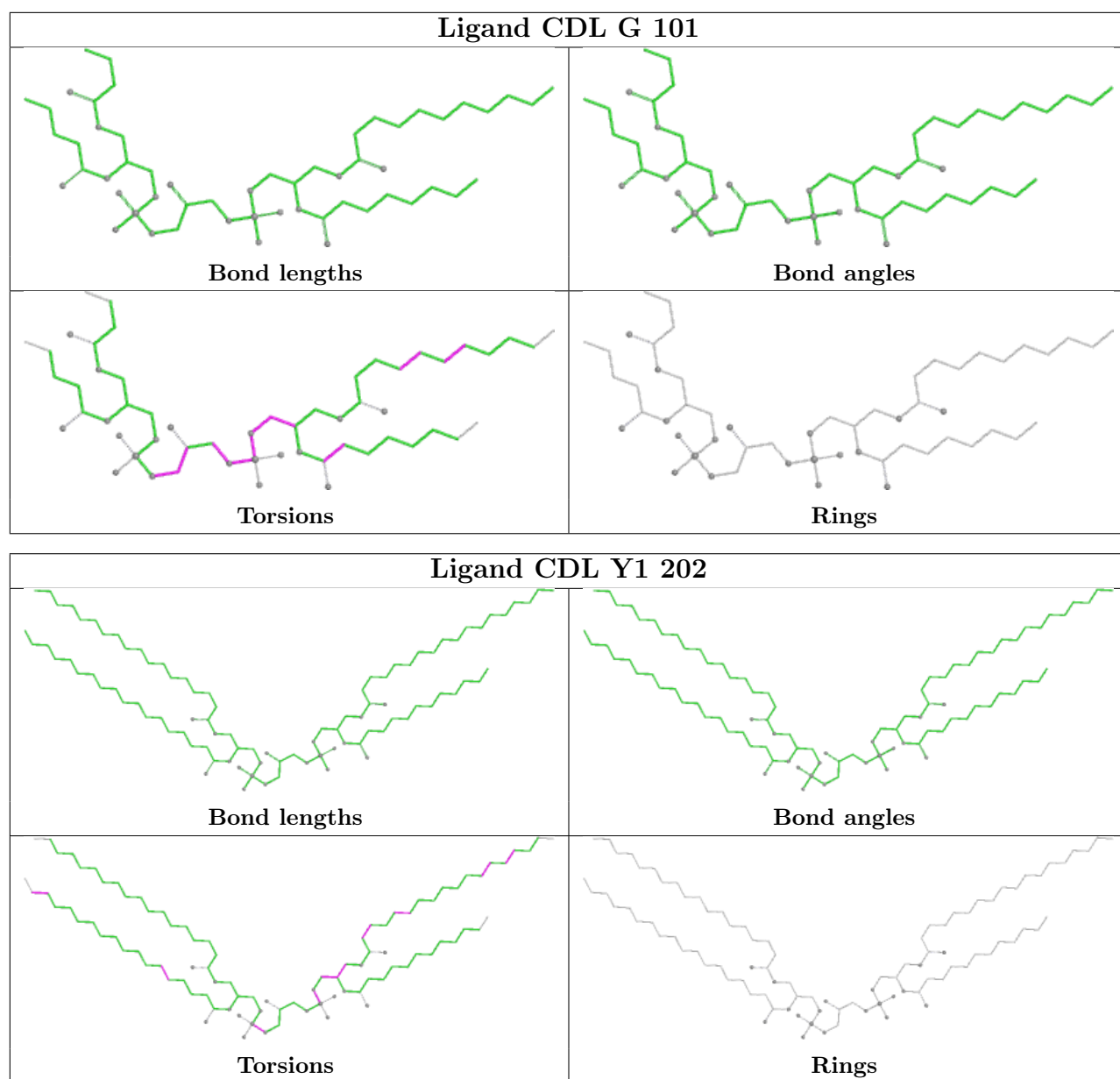


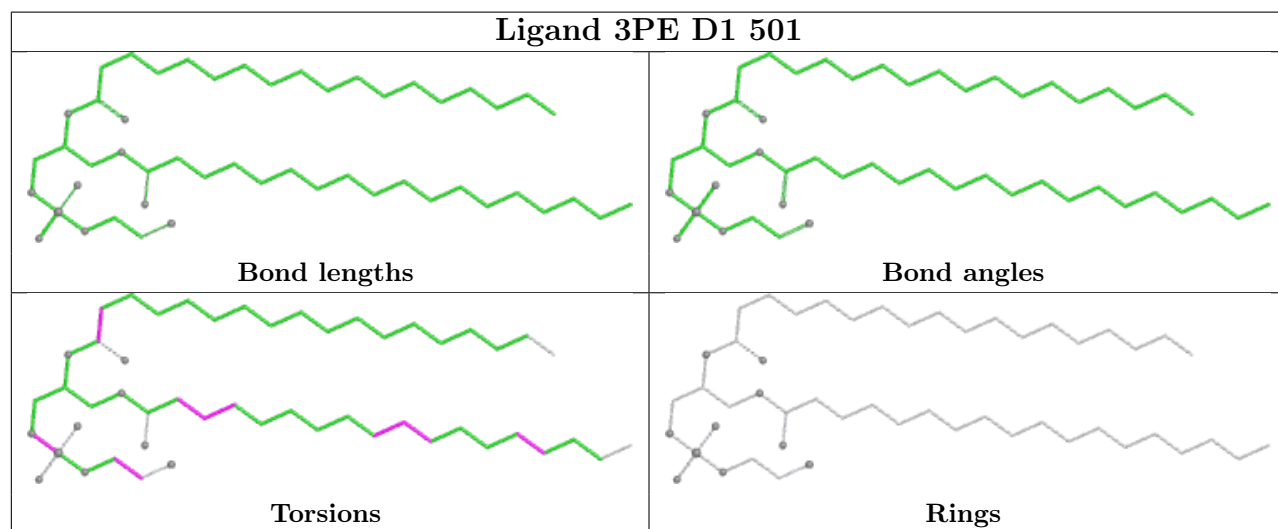
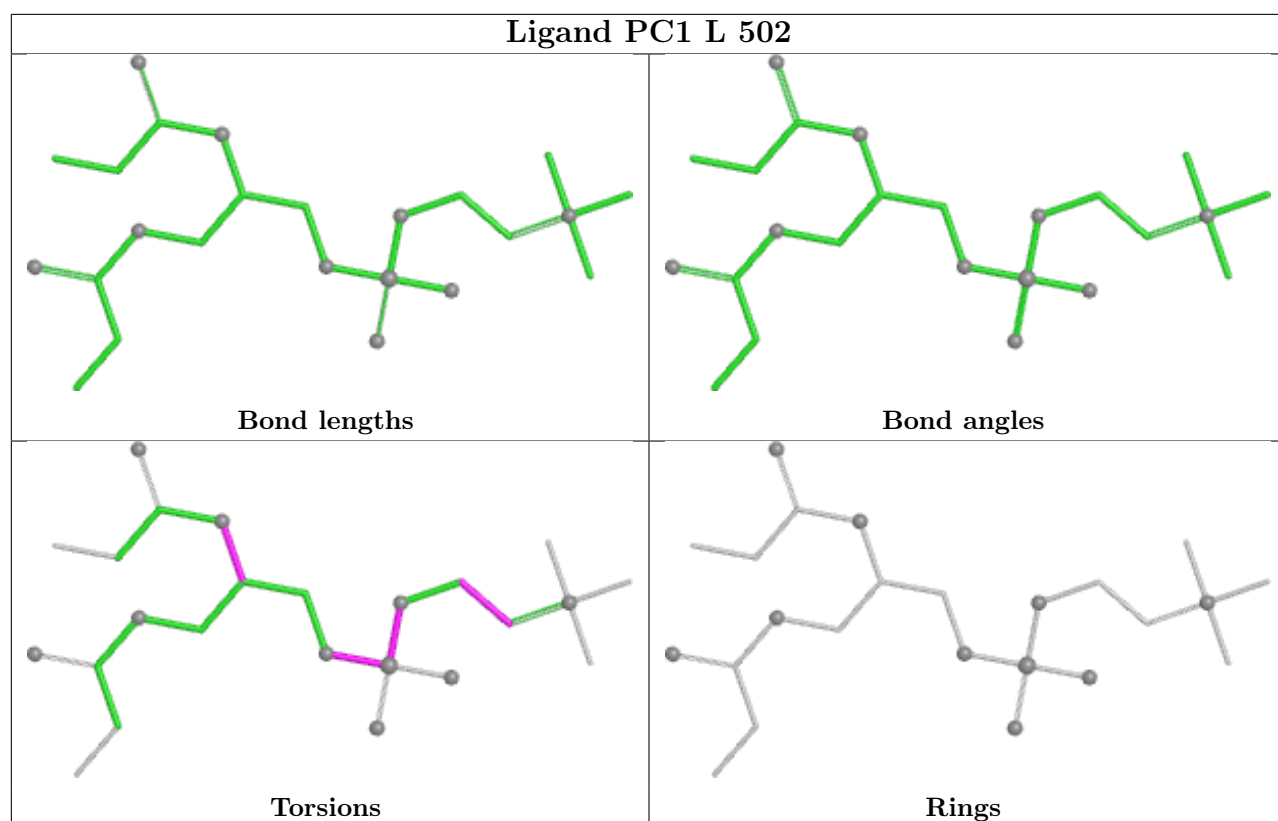


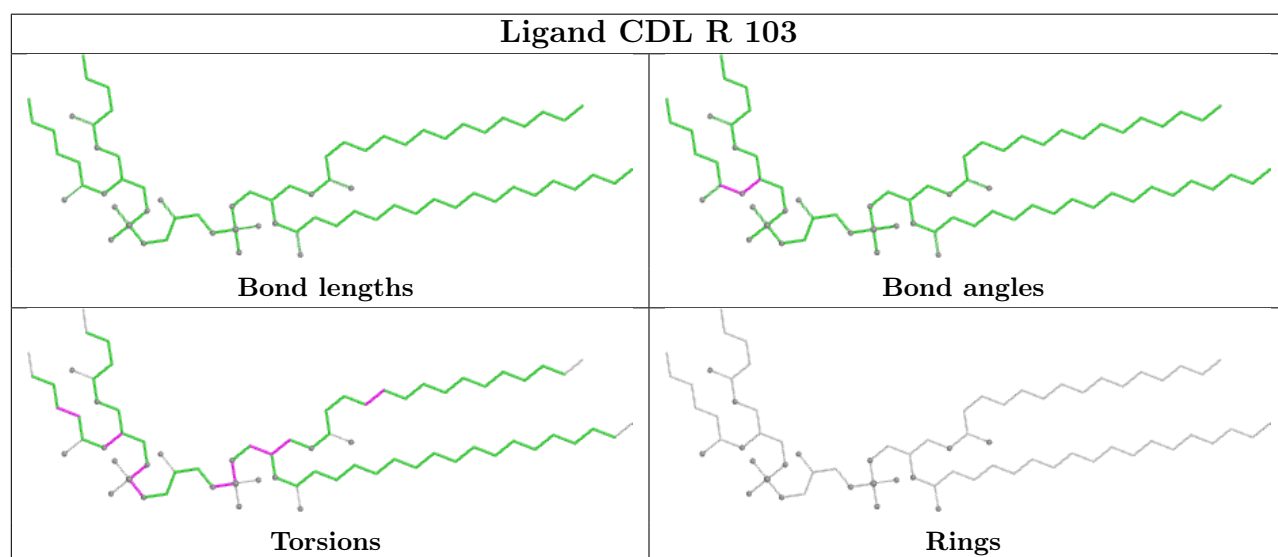
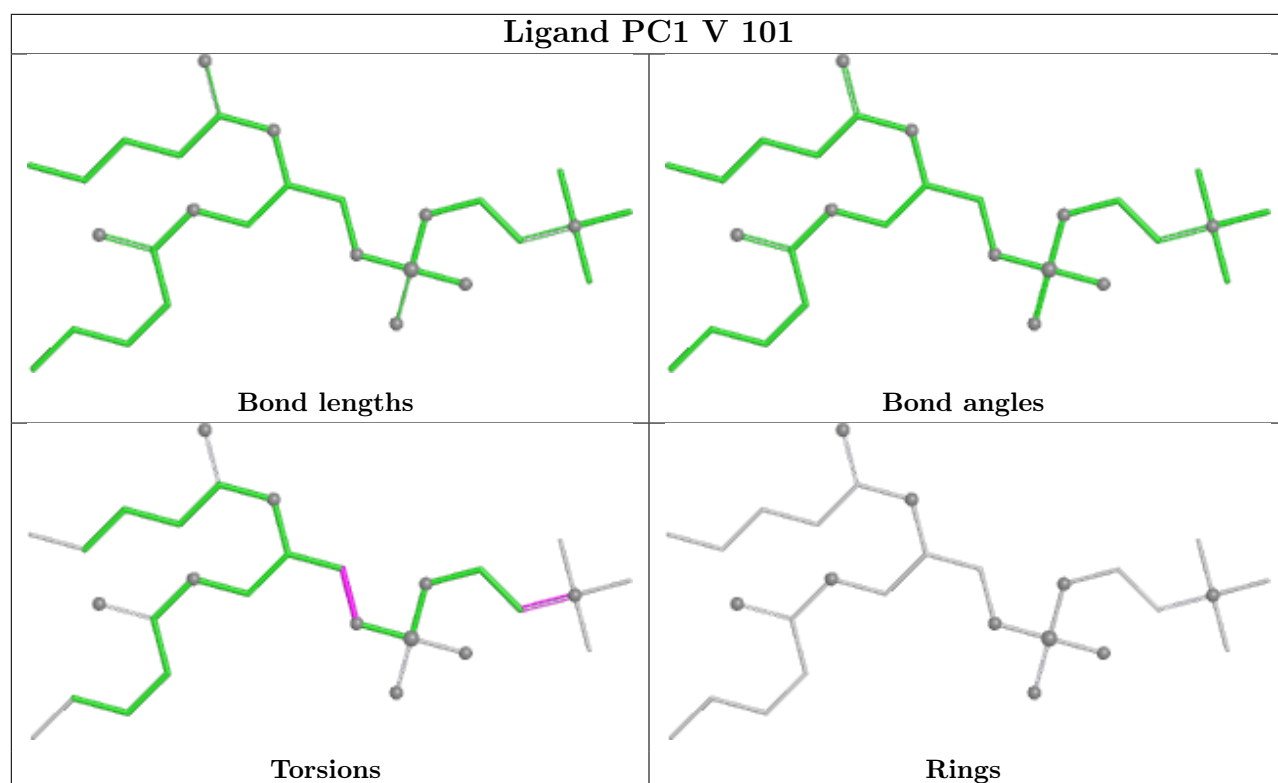


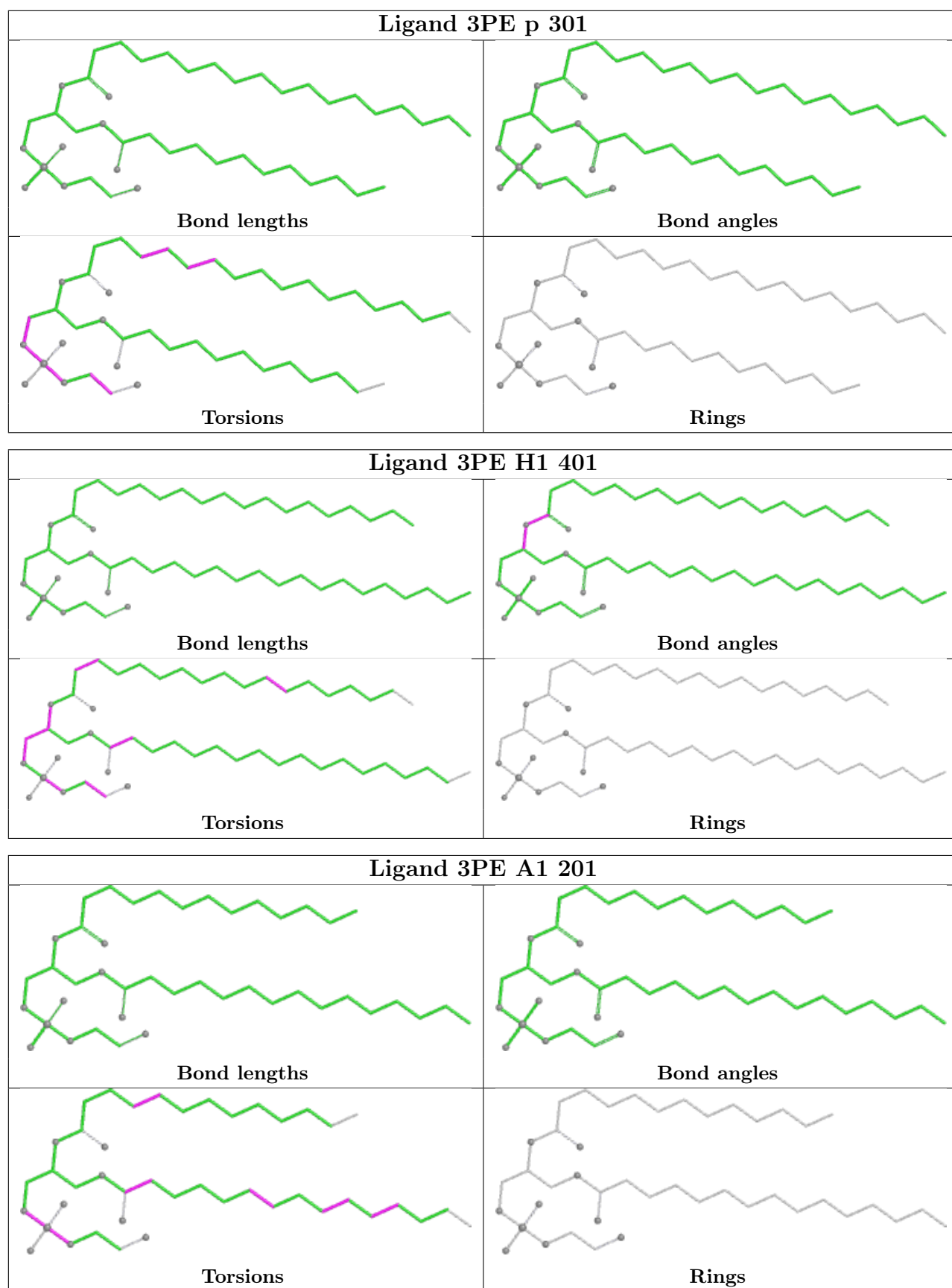


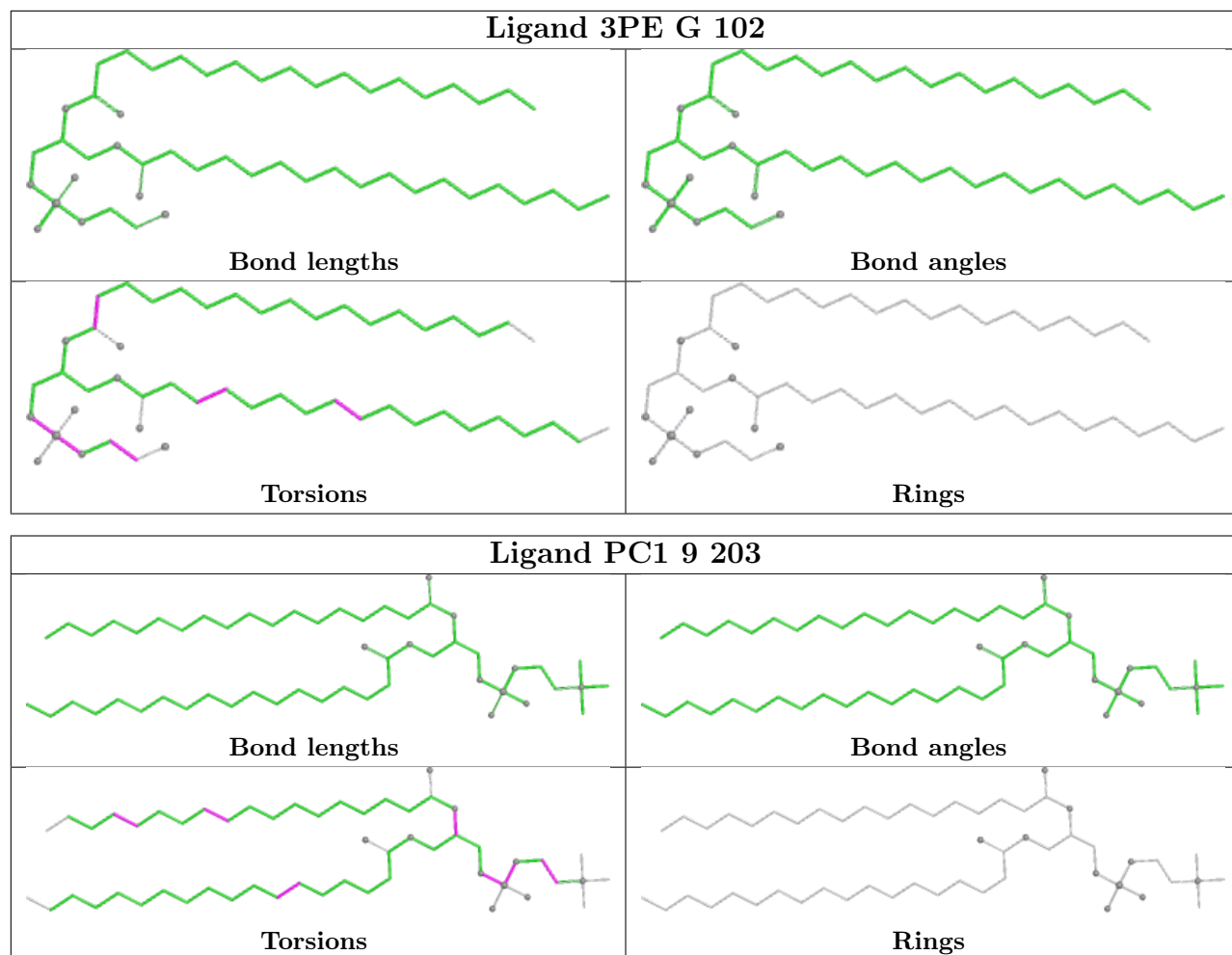


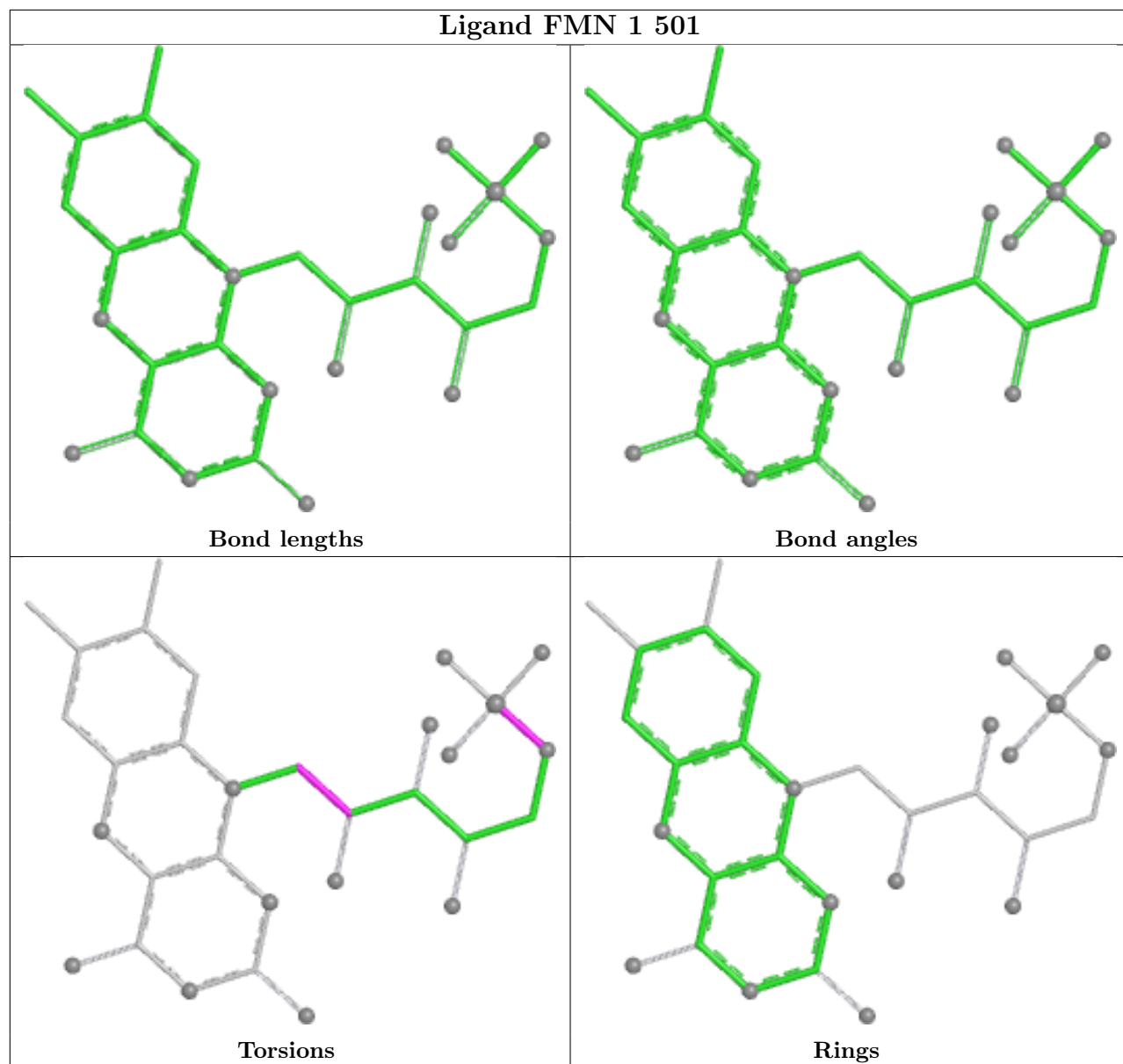


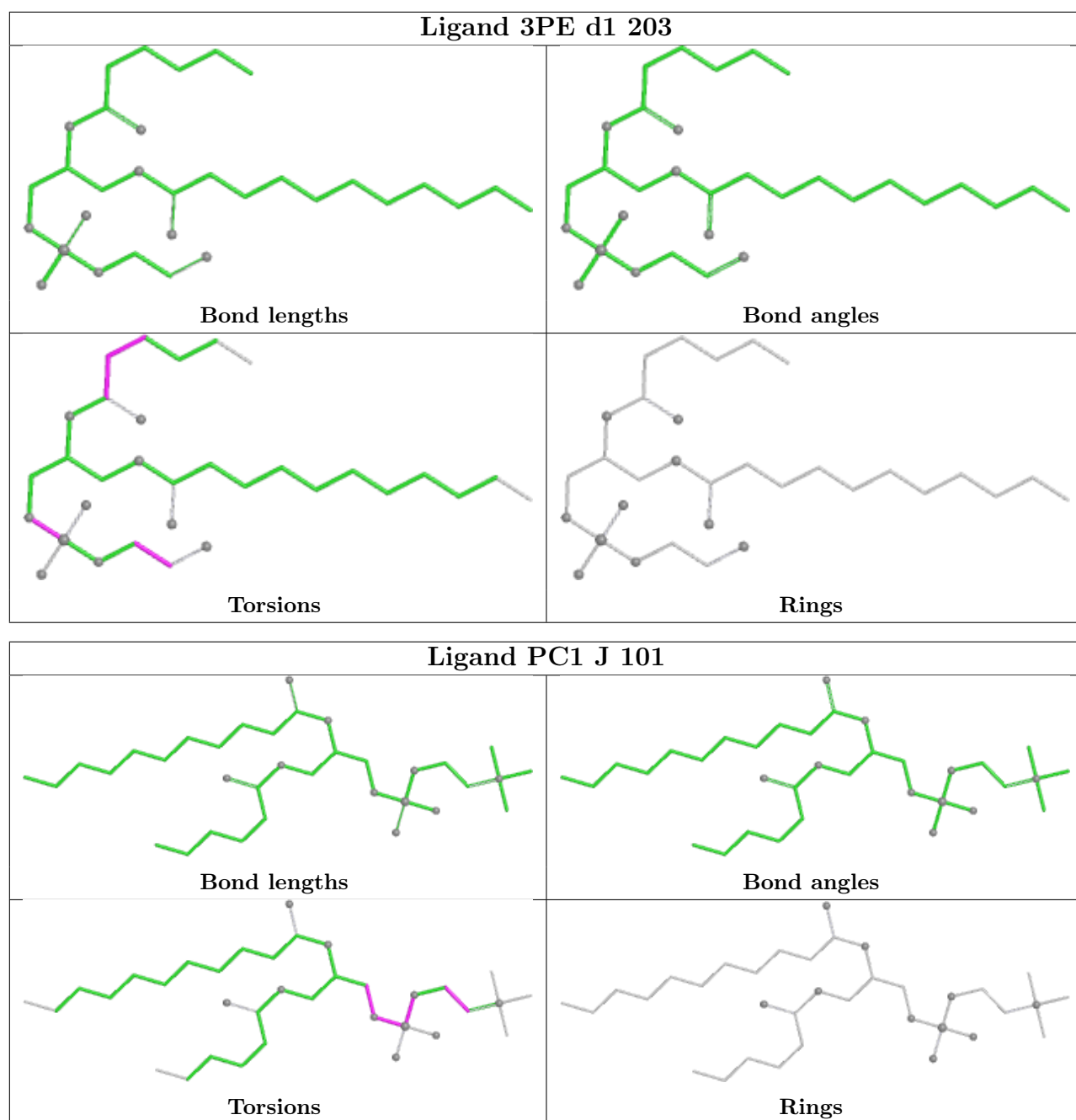


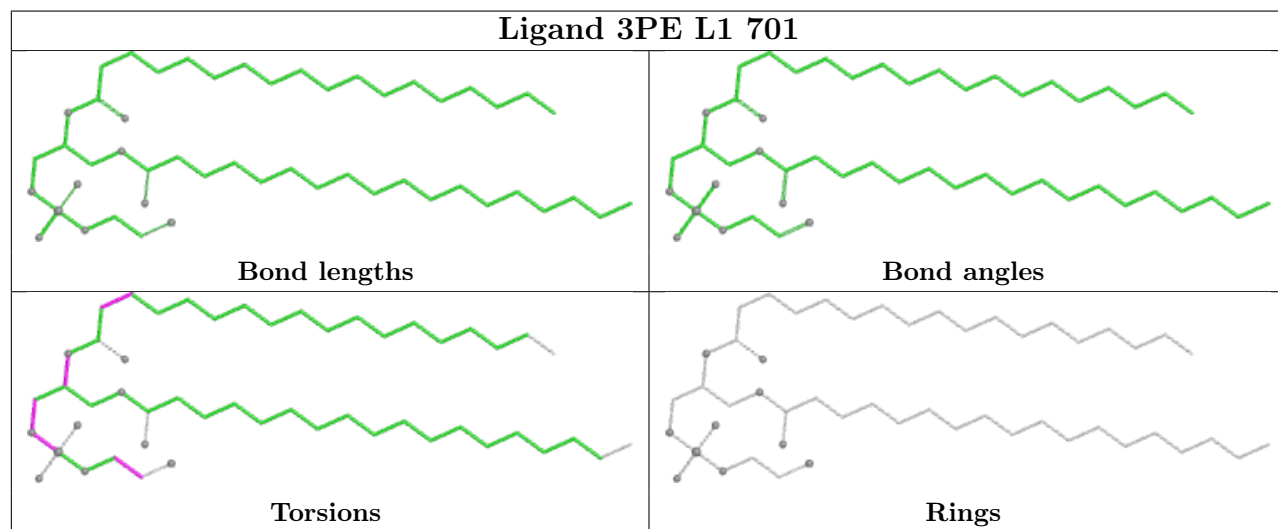
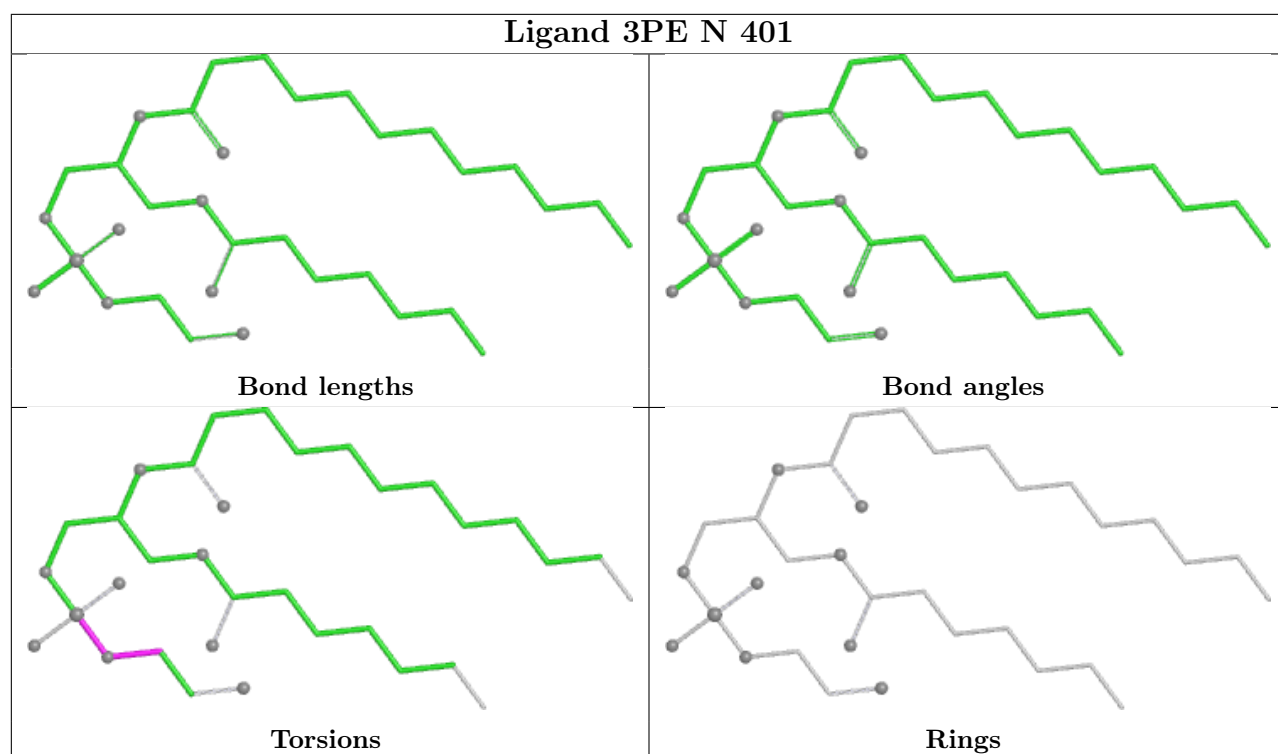


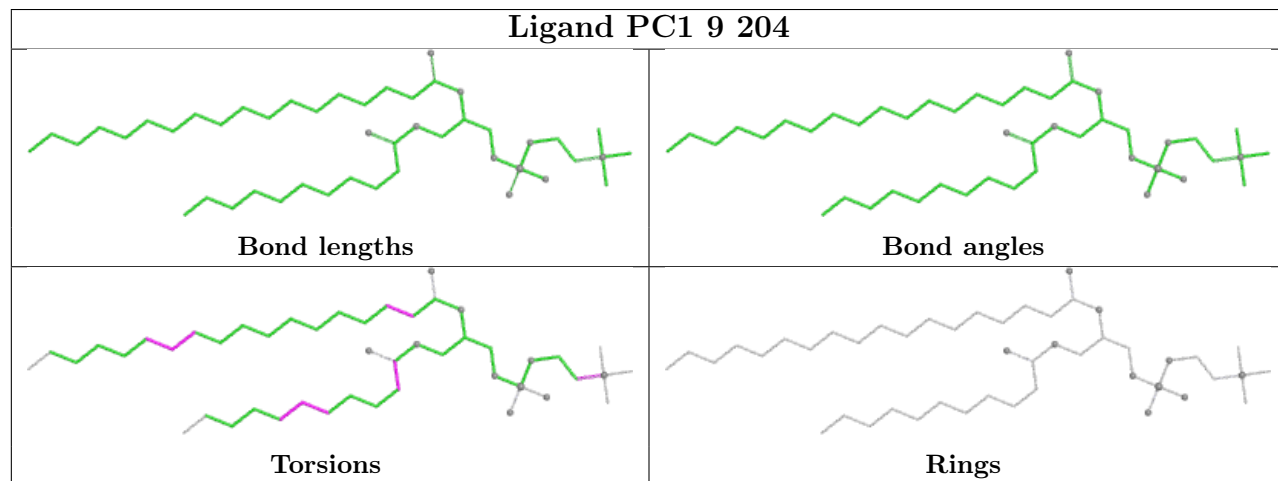
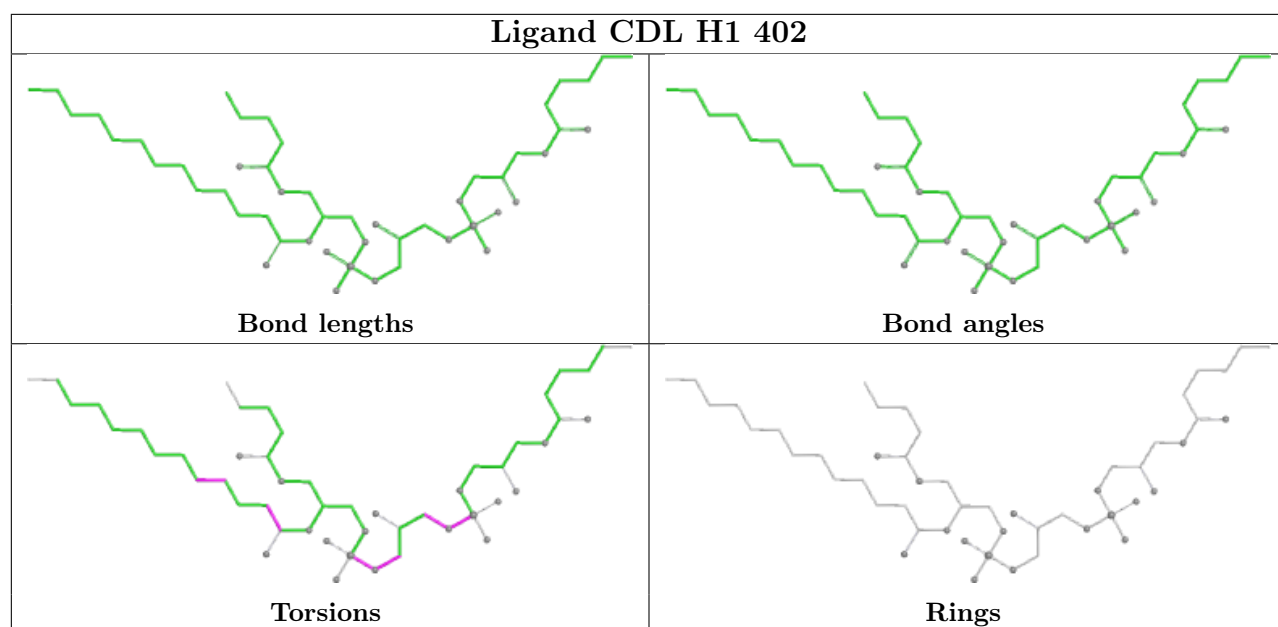




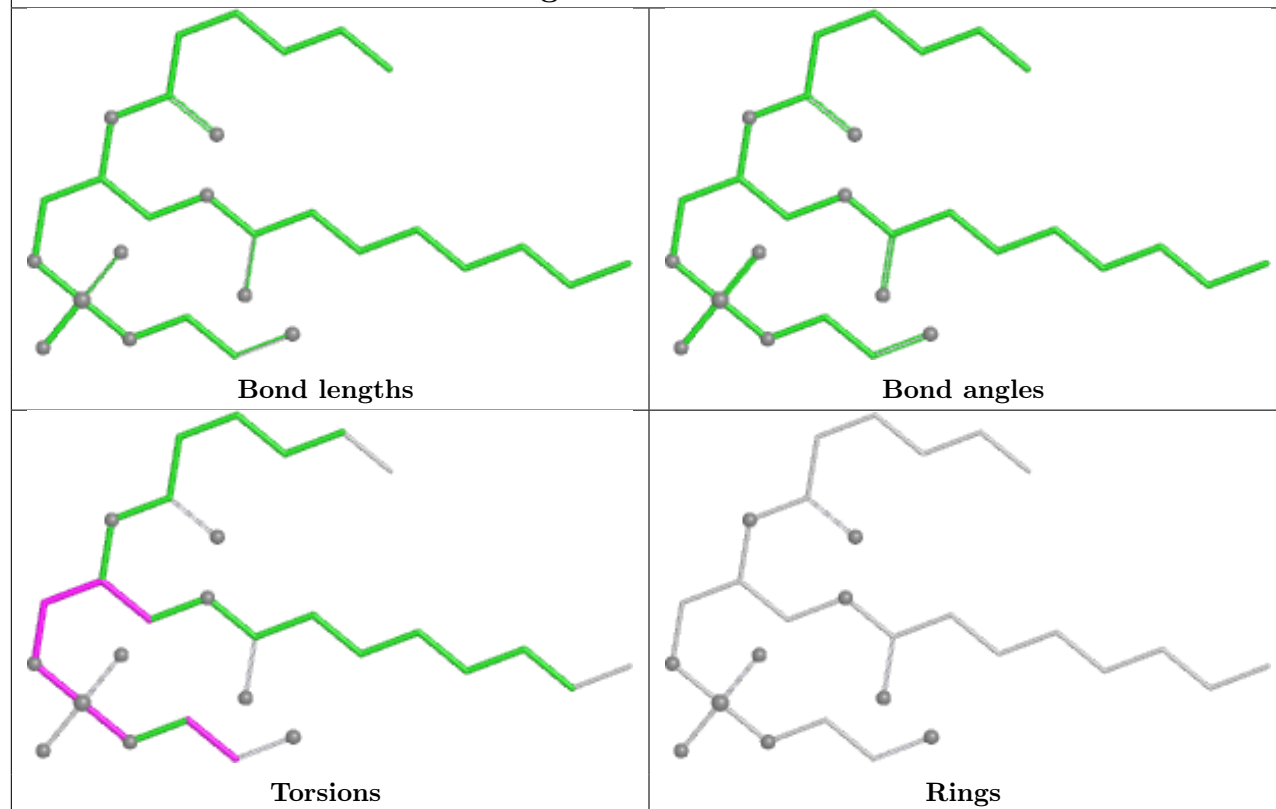




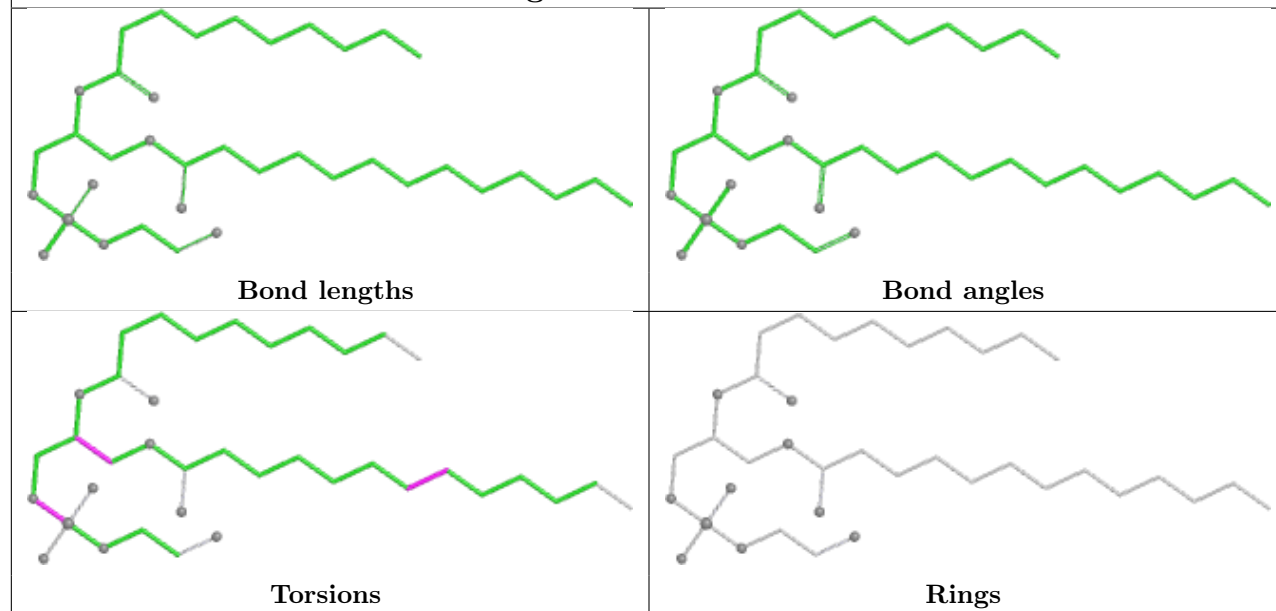


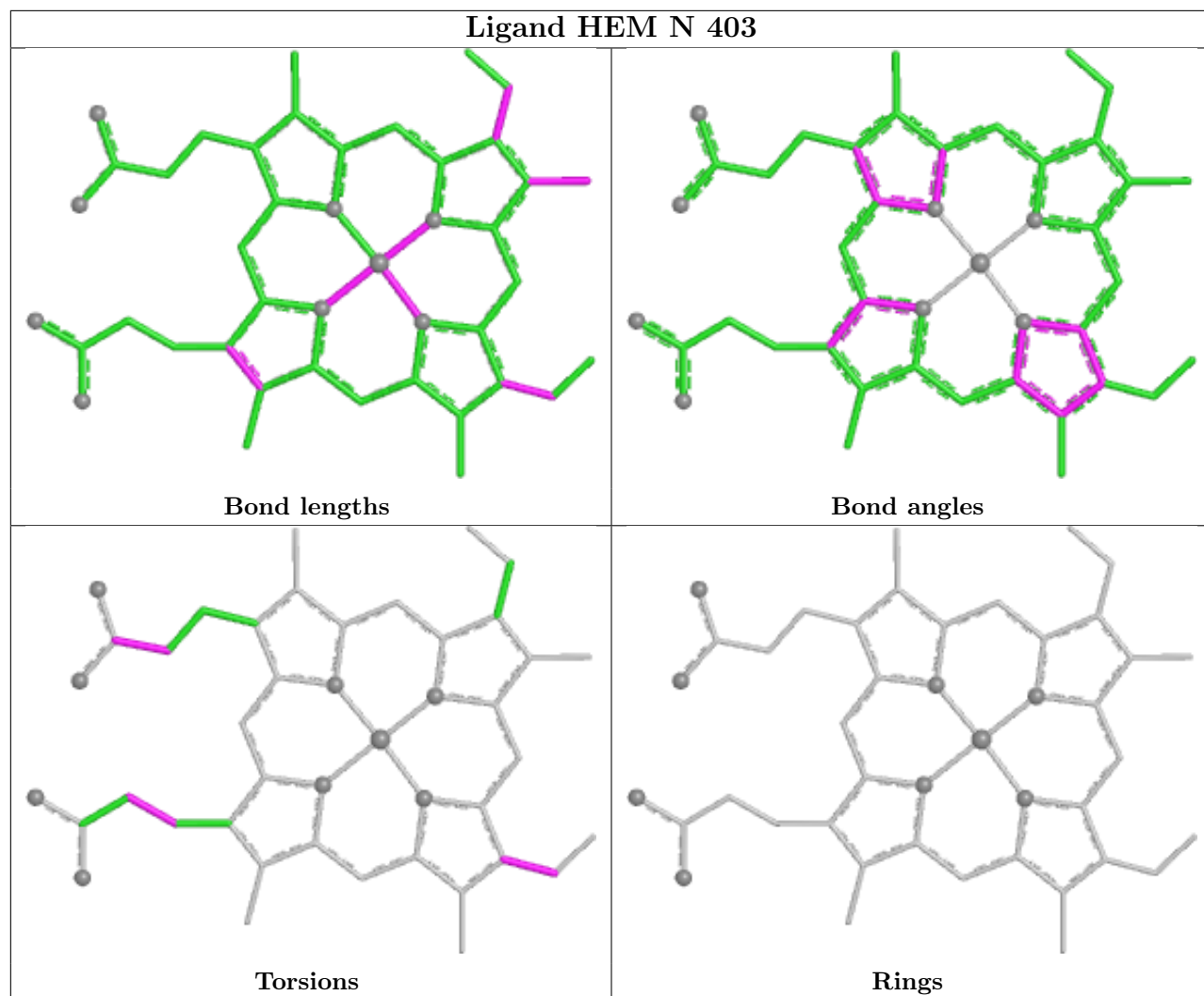


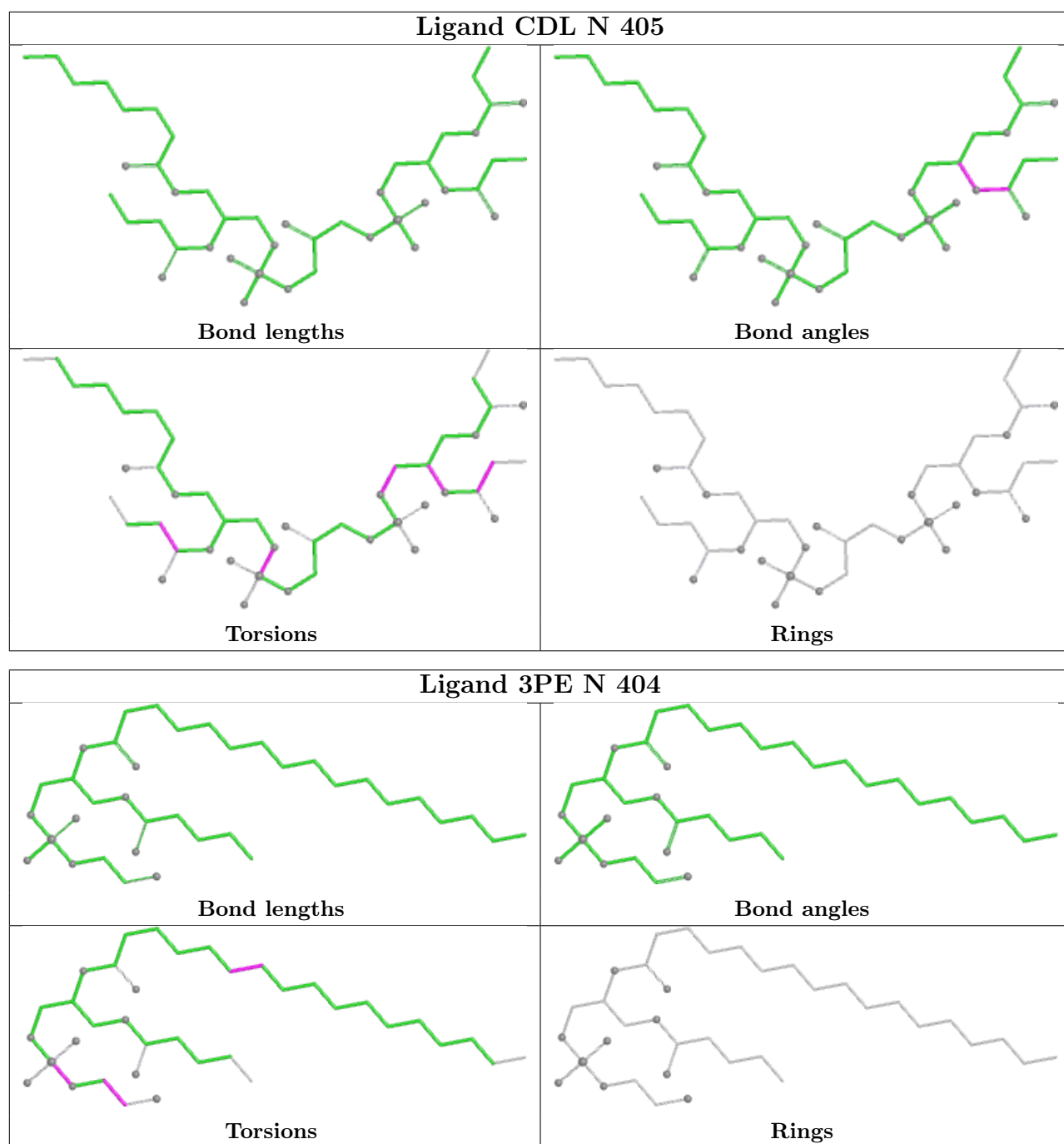
Ligand 3PE o 302

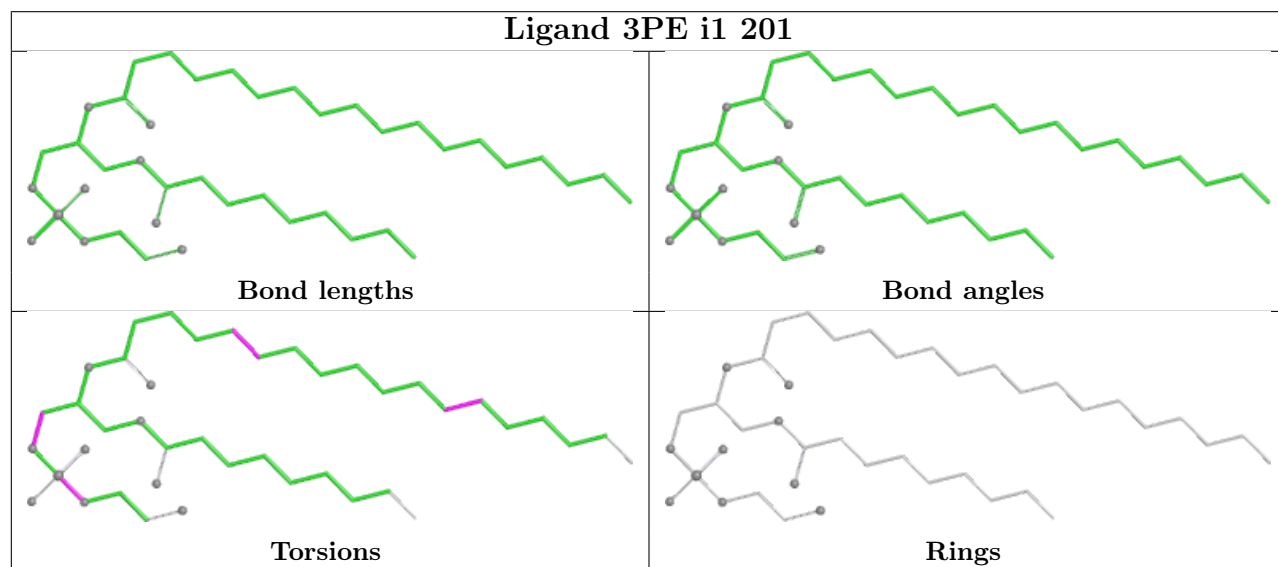
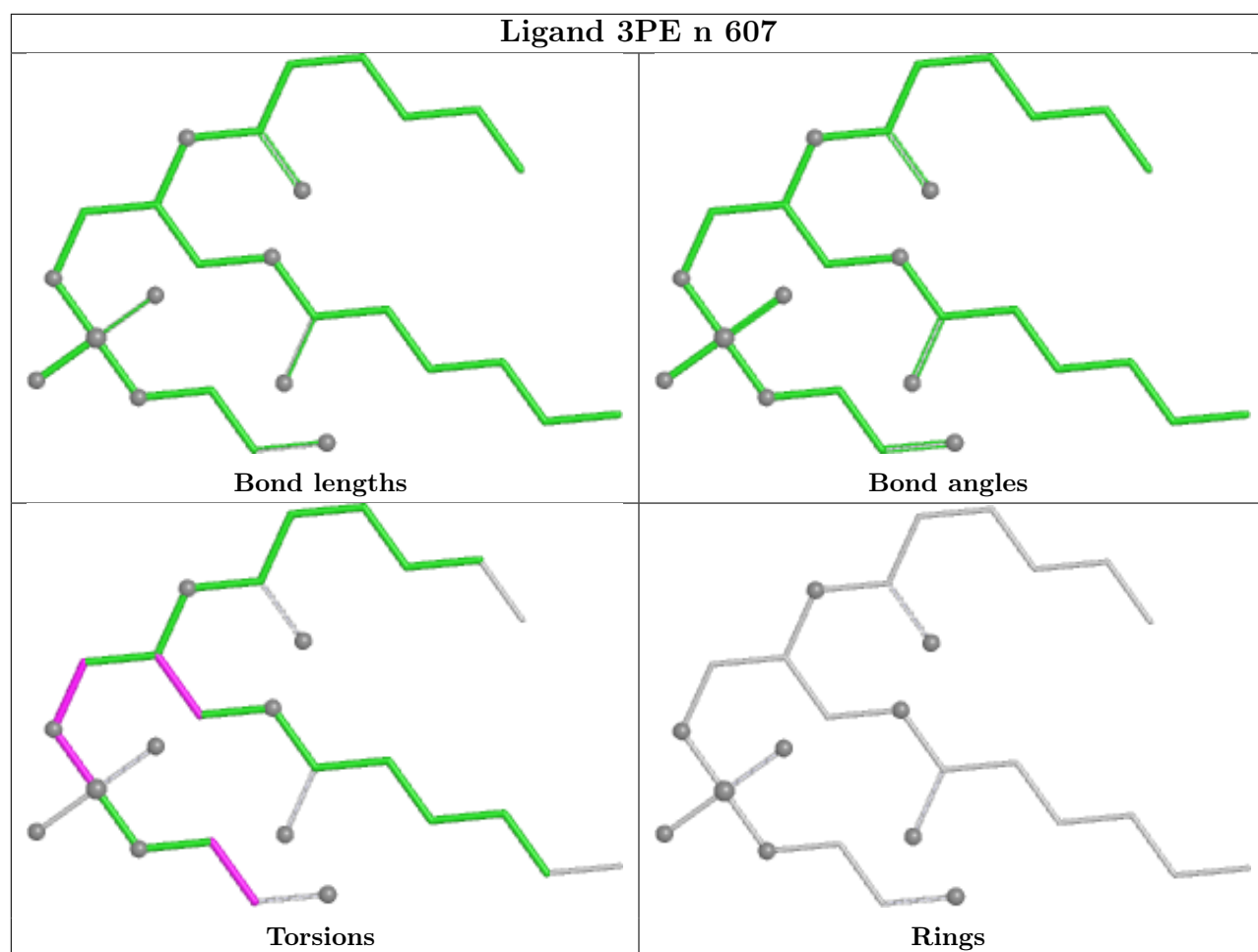


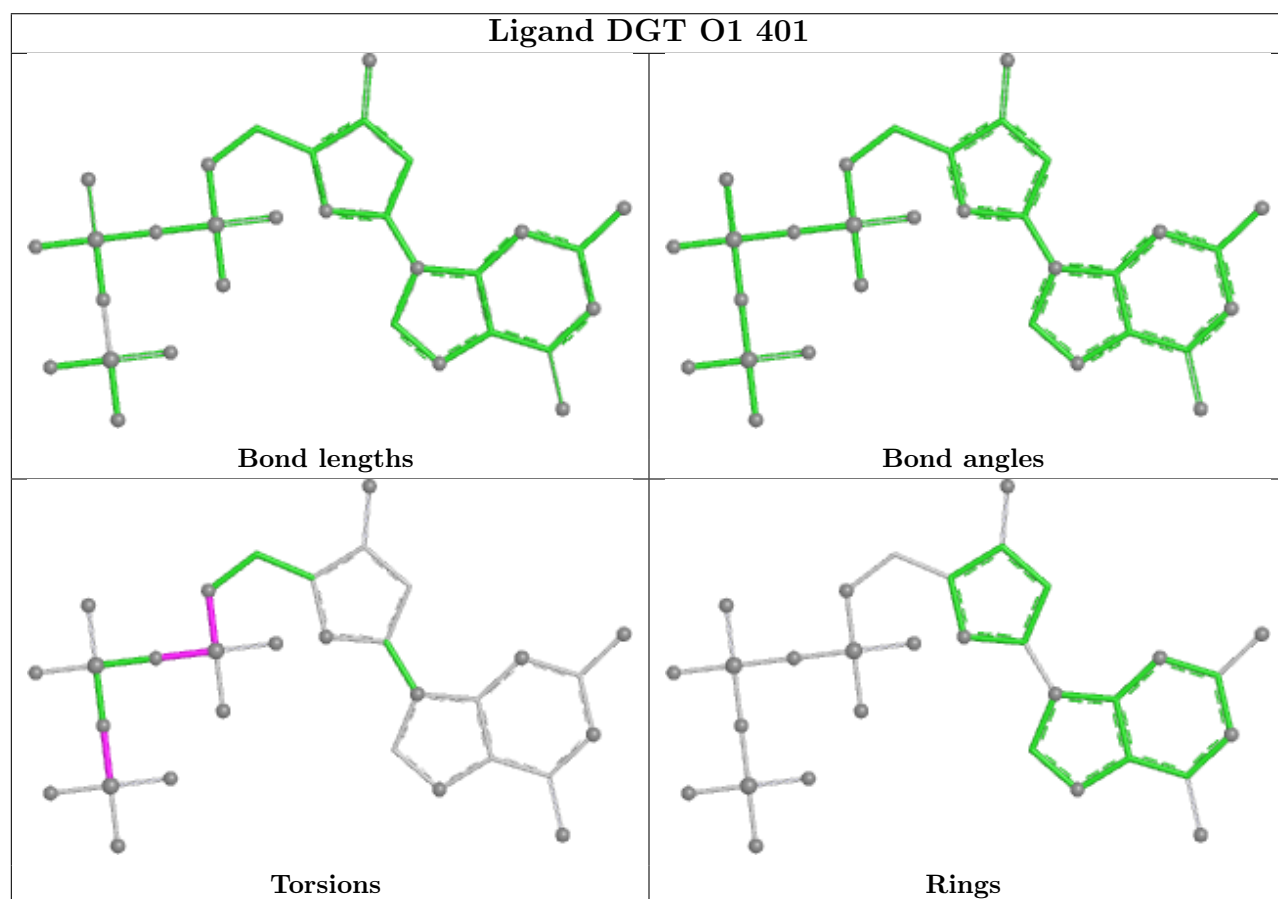
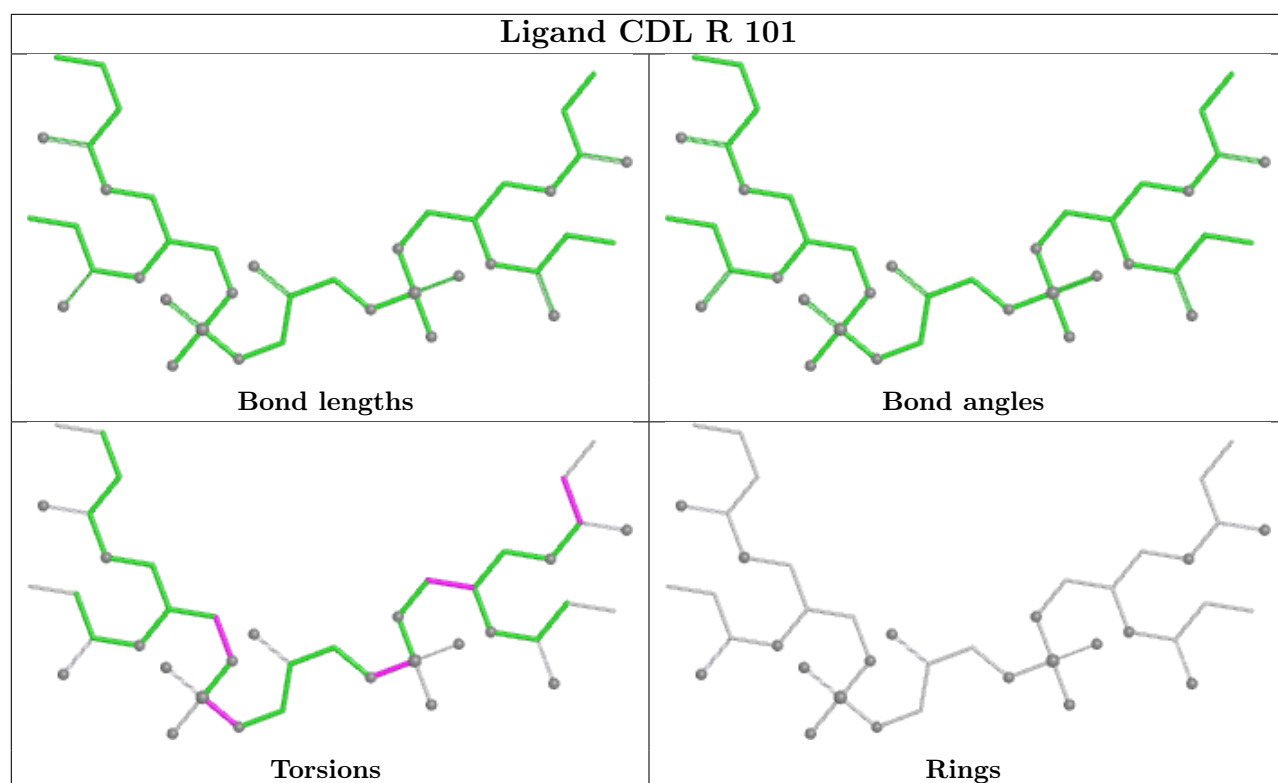
Ligand 3PE N1 402

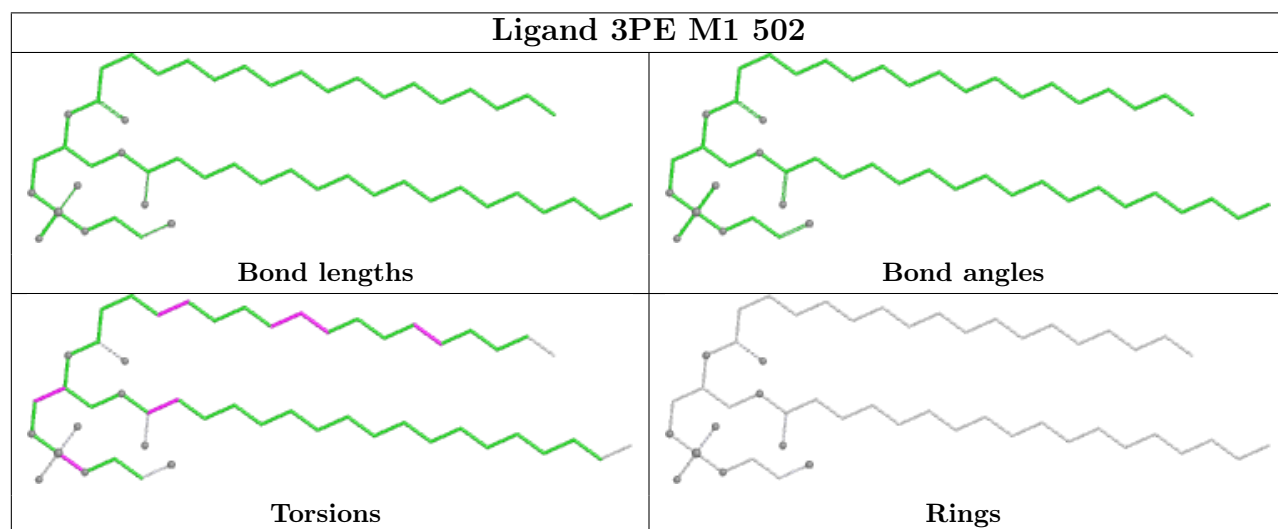
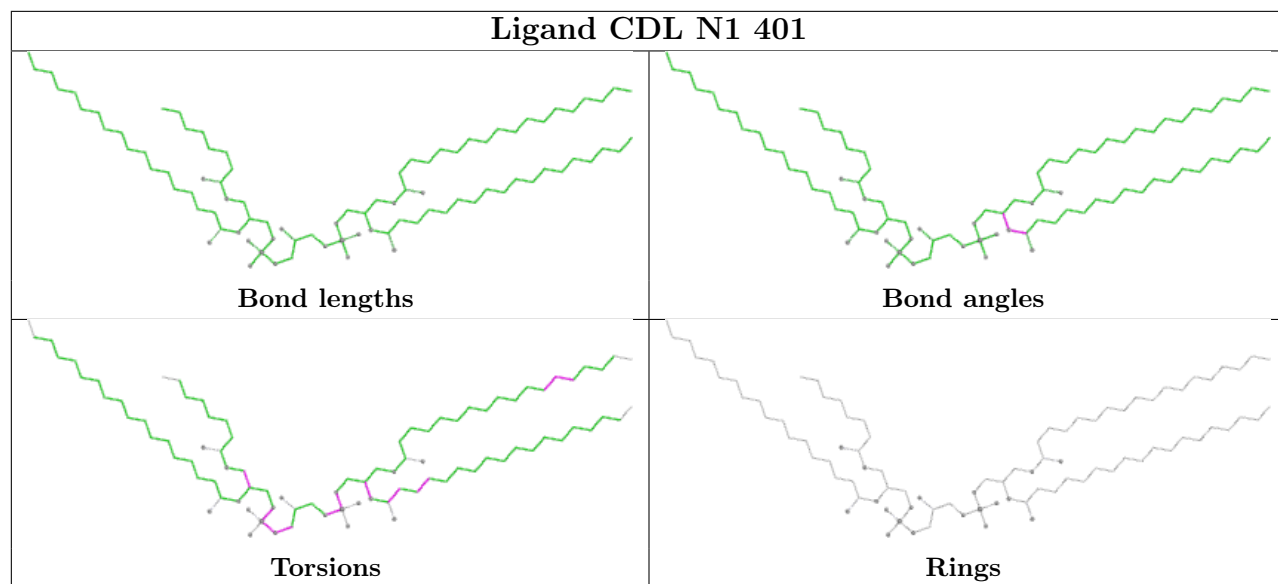


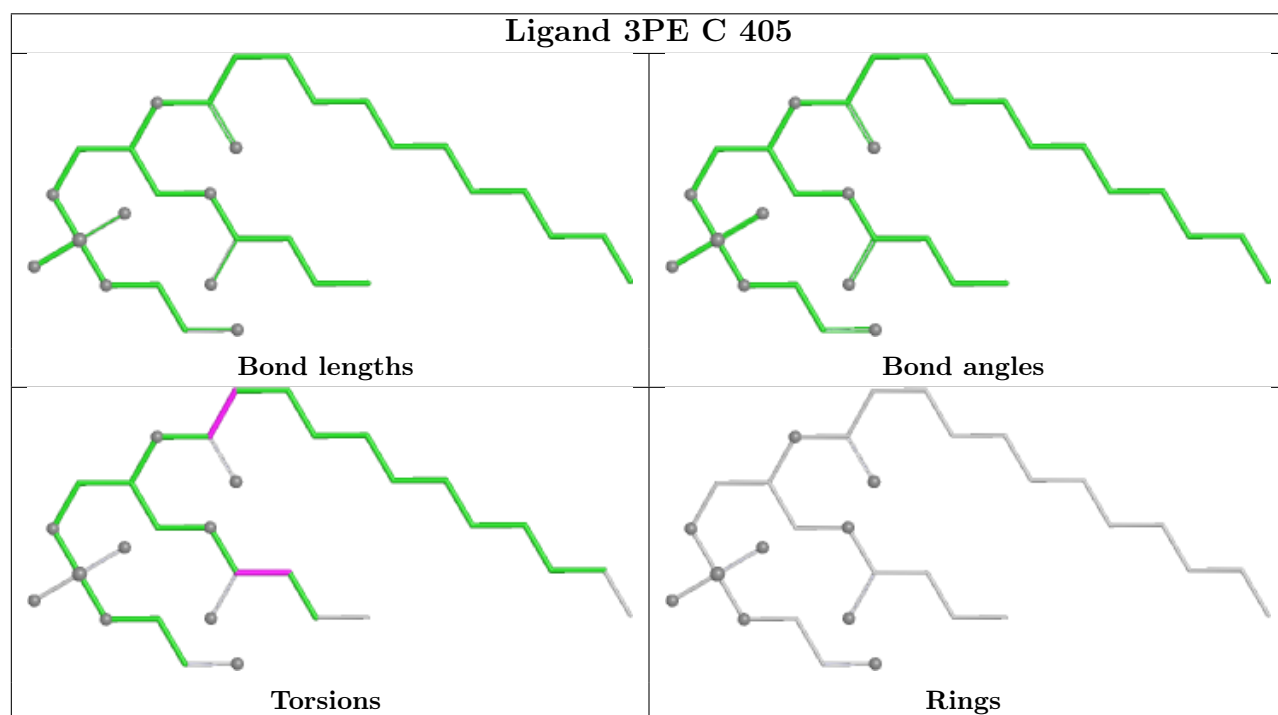
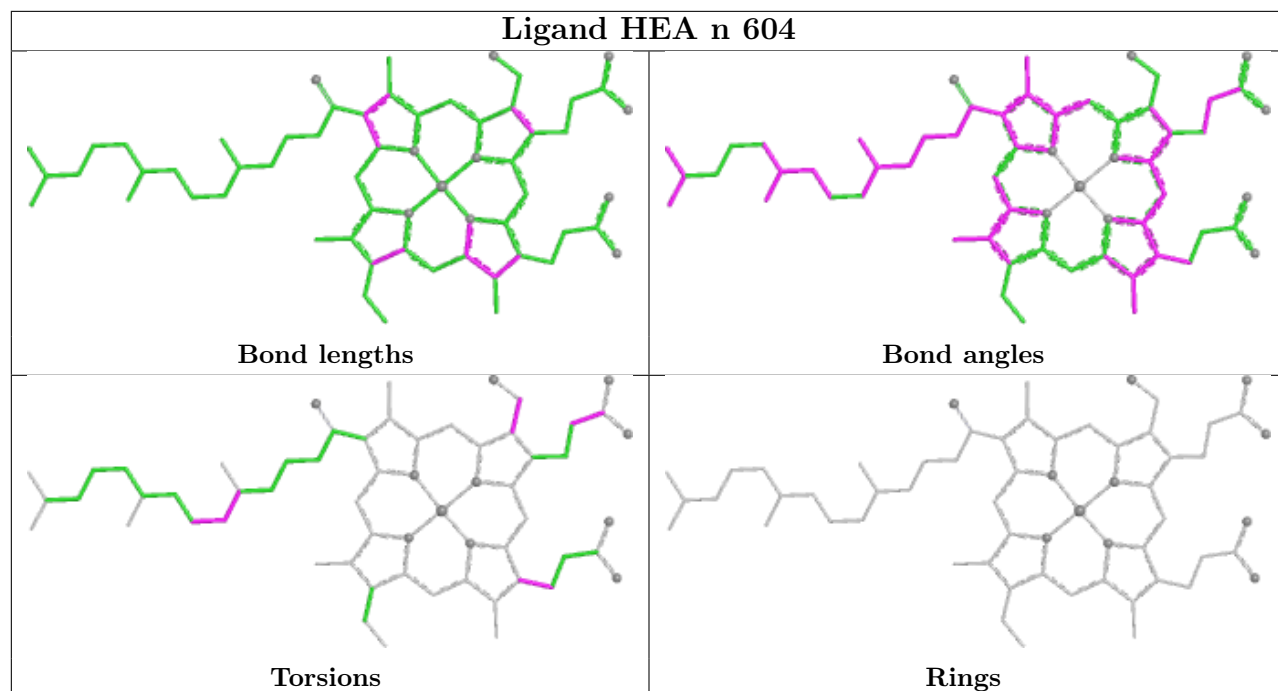


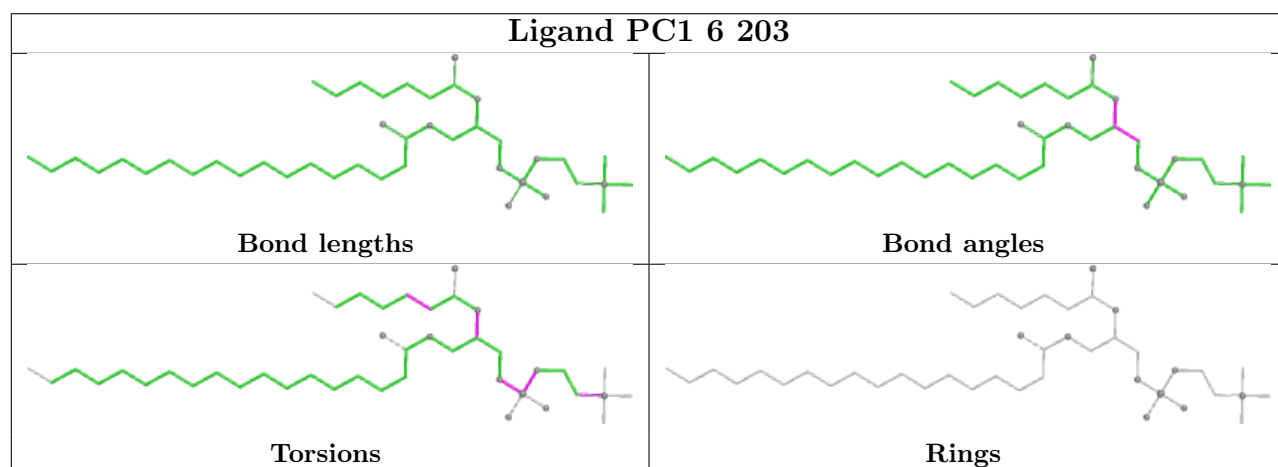
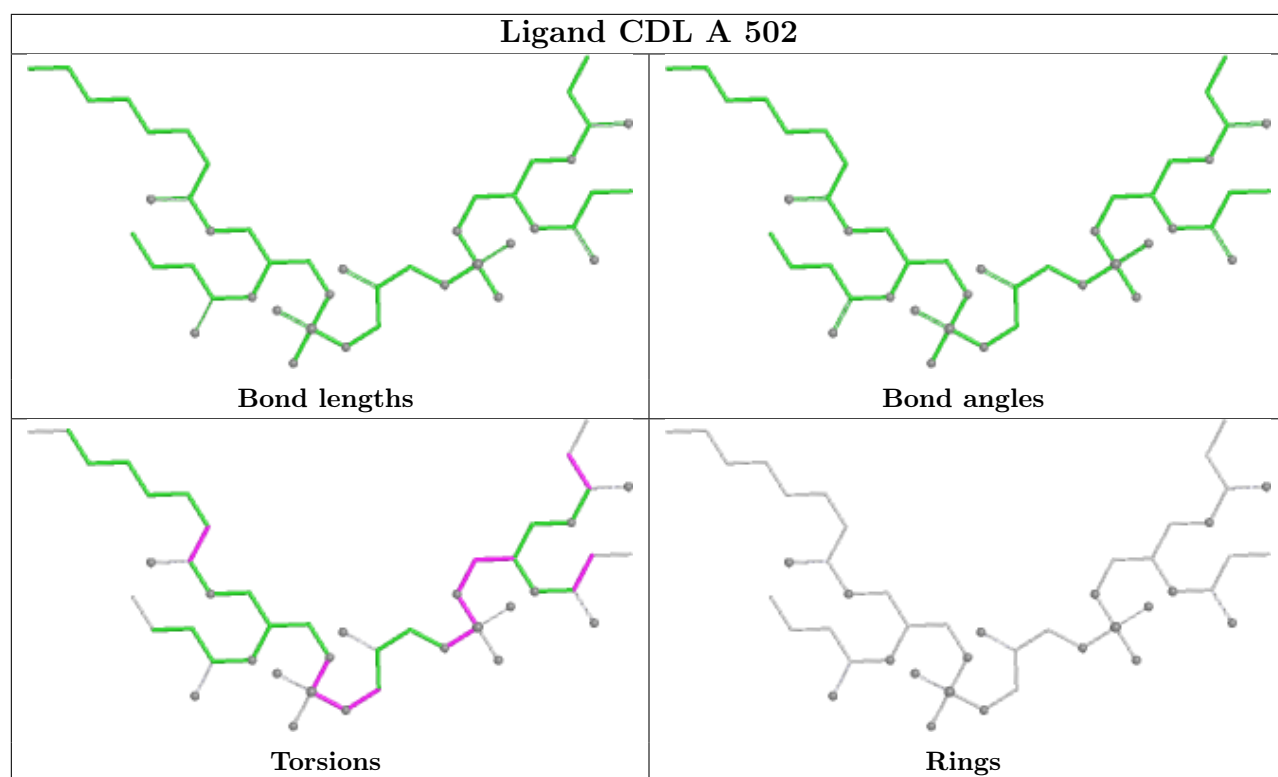


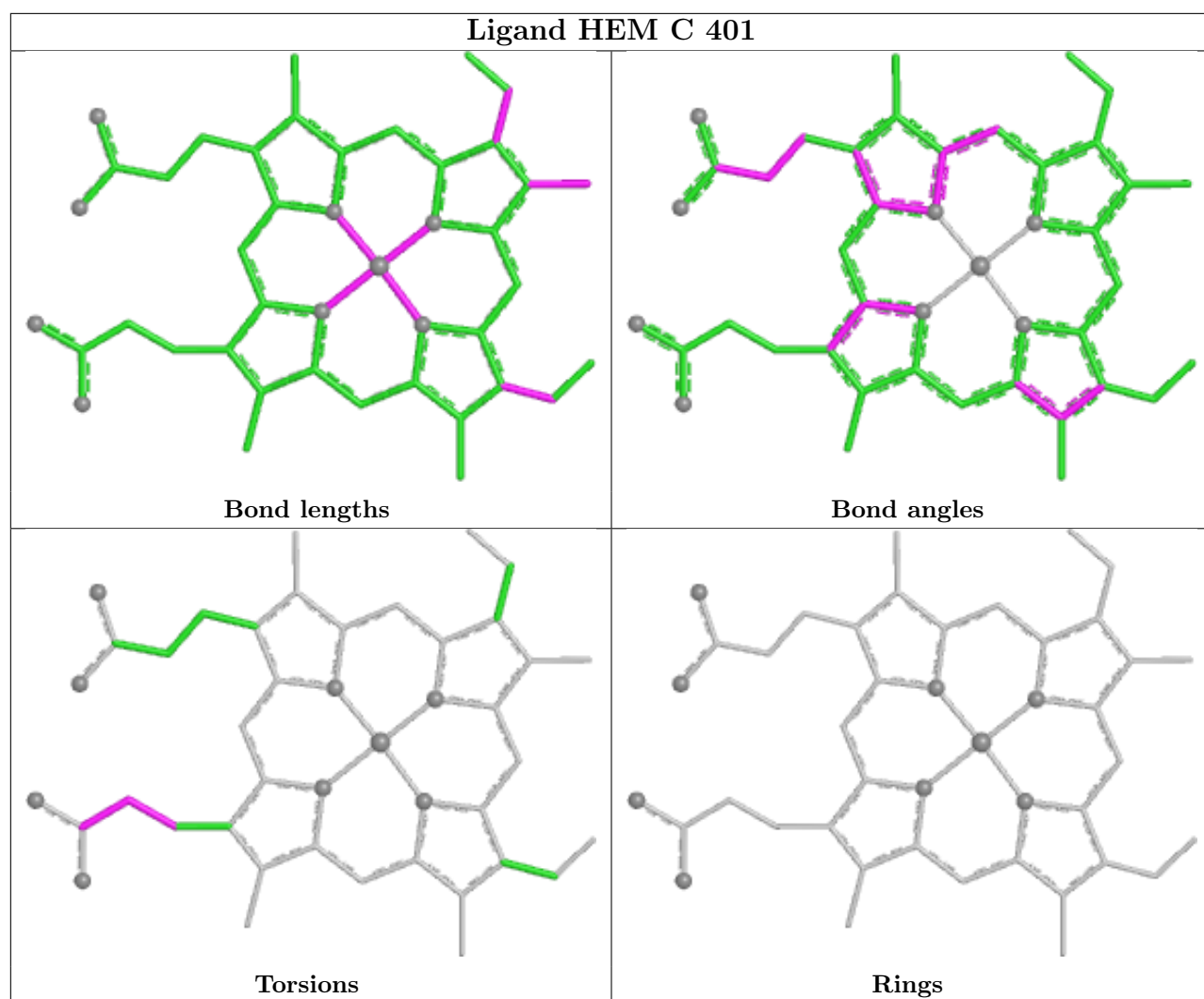












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

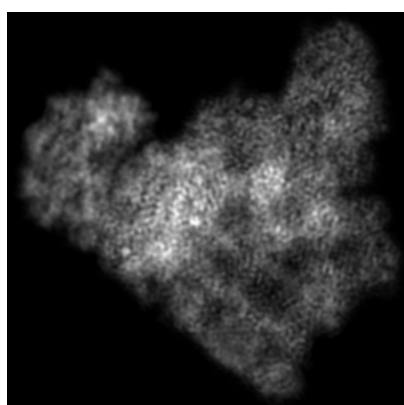
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17991. These allow visual inspection of the internal detail of the map and identification of artifacts.

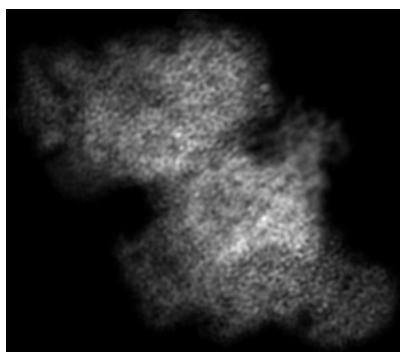
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

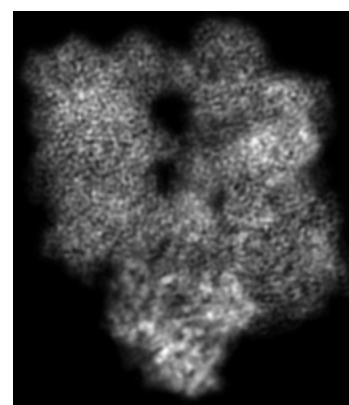
6.1.1 Primary map



X



Y

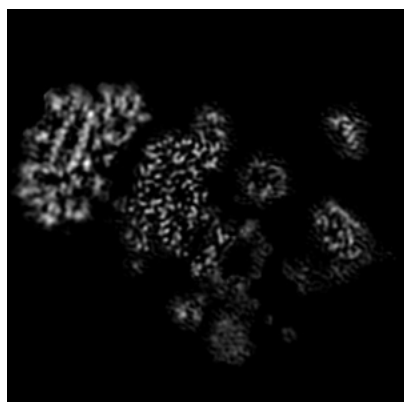


Z

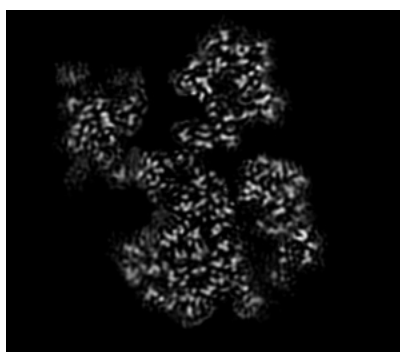
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

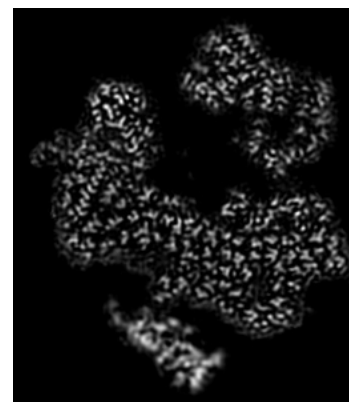
6.2.1 Primary map



X Index: 107



Y Index: 124



Z Index: 124

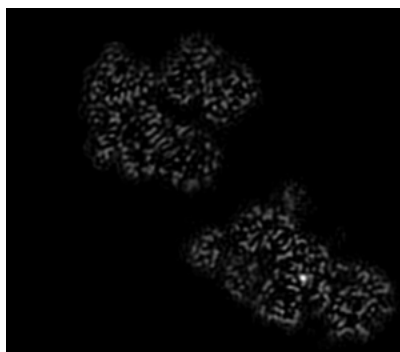
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

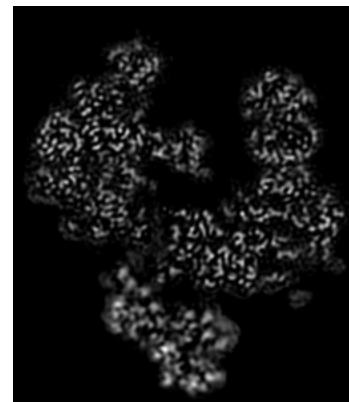
6.3.1 Primary map



X Index: 141



Y Index: 198

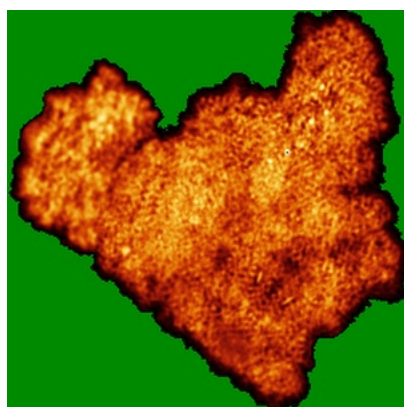


Z Index: 142

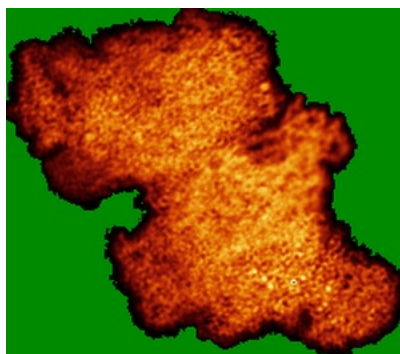
The images above show the largest variance slices of the map in three orthogonal directions.

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

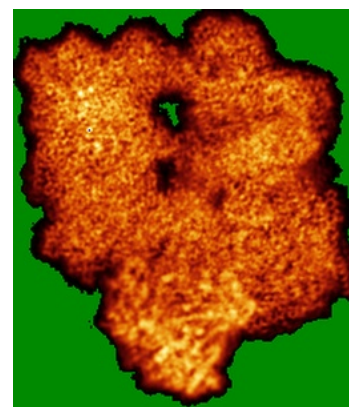
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

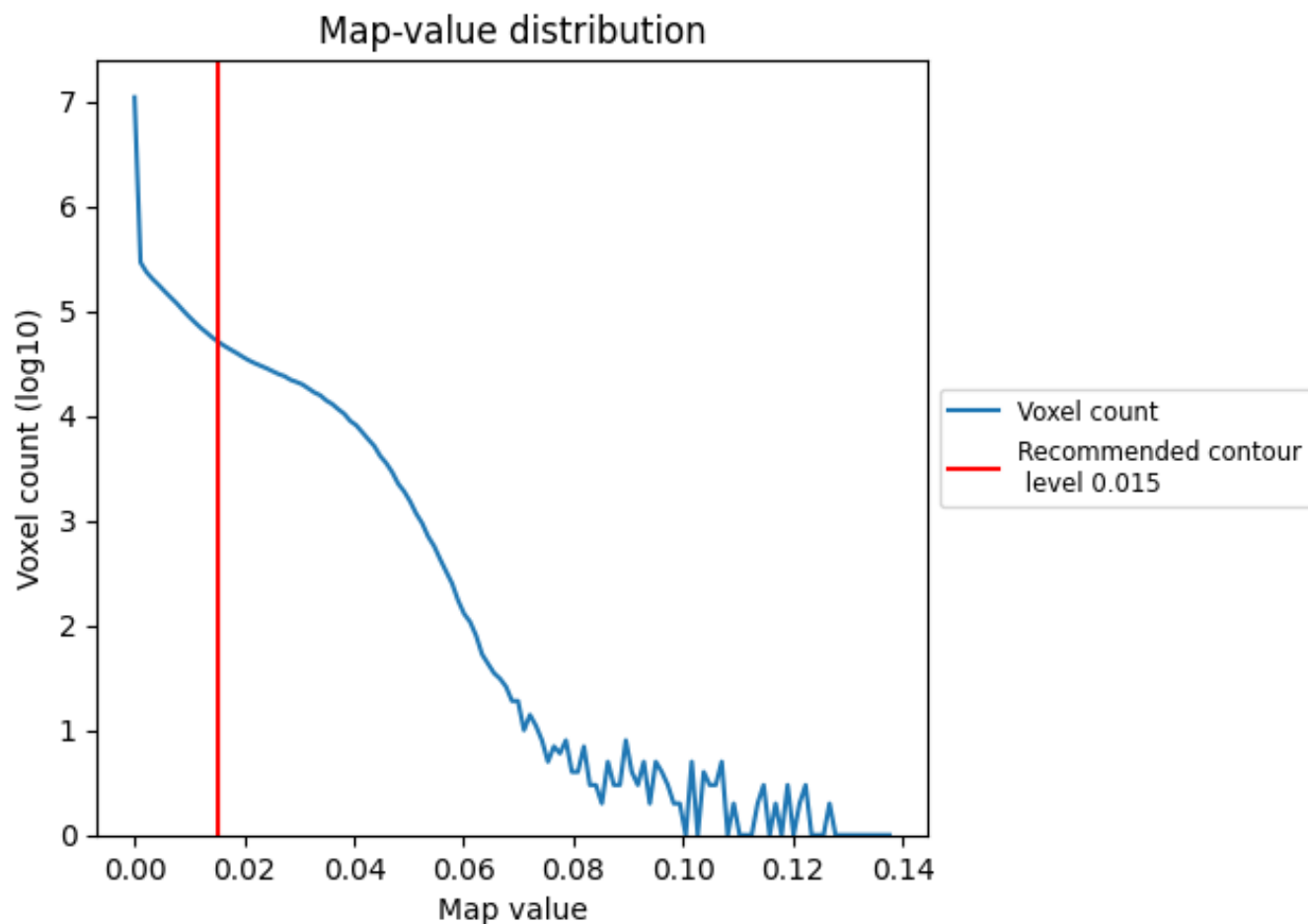
6.6 Mask visualisation

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

7 Map analysis [i](#)

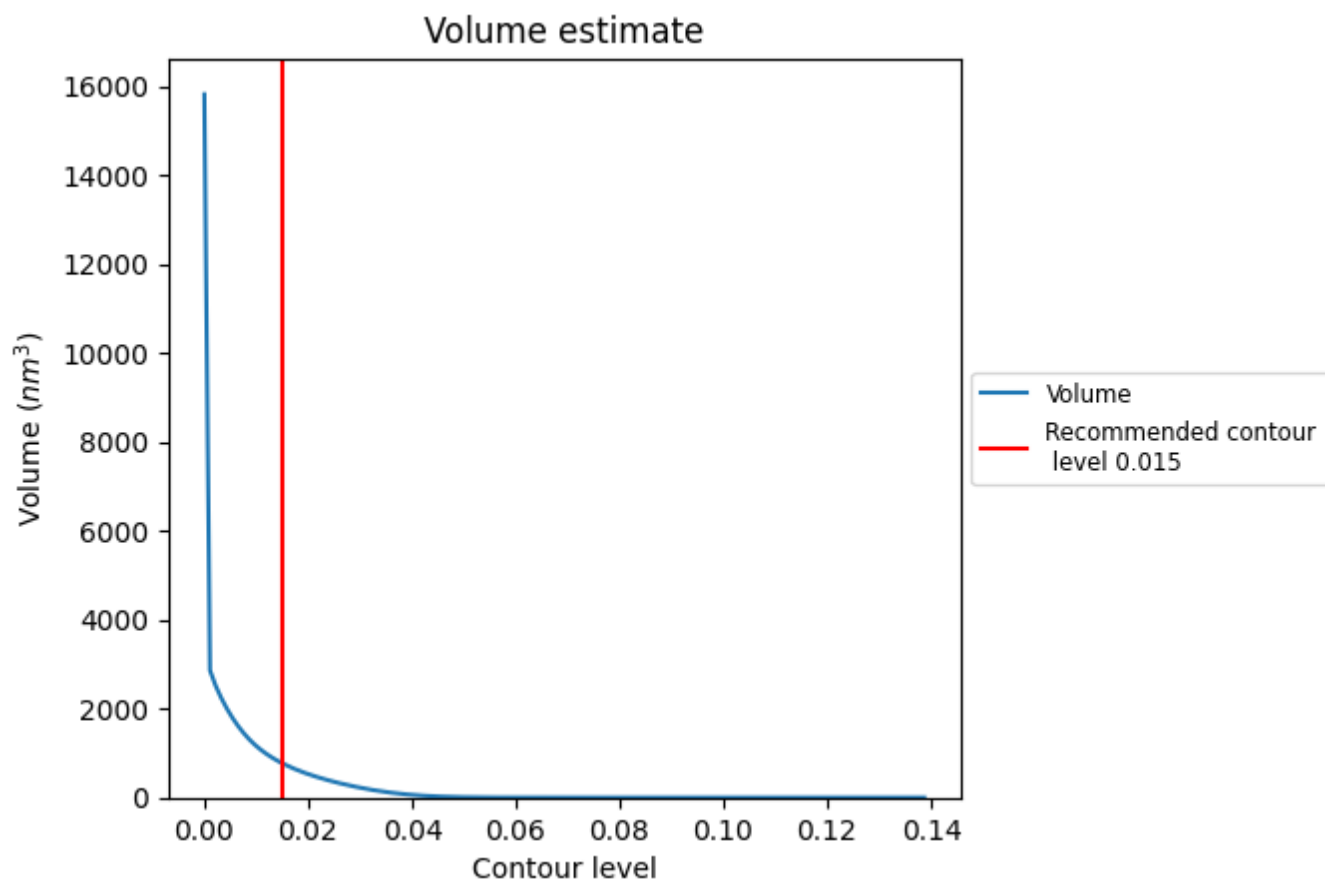
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 772 nm³; this corresponds to an approximate mass of 698 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.

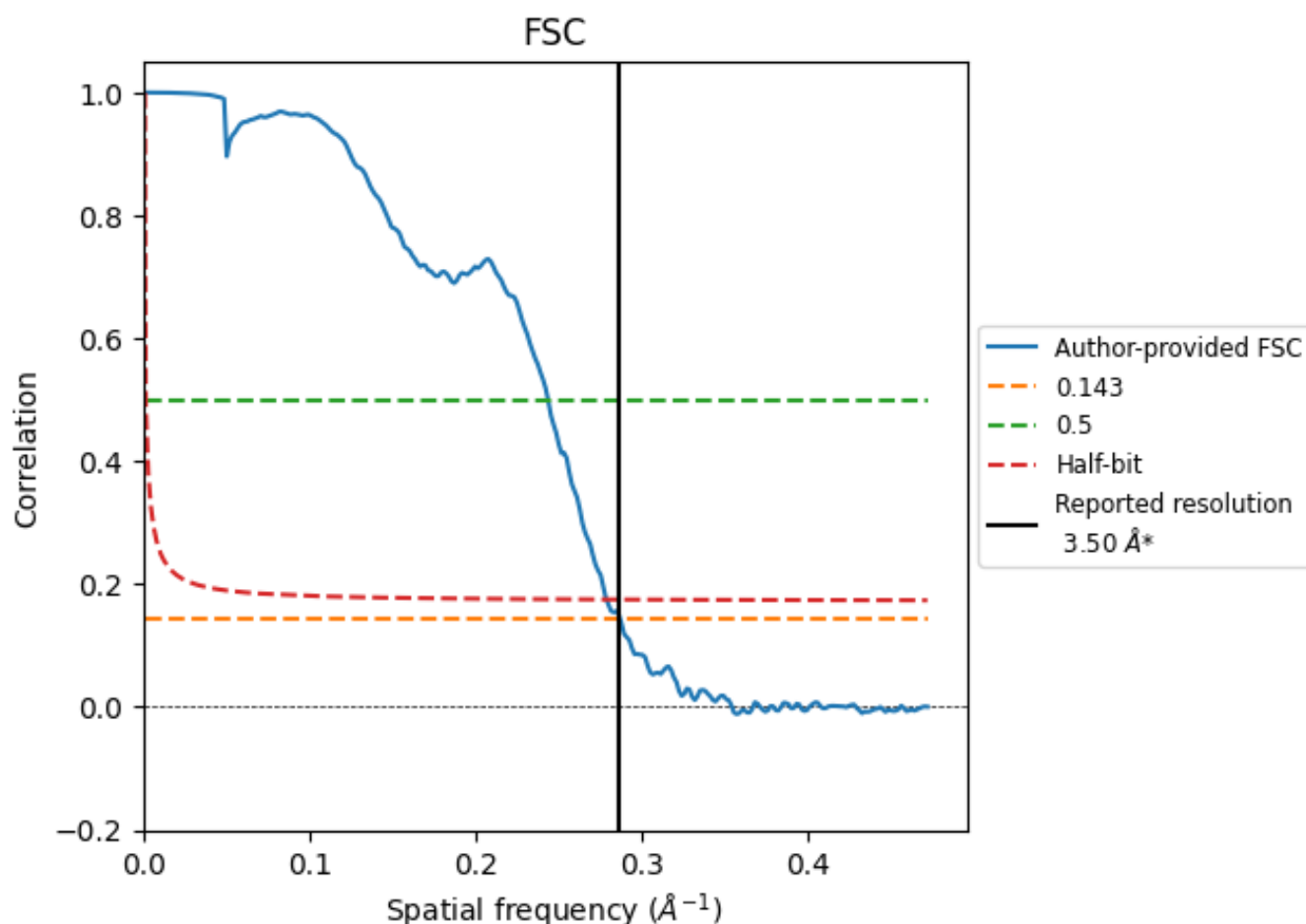
7.3 Rotationally averaged power spectrum [i](#)

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

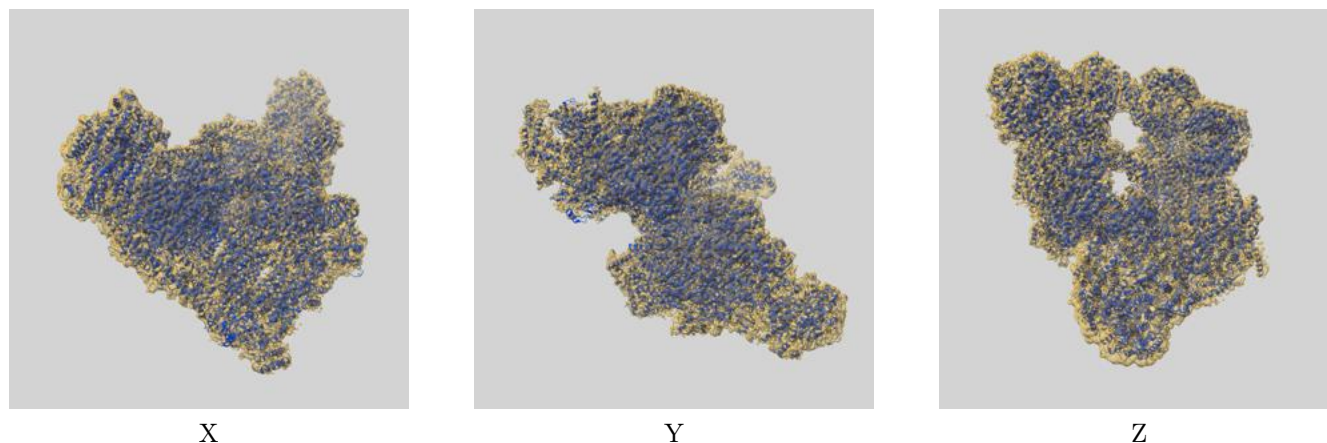
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.11	3.59
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

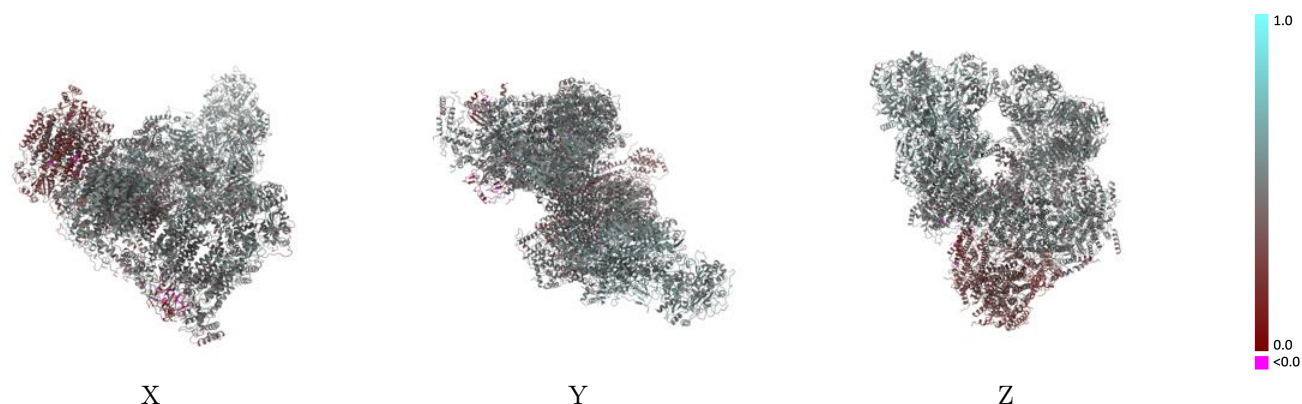
This section contains information regarding the fit between EMDB map EMD-17991 and PDB model 8PW7. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



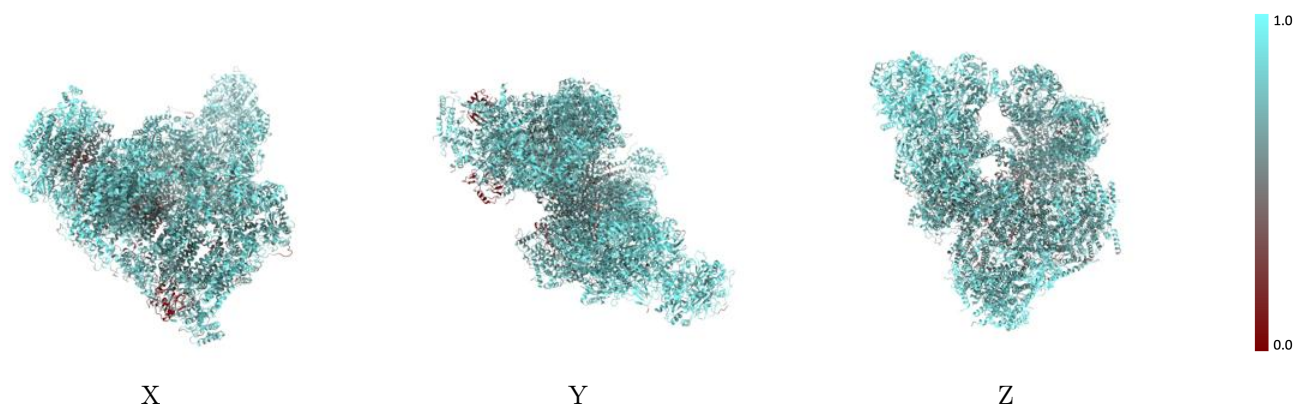
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



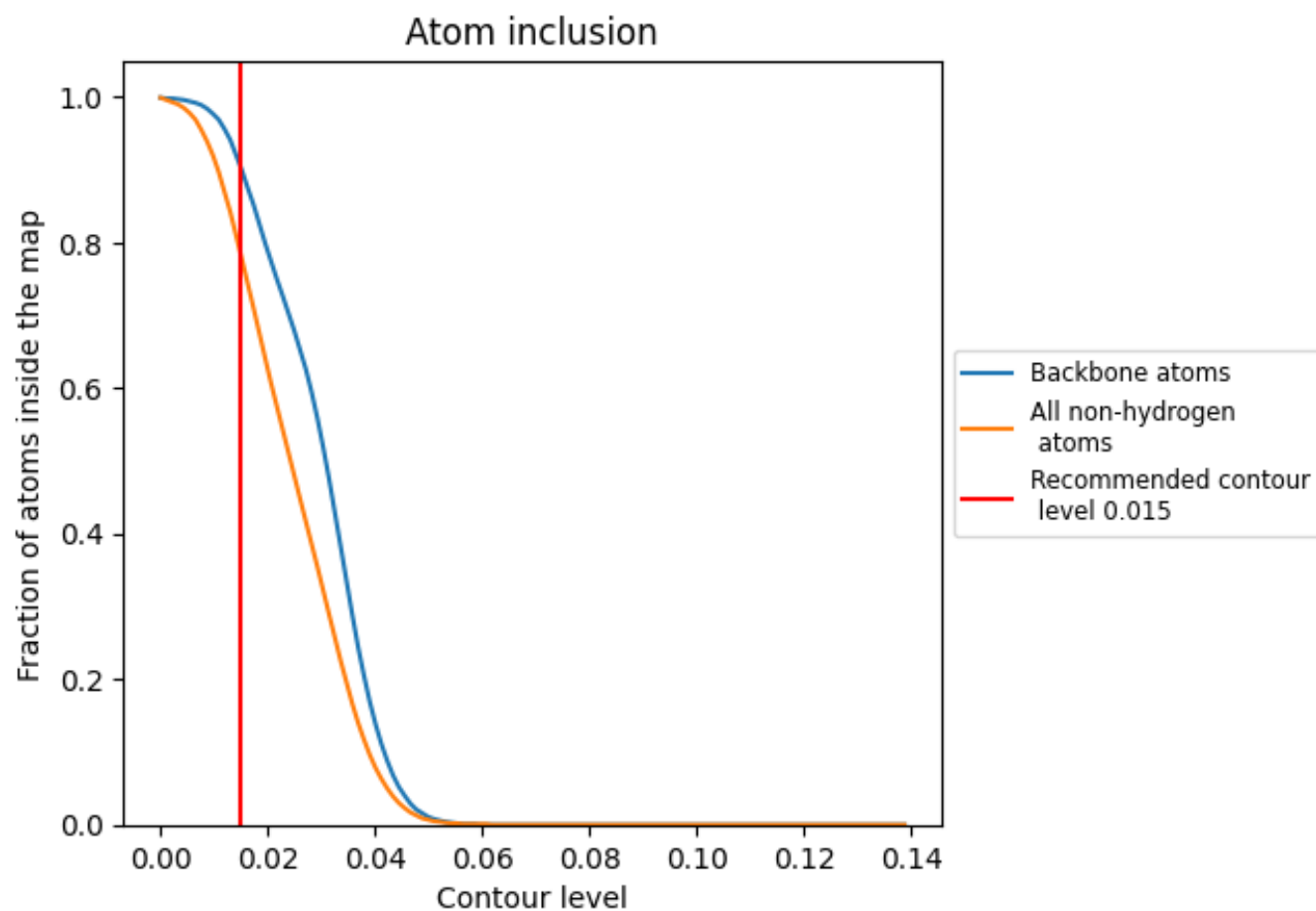
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.7830	 0.4710
1	 0.8740	 0.5240
2	 0.8610	 0.5270
3	 0.8540	 0.5320
6	 0.8450	 0.5240
7	 0.8580	 0.5350
9	 0.8540	 0.5370
A	 0.7730	 0.4960
A1	 0.7010	 0.4750
B	 0.7960	 0.5030
C	 0.7900	 0.5000
C1	 0.8710	 0.5530
D	 0.8200	 0.4890
D1	 0.8040	 0.5120
E	 0.4810	 0.3500
F	 0.8050	 0.4930
G	 0.7560	 0.4890
H	 0.7620	 0.4360
H1	 0.7470	 0.4730
J	 0.7620	 0.4930
J1	 0.6160	 0.4290
K	 0.6280	 0.4510
K1	 0.7050	 0.4750
L	 0.7970	 0.4980
L1	 0.7750	 0.4950
M	 0.7860	 0.4950
M1	 0.7770	 0.5060
N	 0.7770	 0.4960
N1	 0.7370	 0.4940
O	 0.8040	 0.4940
O1	 0.8120	 0.4950
P	 0.4740	 0.3380
P1	 0.7910	 0.5100
Q	 0.7570	 0.5060
Q1	 0.8250	 0.5480



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Chain	Atom inclusion	Q-score
R	 0.6420	 0.4600
S	 0.7110	 0.4250
S1	 0.8250	 0.4910
T	 0.4570	 0.4300
T1	 0.7090	 0.4280
U	 0.7930	 0.5030
U1	 0.7660	 0.4830
V	 0.6770	 0.4710
V1	 0.8330	 0.5180
W1	 0.8280	 0.5200
X1	 0.7920	 0.4770
Y1	 0.6420	 0.4410
Z1	 0.8010	 0.4820
a1	 0.7820	 0.4810
b1	 0.7800	 0.4740
c1	 0.7260	 0.4580
d1	 0.7070	 0.4870
e1	 0.7230	 0.4870
f1	 0.6770	 0.4560
g1	 0.7600	 0.4840
h1	 0.7990	 0.4980
i1	 0.7030	 0.4470
j1	 0.7900	 0.4530
k1	 0.7850	 0.4850
l1	 0.8010	 0.5060
m1	 0.7560	 0.4760
n	 0.7730	 0.3330
n1	 0.8200	 0.4970
o	 0.8290	 0.3160
o1	 0.7730	 0.4550
p	 0.7160	 0.2880
p1	 0.8230	 0.4980
q	 0.9180	 0.3150
q1	 0.8730	 0.5400
r	 0.8890	 0.2870
r1	 0.7980	 0.5290
s	 0.7890	 0.3170
s1	 0.7860	 0.4960
t	 0.7970	 0.2640
u	 0.9120	 0.2960
v	 0.8570	 0.2900
w	 0.8260	 0.3100

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Chain	Atom inclusion	Q-score
x	 0.9440	 0.3210
y	 0.8150	 0.3300
z	 0.7890	 0.2780