



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 7W5Z / pdb_00007w5z
EMDB ID : EMD-32325
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial complex IV, composite dimer model
Authors : Zhou, L.; Maldonado, M.; Padavannil, A.; Letts, J.
Deposited on : 2021-11-30
Resolution : 3.02 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

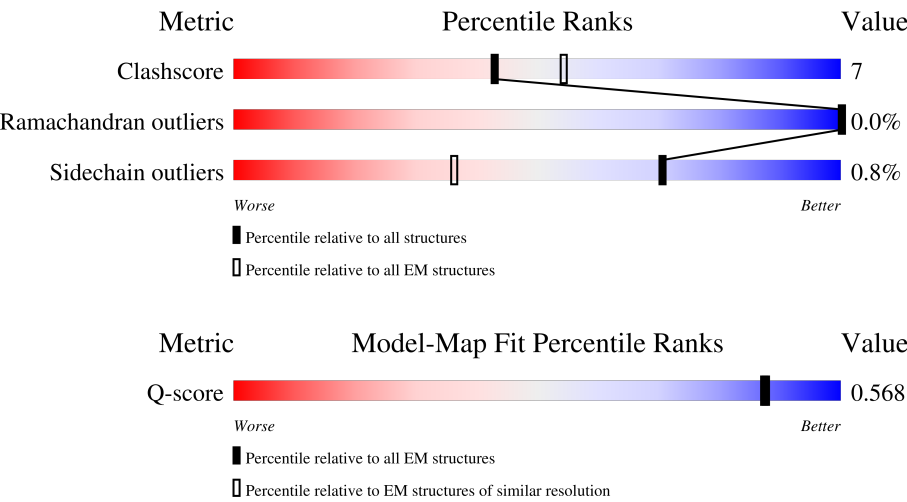
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.02 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	13913 (2.52 - 3.52)

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	U1	98	99% .
1	u1	98	99% .
2	U2	3634	97% .
2	u2	3634	97% .

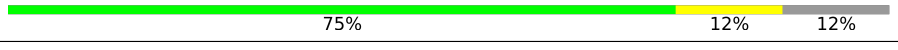
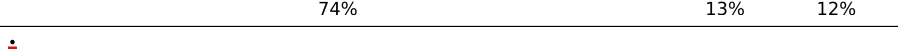
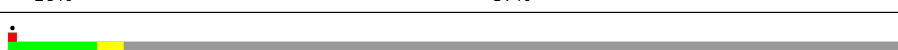
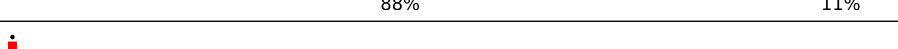
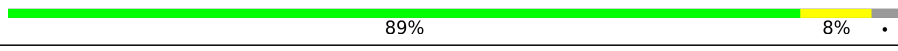
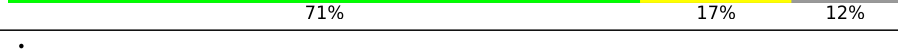
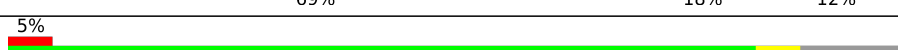
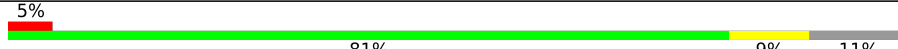
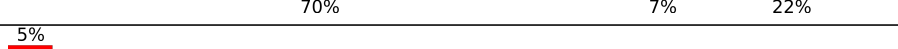
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Mol	Chain	Length	Quality of chain
3	U3	34	85% 100%
3	u3	34	91% 100%
4	U4	30	93% 100%
4	u4	30	100%
5	U5	172	11% 17% 81%
5	u5	172	11% 17% 81%
6	U6	478	8% 91%
6	u6	478	8% 91%
7	C1	688	72% 25%
7	c1	688	75% 23%
8	C2	604	79% 16% 5%
8	c2	604	79% 16% 5%
9	C3	594	10% 76% 18% 5%
9	c3	594	10% 76% 18% 5%
10	5B	637	71% 15% 13%
10	5b	637	72% 14% 13%
11	6A	130	80% 16%
11	6a	130	82% 15%
12	6B	230	81% 14%
12	6b	230	82% 13%
13	6L	88	76% 11% 13%
13	6l	88	76% 11% 13%
14	6C	103	75% 17% 8%
14	6c	103	78% 15% 8%
15	7A	133	70% 30%

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Mol	Chain	Length	Quality of chain
15	7a	133	
16	7C	236	
16	7c	236	
17	7L	990	
17	7l	990	
18	M1	346	
18	m1	346	
19	M2	318	
19	m2	318	
20	M3	330	
20	m3	330	
21	T1	72	
21	t1	72	
22	T2	72	
22	t2	72	
23	T3	93	
23	t3	93	
24	T4	68	
24	t4	68	
25	T5	81	
25	t5	81	
26	T6	72	
26	t6	72	
27	BP	380	
27	bp	380	

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Mol	Chain	Length	Quality of chain
28	FS	188	
28	fs	188	
29	AC	127	
29	ac	127	
30	Y7	453	
30	y7	453	
31	Y0	89	
31	y0	89	
32	Y5	190	
32	y5	190	
33	A	490	
33	a	490	
34	B	473	
34	b	473	
35	C	1471	
35	c	1471	
36	D	402	
36	d	402	
37	E	385	
37	e	385	
38	F	348	
38	f	348	
39	G	318	
39	g	318	
40	H	318	

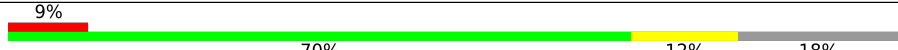
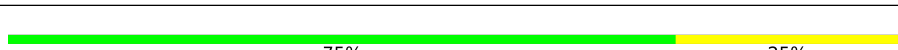
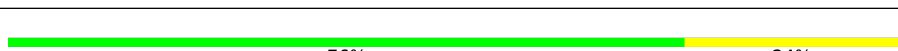
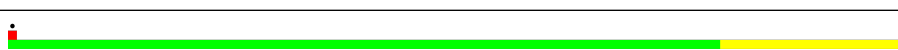
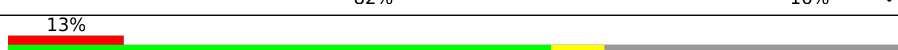
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Mol	Chain	Length	Quality of chain
40	h	318	
41	I	252	
41	i	252	
42	J	234	
42	j	234	
43	K	231	
43	k	231	
44	L	222	
44	l	222	
45	M	220	
45	m	220	
46	N	210	
46	n	210	
47	O	193	
47	o	193	
48	P	175	
48	p	175	
49	Q	173	
49	q	173	
50	R	173	
50	r	173	
51	S	170	
51	s	170	
52	T	158	
52	t	158	

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Mol	Chain	Length	Quality of chain
53	U	154	
53	u	154	
54	V	149	
54	v	149	
55	W	124	
55	w	124	
56	X	122	
56	x	122	
57	Y	105	
57	y	105	
58	Z	90	
58	z	90	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 190448 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 Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	U1	98	Total	C	N	O	0	0
			490	294	98	98		
1	u1	98	Total	C	N	O	0	0
			490	294	98	98		

- Molecule 2 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U2	127	Total	C	N	O	S	0	0
			743	456	139	143	5		
2	u2	127	Total	C	N	O	S	0	0
			743	456	139	143	5		

- Molecule 3 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	U3	34	Total	C	N	O	0	0
			170	102	34	34		
3	u3	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 4 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	U4	30	Total	C	N	O	0	0
			150	90	30	30		
4	u4	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 5 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U5	33	Total	C	N	O	0	0
			242	160	40	42		
5	u5	33	Total	C	N	O	0	0
			242	160	40	42		

- Molecule 6 is a protein called Protein transporter Sec61 alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U6	42	Total	C	N	O	S	0	0
			275	178	45	50	2		
6	u6	42	Total	C	N	O	S	0	0
			275	178	45	50	2		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C1	672	Total	C	N	O	S	0	0
			5563	3722	908	897	36		
7	c1	672	Total	C	N	O	S	0	0
			5563	3722	908	897	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C2	576	Total	C	N	O	S	0	0
			4883	3186	841	846	10		
8	c2	576	Total	C	N	O	S	0	0
			4883	3186	841	846	10		

- Molecule 9 is a protein called Ymf68.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C3	563	Total	C	N	O	S	0	0
			4930	3354	763	805	8		
9	c3	563	Total	C	N	O	S	0	0
			4930	3354	763	805	8		

- Molecule 10 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	5B	554	Total	C	N	O	P	S	0	0
			4624	2915	778	912	2	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	5b	554	Total	C	N	O	P	S	
			4624	2915	778	912	2	17	0
									0

- Molecule 11 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	6A	125	Total	C	N	O	S		
			1074	693	183	196	2	0	0
11	6a	125	Total	C	N	O	S		
			1074	693	183	196	2	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6B	221	Total	C	N	O	S		
			1904	1234	311	346	13	0	0
12	6b	221	Total	C	N	O	S		
			1904	1234	311	346	13	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 6B-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6L	77	Total	C	N	O	S		
			638	408	108	116	6	0	0
13	6l	77	Total	C	N	O	S		
			638	408	108	116	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	6C	95	Total	C	N	O	S		
			841	545	151	143	2	0	0
14	6c	95	Total	C	N	O	S		
			841	545	151	143	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7A	133	Total	C	N	O	S		
			1168	770	197	200	1	0	0
15	7a	133	Total	C	N	O	S		
			1168	770	197	200	1	0	0

- Molecule 16 is a protein called Cytochrome c oxidase subunit 7C.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	7C	207	Total	C	N	O	P	S	0	0
			1789	1139	287	353	2	8		
16	7c	207	Total	C	N	O	P	S	0	0
			1789	1139	287	353	2	8		

- Molecule 17 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7L	130	Total	C	N	O	S	0	0
			1070	693	174	195	8		
17	7l	130	Total	C	N	O	S	0	0
			1070	693	174	195	8		

- Molecule 18 is a protein called Oxoglutarate/malate translocator protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M1	346	Total	C	N	O	S	0	0
			2863	1890	469	491	13		
18	m1	346	Total	C	N	O	S	0	0
			2863	1890	469	491	13		

- Molecule 19 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M2	318	Total	C	N	O	S	0	0
			2560	1666	440	450	4		
19	m2	318	Total	C	N	O	S	0	0
			2560	1666	440	450	4		

- Molecule 20 is a protein called Carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M3	329	Total	C	N	O	S	0	0
			2620	1700	446	470	4		
20	m3	329	Total	C	N	O	S	0	0
			2620	1700	446	470	4		

- Molecule 21 is a protein called Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T1	70	Total	C	N	O	S	0	0
			540	329	98	109	4		
21	t1	70	Total	C	N	O	S	0	0
			540	329	98	109	4		

- Molecule 22 is a protein called Cytochrome c oxidase small TIM subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T2	63	Total	C	N	O	S	0	0
			513	319	90	100	4		
22	t2	63	Total	C	N	O	S	0	0
			513	319	90	100	4		

- Molecule 23 is a protein called Cytochrome c oxidase small TIM subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T3	83	Total	C	N	O	S	0	0
			655	412	109	128	6		
23	t3	83	Total	C	N	O	S	0	0
			655	412	109	128	6		

- Molecule 24 is a protein called Cytochrome c oxidase small TIM subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T4	57	Total	C	N	O	S	0	0
			483	309	80	91	3		
24	t4	57	Total	C	N	O	S	0	0
			483	309	80	91	3		

- Molecule 25 is a protein called Cytochrome c oxidase small TIM subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T5	63	Total	C	N	O	S	0	0
			515	327	90	96	2		
25	t5	63	Total	C	N	O	S	0	0
			515	327	90	96	2		

- Molecule 26 is a protein called Cytochrome c oxidase small TIM subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T6	70	Total	C	N	O	S	0	0
			563	363	90	106	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	t6	70	Total	C	N	O	S	0	0
			563	363	90	106	4		

- Molecule 27 is a protein called Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BP	380	Total	C	N	O	S	0	0
			2916	1856	492	566	2		
27	bp	380	Total	C	N	O	S	0	0
			2916	1856	492	566	2		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BP	413	GLU	-	expression tag	UNP Q22RF2
BP	414	THR	-	expression tag	UNP Q22RF2
BP	415	GLY	-	expression tag	UNP Q22RF2
BP	416	LYS	-	expression tag	UNP Q22RF2
BP	417	ILE	-	expression tag	UNP Q22RF2
BP	418	TYR	-	expression tag	UNP Q22RF2
BP	419	GLN	-	expression tag	UNP Q22RF2
BP	420	PHE	-	expression tag	UNP Q22RF2
BP	421	ASN	-	expression tag	UNP Q22RF2
BP	422	GLU	-	expression tag	UNP Q22RF2
BP	423	PHE	-	expression tag	UNP Q22RF2
BP	424	VAL	-	expression tag	UNP Q22RF2
BP	425	GLY	-	expression tag	UNP Q22RF2
BP	426	VAL	-	expression tag	UNP Q22RF2
BP	427	SER	-	expression tag	UNP Q22RF2
BP	428	THR	-	expression tag	UNP Q22RF2
BP	429	ASN	-	expression tag	UNP Q22RF2
BP	430	GLU	-	expression tag	UNP Q22RF2
BP	431	VAL	-	expression tag	UNP Q22RF2
BP	432	GLY	-	expression tag	UNP Q22RF2
BP	433	ASN	-	expression tag	UNP Q22RF2
BP	434	ASP	-	expression tag	UNP Q22RF2
BP	435	TYR	-	expression tag	UNP Q22RF2
BP	436	ASN	-	expression tag	UNP Q22RF2
BP	437	VAL	-	expression tag	UNP Q22RF2
BP	438	ALA	-	expression tag	UNP Q22RF2
BP	439	ASP	-	expression tag	UNP Q22RF2
BP	440	SER	-	expression tag	UNP Q22RF2

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Chain	Residue	Modelled	Actual	Comment	Reference
BP	441	LYS	-	expression tag	UNP Q22RF2
BP	442	ALA	-	expression tag	UNP Q22RF2
BP	443	PHE	-	expression tag	UNP Q22RF2
BP	444	GLU	-	expression tag	UNP Q22RF2
BP	445	GLY	-	expression tag	UNP Q22RF2
BP	446	LYS	-	expression tag	UNP Q22RF2
BP	447	VAL	-	expression tag	UNP Q22RF2
BP	448	VAL	-	expression tag	UNP Q22RF2
BP	449	ASP	-	expression tag	UNP Q22RF2
BP	450	LEU	-	expression tag	UNP Q22RF2
BP	451	GLY	-	expression tag	UNP Q22RF2
BP	452	GLY	-	expression tag	UNP Q22RF2
BP	453	SER	-	expression tag	UNP Q22RF2
BP	454	TYR	-	expression tag	UNP Q22RF2
BP	455	GLY	-	expression tag	UNP Q22RF2
BP	456	ILE	-	expression tag	UNP Q22RF2
BP	457	ARG	-	expression tag	UNP Q22RF2
BP	458	PHE	-	expression tag	UNP Q22RF2
BP	459	ALA	-	expression tag	UNP Q22RF2
BP	460	ILE	-	expression tag	UNP Q22RF2
BP	461	VAL	-	expression tag	UNP Q22RF2
BP	462	ASN	-	expression tag	UNP Q22RF2
bp	413	GLU	-	expression tag	UNP Q22RF2
bp	414	THR	-	expression tag	UNP Q22RF2
bp	415	GLY	-	expression tag	UNP Q22RF2
bp	416	LYS	-	expression tag	UNP Q22RF2
bp	417	ILE	-	expression tag	UNP Q22RF2
bp	418	TYR	-	expression tag	UNP Q22RF2
bp	419	GLN	-	expression tag	UNP Q22RF2
bp	420	PHE	-	expression tag	UNP Q22RF2
bp	421	ASN	-	expression tag	UNP Q22RF2
bp	422	GLU	-	expression tag	UNP Q22RF2
bp	423	PHE	-	expression tag	UNP Q22RF2
bp	424	VAL	-	expression tag	UNP Q22RF2
bp	425	GLY	-	expression tag	UNP Q22RF2
bp	426	VAL	-	expression tag	UNP Q22RF2
bp	427	SER	-	expression tag	UNP Q22RF2
bp	428	THR	-	expression tag	UNP Q22RF2
bp	429	ASN	-	expression tag	UNP Q22RF2
bp	430	GLU	-	expression tag	UNP Q22RF2
bp	431	VAL	-	expression tag	UNP Q22RF2
bp	432	GLY	-	expression tag	UNP Q22RF2

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Chain	Residue	Modelled	Actual	Comment	Reference
bp	433	ASN	-	expression tag	UNP Q22RF2
bp	434	ASP	-	expression tag	UNP Q22RF2
bp	435	TYR	-	expression tag	UNP Q22RF2
bp	436	ASN	-	expression tag	UNP Q22RF2
bp	437	VAL	-	expression tag	UNP Q22RF2
bp	438	ALA	-	expression tag	UNP Q22RF2
bp	439	ASP	-	expression tag	UNP Q22RF2
bp	440	SER	-	expression tag	UNP Q22RF2
bp	441	LYS	-	expression tag	UNP Q22RF2
bp	442	ALA	-	expression tag	UNP Q22RF2
bp	443	PHE	-	expression tag	UNP Q22RF2
bp	444	GLU	-	expression tag	UNP Q22RF2
bp	445	GLY	-	expression tag	UNP Q22RF2
bp	446	LYS	-	expression tag	UNP Q22RF2
bp	447	VAL	-	expression tag	UNP Q22RF2
bp	448	VAL	-	expression tag	UNP Q22RF2
bp	449	ASP	-	expression tag	UNP Q22RF2
bp	450	LEU	-	expression tag	UNP Q22RF2
bp	451	GLY	-	expression tag	UNP Q22RF2
bp	452	GLY	-	expression tag	UNP Q22RF2
bp	453	SER	-	expression tag	UNP Q22RF2
bp	454	TYR	-	expression tag	UNP Q22RF2
bp	455	GLY	-	expression tag	UNP Q22RF2
bp	456	ILE	-	expression tag	UNP Q22RF2
bp	457	ARG	-	expression tag	UNP Q22RF2
bp	458	PHE	-	expression tag	UNP Q22RF2
bp	459	ALA	-	expression tag	UNP Q22RF2
bp	460	ILE	-	expression tag	UNP Q22RF2
bp	461	VAL	-	expression tag	UNP Q22RF2
bp	462	ASN	-	expression tag	UNP Q22RF2

- Molecule 28 is a protein called Iron-binding zinc finger CDGSH type protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	FS	188	Total	C	N	O	S	0	0
			1509	978	260	257	14		
28	fs	188	Total	C	N	O	S	0	0
			1509	978	260	257	14		

- Molecule 29 is a protein called Cytochrome c oxidase acyl carrier-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AC	100	Total	C	N	O	S	0	0
			816	519	144	151	2		
29	ac	100	Total	C	N	O	S	0	0
			816	519	144	151	2		

- Molecule 30 is a protein called Ymf67.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y7	338	Total	C	N	O	S	0	0
			2895	1936	459	494	6		
30	y7	338	Total	C	N	O	S	0	0
			2895	1936	459	494	6		

- Molecule 31 is a protein called Ymf70.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y0	89	Total	C	N	O	S	0	0
			777	536	115	124	2		
31	y0	89	Total	C	N	O	S	0	0
			777	536	115	124	2		

- Molecule 32 is a protein called Ymf75.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y5	104	Total	C	N	O		0	0
			924	638	140	146			
32	y5	104	Total	C	N	O		0	0
			924	638	140	146			

- Molecule 33 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A	448	Total	C	N	O	S	0	0
			3746	2402	635	700	9		
33	a	448	Total	C	N	O	S	0	0
			3746	2402	635	700	9		

- Molecule 34 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B	214	Total	C	N	O	S	0	0
			1682	1087	287	307	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	214	Total	C	N	O	S	0	0
			1682	1087	287	307	1		

- Molecule 35 is a protein called Cyclic nucleotide-binding domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	46	Total	C	N	O	S	0	0
			383	261	60	60	2		
35	c	46	Total	C	N	O	S	0	0
			383	261	60	60	2		

- Molecule 36 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D	284	Total	C	N	O	S	0	0
			2331	1504	395	427	5		
36	d	284	Total	C	N	O	S	0	0
			2331	1504	395	427	5		

- Molecule 37 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	E	384	Total	C	N	O	S	0	0
			3178	2046	549	576	7		
37	e	384	Total	C	N	O	S	0	0
			3178	2046	549	576	7		

- Molecule 38 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	F	242	Total	C	N	O	S	0	0
			2014	1298	332	379	5		
38	f	242	Total	C	N	O	S	0	0
			2014	1298	332	379	5		

- Molecule 39 is a protein called Cytochrome c oxidase subunit TT7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	281	Total	C	N	O	S	0	0
			2364	1510	395	447	12		
39	g	281	Total	C	N	O	S	0	0
			2364	1510	395	447	12		

- Molecule 40 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	H	239	Total	C	N	O	S	0	0
			1915	1204	330	372	9		
40	h	239	Total	C	N	O	S	0	0
			1915	1204	330	372	9		

- Molecule 41 is a protein called Cytochrome c oxidase subunit TT9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	I	101	Total	C	N	O		0	0
			852	538	150	164			
41	i	101	Total	C	N	O		0	0
			852	538	150	164			

- Molecule 42 is a protein called Cytochrome c oxidase subunit TT10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	187	Total	C	N	O	S	0	0
			1575	1024	276	274	1		
42	j	187	Total	C	N	O	S	0	0
			1575	1024	276	274	1		

- Molecule 43 is a protein called Cytochrome c oxidase subunit TT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	208	Total	C	N	O	S	0	0
			1714	1090	302	319	3		
43	k	208	Total	C	N	O	S	0	0
			1714	1090	302	319	3		

- Molecule 44 is a protein called Cytochrome c oxidase subunit TT12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	194	Total	C	N	O	S	0	0
			1668	1089	284	293	2		
44	l	194	Total	C	N	O	S	0	0
			1668	1089	284	293	2		

- Molecule 45 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	183	Total	C	N	O	S	0	0
			1581	1030	264	276	11		
45	m	183	Total	C	N	O	S	0	0
			1581	1030	264	276	11		

- Molecule 46 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N	206	Total	C	N	O	S	0	0
			1716	1117	286	306	7		
46	n	206	Total	C	N	O	S	0	0
			1716	1117	286	306	7		

- Molecule 47 is a protein called Cytochrome c oxidase subunit TT15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	128	Total	C	N	O	S	0	0
			1073	671	189	207	6		
47	o	128	Total	C	N	O	S	0	0
			1073	671	189	207	6		

- Molecule 48 is a protein called Cytochrome c oxidase subunit TT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	175	Total	C	N	O	S	0	0
			1412	890	247	274	1		
48	p	175	Total	C	N	O	S	0	0
			1412	890	247	274	1		

- Molecule 49 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	173	Total	C	N	O	S	0	0
			1434	927	243	255	9		
49	q	173	Total	C	N	O	S	0	0
			1434	927	243	255	9		

- Molecule 50 is a protein called Cytochrome c oxidase subunit TT18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	159	Total	C	N	O	S	0	0
			1305	854	217	231	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	159	Total	C	N	O	S	0	0
			1305	854	217	231	3		

- Molecule 51 is a protein called Cytochrome c oxidase subunit TT19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	143	Total	C	N	O	S	0	0
			1165	732	204	224	5		
51	s	143	Total	C	N	O	S	0	0
			1165	732	204	224	5		

- Molecule 52 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	157	Total	C	N	O	S	0	0
			1323	864	231	224	4		
52	t	157	Total	C	N	O	S	0	0
			1323	864	231	224	4		

- Molecule 53 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	153	Total	C	N	O	S	0	0
			1304	848	221	230	5		
53	u	153	Total	C	N	O	S	0	0
			1304	848	221	230	5		

- Molecule 54 is a protein called Cytochrome c oxidase subunit TT22.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	146	Total	C	N	O	S	0	0
			1234	802	217	213	2		
54	v	146	Total	C	N	O	S	0	0
			1234	802	217	213	2		

- Molecule 55 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	102	Total	C	N	O	S	0	0
			902	588	146	164	4		
55	w	102	Total	C	N	O	S	0	0
			902	588	146	164	4		

- Molecule 56 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	122	Total	C	N	O	S	0	0
			1012	665	171	172	4		
56	x	122	Total	C	N	O	S	0	0
			1012	665	171	172	4		

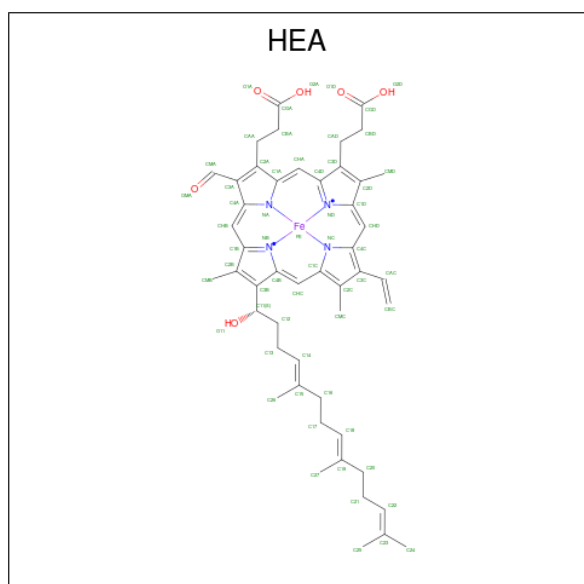
- Molecule 57 is a protein called Cytochrome c oxidase subunit TT25.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Y	105	Total	C	N	O	S	0	0
			859	540	157	153	9		
57	y	105	Total	C	N	O	S	0	0
			859	540	157	153	9		

- Molecule 58 is a protein called Cytochrome c oxidase subunit TT26.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Z	60	Total	C	N	O	0	0
			479	310	85	84		
58	z	60	Total	C	N	O	0	0
			479	310	85	84		

- Molecule 59 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
59	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
59	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
59	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
59	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

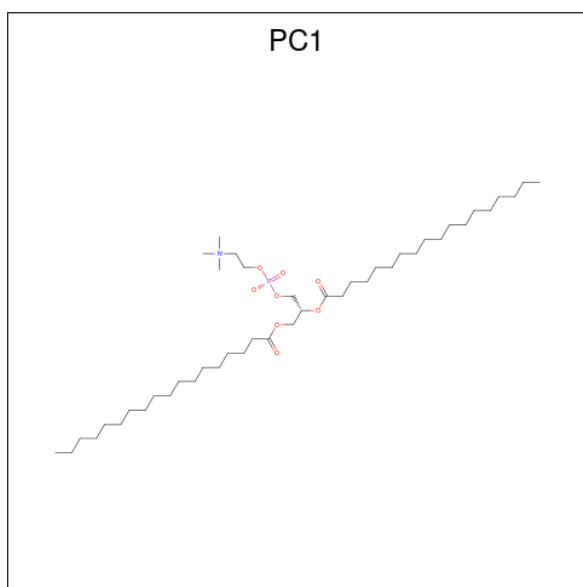
- Molecule 60 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
60	C1	1	Total	Cu	0
			1	1	
60	C2	2	Total	Cu	0
			2	2	
60	c1	1	Total	Cu	0
			1	1	
60	c2	2	Total	Cu	0
			2	2	

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
61	C1	1	Total	Mg	0
			1	1	
61	c1	1	Total	Mg	0
			1	1	

- Molecule 62 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



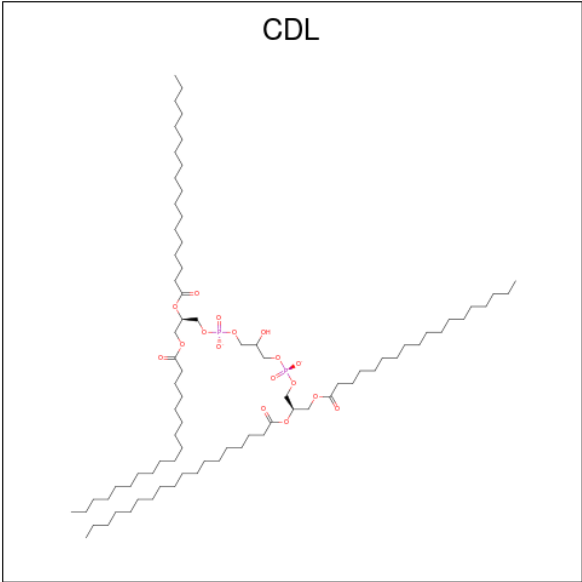
Mol	Chain	Residues	Atoms					AltConf
62	C1	1	Total	C	N	O	P	0
			49	39	1	8	1	
62	C3	1	Total	C	N	O	P	0
			52	42	1	8	1	
62	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
62	C3	1	Total	C	N	O	P	0
			31	21	1	8	1	
62	C3	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	7C	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	7C	1	Total	C	N	O	P	0
			43	33	1	8	1	
62	M1	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	M2	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	M2	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	M2	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
62	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	J	1	Total	C	N	O	P	0
			37	27	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
62	N	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	N	1	Total	C	N	O	P	0
			36	26	1	8	1	
62	V	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	c1	1	Total	C	N	O	P	0
			49	39	1	8	1	
62	c3	1	Total	C	N	O	P	0
			52	42	1	8	1	
62	c3	1	Total	C	N	O	P	0
			39	29	1	8	1	
62	c3	1	Total	C	N	O	P	0
			31	21	1	8	1	
62	c3	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	7c	1	Total	C	N	O	P	0
			43	33	1	8	1	
62	m1	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	m1	1	Total	C	N	O	P	0
			35	25	1	8	1	
62	m2	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	m2	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	m2	1	Total	C	N	O	P	0
			54	44	1	8	1	
62	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
62	a	1	Total	C	N	O	P	0
			41	31	1	8	1	
62	j	1	Total	C	N	O	P	0
			37	27	1	8	1	
62	n	1	Total	C	N	O	P	0
			32	22	1	8	1	
62	n	1	Total	C	N	O	P	0
			36	26	1	8	1	
62	v	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 63 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
63	C1	1	Total	C	O	P	0
			59	40	17	2	
63	C1	1	Total	C	O	P	0
			65	46	17	2	
63	C3	1	Total	C	O	P	0
			68	49	17	2	
63	5B	1	Total	C	O	P	0
			87	68	17	2	
63	5B	1	Total	C	O	P	0
			62	43	17	2	
63	5B	1	Total	C	O	P	0
			67	48	17	2	
63	7A	1	Total	C	O	P	0
			67	48	17	2	
63	7A	1	Total	C	O	P	0
			100	81	17	2	
63	7C	1	Total	C	O	P	0
			85	66	17	2	
63	7C	1	Total	C	O	P	0
			51	32	17	2	
63	M1	1	Total	C	O	P	0
			95	76	17	2	
63	M1	1	Total	C	O	P	0
			66	47	17	2	
63	M1	1	Total	C	O	P	0
			66	47	17	2	
63	M2	1	Total	C	O	P	0
			54	35	17	2	

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Mol	Chain	Residues	Atoms				AltConf
63	M2	1	Total	C	O	P	0
			66	47	17	2	
63	M2	1	Total	C	O	P	0
			74	55	17	2	
63	M3	1	Total	C	O	P	0
			94	75	17	2	
63	M3	1	Total	C	O	P	0
			51	32	17	2	
63	M3	1	Total	C	O	P	0
			63	44	17	2	
63	Y7	1	Total	C	O	P	0
			65	46	17	2	
63	Y0	1	Total	C	O	P	0
			64	45	17	2	
63	Y5	1	Total	C	O	P	0
			81	62	17	2	
63	A	1	Total	C	O	P	0
			51	32	17	2	
63	B	1	Total	C	O	P	0
			62	43	17	2	
63	E	1	Total	C	O	P	0
			60	41	17	2	
63	E	1	Total	C	O	P	0
			72	53	17	2	
63	F	1	Total	C	O	P	0
			100	81	17	2	
63	J	1	Total	C	O	P	0
			70	51	17	2	
63	L	1	Total	C	O	P	0
			74	55	17	2	
63	N	1	Total	C	O	P	0
			95	76	17	2	
63	T	1	Total	C	O	P	0
			68	49	17	2	
63	T	1	Total	C	O	P	0
			75	56	17	2	
63	U	1	Total	C	O	P	0
			82	63	17	2	
63	V	1	Total	C	O	P	0
			91	72	17	2	
63	c1	1	Total	C	O	P	0
			59	40	17	2	

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Mol	Chain	Residues	Atoms				AltConf
63	c1	1	Total	C	O	P	0
			65	46	17	2	
63	c3	1	Total	C	O	P	0
			68	49	17	2	
63	5b	1	Total	C	O	P	0
			87	68	17	2	
63	5b	1	Total	C	O	P	0
			67	48	17	2	
63	7a	1	Total	C	O	P	0
			67	48	17	2	
63	7a	1	Total	C	O	P	0
			100	81	17	2	
63	7c	1	Total	C	O	P	0
			85	66	17	2	
63	7c	1	Total	C	O	P	0
			51	32	17	2	
63	m1	1	Total	C	O	P	0
			95	76	17	2	
63	m1	1	Total	C	O	P	0
			66	47	17	2	
63	m1	1	Total	C	O	P	0
			66	47	17	2	
63	m2	1	Total	C	O	P	0
			54	35	17	2	
63	m2	1	Total	C	O	P	0
			66	47	17	2	
63	m2	1	Total	C	O	P	0
			74	55	17	2	
63	m3	1	Total	C	O	P	0
			94	75	17	2	
63	m3	1	Total	C	O	P	0
			51	32	17	2	
63	m3	1	Total	C	O	P	0
			63	44	17	2	
63	y7	1	Total	C	O	P	0
			65	46	17	2	
63	y0	1	Total	C	O	P	0
			64	45	17	2	
63	y5	1	Total	C	O	P	0
			81	62	17	2	
63	a	1	Total	C	O	P	0
			51	32	17	2	

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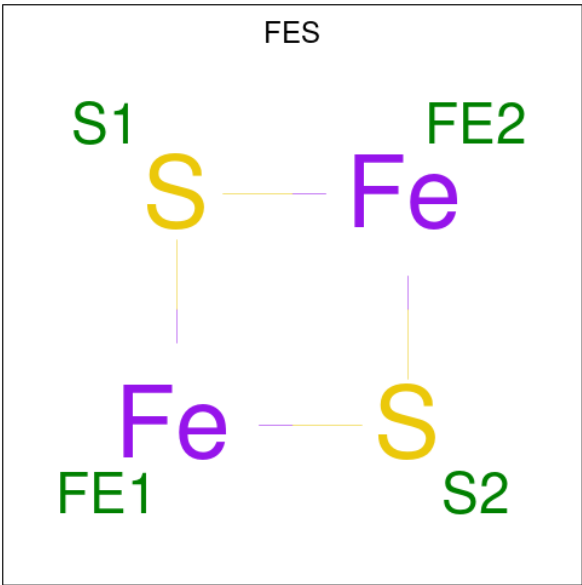
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Mol	Chain	Residues	Atoms				AltConf
63	b	1	Total	C	O	P	0
			62	43	17	2	
63	e	1	Total	C	O	P	0
			60	41	17	2	
63	e	1	Total	C	O	P	0
			72	53	17	2	
63	f	1	Total	C	O	P	0
			100	81	17	2	
63	j	1	Total	C	O	P	0
			70	51	17	2	
63	k	1	Total	C	O	P	0
			62	43	17	2	
63	l	1	Total	C	O	P	0
			74	55	17	2	
63	n	1	Total	C	O	P	0
			95	76	17	2	
63	t	1	Total	C	O	P	0
			68	49	17	2	
63	t	1	Total	C	O	P	0
			75	56	17	2	
63	u	1	Total	C	O	P	0
			82	63	17	2	
63	v	1	Total	C	O	P	0
			91	72	17	2	

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
64	5B	1	Total	Zn	0
			1	1	
64	M	1	Total	Zn	0
			1	1	
64	5b	1	Total	Zn	0
			1	1	
64	m	1	Total	Zn	0
			1	1	

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
65	FS	1	Total	Fe	S	0
			4	2	2	
65	FS	1	Total	Fe	S	0
			4	2	2	
65	fs	1	Total	Fe	S	0
			4	2	2	
65	fs	1	Total	Fe	S	0
			4	2	2	

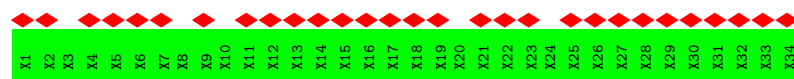




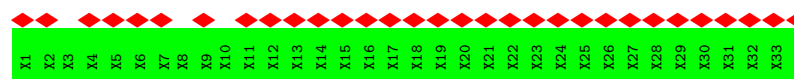
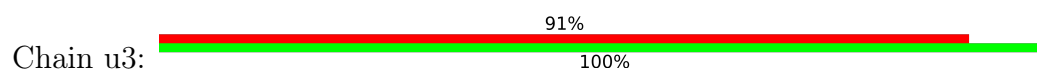




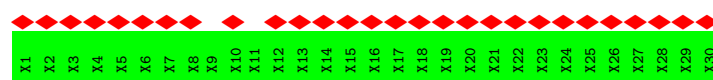




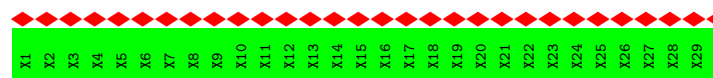
• Molecule 3: Unknown peptide



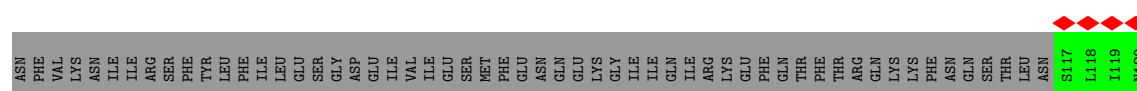
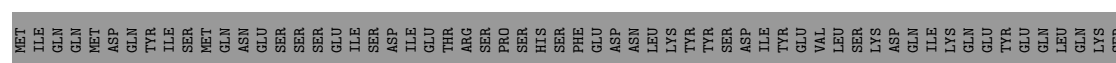
• Molecule 4: Unknown peptide



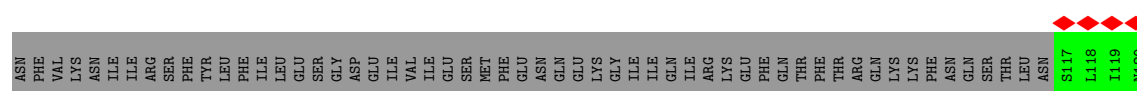
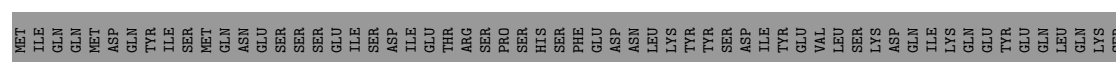
• Molecule 4: Unknown peptide

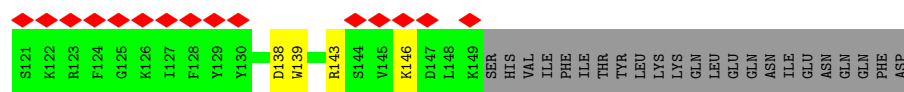


• Molecule 5: Uncharacterized protein



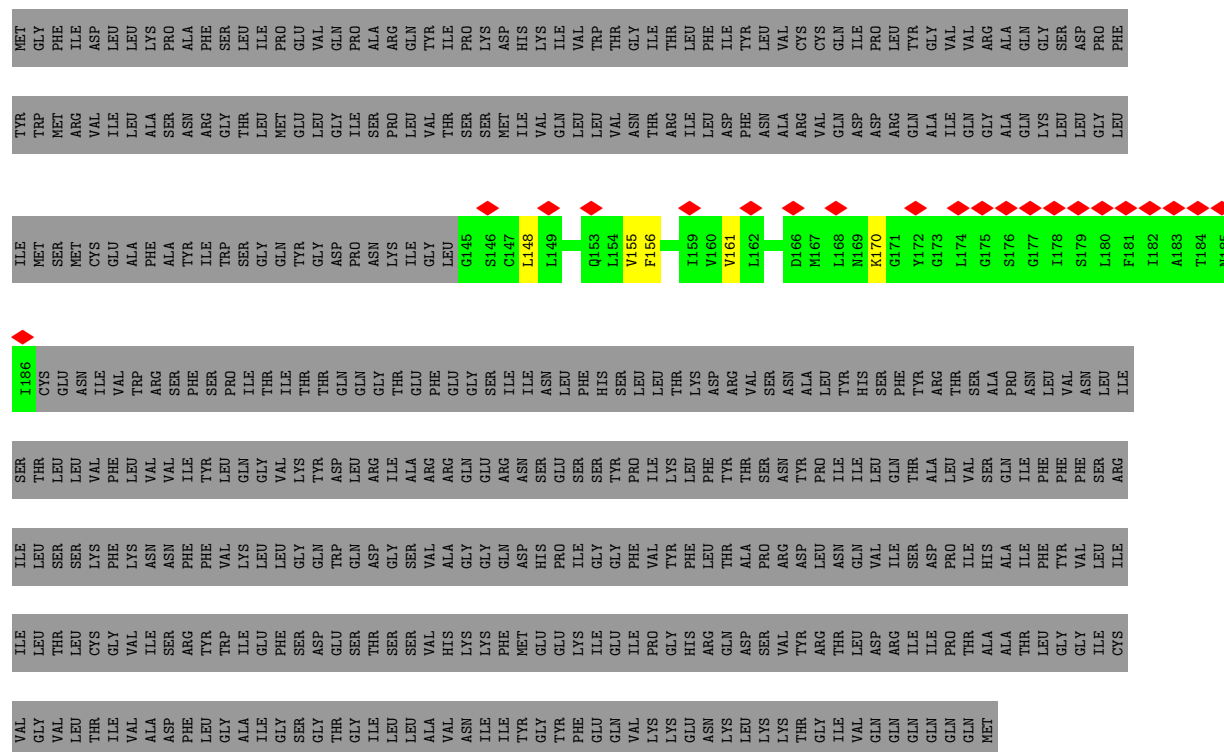
• Molecule 5: Uncharacterized protein





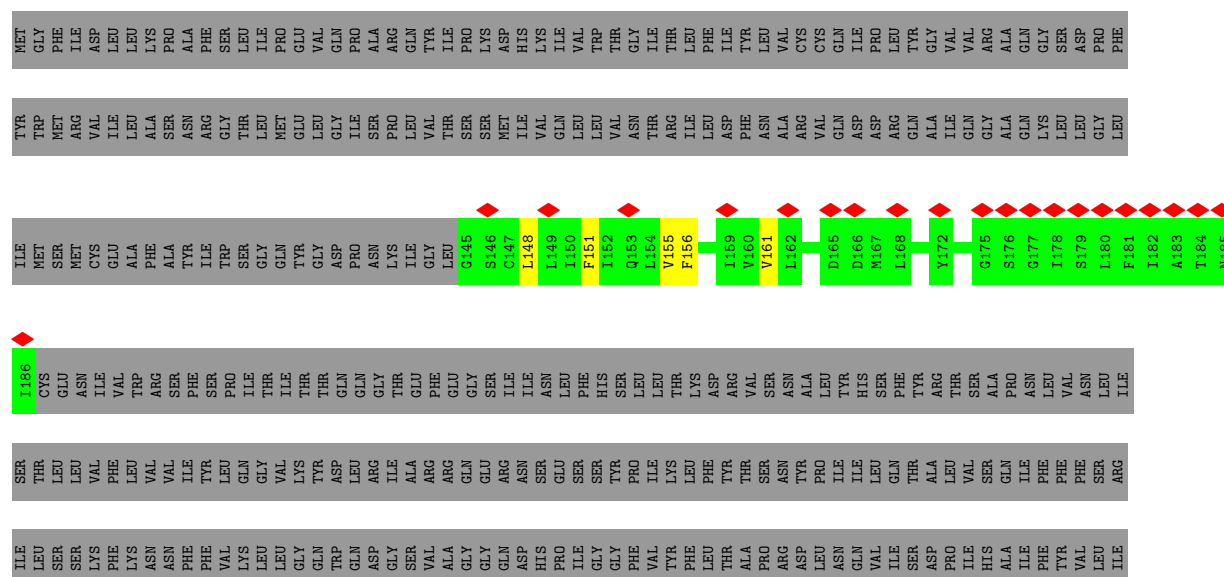
• Molecule 6: Protein transporter Sec61 alpha subunit

Chain U6: 8% 91%



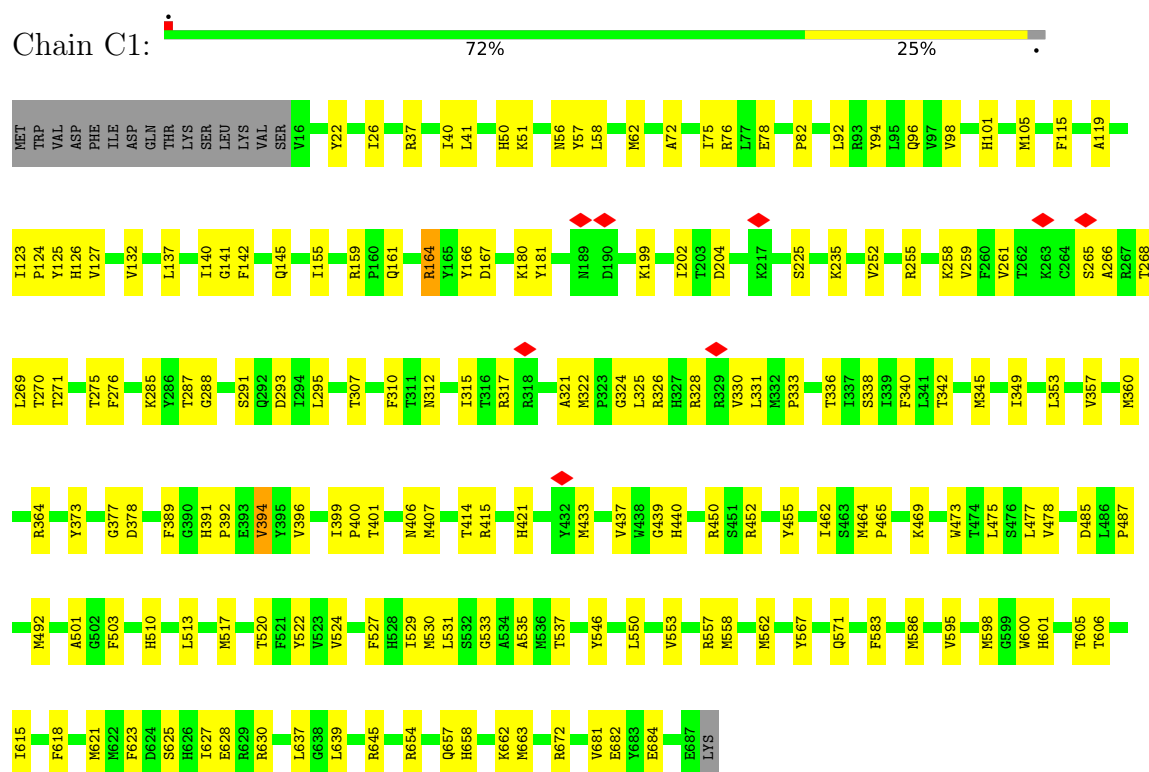
• Molecule 6: Protein transporter Sec61 alpha subunit

Chain u6: 8% 91%

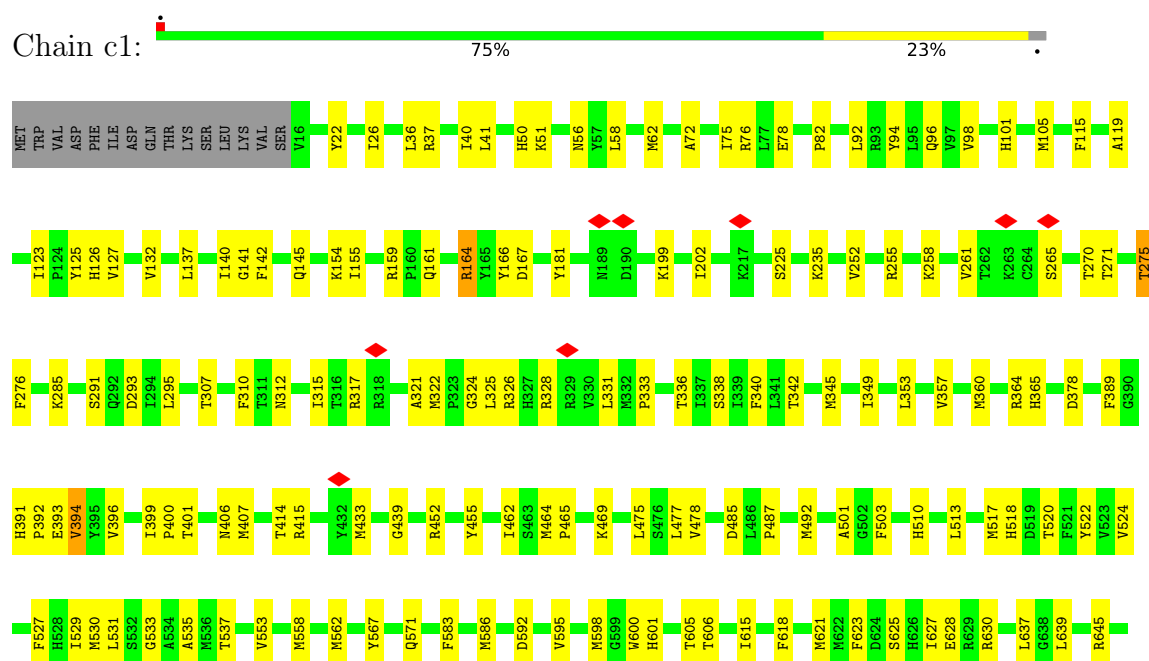


VAL	GLY	GLY	VAL	LEU	THR	ILE	VAL	ALA	ASP	PHE	LEU	GLY	ALA	ILE	GLY	SER	GLY	THR	ILE	LEU	LEU	ALA	VAL	ASN	ILE	ILE	TYR	GLY	THR	PHE	GLU	GLN	VAL	LYS	LYS	GLU	LYS	LYS	LEU	LYS	LYS	THR	GLY	ILE	VAL	GLN	GLN	GLN	GLN	GLN	GLN	GLN	MET
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- Molecule 7: Cytochrome c oxidase subunit 1



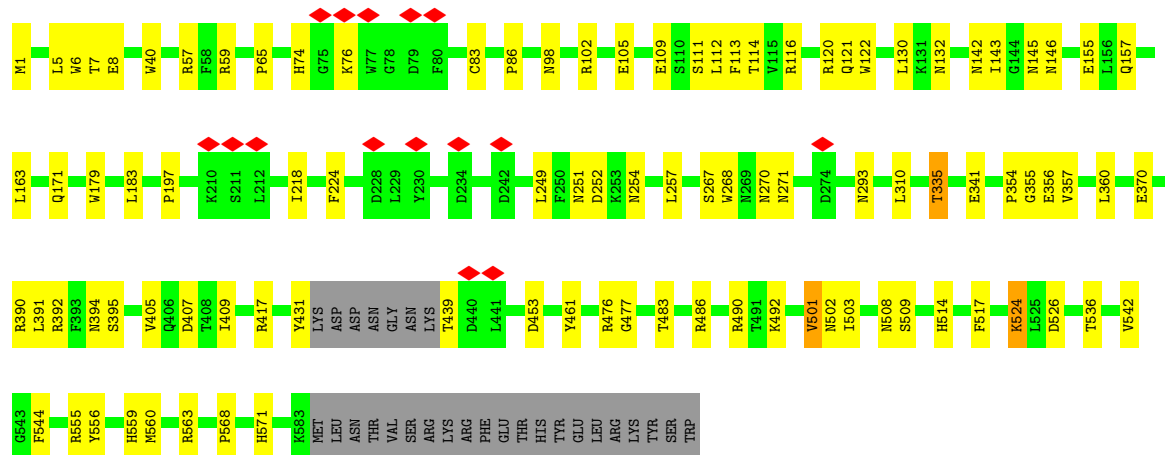
- Molecule 7: Cytochrome c oxidase subunit 1





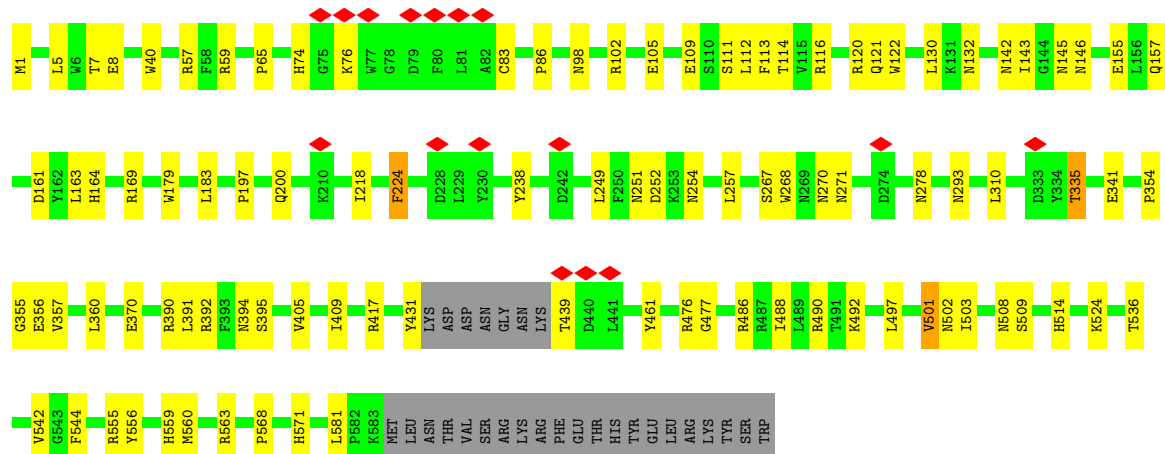
• Molecule 8: Cytochrome c oxidase subunit 2

Chain C2: 79% 16% 5%



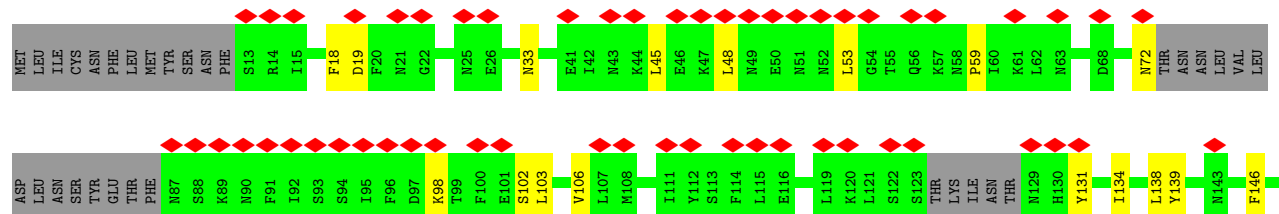
• Molecule 8: Cytochrome c oxidase subunit 2

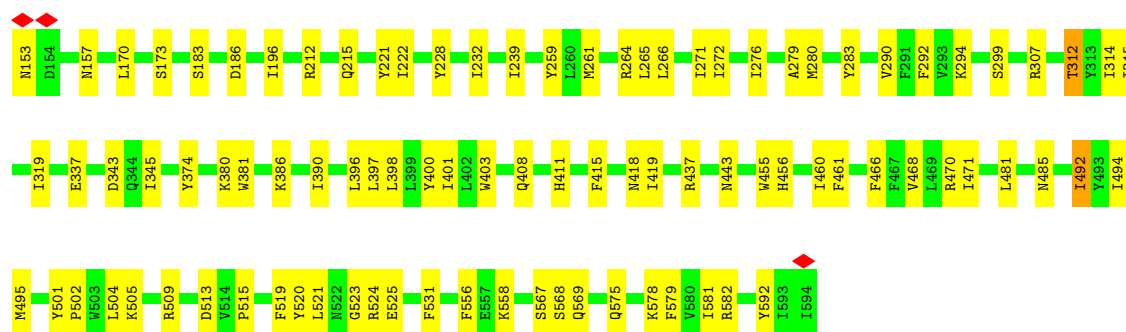
Chain c2: 79% 16% 5%



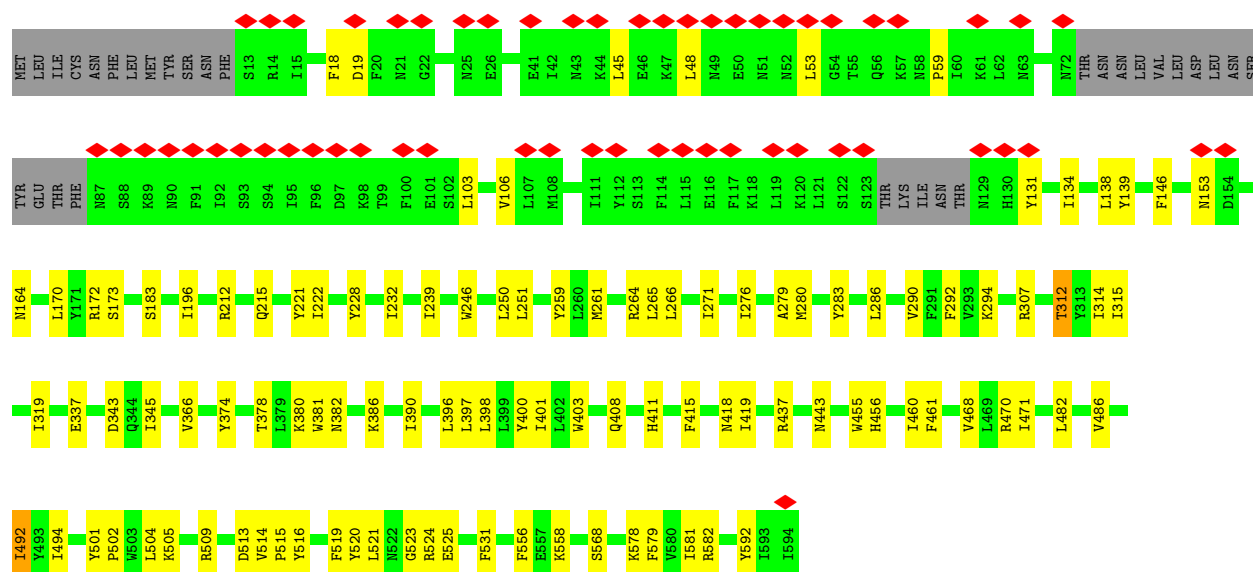
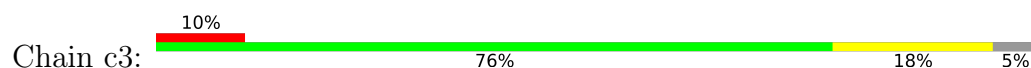
• Molecule 9: Ymf68

Chain C3: 10% 76% 18% 5%

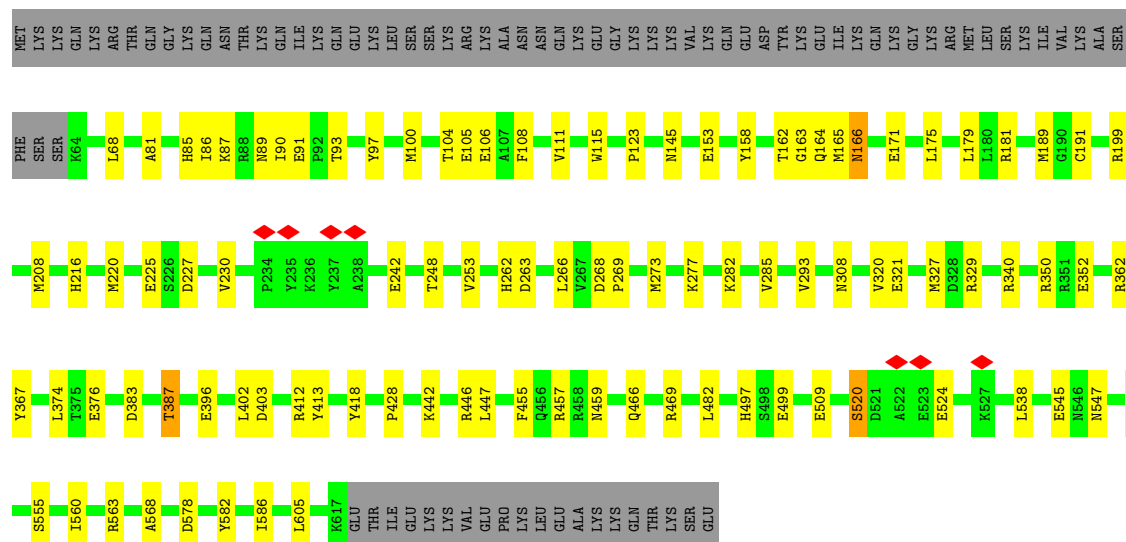




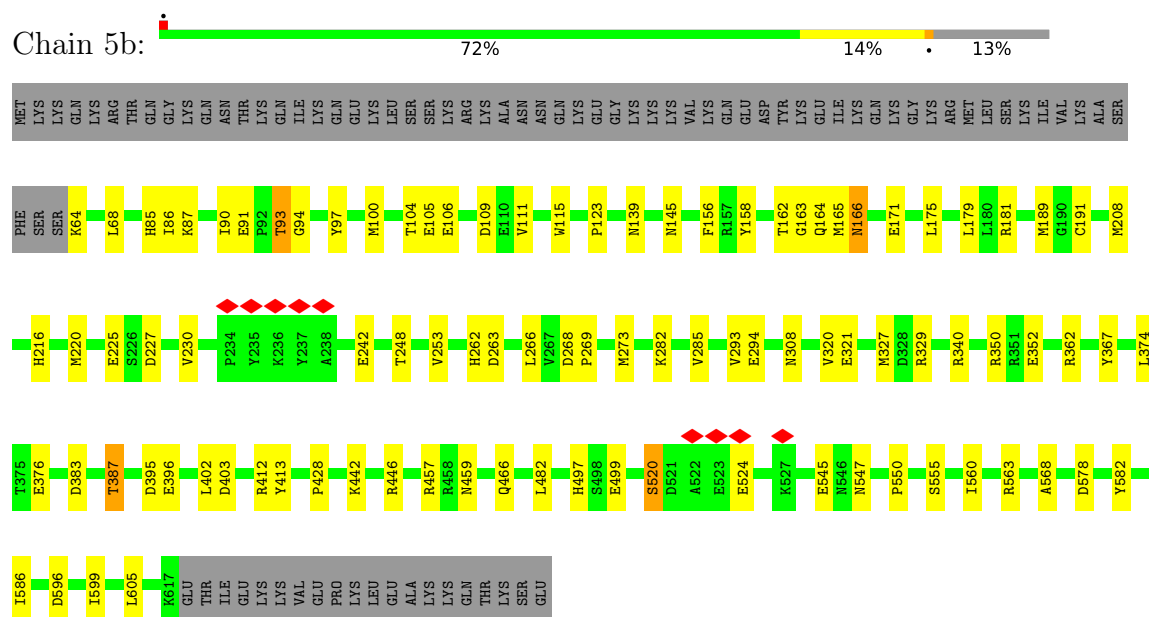
• Molecule 9: Ymf68



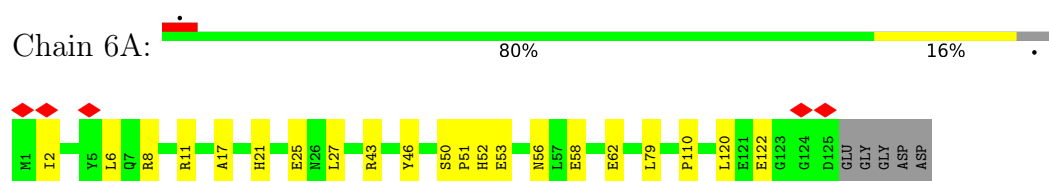
• Molecule 10: Cytochrome C oxidase subunit Vb protein



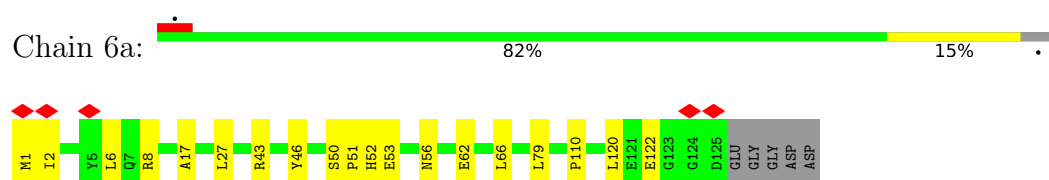
- Molecule 10: Cytochrome C oxidase subunit Vb protein



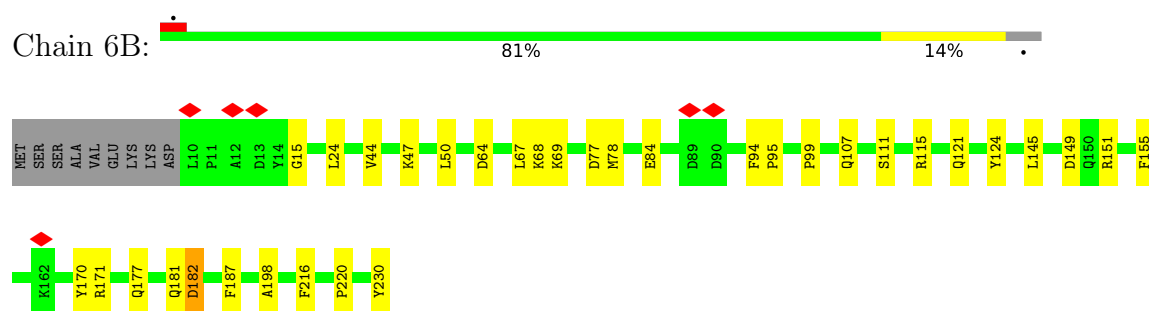
- Molecule 11: Transmembrane protein, putative



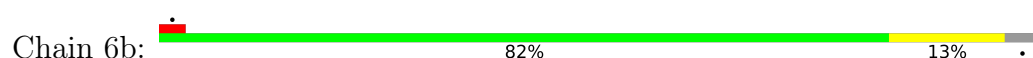
- Molecule 11: Transmembrane protein, putative

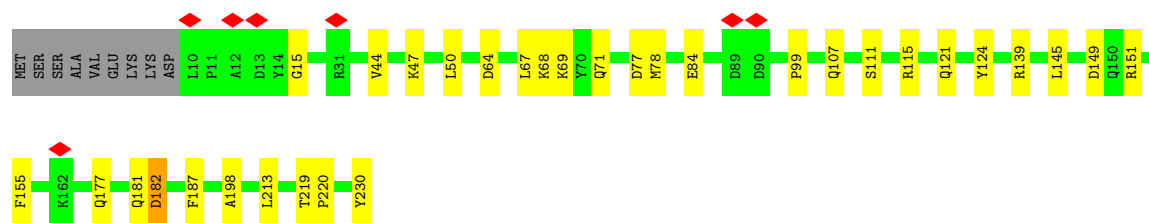


- Molecule 12: Cytochrome c oxidase subunit 6B

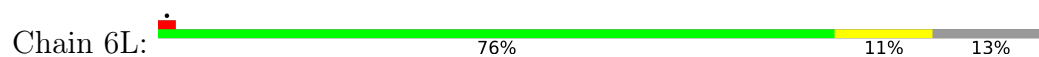


- Molecule 12: Cytochrome c oxidase subunit 6B

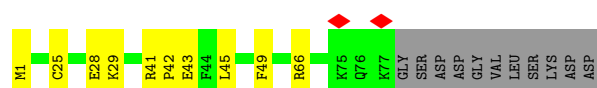
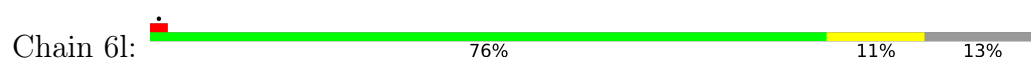




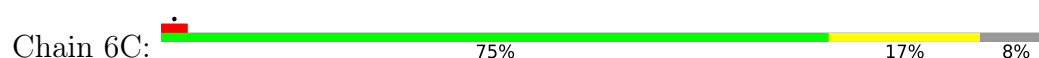
- Molecule 13: Cytochrome c oxidase subunit 6B-like



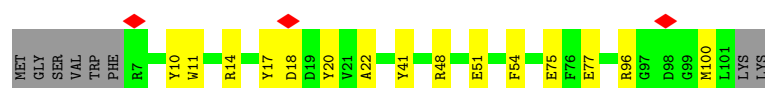
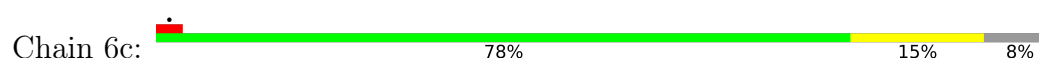
- Molecule 13: Cytochrome c oxidase subunit 6B-like



- Molecule 14: Transmembrane protein, putative



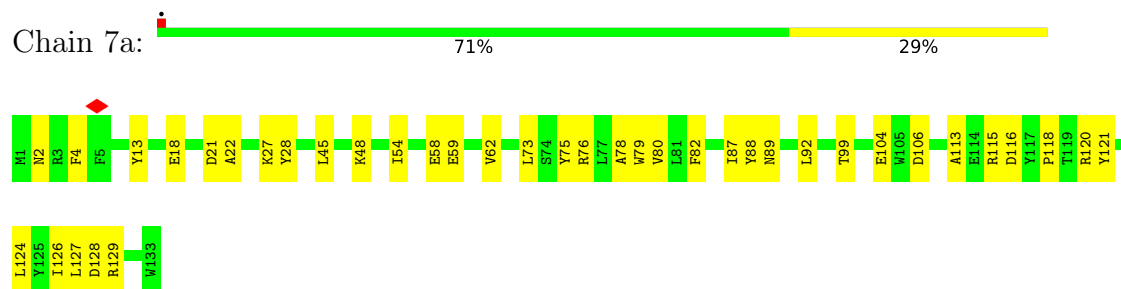
- Molecule 14: Transmembrane protein, putative



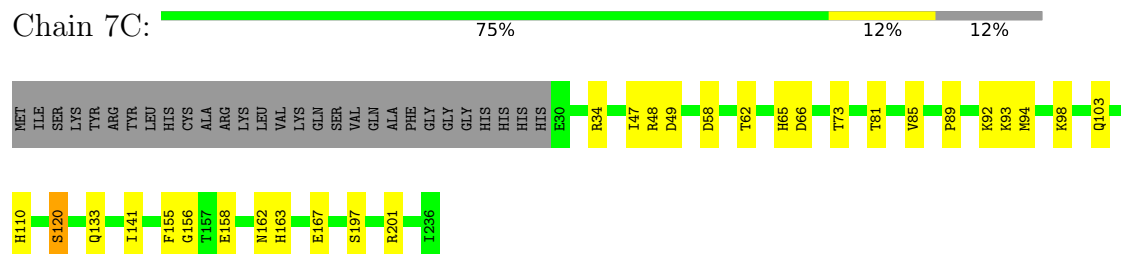
- Molecule 15: Transmembrane protein, putative



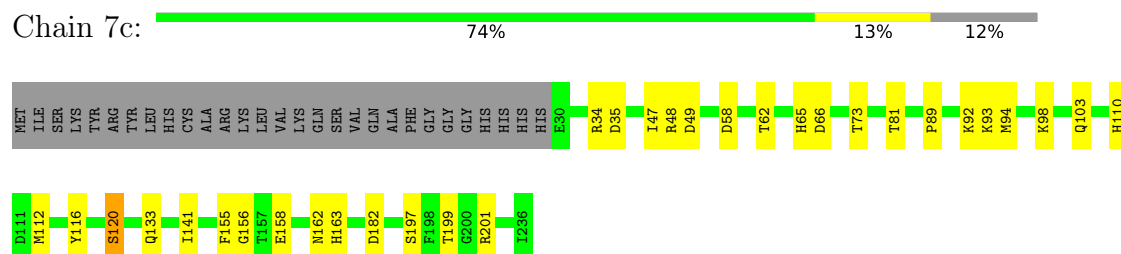
- Molecule 15: Transmembrane protein, putative



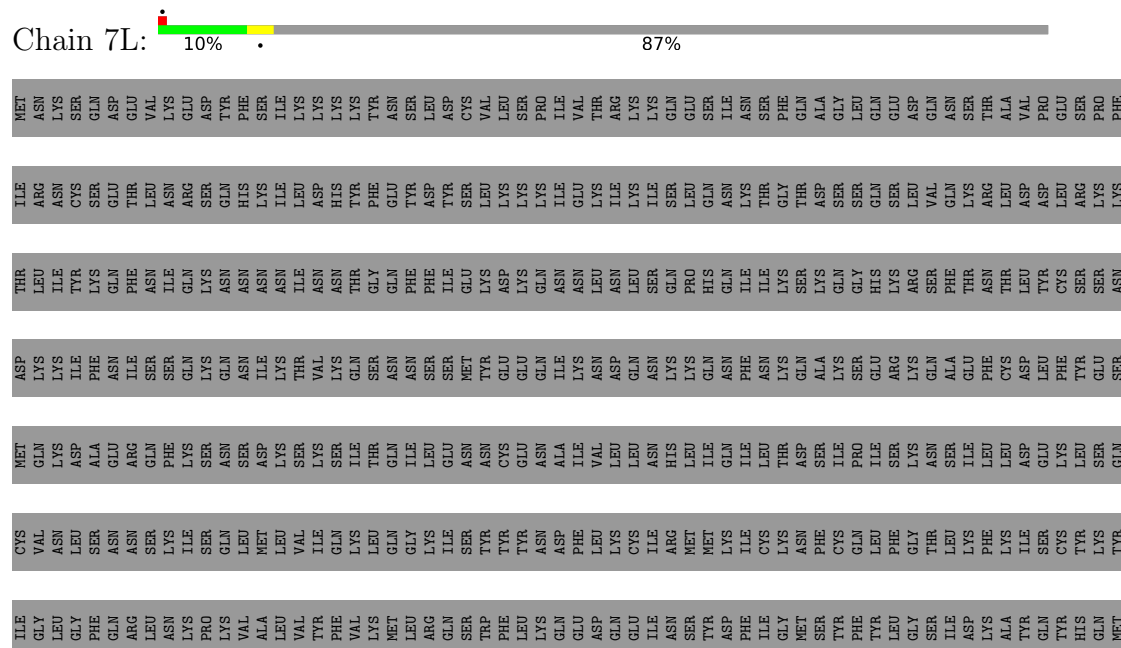
- Molecule 16: Cytochrome c oxidase subunit 7C



- Molecule 16: Cytochrome c oxidase subunit 7C



- Molecule 17: CTF/NF-I domain-containing protein



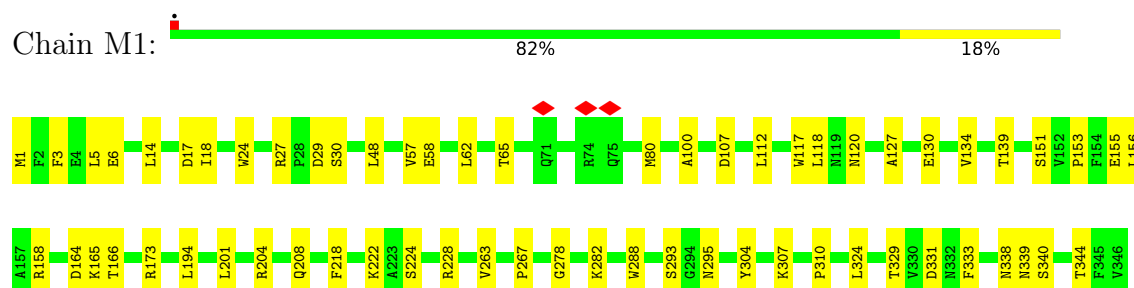
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graph LR
    M939 --- R940
    R940 --- E954
    E954 --- R957
    R957 --- R965
    R965 --- L970
    L970 --- D980
    D980 --- T990
  
```

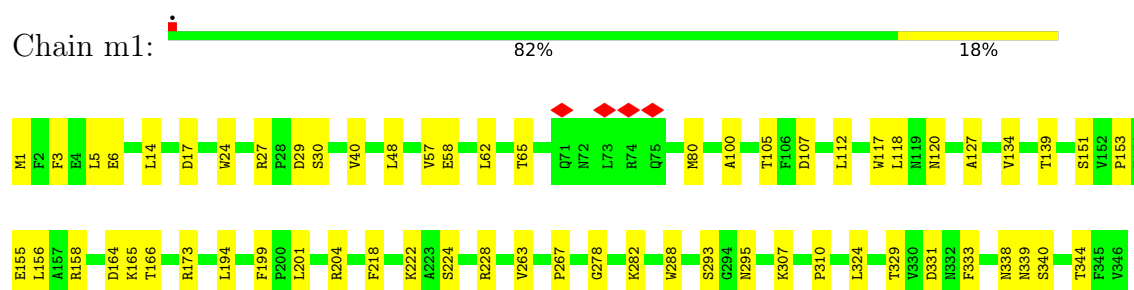
Chain 71: 10% 87%

[illegible]

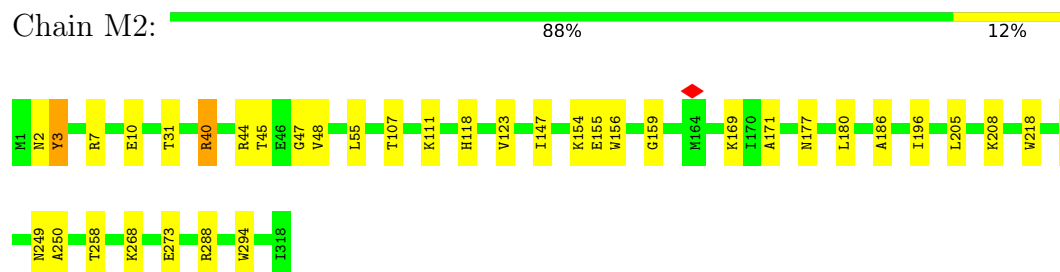
- Molecule 18: Oxoglutarate/malate translocator protein, putative



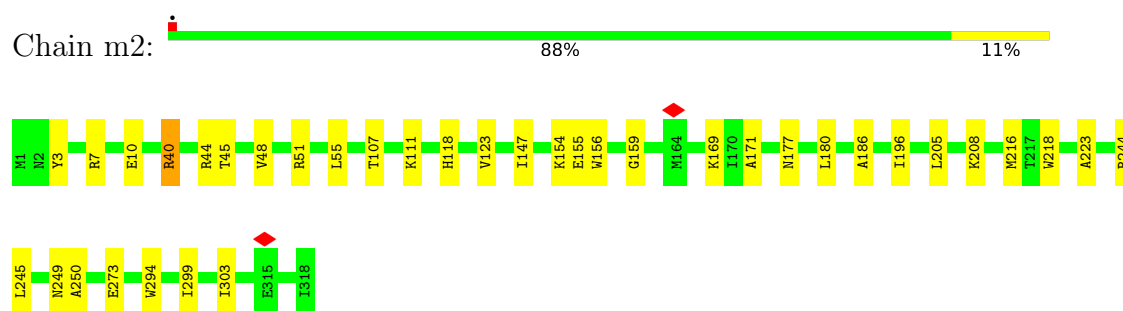
- Molecule 18: Oxoglutarate/malate translocator protein, putative



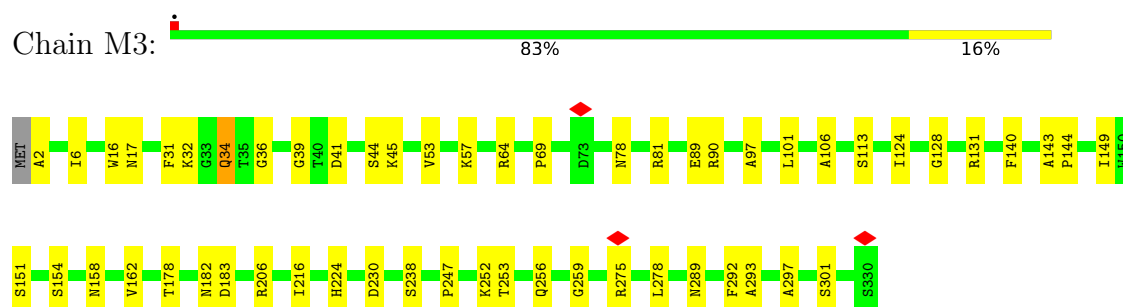
- Molecule 19: 2-oxoglutarate/malate carrier protein



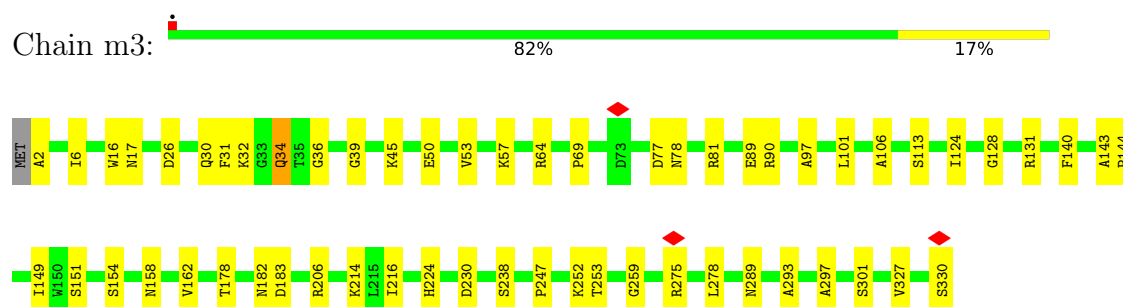
- Molecule 19: 2-oxoglutarate/malate carrier protein



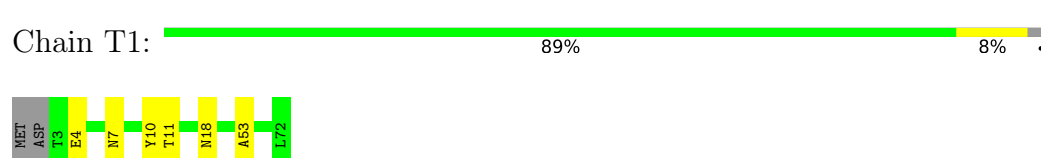
- Molecule 20: Carrier protein



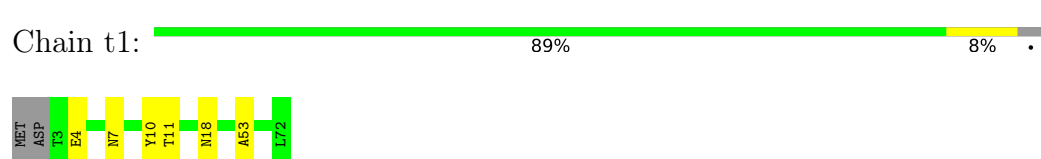
- Molecule 20: Carrier protein



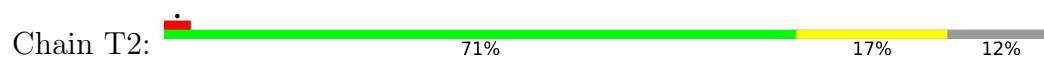
- Molecule 21: Tim10/DDP family zinc finger protein



- Molecule 21: Tim10/DDP family zinc finger protein



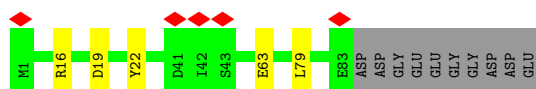
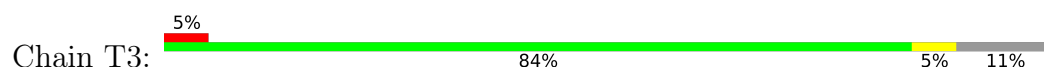
- Molecule 22: Cytochrome c oxidase small TIM subunit 2



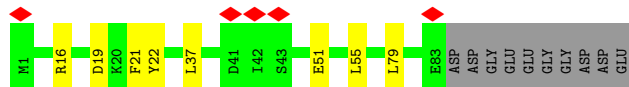
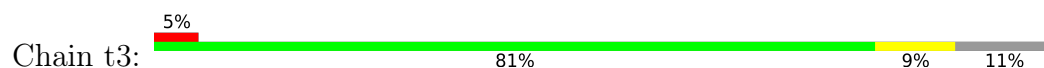
- Molecule 22: Cytochrome c oxidase small TIM subunit 2



- Molecule 23: Cytochrome c oxidase small TIM subunit 3



- Molecule 23: Cytochrome c oxidase small TIM subunit 3



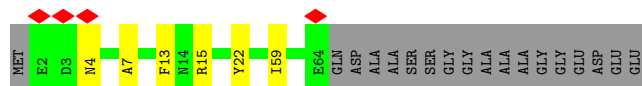
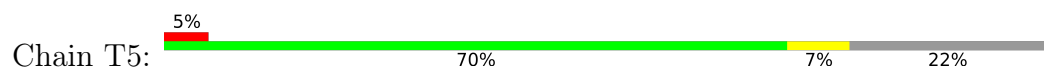
- Molecule 24: Cytochrome c oxidase small TIM subunit 4



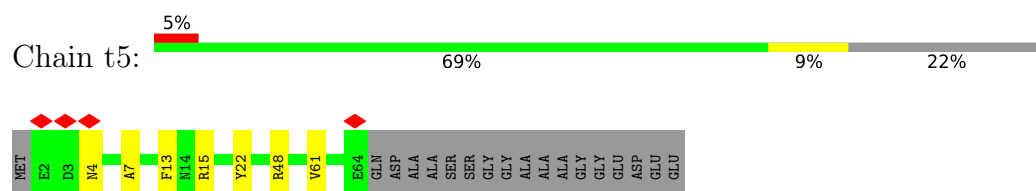
- Molecule 24: Cytochrome c oxidase small TIM subunit 4



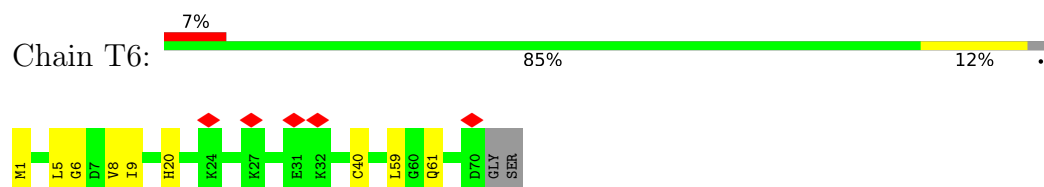
- Molecule 25: Cytochrome c oxidase small TIM subunit 5



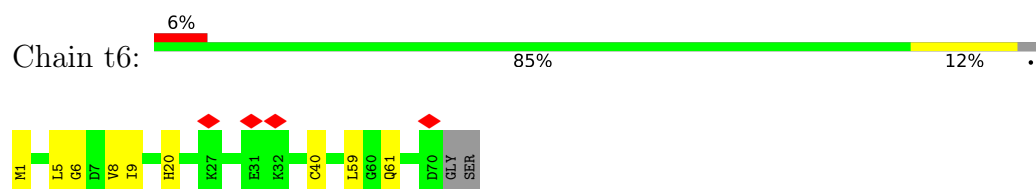
- Molecule 25: Cytochrome c oxidase small TIM subunit 5



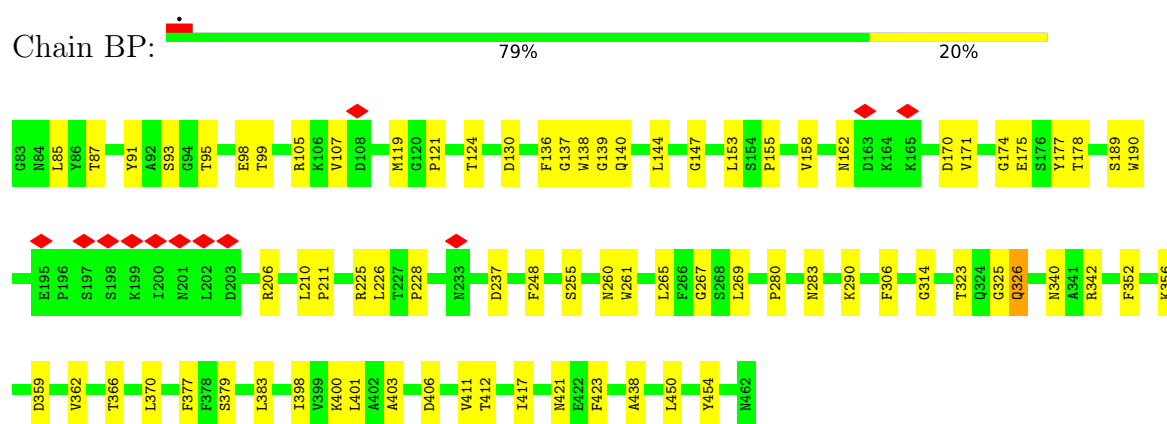
- Molecule 26: Cytochrome c oxidase small TIM subunit 6



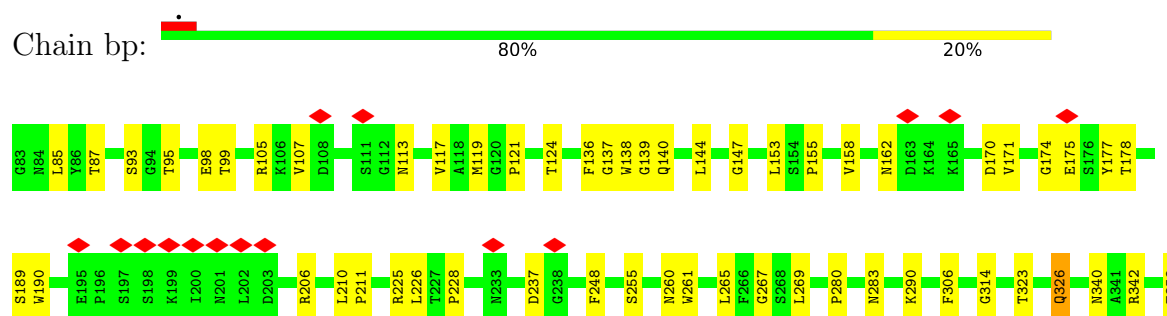
- Molecule 26: Cytochrome c oxidase small TIM subunit 6



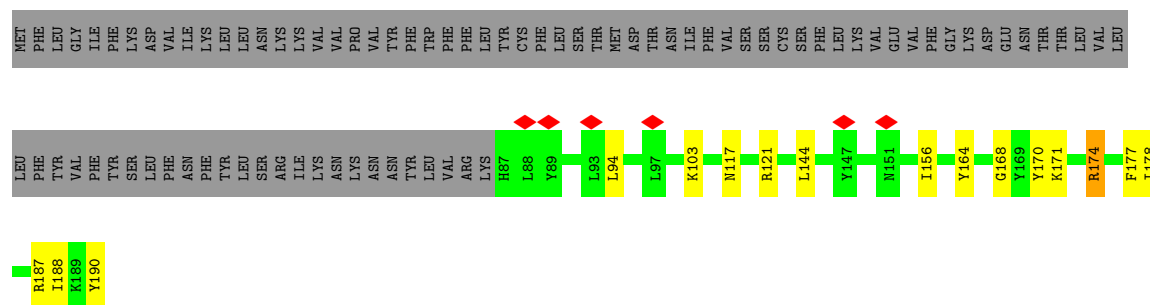
- Molecule 27: Chromosome condensation regulator RCC1 repeat protein



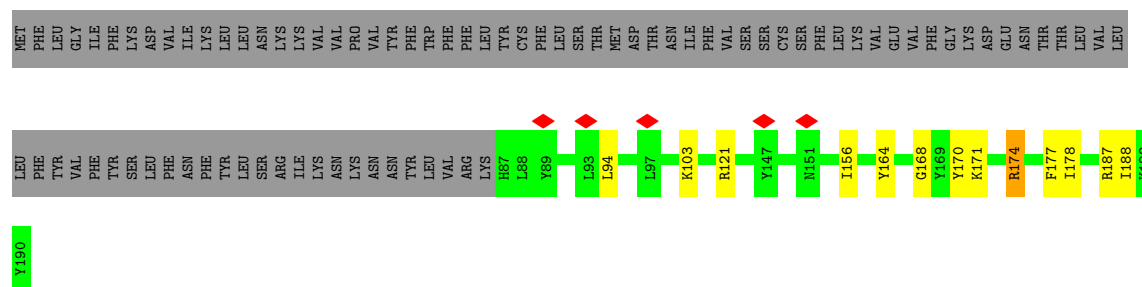
- Molecule 27: Chromosome condensation regulator RCC1 repeat protein



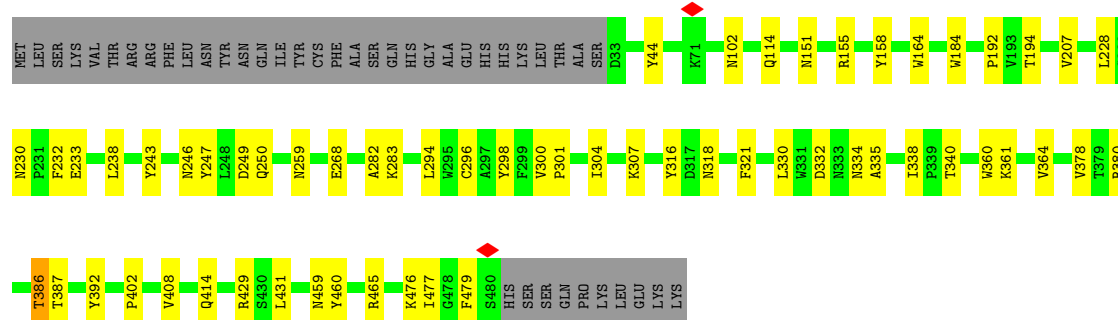
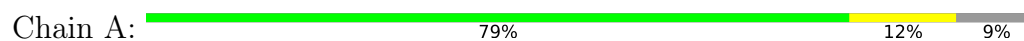




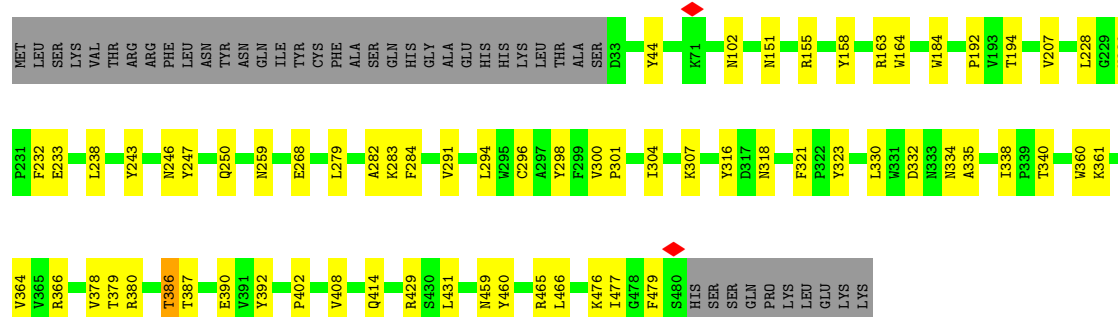
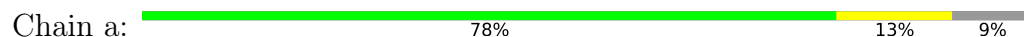
- Molecule 32: Ymf75



- Molecule 33: Transmembrane protein, putative



- Molecule 33: Transmembrane protein, putative





TYR LEU SER TYR GLY VAL SER LYS ARG ARG GLY GLN GLN PHE PRO CYS ASN LYS HIS ASN LEU THR LEU TYR PHE

- Molecule 35: Cyclic nucleotide-binding domain protein

Chain c:  97%

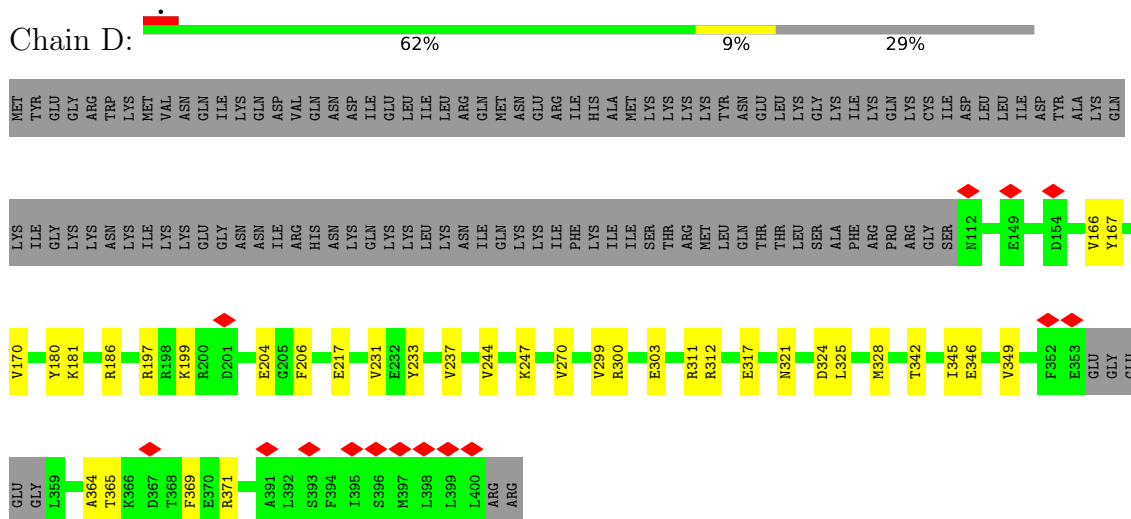
TYR	PHE	LEU	TYR	PHE	TYR	SER	ILE	LEU	LEU	PHE	PHE	ASN	GLN	ASP	ASN	PRO	ASP	THR	GLU	PHE	ILE	LYS	GLU	PHE	TYR	PHE	CYS	THR	PHE	PHE	ILE	PHE	LEU	LEU	ASP	VAL	LEU	VAL	ASN	ASN	PHE	ASN	ASN	LYS	ASP	LEU	ILE	ILE	ILE	ASN	ARG	ARG	GLN	ILE	ALA
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LYS	GLN	TYR	ILE	PHE	SER	THR	VAL	F429	F430	I437	V438	L439	G440	I441	K442	V443	I444	K445	R446	S447	I450	V451	Y452	N453	P454	N455	H456	N457	L458	L459	T460	Y461	C462	F463	N464	M465	L466	I467	F468	F469	K470	V471	N472	G473	I474	SER	SER	LYS	LYS	LYS	GLY	PHE	ASP	TYR	VAL	PHE	THR
-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

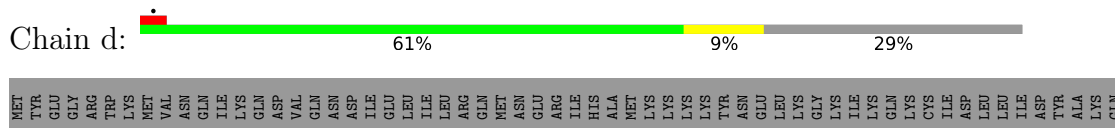
ILE	TYR	SER	SER	PHE	GLN	GLN	ARG	ILE	PHE	PHE	ASP	ARG	THR	TYR	LYS	ASN	ASN	LEU	LYS	PRO	LEU	LEU	ASN	ASN	ILE	GLN	ASP	ASN	ASN	GLN	ASN	VAL	CYS	LYS	ILE	ILE	LYS	LYS	LEU	LEU	GLN	ASN	ASP	ASP	ASN	ASN	ILE	SER	ILE	GLU	ILE	ILE	MET	PHE	ASP	CYS	ASN	ASN	ARG	TYR	THR	GLY	SER
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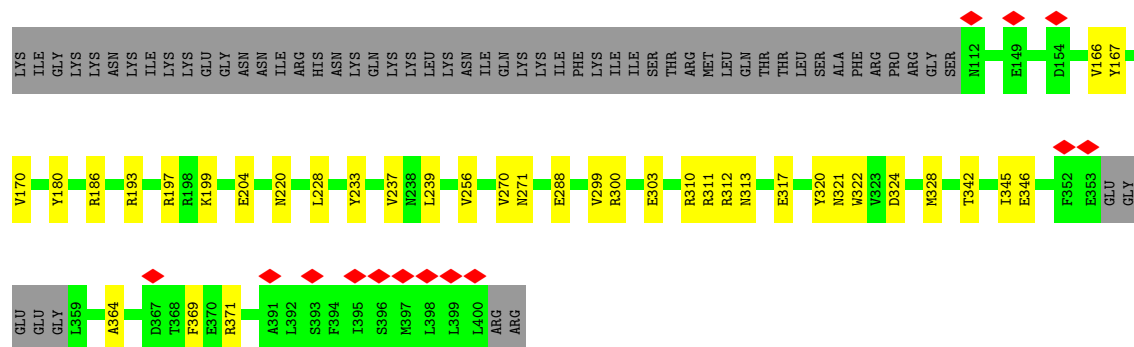
[illegible]

- Molecule 36: SURF1-like protein

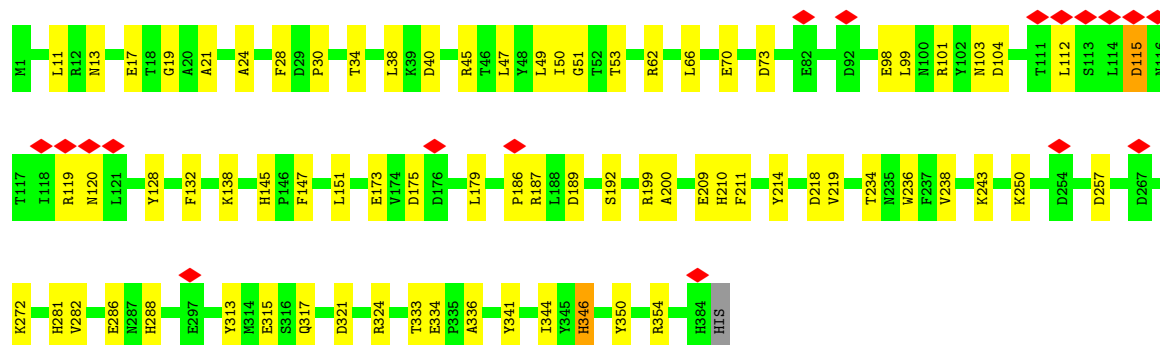
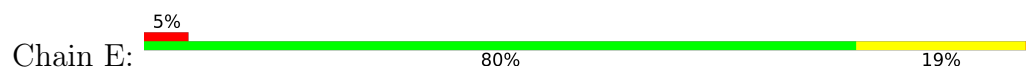


- Molecule 36: SURF1-like protein

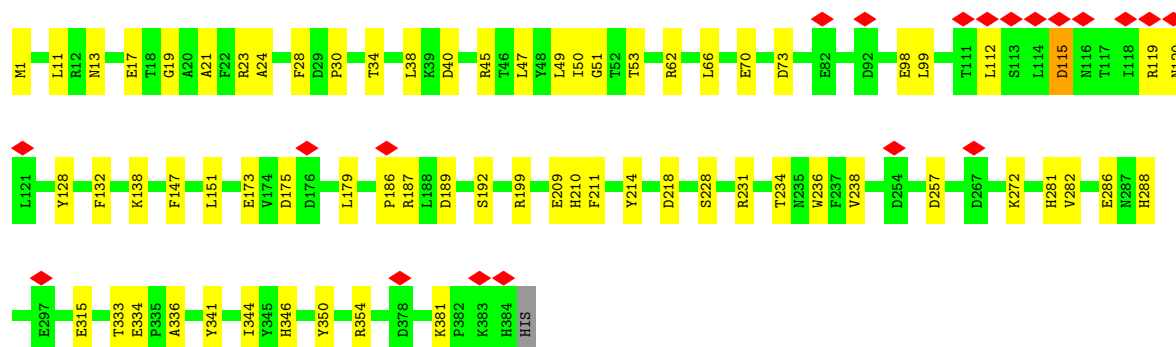
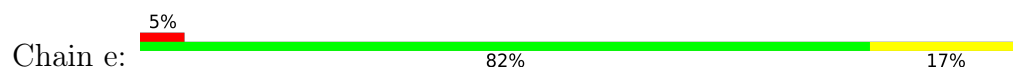




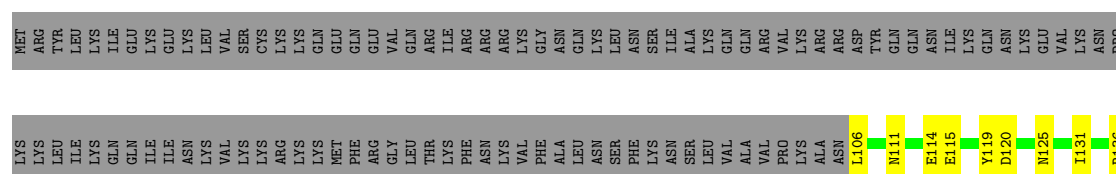
• Molecule 37: TraB family protein



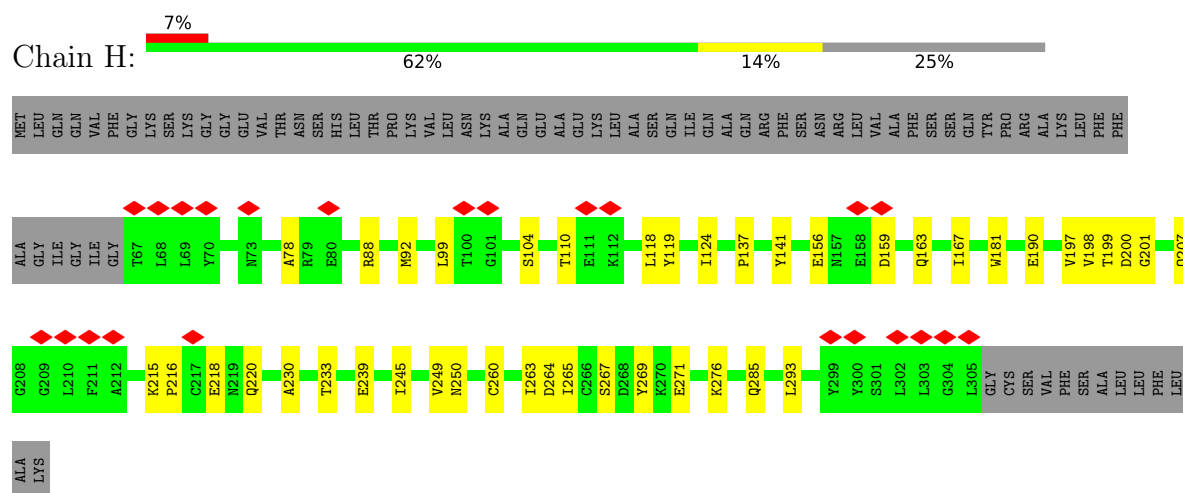
• Molecule 37: TraB family protein



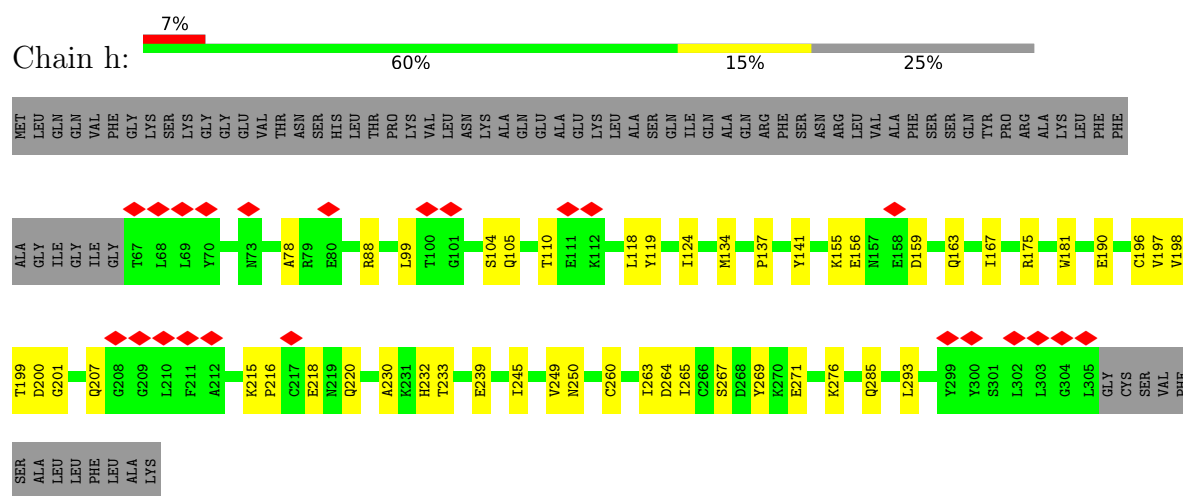
• Molecule 38: Transmembrane protein, putative



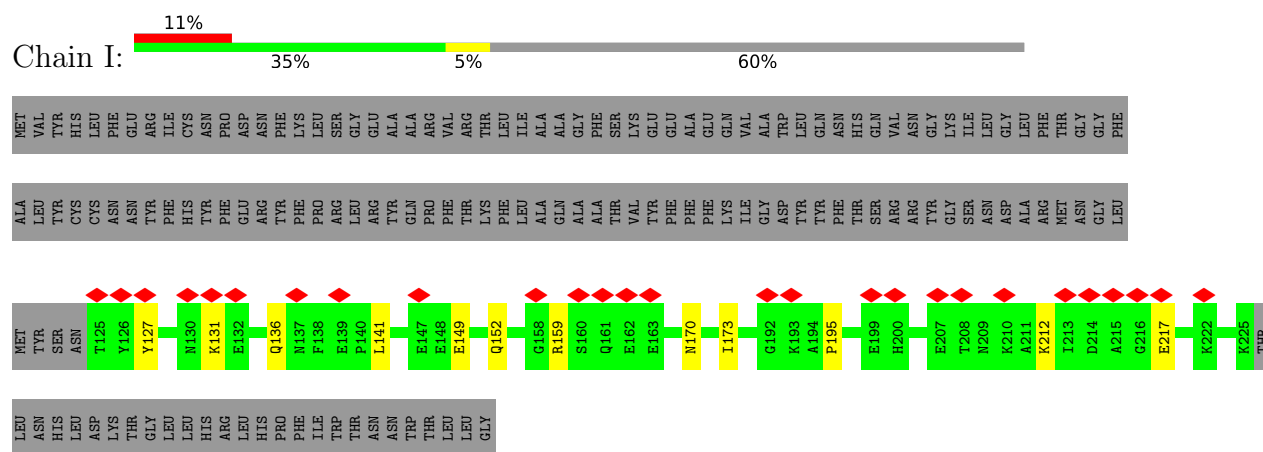
- Molecule 40: SURF1-like protein



- Molecule 40: SURF1-like protein

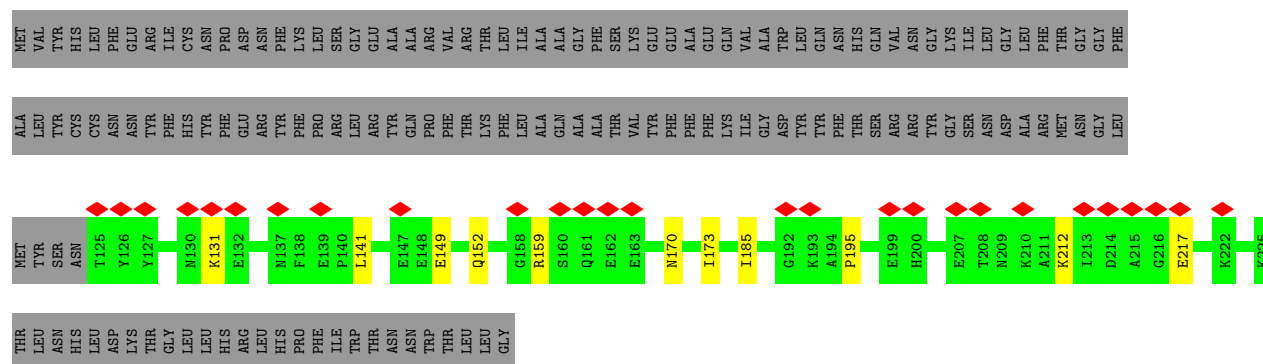


- Molecule 41: Cytochrome c oxidase subunit TT9



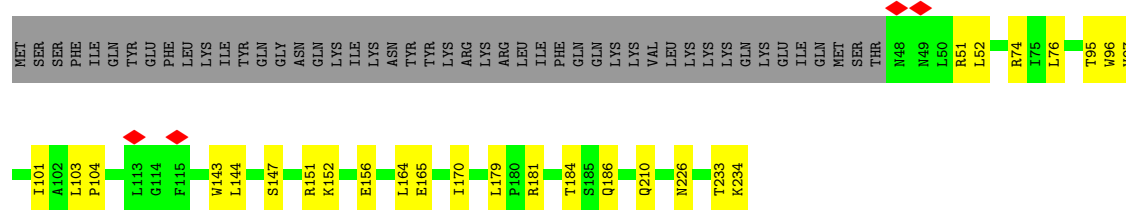
- Molecule 41: Cytochrome c oxidase subunit TT9





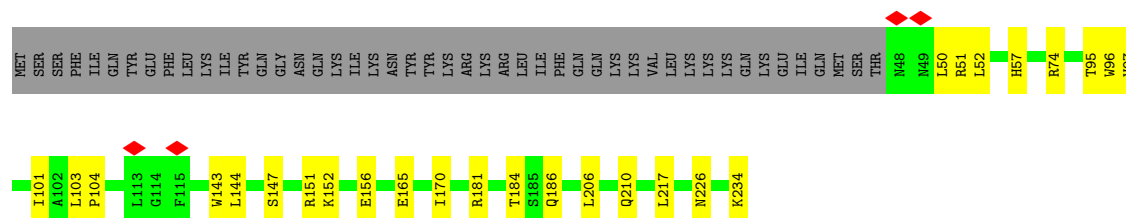
- Molecule 42: Cytochrome c oxidase subunit TT10

Chain J: 68% 12% 20%



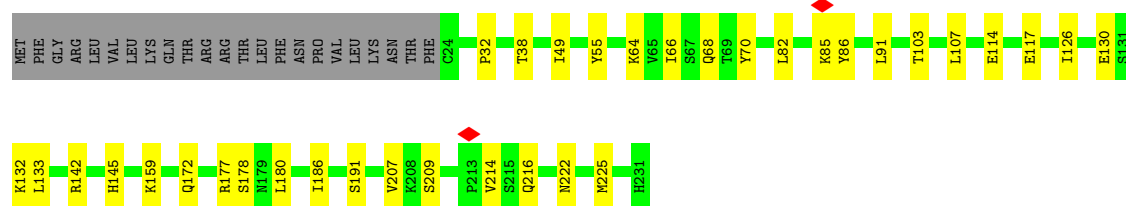
- Molecule 42: Cytochrome c oxidase subunit TT10

Chain j: 68% 12% 20%



- Molecule 43: Cytochrome c oxidase subunit TT11

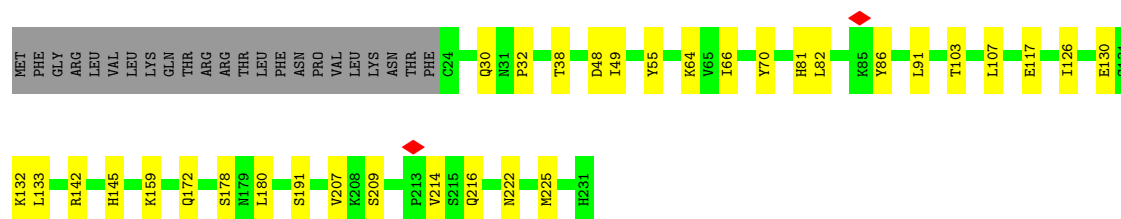
Chain K: 75% 15% 10%



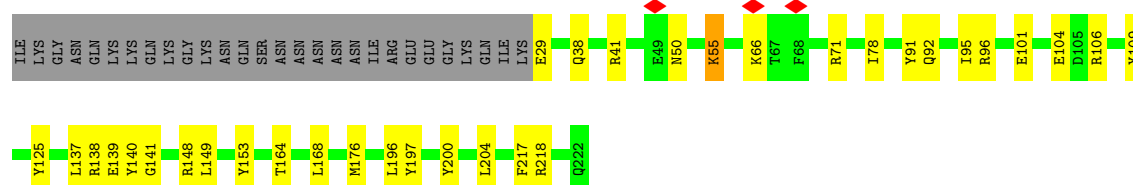
- Molecule 43: Cytochrome c oxidase subunit TT11

Chain k: 76% 14% 10%

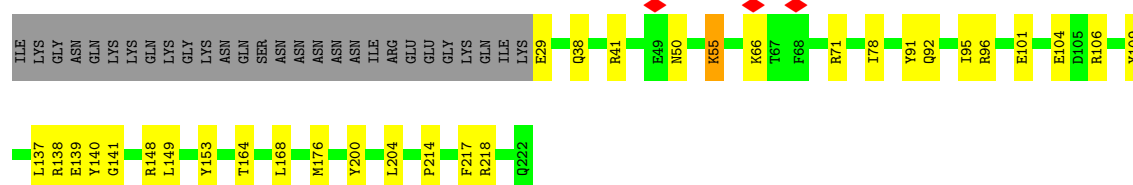




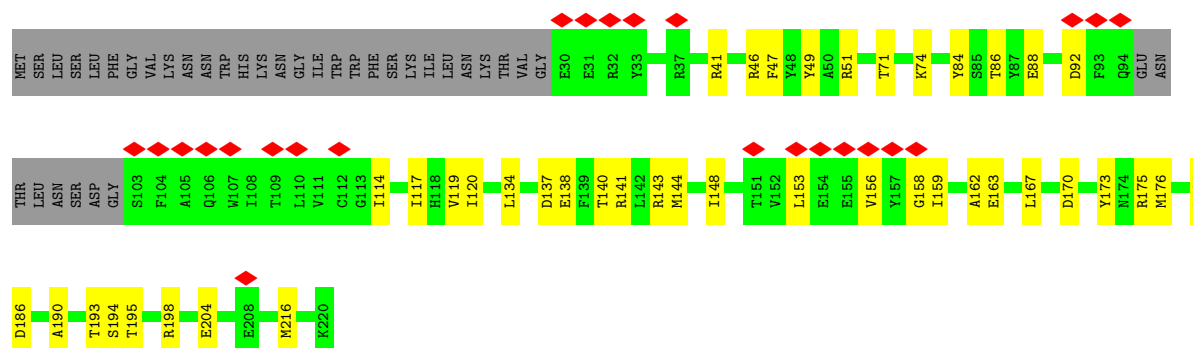
- Molecule 44: Cytochrome c oxidase subunit TT12



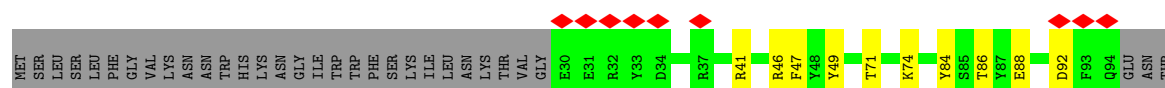
- Molecule 44: Cytochrome c oxidase subunit TT12

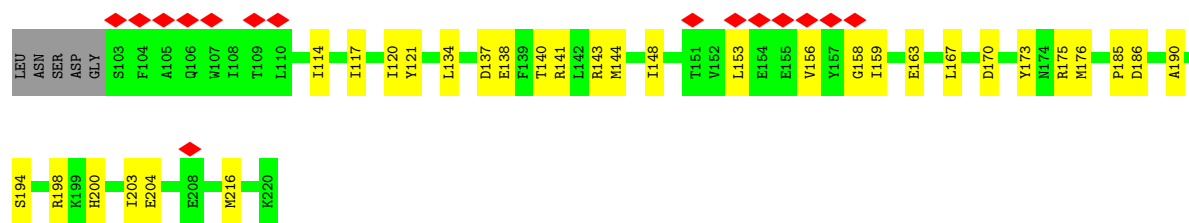


- Molecule 45: Transmembrane protein, putative

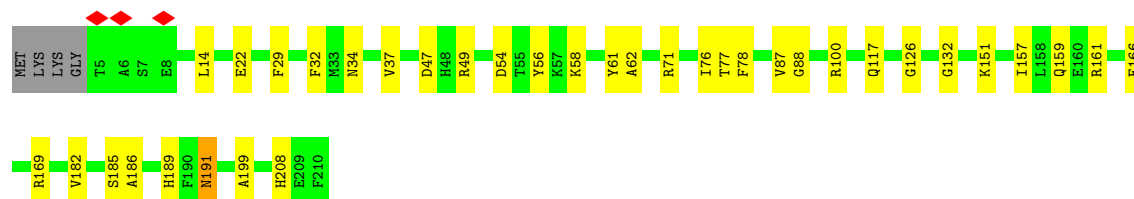
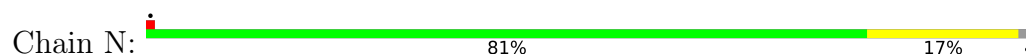


- Molecule 45: Transmembrane protein, putative

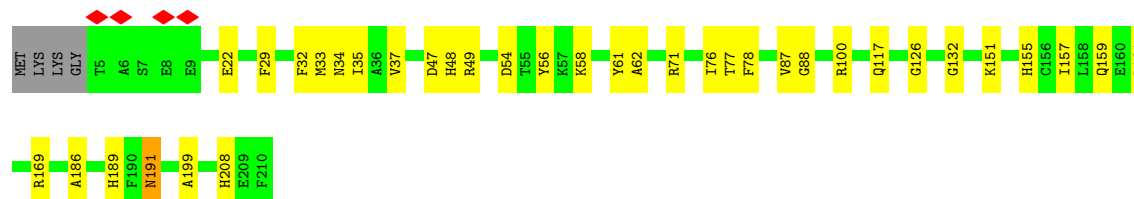
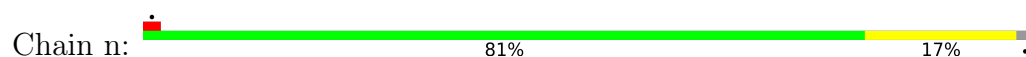




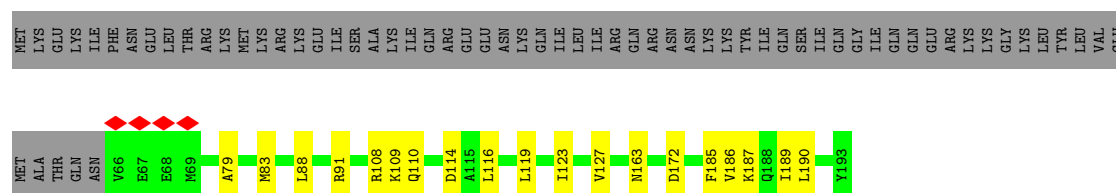
- Molecule 46: Transmembrane protein, putative



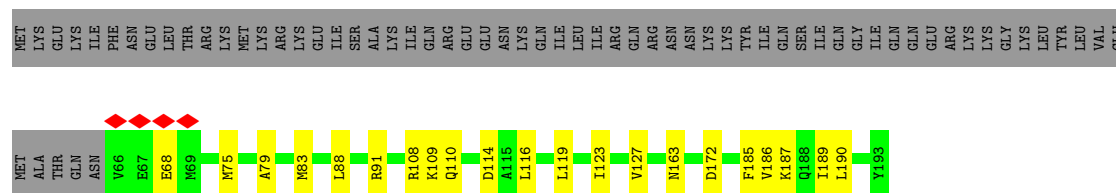
- Molecule 46: Transmembrane protein, putative



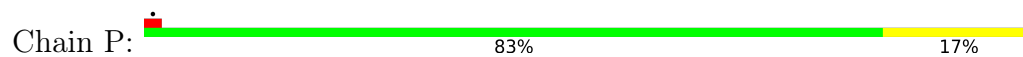
- Molecule 47: Cytochrome c oxidase subunit TT15



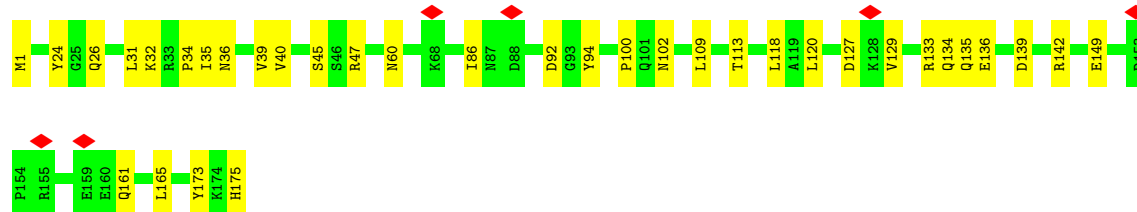
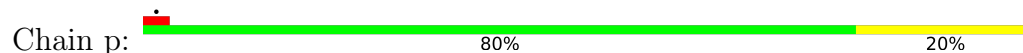
- Molecule 47: Cytochrome c oxidase subunit TT15



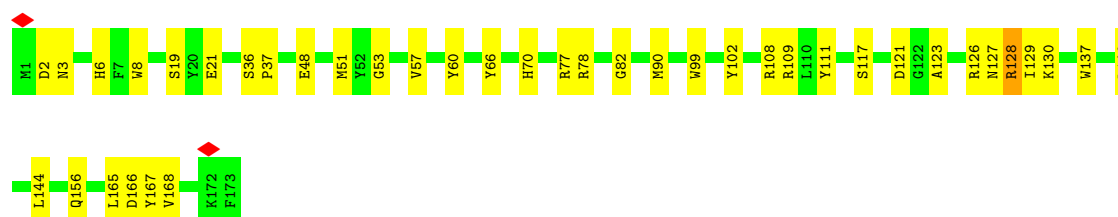
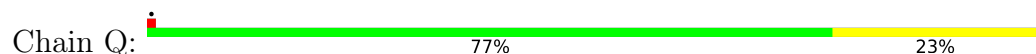
- Molecule 48: Cytochrome c oxidase subunit TT16



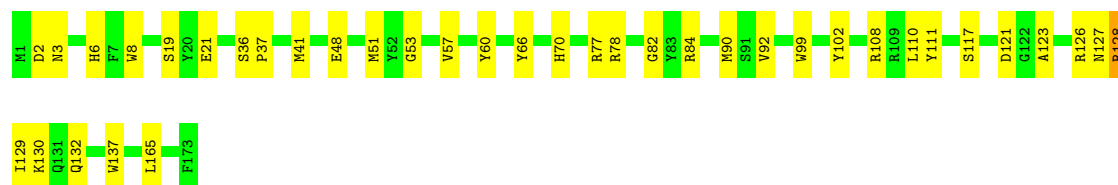
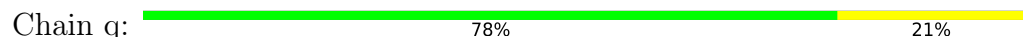
• Molecule 48: Cytochrome c oxidase subunit TT16



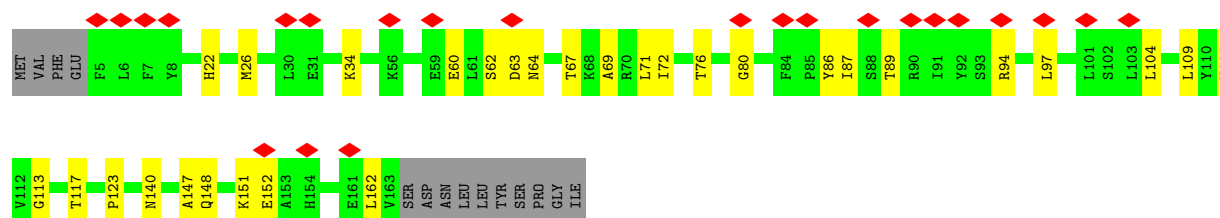
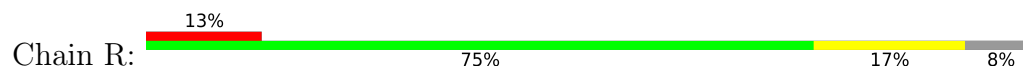
• Molecule 49: Transmembrane protein, putative



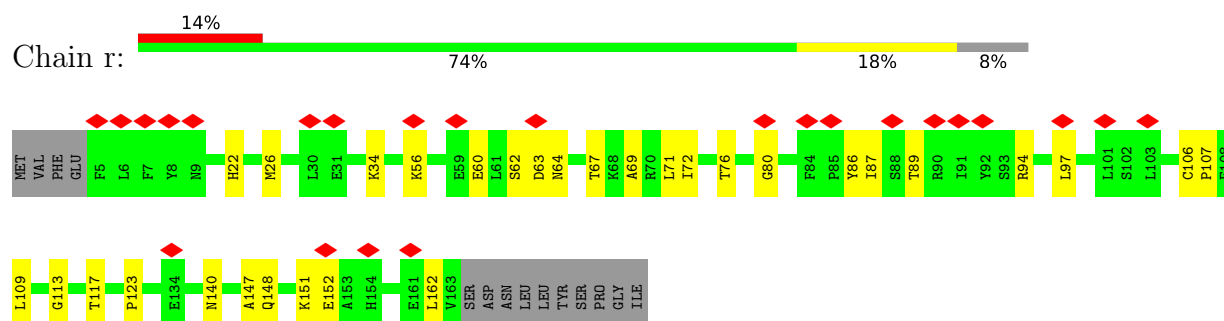
• Molecule 49: Transmembrane protein, putative



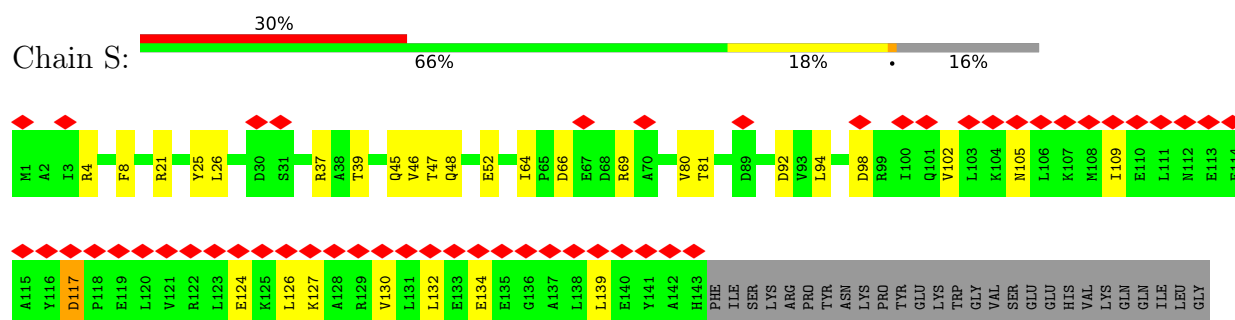
• Molecule 50: Cytochrome c oxidase subunit TT18



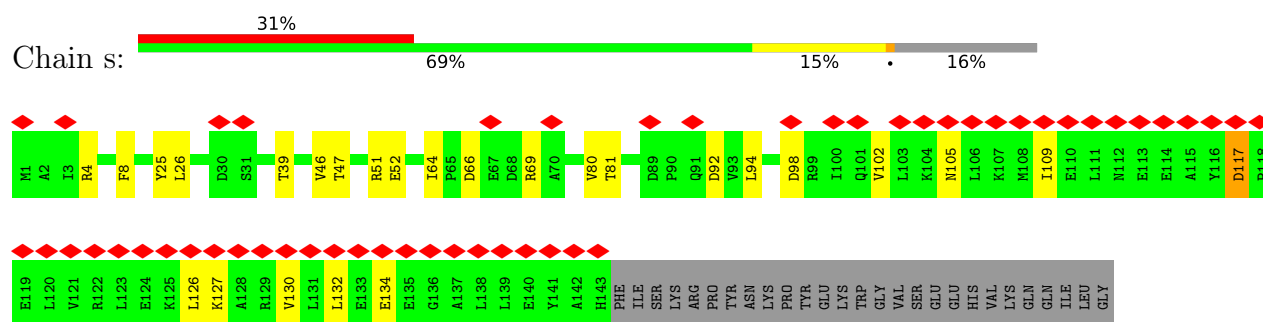
- Molecule 50: Cytochrome c oxidase subunit TT18



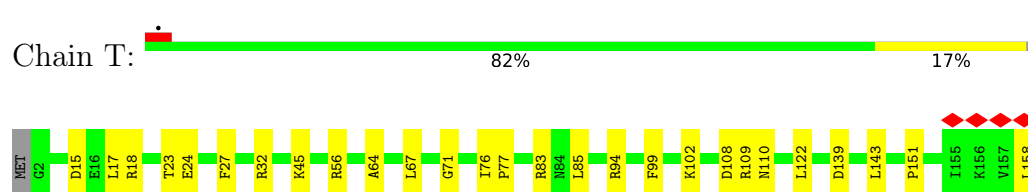
- Molecule 51: Cytochrome c oxidase subunit TT19



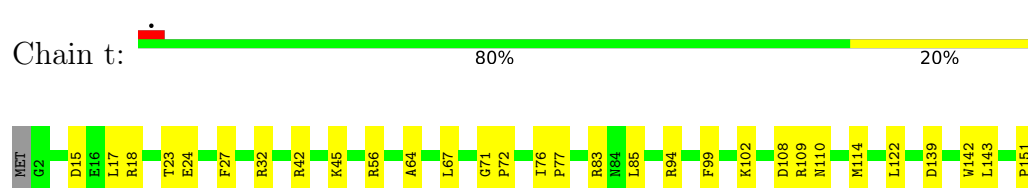
- Molecule 51: Cytochrome c oxidase subunit TT19



- Molecule 52: Transmembrane protein, putative



- Molecule 52: Transmembrane protein, putative



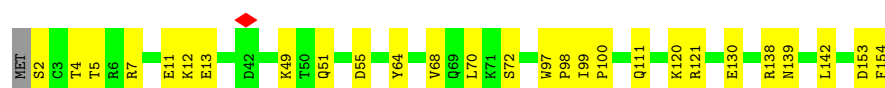
- Molecule 53: Transmembrane protein, putative

Chain U:  82% 17%



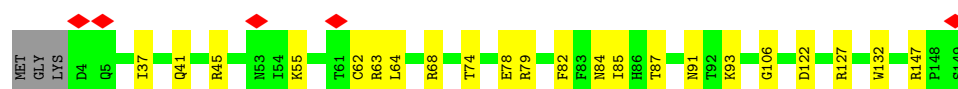
- Molecule 53: Transmembrane protein, putative

Chain u:  82% 18%



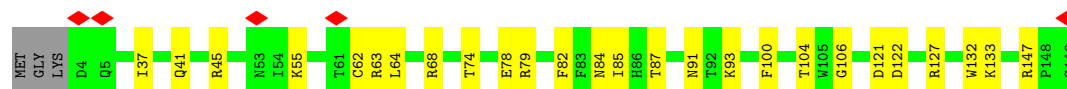
- Molecule 54: Cytochrome c oxidase subunit TT22

Chain V:  83% 15%



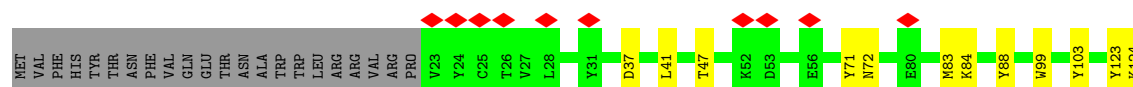
- Molecule 54: Cytochrome c oxidase subunit TT22

Chain v:  81% 17%



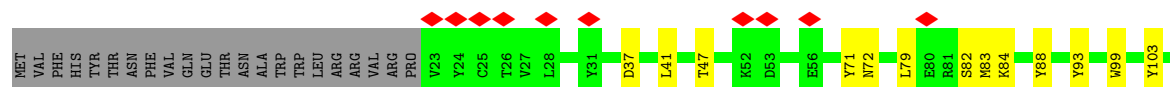
- Molecule 55: Transmembrane protein, putative

Chain W:  8% 73% 10% 18%



- Molecule 55: Transmembrane protein, putative

Chain w:  9% 70% 12% 18%

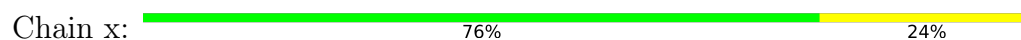


- Molecule 56: Transmembrane protein, putative

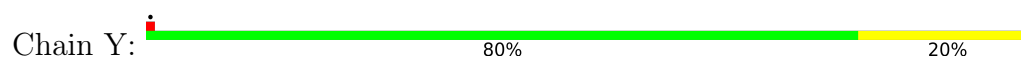
Chain X:  75% 25%



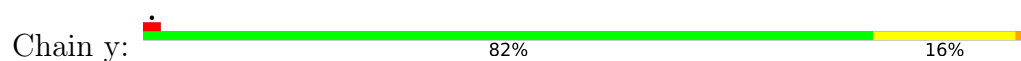
- Molecule 56: Transmembrane protein, putative



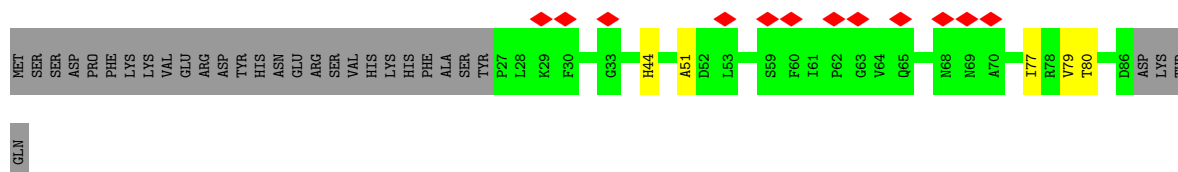
- Molecule 57: Cytochrome c oxidase subunit TT25



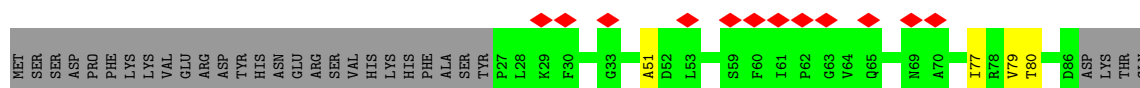
- Molecule 57: Cytochrome c oxidase subunit TT25



- Molecule 58: Cytochrome c oxidase subunit TT26



- Molecule 58: Cytochrome c oxidase subunit TT26



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	394262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	56818	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	33.161	Depositor
Minimum map value	-22.263	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	1.223	Depositor
Recommended contour level	5	Depositor
Map size (Å)	450.56, 450.56, 450.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CDL, CU, FES, MG, PC1, FME, SEP, HEA, TPO

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	$\# Z > 5$
2	U2	0.18	0/749	0.55	4/1031 (0.4%)
2	u2	0.17	0/749	0.55	4/1031 (0.4%)
5	U5	0.14	0/247	0.26	0/335
5	u5	0.12	0/247	0.23	0/335
6	U6	0.15	0/276	0.27	0/373
6	u6	0.14	0/276	0.27	0/373
7	C1	0.17	0/5752	0.31	0/7801
7	c1	0.17	0/5752	0.31	0/7801
8	C2	0.15	0/5027	0.30	0/6818
8	c2	0.16	0/5027	0.30	0/6818
9	C3	0.16	0/5098	0.28	0/6922
9	c3	0.16	0/5098	0.28	0/6922
10	5B	0.14	0/4706	0.23	0/6349
10	5b	0.14	0/4706	0.23	0/6349
11	6A	0.17	0/1107	0.27	0/1500
11	6a	0.16	0/1107	0.26	0/1500
12	6B	0.15	0/1968	0.26	0/2662
12	6b	0.15	0/1968	0.26	0/2662
13	6L	0.13	0/641	0.25	0/861
13	6l	0.13	0/641	0.25	0/861
14	6C	0.15	0/873	0.23	0/1184
14	6c	0.15	0/873	0.23	0/1184
15	7A	0.16	0/1198	0.26	0/1621
15	7a	0.16	0/1198	0.26	0/1621
16	7C	0.15	0/1830	0.24	0/2487
16	7c	0.15	0/1830	0.25	0/2487
17	7L	0.14	0/1099	0.27	0/1495
17	7l	0.15	0/1099	0.28	0/1495
18	M1	0.16	0/2958	0.30	0/4013
18	m1	0.16	0/2958	0.30	0/4013
19	M2	0.15	0/2621	0.26	0/3554
19	m2	0.15	0/2621	0.26	0/3554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	M3	0.14	0/2689	0.26	0/3657
20	m3	0.14	0/2689	0.27	0/3657
21	T1	0.15	0/546	0.22	0/735
21	t1	0.15	0/546	0.21	0/735
22	T2	0.12	0/518	0.23	0/694
22	t2	0.12	0/518	0.23	0/694
23	T3	0.12	0/662	0.24	0/888
23	t3	0.12	0/662	0.24	0/888
24	T4	0.16	0/483	0.29	0/652
24	t4	0.16	0/483	0.28	0/652
25	T5	0.13	0/523	0.25	0/705
25	t5	0.13	0/523	0.24	0/705
26	T6	0.14	0/565	0.26	0/760
26	t6	0.14	0/565	0.26	0/760
27	BP	0.13	0/2984	0.31	0/4047
27	bp	0.13	0/2984	0.31	0/4047
28	FS	0.14	0/1562	0.26	0/2123
28	fs	0.15	0/1562	0.26	0/2123
29	AC	0.14	0/836	0.22	0/1133
29	ac	0.14	0/836	0.23	0/1133
30	Y7	0.13	0/2968	0.23	0/4014
30	y7	0.13	0/2968	0.23	0/4014
31	Y0	0.16	0/793	0.27	0/1077
31	y0	0.16	0/793	0.27	0/1077
32	Y5	0.14	0/951	0.26	0/1284
32	y5	0.14	0/951	0.27	0/1284
33	A	0.16	0/3863	0.27	0/5258
33	a	0.16	0/3863	0.27	0/5258
34	B	0.11	0/1712	0.24	0/2318
34	b	0.11	0/1712	0.23	0/2318
35	C	0.10	0/393	0.26	0/531
35	c	0.10	0/393	0.26	0/531
36	D	0.14	0/2394	0.26	0/3254
36	d	0.14	0/2394	0.26	0/3254
37	E	0.14	0/3258	0.28	0/4425
37	e	0.14	0/3258	0.28	0/4425
38	F	0.15	0/2066	0.28	0/2809
38	f	0.15	0/2066	0.28	0/2809
39	G	0.16	0/2439	0.29	0/3328
39	g	0.16	0/2439	0.29	0/3328
40	H	0.13	0/1960	0.28	0/2656
40	h	0.13	0/1960	0.29	0/2656
41	I	0.09	0/873	0.22	0/1173

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	i	0.09	0/873	0.22	0/1173
42	J	0.14	0/1621	0.27	0/2201
42	j	0.14	0/1621	0.27	0/2201
43	K	0.15	0/1755	0.27	0/2376
43	k	0.14	0/1755	0.27	0/2376
44	L	0.12	0/1718	0.22	0/2333
44	l	0.13	0/1718	0.22	0/2333
45	M	0.14	0/1640	0.27	0/2227
45	m	0.14	0/1640	0.27	0/2227
46	N	0.14	0/1770	0.25	0/2391
46	n	0.14	0/1770	0.25	0/2391
47	O	0.14	0/1090	0.22	0/1466
47	o	0.14	0/1090	0.22	0/1466
48	P	0.13	0/1428	0.25	0/1931
48	p	0.13	0/1428	0.24	0/1931
49	Q	0.17	0/1478	0.31	0/2005
49	q	0.17	0/1478	0.30	0/2005
50	R	0.10	0/1336	0.22	0/1808
50	r	0.10	0/1336	0.22	0/1808
51	S	0.13	0/1178	0.25	0/1588
51	s	0.13	0/1178	0.25	0/1588
52	T	0.16	0/1367	0.29	0/1853
52	t	0.16	0/1367	0.30	0/1853
53	U	0.14	0/1335	0.25	0/1794
53	u	0.15	0/1335	0.25	0/1794
54	V	0.15	0/1277	0.25	0/1735
54	v	0.15	0/1277	0.25	0/1735
55	W	0.12	0/933	0.23	0/1266
55	w	0.12	0/933	0.23	0/1266
56	X	0.16	0/1043	0.25	0/1413
56	x	0.16	0/1043	0.25	0/1413
57	Y	0.15	0/882	0.23	0/1192
57	y	0.15	0/882	0.23	0/1192
58	Z	0.08	0/491	0.19	0/664
58	z	0.09	0/491	0.19	0/664
All	All	0.15	0/187060	0.27	8/253540 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U2	171	PRO	N-CA-CB	7.90	110.34	103.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	u2	171	PRO	N-CA-CB	7.90	110.34	103.31
2	U2	193	PRO	N-CA-CB	6.20	110.15	103.33
2	u2	246	PRO	N-CA-CB	6.17	110.12	103.33
2	U2	240	PRO	N-CA-CB	6.17	110.12	103.33
2	u2	193	PRO	N-CA-CB	6.17	110.12	103.33
2	U2	246	PRO	N-CA-CB	6.17	110.12	103.33
2	u2	240	PRO	N-CA-CB	6.17	110.11	103.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U1	490	0	102	1	0
1	u1	490	0	103	1	0
2	U2	743	0	482	9	0
2	u2	743	0	482	11	0
3	U3	170	0	36	0	0
3	u3	170	0	36	0	0
4	U4	150	0	32	0	0
4	u4	150	0	32	0	0
5	U5	242	0	206	7	0
5	u5	242	0	206	7	0
6	U6	275	0	258	5	0
6	u6	275	0	258	5	0
7	C1	5563	0	5607	131	0
7	c1	5563	0	5607	126	0
8	C2	4883	0	4861	81	0
8	c2	4883	0	4861	85	0
9	C3	4930	0	4914	94	0
9	c3	4930	0	4914	94	0
10	5B	4624	0	4401	83	0
10	5b	4624	0	4401	80	0
11	6A	1074	0	1014	21	0
11	6a	1074	0	1014	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	6B	1904	0	1764	32	0
12	6b	1904	0	1764	32	0
13	6L	638	0	638	6	0
13	6l	638	0	638	6	0
14	6C	841	0	763	17	0
14	6c	841	0	763	16	0
15	7A	1168	0	1128	33	0
15	7a	1168	0	1128	33	0
16	7C	1789	0	1606	25	0
16	7c	1789	0	1606	28	0
17	7L	1070	0	1062	25	0
17	7l	1070	0	1062	30	0
18	M1	2863	0	2781	46	0
18	m1	2863	0	2781	43	0
19	M2	2560	0	2551	27	0
19	m2	2560	0	2551	26	0
20	M3	2620	0	2584	35	0
20	m3	2620	0	2584	36	0
21	T1	540	0	532	7	0
21	t1	540	0	532	8	0
22	T2	513	0	512	9	0
22	t2	513	0	512	11	0
23	T3	655	0	669	4	0
23	t3	655	0	669	6	0
24	T4	483	0	464	9	0
24	t4	483	0	464	12	0
25	T5	515	0	510	7	0
25	t5	515	0	510	8	0
26	T6	563	0	563	10	0
26	t6	563	0	563	10	0
27	BP	2916	0	2814	46	0
27	bp	2916	0	2814	44	0
28	FS	1509	0	1477	24	0
28	fs	1509	0	1477	25	0
29	AC	816	0	795	9	0
29	ac	816	0	795	8	0
30	Y7	2895	0	2953	51	0
30	y7	2895	0	2953	57	0
31	Y0	777	0	797	14	0
31	y0	777	0	797	12	0
32	Y5	924	0	968	15	0
32	y5	924	0	968	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A	3746	0	3550	46	0
33	a	3746	0	3550	52	0
34	B	1682	0	1730	21	0
34	b	1682	0	1730	19	0
35	C	383	0	396	8	0
35	c	383	0	396	7	0
36	D	2331	0	2265	22	0
36	d	2331	0	2265	24	0
37	E	3178	0	3107	56	0
37	e	3178	0	3107	52	0
38	F	2014	0	1951	43	0
38	f	2014	0	1951	40	0
39	G	2364	0	2216	48	0
39	g	2364	0	2216	45	0
40	H	1915	0	1845	32	0
40	h	1915	0	1845	34	0
41	I	852	0	816	10	0
41	i	852	0	816	9	0
42	J	1575	0	1567	22	0
42	j	1575	0	1567	23	0
43	K	1714	0	1678	24	0
43	k	1714	0	1678	24	0
44	L	1668	0	1643	24	0
44	l	1668	0	1643	22	0
45	M	1581	0	1476	36	0
45	m	1581	0	1476	34	0
46	N	1716	0	1648	30	0
46	n	1716	0	1648	30	0
47	O	1073	0	1047	16	0
47	o	1073	0	1047	17	0
48	P	1412	0	1390	17	0
48	p	1412	0	1390	21	0
49	Q	1434	0	1393	27	0
49	q	1434	0	1393	29	0
50	R	1305	0	1323	28	0
50	r	1305	0	1323	28	0
51	S	1165	0	1189	24	0
51	s	1165	0	1189	22	0
52	T	1323	0	1297	25	0
52	t	1323	0	1297	29	0
53	U	1304	0	1299	19	0
53	u	1304	0	1299	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	V	1234	0	1194	21	0
54	v	1234	0	1194	24	0
55	W	902	0	848	9	0
55	w	902	0	848	11	0
56	X	1012	0	1000	23	0
56	x	1012	0	1000	23	0
57	Y	859	0	812	17	0
57	y	859	0	812	14	0
58	Z	479	0	475	4	0
58	z	479	0	475	3	0
59	C1	120	0	108	9	0
59	c1	120	0	108	7	0
60	C1	1	0	0	0	0
60	C2	2	0	0	0	0
60	c1	1	0	0	0	0
60	c2	2	0	0	0	0
61	C1	1	0	0	0	0
61	c1	1	0	0	0	0
62	7C	97	0	151	12	0
62	7c	43	0	63	5	0
62	A	86	0	120	4	0
62	C1	49	0	72	4	0
62	C3	163	0	225	6	0
62	J	37	0	48	0	0
62	M1	35	0	44	0	0
62	M2	127	0	182	8	0
62	N	68	0	84	3	0
62	V	54	0	88	3	0
62	a	86	0	120	5	0
62	c1	49	0	72	4	0
62	c3	163	0	225	6	0
62	j	37	0	48	0	0
62	m1	89	0	132	9	0
62	m2	127	0	182	7	0
62	n	68	0	84	4	0
62	v	54	0	88	3	0
63	5B	216	0	276	14	0
63	5b	154	0	205	9	0
63	7A	167	0	234	11	0
63	7C	136	0	166	9	0
63	7a	167	0	234	14	0
63	7c	136	0	166	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	A	51	0	46	0	0
63	B	62	0	68	0	0
63	C1	124	0	136	6	0
63	C3	68	0	80	0	0
63	E	132	0	158	7	0
63	F	100	0	156	12	0
63	J	70	0	84	6	0
63	L	74	0	95	3	0
63	M1	227	0	295	16	0
63	M2	194	0	220	9	0
63	M3	208	0	254	9	0
63	N	95	0	143	7	0
63	T	143	0	177	7	0
63	U	82	0	111	4	0
63	V	91	0	132	3	0
63	Y0	64	0	72	4	0
63	Y5	81	0	109	2	0
63	Y7	65	0	74	1	0
63	a	51	0	46	0	0
63	b	62	0	68	0	0
63	c1	124	0	136	6	0
63	c3	68	0	80	0	0
63	e	132	0	158	9	0
63	f	100	0	156	9	0
63	j	70	0	84	7	0
63	k	62	0	71	3	0
63	l	74	0	95	2	0
63	m1	227	0	295	15	0
63	m2	194	0	220	11	0
63	m3	208	0	254	12	0
63	n	95	0	143	9	0
63	t	143	0	177	7	0
63	u	82	0	111	4	0
63	v	91	0	132	3	0
63	y0	64	0	72	3	0
63	y5	81	0	109	1	0
63	y7	65	0	74	1	0
64	5B	1	0	0	0	0
64	5b	1	0	0	0	0
64	M	1	0	0	0	0
64	m	1	0	0	0	0
65	FS	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	fs	8	0	0	0	0
All	All	190448	0	186415	2493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2493) 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)
34:b:291:PHE:HB3	34:b:357:LEU:HB3	1.61	0.83
34:B:291:PHE:HB3	34:B:357:LEU:HB3	1.62	0.81
17:7L:936:TYR:HB3	17:7L:939:MET:HB2	1.61	0.81
17:7L:936:TYR:HB3	17:7L:939:MET:HB2	1.61	0.80
13:6L:49:PHE:HB2	14:6c:75:GLU:HG3	1.64	0.79
36:D:170:VAL:HG22	36:D:342:THR:HG21	1.65	0.79
36:d:170:VAL:HG22	36:d:342:THR:HG21	1.65	0.79
11:6a:50:SER:O	32:y5:174:ARG:NH2	2.17	0.78
7:c1:115:PHE:O	7:c1:119:ALA:HB3	1.83	0.78
7:C1:115:PHE:O	7:C1:119:ALA:HB3	1.83	0.78
13:6L:49:PHE:HB2	14:6C:75:GLU:HG3	1.66	0.77
40:H:215:LYS:HB2	40:H:220:GLN:HB2	1.66	0.77
40:h:215:LYS:HB2	40:h:220:GLN:HB2	1.65	0.77
19:m2:118:HIS:HB2	62:m2:405:PC1:H12	1.68	0.76
34:b:291:PHE:HE1	34:b:453:ASN:HD22	1.34	0.76
11:6A:50:SER:O	32:Y5:174:ARG:NH2	2.19	0.75
45:M:185:PRO:HG3	57:Y:64:LEU:HD13	1.69	0.75
34:B:291:PHE:HE1	34:B:453:ASN:HD22	1.35	0.75
53:U:4:THR:HG21	54:V:127:ARG:HG2	1.68	0.75
11:6A:43:ARG:NH1	11:6A:62:GLU:OE1	2.20	0.75
11:6a:43:ARG:NH1	11:6a:62:GLU:OE1	2.20	0.75
10:5b:263:ASP:OD1	30:y7:294:ARG:NH2	2.20	0.75
38:f:202:ILE:HG12	62:v:202:PC1:H271	1.69	0.74
20:M3:31:PHE:O	20:M3:45:LYS:NZ	2.21	0.74
10:5B:263:ASP:OD1	30:Y7:294:ARG:NH2	2.21	0.74
20:m3:31:PHE:O	20:m3:45:LYS:NZ	2.21	0.73
7:c1:331:LEU:HD21	10:5b:171:GLU:HG2	1.70	0.73
18:m1:117:TRP:HE1	63:m2:403:CDL:H1	1.53	0.73
45:m:159:ILE:HG23	45:m:194:SER:HB2	1.69	0.73
7:C1:331:LEU:HD21	10:5B:171:GLU:HG2	1.70	0.73
45:m:185:PRO:HG3	57:y:64:LEU:HD13	1.70	0.73
7:c1:628:GLU:HG2	7:c1:630:ARG:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:96:PHE:HB2	39:g:237:TRP:CZ2	2.23	0.72
45:M:159:ILE:HG23	45:M:194:SER:HB2	1.71	0.72
18:M1:117:TRP:HE1	63:M2:403:CDL:H1	1.54	0.72
39:G:96:PHE:HB2	39:G:237:TRP:CZ2	2.23	0.72
10:5b:139:ASN:ND2	10:5b:145:ASN:OD1	2.23	0.72
15:7a:118:PRO:HD3	15:7a:127:LEU:HD22	1.71	0.72
19:M2:118:HIS:HB2	62:M2:405:PC1:H12	1.71	0.71
7:c1:520:THR:HG23	7:c1:522:TYR:H	1.55	0.71
9:C3:558:LYS:HG2	44:L:104:GLU:HG3	1.72	0.71
53:U:142:LEU:HD11	53:U:153:ASP:HB2	1.70	0.71
9:c3:558:LYS:HG2	44:l:104:GLU:HG3	1.72	0.71
53:u:4:THR:HG21	54:v:127:ARG:HG2	1.73	0.71
9:C3:582:ARG:NH1	56:X:1:MET:O	2.24	0.71
9:c3:582:ARG:NH1	56:x:1:MET:O	2.24	0.71
15:7A:118:PRO:HD3	15:7A:127:LEU:HD22	1.72	0.71
44:L:78:ILE:HG23	44:L:176:MET:HG3	1.71	0.71
53:u:142:LEU:HD11	53:u:153:ASP:HB2	1.71	0.71
7:c1:510:HIS:HD1	7:c1:513:LEU:H	1.38	0.71
7:C1:628:GLU:HG2	7:C1:630:ARG:HG2	1.74	0.70
7:C1:520:THR:HG23	7:C1:522:TYR:H	1.56	0.70
63:e:402:CDL:HA4	63:e:402:CDL:H711	1.73	0.70
27:BP:85:LEU:HB3	27:BP:107:VAL:HB	1.74	0.70
48:p:133:ARG:HG3	48:p:134:GLN:HG3	1.73	0.70
7:C1:433:MET:HE3	7:C1:462:ILE:HD13	1.73	0.69
10:5B:158:TYR:HB2	39:G:215:PRO:HB3	1.74	0.69
63:E:402:CDL:HA4	63:E:402:CDL:H711	1.73	0.69
44:l:78:ILE:HG23	44:l:176:MET:HG3	1.73	0.69
18:M1:293:SER:HB2	63:M1:401:CDL:HB32	1.74	0.69
38:F:202:ILE:HG12	62:V:202:PC1:H271	1.72	0.69
48:P:133:ARG:HG3	48:P:134:GLN:HG3	1.73	0.69
38:F:120:ASP:OD1	54:V:45:ARG:NH2	2.26	0.69
10:5B:403:ASP:OD1	33:A:465:ARG:NH2	2.24	0.69
18:m1:17:ASP:O	18:m1:339:ASN:ND2	2.25	0.69
31:y0:71:LYS:HB3	63:y0:101:CDL:H142	1.74	0.69
10:5B:499:GLU:HG3	51:S:26:LEU:HD21	1.75	0.69
7:c1:518:HIS:O	8:c2:524:LYS:NZ	2.19	0.69
8:c2:270:ASN:HB3	21:t1:4:GLU:HB3	1.75	0.69
7:C1:510:HIS:HD1	7:C1:513:LEU:H	1.40	0.69
10:5b:158:TYR:HB2	39:g:215:PRO:HB3	1.74	0.69
10:5b:403:ASP:OD1	33:a:465:ARG:NH2	2.26	0.69
10:5b:499:GLU:HG3	51:s:26:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:50:ILE:HD11	37:e:66:LEU:HD23	1.74	0.69
7:C1:41:LEU:HD11	63:C1:706:CDL:HB61	1.76	0.68
17:7L:920:LEU:HD12	17:7L:938:TYR:HB2	1.75	0.68
10:5B:482:LEU:HD11	51:S:26:LEU:HD22	1.75	0.68
7:C1:485:ASP:HB3	7:C1:487:PRO:HD2	1.75	0.68
7:c1:92:LEU:HD22	7:c1:270:THR:HB	1.74	0.68
7:c1:485:ASP:HB3	7:c1:487:PRO:HD2	1.76	0.68
7:c1:433:MET:HE3	7:c1:462:ILE:HD13	1.74	0.68
10:5b:482:LEU:HD11	51:s:26:LEU:HD22	1.75	0.68
28:fs:149:ASN:HD22	39:g:259:THR:HG21	1.58	0.68
7:C1:92:LEU:HD22	7:C1:270:THR:HB	1.74	0.68
37:E:50:ILE:HD11	37:E:66:LEU:HD23	1.76	0.68
10:5B:329:ARG:NH2	10:5B:403:ASP:OD2	2.26	0.67
28:FS:149:ASN:HD22	39:G:259:THR:HG21	1.59	0.67
31:Y0:71:LYS:HB3	63:Y0:101:CDL:H142	1.76	0.67
43:K:207:VAL:HG21	44:L:149:LEU:HD11	1.76	0.67
7:c1:82:PRO:HD3	7:c1:598:MET:HB3	1.76	0.67
8:C2:270:ASN:HB3	21:T1:4:GLU:HB3	1.76	0.67
18:m1:310:PRO:HB3	63:m1:404:CDL:H802	1.76	0.67
51:S:102:VAL:HG13	51:S:126:LEU:HD22	1.76	0.67
7:c1:41:LEU:HD11	63:c1:706:CDL:HB61	1.75	0.67
51:s:102:VAL:HG13	51:s:126:LEU:HD22	1.76	0.67
2:u2:253:THR:HB	30:y7:135:SER:HB2	1.75	0.67
63:y0:101:CDL:H721	45:m:47:PHE:HB2	1.76	0.67
2:U2:253:THR:HB	30:Y7:135:SER:HB2	1.74	0.67
7:C1:126:HIS:ND1	7:C1:336:THR:OG1	2.28	0.66
20:m3:113:SER:HB2	63:k:301:CDL:HB31	1.77	0.66
38:f:120:ASP:OD1	54:v:45:ARG:NH2	2.25	0.66
43:k:207:VAL:HG21	44:l:149:LEU:HD11	1.77	0.66
18:M1:17:ASP:O	18:M1:339:ASN:ND2	2.27	0.66
63:Y0:101:CDL:H721	45:M:47:PHE:HB2	1.77	0.66
12:6b:220:PRO:HA	49:q:37:PRO:HB2	1.76	0.66
27:bp:85:LEU:HB3	27:bp:107:VAL:HB	1.76	0.66
10:5b:428:PRO:HG3	37:e:19:GLY:HA2	1.76	0.66
7:C1:181:TYR:OH	46:N:47:ASP:OD2	2.14	0.66
7:C1:672:ARG:NH2	18:M1:295:ASN:O	2.28	0.66
42:J:51:ARG:NH2	42:J:165:GLU:OE2	2.27	0.66
43:k:216:GLN:O	43:k:222:ASN:ND2	2.29	0.66
10:5b:329:ARG:NH2	10:5b:403:ASP:OD2	2.28	0.66
20:m3:178:THR:O	20:m3:182:ASN:ND2	2.27	0.66
42:j:51:ARG:NH2	42:j:165:GLU:OE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:80:VAL:HG12	51:s:81:THR:HG23	1.78	0.66
50:r:69:ALA:HA	50:r:117:THR:HG21	1.78	0.66
43:K:216:GLN:O	43:K:222:ASN:ND2	2.29	0.66
16:7c:89:PRO:HG2	54:v:79:ARG:HD3	1.77	0.66
17:7l:920:LEU:HD12	17:7l:938:TYR:HB2	1.78	0.66
30:Y7:114:PHE:O	30:Y7:118:ASN:ND2	2.29	0.65
51:S:117:ASP:N	51:S:117:ASP:OD1	2.29	0.65
14:6C:14:ARG:NH1	28:FS:105:GLN:OE1	2.29	0.65
43:K:55:TYR:O	46:N:117:GLN:NE2	2.30	0.65
51:S:80:VAL:HG12	51:S:81:THR:HG23	1.79	0.65
7:c1:159:ARG:HE	7:c1:265:SER:HB3	1.60	0.65
14:6c:14:ARG:NH1	28:fs:105:GLN:OE1	2.29	0.65
51:s:117:ASP:N	51:s:117:ASP:OD1	2.29	0.65
50:R:69:ALA:HA	50:R:117:THR:HG21	1.79	0.65
8:C2:271:ASN:ND2	21:T1:7:ASN:OD1	2.29	0.65
12:6B:220:PRO:HA	49:Q:37:PRO:HB2	1.77	0.65
53:U:7:ARG:NH1	54:V:122:ASP:OD2	2.30	0.65
5:U5:138:ASP:OD1	5:U5:146:LYS:NZ	2.30	0.65
7:c1:501:ALA:HB2	7:c1:529:ILE:HG22	1.77	0.65
22:t2:49:GLU:OE2	22:t2:52:ARG:NH2	2.28	0.65
53:u:7:ARG:NH1	54:v:122:ASP:OD2	2.30	0.65
6:U6:155:VAL:HG21	50:R:147:ALA:HA	1.79	0.64
7:C1:501:ALA:HB2	7:C1:529:ILE:HG22	1.78	0.64
20:M3:178:THR:O	20:M3:182:ASN:ND2	2.29	0.64
24:T4:33:GLU:OE2	44:L:218:ARG:NH2	2.28	0.64
30:y7:114:PHE:O	30:y7:118:ASN:ND2	2.31	0.64
8:C2:116:ARG:NH2	12:6B:177:GLN:O	2.29	0.64
7:c1:181:TYR:OH	46:n:47:ASP:OD2	2.16	0.64
18:m1:293:SER:HB2	63:m1:401:CDL:HB32	1.79	0.64
17:7L:899:GLN:NE2	17:7L:940:ARG:O	2.30	0.64
8:c2:8:GLU:OE2	8:c2:486:ARG:NH2	2.31	0.64
30:y7:110:ARG:NH2	35:c:464:ASN:OD1	2.31	0.64
38:f:136:ARG:NH2	38:f:322:LYS:O	2.30	0.64
10:5b:164:GLN:NE2	39:g:226:VAL:O	2.31	0.64
17:7l:899:GLN:NE2	17:7l:940:ARG:O	2.30	0.64
20:m3:32:LYS:NZ	42:j:226:ASN:O	2.30	0.64
7:c1:672:ARG:NH2	18:m1:295:ASN:O	2.29	0.64
16:7C:120:SEP:O	33:A:246:ASN:ND2	2.30	0.64
9:c3:106:VAL:HG22	20:m3:247:PRO:HB2	1.80	0.64
18:M1:1:MET:HG2	18:M1:6:GLU:HB2	1.78	0.64
30:y7:191:ASN:HD21	51:s:47:THR:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5B:428:PRO:HG3	37:E:19:GLY:HA2	1.79	0.63
20:M3:32:LYS:NZ	42:J:226:ASN:O	2.31	0.63
9:c3:419:ILE:HD11	33:a:330:LEU:HD22	1.80	0.63
14:6c:77:GLU:OE2	17:7L:965:ARG:NH1	2.31	0.63
9:C3:106:VAL:HG22	20:M3:247:PRO:HB2	1.80	0.63
53:U:130:GLU:OE1	53:U:139:ASN:ND2	2.31	0.63
42:J:181:ARG:NH1	62:N:302:PC1:O32	2.31	0.63
7:c1:558:MET:HE1	63:m1:401:CDL:H532	1.80	0.63
10:5B:85:HIS:CE1	63:5B:702:CDL:H511	2.34	0.63
8:C2:109:GLU:OE2	12:6B:121:GLN:NE2	2.32	0.63
14:6C:77:GLU:OE2	17:7L:965:ARG:NH1	2.32	0.63
10:5b:85:HIS:CE1	63:5b:702:CDL:H511	2.33	0.63
43:k:55:TYR:O	46:n:117:GLN:NE2	2.32	0.63
10:5B:164:GLN:NE2	39:G:226:VAL:O	2.32	0.63
30:Y7:110:ARG:NH2	35:C:464:ASN:OD1	2.30	0.63
8:c2:271:ASN:ND2	21:t1:7:ASN:OD1	2.30	0.63
18:m1:1:MET:HG2	18:m1:6:GLU:HB2	1.79	0.63
42:j:181:ARG:NH1	62:n:302:PC1:O32	2.32	0.63
22:T2:49:GLU:OE2	22:T2:52:ARG:NH2	2.29	0.63
53:u:130:GLU:OE1	53:u:139:ASN:ND2	2.31	0.63
16:7C:89:PRO:HG2	54:V:79:ARG:HD3	1.80	0.63
8:c2:391:LEU:HG	47:o:116:LEU:HD22	1.80	0.63
17:7L:879:SER:HB2	17:7L:882:MET:HB2	1.81	0.63
10:5b:105:GLU:HG3	10:5b:106:GLU:HG3	1.81	0.63
15:7a:104:GLU:HG3	62:a:501:PC1:H151	1.80	0.63
28:fs:174:LEU:HD12	63:f:401:CDL:H871	1.79	0.63
8:C2:1:MET:HE3	12:6B:78:MET:HG3	1.81	0.62
18:M1:310:PRO:HB3	63:M1:403:CDL:H802	1.78	0.62
7:C1:557:ARG:HH22	18:M1:293:SER:HG	1.46	0.62
9:C3:400:TYR:HA	62:C3:605:PC1:H222	1.81	0.62
28:FS:174:LEU:HD12	63:F:401:CDL:H871	1.79	0.62
39:g:91:ASP:OD2	39:g:118:ARG:NH2	2.32	0.62
8:C2:392:ARG:NH2	12:6B:145:LEU:O	2.27	0.62
15:7A:104:GLU:HG3	62:A:501:PC1:H151	1.81	0.62
63:M3:401:CDL:H782	63:M3:401:CDL:H581	1.81	0.62
14:6c:51:GLU:HG2	45:m:167:LEU:HD13	1.81	0.62
19:m2:111:LYS:NZ	46:n:22:GLU:OE2	2.31	0.62
8:C2:112:LEU:N	8:C2:502:ASN:O	2.32	0.62
8:c2:116:ARG:NH2	12:6b:177:GLN:O	2.32	0.62
9:C3:19:ASP:HB2	9:C3:59:PRO:HB2	1.80	0.62
37:E:173:GLU:OE2	37:E:281:HIS:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:c1:705:PC1:H31	9:c3:292:PHE:HE2	1.64	0.62
8:c2:7:THR:O	8:c2:544:PHE:N	2.30	0.62
24:t4:33:GLU:OE2	44:l:218:ARG:NH2	2.28	0.62
50:r:76:THR:HG22	50:r:109:LEU:HB3	1.81	0.62
19:M2:7:ARG:NH1	19:M2:10:GLU:OE2	2.32	0.62
8:c2:112:LEU:N	8:c2:502:ASN:O	2.33	0.62
10:5b:362:ARG:NH2	10:5b:383:ASP:OD2	2.32	0.62
27:bp:99:THR:O	27:bp:105:ARG:NH2	2.33	0.62
8:C2:7:THR:O	8:C2:544:PHE:N	2.31	0.62
9:c3:19:ASP:HB2	9:c3:59:PRO:HB2	1.81	0.62
9:c3:400:TYR:HA	62:c3:605:PC1:H222	1.81	0.62
54:v:64:LEU:HB3	54:v:68:ARG:HD3	1.80	0.62
14:6C:51:GLU:HG2	45:M:167:LEU:HD13	1.81	0.62
33:A:192:PRO:HB2	33:A:207:VAL:HG21	1.82	0.62
50:R:76:THR:HG22	50:R:109:LEU:HB3	1.82	0.62
54:V:106:GLY:O	54:V:147:ARG:NH2	2.33	0.62
7:c1:155:ILE:HD13	7:c1:295:LEU:HD21	1.81	0.62
8:c2:1:MET:HE3	12:6b:78:MET:HG3	1.82	0.62
10:5b:86:ILE:HG12	63:5b:702:CDL:H602	1.82	0.62
33:a:192:PRO:HB2	33:a:207:VAL:HG21	1.82	0.62
10:5B:86:ILE:HG12	63:5B:702:CDL:H602	1.82	0.61
16:7C:94:MET:HG3	18:M1:267:PRO:HG2	1.82	0.61
8:c2:109:GLU:OE2	12:6b:121:GLN:NE2	2.33	0.61
44:l:66:LYS:O	44:l:71:ARG:NH1	2.34	0.61
37:E:112:LEU:HD22	37:E:179:LEU:HD22	1.83	0.61
45:m:163:GLU:OE2	45:m:198:ARG:NH2	2.33	0.61
21:T1:11:THR:HG23	26:T6:5:LEU:HD22	1.82	0.61
8:c2:568:PRO:HG2	8:c2:571:HIS:HD2	1.65	0.61
62:C1:705:PC1:H31	9:C3:292:PHE:HE2	1.65	0.61
15:7a:76:ARG:NH1	63:7a:202:CDL:OA3	2.33	0.61
5:u5:138:ASP:OD1	5:u5:146:LYS:NZ	2.33	0.61
17:7l:879:SER:HB2	17:7l:882:MET:HB2	1.83	0.61
10:5B:362:ARG:NH2	10:5B:383:ASP:OD2	2.32	0.61
19:M2:111:LYS:NZ	46:N:22:GLU:OE2	2.34	0.61
44:L:66:LYS:O	44:L:71:ARG:NH1	2.34	0.61
45:M:163:GLU:OE2	45:M:198:ARG:NH2	2.34	0.61
54:V:64:LEU:HB3	54:V:68:ARG:HD3	1.81	0.61
37:e:13:ASN:ND2	37:e:24:ALA:O	2.34	0.61
7:c1:645:ARG:NH1	39:g:234:GLU:OE2	2.34	0.61
20:m3:90:ARG:NH1	20:m3:128:GLY:O	2.33	0.61
33:a:268:GLU:HG2	43:k:64:LYS:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:173:GLU:OE2	37:e:281:HIS:NE2	2.33	0.61
38:f:119:TYR:HB2	54:v:41:GLN:HG2	1.83	0.61
7:C1:82:PRO:HD3	7:C1:598:MET:HB3	1.82	0.61
63:m3:401:CDL:H782	63:m3:401:CDL:H581	1.82	0.61
30:y7:171:ASP:OD1	30:y7:172:ASN:ND2	2.33	0.61
8:C2:354:PRO:HD2	12:6B:198:ALA:HB2	1.82	0.61
9:C3:283:TYR:HD1	63:7A:201:CDL:H512	1.65	0.61
30:Y7:171:ASP:OD1	30:Y7:172:ASN:ND2	2.34	0.61
63:E:401:CDL:H511	63:E:401:CDL:H121	1.81	0.61
38:F:136:ARG:NH2	38:F:322:LYS:O	2.31	0.61
41:I:152:GLN:HG2	41:I:195:PRO:HG3	1.83	0.61
7:C1:155:ILE:HD13	7:C1:295:LEU:HD21	1.83	0.60
7:C1:401:THR:HG21	7:C1:535:ALA:HA	1.83	0.60
15:7A:54:ILE:O	16:7C:120:SEP:N	2.34	0.60
20:M3:90:ARG:NH1	20:M3:128:GLY:O	2.33	0.60
21:T1:53:ALA:HB1	26:T6:59:LEU:HG	1.83	0.60
52:T:15:ASP:OD1	52:T:18:ARG:NH2	2.34	0.60
9:c3:173:SER:HB3	48:p:35:ILE:HG21	1.82	0.60
34:b:290:ILE:HD13	34:b:359:LEU:HB2	1.82	0.60
8:C2:391:LEU:HG	47:O:116:LEU:HD22	1.83	0.60
8:C2:431:TYR:O	8:C2:439:THR:N	2.35	0.60
37:E:13:ASN:ND2	37:E:24:ALA:O	2.34	0.60
7:c1:401:THR:HG21	7:c1:535:ALA:HA	1.83	0.60
8:C2:563:ARG:NH1	12:6B:77:ASP:OD2	2.34	0.60
6:u6:155:VAL:HG21	50:r:147:ALA:HA	1.84	0.60
8:c2:476:ARG:NH2	18:m1:331:ASP:OD1	2.34	0.60
21:t1:11:THR:HG23	26:t6:5:LEU:HD22	1.83	0.60
8:C2:476:ARG:NH2	18:M1:331:ASP:OD1	2.34	0.60
34:B:290:ILE:HD13	34:B:359:LEU:HB2	1.82	0.60
8:c2:354:PRO:HD2	12:6b:198:ALA:HB2	1.82	0.60
37:e:112:LEU:HD22	37:e:179:LEU:HD22	1.84	0.60
38:F:119:TYR:HB2	54:V:41:GLN:HG2	1.84	0.60
7:c1:331:LEU:HB3	10:5b:175:LEU:HD22	1.83	0.60
8:c2:431:TYR:O	8:c2:439:THR:N	2.35	0.60
15:7a:54:ILE:O	16:7c:120:SEP:N	2.34	0.60
40:h:216:PRO:C	40:h:218:GLU:H	2.08	0.60
54:v:106:GLY:O	54:v:147:ARG:NH2	2.35	0.60
15:7A:58:GLU:OE2	15:7A:75:TYR:OH	2.19	0.60
8:C2:568:PRO:HG2	8:C2:571:HIS:HD2	1.66	0.60
20:M3:289:ASN:O	20:M3:293:ALA:HB2	2.02	0.60
41:I:131:LYS:HG3	50:R:162:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c3:279:ALA:HA	63:7a:201:CDL:H552	1.84	0.60
15:7a:58:GLU:OE2	15:7a:75:TYR:OH	2.19	0.60
22:t2:52:ARG:NH1	22:t2:56:GLU:OE2	2.35	0.60
63:e:401:CDL:H511	63:e:401:CDL:H121	1.82	0.60
49:q:130:LYS:HE3	49:q:165:LEU:HD12	1.83	0.60
22:T2:52:ARG:NH1	22:T2:56:GLU:OE2	2.35	0.60
40:H:216:PRO:C	40:H:218:GLU:H	2.08	0.60
40:H:250:ASN:ND2	40:H:264:ASP:OD2	2.35	0.60
46:N:58:LYS:HD3	46:N:61:TYR:HA	1.84	0.60
7:c1:338:SER:HB3	7:c1:399:ILE:HG22	1.84	0.60
8:c2:563:ARG:NH1	12:6b:77:ASP:OD2	2.34	0.60
48:p:36:ASN:ND2	48:p:92:ASP:O	2.34	0.60
8:C2:143:ILE:HB	17:7L:893:LEU:HD11	1.84	0.59
29:AC:54:GLY:HA2	29:AC:70:ILE:HD12	1.84	0.59
7:c1:126:HIS:NE2	39:g:187:ASP:OD1	2.35	0.59
8:C2:8:GLU:OE2	8:C2:486:ARG:NH2	2.35	0.59
10:5b:446:ARG:NH1	10:5b:459:ASN:OD1	2.34	0.59
48:p:135:GLN:NE2	48:p:139:ASP:OD1	2.35	0.59
9:C3:173:SER:HB3	48:P:35:ILE:HG21	1.83	0.59
9:C3:265:LEU:HD13	46:N:54:ASP:HB2	1.84	0.59
10:5b:457:ARG:NH1	10:5b:520:SEP:O2P	2.34	0.59
6:U6:155:VAL:HG11	50:R:147:ALA:HB1	1.83	0.59
9:C3:279:ALA:HA	63:7A:201:CDL:H552	1.84	0.59
63:5B:703:CDL:HB31	20:M3:113:SER:HB2	1.84	0.59
9:c3:294:LYS:HD3	15:7a:59:GLU:HG2	1.84	0.59
15:7a:80:VAL:HG11	30:y7:350:LEU:HB2	1.85	0.59
7:C1:558:MET:HE1	63:M1:401:CDL:H532	1.82	0.59
31:Y0:1:FME:HB2	32:Y5:178:ILE:HG12	1.82	0.59
41:I:141:LEU:HD22	50:R:148:GLN:HG2	1.85	0.59
16:7c:120:SEP:O	33:a:246:ASN:ND2	2.34	0.59
20:m3:289:ASN:O	20:m3:293:ALA:HB2	2.02	0.59
41:i:131:LYS:HG3	50:r:162:LEU:HD13	1.83	0.59
7:C1:331:LEU:HB3	10:5B:175:LEU:HD22	1.85	0.59
7:C1:338:SER:HB3	7:C1:399:ILE:HG22	1.85	0.59
9:C3:294:LYS:HD3	15:7A:59:GLU:HG2	1.85	0.59
38:f:194:LYS:NZ	62:v:202:PC1:O12	2.35	0.59
52:t:15:ASP:OD1	52:t:18:ARG:NH2	2.35	0.59
7:C1:645:ARG:NH1	39:G:234:GLU:OE2	2.35	0.59
27:bp:87:THR:HG21	27:bp:95:THR:HA	1.84	0.59
8:C2:157:GLN:NE2	8:C2:370:GLU:OE2	2.36	0.59
10:5B:105:GLU:HG3	10:5B:106:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7A:80:VAL:HG11	30:Y7:350:LEU:HB2	1.85	0.59
19:M2:44:ARG:HG3	19:M2:45:THR:HG23	1.85	0.59
19:M2:244:ARG:NH1	19:M2:273:GLU:OE2	2.36	0.59
33:A:268:GLU:HG2	43:K:64:LYS:HD2	1.84	0.59
21:t1:53:ALA:HB1	26:t6:59:LEU:HG	1.84	0.59
5:u5:143:ARG:HH11	50:r:71:LEU:HD22	1.68	0.59
27:BP:340:ASN:OD1	27:BP:342:ARG:NH1	2.36	0.59
63:5b:702:CDL:H522	33:a:360:TRP:CH2	2.38	0.59
28:fs:145:ALA:HB3	28:fs:146:PRO:HD3	1.83	0.59
36:d:167:TYR:HB2	36:d:170:VAL:HG23	1.85	0.59
41:i:152:GLN:HG2	41:i:195:PRO:HG3	1.85	0.59
10:5B:446:ARG:NH1	10:5B:459:ASN:OD1	2.33	0.58
15:7A:76:ARG:NH1	63:7A:202:CDL:OA3	2.32	0.58
16:7C:34:ARG:HD2	19:M2:48:VAL:HA	1.85	0.58
30:Y7:191:ASN:HD21	51:S:47:THR:HA	1.68	0.58
36:D:369:PHE:O	36:D:371:ARG:NH1	2.36	0.58
40:h:250:ASN:ND2	40:h:264:ASP:OD2	2.36	0.58
16:7c:94:MET:HG3	18:m1:267:PRO:HG2	1.85	0.58
38:f:192:LEU:HB3	38:f:196:ALA:HB3	1.84	0.58
19:m2:244:ARG:NH1	19:m2:273:GLU:OE2	2.36	0.58
38:f:254:GLN:OE1	54:v:79:ARG:NH2	2.36	0.58
63:F:401:CDL:H801	63:F:401:CDL:H362	1.84	0.58
8:c2:390:ARG:HH22	12:6b:149:ASP:CG	2.11	0.58
9:c3:266:LEU:HB3	9:c3:271:ILE:HG21	1.85	0.58
29:ac:54:GLY:HA2	29:ac:70:ILE:HD12	1.85	0.58
7:C1:307:THR:HA	7:C1:310:PHE:CE2	2.38	0.58
7:C1:615:ILE:HD12	59:C1:701:HEA:H18	1.84	0.58
63:5B:702:CDL:H522	33:A:360:TRP:CH2	2.39	0.58
27:BP:87:THR:HG21	27:BP:95:THR:HA	1.84	0.58
25:t5:4:ASN:HB2	25:t5:7:ALA:HB3	1.85	0.58
27:BP:99:THR:O	27:BP:105:ARG:NH2	2.37	0.58
38:F:194:LYS:NZ	62:V:202:PC1:O12	2.37	0.58
28:fs:167:TYR:HB2	63:f:401:CDL:H802	1.86	0.58
30:y7:348:TYR:HE2	63:n:303:CDL:H251	1.68	0.58
63:5B:703:CDL:H331	56:X:79:ILE:HD11	1.84	0.58
39:G:91:ASP:OD2	39:G:118:ARG:NH2	2.36	0.58
48:P:135:GLN:NE2	48:P:139:ASP:OD1	2.36	0.58
22:t2:15:LEU:HD11	24:t4:55:PHE:HE1	1.68	0.58
30:y7:190:ILE:HD11	51:s:46:VAL:HG11	1.85	0.58
38:f:211:ARG:HD2	63:f:401:CDL:H571	1.86	0.58
9:C3:419:ILE:HD11	33:A:330:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:7A:104:GLU:HB3	15:7A:115:ARG:HB2	1.85	0.58
26:T6:20:HIS:ND1	26:T6:40:CYS:SG	2.77	0.58
36:D:317:GLU:OE1	42:J:74:ARG:NH2	2.36	0.58
63:7c:301:CDL:H741	63:7c:301:CDL:H571	1.86	0.58
53:u:51:GLN:NE2	53:u:55:ASP:OD1	2.37	0.58
7:C1:321:ALA:HB3	7:C1:326:ARG:HD2	1.86	0.58
8:C2:360:LEU:HD11	8:C2:391:LEU:HD22	1.85	0.58
9:C3:266:LEU:HB3	9:C3:271:ILE:HG21	1.86	0.58
9:c3:290:VAL:HG22	9:c3:470:ARG:HE	1.69	0.58
19:m2:7:ARG:NH1	19:m2:10:GLU:OE2	2.35	0.58
27:bp:340:ASN:OD1	27:bp:342:ARG:NH1	2.36	0.58
31:y0:61:LYS:HB3	63:t:201:CDL:HB32	1.86	0.58
25:T5:4:ASN:HB2	25:T5:7:ALA:HB3	1.85	0.57
33:A:361:LYS:O	33:A:380:ARG:NH1	2.37	0.57
38:F:211:ARG:HD2	63:F:401:CDL:H571	1.85	0.57
46:N:29:PHE:HA	46:N:32:PHE:HB2	1.84	0.57
8:c2:114:THR:O	8:c2:132:ASN:ND2	2.32	0.57
42:j:186:GLN:HB2	63:j:301:CDL:HB21	1.86	0.57
7:C1:159:ARG:HE	7:C1:265:SER:HB3	1.68	0.57
37:E:354:ARG:NH2	39:G:232:GLU:OE2	2.36	0.57
38:F:192:LEU:HB3	38:F:196:ALA:HB3	1.86	0.57
15:7a:92:LEU:HB3	15:7a:99:THR:HG21	1.85	0.57
8:c2:360:LEU:HD11	8:c2:391:LEU:HD22	1.85	0.57
63:7c:301:CDL:H781	63:7c:301:CDL:H421	1.85	0.57
27:bp:255:SER:O	27:bp:290:LYS:NZ	2.36	0.57
7:C1:126:HIS:NE2	39:G:187:ASP:OD1	2.36	0.57
16:7C:155:PHE:HB3	62:7C:302:PC1:H292	1.86	0.57
28:FS:150:ASN:ND2	37:e:115:ASP:OD1	2.37	0.57
7:c1:615:ILE:HD12	59:c1:701:HEA:H18	1.85	0.57
63:m2:404:CDL:H1	63:n:303:CDL:H741	1.86	0.57
41:I:173:ILE:HG22	47:O:187:LYS:HG2	1.87	0.57
53:U:51:GLN:NE2	53:U:55:ASP:OD1	2.38	0.57
53:U:138:ARG:NH2	53:U:154:PHE:O	2.38	0.57
9:c3:283:TYR:HD2	63:7a:201:CDL:H512	1.69	0.57
9:C3:519:PHE:CE2	45:M:148:ILE:HG21	2.39	0.57
10:5B:179:LEU:HD22	39:G:193:VAL:HG13	1.86	0.57
28:FS:167:TYR:HB2	63:F:401:CDL:H802	1.86	0.57
7:c1:307:THR:HA	7:c1:310:PHE:CE2	2.39	0.57
7:c1:321:ALA:HB3	7:c1:326:ARG:HD2	1.87	0.57
9:c3:265:LEU:HD13	46:n:54:ASP:HB2	1.86	0.57
20:m3:151:SER:HB3	20:m3:162:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:459:ILE:HG23	34:b:469:VAL:HG21	1.87	0.57
40:h:119:TYR:N	40:h:198:VAL:O	2.37	0.57
30:Y7:156:ASP:OD2	35:C:472:ASN:ND2	2.38	0.57
40:H:119:TYR:N	40:H:198:VAL:O	2.37	0.57
52:T:24:GLU:HB2	55:W:47:THR:HG23	1.86	0.57
63:f:401:CDL:H801	63:f:401:CDL:H362	1.85	0.57
63:k:301:CDL:H331	56:x:79:ILE:HD11	1.85	0.57
62:C1:705:PC1:H3E2	62:C1:705:PC1:H391	1.86	0.57
30:Y7:190:ILE:HD11	51:S:46:VAL:HG11	1.87	0.57
43:K:91:LEU:HD21	43:K:107:LEU:HD13	1.87	0.57
8:c:2:65:PRO:HD2	39:g:100:THR:HA	1.86	0.57
33:a:44:TYR:OH	37:e:315:GLU:OE2	2.21	0.57
36:d:369:PHE:O	36:d:371:ARG:NH1	2.37	0.57
43:k:91:LEU:HD21	43:k:107:LEU:HD13	1.87	0.57
5:U5:143:ARG:HH11	50:R:71:LEU:HD22	1.70	0.57
34:B:459:ILE:HG23	34:B:469:VAL:HG21	1.87	0.57
48:P:142:ARG:NH2	48:P:149:GLU:OE2	2.32	0.57
62:m1:402:PC1:H2E2	62:m1:402:PC1:H291	1.87	0.57
38:f:227:LEU:HB2	38:f:320:ILE:HD11	1.87	0.57
2:U2:276:ASN:OD1	30:Y7:145:TYR:OH	2.23	0.56
36:D:167:TYR:HB2	36:D:170:VAL:HG23	1.87	0.56
43:K:82:LEU:O	43:K:86:TYR:N	2.27	0.56
43:K:214:VAL:HG12	43:K:216:GLN:H	1.70	0.56
8:c:2:252:ASP:HB2	24:t4:8:VAL:HG22	1.86	0.56
41:i:170:ASN:HB3	41:i:173:ILE:HG12	1.87	0.56
63:7C:301:CDL:H741	63:7C:301:CDL:H571	1.87	0.56
7:c1:199:LYS:HG2	46:n:208:HIS:HB3	1.87	0.56
8:c:2:143:ILE:HB	17:7l:893:LEU:HD11	1.86	0.56
9:c3:519:PHE:CE2	45:m:148:ILE:HG21	2.39	0.56
30:y7:156:ASP:OD2	35:c:472:ASN:ND2	2.38	0.56
37:e:70:GLU:HG3	37:e:272:LYS:HE2	1.87	0.56
7:C1:553:VAL:HG12	16:7C:103:GLN:HG3	1.87	0.56
8:C2:390:ARG:NH2	12:6B:149:ASP:OD2	2.37	0.56
8:C2:390:ARG:HH22	12:6B:149:ASP:CG	2.12	0.56
10:5B:446:ARG:NH2	10:5B:545:GLU:OE2	2.38	0.56
63:7a:202:CDL:HA22	30:y7:358:ARG:HD2	1.88	0.56
19:m2:44:ARG:HG3	19:m2:45:THR:HG23	1.87	0.56
22:t2:40:GLU:OE1	24:t4:42:ARG:NH2	2.38	0.56
47:o:123:ILE:HG23	47:o:190:LEU:HD21	1.87	0.56
8:C2:293:ASN:ND2	26:T6:61:GLN:OE1	2.37	0.56
15:7A:92:LEU:HB3	15:7A:99:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:M1:403:CDL:H751	63:M1:403:CDL:H182	1.88	0.56
37:E:115:ASP:OD1	28:fs:150:ASN:ND2	2.37	0.56
46:n:29:PHE:HA	46:n:32:PHE:HB2	1.85	0.56
62:7C:302:PC1:H2E2	62:7C:302:PC1:H291	1.88	0.56
43:k:214:VAL:HG12	43:k:216:GLN:H	1.70	0.56
33:A:247:TYR:O	33:A:250:GLN:NE2	2.38	0.56
38:F:254:GLN:OE1	54:V:79:ARG:NH2	2.39	0.56
14:6c:10:TYR:OH	14:6c:14:ARG:NH1	2.38	0.56
21:t1:18:ASN:HD21	26:t6:9:ILE:HG12	1.71	0.56
41:i:141:LEU:HD22	50:r:148:GLN:HG2	1.87	0.56
28:FS:154:LYS:HD2	39:G:256:PRO:HD3	1.87	0.56
38:F:284:LEU:HD21	38:F:321:VAL:HG11	1.87	0.56
63:F:401:CDL:H582	63:F:401:CDL:H372	1.87	0.56
43:K:191:SER:OG	48:P:26:GLN:O	2.20	0.56
7:c1:322:MET:HG2	7:c1:325:LEU:HB2	1.88	0.56
33:a:361:LYS:O	33:a:380:ARG:NH1	2.38	0.56
38:f:284:LEU:HD21	38:f:321:VAL:HG11	1.88	0.56
41:i:149:GLU:HG2	41:i:195:PRO:HB2	1.87	0.56
41:i:173:ILE:HG22	47:o:187:LYS:HG2	1.88	0.56
44:L:138:ARG:NH1	44:L:141:GLY:O	2.37	0.56
18:m1:288:TRP:HZ3	63:m1:401:CDL:H592	1.70	0.56
16:7C:66:ASP:OD1	16:7C:98:LYS:NZ	2.38	0.56
45:M:71:THR:HG23	45:M:74:LYS:HE2	1.88	0.56
27:bp:260:ASN:ND2	27:bp:283:ASN:OD1	2.39	0.56
36:d:180:TYR:N	36:d:299:VAL:O	2.39	0.56
62:7C:302:PC1:H232	62:7C:302:PC1:H272	1.87	0.56
40:H:119:TYR:HA	40:H:198:VAL:O	2.06	0.56
10:5B:181:ARG:NH2	39:G:194:GLY:O	2.38	0.55
14:6C:10:TYR:OH	14:6C:14:ARG:NH1	2.39	0.55
8:c2:357:VAL:O	8:c2:394:ASN:ND2	2.39	0.55
49:q:123:ALA:O	49:q:127:ASN:ND2	2.31	0.55
59:C1:701:HEA:HHC	59:C1:701:HEA:H122	1.88	0.55
63:M3:401:CDL:H592	56:X:58:ILE:HD11	1.88	0.55
32:Y5:187:ARG:NH1	32:Y5:188:ILE:O	2.39	0.55
6:u6:155:VAL:HG11	50:r:147:ALA:HB1	1.87	0.55
7:c1:452:ARG:NH2	8:c2:105:GLU:OE2	2.38	0.55
10:5b:268:ASP:OD1	15:7a:13:TYR:OH	2.18	0.55
63:7c:301:CDL:H802	63:7c:301:CDL:H391	1.89	0.55
7:C1:199:LYS:HG2	46:N:208:HIS:HB3	1.88	0.55
7:C1:345:MET:HE3	7:C1:396:VAL:HG12	1.89	0.55
41:I:170:ASN:HB3	41:I:173:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:V:74:THR:O	54:V:87:THR:OG1	2.21	0.55
7:c1:202:ILE:HD13	42:j:170:ILE:HG22	1.87	0.55
10:5b:350:ARG:NH1	10:5b:387:TPO:O2P	2.39	0.55
10:5b:362:ARG:NH1	10:5b:376:GLU:OE2	2.40	0.55
27:bp:147:GLY:HA2	27:bp:226:LEU:HB3	1.88	0.55
33:a:402:PRO:O	33:a:460:TYR:OH	2.19	0.55
45:m:92:ASP:N	45:m:92:ASP:OD1	2.39	0.55
7:C1:562:MET:HE3	63:M1:401:CDL:H632	1.87	0.55
18:m1:58:GLU:OE2	18:m1:307:LYS:NZ	2.37	0.55
38:f:139:LYS:HD2	38:f:327:ASP:HB3	1.89	0.55
40:h:265:ILE:HA	40:h:271:GLU:HG3	1.89	0.55
63:M2:404:CDL:H312	63:N:303:CDL:H661	1.88	0.55
36:D:312:ARG:O	36:D:321:ASN:ND2	2.40	0.55
8:c2:157:GLN:NE2	8:c2:370:GLU:OE2	2.39	0.55
14:6c:48:ARG:HH12	17:7l:871:SER:HB3	1.71	0.55
26:t6:1:FME:HG2	26:t6:5:LEU:HD23	1.88	0.55
26:t6:20:HIS:ND1	26:t6:40:CYS:SG	2.80	0.55
28:fs:154:LYS:HD2	39:g:256:PRO:HD3	1.87	0.55
36:d:317:GLU:OE1	42:j:74:ARG:NH2	2.39	0.55
37:e:38:LEU:HD12	37:e:47:LEU:HD23	1.89	0.55
42:j:184:THR:HG21	63:j:301:CDL:HA61	1.89	0.55
20:M3:151:SER:HB3	20:M3:162:VAL:HG21	1.88	0.55
37:E:119:ARG:NH1	37:E:120:ASN:OD1	2.40	0.55
41:I:149:GLU:HG2	41:I:195:PRO:HB2	1.88	0.55
59:c1:701:HEA:HHC	59:c1:701:HEA:H122	1.87	0.55
32:Y5:164:TYR:HB3	32:Y5:168:GLY:HA3	1.89	0.55
7:c1:531:LEU:O	7:c1:535:ALA:HB3	2.07	0.55
8:c2:293:ASN:ND2	26:t6:61:GLN:OE1	2.39	0.55
33:a:386:THR:OG1	33:a:387:THR:N	2.35	0.55
40:h:119:TYR:HA	40:h:198:VAL:O	2.07	0.55
7:C1:164:ARG:NH1	7:C1:167:ASP:OD2	2.40	0.55
8:C2:268:TRP:HH2	8:C2:310:LEU:HD12	1.71	0.55
16:7C:158:GLU:O	16:7C:162:ASN:HB2	2.07	0.55
18:M1:156:LEU:HD21	38:F:106:LEU:HD23	1.89	0.55
28:FS:145:ALA:HB3	28:FS:146:PRO:HD3	1.88	0.55
30:Y7:348:TYR:HE2	63:N:303:CDL:H251	1.71	0.55
44:L:38:GLN:HB3	44:L:41:ARG:HB3	1.89	0.55
50:R:148:GLN:NE2	50:R:152:GLU:OE2	2.39	0.55
13:6l:42:PRO:O	13:6l:45:LEU:HB2	2.07	0.55
16:7c:34:ARG:HD2	19:m2:48:VAL:HA	1.88	0.55
37:e:119:ARG:NH1	37:e:120:ASN:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U2:274:LEU:HD22	30:Y7:173:ILE:HG13	1.89	0.55
8:C2:65:PRO:HD2	39:G:100:THR:HA	1.88	0.55
8:C2:252:ASP:HB2	24:T4:8:VAL:HG22	1.88	0.55
13:6L:42:PRO:O	13:6L:45:LEU:HB2	2.07	0.55
28:FS:76:SER:OG	28:FS:119:THR:OG1	2.23	0.55
30:Y7:307:ASN:O	30:Y7:309:GLN:NE2	2.40	0.55
56:X:9:ARG:NH2	56:X:15:GLU:OE2	2.40	0.55
63:m3:401:CDL:H732	33:a:298:TYR:HB3	1.89	0.55
22:t2:58:THR:OG1	25:t5:22:TYR:OH	2.24	0.55
30:y7:412:TYR:OH	34:b:446:GLU:OE1	2.25	0.55
51:s:66:ASP:HA	51:s:69:ARG:HD3	1.89	0.55
9:C3:290:VAL:HG22	9:C3:470:ARG:HE	1.72	0.55
10:5B:362:ARG:NH1	10:5B:376:GLU:OE2	2.40	0.55
17:7L:980:ASP:OD2	53:U:12:LYS:NZ	2.36	0.55
27:BP:260:ASN:ND2	27:BP:283:ASN:OD1	2.40	0.55
38:F:241:LEU:HB3	63:F:401:CDL:H722	1.88	0.55
16:7c:158:GLU:O	16:7c:162:ASN:HB2	2.07	0.55
36:d:312:ARG:O	36:d:321:ASN:ND2	2.40	0.55
38:f:140:PRO:HG3	38:f:144:ILE:HD11	1.88	0.55
7:C1:127:VAL:HG12	7:C1:321:ALA:HA	1.89	0.54
10:5B:350:ARG:NH1	10:5B:387:TPO:O2P	2.39	0.54
33:A:44:TYR:OH	37:E:315:GLU:OE2	2.24	0.54
10:5b:285:VAL:HG22	33:a:477:ILE:HD11	1.89	0.54
15:7a:104:GLU:HB3	15:7a:115:ARG:HB2	1.87	0.54
16:7c:47:ILE:HG12	18:m1:282:LYS:HB3	1.89	0.54
27:bp:189:SER:OG	27:bp:225:ARG:NH1	2.40	0.54
46:n:159:GLN:OE1	46:n:161:ARG:NH2	2.40	0.54
27:BP:260:ASN:HB3	27:BP:269:LEU:HD22	1.88	0.54
27:BP:423:PHE:HE2	27:BP:450:LEU:HD22	1.72	0.54
37:E:70:GLU:HG3	37:E:272:LYS:HE2	1.89	0.54
40:H:78:ALA:HB2	40:H:293:LEU:HB2	1.89	0.54
47:O:123:ILE:HG23	47:O:190:LEU:HD21	1.89	0.54
51:S:66:ASP:HA	51:S:69:ARG:HD3	1.89	0.54
37:e:354:ARG:NH2	39:g:232:GLU:OE2	2.39	0.54
40:h:197:VAL:HG23	40:h:249:VAL:HG11	1.89	0.54
53:u:138:ARG:NH2	53:u:154:PHE:O	2.41	0.54
7:C1:322:MET:HG2	7:C1:325:LEU:HB2	1.90	0.54
18:M1:288:TRP:HZ3	63:M1:401:CDL:H592	1.72	0.54
36:D:180:TYR:N	36:D:299:VAL:O	2.40	0.54
49:Q:130:LYS:HE3	49:Q:165:LEU:HD12	1.89	0.54
7:C1:161:GLN:HB2	7:C1:265:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:F:239:GLN:HE21	38:F:243:GLY:HA2	1.73	0.54
43:K:66:ILE:O	43:K:68:GLN:NE2	2.40	0.54
63:7C:301:CDL:H802	63:7C:301:CDL:H391	1.90	0.54
27:BP:139:GLY:HA2	27:BP:144:LEU:HD13	1.89	0.54
30:Y7:393:LEU:HA	30:Y7:396:LEU:HD12	1.88	0.54
33:A:102:ASN:HB3	33:A:164:TRP:O	2.08	0.54
38:F:140:PRO:HG3	38:F:144:ILE:HD11	1.88	0.54
42:J:234:LYS:NZ	56:X:35:GLU:OE2	2.40	0.54
45:M:92:ASP:OD1	45:M:92:ASP:N	2.40	0.54
10:5b:582:TYR:HA	10:5b:586:ILE:HB	1.89	0.54
18:m1:156:LEU:HD21	38:f:106:LEU:HD23	1.90	0.54
63:j:301:CDL:H542	62:n:301:PC1:H31	1.89	0.54
9:C3:153:ASN:O	9:C3:157:ASN:ND2	2.31	0.54
17:7L:954:GLU:OE2	17:7L:957:ARG:NH1	2.41	0.54
50:r:62:SER:HG	50:r:67:THR:HG1	1.47	0.54
16:7C:47:ILE:HG12	18:M1:282:LYS:HB3	1.90	0.54
63:7C:301:CDL:H781	63:7C:301:CDL:H421	1.89	0.54
38:F:139:LYS:HD2	38:F:327:ASP:HB3	1.90	0.54
39:G:110:MET:HE2	39:G:137:PRO:HB3	1.90	0.54
7:c1:127:VAL:HG12	7:c1:321:ALA:HA	1.89	0.54
31:y0:50:ASN:ND2	33:a:158:TYR:O	2.37	0.54
33:a:102:ASN:HB3	33:a:164:TRP:O	2.07	0.54
63:7A:202:CDL:H241	46:N:132:GLY:HA3	1.90	0.54
40:H:118:LEU:HD11	40:H:200:ASP:HB2	1.89	0.54
20:m3:154:SER:HB3	20:m3:158:ASN:HB3	1.90	0.54
7:C1:452:ARG:NH2	8:C2:105:GLU:OE2	2.39	0.54
8:C2:508:ASN:OD1	8:C2:509:SER:N	2.39	0.54
63:7A:202:CDL:HA22	30:Y7:358:ARG:HD2	1.90	0.54
22:T2:15:LEU:HD11	24:T4:55:PHE:HE1	1.72	0.54
27:BP:147:GLY:HA2	27:BP:226:LEU:HB3	1.89	0.54
27:BP:261:TRP:HB3	27:BP:280:PRO:HA	1.90	0.54
40:H:265:ILE:HA	40:H:271:GLU:HG3	1.89	0.54
42:J:184:THR:HG21	63:J:301:CDL:HA61	1.89	0.54
62:c1:705:PC1:H3E2	62:c1:705:PC1:H391	1.90	0.54
10:5b:181:ARG:NH2	39:g:194:GLY:O	2.40	0.54
30:y7:393:LEU:HA	30:y7:396:LEU:HD12	1.88	0.54
31:y0:36:ARG:NH2	52:t:99:PHE:O	2.39	0.54
9:C3:396:LEU:HD22	62:C3:605:PC1:H271	1.88	0.54
10:5B:340:ARG:NH1	10:5B:352:GLU:OE1	2.40	0.54
63:7C:303:CDL:H521	62:M2:402:PC1:H241	1.90	0.54
52:T:32:ARG:HA	55:W:41:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c1:682:GLU:OE2	18:m1:158:ARG:NH1	2.41	0.54
10:5b:340:ARG:NH1	10:5b:352:GLU:OE1	2.40	0.54
63:m3:401:CDL:H592	56:x:58:ILE:HD11	1.90	0.54
7:C1:531:LEU:O	7:C1:535:ALA:HB3	2.08	0.53
63:C1:706:CDL:H512	15:7A:76:ARG:HA	1.90	0.53
9:C3:283:TYR:CD1	63:7A:201:CDL:H512	2.44	0.53
33:A:386:THR:OG1	33:A:387:THR:N	2.35	0.53
9:c3:153:ASN:O	9:c3:157:ASN:ND2	2.32	0.53
63:7a:202:CDL:H241	46:n:132:GLY:HA3	1.91	0.53
20:m3:206:ARG:HH21	20:m3:259:GLY:H	1.55	0.53
44:l:138:ARG:NH1	44:l:141:GLY:O	2.39	0.53
50:r:148:GLN:NE2	50:r:152:GLU:OE2	2.41	0.53
30:Y7:412:TYR:OH	34:B:446:GLU:OE1	2.24	0.53
40:H:197:VAL:HG23	40:H:249:VAL:HG11	1.90	0.53
8:c2:218:ILE:HD13	24:t4:55:PHE:HZ	1.73	0.53
10:5b:179:LEU:HD22	39:g:193:VAL:HG13	1.91	0.53
46:n:186:ALA:HB3	46:n:189:HIS:HD2	1.73	0.53
50:r:123:PRO:HB3	58:z:77:ILE:HB	1.90	0.53
50:R:60:GLU:O	50:R:64:ASN:ND2	2.38	0.53
56:X:40:ALA:HB2	56:X:102:LYS:HG2	1.90	0.53
9:c3:314:ILE:HB	10:5b:230:VAL:HG11	1.89	0.53
16:7c:155:PHE:HB3	62:m1:402:PC1:H292	1.90	0.53
7:C1:606:THR:HG21	18:M1:222:LYS:HD2	1.90	0.53
16:7C:73:THR:HG22	16:7C:92:LYS:HB2	1.90	0.53
17:7L:894:ASP:OD2	55:W:88:TYR:OH	2.23	0.53
18:M1:57:VAL:HG13	63:M1:403:CDL:H121	1.89	0.53
21:T1:18:ASN:HD21	26:T6:9:ILE:HG12	1.73	0.53
30:Y7:295:LYS:HD3	39:G:40:ILE:HD11	1.89	0.53
28:fs:76:SER:OG	28:fs:119:THR:OG1	2.25	0.53
40:h:118:LEU:HD11	40:h:200:ASP:HB2	1.90	0.53
38:F:227:LEU:HB2	38:F:320:ILE:HD11	1.91	0.53
34:b:345:ASN:O	34:b:349:ASN:ND2	2.33	0.53
43:k:103:THR:HA	43:k:159:LYS:HA	1.90	0.53
49:q:6:HIS:NE2	52:t:139:ASP:OD2	2.36	0.53
50:r:60:GLU:O	50:r:64:ASN:ND2	2.38	0.53
63:M1:401:CDL:H202	63:M1:401:CDL:H372	1.91	0.53
27:BP:87:THR:HG23	27:BP:119:MET:HE1	1.91	0.53
37:E:199:ARG:HH11	63:E:401:CDL:H112	1.72	0.53
40:H:250:ASN:HB2	40:H:276:LYS:HD2	1.89	0.53
7:c1:161:GLN:HB2	7:c1:265:SER:HB2	1.89	0.53
17:7l:980:ASP:OD2	53:u:12:LYS:NZ	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:bp:139:GLY:HA2	27:bp:144:LEU:HD13	1.91	0.53
54:v:74:THR:O	54:v:87:THR:OG1	2.21	0.53
9:C3:307:ARG:NH2	10:5B:242:GLU:OE1	2.41	0.53
63:M1:401:CDL:H561	63:M1:401:CDL:H601	1.91	0.53
29:AC:28:TYR:HB2	37:e:288:HIS:HD2	1.73	0.53
63:J:301:CDL:H542	62:N:301:PC1:H31	1.90	0.53
49:Q:36:SER:OG	49:Q:121:ASP:OD2	2.26	0.53
2:u2:276:ASN:OD1	30:y7:145:TYR:OH	2.25	0.53
45:m:71:THR:HG23	45:m:74:LYS:HE2	1.91	0.53
7:C1:202:ILE:HD13	42:J:170:ILE:HG22	1.89	0.53
7:c1:345:MET:HE3	7:c1:396:VAL:HG12	1.90	0.53
9:c3:266:LEU:HB2	9:c3:271:ILE:HD13	1.91	0.53
9:c3:283:TYR:CD2	63:7a:201:CDL:H512	2.44	0.53
16:7c:141:ILE:HD12	19:m2:55:LEU:HD13	1.91	0.53
38:f:205:ASN:HD21	63:u:201:CDL:H671	1.74	0.53
40:h:199:THR:HG22	40:h:201:GLY:H	1.74	0.53
52:t:102:LYS:NZ	63:t:201:CDL:OB4	2.37	0.53
12:6B:47:LYS:NZ	17:7L:970:LEU:O	2.36	0.53
16:7C:141:ILE:HD12	19:M2:55:LEU:HD13	1.91	0.53
52:T:102:LYS:NZ	63:T:201:CDL:OB4	2.38	0.53
7:C1:75:ILE:HD11	7:C1:98:VAL:HA	1.91	0.53
9:C3:259:TYR:HB2	63:M3:401:CDL:H311	1.89	0.53
9:C3:314:ILE:HB	10:5B:230:VAL:HG11	1.91	0.53
10:5B:374:LEU:HB2	10:5B:555:SER:HB3	1.91	0.53
20:M3:154:SER:HB3	20:M3:158:ASN:HB3	1.90	0.53
10:5b:497:HIS:ND1	30:y7:189:TYR:OH	2.38	0.53
7:C1:342:THR:HB	7:C1:396:VAL:HB	1.90	0.52
17:7L:925:LYS:NZ	17:7L:939:MET:SD	2.82	0.52
63:M2:404:CDL:H1	63:N:303:CDL:H741	1.90	0.52
37:e:209:GLU:OE1	37:e:236:TRP:NE1	2.39	0.52
7:C1:164:ARG:HG3	7:C1:166:TYR:CZ	2.44	0.52
7:C1:663:MET:O	16:7C:92:LYS:NZ	2.29	0.52
9:C3:212:ARG:HH21	43:K:49:ILE:HA	1.75	0.52
62:7C:302:PC1:H2F2	18:M1:134:VAL:HG11	1.92	0.52
18:M1:153:PRO:HG3	62:M2:406:PC1:H3C1	1.91	0.52
54:V:78:GLU:HG3	54:V:82:PHE:HB3	1.91	0.52
7:c1:164:ARG:NH1	7:c1:167:ASP:OD2	2.42	0.52
7:c1:342:THR:HB	7:c1:396:VAL:HB	1.90	0.52
7:c1:392:PRO:O	7:c1:396:VAL:HG13	2.09	0.52
8:c2:392:ARG:NH2	12:6b:145:LEU:O	2.30	0.52
9:c3:212:ARG:HH21	43:k:49:ILE:HA	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:m1:30:SER:OG	18:m1:120:ASN:ND2	2.41	0.52
27:bp:261:TRP:HB3	27:bp:280:PRO:HA	1.91	0.52
37:e:344:ILE:HD11	39:g:223:ASP:HA	1.91	0.52
10:5B:273:MET:HE1	15:7A:28:TYR:HB2	1.92	0.52
63:U:201:CDL:H172	63:U:201:CDL:H802	1.90	0.52
9:c3:261:MET:HE3	9:c3:271:ILE:HD11	1.90	0.52
37:e:186:PRO:HD2	37:e:187:ARG:HH11	1.74	0.52
49:q:36:SER:OG	49:q:121:ASP:OD2	2.27	0.52
15:7A:2:ASN:OD1	33:A:459:ASN:ND2	2.42	0.52
33:A:392:TYR:OH	33:A:429:ARG:NH1	2.42	0.52
7:c1:657:GLN:NE2	39:g:105:TYR:OH	2.42	0.52
8:c2:355:GLY:HA3	9:c3:578:LYS:HD3	1.91	0.52
9:c3:568:SER:HB3	44:l:29:GLU:HA	1.91	0.52
63:f:401:CDL:H582	63:f:401:CDL:H372	1.90	0.52
52:t:85:LEU:HD21	52:t:94:ARG:HH12	1.74	0.52
8:C2:111:SER:HA	8:C2:502:ASN:HB3	1.92	0.52
8:C2:114:THR:O	8:C2:132:ASN:ND2	2.35	0.52
37:E:128:TYR:HB3	63:E:402:CDL:H342	1.92	0.52
45:M:216:MET:HE3	55:W:71:TYR:HB2	1.92	0.52
5:u5:139:TRP:CH2	58:z:51:ALA:HB1	2.45	0.52
7:c1:606:THR:HG21	18:m1:222:LYS:HD2	1.91	0.52
9:c3:396:LEU:HD22	62:c3:605:PC1:H271	1.90	0.52
10:5b:329:ARG:NH1	10:5b:396:GLU:OE2	2.42	0.52
63:m3:401:CDL:H611	33:a:291:VAL:HG13	1.91	0.52
28:fs:154:LYS:HG2	28:fs:157:ARG:HH21	1.75	0.52
52:t:24:GLU:HB2	55:w:47:THR:HG23	1.91	0.52
9:C3:215:GLN:NE2	27:BP:383:LEU:O	2.40	0.52
9:C3:261:MET:HE3	9:C3:271:ILE:HD11	1.90	0.52
9:C3:521:LEU:HD21	45:M:144:MET:HE1	1.92	0.52
50:R:123:PRO:HB3	58:Z:77:ILE:HB	1.91	0.52
8:c2:111:SER:HA	8:c2:502:ASN:HB3	1.92	0.52
8:c2:257:LEU:HD22	26:t6:8:VAL:HG21	1.92	0.52
17:7l:925:LYS:NZ	17:7l:939:MET:SD	2.83	0.52
19:m2:123:VAL:HG22	62:m2:405:PC1:H372	1.92	0.52
43:k:66:ILE:HD11	43:k:172:GLN:HB2	1.91	0.52
48:p:120:LEU:HD21	48:p:165:LEU:HD11	1.92	0.52
52:t:108:ASP:OD1	52:t:109:ARG:N	2.43	0.52
5:U5:139:TRP:CH2	58:Z:51:ALA:HB1	2.45	0.52
8:C2:357:VAL:O	8:C2:394:ASN:ND2	2.42	0.52
16:7C:163:HIS:NE2	62:7C:304:PC1:O14	2.27	0.52
52:T:108:ASP:OD1	52:T:109:ARG:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c1:164:ARG:HG3	7:c1:166:TYR:CZ	2.45	0.52
9:C3:266:LEU:HB2	9:C3:271:ILE:HD13	1.92	0.52
63:5B:702:CDL:OA9	56:X:75:ARG:NH2	2.34	0.52
9:c3:531:PHE:O	49:q:60:TYR:OH	2.21	0.52
62:m1:402:PC1:H232	62:m1:402:PC1:H272	1.91	0.52
63:m2:404:CDL:H312	63:n:303:CDL:H661	1.91	0.52
7:C1:392:PRO:O	7:C1:396:VAL:HG13	2.09	0.52
10:5B:582:TYR:HA	10:5B:586:ILE:HB	1.92	0.52
11:6A:56:ASN:HD22	32:Y5:170:TYR:HE1	1.57	0.52
18:M1:27:ARG:NH1	18:M1:29:ASP:OD2	2.43	0.52
27:BP:366:THR:HG23	27:BP:403:ALA:HB1	1.91	0.52
27:BP:398:ILE:HD13	27:BP:412:THR:HG22	1.92	0.52
9:c3:520:TYR:HB2	52:t:45:LYS:HE2	1.92	0.52
31:y0:19:ILE:O	31:y0:23:ASN:N	2.38	0.52
37:e:73:ASP:H	37:e:272:LYS:HB3	1.75	0.52
48:p:142:ARG:NH2	48:p:149:GLU:OE2	2.33	0.52
53:u:99:ILE:HB	53:u:100:PRO:HD3	1.92	0.52
7:C1:140:ILE:HA	30:Y7:318:CYS:SG	2.50	0.52
26:T6:1:FME:HG2	26:T6:5:LEU:HD23	1.92	0.52
27:BP:400:LYS:HB2	27:BP:411:VAL:HB	1.92	0.52
37:E:186:PRO:HD2	37:E:187:ARG:HH11	1.74	0.52
7:c1:140:ILE:HA	30:y7:318:CYS:SG	2.50	0.52
10:5b:216:HIS:ND1	45:m:84:TYR:O	2.43	0.52
46:n:58:LYS:HD3	46:n:61:TYR:HA	1.92	0.52
52:t:42:ARG:NH1	57:y:21:GLU:OE2	2.40	0.52
40:H:88:ARG:NH1	40:H:285:GLN:OE1	2.43	0.51
49:Q:53:GLY:O	49:Q:57:VAL:HG23	2.10	0.51
7:c1:562:MET:HE3	63:m1:401:CDL:H632	1.92	0.51
8:c2:145:ASN:ND2	17:7l:890:ASP:OD2	2.43	0.51
63:m1:401:CDL:H561	63:m1:401:CDL:H601	1.92	0.51
63:m2:401:CDL:HA22	62:m2:402:PC1:H131	1.91	0.51
27:bp:400:LYS:HB2	27:bp:411:VAL:HB	1.92	0.51
37:e:199:ARG:HH11	63:e:401:CDL:H112	1.74	0.51
40:h:78:ALA:HB2	40:h:293:LEU:HB2	1.91	0.51
47:o:123:ILE:HG22	47:o:127:VAL:HG13	1.92	0.51
7:C1:252:VAL:O	7:C1:255:ARG:NH1	2.42	0.51
8:C2:218:ILE:HD13	24:T4:55:PHE:HZ	1.75	0.51
20:M3:143:ALA:HB3	20:M3:144:PRO:HD3	1.91	0.51
28:FS:154:LYS:HG2	28:FS:157:ARG:HH21	1.75	0.51
40:H:199:THR:HG22	40:H:201:GLY:H	1.75	0.51
42:J:186:GLN:HB2	63:J:301:CDL:HB21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:185:PRO:HG2	57:Y:65:TYR:CE2	2.45	0.51
52:T:64:ALA:HA	52:T:67:LEU:HD12	1.92	0.51
54:V:85:ILE:HG23	63:V:201:CDL:H522	1.91	0.51
7:c1:126:HIS:HD1	7:c1:336:THR:HG1	1.55	0.51
16:7c:58:ASP:OD2	16:7c:62:THR:OG1	2.27	0.51
38:F:166:TYR:HD1	63:F:401:CDL:H391	1.75	0.51
7:c1:225:SER:HB2	46:n:199:ALA:HB2	1.93	0.51
63:m1:403:CDL:HB61	63:m2:401:CDL:HA4	1.90	0.51
27:bp:211:PRO:HG2	27:bp:265:LEU:HD13	1.92	0.51
32:y5:103:LYS:NZ	63:y5:201:CDL:OA9	2.34	0.51
37:e:336:ALA:HB3	39:g:73:PRO:HB2	1.92	0.51
22:T2:40:GLU:OE1	24:T4:42:ARG:NH2	2.42	0.51
43:K:103:THR:HA	43:K:159:LYS:HA	1.92	0.51
8:c2:395:SER:OG	47:o:109:LYS:NZ	2.43	0.51
27:bp:366:THR:HG23	27:bp:403:ALA:HB1	1.91	0.51
27:bp:398:ILE:HD13	27:bp:412:THR:HG22	1.92	0.51
33:a:380:ARG:HH21	33:a:431:LEU:HG	1.75	0.51
33:a:392:TYR:OH	33:a:429:ARG:NH1	2.43	0.51
43:k:81:HIS:NE2	43:k:117:GLU:OE1	2.40	0.51
43:k:82:LEU:O	43:k:86:TYR:N	2.27	0.51
63:u:201:CDL:H172	63:u:201:CDL:H802	1.91	0.51
8:C2:257:LEU:HD22	26:T6:8:VAL:HG21	1.93	0.51
9:C3:276:ILE:HD11	63:Y7:501:CDL:H391	1.92	0.51
63:7A:202:CDL:H791	46:N:126:GLY:HA2	1.93	0.51
63:Y0:101:CDL:OB4	45:M:46:ARG:NH2	2.37	0.51
63:F:401:CDL:HB22	63:F:401:CDL:HB4	1.92	0.51
45:M:175:ARG:NH2	45:M:204:GLU:OE2	2.31	0.51
18:m1:153:PRO:HG3	62:m2:406:PC1:H3C1	1.92	0.51
9:C3:531:PHE:O	49:Q:60:TYR:OH	2.23	0.51
30:Y7:152:ILE:HD11	30:Y7:157:LEU:HD13	1.92	0.51
30:Y7:412:TYR:CZ	30:Y7:416:ILE:HD11	2.46	0.51
46:N:159:GLN:OE1	46:N:161:ARG:NH2	2.43	0.51
46:N:186:ALA:HB3	46:N:189:HIS:HD2	1.75	0.51
53:U:2:SER:HB3	54:V:132:TRP:CE3	2.45	0.51
7:c1:349:ILE:HD13	7:c1:392:PRO:HB2	1.93	0.51
63:7c:302:CDL:H521	62:m2:402:PC1:H241	1.92	0.51
20:m3:143:ALA:HB3	20:m3:144:PRO:HD3	1.91	0.51
63:y0:101:CDL:OB4	45:m:46:ARG:NH2	2.36	0.51
33:a:247:TYR:O	33:a:250:GLN:NE2	2.43	0.51
37:e:132:PHE:HD1	63:e:402:CDL:H311	1.76	0.51
39:g:163:VAL:N	39:g:180:TRP:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:v:74:THR:HG21	63:v:201:CDL:HA61	1.92	0.51
7:C1:349:ILE:HD13	7:C1:392:PRO:HB2	1.93	0.51
10:5B:367:TYR:N	10:5B:560:ILE:O	2.35	0.51
20:M3:16:TRP:CZ3	63:M3:401:CDL:H532	2.46	0.51
27:BP:121:PRO:HA	27:BP:454:TYR:HB2	1.91	0.51
31:Y0:19:ILE:O	31:Y0:23:ASN:N	2.38	0.51
36:D:325:LEU:HD23	36:D:328:MET:HE2	1.93	0.51
40:H:119:TYR:CA	40:H:198:VAL:O	2.58	0.51
63:m1:401:CDL:H202	63:m1:401:CDL:H372	1.93	0.51
39:g:110:MET:HE2	39:g:137:PRO:HB3	1.93	0.51
40:h:119:TYR:CA	40:h:198:VAL:O	2.58	0.51
40:h:250:ASN:HB2	40:h:276:LYS:HD2	1.92	0.51
7:C1:531:LEU:HG	59:C1:702:HEA:HAC	1.93	0.51
10:5B:568:ALA:HA	44:L:139:GLU:HB2	1.92	0.51
63:M2:403:CDL:H782	63:M2:403:CDL:H561	1.92	0.51
32:Y5:103:LYS:NZ	63:Y5:201:CDL:OA9	2.33	0.51
53:U:99:ILE:HB	53:U:100:PRO:HD3	1.93	0.51
9:c3:408:GLN:OE1	33:a:318:ASN:ND2	2.36	0.51
10:5b:282:LYS:HE3	39:g:45:PRO:O	2.11	0.51
16:7c:73:THR:HG22	16:7c:92:LYS:HB2	1.92	0.51
17:7l:894:ASP:OD2	55:w:88:TYR:OH	2.28	0.51
20:m3:16:TRP:CZ3	63:m3:401:CDL:H532	2.46	0.51
27:bp:323:THR:OG1	27:bp:326:GLN:OE1	2.27	0.51
30:y7:277:VAL:HG13	30:y7:280:LEU:HD12	1.92	0.51
43:k:132:LYS:NZ	48:p:32:LYS:O	2.44	0.51
5:U5:143:ARG:HB3	50:R:63:ASP:HA	1.91	0.51
7:C1:94:TYR:OH	59:C1:701:HEA:O2A	2.26	0.51
9:C3:239:ILE:HG12	33:A:232:PHE:HD1	1.76	0.51
9:C3:568:SER:HB3	44:L:29:GLU:HA	1.93	0.51
34:B:345:ASN:O	34:B:349:ASN:ND2	2.32	0.51
9:c3:390:ILE:HD11	63:5b:702:CDL:H662	1.93	0.51
10:5b:374:LEU:HB2	10:5b:555:SER:HB3	1.93	0.51
10:5b:446:ARG:NH2	10:5b:545:GLU:OE2	2.44	0.51
18:m1:153:PRO:HA	18:m1:194:LEU:HB3	1.93	0.51
34:b:366:VAL:HG21	34:b:387:LEU:HD11	1.93	0.51
37:e:147:PHE:HD1	37:e:173:GLU:HG3	1.76	0.51
7:C1:439:GLY:HA3	7:C1:455:TYR:CD2	2.46	0.51
7:C1:477:LEU:HD11	7:C1:492:MET:HE1	1.93	0.51
34:B:366:VAL:HG21	34:B:387:LEU:HD11	1.93	0.51
38:F:136:ARG:NH1	38:F:269:ASP:OD1	2.39	0.51
45:M:134:LEU:HD13	45:M:141:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:O:123:ILE:HG22	47:O:127:VAL:HG13	1.93	0.51
7:c1:663:MET:O	16:7c:92:LYS:NZ	2.30	0.51
18:m1:107:ASP:CG	18:m1:151:SER:HB2	2.36	0.51
42:j:97:VAL:HG12	42:j:101:ILE:HG12	1.93	0.51
53:u:2:SER:HB3	54:v:132:TRP:CE3	2.46	0.51
56:x:40:ALA:HB2	56:x:102:LYS:HG2	1.92	0.51
7:C1:682:GLU:OE2	18:M1:158:ARG:NH1	2.44	0.50
11:6A:2:ILE:O	11:6A:6:LEU:HB3	2.11	0.50
13:6L:41:ARG:NH2	13:6L:43:GLU:OE2	2.44	0.50
18:M1:155:GLU:OE2	18:M1:204:ARG:NH2	2.38	0.50
27:BP:411:VAL:HG22	27:BP:417:ILE:HG12	1.92	0.50
33:A:380:ARG:HH21	33:A:431:LEU:HG	1.76	0.50
40:H:137:PRO:O	40:H:207:GLN:NE2	2.38	0.50
43:K:180:LEU:HD13	48:P:24:TYR:HB2	1.93	0.50
10:5b:165:MET:HE2	39:g:220:ASN:H	1.76	0.50
37:e:257:ASP:OD1	37:e:281:HIS:ND1	2.44	0.50
49:q:53:GLY:O	49:q:57:VAL:HG23	2.11	0.50
10:5B:282:LYS:HE3	39:G:45:PRO:O	2.12	0.50
24:T4:1:FME:HE1	36:D:270:VAL:HG21	1.93	0.50
33:A:249:ASP:O	39:G:34:ARG:NH1	2.31	0.50
40:H:230:ALA:O	40:H:233:THR:OG1	2.27	0.50
9:c3:264:ARG:NH2	33:a:332:ASP:O	2.44	0.50
18:m1:155:GLU:OE2	18:m1:204:ARG:NH2	2.36	0.50
37:e:128:TYR:HB3	63:e:402:CDL:H342	1.93	0.50
63:M3:401:CDL:HB4	63:M3:401:CDL:H121	1.92	0.50
28:FS:102:GLY:HA2	28:FS:140:LYS:HE3	1.93	0.50
7:c1:531:LEU:HG	59:c1:702:HEA:HAC	1.94	0.50
63:m3:401:CDL:H121	63:m3:401:CDL:HB4	1.92	0.50
30:y7:412:TYR:CZ	30:y7:416:ILE:HD11	2.47	0.50
54:v:78:GLU:HG3	54:v:82:PHE:HB3	1.93	0.50
10:5B:285:VAL:HG22	33:A:477:ILE:HD11	1.94	0.50
18:M1:107:ASP:CG	18:M1:151:SER:HB2	2.37	0.50
32:Y5:94:LEU:HD13	50:R:87:ILE:HG13	1.93	0.50
7:c1:439:GLY:HA3	7:c1:455:TYR:CD2	2.47	0.50
8:c2:57:ARG:HE	54:v:91:ASN:HB3	1.77	0.50
9:c3:524:ARG:NH1	49:q:48:GLU:OE2	2.45	0.50
17:7L:988:GLN:HG2	54:v:133:LYS:HD2	1.93	0.50
27:bp:121:PRO:HA	27:bp:454:TYR:HB2	1.93	0.50
27:bp:174:GLY:HA3	27:bp:177:TYR:CE2	2.47	0.50
37:e:147:PHE:CD1	37:e:173:GLU:HG3	2.47	0.50
40:h:230:ALA:O	40:h:233:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:n:76:ILE:HG13	46:n:77:THR:HG23	1.92	0.50
52:t:32:ARG:HA	55:w:41:LEU:HD11	1.94	0.50
12:6B:64:ASP:O	12:6B:68:LYS:N	2.45	0.50
18:M1:153:PRO:HA	18:M1:194:LEU:HB3	1.94	0.50
37:E:147:PHE:HD1	37:E:173:GLU:HG3	1.77	0.50
43:K:66:ILE:HD11	43:K:172:GLN:HB2	1.92	0.50
43:K:132:LYS:NZ	48:P:32:LYS:O	2.42	0.50
44:L:200:TYR:HB3	44:L:204:LEU:HB2	1.94	0.50
46:N:157:ILE:HD13	63:N:303:CDL:H361	1.94	0.50
48:P:120:LEU:HD21	48:P:165:LEU:HD11	1.94	0.50
7:c1:517:MET:HE1	7:c1:583:PHE:HA	1.92	0.50
8:c2:497:LEU:HD22	8:c2:503:ILE:HD13	1.94	0.50
9:c3:516:TYR:OH	45:m:121:TYR:O	2.29	0.50
63:7a:202:CDL:H572	63:7a:202:CDL:H781	1.94	0.50
17:7l:913:ARG:HB2	17:7l:920:LEU:HD23	1.94	0.50
38:f:290:ASN:HB2	54:v:79:ARG:HH21	1.77	0.50
63:f:401:CDL:HB22	63:f:401:CDL:HB4	1.94	0.50
7:C1:342:THR:HG21	7:C1:400:PRO:HD3	1.94	0.50
7:C1:586:MET:HE2	7:C1:601:HIS:HE2	1.75	0.50
10:5B:329:ARG:NH1	10:5B:396:GLU:OE2	2.44	0.50
31:Y0:46:LEU:HD13	37:E:341:TYR:HB2	1.94	0.50
8:c2:508:ASN:OD1	8:c2:509:SER:N	2.42	0.50
9:c3:215:GLN:NE2	27:bp:383:LEU:O	2.41	0.50
10:5b:166:ASN:HB3	37:e:350:TYR:HB2	1.93	0.50
14:6c:20:TYR:CZ	14:6c:22:ALA:HB3	2.46	0.50
20:m3:17:ASN:HD21	63:m3:401:CDL:HB22	1.76	0.50
40:h:269:TYR:OH	53:u:7:ARG:NH2	2.44	0.50
9:C3:509:ARG:HH12	9:C3:513:ASP:HB3	1.76	0.50
14:6C:41:TYR:HB3	63:U:201:CDL:H511	1.94	0.50
27:BP:121:PRO:HD2	27:BP:175:GLU:HA	1.94	0.50
27:BP:352:PHE:HB3	27:BP:377:PHE:CZ	2.46	0.50
32:Y5:156:ILE:HG21	49:Q:77:ARG:HG2	1.94	0.50
39:G:163:VAL:N	39:G:180:TRP:O	2.45	0.50
42:J:97:VAL:HG12	42:J:101:ILE:HG12	1.94	0.50
52:T:56:ARG:HG3	63:T:202:CDL:HB21	1.92	0.50
9:c3:494:ILE:HG12	63:5b:703:CDL:H741	1.94	0.50
10:5b:367:TYR:N	10:5b:560:ILE:O	2.35	0.50
27:bp:158:VAL:O	27:bp:162:ASN:ND2	2.34	0.50
27:bp:423:PHE:HE1	27:bp:450:LEU:HD22	1.77	0.50
10:5B:220:MET:SD	31:Y0:27:TYR:OH	2.69	0.50
18:M1:30:SER:OG	18:M1:120:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BP:136:PHE:HB3	27:BP:155:PRO:HA	1.93	0.50
30:Y7:373:GLU:OE1	46:N:100:ARG:NH1	2.45	0.50
40:H:156:GLU:OE1	40:H:163:GLN:NE2	2.42	0.50
40:H:269:TYR:OH	53:U:7:ARG:NH2	2.45	0.50
49:Q:6:HIS:NE2	52:T:139:ASP:OD2	2.39	0.50
5:u5:143:ARG:HB3	50:r:63:ASP:HA	1.92	0.50
7:c1:477:LEU:HD11	7:c1:492:MET:HE1	1.93	0.50
9:c3:509:ARG:HH12	9:c3:513:ASP:HB3	1.76	0.50
17:7l:954:GLU:OE2	17:7l:957:ARG:NH1	2.44	0.50
20:m3:69:PRO:HG2	20:m3:149:ILE:HG12	1.93	0.50
32:y5:94:LEU:HD13	50:r:87:ILE:HG13	1.93	0.50
7:C1:26:ILE:HG21	63:C1:707:CDL:H141	1.92	0.50
8:C2:355:GLY:HA3	9:C3:578:LYS:HD3	1.94	0.50
9:C3:390:ILE:HD11	63:5B:702:CDL:H662	1.93	0.50
8:c2:130:LEU:HG	8:c2:163:LEU:HD22	1.93	0.50
12:6b:64:ASP:O	12:6b:68:LYS:N	2.44	0.50
17:7l:923:PHE:HA	17:7l:925:LYS:HE3	1.94	0.50
62:m2:405:PC1:O12	46:n:169:ARG:NH2	2.38	0.50
40:h:156:GLU:OE1	40:h:163:GLN:NE2	2.42	0.50
10:5B:166:ASN:HB3	37:E:350:TYR:HB2	1.93	0.49
10:5B:442:LYS:NZ	10:5B:524:GLU:OE1	2.45	0.49
10:5B:466:GLN:OE1	10:5B:547:ASN:ND2	2.34	0.49
15:7A:82:PHE:HE2	63:7C:301:CDL:H822	1.76	0.49
63:M1:402:CDL:HB61	63:M2:401:CDL:HA4	1.93	0.49
31:Y0:36:ARG:NH2	52:T:99:PHE:O	2.42	0.49
40:H:141:TYR:HD1	53:U:11:GLU:HB3	1.77	0.49
43:K:225:MET:HE1	63:L:301:CDL:H202	1.94	0.49
9:c3:196:ILE:HD13	9:c3:232:ILE:HG21	1.93	0.49
9:c3:592:TYR:OH	56:x:21:ARG:NH2	2.45	0.49
20:m3:64:ARG:HB3	20:m3:297:ALA:HB3	1.94	0.49
27:bp:98:GLU:HA	27:bp:153:LEU:HD13	1.94	0.49
27:bp:352:PHE:HB3	27:bp:377:PHE:CZ	2.47	0.49
45:m:185:PRO:HG2	57:y:65:TYR:CE2	2.47	0.49
50:r:148:GLN:O	50:r:152:GLU:HG2	2.12	0.49
52:t:32:ARG:NH1	55:w:37:ASP:OD1	2.44	0.49
8:C2:417:ARG:O	8:C2:492:LYS:NZ	2.44	0.49
9:C3:501:TYR:CD2	9:C3:502:PRO:HD3	2.48	0.49
11:6A:8:ARG:NE	37:E:218:ASP:OD1	2.39	0.49
37:E:115:ASP:H	37:E:120:ASN:HD22	1.59	0.49
44:L:125:TYR:OH	63:L:301:CDL:OA3	2.30	0.49
63:c1:706:CDL:H512	15:7a:76:ARG:HA	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7c:163:HIS:NE2	62:7c:303:PC1:O14	2.27	0.49
27:bp:121:PRO:HD2	27:bp:175:GLU:HA	1.94	0.49
2:U2:273:LEU:O	2:U2:277:PRO:HD3	2.11	0.49
14:6C:20:TYR:CZ	14:6C:22:ALA:HB3	2.47	0.49
17:7L:926:VAL:N	17:7L:927:PRO:HD3	2.27	0.49
37:E:73:ASP:H	37:E:272:LYS:HB3	1.77	0.49
63:J:301:CDL:H142	62:N:301:PC1:H341	1.94	0.49
54:V:74:THR:HG21	63:V:201:CDL:HA61	1.93	0.49
20:m3:78:ASN:HD22	20:m3:140:PHE:HZ	1.59	0.49
40:h:137:PRO:O	40:h:207:GLN:NE2	2.37	0.49
43:k:225:MET:HE1	63:l:301:CDL:H202	1.95	0.49
19:M2:123:VAL:HG22	62:M2:405:PC1:H372	1.93	0.49
27:BP:98:GLU:HA	27:BP:153:LEU:HD13	1.94	0.49
27:BP:211:PRO:HG2	27:BP:265:LEU:HD13	1.93	0.49
37:E:147:PHE:CD1	37:E:173:GLU:HG3	2.48	0.49
37:E:209:GLU:OE1	37:E:236:TRP:NE1	2.39	0.49
8:c2:102:ARG:HE	45:m:158:GLY:HA3	1.77	0.49
9:c3:521:LEU:HD21	45:m:144:MET:HE1	1.93	0.49
10:5b:220:MET:SD	31:y0:27:TYR:OH	2.69	0.49
27:bp:267:GLY:HA3	27:bp:342:ARG:HA	1.94	0.49
34:b:360:HIS:NE2	34:b:367:ASP:OD1	2.37	0.49
39:g:166:GLN:HE21	39:g:168:VAL:HG11	1.77	0.49
44:l:50:ASN:OD1	44:l:55:LYS:NZ	2.46	0.49
45:m:153:LEU:O	45:m:156:VAL:HG12	2.11	0.49
9:C3:520:TYR:HB2	52:T:45:LYS:HE2	1.94	0.49
9:c3:501:TYR:CD2	9:c3:502:PRO:HD3	2.48	0.49
12:6b:47:LYS:NZ	17:7l:970:LEU:O	2.39	0.49
20:m3:97:ALA:HB2	20:m3:253:THR:HG22	1.95	0.49
30:y7:409:ILE:HD13	34:b:432:LEU:HB2	1.95	0.49
33:a:194:THR:HG23	33:a:207:VAL:HG22	1.95	0.49
63:j:301:CDL:H142	62:n:301:PC1:H341	1.95	0.49
10:5B:97:TYR:OH	10:5B:225:GLU:OE1	2.25	0.49
10:5B:216:HIS:ND1	45:M:84:TYR:O	2.46	0.49
17:7L:919:LYS:HG3	17:7L:939:MET:HE1	1.94	0.49
20:M3:97:ALA:HB2	20:M3:253:THR:HG22	1.95	0.49
31:Y0:61:LYS:HB3	63:T:201:CDL:HB32	1.95	0.49
37:E:138:LYS:HG3	63:E:402:CDL:H611	1.93	0.49
37:E:344:ILE:HD11	39:G:223:ASP:HA	1.95	0.49
49:Q:21:GLU:OE2	56:X:6:THR:OG1	2.31	0.49
7:c1:40:ILE:HG23	63:7c:301:CDL:H311	1.95	0.49
8:c2:112:LEU:HD22	8:c2:501:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:6a:2:ILE:O	11:6a:6:LEU:HB3	2.12	0.49
63:m1:404:CDL:H751	63:m1:404:CDL:H182	1.93	0.49
27:bp:260:ASN:HB3	27:bp:269:LEU:HD22	1.93	0.49
36:d:197:ARG:NH1	42:j:210:GLN:OE1	2.44	0.49
38:f:239:GLN:HE21	38:f:243:GLY:HA2	1.77	0.49
7:C1:76:ARG:HB3	7:C1:605:THR:HG23	1.95	0.49
17:7L:913:ARG:HB2	17:7L:920:LEU:HD23	1.94	0.49
23:T3:79:LEU:HD11	26:T6:6:GLY:HA3	1.94	0.49
45:M:153:LEU:O	45:M:156:VAL:HG12	2.11	0.49
6:u6:148:LEU:HA	6:u6:161:VAL:HG11	1.94	0.49
7:c1:75:ILE:HD11	7:c1:98:VAL:HA	1.95	0.49
7:c1:628:GLU:O	16:7c:48:ARG:NH2	2.42	0.49
7:c1:684:GLU:O	18:m1:165:LYS:NZ	2.41	0.49
27:bp:136:PHE:HB3	27:bp:155:PRO:HA	1.94	0.49
32:y5:156:ILE:HG21	49:q:77:ARG:HG2	1.95	0.49
37:e:28:PHE:CD2	37:e:30:PRO:HD3	2.48	0.49
44:l:153:TYR:HB3	63:l:301:CDL:H211	1.94	0.49
7:c1:553:VAL:HG12	16:7c:103:GLN:HG3	1.95	0.49
9:c3:403:TRP:HZ2	33:a:304:ILE:HD11	1.77	0.49
9:c3:455:TRP:HB3	62:a:501:PC1:H3B2	1.94	0.49
15:7a:121:TYR:HD1	15:7a:124:LEU:HD12	1.77	0.49
17:7l:926:VAL:N	17:7l:927:PRO:HD3	2.28	0.49
20:m3:230:ASP:OD1	20:m3:301:SER:OG	2.31	0.49
32:y5:164:TYR:HB3	32:y5:168:GLY:HA3	1.93	0.49
45:m:216:MET:HE3	55:w:71:TYR:HB2	1.94	0.49
6:U6:170:LYS:HD3	41:I:127:TYR:HB2	1.95	0.49
9:C3:592:TYR:OH	56:X:21:ARG:NH2	2.46	0.49
14:6C:14:ARG:NH2	14:6C:18:ASP:OD1	2.46	0.49
14:6C:48:ARG:HH12	17:7L:871:SER:HB3	1.77	0.49
15:7A:21:ASP:OD1	15:7A:22:ALA:N	2.46	0.49
50:R:148:GLN:O	50:R:152:GLU:HG2	2.11	0.49
52:T:17:LEU:HD13	52:t:158:LEU:HG	1.95	0.49
10:5b:568:ALA:HA	44:l:139:GLU:HB2	1.94	0.49
30:y7:152:ILE:HD11	30:y7:157:LEU:HD13	1.95	0.49
54:v:85:ILE:HG23	63:v:201:CDL:H522	1.95	0.49
11:6A:8:ARG:NH2	37:E:214:TYR:HB3	2.27	0.49
11:6A:110:PRO:HB2	56:X:122:VAL:HG22	1.94	0.49
34:B:346:GLN:O	34:B:350:ARG:HG2	2.13	0.49
39:G:135:LEU:HB3	39:G:139:GLU:HB2	1.94	0.49
39:G:162:PHE:HA	39:G:181:ASN:HA	1.94	0.49
49:Q:123:ALA:O	49:Q:127:ASN:ND2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c3:519:PHE:HE2	45:m:148:ILE:HG21	1.78	0.49
10:5b:269:PRO:O	10:5b:273:MET:HG2	2.13	0.49
10:5b:321:GLU:OE2	10:5b:413:TYR:OH	2.28	0.49
10:5b:466:GLN:OE1	10:5b:547:ASN:ND2	2.35	0.49
17:7l:891:CYS:SG	55:w:84:LYS:HD2	2.53	0.49
27:bp:87:THR:HG23	27:bp:119:MET:HE1	1.94	0.49
33:a:230:ASN:HB2	33:a:233:GLU:HG2	1.95	0.49
46:n:157:ILE:HD13	63:n:303:CDL:H361	1.95	0.49
48:p:40:VAL:HG11	48:p:100:PRO:HG2	1.95	0.49
52:t:56:ARG:HG3	63:t:202:CDL:HB21	1.94	0.49
52:t:64:ALA:HA	52:t:67:LEU:HD12	1.94	0.49
20:M3:230:ASP:OD1	20:M3:301:SER:OG	2.30	0.48
27:BP:174:GLY:HA3	27:BP:177:TYR:CE2	2.48	0.48
33:A:364:VAL:HG13	33:A:378:VAL:HG13	1.95	0.48
54:V:62:CYS:SG	54:V:63:ARG:N	2.87	0.48
62:c3:601:PC1:H222	49:q:99:TRP:HA	1.95	0.48
9:C3:519:PHE:HE2	45:M:148:ILE:HG21	1.78	0.48
17:7L:891:CYS:SG	55:W:84:LYS:HD2	2.53	0.48
7:c1:406:ASN:HD21	7:c1:469:LYS:NZ	2.11	0.48
19:m2:40:ARG:NH1	19:m2:147:ILE:O	2.44	0.48
43:k:180:LEU:HD13	48:p:24:TYR:HB2	1.94	0.48
44:l:38:GLN:HB3	44:l:41:ARG:HB3	1.95	0.48
46:n:77:THR:HB	63:n:303:CDL:HA21	1.95	0.48
46:n:191:ASN:OD1	46:n:191:ASN:N	2.39	0.48
7:C1:406:ASN:HD21	7:C1:469:LYS:NZ	2.11	0.48
8:C2:76:LYS:HD3	14:6C:11:TRP:CD1	2.49	0.48
9:C3:276:ILE:O	9:C3:280:MET:HG2	2.13	0.48
10:5B:165:MET:HE2	39:G:220:ASN:H	1.79	0.48
62:M2:405:PC1:O12	46:N:169:ARG:NH2	2.39	0.48
27:BP:119:MET:HG2	27:BP:124:THR:HG23	1.94	0.48
34:B:383:PRO:O	34:B:386:THR:OG1	2.29	0.48
55:W:72:ASN:H	55:W:99:TRP:CD1	2.31	0.48
8:c2:155:GLU:OE2	12:6b:115:ARG:NH1	2.46	0.48
9:c3:276:ILE:O	9:c3:280:MET:HG2	2.12	0.48
19:m2:155:GLU:HG2	19:m2:156:TRP:CD1	2.49	0.48
53:u:13:GLU:OE1	53:u:121:ARG:NH2	2.45	0.48
7:C1:40:ILE:HG23	63:7C:301:CDL:H311	1.96	0.48
17:7L:923:PHE:HA	17:7L:925:LYS:HE3	1.95	0.48
20:M3:81:ARG:NH1	20:M3:292:PHE:O	2.40	0.48
27:BP:267:GLY:HA3	27:BP:342:ARG:HA	1.96	0.48
30:Y7:380:TRP:O	30:Y7:384:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c3:505:LYS:HE3	62:c3:603:PC1:H31	1.96	0.48
22:t2:10:GLU:OE2	25:t5:15:ARG:NH1	2.46	0.48
30:y7:380:TRP:O	30:y7:384:ILE:HG12	2.13	0.48
37:e:49:LEU:HD23	37:e:282:VAL:HG13	1.95	0.48
37:e:98:GLU:OE2	51:s:51:ARG:NH1	2.46	0.48
43:k:191:SER:OG	48:p:26:GLN:O	2.21	0.48
47:o:110:GLN:NE2	47:o:114:ASP:OD1	2.47	0.48
9:C3:418:ASN:HB2	9:C3:437:ARG:HG3	1.95	0.48
10:5B:563:ARG:O	51:S:4:ARG:NH1	2.34	0.48
20:M3:81:ARG:NH2	20:M3:89:GLU:OE2	2.46	0.48
20:M3:131:ARG:NH2	20:M3:183:ASP:OD2	2.45	0.48
11:6a:8:ARG:NH2	37:e:214:TYR:HB3	2.29	0.48
30:y7:373:GLU:OE1	46:n:100:ARG:NH1	2.47	0.48
34:b:346:GLN:O	34:b:350:ARG:HG2	2.14	0.48
39:g:135:LEU:HB3	39:g:139:GLU:HB2	1.96	0.48
52:t:122:LEU:HD12	63:t:202:CDL:H192	1.95	0.48
35:c:461:TYR:HE1	35:c:469:PHE:HB2	1.78	0.48
8:C2:102:ARG:HE	45:M:158:GLY:HA3	1.78	0.48
38:F:198:ASN:HB3	62:V:202:PC1:H221	1.95	0.48
9:C3:18:PHE:HE2	9:C3:134:ILE:HD12	1.78	0.48
9:C3:196:ILE:HD13	9:C3:232:ILE:HG21	1.95	0.48
10:5B:81:ALA:HB2	63:5B:702:CDL:HA31	1.95	0.48
27:BP:190:TRP:HB3	27:BP:228:PRO:HA	1.95	0.48
33:A:408:VAL:O	33:A:414:GLN:NE2	2.40	0.48
35:C:461:TYR:HE1	35:C:469:PHE:HB2	1.78	0.48
37:E:38:LEU:HD12	37:E:47:LEU:HD23	1.96	0.48
44:L:153:TYR:HB3	63:L:301:CDL:H211	1.95	0.48
50:R:89:THR:OG1	51:S:98:ASP:OD2	2.30	0.48
51:S:130:VAL:HG23	51:S:132:LEU:HG	1.95	0.48
7:c1:76:ARG:HB3	7:c1:605:THR:HG23	1.96	0.48
18:m1:263:VAL:HG13	18:m1:278:GLY:HA2	1.96	0.48
20:m3:2:ALA:HA	20:m3:6:ILE:HB	1.96	0.48
22:t2:58:THR:HG1	25:t5:22:TYR:HH	1.54	0.48
27:bp:237:ASP:OD1	27:bp:237:ASP:N	2.47	0.48
37:e:115:ASP:H	37:e:120:ASN:HD22	1.61	0.48
54:v:62:CYS:SG	54:v:63:ARG:N	2.87	0.48
18:M1:263:VAL:HG13	18:M1:278:GLY:HA2	1.95	0.48
27:BP:189:SER:OG	27:BP:225:ARG:NH1	2.46	0.48
42:J:103:LEU:HB3	42:J:104:PRO:HD3	1.96	0.48
46:N:76:ILE:HG13	46:N:77:THR:HG23	1.95	0.48
53:U:68:VAL:O	53:U:72:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7c:66:ASP:OD1	16:7c:98:LYS:NZ	2.39	0.48
63:7c:301:CDL:H521	63:7c:301:CDL:H562	1.94	0.48
37:e:34:THR:HB	37:e:62:ARG:HH12	1.78	0.48
9:C3:455:TRP:HB3	62:A:501:PC1:H3B2	1.95	0.48
9:C3:494:ILE:HG12	63:5B:704:CDL:H741	1.96	0.48
10:5B:216:HIS:CE1	45:M:86:THR:HG22	2.48	0.48
10:5B:412:ARG:HB3	11:6A:52:HIS:CD2	2.49	0.48
43:K:70:TYR:OH	43:K:130:GLU:OE1	2.29	0.48
52:T:122:LEU:HD12	63:T:202:CDL:H192	1.95	0.48
7:c1:533:GLY:O	7:c1:537:THR:OG1	2.23	0.48
9:c3:504:LEU:HG	62:c3:603:PC1:H341	1.95	0.48
63:7c:301:CDL:H721	63:7c:301:CDL:H382	1.95	0.48
42:j:50:LEU:HD22	46:n:35:ILE:HG12	1.96	0.48
44:l:200:TYR:HB3	44:l:204:LEU:HB2	1.96	0.48
53:u:138:ARG:HH12	53:u:142:LEU:HD22	1.79	0.48
6:U6:148:LEU:HA	6:U6:161:VAL:HG11	1.95	0.48
20:M3:64:ARG:HB3	20:M3:297:ALA:HB3	1.96	0.48
33:A:230:ASN:HB2	33:A:233:GLU:HG2	1.95	0.48
48:P:40:VAL:HG11	48:P:100:PRO:HG2	1.96	0.48
7:c1:618:PHE:O	7:c1:621:MET:HG3	2.14	0.48
9:c3:239:ILE:HG12	33:a:232:PHE:HD1	1.79	0.48
12:6b:67:LEU:HB3	12:6b:69:LYS:HG2	1.95	0.48
13:6l:41:ARG:NH2	13:6l:43:GLU:OE2	2.47	0.48
63:7a:202:CDL:H791	46:n:126:GLY:HA2	1.96	0.48
40:h:141:TYR:HD1	53:u:11:GLU:HB3	1.78	0.48
43:k:133:LEU:HD13	43:k:178:SER:HB2	1.96	0.48
45:m:175:ARG:NH2	45:m:204:GLU:OE2	2.32	0.48
51:s:130:VAL:HG23	51:s:132:LEU:HG	1.96	0.48
56:x:30:ASN:OD1	56:x:30:ASN:N	2.44	0.48
20:M3:206:ARG:HH21	20:M3:259:GLY:H	1.61	0.47
27:BP:323:THR:OG1	27:BP:326:GLN:OE1	2.27	0.47
44:L:50:ASN:OD1	44:L:55:LYS:NZ	2.47	0.47
45:M:134:LEU:HB2	45:M:138:GLU:HB2	1.96	0.47
2:u2:274:LEU:HD22	30:y7:173:ILE:HG13	1.96	0.47
10:5b:273:MET:HE1	15:7a:28:TYR:HB2	1.96	0.47
10:5b:442:LYS:NZ	10:5b:524:GLU:OE1	2.46	0.47
14:6c:41:TYR:HB3	63:u:201:CDL:H511	1.96	0.47
40:h:88:ARG:NH1	40:h:285:GLN:OE1	2.47	0.47
8:C2:395:SER:OG	47:O:109:LYS:NZ	2.46	0.47
10:5B:469:ARG:NH2	10:5B:509:GLU:OE2	2.32	0.47
15:7A:56:LEU:O	15:7A:65:LYS:NZ	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:E:132:PHE:HD1	63:E:402:CDL:H311	1.79	0.47
46:N:182:VAL:HB	46:N:185:SER:HB3	1.96	0.47
10:5b:563:ARG:O	51:s:4:ARG:NH1	2.34	0.47
27:bp:119:MET:HG2	27:bp:124:THR:HG23	1.95	0.47
38:f:261:ASP:OD1	38:f:261:ASP:N	2.47	0.47
39:g:91:ASP:N	39:g:91:ASP:OD1	2.48	0.47
45:m:137:ASP:HB3	45:m:140:THR:HB	1.96	0.47
7:C1:598:MET:HE3	18:M1:127:ALA:HB3	1.95	0.47
59:C1:701:HEA:H172	59:C1:701:HEA:H261	1.63	0.47
21:T1:10:TYR:CD1	26:T6:1:FME:HCN	2.49	0.47
7:c1:477:LEU:HD13	63:m1:401:CDL:H241	1.97	0.47
8:c2:76:LYS:HD3	14:6c:11:TRP:CD1	2.50	0.47
9:c3:418:ASN:HB2	9:c3:437:ARG:HG3	1.96	0.47
15:7a:87:ILE:HD12	30:y7:346:LEU:HD11	1.96	0.47
18:m1:155:GLU:CD	18:m1:204:ARG:HH22	2.21	0.47
27:bp:206:ARG:O	27:bp:210:LEU:N	2.42	0.47
38:f:255:PHE:HD2	38:f:286:VAL:HG11	1.79	0.47
43:k:126:ILE:HB	43:k:142:ARG:HH12	1.79	0.47
8:C2:461:TYR:OH	40:H:190:GLU:OE2	2.27	0.47
10:5B:216:HIS:HE1	45:M:86:THR:HG22	1.79	0.47
22:T2:58:THR:OG1	25:T5:22:TYR:OH	2.27	0.47
30:Y7:311:TYR:CE2	30:Y7:314:GLY:HA3	2.50	0.47
34:B:360:HIS:NE2	34:B:367:ASP:OD1	2.38	0.47
36:D:300:ARG:NH1	36:D:346:GLU:OE1	2.47	0.47
44:L:137:LEU:O	44:L:148:ARG:NH1	2.46	0.47
7:c1:291:SER:O	7:c1:295:LEU:HG	2.14	0.47
15:7a:79:TRP:NE1	30:y7:316:TYR:OH	2.44	0.47
18:m1:57:VAL:HG13	63:m1:404:CDL:H121	1.95	0.47
31:y0:1:FME:HB2	32:y5:178:ILE:HG12	1.96	0.47
37:e:147:PHE:HB2	63:e:402:CDL:HB32	1.97	0.47
10:5B:269:PRO:O	10:5B:273:MET:HG2	2.14	0.47
19:M2:3:TYR:HB3	46:N:182:VAL:HG21	1.97	0.47
52:T:158:LEU:HD11	52:t:17:LEU:HB3	1.97	0.47
7:c1:94:TYR:OH	59:c1:701:HEA:O2A	2.28	0.47
63:c1:706:CDL:H742	63:c1:706:CDL:H572	1.96	0.47
9:c3:18:PHE:HE2	9:c3:134:ILE:HD12	1.78	0.47
9:c3:259:TYR:HB2	63:m3:401:CDL:H311	1.94	0.47
31:y0:46:LEU:HD13	37:e:341:TYR:HB2	1.96	0.47
8:C2:112:LEU:HD22	8:C2:501:VAL:HG21	1.95	0.47
9:C3:33:ASN:ND2	9:C3:72:ASN:OD1	2.48	0.47
9:C3:403:TRP:HZ2	33:A:304:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C3:504:LEU:HG	62:C3:603:PC1:H341	1.96	0.47
63:7A:202:CDL:H781	63:7A:202:CDL:H572	1.95	0.47
39:G:121:GLY:HA3	39:G:148:TYR:CZ	2.49	0.47
40:H:267:SER:HB3	53:U:5:THR:HG23	1.96	0.47
52:T:85:LEU:HD21	52:T:94:ARG:HH12	1.79	0.47
7:c1:258:LYS:O	7:c1:261:VAL:HG22	2.15	0.47
8:c2:122:TRP:CG	8:c2:556:TYR:HB2	2.50	0.47
9:c3:509:ARG:NH1	9:c3:513:ASP:HB3	2.29	0.47
10:5b:216:HIS:CE1	45:m:86:THR:HG22	2.49	0.47
42:j:103:LEU:HB3	42:j:104:PRO:HD3	1.96	0.47
45:m:134:LEU:HD13	45:m:141:ARG:HD2	1.97	0.47
7:C1:333:PRO:HB3	7:C1:407:MET:HE3	1.96	0.47
7:C1:621:MET:O	7:C1:625:SER:N	2.46	0.47
8:C2:111:SER:HA	8:C2:502:ASN:CB	2.45	0.47
8:C2:120:ARG:HG2	8:C2:121:GLN:H	1.79	0.47
8:C2:122:TRP:CG	8:C2:556:TYR:HB2	2.50	0.47
8:C2:335:THR:OG1	36:D:217:GLU:OE2	2.33	0.47
10:5B:253:VAL:HB	30:Y7:290:ILE:HD13	1.96	0.47
63:7C:301:CDL:H382	63:7C:301:CDL:H721	1.95	0.47
35:C:437:ILE:HD11	35:C:443:VAL:HG12	1.97	0.47
37:E:34:THR:HB	37:E:62:ARG:HH12	1.80	0.47
38:F:175:GLU:CD	38:F:211:ARG:HE	2.23	0.47
39:G:261:ARG:NH1	39:G:262:ASN:O	2.48	0.47
45:M:193:THR:O	57:Y:1:MET:HG2	2.15	0.47
57:Y:9:ARG:HD2	57:Y:20:ASN:HD21	1.79	0.47
7:c1:96:GLN:HG2	7:c1:271:THR:HG23	1.95	0.47
8:c2:268:TRP:HH2	8:c2:310:LEU:HD12	1.80	0.47
8:c2:514:HIS:ND1	8:c2:560:MET:HE1	2.29	0.47
9:c3:45:LEU:HD11	9:c3:53:LEU:HB2	1.97	0.47
9:c3:337:GLU:HB2	9:c3:343:ASP:HB2	1.96	0.47
10:5b:253:VAL:HB	30:y7:290:ILE:HD13	1.97	0.47
23:t3:79:LEU:HD11	26:t6:6:GLY:HA3	1.96	0.47
34:b:356:GLU:HB2	34:b:369:VAL:HB	1.97	0.47
40:h:99:LEU:HB2	40:h:124:ILE:HA	1.97	0.47
40:h:141:TYR:OH	40:h:260:CYS:O	2.32	0.47
40:h:175:ARG:NH2	54:v:121:ASP:OD1	2.48	0.47
40:h:267:SER:HB3	53:u:5:THR:HG23	1.96	0.47
46:N:77:THR:HB	63:N:303:CDL:HA21	1.97	0.47
7:c1:92:LEU:HD21	8:c2:555:ARG:HG2	1.97	0.47
10:5b:109:ASP:OD1	15:7a:48:LYS:NZ	2.43	0.47
14:6c:14:ARG:NH2	14:6c:18:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:m2:403:CDL:H782	63:m2:403:CDL:H561	1.95	0.47
27:bp:248:PHE:HB2	27:bp:269:LEU:HD21	1.97	0.47
7:C1:533:GLY:O	7:C1:537:THR:OG1	2.23	0.47
18:M1:155:GLU:CD	18:M1:204:ARG:HH22	2.22	0.47
20:M3:69:PRO:HG2	20:M3:149:ILE:HG12	1.96	0.47
27:BP:170:ASP:OD1	27:BP:171:VAL:N	2.45	0.47
37:E:336:ALA:HB3	39:G:73:PRO:HB2	1.95	0.47
38:F:255:PHE:HD2	38:F:286:VAL:HG11	1.80	0.47
47:O:79:ALA:O	47:O:83:MET:HG2	2.14	0.47
10:5b:395:ASP:HB2	30:y7:224:LEU:HD11	1.96	0.47
18:m1:224:SER:HB3	18:m1:228:ARG:HD3	1.97	0.47
27:bp:190:TRP:HB3	27:bp:228:PRO:HA	1.97	0.47
30:y7:295:LYS:HD3	39:g:40:ILE:HD11	1.95	0.47
33:a:364:VAL:HG13	33:a:378:VAL:HG13	1.97	0.47
36:d:300:ARG:NH1	36:d:346:GLU:OE1	2.48	0.47
7:C1:258:LYS:O	7:C1:261:VAL:HG22	2.15	0.47
9:C3:505:LYS:HE3	62:C3:603:PC1:H31	1.97	0.47
12:6B:15:GLY:HA2	55:W:83:MET:SD	2.55	0.47
52:T:158:LEU:HG	52:t:17:LEU:HD13	1.97	0.47
7:c1:621:MET:O	7:c1:625:SER:N	2.47	0.47
9:c3:415:PHE:CZ	9:c3:437:ARG:HD3	2.50	0.47
15:7a:2:ASN:OD1	33:a:459:ASN:ND2	2.48	0.47
22:t2:48:ALA:HB2	24:t4:50:THR:HG23	1.97	0.47
37:e:138:LYS:HG3	63:e:402:CDL:H611	1.95	0.47
49:q:2:ASP:OD1	49:q:3:ASN:N	2.48	0.47
5:U5:143:ARG:NH1	50:R:71:LEU:HD22	2.30	0.46
7:C1:291:SER:O	7:C1:295:LEU:HG	2.14	0.46
9:C3:525:GLU:HB2	63:T:202:CDL:H721	1.96	0.46
27:BP:237:ASP:N	27:BP:237:ASP:OD1	2.48	0.46
29:AC:68:VAL:HG21	37:E:11:LEU:HD23	1.95	0.46
36:D:199:LYS:HG2	36:D:204:GLU:HA	1.97	0.46
39:G:166:GLN:HE21	39:G:168:VAL:HG11	1.80	0.46
7:c1:275:THR:O	7:c1:275:THR:OG1	2.33	0.46
8:c2:5:LEU:HD21	8:c2:542:VAL:HG11	1.97	0.46
8:c2:76:LYS:HE2	28:fs:105:GLN:HE22	1.80	0.46
27:bp:411:VAL:HG22	27:bp:417:ILE:HG12	1.96	0.46
42:j:96:TRP:CH2	63:j:301:CDL:H721	2.50	0.46
9:C3:468:VAL:HA	9:C3:471:ILE:HG12	1.97	0.46
2:u2:277:PRO:HB2	30:y7:206:LEU:HD12	1.97	0.46
7:c1:56:ASN:HB3	7:c1:142:PHE:CZ	2.50	0.46
7:c1:639:LEU:HA	10:5b:189:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:c2:390:ARG:NH2	12:6b:149:ASP:OD2	2.44	0.46
9:c3:492:ILE:HD12	9:c3:492:ILE:HA	1.79	0.46
10:5b:412:ARG:HB3	11:6a:52:HIS:CD2	2.50	0.46
11:6a:8:ARG:NE	11:6a:8:ARG:HA	2.30	0.46
11:6a:56:ASN:HD22	32:y5:170:TYR:HE1	1.64	0.46
63:m1:403:CDL:H732	63:m1:403:CDL:H541	1.96	0.46
28:fs:92:GLN:H	28:fs:131:SER:HB3	1.80	0.46
38:f:136:ARG:NH1	38:f:269:ASP:OD1	2.41	0.46
45:m:143:ARG:HH22	45:m:186:ASP:CG	2.24	0.46
50:r:89:THR:OG1	51:s:98:ASP:OD2	2.30	0.46
51:s:25:TYR:CD2	51:s:39:THR:HG21	2.50	0.46
55:w:123:TYR:CD2	55:w:124:LYS:HB3	2.51	0.46
56:x:11:TRP:HZ3	56:x:19:ILE:HG13	1.80	0.46
6:U6:155:VAL:O	50:R:151:LYS:HG2	2.14	0.46
7:C1:225:SER:HB2	46:N:199:ALA:HB2	1.98	0.46
10:5B:320:VAL:HG11	11:6A:46:TYR:HB2	1.96	0.46
62:7C:304:PC1:H362	62:7C:304:PC1:H292	1.97	0.46
18:M1:3:PHE:CZ	18:M1:5:LEU:HB3	2.49	0.46
37:E:288:HIS:HD2	29:ac:28:TYR:HB2	1.80	0.46
55:W:123:TYR:CD2	55:W:124:LYS:HB3	2.50	0.46
7:C1:517:MET:HE1	7:C1:583:PHE:HA	1.97	0.46
9:C3:509:ARG:NH1	9:C3:513:ASP:HB3	2.29	0.46
63:M3:401:CDL:H732	33:A:298:TYR:HB3	1.98	0.46
28:FS:92:GLN:H	28:FS:131:SER:HB3	1.80	0.46
37:E:147:PHE:HB2	63:E:402:CDL:HB32	1.98	0.46
46:N:191:ASN:OD1	46:N:191:ASN:N	2.40	0.46
49:Q:66:TYR:HA	49:Q:90:MET:HE1	1.97	0.46
7:c1:119:ALA:HA	7:c1:123:ILE:HD13	1.97	0.46
7:c1:524:VAL:HA	7:c1:527:PHE:CE2	2.50	0.46
8:c2:267:SER:HA	21:t1:7:ASN:HB2	1.98	0.46
20:m3:224:HIS:HA	20:m3:238:SER:HB3	1.96	0.46
43:k:70:TYR:OH	43:k:130:GLU:OE1	2.30	0.46
45:m:134:LEU:HB2	45:m:138:GLU:HB2	1.97	0.46
45:m:173:TYR:O	45:m:176:MET:HG3	2.16	0.46
56:x:37:VAL:O	56:x:41:GLU:HG2	2.15	0.46
59:C1:701:HEA:HBA2	59:C1:701:HEA:HMA	1.98	0.46
8:C2:142:ASN:HD21	8:C2:146:ASN:HA	1.80	0.46
8:C2:453:ASP:OD1	8:C2:453:ASP:N	2.42	0.46
8:C2:514:HIS:ND1	8:C2:560:MET:HE1	2.30	0.46
17:7L:907:TRP:CG	17:7L:908:PRO:HD3	2.50	0.46
63:M1:402:CDL:H732	63:M1:402:CDL:H541	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:M:137:ASP:HB3	45:M:140:THR:HB	1.98	0.46
47:O:88:LEU:O	47:O:91:ARG:HG2	2.16	0.46
57:Y:8:ASN:HD22	57:Y:10:TYR:HD2	1.63	0.46
9:c3:411:HIS:CD2	33:a:316:TYR:HB3	2.51	0.46
9:c3:443:ASN:HB3	33:a:321:PHE:CE1	2.50	0.46
10:5b:163:GLY:HA2	10:5b:191:CYS:SG	2.55	0.46
18:m1:134:VAL:HG11	62:m1:402:PC1:H2F2	1.98	0.46
37:e:333:THR:OG1	37:e:334:GLU:N	2.48	0.46
38:f:166:TYR:HD1	63:f:401:CDL:H391	1.81	0.46
55:w:72:ASN:H	55:w:99:TRP:CD1	2.32	0.46
7:C1:623:PHE:CZ	7:C1:627:ILE:HD11	2.50	0.46
63:7C:301:CDL:H562	63:7C:301:CDL:H521	1.96	0.46
18:M1:58:GLU:OE2	18:M1:307:LYS:NZ	2.38	0.46
30:Y7:171:ASP:OD1	30:Y7:172:ASN:N	2.44	0.46
33:A:194:THR:HG23	33:A:207:VAL:HG22	1.98	0.46
33:A:335:ALA:HB1	33:A:338:ILE:HG13	1.97	0.46
37:E:34:THR:HG23	37:E:51:GLY:O	2.15	0.46
45:M:173:TYR:O	45:M:176:MET:HG3	2.15	0.46
7:c1:600:TRP:HA	7:c1:600:TRP:CE3	2.51	0.46
7:c1:623:PHE:CZ	7:c1:627:ILE:HD11	2.51	0.46
16:7c:133:GLN:NE2	39:g:207:GLU:O	2.42	0.46
29:ac:68:VAL:HG21	37:e:11:LEU:HD23	1.97	0.46
47:o:79:ALA:O	47:o:83:MET:HG2	2.15	0.46
7:C1:406:ASN:OD1	7:C1:473:TRP:NE1	2.49	0.46
8:C2:179:TRP:O	8:C2:183:LEU:HB2	2.16	0.46
8:C2:508:ASN:HB2	12:6B:181:GLN:HG3	1.98	0.46
8:C2:517:PHE:HB2	8:C2:524:LYS:HD3	1.96	0.46
10:5B:123:PRO:HG2	10:5B:208:MET:O	2.16	0.46
18:M1:166:THR:HG21	38:F:111:ASN:OD1	2.15	0.46
19:M2:155:GLU:HG2	19:M2:156:TRP:HD1	1.81	0.46
19:M2:218:TRP:HB3	63:M2:403:CDL:H511	1.97	0.46
27:BP:206:ARG:O	27:BP:210:LEU:N	2.43	0.46
48:P:34:PRO:HD3	48:P:173:TYR:HB3	1.97	0.46
50:R:94:ARG:HB3	50:R:97:LEU:HB3	1.97	0.46
7:c1:342:THR:HG21	7:c1:400:PRO:HD3	1.97	0.46
7:c1:391:HIS:O	7:c1:394:VAL:HG22	2.15	0.46
8:c2:508:ASN:HB2	12:6b:181:GLN:HG3	1.98	0.46
17:7l:952:GLU:OE1	55:w:93:TYR:OH	2.33	0.46
56:x:119:LYS:HA	56:x:121:TRP:HZ3	1.80	0.46
57:y:8:ASN:HD22	57:y:10:TYR:HD2	1.63	0.46
7:C1:293:ASP:OD1	7:C1:364:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C1:628:GLU:O	16:7C:48:ARG:NH2	2.44	0.46
9:C3:294:LYS:HD2	15:7A:62:VAL:HA	1.98	0.46
10:5B:327:MET:HE3	11:6A:27:LEU:HD13	1.98	0.46
15:7A:113:ALA:HB3	15:7A:116:ASP:HB2	1.97	0.46
20:M3:224:HIS:HA	20:M3:238:SER:HB3	1.97	0.46
34:B:356:GLU:HB2	34:B:369:VAL:HB	1.98	0.46
50:R:62:SER:OG	50:R:67:THR:OG1	2.24	0.46
10:5b:97:TYR:OH	10:5b:225:GLU:OE1	2.25	0.46
10:5b:227:ASP:OD1	10:5b:227:ASP:N	2.45	0.46
10:5b:293:VAL:HG21	39:g:54:VAL:HG12	1.98	0.46
19:m2:155:GLU:HG2	19:m2:156:TRP:HD1	1.81	0.46
29:ac:104:LYS:HD3	29:ac:107:LEU:HD12	1.98	0.46
38:f:198:ASN:HB3	62:v:202:PC1:H221	1.98	0.46
7:C1:115:PHE:O	7:C1:119:ALA:CB	2.60	0.46
7:C1:391:HIS:O	7:C1:394:VAL:HG22	2.15	0.46
16:7C:133:GLN:NE2	39:G:207:GLU:O	2.43	0.46
39:G:91:ASP:N	39:G:91:ASP:OD1	2.49	0.46
42:J:95:THR:HG23	42:J:144:LEU:HD21	1.97	0.46
53:U:13:GLU:OE1	53:U:121:ARG:NH2	2.48	0.46
59:c1:701:HEA:HBA2	59:c1:701:HEA:HMA	1.98	0.46
9:c3:374:TYR:CE1	11:6a:79:LEU:HB2	2.51	0.46
39:g:121:GLY:HA3	39:g:148:TYR:CZ	2.51	0.46
49:q:128:ARG:HH12	49:q:132:GLN:HE21	1.64	0.46
7:C1:524:VAL:HA	7:C1:527:PHE:CE2	2.51	0.46
7:C1:567:TYR:O	7:C1:571:GLN:HG2	2.16	0.46
9:C3:408:GLN:OE1	33:A:318:ASN:ND2	2.37	0.46
62:7C:302:PC1:H322	19:M2:218:TRP:CZ2	2.51	0.46
33:A:361:LYS:HG2	33:A:429:ARG:HH22	1.80	0.46
38:F:178:ILE:HD11	38:F:207:ALA:HB3	1.97	0.46
56:X:37:VAL:O	56:X:41:GLU:HG2	2.15	0.46
6:u6:151:PHE:HD2	6:u6:161:VAL:HG13	1.80	0.46
8:c2:111:SER:HA	8:c2:502:ASN:CB	2.46	0.46
11:6a:51:PRO:HB3	32:y5:177:PHE:CD1	2.51	0.46
15:7a:128:ASP:OD1	15:7a:129:ARG:N	2.45	0.46
27:bp:170:ASP:OD1	27:bp:171:VAL:N	2.47	0.46
54:v:37:ILE:O	54:v:41:GLN:HB2	2.16	0.46
5:U5:146:LYS:HB2	5:U5:146:LYS:HE3	1.69	0.45
7:C1:353:LEU:O	7:C1:357:VAL:HG22	2.15	0.45
7:C1:618:PHE:O	7:C1:621:MET:HG3	2.16	0.45
7:C1:657:GLN:NE2	39:G:105:TYR:OH	2.49	0.45
10:5B:227:ASP:OD1	10:5B:227:ASP:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:K:133:LEU:HD13	43:K:178:SER:HB2	1.97	0.45
7:c1:637:LEU:HD22	39:g:199:LEU:HD13	1.98	0.45
8:c2:197:PRO:HD2	20:m3:39:GLY:HA2	1.99	0.45
15:7a:21:ASP:OD1	15:7a:22:ALA:N	2.48	0.45
15:7a:82:PHE:HE2	63:7c:301:CDL:H822	1.81	0.45
37:e:34:THR:HG23	37:e:51:GLY:O	2.16	0.45
38:f:175:GLU:CD	38:f:211:ARG:HE	2.24	0.45
38:f:183:TRP:CH2	38:f:189:PRO:HG3	2.51	0.45
44:l:106:ARG:HG2	44:l:168:LEU:HD13	1.97	0.45
9:C3:337:GLU:HB2	9:C3:343:ASP:HB2	1.97	0.45
18:M1:224:SER:HB3	18:M1:228:ARG:HD3	1.98	0.45
18:M1:333:PHE:HB3	18:M1:344:THR:HG23	1.97	0.45
20:M3:2:ALA:HA	20:M3:6:ILE:HB	1.98	0.45
24:T4:38:ASN:O	24:T4:42:ARG:HG3	2.15	0.45
40:H:263:ILE:HG13	40:H:265:ILE:HG12	1.98	0.45
8:c2:278:ASN:O	21:t1:10:TYR:OH	2.28	0.45
9:c3:556:PHE:CD1	44:l:101:GLU:HG3	2.51	0.45
50:r:63:ASP:OD1	50:r:64:ASN:ND2	2.49	0.45
7:C1:464:MET:HG2	8:C2:86:PRO:HB2	1.98	0.45
8:C2:171:GLN:NE2	8:C2:407:ASP:OD1	2.50	0.45
20:M3:41:ASP:OD1	20:M3:44:SER:OG	2.32	0.45
37:E:49:LEU:HD23	37:E:282:VAL:HG13	1.97	0.45
49:Q:117:SER:O	49:Q:126:ARG:NH2	2.49	0.45
56:X:28:HIS:O	56:X:114:HIS:NE2	2.41	0.45
8:c2:120:ARG:HG2	8:c2:121:GLN:H	1.81	0.45
9:c3:386:LYS:NZ	10:5b:91:GLU:O	2.45	0.45
10:5b:457:ARG:HH12	10:5b:520:SEP:P	2.38	0.45
11:6a:62:GLU:OE2	30:y7:283:LYS:NZ	2.32	0.45
16:7c:58:ASP:OD1	16:7c:58:ASP:N	2.46	0.45
24:t4:38:ASN:O	24:t4:42:ARG:HG3	2.16	0.45
34:b:298:TYR:HB2	34:b:349:ASN:HD21	1.81	0.45
38:f:257:PRO:HG3	38:f:321:VAL:HG12	1.98	0.45
43:k:32:PRO:HB3	43:k:38:THR:HG21	1.98	0.45
35:c:437:ILE:HD11	35:c:443:VAL:HG12	1.98	0.45
7:C1:477:LEU:HD13	63:M1:401:CDL:H241	1.99	0.45
7:C1:600:TRP:CE3	7:C1:600:TRP:HA	2.51	0.45
8:C2:145:ASN:ND2	17:7L:890:ASP:OD2	2.49	0.45
9:C3:45:LEU:HD11	9:C3:53:LEU:HB2	1.98	0.45
12:6B:99:PRO:HB2	17:7L:921:LEU:HD11	1.98	0.45
62:7C:302:PC1:H371	62:7C:302:PC1:H271	1.99	0.45
18:M1:112:LEU:HB3	18:M1:324:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M1:208:GLN:NE2	18:M1:304:TYR:OH	2.32	0.45
30:Y7:201:GLU:HB2	35:C:442:LYS:HB3	1.99	0.45
46:N:34:ASN:O	46:N:37:VAL:HG22	2.16	0.45
51:S:25:TYR:CD2	51:S:39:THR:HG21	2.51	0.45
58:Z:79:VAL:HG23	58:Z:80:THR:HG23	1.98	0.45
17:7l:919:LYS:HG3	17:7l:939:MET:HE1	1.97	0.45
19:m2:218:TRP:HB3	63:m2:403:CDL:H511	1.97	0.45
30:y7:311:TYR:CE2	30:y7:314:GLY:HA3	2.51	0.45
39:g:162:PHE:HA	39:g:181:ASN:HA	1.97	0.45
42:j:95:THR:HG23	42:j:144:LEU:HD21	1.98	0.45
49:q:21:GLU:OE2	56:x:6:THR:OG1	2.27	0.45
49:q:129:ILE:HG22	49:q:137:TRP:HB2	1.98	0.45
5:U5:139:TRP:HD1	50:R:72:ILE:HG13	1.82	0.45
63:C1:706:CDL:OA3	30:Y7:357:SER:OG	2.33	0.45
9:C3:415:PHE:CZ	9:C3:437:ARG:HD3	2.52	0.45
15:7A:128:ASP:OD1	15:7A:129:ARG:N	2.44	0.45
40:H:99:LEU:HB2	40:H:124:ILE:HA	1.99	0.45
44:L:106:ARG:HG2	44:L:168:LEU:HD13	1.97	0.45
45:M:143:ARG:HH22	45:M:186:ASP:CG	2.25	0.45
7:c1:115:PHE:O	7:c1:119:ALA:CB	2.60	0.45
7:c1:328:ARG:HG2	45:m:88:GLU:OE2	2.17	0.45
7:c1:353:LEU:O	7:c1:357:VAL:HG22	2.15	0.45
7:c1:598:MET:HE3	18:m1:127:ALA:HB3	1.96	0.45
8:c2:252:ASP:C	8:c2:254:ASN:H	2.25	0.45
11:6a:110:PRO:HB2	56:x:122:VAL:HG22	1.99	0.45
12:6b:230:TYR:O	57:y:102:ARG:NH2	2.43	0.45
17:7l:927:PRO:O	17:7l:928:PHE:HB2	2.16	0.45
28:fs:95:VAL:HB	29:ac:125:ASP:HB2	1.97	0.45
42:j:234:LYS:NZ	56:x:35:GLU:OE2	2.42	0.45
53:u:120:LYS:HB3	53:u:120:LYS:HE2	1.83	0.45
8:C2:130:LEU:HG	8:C2:163:LEU:HD22	1.98	0.45
8:C2:405:VAL:HG21	47:O:83:MET:HE1	1.98	0.45
9:C3:345:ILE:HD11	56:X:120:LEU:HD23	1.98	0.45
62:C3:601:PC1:H222	49:Q:99:TRP:HA	1.97	0.45
11:6A:58:GLU:OE2	30:Y7:281:SER:OG	2.29	0.45
19:M2:155:GLU:HG2	19:M2:156:TRP:CD1	2.52	0.45
37:E:250:LYS:HB3	37:E:250:LYS:HE2	1.83	0.45
57:Y:1:MET:HB3	57:Y:34:TRP:CZ3	2.52	0.45
6:u6:155:VAL:O	50:r:151:LYS:HG2	2.16	0.45
9:c3:103:LEU:HD21	20:m3:216:ILE:HD13	1.98	0.45
9:c3:468:VAL:HA	9:c3:471:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6b:64:ASP:O	12:6b:68:LYS:HA	2.16	0.45
18:m1:3:PHE:CZ	18:m1:5:LEU:HB3	2.50	0.45
19:m2:294:TRP:NE1	63:m2:403:CDL:OA7	2.46	0.45
30:y7:171:ASP:OD1	30:y7:172:ASN:N	2.44	0.45
33:a:335:ALA:HB1	33:a:338:ILE:HG13	1.98	0.45
36:d:271:ASN:ND2	36:d:288:GLU:OE1	2.47	0.45
47:o:88:LEU:O	47:o:91:ARG:HG2	2.17	0.45
7:C1:630:ARG:NH2	16:7C:49:ASP:OD1	2.30	0.45
10:5B:497:HIS:ND1	30:Y7:189:TYR:OH	2.40	0.45
15:7A:79:TRP:NE1	30:Y7:316:TYR:OH	2.46	0.45
62:7C:304:PC1:H31	19:M2:208:LYS:HD3	1.99	0.45
17:7L:927:PRO:O	17:7L:928:PHE:HB2	2.16	0.45
38:F:257:PRO:HG3	38:F:321:VAL:HG12	1.98	0.45
9:c3:307:ARG:NH2	10:5b:242:GLU:OE1	2.42	0.45
11:6a:53:GLU:HG3	32:y5:170:TYR:OH	2.17	0.45
19:m2:177:ASN:HA	19:m2:180:LEU:HD23	1.98	0.45
52:t:72:PRO:HA	52:t:76:ILE:HD12	1.99	0.45
8:C2:142:ASN:HB3	12:6B:107:GLN:HB3	1.99	0.45
9:C3:481:LEU:O	9:C3:485:ASN:ND2	2.37	0.45
10:5B:293:VAL:HG21	39:G:54:VAL:HG12	1.99	0.45
14:6C:96:ARG:HH21	14:6C:100:MET:HA	1.82	0.45
19:M2:196:ILE:HB	62:M2:405:PC1:H332	1.99	0.45
20:M3:140:PHE:O	20:M3:144:PRO:HD2	2.17	0.45
28:FS:72:TYR:O	39:G:255:ARG:NH2	2.45	0.45
33:A:184:TRP:HB2	39:G:41:PRO:HB3	1.99	0.45
34:B:298:TYR:HB2	34:B:349:ASN:HD21	1.82	0.45
38:F:168:LYS:HB3	38:F:171:TYR:HD2	1.81	0.45
42:J:76:LEU:HG	42:J:164:LEU:HD21	1.99	0.45
47:O:185:PHE:CE2	47:O:189:ILE:HD11	2.52	0.45
12:6b:15:GLY:HA2	55:w:83:MET:SD	2.56	0.45
15:7a:121:TYR:CE1	46:n:71:ARG:HD3	2.52	0.45
20:m3:140:PHE:O	20:m3:144:PRO:HD2	2.17	0.45
36:d:303:GLU:HB3	36:d:311:ARG:HH21	1.81	0.45
48:p:109:LEU:O	48:p:113:THR:OG1	2.33	0.45
56:x:28:HIS:O	56:x:114:HIS:NE2	2.41	0.45
56:x:33:THR:HG23	56:x:106:ALA:HB1	1.97	0.45
12:6B:67:LEU:HB3	12:6B:69:LYS:HG2	1.98	0.45
18:M1:24:TRP:CZ2	63:M2:403:CDL:HB61	2.52	0.45
19:M2:186:ALA:HB2	19:M2:245:LEU:HD12	1.98	0.45
23:T3:63:GLU:HG2	25:T5:59:ILE:HG23	1.99	0.45
27:BP:255:SER:O	27:BP:290:LYS:NZ	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:O:119:LEU:O	47:O:123:ILE:HG13	2.16	0.45
5:u5:139:TRP:HD1	50:r:72:ILE:HG13	1.82	0.45
7:c1:26:ILE:HG21	63:c1:707:CDL:H141	1.97	0.45
7:c1:315:ILE:HG13	9:c3:315:ILE:HD13	1.98	0.45
15:7a:4:PHE:HB3	15:7a:18:GLU:HA	1.99	0.45
15:7a:88:TYR:OH	30:y7:339:ASN:O	2.25	0.45
16:7c:201:ARG:NH1	40:h:159:ASP:O	2.50	0.45
24:t4:1:FME:HE1	36:d:270:VAL:HG11	1.99	0.45
33:a:408:VAL:O	33:a:414:GLN:NE2	2.43	0.45
9:C3:492:ILE:HD12	9:C3:492:ILE:HA	1.83	0.45
9:C3:523:GLY:O	63:T:202:CDL:H562	2.17	0.45
17:7L:908:PRO:HG2	17:7L:957:ARG:NH2	2.32	0.45
27:BP:248:PHE:HB2	27:BP:269:LEU:HD21	1.99	0.45
36:D:303:GLU:HB3	36:D:311:ARG:HH21	1.81	0.45
38:F:208:TRP:CE3	63:F:401:CDL:H531	2.52	0.45
43:K:32:PRO:HB3	43:K:38:THR:HG21	1.99	0.45
46:N:166:GLU:OE1	46:N:169:ARG:NH1	2.50	0.45
51:S:127:LYS:HD2	51:S:134:GLU:HG3	1.98	0.45
8:c2:74:HIS:HB2	14:6c:14:ARG:NH2	2.32	0.45
8:c2:161:ASP:O	8:c2:164:HIS:ND1	2.47	0.45
8:c2:490:ARG:HH22	12:6b:84:GLU:CD	2.25	0.45
8:c2:568:PRO:HG2	8:c2:571:HIS:CD2	2.49	0.45
7:C1:235:LYS:HE3	42:J:52:LEU:HD21	1.97	0.44
7:C1:378:ASP:OD1	7:C1:378:ASP:N	2.48	0.44
8:C2:76:LYS:HE2	28:FS:105:GLN:HE22	1.82	0.44
8:C2:335:THR:HG23	36:D:233:TYR:OH	2.16	0.44
9:C3:386:LYS:NZ	10:5B:91:GLU:O	2.44	0.44
63:5B:702:CDL:H522	33:A:360:TRP:CZ3	2.52	0.44
12:6B:115:ARG:HH21	57:Y:71:GLU:CD	2.25	0.44
27:BP:91:TYR:OH	27:BP:121:PRO:O	2.26	0.44
30:Y7:125:ILE:HD12	30:Y7:133:ILE:HA	1.99	0.44
37:E:151:LEU:HD23	37:E:151:LEU:HA	1.87	0.44
38:F:216:ARG:HB2	63:F:401:CDL:HB31	1.98	0.44
7:c1:252:VAL:O	7:c1:255:ARG:NH1	2.48	0.44
18:m1:166:THR:HG21	38:f:111:ASN:OD1	2.16	0.44
62:m1:402:PC1:H322	19:m2:218:TRP:CZ2	2.52	0.44
24:t4:29:VAL:H	24:t4:32:ASP:HB2	1.81	0.44
30:y7:138:LEU:O	30:y7:142:ASN:ND2	2.28	0.44
34:b:391:ARG:O	43:k:117:GLU:HG2	2.17	0.44
46:n:34:ASN:O	46:n:37:VAL:HG22	2.16	0.44
7:C1:56:ASN:HB3	7:C1:142:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T2:48:ALA:HB2	24:T4:50:THR:HG23	1.99	0.44
37:E:101:ARG:NH2	51:S:45:GLN:OE1	2.50	0.44
44:L:109:TYR:HD2	44:L:168:LEU:HG	1.81	0.44
49:Q:90:MET:HE2	49:Q:90:MET:HB2	1.78	0.44
50:R:63:ASP:OD1	50:R:64:ASN:ND2	2.50	0.44
7:c1:72:ALA:HB2	7:c1:101:HIS:CE1	2.53	0.44
7:c1:333:PRO:HB3	7:c1:407:MET:HE3	1.98	0.44
8:c2:142:ASN:HD21	8:c2:146:ASN:HA	1.82	0.44
30:y7:379:MET:O	30:y7:383:ILE:HG13	2.17	0.44
36:d:199:LYS:HG2	36:d:204:GLU:HA	1.98	0.44
7:C1:266:ALA:HB3	7:C1:269:LEU:HG	1.99	0.44
10:5B:90:ILE:HG12	63:5B:702:CDL:H672	1.98	0.44
10:5B:220:MET:HE1	10:5B:248:THR:HG21	1.98	0.44
10:5B:457:ARG:NH1	10:5B:520:SEP:O1P	2.46	0.44
15:7A:108:ARG:NH1	15:7A:130:THR:O	2.50	0.44
16:7C:58:ASP:OD1	16:7C:58:ASP:N	2.46	0.44
19:M2:40:ARG:NH1	19:M2:147:ILE:O	2.46	0.44
40:H:119:TYR:CZ	40:H:199:THR:HG23	2.52	0.44
50:R:87:ILE:HG23	51:S:94:LEU:HD21	1.98	0.44
56:X:20:THR:HG22	56:X:24:LYS:HE2	1.98	0.44
5:u5:143:ARG:NH1	50:r:71:LEU:HD22	2.31	0.44
63:7a:202:CDL:H141	63:7a:202:CDL:H532	1.99	0.44
17:7l:907:TRP:CG	17:7l:908:PRO:HD3	2.52	0.44
63:n:303:CDL:H211	63:n:303:CDL:H541	2.00	0.44
7:C1:475:LEU:HD12	14:6C:17:TYR:HD2	1.83	0.44
7:C1:501:ALA:HB1	7:C1:530:MET:HB2	1.98	0.44
9:C3:515:PRO:HG3	9:C3:521:LEU:HD12	2.00	0.44
28:FS:90:LEU:HD11	28:FS:136:ILE:HD11	1.99	0.44
38:F:205:ASN:HD21	63:U:201:CDL:H671	1.81	0.44
53:U:120:LYS:HE2	53:U:120:LYS:HB3	1.81	0.44
9:c3:294:LYS:HD2	15:7a:62:VAL:HA	2.00	0.44
10:5b:123:PRO:HG2	10:5b:208:MET:O	2.17	0.44
10:5b:320:VAL:HG11	11:6a:46:TYR:HB2	1.99	0.44
63:m1:403:CDL:HA21	63:m1:403:CDL:HB31	1.99	0.44
31:y0:62:ASN:O	52:t:110:ASN:ND2	2.45	0.44
57:y:64:LEU:HD12	57:y:92:VAL:HG11	2.00	0.44
7:C1:328:ARG:HG2	45:M:88:GLU:OE2	2.18	0.44
8:C2:267:SER:HA	21:T1:7:ASN:HB2	2.00	0.44
28:FS:86:TYR:CD2	28:FS:108:PRO:HG3	2.52	0.44
40:H:141:TYR:OH	40:H:260:CYS:O	2.35	0.44
47:O:119:LEU:HD23	47:O:119:LEU:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c1:235:LYS:HE3	42:j:52:LEU:HD21	1.98	0.44
7:c1:378:ASP:OD1	7:c1:378:ASP:N	2.48	0.44
7:c1:630:ARG:NH2	16:7c:49:ASP:OD1	2.32	0.44
9:c3:170:LEU:HB2	20:m3:106:ALA:HB2	1.99	0.44
9:c3:366:VAL:HG11	49:q:92:VAL:HG21	1.99	0.44
14:6c:51:GLU:HB3	17:7l:872:VAL:HG11	1.98	0.44
63:7a:202:CDL:H741	63:7a:202:CDL:H712	1.83	0.44
18:m1:24:TRP:CZ2	63:m2:403:CDL:HB61	2.53	0.44
19:m2:171:ALA:HB2	19:m2:180:LEU:HD21	2.00	0.44
21:t1:10:TYR:CD1	26:t6:1:FME:HCN	2.53	0.44
30:y7:201:GLU:HB2	35:c:442:LYS:HB3	2.00	0.44
9:C3:170:LEU:HB2	20:M3:106:ALA:HB2	2.00	0.44
9:C3:280:MET:HG3	30:Y7:320:TYR:CZ	2.51	0.44
9:C3:374:TYR:CE1	11:6A:79:LEU:HB2	2.53	0.44
10:5B:402:LEU:HD22	30:Y7:244:LEU:HB2	2.00	0.44
11:6A:8:ARG:NE	11:6A:8:ARG:HA	2.32	0.44
63:7A:202:CDL:H741	63:7A:202:CDL:H712	1.84	0.44
17:7L:927:PRO:HG2	17:7L:936:TYR:CE1	2.53	0.44
51:S:64:ILE:HG13	51:S:69:ARG:HD2	2.00	0.44
9:c3:222:ILE:HD11	33:a:259:ASN:ND2	2.32	0.44
49:q:19:SER:HB2	49:q:102:TYR:O	2.18	0.44
51:s:64:ILE:HG13	51:s:69:ARG:HD2	2.00	0.44
7:C1:132:VAL:HG21	7:C1:312:ASN:HD21	1.82	0.44
7:C1:639:LEU:HA	10:5B:189:MET:HE1	1.99	0.44
8:C2:197:PRO:HD2	20:M3:39:GLY:HA2	2.00	0.44
9:C3:411:HIS:CD2	33:A:316:TYR:HB3	2.53	0.44
10:5B:163:GLY:HA2	10:5B:191:CYS:SG	2.58	0.44
10:5B:418:TYR:OH	11:6A:52:HIS:NE2	2.44	0.44
10:5B:563:ARG:NH1	10:5B:578:ASP:OD1	2.51	0.44
15:7A:87:ILE:HD12	30:Y7:346:LEU:HD11	2.00	0.44
27:BP:359:ASP:OD1	27:BP:370:LEU:HB3	2.18	0.44
29:AC:122:SER:O	37:E:346:HIS:NE2	2.47	0.44
57:Y:1:MET:HB3	57:Y:34:TRP:HZ3	1.82	0.44
63:c1:706:CDL:OA3	30:y7:357:SER:OG	2.34	0.44
8:c2:113:PHE:O	8:c2:503:ILE:HA	2.18	0.44
8:c2:356:GLU:HG2	9:c3:581:ILE:HD11	1.99	0.44
10:5b:87:LYS:O	10:5b:91:GLU:HG3	2.18	0.44
12:6b:115:ARG:HH21	57:y:71:GLU:CD	2.25	0.44
12:6b:151:ARG:HA	12:6b:155:PHE:HB2	1.99	0.44
37:e:175:ASP:OD1	37:e:175:ASP:N	2.51	0.44
39:g:160:GLN:HG2	39:g:199:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:p:45:SER:HB2	48:p:127:ASP:HB3	2.00	0.44
2:U2:270:ASN:O	2:U2:274:LEU:HG	2.18	0.44
9:C3:556:PHE:CD1	44:L:101:GLU:HG3	2.53	0.44
27:BP:406:ASP:O	27:BP:421:ASN:ND2	2.30	0.44
28:FS:71:LYS:HB3	39:G:257:TYR:OH	2.18	0.44
30:Y7:409:ILE:HD13	34:B:432:LEU:HB2	1.99	0.44
36:D:237:VAL:HA	36:D:345:ILE:O	2.18	0.44
38:F:290:ASN:HB2	54:V:79:ARG:HH21	1.83	0.44
44:L:217:PHE:CD2	47:O:88:LEU:HB2	2.52	0.44
7:c1:126:HIS:ND1	7:c1:336:THR:OG1	2.29	0.44
7:c1:293:ASP:OD1	7:c1:364:ARG:NE	2.50	0.44
18:m1:27:ARG:NH1	18:m1:29:ASP:OD2	2.50	0.44
27:bp:406:ASP:O	27:bp:421:ASN:ND2	2.29	0.44
40:h:119:TYR:CZ	40:h:199:THR:HG23	2.52	0.44
7:C1:119:ALA:HA	7:C1:123:ILE:HD13	2.00	0.44
7:C1:276:PHE:HB2	7:C1:360:MET:HE1	2.00	0.44
37:E:28:PHE:CD2	37:E:30:PRO:HD3	2.52	0.44
42:J:143:TRP:O	42:J:147:SER:HB2	2.18	0.44
49:Q:19:SER:HB2	49:Q:102:TYR:O	2.18	0.44
7:c1:567:TYR:O	7:c1:571:GLN:HG2	2.17	0.44
17:7l:908:PRO:HG2	17:7l:957:ARG:NH2	2.33	0.44
18:m1:338:ASN:ND2	18:m1:340:SER:O	2.50	0.44
22:t2:3:ASP:OD1	22:t2:4:LYS:N	2.50	0.44
28:fs:102:GLY:HA2	28:fs:140:LYS:HE3	1.99	0.44
30:y7:311:TYR:CD2	30:y7:314:GLY:HA3	2.53	0.44
48:p:31:LEU:O	48:p:175:HIS:NE2	2.47	0.44
2:U2:259:GLU:HB3	2:U2:260:PRO:HD3	1.98	0.43
7:C1:92:LEU:HD21	8:C2:555:ARG:HG2	2.00	0.43
7:C1:315:ILE:HG13	9:C3:315:ILE:HD13	1.99	0.43
20:M3:78:ASN:HD22	20:M3:140:PHE:HZ	1.64	0.43
36:D:324:ASP:O	36:D:328:MET:HG3	2.18	0.43
37:E:321:ASP:OD1	37:E:324:ARG:NH2	2.50	0.43
56:X:30:ASN:OD1	56:X:30:ASN:N	2.47	0.43
8:c2:142:ASN:HB3	12:6b:107:GLN:HB3	2.00	0.43
10:5b:294:GLU:HG3	30:y7:278:LYS:HD2	2.01	0.43
19:m2:216:MET:SD	19:m2:218:TRP:NE1	2.80	0.43
40:h:99:LEU:O	40:h:104:SER:OG	2.36	0.43
44:l:109:TYR:HB3	44:l:164:THR:HG23	2.00	0.43
50:r:94:ARG:HB3	50:r:97:LEU:HB3	2.00	0.43
7:C1:595:VAL:O	7:C1:598:MET:HG2	2.18	0.43
7:C1:658:HIS:CE1	7:C1:662:LYS:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C2:74:HIS:HB2	14:6C:14:ARG:NH2	2.33	0.43
30:Y7:379:MET:O	30:Y7:383:ILE:HG13	2.18	0.43
30:Y7:419:THR:HB	34:B:445:THR:HG22	1.99	0.43
36:D:197:ARG:NH1	42:J:210:GLN:OE1	2.50	0.43
44:L:109:TYR:HB3	44:L:164:THR:HG23	2.00	0.43
7:c1:276:PHE:HB2	7:c1:360:MET:HE1	2.01	0.43
7:c1:324:GLY:HA3	39:g:217:LYS:HB3	2.00	0.43
9:c3:164:ASN:OD1	9:c3:172:ARG:NH2	2.42	0.43
20:m3:275:ARG:HA	20:m3:278:LEU:HD13	1.99	0.43
27:bp:359:ASP:OD1	27:bp:370:LEU:HB3	2.18	0.43
40:h:263:ILE:HG13	40:h:265:ILE:HG12	2.00	0.43
48:p:39:VAL:HA	48:p:118:LEU:O	2.18	0.43
50:r:87:ILE:HG23	51:s:94:LEU:HD21	1.99	0.43
1:U1:93:UNK:O	41:I:159:ARG:NH2	2.52	0.43
7:C1:259:VAL:HG22	18:M1:18:ILE:HD13	1.99	0.43
8:C2:568:PRO:HG2	8:C2:571:HIS:CD2	2.51	0.43
15:7A:4:PHE:HB3	15:7A:18:GLU:HA	2.00	0.43
27:BP:158:VAL:O	27:BP:162:ASN:ND2	2.35	0.43
42:J:96:TRP:CH2	63:J:301:CDL:H721	2.53	0.43
49:Q:129:ILE:HG22	49:Q:137:TRP:HB2	1.99	0.43
54:V:37:ILE:O	54:V:41:GLN:HB2	2.17	0.43
7:c1:464:MET:HG2	8:c2:86:PRO:HB2	1.99	0.43
7:c1:595:VAL:O	7:c1:598:MET:HG2	2.18	0.43
11:6a:120:LEU:HB3	12:6b:187:PHE:HE1	1.84	0.43
12:6b:64:ASP:OD2	12:6b:71:GLN:NE2	2.51	0.43
15:7a:126:ILE:HG12	46:n:49:ARG:NH2	2.34	0.43
18:m1:62:LEU:O	18:m1:65:THR:HG22	2.17	0.43
28:fs:86:TYR:CD2	28:fs:108:PRO:HG3	2.53	0.43
48:p:34:PRO:HD3	48:p:173:TYR:HB3	2.00	0.43
49:q:90:MET:HE2	49:q:90:MET:HB2	1.75	0.43
49:q:128:ARG:NE	49:q:128:ARG:HA	2.32	0.43
7:C1:684:GLU:O	18:M1:165:LYS:NZ	2.47	0.43
8:C2:113:PHE:O	8:C2:503:ILE:HA	2.19	0.43
8:C2:251:ASN:HA	23:T3:22:TYR:OH	2.18	0.43
16:7C:34:ARG:NH1	19:M2:47:GLY:O	2.47	0.43
18:M1:48:LEU:HD23	18:M1:100:ALA:HB3	2.01	0.43
18:M1:218:PHE:O	18:M1:222:LYS:HG2	2.17	0.43
19:M2:294:TRP:NE1	63:M2:403:CDL:OA7	2.48	0.43
31:Y0:62:ASN:O	52:T:110:ASN:ND2	2.45	0.43
57:Y:59:ARG:NE	57:Y:63:GLU:OE2	2.45	0.43
7:c1:317:ARG:HB2	7:c1:340:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:6a:43:ARG:HE	11:6a:66:LEU:HD11	1.84	0.43
12:6b:64:ASP:O	12:6b:68:LYS:CA	2.67	0.43
14:6c:54:PHE:CD2	45:m:170:ASP:HB2	2.53	0.43
27:bp:449:ASP:HB3	27:bp:460:ILE:HB	2.00	0.43
63:e:401:CDL:H312	63:e:401:CDL:HB31	2.00	0.43
38:f:112:MET:HE3	38:f:115:GLU:HB2	2.01	0.43
42:j:143:TRP:O	42:j:147:SER:HB2	2.18	0.43
7:C1:450:ARG:HH21	45:M:119:VAL:HA	1.84	0.43
7:C1:464:MET:HB2	7:C1:465:PRO:HD3	2.00	0.43
59:C1:701:HEA:H271	59:C1:701:HEA:H211	1.68	0.43
8:C2:249:LEU:HD13	25:T5:13:PHE:HE1	1.83	0.43
12:6B:64:ASP:O	12:6B:68:LYS:HA	2.18	0.43
14:6C:54:PHE:CD2	45:M:170:ASP:HB2	2.53	0.43
19:M2:258:THR:O	19:M2:268:LYS:NZ	2.35	0.43
20:M3:275:ARG:HA	20:M3:278:LEU:HD13	2.00	0.43
22:T2:3:ASP:OD1	22:T2:4:LYS:N	2.51	0.43
37:E:333:THR:OG1	37:E:334:GLU:N	2.51	0.43
42:J:179:LEU:O	46:N:58:LYS:NZ	2.45	0.43
57:Y:52:GLU:O	57:Y:56:MET:HG3	2.18	0.43
7:c1:464:MET:HB2	7:c1:465:PRO:HD3	2.00	0.43
7:c1:518:HIS:HB3	8:c2:524:LYS:HE3	1.99	0.43
9:c3:131:TYR:HB3	9:c3:138:LEU:HD11	2.00	0.43
28:fs:130:GLN:O	28:fs:134:TYR:OH	2.34	0.43
36:d:364:ALA:HB1	36:d:369:PHE:HA	2.00	0.43
37:e:38:LEU:HD21	37:e:286:GLU:HG3	1.99	0.43
38:f:252:THR:O	38:f:323:GLY:HA2	2.18	0.43
44:l:109:TYR:HD2	44:l:168:LEU:HG	1.82	0.43
47:o:119:LEU:O	47:o:123:ILE:HG13	2.17	0.43
57:y:59:ARG:NE	57:y:63:GLU:OE2	2.45	0.43
7:C1:546:TYR:OH	39:G:187:ASP:OD2	2.23	0.43
8:C2:252:ASP:C	8:C2:254:ASN:H	2.27	0.43
37:E:175:ASP:OD1	37:E:175:ASP:N	2.52	0.43
63:U:201:CDL:H311	63:U:201:CDL:H711	2.00	0.43
56:X:11:TRP:HZ3	56:X:19:ILE:HG13	1.84	0.43
8:c2:251:ASN:HA	23:t3:22:TYR:OH	2.18	0.43
16:7c:65:HIS:CE1	39:g:198:VAL:HG11	2.54	0.43
23:t3:16:ARG:HA	23:t3:19:ASP:OD2	2.18	0.43
26:t6:59:LEU:HD23	26:t6:59:LEU:HA	1.84	0.43
28:fs:164:ARG:HH12	39:g:246:ASP:HA	1.81	0.43
38:f:178:ILE:HD11	38:f:207:ALA:HB3	1.99	0.43
49:q:117:SER:O	49:q:126:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:t:139:ASP:HA	63:t:202:CDL:H572	2.00	0.43
53:u:68:VAL:O	53:u:72:SER:OG	2.28	0.43
56:x:20:THR:HG22	56:x:24:LYS:HE2	1.99	0.43
57:y:4:THR:HG22	57:y:5:ALA:H	1.82	0.43
2:U2:279:VAL:HG21	2:U2:283:ILE:HB	2.00	0.43
8:C2:155:GLU:OE2	12:6B:115:ARG:NH1	2.52	0.43
8:C2:335:THR:HG21	36:D:231:VAL:HG11	2.00	0.43
15:7A:121:TYR:HD1	15:7A:124:LEU:HD12	1.83	0.43
22:T2:10:GLU:OE2	25:T5:15:ARG:NH1	2.52	0.43
27:BP:130:ASP:OD1	27:BP:130:ASP:N	2.42	0.43
30:Y7:277:VAL:HG13	30:Y7:280:LEU:HD12	2.01	0.43
34:B:402:ASP:HB2	34:B:409:LYS:HG3	2.01	0.43
46:N:78:PHE:HA	46:N:151:LYS:HG2	2.00	0.43
56:X:119:LYS:HA	56:X:121:TRP:HZ3	1.82	0.43
7:c1:353:LEU:HD22	7:c1:389:PHE:CZ	2.54	0.43
7:c1:517:MET:O	7:c1:520:THR:HG22	2.19	0.43
62:c1:705:PC1:H232	9:c3:312:THR:HG23	1.99	0.43
20:m3:17:ASN:ND2	63:m3:401:CDL:HB22	2.33	0.43
20:m3:124:ILE:HD11	63:k:301:CDL:H832	2.01	0.43
39:g:127:ALA:O	39:g:131:THR:HG23	2.18	0.43
46:n:155:HIS:O	46:n:161:ARG:NH1	2.45	0.43
55:w:79:LEU:HB3	55:w:82:SER:HB2	2.01	0.43
7:C1:72:ALA:HB2	7:C1:101:HIS:CE1	2.54	0.43
9:C3:222:ILE:HD11	33:A:259:ASN:ND2	2.34	0.43
9:C3:443:ASN:HB3	33:A:321:PHE:CE1	2.53	0.43
10:5B:87:LYS:O	10:5B:91:GLU:HG3	2.18	0.43
10:5B:273:MET:HE2	15:7A:25:LEU:HD23	2.01	0.43
10:5B:277:LYS:HD3	15:7A:20:TYR:HD1	1.84	0.43
16:7C:156:GLY:HA3	62:7C:302:PC1:H3B1	2.00	0.43
62:7C:304:PC1:H292	62:7C:304:PC1:H252	2.00	0.43
63:M1:401:CDL:H511	63:V:201:CDL:H742	2.00	0.43
63:M2:401:CDL:HA22	62:M2:402:PC1:H131	1.99	0.43
27:BP:325:GLY:O	27:BP:379:SER:OG	2.32	0.43
31:Y0:27:TYR:O	31:Y0:30:LEU:HG	2.19	0.43
63:Y0:101:CDL:H562	45:M:51:ARG:HG3	2.00	0.43
37:E:234:THR:O	37:E:238:VAL:HG13	2.18	0.43
37:E:257:ASP:OD1	37:E:281:HIS:ND1	2.40	0.43
38:F:208:TRP:HB2	63:F:401:CDL:H572	2.01	0.43
47:O:108:ARG:NH1	47:O:172:ASP:OD1	2.52	0.43
49:Q:166:ASP:OD1	49:Q:167:TYR:N	2.47	0.43
52:T:32:ARG:NH1	55:W:37:ASP:OD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:u5:146:LYS:HB2	5:u5:146:LYS:HE3	1.71	0.43
7:c1:501:ALA:HB1	7:c1:530:MET:HB2	1.99	0.43
9:c3:183:SER:HA	43:k:145:HIS:CE1	2.54	0.43
12:6b:182:ASP:OD1	12:6b:182:ASP:N	2.48	0.43
18:m1:112:LEU:HB3	18:m1:324:LEU:HD13	2.00	0.43
28:fs:117:VAL:HG13	28:fs:119:THR:HG22	2.01	0.43
30:y7:125:ILE:HD12	30:y7:133:ILE:HA	2.01	0.43
30:y7:307:ASN:O	30:y7:309:GLN:NE2	2.52	0.43
34:b:352:PRO:HB3	34:b:372:VAL:HG22	2.00	0.43
37:e:99:LEU:HD12	37:e:99:LEU:HA	1.84	0.43
8:C2:6:TRP:CE3	13:6L:4:LYS:HE3	2.53	0.43
8:C2:249:LEU:HD22	25:T5:13:PHE:HD1	1.83	0.43
8:C2:356:GLU:HG2	9:C3:581:ILE:HD11	2.01	0.43
9:C3:460:ILE:HG13	9:C3:461:PHE:N	2.33	0.43
19:M2:177:ASN:HA	19:M2:180:LEU:HD23	2.00	0.43
20:M3:34:GLN:HG2	20:M3:36:GLY:H	1.84	0.43
28:FS:164:ARG:HH22	39:G:246:ASP:C	2.27	0.43
30:Y7:273:ALA:O	30:Y7:278:LYS:NZ	2.39	0.43
32:Y5:174:ARG:O	32:Y5:178:ILE:HG13	2.19	0.43
36:D:364:ALA:HB1	36:D:369:PHE:HA	2.01	0.43
37:E:38:LEU:HD21	37:E:286:GLU:HG3	2.01	0.43
2:u2:278:ARG:O	30:y7:164:ASN:ND2	2.32	0.43
9:c3:415:PHE:O	9:c3:437:ARG:HD2	2.19	0.43
10:5b:90:ILE:HG12	63:5b:702:CDL:H672	1.99	0.43
10:5b:563:ARG:NH1	10:5b:578:ASP:OD1	2.52	0.43
15:7a:73:LEU:HD22	63:7a:201:CDL:H391	2.00	0.43
28:fs:164:ARG:HH22	39:g:246:ASP:C	2.26	0.43
33:a:323:TYR:CE1	56:x:102:LYS:HD2	2.54	0.43
37:e:234:THR:O	37:e:238:VAL:HG13	2.19	0.43
38:f:111:ASN:O	38:f:115:GLU:HG2	2.19	0.43
47:o:186:VAL:O	47:o:190:LEU:HG	2.19	0.43
7:C1:50:HIS:CE1	7:C1:51:LYS:HG2	2.54	0.43
7:C1:268:THR:O	7:C1:288:GLY:N	2.28	0.43
62:C1:705:PC1:H261	9:C3:319:ILE:HD12	1.99	0.43
9:C3:139:TYR:HB3	9:C3:146:PHE:HB3	2.01	0.43
10:5B:111:VAL:O	10:5B:115:TRP:HD1	2.02	0.43
11:6A:51:PRO:HB3	32:Y5:177:PHE:CD1	2.54	0.43
13:6L:66:ARG:NH1	14:6C:100:MET:HE3	2.34	0.43
18:M1:118:LEU:HB3	18:M1:139:THR:CG2	2.49	0.43
38:F:111:ASN:O	38:F:115:GLU:HG2	2.18	0.43
47:O:186:VAL:O	47:O:190:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c1:586:MET:HE2	7:c1:601:HIS:HE2	1.82	0.43
12:6b:99:PRO:HB2	17:7l:921:LEU:HD11	1.99	0.43
14:6c:96:ARG:HH21	14:6c:100:MET:HA	1.84	0.43
15:7a:78:ALA:HB2	30:y7:320:TYR:CE2	2.53	0.43
62:7c:303:PC1:H252	62:7c:303:PC1:H292	2.01	0.43
17:7l:927:PRO:HG2	17:7l:936:TYR:CE1	2.54	0.43
18:m1:48:LEU:HD23	18:m1:100:ALA:HB3	2.01	0.43
62:m1:402:PC1:H371	62:m1:402:PC1:H271	2.01	0.43
19:m2:159:GLY:O	19:m2:169:LYS:NZ	2.48	0.43
19:m2:196:ILE:HB	62:m2:405:PC1:H332	2.00	0.43
20:m3:97:ALA:O	20:m3:101:LEU:HB2	2.18	0.43
36:d:193:ARG:HB2	42:j:217:LEU:HB3	2.00	0.43
36:d:313:ASN:OD1	36:d:322:TRP:NE1	2.52	0.43
39:g:261:ARG:NH1	39:g:262:ASN:O	2.52	0.43
47:o:185:PHE:CE2	47:o:189:ILE:HD11	2.54	0.43
51:s:105:ASN:O	51:s:109:ILE:HG13	2.19	0.43
7:C1:37:ARG:NH1	63:C1:706:CDL:HB31	2.34	0.42
63:5B:704:CDL:H821	63:5B:704:CDL:H862	2.02	0.42
11:6A:53:GLU:HG3	32:Y5:170:TYR:OH	2.19	0.42
42:J:152:LYS:O	42:J:156:GLU:HG2	2.19	0.42
43:K:85:LYS:NZ	43:K:114:GLU:OE2	2.48	0.42
2:u2:259:GLU:HB3	2:u2:260:PRO:HD3	1.99	0.42
9:c3:345:ILE:HD11	56:x:120:LEU:HD23	2.00	0.42
9:c3:397:LEU:O	9:c3:401:ILE:HG13	2.19	0.42
15:7a:27:LYS:HD3	30:y7:289:VAL:HG22	2.01	0.42
20:m3:53:VAL:HG12	20:m3:57:LYS:HE3	2.01	0.42
27:bp:113:ASN:OD1	27:bp:113:ASN:N	2.51	0.42
27:bp:306:PHE:CE2	27:bp:362:VAL:HG13	2.54	0.42
29:ac:77:ARG:HH21	37:e:17:GLU:HG2	1.84	0.42
33:a:390:GLU:OE1	33:a:429:ARG:NH1	2.52	0.42
63:f:401:CDL:H791	63:f:401:CDL:H382	2.00	0.42
43:k:209:SER:O	44:l:140:TYR:OH	2.37	0.42
49:q:66:TYR:HA	49:q:90:MET:HE1	2.00	0.42
7:C1:141:GLY:O	7:C1:145:GLN:HG2	2.19	0.42
62:C1:705:PC1:H232	9:C3:312:THR:HG23	2.00	0.42
11:6A:120:LEU:HB3	12:6B:187:PHE:HE1	1.84	0.42
12:6B:64:ASP:O	12:6B:68:LYS:CA	2.68	0.42
15:7A:82:PHE:CE2	63:7C:301:CDL:H822	2.54	0.42
15:7A:88:TYR:OH	30:Y7:339:ASN:O	2.25	0.42
63:7A:201:CDL:H771	33:A:340:THR:HA	2.01	0.42
30:Y7:345:TRP:CD1	63:N:303:CDL:H592	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:A:238:LEU:O	33:A:243:TYR:OH	2.29	0.42
33:A:307:LYS:HD3	56:X:46:TYR:CZ	2.54	0.42
38:F:183:TRP:CH2	38:F:189:PRO:HG3	2.54	0.42
38:F:258:LEU:C	38:F:266:ASP:HB2	2.43	0.42
63:F:401:CDL:H791	63:F:401:CDL:H382	2.01	0.42
39:G:95:VAL:HG21	39:G:142:ASP:HB2	2.01	0.42
41:I:136:GLN:O	53:u:49:LYS:NZ	2.51	0.42
43:K:126:ILE:HB	43:K:142:ARG:HH12	1.84	0.42
7:c1:336:THR:HG22	7:c1:340:PHE:CE2	2.54	0.42
9:c3:398:LEU:HD23	9:c3:398:LEU:HA	1.88	0.42
18:m1:218:PHE:O	18:m1:222:LYS:HG2	2.19	0.42
20:m3:131:ARG:NH2	20:m3:183:ASP:OD2	2.45	0.42
30:y7:345:TRP:CD1	63:n:303:CDL:H592	2.53	0.42
30:y7:419:THR:HB	34:b:445:THR:HG22	2.00	0.42
34:b:402:ASP:HB2	34:b:409:LYS:HG3	2.01	0.42
42:j:144:LEU:HD11	63:j:301:CDL:H541	2.01	0.42
44:l:217:PHE:CD2	47:o:88:LEU:HB2	2.54	0.42
48:p:102:ASN:HA	48:p:136:GLU:HB2	2.02	0.42
54:v:55:LYS:HE2	54:v:55:LYS:HB3	1.89	0.42
2:U2:261:ILE:HG22	51:S:92:ASP:OD2	2.19	0.42
12:6B:182:ASP:OD1	12:6B:182:ASP:N	2.47	0.42
18:M1:338:ASN:ND2	18:M1:340:SER:O	2.53	0.42
20:M3:32:LYS:NZ	42:J:233:THR:OG1	2.50	0.42
27:BP:178:THR:HB	27:BP:190:TRP:CE2	2.54	0.42
27:BP:306:PHE:CE2	27:BP:362:VAL:HG13	2.54	0.42
30:Y7:420:LEU:HD23	34:B:379:LYS:HE3	2.01	0.42
34:B:391:ARG:O	43:K:117:GLU:HG2	2.19	0.42
41:I:212:LYS:O	41:I:217:GLU:HB2	2.19	0.42
8:c2:179:TRP:O	8:c2:183:LEU:HB2	2.18	0.42
9:c3:460:ILE:HG13	9:c3:461:PHE:N	2.34	0.42
13:6l:1:FME:HCN	13:6l:1:FME:HB3	1.70	0.42
16:7c:156:GLY:HA3	62:m1:402:PC1:H3B1	2.00	0.42
30:y7:439:LYS:HE2	30:y7:439:LYS:HB3	1.89	0.42
44:l:92:GLN:HG2	44:l:95:ILE:HG12	2.01	0.42
44:l:137:LEU:O	44:l:148:ARG:NH1	2.52	0.42
50:r:80:GLY:O	50:r:86:TYR:OH	2.38	0.42
7:C1:285:LYS:NZ	11:6A:122:GLU:HG3	2.33	0.42
10:5B:104:THR:O	10:5B:262:HIS:NE2	2.43	0.42
16:7C:201:ARG:NH1	40:H:159:ASP:O	2.52	0.42
18:M1:62:LEU:O	18:M1:65:THR:HG22	2.18	0.42
63:M1:403:CDL:H722	63:M1:403:CDL:H122	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T3:16:ARG:HA	23:T3:19:ASP:OD2	2.19	0.42
27:BP:314:GLY:HA3	27:BP:356:LYS:HB3	2.02	0.42
28:FS:95:VAL:HB	29:AC:125:ASP:HB2	2.01	0.42
29:AC:77:ARG:HH21	37:E:17:GLU:HG2	1.84	0.42
29:AC:105:ASP:OD2	45:M:41:ARG:HD2	2.19	0.42
30:Y7:311:TYR:CD2	30:Y7:314:GLY:HA3	2.55	0.42
31:Y0:64:TYR:CE1	31:Y0:66:ASP:HB2	2.54	0.42
39:G:160:GLN:HG2	39:G:199:LEU:HA	2.01	0.42
47:O:123:ILE:O	47:O:127:VAL:HG22	2.20	0.42
2:u2:261:ILE:HG22	51:s:92:ASP:OD2	2.20	0.42
7:c1:141:GLY:O	7:c1:145:GLN:HG2	2.19	0.42
8:c2:524:LYS:HB2	8:c2:524:LYS:HE2	1.79	0.42
9:c3:276:ILE:HD11	63:y7:501:CDL:H391	2.02	0.42
63:5b:703:CDL:H862	63:5b:703:CDL:H821	2.01	0.42
63:7a:202:CDL:H381	46:n:88:GLY:HA2	2.01	0.42
41:i:212:LYS:O	41:i:217:GLU:HB2	2.19	0.42
48:p:47:ARG:NH1	48:p:161:GLN:OE1	2.43	0.42
52:t:27:PHE:CE1	57:y:21:GLU:HG3	2.54	0.42
52:t:114:MET:HE2	52:t:114:MET:HB3	1.96	0.42
7:C1:125:TYR:CE1	39:G:208:ILE:HG21	2.55	0.42
7:C1:180:LYS:NZ	7:C1:204:ASP:O	2.52	0.42
7:C1:270:THR:HG23	7:C1:287:THR:HG22	2.01	0.42
7:C1:336:THR:HG22	7:C1:340:PHE:CE2	2.54	0.42
10:5B:497:HIS:CD2	30:Y7:205:ILE:HD12	2.54	0.42
19:M2:159:GLY:O	19:M2:169:LYS:NZ	2.49	0.42
36:D:206:PHE:CE2	36:D:244:VAL:HG12	2.55	0.42
40:H:92:MET:HE3	40:H:197:VAL:HG21	2.00	0.42
45:M:159:ILE:HD12	45:M:162:ALA:HB2	2.01	0.42
46:N:47:ASP:OD1	46:N:49:ARG:HD3	2.19	0.42
7:c1:105:MET:HB3	59:c1:701:HEA:CBC	2.49	0.42
7:c1:365:HIS:CD2	62:a:501:PC1:H221	2.55	0.42
8:c2:59:ARG:HD3	8:c2:59:ARG:HA	1.64	0.42
8:c2:514:HIS:CE1	8:c2:560:MET:HE1	2.54	0.42
9:c3:139:TYR:HB3	9:c3:146:PHE:HB3	2.02	0.42
12:6b:219:THR:HG22	52:t:142:TRP:O	2.19	0.42
20:m3:327:VAL:HG23	20:m3:330:SER:HB3	2.02	0.42
63:m3:401:CDL:H811	33:a:294:LEU:HD23	2.02	0.42
23:t3:51:GLU:OE1	25:t5:48:ARG:NH2	2.51	0.42
28:fs:129:SER:N	39:g:264:HIS:O	2.46	0.42
33:a:332:ASP:N	62:a:502:PC1:O12	2.44	0.42
33:a:361:LYS:HG2	33:a:429:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:p:60:ASN:HB2	48:p:94:TYR:CD1	2.55	0.42
48:p:86:ILE:HG12	48:p:92:ASP:HB3	2.02	0.42
7:C1:96:GLN:HG2	7:C1:271:THR:HG23	2.00	0.42
63:C1:706:CDL:H742	63:C1:706:CDL:H572	2.01	0.42
9:C3:299:SER:HB3	10:5B:108:PHE:HB2	2.02	0.42
10:5B:100:MET:HE3	10:5B:115:TRP:HH2	1.84	0.42
15:7A:78:ALA:HB2	30:Y7:320:TYR:CE2	2.54	0.42
31:Y0:33:PHE:HB3	32:Y5:171:LYS:HG3	2.01	0.42
34:B:350:ARG:HD3	34:B:373:ASN:HB2	2.00	0.42
35:C:446:ARG:O	35:C:450:ILE:HG13	2.19	0.42
47:O:110:GLN:NE2	47:O:114:ASP:OD1	2.52	0.42
50:R:111:TYR:OH	58:Z:44:HIS:NE2	2.40	0.42
7:c1:22:TYR:O	7:c1:26:ILE:HG12	2.20	0.42
7:c1:36:LEU:HD13	16:7c:112:MET:HE2	2.01	0.42
8:c2:477:GLY:HA3	40:h:181:TRP:CE2	2.55	0.42
16:7c:35:ASP:OD1	19:m2:51:ARG:NH1	2.50	0.42
16:7c:182:ASP:OD1	16:7c:182:ASP:N	2.52	0.42
32:y5:187:ARG:NH1	32:y5:188:ILE:O	2.53	0.42
36:d:237:VAL:HA	36:d:345:ILE:O	2.20	0.42
47:o:123:ILE:O	47:o:127:VAL:HG22	2.19	0.42
53:u:64:TYR:OH	53:u:111:GLN:NE2	2.50	0.42
7:C1:317:ARG:HB2	7:C1:340:PHE:CZ	2.55	0.42
9:C3:264:ARG:NH2	33:A:332:ASP:O	2.52	0.42
9:C3:272:ILE:HD12	9:C3:272:ILE:HA	1.91	0.42
10:5B:367:TYR:HB3	51:S:8:PHE:CZ	2.54	0.42
63:7A:202:CDL:H381	46:N:88:GLY:HA2	2.02	0.42
37:E:99:LEU:HD12	37:E:99:LEU:HA	1.84	0.42
37:E:200:ALA:O	37:E:243:LYS:NZ	2.41	0.42
45:M:195:THR:HA	57:Y:2:ALA:HA	2.01	0.42
52:T:76:ILE:HB	52:T:77:PRO:HD3	2.02	0.42
52:T:139:ASP:HA	63:T:202:CDL:H572	2.01	0.42
54:V:55:LYS:HE2	54:V:55:LYS:HB3	1.88	0.42
56:X:80:GLY:O	56:X:83:PRO:HD2	2.20	0.42
7:c1:58:LEU:O	7:c1:62:MET:HG3	2.20	0.42
10:5b:497:HIS:CD2	30:y7:205:ILE:HD12	2.55	0.42
16:7c:93:LYS:HG2	38:f:125:ASN:O	2.19	0.42
63:m1:401:CDL:H511	63:v:201:CDL:H742	2.01	0.42
19:m2:186:ALA:HB2	19:m2:245:LEU:HD12	2.01	0.42
33:a:340:THR:HG21	62:a:502:PC1:H252	2.01	0.42
36:d:324:ASP:O	36:d:328:MET:HG3	2.20	0.42
37:e:40:ASP:HB3	37:e:45:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:381:LYS:HD3	37:e:381:LYS:HA	1.87	0.42
41:i:185:ILE:HD13	41:i:185:ILE:HA	1.92	0.42
50:r:34:LYS:HE3	50:r:140:ASN:HA	2.00	0.42
56:x:80:GLY:O	56:x:83:PRO:HD2	2.20	0.42
57:y:44:VAL:HG21	57:y:103:GLN:O	2.20	0.42
35:c:446:ARG:O	35:c:450:ILE:HG13	2.18	0.42
7:C1:105:MET:HB3	59:C1:701:HEA:CBC	2.50	0.42
8:C2:57:ARG:HE	54:V:91:ASN:HB3	1.84	0.42
9:C3:524:ARG:NH1	49:Q:48:GLU:OE2	2.52	0.42
19:M2:205:LEU:HD23	19:M2:223:ALA:HA	2.02	0.42
63:M3:401:CDL:H781	33:A:294:LEU:HD23	2.02	0.42
28:FS:74:PRO:O	38:F:340:ARG:NH1	2.53	0.42
31:Y0:50:ASN:ND2	33:A:158:TYR:O	2.41	0.42
40:H:216:PRO:C	40:H:218:GLU:N	2.77	0.42
49:Q:78:ARG:O	49:Q:82:GLY:N	2.44	0.42
50:R:34:LYS:HE3	50:R:140:ASN:HA	2.00	0.42
7:c1:132:VAL:HG21	7:c1:312:ASN:HD21	1.85	0.42
10:5b:104:THR:O	10:5b:262:HIS:NE2	2.45	0.42
10:5b:220:MET:HE1	10:5b:248:THR:HG21	2.01	0.42
18:m1:80:MET:HE1	63:m1:404:CDL:H152	2.01	0.42
39:g:45:PRO:HG2	39:g:50:ILE:HD11	2.01	0.42
40:h:216:PRO:C	40:h:218:GLU:N	2.77	0.42
46:n:186:ALA:HB3	46:n:189:HIS:CD2	2.54	0.42
51:s:127:LYS:HD2	51:s:134:GLU:HG3	2.00	0.42
8:C2:98:ASN:O	8:C2:102:ARG:HG2	2.20	0.42
10:5B:457:ARG:HH12	10:5B:520:SEP:P	2.42	0.42
12:6B:111:SER:HB2	57:Y:66:TRP:CZ2	2.55	0.42
15:7A:121:TYR:CE1	46:N:71:ARG:HD3	2.55	0.42
16:7C:58:ASP:OD2	16:7C:62:THR:OG1	2.36	0.42
18:M1:80:MET:HE1	63:M1:403:CDL:H152	2.01	0.42
37:E:40:ASP:HB3	37:E:45:ARG:HB2	2.02	0.42
39:G:146:ILE:O	39:G:150:ILE:HG12	2.20	0.42
48:P:109:LEU:O	48:P:113:THR:OG1	2.30	0.42
48:P:129:VAL:O	48:P:133:ARG:HG2	2.20	0.42
52:T:23:THR:HG22	52:T:151:PRO:HG2	2.01	0.42
53:U:97:TRP:CD1	53:U:98:PRO:HD3	2.54	0.42
7:c1:415:ARG:NH1	7:c1:478:VAL:O	2.43	0.42
18:m1:333:PHE:HB3	18:m1:344:THR:HG23	2.02	0.42
27:bp:117:VAL:HG23	27:bp:460:ILE:HD11	2.02	0.42
37:e:189:ASP:HB3	37:e:192:SER:HG	1.85	0.42
49:q:108:ARG:HB2	49:q:111:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C1:22:TYR:O	7:C1:26:ILE:HG12	2.20	0.42
7:C1:324:GLY:HA3	39:G:217:LYS:HB3	2.02	0.42
8:C2:249:LEU:HD22	25:T5:13:PHE:CD1	2.55	0.42
8:C2:490:ARG:HH22	12:6B:84:GLU:CD	2.28	0.42
10:5B:447:LEU:HD13	10:5B:455:PHE:CG	2.55	0.42
20:M3:252:LYS:NZ	20:M3:256:GLN:OE1	2.49	0.42
22:T2:18:TYR:CD1	22:T2:51:ILE:HD13	2.55	0.42
32:Y5:117:ASN:ND2	37:E:104:ASP:OD2	2.53	0.42
32:Y5:121:ARG:NH2	51:S:52:GLU:OE2	2.52	0.42
39:G:180:TRP:N	39:G:180:TRP:CD1	2.88	0.42
49:Q:2:ASP:OD1	49:Q:3:ASN:N	2.51	0.42
51:S:105:ASN:O	51:S:109:ILE:HG13	2.20	0.42
9:c3:378:THR:O	9:c3:382:ASN:HB2	2.20	0.42
11:6a:8:ARG:NE	37:e:218:ASP:OD1	2.44	0.42
13:6l:66:ARG:NH1	14:6c:100:MET:HE3	2.35	0.42
62:7c:303:PC1:H31	19:m2:208:LYS:HD3	2.02	0.42
25:t5:4:ASN:O	25:t5:4:ASN:ND2	2.53	0.42
32:y5:174:ARG:O	32:y5:178:ILE:HG13	2.20	0.42
33:a:307:LYS:HD3	56:x:46:TYR:CZ	2.55	0.42
36:d:303:GLU:HB3	36:d:311:ARG:NH2	2.34	0.42
63:n:303:CDL:H472	63:n:303:CDL:H421	2.02	0.42
47:o:108:ARG:NH1	47:o:172:ASP:OD1	2.53	0.42
53:u:70:LEU:HD23	53:u:70:LEU:HA	1.92	0.42
7:C1:637:LEU:HD22	39:G:199:LEU:HD13	2.02	0.41
8:C2:8:GLU:HG2	8:C2:483:THR:HG22	2.01	0.41
62:C3:605:PC1:H232	33:A:296:CYS:O	2.20	0.41
36:D:303:GLU:HB3	36:D:311:ARG:NH2	2.35	0.41
56:X:33:THR:HG23	56:X:106:ALA:HB1	2.02	0.41
7:c1:285:LYS:NZ	11:6a:122:GLU:HG3	2.35	0.41
8:c2:40:TRP:CH2	28:fs:182:MET:HE1	2.54	0.41
8:c2:581:LEU:HD23	8:c2:581:LEU:HA	1.87	0.41
9:c3:525:GLU:HB2	63:t:202:CDL:H721	2.02	0.41
10:5b:111:VAL:O	10:5b:115:TRP:HD1	2.03	0.41
18:m1:164:ASP:OD1	18:m1:173:ARG:N	2.37	0.41
63:m2:404:CDL:H511	63:n:303:CDL:H601	2.02	0.41
28:fs:74:PRO:O	38:f:340:ARG:NH1	2.53	0.41
36:d:310:ARG:HE	42:j:206:LEU:HD12	1.85	0.41
40:h:105:GLN:HB3	40:h:155:LYS:HB2	2.02	0.41
42:j:57:HIS:CE1	46:n:48:HIS:HB3	2.55	0.41
2:U2:273:LEU:HD21	30:Y7:177:LYS:HG2	2.02	0.41
7:C1:58:LEU:O	7:C1:62:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:5B:703:CDL:H832	20:M3:124:ILE:HD11	2.02	0.41
19:M2:249:ASN:OD1	19:M2:250:ALA:N	2.53	0.41
20:M3:97:ALA:O	20:M3:101:LEU:HB2	2.20	0.41
33:A:340:THR:HG21	62:A:502:PC1:H252	2.02	0.41
38:F:261:ASP:OD1	38:F:261:ASP:N	2.46	0.41
42:J:181:ARG:NH1	46:N:62:ALA:O	2.52	0.41
45:M:117:ILE:HA	45:M:120:ILE:HG22	2.01	0.41
46:N:14:LEU:HD21	46:N:191:ASN:HD21	1.85	0.41
48:P:31:LEU:O	48:P:175:HIS:NE2	2.48	0.41
49:Q:36:SER:HG	49:Q:121:ASP:CG	2.26	0.41
49:Q:48:GLU:HA	49:Q:51:MET:HG2	2.02	0.41
49:Q:108:ARG:HB2	49:Q:111:TYR:CD2	2.55	0.41
52:T:27:PHE:CE1	57:Y:21:GLU:HG3	2.54	0.41
57:Y:1:MET:HB2	57:Y:4:THR:OG1	2.20	0.41
8:c2:98:ASN:O	8:c2:102:ARG:HG2	2.20	0.41
8:c2:335:THR:HG23	36:d:233:TYR:OH	2.19	0.41
10:5b:100:MET:HE3	10:5b:115:TRP:HH2	1.84	0.41
10:5b:321:GLU:OE1	10:5b:412:ARG:NH2	2.53	0.41
63:7a:201:CDL:H771	33:a:340:THR:HA	2.02	0.41
62:7c:303:PC1:H292	62:7c:303:PC1:H362	2.02	0.41
17:7l:873:PRO:HB3	53:u:55:ASP:HB3	2.03	0.41
62:m1:402:PC1:H291	62:m1:402:PC1:H2H2	2.01	0.41
20:m3:34:GLN:HG2	20:m3:36:GLY:H	1.85	0.41
24:t4:24:LYS:HE2	24:t4:26:LYS:HE2	2.01	0.41
30:y7:234:LEU:HG	30:y7:235:VAL:HG13	2.01	0.41
30:y7:420:LEU:HD23	34:b:379:LYS:HE3	2.01	0.41
38:f:208:TRP:CE3	63:f:401:CDL:H531	2.56	0.41
42:j:152:LYS:O	42:j:156:GLU:HG2	2.20	0.41
7:C1:353:LEU:HD22	7:C1:389:PHE:CZ	2.55	0.41
7:C1:557:ARG:NH2	18:M1:293:SER:HG	2.13	0.41
10:5B:216:HIS:CE1	45:M:86:THR:H	2.38	0.41
12:6B:78:MET:HE3	12:6B:78:MET:HB2	1.85	0.41
16:7C:65:HIS:CE1	39:G:198:VAL:HG11	2.54	0.41
18:M1:164:ASP:OD1	18:M1:173:ARG:N	2.37	0.41
27:BP:138:TRP:CE2	27:BP:140:GLN:HB3	2.55	0.41
40:H:99:LEU:O	40:H:104:SER:OG	2.38	0.41
7:c1:125:TYR:CE1	39:g:208:ILE:HG21	2.55	0.41
7:c1:342:THR:HG22	7:c1:396:VAL:HA	2.02	0.41
9:c3:280:MET:HG3	30:y7:320:TYR:CZ	2.54	0.41
10:5b:327:MET:HE3	11:6a:27:LEU:HD13	2.01	0.41
10:5b:367:TYR:HB3	51:s:8:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:5b:702:CDL:H522	33:a:360:TRP:CZ3	2.55	0.41
15:7a:113:ALA:HB3	15:7a:116:ASP:HB2	2.02	0.41
17:7l:927:PRO:HG3	17:7l:938:TYR:OH	2.19	0.41
20:m3:81:ARG:NH2	20:m3:89:GLU:OE2	2.52	0.41
31:y0:69:TYR:CE1	52:t:71:GLY:HA3	2.55	0.41
33:a:300:VAL:HB	33:a:301:PRO:HD3	2.01	0.41
37:e:231:ARG:NH1	37:e:286:GLU:OE1	2.34	0.41
39:g:146:ILE:O	39:g:150:ILE:HG12	2.21	0.41
44:l:91:TYR:HA	44:l:96:ARG:HD2	2.03	0.41
46:n:47:ASP:OD1	46:n:49:ARG:HD3	2.20	0.41
8:C2:59:ARG:HA	8:C2:59:ARG:HD3	1.64	0.41
8:C2:341:GLU:OE1	56:X:113:TYR:OH	2.35	0.41
9:C3:103:LEU:HD21	20:M3:216:ILE:HD13	2.02	0.41
12:6B:94:PHE:HA	12:6B:95:PRO:HD3	1.93	0.41
62:M2:402:PC1:H112	62:M2:402:PC1:H153	1.74	0.41
24:T4:31:HIS:O	24:T4:35:ARG:HG3	2.19	0.41
27:BP:93:SER:O	27:BP:137:GLY:HA2	2.20	0.41
28:FS:141:PHE:O	39:G:255:ARG:NH1	2.45	0.41
33:A:402:PRO:O	33:A:460:TYR:OH	2.21	0.41
39:G:127:ALA:O	39:G:131:THR:HG23	2.20	0.41
7:c1:105:MET:HB3	59:c1:701:HEA:HBC1	2.03	0.41
7:c1:310:PHE:CD1	7:c1:310:PHE:C	2.98	0.41
8:c2:224:PHE:HD1	8:c2:224:PHE:H	1.68	0.41
10:5b:162:THR:HB	10:5b:171:GLU:HB3	2.02	0.41
12:6b:121:GLN:HA	12:6b:124:TYR:HB2	2.02	0.41
12:6b:139:ARG:NH2	45:m:138:GLU:OE1	2.50	0.41
18:m1:118:LEU:HB3	18:m1:139:THR:CG2	2.51	0.41
24:t4:31:HIS:O	24:t4:35:ARG:HG3	2.19	0.41
29:ac:105:ASP:OD2	45:m:41:ARG:HD2	2.19	0.41
30:y7:187:ILE:HG23	51:s:46:VAL:HG13	2.02	0.41
38:f:258:LEU:C	38:f:266:ASP:HB2	2.45	0.41
49:q:36:SER:HG	49:q:121:ASP:CG	2.25	0.41
50:r:113:GLY:O	50:r:117:THR:HG22	2.20	0.41
57:y:52:GLU:O	57:y:56:MET:HG3	2.21	0.41
58:z:79:VAL:HG23	58:z:80:THR:HG23	2.01	0.41
9:C3:186:ASP:OD1	43:K:177:ARG:NH2	2.32	0.41
10:5B:162:THR:HB	10:5B:171:GLU:HB3	2.02	0.41
27:BP:417:ILE:HB	27:BP:438:ALA:HB3	2.03	0.41
33:A:44:TYR:O	33:A:114:GLN:NE2	2.54	0.41
33:A:300:VAL:HB	33:A:301:PRO:HD3	2.02	0.41
38:F:146:PHE:HB2	38:F:333:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L:91:TYR:HA	44:L:96:ARG:HD2	2.03	0.41
63:N:303:CDL:H472	63:N:303:CDL:H421	2.02	0.41
48:P:102:ASN:HA	48:P:136:GLU:HB2	2.03	0.41
51:S:124:GLU:HB3	51:S:139:LEU:HB3	2.02	0.41
8:c2:112:LEU:HB2	8:c2:501:VAL:HG22	2.02	0.41
10:5b:93:THR:HG22	10:5b:94:GLY:H	1.86	0.41
10:5b:216:HIS:HE1	45:m:86:THR:HG22	1.83	0.41
10:5b:266:LEU:HD12	15:7a:45:LEU:HD21	2.01	0.41
27:bp:93:SER:O	27:bp:137:GLY:HA2	2.21	0.41
12:6B:151:ARG:HA	12:6B:155:PHE:HB2	2.01	0.41
14:6C:64:GLY:O	14:6C:68:ASN:ND2	2.54	0.41
16:7C:85:VAL:HG13	38:F:131:ILE:HG23	2.02	0.41
27:BP:370:LEU:HB2	27:BP:401:LEU:HD11	2.02	0.41
33:A:151:ASN:HB3	33:A:155:ARG:HH21	1.85	0.41
39:G:280:GLU:HB2	37:e:1:FME:HE2	2.01	0.41
40:H:239:GLU:H	40:H:239:GLU:CD	2.29	0.41
48:P:60:ASN:HB2	48:P:94:TYR:CD1	2.55	0.41
49:Q:8:TRP:HA	49:Q:109:ARG:HH11	1.85	0.41
49:Q:128:ARG:HA	49:Q:128:ARG:NE	2.35	0.41
53:U:121:ARG:O	53:U:125:MET:HG3	2.21	0.41
7:c1:439:GLY:HA3	7:c1:455:TYR:CE2	2.56	0.41
62:c1:705:PC1:H261	9:c3:319:ILE:HD12	2.02	0.41
9:c3:286:LEU:HD12	63:7a:201:CDL:H511	2.03	0.41
9:c3:470:ARG:HA	9:c3:470:ARG:HD3	1.79	0.41
63:5b:703:CDL:OB9	49:q:84:ARG:HA	2.19	0.41
62:7c:303:PC1:H342	62:m1:402:PC1:H3C1	2.02	0.41
27:bp:138:TRP:CE2	27:bp:140:GLN:HB3	2.55	0.41
27:bp:178:THR:HB	27:bp:190:TRP:CE2	2.56	0.41
29:ac:105:ASP:O	45:m:49:TYR:OH	2.23	0.41
33:a:238:LEU:O	33:a:243:TYR:OH	2.30	0.41
38:f:231:GLY:HA3	38:f:326:ILE:O	2.20	0.41
46:n:78:PHE:HA	46:n:151:LYS:HG2	2.02	0.41
49:q:8:TRP:HD1	49:q:110:LEU:HD11	1.84	0.41
50:r:72:ILE:HD13	50:r:72:ILE:HA	1.90	0.41
59:C1:702:HEA:H211	59:C1:702:HEA:H271	1.81	0.41
8:C2:40:TRP:CH2	28:FS:182:MET:HE1	2.55	0.41
9:C3:183:SER:HA	43:K:145:HIS:CE1	2.56	0.41
20:M3:53:VAL:HG12	20:M3:57:LYS:HE3	2.03	0.41
63:Y5:201:CDL:H431	50:R:104:LEU:HB3	2.01	0.41
33:A:476:LYS:HB3	33:A:479:PHE:CD1	2.55	0.41
62:A:501:PC1:H252	62:A:502:PC1:H331	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:E:189:ASP:HB3	37:E:192:SER:OG	2.21	0.41
37:E:313:TYR:O	37:E:317:GLN:HG2	2.21	0.41
44:L:92:GLN:HG2	44:L:95:ILE:HG12	2.03	0.41
50:R:80:GLY:O	50:R:86:TYR:OH	2.38	0.41
7:c1:654:ARG:HD2	7:c1:654:ARG:HA	1.84	0.41
8:c2:249:LEU:HD22	25:t5:13:PHE:HD1	1.85	0.41
9:c3:456:HIS:O	9:c3:460:ILE:HG23	2.21	0.41
10:5b:216:HIS:CE1	45:m:86:THR:H	2.39	0.41
10:5b:308:ASN:HB3	37:e:21:ALA:HB2	2.02	0.41
22:t2:18:TYR:CD1	22:t2:51:ILE:HD13	2.55	0.41
23:t3:37:LEU:HD21	23:t3:55:LEU:HD11	2.03	0.41
31:y0:27:TYR:O	31:y0:30:LEU:HG	2.21	0.41
33:a:184:TRP:HB2	39:g:41:PRO:HB3	2.02	0.41
33:a:476:LYS:HB3	33:a:479:PHE:CD1	2.55	0.41
34:b:350:ARG:HD3	34:b:373:ASN:HB2	2.01	0.41
39:g:180:TRP:N	39:g:180:TRP:CD1	2.88	0.41
40:h:269:TYR:HB3	54:v:127:ARG:HB3	2.03	0.41
52:t:76:ILE:HB	52:t:77:PRO:HD3	2.03	0.41
56:x:19:ILE:HD13	56:x:19:ILE:HA	1.95	0.41
7:C1:50:HIS:CG	7:C1:124:PRO:HG2	2.56	0.41
9:C3:397:LEU:O	9:C3:401:ILE:HG13	2.21	0.41
9:C3:456:HIS:O	9:C3:460:ILE:HG23	2.21	0.41
10:5B:538:LEU:HD22	51:S:37:ARG:HB3	2.03	0.41
10:5B:550:PRO:HG3	10:5B:605:LEU:HD21	2.01	0.41
11:6A:11:ARG:HG3	37:E:219:VAL:HA	2.02	0.41
20:M3:17:ASN:HD21	63:M3:401:CDL:HB22	1.84	0.41
37:E:103:ASN:HD21	37:E:145:HIS:CD2	2.39	0.41
37:E:210:HIS:O	37:E:211:PHE:C	2.64	0.41
42:J:144:LEU:HD11	63:J:301:CDL:H541	2.02	0.41
49:Q:156:GLN:HG3	49:Q:168:VAL:HG13	2.02	0.41
53:U:64:TYR:OH	53:U:111:GLN:NE2	2.50	0.41
56:X:19:ILE:HD13	56:X:19:ILE:HA	1.92	0.41
2:u2:273:LEU:HD21	30:y7:177:LYS:HG2	2.03	0.41
7:c1:154:LYS:HE2	15:7a:89:ASN:O	2.21	0.41
8:c2:169:ARG:HD2	47:o:75:MET:HE2	2.02	0.41
8:c2:461:TYR:OH	40:h:190:GLU:OE2	2.26	0.41
11:6a:1:MET:HB2	63:e:402:CDL:H122	2.03	0.41
31:y0:64:TYR:CE1	31:y0:66:ASP:HB2	2.55	0.41
39:g:105:TYR:HB2	39:g:107:TYR:CZ	2.56	0.41
45:m:190:ALA:O	57:y:1:MET:N	2.42	0.41
54:v:78:GLU:CD	54:v:84:ASN:HD21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C1:140:ILE:HG12	30:Y7:318:CYS:SG	2.60	0.41
7:C1:310:PHE:CD1	7:C1:310:PHE:C	2.99	0.41
7:C1:373:TYR:HA	7:C1:377:GLY:O	2.21	0.41
7:C1:437:VAL:O	7:C1:440:HIS:ND1	2.54	0.41
7:C1:681:VAL:HG21	38:F:114:GLU:HG3	2.03	0.41
8:C2:5:LEU:HD21	8:C2:542:VAL:HG11	2.02	0.41
8:C2:83:CYS:C	8:C2:86:PRO:HD2	2.45	0.41
9:C3:131:TYR:HB3	9:C3:138:LEU:HD11	2.03	0.41
9:C3:415:PHE:O	9:C3:437:ARG:HD2	2.21	0.41
9:C3:495:MET:HE2	9:C3:495:MET:HB3	1.86	0.41
11:6A:17:ALA:HB2	52:T:83:ARG:HB3	2.03	0.41
11:6A:21:HIS:O	11:6A:25:GLU:HG3	2.20	0.41
12:6B:121:GLN:HA	12:6B:124:TYR:HB2	2.01	0.41
14:6C:51:GLU:HB3	17:7L:872:VAL:HG11	2.03	0.41
18:M1:130:GLU:O	18:M1:222:LYS:HE3	2.20	0.41
18:M1:333:PHE:HD1	18:M1:333:PHE:HA	1.77	0.41
28:FS:92:GLN:NE2	28:FS:129:SER:O	2.51	0.41
28:FS:164:ARG:HH12	39:G:246:ASP:HA	1.84	0.41
38:F:201:LEU:O	38:F:204:PRO:HD2	2.21	0.41
40:H:167:ILE:HB	40:H:245:ILE:HG22	2.02	0.41
50:R:22:HIS:O	50:R:26:MET:HG3	2.20	0.41
53:U:138:ARG:HH12	53:U:142:LEU:HD22	1.86	0.41
54:V:78:GLU:CD	54:V:84:ASN:HD21	2.28	0.41
56:X:33:THR:O	56:X:37:VAL:HG23	2.20	0.41
57:Y:12:GLY:HA3	57:Y:16:TYR:CD2	2.56	0.41
2:u2:270:ASN:O	2:u2:274:LEU:HG	2.21	0.41
2:u2:276:ASN:O	2:u2:279:VAL:HG22	2.21	0.41
7:c1:50:HIS:CE1	7:c1:51:LYS:HG2	2.56	0.41
7:c1:307:THR:HA	7:c1:310:PHE:CD2	2.56	0.41
9:c3:212:ARG:NH2	43:k:48:ASP:O	2.54	0.41
10:5b:550:PRO:HG3	10:5b:605:LEU:HD21	2.02	0.41
11:6a:17:ALA:HB2	52:t:83:ARG:HB3	2.03	0.41
15:7a:106:ASP:O	15:7a:129:ARG:NH2	2.51	0.41
16:7c:116:TYR:OH	43:k:30:GLN:NE2	2.54	0.41
18:m1:40:VAL:HG13	18:m1:105:THR:HG22	2.02	0.41
18:m1:201:LEU:HD11	38:f:106:LEU:HD21	2.02	0.41
63:m3:401:CDL:H792	63:m3:401:CDL:H761	1.94	0.41
22:t2:30:LYS:H	24:t4:42:ARG:HD3	1.85	0.41
23:t3:21:PHE:HA	25:t5:61:VAL:HG22	2.03	0.41
28:fs:22:GLU:HB3	28:fs:24:HIS:CE1	2.56	0.41
30:y7:191:ASN:ND2	51:s:47:THR:HA	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:y5:156:ILE:CG2	49:q:77:ARG:HG2	2.51	0.41
33:a:366:ARG:HB3	33:a:379:THR:HB	2.02	0.41
34:b:383:PRO:O	34:b:386:THR:OG1	2.28	0.41
37:e:228:SER:O	37:e:228:SER:OG	2.35	0.41
38:f:201:LEU:O	38:f:204:PRO:HD2	2.21	0.41
45:m:200:HIS:HB3	45:m:203:ILE:O	2.21	0.41
49:q:48:GLU:HA	49:q:51:MET:HG2	2.03	0.41
50:r:22:HIS:O	50:r:26:MET:HG3	2.21	0.41
63:u:201:CDL:H711	63:u:201:CDL:H311	2.02	0.41
35:c:470:LYS:O	35:c:474:ILE:HG13	2.21	0.41
9:C3:380:LYS:HB3	9:C3:381:TRP:CE3	2.55	0.41
9:C3:466:PHE:O	9:C3:470:ARG:HG2	2.21	0.41
10:5B:268:ASP:OD1	15:7A:13:TYR:OH	2.18	0.41
62:7C:302:PC1:H3C1	62:7C:304:PC1:H342	2.03	0.41
18:M1:201:LEU:HD11	38:F:106:LEU:HD21	2.02	0.41
19:M2:154:LYS:HE3	19:M2:154:LYS:HB3	1.92	0.41
19:M2:171:ALA:HB2	19:M2:180:LEU:HD21	2.03	0.41
63:M3:401:CDL:H562	63:M3:401:CDL:H531	1.86	0.41
37:E:98:GLU:HG2	51:S:48:GLN:HG2	2.03	0.41
39:G:142:ASP:O	39:G:146:ILE:HG13	2.21	0.41
40:H:269:TYR:HB3	54:V:127:ARG:HB3	2.03	0.41
42:J:147:SER:O	42:J:151:ARG:HG2	2.21	0.41
45:M:190:ALA:O	57:Y:1:MET:N	2.44	0.41
50:R:72:ILE:HD13	50:R:72:ILE:HA	1.90	0.41
1:u1:93:UNK:O	41:i:159:ARG:NH2	2.54	0.41
2:u2:280:CYS:HB2	2:u2:282:ARG:HG2	2.03	0.41
7:c1:37:ARG:NH1	63:c1:706:CDL:HB31	2.36	0.41
8:c2:341:GLU:OE1	56:x:113:TYR:OH	2.35	0.41
8:c2:417:ARG:O	8:c2:492:LYS:NZ	2.54	0.41
8:c2:461:TYR:HB3	16:7c:199:THR:HG23	2.02	0.41
9:c3:380:LYS:HB3	9:c3:381:TRP:CE3	2.55	0.41
9:c3:515:PRO:HG3	9:c3:521:LEU:HD12	2.03	0.41
13:6l:25:CYS:O	13:6l:29:LYS:HG2	2.21	0.41
17:7l:927:PRO:HG2	17:7l:936:TYR:CD1	2.55	0.41
19:m2:205:LEU:HD23	19:m2:223:ALA:HA	2.03	0.41
20:m3:50:GLU:OE2	56:x:25:TYR:OH	2.28	0.41
33:a:279:LEU:HD11	33:a:387:THR:HG22	2.03	0.41
37:e:23:ARG:HE	37:e:23:ARG:HB2	1.53	0.41
38:f:293:GLU:H	38:f:293:GLU:HG2	1.72	0.41
42:j:147:SER:O	42:j:151:ARG:HG2	2.21	0.41
45:m:117:ILE:HA	45:m:120:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:t:23:THR:HG22	52:t:151:PRO:HG2	2.02	0.41
7:C1:517:MET:O	7:C1:520:THR:HG22	2.21	0.40
7:C1:654:ARG:HD2	7:C1:654:ARG:HA	1.83	0.40
9:C3:470:ARG:HA	9:C3:470:ARG:HD3	1.80	0.40
12:6B:230:TYR:O	57:Y:102:ARG:NH2	2.47	0.40
17:7L:927:PRO:HG3	17:7L:938:TYR:OH	2.20	0.40
30:Y7:411:TYR:CZ	34:B:398:VAL:HG13	2.56	0.40
32:Y5:144:LEU:HD23	51:S:21:ARG:HD2	2.03	0.40
34:B:352:PRO:HB3	34:B:372:VAL:HG22	2.02	0.40
34:B:389:LEU:HD22	34:B:464:PHE:CD2	2.56	0.40
38:F:231:GLY:HA3	38:F:326:ILE:O	2.20	0.40
48:P:45:SER:HB2	48:P:127:ASP:HB3	2.03	0.40
49:Q:140:LEU:O	49:Q:144:LEU:HG	2.21	0.40
9:c3:523:GLY:O	63:t:202:CDL:H562	2.21	0.40
10:5b:402:LEU:HD22	30:y7:244:LEU:HB2	2.03	0.40
10:5b:596:ASP:HA	10:5b:599:ILE:HG22	2.02	0.40
12:6b:47:LYS:O	12:6b:50:LEU:HB2	2.21	0.40
15:7a:82:PHE:CE2	63:7c:301:CDL:H822	2.56	0.40
19:m2:154:LYS:HE3	19:m2:154:LYS:HB3	1.90	0.40
19:m2:249:ASN:OD1	19:m2:250:ALA:N	2.54	0.40
20:m3:214:LYS:HB2	20:m3:252:LYS:HD2	2.04	0.40
28:fs:118:VAL:HG22	39:g:233:TYR:HD1	1.86	0.40
28:fs:182:MET:HE2	28:fs:182:MET:HB3	1.87	0.40
32:y5:121:ARG:NH2	51:s:52:GLU:OE2	2.54	0.40
33:a:282:ALA:O	33:a:283:LYS:C	2.64	0.40
37:e:210:HIS:O	37:e:211:PHE:C	2.64	0.40
49:q:78:ARG:O	49:q:82:GLY:N	2.48	0.40
53:u:97:TRP:CD1	53:u:98:PRO:HD3	2.56	0.40
7:C1:330:VAL:HG11	7:C1:421:HIS:CE1	2.56	0.40
8:C2:477:GLY:HA3	40:H:181:TRP:CE2	2.56	0.40
9:C3:398:LEU:HD23	9:C3:398:LEU:HA	1.90	0.40
9:C3:569:GLN:HG2	44:L:196:LEU:HD11	2.02	0.40
10:5B:308:ASN:HB3	37:E:21:ALA:HB2	2.03	0.40
13:6L:25:CYS:O	13:6L:29:LYS:HG2	2.21	0.40
36:D:349:VAL:HG23	36:D:365:THR:HG22	2.03	0.40
38:F:185:TRP:CG	38:F:201:LEU:HG	2.57	0.40
43:K:209:SER:O	44:L:140:TYR:OH	2.39	0.40
9:c3:251:LEU:HA	63:m3:401:CDL:H412	2.02	0.40
62:c3:605:PC1:H232	33:a:296:CYS:O	2.22	0.40
27:bp:314:GLY:HA3	27:bp:356:LYS:HB3	2.03	0.40
30:y7:359:ALA:HB1	30:y7:364:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:151:ASN:HB3	33:a:155:ARG:HH21	1.87	0.40
38:f:168:LYS:HB3	38:f:171:TYR:HD2	1.85	0.40
40:h:239:GLU:CD	40:h:239:GLU:H	2.29	0.40
63:j:301:CDL:H391	62:n:301:PC1:H342	2.03	0.40
49:q:41:MET:HE1	52:t:143:LEU:HD12	2.02	0.40
54:v:74:THR:HB	54:v:93:LYS:HD2	2.02	0.40
9:C3:221:TYR:CE1	33:A:228:LEU:HD23	2.56	0.40
9:C3:567:SER:OG	9:C3:575:GLN:NE2	2.54	0.40
12:6B:47:LYS:O	12:6B:50:LEU:HB2	2.21	0.40
12:6B:170:TYR:OH	12:6B:171:ARG:NH1	2.54	0.40
12:6B:216:PHE:CD1	52:T:143:LEU:HB3	2.56	0.40
15:7A:27:LYS:HD3	30:Y7:289:VAL:HG22	2.03	0.40
28:FS:129:SER:N	39:G:264:HIS:O	2.48	0.40
29:AC:105:ASP:O	45:M:49:TYR:OH	2.24	0.40
35:C:453:ASN:HB2	35:C:454:PRO:HD3	2.03	0.40
35:C:461:TYR:OH	35:C:467:ILE:O	2.32	0.40
38:F:201:LEU:HA	38:F:201:LEU:HD23	1.83	0.40
50:R:113:GLY:O	50:R:117:THR:HG22	2.20	0.40
52:T:17:LEU:HB3	52:t:158:LEU:HD11	2.04	0.40
8:c2:200:GLN:HE21	8:c2:200:GLN:HB2	1.63	0.40
18:m1:199:PHE:HZ	63:m2:401:CDL:H722	1.87	0.40
28:fs:71:LYS:HB3	39:g:257:TYR:OH	2.22	0.40
30:y7:234:LEU:HD22	33:a:466:LEU:HD11	2.03	0.40
36:d:228:LEU:HD23	36:d:228:LEU:HA	1.90	0.40
37:e:151:LEU:HD23	37:e:151:LEU:HA	1.89	0.40
44:l:214:PRO:HB2	47:o:91:ARG:HH12	1.86	0.40
48:p:129:VAL:O	48:p:133:ARG:HG2	2.21	0.40
50:r:56:LYS:HE2	50:r:56:LYS:HB3	1.89	0.40
10:5B:153:GLU:HA	10:5B:199:ARG:HE	1.86	0.40
10:5B:266:LEU:HD12	15:7A:45:LEU:HD21	2.02	0.40
63:M1:402:CDL:HB31	63:M1:402:CDL:HA21	2.04	0.40
29:AC:82:TYR:CE1	31:Y0:57:LYS:HE2	2.57	0.40
30:Y7:180:ILE:HG23	30:Y7:186:TYR:HD1	1.86	0.40
36:D:206:PHE:CE2	36:D:247:LYS:HD2	2.57	0.40
44:L:197:TYR:CE1	49:Q:165:LEU:HD21	2.56	0.40
46:N:186:ALA:HB3	46:N:189:HIS:CD2	2.55	0.40
8:c2:83:CYS:C	8:c2:86:PRO:HD2	2.46	0.40
8:c2:405:VAL:HG21	47:o:83:MET:HE1	2.02	0.40
9:c3:482:LEU:O	9:c3:486:VAL:HG23	2.22	0.40
9:c3:514:VAL:HG22	12:6b:213:LEU:HD11	2.03	0.40
10:5b:156:PHE:CD1	10:5b:179:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:6b:111:SER:HB2	57:y:66:TRP:CZ2	2.57	0.40
19:m2:299:ILE:O	19:m2:303:ILE:HG12	2.22	0.40
20:m3:26:ASP:O	20:m3:30:GLN:HG3	2.22	0.40
33:a:283:LYS:O	33:a:284:PHE:C	2.64	0.40
36:d:220:ASN:HB2	36:d:228:LEU:HB2	2.04	0.40
36:d:313:ASN:CB	36:d:320:TYR:HA	2.51	0.40
40:h:134:MET:HE3	40:h:232:HIS:ND1	2.37	0.40
40:h:167:ILE:HB	40:h:245:ILE:HG22	2.02	0.40
42:j:181:ARG:NH1	46:n:62:ALA:O	2.54	0.40
46:n:33:MET:O	46:n:37:VAL:HG13	2.21	0.40
7:C1:78:GLU:HG2	7:C1:94:TYR:CD1	2.56	0.40
7:C1:415:ARG:NH1	7:C1:478:VAL:O	2.46	0.40
7:C1:546:TYR:HB3	7:C1:550:LEU:HD13	2.03	0.40
9:C3:98:LYS:O	9:C3:102:SER:OG	2.33	0.40
10:5B:89:ASN:OD1	63:5B:702:CDL:H571	2.22	0.40
10:5B:273:MET:HE3	15:7A:24:PHE:CE2	2.56	0.40
10:5B:321:GLU:OE2	10:5B:413:TYR:OH	2.29	0.40
16:7C:93:LYS:HG2	38:F:125:ASN:O	2.21	0.40
19:M2:31:THR:HB	19:M2:288:ARG:HG3	2.02	0.40
26:T6:59:LEU:HD23	26:T6:59:LEU:HA	1.86	0.40
30:Y7:393:LEU:HD22	30:Y7:449:LEU:HD22	2.04	0.40
31:Y0:69:TYR:CE1	52:T:71:GLY:HA3	2.56	0.40
33:A:282:ALA:O	33:A:283:LYS:C	2.64	0.40
48:P:56:PHE:HB3	48:P:59:PHE:HB2	2.03	0.40
54:V:74:THR:HB	54:V:93:LYS:HD2	2.03	0.40
7:c1:78:GLU:HG2	7:c1:94:TYR:CD1	2.56	0.40
7:c1:393:GLU:O	7:c1:396:VAL:HG22	2.22	0.40
7:c1:475:LEU:HD12	14:6c:17:TYR:HD2	1.87	0.40
7:c1:656:LEU:HD13	39:g:134:GLY:HA3	2.04	0.40
9:c3:221:TYR:CE1	33:a:228:LEU:HD23	2.57	0.40
9:c3:246:TRP:O	9:c3:250:LEU:HB2	2.21	0.40
17:7l:978:SER:O	17:7l:978:SER:OG	2.36	0.40
18:m1:333:PHE:HD1	18:m1:333:PHE:HA	1.77	0.40
32:y5:171:LYS:HD2	32:y5:171:LYS:HA	1.91	0.40
36:d:239:LEU:HD22	36:d:256:VAL:HG11	2.03	0.40
38:f:222:ILE:HD11	38:f:303:ILE:HB	2.03	0.40
38:f:290:ASN:OD1	38:f:299:GLN:NE2	2.55	0.40
48:p:1:FME:HE3	48:p:1:FME:HB2	1.85	0.40
49:q:48:GLU:O	49:q:51:MET:HG2	2.22	0.40
50:r:106:CYS:HB2	50:r:107:PRO:HD3	2.02	0.40
54:v:100:PHE:HA	54:v:104:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:x:11:TRP:CZ3	56:x:19:ILE:HG13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U2	125/3634 (3%)	115 (92%)	9 (7%)	1 (1%)	16	48
2	u2	125/3634 (3%)	114 (91%)	10 (8%)	1 (1%)	16	48
5	U5	31/172 (18%)	31 (100%)	0	0	100	100
5	u5	31/172 (18%)	31 (100%)	0	0	100	100
6	U6	40/478 (8%)	39 (98%)	1 (2%)	0	100	100
6	u6	40/478 (8%)	39 (98%)	1 (2%)	0	100	100
7	C1	670/688 (97%)	638 (95%)	32 (5%)	0	100	100
7	c1	670/688 (97%)	638 (95%)	32 (5%)	0	100	100
8	C2	572/604 (95%)	547 (96%)	25 (4%)	0	100	100
8	c2	572/604 (95%)	547 (96%)	25 (4%)	0	100	100
9	C3	557/594 (94%)	542 (97%)	15 (3%)	0	100	100
9	c3	557/594 (94%)	543 (98%)	14 (2%)	0	100	100
10	5B	550/637 (86%)	539 (98%)	11 (2%)	0	100	100
10	5b	550/637 (86%)	540 (98%)	10 (2%)	0	100	100
11	6A	123/130 (95%)	117 (95%)	6 (5%)	0	100	100
11	6a	123/130 (95%)	117 (95%)	6 (5%)	0	100	100
12	6B	219/230 (95%)	215 (98%)	4 (2%)	0	100	100
12	6b	219/230 (95%)	216 (99%)	3 (1%)	0	100	100
13	6L	75/88 (85%)	75 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	6l	75/88 (85%)	75 (100%)	0	0	100	100
14	6C	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
14	6c	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
15	7A	131/133 (98%)	124 (95%)	7 (5%)	0	100	100
15	7a	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
16	7C	203/236 (86%)	198 (98%)	5 (2%)	0	100	100
16	7c	203/236 (86%)	198 (98%)	5 (2%)	0	100	100
17	7L	128/990 (13%)	120 (94%)	8 (6%)	0	100	100
17	7l	128/990 (13%)	120 (94%)	8 (6%)	0	100	100
18	M1	344/346 (99%)	330 (96%)	14 (4%)	0	100	100
18	m1	344/346 (99%)	330 (96%)	14 (4%)	0	100	100
19	M2	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
19	m2	316/318 (99%)	311 (98%)	5 (2%)	0	100	100
20	M3	327/330 (99%)	312 (95%)	15 (5%)	0	100	100
20	m3	327/330 (99%)	313 (96%)	14 (4%)	0	100	100
21	T1	68/72 (94%)	68 (100%)	0	0	100	100
21	t1	68/72 (94%)	68 (100%)	0	0	100	100
22	T2	61/72 (85%)	61 (100%)	0	0	100	100
22	t2	61/72 (85%)	61 (100%)	0	0	100	100
23	T3	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
23	t3	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
24	T4	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
24	t4	55/68 (81%)	53 (96%)	2 (4%)	0	100	100
25	T5	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
25	t5	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
26	T6	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
26	t6	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
27	BP	378/380 (100%)	361 (96%)	17 (4%)	0	100	100
27	bp	378/380 (100%)	359 (95%)	19 (5%)	0	100	100
28	FS	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
28	fs	186/188 (99%)	178 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AC	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
29	ac	98/127 (77%)	98 (100%)	0	0	100	100
30	Y7	332/453 (73%)	326 (98%)	6 (2%)	0	100	100
30	y7	332/453 (73%)	325 (98%)	7 (2%)	0	100	100
31	Y0	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
31	y0	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
32	Y5	102/190 (54%)	99 (97%)	3 (3%)	0	100	100
32	y5	102/190 (54%)	99 (97%)	3 (3%)	0	100	100
33	A	446/490 (91%)	431 (97%)	15 (3%)	0	100	100
33	a	446/490 (91%)	432 (97%)	14 (3%)	0	100	100
34	B	212/473 (45%)	203 (96%)	9 (4%)	0	100	100
34	b	212/473 (45%)	203 (96%)	9 (4%)	0	100	100
35	C	44/1471 (3%)	43 (98%)	1 (2%)	0	100	100
35	c	44/1471 (3%)	43 (98%)	1 (2%)	0	100	100
36	D	280/402 (70%)	275 (98%)	5 (2%)	0	100	100
36	d	280/402 (70%)	275 (98%)	5 (2%)	0	100	100
37	E	382/385 (99%)	361 (94%)	21 (6%)	0	100	100
37	e	382/385 (99%)	361 (94%)	21 (6%)	0	100	100
38	F	240/348 (69%)	232 (97%)	8 (3%)	0	100	100
38	f	240/348 (69%)	233 (97%)	7 (3%)	0	100	100
39	G	279/318 (88%)	270 (97%)	9 (3%)	0	100	100
39	g	279/318 (88%)	271 (97%)	8 (3%)	0	100	100
40	H	237/318 (74%)	233 (98%)	4 (2%)	0	100	100
40	h	237/318 (74%)	234 (99%)	3 (1%)	0	100	100
41	I	99/252 (39%)	98 (99%)	1 (1%)	0	100	100
41	i	99/252 (39%)	98 (99%)	1 (1%)	0	100	100
42	J	185/234 (79%)	182 (98%)	3 (2%)	0	100	100
42	j	185/234 (79%)	182 (98%)	3 (2%)	0	100	100
43	K	206/231 (89%)	194 (94%)	12 (6%)	0	100	100
43	k	206/231 (89%)	195 (95%)	11 (5%)	0	100	100
44	L	192/222 (86%)	186 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	l	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
45	M	179/220 (81%)	176 (98%)	3 (2%)	0	100	100
45	m	179/220 (81%)	176 (98%)	3 (2%)	0	100	100
46	N	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
46	n	204/210 (97%)	198 (97%)	6 (3%)	0	100	100
47	O	126/193 (65%)	125 (99%)	1 (1%)	0	100	100
47	o	126/193 (65%)	126 (100%)	0	0	100	100
48	P	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
48	p	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
49	Q	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
49	q	171/173 (99%)	170 (99%)	1 (1%)	0	100	100
50	R	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
50	r	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
51	S	141/170 (83%)	137 (97%)	4 (3%)	0	100	100
51	s	141/170 (83%)	137 (97%)	4 (3%)	0	100	100
52	T	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
52	t	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
53	U	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
53	u	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
54	V	144/149 (97%)	139 (96%)	5 (4%)	0	100	100
54	v	144/149 (97%)	139 (96%)	5 (4%)	0	100	100
55	W	100/124 (81%)	99 (99%)	1 (1%)	0	100	100
55	w	100/124 (81%)	100 (100%)	0	0	100	100
56	X	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
56	x	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
57	Y	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
57	y	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
58	Z	58/90 (64%)	58 (100%)	0	0	100	100
58	z	58/90 (64%)	58 (100%)	0	0	100	100
All	All	21730/37912 (57%)	21056 (97%)	672 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U2	175	ILE
2	u2	175	ILE

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	
2	U2	35/3358 (1%)	35 (100%)	0	100	100
2	u2	35/3358 (1%)	35 (100%)	0	100	100
5	U5	19/169 (11%)	19 (100%)	0	100	100
5	u5	19/169 (11%)	19 (100%)	0	100	100
6	U6	24/419 (6%)	23 (96%)	1 (4%)	26	59
6	u6	24/419 (6%)	23 (96%)	1 (4%)	26	59
7	C1	597/613 (97%)	590 (99%)	7 (1%)	63	81
7	c1	597/613 (97%)	590 (99%)	7 (1%)	63	81
8	C2	542/569 (95%)	534 (98%)	8 (2%)	57	79
8	c2	542/569 (95%)	534 (98%)	8 (2%)	57	79
9	C3	534/565 (94%)	529 (99%)	5 (1%)	70	84
9	c3	534/565 (94%)	529 (99%)	5 (1%)	70	84
10	5B	502/579 (87%)	498 (99%)	4 (1%)	73	85
10	5b	502/579 (87%)	498 (99%)	4 (1%)	73	85
11	6A	113/116 (97%)	113 (100%)	0	100	100
11	6a	113/116 (97%)	113 (100%)	0	100	100
12	6B	199/207 (96%)	196 (98%)	3 (2%)	57	79
12	6b	199/207 (96%)	197 (99%)	2 (1%)	68	83
13	6L	71/80 (89%)	70 (99%)	1 (1%)	59	79
13	6l	71/80 (89%)	70 (99%)	1 (1%)	59	79
14	6C	81/88 (92%)	80 (99%)	1 (1%)	63	81
14	6c	81/88 (92%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	7A	119/119 (100%)	119 (100%)	0	100	100
15	7a	119/119 (100%)	118 (99%)	1 (1%)	73	85
16	7C	193/217 (89%)	190 (98%)	3 (2%)	55	78
16	7c	193/217 (89%)	191 (99%)	2 (1%)	68	83
17	7L	121/943 (13%)	120 (99%)	1 (1%)	73	85
17	7l	121/943 (13%)	120 (99%)	1 (1%)	73	85
18	M1	294/294 (100%)	292 (99%)	2 (1%)	76	85
18	m1	294/294 (100%)	292 (99%)	2 (1%)	76	85
19	M2	259/259 (100%)	255 (98%)	4 (2%)	57	79
19	m2	259/259 (100%)	256 (99%)	3 (1%)	63	81
20	M3	275/276 (100%)	274 (100%)	1 (0%)	84	89
20	m3	275/276 (100%)	273 (99%)	2 (1%)	76	85
21	T1	61/63 (97%)	61 (100%)	0	100	100
21	t1	61/63 (97%)	61 (100%)	0	100	100
22	T2	58/67 (87%)	58 (100%)	0	100	100
22	t2	58/67 (87%)	58 (100%)	0	100	100
23	T3	76/83 (92%)	76 (100%)	0	100	100
23	t3	76/83 (92%)	76 (100%)	0	100	100
24	T4	53/62 (86%)	53 (100%)	0	100	100
24	t4	53/62 (86%)	53 (100%)	0	100	100
25	T5	57/66 (86%)	57 (100%)	0	100	100
25	t5	57/66 (86%)	57 (100%)	0	100	100
26	T6	61/62 (98%)	61 (100%)	0	100	100
26	t6	61/62 (98%)	61 (100%)	0	100	100
27	BP	308/308 (100%)	307 (100%)	1 (0%)	86	90
27	bp	308/308 (100%)	307 (100%)	1 (0%)	86	90
28	FS	164/164 (100%)	163 (99%)	1 (1%)	78	87
28	fs	164/164 (100%)	162 (99%)	2 (1%)	63	81
29	AC	87/113 (77%)	87 (100%)	0	100	100
29	ac	87/113 (77%)	87 (100%)	0	100	100
30	Y7	328/442 (74%)	325 (99%)	3 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	y7	328/442 (74%)	324 (99%)	4 (1%)	63	81
31	Y0	83/83 (100%)	83 (100%)	0	100	100
31	y0	83/83 (100%)	83 (100%)	0	100	100
32	Y5	101/185 (55%)	99 (98%)	2 (2%)	48	75
32	y5	101/185 (55%)	100 (99%)	1 (1%)	68	83
33	A	409/447 (92%)	407 (100%)	2 (0%)	81	88
33	a	409/447 (92%)	406 (99%)	3 (1%)	76	85
34	B	182/413 (44%)	182 (100%)	0	100	100
34	b	182/413 (44%)	182 (100%)	0	100	100
35	C	44/1405 (3%)	40 (91%)	4 (9%)	9	32
35	c	44/1405 (3%)	40 (91%)	4 (9%)	9	32
36	D	250/358 (70%)	247 (99%)	3 (1%)	63	81
36	d	250/358 (70%)	248 (99%)	2 (1%)	73	85
37	E	341/342 (100%)	338 (99%)	3 (1%)	70	84
37	e	341/342 (100%)	338 (99%)	3 (1%)	70	84
38	F	218/318 (69%)	218 (100%)	0	100	100
38	f	218/318 (69%)	218 (100%)	0	100	100
39	G	260/289 (90%)	257 (99%)	3 (1%)	63	81
39	g	260/289 (90%)	256 (98%)	4 (2%)	57	79
40	H	209/272 (77%)	208 (100%)	1 (0%)	81	88
40	h	209/272 (77%)	207 (99%)	2 (1%)	68	83
41	I	90/219 (41%)	90 (100%)	0	100	100
41	i	90/219 (41%)	90 (100%)	0	100	100
42	J	170/216 (79%)	170 (100%)	0	100	100
42	j	170/216 (79%)	170 (100%)	0	100	100
43	K	191/213 (90%)	190 (100%)	1 (0%)	81	88
43	k	191/213 (90%)	191 (100%)	0	100	100
44	L	181/206 (88%)	180 (99%)	1 (1%)	78	87
44	l	181/206 (88%)	180 (99%)	1 (1%)	78	87
45	M	166/199 (83%)	165 (99%)	1 (1%)	78	87
45	m	166/199 (83%)	165 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	N	178/181 (98%)	175 (98%)	3 (2%)	53	77
46	n	178/181 (98%)	175 (98%)	3 (2%)	53	77
47	O	119/180 (66%)	118 (99%)	1 (1%)	73	85
47	o	119/180 (66%)	117 (98%)	2 (2%)	53	77
48	P	156/156 (100%)	156 (100%)	0	100	100
48	p	156/156 (100%)	156 (100%)	0	100	100
49	Q	157/157 (100%)	155 (99%)	2 (1%)	61	80
49	q	157/157 (100%)	155 (99%)	2 (1%)	61	80
50	R	144/157 (92%)	144 (100%)	0	100	100
50	r	144/157 (92%)	144 (100%)	0	100	100
51	S	129/154 (84%)	128 (99%)	1 (1%)	73	85
51	s	129/154 (84%)	128 (99%)	1 (1%)	73	85
52	T	138/139 (99%)	138 (100%)	0	100	100
52	t	138/139 (99%)	138 (100%)	0	100	100
53	U	137/138 (99%)	137 (100%)	0	100	100
53	u	137/138 (99%)	137 (100%)	0	100	100
54	V	133/135 (98%)	133 (100%)	0	100	100
54	v	133/135 (98%)	133 (100%)	0	100	100
55	W	92/113 (81%)	91 (99%)	1 (1%)	65	82
55	w	92/113 (81%)	91 (99%)	1 (1%)	65	82
56	X	105/105 (100%)	104 (99%)	1 (1%)	68	83
56	x	105/105 (100%)	104 (99%)	1 (1%)	68	83
57	Y	88/88 (100%)	87 (99%)	1 (1%)	65	82
57	y	88/88 (100%)	85 (97%)	3 (3%)	32	64
58	Z	51/80 (64%)	51 (100%)	0	100	100
58	z	51/80 (64%)	51 (100%)	0	100	100
All	All	19506/34498 (56%)	19349 (99%)	157 (1%)	70	85

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	U6	156	PHE
7	C1	57	TYR

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Mol	Chain	Res	Type
7	C1	137	LEU
7	C1	164	ARG
7	C1	275	THR
7	C1	394	VAL
7	C1	414	THR
7	C1	503	PHE
8	C2	224	PHE
8	C2	335	THR
8	C2	409	ILE
8	C2	501	VAL
8	C2	524	LYS
8	C2	526	ASP
8	C2	536	THR
8	C2	559	HIS
9	C3	48	LEU
9	C3	228	TYR
9	C3	312	THR
9	C3	492	ILE
9	C3	579	PHE
10	5B	68	LEU
10	5B	93	THR
10	5B	145	ASN
10	5B	166	ASN
12	6B	24	LEU
12	6B	44	VAL
12	6B	182	ASP
13	6L	28	GLU
14	6C	31	ILE
16	7C	81	THR
16	7C	110	HIS
16	7C	167	GLU
17	7L	872	VAL
18	M1	14	LEU
18	M1	329	THR
19	M2	2	ASN
19	M2	3	TYR
19	M2	40	ARG
19	M2	107	THR
20	M3	34	GLN
27	BP	326	GLN
28	FS	18	LEU
30	Y7	208	LEU

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Mol	Chain	Res	Type
30	Y7	297	LYS
30	Y7	400	TYR
32	Y5	174	ARG
32	Y5	190	TYR
33	A	334	ASN
33	A	386	THR
35	C	460	THR
35	C	464	ASN
35	C	467	ILE
35	C	468	PHE
36	D	166	VAL
36	D	181	LYS
36	D	186	ARG
37	E	53	THR
37	E	115	ASP
37	E	346	HIS
39	G	169	THR
39	G	208	ILE
39	G	279	GLU
40	H	110	THR
43	K	186	ILE
44	L	55	LYS
45	M	114	ILE
46	N	56	TYR
46	N	87	VAL
46	N	191	ASN
47	O	163	ASN
49	Q	70	HIS
49	Q	128	ARG
51	S	117	ASP
55	W	103	TYR
56	X	65	PHE
57	Y	67	THR
6	u6	156	PHE
7	c1	137	LEU
7	c1	164	ARG
7	c1	275	THR
7	c1	394	VAL
7	c1	414	THR
7	c1	503	PHE
7	c1	592	ASP
8	c2	224	PHE

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Mol	Chain	Res	Type
8	c2	238	TYR
8	c2	335	THR
8	c2	409	ILE
8	c2	488	ILE
8	c2	501	VAL
8	c2	536	THR
8	c2	559	HIS
9	c3	48	LEU
9	c3	228	TYR
9	c3	312	THR
9	c3	492	ILE
9	c3	579	PHE
10	5b	64	LYS
10	5b	68	LEU
10	5b	93	THR
10	5b	166	ASN
12	6b	44	VAL
12	6b	182	ASP
13	6l	28	GLU
15	7a	120	ARG
16	7c	81	THR
16	7c	110	HIS
17	7l	872	VAL
18	m1	14	LEU
18	m1	329	THR
19	m2	3	TYR
19	m2	40	ARG
19	m2	107	THR
20	m3	34	GLN
20	m3	77	ASP
27	bp	326	GLN
28	fs	1	MET
28	fs	18	LEU
30	y7	106	LYS
30	y7	208	LEU
30	y7	297	LYS
30	y7	400	TYR
32	y5	174	ARG
33	a	163	ARG
33	a	334	ASN
33	a	386	THR
36	d	166	VAL

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Mol	Chain	Res	Type
36	d	186	ARG
37	e	53	THR
37	e	115	ASP
37	e	346	HIS
39	g	91	ASP
39	g	169	THR
39	g	208	ILE
39	g	279	GLU
40	h	110	THR
40	h	196	CYS
44	l	55	LYS
45	m	114	ILE
46	n	56	TYR
46	n	87	VAL
46	n	191	ASN
47	o	68	GLU
47	o	163	ASN
49	q	70	HIS
49	q	128	ARG
51	s	117	ASP
55	w	103	TYR
56	x	65	PHE
57	y	1	MET
57	y	4	THR
57	y	67	THR
35	c	460	THR
35	c	464	ASN
35	c	467	ILE
35	c	468	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
7	C1	17	ASN
7	C1	161	GLN
7	C1	312	ASN
7	C1	327	HIS
7	C1	412	ASN
7	C1	526	HIS
7	C1	657	GLN
8	C2	34	GLN
8	C2	96	ASN

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Mol	Chain	Res	Type
8	C2	146	ASN
8	C2	293	ASN
8	C2	379	ASN
8	C2	427	GLN
9	C3	33	ASN
9	C3	129	ASN
9	C3	130	HIS
9	C3	223	ASN
9	C3	224	ASN
9	C3	333	ASN
9	C3	444	ASN
9	C3	574	ASN
10	5B	67	ASN
10	5B	164	GLN
10	5B	216	HIS
10	5B	449	ASN
10	5B	477	HIS
10	5B	531	ASN
12	6B	71	GLN
12	6B	163	ASN
12	6B	181	GLN
14	6C	68	ASN
15	7A	12	GLN
16	7C	65	HIS
16	7C	114	HIS
17	7L	867	ASN
18	M1	119	ASN
18	M1	120	ASN
18	M1	208	GLN
18	M1	338	ASN
19	M2	73	ASN
19	M2	143	ASN
20	M3	17	ASN
20	M3	56	HIS
21	T1	9	ASN
21	T1	18	ASN
24	T4	48	ASN
25	T5	51	GLN
26	T6	61	GLN
27	BP	260	ASN
27	BP	283	ASN
28	FS	68	GLN

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Mol	Chain	Res	Type
28	FS	87	ASN
28	FS	130	GLN
28	FS	160	HIS
28	FS	185	ASN
30	Y7	172	ASN
30	Y7	191	ASN
30	Y7	202	ASN
33	A	67	HIS
33	A	70	HIS
33	A	246	ASN
36	D	304	GLN
37	E	33	ASN
37	E	97	GLN
37	E	103	ASN
37	E	311	ASN
38	F	162	ASN
38	F	239	GLN
38	F	254	GLN
39	G	55	GLN
39	G	98	ASN
39	G	220	ASN
39	G	247	GLN
39	G	262	ASN
39	G	264	HIS
40	H	81	ASN
40	H	284	GLN
41	I	172	HIS
41	I	209	ASN
42	J	65	HIS
42	J	193	GLN
42	J	197	ASN
43	K	31	ASN
43	K	58	GLN
43	K	168	ASN
43	K	179	ASN
43	K	200	GLN
46	N	117	GLN
46	N	155	HIS
46	N	208	HIS
47	O	105	GLN
48	P	29	HIS
48	P	60	ASN

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Mol	Chain	Res	Type
48	P	75	GLN
48	P	134	GLN
50	R	114	ASN
50	R	128	ASN
52	T	101	GLN
53	U	91	ASN
53	U	146	ASN
54	V	111	GLN
54	V	141	GLN
55	W	119	ASN
57	Y	103	GLN
7	c1	17	ASN
7	c1	50	HIS
7	c1	161	GLN
7	c1	327	HIS
7	c1	412	ASN
7	c1	449	HIS
7	c1	526	HIS
7	c1	657	GLN
8	c2	16	ASN
8	c2	34	GLN
8	c2	96	ASN
8	c2	146	ASN
8	c2	293	ASN
8	c2	463	GLN
9	c3	129	ASN
9	c3	130	HIS
9	c3	223	ASN
9	c3	224	ASN
9	c3	333	ASN
9	c3	444	ASN
10	5b	67	ASN
10	5b	85	HIS
10	5b	164	GLN
10	5b	449	ASN
10	5b	531	ASN
11	6a	112	HIS
12	6b	163	ASN
12	6b	181	GLN
15	7a	12	GLN
16	7c	114	HIS
17	7l	867	ASN

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Mol	Chain	Res	Type
18	m1	119	ASN
18	m1	120	ASN
18	m1	338	ASN
19	m2	73	ASN
19	m2	143	ASN
20	m3	17	ASN
20	m3	56	HIS
21	t1	9	ASN
21	t1	18	ASN
22	t2	24	GLN
25	t5	51	GLN
26	t6	61	GLN
27	bp	222	ASN
27	bp	260	ASN
27	bp	283	ASN
28	fs	130	GLN
28	fs	160	HIS
28	fs	185	ASN
30	y7	172	ASN
30	y7	191	ASN
30	y7	202	ASN
30	y7	300	ASN
32	y5	151	ASN
32	y5	154	ASN
33	a	70	HIS
33	a	250	GLN
36	d	304	GLN
37	e	33	ASN
37	e	97	GLN
37	e	311	ASN
38	f	162	ASN
38	f	239	GLN
39	g	55	GLN
39	g	57	GLN
39	g	98	ASN
39	g	220	ASN
39	g	247	GLN
39	g	262	ASN
39	g	264	HIS
40	h	81	ASN
40	h	248	HIS
40	h	284	GLN

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Mol	Chain	Res	Type
41	i	172	HIS
41	i	209	ASN
42	j	65	HIS
42	j	193	GLN
42	j	197	ASN
43	k	30	GLN
43	k	31	ASN
43	k	168	ASN
43	k	179	ASN
45	m	39	GLN
46	n	117	GLN
46	n	155	HIS
46	n	208	HIS
47	o	110	GLN
47	o	179	ASN
48	p	29	HIS
48	p	60	ASN
48	p	77	ASN
49	q	132	GLN
52	t	101	GLN
53	u	91	ASN
53	u	146	ASN
54	v	141	GLN
55	w	119	ASN
57	y	81	HIS
57	y	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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
15	FME	7a	1	15	8,9,10	0.98	0	8,9,11	0.87	0
15	FME	7A	1	15	8,9,10	0.99	0	8,9,11	0.87	0
26	FME	T6	1	26	8,9,10	0.97	0	8,9,11	0.81	0
10	SEP	5B	520	10	8,9,10	1.58	1 (12%)	7,12,14	1.25	1 (14%)
16	SEP	7c	197	16	8,9,10	1.57	1 (12%)	7,12,14	1.81	1 (14%)
16	SEP	7C	120	16	8,9,10	1.55	1 (12%)	7,12,14	1.33	1 (14%)
19	FME	m2	1	19	8,9,10	0.98	0	8,9,11	0.95	0
37	FME	E	1	37	8,9,10	0.98	0	8,9,11	0.95	0
48	FME	P	1	48	8,9,10	0.96	0	8,9,11	1.01	0
31	FME	y0	1	31	8,9,10	0.98	0	8,9,11	0.87	0
19	FME	M2	1	19	8,9,10	0.98	0	8,9,11	0.99	0
10	TPO	5b	387	10	8,10,11	1.60	1 (12%)	10,14,16	2.11	1 (10%)
48	FME	p	1	48	8,9,10	0.95	0	8,9,11	1.03	0
31	FME	Y0	1	31	8,9,10	1.00	0	8,9,11	0.86	0
10	TPO	5B	387	10	8,10,11	1.06	0	10,14,16	2.09	1 (10%)
13	FME	6L	1	13	8,9,10	0.99	0	8,9,11	0.91	0
24	FME	T4	1	24	8,9,10	0.96	0	8,9,11	0.87	0
10	SEP	5b	520	10	8,9,10	1.59	1 (12%)	7,12,14	1.26	1 (14%)
26	FME	t6	1	26	8,9,10	0.97	0	8,9,11	0.79	0
13	FME	6l	1	13	8,9,10	0.97	0	8,9,11	0.93	0
37	FME	e	1	37	8,9,10	0.98	0	8,9,11	0.96	0
24	FME	t4	1	24	8,9,10	0.96	0	8,9,11	0.89	0
16	SEP	7C	197	16	8,9,10	1.59	1 (12%)	7,12,14	1.85	1 (14%)
16	SEP	7c	120	16	8,9,10	1.56	1 (12%)	7,12,14	1.25	1 (14%)

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
15	FME	7a	1	15	-	4/7/9/11	-
15	FME	7A	1	15	-	4/7/9/11	-
26	FME	T6	1	26	-	5/7/9/11	-
10	SEP	5B	520	10	-	3/6/8/10	-
16	SEP	7c	197	16	-	0/6/8/10	-
16	SEP	7C	120	16	-	0/6/8/10	-
19	FME	m2	1	19	-	4/7/9/11	-
37	FME	E	1	37	-	5/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FME	P	1	48	-	3/7/9/11	-
31	FME	y0	1	31	-	5/7/9/11	-
19	FME	M2	1	19	-	4/7/9/11	-
10	TPO	5b	387	10	-	1/9/11/13	-
48	FME	p	1	48	-	3/7/9/11	-
31	FME	Y0	1	31	-	5/7/9/11	-
10	TPO	5B	387	10	-	1/9/11/13	-
13	FME	6L	1	13	-	5/7/9/11	-
24	FME	T4	1	24	-	4/7/9/11	-
10	SEP	5b	520	10	-	3/6/8/10	-
26	FME	t6	1	26	-	5/7/9/11	-
13	FME	6l	1	13	-	6/7/9/11	-
37	FME	e	1	37	-	5/7/9/11	-
24	FME	t4	1	24	-	4/7/9/11	-
16	SEP	7C	197	16	-	2/6/8/10	-
16	SEP	7c	120	16	-	0/6/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	7C	197	SEP	P-O1P	3.49	1.61	1.50
10	5b	520	SEP	P-O1P	3.47	1.61	1.50
10	5B	520	SEP	P-O1P	3.46	1.61	1.50
16	7c	120	SEP	P-O1P	3.43	1.61	1.50
10	5b	387	TPO	P-O1P	3.41	1.61	1.50
16	7C	120	SEP	P-O1P	3.41	1.61	1.50
16	7c	197	SEP	P-O1P	3.39	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5b	387	TPO	P-OG1-CB	-6.12	106.70	123.33
10	5B	387	TPO	P-OG1-CB	-6.02	106.97	123.33
16	7C	197	SEP	OG-CB-CA	4.32	112.35	108.14
16	7c	197	SEP	OG-CB-CA	4.18	112.21	108.14
16	7C	120	SEP	OG-CB-CA	2.99	111.05	108.14
16	7c	120	SEP	OG-CB-CA	2.84	110.91	108.14
10	5b	520	SEP	OG-CB-CA	2.75	110.82	108.14
10	5B	520	SEP	OG-CB-CA	2.66	110.73	108.14

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	5B	387	TPO	O-C-CA-CB
10	5B	520	SEP	CB-OG-P-O1P
10	5B	520	SEP	CB-OG-P-O2P
10	5B	520	SEP	CB-OG-P-O3P
13	6L	1	FME	O1-CN-N-CA
13	6L	1	FME	N-CA-CB-CG
13	6L	1	FME	C-CA-CB-CG
13	6L	1	FME	O-C-CA-CB
15	7A	1	FME	O1-CN-N-CA
15	7A	1	FME	C-CA-CB-CG
15	7A	1	FME	O-C-CA-CB
16	7C	197	SEP	CB-OG-P-O1P
16	7C	197	SEP	CB-OG-P-O2P
19	M2	1	FME	O1-CN-N-CA
19	M2	1	FME	N-CA-CB-CG
24	T4	1	FME	O1-CN-N-CA
24	T4	1	FME	CB-CA-N-CN
26	T6	1	FME	O1-CN-N-CA
26	T6	1	FME	CB-CA-N-CN
31	Y0	1	FME	O1-CN-N-CA
31	Y0	1	FME	C-CA-CB-CG
37	E	1	FME	O1-CN-N-CA
37	E	1	FME	CB-CA-N-CN
37	E	1	FME	N-CA-CB-CG
48	P	1	FME	O1-CN-N-CA
10	5b	387	TPO	O-C-CA-CB
10	5b	520	SEP	CB-OG-P-O1P
10	5b	520	SEP	CB-OG-P-O2P
10	5b	520	SEP	CB-OG-P-O3P
13	6l	1	FME	O1-CN-N-CA
13	6l	1	FME	CB-CA-N-CN
13	6l	1	FME	C-CA-CB-CG
13	6l	1	FME	O-C-CA-CB
15	7a	1	FME	O1-CN-N-CA
15	7a	1	FME	C-CA-CB-CG
15	7a	1	FME	O-C-CA-CB
19	m2	1	FME	O1-CN-N-CA
19	m2	1	FME	N-CA-CB-CG
24	t4	1	FME	O1-CN-N-CA
24	t4	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
26	t6	1	FME	O1-CN-N-CA
26	t6	1	FME	CB-CA-N-CN
31	y0	1	FME	O1-CN-N-CA
31	y0	1	FME	C-CA-CB-CG
37	e	1	FME	O1-CN-N-CA
37	e	1	FME	CB-CA-N-CN
37	e	1	FME	N-CA-CB-CG
48	p	1	FME	O1-CN-N-CA
31	y0	1	FME	CA-CB-CG-SD
13	6L	1	FME	CA-CB-CG-SD
31	Y0	1	FME	CA-CB-CG-SD
15	7A	1	FME	N-CA-CB-CG
13	6l	1	FME	N-CA-CB-CG
15	7a	1	FME	N-CA-CB-CG
37	E	1	FME	CB-CG-SD-CE
48	P	1	FME	N-CA-CB-CG
24	t4	1	FME	N-CA-CB-CG
31	y0	1	FME	N-CA-CB-CG
48	p	1	FME	N-CA-CB-CG
24	t4	1	FME	CB-CG-SD-CE
37	e	1	FME	CB-CG-SD-CE
24	T4	1	FME	CB-CG-SD-CE
13	6l	1	FME	CB-CG-SD-CE
24	T4	1	FME	N-CA-CB-CG
26	T6	1	FME	CB-CG-SD-CE
19	M2	1	FME	C-CA-CB-CG
37	E	1	FME	C-CA-CB-CG
19	m2	1	FME	C-CA-CB-CG
26	t6	1	FME	C-CA-CB-CG
37	e	1	FME	C-CA-CB-CG
19	M2	1	FME	CB-CA-N-CN
31	Y0	1	FME	CB-CA-N-CN
19	m2	1	FME	CB-CA-N-CN
26	t6	1	FME	N-CA-CB-CG
26	t6	1	FME	CB-CG-SD-CE
26	T6	1	FME	C-CA-CB-CG
26	T6	1	FME	N-CA-CB-CG
48	P	1	FME	CB-CA-N-CN
48	p	1	FME	CB-CA-N-CN
31	Y0	1	FME	N-CA-CB-CG
31	y0	1	FME	CB-CG-SD-CE

There are no ring outliers.

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	T6	1	FME	2	0
10	5B	520	SEP	2	0
16	7C	120	SEP	2	0
31	y0	1	FME	1	0
10	5b	387	TPO	1	0
48	p	1	FME	1	0
31	Y0	1	FME	1	0
10	5B	387	TPO	1	0
24	T4	1	FME	1	0
10	5b	520	SEP	2	0
26	t6	1	FME	2	0
13	6l	1	FME	1	0
37	e	1	FME	1	0
24	t4	1	FME	1	0
16	7c	120	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 122 ligands modelled in this entry, 12 are monoatomic - leaving 110 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	$\# Z > 2$
63	CDL	m3	401	-	93,93,99	0.30	0	99,105,111	0.33	0
62	PC1	C3	601	-	51,51,53	0.29	0	57,59,61	0.38	0
63	CDL	e	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	7C	303	-	50,50,99	0.41	0	56,62,111	0.35	0
65	FES	fs	201	28	0,4,4	-	-	-	-	-
62	PC1	M2	405	-	40,40,53	0.33	0	46,48,61	0.34	0
63	CDL	y7	501	-	64,64,99	0.37	0	70,76,111	0.37	0
65	FES	fs	202	28	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	CDL	t	201	-	67,67,99	0.36	0	73,79,111	0.35	0
59	HEA	c1	702	7	67,67,67	1.23	10 (14%)	81,103,103	1.53	16 (19%)
63	CDL	M3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
62	PC1	c3	602	-	38,38,53	0.33	0	44,46,61	0.34	0
63	CDL	M2	401	-	53,53,99	0.40	0	59,65,111	0.39	0
63	CDL	A	503	-	50,50,99	0.41	0	56,62,111	0.50	0
62	PC1	v	202	-	53,53,53	0.29	0	59,61,61	0.33	0
62	PC1	j	302	-	36,36,53	0.34	0	42,44,61	0.33	0
63	CDL	m2	404	-	73,73,99	0.34	0	79,85,111	0.35	0
63	CDL	7A	202	-	99,99,99	0.30	0	105,111,111	0.29	0
63	CDL	7C	301	-	84,84,99	0.32	0	90,96,111	0.34	0
63	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.32	0
62	PC1	A	501	-	44,44,53	0.31	0	50,52,61	0.36	0
62	PC1	C3	605	-	40,40,53	0.33	0	46,48,61	0.42	0
63	CDL	m3	403	-	62,62,99	0.37	0	68,74,111	0.34	0
62	PC1	n	301	-	31,31,53	0.36	0	37,39,61	0.36	0
63	CDL	C3	604	-	67,67,99	0.36	0	73,79,111	0.30	0
62	PC1	a	502	-	40,40,53	0.34	0	46,48,61	0.40	0
63	CDL	Y7	501	-	64,64,99	0.37	0	70,76,111	0.37	0
62	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.38	0
62	PC1	m2	402	-	31,31,53	0.37	0	37,39,61	0.37	0
63	CDL	E	402	-	71,71,99	0.34	0	77,83,111	0.34	0
63	CDL	c1	706	-	58,58,99	0.38	0	64,70,111	0.41	0
59	HEA	c1	701	7	67,67,67	1.20	9 (13%)	81,103,103	1.51	16 (19%)
62	PC1	M1	404	-	34,34,53	0.35	0	40,42,61	0.33	0
62	PC1	c1	705	-	48,48,53	0.31	0	54,56,61	0.31	0
63	CDL	M1	403	-	65,65,99	0.36	0	71,77,111	0.30	0
63	CDL	5b	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	5B	702	-	86,86,99	0.32	0	92,98,111	0.33	0
63	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	m2	406	-	53,53,53	0.29	0	59,61,61	0.28	0
59	HEA	C1	702	7	67,67,67	1.23	10 (14%)	81,103,103	1.54	16 (19%)
63	CDL	l	301	-	73,73,99	0.34	0	79,85,111	0.29	0
63	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0
63	CDL	7a	202	-	99,99,99	0.30	0	105,111,111	0.30	0
62	PC1	V	202	-	53,53,53	0.29	0	59,61,61	0.33	0
63	CDL	7c	302	-	50,50,99	0.40	0	56,62,111	0.34	0
63	CDL	7A	201	-	66,66,99	0.36	0	72,78,111	0.38	0
62	PC1	N	302	-	35,35,53	0.36	0	41,43,61	0.35	0
63	CDL	c1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
63	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	a	501	-	44,44,53	0.31	0	50,52,61	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	CDL	u	201	-	81,81,99	0.32	0	87,93,111	0.32	0
63	CDL	v	201	-	90,90,99	0.32	0	96,102,111	0.37	0
63	CDL	C1	706	-	58,58,99	0.38	0	64,70,111	0.40	0
63	CDL	m1	401	-	94,94,99	0.31	0	100,106,111	0.32	0
62	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.39	0
63	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.30	0
59	HEA	C1	701	7	67,67,67	1.20	9 (13%)	81,103,103	1.53	17 (20%)
62	PC1	C1	705	-	48,48,53	0.31	0	54,56,61	0.31	0
63	CDL	m2	401	-	53,53,99	0.40	0	59,65,111	0.40	0
63	CDL	U	201	-	81,81,99	0.32	0	87,93,111	0.32	0
63	CDL	5B	704	-	66,66,99	0.36	0	72,78,111	0.34	0
62	PC1	N	301	-	31,31,53	0.36	0	37,39,61	0.36	0
63	CDL	n	303	-	94,94,99	0.31	0	100,106,111	0.37	0
62	PC1	m2	405	-	40,40,53	0.33	0	46,48,61	0.33	0
62	PC1	7C	304	-	42,42,53	0.32	0	48,50,61	0.30	0
62	PC1	C3	602	-	38,38,53	0.33	0	44,46,61	0.34	0
63	CDL	m1	403	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	f	401	-	99,99,99	0.29	0	105,111,111	0.35	0
65	FES	FS	202	28	0,4,4	-	-	-	-	-
63	CDL	Y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
63	CDL	E	401	-	59,59,99	0.38	0	65,71,111	0.38	0
63	CDL	m3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
63	CDL	N	303	-	94,94,99	0.31	0	100,106,111	0.36	0
63	CDL	7c	301	-	84,84,99	0.32	0	90,96,111	0.34	0
63	CDL	k	301	-	61,61,99	0.37	0	67,73,111	0.33	0
63	CDL	7a	201	-	66,66,99	0.36	0	72,78,111	0.38	0
63	CDL	e	401	-	59,59,99	0.38	0	65,71,111	0.38	0
62	PC1	7c	303	-	42,42,53	0.32	0	48,50,61	0.30	0
63	CDL	M3	401	-	93,93,99	0.30	0	99,105,111	0.34	0
62	PC1	A	502	-	40,40,53	0.33	0	46,48,61	0.39	0
63	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
62	PC1	m1	402	-	53,53,53	0.29	0	59,61,61	0.35	0
63	CDL	V	201	-	90,90,99	0.32	0	96,102,111	0.37	0
65	FES	FS	201	28	0,4,4	-	-	-	-	-
63	CDL	M3	402	-	50,50,99	0.41	0	56,62,111	0.35	0
62	PC1	n	302	-	35,35,53	0.36	0	41,43,61	0.35	0
63	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.32	0
63	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.35	0
62	PC1	J	302	-	36,36,53	0.34	0	42,44,61	0.33	0
63	CDL	T	201	-	67,67,99	0.36	0	73,79,111	0.35	0
63	CDL	m1	404	-	65,65,99	0.36	0	71,77,111	0.30	0
63	CDL	T	202	-	74,74,99	0.34	0	80,86,111	0.35	0
63	CDL	M1	401	-	94,94,99	0.31	0	100,106,111	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	CDL	5b	703	-	66,66,99	0.36	0	72,78,111	0.33	0
62	PC1	m1	405	-	34,34,53	0.35	0	40,42,61	0.32	0
62	PC1	7C	302	-	53,53,53	0.29	0	59,61,61	0.36	0
63	CDL	a	503	-	50,50,99	0.41	0	56,62,111	0.51	0
63	CDL	5B	703	-	61,61,99	0.37	0	67,73,111	0.33	0
62	PC1	M2	406	-	53,53,53	0.29	0	59,61,61	0.28	0
62	PC1	c3	605	-	40,40,53	0.33	0	46,48,61	0.42	0
62	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.39	0
63	CDL	y5	201	-	80,80,99	0.33	0	86,92,111	0.28	0
63	CDL	y0	101	-	63,63,99	0.37	0	69,75,111	0.34	0
63	CDL	c3	604	-	67,67,99	0.36	0	73,79,111	0.31	0
63	CDL	Y0	101	-	63,63,99	0.37	0	69,75,111	0.34	0
63	CDL	t	202	-	74,74,99	0.34	0	80,86,111	0.35	0
62	PC1	M2	402	-	31,31,53	0.37	0	37,39,61	0.37	0
63	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.30	0
63	CDL	F	401	-	99,99,99	0.29	0	105,111,111	0.36	0
63	CDL	M2	403	-	65,65,99	0.36	0	71,77,111	0.32	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
63	CDL	m3	401	-	-	19/104/104/110	-
62	PC1	C3	601	-	-	12/55/55/57	-
63	CDL	e	402	-	-	14/82/82/110	-
63	CDL	7C	303	-	-	15/61/61/110	-
65	FES	fs	201	28	-	-	0/1/1/1
62	PC1	M2	405	-	-	11/44/44/57	-
63	CDL	y7	501	-	-	10/75/75/110	-
65	FES	fs	202	28	-	-	0/1/1/1
63	CDL	t	201	-	-	10/78/78/110	-
59	HEA	c1	702	7	-	14/36/76/76	-
63	CDL	M3	403	-	-	17/73/73/110	-
62	PC1	c3	602	-	-	9/42/42/57	-
63	CDL	M2	401	-	-	15/64/64/110	-
63	CDL	A	503	-	-	8/61/61/110	-
62	PC1	v	202	-	-	9/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	j	302	-	-	8/40/40/57	-
63	CDL	m2	404	-	-	16/84/84/110	-
63	CDL	7A	202	-	-	19/110/110/110	-
63	CDL	7C	301	-	-	22/95/95/110	-
63	CDL	M1	402	-	-	15/76/76/110	-
62	PC1	A	501	-	-	11/48/48/57	-
62	PC1	C3	605	-	-	10/44/44/57	-
63	CDL	m3	403	-	-	18/73/73/110	-
62	PC1	n	301	-	-	13/35/35/57	-
63	CDL	C3	604	-	-	9/78/78/110	-
62	PC1	a	502	-	-	9/44/44/57	-
63	CDL	Y7	501	-	-	11/75/75/110	-
62	PC1	c3	601	-	-	12/55/55/57	-
62	PC1	m2	402	-	-	3/35/35/57	-
63	CDL	E	402	-	-	14/82/82/110	-
63	CDL	c1	706	-	-	19/69/69/110	-
59	HEA	c1	701	7	-	18/36/76/76	-
62	PC1	M1	404	-	-	8/38/38/57	-
62	PC1	c1	705	-	-	9/52/52/57	-
63	CDL	M1	403	-	-	9/76/76/110	-
63	CDL	5b	702	-	-	23/97/97/110	-
63	CDL	5B	702	-	-	23/97/97/110	-
63	CDL	b	501	-	-	14/72/72/110	-
62	PC1	m2	406	-	-	8/57/57/57	-
59	HEA	C1	702	7	-	14/36/76/76	-
63	CDL	l	301	-	-	21/84/84/110	-
63	CDL	L	301	-	-	21/84/84/110	-
63	CDL	7a	202	-	-	23/110/110/110	-
62	PC1	V	202	-	-	10/57/57/57	-
63	CDL	7c	302	-	-	15/61/61/110	-
63	CDL	7A	201	-	-	12/77/77/110	-
62	PC1	N	302	-	-	4/39/39/57	-
63	CDL	c1	707	-	-	10/75/75/110	-
63	CDL	B	501	-	-	14/72/72/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PC1	a	501	-	-	13/48/48/57	-
63	CDL	u	201	-	-	15/92/92/110	-
63	CDL	v	201	-	-	13/101/101/110	-
63	CDL	C1	706	-	-	17/69/69/110	-
63	CDL	m1	401	-	-	26/105/105/110	-
62	PC1	c3	603	-	-	10/34/34/57	-
63	CDL	j	301	-	-	13/80/80/110	-
59	HEA	C1	701	7	-	17/36/76/76	-
62	PC1	C1	705	-	-	12/52/52/57	-
63	CDL	m2	401	-	-	18/64/64/110	-
63	CDL	U	201	-	-	17/92/92/110	-
63	CDL	5B	704	-	-	9/77/77/110	-
62	PC1	N	301	-	-	13/35/35/57	-
63	CDL	n	303	-	-	22/105/105/110	-
62	PC1	m2	405	-	-	6/44/44/57	-
62	PC1	7C	304	-	-	12/46/46/57	-
62	PC1	C3	602	-	-	10/42/42/57	-
63	CDL	m1	403	-	-	15/76/76/110	-
63	CDL	f	401	-	-	17/110/110/110	-
65	FES	FS	202	28	-	-	0/1/1/1
63	CDL	Y5	201	-	-	16/91/91/110	-
63	CDL	E	401	-	-	17/70/70/110	-
63	CDL	m3	402	-	-	13/61/61/110	-
63	CDL	N	303	-	-	22/105/105/110	-
63	CDL	7c	301	-	-	24/95/95/110	-
63	CDL	k	301	-	-	14/72/72/110	-
63	CDL	7a	201	-	-	13/77/77/110	-
63	CDL	e	401	-	-	16/70/70/110	-
62	PC1	7c	303	-	-	13/46/46/57	-
63	CDL	M3	401	-	-	20/104/104/110	-
62	PC1	A	502	-	-	11/44/44/57	-
63	CDL	C1	707	-	-	11/75/75/110	-
62	PC1	m1	402	-	-	16/57/57/57	-
63	CDL	V	201	-	-	14/101/101/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	FES	FS	201	28	-	-	0/1/1/1
63	CDL	M3	402	-	-	13/61/61/110	-
62	PC1	n	302	-	-	4/39/39/57	-
63	CDL	m2	403	-	-	15/76/76/110	-
63	CDL	M2	404	-	-	17/84/84/110	-
62	PC1	J	302	-	-	7/40/40/57	-
63	CDL	T	201	-	-	12/78/78/110	-
63	CDL	m1	404	-	-	10/76/76/110	-
63	CDL	T	202	-	-	13/85/85/110	-
63	CDL	M1	401	-	-	27/105/105/110	-
63	CDL	5b	703	-	-	11/77/77/110	-
62	PC1	m1	405	-	-	8/38/38/57	-
62	PC1	7C	302	-	-	17/57/57/57	-
63	CDL	a	503	-	-	12/61/61/110	-
63	CDL	5B	703	-	-	14/72/72/110	-
62	PC1	M2	406	-	-	8/57/57/57	-
62	PC1	c3	605	-	-	9/44/44/57	-
62	PC1	C3	603	-	-	10/34/34/57	-
63	CDL	y5	201	-	-	15/91/91/110	-
63	CDL	y0	101	-	-	21/74/74/110	-
63	CDL	c3	604	-	-	9/78/78/110	-
63	CDL	Y0	101	-	-	17/74/74/110	-
63	CDL	t	202	-	-	14/85/85/110	-
62	PC1	M2	402	-	-	4/35/35/57	-
63	CDL	J	301	-	-	12/80/80/110	-
63	CDL	F	401	-	-	19/110/110/110	-
63	CDL	M2	403	-	-	15/76/76/110	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	702	HEA	C4D-C3D	3.26	1.50	1.45
59	C1	702	HEA	C4D-C3D	3.25	1.50	1.45
59	C1	702	HEA	C3A-C4A	-3.20	1.40	1.46
59	c1	702	HEA	C3A-C4A	-3.17	1.40	1.46
59	C1	702	HEA	FE-NB	3.09	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	c1	702	HEA	FE-NB	3.08	2.04	1.94
59	C1	702	HEA	FE-ND	3.03	2.04	1.94
59	c1	702	HEA	FE-ND	3.02	2.04	1.94
59	c1	701	HEA	FE-ND	2.94	2.04	1.94
59	C1	701	HEA	C4D-C3D	2.93	1.50	1.45
59	C1	701	HEA	C1D-ND	-2.92	1.35	1.40
59	C1	701	HEA	FE-ND	2.92	2.03	1.94
59	c1	701	HEA	C1D-ND	-2.92	1.35	1.40
59	c1	701	HEA	C4D-C3D	2.91	1.50	1.45
59	c1	701	HEA	FE-NB	2.82	2.03	1.94
59	c1	702	HEA	C1D-ND	-2.82	1.35	1.40
59	C1	702	HEA	C1D-ND	-2.80	1.35	1.40
59	C1	701	HEA	FE-NB	2.80	2.03	1.94
59	c1	701	HEA	C3A-C4A	-2.70	1.41	1.46
59	C1	701	HEA	C3A-C4A	-2.70	1.41	1.46
59	c1	701	HEA	C1A-C2A	-2.64	1.40	1.45
59	C1	701	HEA	C1A-C2A	-2.63	1.40	1.45
59	C1	701	HEA	CMA-C3A	2.56	1.51	1.45
59	c1	701	HEA	CMA-C3A	2.55	1.51	1.45
59	c1	702	HEA	FE-NC	2.46	2.03	1.95
59	c1	702	HEA	CMA-C3A	2.46	1.50	1.45
59	C1	702	HEA	CMA-C3A	2.46	1.50	1.45
59	C1	702	HEA	FE-NC	2.45	2.03	1.95
59	C1	701	HEA	C4B-NB	-2.44	1.36	1.40
59	c1	701	HEA	C4B-NB	-2.43	1.36	1.40
59	c1	702	HEA	C4B-NB	-2.41	1.36	1.40
59	C1	702	HEA	C4B-NB	-2.41	1.36	1.40
59	c1	701	HEA	FE-NC	2.37	2.03	1.95
59	C1	701	HEA	FE-NC	2.35	2.02	1.95
59	C1	702	HEA	C1A-C2A	-2.20	1.41	1.45
59	c1	702	HEA	C1A-C2A	-2.19	1.41	1.45
59	c1	702	HEA	FE-NA	2.01	2.01	1.95
59	C1	702	HEA	FE-NA	2.00	2.01	1.95

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	C1	702	HEA	C13-C12-C11	-4.84	106.65	114.39
59	c1	702	HEA	C13-C12-C11	-4.80	106.73	114.39
59	C1	701	HEA	C13-C12-C11	-3.67	108.53	114.39
59	c1	701	HEA	C13-C12-C11	-3.61	108.63	114.39
59	C1	702	HEA	CHB-C4A-NA	3.61	128.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c1	702	HEA	CHB-C4A-NA	3.55	128.32	124.45
59	C1	702	HEA	C13-C14-C15	-3.30	120.06	127.62
59	c1	702	HEA	C13-C14-C15	-3.28	120.13	127.62
59	C1	701	HEA	C4B-NB-C1B	3.21	109.01	105.21
59	C1	702	HEA	C17-C18-C19	-3.20	120.29	127.62
59	c1	702	HEA	C17-C18-C19	-3.19	120.33	127.62
59	C1	701	HEA	CAA-CBA-CGA	-3.15	105.30	113.67
59	c1	701	HEA	CAA-CBA-CGA	-3.15	105.30	113.67
59	c1	701	HEA	C4B-NB-C1B	3.12	108.90	105.21
59	C1	701	HEA	C3C-C4C-NC	-3.10	107.19	109.80
59	c1	701	HEA	C3C-C4C-NC	-3.01	107.26	109.80
59	C1	701	HEA	C13-C14-C15	-2.96	120.84	127.62
59	C1	702	HEA	C3C-C4C-NC	-2.94	107.33	109.80
59	C1	701	HEA	C1D-ND-C4D	2.92	108.67	105.21
59	c1	701	HEA	C13-C14-C15	-2.92	120.94	127.62
59	c1	701	HEA	C17-C18-C19	-2.91	120.95	127.62
59	C1	701	HEA	C17-C18-C19	-2.90	120.99	127.62
59	c1	702	HEA	C3C-C4C-NC	-2.87	107.38	109.80
59	c1	701	HEA	C1D-ND-C4D	2.83	108.56	105.21
59	c1	702	HEA	C1D-ND-C4D	2.73	108.44	105.21
59	C1	702	HEA	C1D-ND-C4D	2.69	108.39	105.21
59	C1	702	HEA	C26-C15-C16	2.60	119.73	115.23
59	c1	701	HEA	C27-C19-C20	2.55	119.65	115.23
59	c1	702	HEA	C26-C15-C16	2.52	119.61	115.23
59	c1	702	HEA	C3D-C4D-ND	-2.50	107.94	110.35
59	c1	702	HEA	OMA-CMA-C3A	-2.48	120.03	125.62
59	C1	702	HEA	C3D-C4D-ND	-2.45	107.98	110.35
59	C1	701	HEA	C27-C19-C20	2.45	119.48	115.23
59	C1	702	HEA	OMA-CMA-C3A	-2.44	120.12	125.62
59	c1	701	HEA	CHB-C4A-NA	2.41	127.08	124.45
59	c1	702	HEA	C27-C19-C20	2.35	119.31	115.23
59	C1	701	HEA	CHB-C4A-NA	2.35	127.01	124.45
59	C1	701	HEA	CMB-C2B-C3B	-2.33	125.78	130.28
59	C1	702	HEA	C27-C19-C20	2.32	119.26	115.23
59	C1	701	HEA	C3D-C4D-ND	-2.31	108.12	110.35
59	c1	701	HEA	CMB-C2B-C3B	-2.30	125.82	130.28
59	C1	701	HEA	C26-C15-C16	2.29	119.21	115.23
59	c1	701	HEA	OMA-CMA-C3A	-2.29	120.45	125.62
59	C1	702	HEA	CMB-C2B-C3B	-2.28	125.88	130.28
59	c1	702	HEA	CMB-C2B-C3B	-2.25	125.92	130.28
59	c1	701	HEA	C26-C15-C16	2.25	119.14	115.23
59	C1	701	HEA	OMA-CMA-C3A	-2.25	120.54	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c1	701	HEA	C3D-C4D-ND	-2.25	108.18	110.35
59	c1	702	HEA	CAD-CBD-CGD	-2.18	107.88	113.67
59	C1	702	HEA	CAD-CBD-CGD	-2.17	107.90	113.67
59	c1	702	HEA	CAD-C3D-C4D	2.17	128.47	124.70
59	C1	702	HEA	C25-C23-C24	2.17	119.57	114.59
59	C1	702	HEA	CAA-CBA-CGA	-2.17	107.92	113.67
59	C1	702	HEA	CAD-C3D-C4D	2.14	128.43	124.70
59	c1	702	HEA	C21-C22-C23	-2.14	120.52	127.64
59	C1	702	HEA	C21-C22-C23	-2.13	120.54	127.64
59	c1	702	HEA	C25-C23-C24	2.12	119.47	114.59
59	c1	702	HEA	CAA-CBA-CGA	-2.11	108.07	113.67
59	C1	701	HEA	C3B-C4B-NB	-2.08	107.45	109.84
59	c1	701	HEA	C21-C22-C23	-2.07	120.73	127.64
59	C1	701	HEA	CAD-CBD-CGD	-2.07	108.17	113.67
59	c1	701	HEA	CAD-CBD-CGD	-2.05	108.22	113.67
59	C1	701	HEA	C21-C22-C23	-2.05	120.80	127.64
59	c1	701	HEA	C3B-C4B-NB	-2.02	107.52	109.84
59	C1	701	HEA	C4C-NC-C1C	2.02	109.11	105.82

There are no chirality outliers.

All (1456) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	C1	701	HEA	C2A-C3A-CMA-OMA
59	C1	701	HEA	C4A-C3A-CMA-OMA
59	C1	701	HEA	C26-C15-C16-C17
59	C1	701	HEA	C15-C16-C17-C18
59	C1	701	HEA	C17-C18-C19-C20
59	C1	701	HEA	C17-C18-C19-C27
59	C1	702	HEA	C2A-C3A-CMA-OMA
59	C1	702	HEA	C4A-C3A-CMA-OMA
59	C1	702	HEA	C13-C14-C15-C16
59	C1	702	HEA	C13-C14-C15-C26
59	C1	702	HEA	C17-C18-C19-C27
59	c1	701	HEA	C2A-C3A-CMA-OMA
59	c1	701	HEA	C4A-C3A-CMA-OMA
59	c1	701	HEA	C15-C16-C17-C18
59	c1	701	HEA	C17-C18-C19-C20
59	c1	701	HEA	C17-C18-C19-C27
59	c1	702	HEA	C2A-C3A-CMA-OMA
59	c1	702	HEA	C4A-C3A-CMA-OMA
59	c1	702	HEA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
59	c1	702	HEA	C13-C14-C15-C26
59	c1	702	HEA	C17-C18-C19-C27
62	C1	705	PC1	C11-O13-P-O12
62	C3	601	PC1	C1-O11-P-O14
62	C3	601	PC1	C1-O11-P-O13
62	C3	601	PC1	C2-C1-O11-P
62	C3	602	PC1	C1-O11-P-O12
62	C3	602	PC1	O21-C2-C3-O31
62	C3	603	PC1	C11-O13-P-O12
62	7C	302	PC1	C11-O13-P-O14
62	7C	302	PC1	C11-O13-P-O11
62	7C	302	PC1	C1-O11-P-O12
62	7C	302	PC1	C1-O11-P-O14
62	7C	302	PC1	C1-O11-P-O13
62	7C	304	PC1	C11-O13-P-O12
62	7C	304	PC1	C11-O13-P-O14
62	7C	304	PC1	C11-O13-P-O11
62	7C	304	PC1	C1-O11-P-O14
62	M1	404	PC1	C11-O13-P-O12
62	M1	404	PC1	C11-O13-P-O11
62	M2	405	PC1	C11-O13-P-O12
62	M2	406	PC1	C1-O11-P-O12
62	M2	406	PC1	C1-O11-P-O13
62	A	501	PC1	C11-O13-P-O12
62	A	501	PC1	C11-O13-P-O11
62	A	501	PC1	C1-O11-P-O12
62	A	501	PC1	C1-O11-P-O13
62	A	501	PC1	C2-C1-O11-P
62	A	502	PC1	C11-O13-P-O11
62	A	502	PC1	C1-O11-P-O13
62	J	302	PC1	C1-O11-P-O12
62	J	302	PC1	C1-O11-P-O14
62	J	302	PC1	C1-O11-P-O13
62	N	301	PC1	C11-O13-P-O14
62	N	301	PC1	C1-O11-P-O12
62	N	301	PC1	C1-O11-P-O14
62	N	302	PC1	C1-O11-P-O13
62	N	302	PC1	O13-C11-C12-N
62	V	202	PC1	C11-O13-P-O12
62	V	202	PC1	C11-O13-P-O14
62	V	202	PC1	C11-O13-P-O11
62	V	202	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
62	V	202	PC1	C1-O11-P-O13
62	c1	705	PC1	C11-O13-P-O12
62	c1	705	PC1	C11-O13-P-O11
62	c3	601	PC1	C1-O11-P-O14
62	c3	601	PC1	C1-O11-P-O13
62	c3	601	PC1	C2-C1-O11-P
62	c3	602	PC1	C1-O11-P-O12
62	c3	602	PC1	C1-O11-P-O13
62	c3	602	PC1	O21-C2-C3-O31
62	c3	603	PC1	C11-O13-P-O12
62	c3	603	PC1	C11-O13-P-O11
62	7c	303	PC1	C11-O13-P-O12
62	7c	303	PC1	C11-O13-P-O14
62	7c	303	PC1	C11-O13-P-O11
62	7c	303	PC1	C1-O11-P-O14
62	7c	303	PC1	C1-O11-P-O13
62	m1	402	PC1	C11-O13-P-O12
62	m1	402	PC1	C11-O13-P-O14
62	m1	402	PC1	C11-O13-P-O11
62	m1	402	PC1	C1-O11-P-O12
62	m1	402	PC1	C1-O11-P-O14
62	m1	402	PC1	C1-O11-P-O13
62	m1	405	PC1	C11-O13-P-O12
62	m1	405	PC1	C11-O13-P-O14
62	m1	405	PC1	C11-O13-P-O11
62	m2	405	PC1	C11-O13-P-O11
62	m2	406	PC1	C1-O11-P-O12
62	m2	406	PC1	C1-O11-P-O13
62	a	501	PC1	C11-O13-P-O12
62	a	501	PC1	C1-O11-P-O12
62	a	502	PC1	C11-O13-P-O11
62	a	502	PC1	C1-O11-P-O13
62	j	302	PC1	C1-O11-P-O12
62	j	302	PC1	C1-O11-P-O14
62	j	302	PC1	C1-O11-P-O13
62	n	301	PC1	C11-O13-P-O14
62	n	301	PC1	C1-O11-P-O12
62	n	301	PC1	C1-O11-P-O14
62	n	302	PC1	C1-O11-P-O13
62	n	302	PC1	O13-C11-C12-N
62	v	202	PC1	C11-O13-P-O12
62	v	202	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
62	v	202	PC1	C1-O11-P-O13
63	C1	706	CDL	CA2-OA2-PA1-OA3
63	C1	706	CDL	CA2-OA2-PA1-OA5
63	C1	706	CDL	CA3-OA5-PA1-OA2
63	C1	706	CDL	CB2-OB2-PB2-OB3
63	C1	706	CDL	CB3-OB5-PB2-OB2
63	C1	706	CDL	CB3-OB5-PB2-OB3
63	C1	707	CDL	CA2-OA2-PA1-OA3
63	C1	707	CDL	CA3-OA5-PA1-OA2
63	C1	707	CDL	CA3-OA5-PA1-OA3
63	C1	707	CDL	CA3-OA5-PA1-OA4
63	C3	604	CDL	CA2-OA2-PA1-OA3
63	C3	604	CDL	CA2-OA2-PA1-OA4
63	C3	604	CDL	CA2-OA2-PA1-OA5
63	5B	702	CDL	CA2-C1-CB2-OB2
63	5B	702	CDL	CA2-OA2-PA1-OA3
63	5B	702	CDL	CA2-OA2-PA1-OA4
63	5B	702	CDL	CA2-OA2-PA1-OA5
63	5B	702	CDL	CA3-OA5-PA1-OA2
63	5B	702	CDL	CA3-OA5-PA1-OA3
63	5B	702	CDL	CA3-OA5-PA1-OA4
63	5B	703	CDL	CA2-OA2-PA1-OA3
63	5B	703	CDL	CA2-OA2-PA1-OA5
63	5B	703	CDL	CA3-OA5-PA1-OA4
63	5B	704	CDL	CA3-OA5-PA1-OA2
63	5B	704	CDL	CB2-OB2-PB2-OB3
63	7A	201	CDL	CA2-OA2-PA1-OA4
63	7A	201	CDL	CA2-OA2-PA1-OA5
63	7A	201	CDL	CB2-OB2-PB2-OB4
63	7A	201	CDL	CB2-OB2-PB2-OB5
63	7A	202	CDL	CA3-OA5-PA1-OA3
63	7A	202	CDL	CB2-OB2-PB2-OB3
63	7A	202	CDL	CB2-OB2-PB2-OB5
63	7C	301	CDL	CA3-OA5-PA1-OA2
63	7C	301	CDL	CA3-OA5-PA1-OA3
63	7C	301	CDL	CB2-OB2-PB2-OB4
63	7C	301	CDL	CB3-OB5-PB2-OB2
63	7C	301	CDL	CB3-OB5-PB2-OB3
63	7C	301	CDL	CB3-OB5-PB2-OB4
63	7C	303	CDL	CA2-OA2-PA1-OA3
63	7C	303	CDL	CA2-OA2-PA1-OA4
63	7C	303	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
63	7C	303	CDL	CA3-OA5-PA1-OA2
63	7C	303	CDL	CA3-OA5-PA1-OA3
63	7C	303	CDL	CA3-OA5-PA1-OA4
63	7C	303	CDL	CB2-OB2-PB2-OB3
63	M1	401	CDL	CA2-OA2-PA1-OA4
63	M1	401	CDL	CB2-OB2-PB2-OB4
63	M1	401	CDL	CB3-OB5-PB2-OB2
63	M1	401	CDL	CB3-OB5-PB2-OB3
63	M1	401	CDL	CB3-OB5-PB2-OB4
63	M1	403	CDL	CA2-OA2-PA1-OA3
63	M1	403	CDL	CA3-OA5-PA1-OA2
63	M1	403	CDL	CA3-OA5-PA1-OA3
63	M1	403	CDL	CA3-OA5-PA1-OA4
63	M1	403	CDL	CB2-OB2-PB2-OB4
63	M2	401	CDL	CA2-OA2-PA1-OA3
63	M2	401	CDL	CA3-OA5-PA1-OA4
63	M2	401	CDL	CB3-OB5-PB2-OB3
63	M2	403	CDL	CA2-OA2-PA1-OA3
63	M2	403	CDL	CA2-OA2-PA1-OA4
63	M2	403	CDL	CA2-OA2-PA1-OA5
63	M2	403	CDL	CB2-OB2-PB2-OB5
63	M2	403	CDL	CB3-OB5-PB2-OB2
63	M2	404	CDL	CA2-OA2-PA1-OA3
63	M2	404	CDL	CA2-OA2-PA1-OA5
63	M2	404	CDL	CB2-OB2-PB2-OB3
63	M2	404	CDL	CB2-OB2-PB2-OB4
63	M2	404	CDL	CB2-OB2-PB2-OB5
63	M3	401	CDL	CB2-OB2-PB2-OB4
63	M3	401	CDL	CB2-OB2-PB2-OB5
63	M3	401	CDL	CB3-OB5-PB2-OB2
63	M3	401	CDL	CB3-OB5-PB2-OB3
63	M3	402	CDL	CA2-OA2-PA1-OA5
63	M3	402	CDL	CA3-OA5-PA1-OA4
63	M3	402	CDL	CB2-OB2-PB2-OB3
63	M3	402	CDL	CB2-OB2-PB2-OB4
63	M3	402	CDL	CB2-OB2-PB2-OB5
63	M3	402	CDL	CB3-OB5-PB2-OB2
63	M3	403	CDL	CA2-OA2-PA1-OA5
63	Y7	501	CDL	CA2-OA2-PA1-OA3
63	Y7	501	CDL	CA2-OA2-PA1-OA4
63	Y7	501	CDL	CA2-OA2-PA1-OA5
63	Y7	501	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
63	Y0	101	CDL	CA2-OA2-PA1-OA5
63	Y0	101	CDL	CA3-OA5-PA1-OA3
63	Y0	101	CDL	CB2-OB2-PB2-OB3
63	Y0	101	CDL	CB3-OB5-PB2-OB2
63	Y0	101	CDL	CB3-OB5-PB2-OB3
63	Y5	201	CDL	CA2-OA2-PA1-OA4
63	Y5	201	CDL	CA2-OA2-PA1-OA5
63	Y5	201	CDL	CA3-OA5-PA1-OA4
63	Y5	201	CDL	CB2-OB2-PB2-OB4
63	Y5	201	CDL	CB3-OB5-PB2-OB3
63	A	503	CDL	CA2-OA2-PA1-OA3
63	A	503	CDL	CB3-OB5-PB2-OB2
63	A	503	CDL	CB3-OB5-PB2-OB3
63	B	501	CDL	CA2-OA2-PA1-OA3
63	B	501	CDL	CA2-OA2-PA1-OA4
63	B	501	CDL	CA2-OA2-PA1-OA5
63	B	501	CDL	CA3-OA5-PA1-OA2
63	B	501	CDL	CA3-OA5-PA1-OA3
63	B	501	CDL	CA3-OA5-PA1-OA4
63	E	401	CDL	CA2-OA2-PA1-OA3
63	E	401	CDL	CA2-OA2-PA1-OA5
63	E	401	CDL	CA3-OA5-PA1-OA2
63	E	401	CDL	CA3-OA5-PA1-OA4
63	E	401	CDL	CB3-OB5-PB2-OB2
63	E	401	CDL	CB3-OB5-PB2-OB3
63	E	402	CDL	CA2-OA2-PA1-OA3
63	E	402	CDL	CA2-OA2-PA1-OA4
63	E	402	CDL	CA2-OA2-PA1-OA5
63	E	402	CDL	CB2-OB2-PB2-OB3
63	F	401	CDL	CA3-OA5-PA1-OA2
63	F	401	CDL	CA3-OA5-PA1-OA3
63	F	401	CDL	CB3-OB5-PB2-OB2
63	F	401	CDL	CB3-OB5-PB2-OB3
63	F	401	CDL	CB3-OB5-PB2-OB4
63	J	301	CDL	CA2-OA2-PA1-OA3
63	L	301	CDL	CA2-OA2-PA1-OA3
63	L	301	CDL	CA2-OA2-PA1-OA5
63	L	301	CDL	CA3-OA5-PA1-OA2
63	L	301	CDL	CA3-OA5-PA1-OA4
63	L	301	CDL	CB2-OB2-PB2-OB5
63	L	301	CDL	CB3-OB5-PB2-OB2
63	L	301	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
63	N	303	CDL	CA2-OA2-PA1-OA4
63	N	303	CDL	CA2-OA2-PA1-OA5
63	N	303	CDL	CA3-OA5-PA1-OA2
63	N	303	CDL	CA3-OA5-PA1-OA3
63	N	303	CDL	CA3-OA5-PA1-OA4
63	N	303	CDL	CB2-OB2-PB2-OB3
63	N	303	CDL	CB2-OB2-PB2-OB4
63	N	303	CDL	CB2-OB2-PB2-OB5
63	N	303	CDL	CB3-OB5-PB2-OB2
63	N	303	CDL	CB3-OB5-PB2-OB3
63	N	303	CDL	CB3-OB5-PB2-OB4
63	T	201	CDL	CA2-OA2-PA1-OA5
63	T	201	CDL	CB2-OB2-PB2-OB3
63	T	201	CDL	CB2-OB2-PB2-OB5
63	T	201	CDL	CB3-OB5-PB2-OB3
63	T	202	CDL	CB3-OB5-PB2-OB2
63	T	202	CDL	CB3-OB5-PB2-OB3
63	T	202	CDL	CB3-OB5-PB2-OB4
63	U	201	CDL	CA3-OA5-PA1-OA2
63	U	201	CDL	CA3-OA5-PA1-OA3
63	U	201	CDL	CA3-OA5-PA1-OA4
63	U	201	CDL	CB3-OB5-PB2-OB2
63	V	201	CDL	CB2-OB2-PB2-OB3
63	V	201	CDL	CB3-OB5-PB2-OB2
63	V	201	CDL	CB3-OB5-PB2-OB3
63	c1	706	CDL	CA2-OA2-PA1-OA3
63	c1	706	CDL	CA2-OA2-PA1-OA5
63	c1	706	CDL	CA3-OA5-PA1-OA2
63	c1	706	CDL	CB2-OB2-PB2-OB3
63	c1	706	CDL	CB2-OB2-PB2-OB5
63	c1	706	CDL	CB3-OB5-PB2-OB2
63	c1	706	CDL	CB3-OB5-PB2-OB3
63	c1	707	CDL	CA2-OA2-PA1-OA3
63	c1	707	CDL	CA3-OA5-PA1-OA2
63	c1	707	CDL	CA3-OA5-PA1-OA3
63	c1	707	CDL	CA3-OA5-PA1-OA4
63	c3	604	CDL	CA2-OA2-PA1-OA3
63	c3	604	CDL	CA2-OA2-PA1-OA4
63	c3	604	CDL	CA2-OA2-PA1-OA5
63	5b	702	CDL	CA2-OA2-PA1-OA3
63	5b	702	CDL	CA2-OA2-PA1-OA4
63	5b	702	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
63	5b	702	CDL	CA3-OA5-PA1-OA2
63	5b	702	CDL	CA3-OA5-PA1-OA3
63	5b	702	CDL	CA3-OA5-PA1-OA4
63	5b	702	CDL	CB3-OB5-PB2-OB2
63	5b	702	CDL	CB3-OB5-PB2-OB4
63	5b	703	CDL	CA3-OA5-PA1-OA2
63	5b	703	CDL	CB2-OB2-PB2-OB3
63	7a	201	CDL	CA2-OA2-PA1-OA4
63	7a	201	CDL	CA2-OA2-PA1-OA5
63	7a	201	CDL	CB2-OB2-PB2-OB4
63	7a	201	CDL	CB2-OB2-PB2-OB5
63	7a	202	CDL	CA2-OA2-PA1-OA4
63	7a	202	CDL	CA3-OA5-PA1-OA3
63	7a	202	CDL	CB2-OB2-PB2-OB3
63	7a	202	CDL	CB2-OB2-PB2-OB5
63	7c	301	CDL	CA3-OA5-PA1-OA2
63	7c	301	CDL	CA3-OA5-PA1-OA3
63	7c	301	CDL	CB2-OB2-PB2-OB3
63	7c	301	CDL	CB2-OB2-PB2-OB4
63	7c	301	CDL	CB2-OB2-PB2-OB5
63	7c	301	CDL	CB3-OB5-PB2-OB2
63	7c	301	CDL	CB3-OB5-PB2-OB4
63	7c	302	CDL	CA2-OA2-PA1-OA3
63	7c	302	CDL	CA2-OA2-PA1-OA4
63	7c	302	CDL	CA2-OA2-PA1-OA5
63	7c	302	CDL	CA3-OA5-PA1-OA2
63	7c	302	CDL	CA3-OA5-PA1-OA3
63	7c	302	CDL	CA3-OA5-PA1-OA4
63	7c	302	CDL	CB2-OB2-PB2-OB3
63	m1	401	CDL	CA2-OA2-PA1-OA4
63	m1	401	CDL	CB2-OB2-PB2-OB4
63	m1	401	CDL	CB2-OB2-PB2-OB5
63	m1	401	CDL	CB3-OB5-PB2-OB2
63	m1	401	CDL	CB3-OB5-PB2-OB3
63	m1	401	CDL	CB3-OB5-PB2-OB4
63	m1	404	CDL	CA2-OA2-PA1-OA3
63	m1	404	CDL	CA3-OA5-PA1-OA2
63	m1	404	CDL	CA3-OA5-PA1-OA3
63	m1	404	CDL	CA3-OA5-PA1-OA4
63	m1	404	CDL	CB2-OB2-PB2-OB4
63	m2	401	CDL	CA2-OA2-PA1-OA3
63	m2	401	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
63	m2	401	CDL	CA3-OA5-PA1-OA4
63	m2	401	CDL	CB3-OB5-PB2-OB2
63	m2	401	CDL	CB3-OB5-PB2-OB3
63	m2	403	CDL	CA2-OA2-PA1-OA3
63	m2	403	CDL	CA2-OA2-PA1-OA4
63	m2	403	CDL	CA2-OA2-PA1-OA5
63	m2	403	CDL	CB2-OB2-PB2-OB5
63	m2	404	CDL	CA2-OA2-PA1-OA3
63	m2	404	CDL	CA2-OA2-PA1-OA5
63	m2	404	CDL	CB2-OB2-PB2-OB3
63	m2	404	CDL	CB2-OB2-PB2-OB4
63	m2	404	CDL	CB2-OB2-PB2-OB5
63	m3	401	CDL	CB2-OB2-PB2-OB4
63	m3	401	CDL	CB2-OB2-PB2-OB5
63	m3	401	CDL	CB3-OB5-PB2-OB2
63	m3	401	CDL	CB3-OB5-PB2-OB3
63	m3	401	CDL	CB3-OB5-PB2-OB4
63	m3	402	CDL	CA2-OA2-PA1-OA5
63	m3	402	CDL	CA3-OA5-PA1-OA2
63	m3	402	CDL	CA3-OA5-PA1-OA3
63	m3	402	CDL	CA3-OA5-PA1-OA4
63	m3	402	CDL	CB2-OB2-PB2-OB3
63	m3	402	CDL	CB2-OB2-PB2-OB4
63	m3	402	CDL	CB2-OB2-PB2-OB5
63	m3	402	CDL	CB3-OB5-PB2-OB2
63	m3	403	CDL	CA2-OA2-PA1-OA5
63	y7	501	CDL	CA2-OA2-PA1-OA3
63	y7	501	CDL	CA2-OA2-PA1-OA4
63	y7	501	CDL	CA2-OA2-PA1-OA5
63	y7	501	CDL	CB2-OB2-PB2-OB5
63	y0	101	CDL	CA2-OA2-PA1-OA4
63	y0	101	CDL	CA2-OA2-PA1-OA5
63	y0	101	CDL	CA3-OA5-PA1-OA3
63	y0	101	CDL	CB2-OB2-PB2-OB3
63	y0	101	CDL	CB3-OB5-PB2-OB2
63	y0	101	CDL	CB3-OB5-PB2-OB3
63	y5	201	CDL	CA2-OA2-PA1-OA4
63	y5	201	CDL	CA2-OA2-PA1-OA5
63	y5	201	CDL	CA3-OA5-PA1-OA4
63	y5	201	CDL	CB2-OB2-PB2-OB4
63	y5	201	CDL	CB2-OB2-PB2-OB5
63	y5	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
63	y5	201	CDL	CB3-OB5-PB2-OB3
63	a	503	CDL	CA2-OA2-PA1-OA3
63	a	503	CDL	CB2-OB2-PB2-OB4
63	a	503	CDL	CB3-OB5-PB2-OB3
63	b	501	CDL	CA2-OA2-PA1-OA3
63	b	501	CDL	CA2-OA2-PA1-OA4
63	b	501	CDL	CA2-OA2-PA1-OA5
63	b	501	CDL	CA3-OA5-PA1-OA2
63	b	501	CDL	CA3-OA5-PA1-OA3
63	b	501	CDL	CA3-OA5-PA1-OA4
63	e	401	CDL	CA2-OA2-PA1-OA3
63	e	401	CDL	CA2-OA2-PA1-OA5
63	e	401	CDL	CA3-OA5-PA1-OA2
63	e	401	CDL	CA3-OA5-PA1-OA4
63	e	401	CDL	CB3-OB5-PB2-OB2
63	e	401	CDL	CB3-OB5-PB2-OB3
63	e	402	CDL	CA2-OA2-PA1-OA3
63	e	402	CDL	CA2-OA2-PA1-OA4
63	e	402	CDL	CA2-OA2-PA1-OA5
63	e	402	CDL	CB3-OB5-PB2-OB4
63	f	401	CDL	CA2-C1-CB2-OB2
63	f	401	CDL	CA3-OA5-PA1-OA3
63	f	401	CDL	CB3-OB5-PB2-OB2
63	f	401	CDL	CB3-OB5-PB2-OB3
63	f	401	CDL	CB3-OB5-PB2-OB4
63	k	301	CDL	CA2-OA2-PA1-OA3
63	k	301	CDL	CA2-OA2-PA1-OA5
63	k	301	CDL	CA3-OA5-PA1-OA4
63	l	301	CDL	CA2-OA2-PA1-OA3
63	l	301	CDL	CA2-OA2-PA1-OA5
63	l	301	CDL	CA3-OA5-PA1-OA2
63	l	301	CDL	CA3-OA5-PA1-OA4
63	l	301	CDL	CB2-OB2-PB2-OB5
63	l	301	CDL	CB3-OB5-PB2-OB2
63	l	301	CDL	CB3-OB5-PB2-OB3
63	n	303	CDL	CA2-OA2-PA1-OA4
63	n	303	CDL	CA2-OA2-PA1-OA5
63	n	303	CDL	CA3-OA5-PA1-OA2
63	n	303	CDL	CA3-OA5-PA1-OA3
63	n	303	CDL	CA3-OA5-PA1-OA4
63	n	303	CDL	CB2-OB2-PB2-OB3
63	n	303	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
63	n	303	CDL	CB2-OB2-PB2-OB5
63	n	303	CDL	CB3-OB5-PB2-OB2
63	n	303	CDL	CB3-OB5-PB2-OB3
63	n	303	CDL	CB3-OB5-PB2-OB4
63	t	201	CDL	CA2-OA2-PA1-OA5
63	t	201	CDL	CB2-OB2-PB2-OB3
63	t	201	CDL	CB3-OB5-PB2-OB3
63	t	202	CDL	CB3-OB5-PB2-OB2
63	t	202	CDL	CB3-OB5-PB2-OB3
63	t	202	CDL	CB3-OB5-PB2-OB4
63	u	201	CDL	CA3-OA5-PA1-OA2
63	u	201	CDL	CA3-OA5-PA1-OA3
63	u	201	CDL	CA3-OA5-PA1-OA4
63	u	201	CDL	CB2-OB2-PB2-OB3
63	u	201	CDL	CB2-OB2-PB2-OB5
63	u	201	CDL	CB3-OB5-PB2-OB2
63	u	201	CDL	CB3-OB5-PB2-OB3
63	u	201	CDL	CB3-OB5-PB2-OB4
63	v	201	CDL	CB2-OB2-PB2-OB3
63	v	201	CDL	CB3-OB5-PB2-OB2
63	v	201	CDL	CB3-OB5-PB2-OB3
59	c1	701	HEA	C21-C22-C23-C25
59	C1	701	HEA	C18-C19-C20-C21
59	c1	701	HEA	C18-C19-C20-C21
59	C1	701	HEA	C1A-C2A-CAA-CBA
63	5B	702	CDL	O1-C1-CB2-OB2
63	F	401	CDL	O1-C1-CB2-OB2
63	5b	702	CDL	O1-C1-CB2-OB2
63	f	401	CDL	O1-C1-CB2-OB2
59	C1	701	HEA	C21-C22-C23-C25
59	c1	701	HEA	C26-C15-C16-C17
59	c1	701	HEA	C14-C15-C16-C17
59	c1	702	HEA	C18-C19-C20-C21
62	a	501	PC1	C2-C1-O11-P
63	M1	401	CDL	C1-CB2-OB2-PB2
63	m1	401	CDL	C1-CB2-OB2-PB2
59	C1	701	HEA	C3A-C2A-CAA-CBA
59	C1	702	HEA	C17-C18-C19-C20
59	c1	702	HEA	C17-C18-C19-C20
59	c1	701	HEA	C1A-C2A-CAA-CBA
63	5b	702	CDL	CA2-C1-CB2-OB2
62	C3	601	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
62	c3	601	PC1	C11-C12-N-C13
59	C1	701	HEA	C14-C15-C16-C17
59	C1	702	HEA	C18-C19-C20-C21
59	c1	701	HEA	C3A-C2A-CAA-CBA
63	5b	702	CDL	OB5-CB3-CB4-OB6
62	C3	602	PC1	C21-C22-C23-C24
62	V	202	PC1	C31-C32-C33-C34
62	v	202	PC1	C31-C32-C33-C34
62	c3	602	PC1	C21-C22-C23-C24
63	v	201	CDL	CB5-C51-C52-C53
62	C3	601	PC1	C11-C12-N-C14
62	J	302	PC1	C11-C12-N-C15
62	c3	602	PC1	C11-C12-N-C15
62	j	302	PC1	C11-C12-N-C15
62	M2	406	PC1	C21-C22-C23-C24
62	m2	406	PC1	C21-C22-C23-C24
63	U	201	CDL	CB5-C51-C52-C53
63	V	201	CDL	CB5-C51-C52-C53
63	u	201	CDL	CB5-C51-C52-C53
63	C3	604	CDL	CA7-C31-C32-C33
63	M1	401	CDL	CB7-C71-C72-C73
63	m1	401	CDL	CB7-C71-C72-C73
63	c3	604	CDL	CA7-C31-C32-C33
63	F	401	CDL	CA2-C1-CB2-OB2
62	C3	602	PC1	C11-C12-N-C15
62	C3	605	PC1	C11-C12-N-C15
62	7C	302	PC1	C11-C12-N-C15
62	M2	405	PC1	C11-C12-N-C13
62	M2	405	PC1	C11-C12-N-C14
62	N	301	PC1	C11-C12-N-C14
62	c3	601	PC1	C11-C12-N-C14
62	c3	605	PC1	C11-C12-N-C15
62	m1	402	PC1	C11-C12-N-C15
62	n	301	PC1	C11-C12-N-C14
63	Y0	101	CDL	O1-C1-CA2-OA2
63	M1	401	CDL	CB5-C51-C52-C53
63	Y0	101	CDL	CA4-CA3-OA5-PA1
63	7A	202	CDL	C76-C77-C78-C79
63	7a	202	CDL	CA7-C31-C32-C33
59	C1	701	HEA	O11-C11-C12-C13
59	c1	701	HEA	O11-C11-C12-C13
62	M2	405	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
62	J	302	PC1	C11-C12-N-C14
63	e	402	CDL	C54-C55-C56-C57
63	7A	202	CDL	C52-C53-C54-C55
63	M2	403	CDL	C11-C12-C13-C14
63	m2	403	CDL	C11-C12-C13-C14
63	m3	401	CDL	CA5-C11-C12-C13
63	7a	202	CDL	OB5-CB3-CB4-CB6
63	J	301	CDL	O1-C1-CA2-OA2
63	j	301	CDL	O1-C1-CA2-OA2
59	c1	701	HEA	C21-C22-C23-C24
63	7A	202	CDL	CA7-C31-C32-C33
63	M3	401	CDL	CA5-C11-C12-C13
63	E	401	CDL	CA5-C11-C12-C13
63	e	401	CDL	CA5-C11-C12-C13
63	7a	202	CDL	C76-C77-C78-C79
63	7a	202	CDL	C52-C53-C54-C55
63	M1	401	CDL	C77-C78-C79-C80
63	m1	401	CDL	C77-C78-C79-C80
63	C3	604	CDL	CB5-C51-C52-C53
63	5B	703	CDL	CA5-C11-C12-C13
63	k	301	CDL	CA5-C11-C12-C13
62	7C	304	PC1	C22-C23-C24-C25
63	V	201	CDL	C56-C57-C58-C59
63	n	303	CDL	C39-C40-C41-C42
63	N	303	CDL	C39-C40-C41-C42
63	t	202	CDL	C75-C76-C77-C78
63	E	402	CDL	C54-C55-C56-C57
62	C3	601	PC1	C11-C12-N-C15
62	C3	602	PC1	C11-C12-N-C13
62	C3	605	PC1	C11-C12-N-C13
62	7C	302	PC1	C11-C12-N-C14
62	c3	601	PC1	C11-C12-N-C15
62	c3	602	PC1	C11-C12-N-C13
62	m1	402	PC1	C11-C12-N-C14
62	j	302	PC1	C11-C12-N-C13
62	j	302	PC1	C11-C12-N-C14
63	T	202	CDL	C75-C76-C77-C78
63	5B	702	CDL	C73-C74-C75-C76
63	7A	202	CDL	C62-C63-C64-C65
63	7a	202	CDL	C62-C63-C64-C65
63	m3	401	CDL	C58-C59-C60-C61
62	7c	303	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
63	M3	401	CDL	C73-C74-C75-C76
62	v	202	PC1	C3B-C3C-C3D-C3E
63	5b	702	CDL	C73-C74-C75-C76
62	V	202	PC1	C3B-C3C-C3D-C3E
63	m3	401	CDL	C72-C73-C74-C75
62	V	202	PC1	C3E-C3F-C3G-C3H
63	m1	401	CDL	CB5-C51-C52-C53
63	7C	301	CDL	C81-C82-C83-C84
63	f	401	CDL	CB7-C71-C72-C73
59	c1	701	HEA	C27-C19-C20-C21
62	C3	602	PC1	C11-C12-N-C14
62	C3	605	PC1	C11-C12-N-C14
62	7C	302	PC1	C11-C12-N-C13
62	J	302	PC1	C11-C12-N-C13
62	N	301	PC1	C11-C12-N-C13
62	N	301	PC1	C11-C12-N-C15
62	c3	602	PC1	C11-C12-N-C14
62	c3	605	PC1	C11-C12-N-C13
62	c3	605	PC1	C11-C12-N-C14
62	7c	303	PC1	C11-C12-N-C13
62	m1	402	PC1	C11-C12-N-C13
62	n	301	PC1	C11-C12-N-C13
62	n	301	PC1	C11-C12-N-C15
59	c1	702	HEA	C21-C22-C23-C25
63	m3	401	CDL	C73-C74-C75-C76
63	J	301	CDL	C52-C53-C54-C55
62	7C	304	PC1	C31-C32-C33-C34
63	T	202	CDL	C14-C15-C16-C17
63	7c	301	CDL	C81-C82-C83-C84
63	t	202	CDL	C14-C15-C16-C17
63	Y5	201	CDL	CA4-CA3-OA5-PA1
63	y0	101	CDL	CA4-CA3-OA5-PA1
63	y5	201	CDL	CA4-CA3-OA5-PA1
63	U	201	CDL	C74-C75-C76-C77
62	7C	302	PC1	C2B-C2C-C2D-C2E
59	C1	701	HEA	C21-C22-C23-C24
63	j	301	CDL	C52-C53-C54-C55
63	v	201	CDL	C56-C57-C58-C59
63	y5	201	CDL	C41-C42-C43-C44
62	7C	304	PC1	C11-C12-N-C13
63	Y5	201	CDL	C41-C42-C43-C44
63	5B	703	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
63	5B	704	CDL	OB5-CB3-CB4-CB6
63	Y0	101	CDL	OA5-CA3-CA4-CA6
63	N	303	CDL	OA5-CA3-CA4-CA6
63	c1	706	CDL	OB5-CB3-CB4-CB6
63	5b	703	CDL	OB5-CB3-CB4-CB6
63	m2	403	CDL	OB5-CB3-CB4-CB6
63	y0	101	CDL	OA5-CA3-CA4-CA6
63	f	401	CDL	OB5-CB3-CB4-CB6
63	M3	401	CDL	C72-C73-C74-C75
63	F	401	CDL	CB7-C71-C72-C73
62	m1	402	PC1	C2B-C2C-C2D-C2E
63	M3	401	CDL	C58-C59-C60-C61
62	7c	303	PC1	C31-C32-C33-C34
63	u	201	CDL	C74-C75-C76-C77
63	j	301	CDL	C16-C17-C18-C19
63	M1	402	CDL	C71-C72-C73-C74
63	M1	402	CDL	C51-C52-C53-C54
63	c3	604	CDL	CB5-C51-C52-C53
62	C3	602	PC1	C1-C2-C3-O31
62	c3	602	PC1	C1-C2-C3-O31
63	M1	402	CDL	CA3-CA4-CA6-OA8
63	m1	403	CDL	CA3-CA4-CA6-OA8
63	m3	401	CDL	CB3-CB4-CB6-OB8
63	b	501	CDL	CB3-CB4-CB6-OB8
62	n	302	PC1	C33-C34-C35-C36
63	m1	403	CDL	C71-C72-C73-C74
63	m1	403	CDL	C51-C52-C53-C54
62	C3	605	PC1	C21-C22-C23-C24
62	N	302	PC1	C33-C34-C35-C36
63	5B	702	CDL	OB5-CB3-CB4-OB6
63	M3	403	CDL	OB5-CB3-CB4-OB6
63	N	303	CDL	OB5-CB3-CB4-OB6
63	m1	403	CDL	OB5-CB3-CB4-OB6
63	m3	403	CDL	OB5-CB3-CB4-OB6
63	j	301	CDL	OB5-CB3-CB4-OB6
63	J	301	CDL	C16-C17-C18-C19
63	7c	301	CDL	C34-C35-C36-C37
62	7c	303	PC1	C11-C12-N-C15
63	7a	202	CDL	C32-C31-CA7-OA8
59	C1	701	HEA	C3B-C11-C12-C13
59	c1	701	HEA	C3B-C11-C12-C13
63	t	201	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
62	c3	605	PC1	C21-C22-C23-C24
63	v	201	CDL	C74-C75-C76-C77
63	Y5	201	CDL	C39-C40-C41-C42
63	m3	401	CDL	C52-C53-C54-C55
63	7C	301	CDL	C34-C35-C36-C37
63	y5	201	CDL	C39-C40-C41-C42
63	M1	401	CDL	CB4-CB3-OB5-PB2
63	F	401	CDL	CB4-CB3-OB5-PB2
63	T	202	CDL	CA4-CA3-OA5-PA1
63	7a	201	CDL	CB4-CB3-OB5-PB2
63	m1	401	CDL	CB4-CB3-OB5-PB2
63	t	202	CDL	CA4-CA3-OA5-PA1
62	N	301	PC1	C23-C24-C25-C26
63	V	201	CDL	C74-C75-C76-C77
62	v	202	PC1	C3E-C3F-C3G-C3H
63	V	201	CDL	C53-C54-C55-C56
63	m2	404	CDL	C34-C35-C36-C37
63	7A	202	CDL	OB5-CB3-CB4-CB6
63	M2	401	CDL	OB5-CB3-CB4-CB6
63	B	501	CDL	OB5-CB3-CB4-CB6
63	F	401	CDL	OB5-CB3-CB4-CB6
63	J	301	CDL	OB5-CB3-CB4-CB6
63	5b	702	CDL	OB5-CB3-CB4-CB6
63	y7	501	CDL	OB5-CB3-CB4-CB6
63	b	501	CDL	OB5-CB3-CB4-CB6
63	n	303	CDL	OA5-CA3-CA4-CA6
62	n	301	PC1	C23-C24-C25-C26
63	m3	403	CDL	O1-C1-CA2-OA2
63	v	201	CDL	C53-C54-C55-C56
63	T	201	CDL	C19-C20-C21-C22
63	m1	401	CDL	C74-C75-C76-C77
63	M3	401	CDL	C32-C33-C34-C35
63	M1	401	CDL	C74-C75-C76-C77
62	m1	402	PC1	C24-C25-C26-C27
63	M2	404	CDL	C34-C35-C36-C37
63	7A	201	CDL	CA5-C11-C12-C13
63	7a	201	CDL	CA5-C11-C12-C13
63	m2	404	CDL	CA7-C31-C32-C33
63	M3	401	CDL	C52-C53-C54-C55
63	7C	301	CDL	CA3-CA4-CA6-OA8
63	M1	402	CDL	CB3-CB4-CB6-OB8
63	M3	401	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
63	B	501	CDL	CB3-CB4-CB6-OB8
63	7c	301	CDL	CA3-CA4-CA6-OA8
63	N	303	CDL	C42-C43-C44-C45
63	n	303	CDL	C44-C45-C46-C47
63	N	303	CDL	C44-C45-C46-C47
63	n	303	CDL	C42-C43-C44-C45
62	7C	304	PC1	C11-C12-N-C15
63	C1	706	CDL	OB5-CB3-CB4-OB6
63	M2	403	CDL	OB5-CB3-CB4-OB6
63	F	401	CDL	OB5-CB3-CB4-OB6
63	J	301	CDL	OB5-CB3-CB4-OB6
63	5b	702	CDL	OA5-CA3-CA4-OA6
63	7a	202	CDL	OB5-CB3-CB4-OB6
63	m2	403	CDL	OB5-CB3-CB4-OB6
63	M3	403	CDL	O1-C1-CA2-OA2
63	5B	702	CDL	C1-CB2-OB2-PB2
63	7A	201	CDL	CB4-CB3-OB5-PB2
63	B	501	CDL	CB4-CB3-OB5-PB2
63	L	301	CDL	CA4-CA3-OA5-PA1
63	5b	702	CDL	C1-CB2-OB2-PB2
63	b	501	CDL	CB4-CB3-OB5-PB2
63	f	401	CDL	CB4-CB3-OB5-PB2
63	l	301	CDL	CA4-CA3-OA5-PA1
63	m3	401	CDL	C32-C33-C34-C35
63	7C	303	CDL	OA6-CA4-CA6-OA8
63	E	402	CDL	OA6-CA4-CA6-OA8
63	7c	301	CDL	OA6-CA4-CA6-OA8
63	7c	302	CDL	OA6-CA4-CA6-OA8
63	e	402	CDL	OA6-CA4-CA6-OA8
63	F	401	CDL	C80-C81-C82-C83
62	C1	705	PC1	C3B-C3C-C3D-C3E
62	M2	406	PC1	C11-C12-N-C14
62	c1	705	PC1	C3B-C3C-C3D-C3E
62	m1	402	PC1	C29-C2A-C2B-C2C
63	f	401	CDL	C80-C81-C82-C83
62	C3	601	PC1	O31-C31-C32-C33
62	m1	402	PC1	C3B-C3C-C3D-C3E
63	7c	301	CDL	CA2-C1-CB2-OB2
63	T	202	CDL	C56-C57-C58-C59
63	7A	202	CDL	C32-C31-CA7-OA8
62	7C	302	PC1	C24-C25-C26-C27
63	C1	706	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
63	5B	702	CDL	OA5-CA3-CA4-CA6
63	M2	403	CDL	OB5-CB3-CB4-CB6
63	Y7	501	CDL	OB5-CB3-CB4-CB6
63	5b	702	CDL	OA5-CA3-CA4-CA6
63	m2	401	CDL	OB5-CB3-CB4-CB6
63	m3	403	CDL	OB5-CB3-CB4-CB6
63	j	301	CDL	OB5-CB3-CB4-CB6
63	k	301	CDL	OB5-CB3-CB4-CB6
63	n	303	CDL	OB5-CB3-CB4-CB6
63	t	202	CDL	OB5-CB3-CB4-CB6
63	M2	403	CDL	C52-C53-C54-C55
63	n	303	CDL	CB7-C71-C72-C73
62	c1	705	PC1	C39-C3A-C3B-C3C
59	C1	701	HEA	C27-C19-C20-C21
62	7C	302	PC1	C29-C2A-C2B-C2C
63	y0	101	CDL	O1-C1-CA2-OA2
63	m1	403	CDL	CB7-C71-C72-C73
63	M1	401	CDL	C19-C20-C21-C22
63	t	202	CDL	C56-C57-C58-C59
63	m3	401	CDL	C20-C21-C22-C23
63	7A	202	CDL	OB5-CB3-CB4-OB6
63	7C	301	CDL	OB5-CB3-CB4-OB6
63	M1	402	CDL	OB5-CB3-CB4-OB6
63	M2	401	CDL	OB5-CB3-CB4-OB6
63	Y7	501	CDL	OB5-CB3-CB4-OB6
63	5b	703	CDL	OB5-CB3-CB4-OB6
63	m2	401	CDL	OB5-CB3-CB4-OB6
63	m3	403	CDL	OA5-CA3-CA4-OA6
63	b	501	CDL	OB5-CB3-CB4-OB6
63	f	401	CDL	OB5-CB3-CB4-OB6
63	n	303	CDL	OB5-CB3-CB4-OB6
63	E	402	CDL	CA3-CA4-CA6-OA8
63	e	402	CDL	CA3-CA4-CA6-OA8
62	C1	705	PC1	C39-C3A-C3B-C3C
63	7C	301	CDL	OA6-CA4-CA6-OA8
63	M1	402	CDL	OB6-CB4-CB6-OB8
63	b	501	CDL	OB6-CB4-CB6-OB8
63	l	301	CDL	OB6-CB4-CB6-OB8
63	m2	403	CDL	C52-C53-C54-C55
62	M2	406	PC1	C11-C12-N-C15
62	m2	402	PC1	C11-C12-N-C13
62	m2	402	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
62	m2	406	PC1	C11-C12-N-C14
62	m2	406	PC1	C11-C12-N-C15
62	m2	405	PC1	C32-C33-C34-C35
63	V	201	CDL	C51-C52-C53-C54
63	7C	301	CDL	CA5-C11-C12-C13
63	v	201	CDL	C51-C52-C53-C54
62	C3	603	PC1	O13-C11-C12-N
62	M2	402	PC1	O13-C11-C12-N
62	M2	405	PC1	O13-C11-C12-N
62	A	501	PC1	O13-C11-C12-N
62	A	502	PC1	O13-C11-C12-N
62	V	202	PC1	O13-C11-C12-N
62	c3	603	PC1	O13-C11-C12-N
62	m2	405	PC1	O13-C11-C12-N
62	a	501	PC1	O13-C11-C12-N
62	a	502	PC1	O13-C11-C12-N
62	v	202	PC1	O13-C11-C12-N
63	m1	401	CDL	C19-C20-C21-C22
62	7C	302	PC1	C3B-C3C-C3D-C3E
63	7c	301	CDL	CA5-C11-C12-C13
63	M3	401	CDL	C20-C21-C22-C23
63	U	201	CDL	C32-C33-C34-C35
63	7C	301	CDL	C53-C54-C55-C56
63	u	201	CDL	C53-C54-C55-C56
62	M1	404	PC1	O11-C1-C2-C3
63	7C	303	CDL	OA5-CA3-CA4-CA6
63	M1	402	CDL	OB5-CB3-CB4-CB6
63	M3	403	CDL	OA5-CA3-CA4-CA6
63	M3	403	CDL	OB5-CB3-CB4-CB6
63	N	303	CDL	OB5-CB3-CB4-CB6
63	T	202	CDL	OB5-CB3-CB4-CB6
63	7c	302	CDL	OA5-CA3-CA4-CA6
63	m1	403	CDL	OB5-CB3-CB4-CB6
63	m3	403	CDL	OA5-CA3-CA4-CA6
63	U	201	CDL	C53-C54-C55-C56
63	7c	301	CDL	C35-C36-C37-C38
63	7a	202	CDL	C21-C22-C23-C24
63	u	201	CDL	C32-C33-C34-C35
63	7C	301	CDL	C35-C36-C37-C38
63	7c	301	CDL	C53-C54-C55-C56
63	M2	404	CDL	C1-CA2-OA2-PA1
63	A	503	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
63	l	301	CDL	C1-CA2-OA2-PA1
63	m1	401	CDL	C61-C62-C63-C64
62	M1	404	PC1	O11-C1-C2-O21
62	m1	405	PC1	O11-C1-C2-O21
63	C1	706	CDL	OA5-CA3-CA4-OA6
63	5B	702	CDL	OA5-CA3-CA4-OA6
63	5B	703	CDL	OB5-CB3-CB4-OB6
63	5B	704	CDL	OB5-CB3-CB4-OB6
63	7C	303	CDL	OA5-CA3-CA4-OA6
63	M3	403	CDL	OA5-CA3-CA4-OA6
63	B	501	CDL	OB5-CB3-CB4-OB6
63	N	303	CDL	OA5-CA3-CA4-OA6
63	T	202	CDL	OB5-CB3-CB4-OB6
63	c1	706	CDL	OA5-CA3-CA4-OA6
63	c1	706	CDL	OB5-CB3-CB4-OB6
63	7c	302	CDL	OA5-CA3-CA4-OA6
63	y7	501	CDL	OB5-CB3-CB4-OB6
63	y0	101	CDL	OA5-CA3-CA4-OA6
63	k	301	CDL	OB5-CB3-CB4-OB6
63	n	303	CDL	OA5-CA3-CA4-OA6
63	t	202	CDL	OB5-CB3-CB4-OB6
63	M3	401	CDL	C23-C24-C25-C26
62	7c	303	PC1	C11-C12-N-C14
62	m1	405	PC1	C11-C12-N-C13
63	M3	403	CDL	CA5-C11-C12-C13
63	M1	402	CDL	OA6-CA4-CA6-OA8
63	M3	401	CDL	OB6-CB4-CB6-OB8
63	B	501	CDL	OB6-CB4-CB6-OB8
63	L	301	CDL	OB6-CB4-CB6-OB8
63	m3	401	CDL	OB6-CB4-CB6-OB8
63	M3	403	CDL	C74-C75-C76-C77
63	M3	403	CDL	CB2-C1-CA2-OA2
63	m3	403	CDL	CB2-C1-CA2-OA2
63	M2	404	CDL	CB3-CB4-CB6-OB8
63	m1	403	CDL	CB3-CB4-CB6-OB8
63	m2	404	CDL	CB3-CB4-CB6-OB8
63	M3	403	CDL	C71-C72-C73-C74
63	m3	403	CDL	C74-C75-C76-C77
62	C1	705	PC1	C26-C27-C28-C29
62	M2	405	PC1	C32-C33-C34-C35
63	u	201	CDL	C55-C56-C57-C58
63	7A	202	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
63	F	401	CDL	C36-C37-C38-C39
63	U	201	CDL	C55-C56-C57-C58
62	C1	705	PC1	C11-O13-P-O14
62	C1	705	PC1	C11-O13-P-O11
62	C1	705	PC1	C11-C12-N-C14
62	C3	601	PC1	C1-O11-P-O12
62	C3	602	PC1	C1-O11-P-O14
62	C3	602	PC1	C1-O11-P-O13
62	C3	603	PC1	C11-O13-P-O14
62	C3	603	PC1	C11-O13-P-O11
62	C3	603	PC1	C1-O11-P-O12
62	C3	603	PC1	C1-O11-P-O14
62	C3	603	PC1	C1-O11-P-O13
62	7C	302	PC1	C11-O13-P-O12
62	7C	304	PC1	C1-O11-P-O13
62	7C	304	PC1	C11-C12-N-C14
62	M1	404	PC1	C11-O13-P-O14
62	M2	402	PC1	C11-C12-N-C15
62	M2	405	PC1	C11-O13-P-O14
62	M2	405	PC1	C11-O13-P-O11
62	A	502	PC1	C11-O13-P-O14
62	A	502	PC1	C1-O11-P-O14
62	N	301	PC1	C11-O13-P-O12
62	N	301	PC1	C11-O13-P-O11
62	N	301	PC1	C1-O11-P-O13
62	V	202	PC1	C1-O11-P-O12
62	c1	705	PC1	C11-O13-P-O14
62	c3	601	PC1	C1-O11-P-O12
62	c3	602	PC1	C1-O11-P-O14
62	c3	603	PC1	C11-O13-P-O14
62	c3	603	PC1	C1-O11-P-O12
62	c3	603	PC1	C1-O11-P-O14
62	c3	603	PC1	C1-O11-P-O13
62	a	501	PC1	C1-O11-P-O13
62	a	502	PC1	C11-O13-P-O14
62	a	502	PC1	C1-O11-P-O14
62	n	301	PC1	C11-O13-P-O12
62	n	301	PC1	C11-O13-P-O11
62	n	301	PC1	C1-O11-P-O13
62	v	202	PC1	C11-O13-P-O14
62	v	202	PC1	C11-O13-P-O11
63	C1	706	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
63	C1	706	CDL	CB3-OB5-PB2-OB4
63	C1	707	CDL	CA2-OA2-PA1-OA5
63	5B	702	CDL	CB2-OB2-PB2-OB3
63	5B	702	CDL	CB3-OB5-PB2-OB2
63	5B	702	CDL	CB3-OB5-PB2-OB3
63	5B	702	CDL	CB3-OB5-PB2-OB4
63	5B	703	CDL	CA2-OA2-PA1-OA4
63	5B	703	CDL	CA3-OA5-PA1-OA2
63	5B	703	CDL	CA3-OA5-PA1-OA3
63	5B	703	CDL	CB3-OB5-PB2-OB3
63	5B	704	CDL	CA3-OA5-PA1-OA3
63	7A	202	CDL	CA3-OA5-PA1-OA2
63	7A	202	CDL	CB2-OB2-PB2-OB4
63	7A	202	CDL	CB3-OB5-PB2-OB3
63	7C	301	CDL	CB2-OB2-PB2-OB3
63	7C	301	CDL	CB2-OB2-PB2-OB5
63	7C	303	CDL	CB2-OB2-PB2-OB4
63	M1	401	CDL	CA2-OA2-PA1-OA3
63	M1	401	CDL	CA2-OA2-PA1-OA5
63	M1	401	CDL	CB2-OB2-PB2-OB3
63	M1	401	CDL	CB2-OB2-PB2-OB5
63	M1	403	CDL	CA2-OA2-PA1-OA5
63	M1	403	CDL	CB2-OB2-PB2-OB3
63	M1	403	CDL	CB2-OB2-PB2-OB5
63	M2	401	CDL	CA2-OA2-PA1-OA4
63	M2	401	CDL	CA2-OA2-PA1-OA5
63	M2	401	CDL	CA3-OA5-PA1-OA2
63	M2	401	CDL	CA3-OA5-PA1-OA3
63	M2	401	CDL	CB2-OB2-PB2-OB3
63	M2	401	CDL	CB3-OB5-PB2-OB2
63	M2	401	CDL	CB3-OB5-PB2-OB4
63	M2	403	CDL	CA3-OA5-PA1-OA3
63	M2	403	CDL	CB2-OB2-PB2-OB3
63	M2	404	CDL	CA2-OA2-PA1-OA4
63	M3	401	CDL	CB3-OB5-PB2-OB4
63	M3	402	CDL	CA2-OA2-PA1-OA3
63	M3	402	CDL	CA3-OA5-PA1-OA2
63	M3	402	CDL	CA3-OA5-PA1-OA3
63	M3	402	CDL	CB3-OB5-PB2-OB3
63	M3	403	CDL	CA2-OA2-PA1-OA3
63	M3	403	CDL	CA3-OA5-PA1-OA3
63	Y7	501	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
63	Y0	101	CDL	CA3-OA5-PA1-OA2
63	Y0	101	CDL	CB2-OB2-PB2-OB5
63	Y0	101	CDL	CB3-OB5-PB2-OB4
63	Y5	201	CDL	CA3-OA5-PA1-OA2
63	Y5	201	CDL	CA3-OA5-PA1-OA3
63	Y5	201	CDL	CB2-OB2-PB2-OB3
63	Y5	201	CDL	CB2-OB2-PB2-OB5
63	Y5	201	CDL	CB3-OB5-PB2-OB2
63	A	503	CDL	CB3-OB5-PB2-OB4
63	E	401	CDL	CA2-OA2-PA1-OA4
63	E	401	CDL	CB3-OB5-PB2-OB4
63	F	401	CDL	CA3-OA5-PA1-OA4
63	J	301	CDL	CA2-OA2-PA1-OA4
63	J	301	CDL	CA2-OA2-PA1-OA5
63	J	301	CDL	CB2-OB2-PB2-OB3
63	L	301	CDL	CA2-OA2-PA1-OA4
63	L	301	CDL	CB2-OB2-PB2-OB3
63	T	201	CDL	CA2-OA2-PA1-OA3
63	T	201	CDL	CB2-OB2-PB2-OB4
63	U	201	CDL	CB2-OB2-PB2-OB3
63	U	201	CDL	CB2-OB2-PB2-OB4
63	U	201	CDL	CB2-OB2-PB2-OB5
63	U	201	CDL	CB3-OB5-PB2-OB3
63	V	201	CDL	CB3-OB5-PB2-OB4
63	c1	706	CDL	CA3-OA5-PA1-OA3
63	c1	706	CDL	CB2-OB2-PB2-OB4
63	c1	706	CDL	CB3-OB5-PB2-OB4
63	c1	707	CDL	CA2-OA2-PA1-OA5
63	5b	702	CDL	CB3-OB5-PB2-OB3
63	5b	703	CDL	CA3-OA5-PA1-OA3
63	5b	703	CDL	CB2-OB2-PB2-OB5
63	7a	201	CDL	CB3-OB5-PB2-OB3
63	7a	202	CDL	CA3-OA5-PA1-OA2
63	7a	202	CDL	CA3-OA5-PA1-OA4
63	7a	202	CDL	CB2-OB2-PB2-OB4
63	7a	202	CDL	CB3-OB5-PB2-OB3
63	7c	301	CDL	CB3-OB5-PB2-OB3
63	7c	302	CDL	CB2-OB2-PB2-OB5
63	m1	401	CDL	CA2-OA2-PA1-OA3
63	m1	401	CDL	CA2-OA2-PA1-OA5
63	m1	401	CDL	CB2-OB2-PB2-OB3
63	m1	404	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
63	m1	404	CDL	CB2-OB2-PB2-OB3
63	m1	404	CDL	CB2-OB2-PB2-OB5
63	m1	404	CDL	CB3-OB5-PB2-OB3
63	m2	401	CDL	CA2-OA2-PA1-OA4
63	m2	401	CDL	CA3-OA5-PA1-OA2
63	m2	401	CDL	CA3-OA5-PA1-OA3
63	m2	401	CDL	CB2-OB2-PB2-OB3
63	m2	403	CDL	CA3-OA5-PA1-OA3
63	m2	403	CDL	CB2-OB2-PB2-OB3
63	m2	403	CDL	CB3-OB5-PB2-OB2
63	m2	404	CDL	CA2-OA2-PA1-OA4
63	m3	402	CDL	CA2-OA2-PA1-OA3
63	m3	402	CDL	CB3-OB5-PB2-OB3
63	m3	403	CDL	CA2-OA2-PA1-OA3
63	m3	403	CDL	CA3-OA5-PA1-OA3
63	y7	501	CDL	CB2-OB2-PB2-OB3
63	y0	101	CDL	CA2-OA2-PA1-OA3
63	y0	101	CDL	CA3-OA5-PA1-OA2
63	y0	101	CDL	CA3-OA5-PA1-OA4
63	y0	101	CDL	CB2-OB2-PB2-OB5
63	y0	101	CDL	CB3-OB5-PB2-OB4
63	y5	201	CDL	CA3-OA5-PA1-OA2
63	y5	201	CDL	CA3-OA5-PA1-OA3
63	y5	201	CDL	CB2-OB2-PB2-OB3
63	a	503	CDL	CA2-OA2-PA1-OA5
63	a	503	CDL	CB2-OB2-PB2-OB5
63	a	503	CDL	CB3-OB5-PB2-OB2
63	a	503	CDL	CB3-OB5-PB2-OB4
63	e	401	CDL	CA2-OA2-PA1-OA4
63	e	401	CDL	CB3-OB5-PB2-OB4
63	e	402	CDL	CB3-OB5-PB2-OB2
63	j	301	CDL	CA2-OA2-PA1-OA3
63	j	301	CDL	CA2-OA2-PA1-OA4
63	j	301	CDL	CA2-OA2-PA1-OA5
63	j	301	CDL	CB2-OB2-PB2-OB3
63	k	301	CDL	CA2-OA2-PA1-OA4
63	k	301	CDL	CA3-OA5-PA1-OA2
63	k	301	CDL	CA3-OA5-PA1-OA3
63	k	301	CDL	CB3-OB5-PB2-OB3
63	l	301	CDL	CA2-OA2-PA1-OA4
63	l	301	CDL	CB2-OB2-PB2-OB3
63	t	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
63	t	201	CDL	CB2-OB2-PB2-OB5
63	v	201	CDL	CB3-OB5-PB2-OB4
63	m3	401	CDL	C23-C24-C25-C26
63	M1	401	CDL	C61-C62-C63-C64
62	M2	405	PC1	C2-C1-O11-P
63	M2	401	CDL	CB4-CB3-OB5-PB2
63	M2	404	CDL	CA4-CA3-OA5-PA1
63	M2	404	CDL	CB4-CB3-OB5-PB2
63	M3	403	CDL	C1-CB2-OB2-PB2
63	Y7	501	CDL	CB4-CB3-OB5-PB2
63	B	501	CDL	C1-CA2-OA2-PA1
63	E	401	CDL	CA4-CA3-OA5-PA1
63	E	401	CDL	C1-CB2-OB2-PB2
63	J	301	CDL	C1-CA2-OA2-PA1
63	L	301	CDL	C1-CA2-OA2-PA1
63	L	301	CDL	CB4-CB3-OB5-PB2
63	N	303	CDL	CA4-CA3-OA5-PA1
63	7c	302	CDL	C1-CA2-OA2-PA1
63	m2	401	CDL	CB4-CB3-OB5-PB2
63	m2	404	CDL	C1-CA2-OA2-PA1
63	m2	404	CDL	CA4-CA3-OA5-PA1
63	m2	404	CDL	CB4-CB3-OB5-PB2
63	m3	403	CDL	C1-CB2-OB2-PB2
63	y7	501	CDL	CB4-CB3-OB5-PB2
63	a	503	CDL	CA4-CA3-OA5-PA1
63	e	401	CDL	C1-CA2-OA2-PA1
63	e	401	CDL	CA4-CA3-OA5-PA1
63	e	401	CDL	C1-CB2-OB2-PB2
63	j	301	CDL	C1-CA2-OA2-PA1
63	l	301	CDL	CB4-CB3-OB5-PB2
63	n	303	CDL	CA4-CA3-OA5-PA1
63	m3	403	CDL	CA5-C11-C12-C13
62	c1	705	PC1	C2A-C2B-C2C-C2D
63	m1	401	CDL	C18-C19-C20-C21
63	M1	401	CDL	C18-C19-C20-C21
63	y7	501	CDL	CA6-CA4-OA6-CA5
63	M1	401	CDL	C72-C71-CB7-OB8
62	C1	705	PC1	C2A-C2B-C2C-C2D
63	L	301	CDL	C12-C13-C14-C15
63	m3	403	CDL	C71-C72-C73-C74
62	7C	304	PC1	C2A-C2B-C2C-C2D
62	M2	406	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
62	m1	405	PC1	C11-C12-N-C14
62	A	501	PC1	O11-C1-C2-C3
62	a	501	PC1	O11-C1-C2-C3
63	e	402	CDL	OB5-CB3-CB4-CB6
62	7c	303	PC1	C2A-C2B-C2C-C2D
63	N	303	CDL	CB7-C71-C72-C73
63	5b	703	CDL	CA7-C31-C32-C33
63	C1	707	CDL	OB5-CB3-CB4-OB6
63	Y0	101	CDL	OA5-CA3-CA4-OA6
63	c1	707	CDL	OB5-CB3-CB4-OB6
63	M1	401	CDL	C52-C51-CB5-OB6
63	B	501	CDL	C51-C52-C53-C54
63	5b	702	CDL	C35-C36-C37-C38
63	7C	303	CDL	C1-CA2-OA2-PA1
63	M1	403	CDL	CB4-CB3-OB5-PB2
63	m3	402	CDL	C1-CA2-OA2-PA1
63	b	501	CDL	C1-CA2-OA2-PA1
63	5B	702	CDL	C35-C36-C37-C38
63	v	201	CDL	C16-C17-C18-C19
63	m1	403	CDL	OA6-CA4-CA6-OA8
63	m1	403	CDL	OB6-CB4-CB6-OB8
62	c3	601	PC1	O31-C31-C32-C33
63	m1	401	CDL	C52-C51-CB5-OB6
62	c1	705	PC1	C26-C27-C28-C29
63	m3	403	CDL	C73-C74-C75-C76
62	N	301	PC1	C21-C22-C23-C24
63	F	401	CDL	C52-C53-C54-C55
63	M3	403	CDL	C73-C74-C75-C76
63	y0	101	CDL	C52-C51-CB5-OB6
63	L	301	CDL	CB3-CB4-CB6-OB8
63	l	301	CDL	CB3-CB4-CB6-OB8
63	5B	704	CDL	C72-C71-CB7-OB8
63	f	401	CDL	C36-C37-C38-C39
63	c1	706	CDL	CA7-C31-C32-C33
62	C3	601	PC1	C39-C3A-C3B-C3C
63	e	402	CDL	C53-C54-C55-C56
63	5B	704	CDL	CA7-C31-C32-C33
63	7c	301	CDL	C82-C83-C84-C85
63	7C	301	CDL	CA2-C1-CB2-OB2
63	E	401	CDL	C1-CA2-OA2-PA1
63	5B	702	CDL	CA7-C31-C32-C33
63	M2	404	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
63	f	401	CDL	C52-C53-C54-C55
63	m1	401	CDL	C51-C52-C53-C54
62	C3	605	PC1	C35-C36-C37-C38
62	c3	601	PC1	C38-C39-C3A-C3B
63	V	201	CDL	C16-C17-C18-C19
63	C1	706	CDL	CA7-C31-C32-C33
63	Y0	101	CDL	C72-C71-CB7-OB8
63	E	402	CDL	C53-C54-C55-C56
63	m1	403	CDL	C11-C12-C13-C14
62	M2	402	PC1	C11-C12-N-C13
62	m2	402	PC1	C11-C12-N-C14
62	m2	406	PC1	C11-C12-N-C13
63	C1	706	CDL	C52-C51-CB5-OB6
63	7a	202	CDL	C32-C31-CA7-OA9
63	l	301	CDL	C12-C13-C14-C15
63	A	503	CDL	OB6-CB4-CB6-OB8
63	5b	703	CDL	C71-C72-C73-C74
63	m3	401	CDL	C53-C54-C55-C56
63	m1	403	CDL	C31-C32-C33-C34
63	b	501	CDL	C51-C52-C53-C54
62	m2	405	PC1	C2-C1-O11-P
63	7C	303	CDL	CB4-CB3-OB5-PB2
63	7c	302	CDL	CB4-CB3-OB5-PB2
63	Y0	101	CDL	C52-C51-CB5-OB6
63	y0	101	CDL	C72-C71-CB7-OB8
63	M1	402	CDL	C31-C32-C33-C34
62	m2	406	PC1	C2E-C2F-C2G-C2H
63	l	301	CDL	C22-C23-C24-C25
63	A	503	CDL	CB3-CB4-CB6-OB8
63	M3	401	CDL	C36-C37-C38-C39
62	C3	601	PC1	C38-C39-C3A-C3B
62	c3	601	PC1	C39-C3A-C3B-C3C
63	7a	202	CDL	C40-C41-C42-C43
62	C3	601	PC1	C1-C2-O21-C21
62	C3	605	PC1	C1-C2-O21-C21
62	A	502	PC1	C3-C2-O21-C21
62	c3	601	PC1	C1-C2-O21-C21
62	c3	605	PC1	C1-C2-O21-C21
62	a	502	PC1	C3-C2-O21-C21
63	7A	201	CDL	CA6-CA4-OA6-CA5
63	7C	301	CDL	CB6-CB4-OB6-CB5
63	Y7	501	CDL	CA6-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
63	A	503	CDL	CA3-CA4-OA6-CA5
63	N	303	CDL	CA6-CA4-OA6-CA5
63	7a	201	CDL	CA6-CA4-OA6-CA5
63	a	503	CDL	CA3-CA4-OA6-CA5
63	n	303	CDL	CA6-CA4-OA6-CA5
63	t	201	CDL	CA6-CA4-OA6-CA5
63	M3	401	CDL	C53-C54-C55-C56
63	m1	401	CDL	C72-C71-CB7-OB8
63	5B	703	CDL	C75-C76-C77-C78
63	M1	402	CDL	CB7-C71-C72-C73
63	L	301	CDL	C14-C15-C16-C17
63	u	201	CDL	C11-C12-C13-C14
63	7c	301	CDL	OB5-CB3-CB4-OB6
63	M1	402	CDL	C11-C12-C13-C14
63	V	201	CDL	O1-C1-CA2-OA2
63	v	201	CDL	O1-C1-CA2-OA2
63	M1	401	CDL	C51-C52-C53-C54
62	m2	406	PC1	C2-C1-O11-P
63	M3	403	CDL	C1-CA2-OA2-PA1
63	m1	404	CDL	CB4-CB3-OB5-PB2
62	m1	405	PC1	O11-C1-C2-C3
63	U	201	CDL	OB5-CB3-CB4-CB6
63	U	201	CDL	C11-C12-C13-C14
63	M1	402	CDL	C13-C14-C15-C16
63	7c	301	CDL	C39-C40-C41-C42
63	m2	401	CDL	OA6-CA4-CA6-OA8
63	a	503	CDL	OB6-CB4-CB6-OB8
62	M2	405	PC1	C24-C25-C26-C27
63	L	301	CDL	C22-C23-C24-C25
59	C1	702	HEA	CAD-CBD-CGD-O1D
63	5B	704	CDL	C74-C75-C76-C77
62	M1	404	PC1	C11-C12-N-C13
62	m1	405	PC1	C11-C12-N-C15
62	a	501	PC1	C11-C12-N-C15
63	7A	202	CDL	C40-C41-C42-C43
63	m1	403	CDL	C13-C14-C15-C16
59	c1	702	HEA	CAD-CBD-CGD-O1D
62	C3	605	PC1	O31-C31-C32-C33
63	c1	706	CDL	C52-C51-CB5-OB6
63	m3	401	CDL	C51-C52-C53-C54
62	C1	705	PC1	C28-C29-C2A-C2B
62	M2	406	PC1	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
62	m1	402	PC1	C39-C3A-C3B-C3C
62	m2	405	PC1	C24-C25-C26-C27
59	C1	701	HEA	CAD-CBD-CGD-O2D
59	c1	701	HEA	CAD-CBD-CGD-O2D
63	c3	604	CDL	C52-C53-C54-C55
62	m2	405	PC1	C22-C23-C24-C25
63	5b	703	CDL	C74-C75-C76-C77
62	M2	406	PC1	C2-C1-O11-P
63	c3	604	CDL	CB4-CB3-OB5-PB2
63	m3	403	CDL	C1-CA2-OA2-PA1
63	t	201	CDL	CA4-CA3-OA5-PA1
62	M2	405	PC1	C22-C23-C24-C25
63	k	301	CDL	C75-C76-C77-C78
63	m3	403	CDL	C16-C17-C18-C19
62	C1	705	PC1	C11-C12-N-C13
63	f	401	CDL	C38-C39-C40-C41
63	M3	401	CDL	C77-C78-C79-C80
63	m3	402	CDL	C53-C54-C55-C56
63	C1	706	CDL	CA3-CA4-CA6-OA8
63	m2	401	CDL	CA3-CA4-CA6-OA8
63	a	503	CDL	CB3-CB4-CB6-OB8
63	t	202	CDL	CB3-CB4-CB6-OB8
63	N	303	CDL	C73-C74-C75-C76
63	l	301	CDL	C14-C15-C16-C17
63	M1	401	CDL	C12-C11-CA5-OA6
62	c3	605	PC1	C36-C37-C38-C39
62	m1	402	PC1	C2A-C2B-C2C-C2D
63	E	401	CDL	OB5-CB3-CB4-OB6
63	U	201	CDL	OB5-CB3-CB4-OB6
63	7C	301	CDL	C82-C83-C84-C85
63	C1	707	CDL	CB7-C71-C72-C73
63	c1	707	CDL	CB7-C71-C72-C73
62	A	501	PC1	C36-C37-C38-C39
62	c3	605	PC1	O31-C31-C32-C33
63	7A	201	CDL	C72-C71-CB7-OB8
63	m1	401	CDL	C12-C11-CA5-OA6
62	c1	705	PC1	C28-C29-C2A-C2B
63	m1	403	CDL	C32-C31-CA7-OA8
63	5B	702	CDL	OB5-CB3-CB4-CB6
63	E	401	CDL	OB5-CB3-CB4-CB6
62	c3	605	PC1	C35-C36-C37-C38
63	5B	702	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
63	u	201	CDL	C62-C63-C64-C65
63	C3	604	CDL	CB4-CB3-OB5-PB2
63	5B	703	CDL	C1-CA2-OA2-PA1
63	M3	402	CDL	C1-CA2-OA2-PA1
63	T	201	CDL	CA4-CA3-OA5-PA1
63	k	301	CDL	CB4-CB3-OB5-PB2
63	M3	402	CDL	C53-C54-C55-C56
63	m3	401	CDL	C36-C37-C38-C39
62	a	501	PC1	C36-C37-C38-C39
62	C3	603	PC1	O21-C21-C22-C23
63	M3	403	CDL	C16-C17-C18-C19
62	c3	603	PC1	O21-C21-C22-C23
62	n	301	PC1	C21-C22-C23-C24
62	C1	705	PC1	C11-C12-N-C15
63	M3	401	CDL	C51-C52-C53-C54
62	n	302	PC1	O31-C31-C32-C33
63	5b	703	CDL	C72-C71-CB7-OB8
63	7a	201	CDL	C72-C71-CB7-OB8
63	7a	202	CDL	C72-C71-CB7-OB8
63	m3	402	CDL	C32-C31-CA7-OA8
63	7a	202	CDL	C41-C42-C43-C44
63	M1	401	CDL	CB3-CB4-OB6-CB5
63	M2	401	CDL	CB3-CB4-OB6-CB5
63	M2	404	CDL	CB3-CB4-OB6-CB5
63	E	402	CDL	CB3-CB4-OB6-CB5
63	T	201	CDL	CA6-CA4-OA6-CA5
63	T	202	CDL	CA6-CA4-OA6-CA5
63	7c	301	CDL	CB6-CB4-OB6-CB5
63	m2	401	CDL	CB3-CB4-OB6-CB5
63	m2	404	CDL	CB3-CB4-OB6-CB5
63	e	402	CDL	CB3-CB4-OB6-CB5
63	t	202	CDL	CA6-CA4-OA6-CA5
63	n	303	CDL	C73-C74-C75-C76
62	7C	302	PC1	C39-C3A-C3B-C3C
63	f	401	CDL	C77-C78-C79-C80
62	7C	302	PC1	C2A-C2B-C2C-C2D
63	5b	702	CDL	C56-C57-C58-C59
59	c1	702	HEA	C4D-C3D-CAD-CBD
63	5B	703	CDL	CB4-CB3-OB5-PB2
63	k	301	CDL	C1-CA2-OA2-PA1
63	7c	301	CDL	CB2-C1-CA2-OA2
59	C1	702	HEA	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
63	7C	303	CDL	CA3-CA4-CA6-OA8
63	7c	302	CDL	CA3-CA4-CA6-OA8
63	M3	401	CDL	C71-C72-C73-C74
62	A	502	PC1	O31-C31-C32-C33
63	c1	706	CDL	C32-C31-CA7-OA8
62	c3	605	PC1	C24-C25-C26-C27
63	f	401	CDL	C34-C35-C36-C37
63	7A	202	CDL	C39-C40-C41-C42
62	A	502	PC1	O21-C2-C3-O31
63	L	301	CDL	C23-C24-C25-C26
62	a	502	PC1	O31-C31-C32-C33
63	M1	402	CDL	C12-C11-CA5-OA6
63	J	301	CDL	C32-C31-CA7-OA8
63	7A	202	CDL	C32-C31-CA7-OA9
63	M1	401	CDL	C78-C79-C80-C81
62	M2	402	PC1	C11-C12-N-C14
62	C3	601	PC1	O32-C31-C32-C33
63	C1	706	CDL	C32-C31-CA7-OA8
63	7a	201	CDL	C32-C31-CA7-OA8
63	T	201	CDL	C24-C25-C26-C27
63	t	201	CDL	C24-C25-C26-C27
59	C1	702	HEA	C2C-C3C-CAC-CBC
59	c1	702	HEA	C2C-C3C-CAC-CBC
63	5b	703	CDL	C83-C84-C85-C86
63	M1	402	CDL	C32-C31-CA7-OA8
63	M2	403	CDL	C72-C71-CB7-OB8
62	7c	303	PC1	C26-C27-C28-C29
63	C3	604	CDL	C1-CB2-OB2-PB2
62	c3	601	PC1	C3A-C3B-C3C-C3D
63	F	401	CDL	C38-C39-C40-C41
59	c1	701	HEA	C19-C20-C21-C22
59	C1	702	HEA	CAA-CBA-CGA-O2A
63	L	301	CDL	C13-C14-C15-C16
62	c1	705	PC1	O13-C11-C12-N
63	m1	401	CDL	C56-C57-C58-C59
62	A	501	PC1	O31-C31-C32-C33
62	N	302	PC1	O31-C31-C32-C33
63	E	402	CDL	C72-C71-CB7-OB8
63	j	301	CDL	C32-C31-CA7-OA8
62	7C	304	PC1	C2D-C2E-C2F-C2G
59	c1	702	HEA	CAA-CBA-CGA-O2A
63	C3	604	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
63	m1	403	CDL	C12-C11-CA5-OA6
63	5b	702	CDL	C58-C59-C60-C61
63	l	301	CDL	C13-C14-C15-C16
62	M1	404	PC1	C11-C12-N-C14
63	F	401	CDL	C77-C78-C79-C80
63	c1	707	CDL	C52-C53-C54-C55
63	m2	404	CDL	C33-C34-C35-C36
62	N	301	PC1	O21-C21-C22-C23
62	a	501	PC1	O31-C31-C32-C33
62	n	301	PC1	O21-C21-C22-C23
63	c3	604	CDL	C12-C11-CA5-OA6
63	e	402	CDL	C72-C71-CB7-OB8
63	l	301	CDL	C12-C11-CA5-OA6
63	C1	707	CDL	C52-C53-C54-C55
63	Y5	201	CDL	CB7-C71-C72-C73
63	M2	404	CDL	C52-C51-CB5-OB6
63	M1	401	CDL	C57-C58-C59-C60
63	l	301	CDL	C23-C24-C25-C26
63	7a	202	CDL	C39-C40-C41-C42
63	E	401	CDL	C16-C17-C18-C19
63	7A	201	CDL	C32-C31-CA7-OA8
63	L	301	CDL	C12-C11-CA5-OA6
63	m2	403	CDL	C72-C71-CB7-OB8
63	y0	101	CDL	C12-C11-CA5-OA6
63	t	202	CDL	C12-C11-CA5-OA6
63	5B	704	CDL	C82-C83-C84-C85
63	F	401	CDL	C34-C35-C36-C37
59	C1	701	HEA	C19-C20-C21-C22
63	M2	403	CDL	CA3-CA4-CA6-OA8
63	Y7	501	CDL	CB3-CB4-CB6-OB8
63	c1	706	CDL	CA3-CA4-CA6-OA8
63	m2	403	CDL	CA3-CA4-CA6-OA8
63	y7	501	CDL	CB3-CB4-CB6-OB8
59	C1	702	HEA	C4C-C3C-CAC-CBC
62	a	501	PC1	C11-C12-N-C13
62	7C	302	PC1	O21-C21-C22-C23
63	T	202	CDL	C12-C11-CA5-OA6
63	m2	404	CDL	C52-C51-CB5-OB6
63	C1	706	CDL	C33-C34-C35-C36
62	j	302	PC1	O21-C2-C3-O31
63	V	201	CDL	OB6-CB4-CB6-OB8
63	v	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
63	7a	202	CDL	C60-C61-C62-C63
62	C3	603	PC1	O31-C31-C32-C33
63	5B	702	CDL	C58-C59-C60-C61
63	k	301	CDL	C77-C78-C79-C80
63	M2	404	CDL	CA5-C11-C12-C13
63	C1	707	CDL	OB5-CB3-CB4-CB6
63	c1	707	CDL	OB5-CB3-CB4-CB6
59	C1	702	HEA	CAD-CBD-CGD-O2D
62	C3	605	PC1	C24-C25-C26-C27
63	m3	401	CDL	C34-C35-C36-C37
62	a	501	PC1	C2A-C2B-C2C-C2D
63	M2	403	CDL	CB7-C71-C72-C73
63	7A	202	CDL	C60-C61-C62-C63
63	7C	301	CDL	C39-C40-C41-C42
63	Y0	101	CDL	C15-C16-C17-C18
62	A	502	PC1	C1-C2-O21-C21
62	a	502	PC1	C1-C2-O21-C21
63	7A	201	CDL	CA3-CA4-OA6-CA5
63	M1	401	CDL	CB6-CB4-OB6-CB5
63	M2	401	CDL	CB6-CB4-OB6-CB5
63	E	401	CDL	CA3-CA4-OA6-CA5
63	E	401	CDL	CA6-CA4-OA6-CA5
63	E	402	CDL	CB6-CB4-OB6-CB5
63	T	202	CDL	CA3-CA4-OA6-CA5
63	7a	201	CDL	CA3-CA4-OA6-CA5
63	7c	301	CDL	CB3-CB4-OB6-CB5
63	m1	401	CDL	CB3-CB4-OB6-CB5
63	m1	401	CDL	CB6-CB4-OB6-CB5
63	m2	401	CDL	CB6-CB4-OB6-CB5
63	e	401	CDL	CA3-CA4-OA6-CA5
63	e	401	CDL	CA6-CA4-OA6-CA5
63	e	402	CDL	CB6-CB4-OB6-CB5
63	t	202	CDL	CA3-CA4-OA6-CA5
63	7c	302	CDL	C51-C52-C53-C54
63	M1	401	CDL	C56-C57-C58-C59
59	c1	702	HEA	CAD-CBD-CGD-O2D
63	y5	201	CDL	C72-C71-CB7-OB8
62	C3	605	PC1	C36-C37-C38-C39
63	7C	303	CDL	C51-C52-C53-C54
63	F	401	CDL	C72-C73-C74-C75
63	b	501	CDL	C15-C16-C17-C18
63	T	201	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
62	c3	603	PC1	O31-C31-C32-C33
63	7A	202	CDL	C72-C71-CB7-OB8
63	c1	707	CDL	C32-C31-CA7-OA8
63	c1	706	CDL	C33-C34-C35-C36
63	M2	403	CDL	C1-CB2-OB2-PB2
63	Y0	101	CDL	CB4-CB3-OB5-PB2
63	E	402	CDL	CA4-CA3-OA5-PA1
62	a	501	PC1	O32-C31-C32-C33
63	J	301	CDL	C32-C31-CA7-OA9
63	j	301	CDL	C32-C31-CA7-OA9
63	C1	707	CDL	C32-C31-CA7-OA8
59	C1	702	HEA	C4D-C3D-CAD-CBD
63	7a	201	CDL	C32-C31-CA7-OA9
63	e	401	CDL	C16-C17-C18-C19
63	m1	401	CDL	C57-C58-C59-C60
63	M3	402	CDL	C32-C31-CA7-OA8
63	Y0	101	CDL	C12-C11-CA5-OA6
63	E	402	CDL	C72-C71-CB7-OB9
63	c3	604	CDL	C12-C11-CA5-OA7
63	m1	403	CDL	C12-C11-CA5-OA7
62	M1	404	PC1	C11-C12-N-C15
62	N	301	PC1	O22-C21-C22-C23
63	M2	404	CDL	C52-C51-CB5-OB7
63	t	202	CDL	C12-C11-CA5-OA7
63	Y7	501	CDL	C71-C72-C73-C74
63	M1	402	CDL	C12-C11-CA5-OA7
63	M2	404	CDL	C33-C34-C35-C36
63	y5	201	CDL	CB7-C71-C72-C73
62	a	502	PC1	O32-C31-C32-C33
63	C1	706	CDL	C32-C31-CA7-OA9
63	5B	703	CDL	C77-C78-C79-C80
62	C3	602	PC1	C28-C29-C2A-C2B
62	A	501	PC1	C2A-C2B-C2C-C2D
59	c1	702	HEA	C2D-C3D-CAD-CBD
63	m2	403	CDL	OA6-CA4-CA6-OA8
63	B	501	CDL	C15-C16-C17-C18
63	5b	702	CDL	C31-C32-C33-C34
62	A	502	PC1	O32-C31-C32-C33
63	C3	604	CDL	C12-C11-CA5-OA7
63	c1	706	CDL	C32-C31-CA7-OA9
63	m2	404	CDL	C52-C51-CB5-OB7
63	e	402	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
62	J	302	PC1	O31-C31-C32-C33
63	Y5	201	CDL	C72-C71-CB7-OB8
63	y0	101	CDL	C15-C16-C17-C18
62	A	502	PC1	C1-C2-C3-O31
63	E	402	CDL	CB3-CB4-CB6-OB8
63	V	201	CDL	CB3-CB4-CB6-OB8
63	v	201	CDL	CB3-CB4-CB6-OB8
63	L	301	CDL	C12-C11-CA5-OA7
62	C3	605	PC1	C2-C1-O11-P
63	m2	401	CDL	C1-CA2-OA2-PA1
63	m2	403	CDL	C1-CB2-OB2-PB2
63	y0	101	CDL	CB4-CB3-OB5-PB2
63	T	201	CDL	C52-C51-CB5-OB6
63	f	401	CDL	C72-C71-CB7-OB8
63	t	201	CDL	C52-C51-CB5-OB6
62	a	501	PC1	C11-C12-N-C14
59	c1	701	HEA	CAD-CBD-CGD-O1D
62	7C	302	PC1	O22-C21-C22-C23
62	A	501	PC1	O32-C31-C32-C33
62	n	301	PC1	O22-C21-C22-C23
63	l	301	CDL	C12-C11-CA5-OA7
62	m1	402	PC1	O21-C21-C22-C23
63	7A	201	CDL	C12-C11-CA5-OA6
63	7c	301	CDL	C52-C51-CB5-OB6
62	7c	303	PC1	C2D-C2E-C2F-C2G
62	C3	603	PC1	O32-C31-C32-C33
63	m2	401	CDL	C32-C31-CA7-OA8
63	m3	403	CDL	C72-C71-CB7-OB8
63	j	301	CDL	C72-C71-CB7-OB8
63	U	201	CDL	C62-C63-C64-C65
62	C1	705	PC1	C3A-C3B-C3C-C3D
62	c3	603	PC1	O32-C31-C32-C33
63	T	202	CDL	C12-C11-CA5-OA7
63	5b	702	CDL	CA7-C31-C32-C33
63	7a	202	CDL	C57-C58-C59-C60
62	j	302	PC1	O31-C31-C32-C33
63	7C	301	CDL	C12-C11-CA5-OA6
63	M3	403	CDL	C72-C71-CB7-OB8
63	7a	201	CDL	C12-C11-CA5-OA6
63	7c	301	CDL	C12-C11-CA5-OA6
63	e	401	CDL	C72-C71-CB7-OB8
63	5B	702	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
63	C1	707	CDL	C32-C31-CA7-OA9
63	7A	201	CDL	C32-C31-CA7-OA9
63	Y5	201	CDL	C72-C71-CB7-OB9
63	7C	301	CDL	C52-C51-CB5-OB6
63	5b	702	CDL	C12-C11-CA5-OA6
63	m3	403	CDL	C12-C11-CA5-OA6
63	a	503	CDL	C12-C11-CA5-OA6
63	y0	101	CDL	C12-C11-CA5-OA7
63	V	201	CDL	C72-C73-C74-C75

There are no ring outliers.

90 monomers are involved in 344 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	m3	401	CDL	12	0
62	C3	601	PC1	1	0
63	e	402	CDL	6	0
63	7C	303	CDL	1	0
62	M2	405	PC1	4	0
63	y7	501	CDL	1	0
63	t	201	CDL	2	0
59	c1	702	HEA	1	0
63	M2	401	CDL	2	0
62	v	202	PC1	3	0
63	m2	404	CDL	3	0
63	7A	202	CDL	7	0
63	7C	301	CDL	8	0
63	M1	402	CDL	3	0
62	A	501	PC1	3	0
62	C3	605	PC1	3	0
62	n	301	PC1	3	0
62	a	502	PC1	2	0
63	Y7	501	CDL	1	0
62	c3	601	PC1	1	0
62	m2	402	PC1	2	0
63	E	402	CDL	5	0
63	c1	706	CDL	5	0
59	c1	701	HEA	6	0
62	c1	705	PC1	4	0
63	M1	403	CDL	5	0
63	5b	702	CDL	6	0
63	5B	702	CDL	9	0

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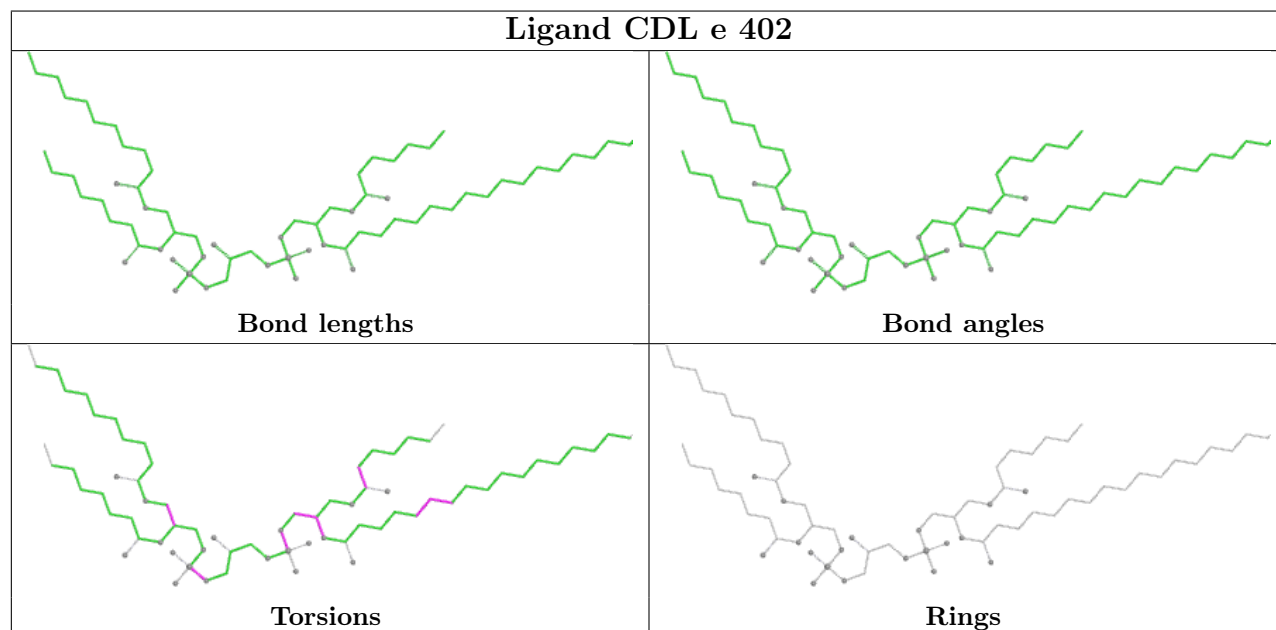
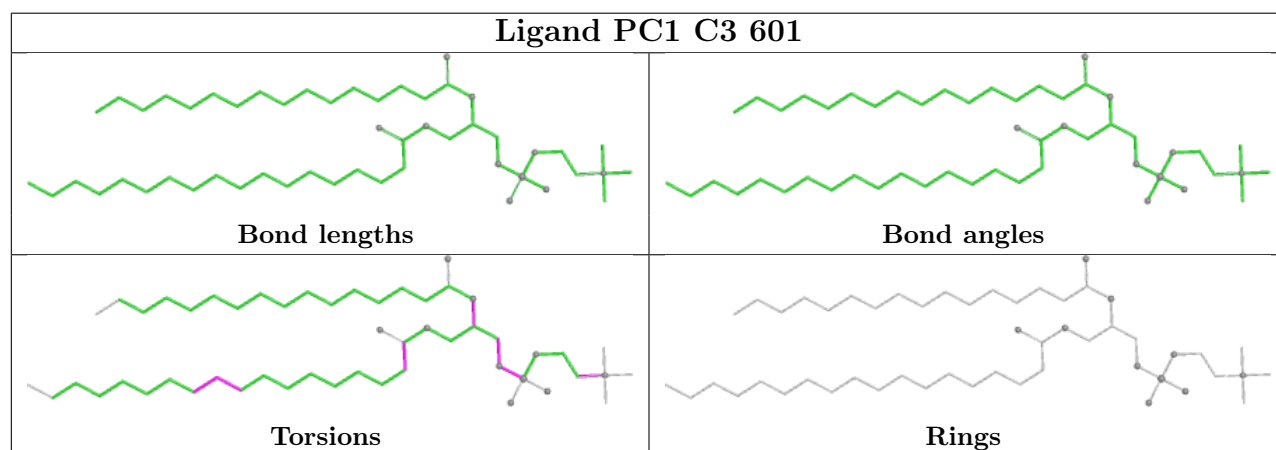
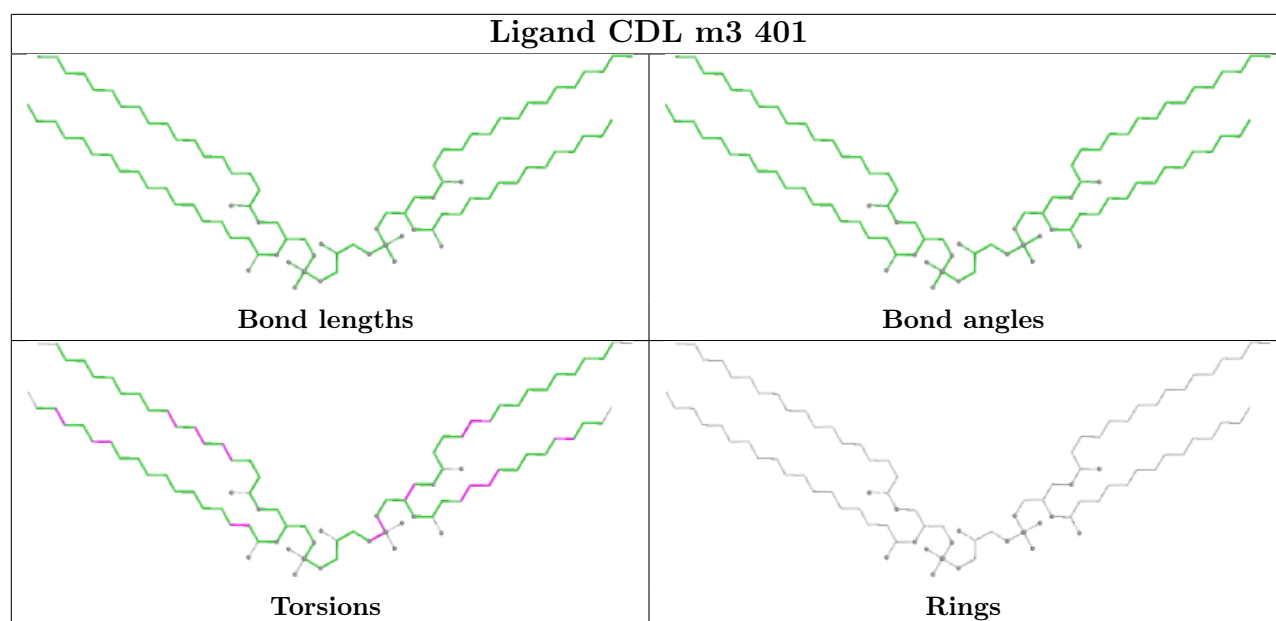
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	m2	406	PC1	1	0
59	C1	702	HEA	2	0
63	l	301	CDL	2	0
63	L	301	CDL	3	0
63	7a	202	CDL	8	0
62	V	202	PC1	3	0
63	7c	302	CDL	1	0
63	7A	201	CDL	4	0
62	N	302	PC1	1	0
63	c1	707	CDL	1	0
62	a	501	PC1	3	0
63	u	201	CDL	4	0
63	v	201	CDL	3	0
63	C1	706	CDL	5	0
63	m1	401	CDL	8	0
62	c3	603	PC1	2	0
63	j	301	CDL	7	0
59	C1	701	HEA	7	0
62	C1	705	PC1	4	0
63	m2	401	CDL	3	0
63	U	201	CDL	4	0
63	5B	704	CDL	2	0
62	N	301	PC1	2	0
63	n	303	CDL	9	0
62	m2	405	PC1	4	0
62	7C	304	PC1	5	0
63	m1	403	CDL	3	0
63	f	401	CDL	9	0
63	Y5	201	CDL	2	0
63	E	401	CDL	2	0
63	N	303	CDL	7	0
63	7c	301	CDL	8	0
63	k	301	CDL	3	0
63	7a	201	CDL	6	0
63	e	401	CDL	3	0
62	7c	303	PC1	5	0
63	M3	401	CDL	9	0
62	A	502	PC1	2	0
63	C1	707	CDL	1	0
62	m1	402	PC1	9	0
63	V	201	CDL	3	0
62	n	302	PC1	1	0

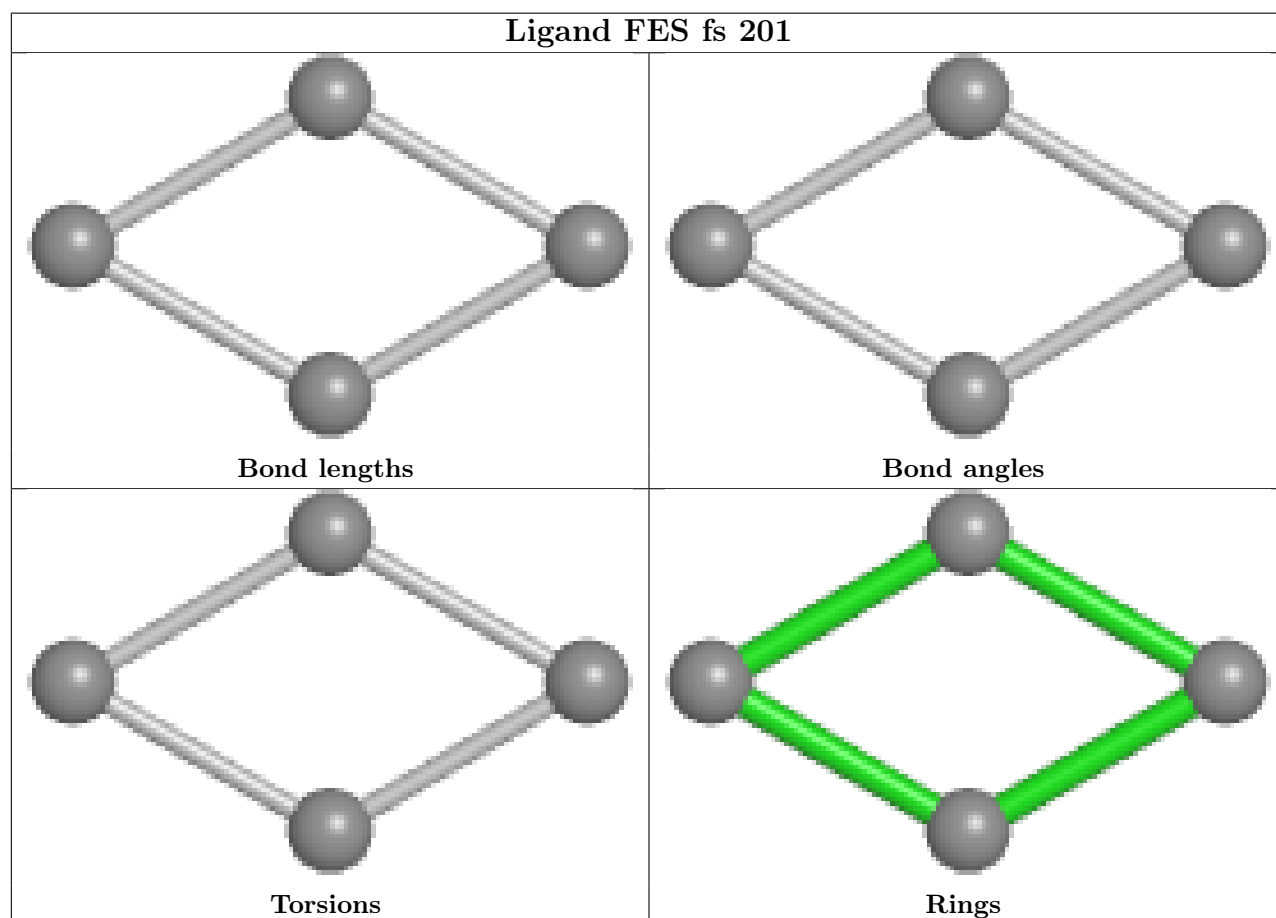
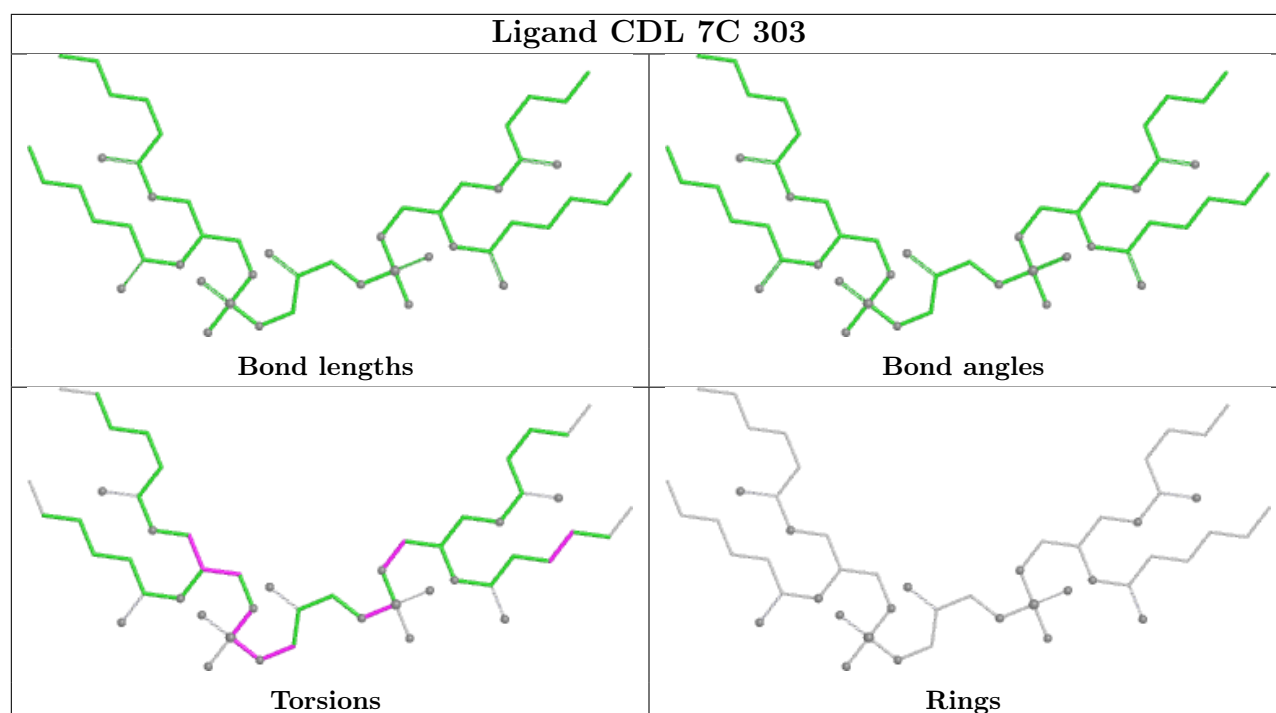
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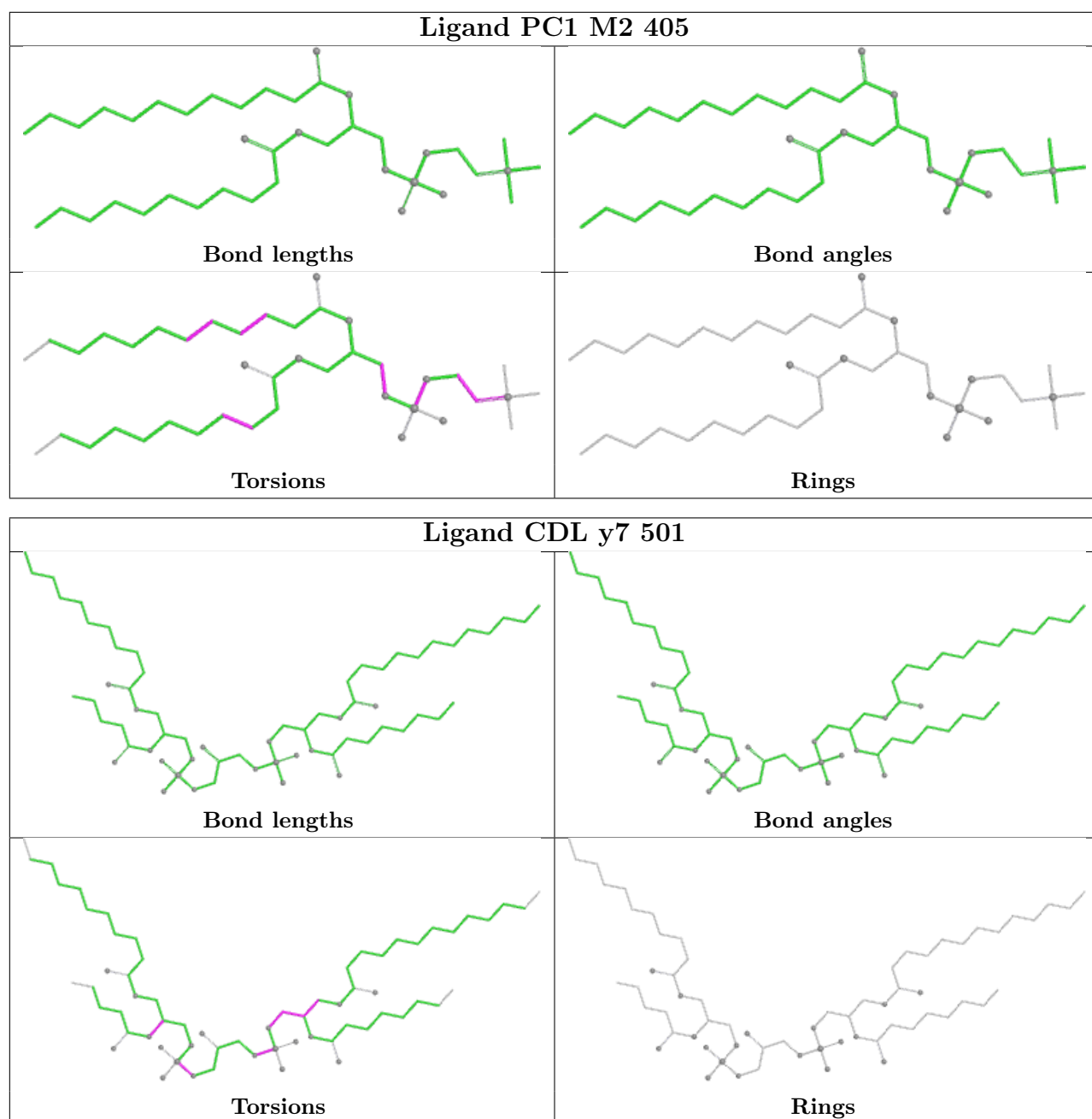
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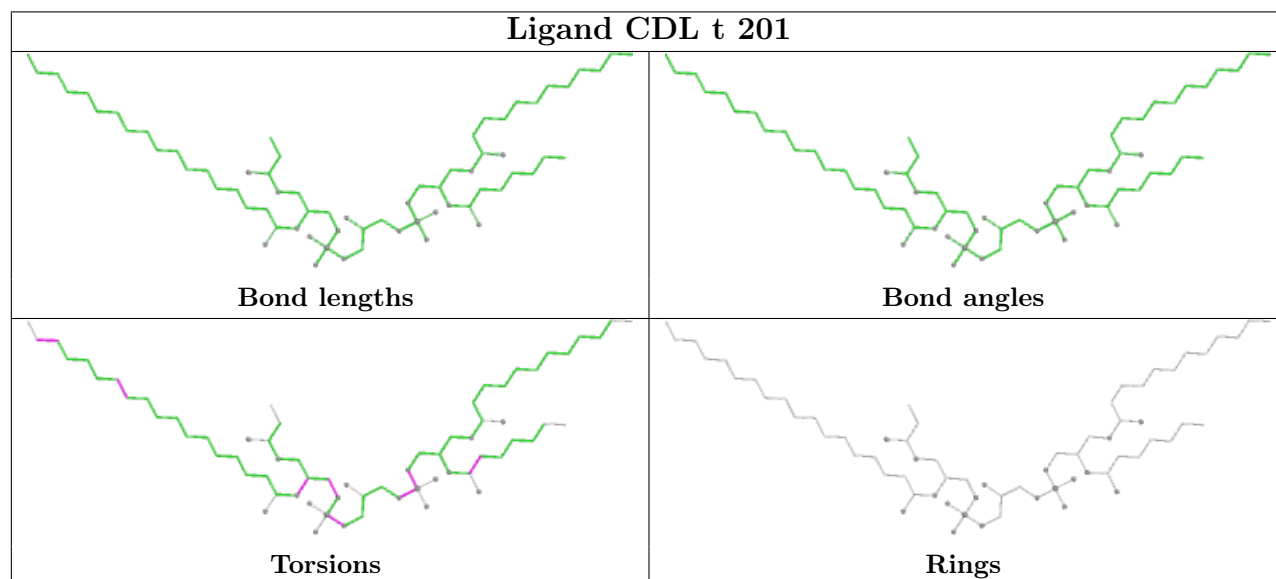
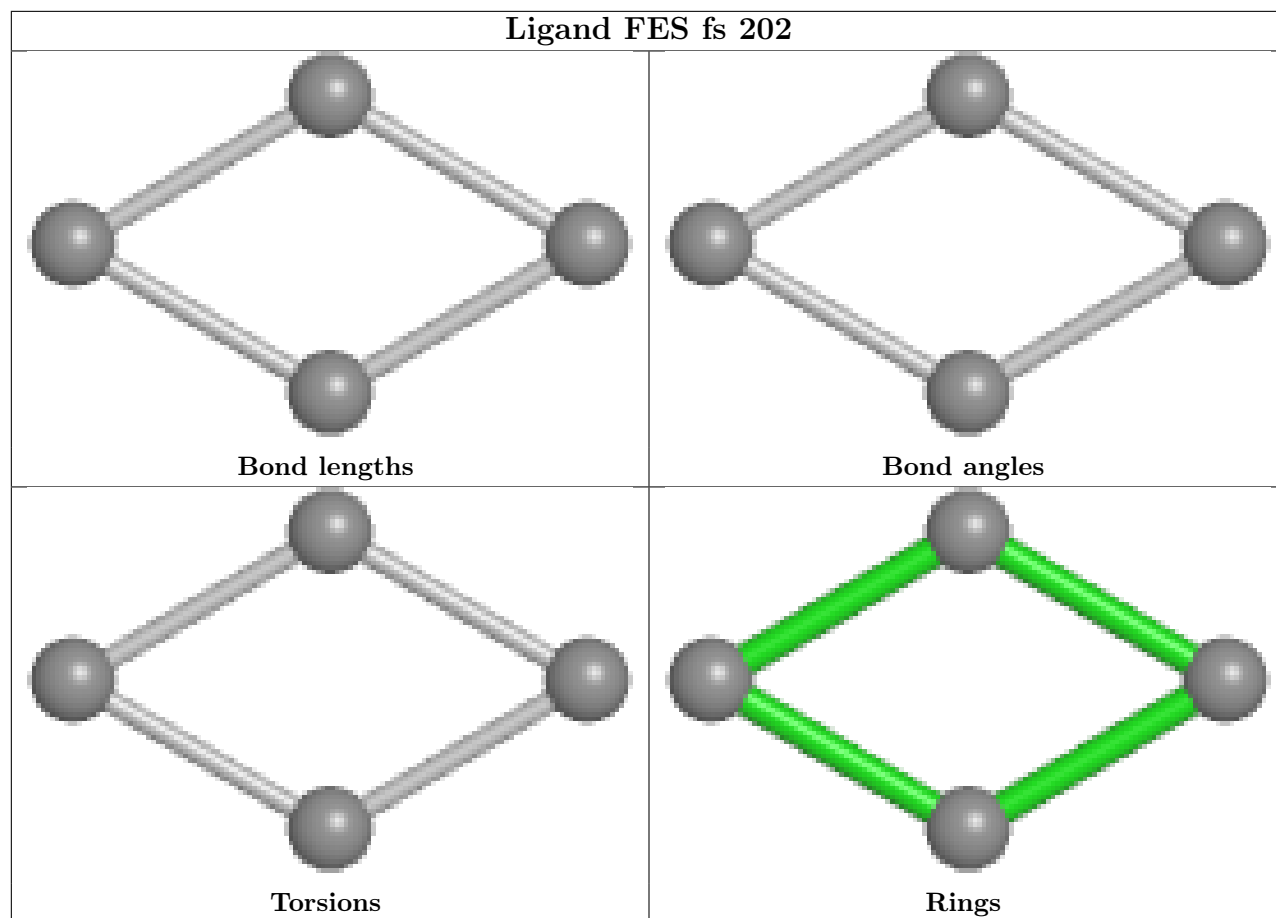
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	m2	403	CDL	5	0
63	M2	404	CDL	2	0
63	T	201	CDL	2	0
63	m1	404	CDL	4	0
63	T	202	CDL	5	0
63	M1	401	CDL	8	0
63	5b	703	CDL	3	0
62	7C	302	PC1	8	0
63	5B	703	CDL	3	0
62	M2	406	PC1	1	0
62	c3	605	PC1	3	0
62	C3	603	PC1	2	0
63	y5	201	CDL	1	0
63	y0	101	CDL	3	0
63	Y0	101	CDL	4	0
63	t	202	CDL	5	0
62	M2	402	PC1	3	0
63	J	301	CDL	6	0
63	F	401	CDL	12	0
63	M2	403	CDL	5	0

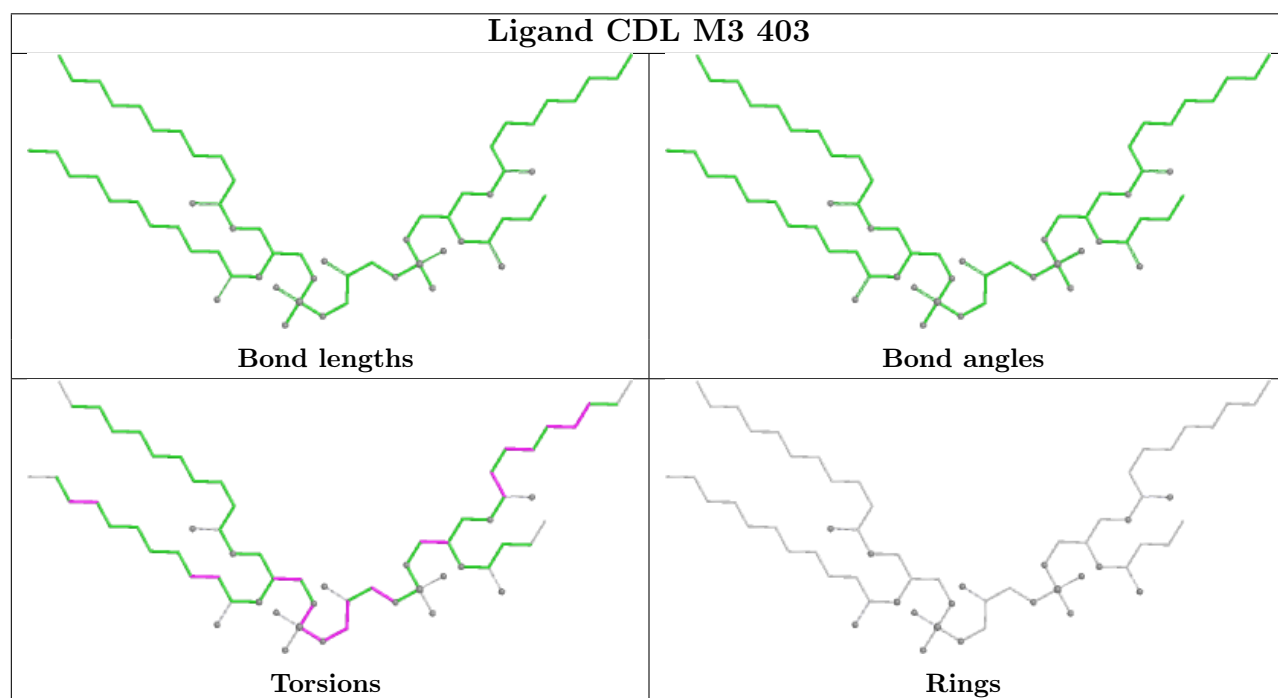
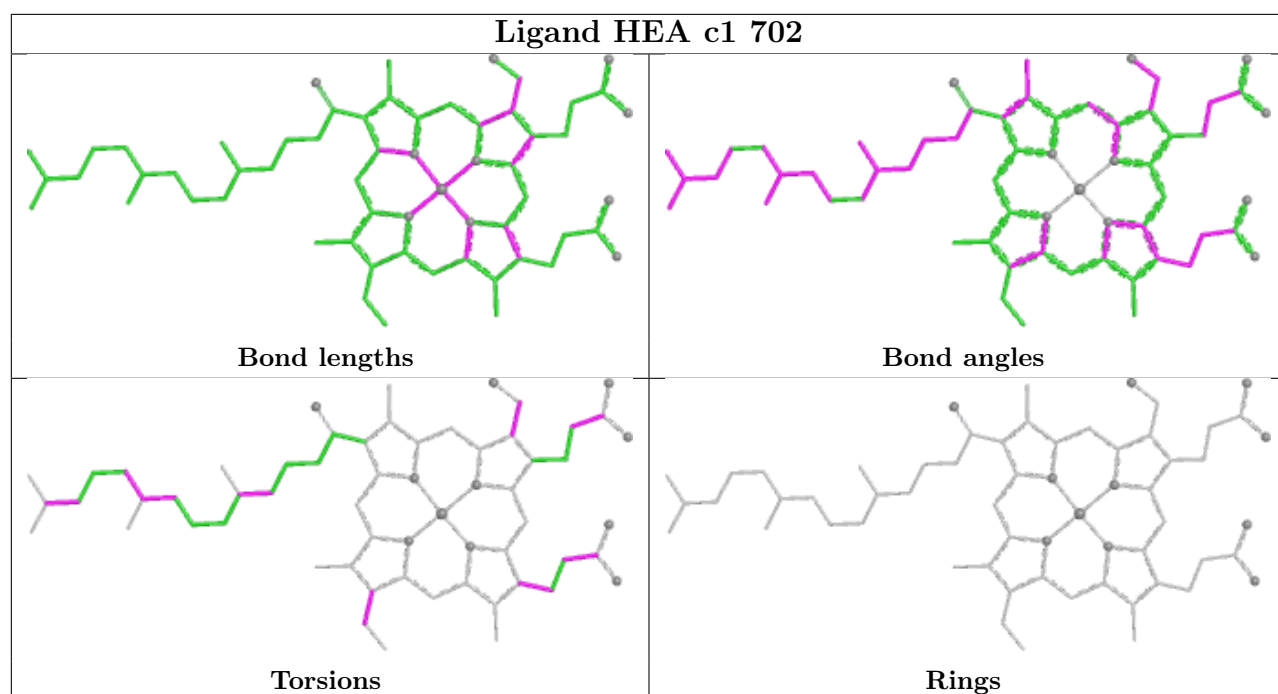
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

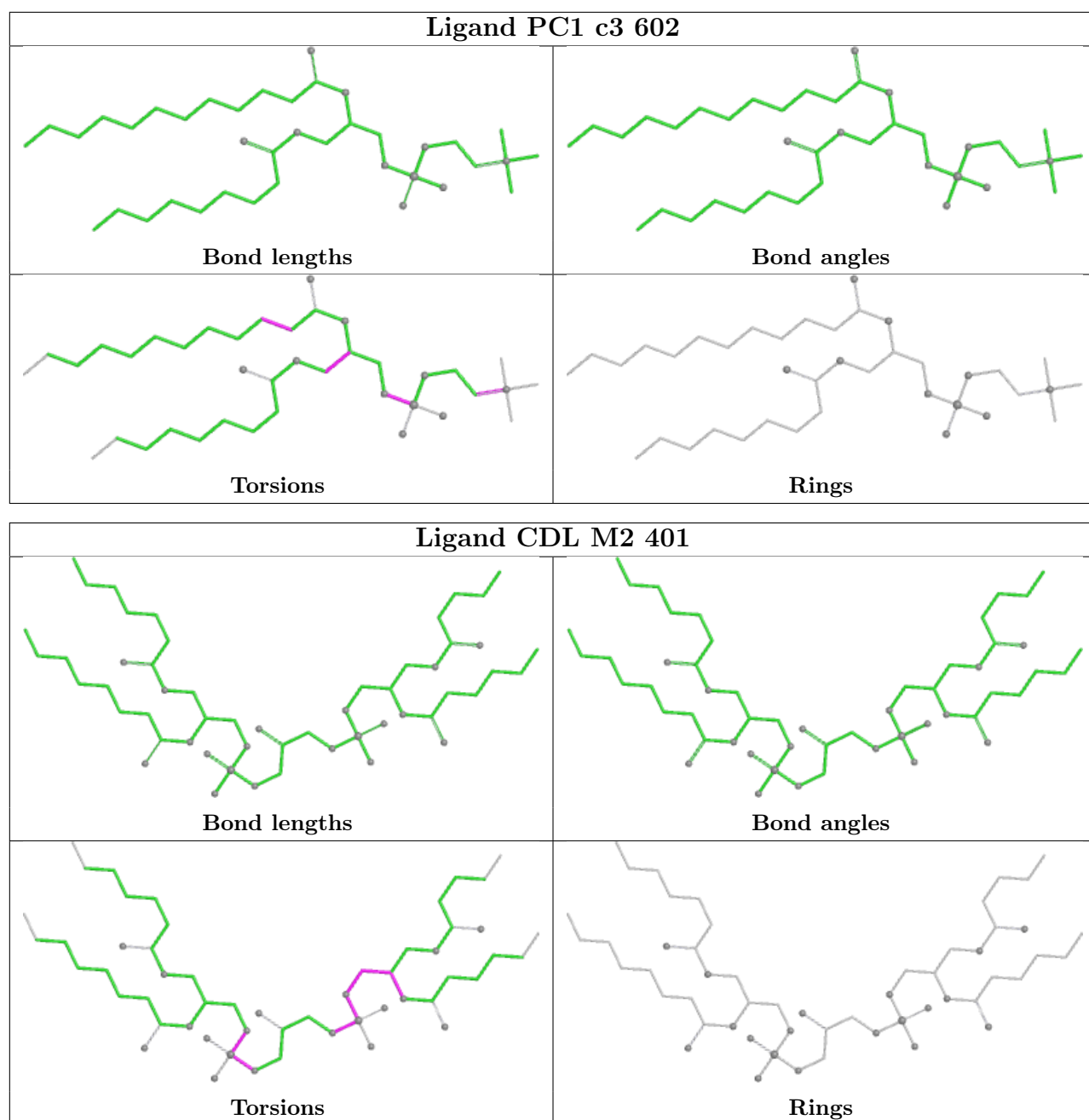


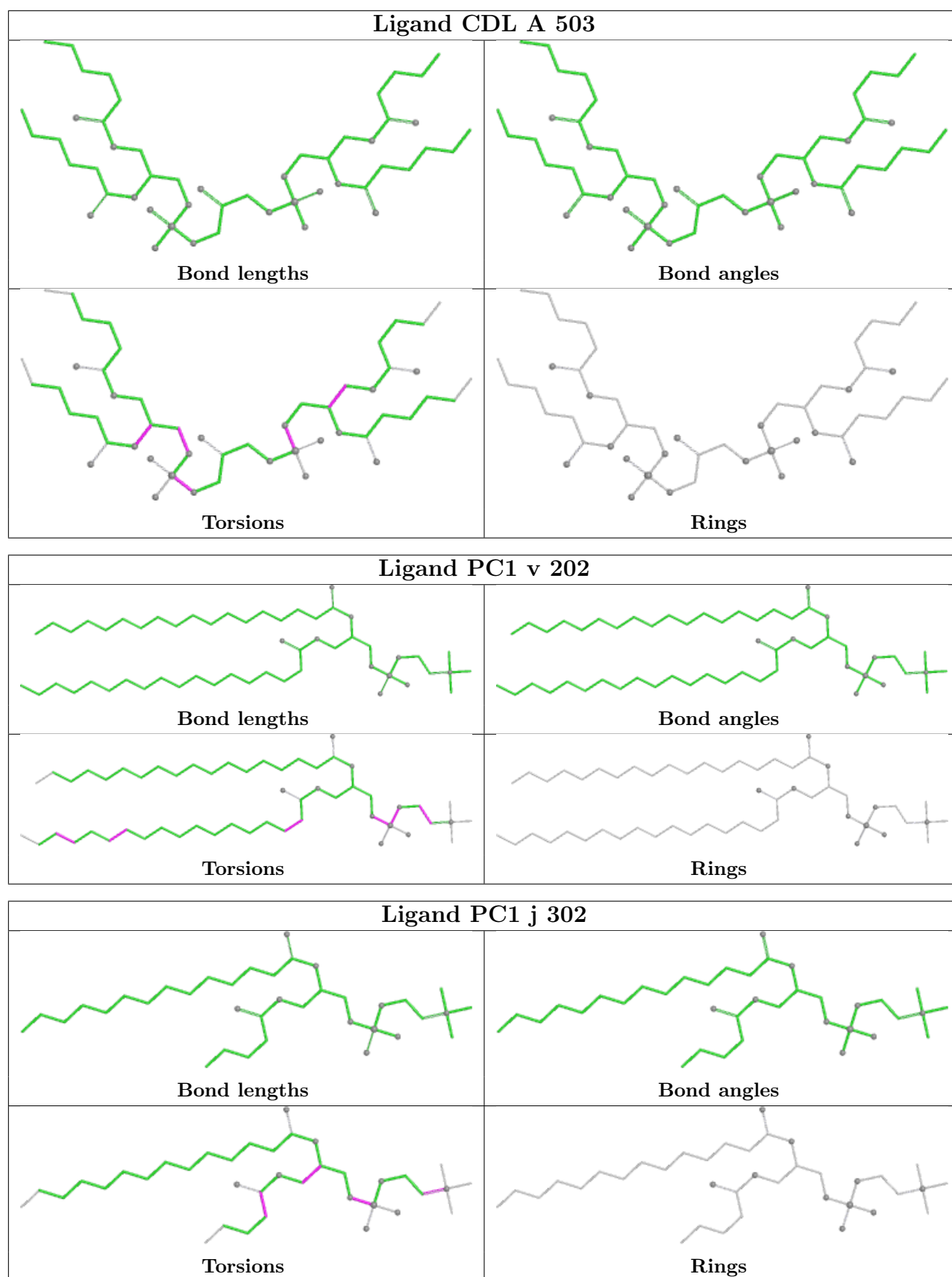


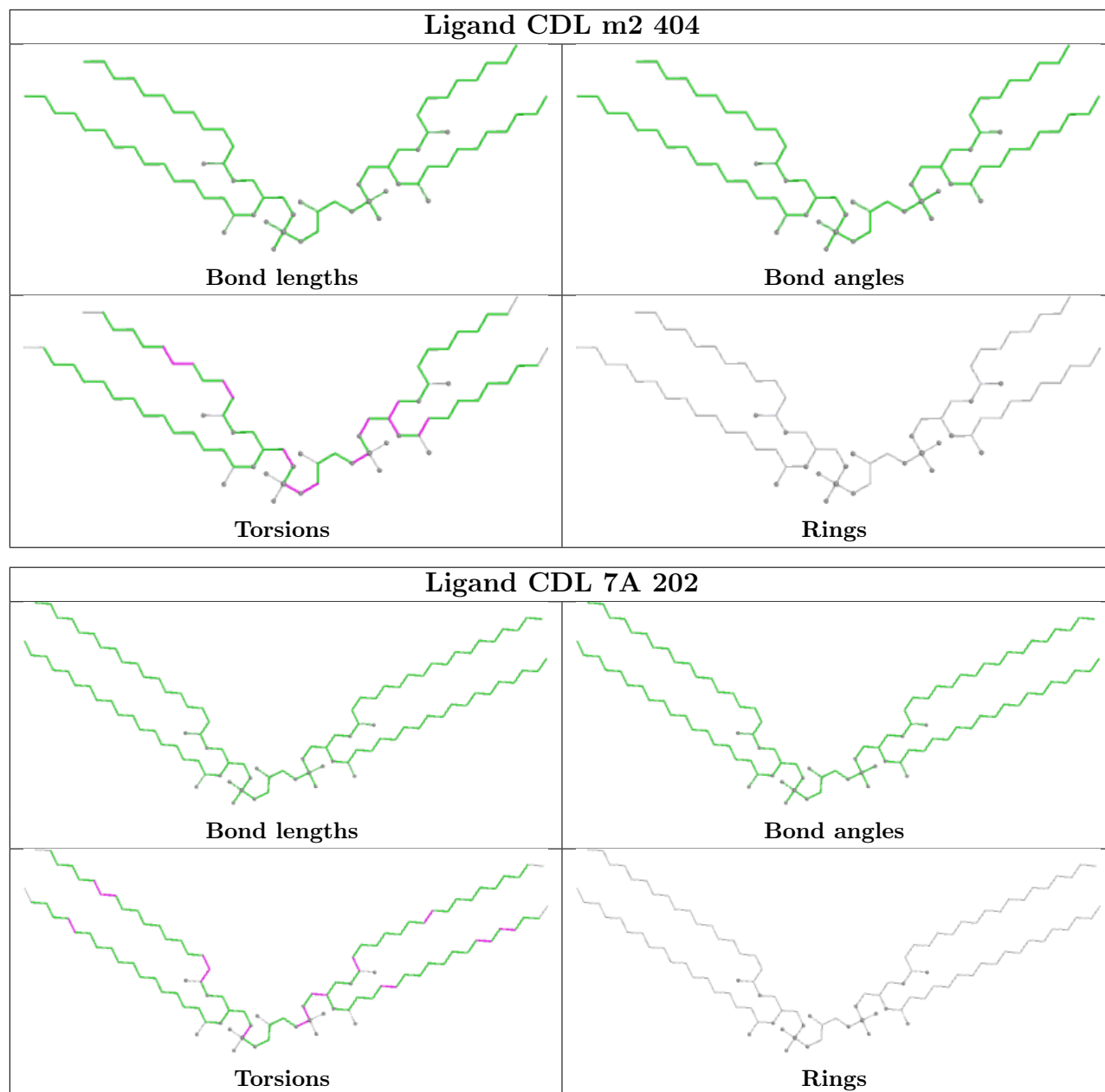


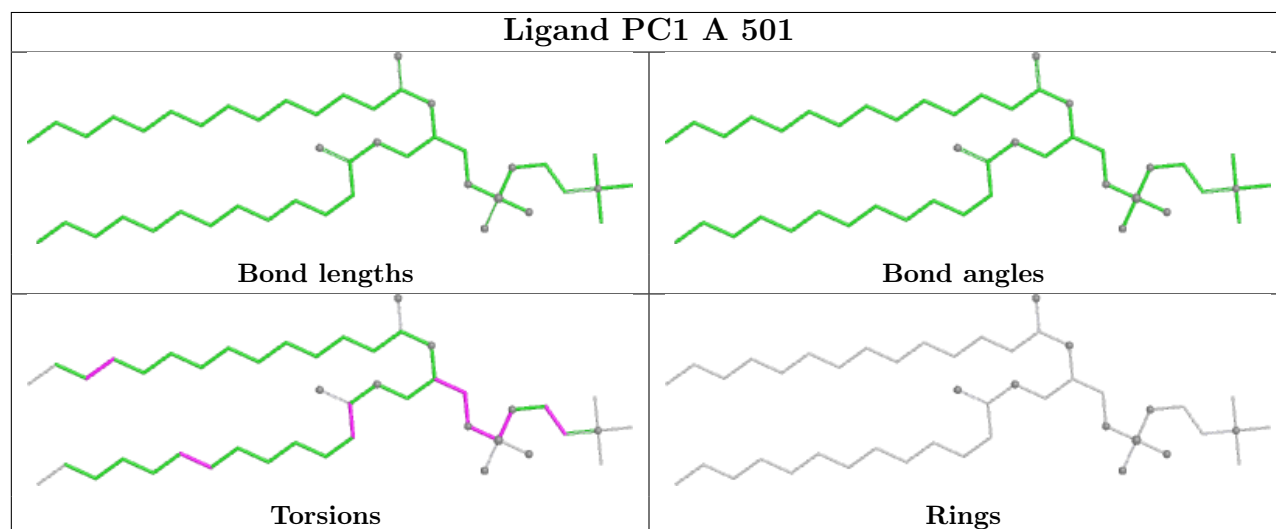
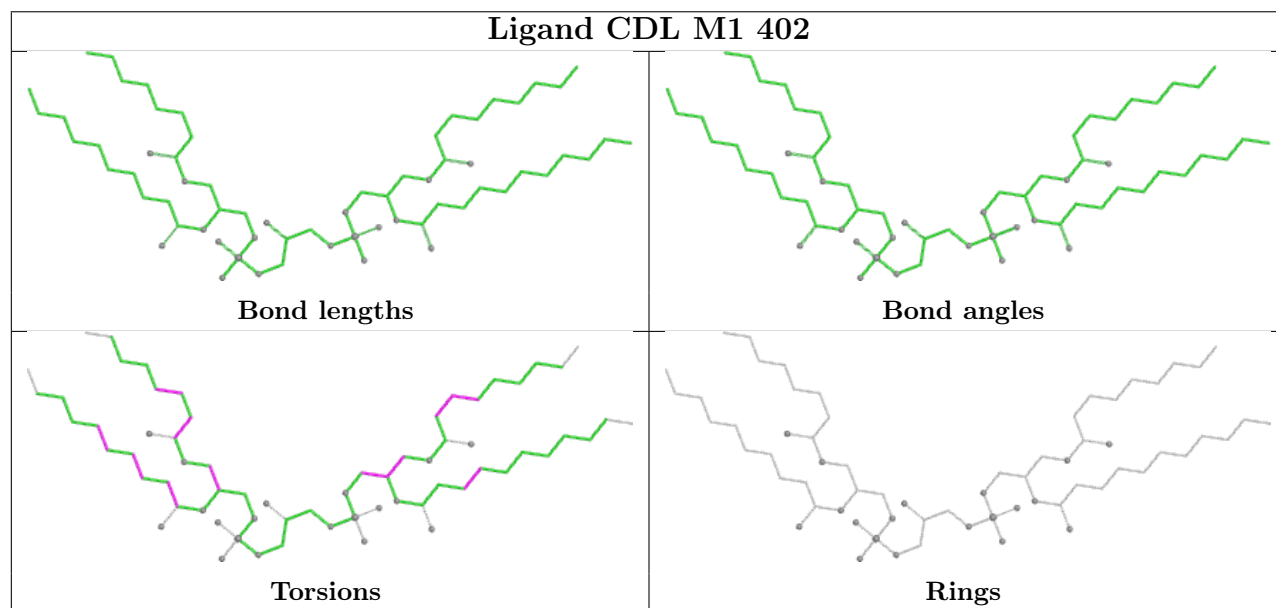
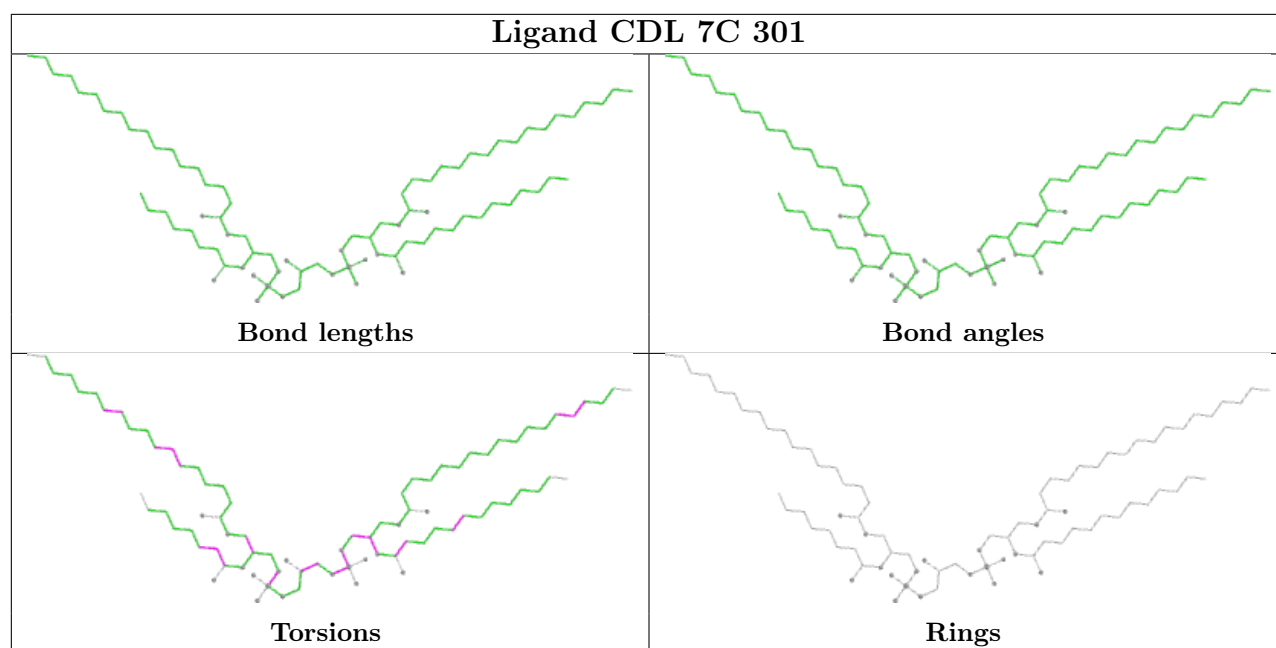


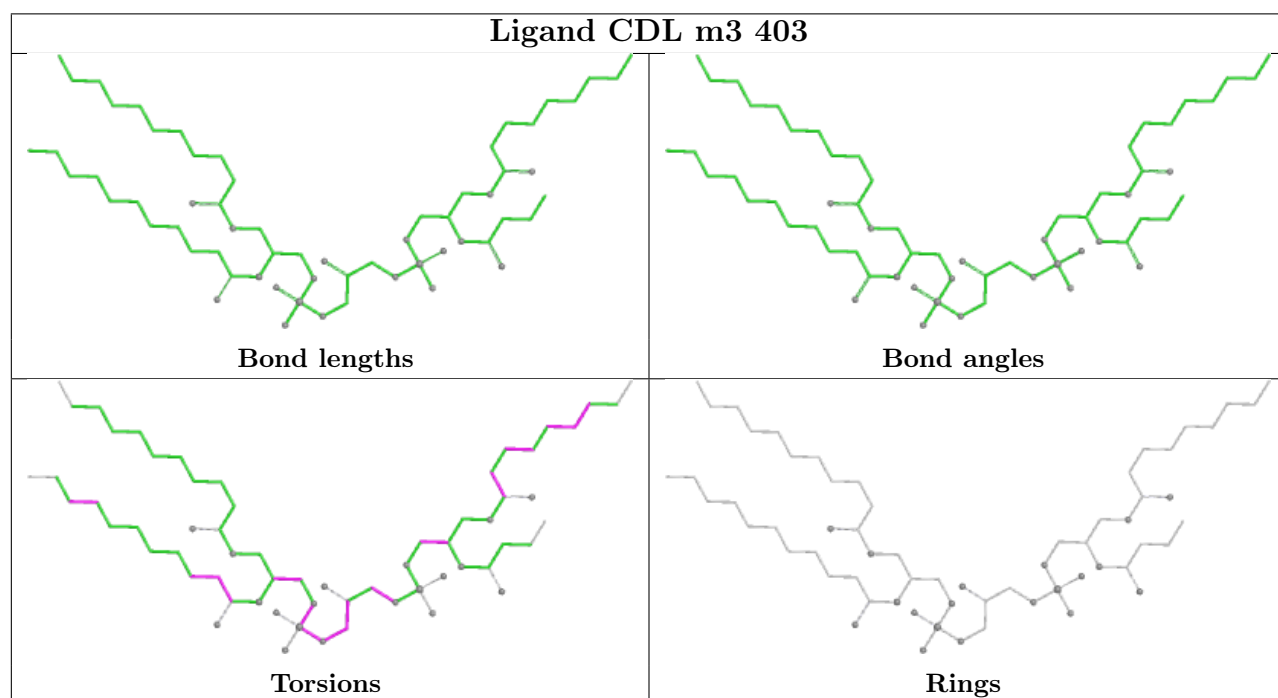
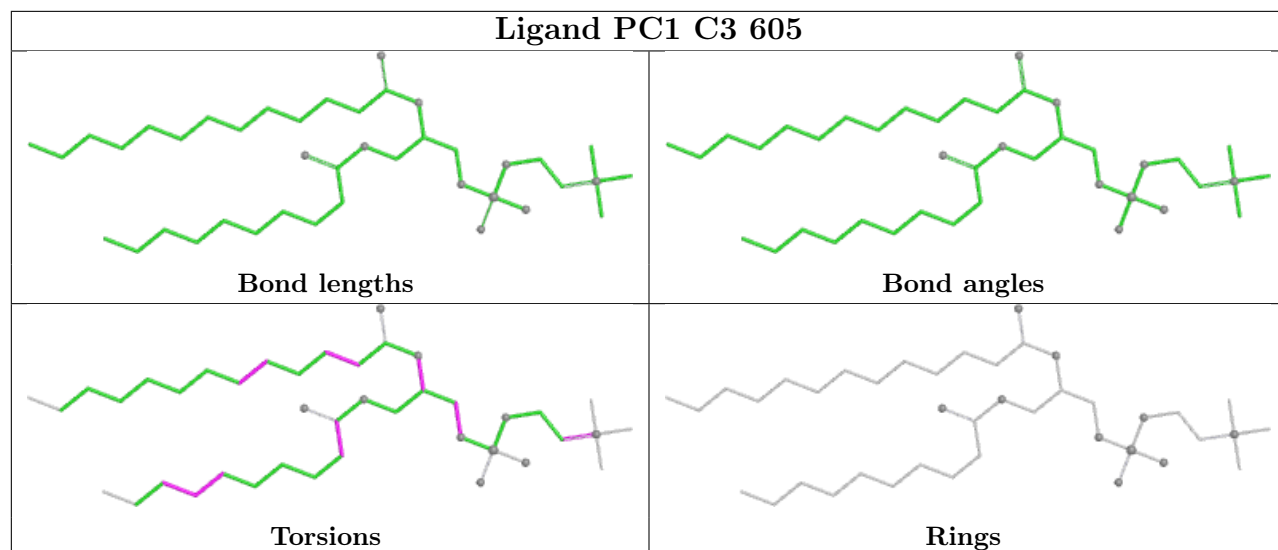


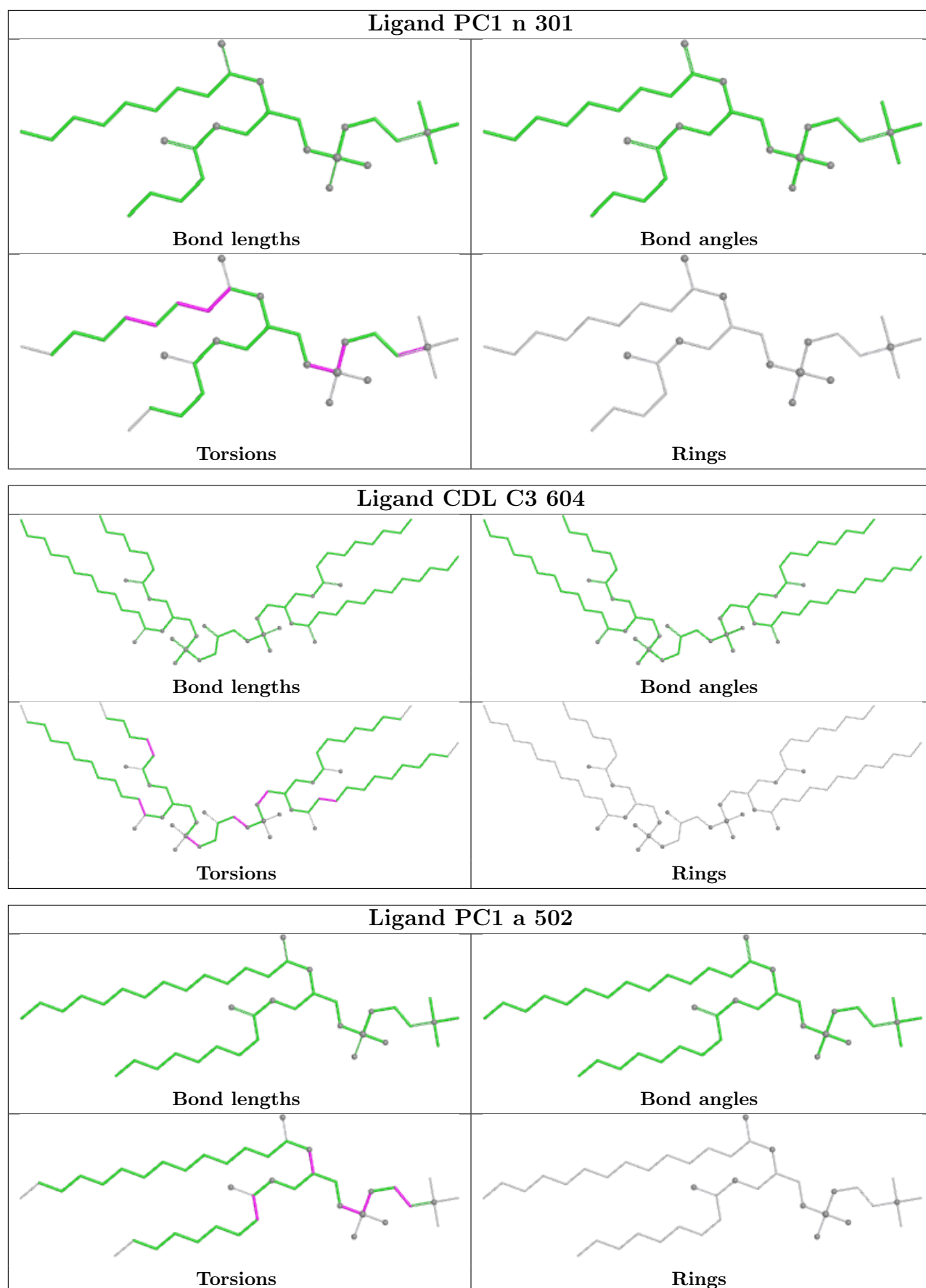


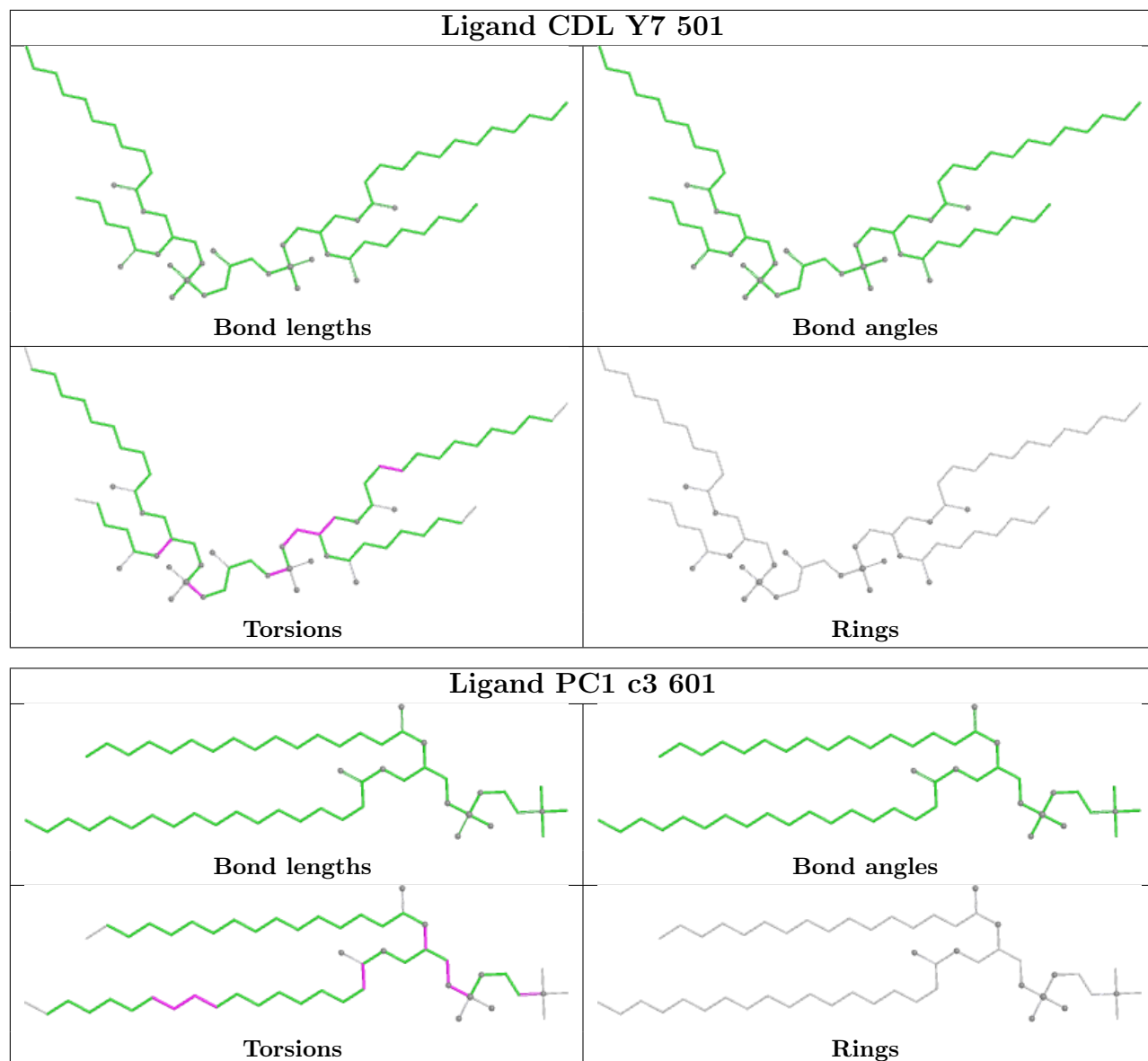


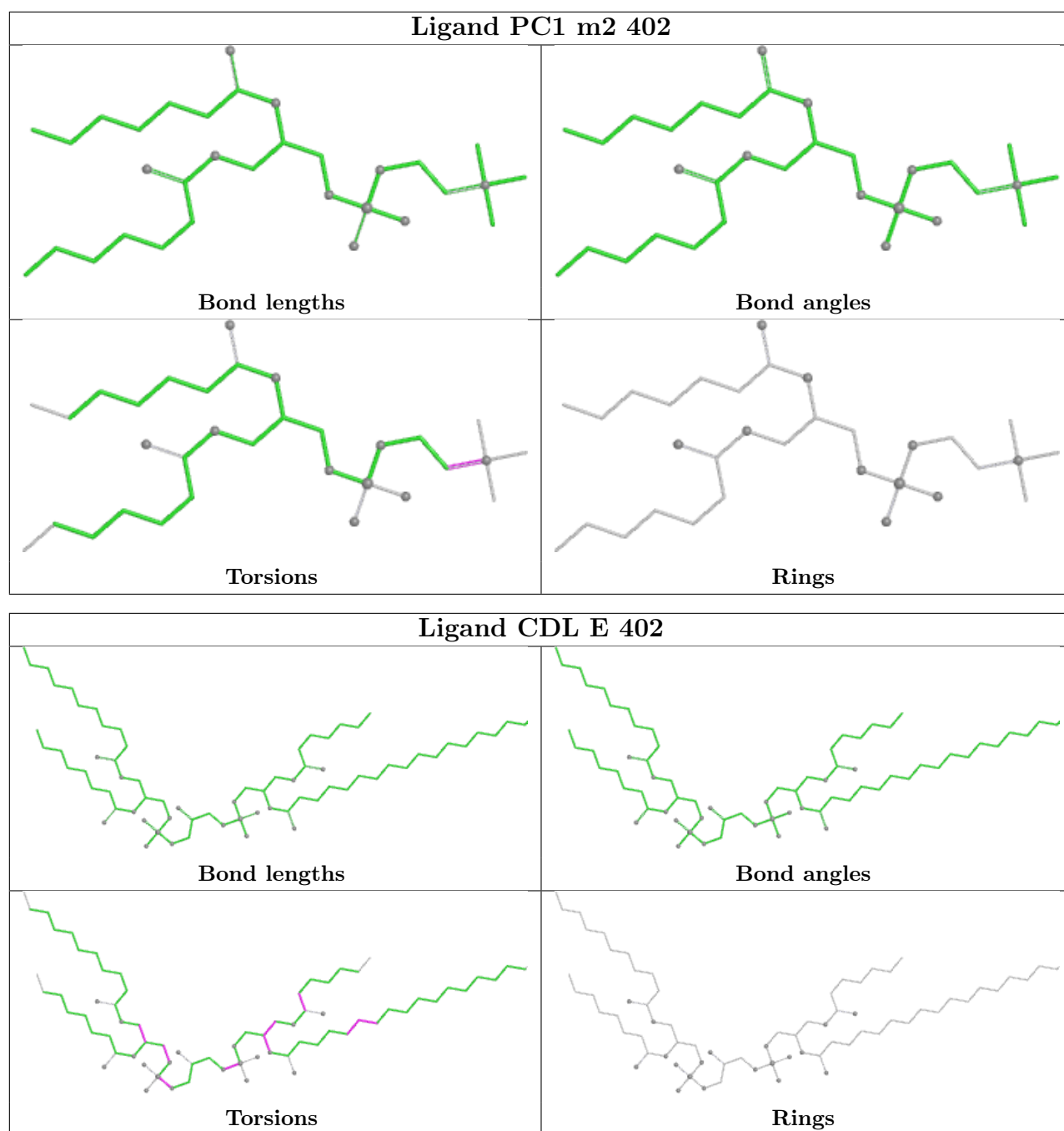


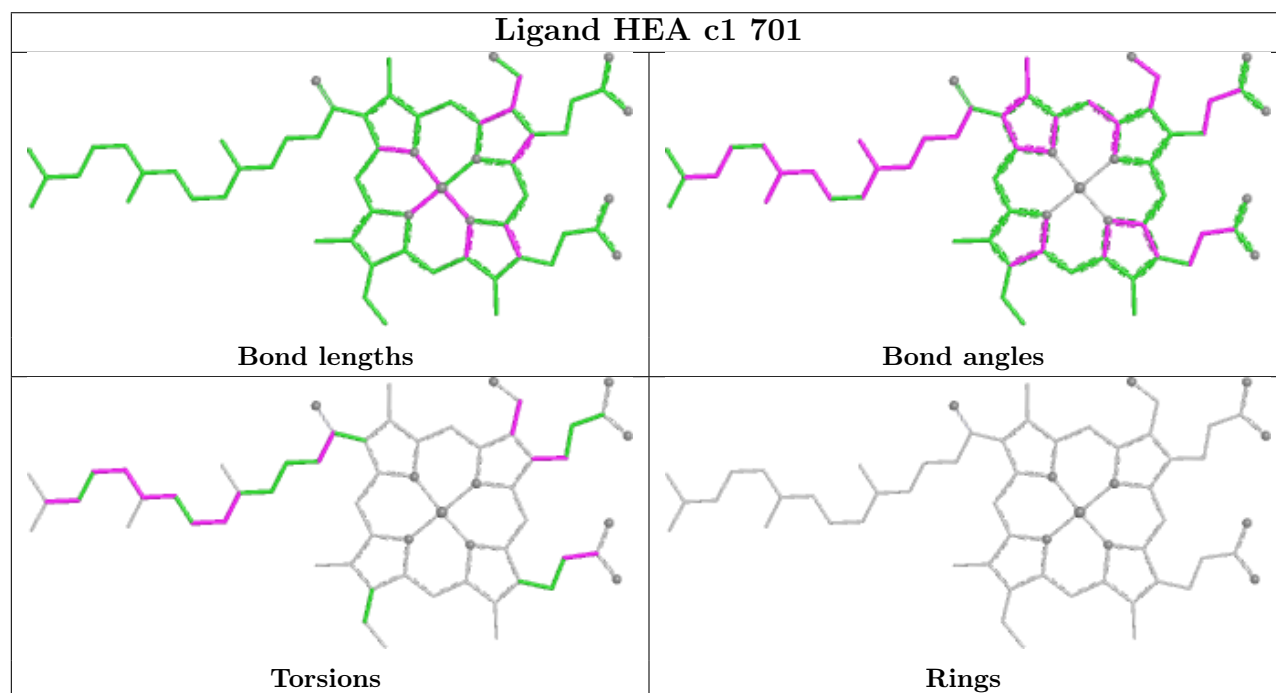
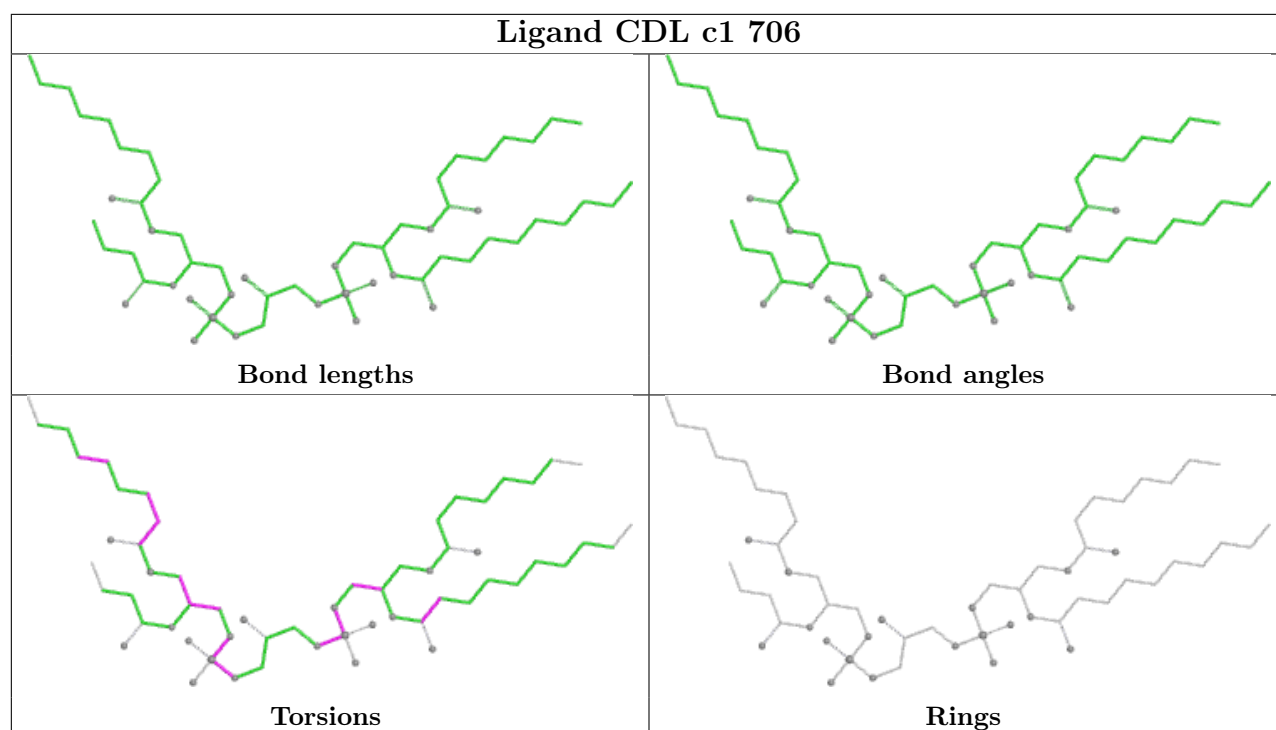


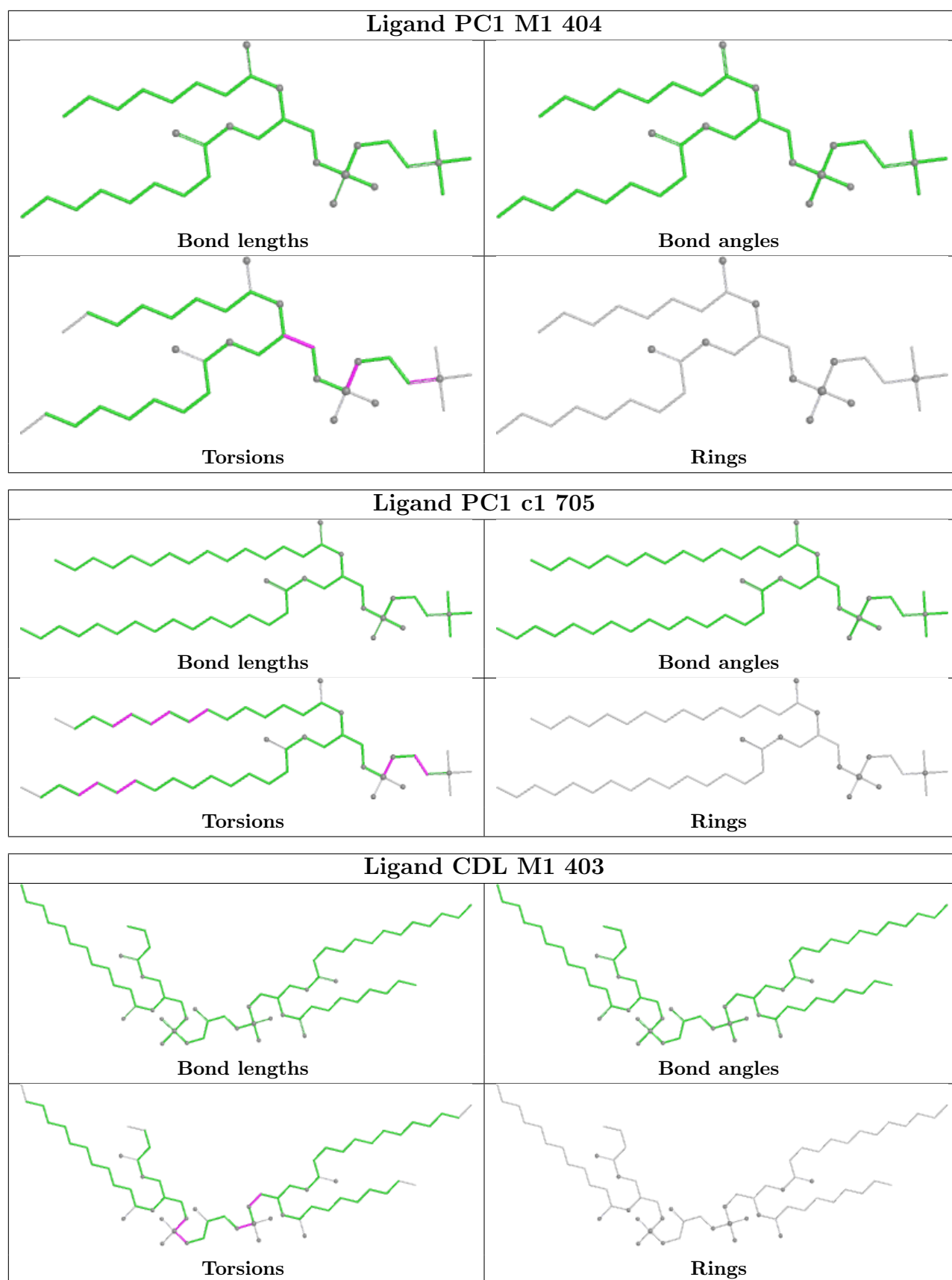


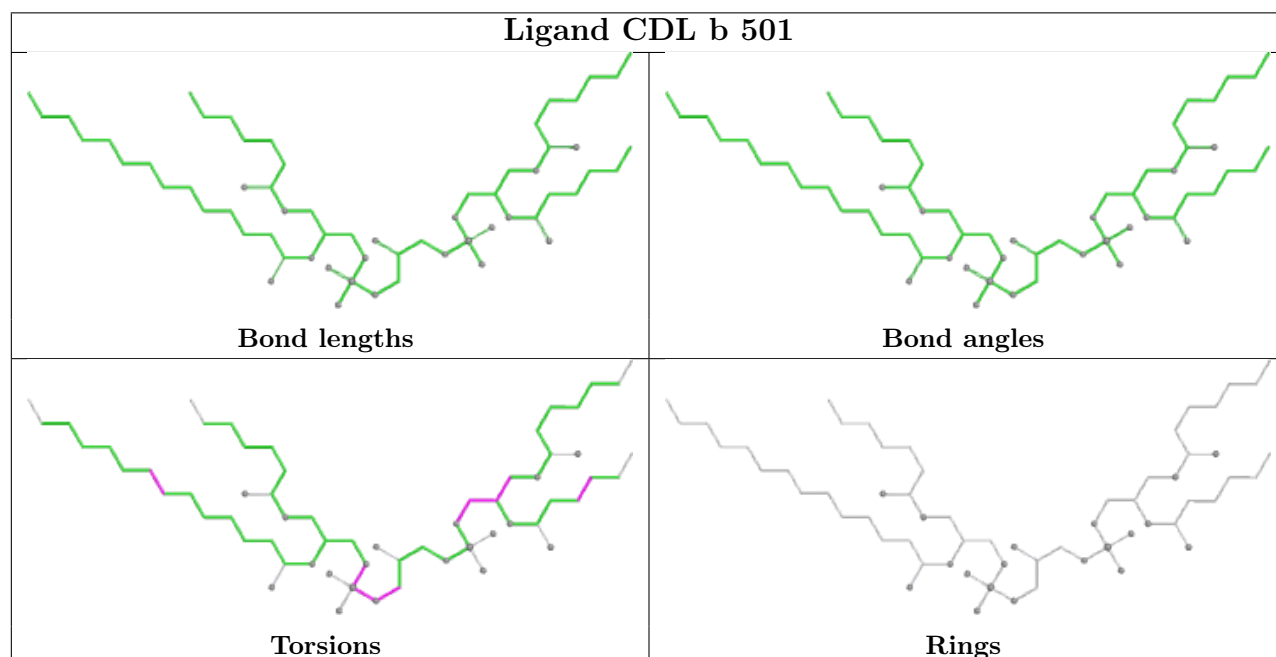
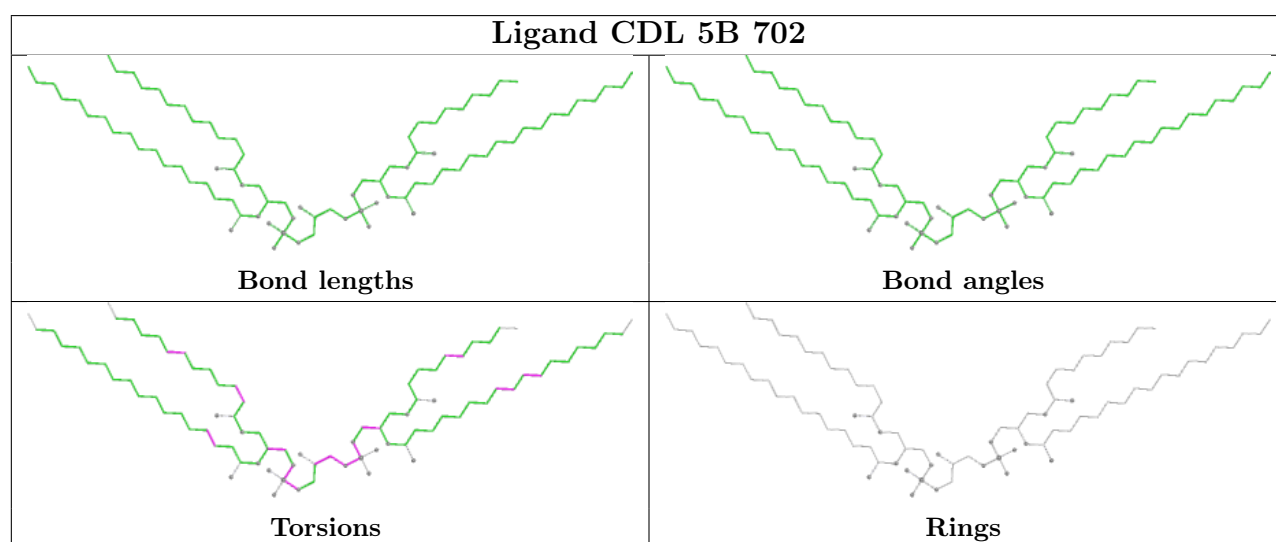
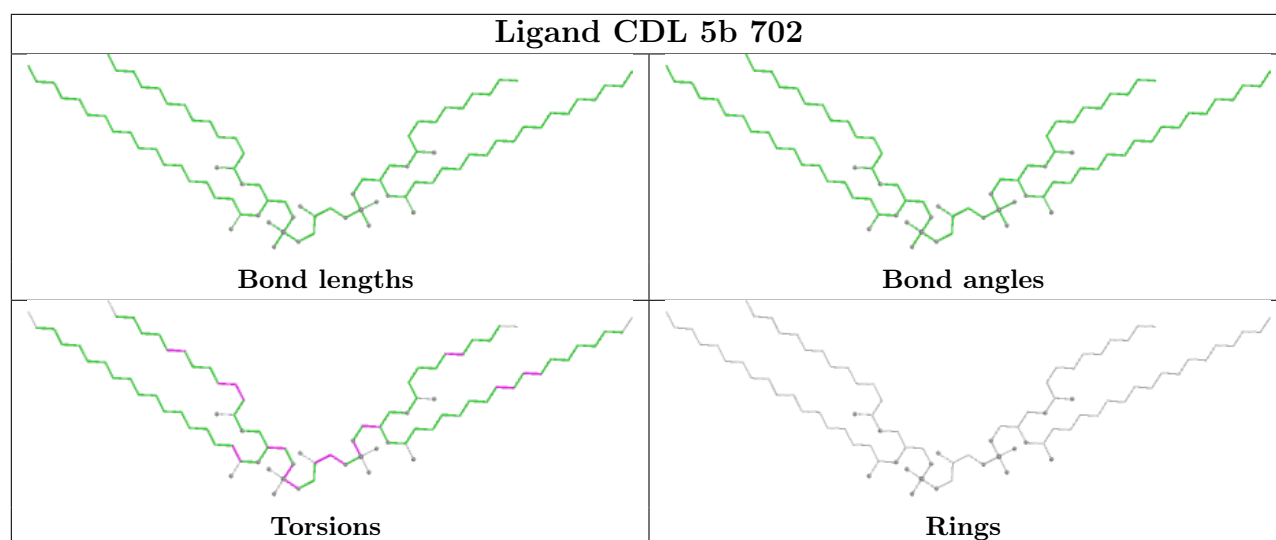


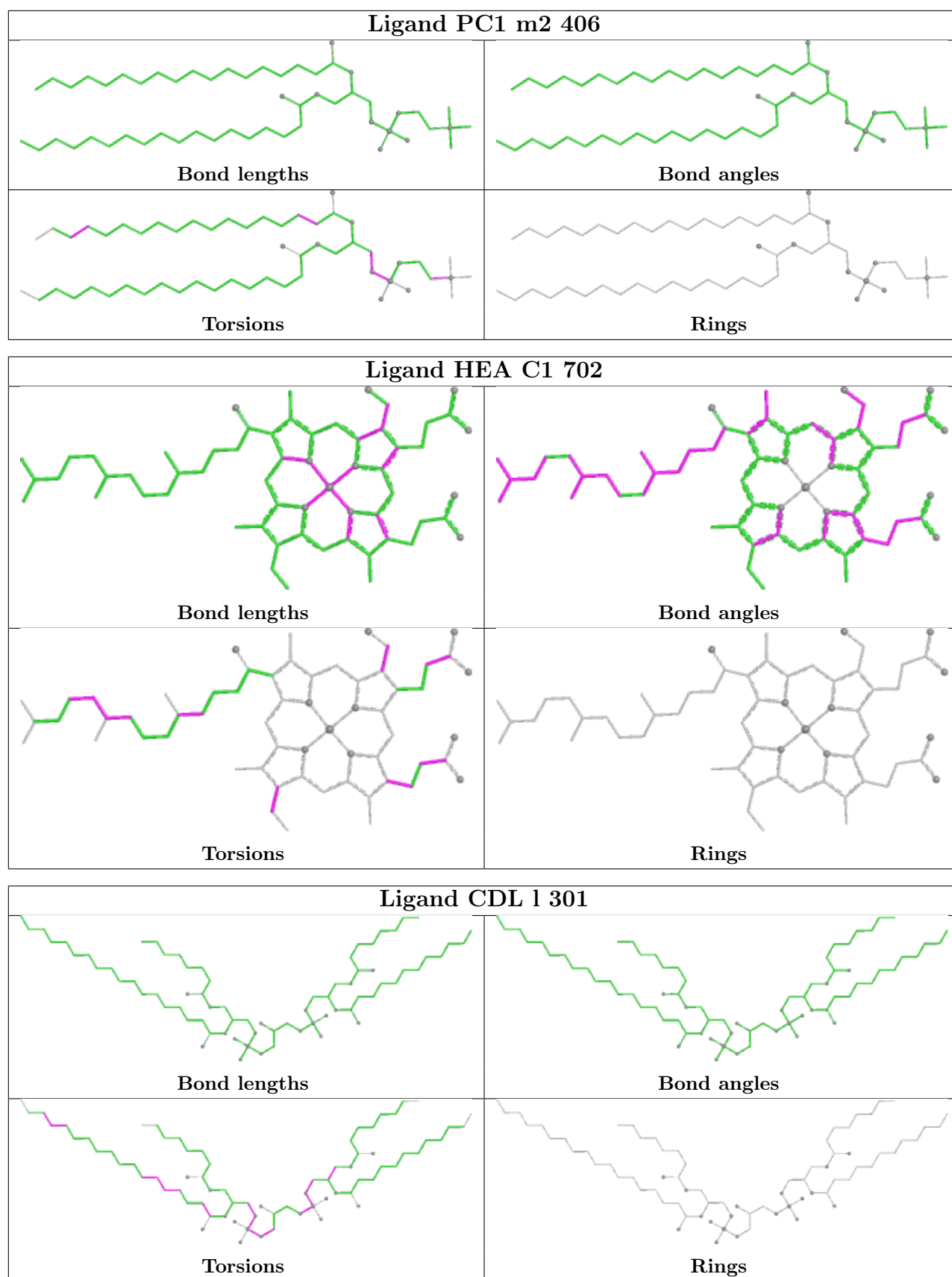


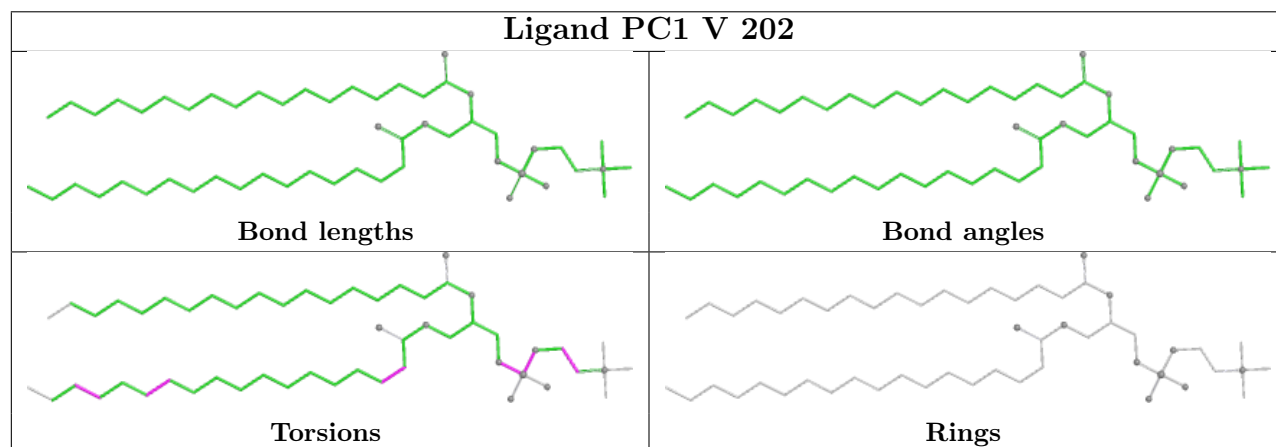
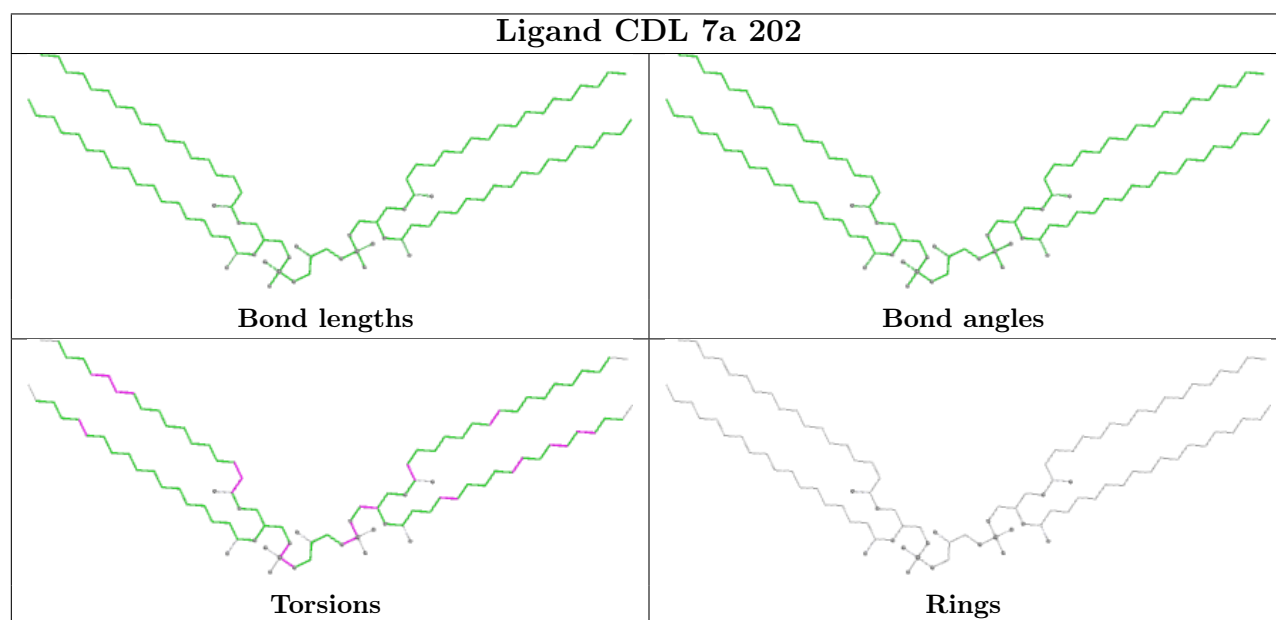
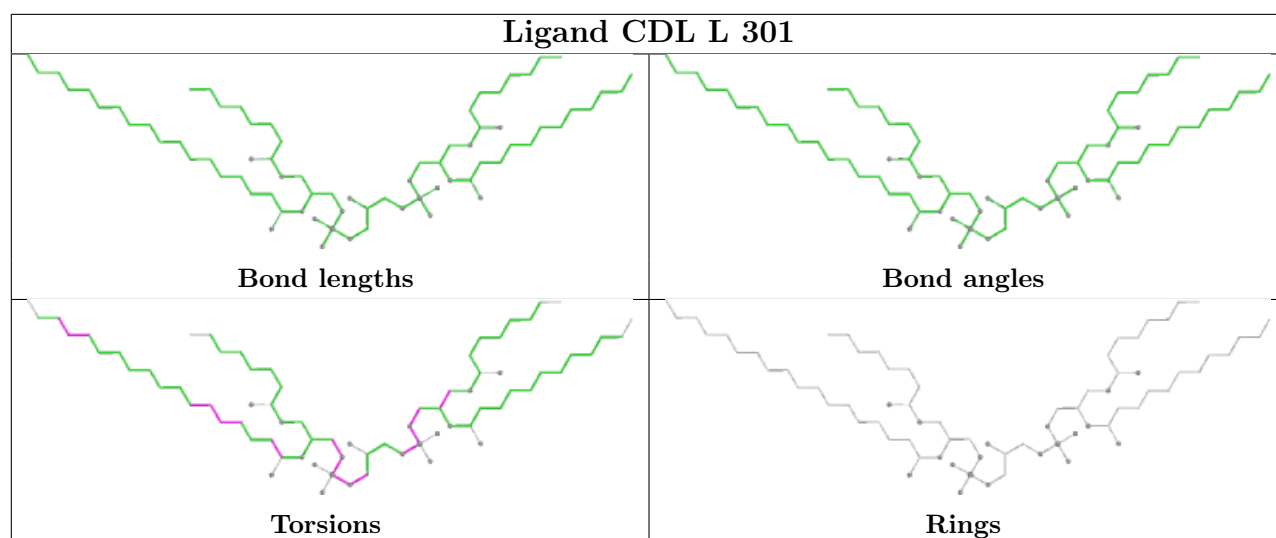


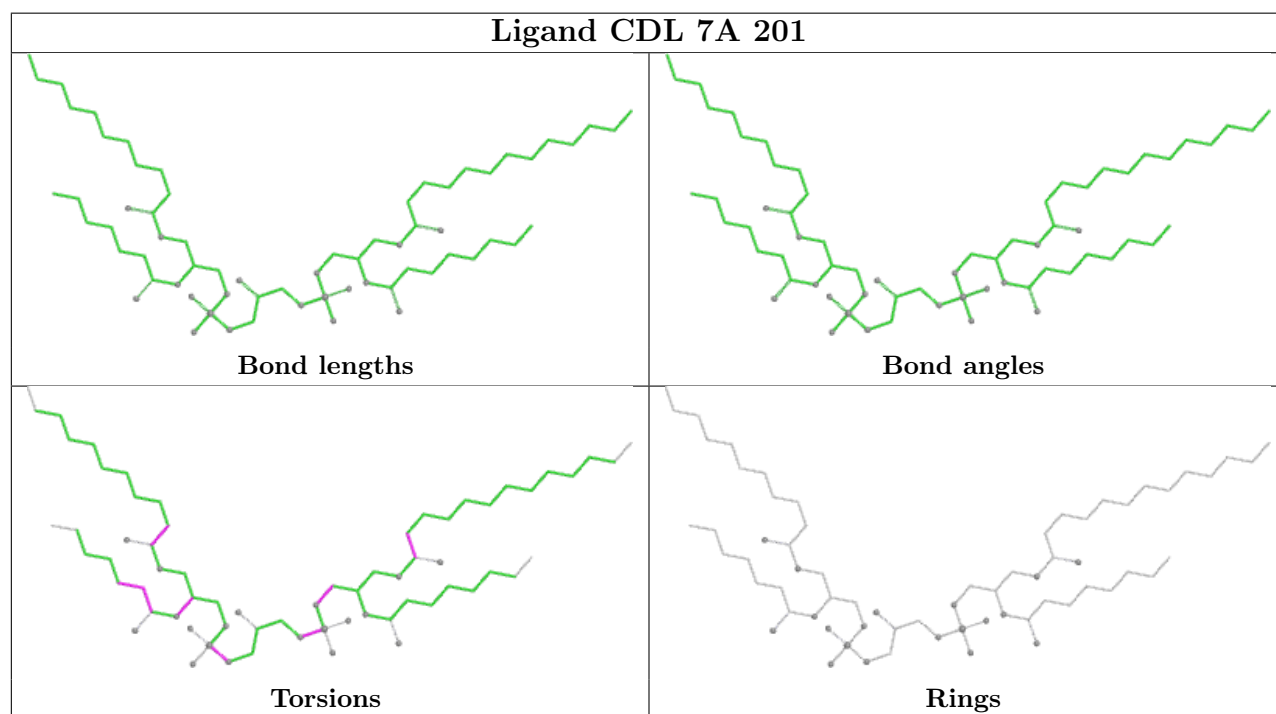
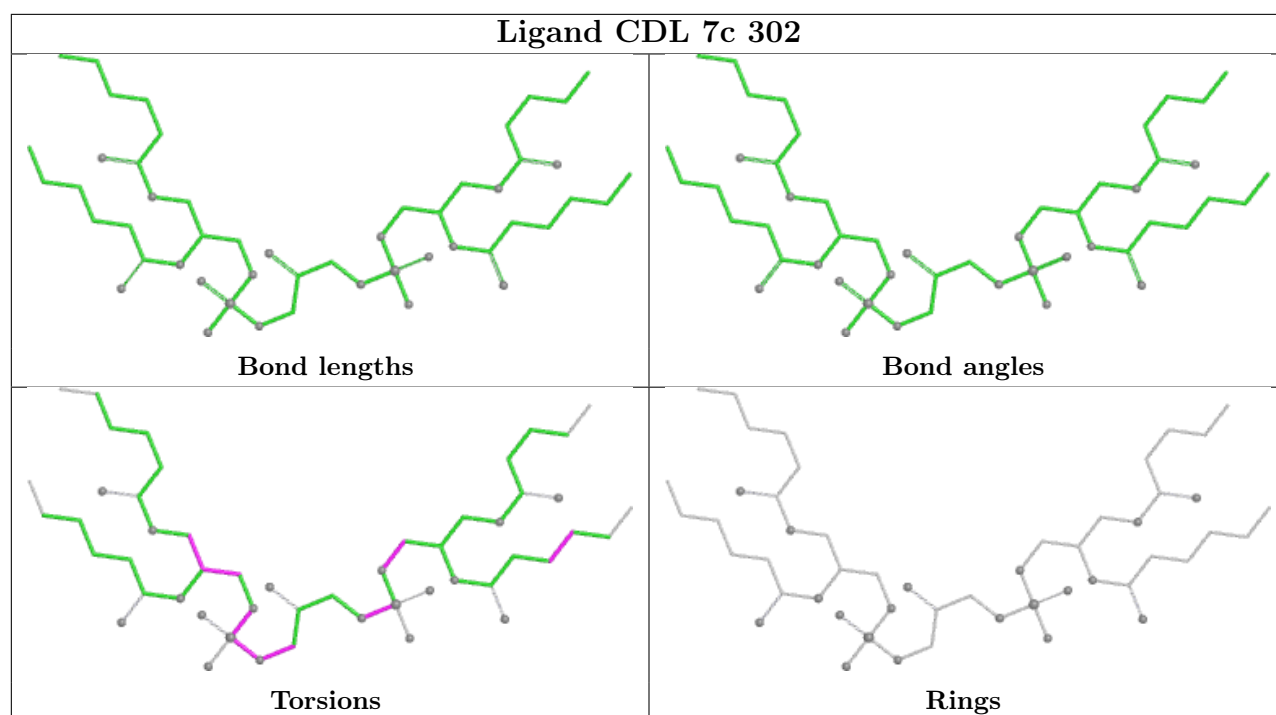


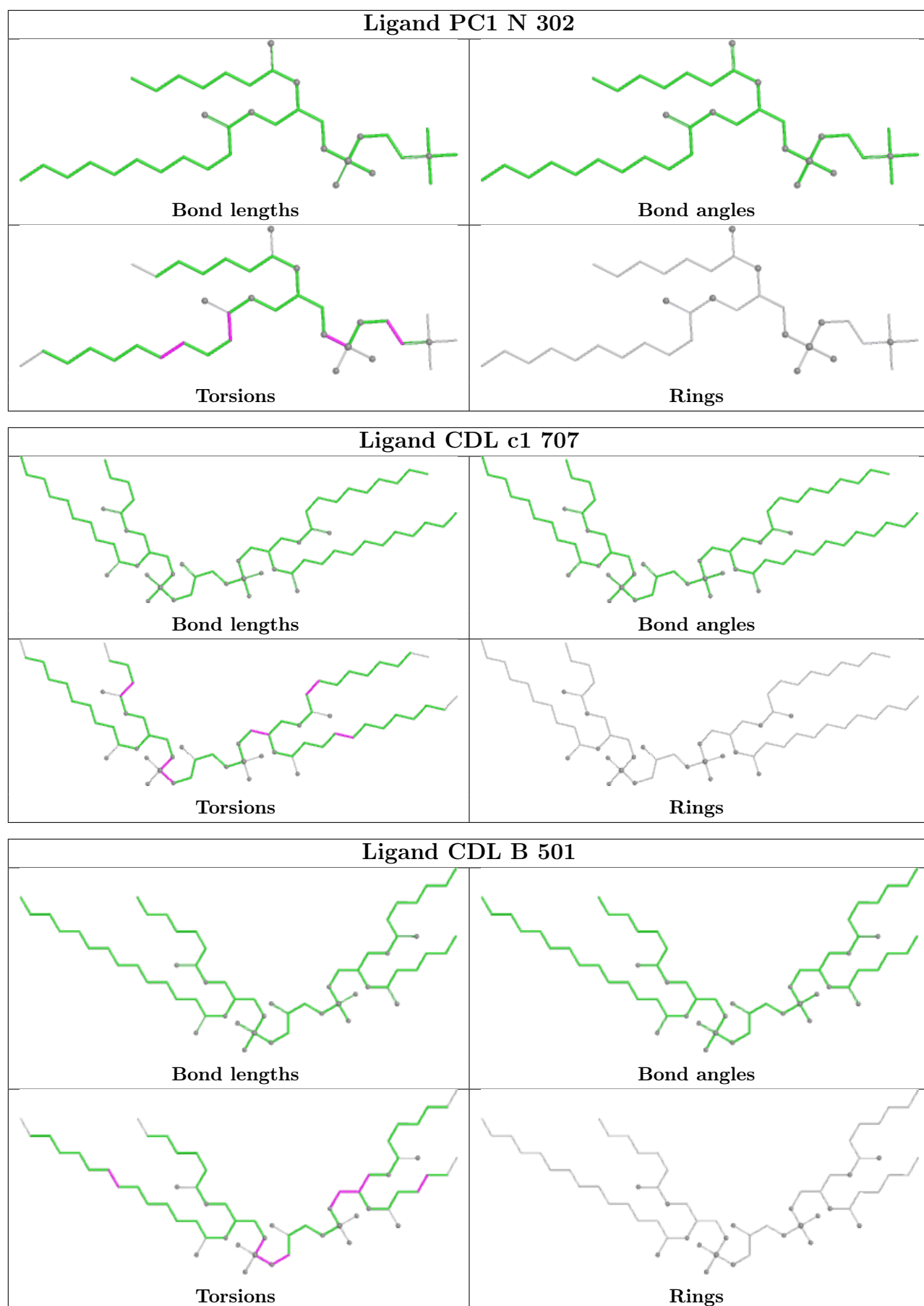


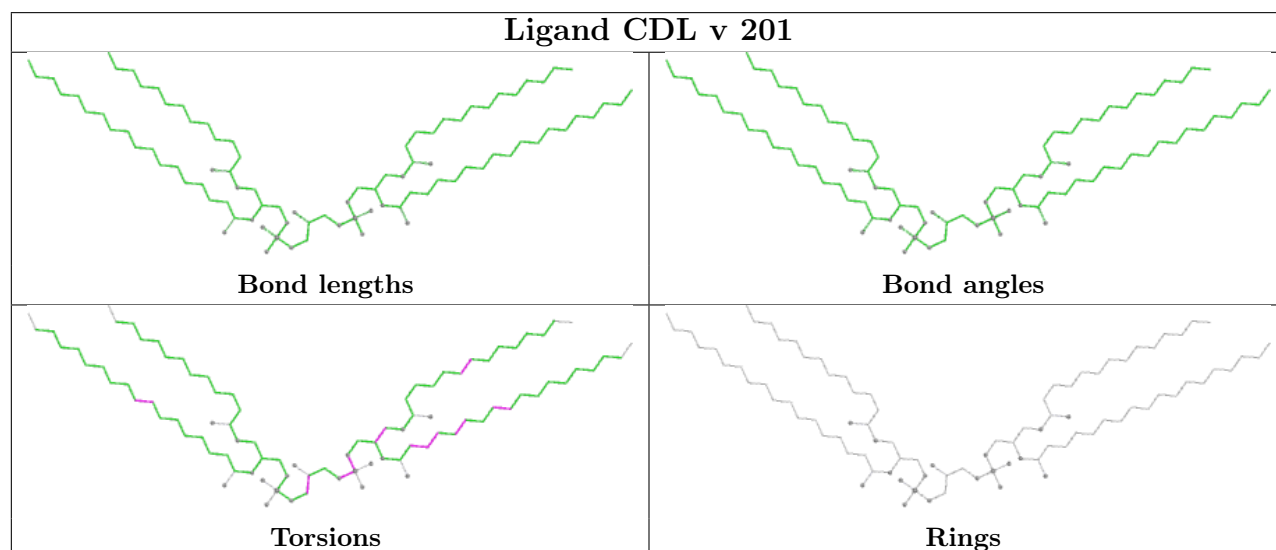
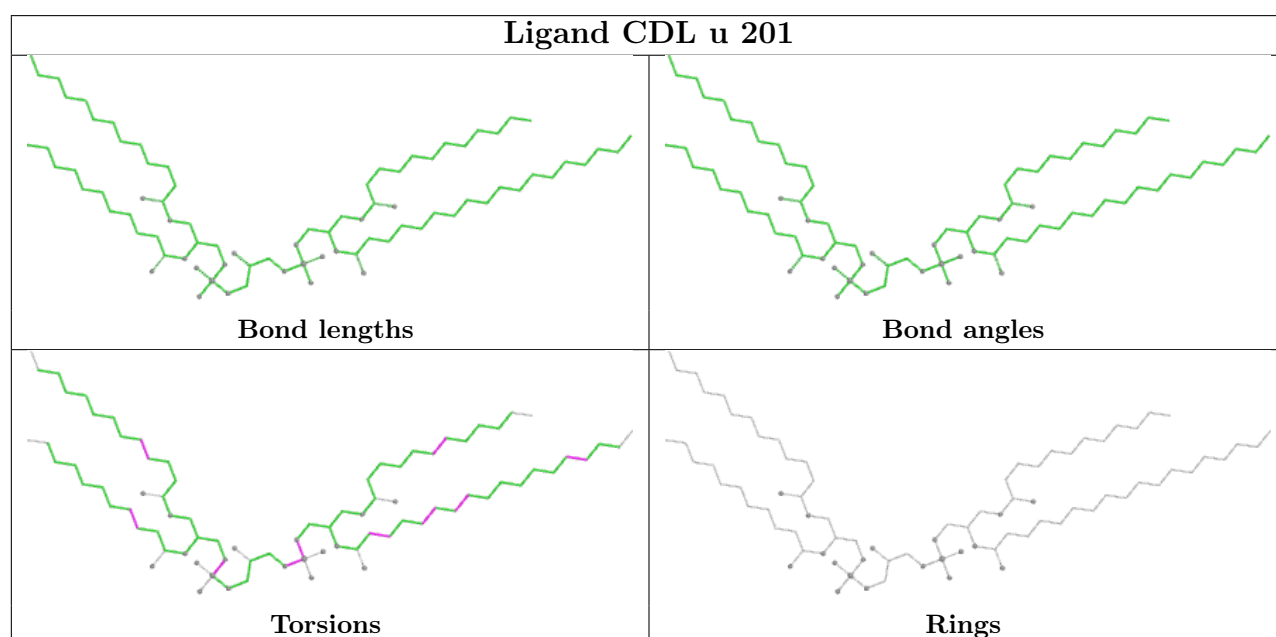
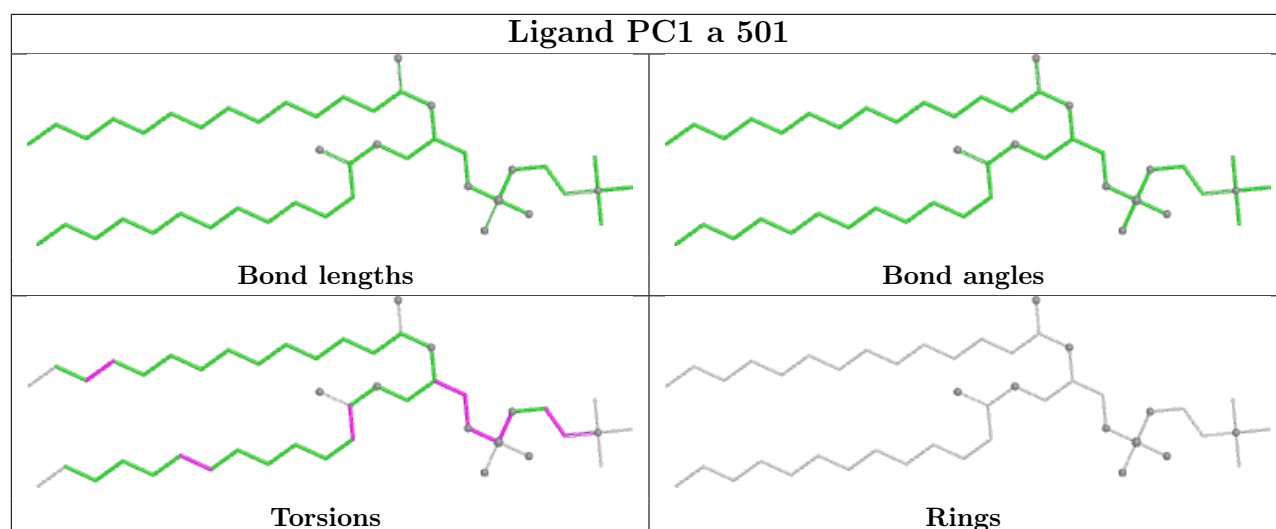


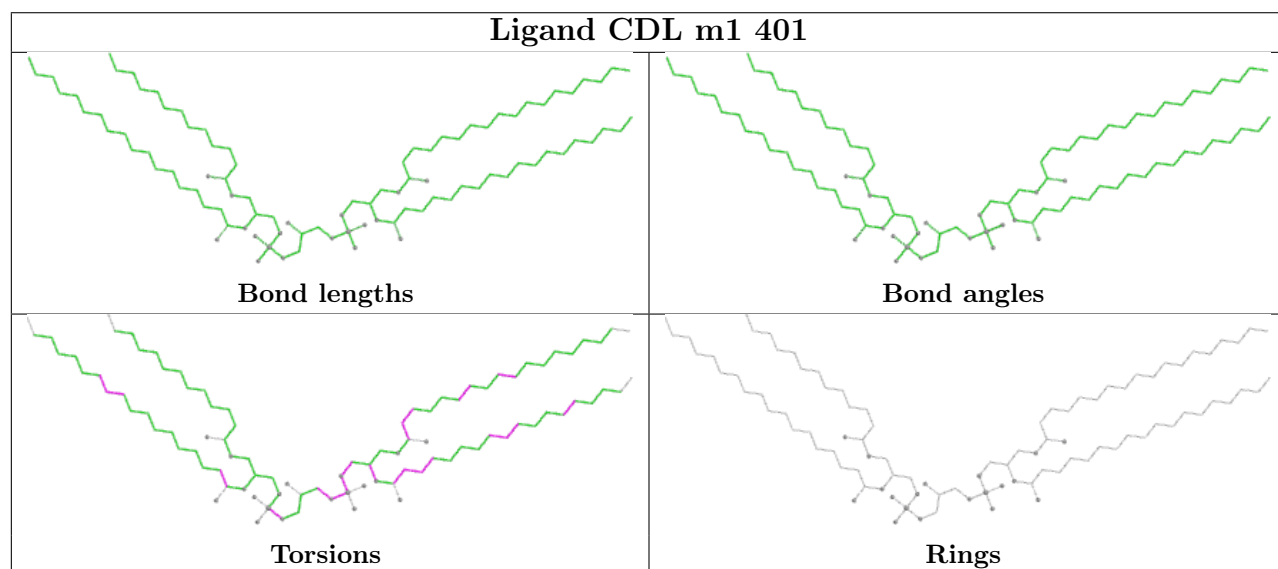
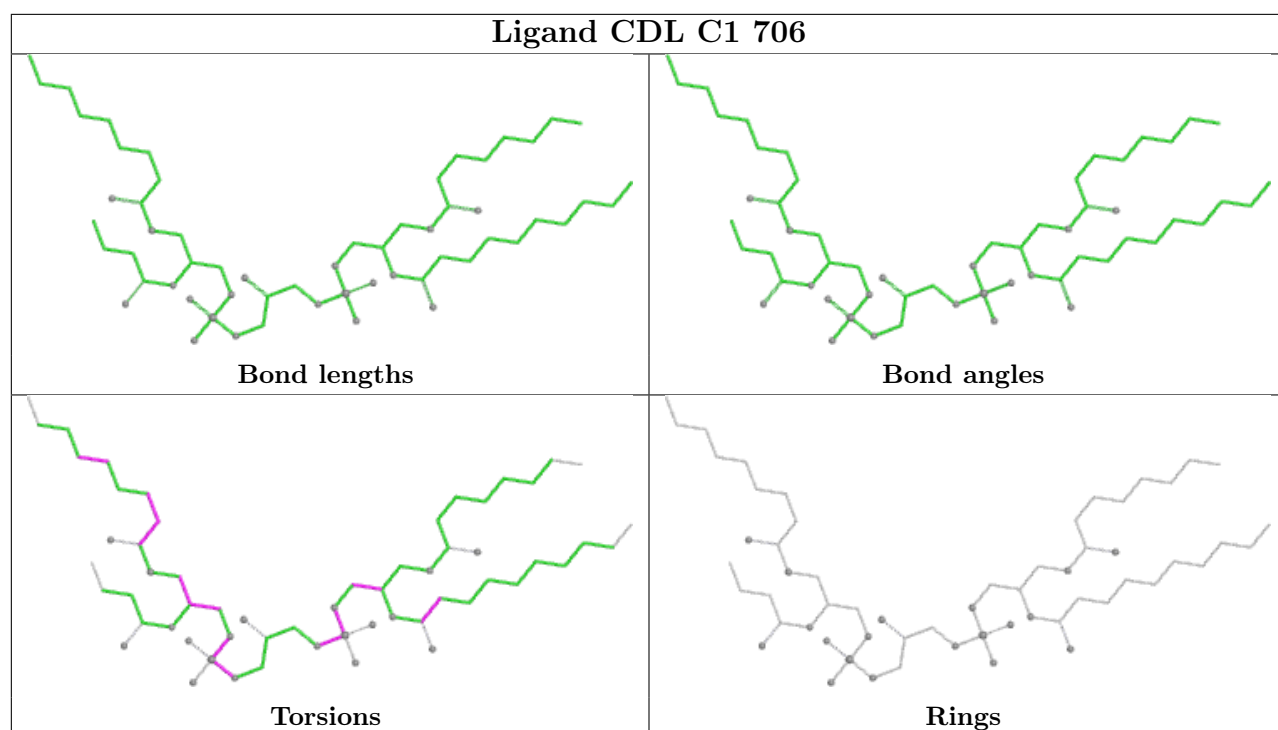


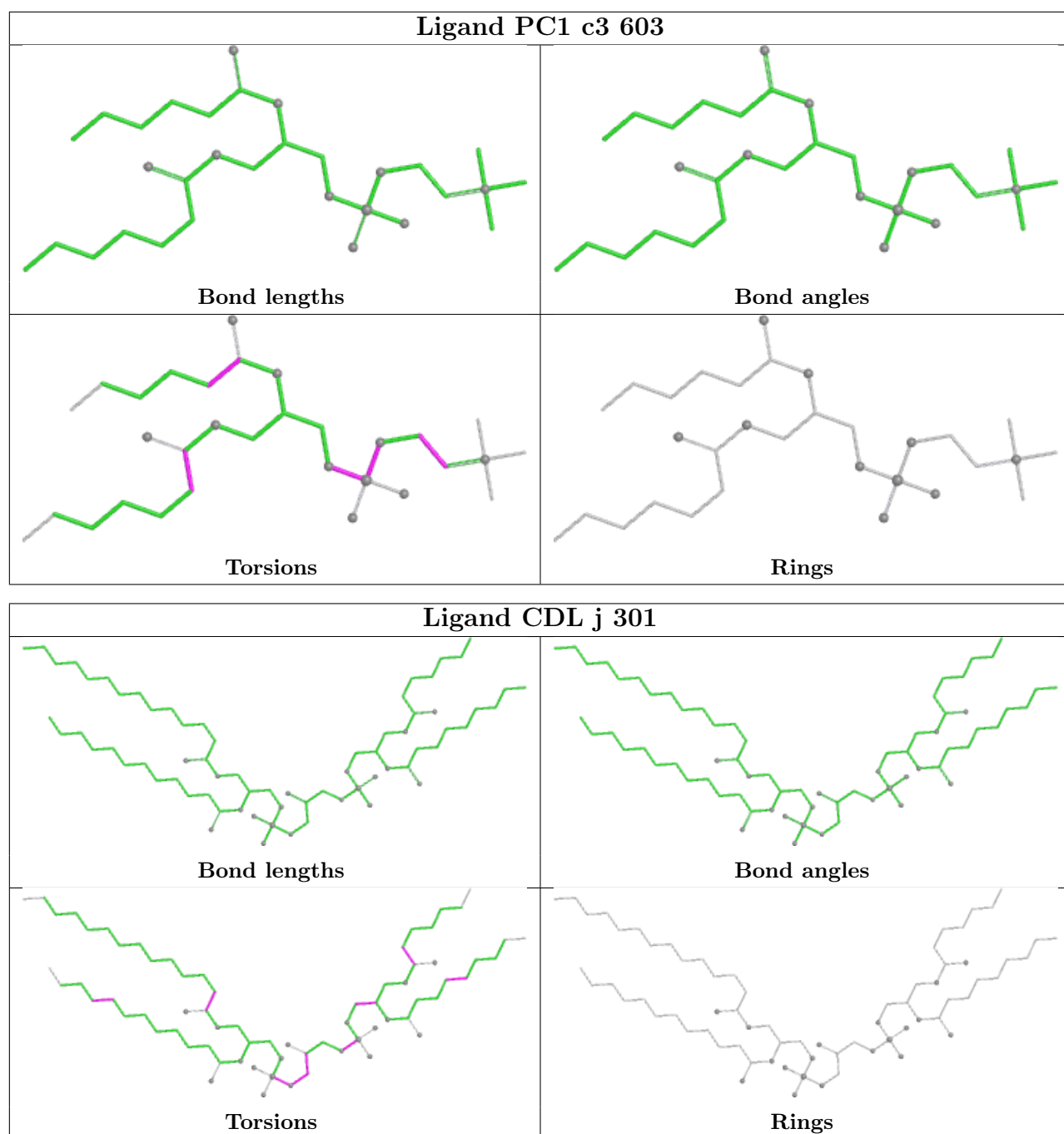


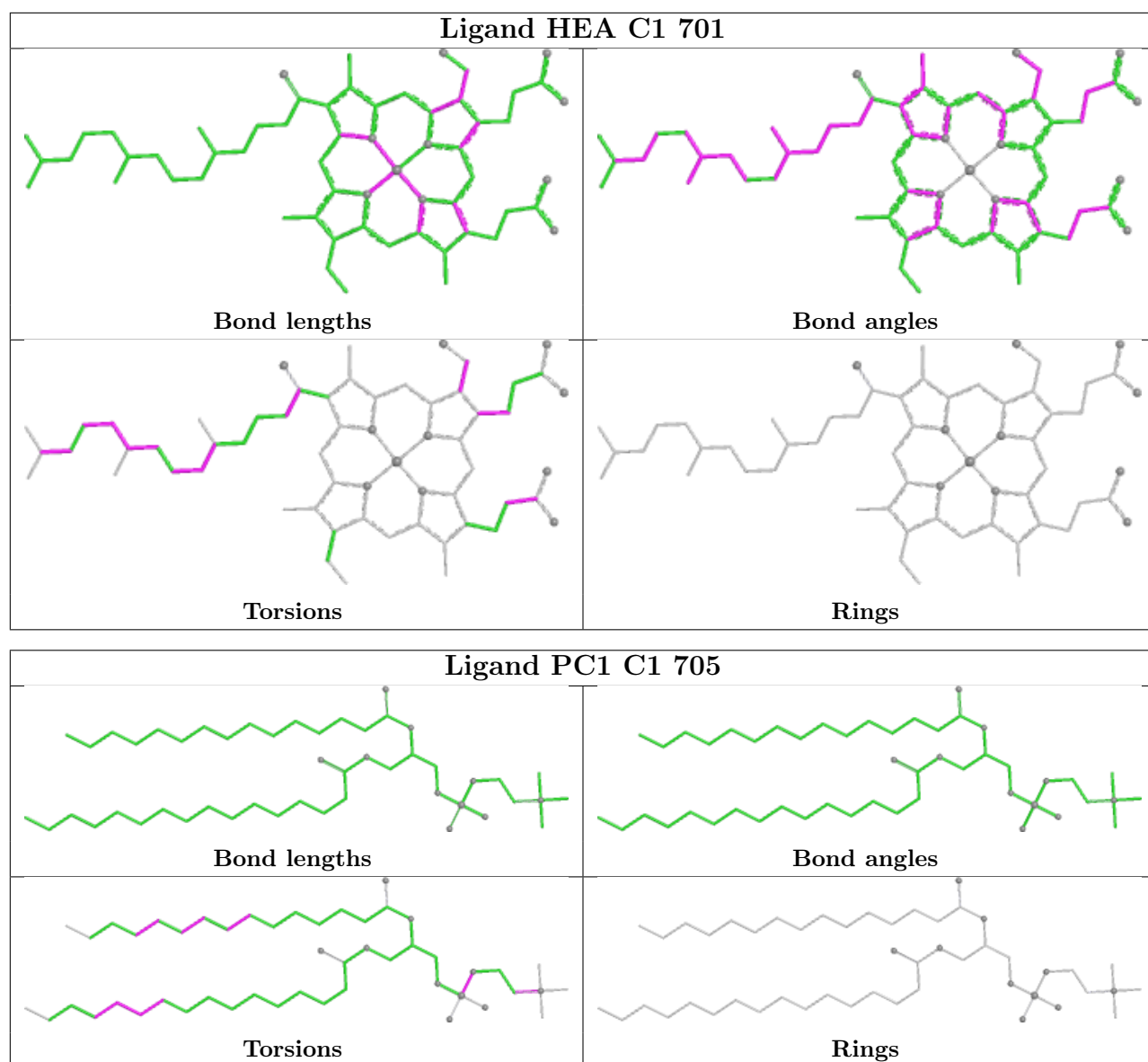


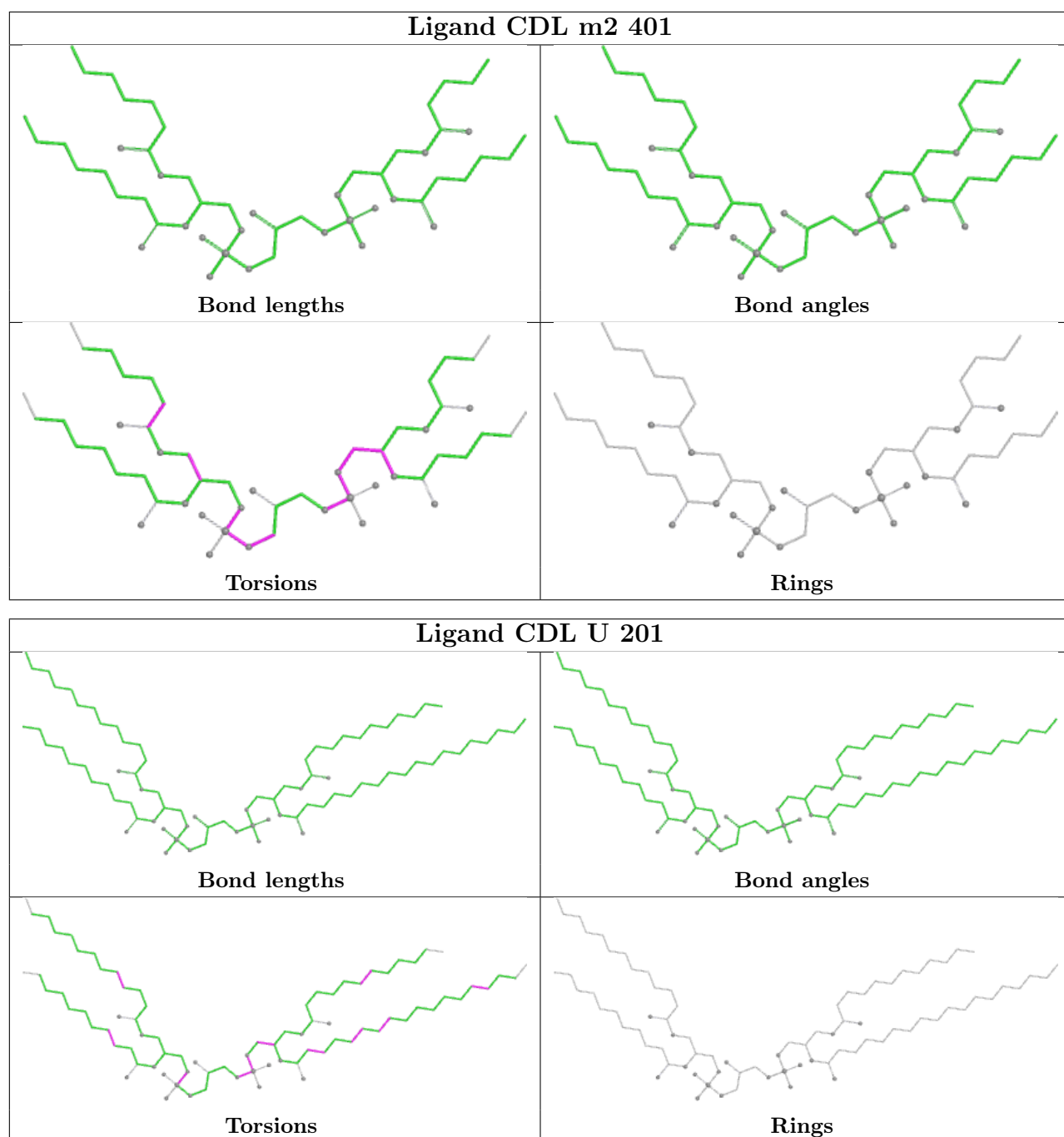


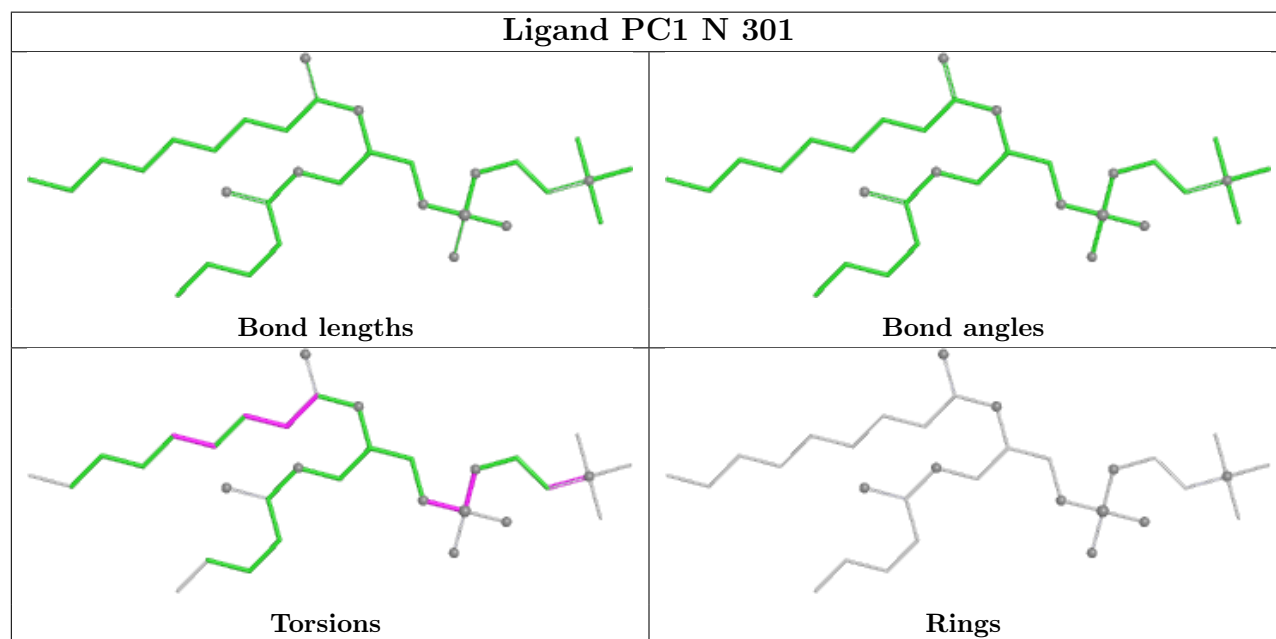
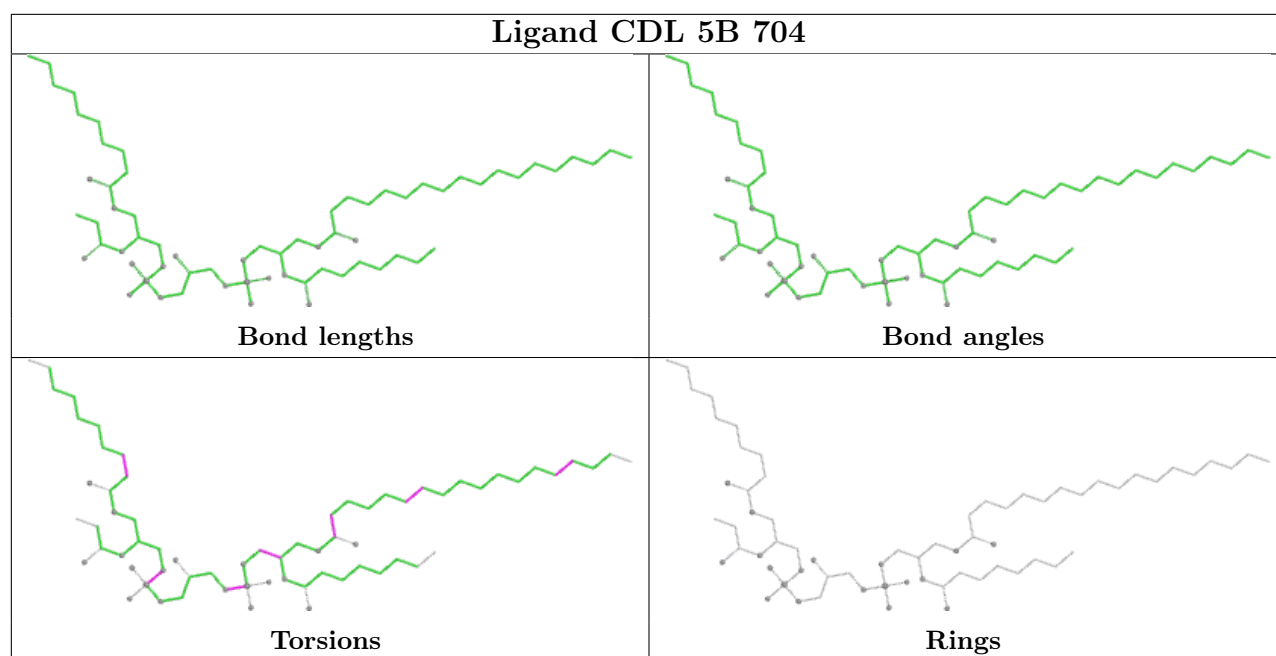


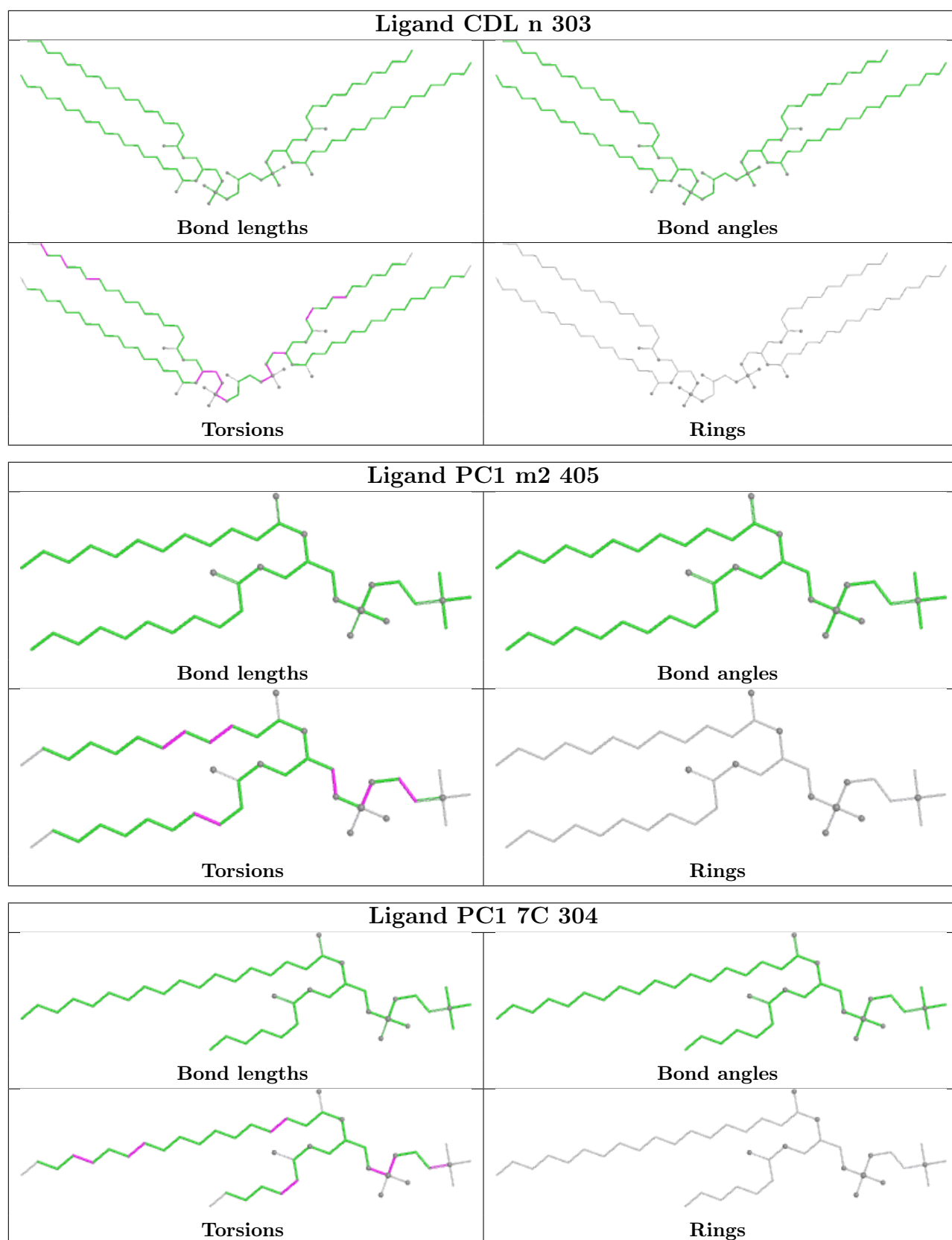


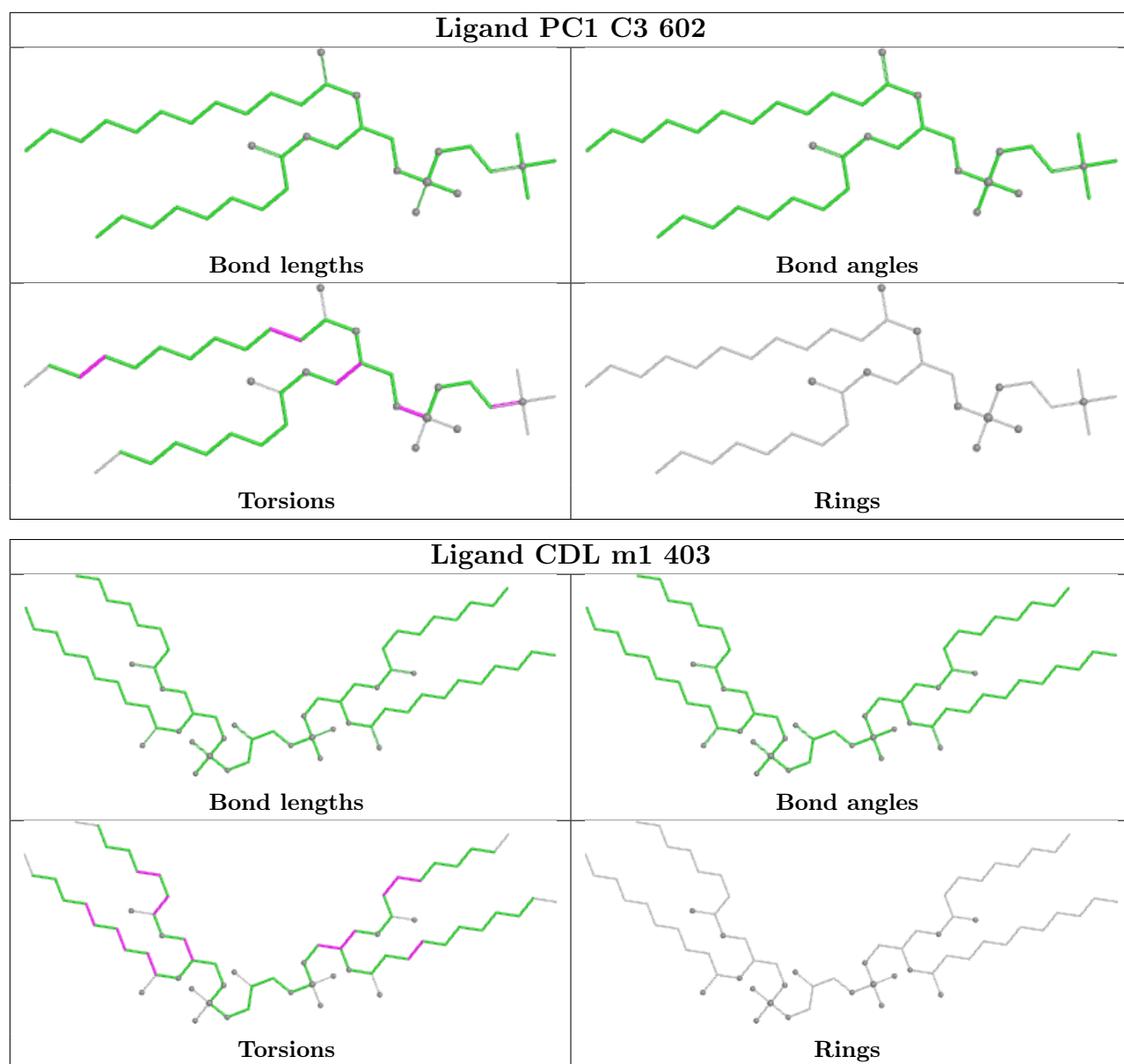


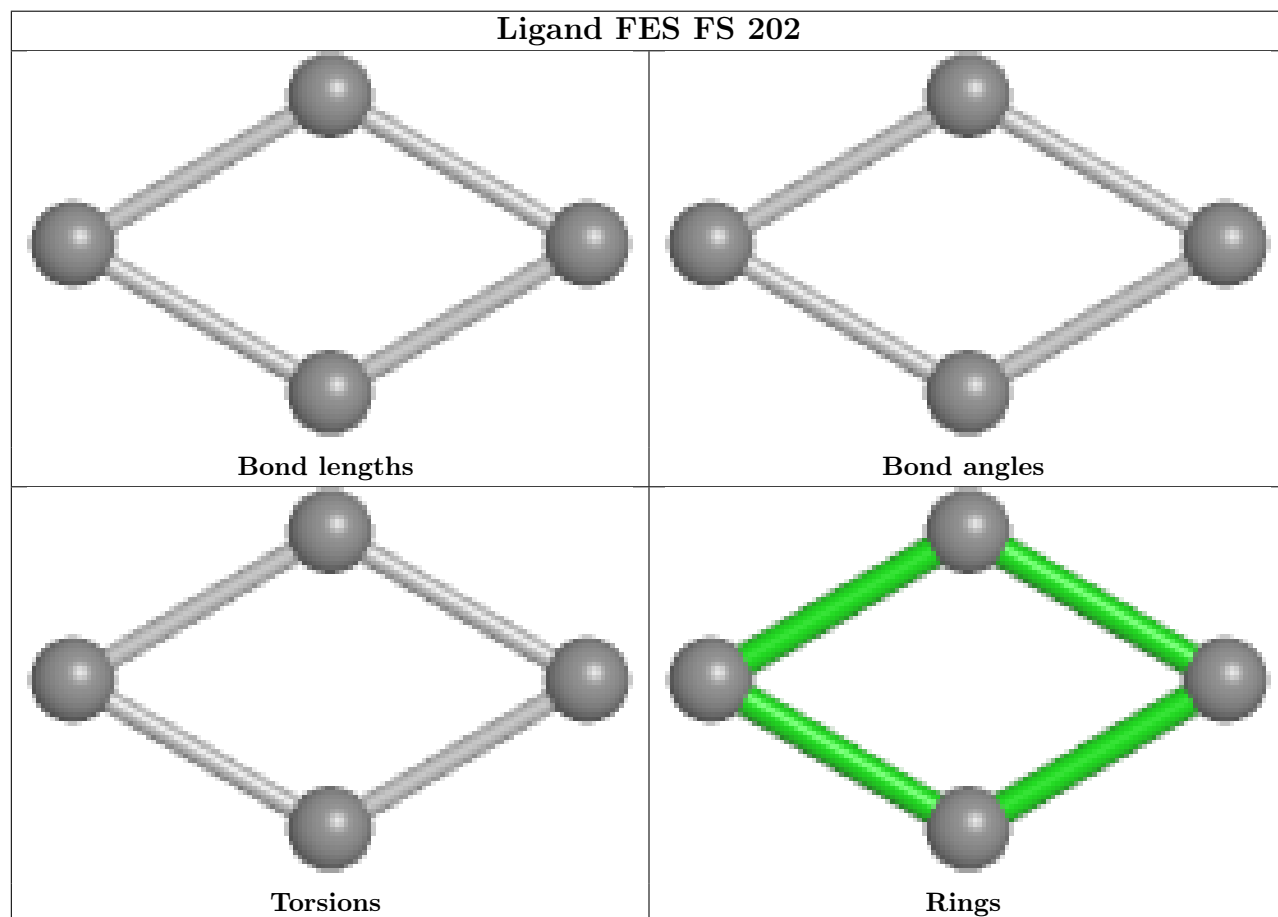
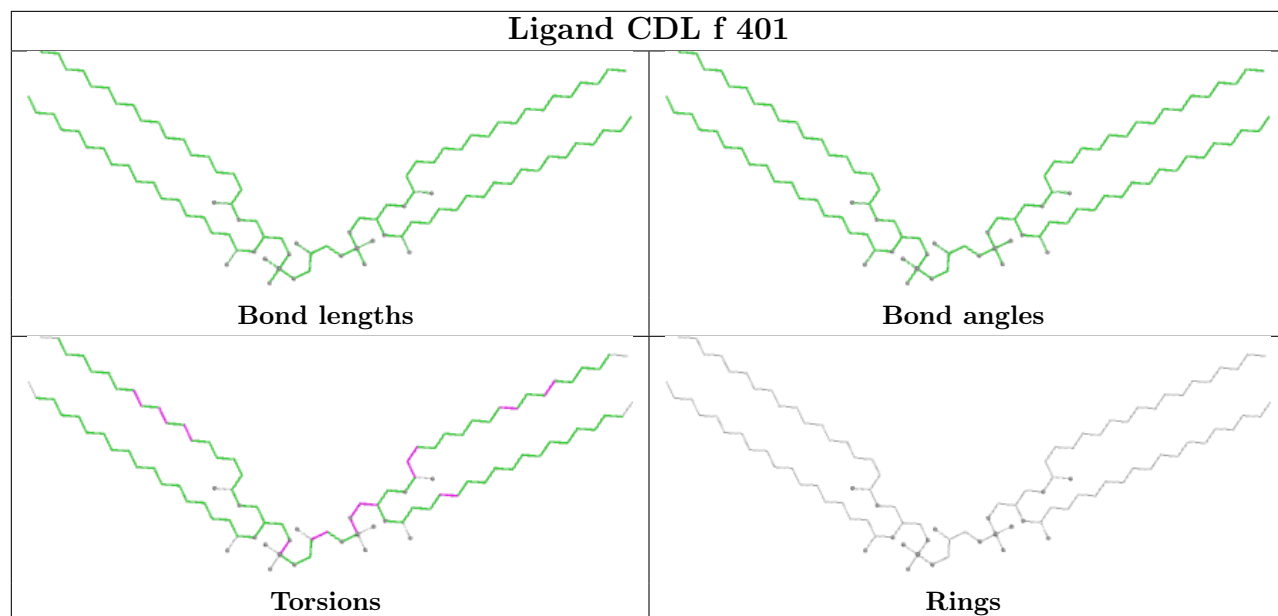


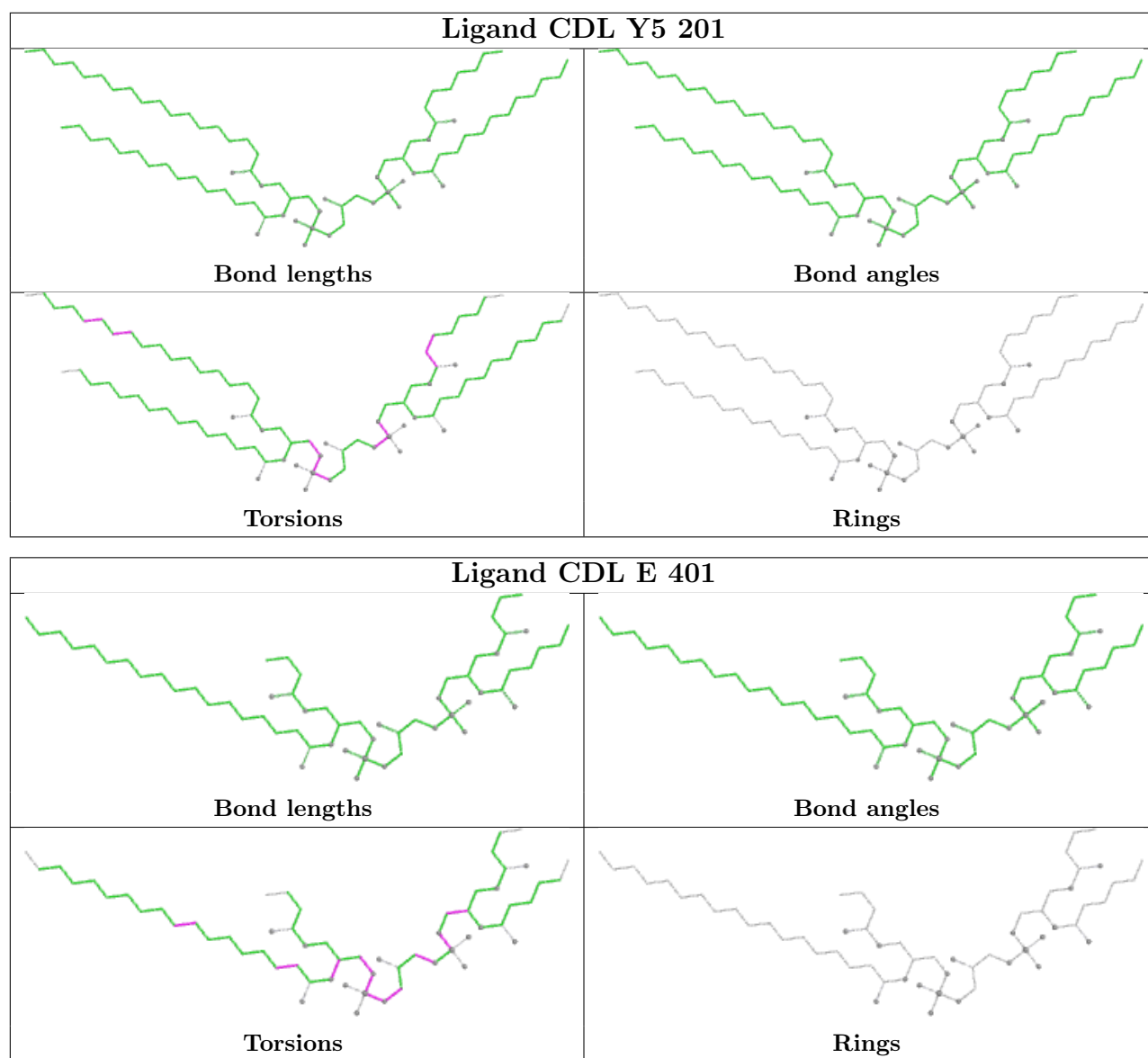


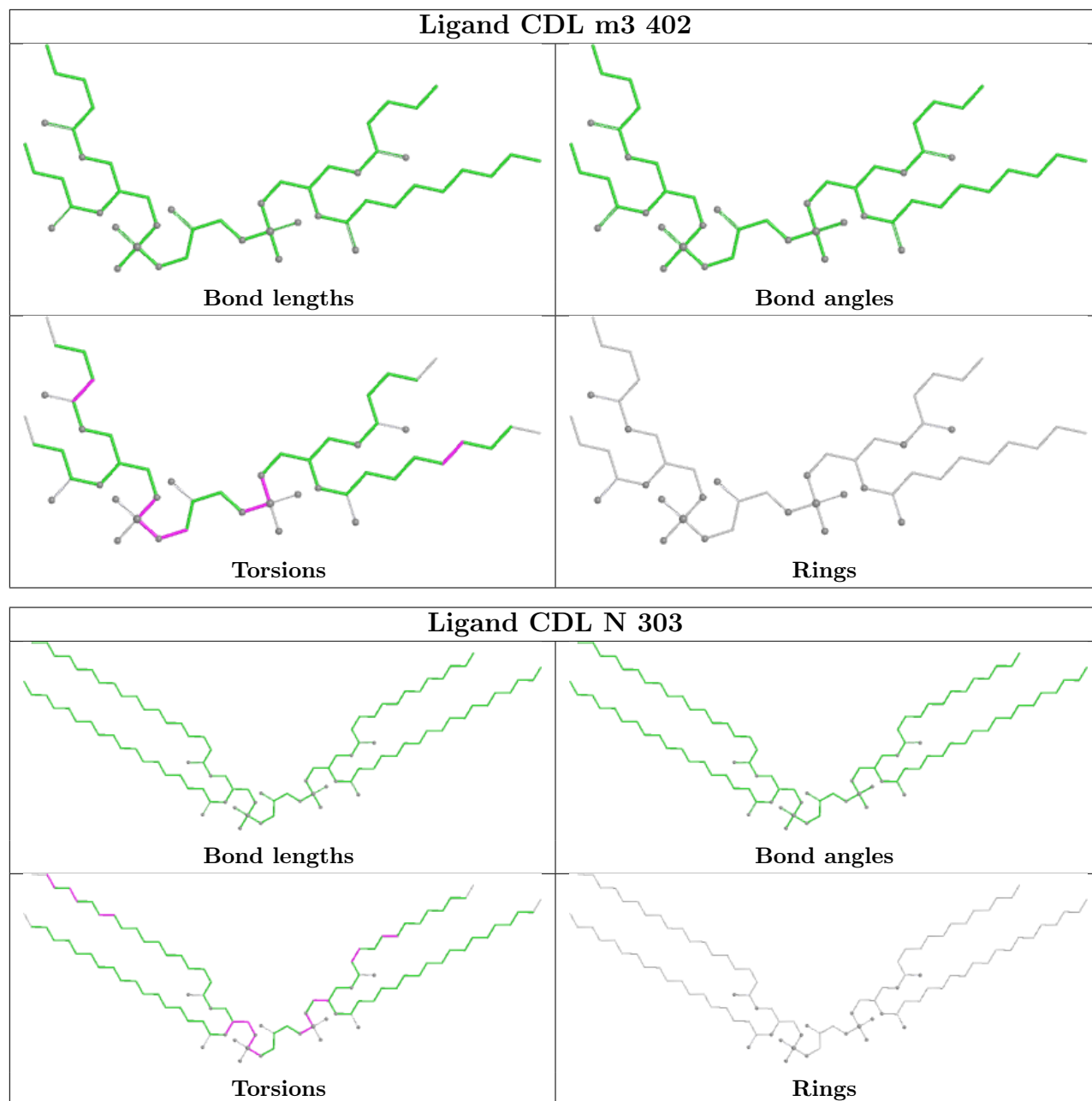


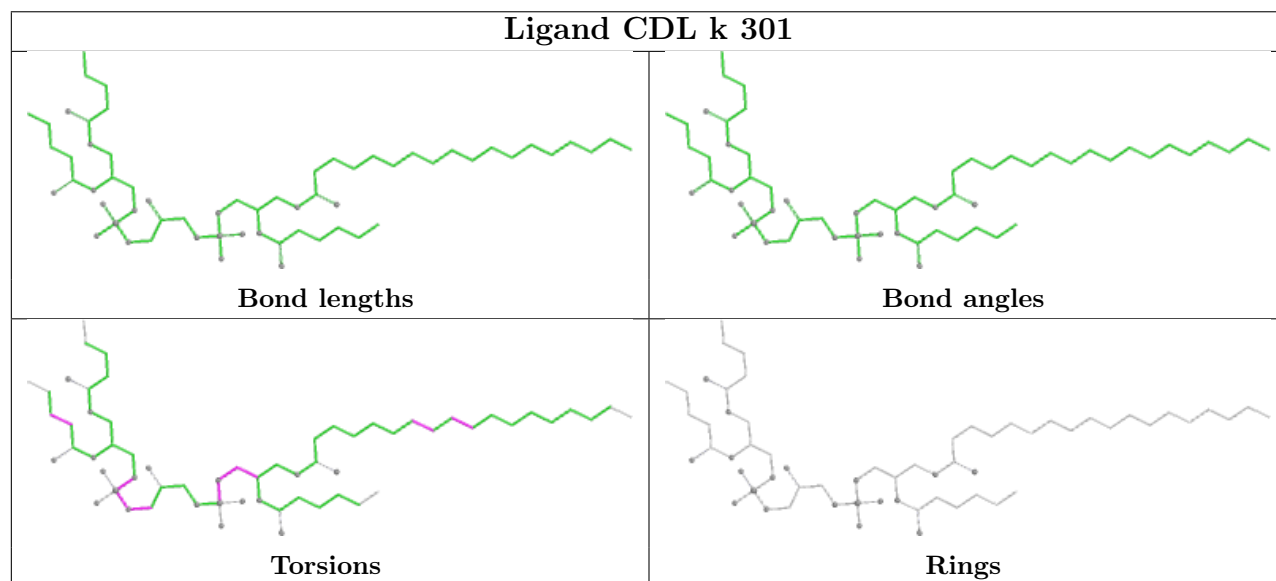
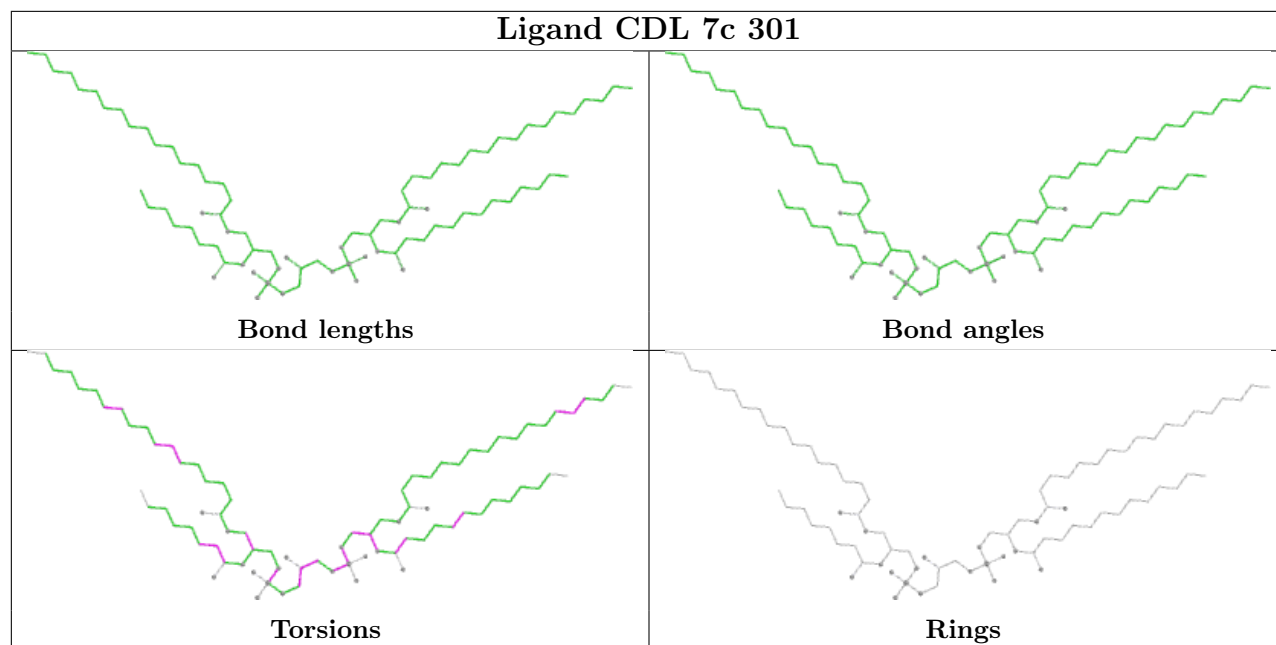


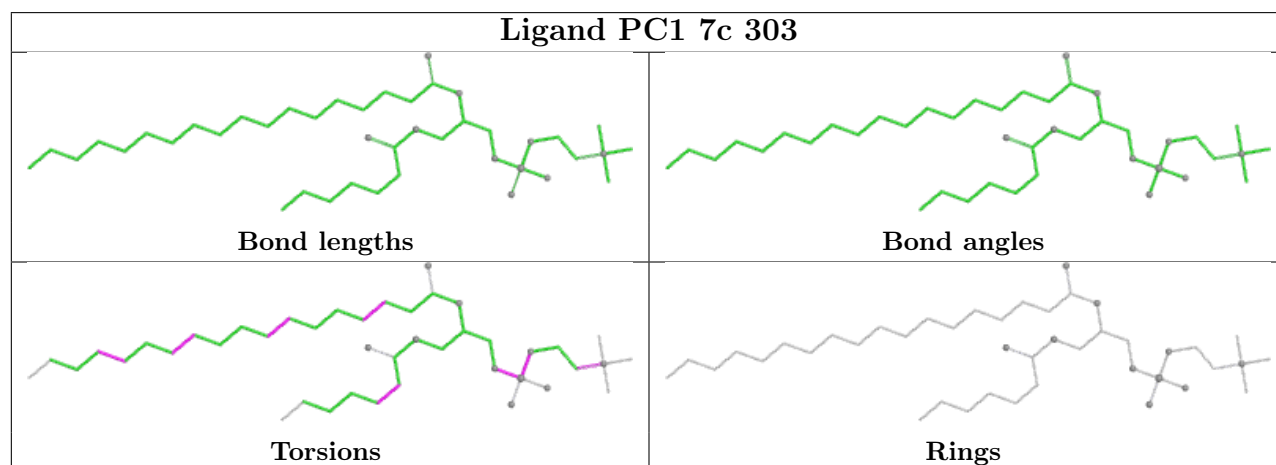
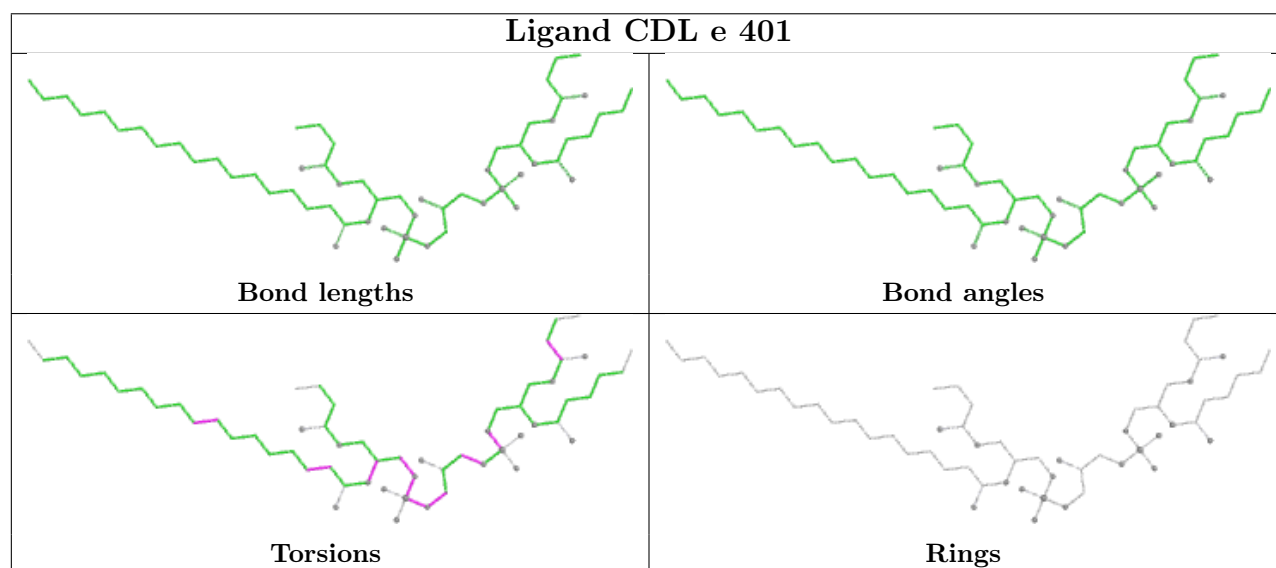
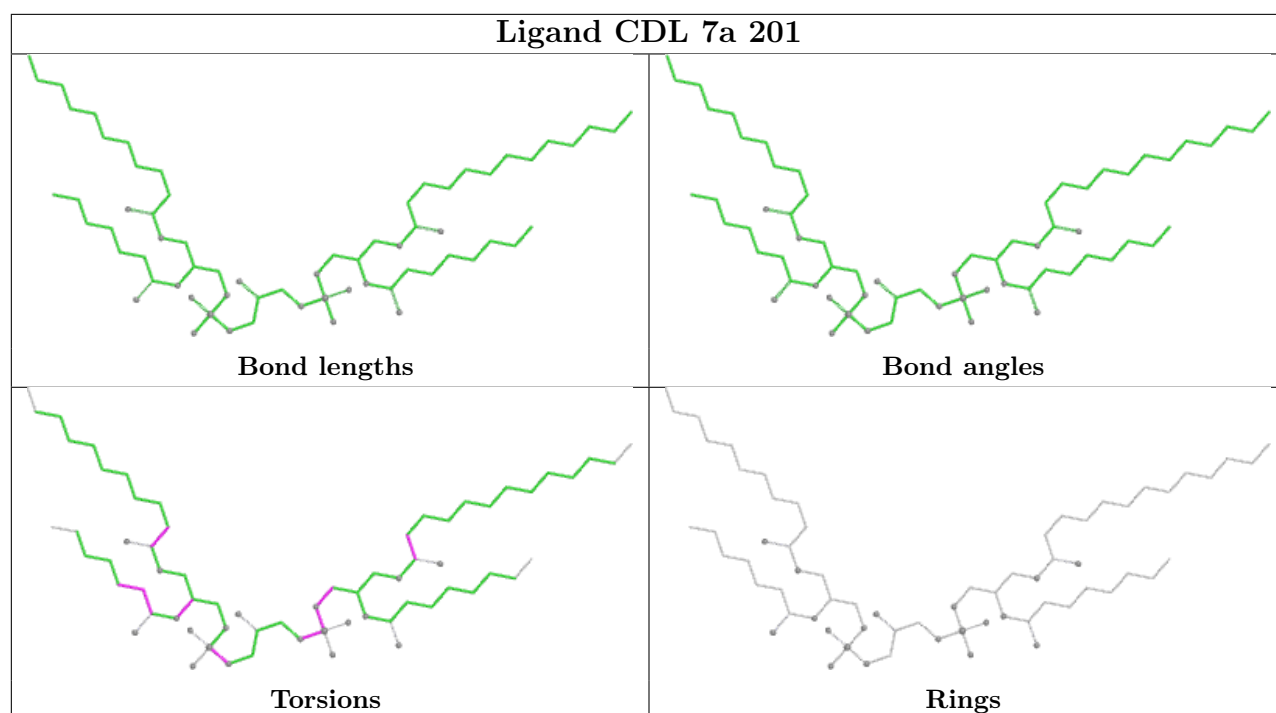


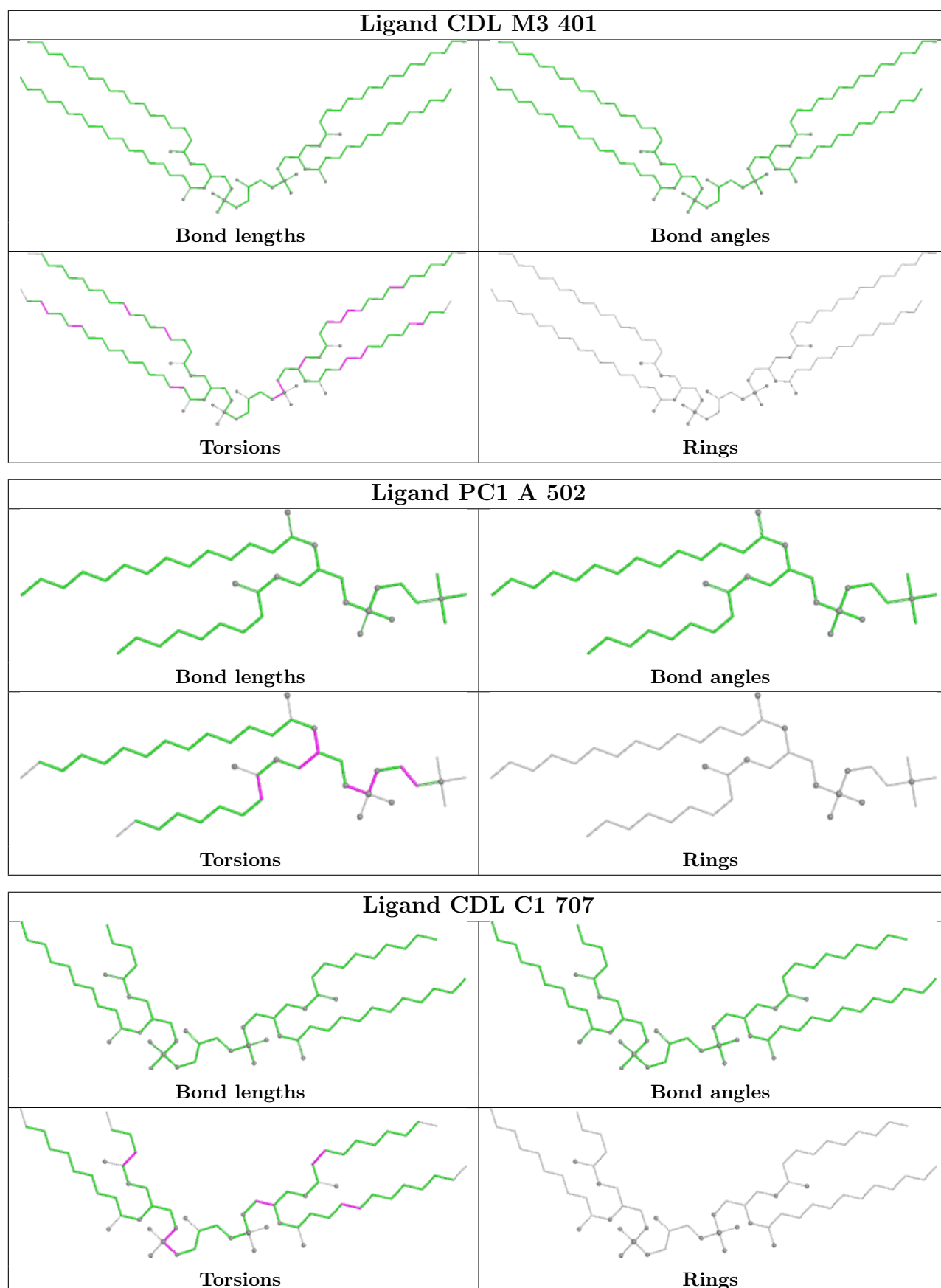


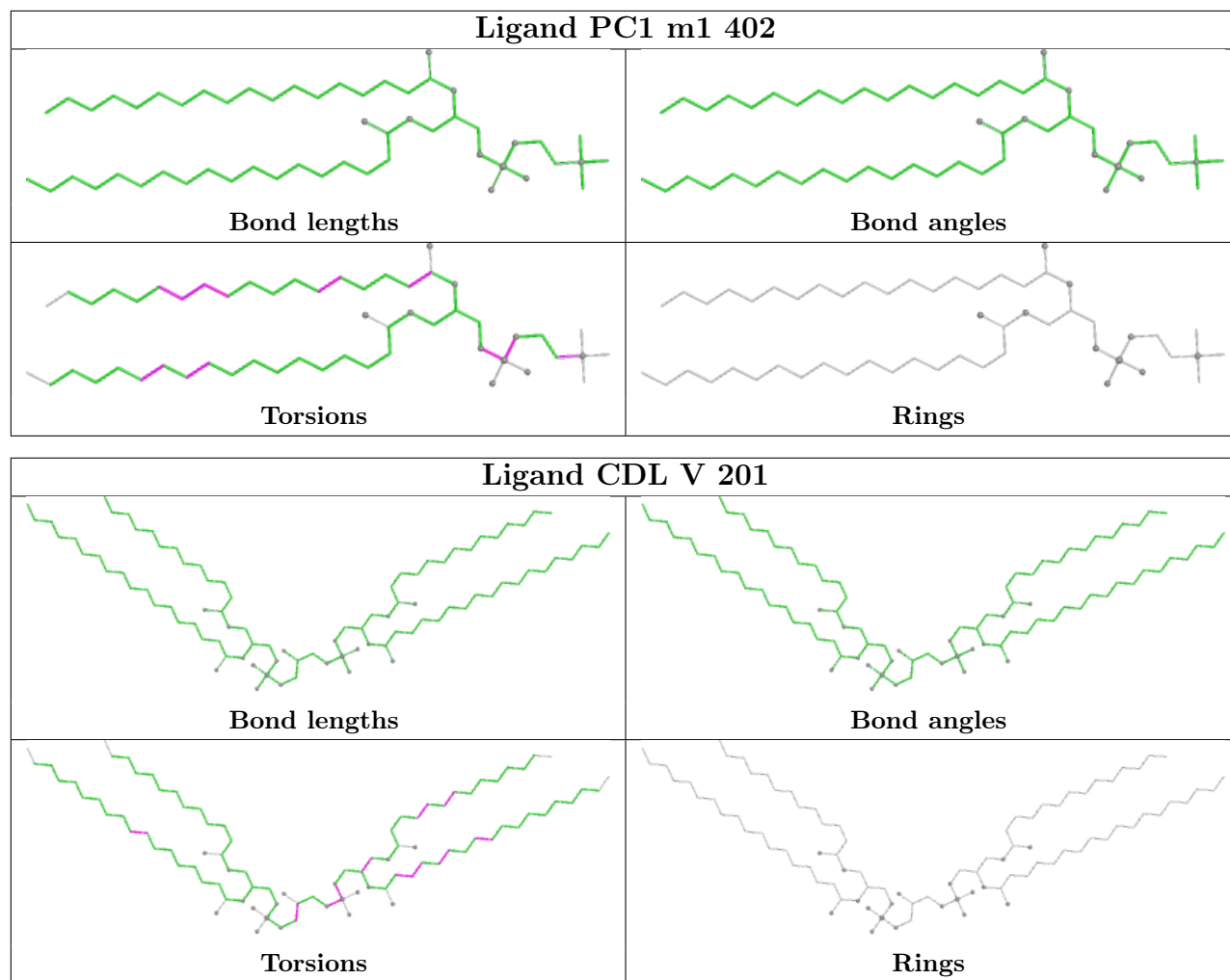


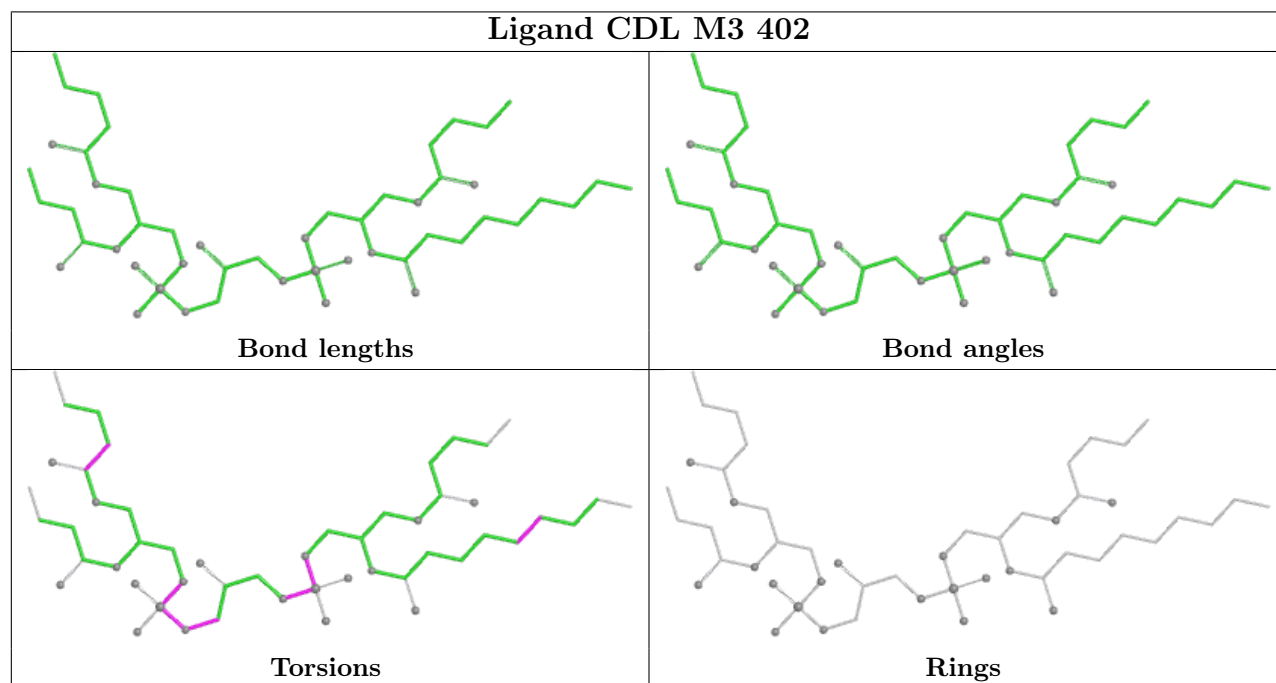
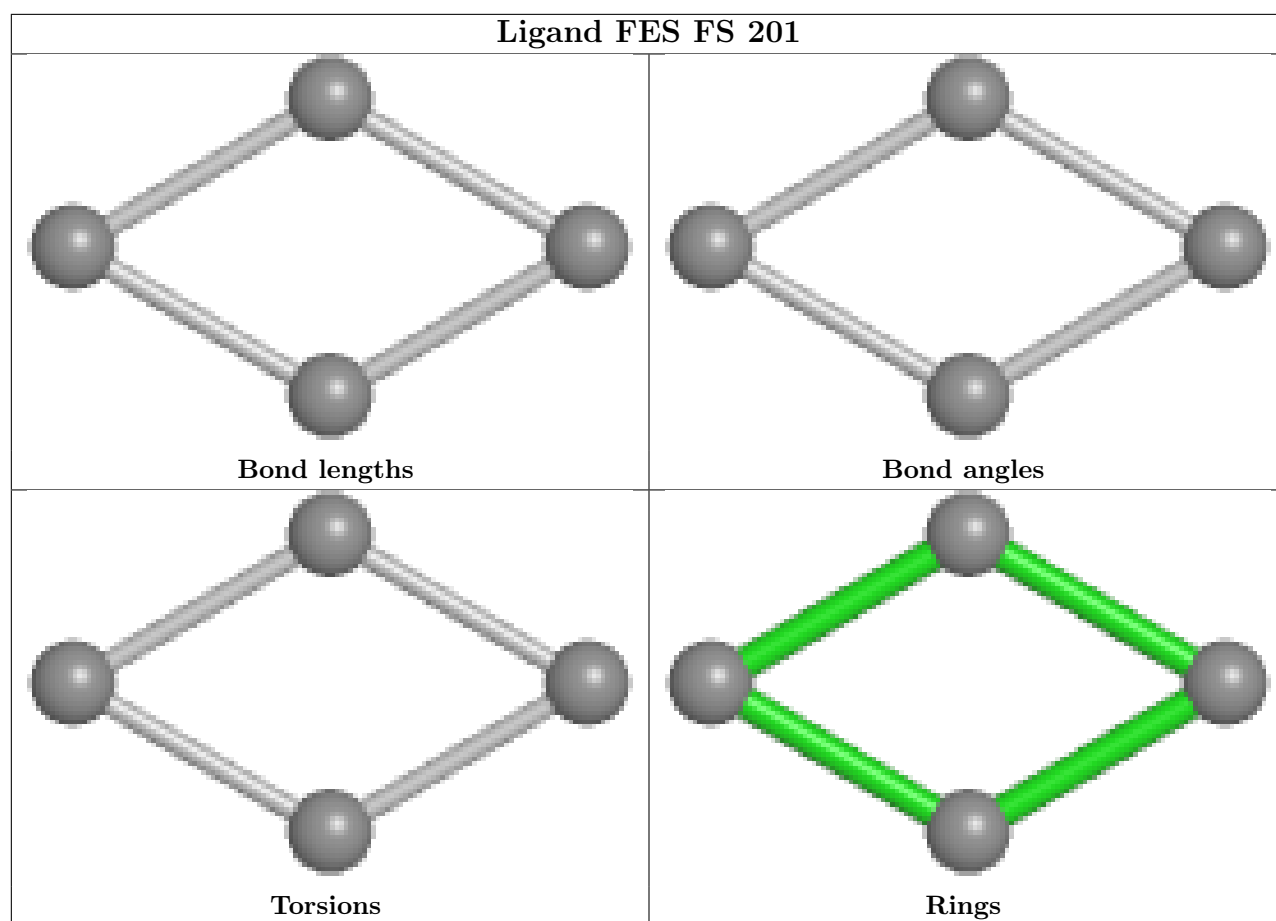


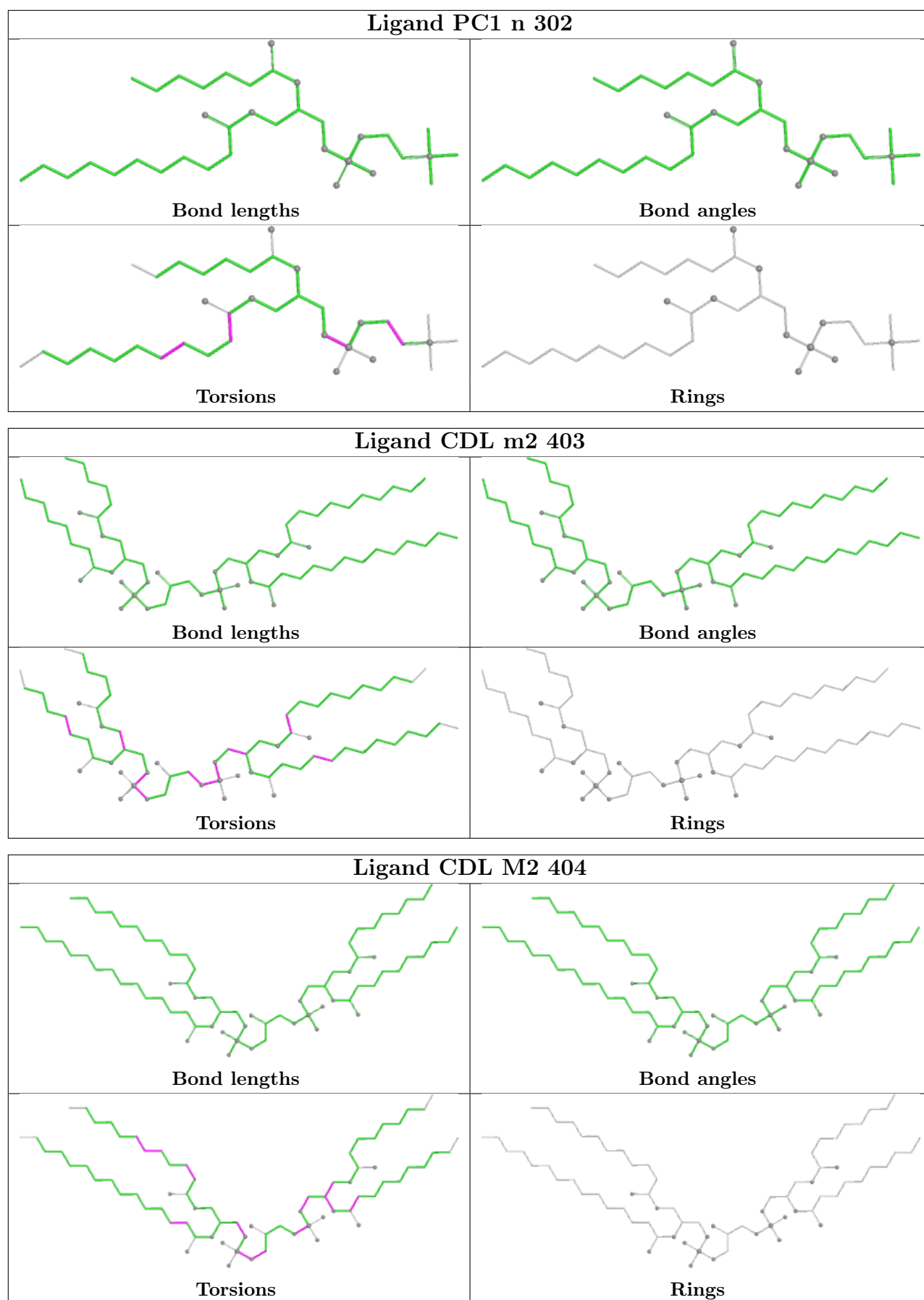


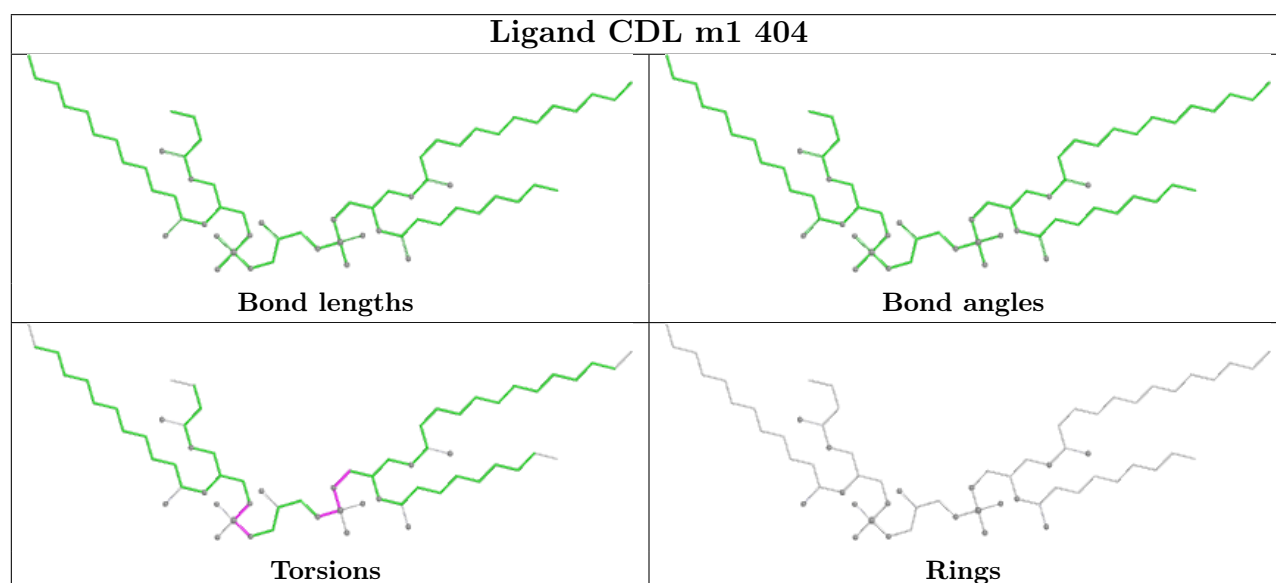
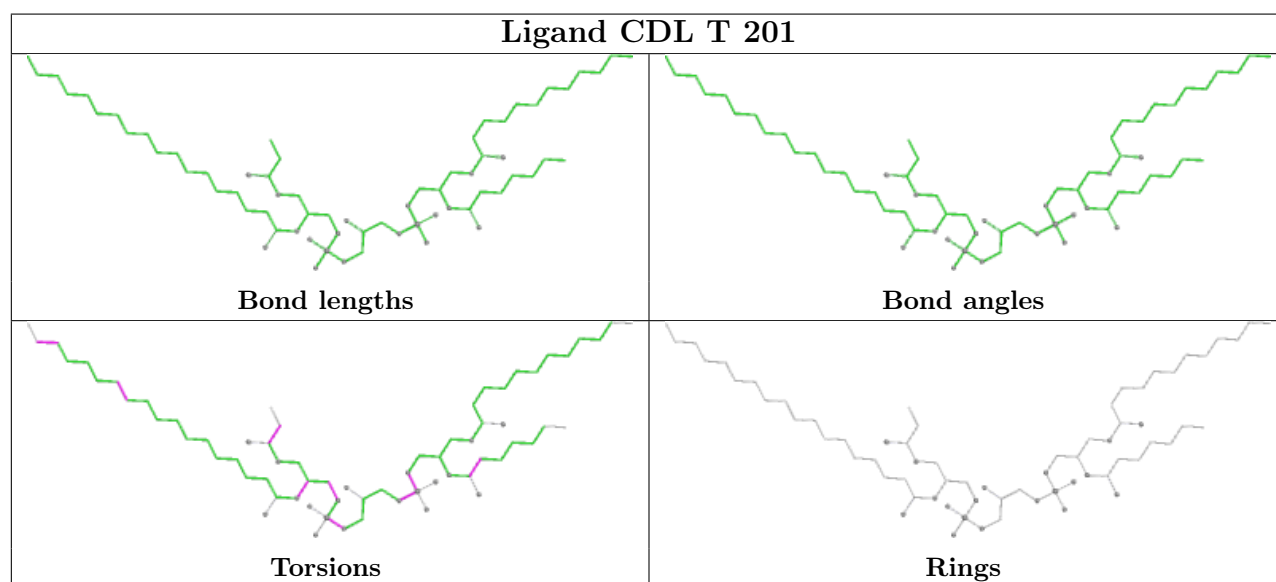
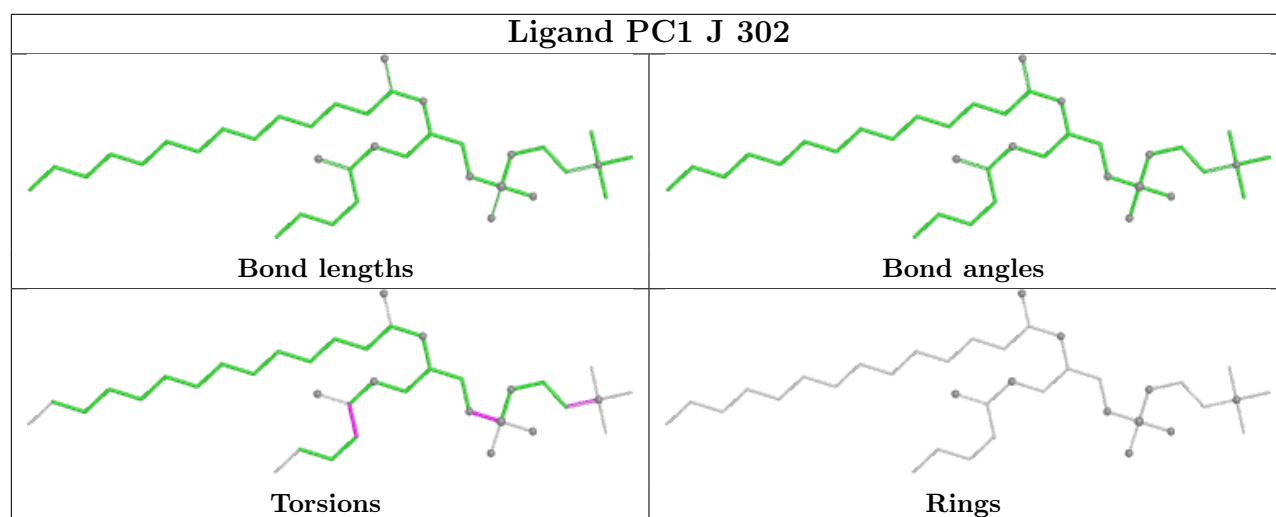


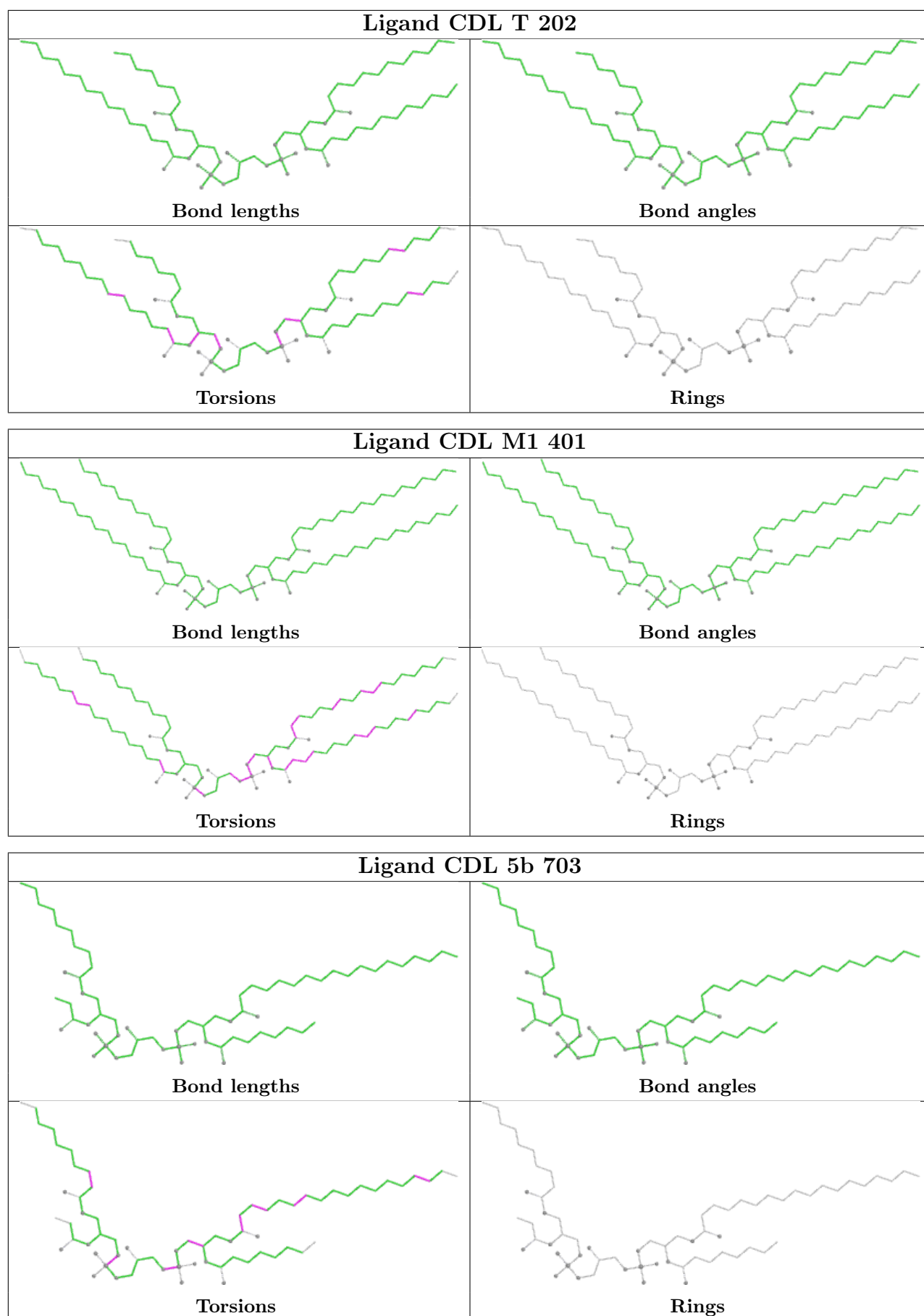


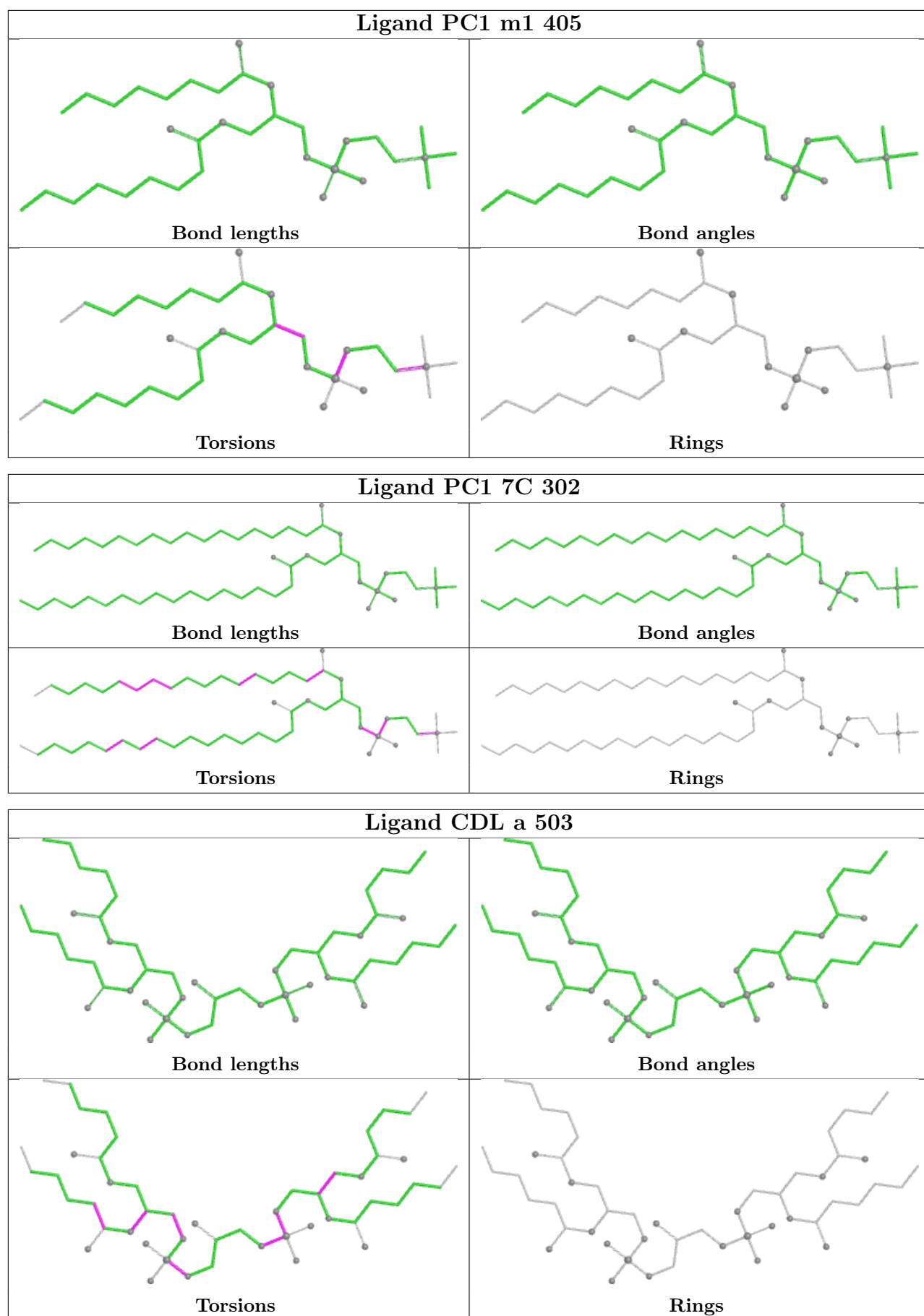


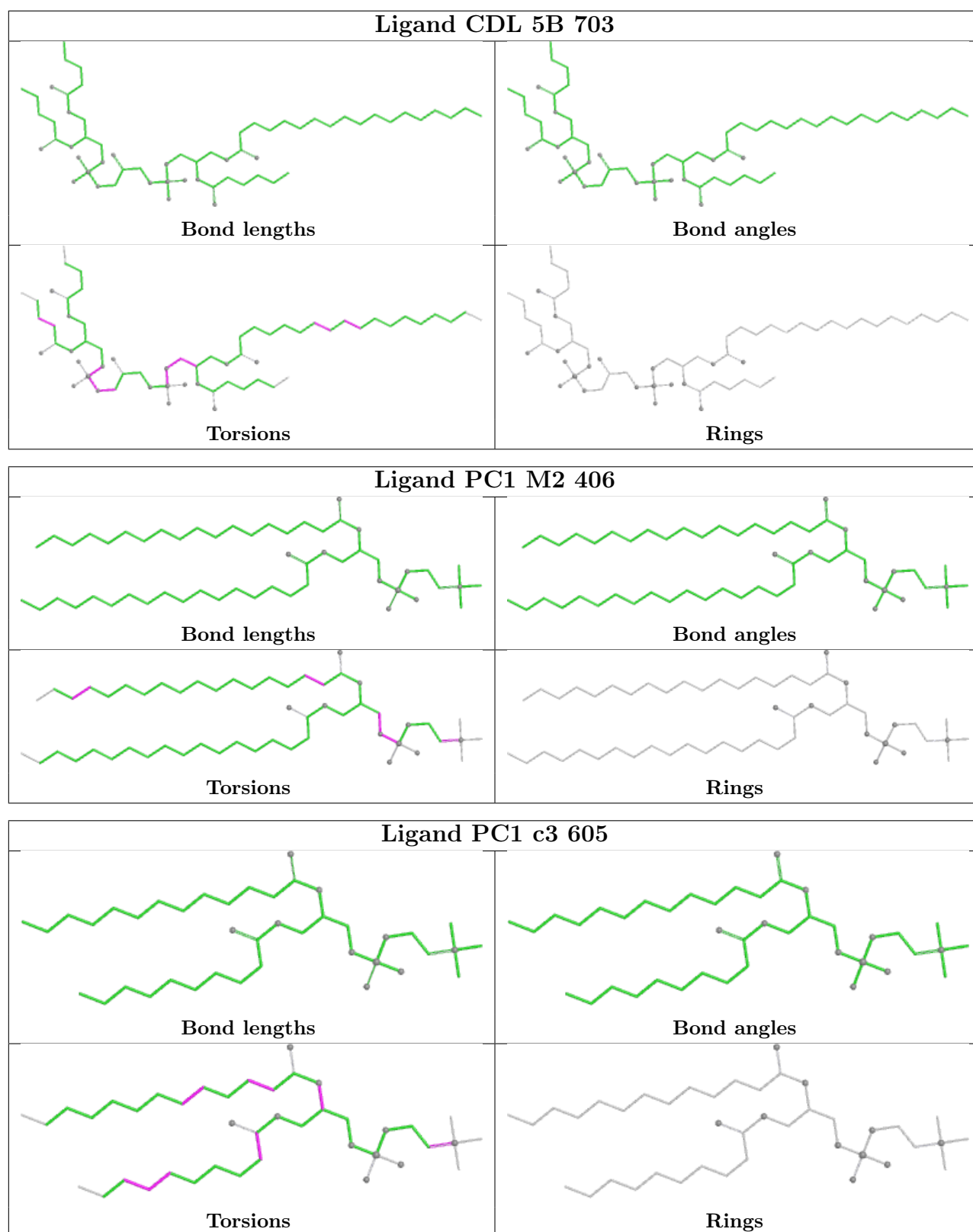


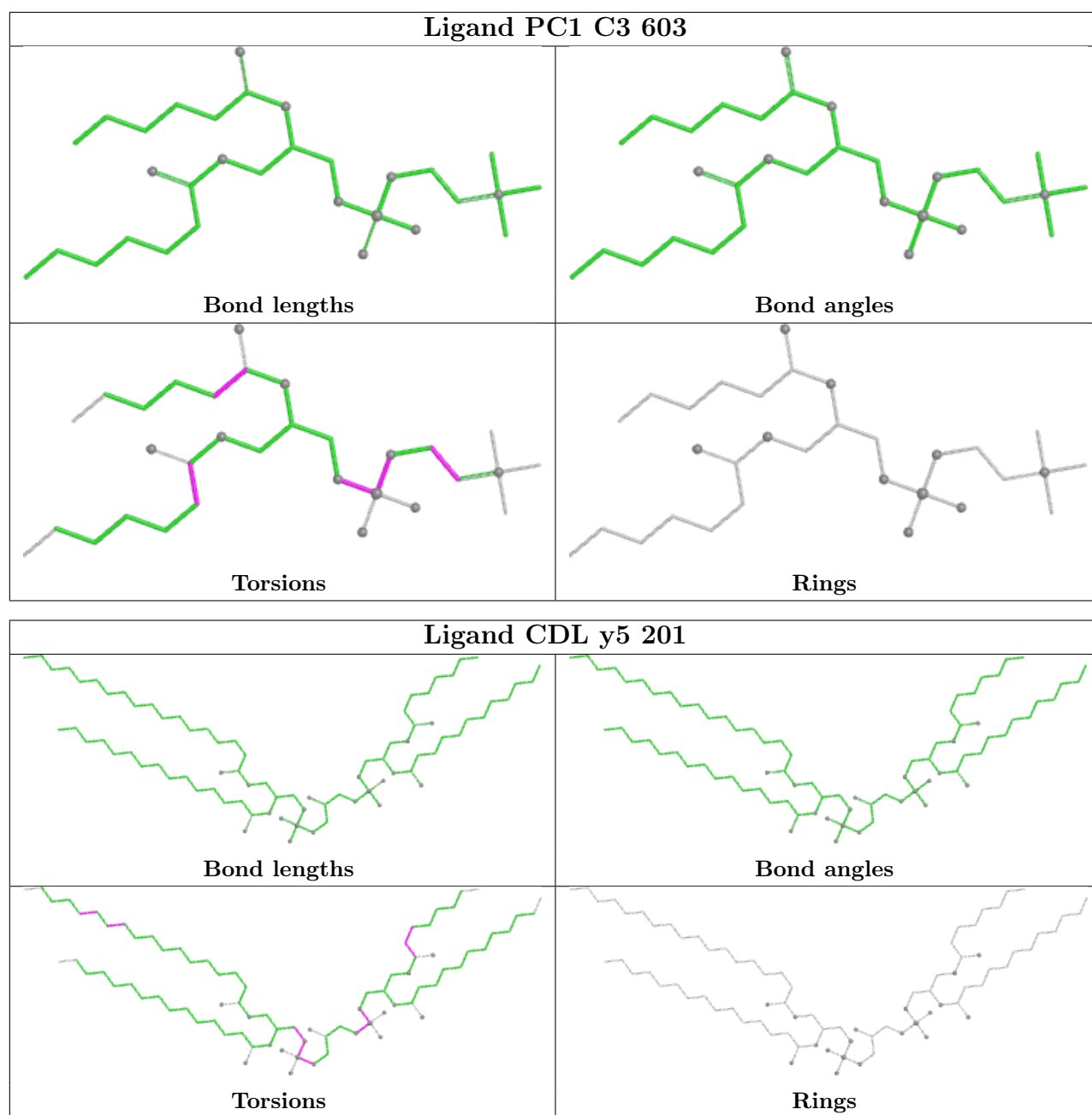


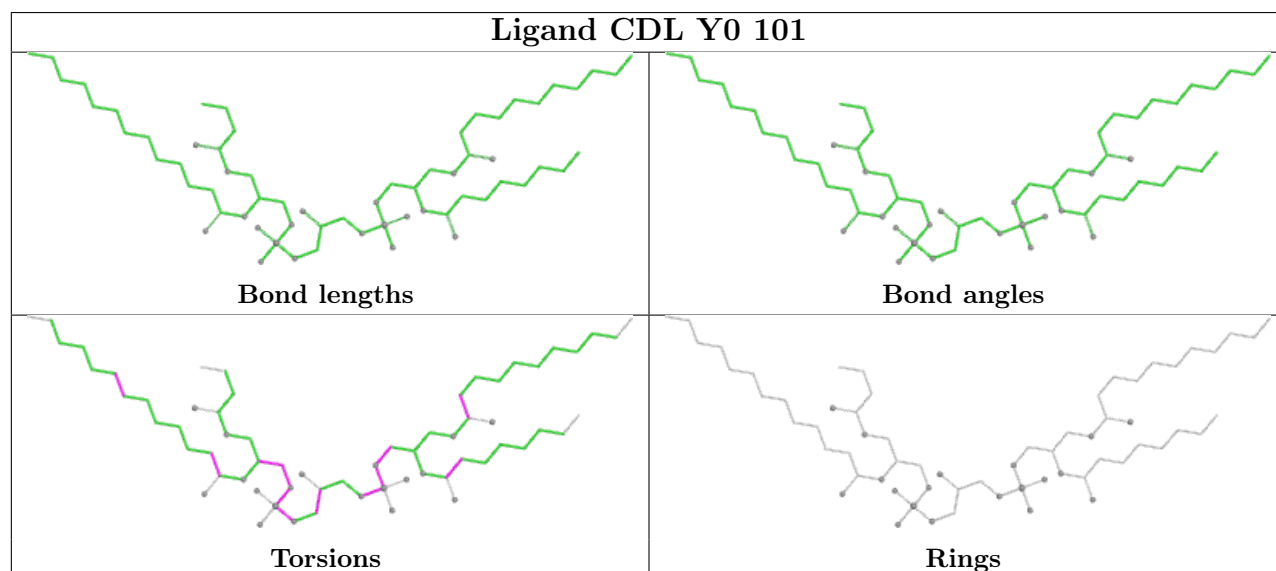
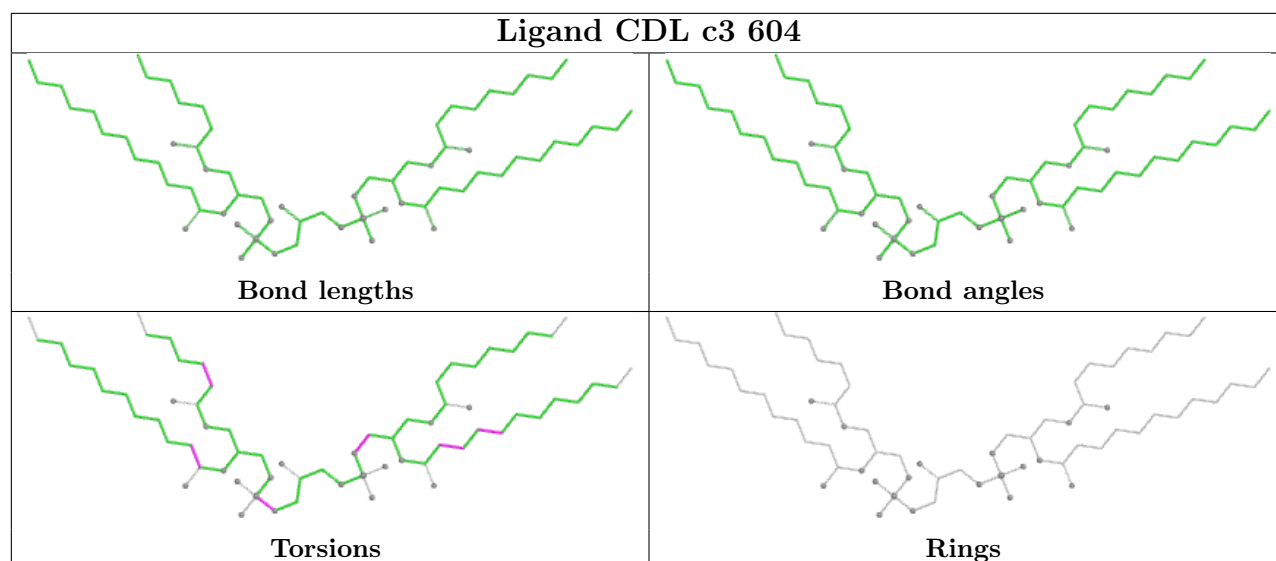
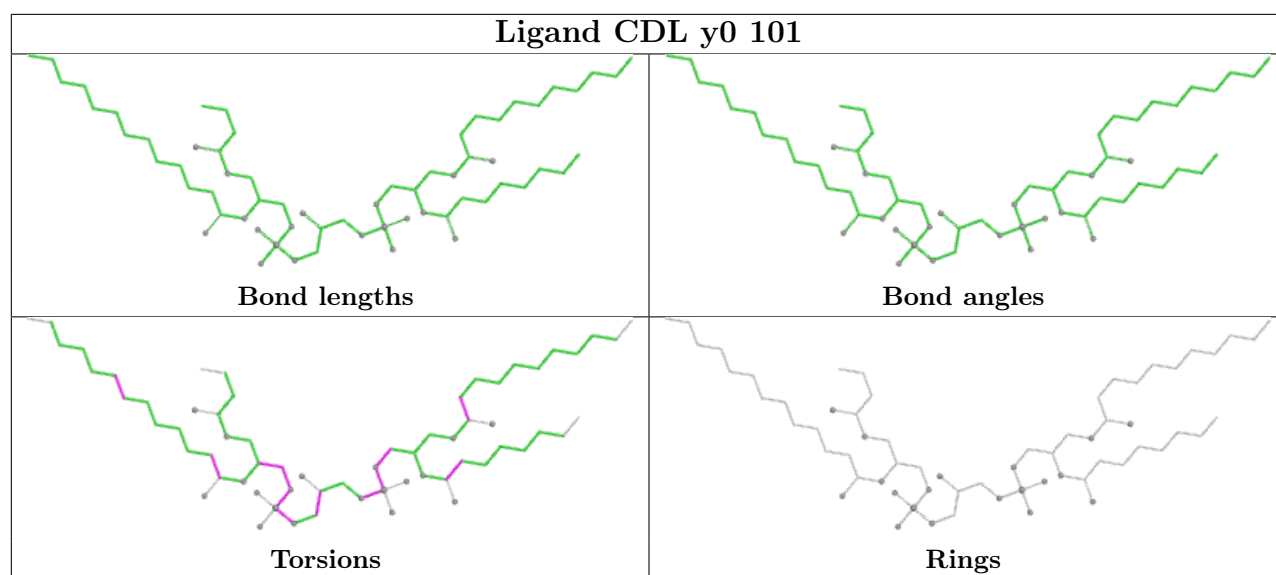


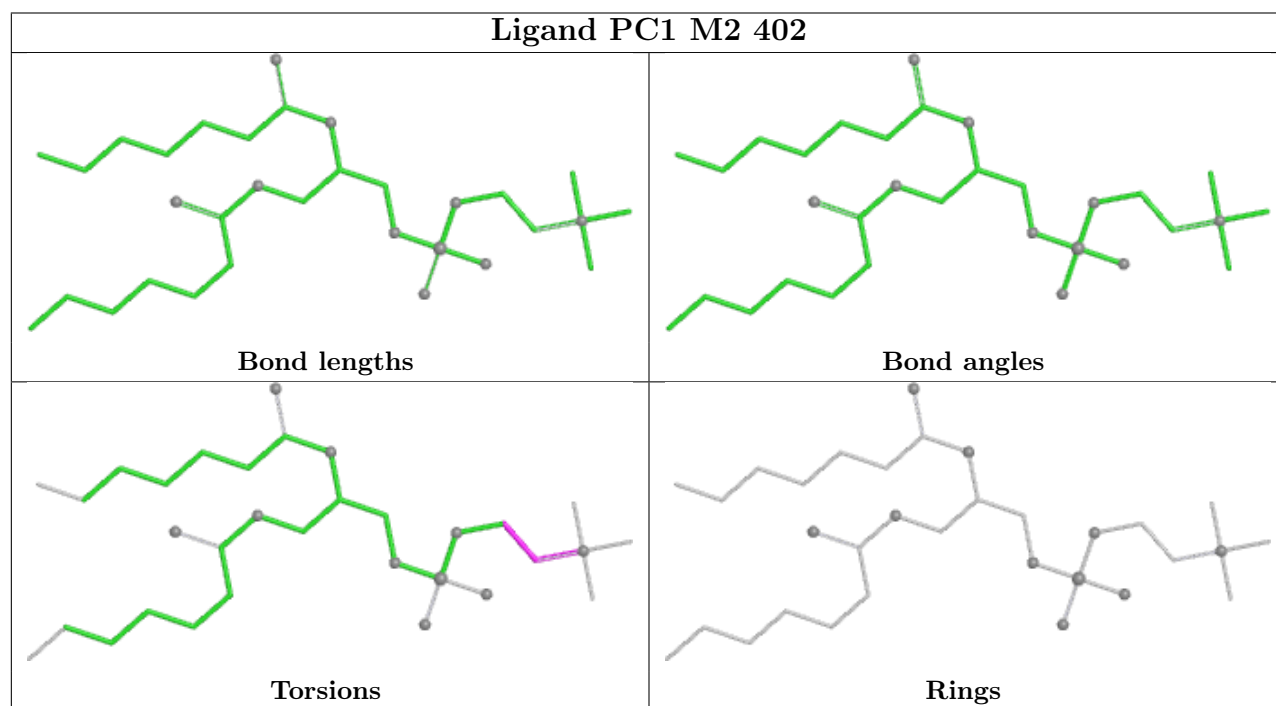
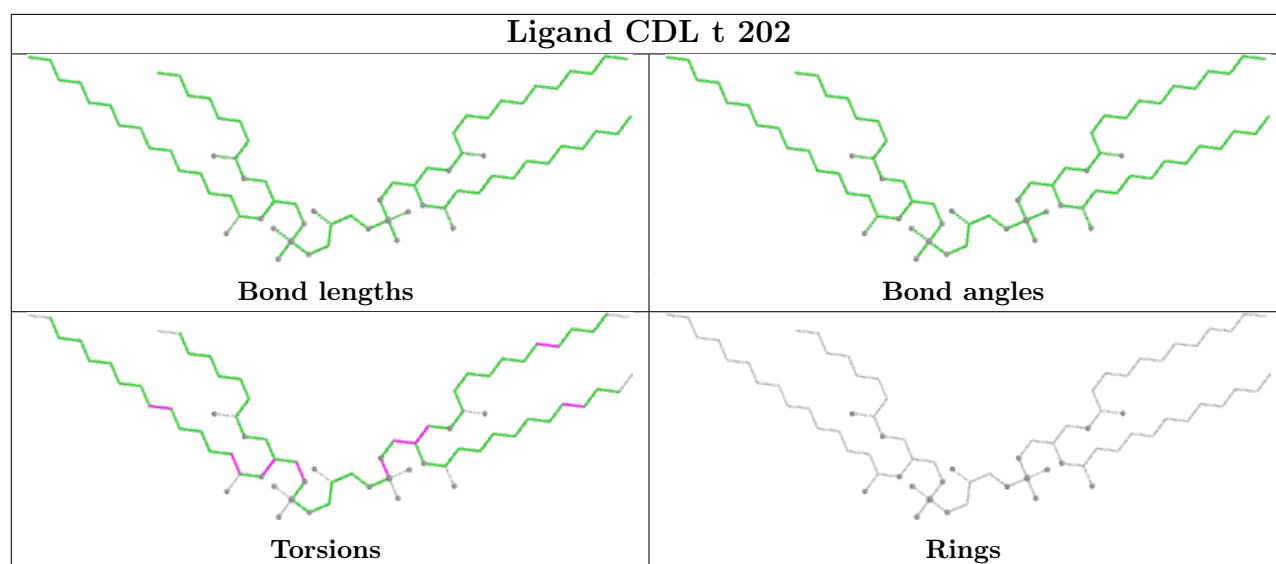


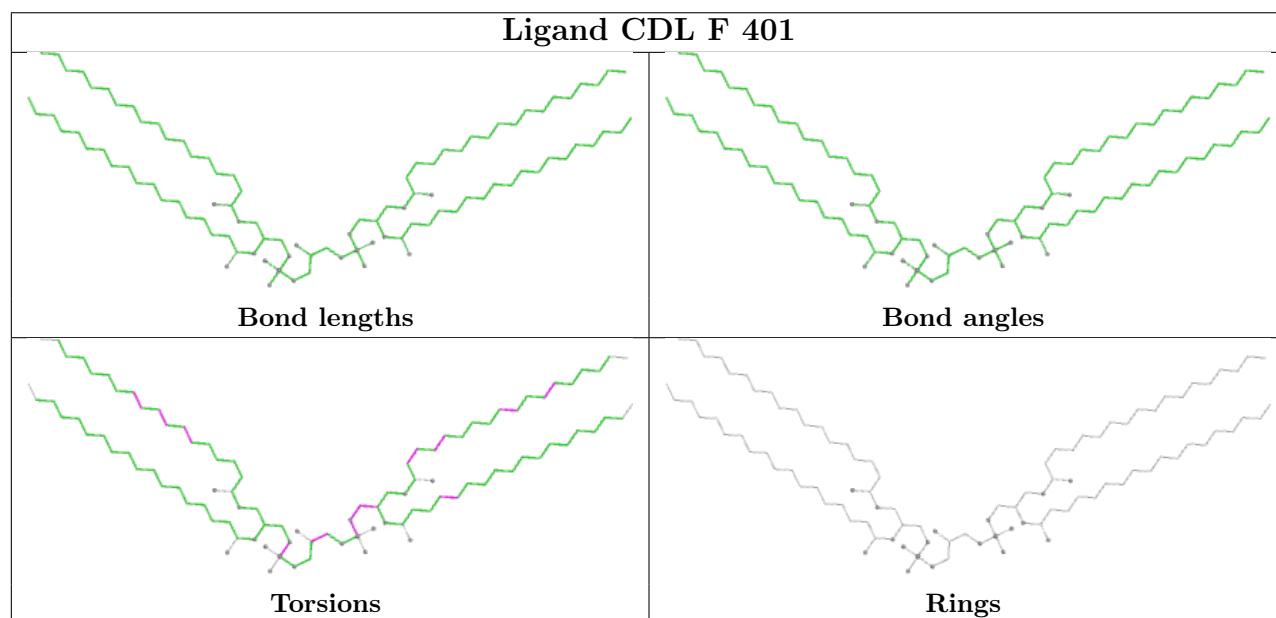
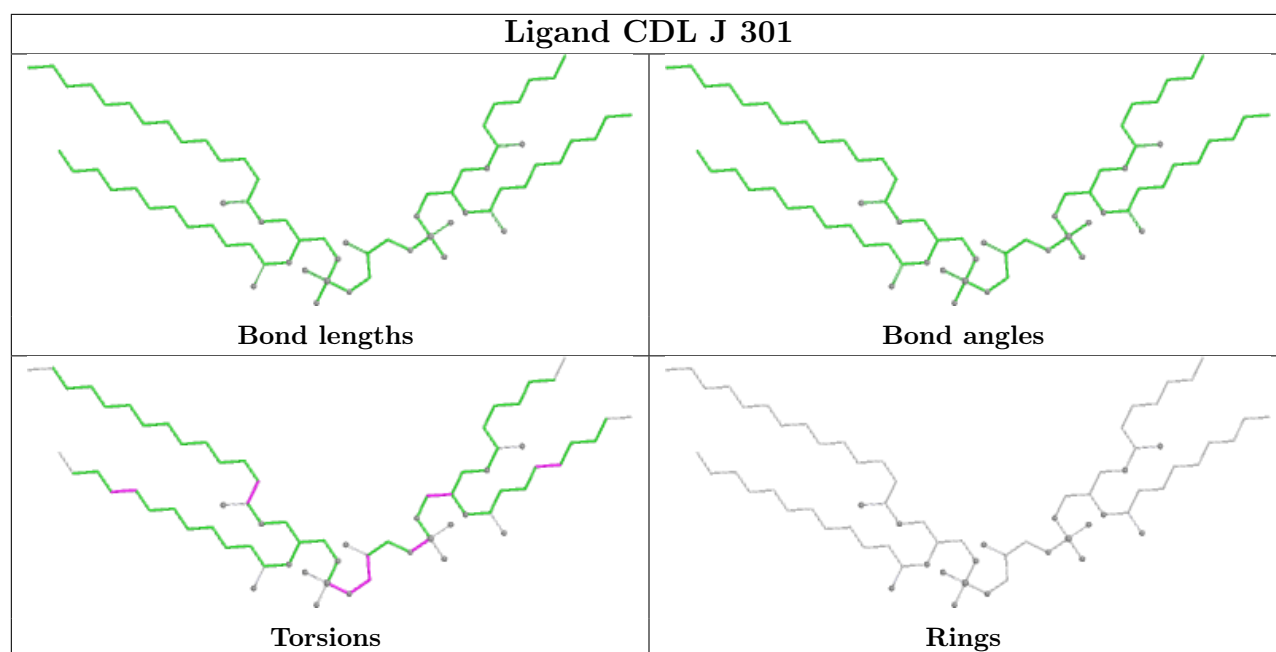


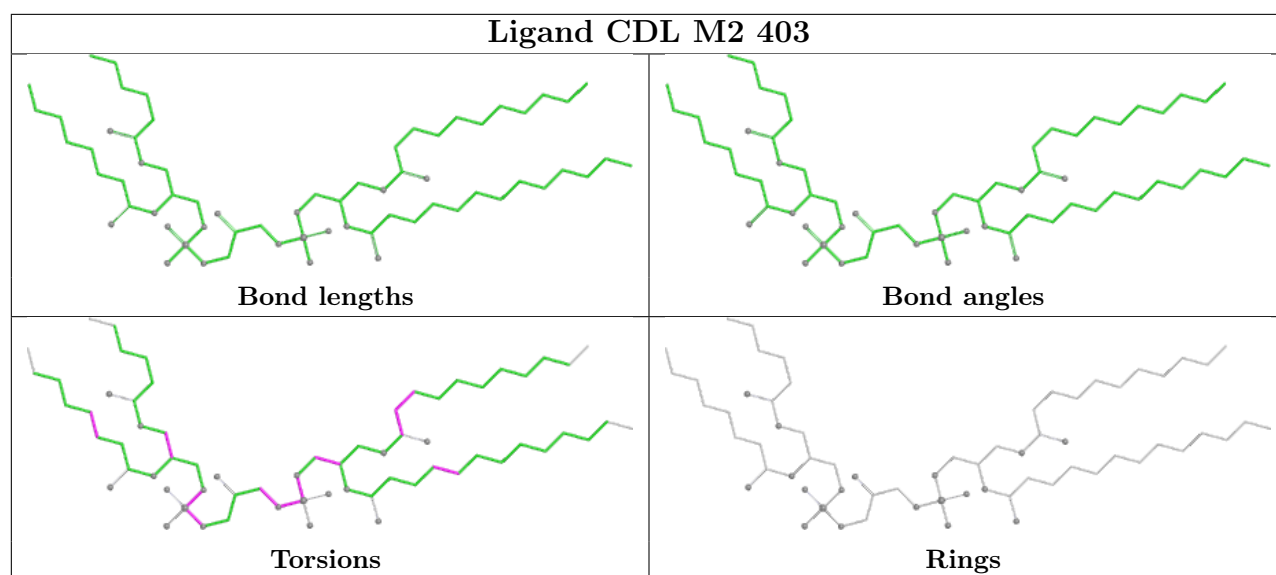












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

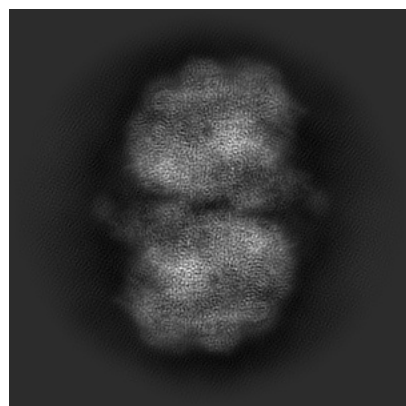
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32325. These allow visual inspection of the internal detail of the map and identification of artifacts.

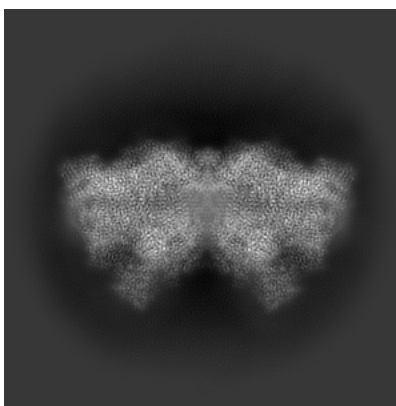
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

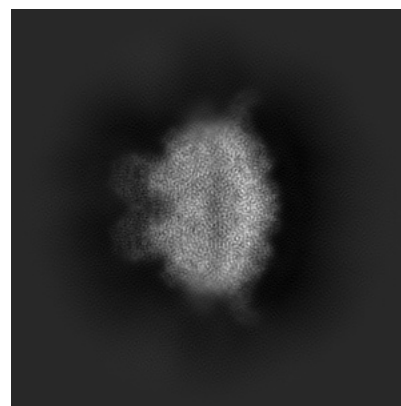
6.1.1 Primary map



X

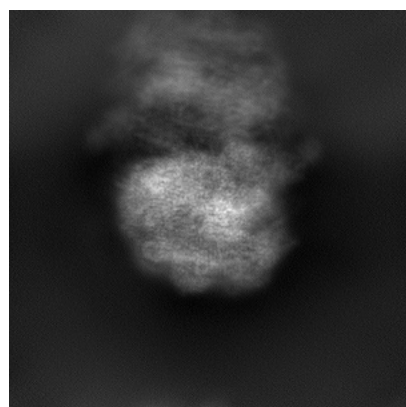


Y

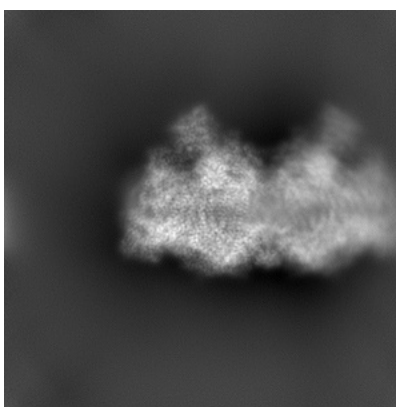


Z

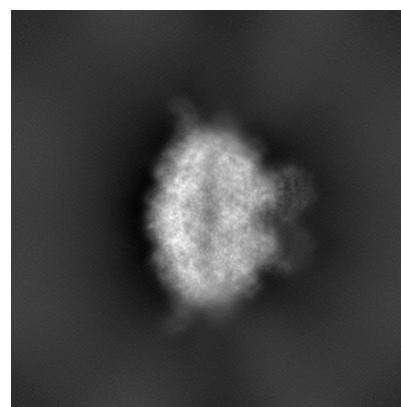
6.1.2 Raw map



X



Y

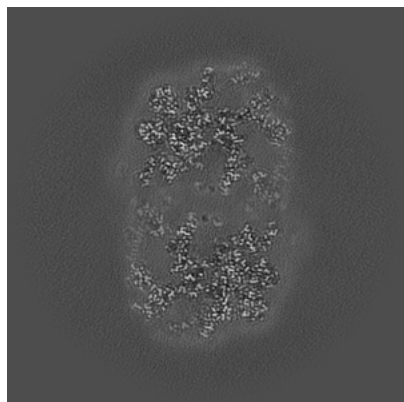


Z

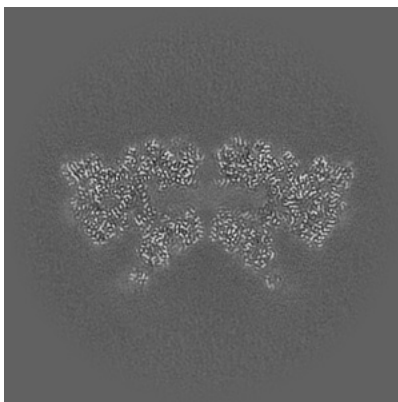
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

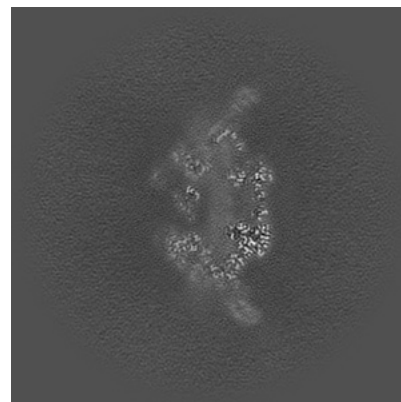
6.2.1 Primary map



X Index: 256

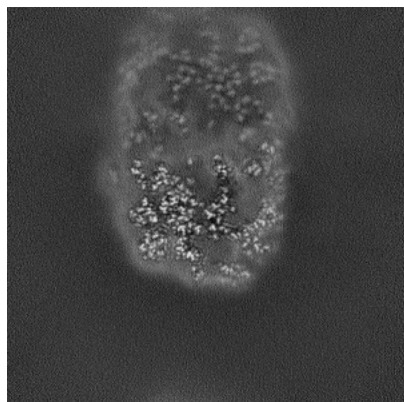


Y Index: 256

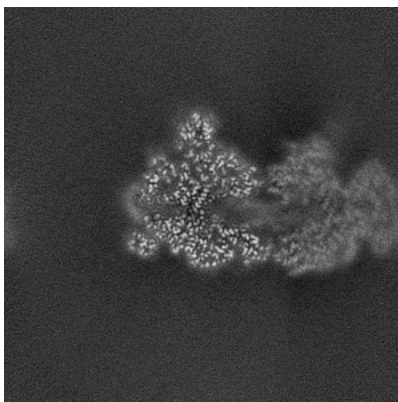


Z Index: 256

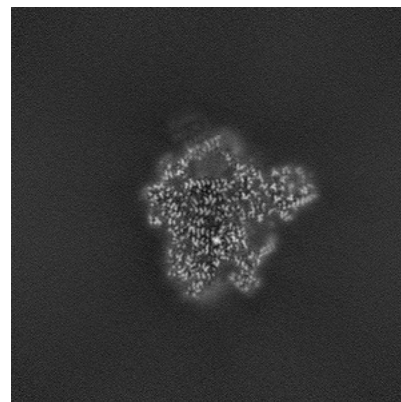
6.2.2 Raw map



X Index: 256



Y Index: 256

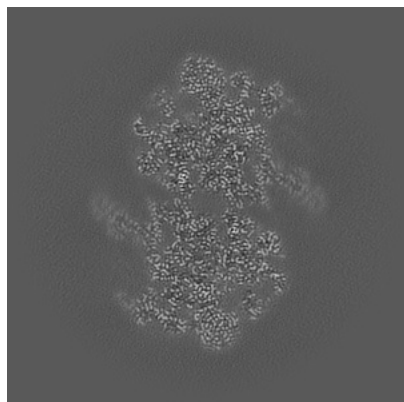


Z Index: 256

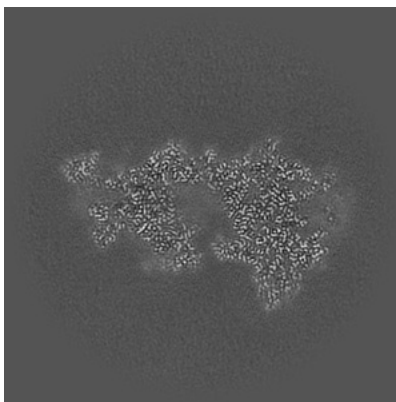
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

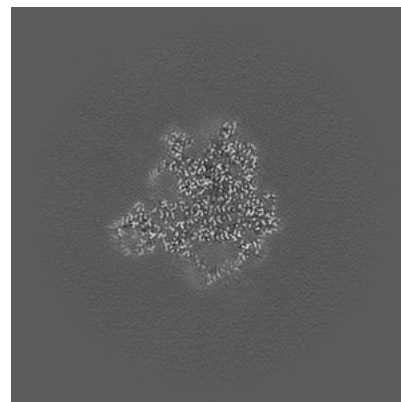
6.3.1 Primary map



X Index: 297

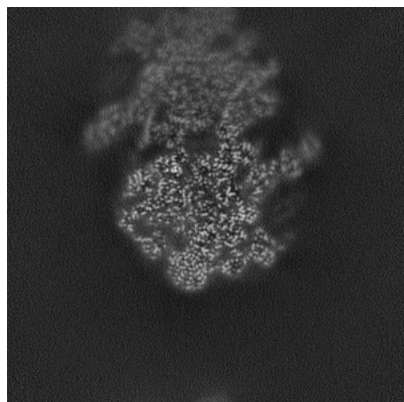


Y Index: 286

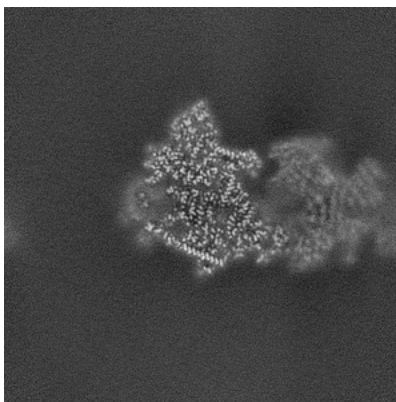


Z Index: 180

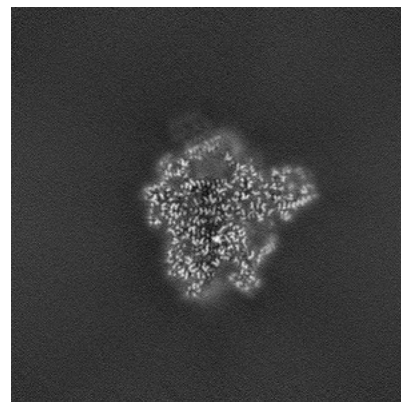
6.3.2 Raw map



X Index: 217



Y Index: 273

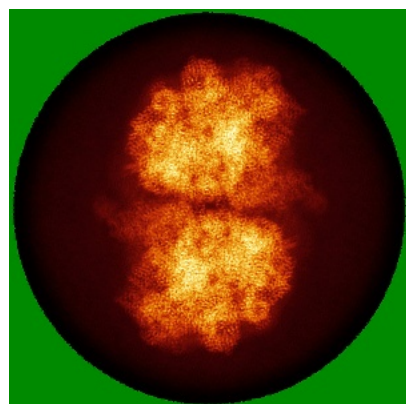


Z Index: 257

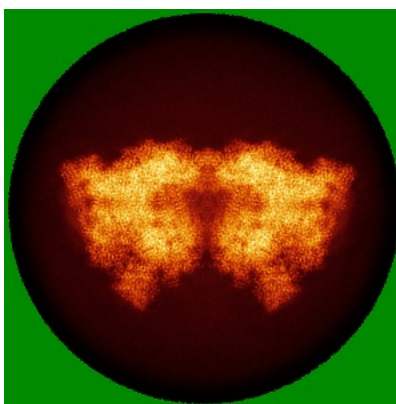
The images above show the largest variance slices of the map in three orthogonal directions.

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

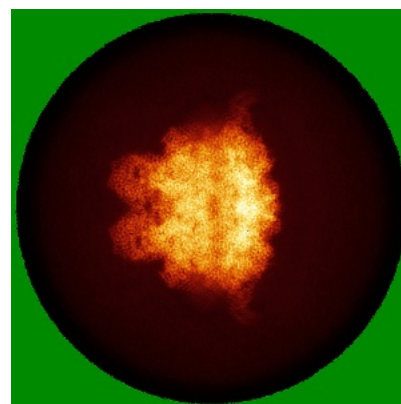
6.4.1 Primary map



X

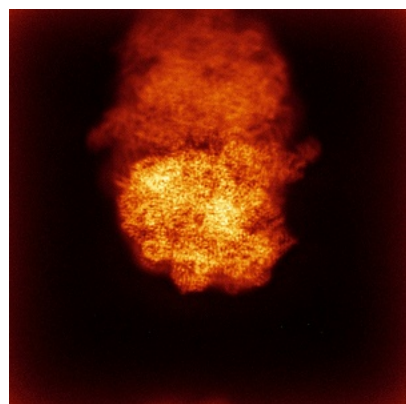


Y

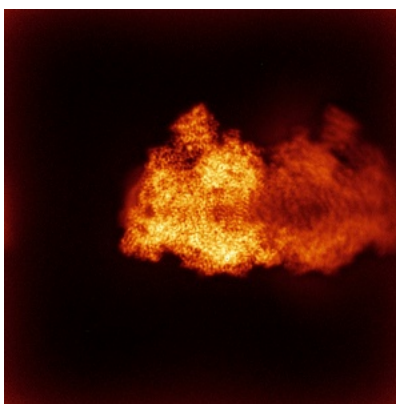


Z

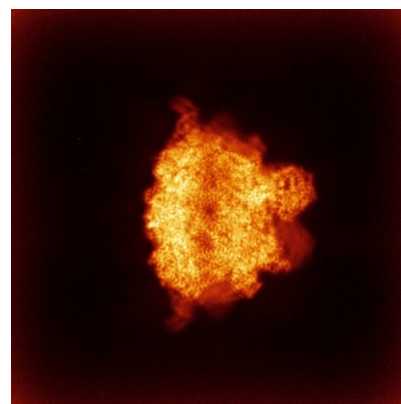
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

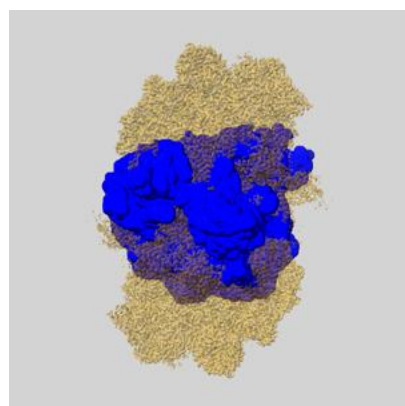
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

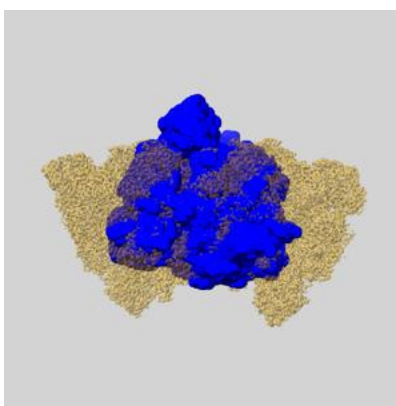
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

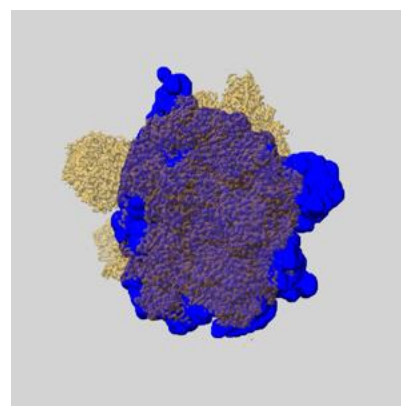
6.6.1 emd_32325_msk_1.map [i](#)



X



Y

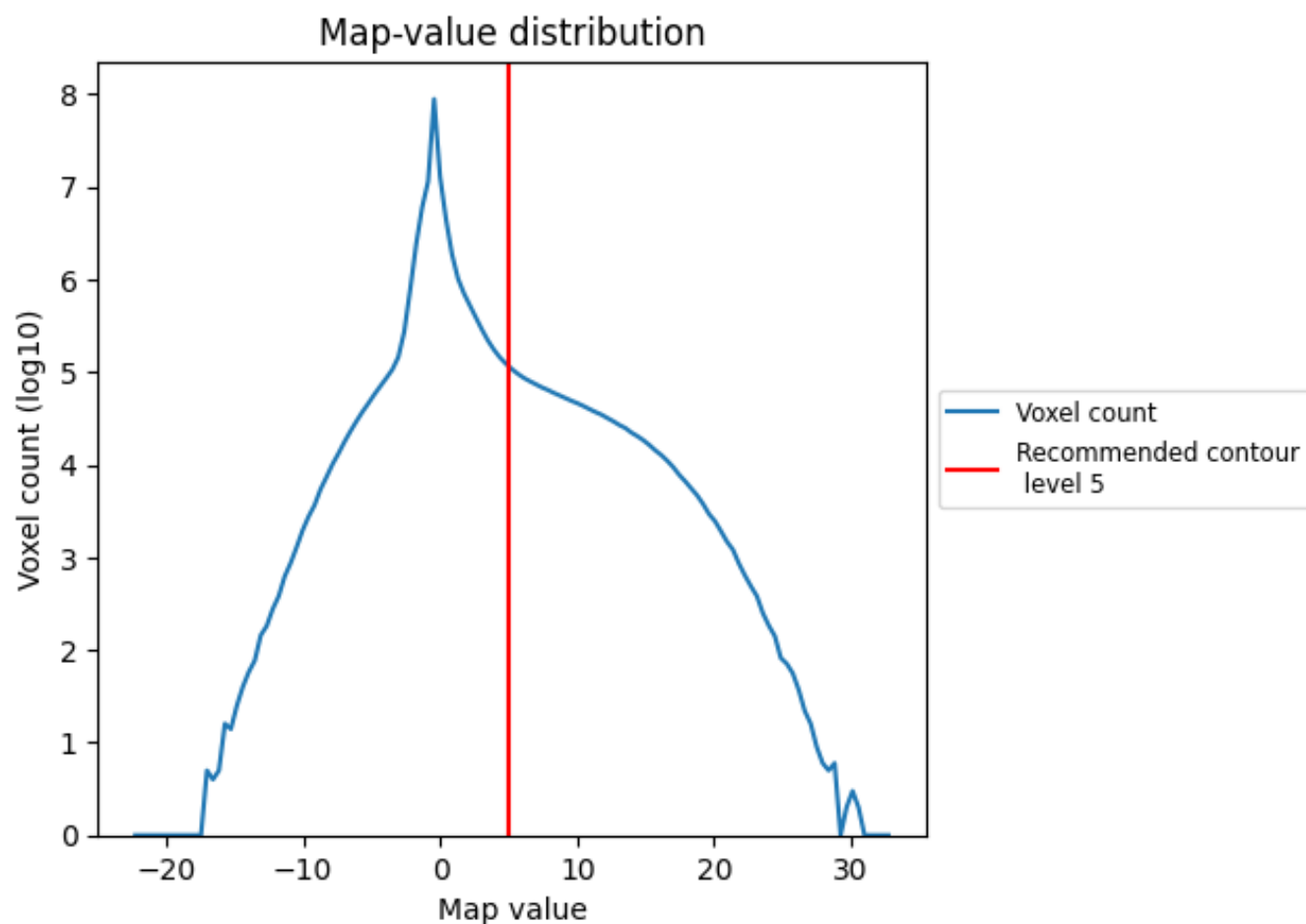


Z

7 Map analysis [i](#)

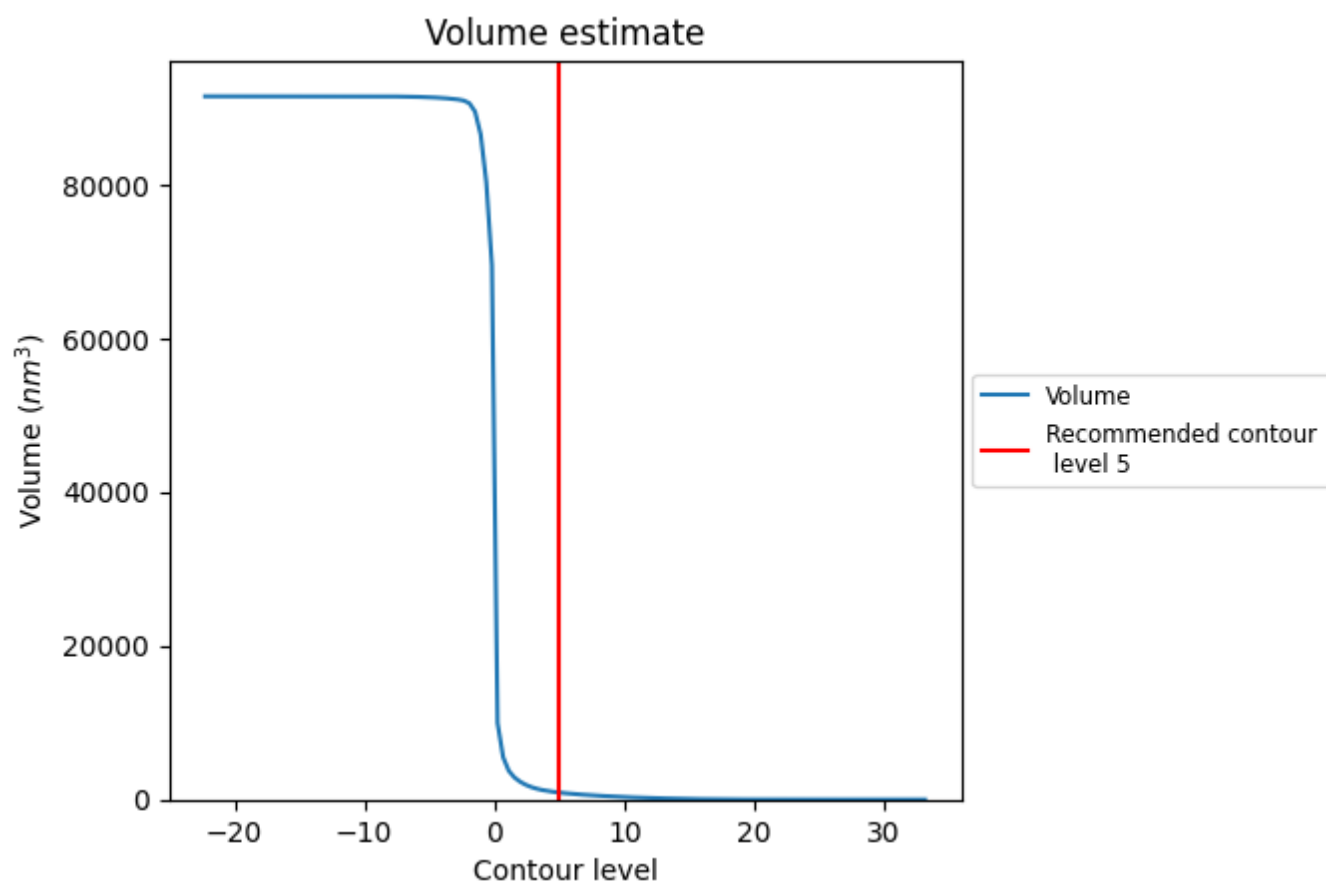
This section contains the results of statistical analysis of the map.

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.

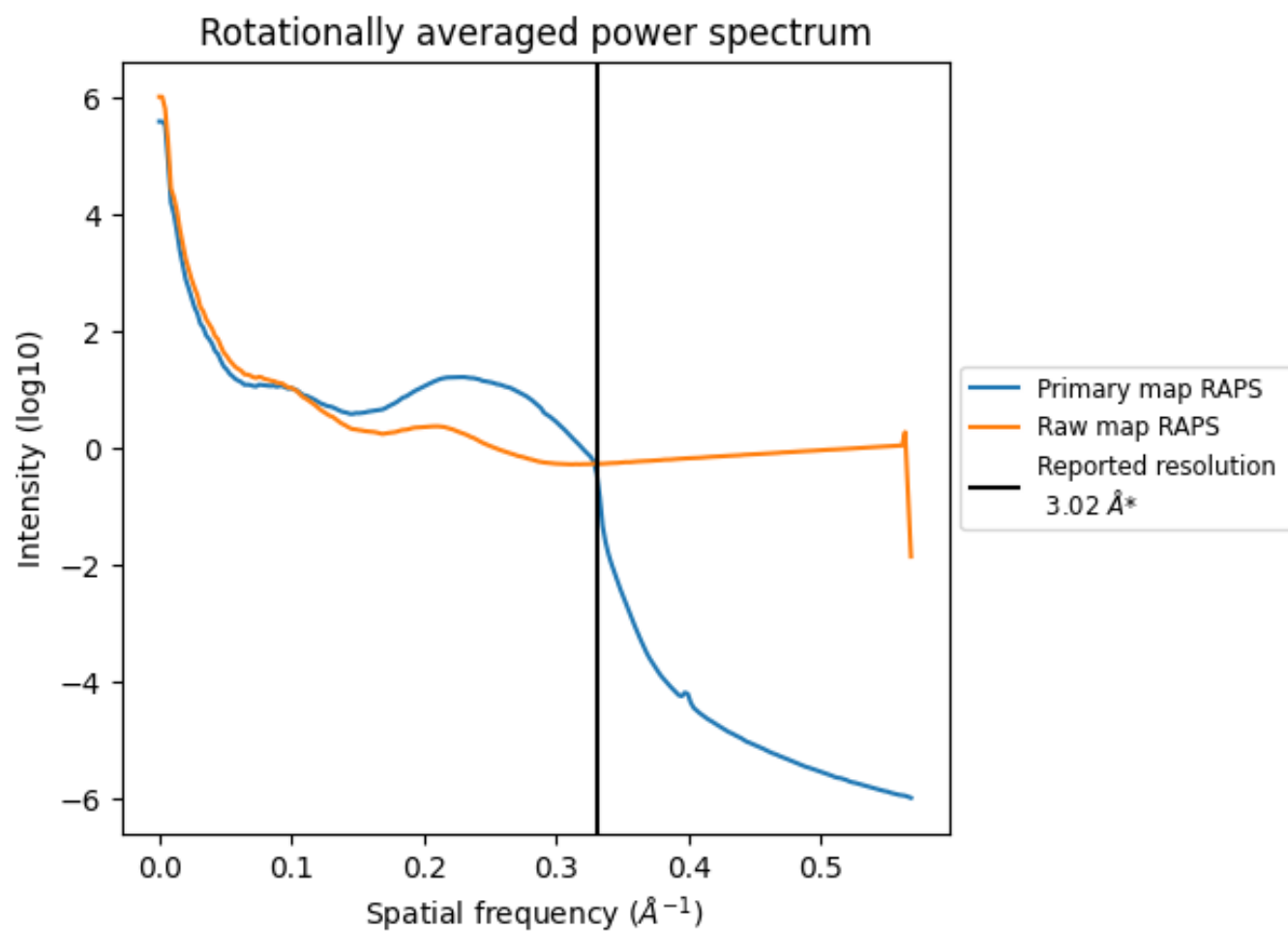
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm³; this corresponds to an approximate mass of 823 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

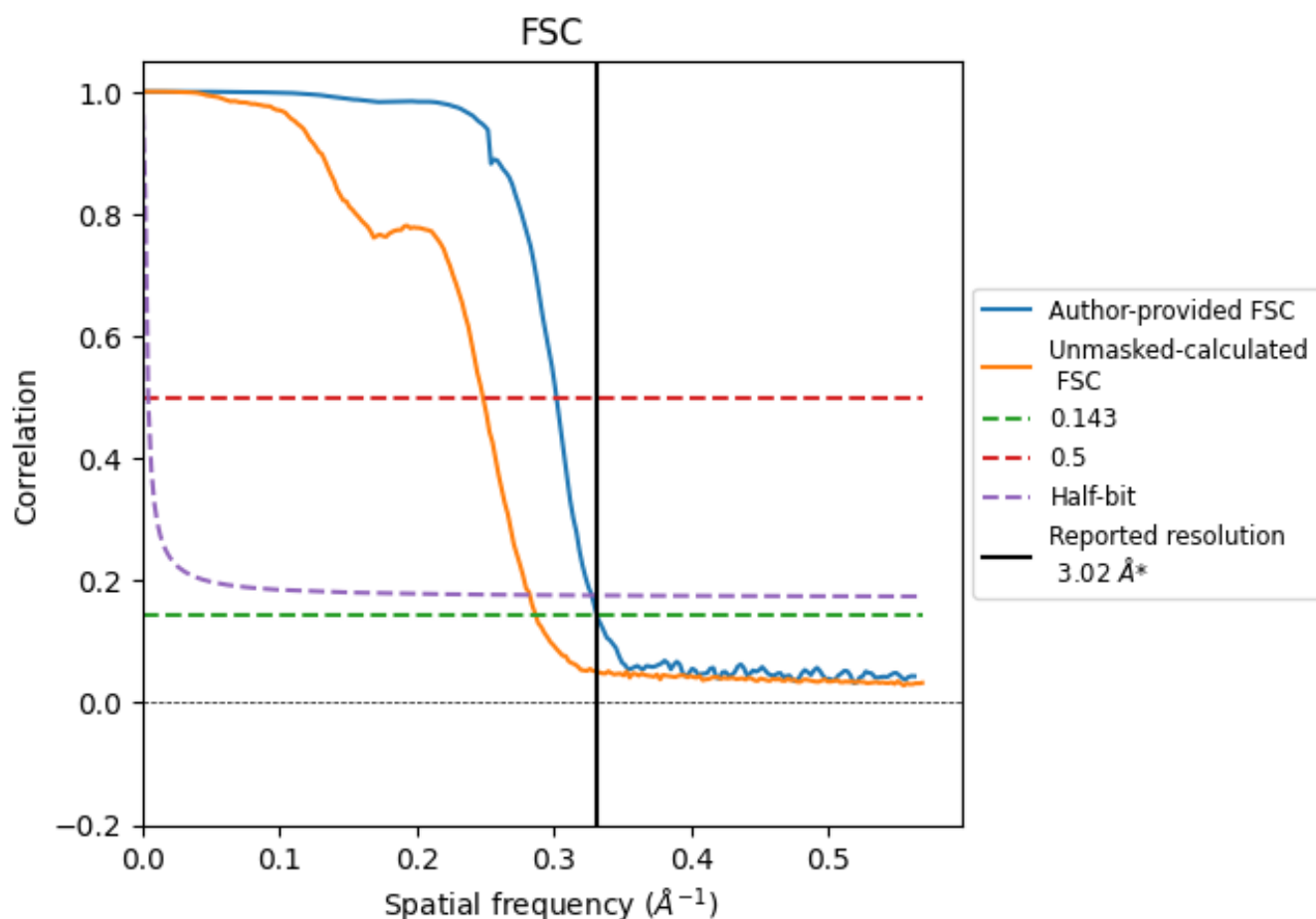


*Reported resolution corresponds to spatial frequency of 0.331 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.331 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

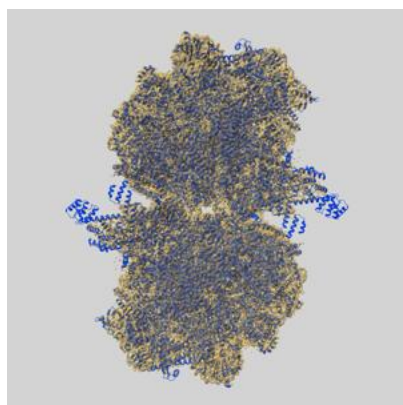
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.31	3.05
Unmasked-calculated*	3.49	4.03	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 3.02 by more than 10 %

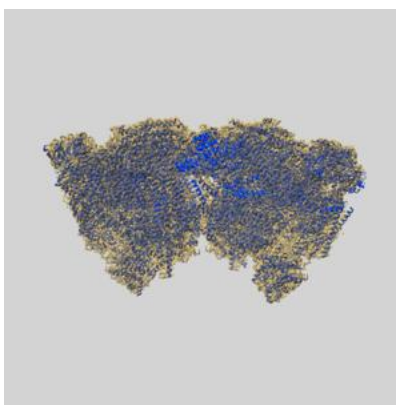
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32325 and PDB model 7W5Z. Per-residue inclusion information can be found in section 3 on page 30.

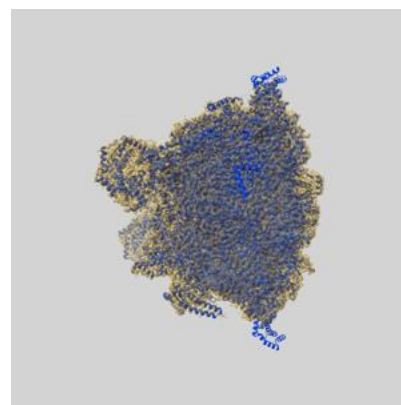
9.1 Map-model overlay [i](#)



X



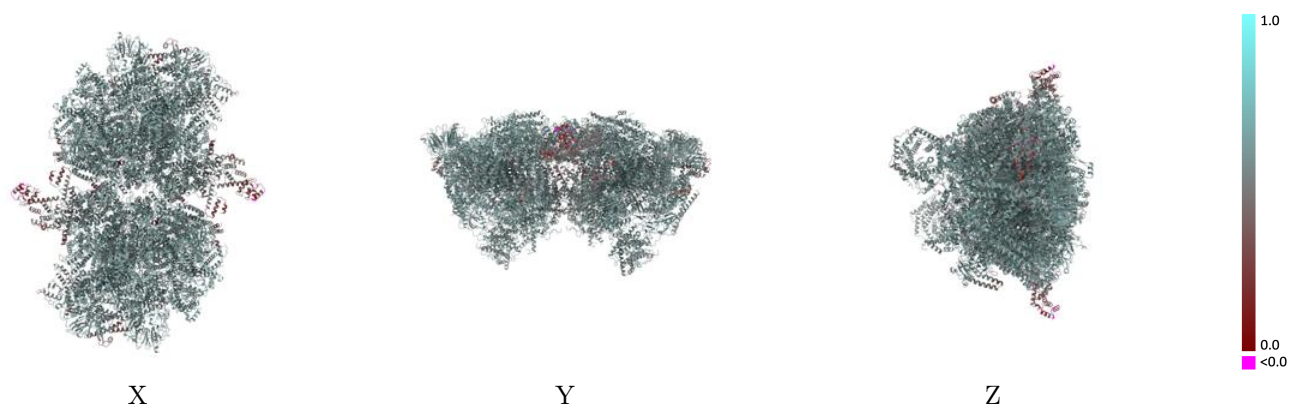
Y



Z

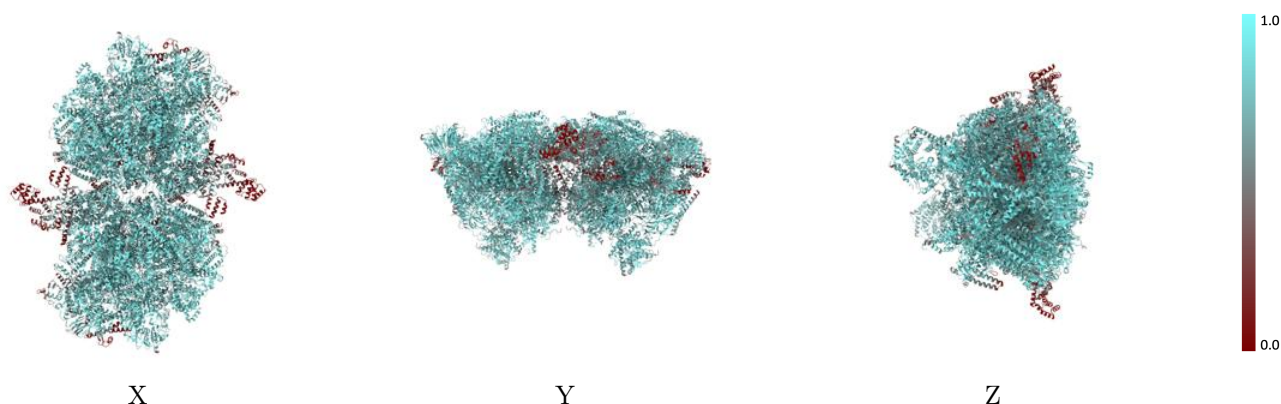
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



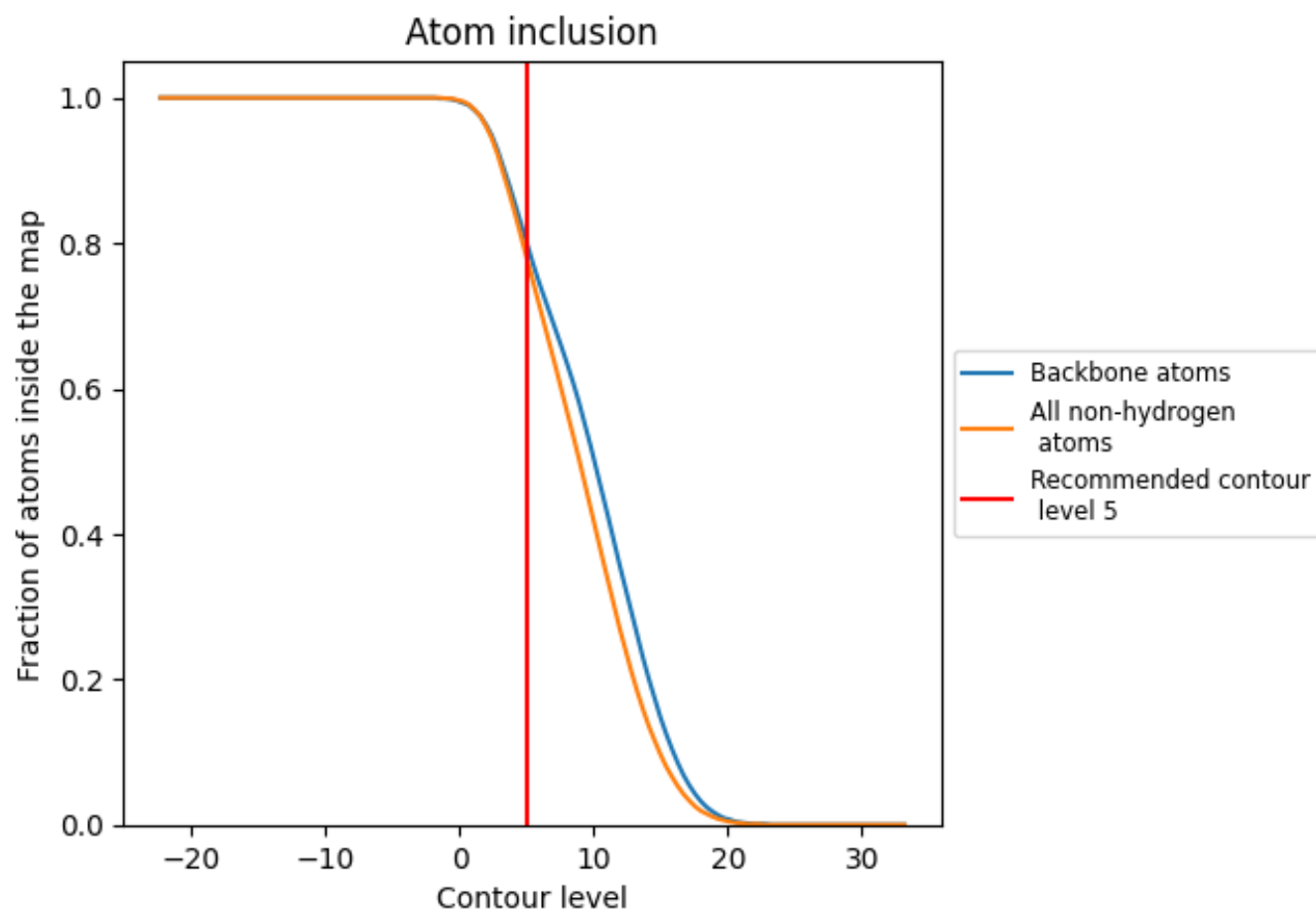
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7810	 0.5680
5B	 0.8080	 0.5800
5b	 0.8080	 0.5790
6A	 0.8120	 0.5890
6B	 0.8530	 0.5890
6C	 0.8020	 0.5790
6L	 0.8290	 0.5640
6a	 0.8100	 0.5880
6b	 0.8580	 0.5900
6c	 0.8000	 0.5790
6l	 0.8230	 0.5640
7A	 0.8530	 0.6040
7C	 0.8460	 0.5920
7L	 0.8010	 0.5590
7a	 0.8500	 0.6030
7c	 0.8420	 0.5900
7l	 0.8010	 0.5590
A	 0.8400	 0.5910
AC	 0.8350	 0.5970
B	 0.5960	 0.5200
BP	 0.8080	 0.5750
C	 0.2690	 0.4150
C1	 0.8480	 0.5900
C2	 0.8260	 0.5800
C3	 0.7670	 0.5690
D	 0.7750	 0.5640
E	 0.7780	 0.5730
F	 0.8510	 0.5820
FS	 0.8390	 0.5810
G	 0.8750	 0.5890
H	 0.7430	 0.5450
I	 0.5910	 0.5130
J	 0.8190	 0.5820
K	 0.8380	 0.5780
L	 0.7810	 0.5690



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Chain	Atom inclusion	Q-score
M	 0.7180	 0.5520
M1	 0.8400	 0.5800
M2	 0.8440	 0.5870
M3	 0.7890	 0.5770
N	 0.8300	 0.5870
O	 0.8080	 0.5760
P	 0.7950	 0.5670
Q	 0.8470	 0.5900
R	 0.6280	 0.5160
S	 0.4690	 0.4540
T	 0.7560	 0.5810
T1	 0.8120	 0.5690
T2	 0.7560	 0.5490
T3	 0.7430	 0.5210
T4	 0.8170	 0.5560
T5	 0.7710	 0.5390
T6	 0.7910	 0.5410
U	 0.8170	 0.5790
U1	 0.7550	 0.5310
U2	 0.1760	 0.3210
U3	 0.2820	 0.3910
U4	 0.1600	 0.3930
U5	 0.4150	 0.4690
U6	 0.4110	 0.4220
V	 0.8100	 0.5780
W	 0.7220	 0.5520
X	 0.8520	 0.5930
Y	 0.8760	 0.5940
Y0	 0.8460	 0.5900
Y5	 0.7020	 0.5520
Y7	 0.6180	 0.5230
Z	 0.5880	 0.5160
a	 0.8440	 0.5900
ac	 0.8330	 0.5960
b	 0.6000	 0.5200
bp	 0.8060	 0.5740
c	 0.2800	 0.4160
c1	 0.8500	 0.5910
c2	 0.8300	 0.5800
c3	 0.7680	 0.5690
d	 0.7740	 0.5670
e	 0.7800	 0.5730

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Chain	Atom inclusion	Q-score
f	 0.8550	 0.5840
fs	 0.8410	 0.5810
g	 0.8760	 0.5890
h	 0.7450	 0.5470
i	 0.5980	 0.5140
j	 0.8190	 0.5810
k	 0.8340	 0.5780
l	 0.7790	 0.5700
m	 0.7250	 0.5520
m1	 0.8330	 0.5810
m2	 0.8420	 0.5870
m3	 0.7920	 0.5760
n	 0.8300	 0.5870
o	 0.8090	 0.5760
p	 0.7900	 0.5680
q	 0.8470	 0.5880
r	 0.6350	 0.5160
s	 0.4680	 0.4530
t	 0.7560	 0.5810
t1	 0.8180	 0.5640
t2	 0.7680	 0.5500
t3	 0.7380	 0.5210
t4	 0.8100	 0.5580
t5	 0.7790	 0.5430
t6	 0.7870	 0.5420
u	 0.8080	 0.5770
u1	 0.7470	 0.5330
u2	 0.1820	 0.3190
u3	 0.2530	 0.4000
u4	 0.1530	 0.4160
u5	 0.4190	 0.4830
u6	 0.4070	 0.4350
v	 0.8090	 0.5800
w	 0.7230	 0.5530
x	 0.8560	 0.5950
y	 0.8800	 0.5940
y0	 0.8370	 0.5880
y5	 0.7010	 0.5510
y7	 0.6150	 0.5240
z	 0.5940	 0.5200