Full wwPDB EM Validation Report

Mar 20, 2026 – 02:36 PM EDT

PDB ID	:	8GYM / pdb_00008gym
EMDB ID	:	EMD-34373
Title	:	Cryo-EM structure of Tetrahymena thermophila respiratory mega-complex MC IV2+(I+III2+II)2
Authors	:	Wu, M.C.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on	:	2022-09-23
Resolution	:	2.96 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:

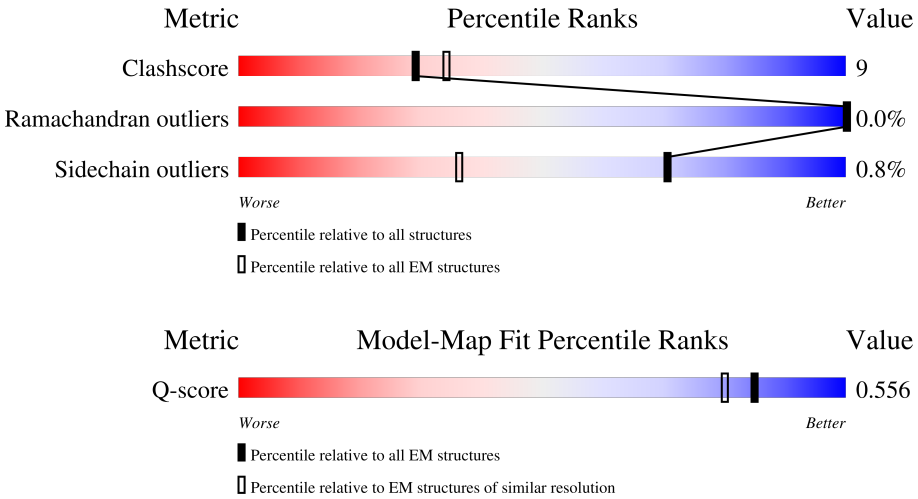
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.96 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	13155 (2.46 - 3.46)

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 <=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	1T	72	82% 15%
1	1t	72	82% 15%
2	2E	322	6% 72% 26%
2	2e	322	6% 73% 26%

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Mol	Chain	Length	Quality of chain
3	2F	296	51% 22% 27%
3	2f	296	51% 22% 27%
4	2G	198	75% 24%
4	2g	198	75% 25%
5	2H	195	39% 13% 48%
5	2h	195	38% 14% 48%
6	2I	114	86% 13%
6	2i	114	86% 13%
7	2J	103	76% 23%
7	2j	103	75% 24%
8	2K	93	75% 25%
8	2k	93	77% 23%
9	2L	89	71% 22% 7%
9	2l	89	74% 19% 7%
10	2M	76	78% 21%
10	2m	76	76% 22%
11	2N	62	73% 24%
11	2n	62	71% 27%
12	2O	46	72% 20% 9%
12	2o	46	76% 15% 9%
13	2T	72	10% 74% 24%
13	2t	72	10% 71% 26%
14	3T	93	14% 68% 22% 11%
14	3t	93	14% 72% 17% 11%
15	4A	127	68% 11% 21%

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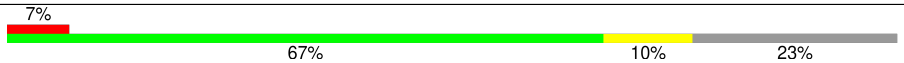
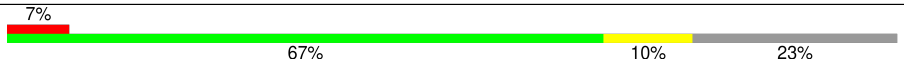
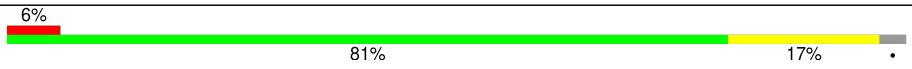
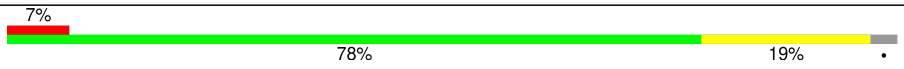
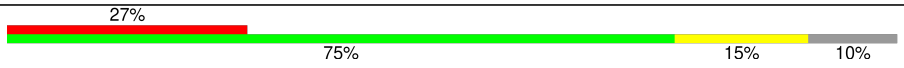
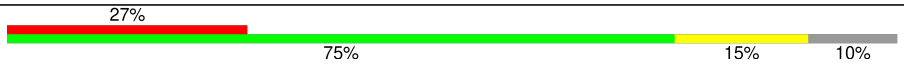
Mol	Chain	Length	Quality of chain
15	4a	127	
16	4T	68	
16	4t	68	
17	5T	81	
17	5t	81	
18	6A	130	
18	6a	130	
19	6B	230	
19	6b	230	
20	6C	103	
20	6c	103	
21	6L	88	
21	6l	88	
22	6T	72	
22	6t	72	
23	7A	133	
23	7a	133	
24	7C	236	
24	7c	236	
25	7L	990	
25	7l	990	
26	A	490	
26	a	490	
27	B	473	
27	b	473	

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Mol	Chain	Length	Quality of chain
28	BP	462	7% 61% 22% 18%
28	bp	462	7% 61% 22% 18%
29	C1	688	69% 29%
29	c1	688	68% 30%
30	C2	604	73% 26%
30	c2	604	72% 27%
31	C3	594	9% 75% 23%
31	c3	594	8% 75% 23%
32	D	402	61% 11% 28%
32	d	402	60% 12% 28%
33	E	385	74% 26%
33	e	385	74% 26%
34	F	348	51% 19% 30%
34	f	348	51% 19% 30%
35	FS	188	5% 79% 21%
35	fs	188	5% 78% 22%
36	G	318	68% 24% 8%
36	g	318	68% 24% 8%
37	H	318	11% 74% 19% 6%
37	h	318	11% 72% 21% 6%
38	I	252	68% 23% 8%
38	i	252	67% 24% 8%
39	J	234	64% 16% 20%
39	j	234	66% 14% 20%
40	K	231	68% 22% 10%

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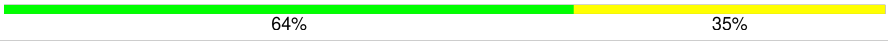
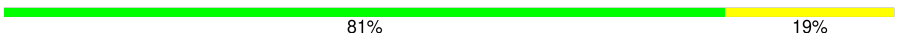
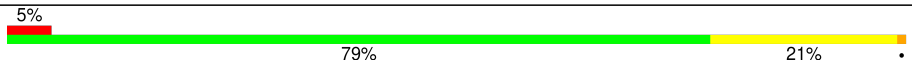
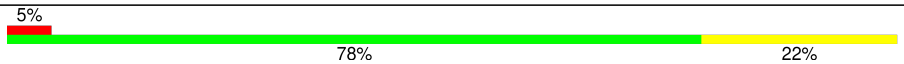
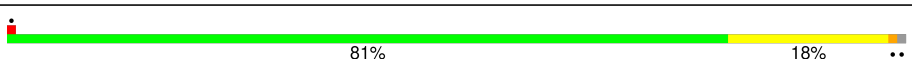
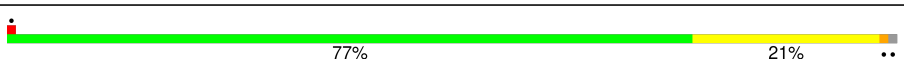
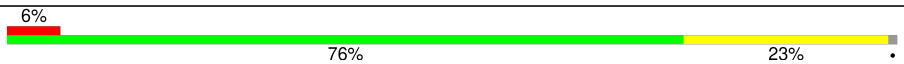
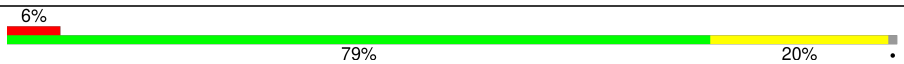
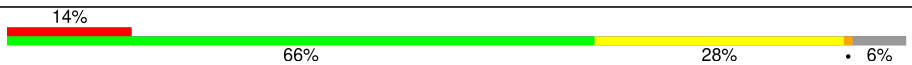
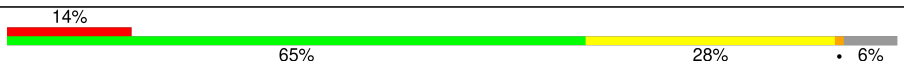
Mol	Chain	Length	Quality of chain
40	k	231	
41	L	222	
41	l	222	
42	M	220	
42	m	220	
43	M1	346	
43	m1	346	
44	M2	318	
44	m2	318	
45	M3	330	
45	m3	330	
46	N	210	
46	n	210	
47	O	193	
47	o	193	
48	P	175	
48	p	175	
49	Q	173	
49	q	173	
50	R	173	
50	r	173	
51	S	170	
51	s	170	
52	SA	636	
52	sa	636	

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Mol	Chain	Length	Quality of chain
53	SB	312	5% 63% 25% 11%
53	sb	312	5% 64% 24% 11%
54	SC	60	62% 35%
54	sc	60	62% 35%
55	SD	44	70% 30%
55	sd	44	68% 32%
56	T	158	81% 18%
56	t	158	80% 19%
57	U	154	72% 27%
57	u	154	72% 27%
58	V	149	77% 21%
58	v	149	77% 21%
59	VB	637	66% 21% 13%
59	vb	637	66% 20% 13%
60	W	124	76% 23%
60	w	124	76% 23%
61	X	122	83% 17%
61	x	122	85% 15%
62	Y	105	74% 26%
62	y	105	71% 29%
63	Y0	89	67% 33%
63	y0	89	63% 37%
64	Y5	190	8% 81% 19%
64	y5	190	8% 80% 20%
65	Y7	453	7% 59% 17% 24%

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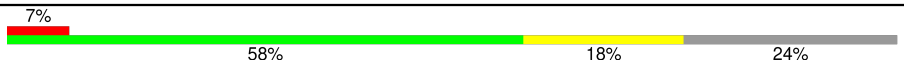
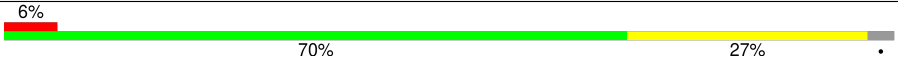
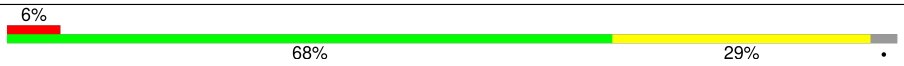
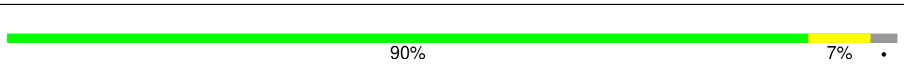
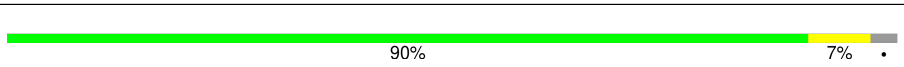
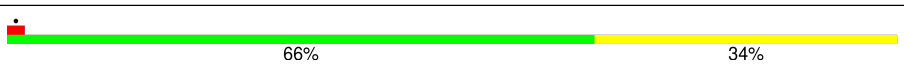
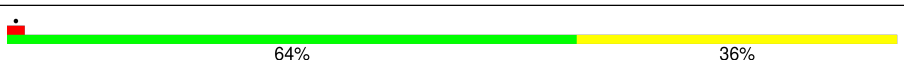
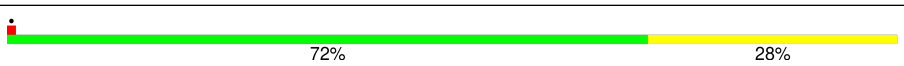
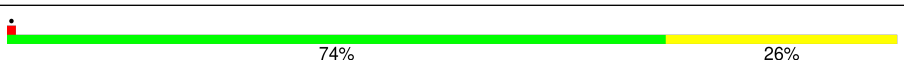
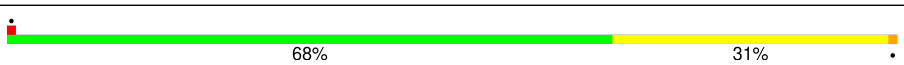
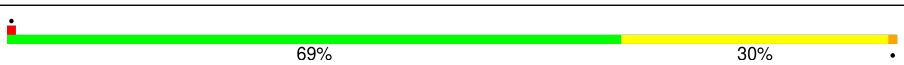
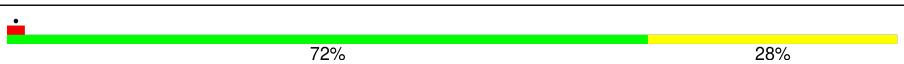
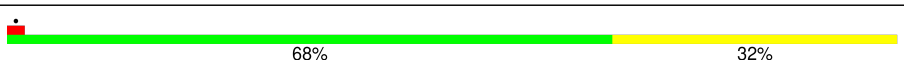
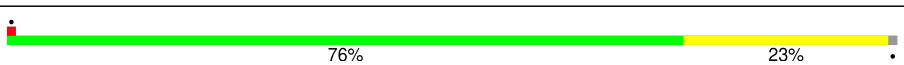
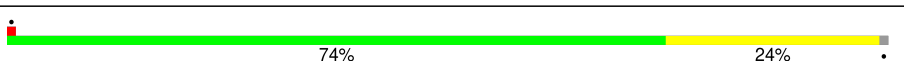
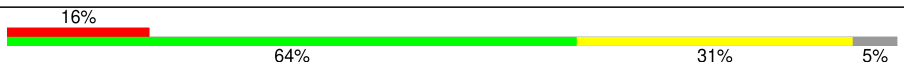
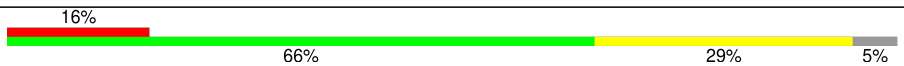
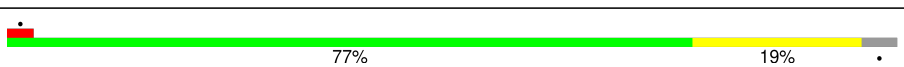
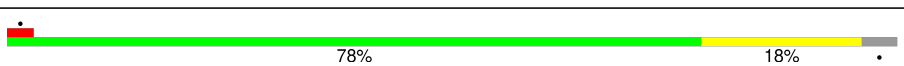
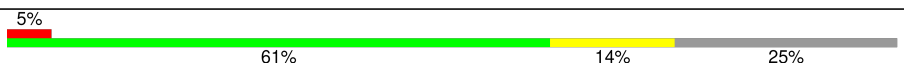
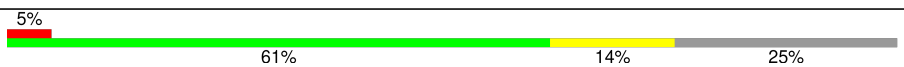
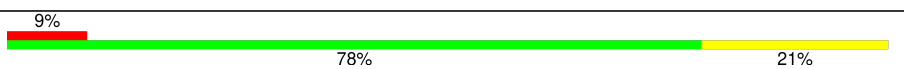
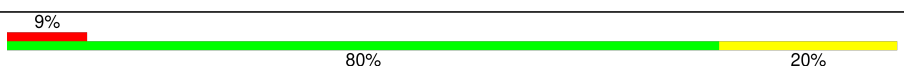
Mol	Chain	Length	Quality of chain
65	y7	453	
66	Z	90	
66	z	90	
67	Z1	100	
67	z1	100	
68	1B	59	
68	1b	59	
69	2B	178	
69	2b	178	
70	4L	116	
70	4l	116	
71	5B	100	
71	5b	100	
72	A1	94	
72	a1	94	
73	A2	103	
73	a2	103	
74	A3	135	
74	a3	135	
75	A5	206	
75	a5	206	
76	A6	172	
76	a6	172	
77	A7	282	
77	a7	282	

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Mol	Chain	Length	Quality of chain
78	A8	238	44% 11% 45%
78	a8	238	44% 11% 45%
79	A9	362	75% 19% 6%
79	a9	362	75% 19% 6%
80	AB	138	5% 70% 12% 19%
80	ab	138	5% 70% 12% 19%
81	AC	133	60% 14% 26%
81	ac	133	60% 14% 26%
82	AL	194	9% 74% 25%
82	al	194	9% 76% 24%
83	AM	175	65% 27% 9%
83	am	175	66% 26% 9%
84	AN	231	84% 16%
84	an	231	84% 16%
85	B2	126	10% 80% 14% 5%
85	b2	126	13% 82% 12% 5%
86	B3	83	6% 64% 19% 17%
86	b3	83	6% 65% 18% 17%
87	B4	147	62% 16% 22%
87	b4	147	62% 16% 22%
88	B6	129	46% 8% 46%
88	b6	129	43% 10% 46%
89	B7	120	84% 12%
89	b7	120	83% 13%
90	B8	207	6% 63% 22% 15%

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Mol	Chain	Length	Quality of chain
90	b8	207	6% 63% 22% 15%
91	B9	189	84% 15%
91	b9	189	85% 15%
92	BL	188	72% 21% 7%
92	bl	188	69% 24% 7%
93	BM	214	9% 62% 15% 23%
93	bm	214	10% 62% 15% 23%
94	C4	102	78% 21%
94	c4	102	81% 19%
95	FX	172	58% 27% 15%
95	fx	172	59% 26% 15%
96	G1	257	69% 20% 11%
96	g1	257	68% 20% 11%
97	G2	233	73% 25%
97	g2	233	75% 24%
98	G3	346	83% 17%
98	g3	346	83% 17%
99	J1	317	7% 68% 16% 16%
99	j1	317	7% 67% 16% 16%
100	N1	284	62% 37%
100	n1	284	62% 38%
101	N2	360	72% 27%
101	n2	360	72% 27%
102	N3	121	71% 28%
102	n3	121	70% 29%

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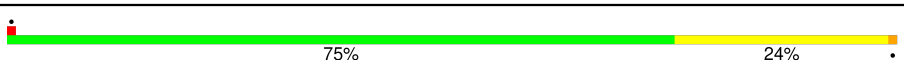
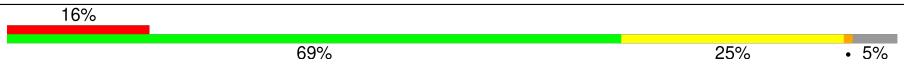
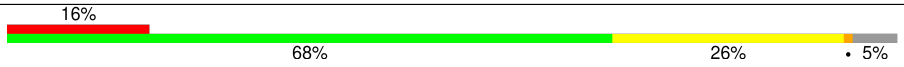
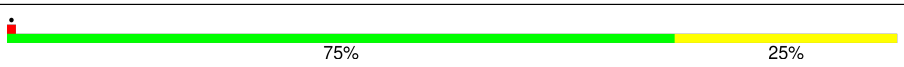
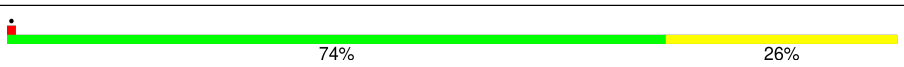
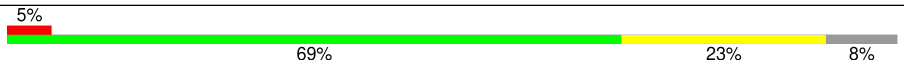
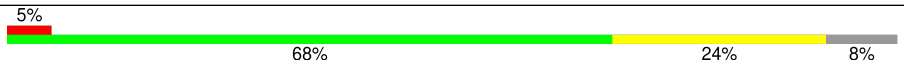
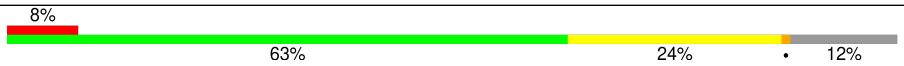
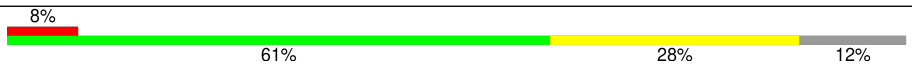
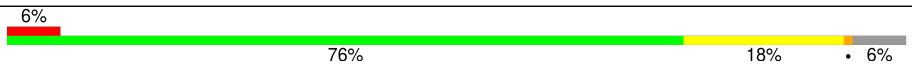
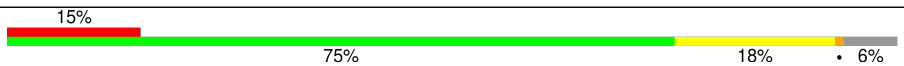
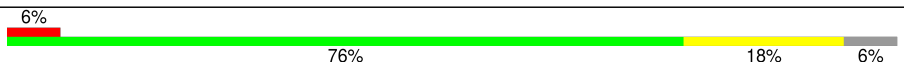
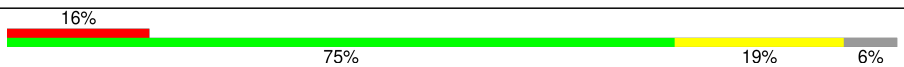
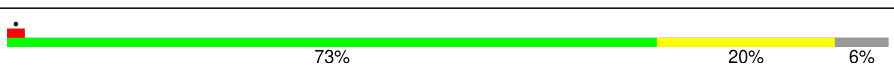
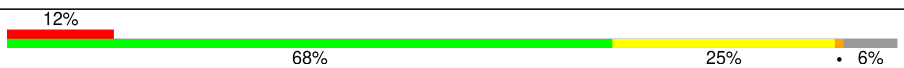
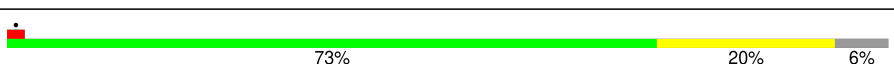
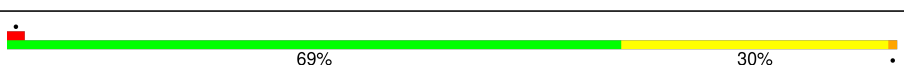
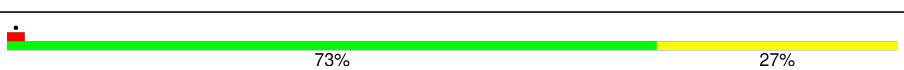
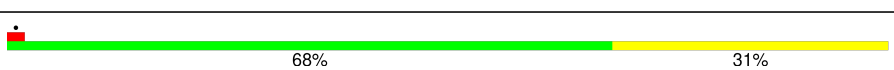
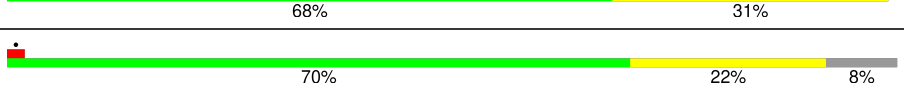
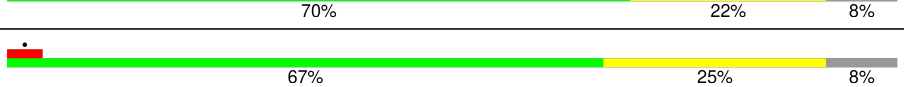
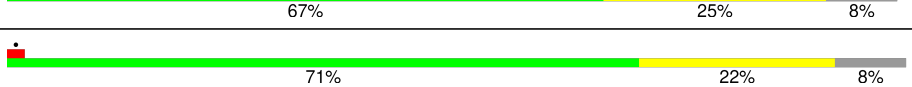
Mol	Chain	Length	Quality of chain
103	N4	505	
103	n4	505	
104	N5	750	
104	n5	750	
105	N6	255	
105	n6	255	
106	P1	251	
106	p1	251	
107	P2	189	
107	p2	189	
108	QA	482	
108	Qa	482	
108	qA	482	
108	qa	482	
109	QB	513	
109	Qb	513	
109	qB	513	
109	qb	513	
110	QC	426	
110	Qc	426	
110	qC	426	
110	qc	426	
111	QD	319	
111	Qd	319	
111	qD	319	

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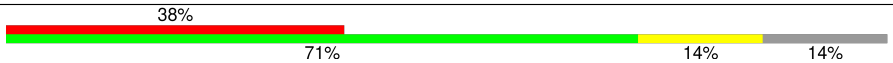
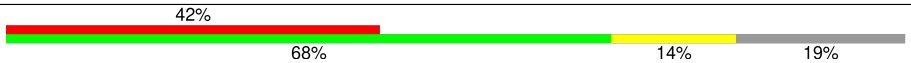
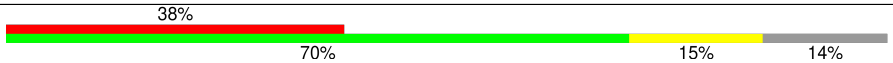
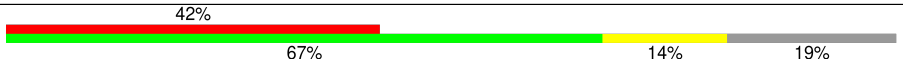
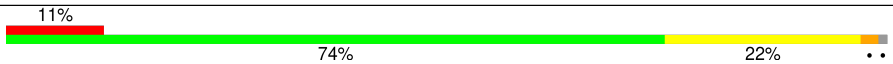
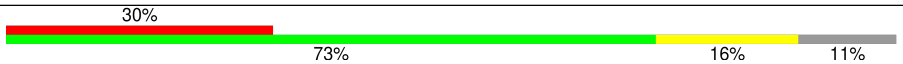
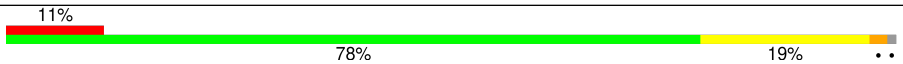
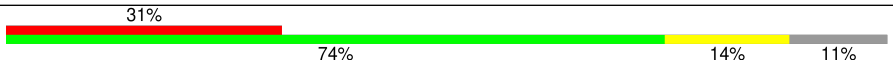
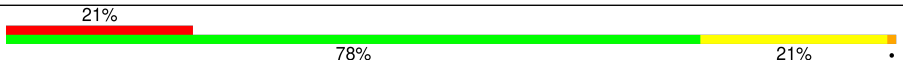
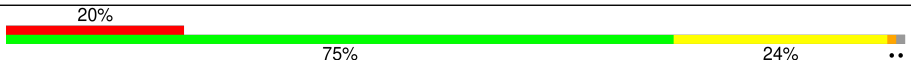
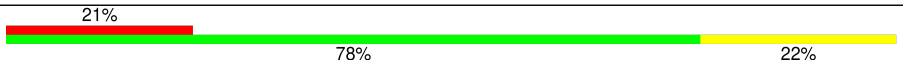
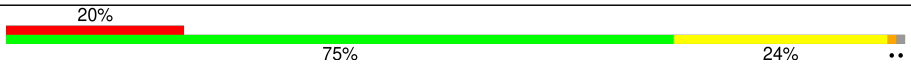
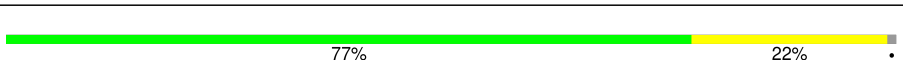
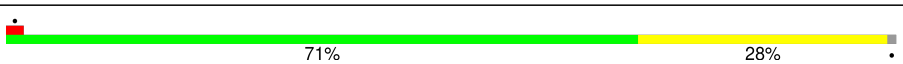
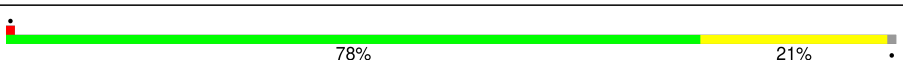
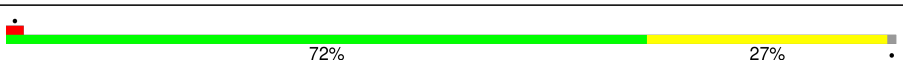
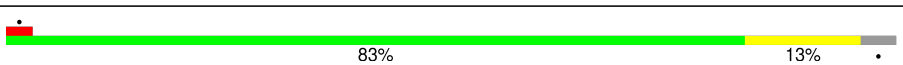
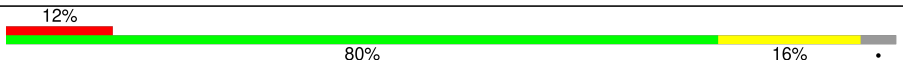
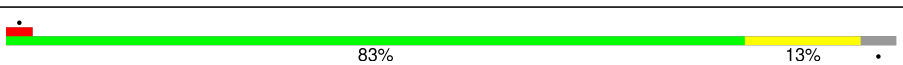
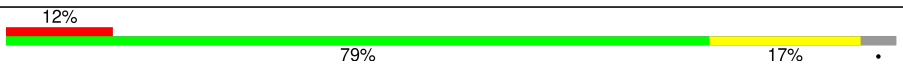
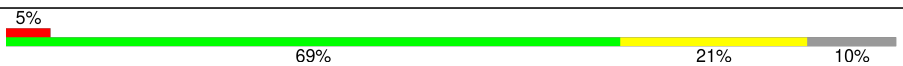
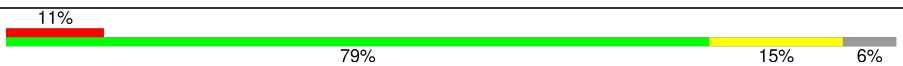
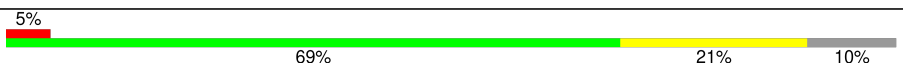
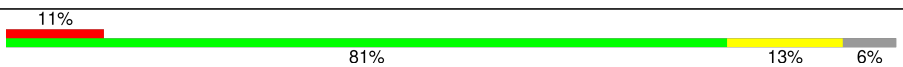
Mol	Chain	Length	Quality of chain
111	qd	319	
112	QE	269	
112	Qe	269	
112	qE	269	
112	qe	269	
113	QF	90	
113	Qf	90	
113	qF	90	
113	qf	90	
114	QG	328	
114	Qg	328	
114	qG	328	
114	qg	328	
115	QH	130	
115	Qh	130	
115	qH	130	
115	qh	130	
116	QI	119	
116	Qi	119	
116	qI	119	
116	qi	119	
117	QJ	62	
117	Qj	62	
117	qJ	62	
117	qj	62	

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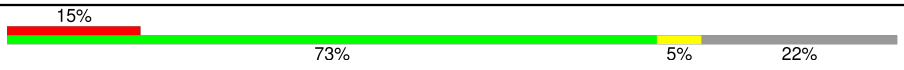
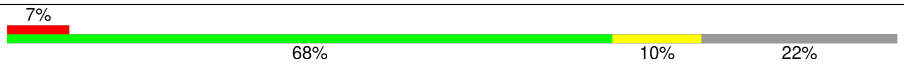
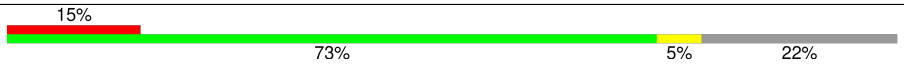
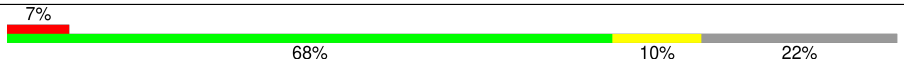
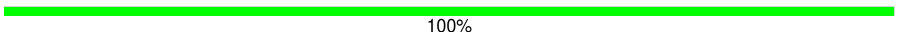
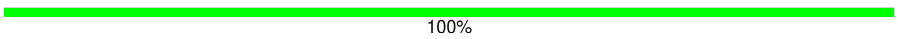
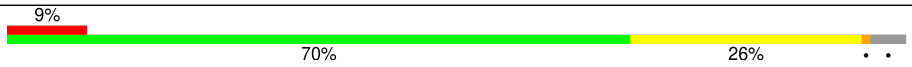
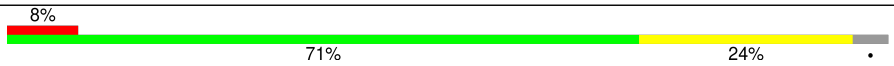
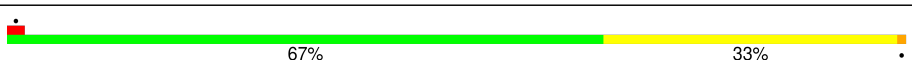
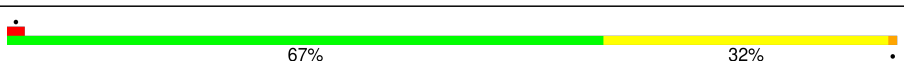
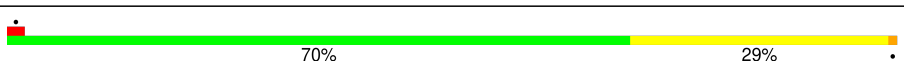
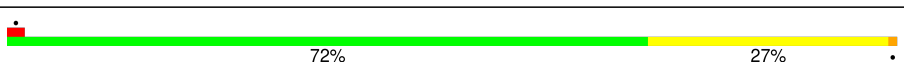
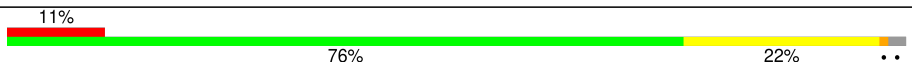
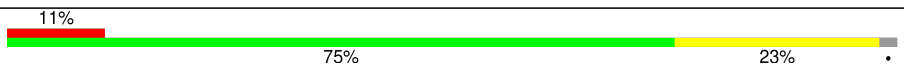
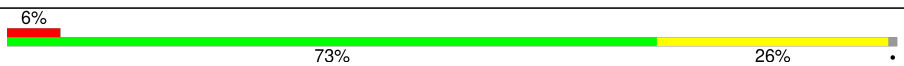
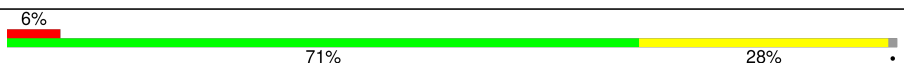
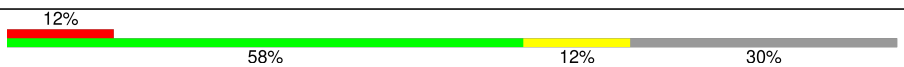
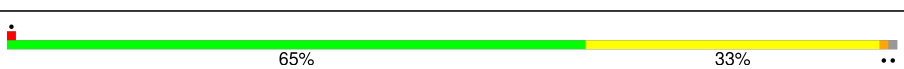
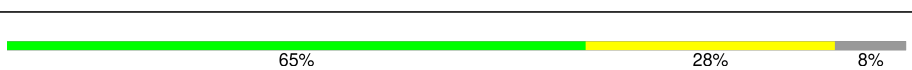
Mol	Chain	Length	Quality of chain
118	QL	41	
118	Ql	41	
118	qL	41	
118	ql	41	
119	QM	17	
119	Qm	17	
119	U2	17	
119	qM	17	
119	qm	17	
119	u2	17	
120	S1	718	
120	s1	718	
121	S2	442	
121	s2	442	
122	S3	198	
122	s3	198	
123	S4	185	
123	s4	185	
124	S5	94	
124	s5	94	
125	S6	132	
125	s6	132	
126	S7	162	
126	s7	162	
127	S8	236	

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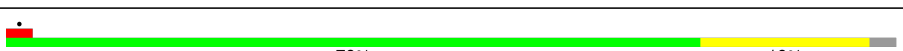
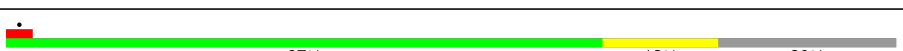
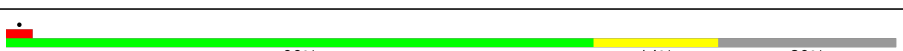
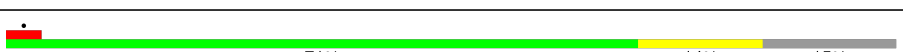
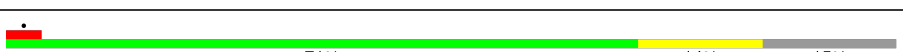
Mol	Chain	Length	Quality of chain
127	s8	236	
128	T1	516	
128	t1	516	
129	T2	333	
129	t2	333	
130	T3	311	
130	t3	311	
131	T4	212	
131	t4	212	
132	T5	205	
132	t5	205	
133	T6	144	
133	t6	144	
134	T7	143	
134	t7	143	
135	T8	135	
135	t8	135	
136	T9	136	
136	t9	136	
137	TA	127	
137	ta	127	
138	TB	113	
138	tb	113	
139	TC	93	
139	tc	93	

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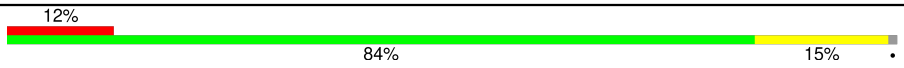
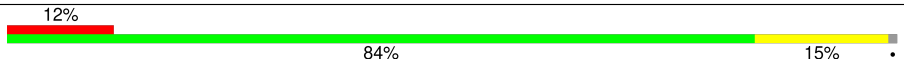
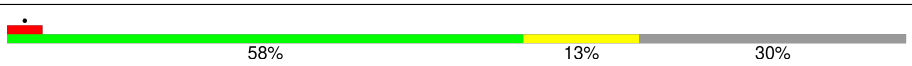
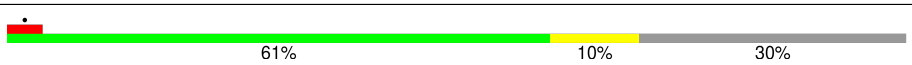
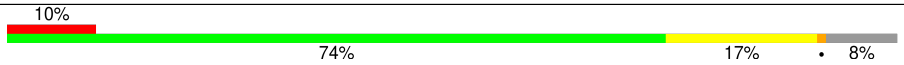
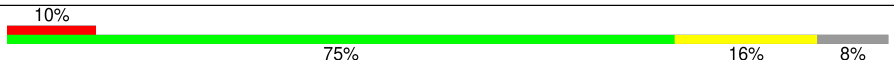
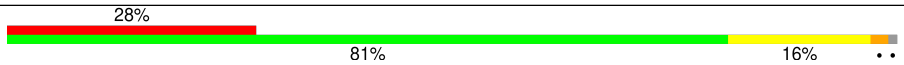
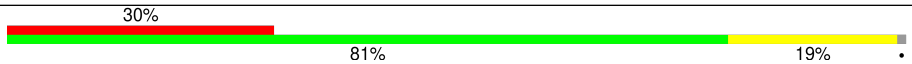
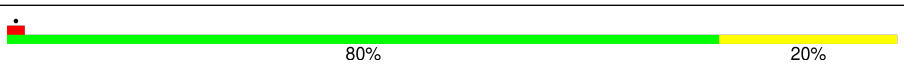
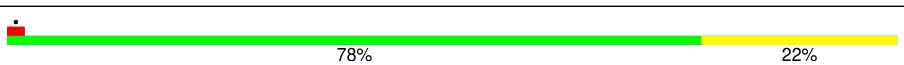
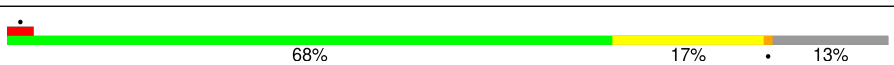
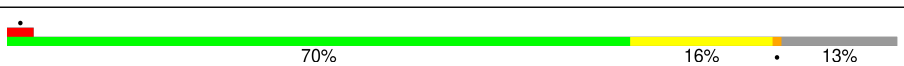
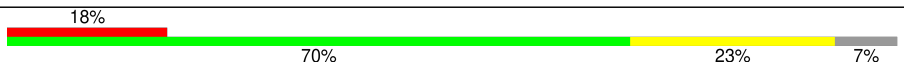
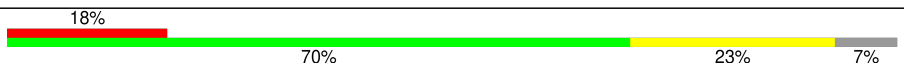
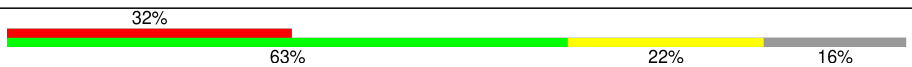
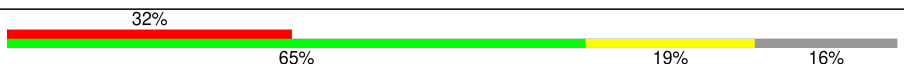
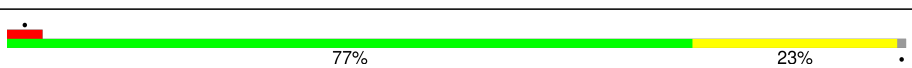
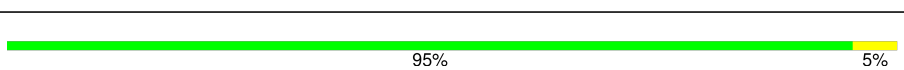
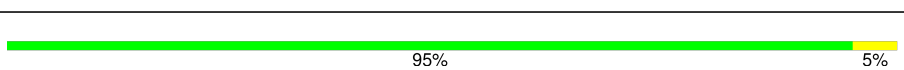
Mol	Chain	Length	Quality of chain
140	TD	73	
140	td	73	
141	TE	71	
141	te	71	
142	TF	236	
142	tf	236	
143	TG	135	
143	tg	135	
144	TH	124	
144	th	124	
145	TX	166	
145	tx	166	
146	V1	474	
146	v1	474	
147	V2	274	
147	v2	274	
148	X1	150	
148	x1	150	
149	C	212	
149	c	212	
150	U1	92	
150	u1	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
162	SF4	S1	801	-	-	X	-
162	SF4	S7	201	-	-	X	-
162	SF4	S8	302	-	-	X	-
162	SF4	s1	801	-	-	X	-
162	SF4	s7	201	-	-	X	-
162	SF4	s8	302	-	-	X	-

2 Entry composition (i)

There are 171 unique types of molecules in this entry. The entry contains 568568 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 Tim10/DDP family zinc finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1t	70	Total	C	N	O	S	0	0
			540	329	98	109	4		
1	1T	70	Total	C	N	O	S	0	0
			540	329	98	109	4		

- Molecule 2 is a protein called NmrA domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2e	321	Total	C	N	O	S	0	0
			2560	1623	449	487	1		
2	2E	321	Total	C	N	O	S	0	0
			2560	1623	449	487	1		

- Molecule 3 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2f	217	Total	C	N	O	S	0	0
			1803	1166	305	328	4		
3	2F	217	Total	C	N	O	S	0	0
			1803	1166	305	328	4		

- Molecule 4 is a protein called SDHTT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2g	198	Total	C	N	O	S	0	0
			1671	1083	276	307	5		
4	2G	198	Total	C	N	O	S	0	0
			1671	1083	276	307	5		

- Molecule 5 is a protein called Diphthamide synthesis protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2h	102	Total	C	N	O	S	0	0
			801	497	139	157	8		
5	2H	102	Total	C	N	O	S	0	0
			801	497	139	157	8		

- Molecule 6 is a protein called DUF4885 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	2i	114	Total	C	N	O	S	0	0
			915	580	153	180	2		
6	2I	114	Total	C	N	O	S	0	0
			915	580	153	180	2		

- Molecule 7 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2j	102	Total	C	N	O	S	0	0
			839	549	139	149	2		
7	2J	102	Total	C	N	O	S	0	0
			839	549	139	149	2		

- Molecule 8 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2k	93	Total	C	N	O	S	0	0
			795	530	129	134	2		
8	2K	93	Total	C	N	O	S	0	0
			795	530	129	134	2		

- Molecule 9 is a protein called Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2l	83	Total	C	N	O	S	0	0
			722	467	120	134	1		
9	2L	83	Total	C	N	O	S	0	0
			722	467	120	134	1		

- Molecule 10 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2m	75	Total	C	N	O	S	0	0
			640	412	116	110	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2M	75	Total 640	C 412	N 116	O 110	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2n	61	Total 505	C 341	N 78	O 84	S 2	0	0
11	2N	61	Total 505	C 341	N 78	O 84	S 2	0	0

- Molecule 12 is a protein called SDHTT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2o	42	Total 356	C 239	N 59	O 56	S 2	0	0
12	2O	42	Total 356	C 239	N 59	O 56	S 2	0	0

- Molecule 13 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2t	70	Total 567	C 353	N 100	O 110	S 4	0	0
13	2T	70	Total 567	C 353	N 100	O 110	S 4	0	0

- Molecule 14 is a protein called Zf-Tim10_DDP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3t	83	Total 655	C 412	N 109	O 128	S 6	0	0
14	3T	83	Total 655	C 412	N 109	O 128	S 6	0	0

- Molecule 15 is a protein called Phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4a	100	Total 816	C 519	N 144	O 151	S 2	0	0
15	4A	100	Total 816	C 519	N 144	O 151	S 2	0	0

- Molecule 16 is a protein called Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4t	57	Total	C	N	O	S	0	0
			481	308	80	90	3		
16	4T	57	Total	C	N	O	S	0	0
			481	308	80	90	3		

- Molecule 17 is a protein called Cullin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5t	62	Total	C	N	O	S	0	0
			506	322	89	93	2		
17	5T	62	Total	C	N	O	S	0	0
			506	322	89	93	2		

- Molecule 18 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6a	126	Total	C	N	O	S	0	0
			1083	698	184	199	2		
18	6A	126	Total	C	N	O	S	0	0
			1083	698	184	199	2		

- Molecule 19 is a protein called Structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6b	222	Total	C	N	O	S	0	0
			1912	1238	312	349	13		
19	6B	222	Total	C	N	O	S	0	0
			1912	1238	312	349	13		

- Molecule 20 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6c	101	Total	C	N	O	S	0	0
			891	580	158	150	3		
20	6C	101	Total	C	N	O	S	0	0
			891	580	158	150	3		

- Molecule 21 is a protein called Decapping nuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6l	77	Total	C	N	O	S	0	0
			636	407	108	115	6		
21	6L	77	Total	C	N	O	S	0	0
			636	407	108	115	6		

- Molecule 22 is a protein called Annexin.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6t	70	Total	C	N	O	S	0	0
			561	362	90	105	4		
22	6T	70	Total	C	N	O	S	0	0
			561	362	90	105	4		

- Molecule 23 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	7a	133	Total	C	N	O	S	0	0
			1166	769	197	199	1		
23	7A	133	Total	C	N	O	S	0	0
			1166	769	197	199	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	7c	211	Total	C	N	O	P	S	0	0
			1825	1163	299	354	1	8		
24	7C	211	Total	C	N	O	P	S	0	0
			1825	1163	299	354	1	8		

- Molecule 25 is a protein called CTF/NF-I domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	7l	131	Total	C	N	O	S	0	0
			1078	698	175	196	9		
25	7L	131	Total	C	N	O	S	0	0
			1078	698	175	196	9		

- Molecule 26 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	449	Total	C	N	O	S	0	0
			3756	2408	638	701	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	449	Total	C	N	O	S	0	0
			3756	2408	638	701	9		

- Molecule 27 is a protein called Protein phosphatase 2C, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	428	Total	C	N	O	S	0	0
			3398	2164	593	638	3		
27	B	428	Total	C	N	O	S	0	0
			3398	2164	593	638	3		

- Molecule 28 is a protein called Chromosome condensation regulator RCC1 repeat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	bp	381	Total	C	N	O	S	0	0
			2920	1858	493	567	2		
28	BP	381	Total	C	N	O	S	0	0
			2920	1858	493	567	2		

- Molecule 29 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	674	Total	C	N	O	S	0	0
			5576	3730	910	900	36		
29	C1	674	Total	C	N	O	S	0	0
			5576	3730	910	900	36		

- Molecule 30 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c2	599	Total	C	N	O	S	0	0
			5094	3322	881	880	11		
30	C2	599	Total	C	N	O	S	0	0
			5094	3322	881	880	11		

- Molecule 31 is a protein called Ymf68.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c3	582	Total	C	N	O	S	0	0
			5084	3451	787	838	8		
31	C3	582	Total	C	N	O	S	0	0
			5084	3451	787	838	8		

- Molecule 32 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	289	Total	C	N	O	S	0	0
			2366	1523	400	438	5		
32	D	289	Total	C	N	O	S	0	0
			2366	1523	400	438	5		

- Molecule 33 is a protein called TraB family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	384	Total	C	N	O	S	0	0
			3176	2045	549	575	7		
33	E	384	Total	C	N	O	S	0	0
			3176	2045	549	575	7		

- Molecule 34 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	243	Total	C	N	O	S	0	0
			2024	1304	335	380	5		
34	F	243	Total	C	N	O	S	0	0
			2024	1304	335	380	5		

- Molecule 35 is a protein called Iron-binding zinc finger CDGSH type protein.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	293	Total	C	N	O	S	0	0
			2442	1555	410	465	12		
36	G	293	Total	C	N	O	S	0	0
			2442	1555	410	465	12		

- Molecule 37 is a protein called SURF1-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	298	Total	C	N	O	S	0	0
			2369	1500	409	450	10		
37	H	298	Total	C	N	O	S	0	0
			2369	1500	409	450	10		

- Molecule 38 is a protein called COXTT9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	231	Total	C	N	O	S	0	0
			1943	1253	340	346	4		
38	I	231	Total	C	N	O	S	0	0
			1943	1253	340	346	4		

- Molecule 39 is a protein called COXTT10.

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

- Molecule 40 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 41 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

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

- Molecule 42 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	219	Total	C	N	O	S	0	0
			1872	1218	315	328	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	M	219	Total	C	N	O	S	0	0
			1872	1218	315	328	11		

- Molecule 43 is a protein called Oxoglutarate/malate translocator protein, putative.

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

- Molecule 44 is a protein called 2-oxoglutarate/malate carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m2	318	Total	C	N	O	S	0	0
			2558	1665	440	449	4		
44	M2	318	Total	C	N	O	S	0	0
			2558	1665	440	449	4		

- Molecule 45 is a protein called Carrier protein.

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

- 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 Mobilization protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	129	Total	C	N	O	S	0	0
			1081	675	191	209	6		
47	O	129	Total	C	N	O	S	0	0
			1081	675	191	209	6		

- Molecule 48 is a protein called YflT domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	175	Total	C	N	O	S	0	0
			1410	889	247	273	1		
48	P	175	Total	C	N	O	S	0	0
			1410	889	247	273	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 Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	172	Total	C	N	O	S	0	0
			1407	921	231	252	3		
50	R	172	Total	C	N	O	S	0	0
			1407	921	231	252	3		

- Molecule 51 is a protein called Complex III subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	169	Total	C	N	O	S	0	0
			1388	878	243	263	4		
51	S	169	Total	C	N	O	S	0	0
			1388	878	243	263	4		

- Molecule 52 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	sa	599	Total	C	N	O	S	0	0
			4624	2907	825	866	26		
52	SA	599	Total	C	N	O	S	0	0
			4624	2907	825	866	26		

- Molecule 53 is a protein called Succinate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sb	279	Total	C	N	O	S	0	0
			2260	1437	385	417	21		
53	SB	279	Total	C	N	O	S	0	0
			2260	1437	385	417	21		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	sc	58	Total	C	N	O	0	0
			481	314	85	82		
54	SC	58	Total	C	N	O	0	0
			481	314	85	82		

- Molecule 55 is a protein called SDHD.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	sd	44	Total	C	N	O	S	0	0
			393	271	60	60	2		
55	SD	44	Total	C	N	O	S	0	0
			393	271	60	60	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
56	t	156	Total	C	N	O	S	0	0
			1315	858	230	223	4		
56	T	156	Total	C	N	O	S	0	0
			1315	858	230	223	4		

- Molecule 57 is a protein called Transmembrane protein, putative.

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

- Molecule 58 is a protein called COXTT22.

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

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

- Molecule 59 is a protein called Cytochrome C oxidase subunit Vb protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	vb	555	Total 4630	C 2918	N 779	O 914	P 2	S 17	0	0
59	VB	555	Total 4630	C 2918	N 779	O 914	P 2	S 17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	w	123	Total 1096	C 716	N 183	O 193	S 4	0	0
60	W	123	Total 1096	C 716	N 183	O 193	S 4	0	0

- Molecule 61 is a protein called Transmembrane protein, putative.

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

- Molecule 62 is a protein called Lysozyme.

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

- Molecule 63 is a protein called Ymf70.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	y0	89	Total 775	C 535	N 115	O 123	S 2	0	0
63	Y0	89	Total 775	C 535	N 115	O 123	S 2	0	0

- Molecule 64 is a protein called Ymf75.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	y5	190	Total	C	N	O	S	0	0
			1659	1141	249	265	4		
64	Y5	190	Total	C	N	O	S	0	0
			1659	1141	249	265	4		

- Molecule 65 is a protein called Ymf67.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	y7	343	Total	C	N	O	S	0	0
			2938	1964	468	500	6		
65	Y7	343	Total	C	N	O	S	0	0
			2938	1964	468	500	6		

- Molecule 66 is a protein called ABC transporter.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	z	87	Total	C	N	O	0	0
			717	459	130	128		
66	Z	87	Total	C	N	O	0	0
			717	459	130	128		

- Molecule 67 is a protein called COXTT28.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	z1	97	Total	C	N	O	S	0	0
			766	489	135	140	2		
67	Z1	97	Total	C	N	O	S	0	0
			766	489	135	140	2		

- Molecule 68 is a protein called NADH dehydrogenase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	1b	59	Total	C	N	O	S	0	0
			516	362	78	73	3		
68	1B	59	Total	C	N	O	S	0	0
			516	362	78	73	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1b	49	VAL	LEU	conflict	UNP Q09FB0

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

- Molecule 69 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	2b	178	Total	C	N	O	S	0	0
			1483	1015	215	248	5		
69	2B	178	Total	C	N	O	S	0	0
			1483	1015	215	248	5		

- Molecule 70 is a protein called Ymf58.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	4l	116	Total	C	N	O	S	0	0
			957	648	142	163	4		
70	4L	116	Total	C	N	O	S	0	0
			957	648	142	163	4		

- Molecule 71 is a protein called Ymf57.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	5b	100	Total	C	N	O	S	0	0
			888	620	128	137	3		
71	5B	100	Total	C	N	O	S	0	0
			888	620	128	137	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
72	a1	93	Total	C	N	O	0	0
			806	531	139	136		
72	A1	93	Total	C	N	O	0	0
			806	531	139	136		

- Molecule 73 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	a2	98	Total	C	N	O	S	0	0
			811	512	146	151	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
73	A2	98	Total	C	N	O	S	0	0
			811	512	146	151	2		

- Molecule 74 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a3	129	Total	C	N	O	S	0	0
			1077	697	195	182	3		
74	A3	129	Total	C	N	O	S	0	0
			1077	697	195	182	3		

- Molecule 75 is a protein called ETC complex I subunit motif protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	a5	155	Total	C	N	O	S	0	0
			1307	838	219	244	6		
75	A5	155	Total	C	N	O	S	0	0
			1307	838	219	244	6		

- Molecule 76 is a protein called NADH dehydrogenase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	a6	172	Total	C	N	O	S	0	0
			1421	903	253	257	8		
76	A6	172	Total	C	N	O	S	0	0
			1421	903	253	257	8		

- Molecule 77 is a protein called 37S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	a7	282	Total	C	N	O	S	0	0
			2347	1478	413	453	3		
77	A7	282	Total	C	N	O	S	0	0
			2347	1478	413	453	3		

- Molecule 78 is a protein called CX9C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	a8	132	Total	C	N	O	S	0	0
			1075	676	180	208	11		
78	A8	132	Total	C	N	O	S	0	0
			1075	676	180	208	11		

- Molecule 79 is a protein called NAD-dependent epimerase/dehydratase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	a9	340	Total	C	N	O	S	0	0
			2736	1747	479	498	12		
79	A9	340	Total	C	N	O	S	0	0
			2736	1747	479	498	12		

- Molecule 80 is a protein called Acyl carrier protein.

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

- Molecule 81 is a protein called Acyl carrier protein.

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

- Molecule 82 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 83 is a protein called NDUA13.

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

- Molecule 84 is a protein called Transmembrane protein, putative.

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

- Molecule 85 is a protein called NDUB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	b2	120	Total	C	N	O	S	0	0
			966	621	167	175	3		
85	B2	120	Total	C	N	O	S	0	0
			966	621	167	175	3		

- Molecule 86 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	b3	69	Total	C	N	O	S	0	0
			602	396	105	100	1		
86	B3	69	Total	C	N	O	S	0	0
			602	396	105	100	1		

- Molecule 87 is a protein called NDUB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	b4	115	Total	C	N	O	S	0	0
			976	641	156	175	4		
87	B4	115	Total	C	N	O	S	0	0
			976	641	156	175	4		

- Molecule 88 is a protein called NDUB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	b6	70	Total	C	N	O	S	0	0
			596	400	98	94	4		
88	B6	70	Total	C	N	O	S	0	0
			596	400	98	94	4		

- Molecule 89 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	b7	116	Total	C	N	O	S	0	0
			941	595	163	177	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
89	B7	116	Total	C	N	O	S	0	0
			941	595	163	177	6		

- Molecule 90 is a protein called NDUB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	b8	175	Total	C	N	O	S	0	0
			1456	936	248	266	6		
90	B8	175	Total	C	N	O	S	0	0
			1456	936	248	266	6		

- Molecule 91 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	b9	188	Total	C	N	O	S	0	0
			1596	1032	255	304	5		
91	B9	188	Total	C	N	O	S	0	0
			1596	1032	255	304	5		

- Molecule 92 is a protein called NDUB10.

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

- Molecule 93 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	bm	164	Total	C	N	O	S	0	0
			1321	834	223	259	5		
93	BM	164	Total	C	N	O	S	0	0
			1321	834	223	259	5		

- Molecule 94 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	c4	102	Total	C	N	O	S	0	0
			850	553	139	150	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
94	C4	102	Total 850	C 553	N 139	O 150	S 8	0	0

- Molecule 95 is a protein called 2 iron, 2 sulfur cluster-binding protein.

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

- Molecule 96 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	g1	229	Total 1773	C 1113	N 305	O 350	S 5	0	0
96	G1	229	Total 1773	C 1113	N 305	O 350	S 5	0	0

- Molecule 97 is a protein called Gamma-carbonic anhydrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	g2	230	Total 1762	C 1106	N 315	O 334	S 7	0	0
97	G2	230	Total 1762	C 1106	N 315	O 334	S 7	0	0

- Molecule 98 is a protein called Transcription factor apfi protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	g3	346	Total 2804	C 1766	N 481	O 549	S 8	0	0
98	G3	346	Total 2804	C 1766	N 481	O 549	S 8	0	0

- Molecule 99 is a protein called DnaJ domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	j1	265	Total 2170	C 1375	N 402	O 390	S 3	0	0
99	J1	265	Total 2170	C 1375	N 402	O 390	S 3	0	0

- Molecule 100 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	n1	283	Total	C	N	O	S	0	0
			2305	1581	334	378	12		
100	N1	283	Total	C	N	O	S	0	0
			2305	1581	334	378	12		

- Molecule 101 is a protein called Ymf65.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	n2	360	Total	C	N	O	S	0	0
			3073	2134	436	495	8		
101	N2	360	Total	C	N	O	S	0	0
			3073	2134	436	495	8		

- Molecule 102 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	n3	120	Total	C	N	O	S	0	0
			1017	705	142	166	4		
102	N3	120	Total	C	N	O	S	0	0
			1017	705	142	166	4		

- Molecule 103 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	n4	505	Total	C	N	O	S	0	0
			4170	2859	601	692	18		
103	N4	505	Total	C	N	O	S	0	0
			4170	2859	601	692	18		

- Molecule 104 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	n5	709	Total	C	N	O	S	0	0
			5908	4044	850	998	16		
104	N5	709	Total	C	N	O	S	0	0
			5908	4044	850	998	16		

- Molecule 105 is a protein called Ymf62.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	n6	255	Total	C	N	O	S	0	0
			2168	1483	306	374	5		
105	N6	255	Total	C	N	O	S	0	0
			2168	1483	306	374	5		

- Molecule 106 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	p1	230	Total	C	N	O	S	0	0
			1908	1241	322	340	5		
106	P1	230	Total	C	N	O	S	0	0
			1908	1241	322	340	5		

- Molecule 107 is a protein called NDUPH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	p2	167	Total	C	N	O	S	0	0
			1414	926	225	258	5		
107	P2	167	Total	C	N	O	S	0	0
			1414	926	225	258	5		

- Molecule 108 is a protein called M16 family peptidase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	qA	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		
108	qa	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		
108	QA	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		
108	Qa	454	Total	C	N	O	S	0	0
			3517	2213	599	699	6		

- Molecule 109 is a protein called Peptidase M16 inactive domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	qB	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		
109	qb	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		
109	QB	480	Total	C	N	O	S	0	0
			3835	2431	668	731	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
109	Qb	480	Total 3835	C 2431	N 668	O 731	S 5	0	0

- Molecule 110 is a protein called Apocytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	qC	426	Total 3589	C 2417	N 541	O 609	S 22	0	0
110	qc	425	Total 3580	C 2411	N 539	O 608	S 22	0	0
110	QC	426	Total 3589	C 2417	N 541	O 609	S 22	0	0
110	Qc	425	Total 3580	C 2411	N 539	O 608	S 22	0	0

- Molecule 111 is a protein called Cytochrome protein c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	qD	295	Total 2489	C 1627	N 418	O 431	S 13	0	0
111	qd	295	Total 2489	C 1627	N 418	O 431	S 13	0	0
111	QD	295	Total 2489	C 1627	N 418	O 431	S 13	0	0
111	Qd	295	Total 2489	C 1627	N 418	O 431	S 13	0	0

- Molecule 112 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	qE	230	Total 1559	C 971	N 294	O 292	S 2	0	0
112	qe	219	Total 1471	C 917	N 278	O 274	S 2	0	0
112	QE	230	Total 1559	C 971	N 294	O 292	S 2	0	0
112	Qe	219	Total 1471	C 917	N 278	O 274	S 2	0	0

- Molecule 113 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	qF	89	Total	C	N	O	S	0	0
			702	439	125	129	9		
113	qf	80	Total	C	N	O	S	0	0
			630	393	112	116	9		
113	QF	89	Total	C	N	O	S	0	0
			702	439	125	129	9		
113	Qf	80	Total	C	N	O	S	0	0
			630	393	112	116	9		

- Molecule 114 is a protein called Sulphotransf domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	qG	327	Total	C	N	O	S	0	0
			2767	1789	482	490	6		
114	qg	326	Total	C	N	O	S	0	0
			2760	1784	481	489	6		
114	QG	327	Total	C	N	O	S	0	0
			2767	1789	482	490	6		
114	Qg	326	Total	C	N	O	S	0	0
			2760	1784	481	489	6		

- Molecule 115 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	qH	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
115	qh	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
115	QH	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		
115	Qh	129	Total	C	N	O	S	0	0
			1098	708	195	187	8		

- Molecule 116 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	qI	114	Total	C	N	O	S	0	0
			971	651	161	158	1		
116	qi	114	Total	C	N	O	S	0	0
			971	651	161	158	1		
116	QI	114	Total	C	N	O	S	0	0
			971	651	161	158	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
116	Qi	114	Total	C	N	O	S	0	0
			971	651	161	158	1		

- Molecule 117 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	qJ	56	Total	C	N	O	S	0	0
			481	329	73	77	2		
117	qj	58	Total	C	N	O	S	0	0
			501	341	79	79	2		
117	QJ	56	Total	C	N	O	S	0	0
			481	329	73	77	2		
117	Qj	58	Total	C	N	O	S	0	0
			501	341	79	79	2		

- Molecule 118 is a protein called UQCRTT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	qL	32	Total	C	N	O	S	0	0
			266	181	41	42	2		
118	ql	32	Total	C	N	O	S	0	0
			266	181	41	42	2		
118	QL	32	Total	C	N	O	S	0	0
			266	181	41	42	2		
118	Ql	32	Total	C	N	O	S	0	0
			266	181	41	42	2		

- Molecule 119 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
119	qM	17	Total	C	N	O	0	0
			85	51	17	17		
119	qm	17	Total	C	N	O	0	0
			85	51	17	17		
119	Qm	17	Total	C	N	O	0	0
			85	51	17	17		
119	u2	17	Total	C	N	O	0	0
			85	51	17	17		
119	U2	17	Total	C	N	O	0	0
			85	51	17	17		
119	QM	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 120 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	s1	689	Total	C	N	O	S	0	0
			5410	3414	937	1031	28		
120	S1	689	Total	C	N	O	S	0	0
			5410	3414	937	1031	28		

- Molecule 121 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
121	s2	442	Total	C	N	O	S	0	0
			3598	2291	624	659	24		
121	S2	442	Total	C	N	O	S	0	0
			3598	2291	624	659	24		

- Molecule 122 is a protein called NADH dehydrogenase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
122	s3	198	Total	C	N	O	S	0	0
			1681	1096	267	312	6		
122	S3	198	Total	C	N	O	S	0	0
			1681	1096	267	312	6		

- Molecule 123 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
123	s4	182	Total	C	N	O	S	0	0
			1500	952	268	272	8		
123	S4	182	Total	C	N	O	S	0	0
			1500	952	268	272	8		

- Molecule 124 is a protein called GRAM domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
124	s5	93	Total	C	N	O	S	0	0
			756	480	129	141	6		
124	S5	93	Total	C	N	O	S	0	0
			756	480	129	141	6		

- Molecule 125 is a protein called Zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
125	s6	92	Total	C	N	O	S	0	0
			738	464	131	139	4		
125	S6	92	Total	C	N	O	S	0	0
			738	464	131	139	4		

- Molecule 126 is a protein called NADH dehydrogenase subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	s7	161	Total	C	N	O	S	0	0
			1278	822	220	226	10		
126	S7	161	Total	C	N	O	S	0	0
			1278	822	220	226	10		

- Molecule 127 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	s8	218	Total	C	N	O	S	0	0
			1812	1155	299	347	11		
127	S8	218	Total	C	N	O	S	0	0
			1812	1155	299	347	11		

- Molecule 128 is a protein called Lipid-A-disaccharide synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
128	t1	502	Total	C	N	O	S	0	0
			4059	2600	698	748	13		
128	T1	502	Total	C	N	O	S	0	0
			4059	2600	698	748	13		

- Molecule 129 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

Mol	Chain	Residues	Atoms					AltConf	Trace
129	t2	279	Total	C	N	O	S	0	0
			2180	1386	375	418	1		
129	T2	279	Total	C	N	O	S	0	0
			2180	1386	375	418	1		

- Molecule 130 is a protein called RNase III domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
130	t3	310	Total	C	N	O	S	0	0
			2479	1576	432	464	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
130	T3	310	Total 2479	C 1576	N 432	O 464	S 7	0	0

- Molecule 131 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
131	t4	198	Total 1644	C 1068	N 284	O 289	S 3	0	0
131	T4	198	Total 1644	C 1068	N 284	O 289	S 3	0	0

- Molecule 132 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
132	t5	141	Total 1138	C 730	N 202	O 204	S 2	0	0
132	T5	141	Total 1138	C 730	N 202	O 204	S 2	0	0

- Molecule 133 is a protein called COX assembly mitochondrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
133	t6	109	Total 903	C 562	N 161	O 174	S 6	0	0
133	T6	109	Total 903	C 562	N 161	O 174	S 6	0	0

- Molecule 134 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
134	t7	142	Total 1187	C 770	N 202	O 209	S 6	0	0
134	T7	142	Total 1187	C 770	N 202	O 209	S 6	0	0

- Molecule 135 is a protein called PH domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
135	t8	131	Total 1084	C 705	N 191	O 188	0	0
135	T8	131	Total 1084	C 705	N 191	O 188	0	0

- Molecule 136 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
136	t9	132	Total	C	N	O	S	0	0
			1066	670	185	201	10		
136	T9	132	Total	C	N	O	S	0	0
			1066	670	185	201	10		

- Molecule 137 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 138 is a protein called Transmembrane protein, putative.

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

- Molecule 139 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
139	tc	92	Total	C	N	O	S	0	0
			789	497	146	145	1		
139	TC	92	Total	C	N	O	S	0	0
			789	497	146	145	1		

- Molecule 140 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
140	td	72	Total	C	N	O	0	0
			616	403	110	103		
140	TD	72	Total	C	N	O	0	0
			616	403	110	103		

- Molecule 141 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
141	te	50	Total	C	N	O	S	0	0
			420	282	64	72	2		
141	TE	50	Total	C	N	O	S	0	0
			420	282	64	72	2		

- Molecule 142 is a protein called NDUTT15.

Mol	Chain	Residues	Atoms					AltConf	Trace
142	tf	216	Total	C	N	O	S	0	0
			1789	1150	304	327	8		
142	TF	216	Total	C	N	O	S	0	0
			1789	1150	304	327	8		

- Molecule 143 is a protein called NDUTT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
143	tg	134	Total	C	N	O	S	0	0
			1081	683	194	203	1		
143	TG	134	Total	C	N	O	S	0	0
			1081	683	194	203	1		

- Molecule 144 is a protein called NDUTT17.

Mol	Chain	Residues	Atoms					AltConf	Trace
144	th	124	Total	C	N	O	S	0	0
			996	639	178	177	2		
144	TH	124	Total	C	N	O	S	0	0
			996	639	178	177	2		

- Molecule 145 is a protein called Thioredoxin.

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

- Molecule 146 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
146	v1	442	Total	C	N	O	S	0	0
			3410	2146	600	640	24		

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

- Molecule 147 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
147	v2	231	Total	C	N	O	S	0	0
			1858	1173	318	357	10		
147	V2	231	Total	C	N	O	S	0	0
			1858	1173	318	357	10		

- Molecule 148 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
148	x1	149	Total	C	N	O	0	0
			1227	800	213	214		
148	X1	149	Total	C	N	O	0	0
			1227	800	213	214		

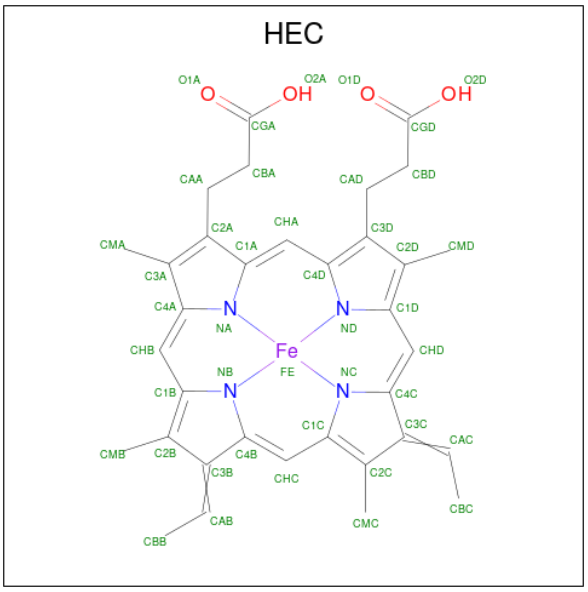
- Molecule 149 is a protein called COXTT3.

Mol	Chain	Residues	Atoms				AltConf	Trace
149	C	203	Total	C	N	O	0	0
			1368	851	246	271		
149	c	203	Total	C	N	O	0	0
			1368	851	246	271		

- Molecule 150 is a protein called Unknown peptide.

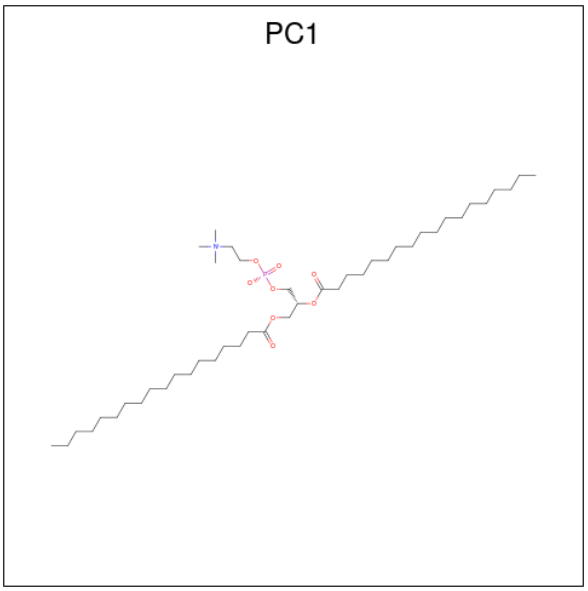
Mol	Chain	Residues	Atoms				AltConf	Trace
150	u1	92	Total	C	N	O	0	0
			460	276	92	92		
150	U1	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 151 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
151	2e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
151	qD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
151	qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
151	2E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
151	QD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
151	Qd	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 152 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
152	2f	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	2f	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	2f	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	2g	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	2j	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	6a	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	6c	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	7a	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	7c	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	a	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	a	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	c1	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	c1	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	c1	1	Total	C	N	O	P	0
			38	28	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	c1	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	c2	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	c3	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	c3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	c3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	c3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	c3	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	f	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	fs	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	i	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	j	1	Total	C	N	O	P	0
			37	27	1	8	1	
152	m	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	m	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	m	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	m1	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	m1	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	m2	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	m2	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	m2	1	Total	C	N	O	P	0
			46	36	1	8	1	
152	n	1	Total	C	N	O	P	0
			41	31	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	n	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	n	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	v	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	v	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	w	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	w	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	w	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	5b	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	al	1	Total	C	N	O	P	0
			26	16	1	8	1	
152	am	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	an	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	b9	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	c4	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	j1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	n1	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	n3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	n5	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	n5	1	Total	C	N	O	P	0
			53	43	1	8	1	
152	n5	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	n5	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	n6	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	p1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	qB	1	Total	C	N	O	P	0
			44	34	1	8	1	
152	qC	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	qC	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	qC	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	qE	1	Total	C	N	O	P	0
			24	14	1	8	1	
152	qE	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	qE	1	Total	C	N	O	P	0
			28	18	1	8	1	
152	qG	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	qI	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	qI	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	qJ	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	qb	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	qc	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	qc	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	qe	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	qe	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	qg	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	qi	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	qi	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	qj	1	Total	C	N	O	P	0
			36	26	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	s8	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	t1	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	t4	1	Total	C	N	O	P	0
			48	38	1	8	1	
152	t4	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	tc	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	tc	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	te	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	2F	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	2F	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	2F	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	2G	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	2J	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	6A	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	6C	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	7A	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	7C	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	C1	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	C1	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	C1	1	Total	C	N	O	P	0
			38	28	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	C1	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	C2	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	C3	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	C3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	C3	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	D	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	F	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	FS	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	I	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	J	1	Total	C	N	O	P	0
			37	27	1	8	1	
152	M	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
152	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	M1	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	M2	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	M2	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	M2	1	Total	C	N	O	P	0
			46	36	1	8	1	
152	N	1	Total	C	N	O	P	0
			41	31	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	N	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	N	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
152	V	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	W	1	Total	C	N	O	P	0
			49	39	1	8	1	
152	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	W	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	5B	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	AL	1	Total	C	N	O	P	0
			26	16	1	8	1	
152	AM	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	AN	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	B9	1	Total	C	N	O	P	0
			34	24	1	8	1	
152	C4	1	Total	C	N	O	P	0
			41	31	1	8	1	
152	J1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	N1	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	N3	1	Total	C	N	O	P	0
			31	21	1	8	1	
152	N5	1	Total	C	N	O	P	0
			52	42	1	8	1	
152	N5	1	Total	C	N	O	P	0
			53	43	1	8	1	
152	N5	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	N5	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	N6	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
152	P1	1	Total	C	N	O	P	0
			40	30	1	8	1	
152	QB	1	Total	C	N	O	P	0
			44	34	1	8	1	
152	QC	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	QC	1	Total	C	N	O	P	0
			50	40	1	8	1	
152	QC	1	Total	C	N	O	P	0
			36	26	1	8	1	
152	QE	1	Total	C	N	O	P	0
			24	14	1	8	1	
152	QE	1	Total	C	N	O	P	0
			39	29	1	8	1	
152	QG	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	QI	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	QI	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	QJ	1	Total	C	N	O	P	0
			28	18	1	8	1	
152	QJ	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	Qb	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	Qc	1	Total	C	N	O	P	0
			38	28	1	8	1	
152	Qc	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	Qe	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	Qe	1	Total	C	N	O	P	0
			43	33	1	8	1	
152	Qg	1	Total	C	N	O	P	0
			32	22	1	8	1	
152	Qi	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	Qi	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	Qj	1	Total	C	N	O	P	0
			36	26	1	8	1	

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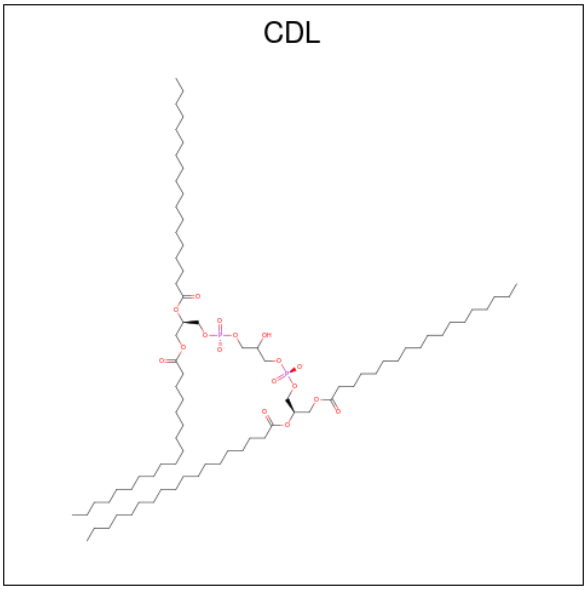
Mol	Chain	Residues	Atoms					AltConf
152	S8	1	Total	C	N	O	P	0
			30	20	1	8	1	
152	T1	1	Total	C	N	O	P	0
			33	23	1	8	1	
152	T4	1	Total	C	N	O	P	0
			48	38	1	8	1	
152	T4	1	Total	C	N	O	P	0
			54	44	1	8	1	
152	TC	1	Total	C	N	O	P	0
			42	32	1	8	1	
152	TC	1	Total	C	N	O	P	0
			47	37	1	8	1	
152	TE	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 153 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
153	2g	1	Total	C	O	P	0
			89	70	17	2	
153	2g	1	Total	C	O	P	0
			55	36	17	2	
153	2g	1	Total	C	O	P	0
			63	44	17	2	
153	2k	1	Total	C	O	P	0
			98	79	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	2m	1	Total	C	O	P	0
			96	77	17	2	
153	2o	1	Total	C	O	P	0
			50	31	17	2	
153	6a	1	Total	C	O	P	0
			74	55	17	2	
153	6c	1	Total	C	O	P	0
			75	56	17	2	
153	6c	1	Total	C	O	P	0
			82	63	17	2	
153	7a	1	Total	C	O	P	0
			100	81	17	2	
153	7a	1	Total	C	O	P	0
			62	43	17	2	
153	7c	1	Total	C	O	P	0
			85	66	17	2	
153	7c	1	Total	C	O	P	0
			51	32	17	2	
153	a	1	Total	C	O	P	0
			51	32	17	2	
153	a	1	Total	C	O	P	0
			94	75	17	2	
153	a	1	Total	C	O	P	0
			82	63	17	2	
153	b	1	Total	C	O	P	0
			62	43	17	2	
153	c1	1	Total	C	O	P	0
			79	60	17	2	
153	c1	1	Total	C	O	P	0
			65	46	17	2	
153	c1	1	Total	C	O	P	0
			63	44	17	2	
153	c1	1	Total	C	O	P	0
			95	76	17	2	
153	c3	1	Total	C	O	P	0
			68	49	17	2	
153	e	1	Total	C	O	P	0
			60	41	17	2	
153	e	1	Total	C	O	P	0
			72	53	17	2	
153	e	1	Total	C	O	P	0
			63	44	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	f	1	Total	C	O	P	0
			100	81	17	2	
153	fs	1	Total	C	O	P	0
			47	28	17	2	
153	i	1	Total	C	O	P	0
			77	58	17	2	
153	i	1	Total	C	O	P	0
			75	56	17	2	
153	j	1	Total	C	O	P	0
			70	51	17	2	
153	l	1	Total	C	O	P	0
			74	55	17	2	
153	m	1	Total	C	O	P	0
			64	45	17	2	
153	m	1	Total	C	O	P	0
			83	64	17	2	
153	m	1	Total	C	O	P	0
			64	45	17	2	
153	m	1	Total	C	O	P	0
			66	47	17	2	
153	m1	1	Total	C	O	P	0
			66	47	17	2	
153	m1	1	Total	C	O	P	0
			91	72	17	2	
153	m1	1	Total	C	O	P	0
			57	38	17	2	
153	m2	1	Total	C	O	P	0
			54	35	17	2	
153	m2	1	Total	C	O	P	0
			66	47	17	2	
153	m2	1	Total	C	O	P	0
			74	55	17	2	
153	m3	1	Total	C	O	P	0
			63	44	17	2	
153	m3	1	Total	C	O	P	0
			55	36	17	2	
153	n	1	Total	C	O	P	0
			84	65	17	2	
153	q	1	Total	C	O	P	0
			63	44	17	2	
153	q	1	Total	C	O	P	0
			72	53	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	q	1	Total	C	O	P	0
			86	67	17	2	
153	r	1	Total	C	O	P	0
			65	46	17	2	
153	sd	1	Total	C	O	P	0
			76	57	17	2	
153	t	1	Total	C	O	P	0
			59	40	17	2	
153	t	1	Total	C	O	P	0
			75	56	17	2	
153	t	1	Total	C	O	P	0
			71	52	17	2	
153	t	1	Total	C	O	P	0
			90	71	17	2	
153	u	1	Total	C	O	P	0
			60	41	17	2	
153	vb	1	Total	C	O	P	0
			62	43	17	2	
153	vb	1	Total	C	O	P	0
			67	48	17	2	
153	w	1	Total	C	O	P	0
			84	65	17	2	
153	y5	1	Total	C	O	P	0
			70	51	17	2	
153	y7	1	Total	C	O	P	0
			65	46	17	2	
153	z	1	Total	C	O	P	0
			67	48	17	2	
153	2b	1	Total	C	O	P	0
			87	68	17	2	
153	5b	1	Total	C	O	P	0
			81	62	17	2	
153	a1	1	Total	C	O	P	0
			67	48	17	2	
153	a9	1	Total	C	O	P	0
			76	57	17	2	
153	a9	1	Total	C	O	P	0
			87	68	17	2	
153	al	1	Total	C	O	P	0
			53	34	17	2	
153	am	1	Total	C	O	P	0
			56	37	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	an	1	Total	C	O	P	0
			87	68	17	2	
153	b3	1	Total	C	O	P	0
			58	39	17	2	
153	b3	1	Total	C	O	P	0
			82	63	17	2	
153	b4	1	Total	C	O	P	0
			37	18	17	2	
153	b8	1	Total	C	O	P	0
			69	50	17	2	
153	bm	1	Total	C	O	P	0
			86	67	17	2	
153	c4	1	Total	C	O	P	0
			98	79	17	2	
153	n5	1	Total	C	O	P	0
			90	71	17	2	
153	n6	1	Total	C	O	P	0
			90	71	17	2	
153	p1	1	Total	C	O	P	0
			63	44	17	2	
153	p1	1	Total	C	O	P	0
			58	39	17	2	
153	qB	1	Total	C	O	P	0
			68	49	17	2	
153	qC	1	Total	C	O	P	0
			64	45	17	2	
153	qC	1	Total	C	O	P	0
			56	37	17	2	
153	qD	1	Total	C	O	P	0
			61	42	17	2	
153	qG	1	Total	C	O	P	0
			86	67	17	2	
153	qH	1	Total	C	O	P	0
			94	75	17	2	
153	qI	1	Total	C	O	P	0
			71	52	17	2	
153	qb	1	Total	C	O	P	0
			68	49	17	2	
153	qc	1	Total	C	O	P	0
			64	45	17	2	
153	qc	1	Total	C	O	P	0
			56	37	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	qc	1	Total	C	O	P	0
			47	28	17	2	
153	qg	1	Total	C	O	P	0
			100	81	17	2	
153	qi	1	Total	C	O	P	0
			71	52	17	2	
153	t1	1	Total	C	O	P	0
			55	36	17	2	
153	t5	1	Total	C	O	P	0
			96	77	17	2	
153	t7	1	Total	C	O	P	0
			73	54	17	2	
153	td	1	Total	C	O	P	0
			66	47	17	2	
153	te	1	Total	C	O	P	0
			53	34	17	2	
153	th	1	Total	C	O	P	0
			84	65	17	2	
153	2G	1	Total	C	O	P	0
			89	70	17	2	
153	2G	1	Total	C	O	P	0
			55	36	17	2	
153	2G	1	Total	C	O	P	0
			63	44	17	2	
153	2K	1	Total	C	O	P	0
			98	79	17	2	
153	2M	1	Total	C	O	P	0
			96	77	17	2	
153	2O	1	Total	C	O	P	0
			50	31	17	2	
153	6A	1	Total	C	O	P	0
			74	55	17	2	
153	6C	1	Total	C	O	P	0
			75	56	17	2	
153	6C	1	Total	C	O	P	0
			82	63	17	2	
153	7A	1	Total	C	O	P	0
			100	81	17	2	
153	7A	1	Total	C	O	P	0
			62	43	17	2	
153	7C	1	Total	C	O	P	0
			85	66	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	7C	1	Total	C	O	P	0
			51	32	17	2	
153	A	1	Total	C	O	P	0
			51	32	17	2	
153	A	1	Total	C	O	P	0
			94	75	17	2	
153	B	1	Total	C	O	P	0
			62	43	17	2	
153	C1	1	Total	C	O	P	0
			79	60	17	2	
153	C1	1	Total	C	O	P	0
			65	46	17	2	
153	C1	1	Total	C	O	P	0
			63	44	17	2	
153	C1	1	Total	C	O	P	0
			95	76	17	2	
153	C3	1	Total	C	O	P	0
			68	49	17	2	
153	E	1	Total	C	O	P	0
			60	41	17	2	
153	E	1	Total	C	O	P	0
			72	53	17	2	
153	E	1	Total	C	O	P	0
			63	44	17	2	
153	F	1	Total	C	O	P	0
			100	81	17	2	
153	FS	1	Total	C	O	P	0
			47	28	17	2	
153	I	1	Total	C	O	P	0
			77	58	17	2	
153	I	1	Total	C	O	P	0
			75	56	17	2	
153	J	1	Total	C	O	P	0
			70	51	17	2	
153	L	1	Total	C	O	P	0
			74	55	17	2	
153	M	1	Total	C	O	P	0
			66	47	17	2	
153	M	1	Total	C	O	P	0
			64	45	17	2	
153	M	1	Total	C	O	P	0
			83	64	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	M	1	Total	C	O	P	0
			64	45	17	2	
153	M1	1	Total	C	O	P	0
			66	47	17	2	
153	M1	1	Total	C	O	P	0
			91	72	17	2	
153	M1	1	Total	C	O	P	0
			57	38	17	2	
153	M2	1	Total	C	O	P	0
			54	35	17	2	
153	M2	1	Total	C	O	P	0
			66	47	17	2	
153	M2	1	Total	C	O	P	0
			74	55	17	2	
153	M3	1	Total	C	O	P	0
			63	44	17	2	
153	M3	1	Total	C	O	P	0
			55	36	17	2	
153	N	1	Total	C	O	P	0
			84	65	17	2	
153	Q	1	Total	C	O	P	0
			63	44	17	2	
153	Q	1	Total	C	O	P	0
			72	53	17	2	
153	R	1	Total	C	O	P	0
			65	46	17	2	
153	SD	1	Total	C	O	P	0
			76	57	17	2	
153	T	1	Total	C	O	P	0
			59	40	17	2	
153	T	1	Total	C	O	P	0
			75	56	17	2	
153	T	1	Total	C	O	P	0
			71	52	17	2	
153	T	1	Total	C	O	P	0
			90	71	17	2	
153	U	1	Total	C	O	P	0
			60	41	17	2	
153	VB	1	Total	C	O	P	0
			62	43	17	2	
153	VB	1	Total	C	O	P	0
			86	67	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	VB	1	Total	C	O	P	0
			82	63	17	2	
153	VB	1	Total	C	O	P	0
			67	48	17	2	
153	W	1	Total	C	O	P	0
			84	65	17	2	
153	Y5	1	Total	C	O	P	0
			70	51	17	2	
153	Y7	1	Total	C	O	P	0
			65	46	17	2	
153	Z	1	Total	C	O	P	0
			67	48	17	2	
153	2B	1	Total	C	O	P	0
			87	68	17	2	
153	5B	1	Total	C	O	P	0
			81	62	17	2	
153	A1	1	Total	C	O	P	0
			66	47	17	2	
153	A1	1	Total	C	O	P	0
			67	48	17	2	
153	A9	1	Total	C	O	P	0
			76	57	17	2	
153	A9	1	Total	C	O	P	0
			87	68	17	2	
153	AL	1	Total	C	O	P	0
			53	34	17	2	
153	AM	1	Total	C	O	P	0
			56	37	17	2	
153	AN	1	Total	C	O	P	0
			87	68	17	2	
153	B3	1	Total	C	O	P	0
			58	39	17	2	
153	B3	1	Total	C	O	P	0
			82	63	17	2	
153	B4	1	Total	C	O	P	0
			37	18	17	2	
153	B8	1	Total	C	O	P	0
			69	50	17	2	
153	BM	1	Total	C	O	P	0
			86	67	17	2	
153	C4	1	Total	C	O	P	0
			98	79	17	2	

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Mol	Chain	Residues	Atoms				AltConf
153	N5	1	Total	C	O	P	0
			90	71	17	2	
153	N6	1	Total	C	O	P	0
			90	71	17	2	
153	P1	1	Total	C	O	P	0
			63	44	17	2	
153	P1	1	Total	C	O	P	0
			58	39	17	2	
153	QB	1	Total	C	O	P	0
			68	49	17	2	
153	QC	1	Total	C	O	P	0
			64	45	17	2	
153	QC	1	Total	C	O	P	0
			56	37	17	2	
153	QD	1	Total	C	O	P	0
			61	42	17	2	
153	QG	1	Total	C	O	P	0
			86	67	17	2	
153	QH	1	Total	C	O	P	0
			94	75	17	2	
153	QI	1	Total	C	O	P	0
			71	52	17	2	
153	Qb	1	Total	C	O	P	0
			68	49	17	2	
153	Qc	1	Total	C	O	P	0
			64	45	17	2	
153	Qc	1	Total	C	O	P	0
			56	37	17	2	
153	Qc	1	Total	C	O	P	0
			47	28	17	2	
153	Qg	1	Total	C	O	P	0
			100	81	17	2	
153	Qi	1	Total	C	O	P	0
			71	52	17	2	
153	T1	1	Total	C	O	P	0
			55	36	17	2	
153	T5	1	Total	C	O	P	0
			96	77	17	2	
153	T7	1	Total	C	O	P	0
			73	54	17	2	
153	TE	1	Total	C	O	P	0
			53	34	17	2	

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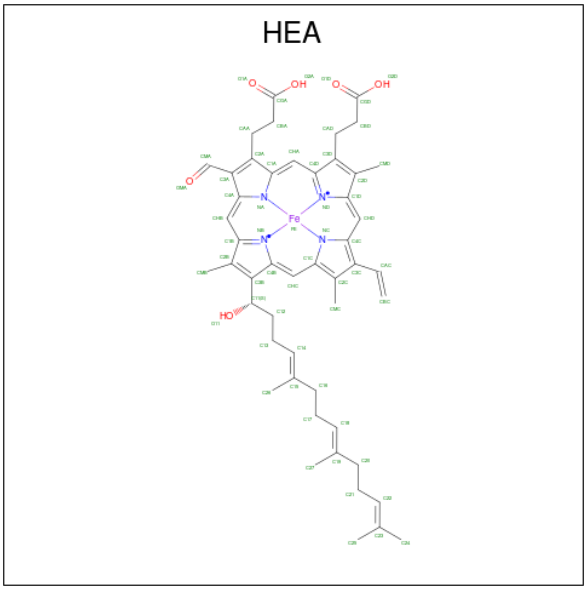
Mol	Chain	Residues	Atoms				AltConf
153	TH	1	Total	C	O	P	0
			84	65	17	2	
153	C	1	Total	C	O	P	0
			64	45	17	2	
153	c	1	Total	C	O	P	0
			64	45	17	2	
153	u1	1	Total	C	O	P	0
			57	38	17	2	
153	U1	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 154 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
154	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
154	c1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
154	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
154	C1	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

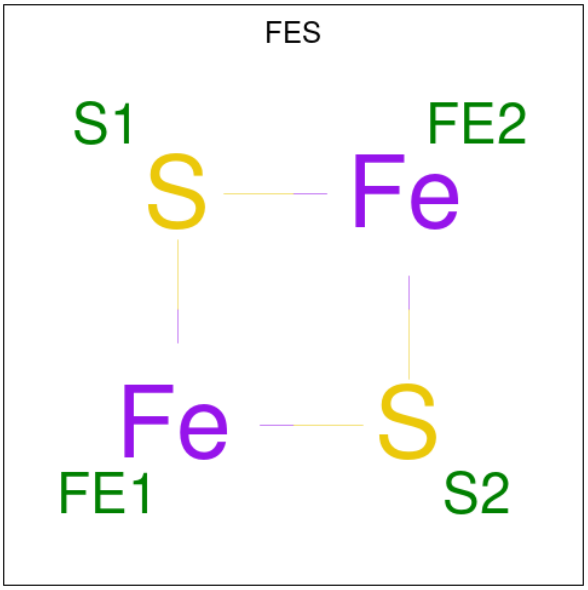
- Molecule 155 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 156 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 157 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
157	fs	1	Total Fe S 4 2 2	0
157	fs	1	Total Fe S 4 2 2	0
157	sb	1	Total Fe S 4 2 2	0

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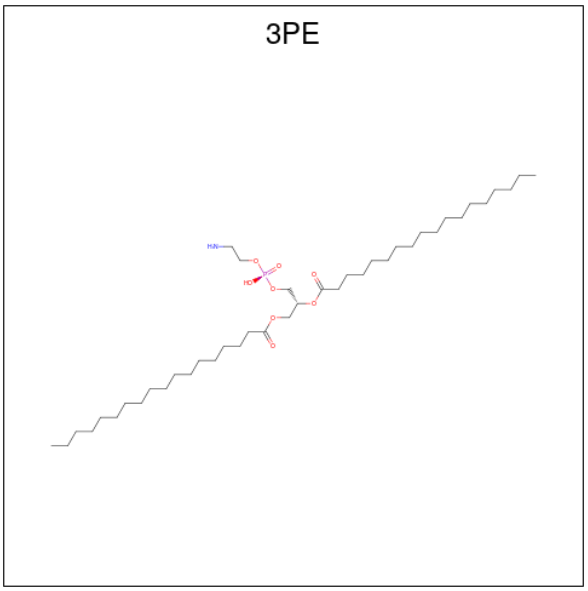
Mol	Chain	Residues	Atoms			AltConf
157	fx	1	Total 4	Fe 2	S 2	0
157	qE	1	Total 4	Fe 2	S 2	0
157	qe	1	Total 4	Fe 2	S 2	0
157	s1	1	Total 4	Fe 2	S 2	0
157	v2	1	Total 4	Fe 2	S 2	0
157	FS	1	Total 4	Fe 2	S 2	0
157	FS	1	Total 4	Fe 2	S 2	0
157	SB	1	Total 4	Fe 2	S 2	0
157	FX	1	Total 4	Fe 2	S 2	0
157	QE	1	Total 4	Fe 2	S 2	0
157	Qe	1	Total 4	Fe 2	S 2	0
157	S1	1	Total 4	Fe 2	S 2	0
157	V2	1	Total 4	Fe 2	S 2	0

- Molecule 158 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
158	i	1	Total	C	N	O	P	0
			32	22	1	8	1	
158	m2	1	Total	C	N	O	P	0
			31	21	1	8	1	
158	m3	1	Total	C	N	O	P	0
			38	28	1	8	1	
158	sc	1	Total	C	N	O	P	0
			40	30	1	8	1	
158	vb	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	w	1	Total	C	N	O	P	0
			34	24	1	8	1	
158	y5	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	a3	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	a3	1	Total	C	N	O	P	0
			44	34	1	8	1	
158	an	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	an	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	an	1	Total	C	N	O	P	0
			33	23	1	8	1	
158	an	1	Total	C	N	O	P	0
			29	19	1	8	1	
158	b4	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
158	bm	1	Total	C	N	O	P	0
			30	20	1	8	1	
158	c4	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	g2	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	n4	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	n5	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	s8	1	Total	C	N	O	P	0
			41	31	1	8	1	
158	t4	1	Total	C	N	O	P	0
			25	15	1	8	1	
158	t8	1	Total	C	N	O	P	0
			47	37	1	8	1	
158	t8	1	Total	C	N	O	P	0
			39	29	1	8	1	
158	ta	1	Total	C	N	O	P	0
			26	16	1	8	1	
158	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
158	M2	1	Total	C	N	O	P	0
			31	21	1	8	1	
158	M3	1	Total	C	N	O	P	0
			38	28	1	8	1	
158	SC	1	Total	C	N	O	P	0
			40	30	1	8	1	
158	VB	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
158	Y5	1	Total	C	N	O	P	0
			28	18	1	8	1	
158	A3	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	A3	1	Total	C	N	O	P	0
			44	34	1	8	1	
158	AN	1	Total	C	N	O	P	0
			45	35	1	8	1	
158	AN	1	Total	C	N	O	P	0
			45	35	1	8	1	

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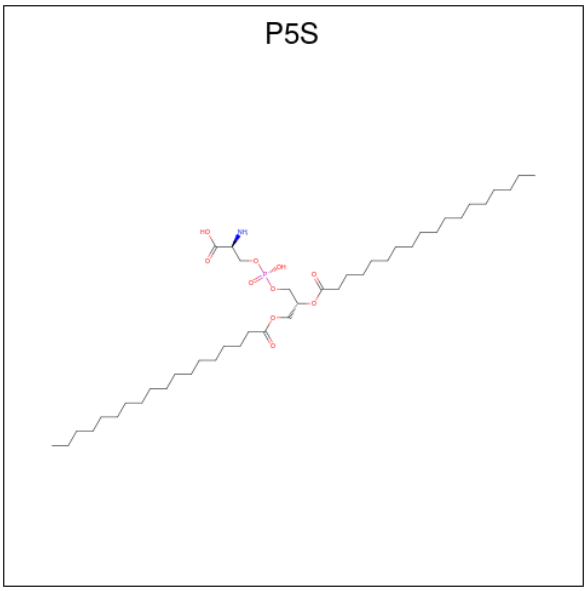
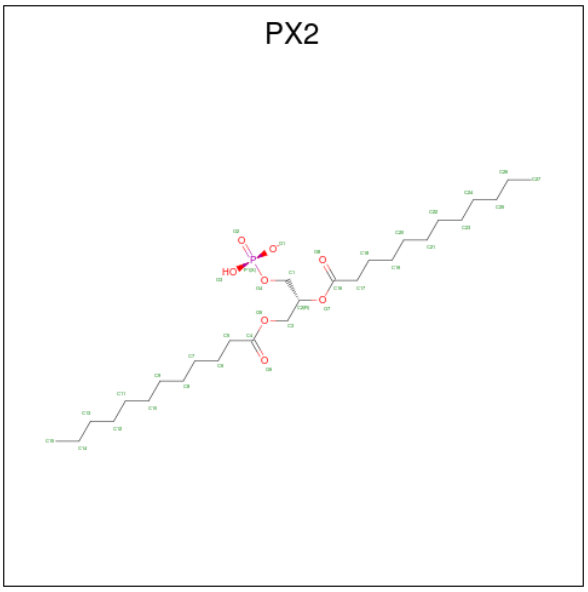
Mol	Chain	Residues	Atoms					AltConf
158	AN	1	Total	C	N	O	P	0
			33	23	1	8	1	
158	AN	1	Total	C	N	O	P	0
			29	19	1	8	1	
158	B4	1	Total	C	N	O	P	0
			48	38	1	8	1	
158	BM	1	Total	C	N	O	P	0
			30	20	1	8	1	
158	C4	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	G2	1	Total	C	N	O	P	0
			51	41	1	8	1	
158	N4	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	N5	1	Total	C	N	O	P	0
			36	26	1	8	1	
158	S8	1	Total	C	N	O	P	0
			41	31	1	8	1	
158	T4	1	Total	C	N	O	P	0
			25	15	1	8	1	
158	T8	1	Total	C	N	O	P	0
			47	37	1	8	1	
158	T8	1	Total	C	N	O	P	0
			39	29	1	8	1	
158	TA	1	Total	C	N	O	P	0
			26	16	1	8	1	

- Molecule 159 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



Mol	Chain	Residues	Atoms					AltConf
159	m2	1	Total	C	N	O	P	0
			36	24	1	10	1	
159	M2	1	Total	C	N	O	P	0
			36	24	1	10	1	

- Molecule 160 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
160	r	1	Total	C	O	P	0
			33	24	8	1	

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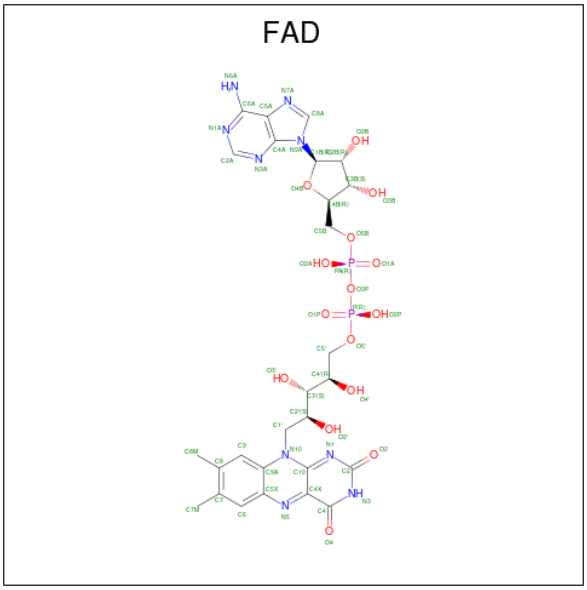
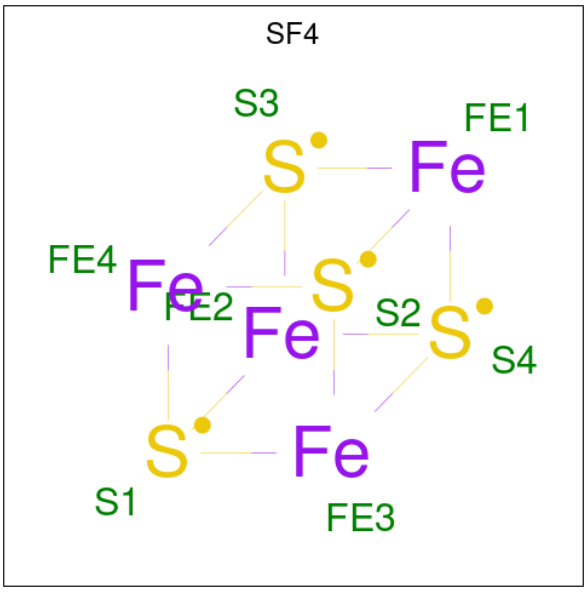
Mol	Chain	Residues	Atoms				AltConf
160	y5	1	Total	C	O	P	0
			21	12	8	1	
160	qh	1	Total	C	O	P	0
			36	27	8	1	
160	R	1	Total	C	O	P	0
			33	24	8	1	
160	Y5	1	Total	C	O	P	0
			21	12	8	1	
160	Qh	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 161 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



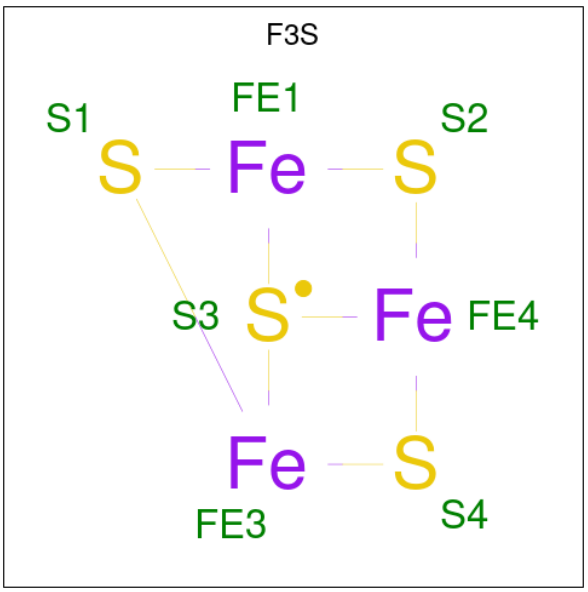
Mol	Chain	Residues	Atoms					AltConf
161	sa	1	Total	C	N	O	P	0
			53	27	9	15	2	
161	SA	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 162 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



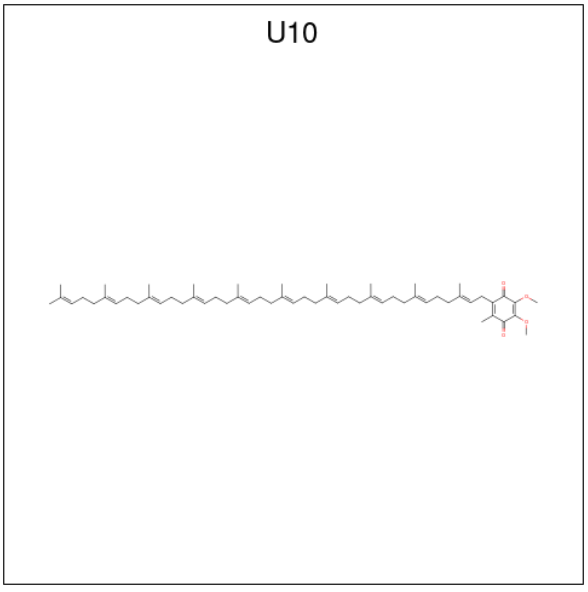
Mol	Chain	Residues	Atoms			AltConf
162	sb	1	Total 8	Fe 4	S 4	0
162	s1	1	Total 8	Fe 4	S 4	0
162	s1	1	Total 8	Fe 4	S 4	0
162	s7	1	Total 8	Fe 4	S 4	0
162	s8	1	Total 8	Fe 4	S 4	0
162	s8	1	Total 8	Fe 4	S 4	0
162	v1	1	Total 8	Fe 4	S 4	0
162	SB	1	Total 8	Fe 4	S 4	0
162	S1	1	Total 8	Fe 4	S 4	0
162	S1	1	Total 8	Fe 4	S 4	0
162	S7	1	Total 8	Fe 4	S 4	0
162	S8	1	Total 8	Fe 4	S 4	0
162	S8	1	Total 8	Fe 4	S 4	0
162	V1	1	Total 8	Fe 4	S 4	0

- Molecule 163 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms	AltConf
163	sb	1	Total Fe S 7 3 4	0
163	SB	1	Total Fe S 7 3 4	0

- Molecule 164 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

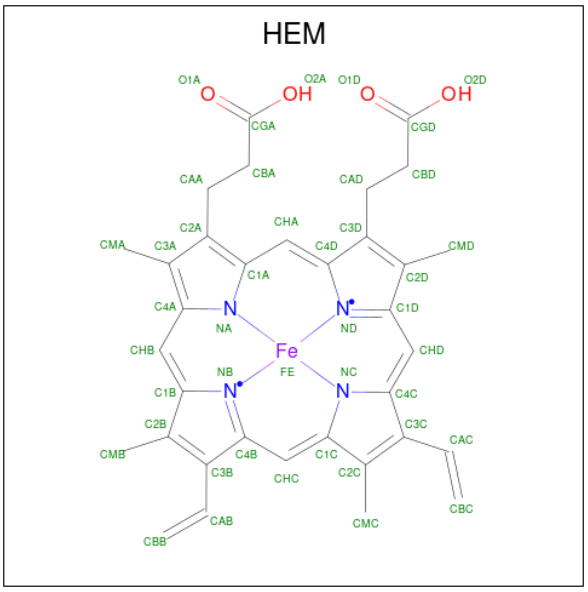


Mol	Chain	Residues	Atoms	AltConf
164	sc	1	Total C O 63 59 4	0
164	b8	1	Total C O 63 59 4	0
164	qC	1	Total C O 29 25 4	0
164	qc	1	Total C 26 26	0
164	qc	1	Total C O 29 25 4	0
164	SC	1	Total C O 63 59 4	0
164	B8	1	Total C O 63 59 4	0
164	QC	1	Total C O 29 25 4	0
164	Qc	1	Total C 26 26	0
164	Qc	1	Total C O 29 25 4	0

- Molecule 165 is ZINC ION (CCD ID: ZN) (formula: Zn).

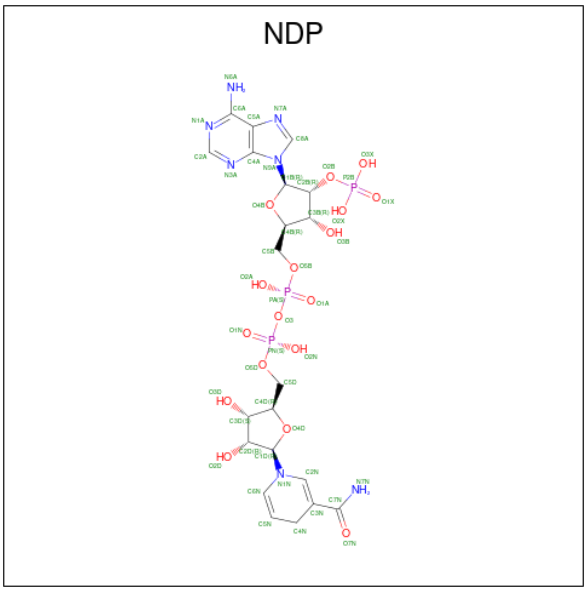
Mol	Chain	Residues	Atoms	AltConf
165	vb	2	Total Zn 2 2	0
165	s6	1	Total Zn 1 1	0
165	VB	2	Total Zn 2 2	0
165	S6	1	Total Zn 1 1	0

- Molecule 166 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



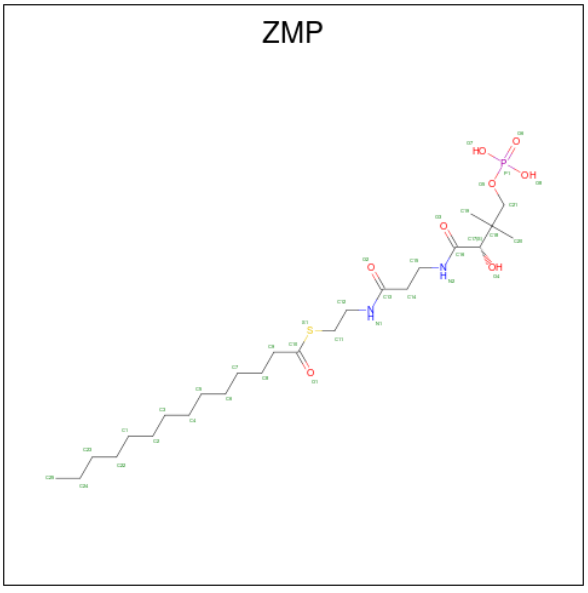
Mol	Chain	Residues	Atoms					AltConf
166	y5	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	Y5	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
166	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 167 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
167	a9	1	Total	C	N	O	P	0
			48	21	7	17	3	
167	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 168 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
168	ab	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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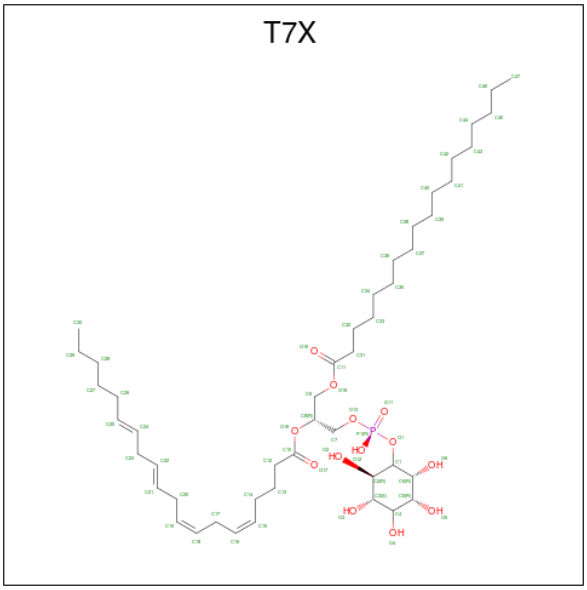
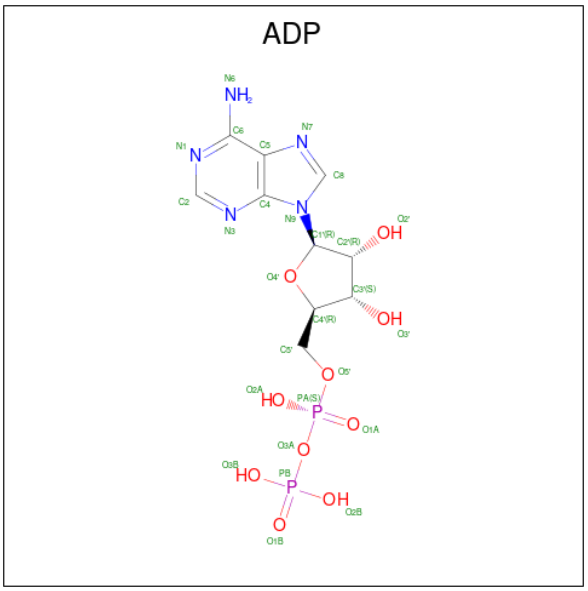
Mol	Chain	Residues	Atoms						AltConf
168	AB	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 169 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



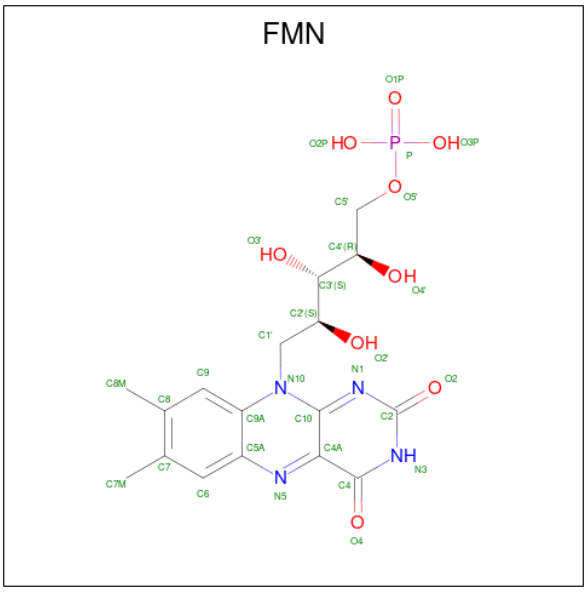
Mol	Chain	Residues	Atoms				AltConf
169	b6	1	Total	C	O	P	0
			55	41	13	1	
169	B6	1	Total	C	O	P	0
			55	41	13	1	

- Molecule 170 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
170	b9	1	Total	C	N	O	P	0
			27	10	5	10	2	
170	B9	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 171 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
171	v1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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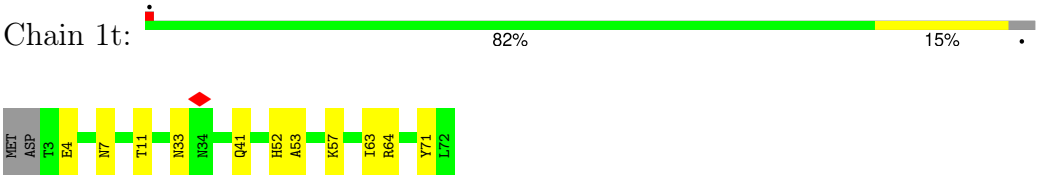
Mol	Chain	Residues	Atoms					AltConf
171	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

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

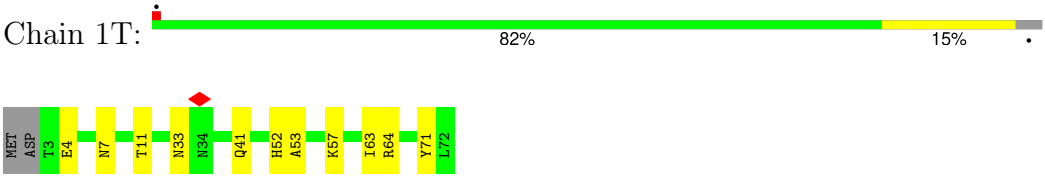
• Molecule 1: Tim10/DDP family zinc finger protein

Chain 1t:



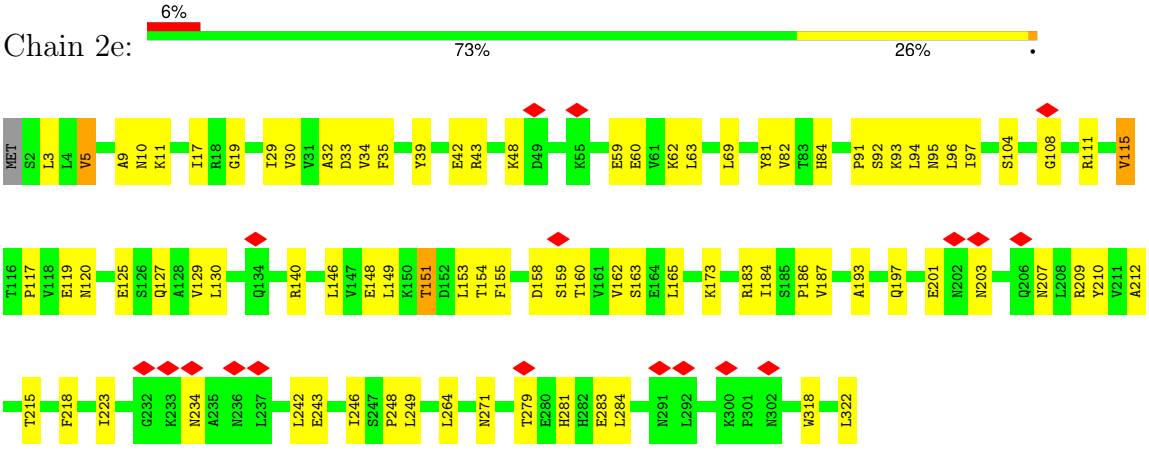
• Molecule 1: Tim10/DDP family zinc finger protein

Chain 1T:



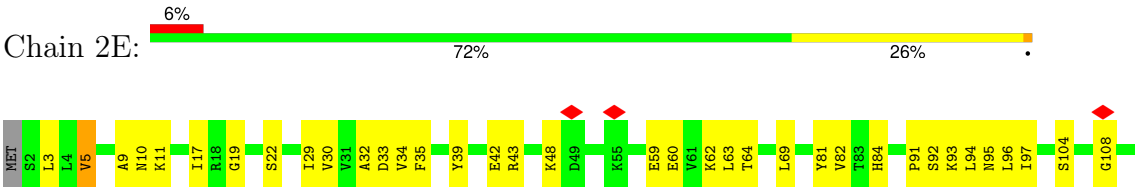
• Molecule 2: NmrA domain-containing protein

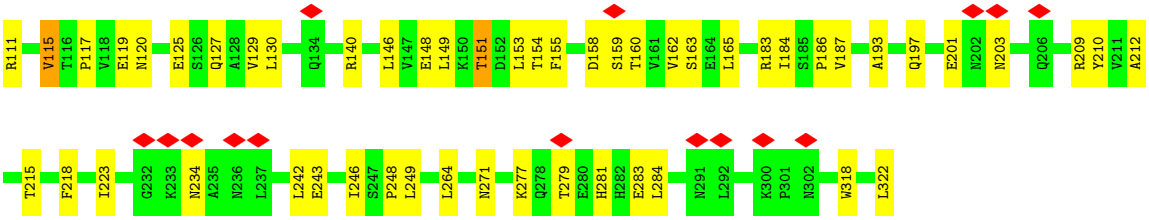
Chain 2e:



• Molecule 2: NmrA domain-containing protein

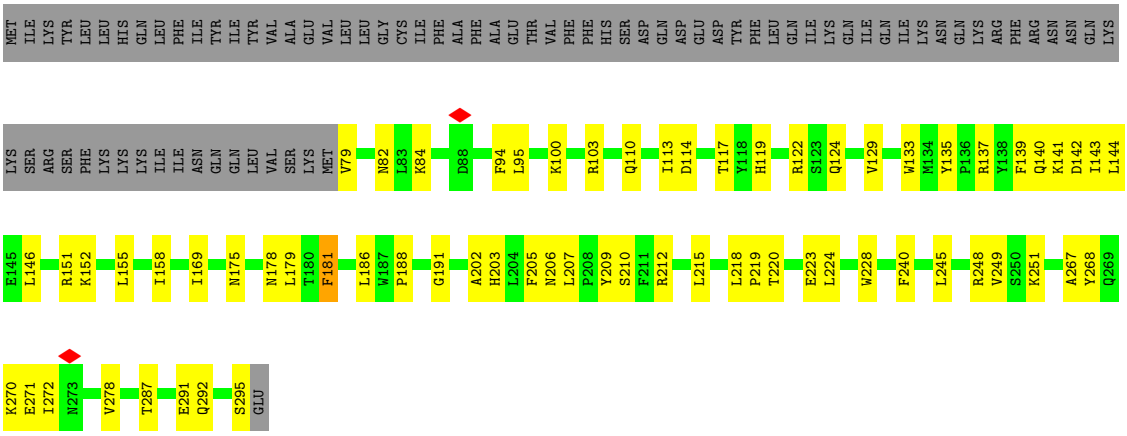
Chain 2E:





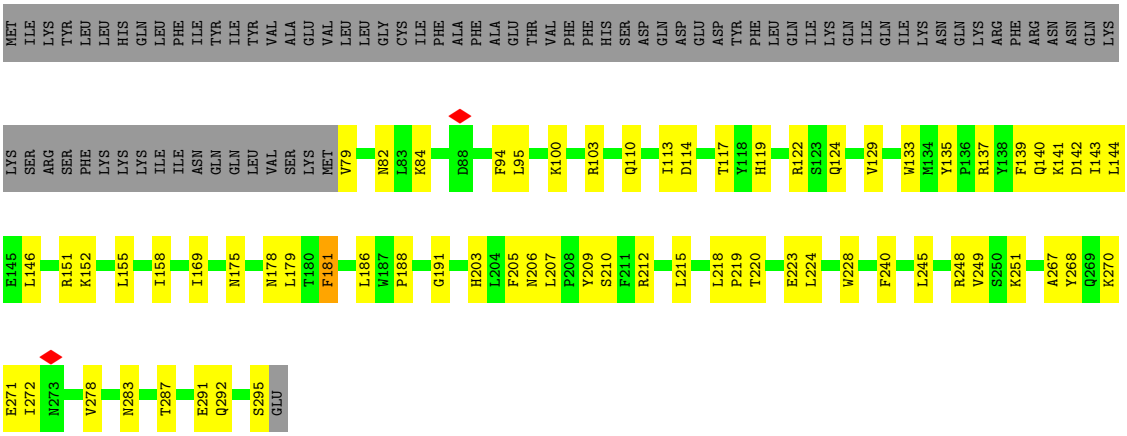
• Molecule 3: Transmembrane protein, putative

Chain 2f:



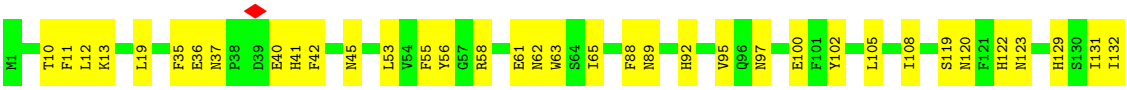
• Molecule 3: Transmembrane protein, putative

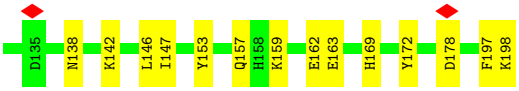
Chain 2F:



• Molecule 4: SDHTT3

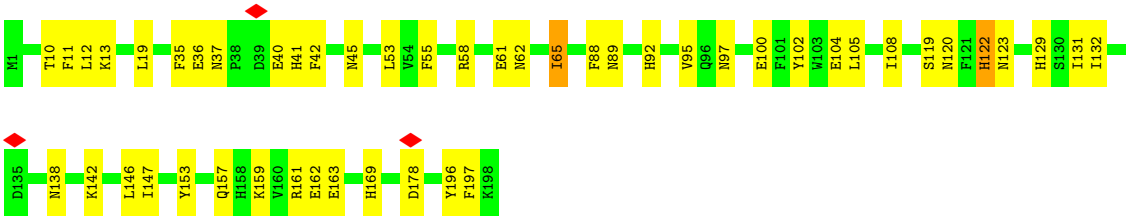
Chain 2g:





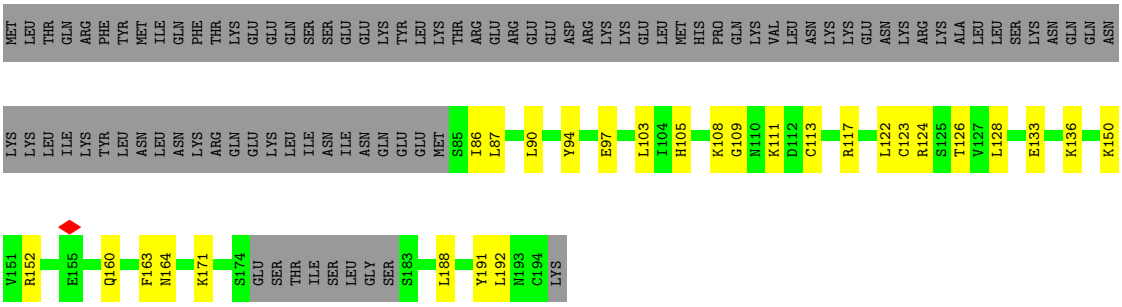
• Molecule 4: SDHTT3

Chain 2G:



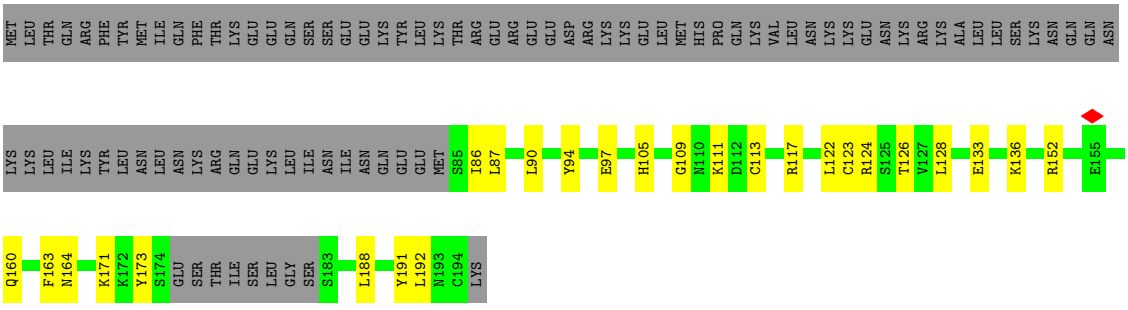
• Molecule 5: Diphthamide synthesis protein

Chain 2h:



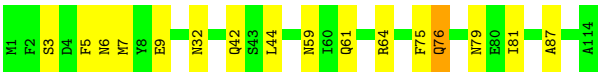
• Molecule 5: Diphthamide synthesis protein

Chain 2H:



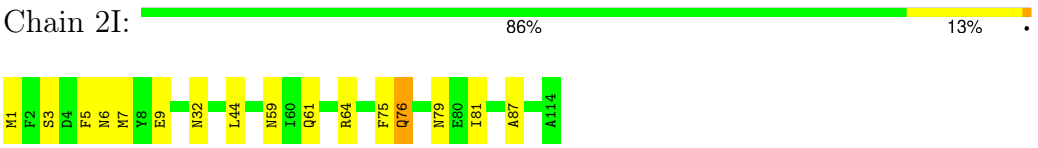
• Molecule 6: DUF4885 domain-containing protein

Chain 2i:



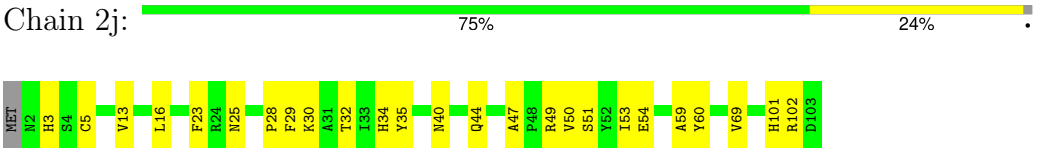
• Molecule 6: DUF4885 domain-containing protein

Chain 2I:



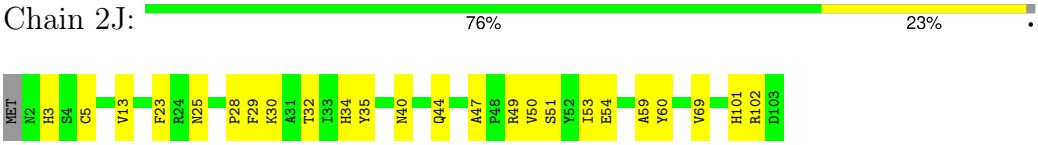
• Molecule 7: Transmembrane protein, putative

Chain 2j:



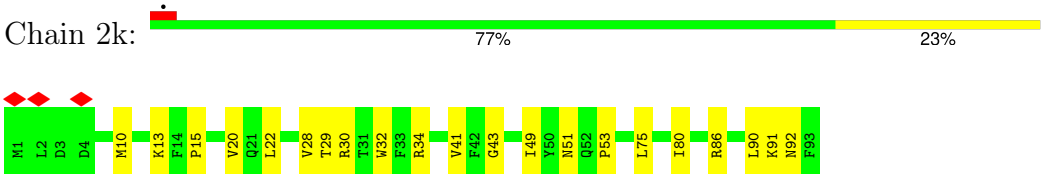
• Molecule 7: Transmembrane protein, putative

Chain 2J:



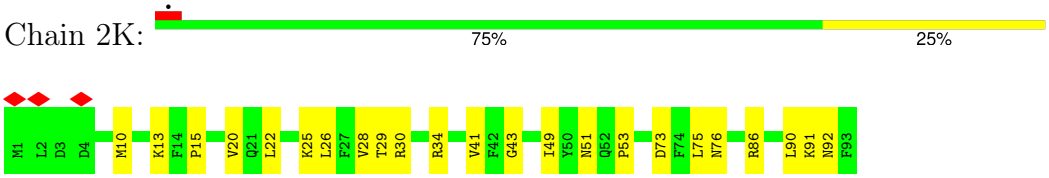
• Molecule 8: Transmembrane protein, putative

Chain 2k:



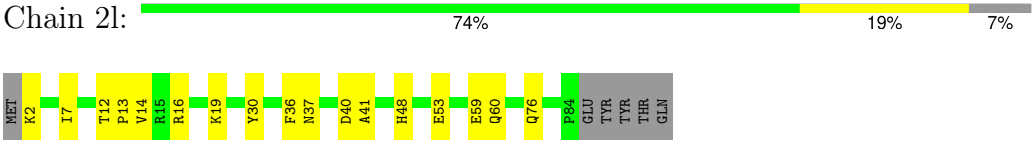
• Molecule 8: Transmembrane protein, putative

Chain 2K:



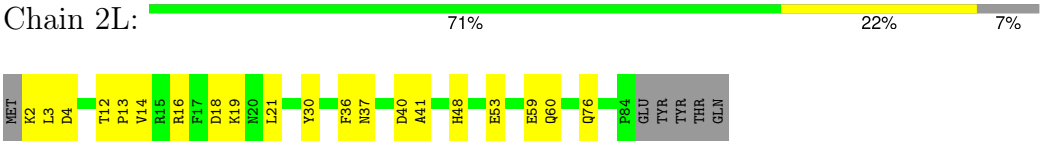
• Molecule 9: Transposase

Chain 2l:



• Molecule 9: Transposase

Chain 2L:

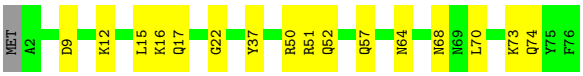


• Molecule 10: Transmembrane protein, putative

Chain 2m:

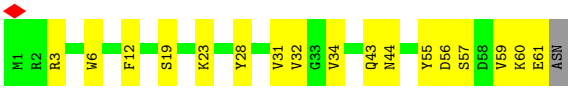
• Molecule 10: Transmembrane protein, putative

Chain 2M:



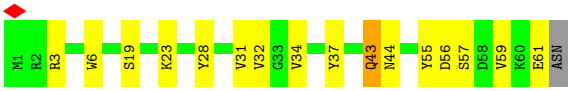
• Molecule 11: Transmembrane protein, putative

Chain 2n:



• Molecule 11: Transmembrane protein, putative

Chain 2N:



• Molecule 12: SDHTT11

Chain 2o:

• Molecule 12: SDHTT11

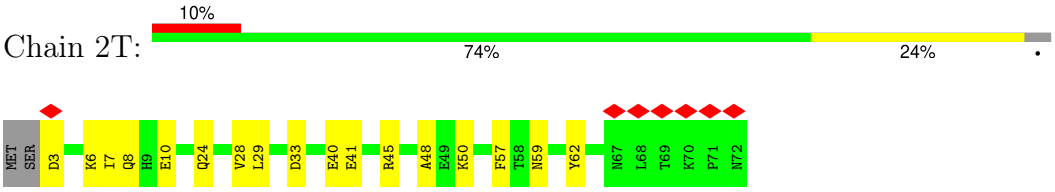
Chain 2O:

• Molecule 13: Zf-Tim10_DDP domain-containing protein

Chain 2t:

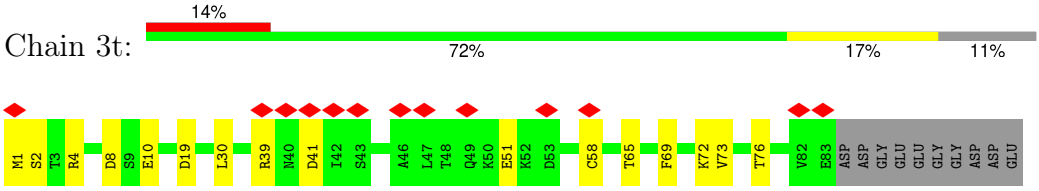
• Molecule 13: Zf-Tim10_DDP domain-containing protein

Chain 2T:



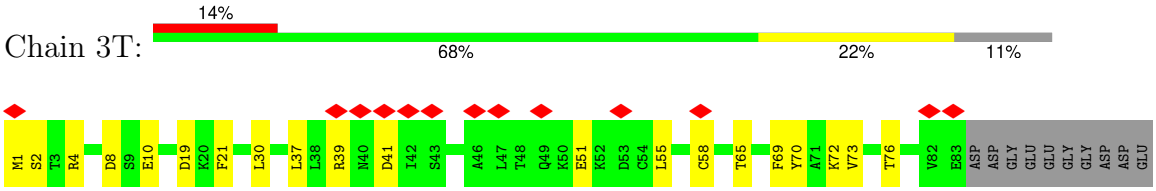
• Molecule 14: Zf-Tim10_DDP domain-containing protein

Chain 3t:



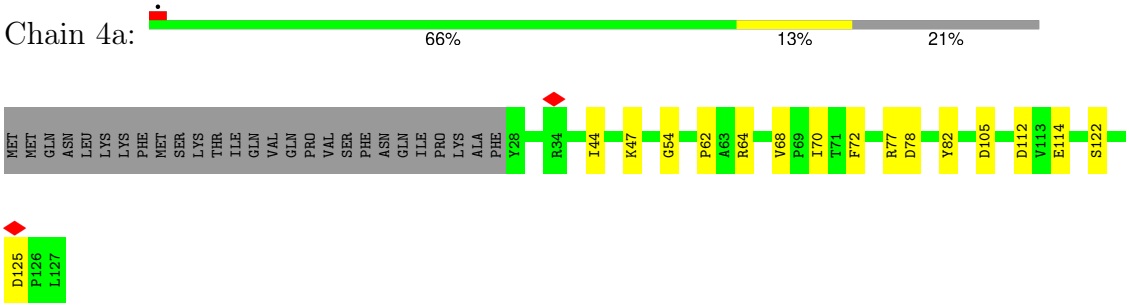
• Molecule 14: Zf-Tim10_DDP domain-containing protein

Chain 3T:



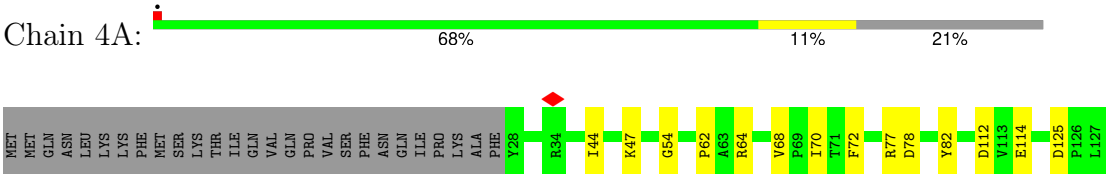
• Molecule 15: Phage protein

Chain 4a:



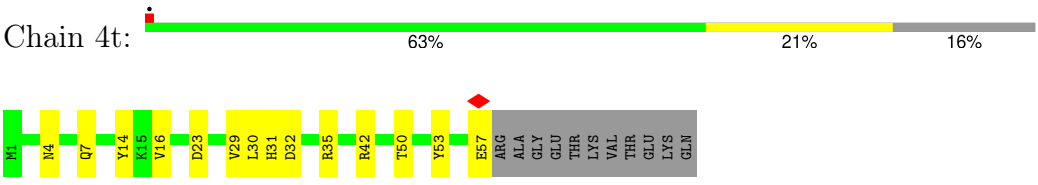
• Molecule 15: Phage protein

Chain 4A:



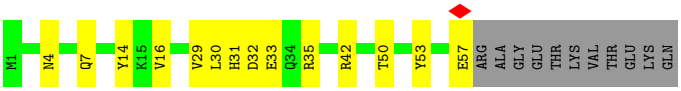
• Molecule 16: Transposase

Chain 4t:



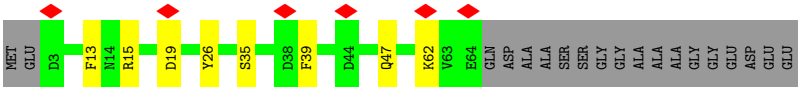
• Molecule 16: Transposase

Chain 4T:



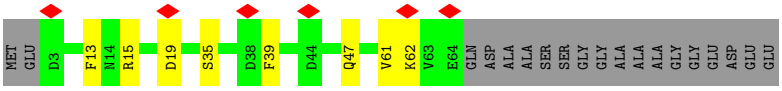
• Molecule 17: Cullin domain-containing protein

Chain 5t:



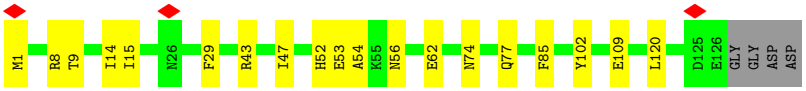
• Molecule 17: Cullin domain-containing protein

Chain 5T:



• Molecule 18: Transmembrane protein, putative

Chain 6a:

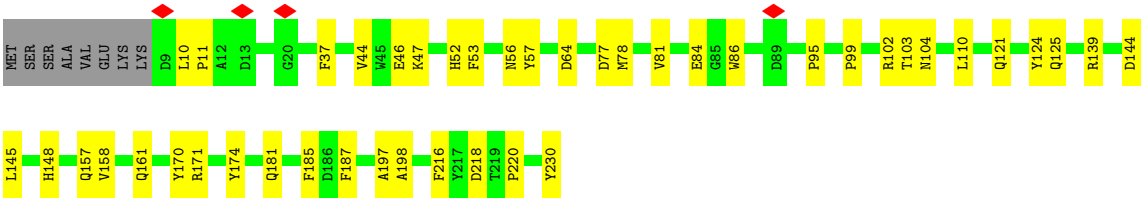


• Molecule 18: Transmembrane protein, putative

Chain 6A:

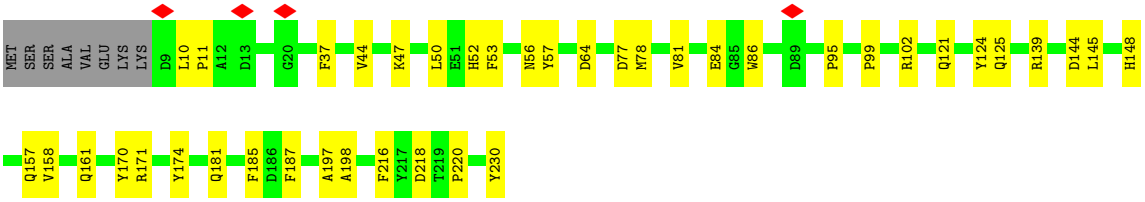
• Molecule 19: Structural protein

Chain 6b:



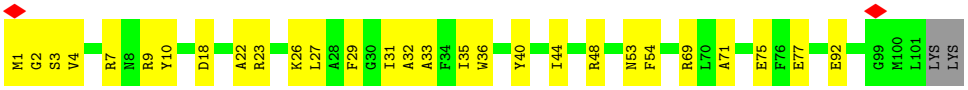
• Molecule 19: Structural protein

Chain 6B:



• Molecule 20: Transmembrane protein, putative

Chain 6c:

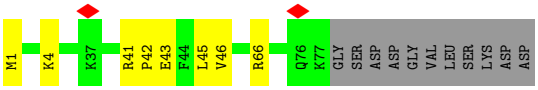


• Molecule 20: Transmembrane protein, putative

Chain 6C:

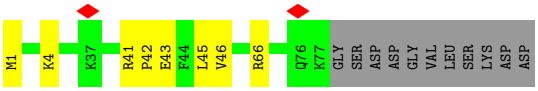
• Molecule 21: Decapping nuclease

Chain 6l:



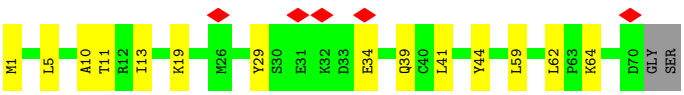
• Molecule 21: Decapping nuclease

Chain 6L:



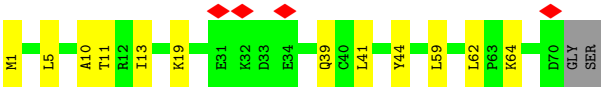
• Molecule 22: Annexin

Chain 6t:



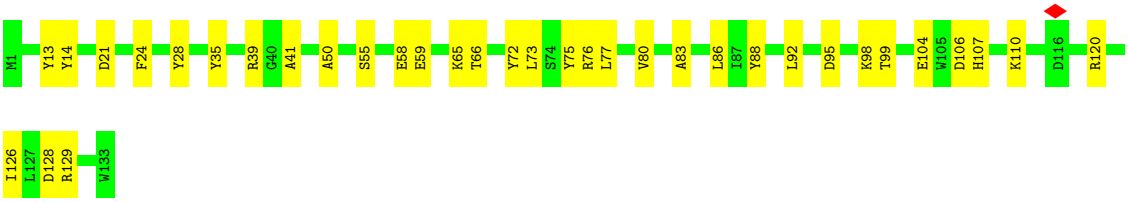
• Molecule 22: Annexin

Chain 6T:



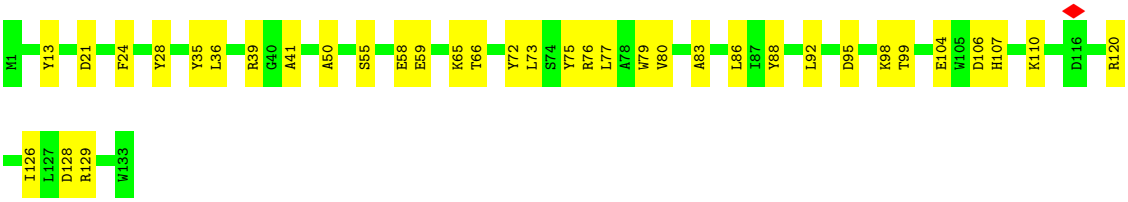
• Molecule 23: Transmembrane protein, putative

Chain 7a:



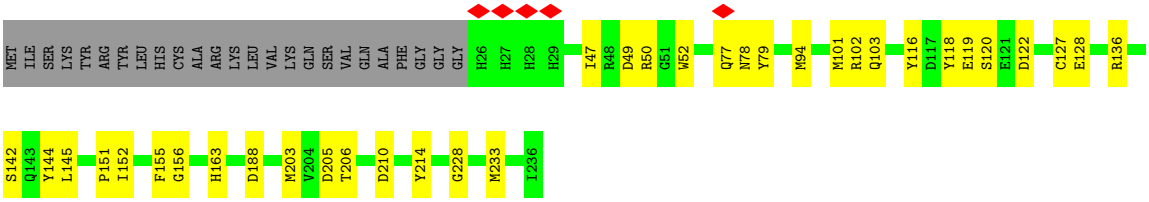
• Molecule 23: Transmembrane protein, putative

Chain 7A:



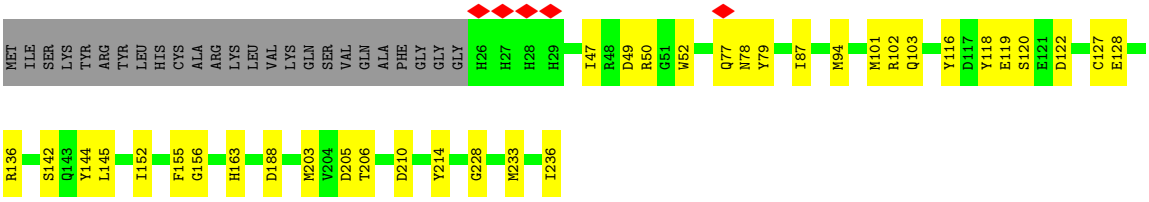
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 7c:



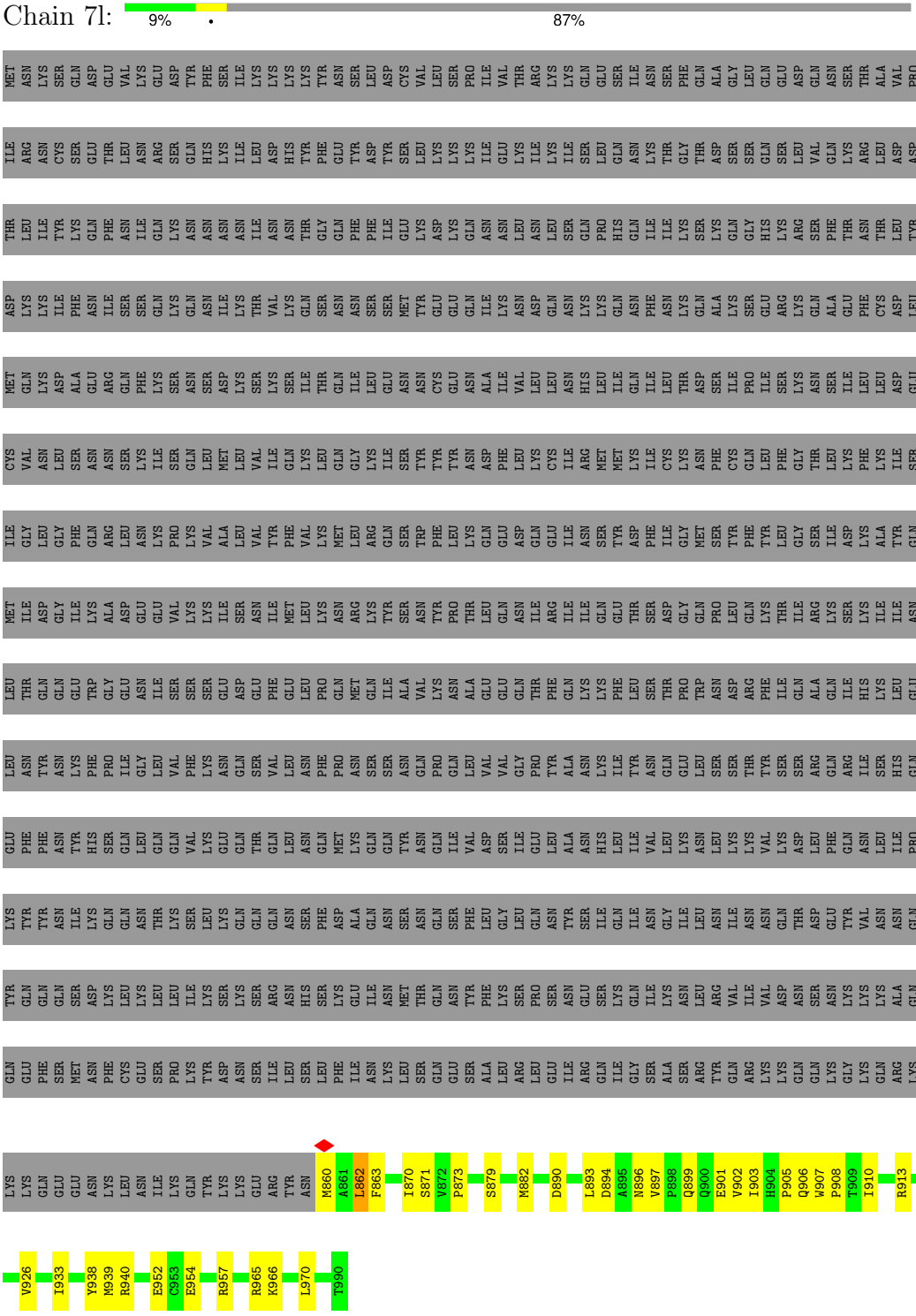
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 7C:



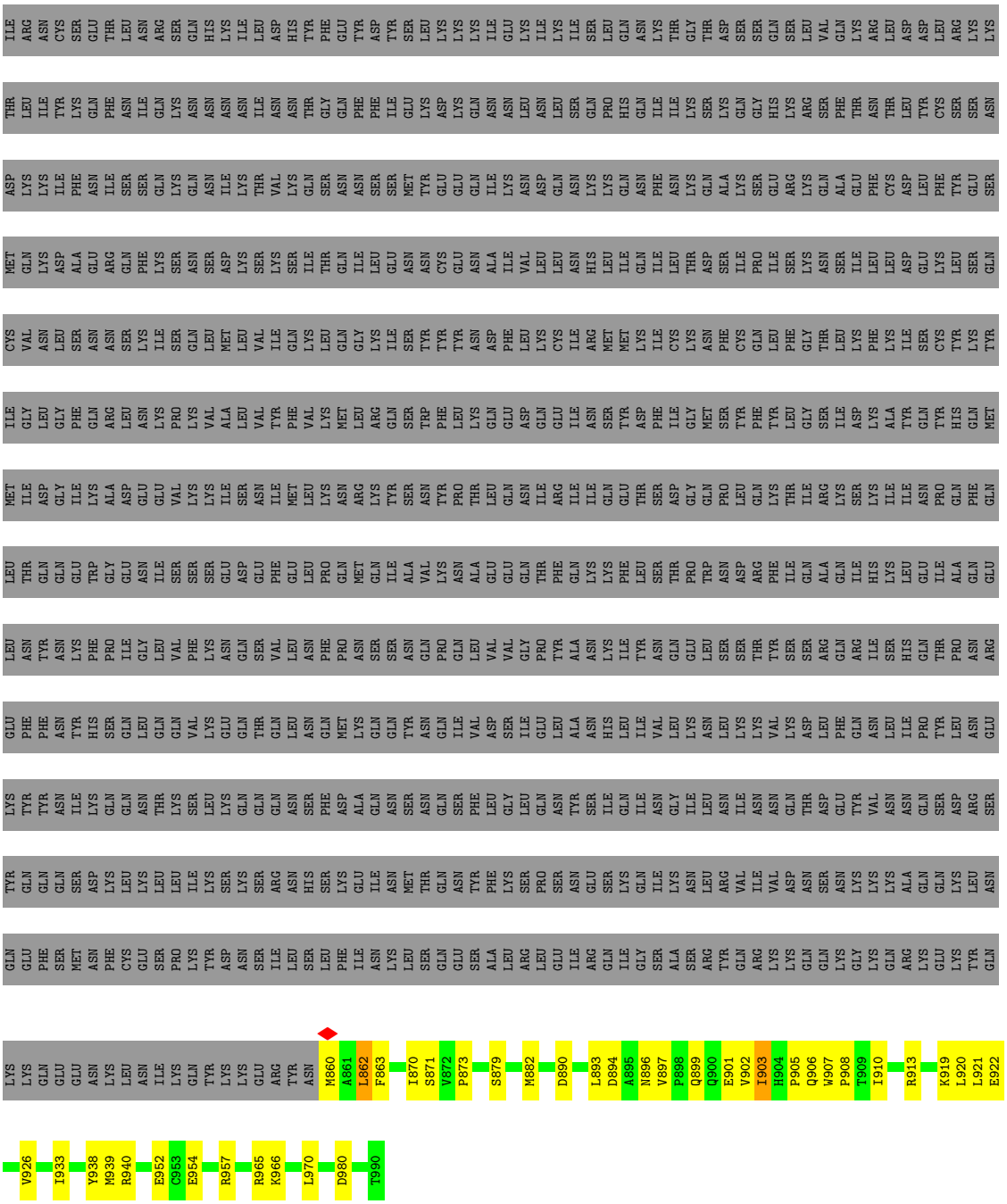
• Molecule 25: CTF/NF-I domain-containing protein

Chain 7l:



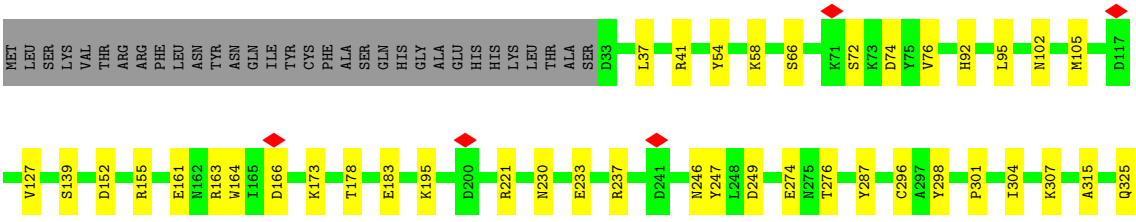
• Molecule 25: CTF/NF-I domain-containing protein

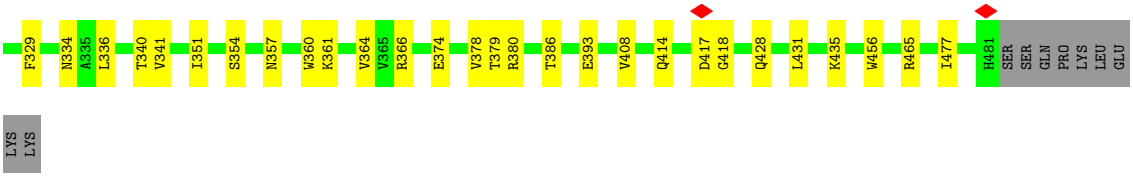
Chain 7L:



• Molecule 26: Transmembrane protein, putative

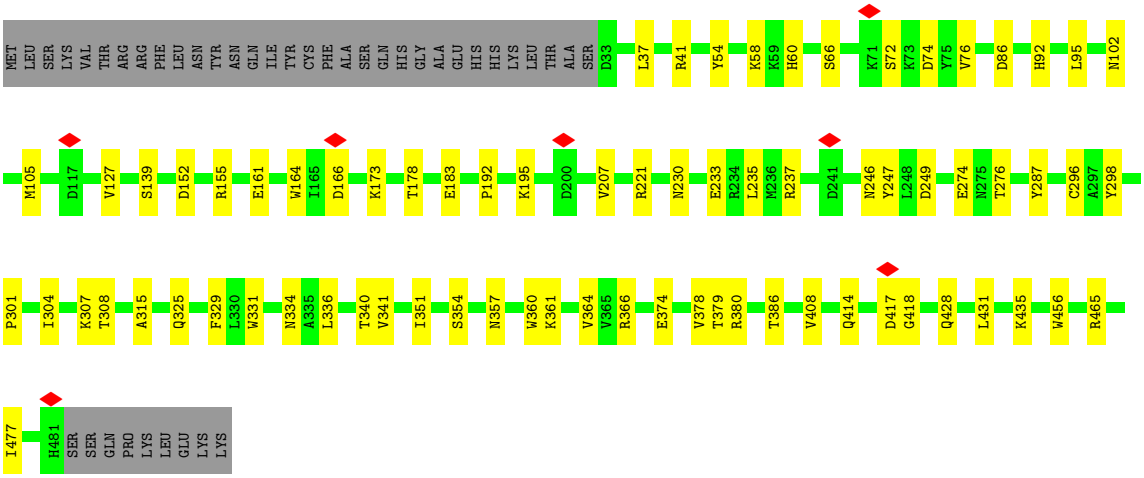
Chain a:





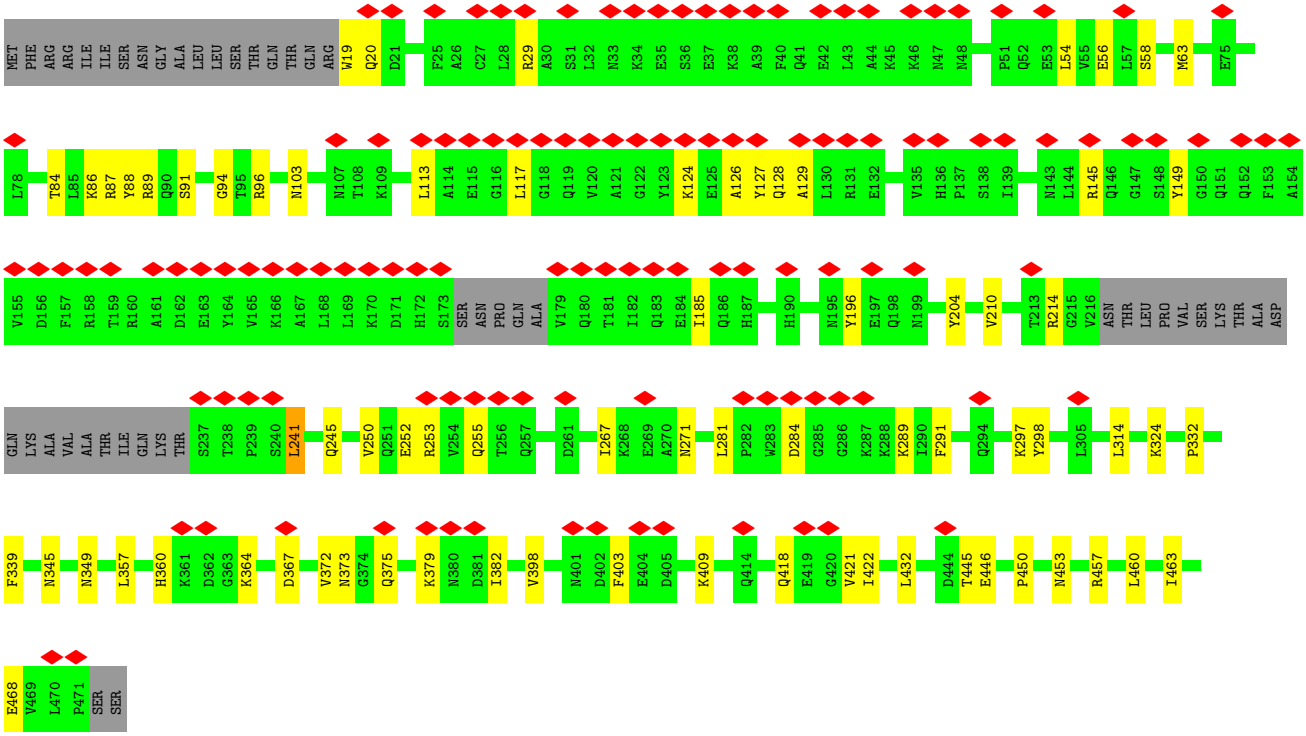
• Molecule 26: Transmembrane protein, putative

Chain A:



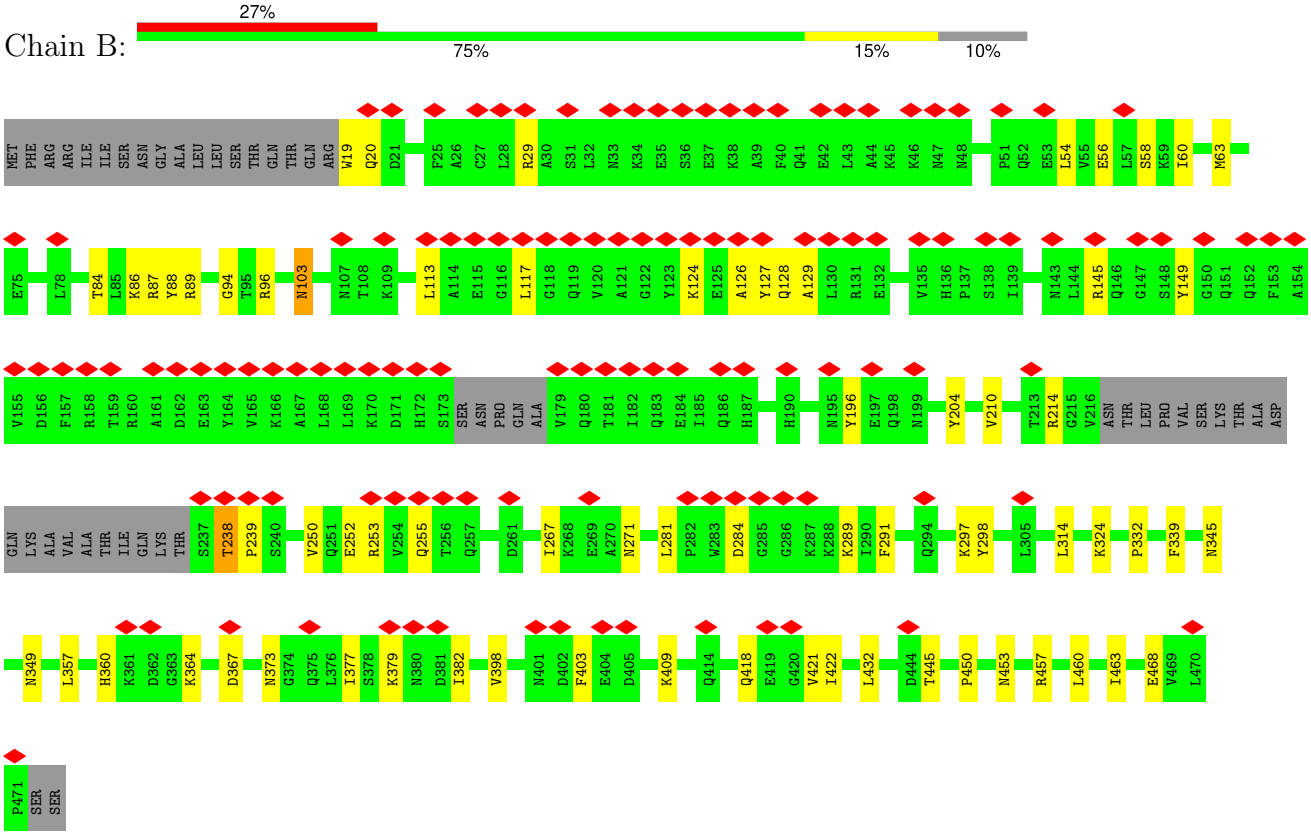
• Molecule 27: Protein phosphatase 2C, putative

Chain b:



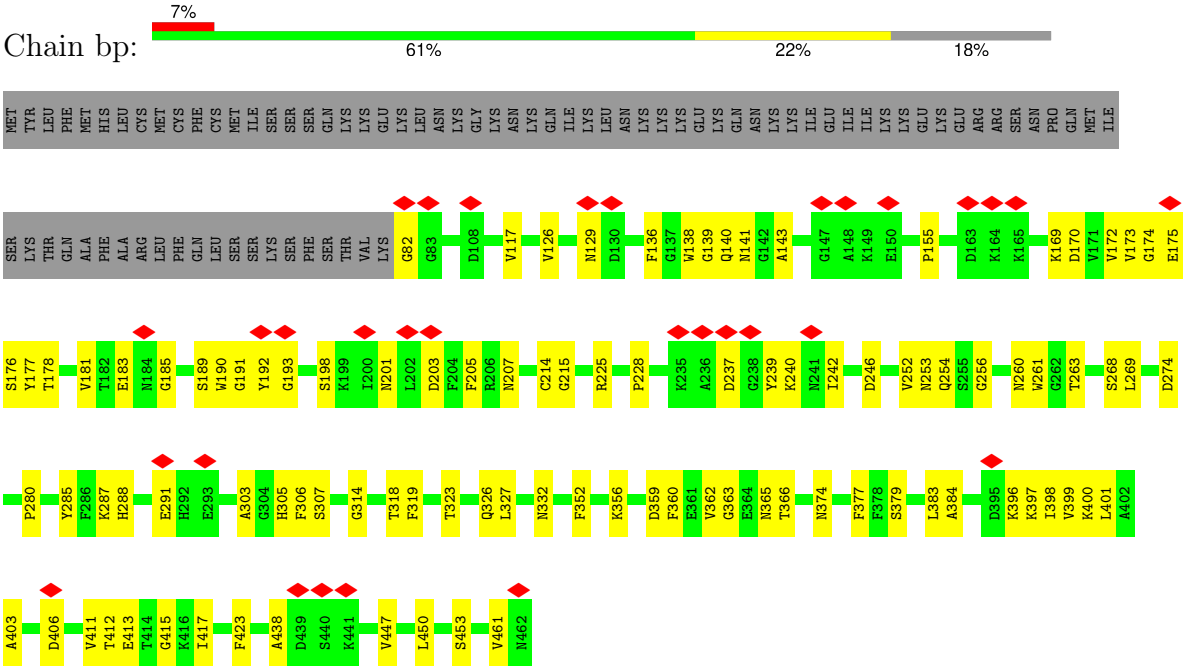
• Molecule 27: Protein phosphatase 2C, putative

Chain B:



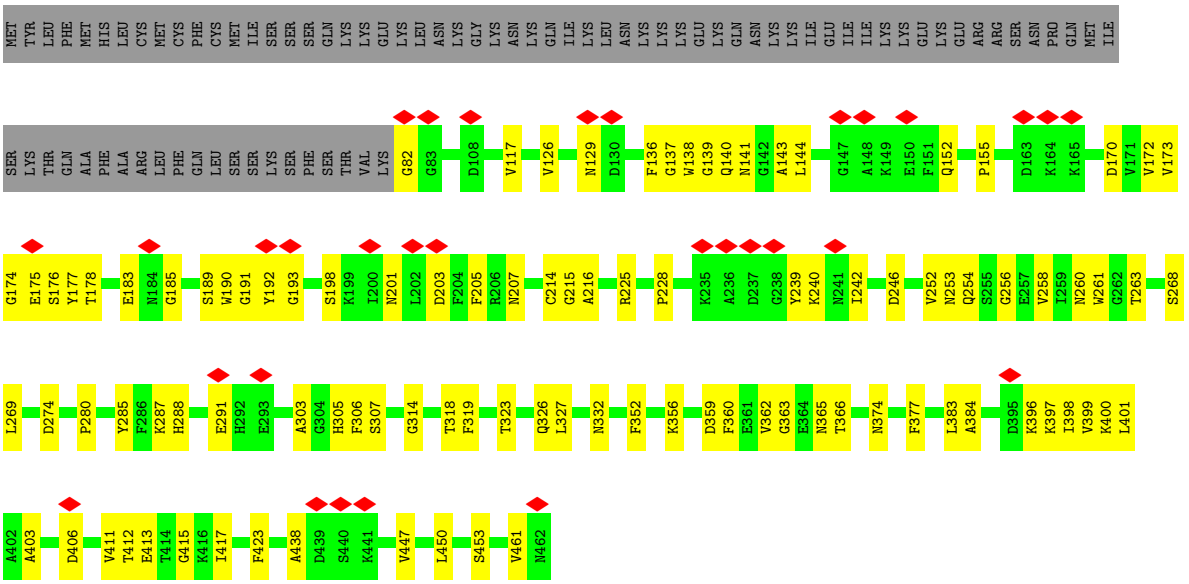
• Molecule 28: Chromosome condensation regulator RCC1 repeat protein

Chain bp:



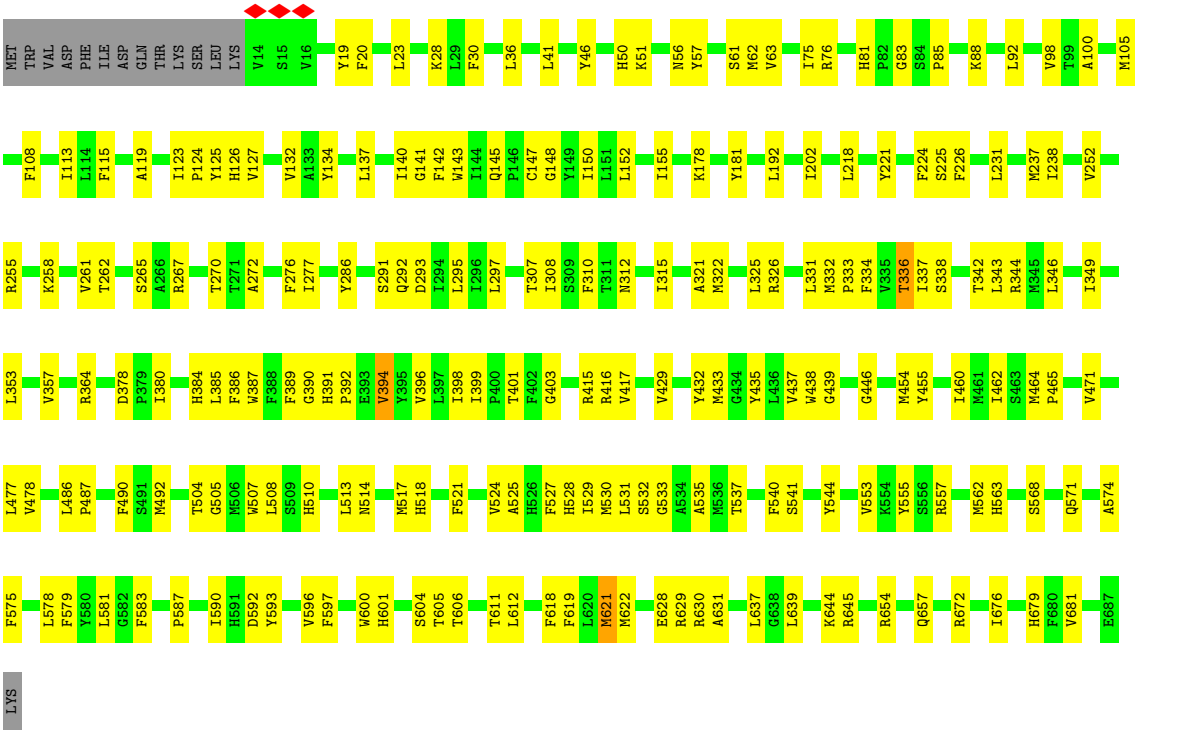
• Molecule 28: Chromosome condensation regulator RCC1 repeat protein

Chain BP:



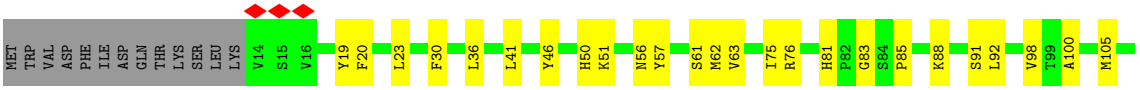
• Molecule 29: Cytochrome c oxidase subunit 1

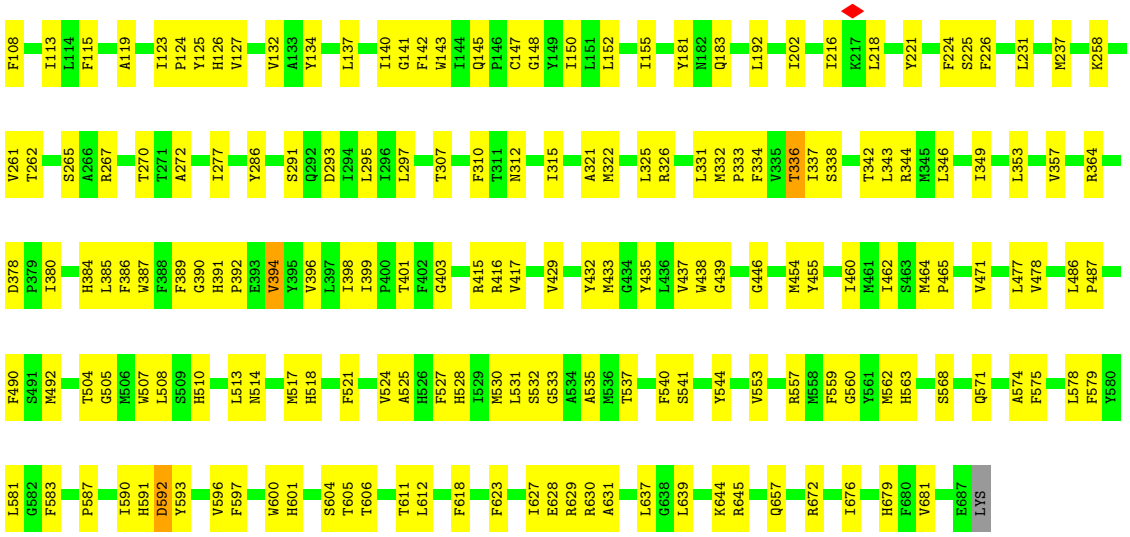
Chain c1:



• Molecule 29: Cytochrome c oxidase subunit 1

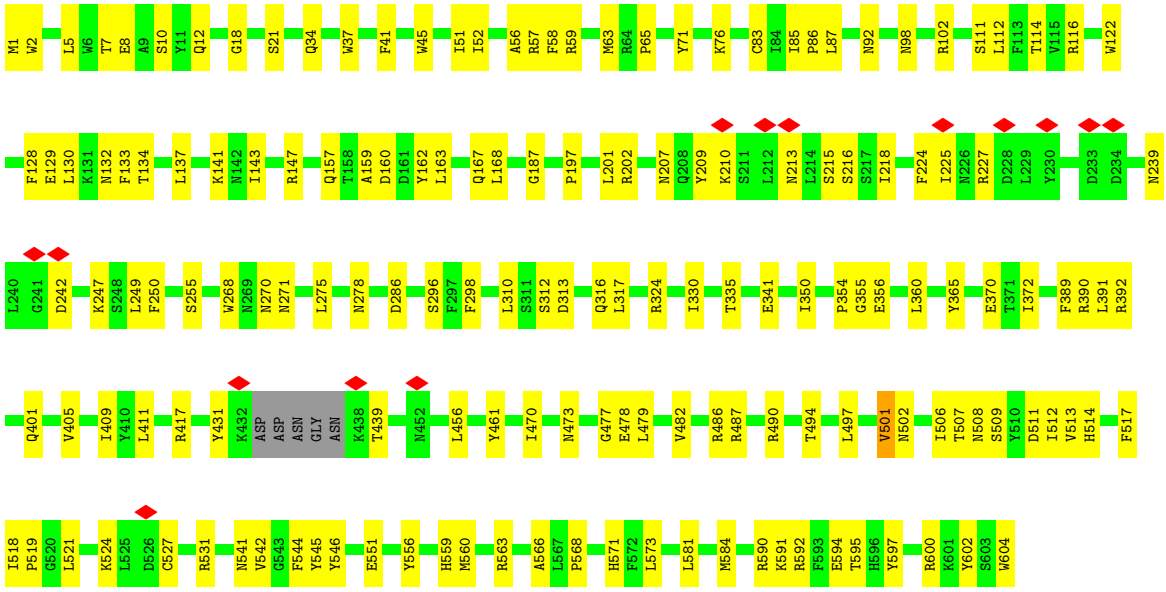
Chain C1:





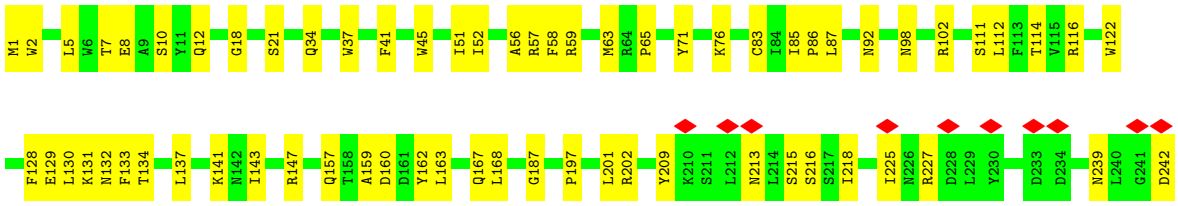
• Molecule 30: Cytochrome c oxidase subunit 2

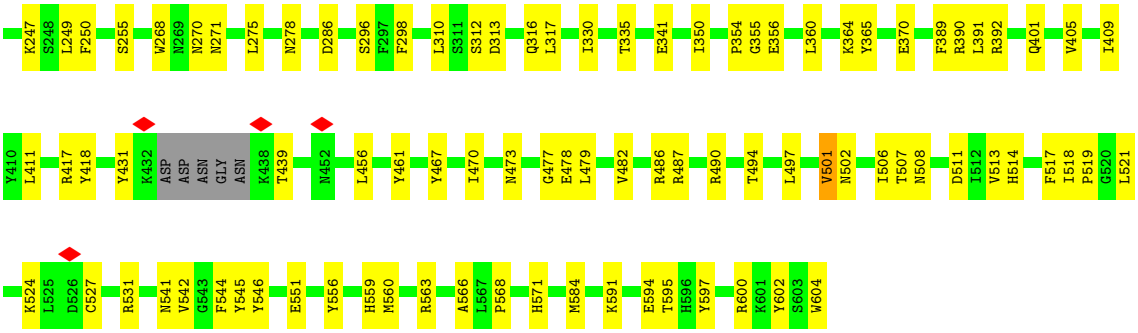
Chain c2:



• Molecule 30: Cytochrome c oxidase subunit 2

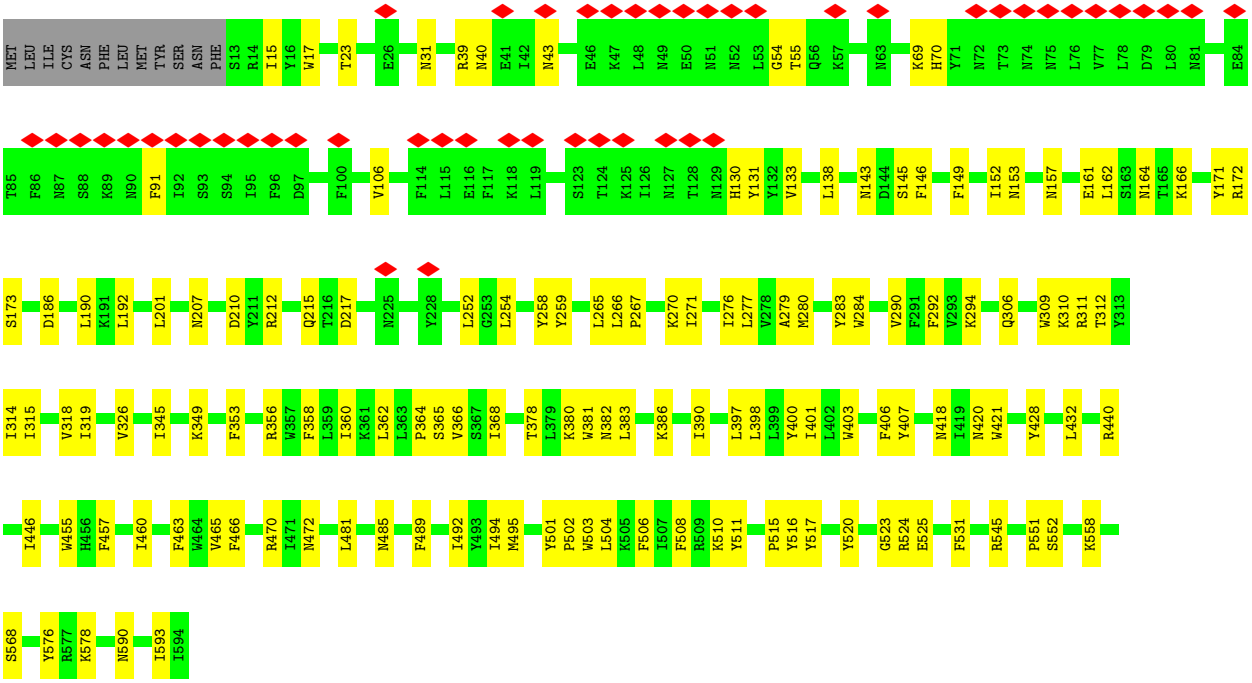
Chain C2:





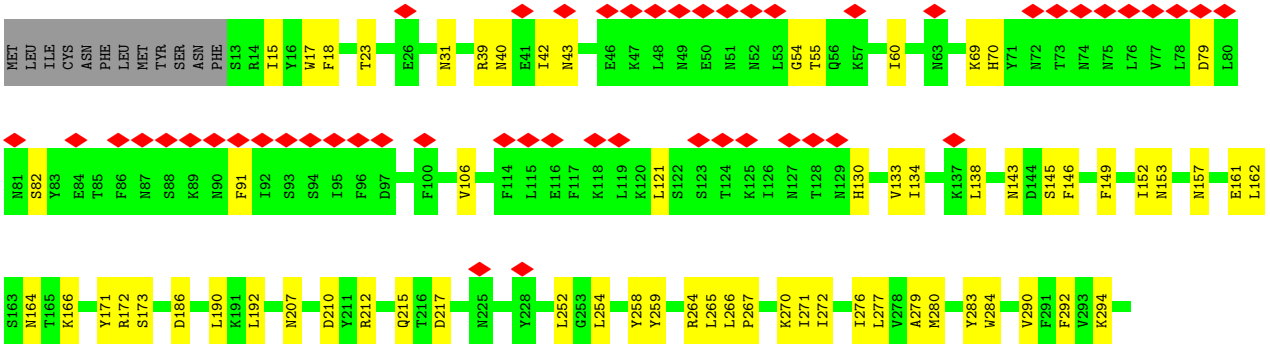
• Molecule 31: Ymf68

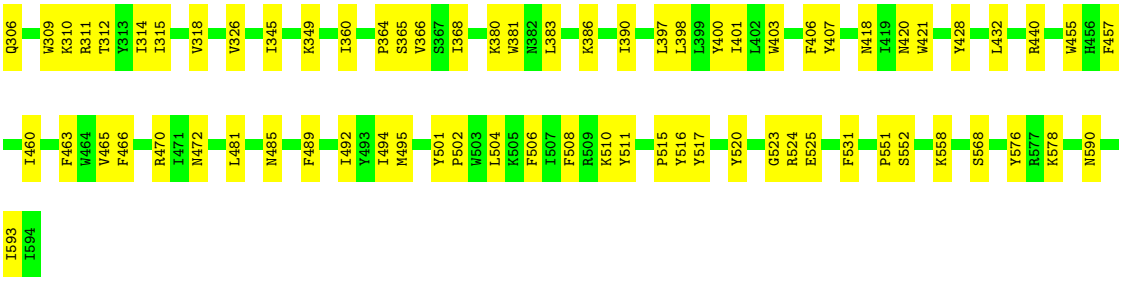
Chain c3:



• Molecule 31: Ymf68

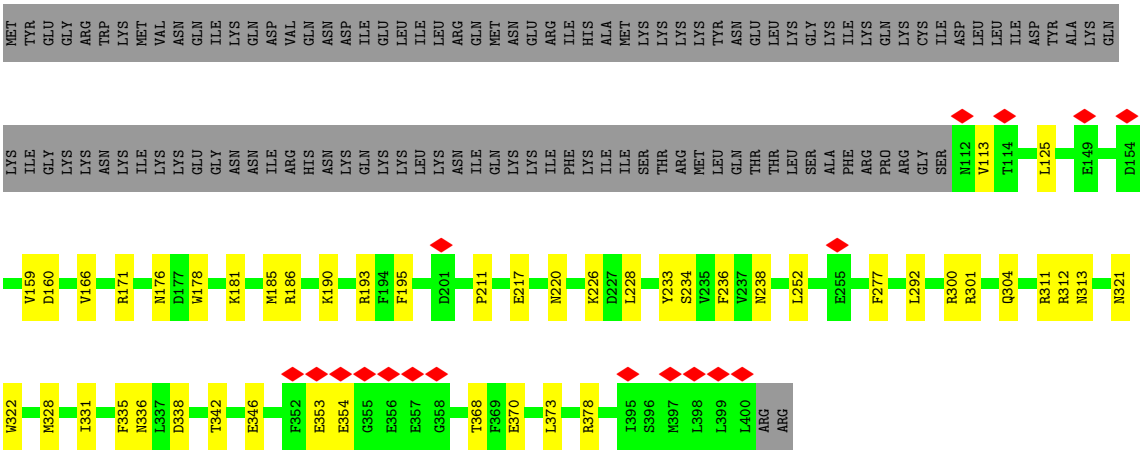
Chain C3:





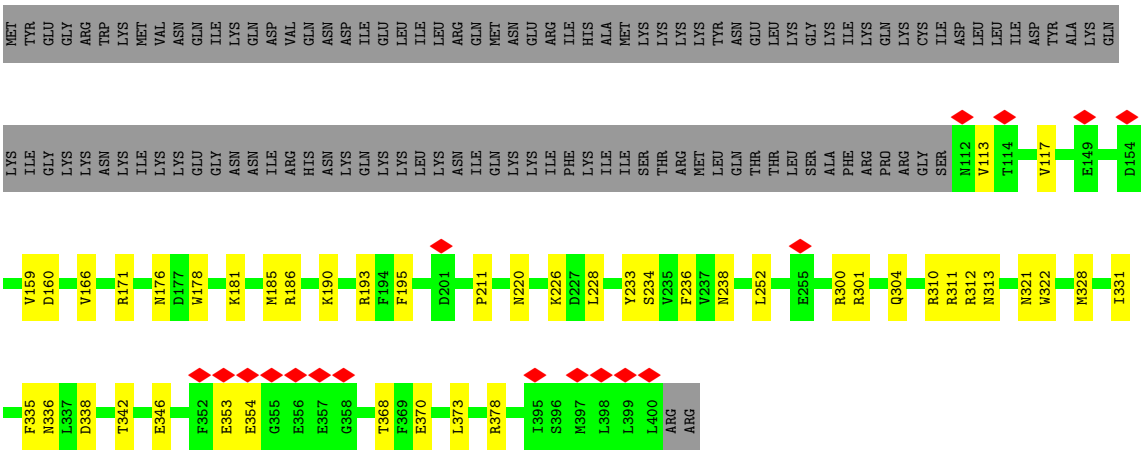
• Molecule 32: SURF1-like protein

Chain d:



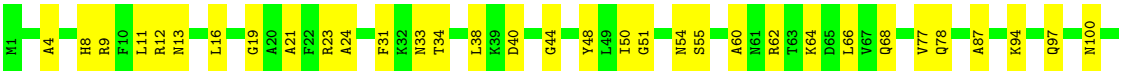
• Molecule 32: SURF1-like protein

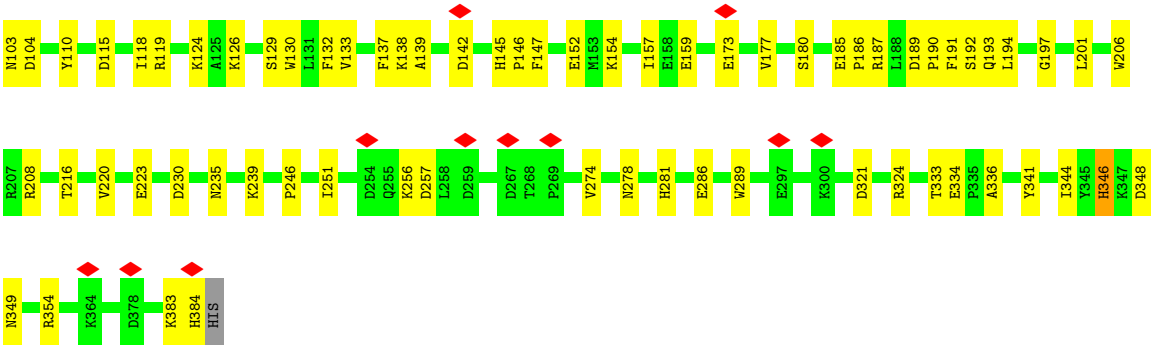
Chain D:



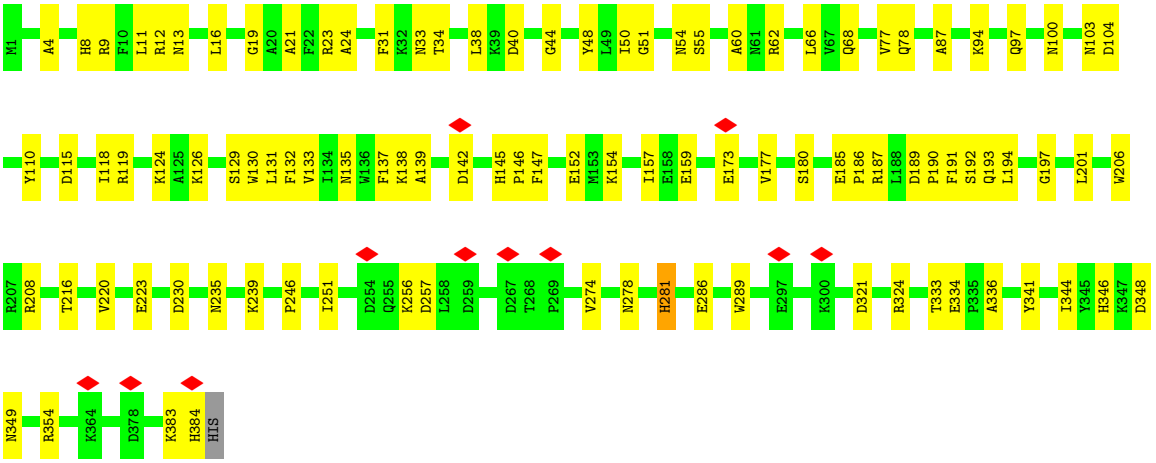
• Molecule 33: TraB family protein

Chain e:

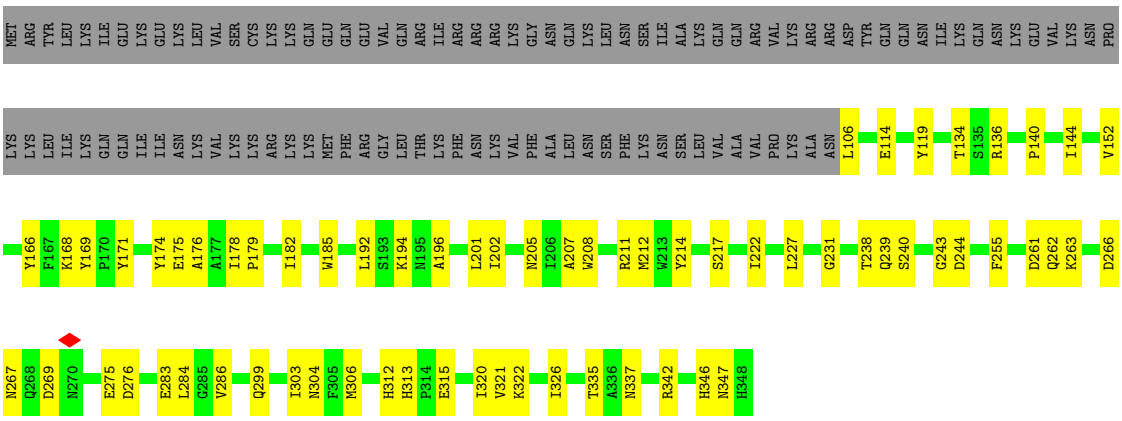




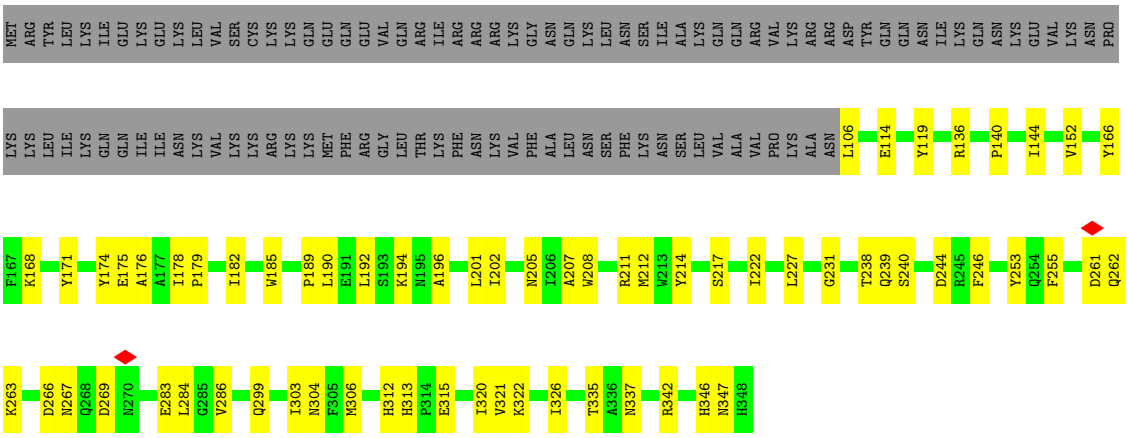
• Molecule 33: TraB family protein



• Molecule 34: Transmembrane protein, putative

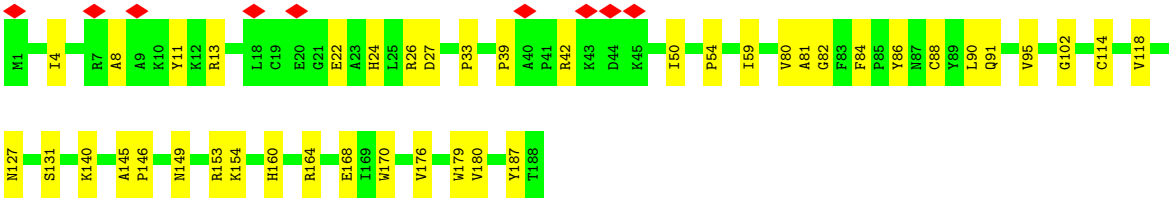


• Molecule 34: Transmembrane protein, putative



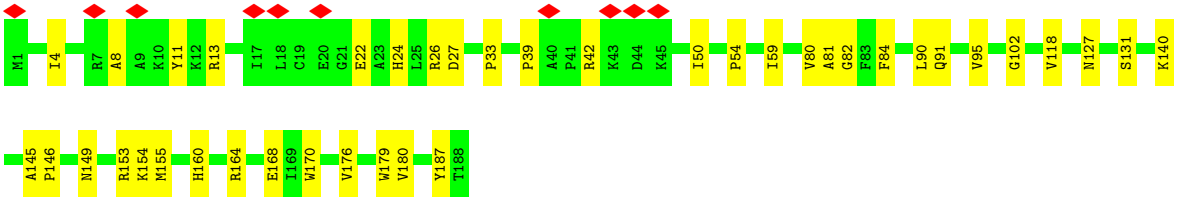
• Molecule 35: Iron-binding zinc finger CDGSH type protein

Chain fs:



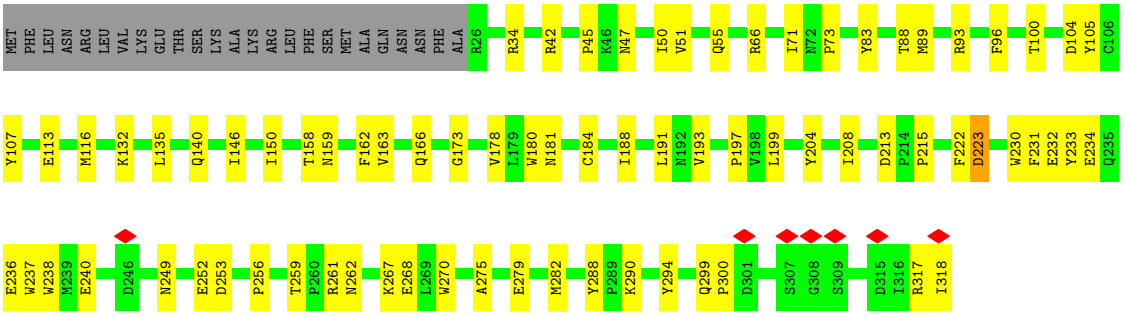
• Molecule 35: Iron-binding zinc finger CDGSH type protein

Chain FS:



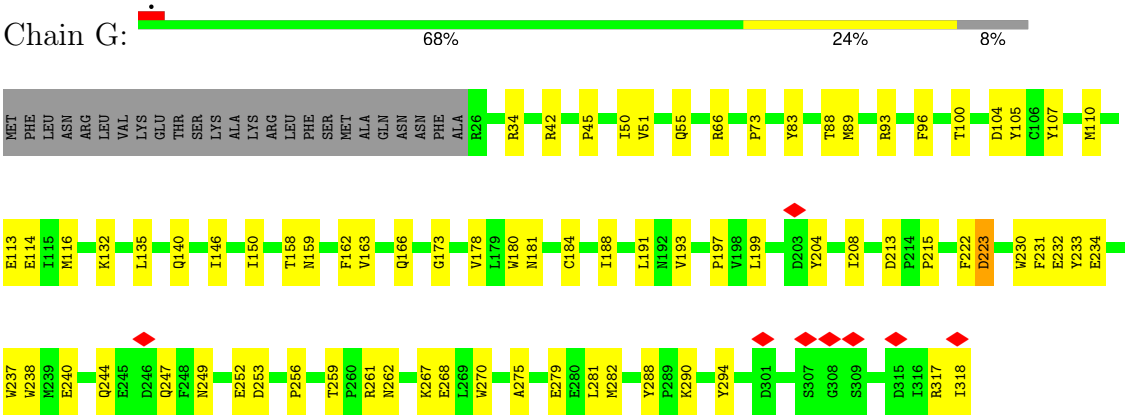
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain g:



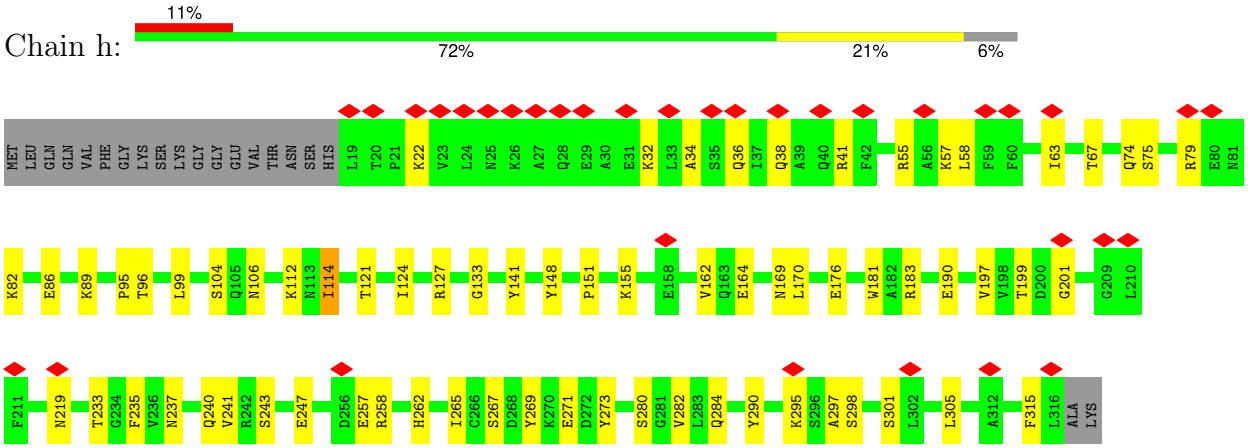
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain G:



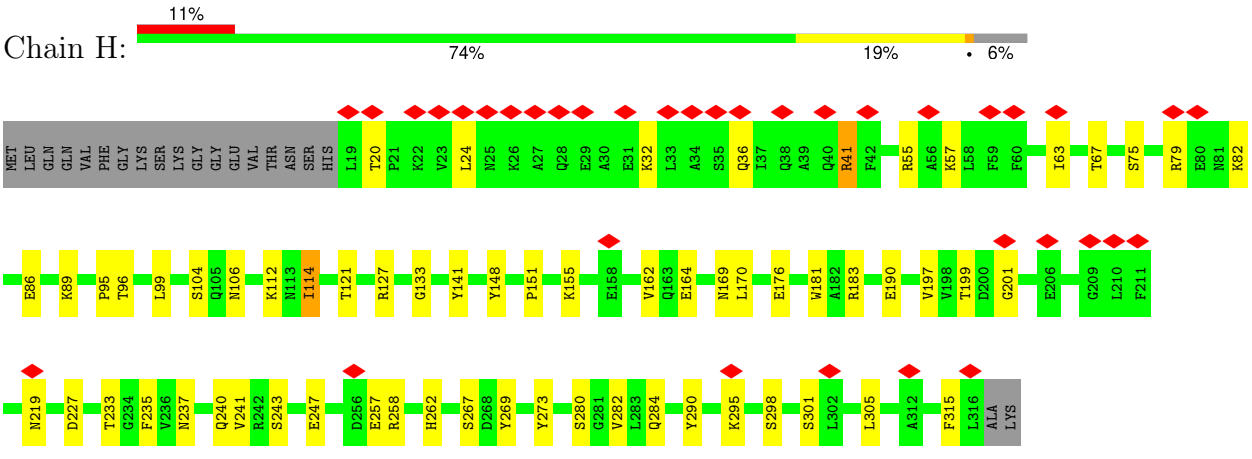
• Molecule 37: SURF1-like protein

Chain h:



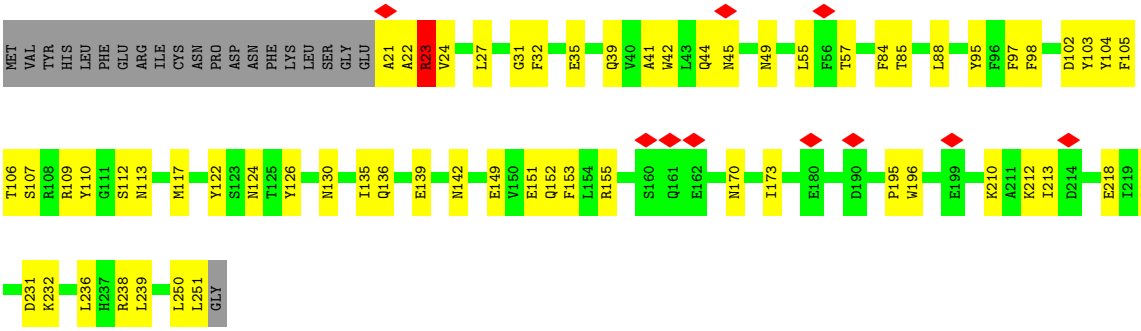
• Molecule 37: SURF1-like protein

Chain H:

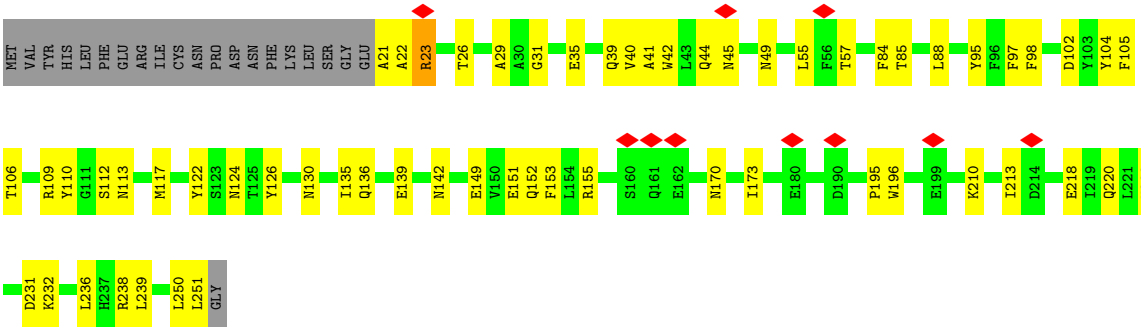


• Molecule 38: COXTT9

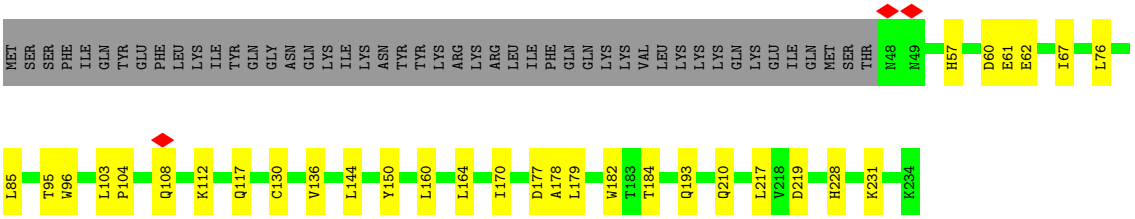
Chain i:



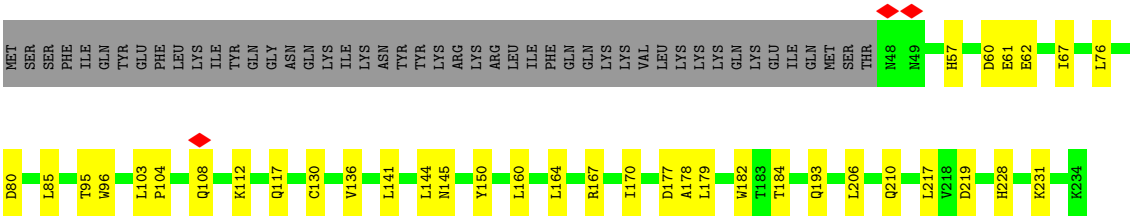
• Molecule 38: COXTT9



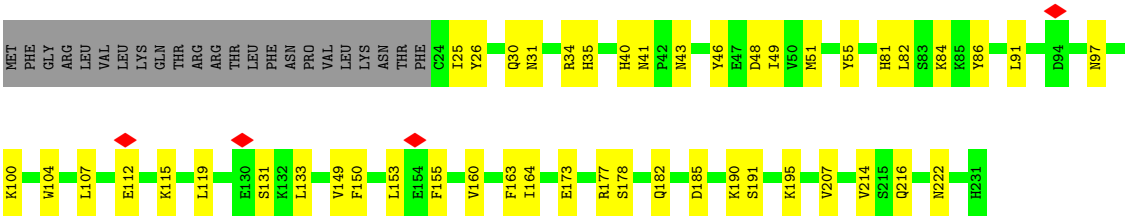
• Molecule 39: COXTT10



• Molecule 39: COXTT10

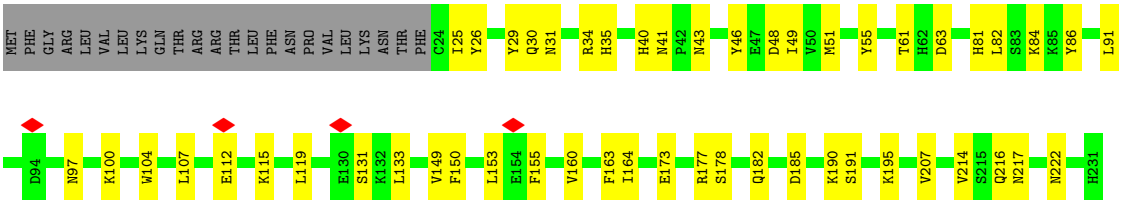


• Molecule 40: 39S ribosomal protein L9, mitochondrial



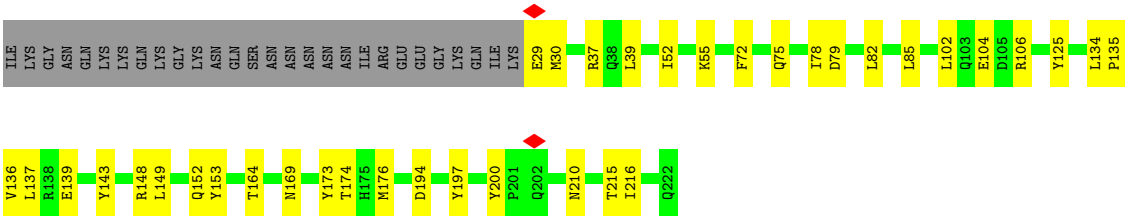
• Molecule 40: 39S ribosomal protein L9, mitochondrial

Chain K:



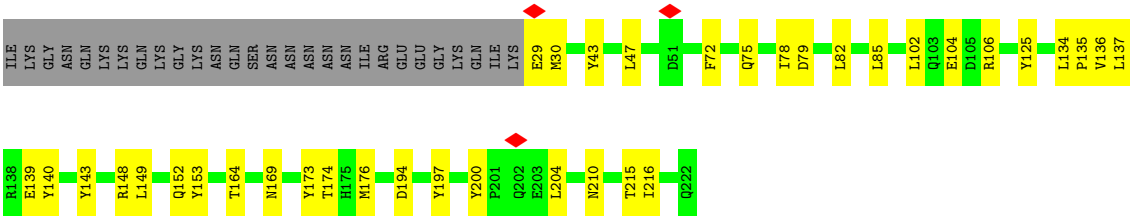
• Molecule 41: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain l:



• Molecule 41: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C

Chain L:



• Molecule 42: Transmembrane protein, putative

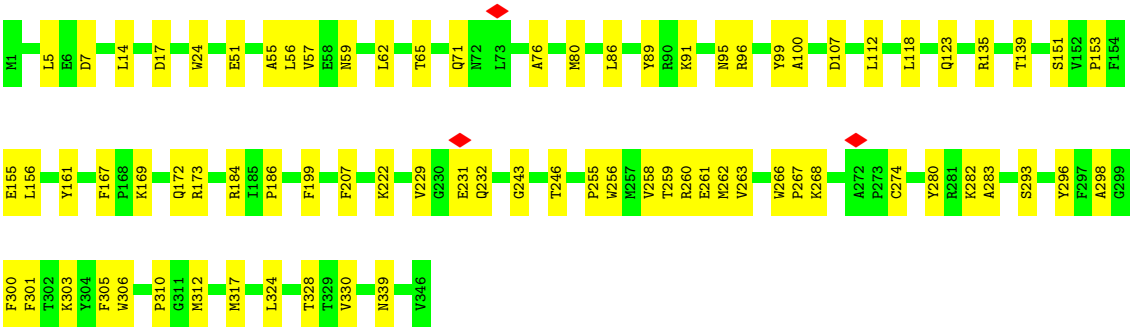
Chain m:

• Molecule 42: Transmembrane protein, putative

Chain M:

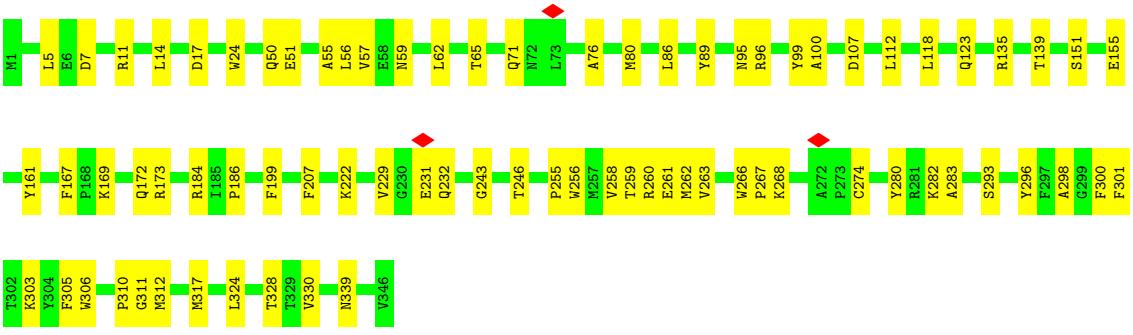
• Molecule 43: Oxoglutarate/malate translocator protein, putative

Chain m1:



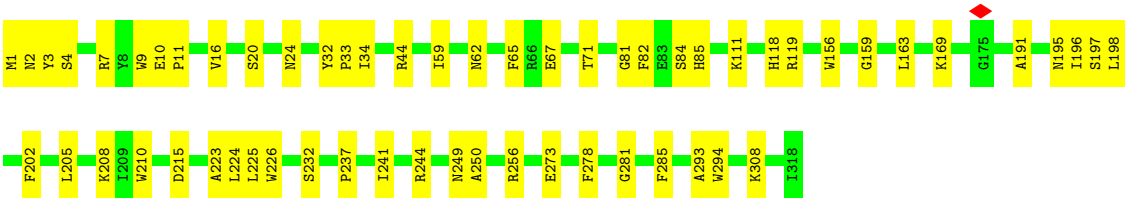
• Molecule 43: Oxoglutarate/malate translocator protein, putative

Chain M1:



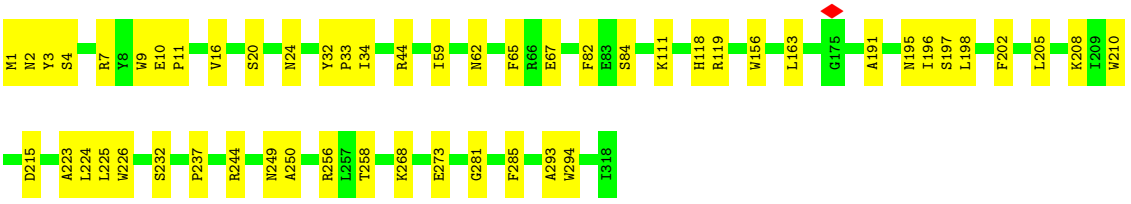
• Molecule 44: 2-oxoglutarate/malate carrier protein

Chain m2:



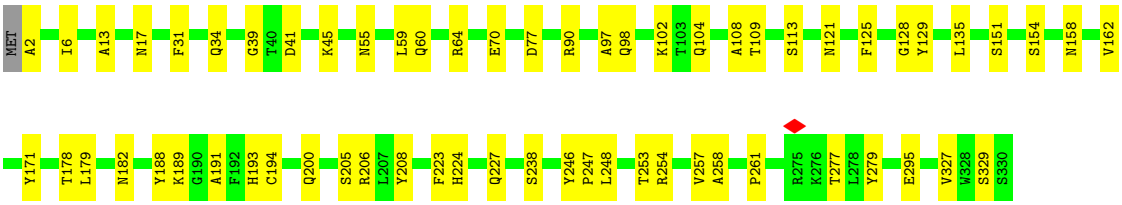
• Molecule 44: 2-oxoglutarate/malate carrier protein

Chain M2:



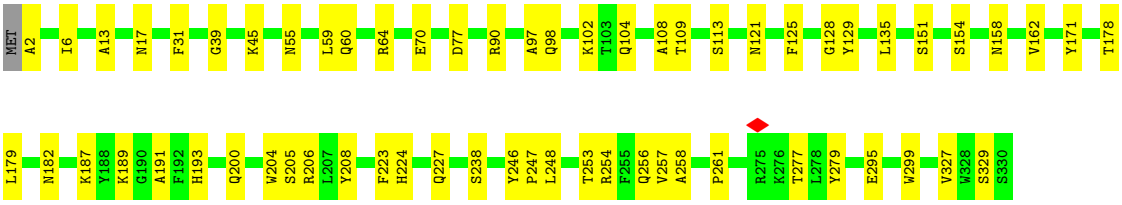
• Molecule 45: Carrier protein

Chain m3:



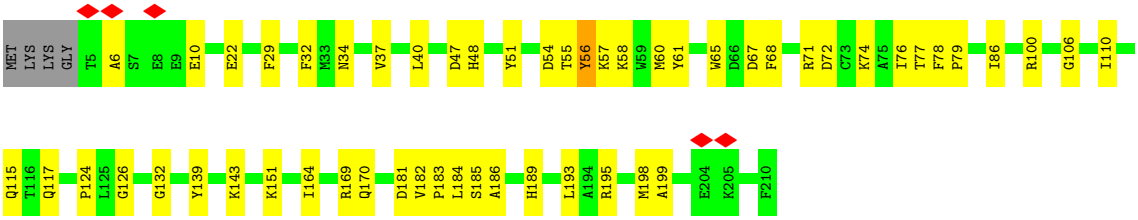
• Molecule 45: Carrier protein

Chain M3:



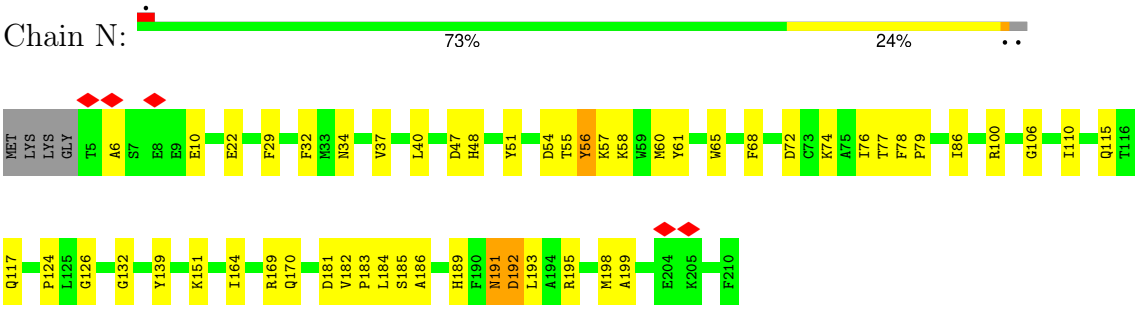
• Molecule 46: Transmembrane protein, putative

Chain n:



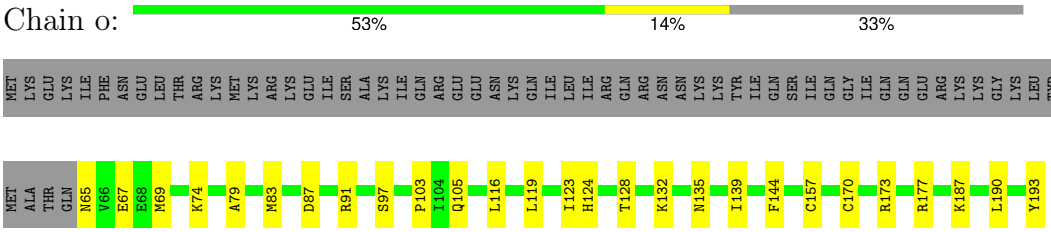
• Molecule 46: Transmembrane protein, putative

Chain N:



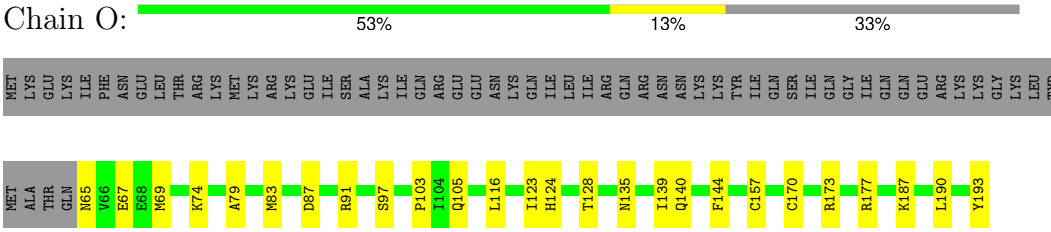
• Molecule 47: Mobilization protein

Chain o:



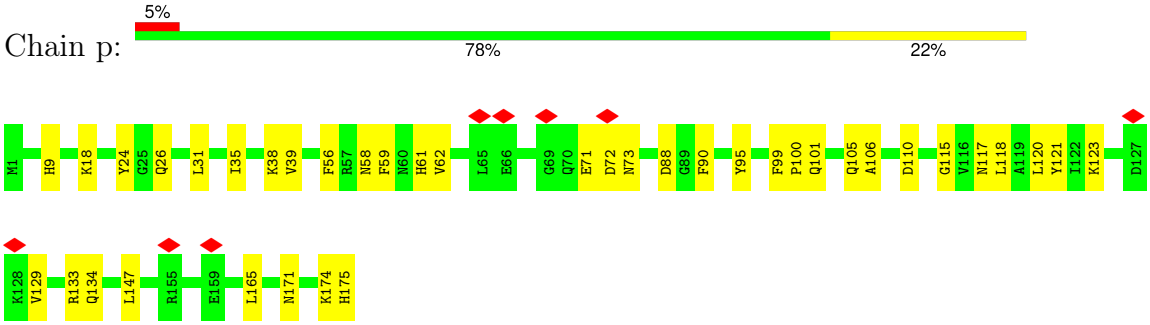
• Molecule 47: Mobilization protein

Chain O:



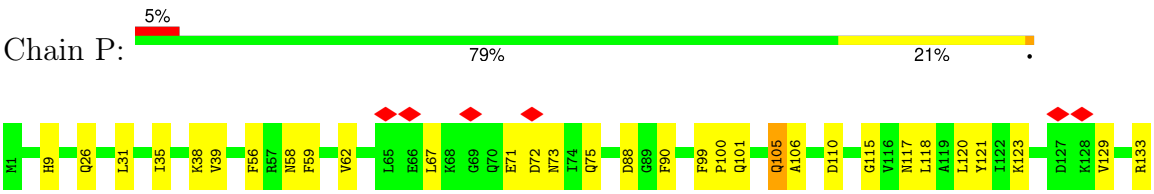
• Molecule 48: YflT domain-containing protein

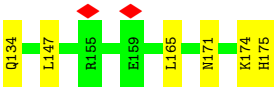
Chain p:



• Molecule 48: YflT domain-containing protein

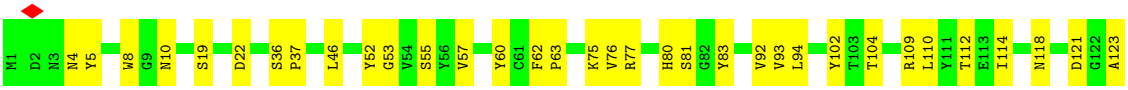
Chain P:

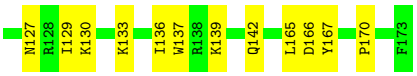




• Molecule 49: Transmembrane protein, putative

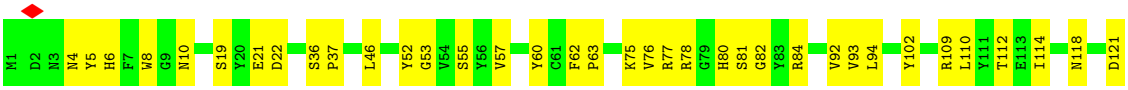
Chain q:

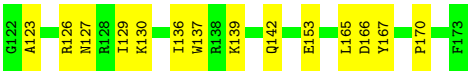




• Molecule 49: Transmembrane protein, putative

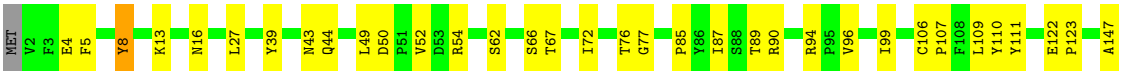
Chain Q:

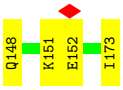




• Molecule 50: Transmembrane protein

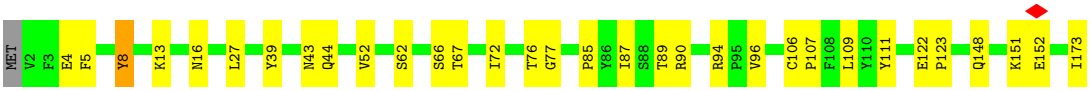
Chain r:





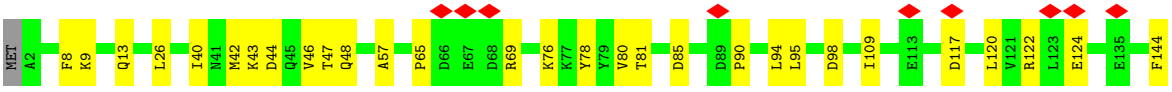
• Molecule 50: Transmembrane protein

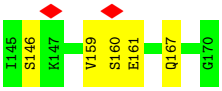
Chain R:



• Molecule 51: Complex III subunit VII

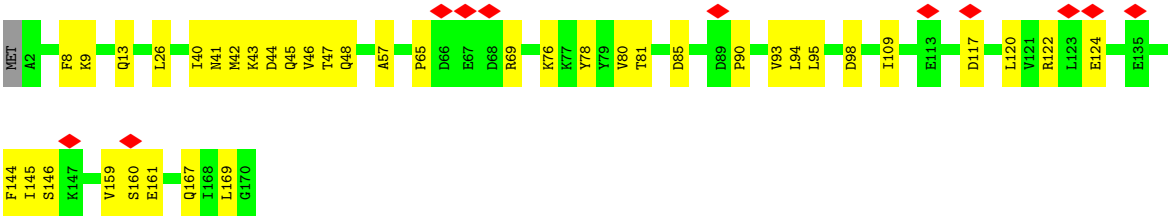
Chain s:





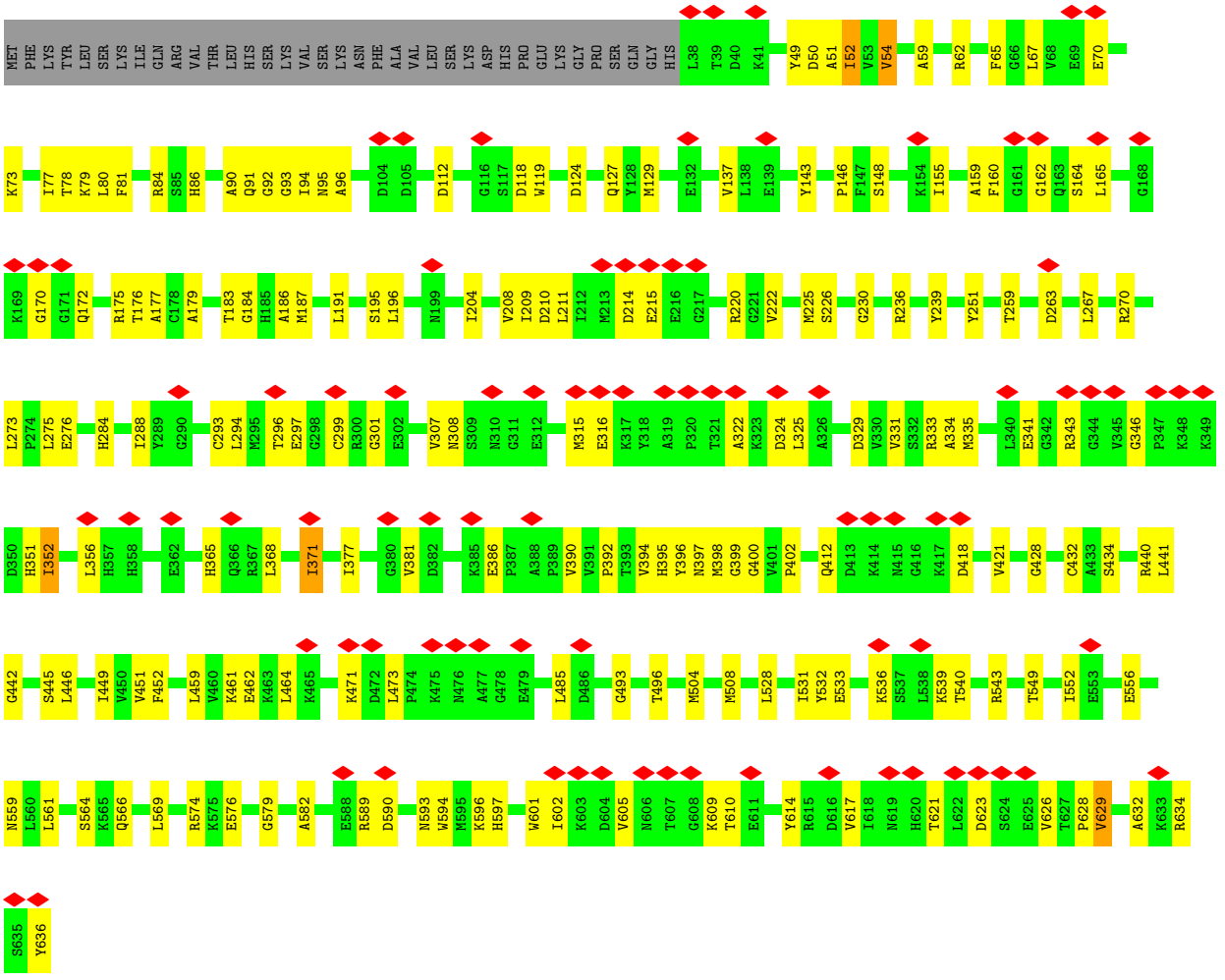
• Molecule 51: Complex III subunit VII

Chain S:



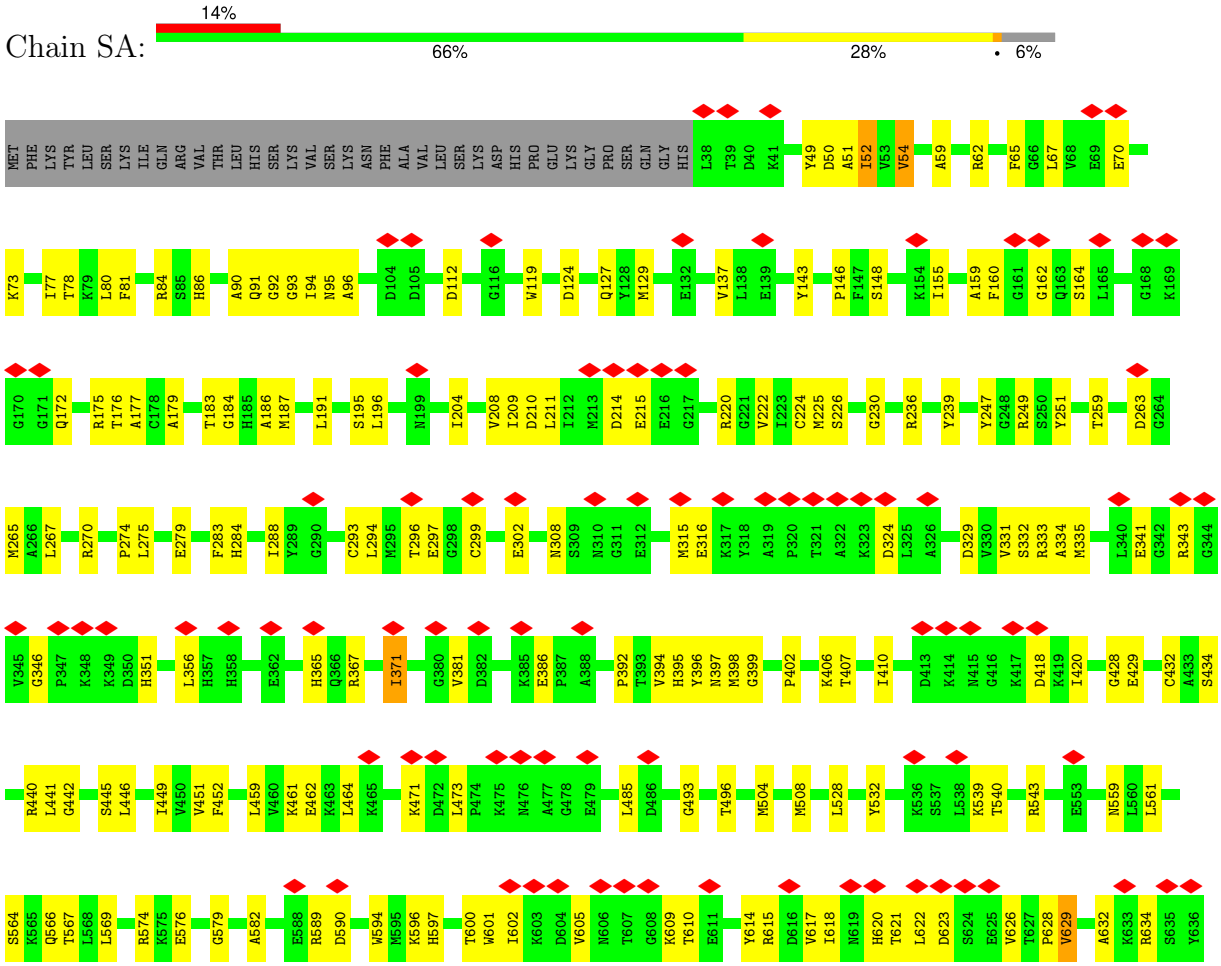
• Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain sa:



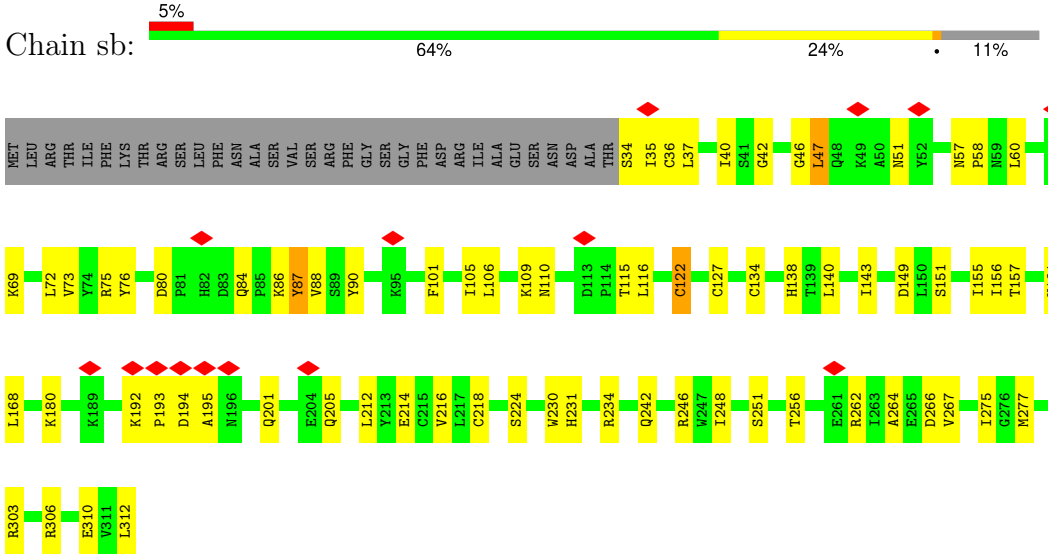
• Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

Chain SA:



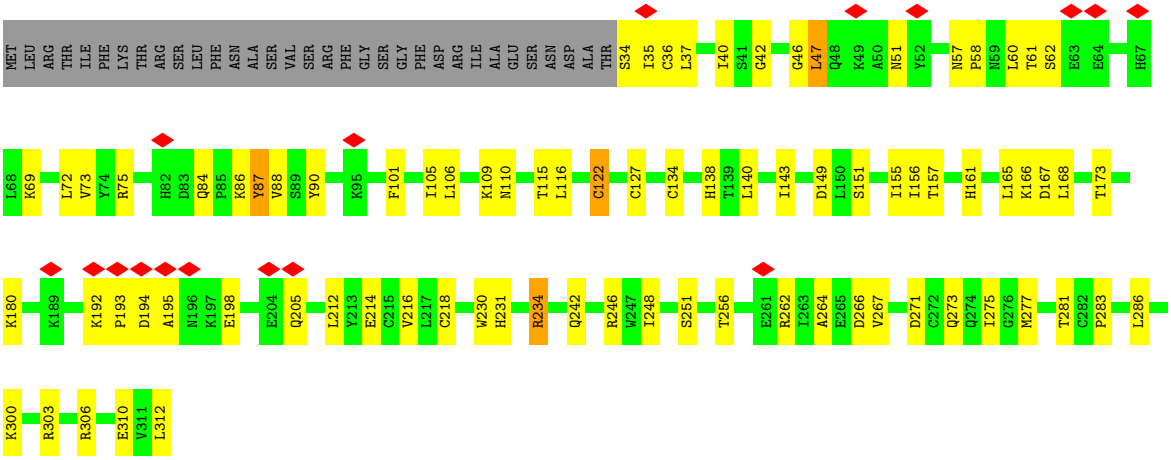
• Molecule 53: Succinate dehydrogenase (quinone)

Chain sb:



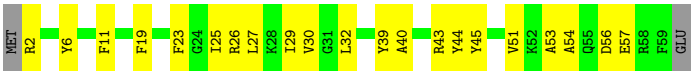
• Molecule 53: Succinate dehydrogenase (quinone)

Chain SB:



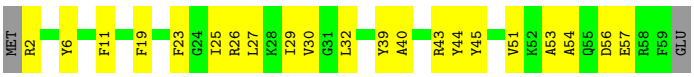
• Molecule 54: Cytochrome b-c1 complex subunit 8

Chain sc:



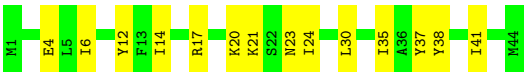
• Molecule 54: Cytochrome b-c1 complex subunit 8

Chain SC:



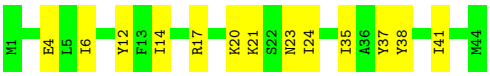
• Molecule 55: SDHD

Chain sd:



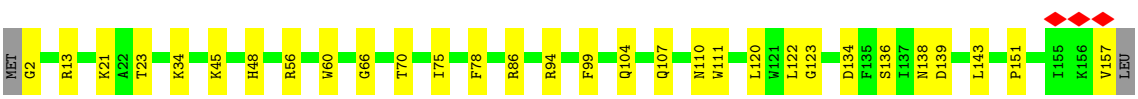
• Molecule 55: SDHD

Chain SD:



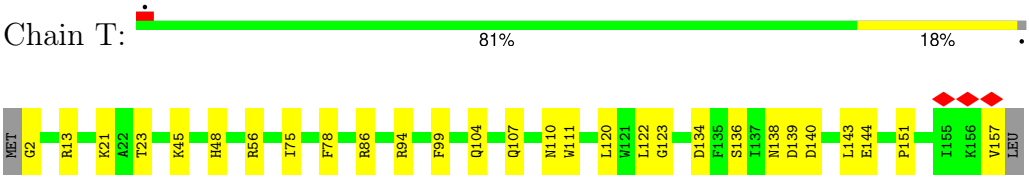
• Molecule 56: Transmembrane protein, putative

Chain t:



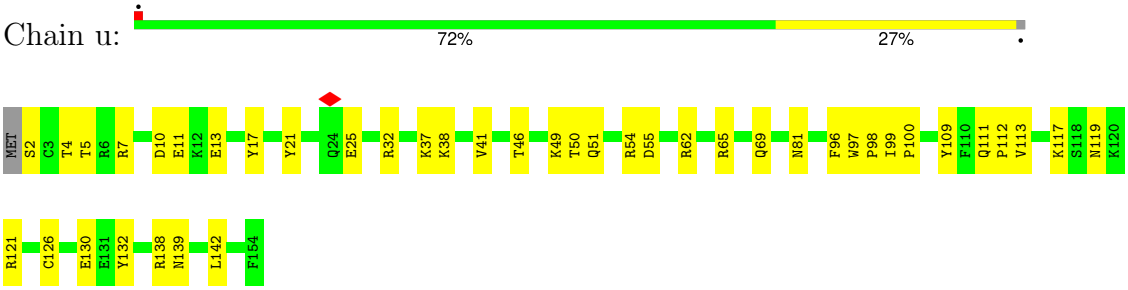
• Molecule 56: Transmembrane protein, putative

Chain T:



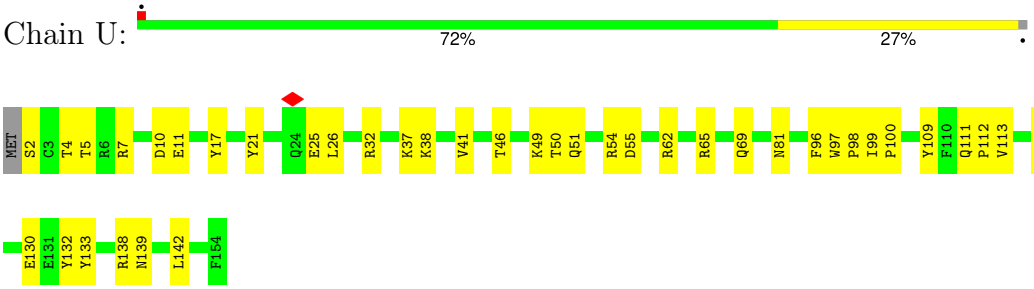
• Molecule 57: Transmembrane protein, putative

Chain u:



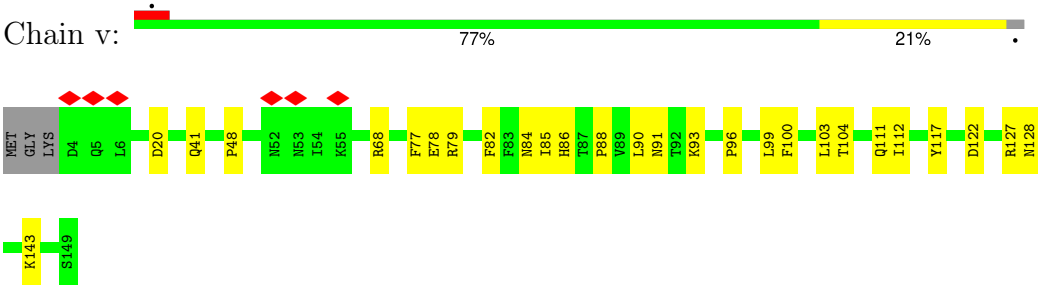
• Molecule 57: Transmembrane protein, putative

Chain U:



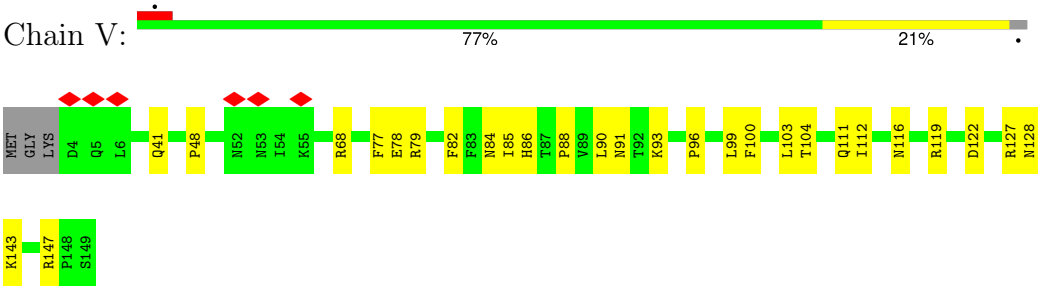
• Molecule 58: COXTT22

Chain v:



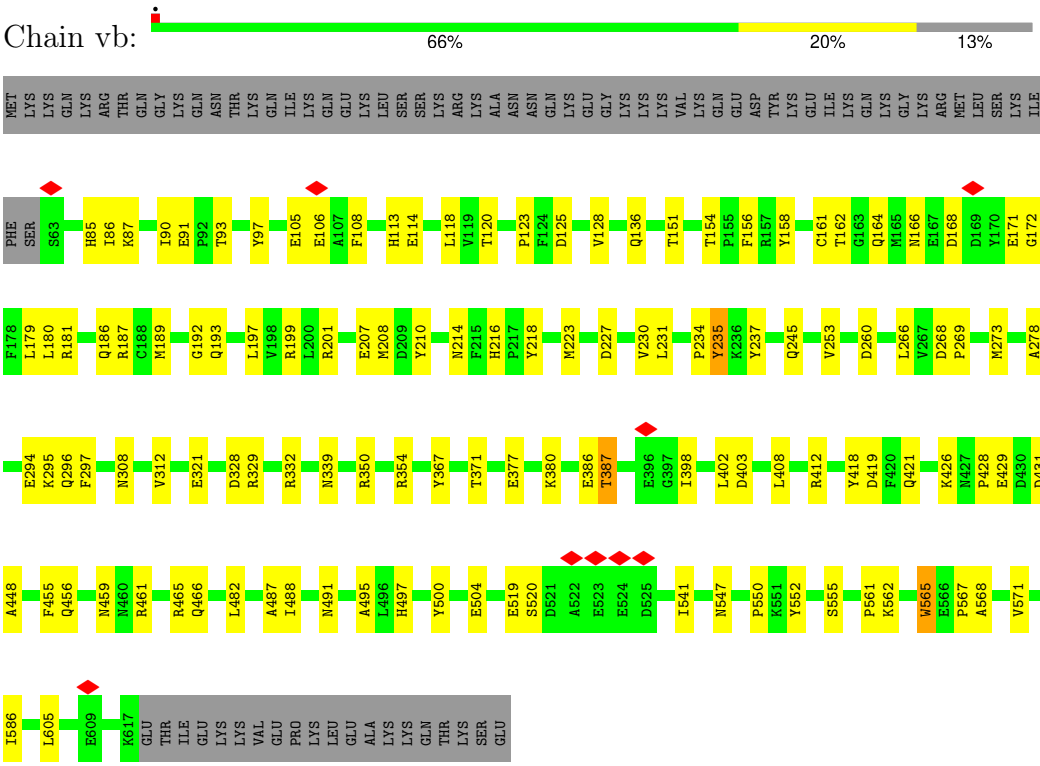
• Molecule 58: COXTT22

Chain V:



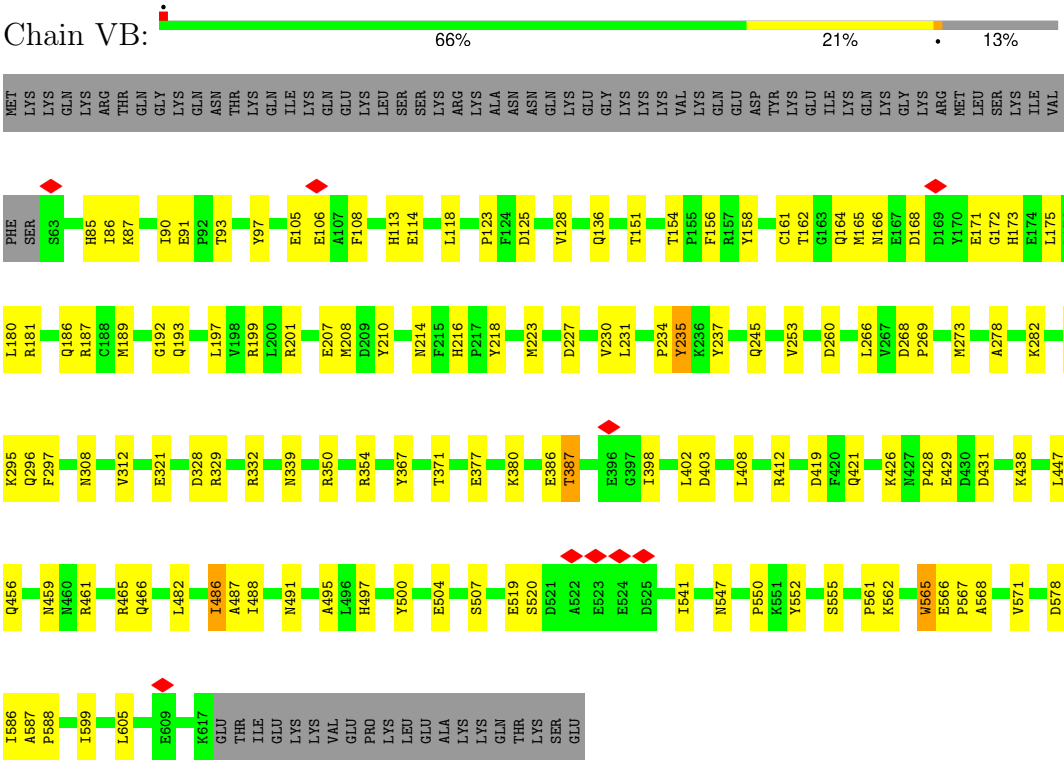
• Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain vb:



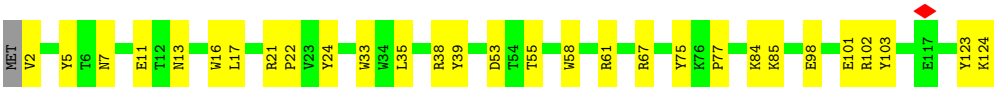
• Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain VB:

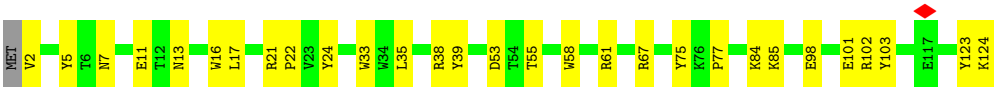


• Molecule 60: Transmembrane protein, putative

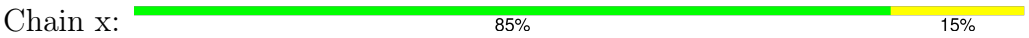
Chain w:

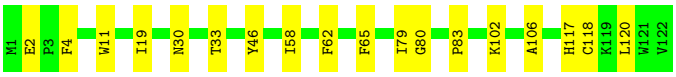


• Molecule 60: Transmembrane protein, putative

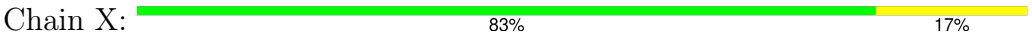


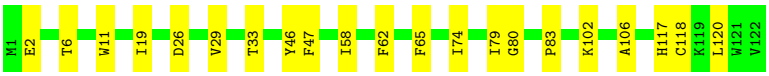
• Molecule 61: Transmembrane protein, putative



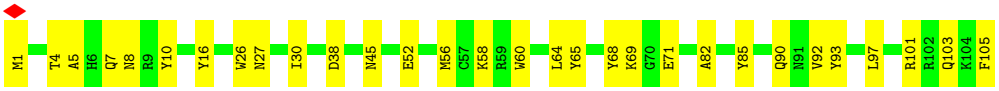


• Molecule 61: Transmembrane protein, putative

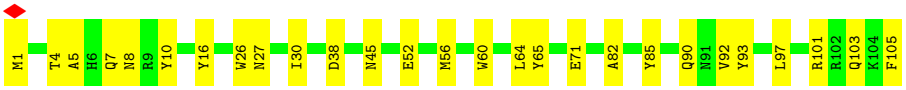




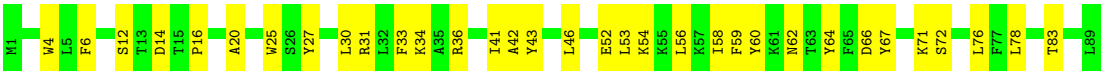
• Molecule 62: Lysozyme



• Molecule 62: Lysozyme

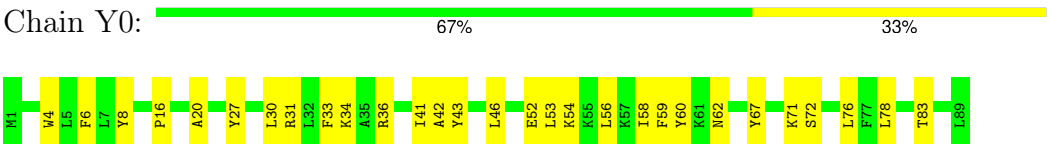


• Molecule 63: Ymf70



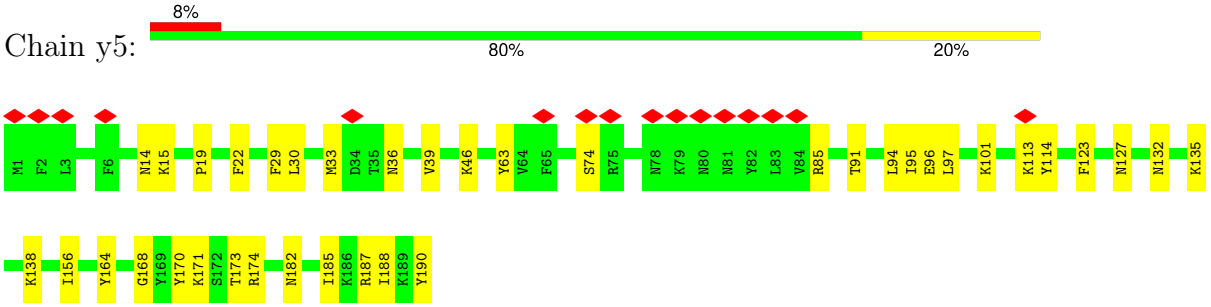
• Molecule 63: Ymf70

Chain Y0:



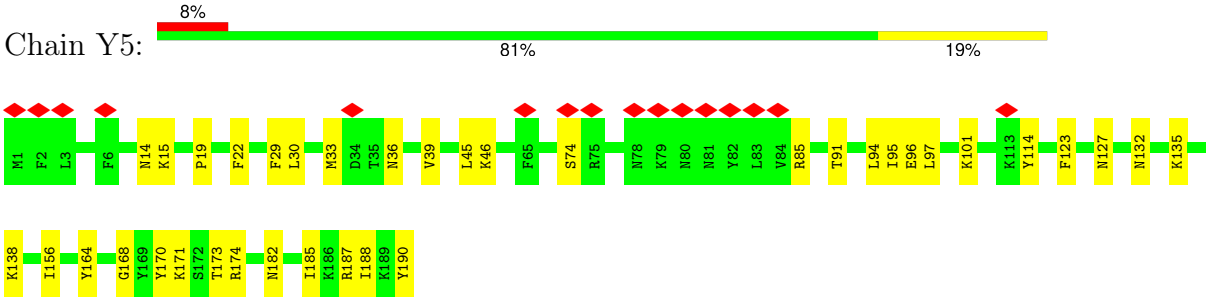
• Molecule 64: Ymf75

Chain y5:



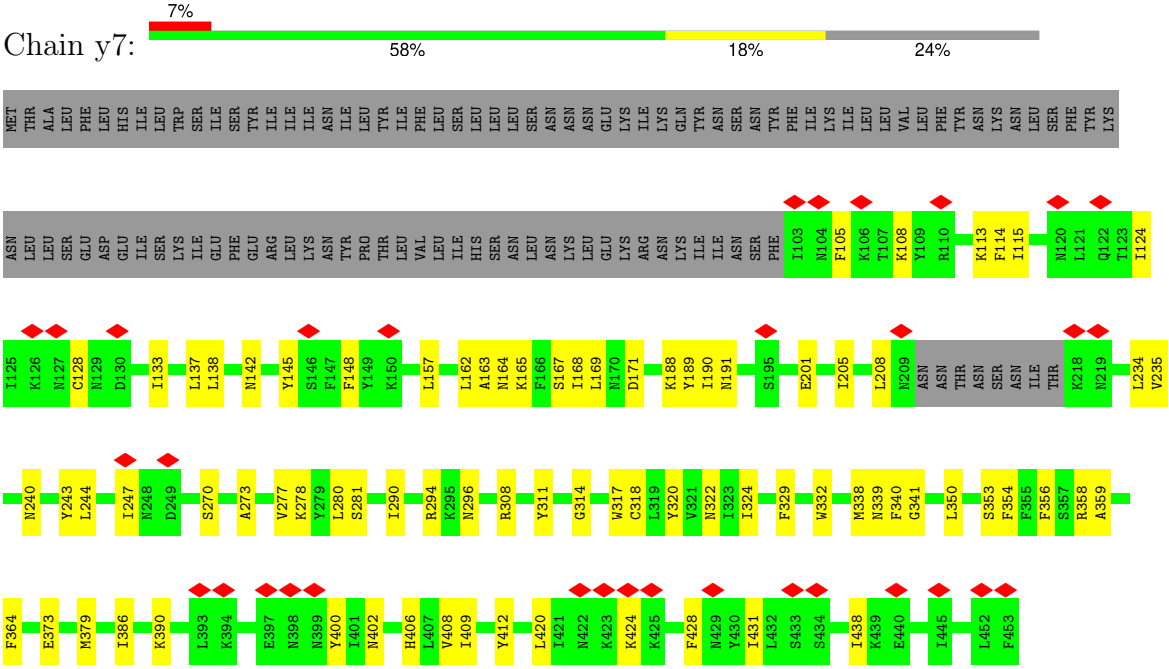
• Molecule 64: Ymf75

Chain Y5:



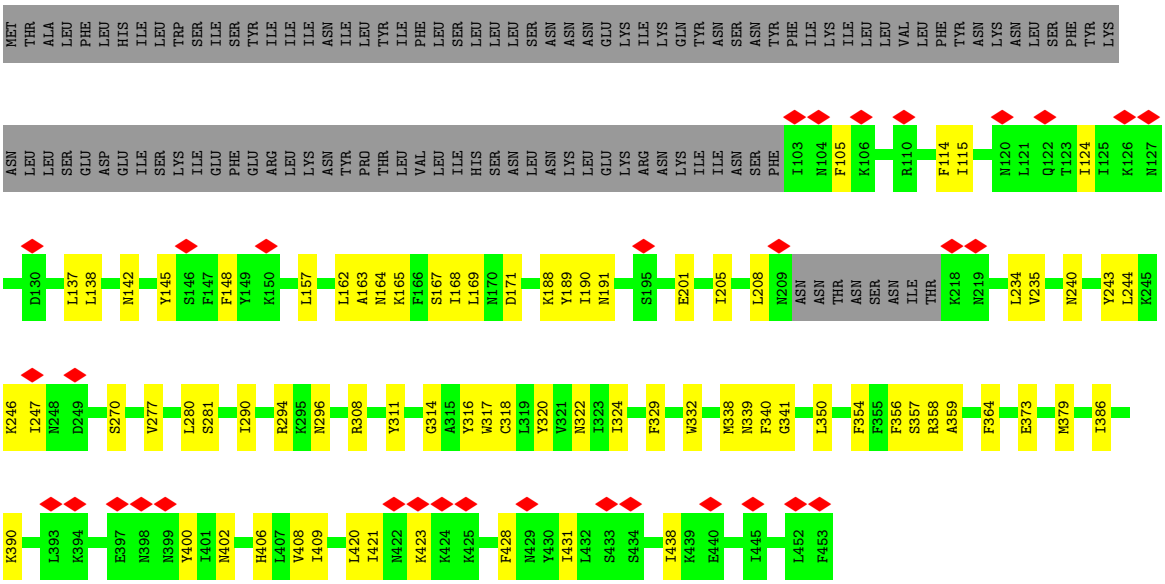
• Molecule 65: Ymf67

Chain y7:

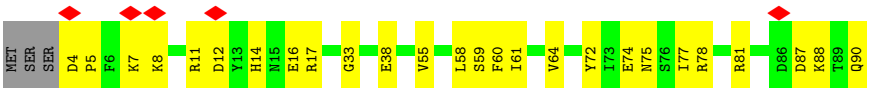


• Molecule 65: Ymf67

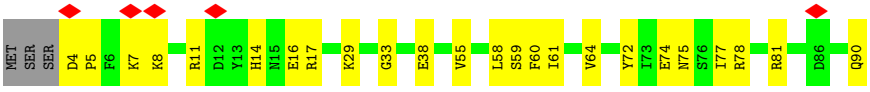
Chain Y7:



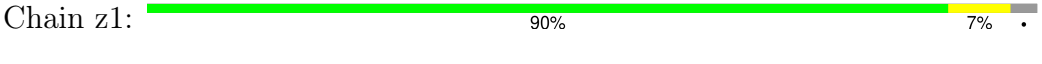
• Molecule 66: ABC transporter

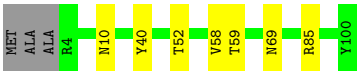


• Molecule 66: ABC transporter

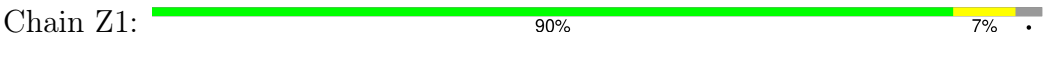


• Molecule 67: COXTT28

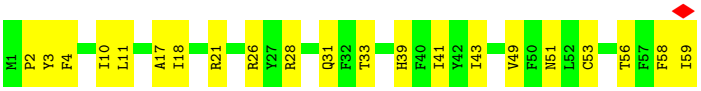




• Molecule 67: COXTT28

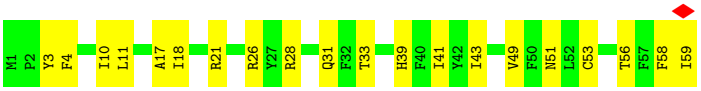


• Molecule 68: NADH dehydrogenase subunit 1



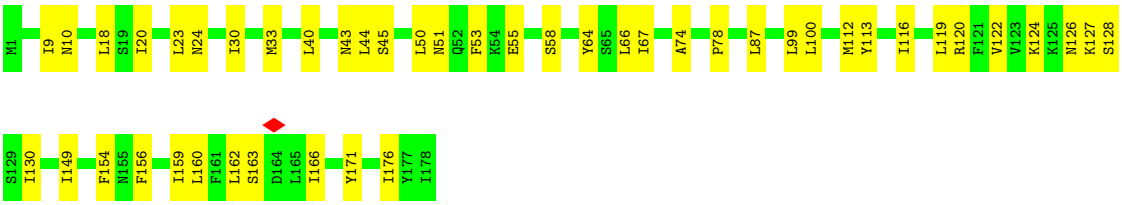
• Molecule 68: NADH dehydrogenase subunit 1

Chain 1B:



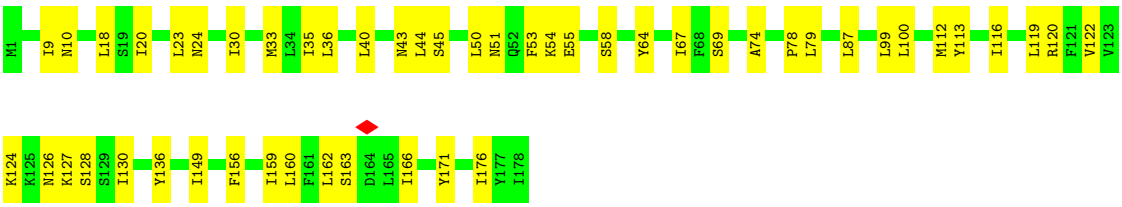
• Molecule 69: NADH dehydrogenase subunit 2

Chain 2b:



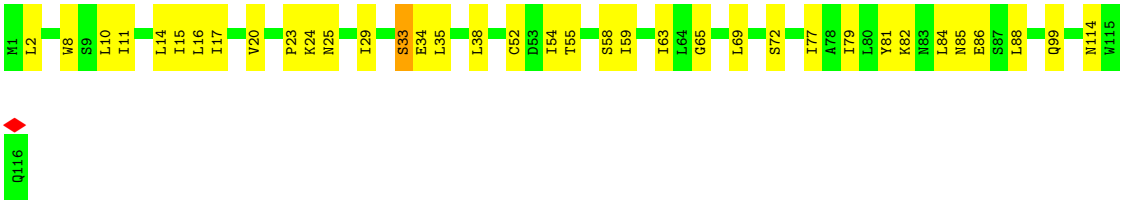
• Molecule 69: NADH dehydrogenase subunit 2

Chain 2B:



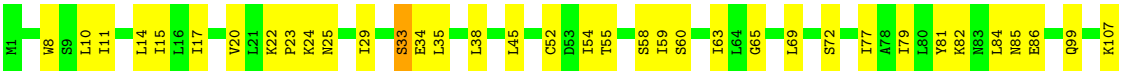
• Molecule 70: Ymf58

Chain 4l:



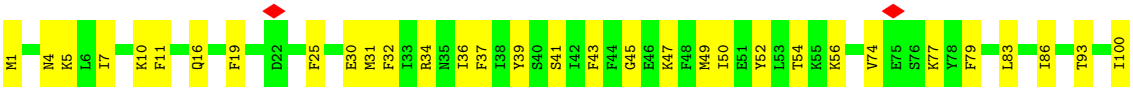
• Molecule 70: Ymf58

Chain 4L:



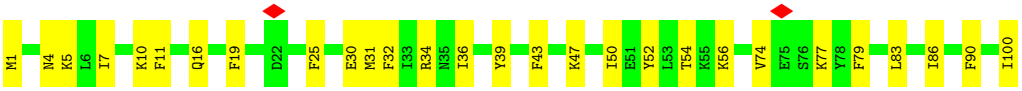
• Molecule 71: Ymf57

Chain 5b:



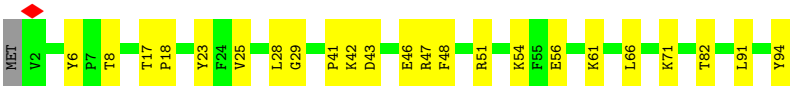
• Molecule 71: Ymf57

Chain 5B:



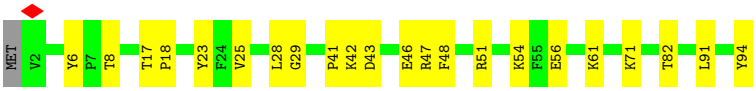
• Molecule 72: Transmembrane protein, putative

Chain a1:



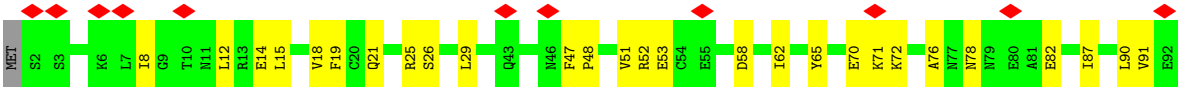
• Molecule 72: Transmembrane protein, putative

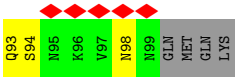
Chain A1:



• Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

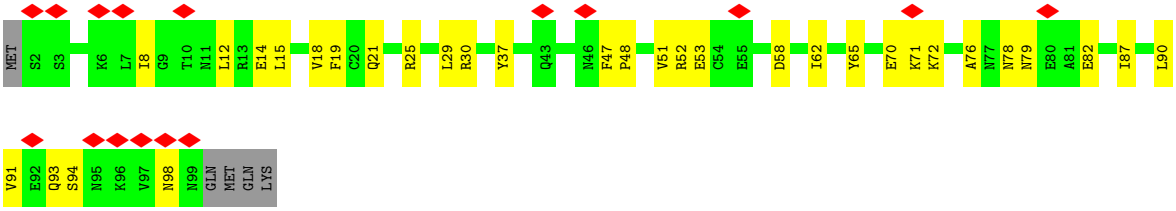
Chain a2:



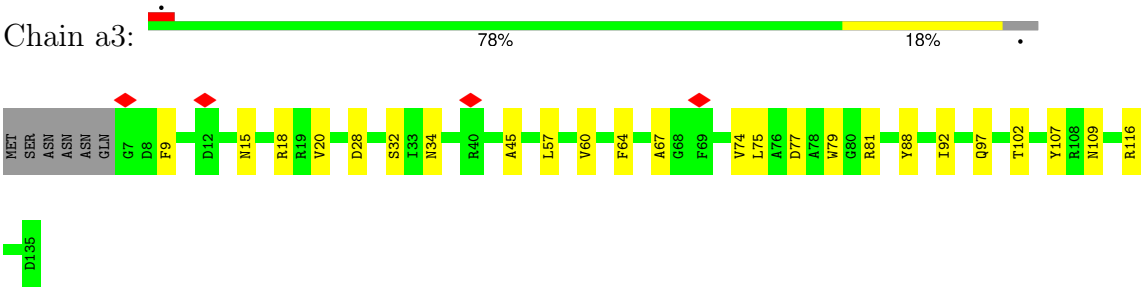


• Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

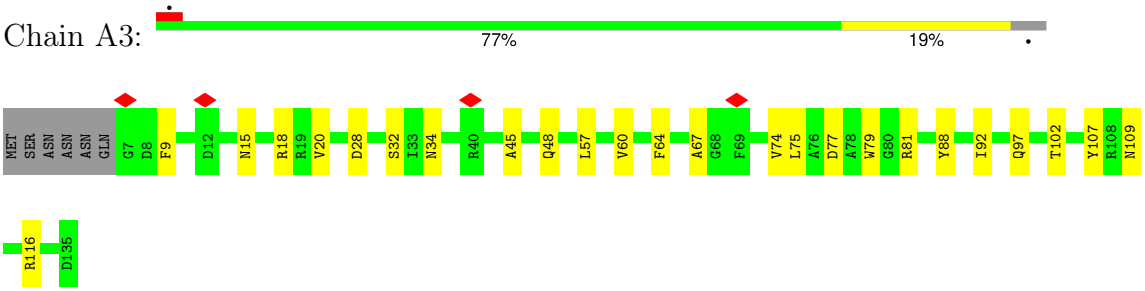
Chain A2:



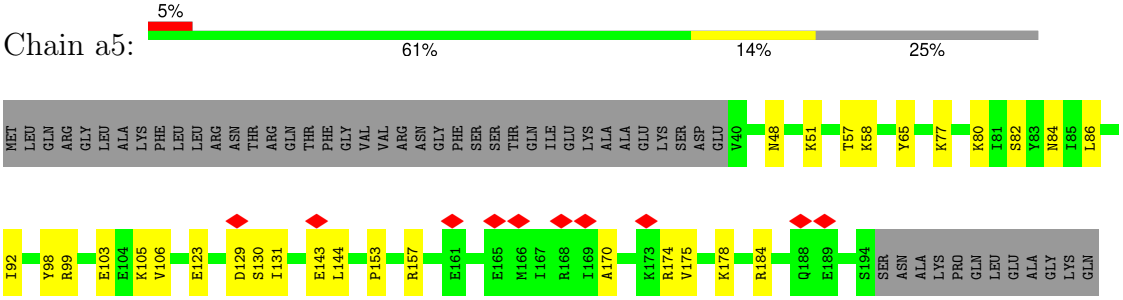
• Molecule 74: Transmembrane protein, putative



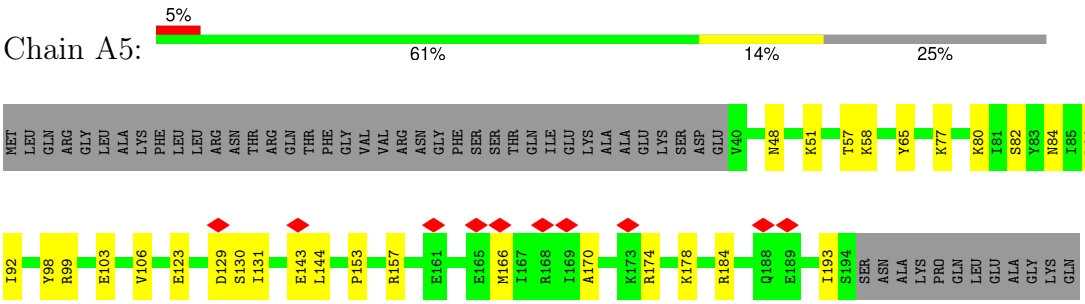
• Molecule 74: Transmembrane protein, putative



• Molecule 75: ETC complex I subunit motif protein

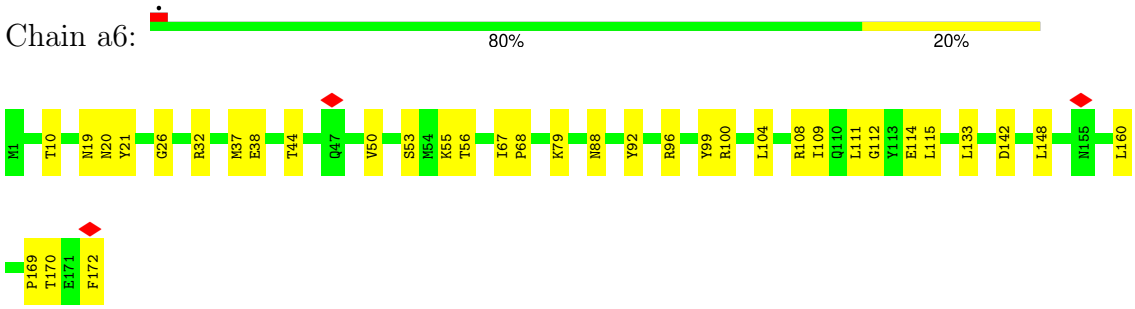


• Molecule 75: ETC complex I subunit motif protein



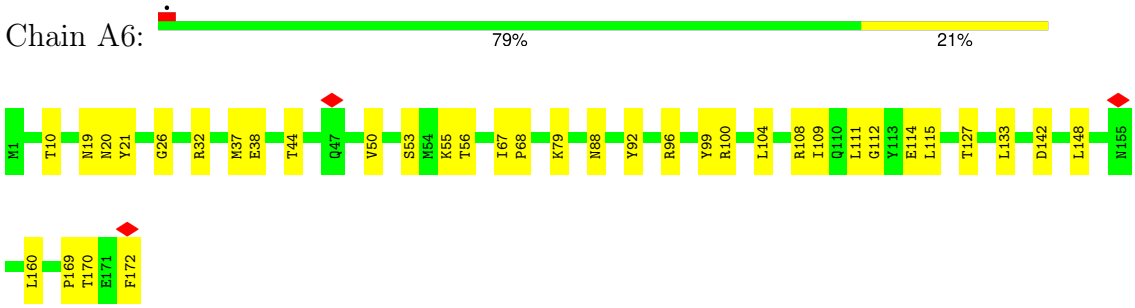
• Molecule 76: NADH dehydrogenase, putative

Chain a6:



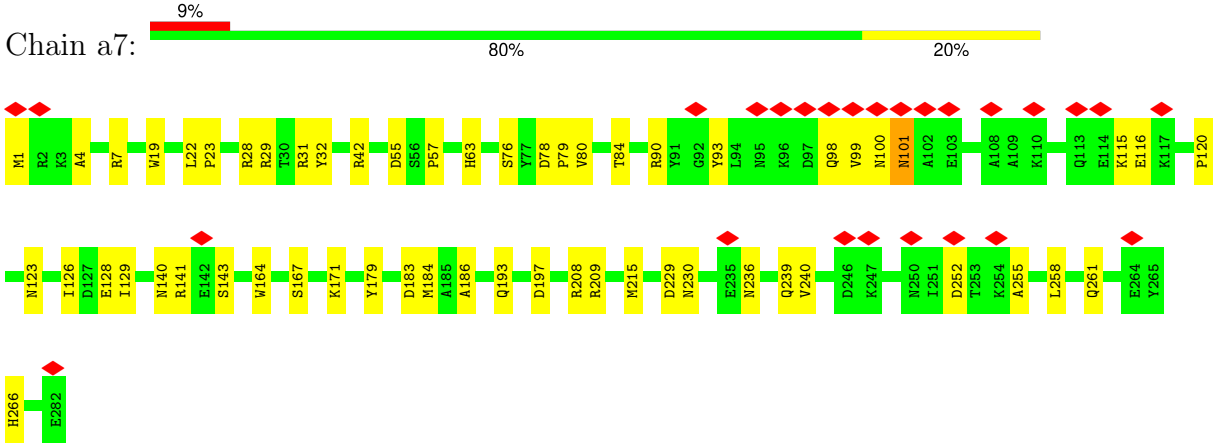
• Molecule 76: NADH dehydrogenase, putative

Chain A6:



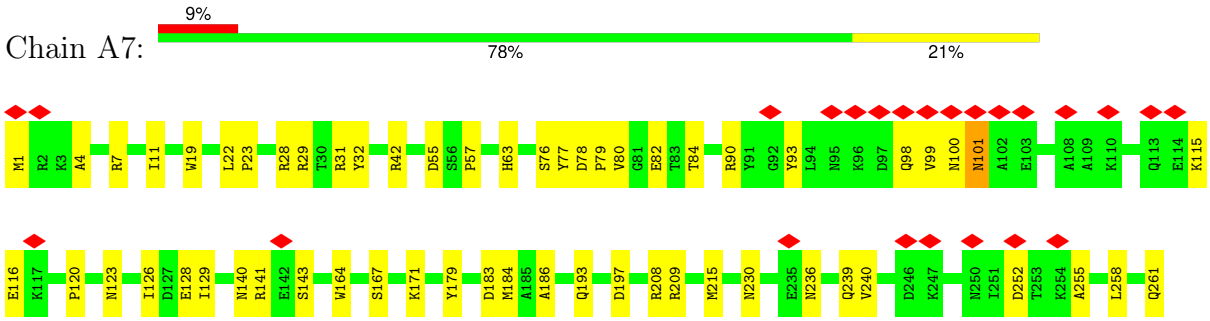
• Molecule 77: 37S ribosomal protein S25, mitochondrial

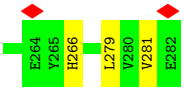
Chain a7:



• Molecule 77: 37S ribosomal protein S25, mitochondrial

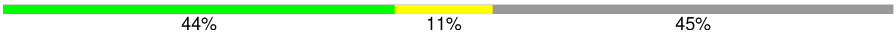
Chain A7:

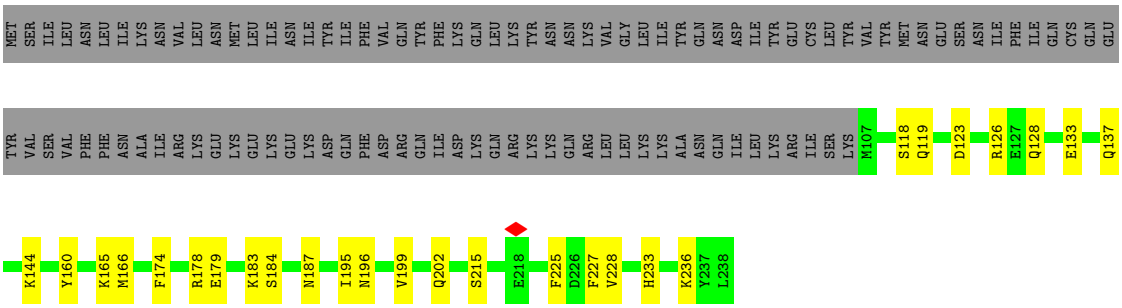




• Molecule 78: CX9C domain-containing protein

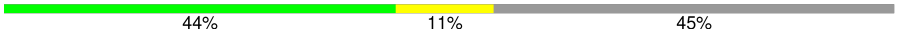
Chain a8:

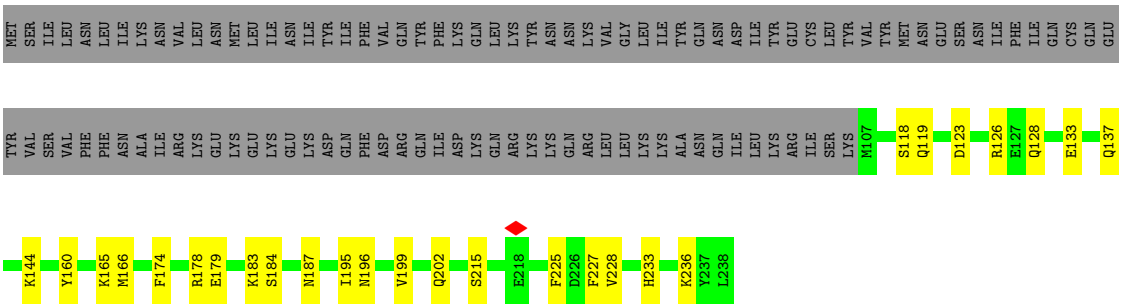




• Molecule 78: CX9C domain-containing protein

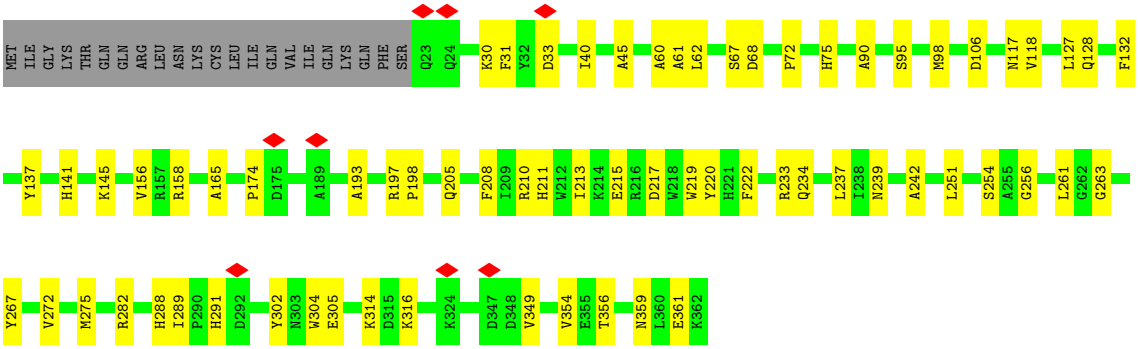
Chain A8:





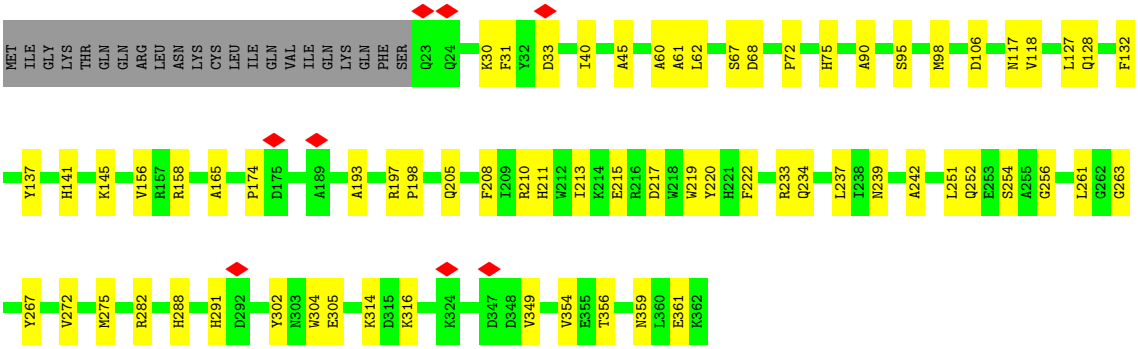
• Molecule 79: NAD-dependent epimerase/dehydratase family protein

Chain a9:



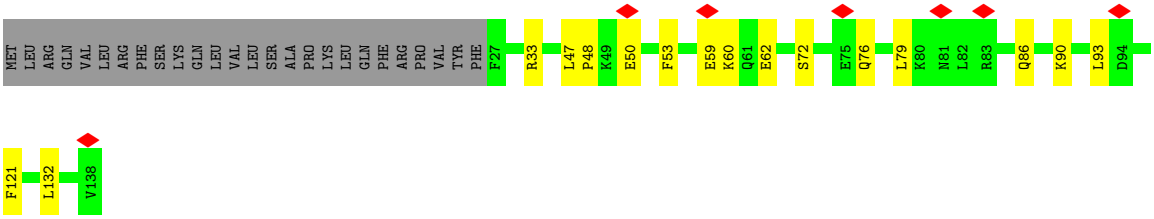
• Molecule 79: NAD-dependent epimerase/dehydratase family protein

Chain A9:



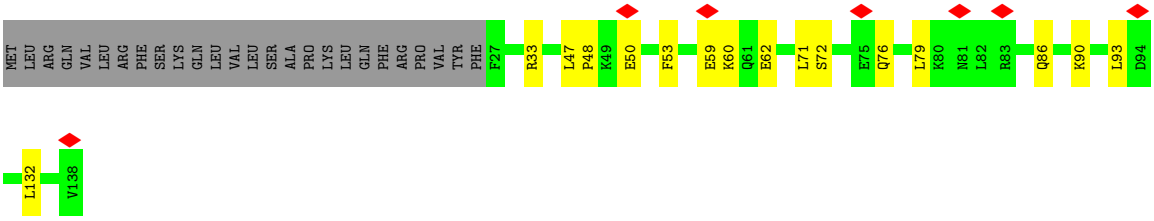
• Molecule 80: Acyl carrier protein

Chain ab:



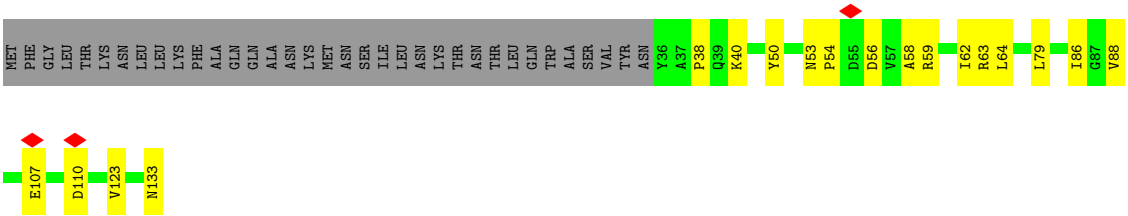
• Molecule 80: Acyl carrier protein

Chain AB:



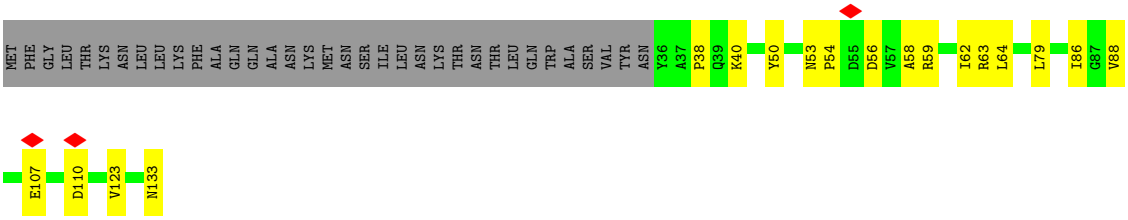
• Molecule 81: Acyl carrier protein

Chain ac:

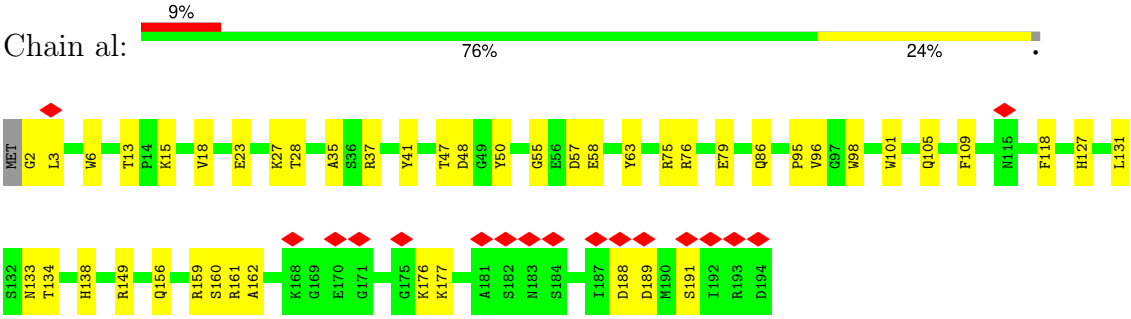


• Molecule 81: Acyl carrier protein

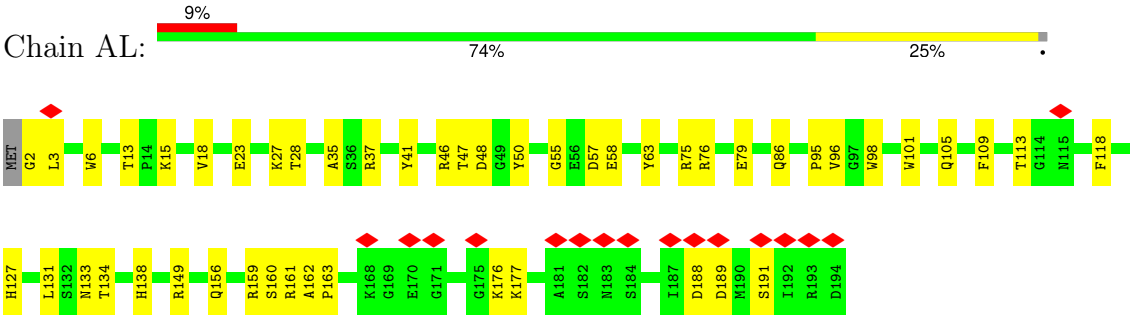
Chain AC:



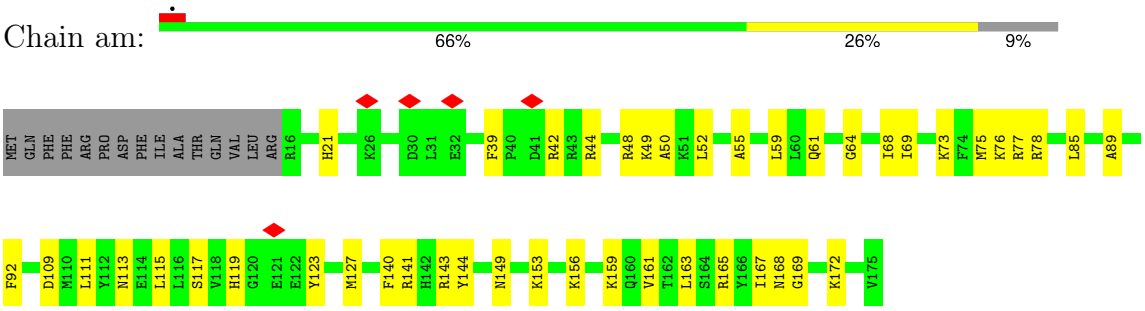
• Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



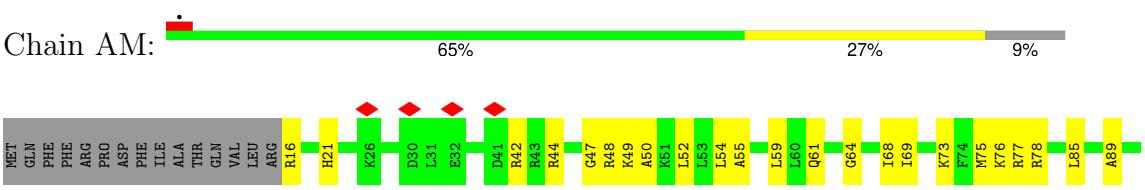
• Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



• Molecule 83: NDUA13

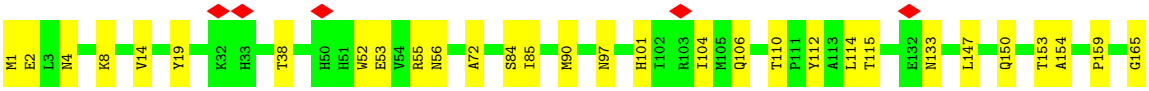


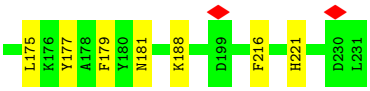
• Molecule 83: NDUA13



• Molecule 84: Transmembrane protein, putative

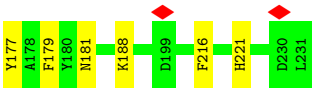
Chain an:





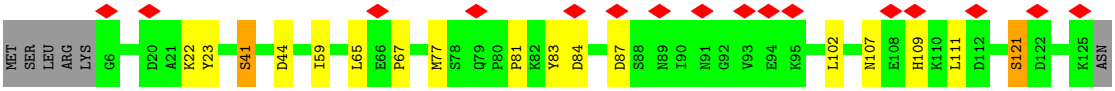
• Molecule 84: Transmembrane protein, putative

Chain AN:



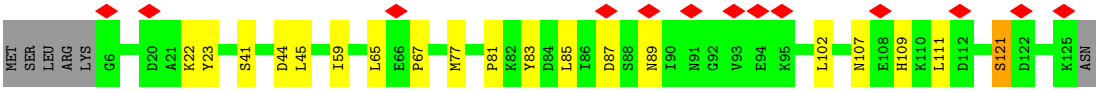
• Molecule 85: NDUB2

Chain b2:



• Molecule 85: NDUB2

Chain B2:

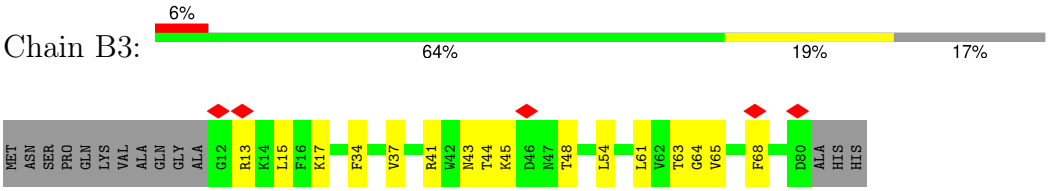


• Molecule 86: Transmembrane protein, putative

Chain b3:

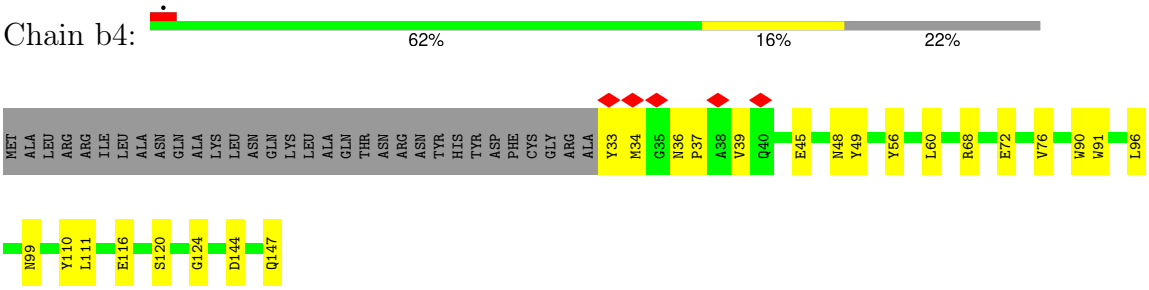
• Molecule 86: Transmembrane protein, putative

Chain B3:



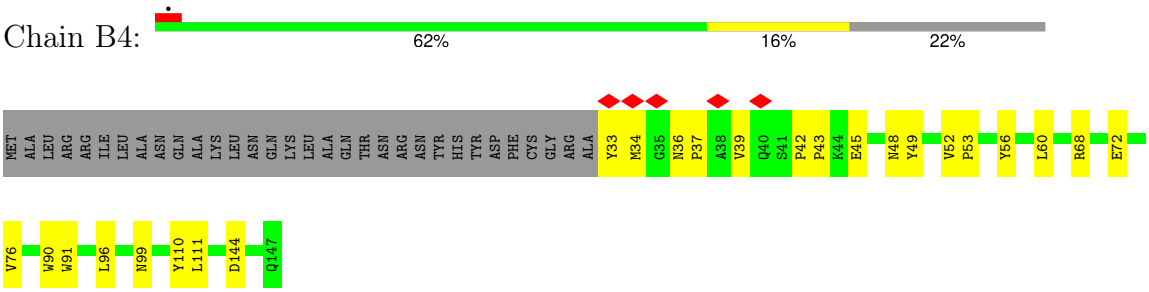
• Molecule 87: NDUB4

Chain b4:



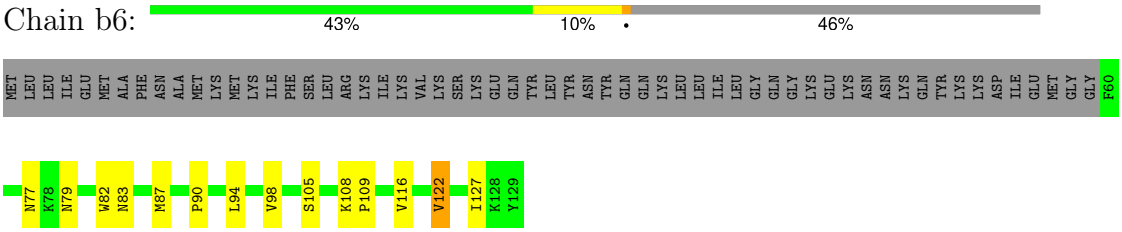
• Molecule 87: NDUB4

Chain B4:



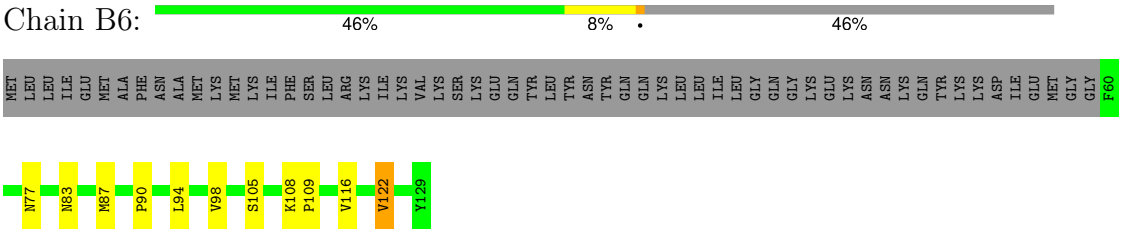
• Molecule 88: NDUB6

Chain b6:



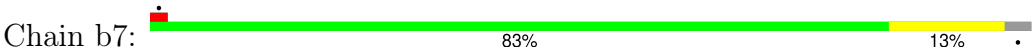
• Molecule 88: NDUB6

Chain B6:



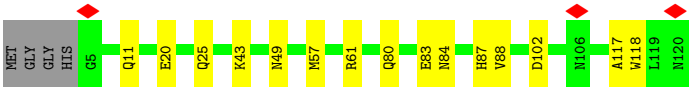
• Molecule 89: CHCH domain-containing protein

Chain b7:



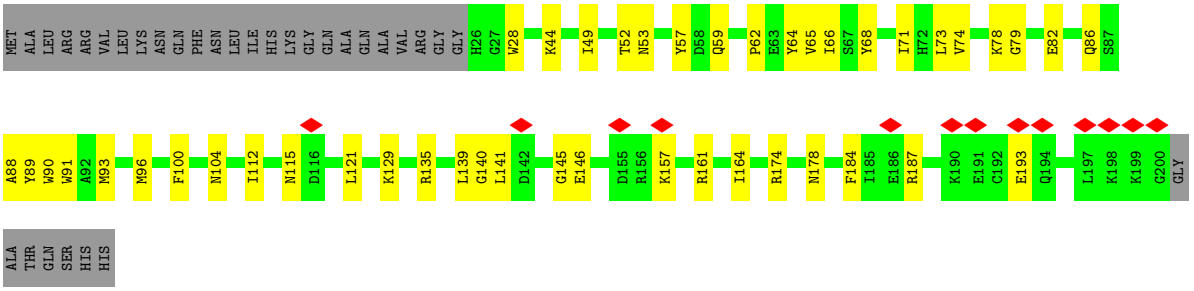
• Molecule 89: CHCH domain-containing protein

Chain B7:



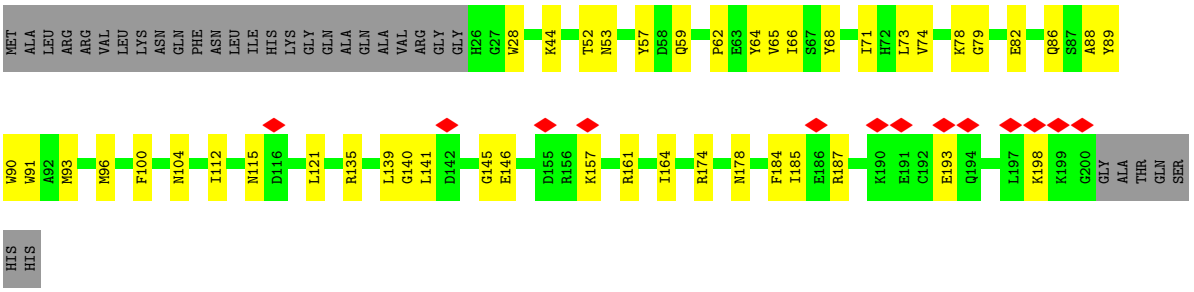
• Molecule 90: NDUB8

Chain b8:



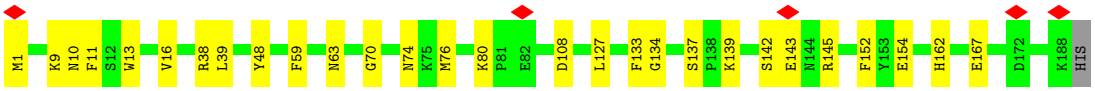
• Molecule 90: NDUB8

Chain B8:



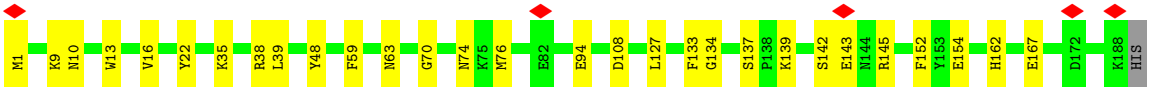
• Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain b9:



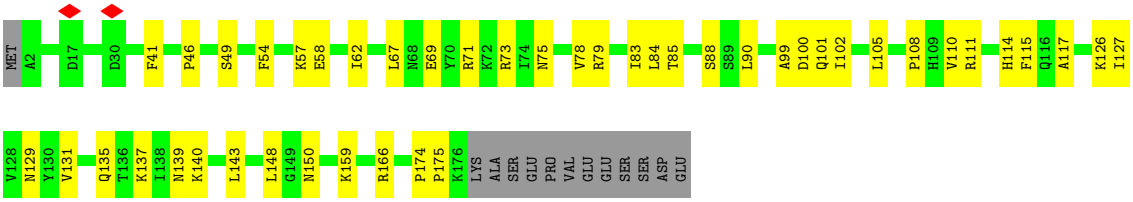
• Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain B9:



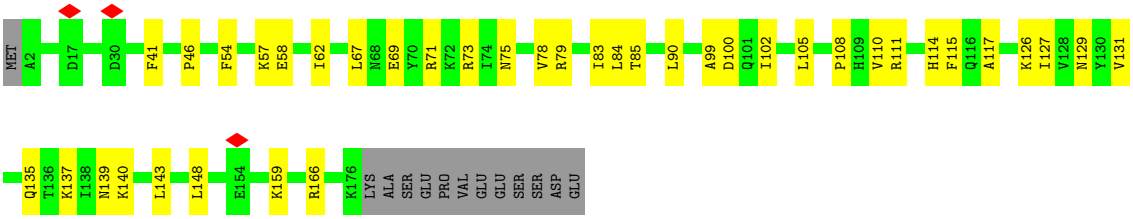
• Molecule 92: NDUB10

Chain bl:



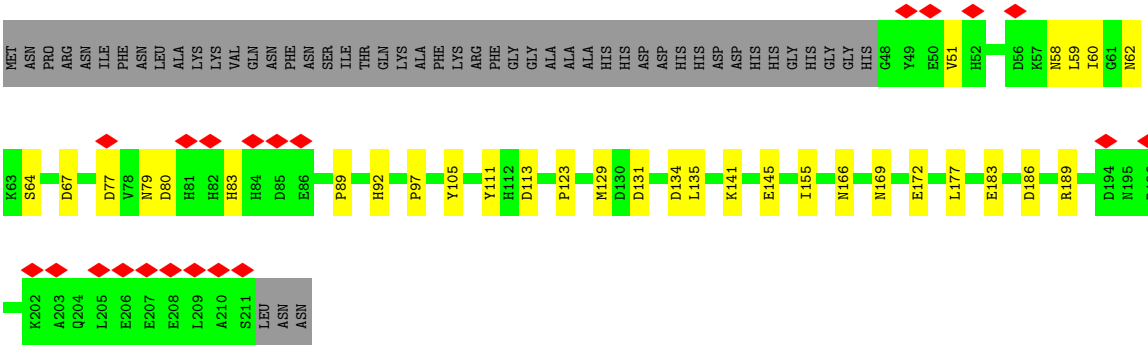
• Molecule 92: NDUB10

Chain BL:



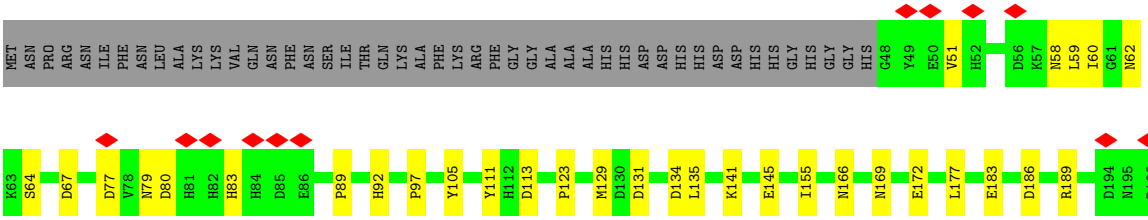
• Molecule 93: Transmembrane protein, putative

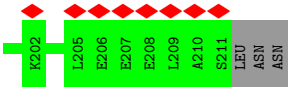
Chain bm:



• Molecule 93: Transmembrane protein, putative

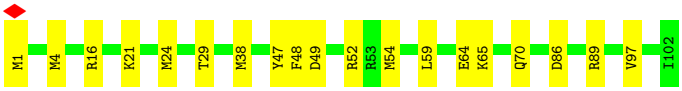
Chain BM:





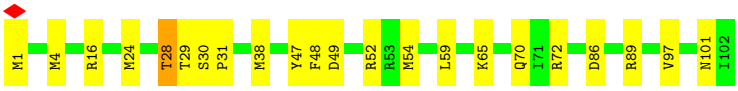
• Molecule 94: Complex I-MNLL

Chain c4:



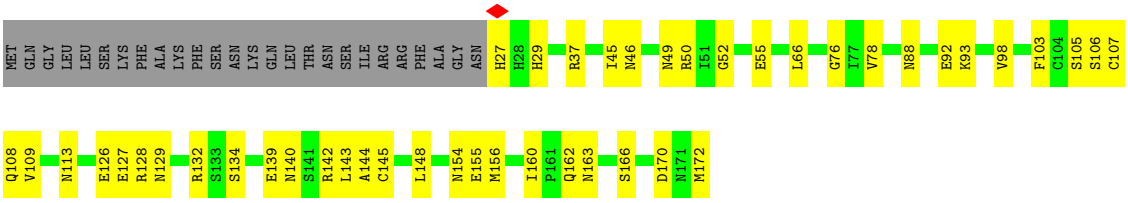
• Molecule 94: Complex I-MNLL

Chain C4:



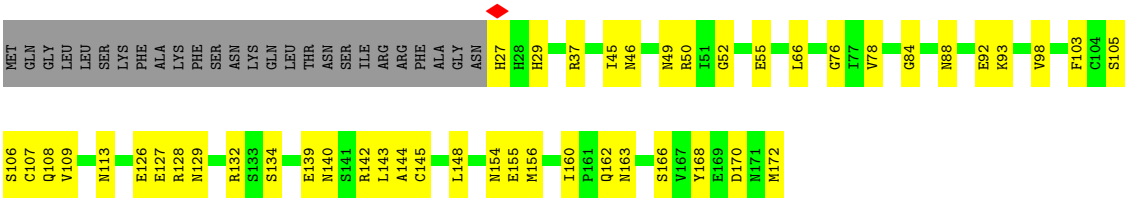
• Molecule 95: 2 iron, 2 sulfur cluster-binding protein

Chain fx:



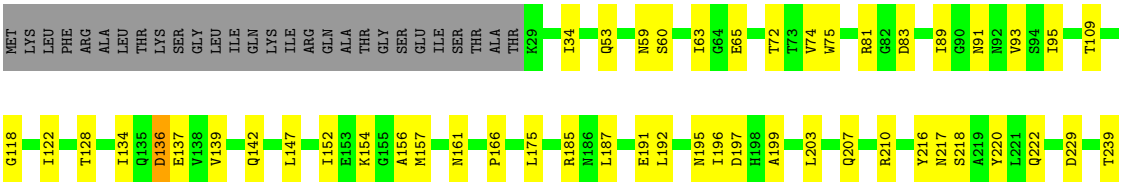
• Molecule 95: 2 iron, 2 sulfur cluster-binding protein

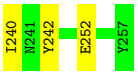
Chain FX:



• Molecule 96: Gamma-carbonic anhydrase

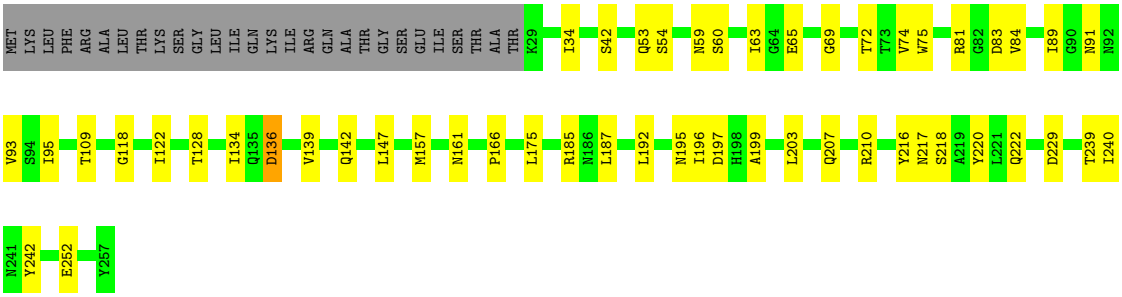
Chain g1:





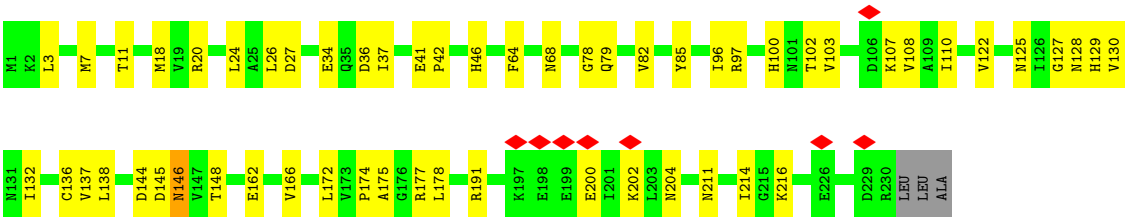
• Molecule 96: Gamma-carbonic anhydrase

Chain G1:



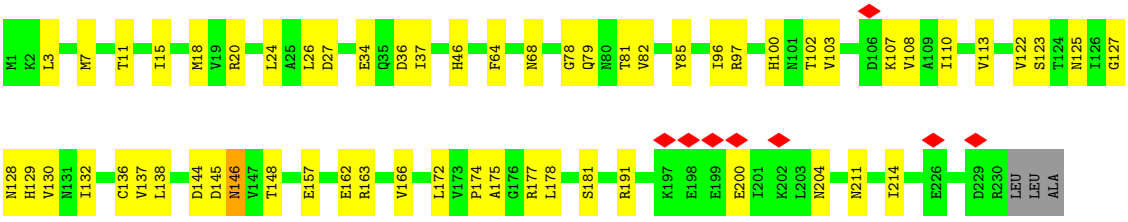
• Molecule 97: Gamma-carbonic anhydrase

Chain g2:



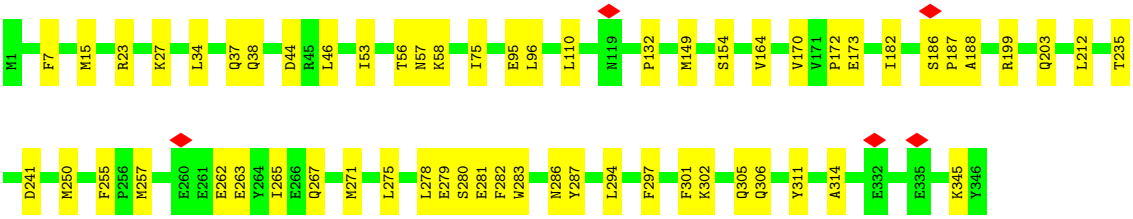
• Molecule 97: Gamma-carbonic anhydrase

Chain G2:



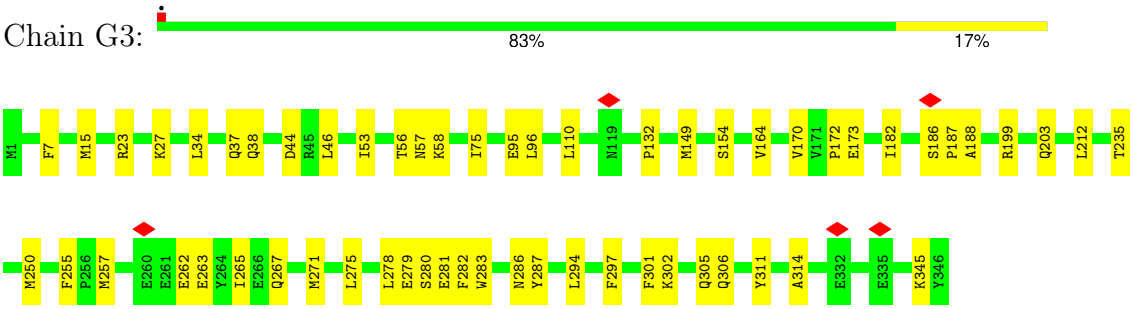
• Molecule 98: Transcription factor apfi protein, putative

Chain g3:



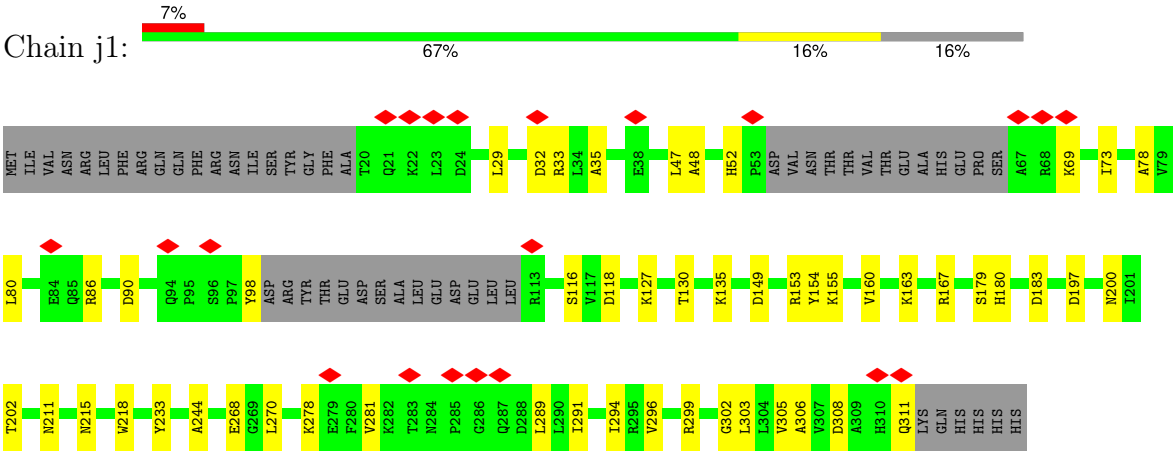
• Molecule 98: Transcription factor apfi protein, putative

Chain G3:



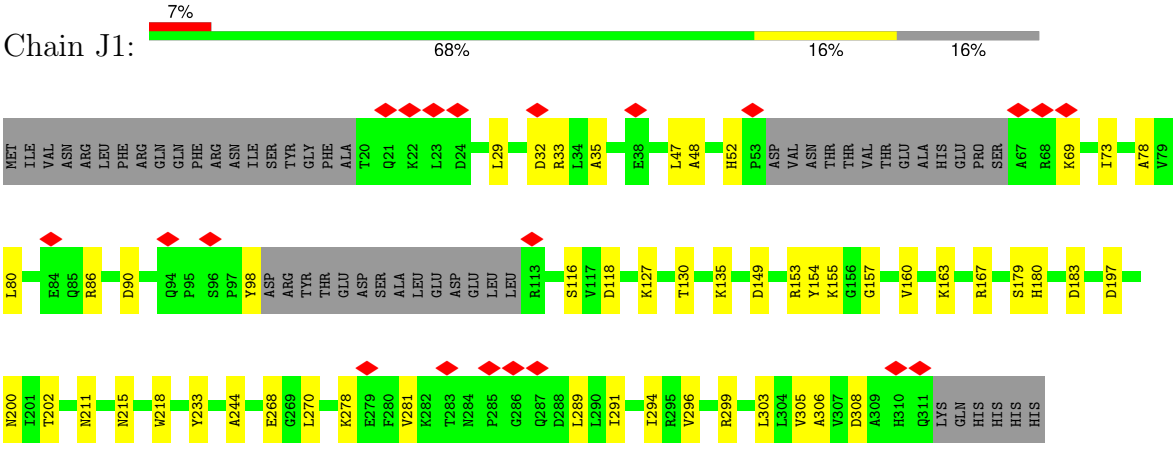
• Molecule 99: DnaJ domain protein

Chain j1:



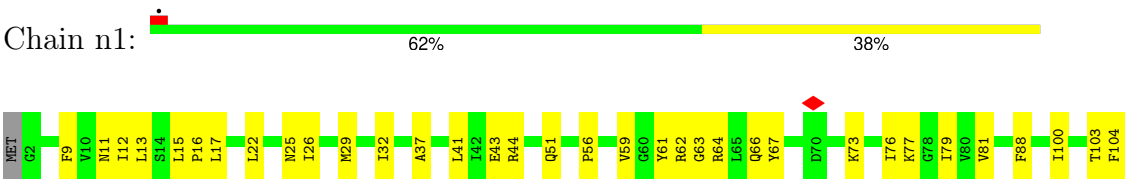
• Molecule 99: DnaJ domain protein

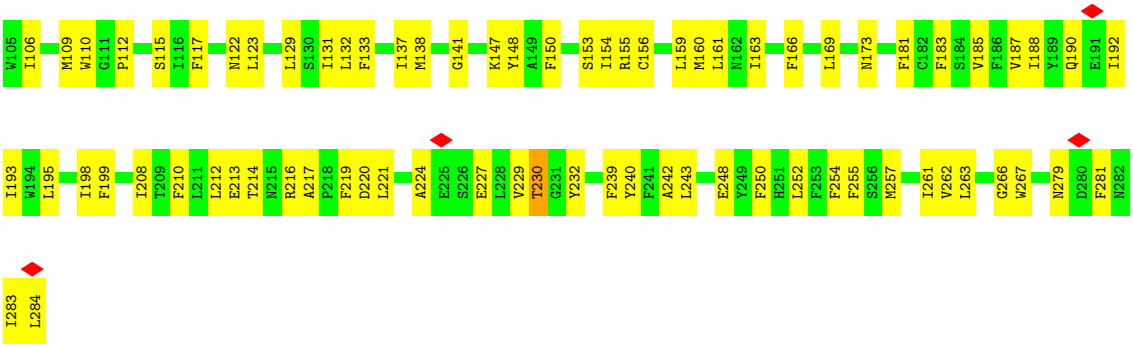
Chain J1:



• Molecule 100: NADH-ubiquinone oxidoreductase chain 1

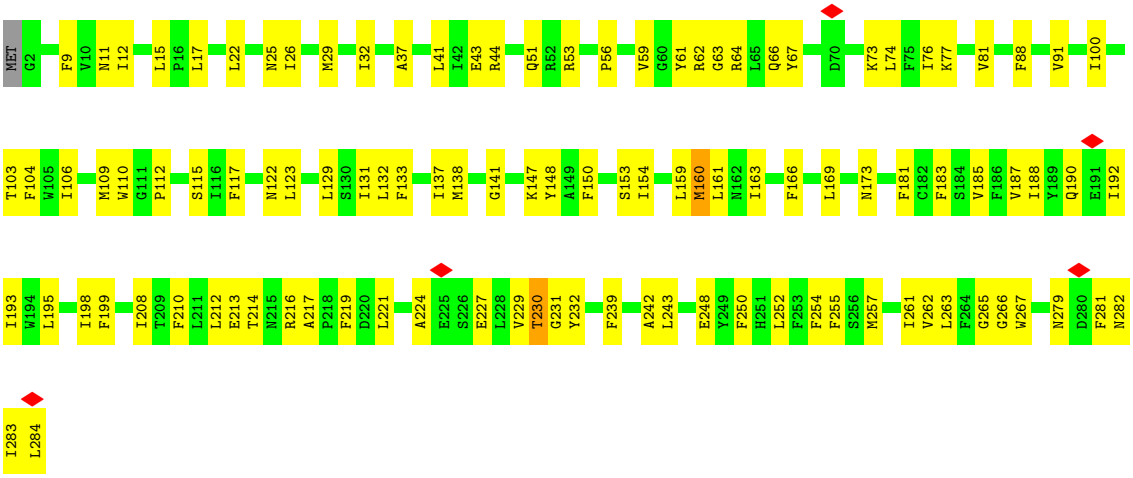
Chain n1:





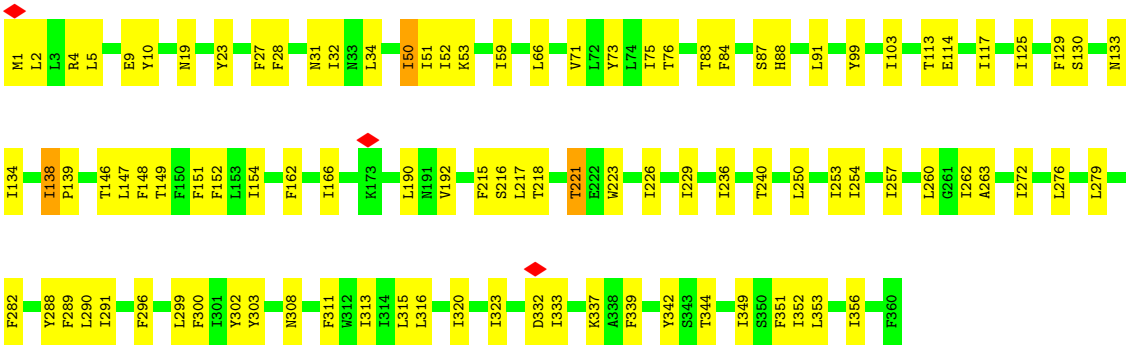
• Molecule 100: NADH-ubiquinone oxidoreductase chain 1

Chain N1:



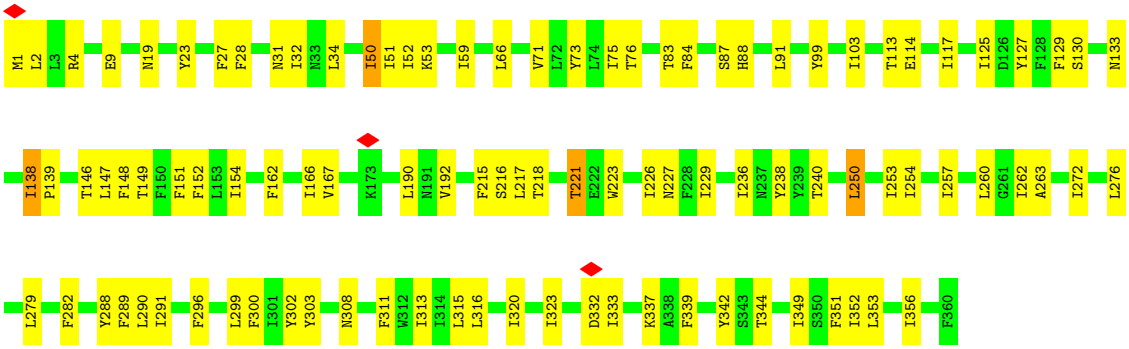
• Molecule 101: Ymf65

Chain n2:



• Molecule 101: Ymf65

Chain N2:

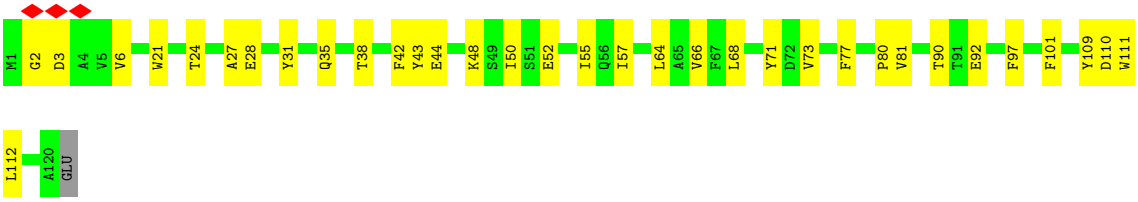


• Molecule 102: NADH-ubiquinone oxidoreductase chain 3

Chain n3:

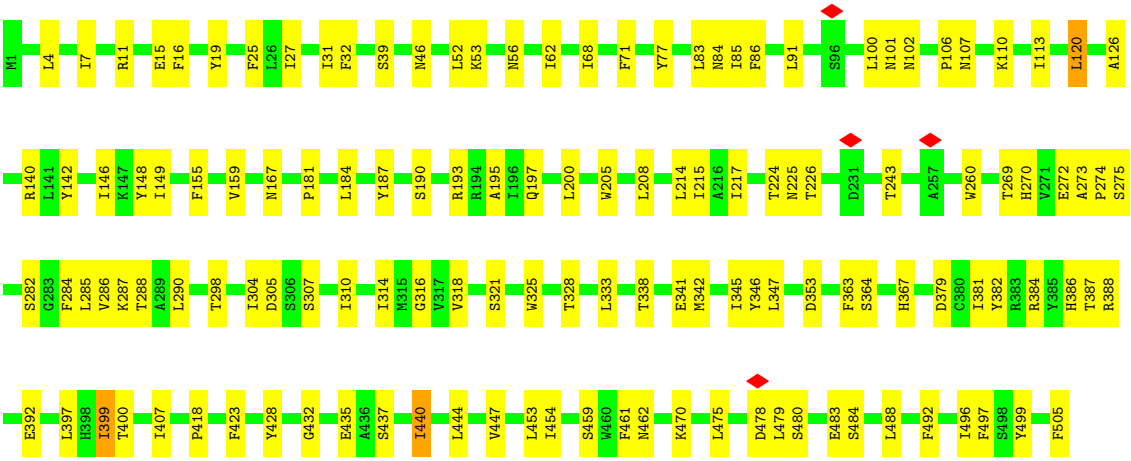
• Molecule 102: NADH-ubiquinone oxidoreductase chain 3

Chain N3:



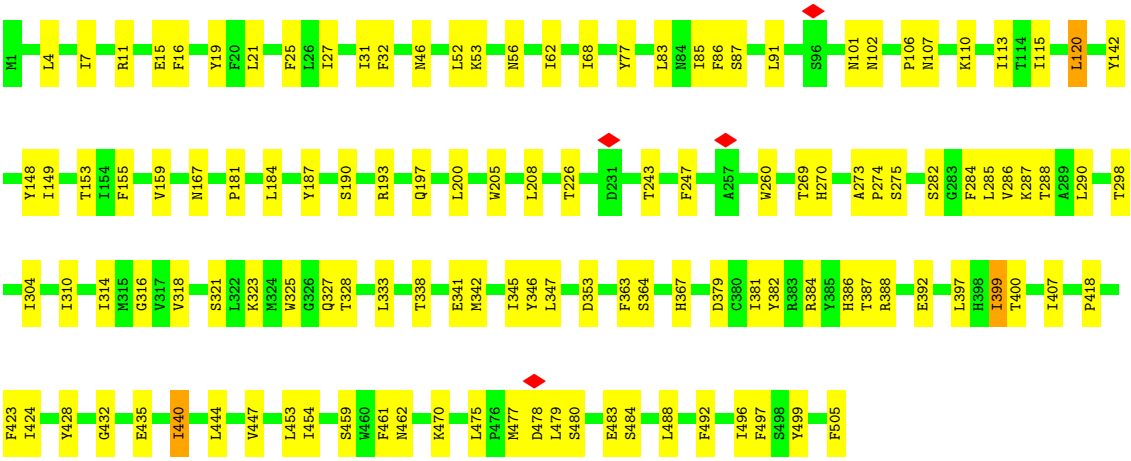
• Molecule 103: NADH-ubiquinone oxidoreductase chain 4

Chain n4:



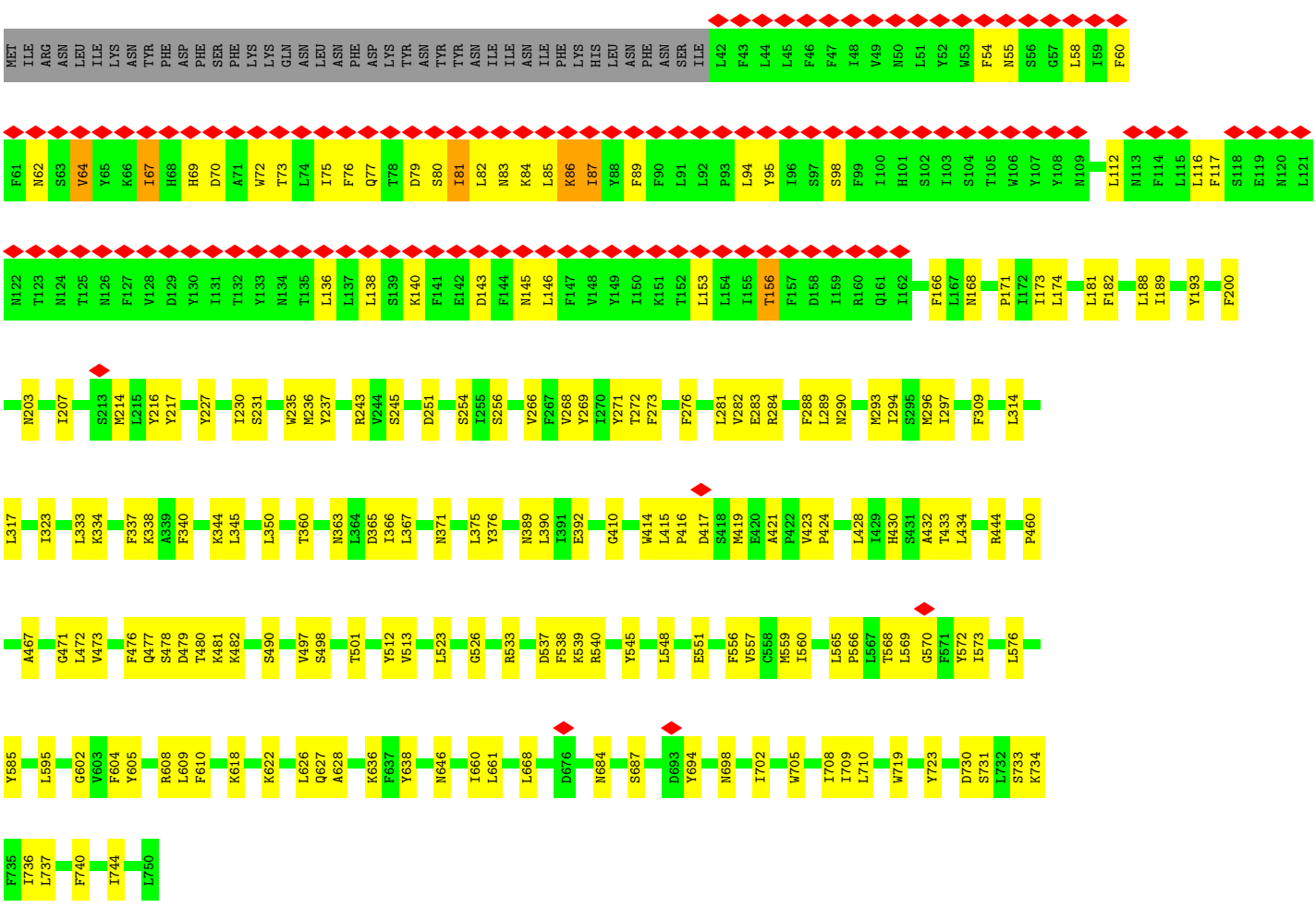
• Molecule 103: NADH-ubiquinone oxidoreductase chain 4

Chain N4:



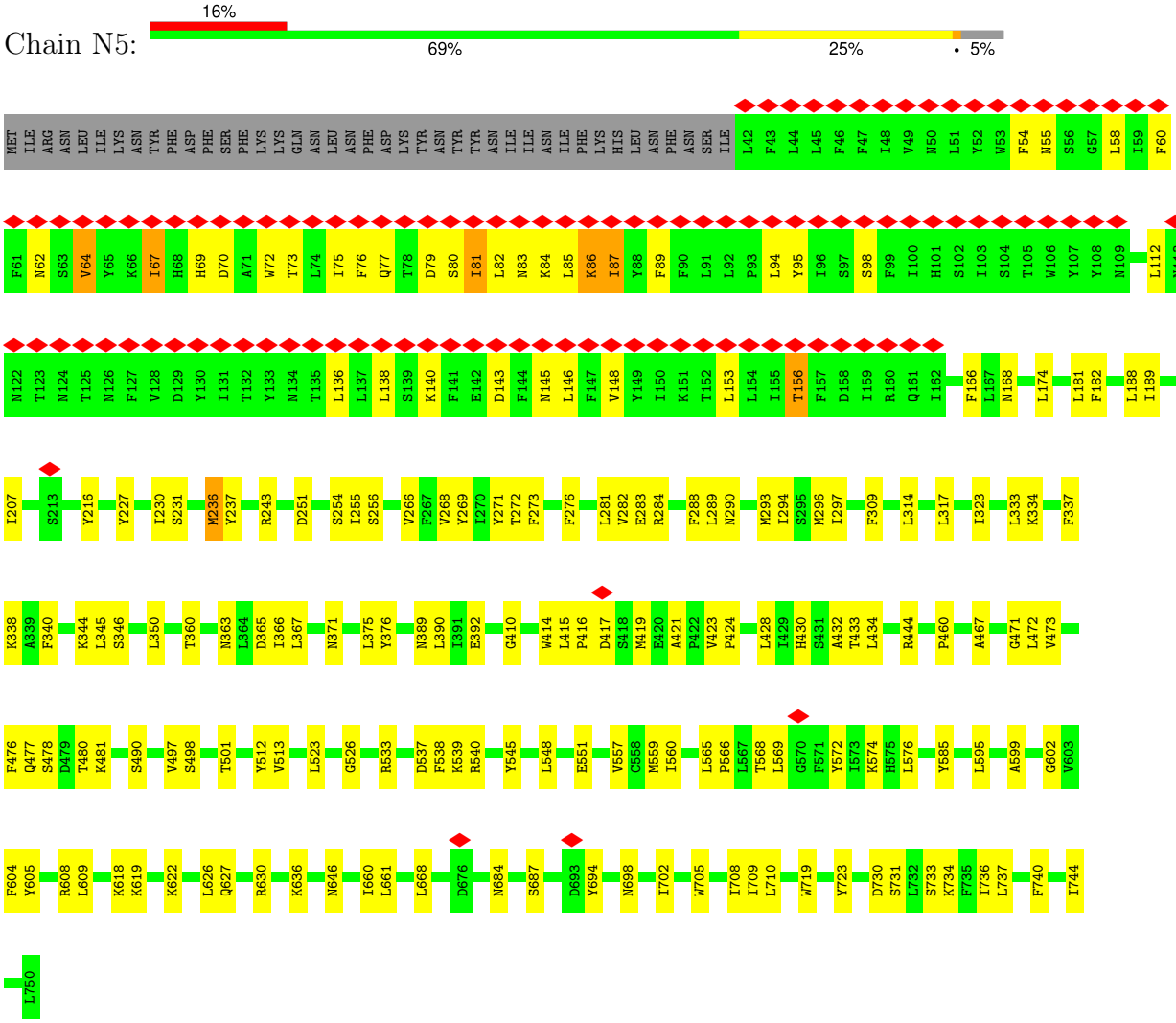
• Molecule 104: NADH dehydrogenase subunit 5

Chain n5:



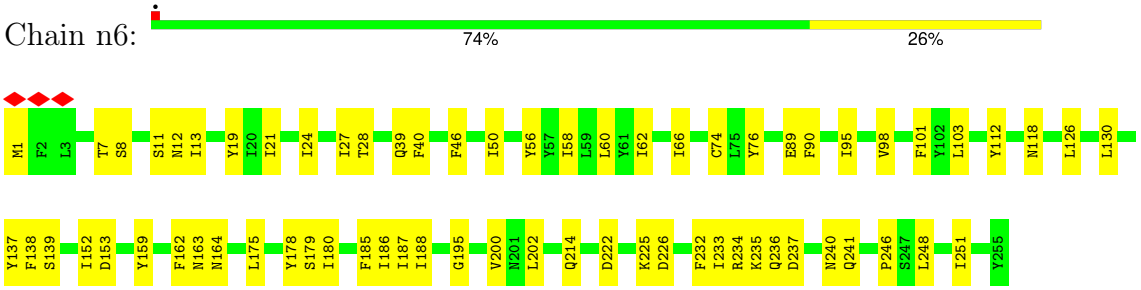
• Molecule 104: NADH dehydrogenase subunit 5

Chain N5:



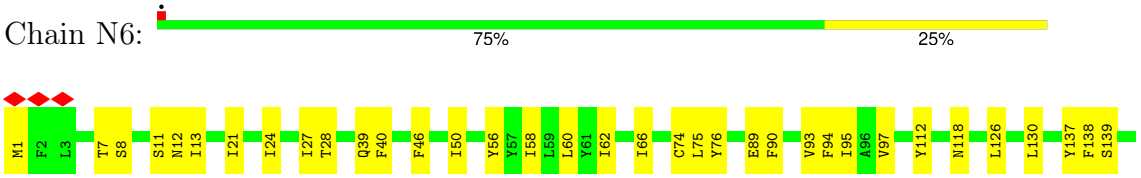
• Molecule 105: Ymf62

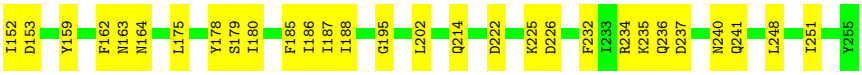
Chain n6:



• Molecule 105: Ymf62

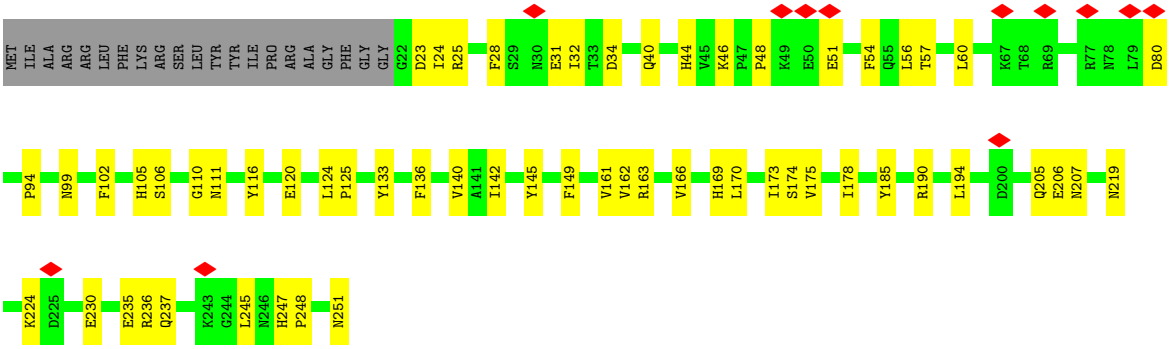
Chain N6:





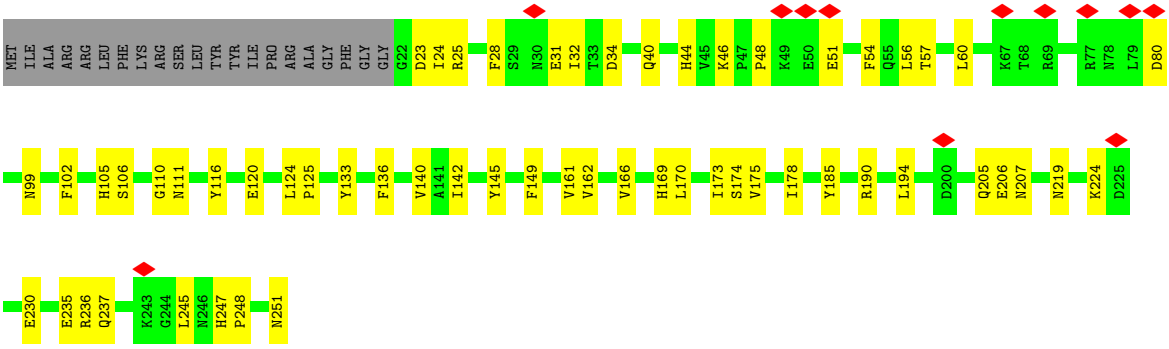
• Molecule 106: Transmembrane protein, putative

Chain p1:



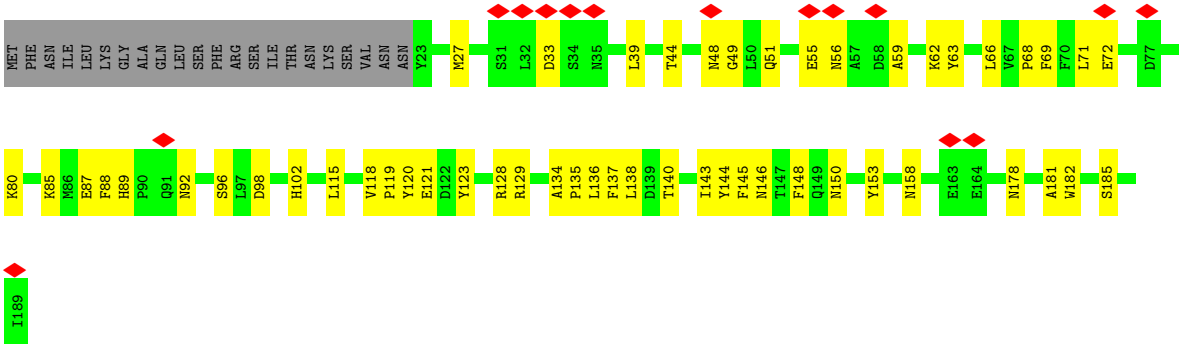
• Molecule 106: Transmembrane protein, putative

Chain P1:



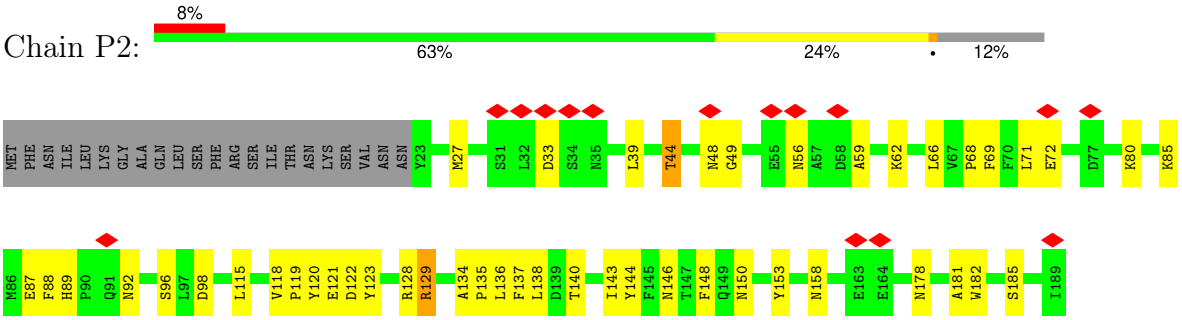
• Molecule 107: NDUPH2

Chain p2:



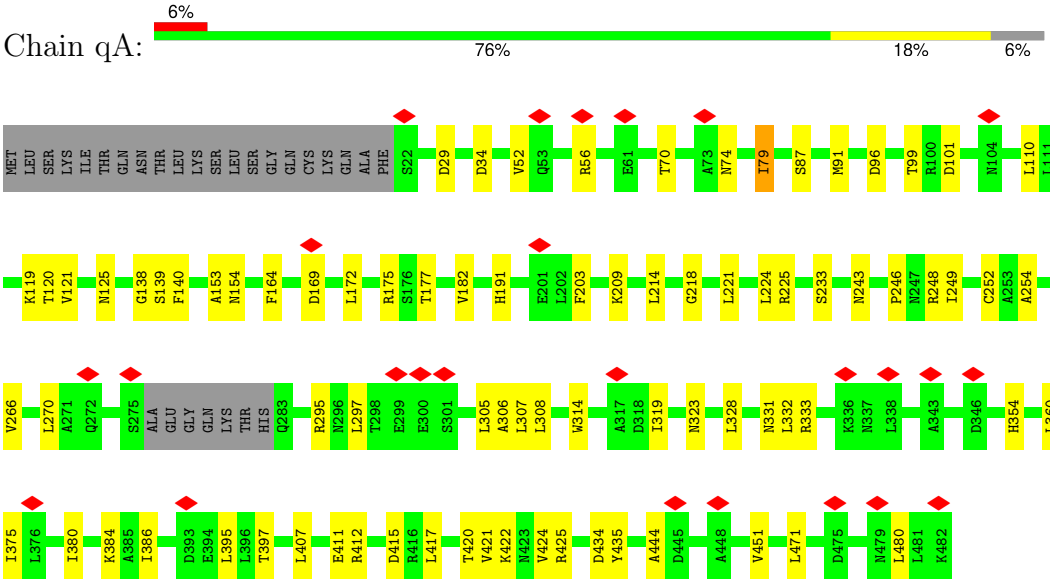
• Molecule 107: NDUPH2

Chain P2:



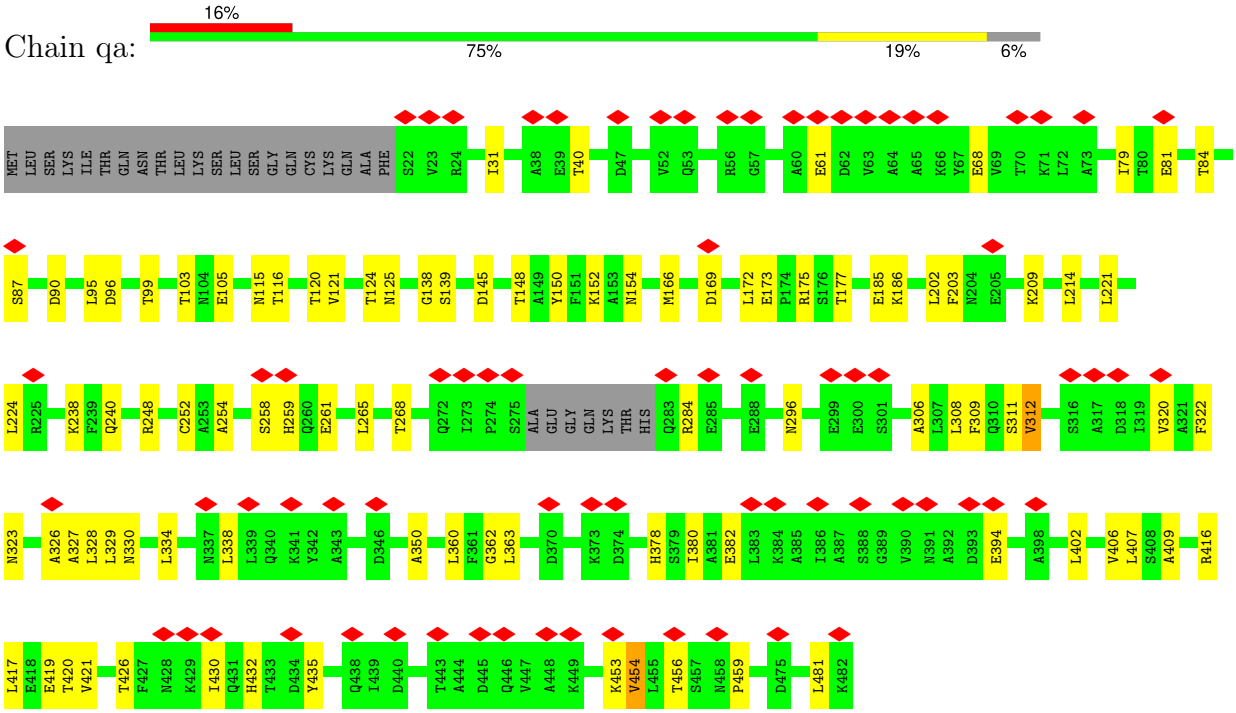
• Molecule 108: M16 family peptidase, putative

Chain qA:



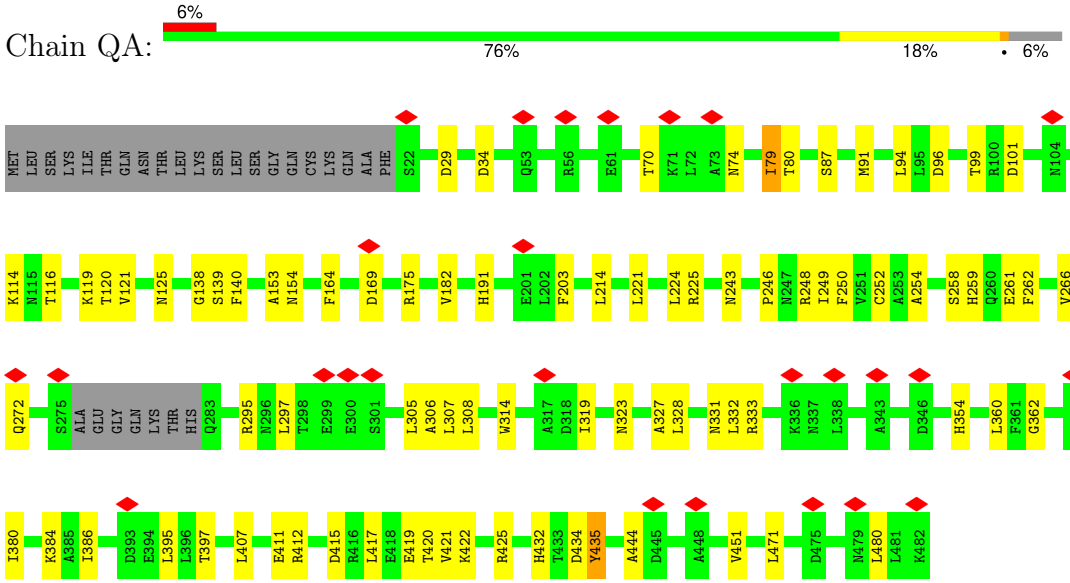
• Molecule 108: M16 family peptidase, putative

Chain qa:



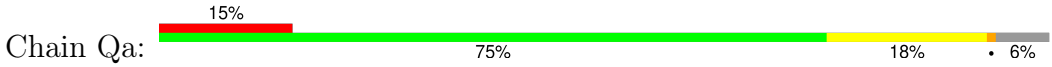
• Molecule 108: M16 family peptidase, putative

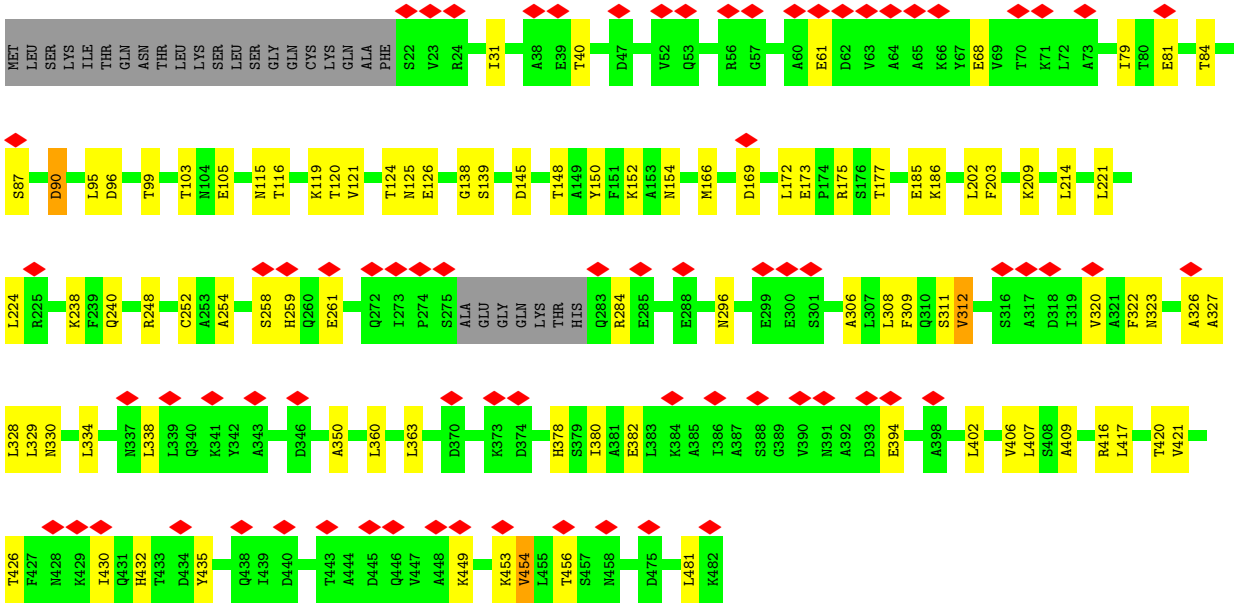
Chain QA:



• Molecule 108: M16 family peptidase, putative

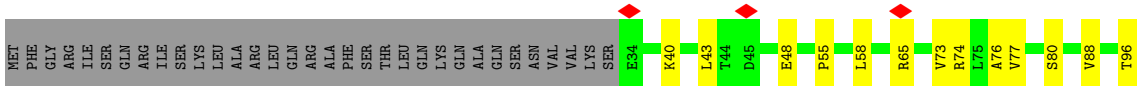
Chain Qa:

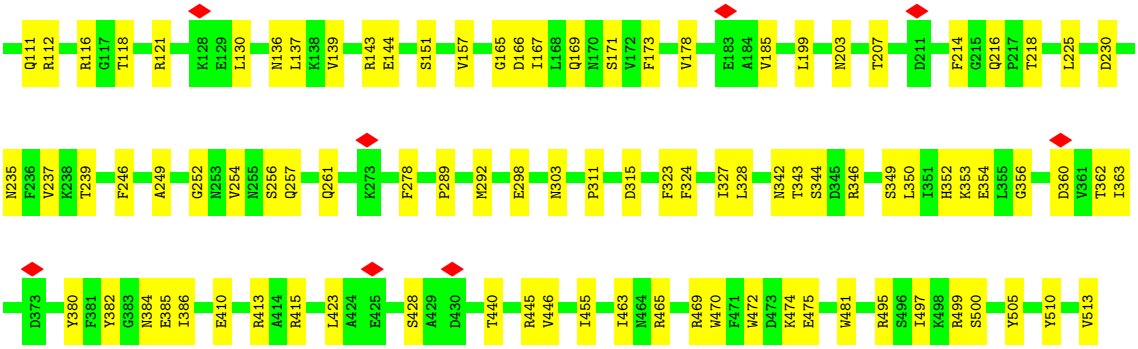




• Molecule 109: Peptidase M16 inactive domain protein

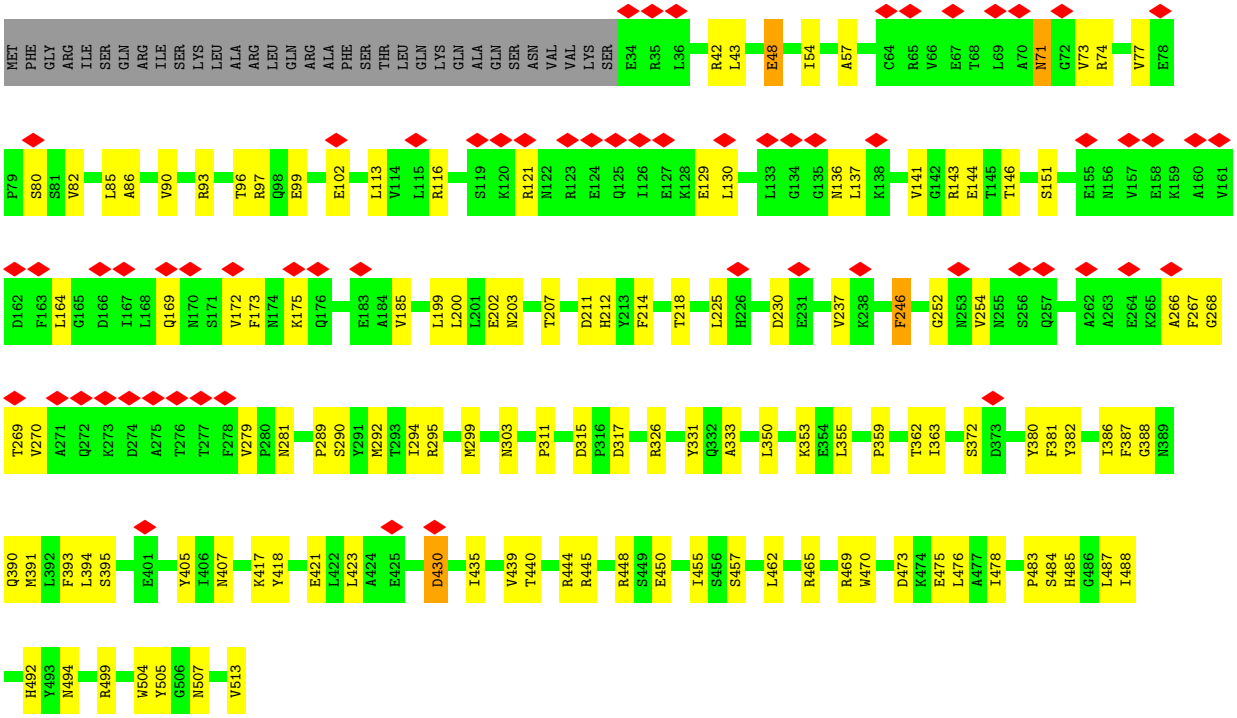
Chain qB:





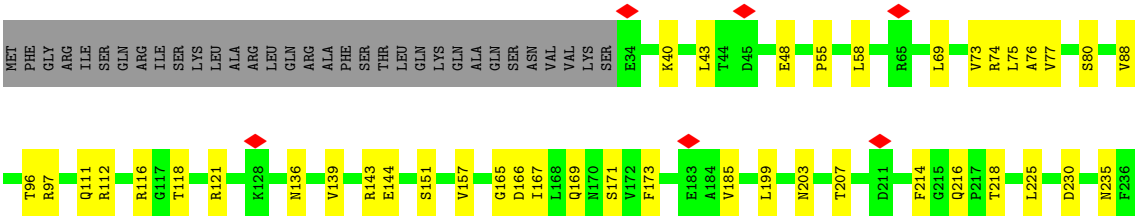
• Molecule 109: Peptidase M16 inactive domain protein

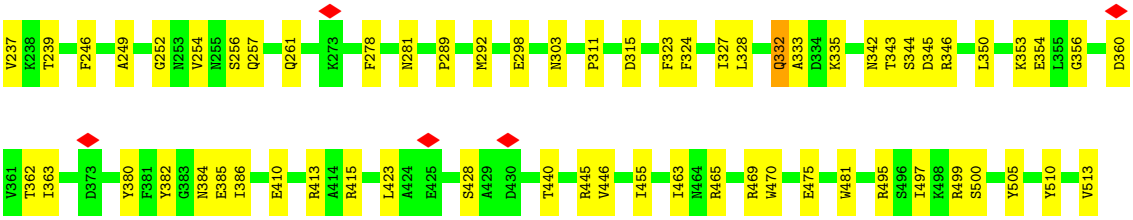
Chain qb:



• Molecule 109: Peptidase M16 inactive domain protein

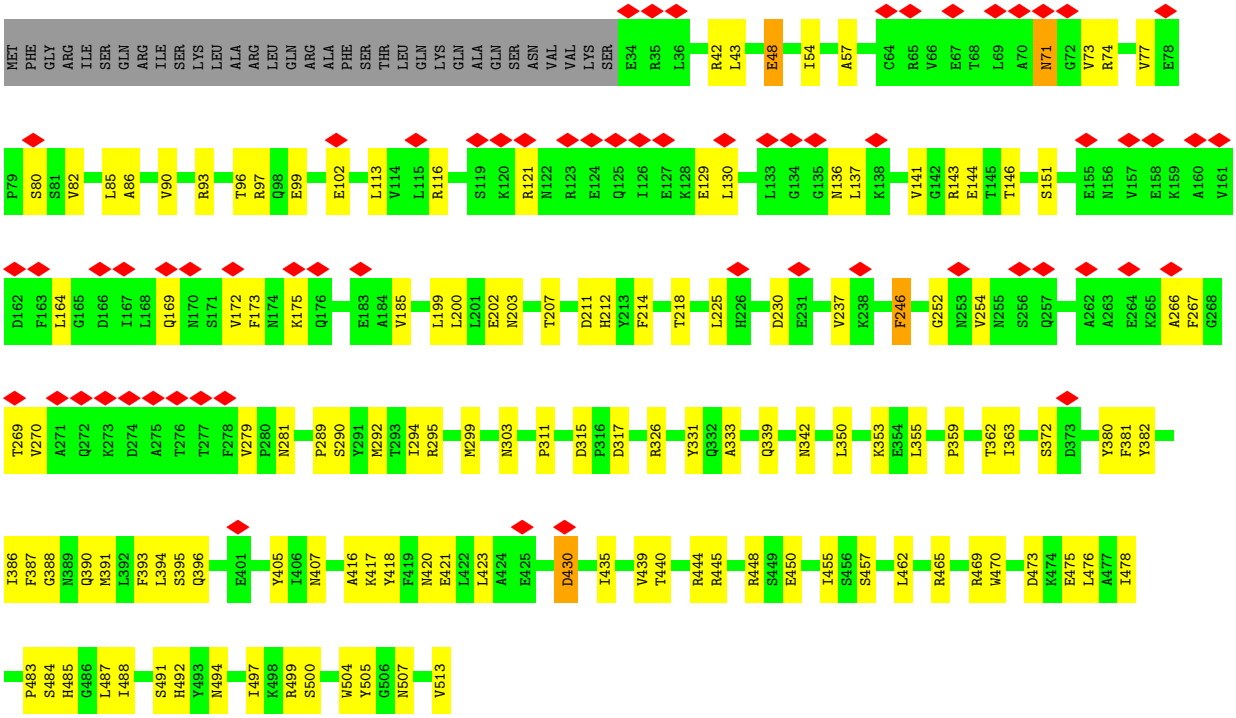
Chain QB:





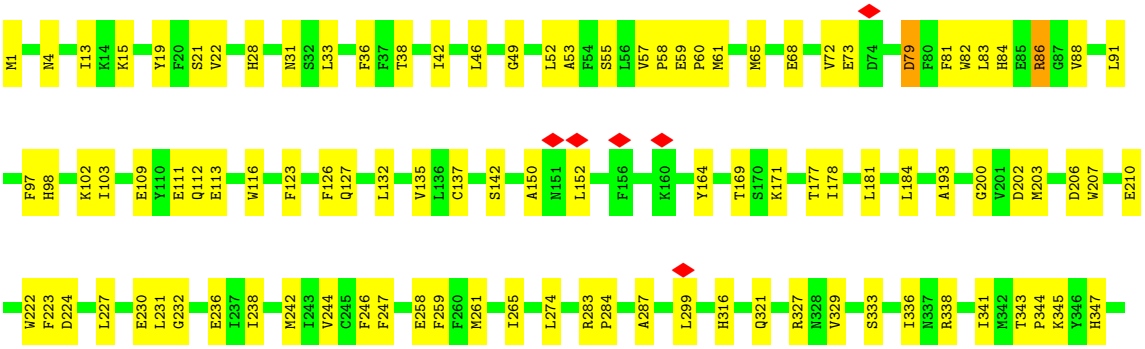
• Molecule 109: Peptidase M16 inactive domain protein

Chain Qb:



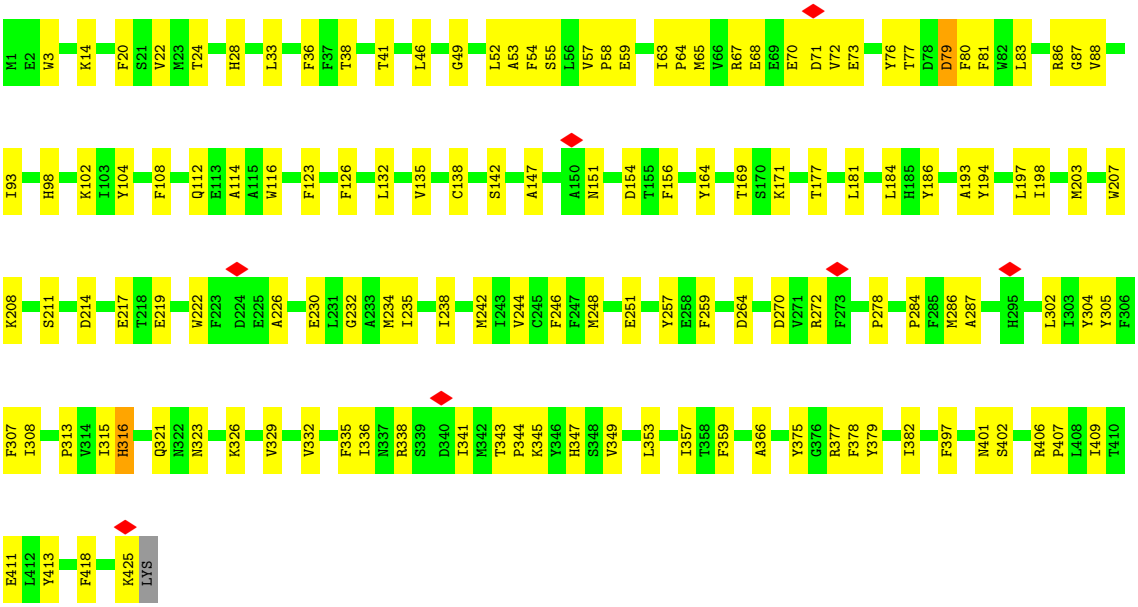
• Molecule 110: Apocytochrome b

Chain qC:



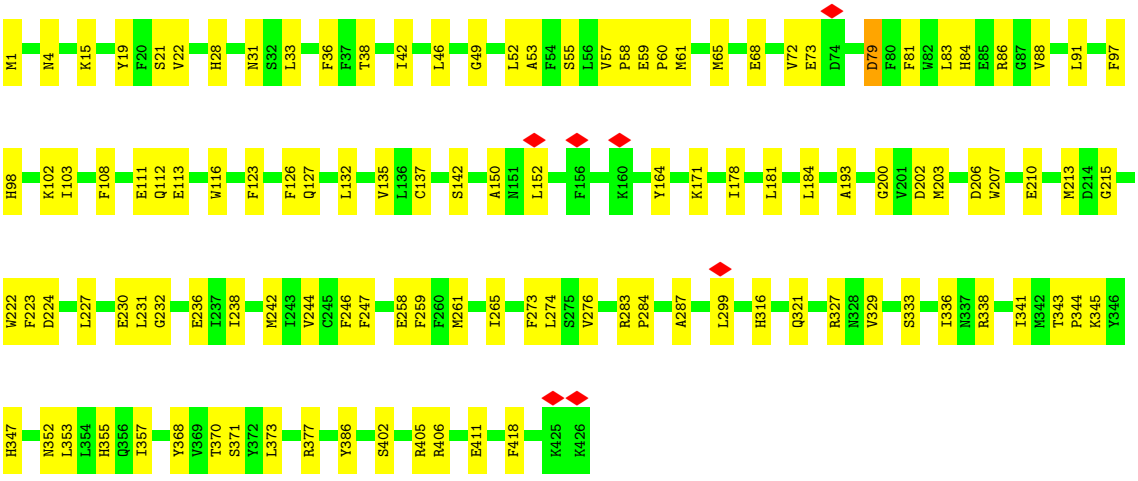
• Molecule 110: Apocytochrome b

Chain qc:



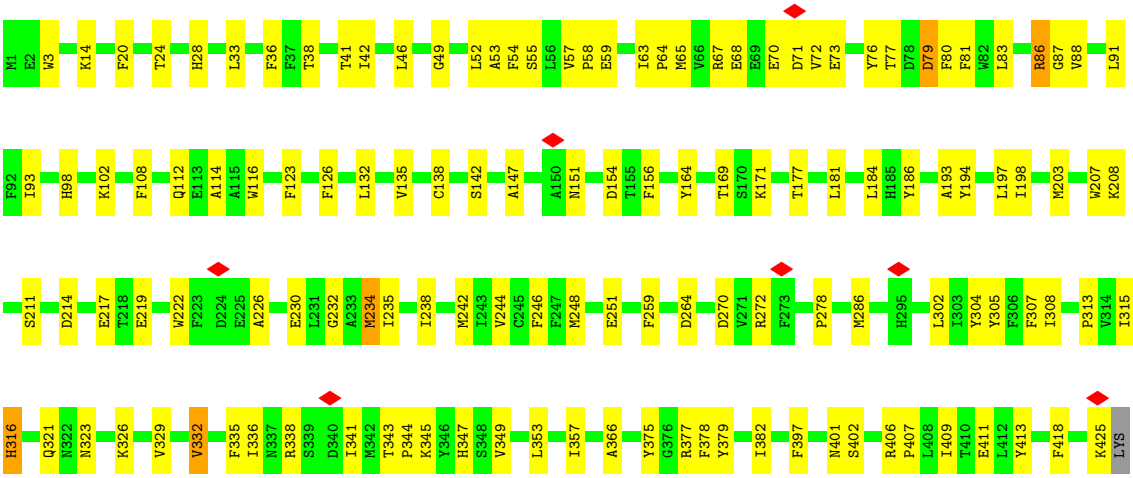
• Molecule 110: Apocytochrome b

Chain QC:



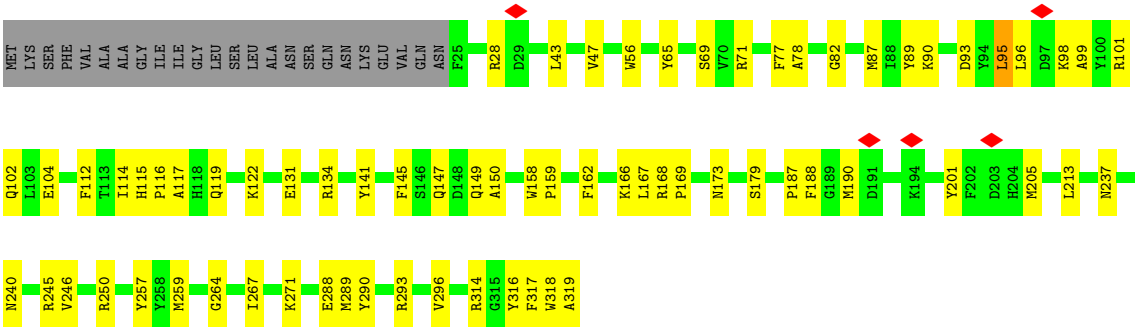
• Molecule 110: Apocytochrome b

Chain Qc:



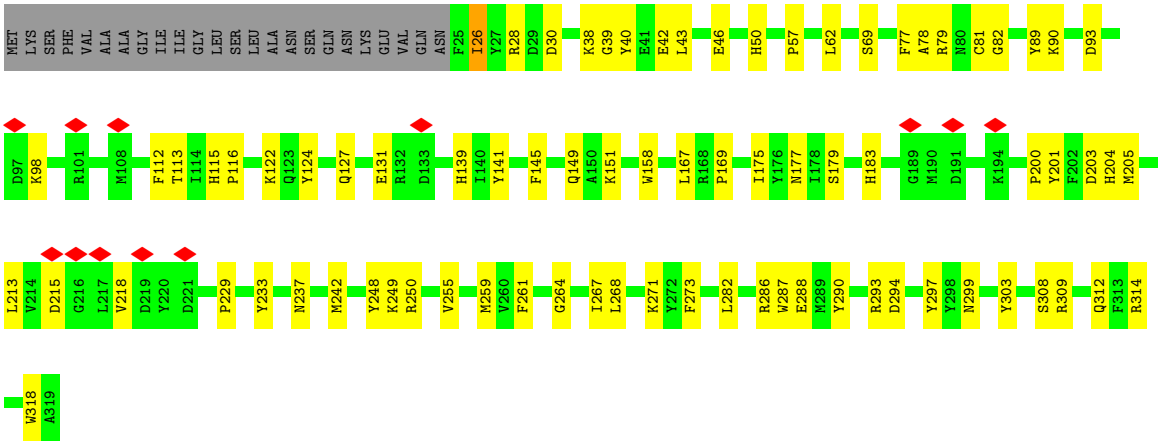
• Molecule 111: Cytochrome protein c1

Chain qD:



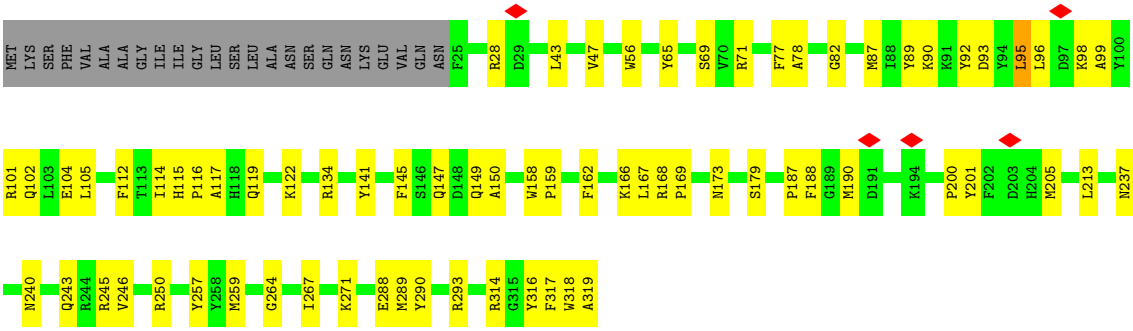
• Molecule 111: Cytochrome protein c1

Chain qd:



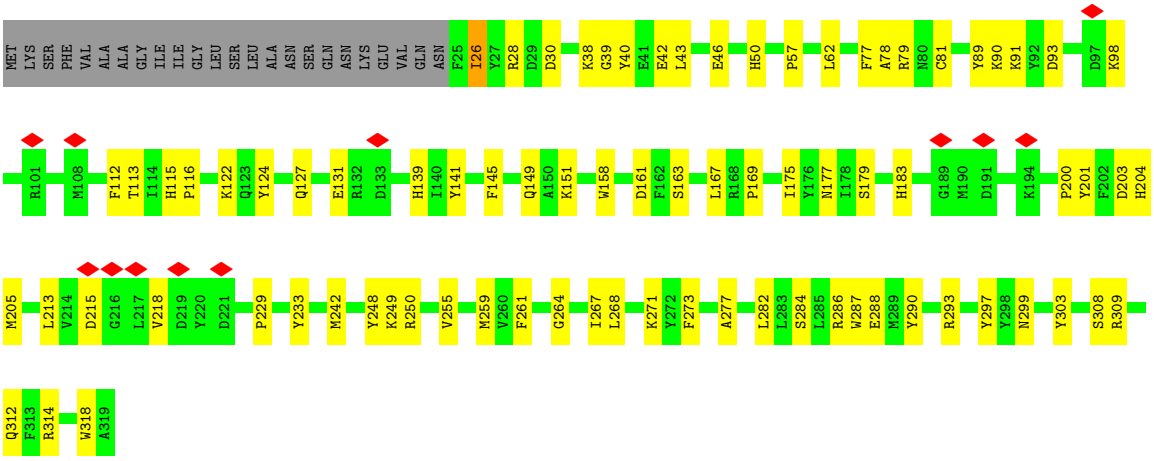
• Molecule 111: Cytochrome protein c1

Chain QD:



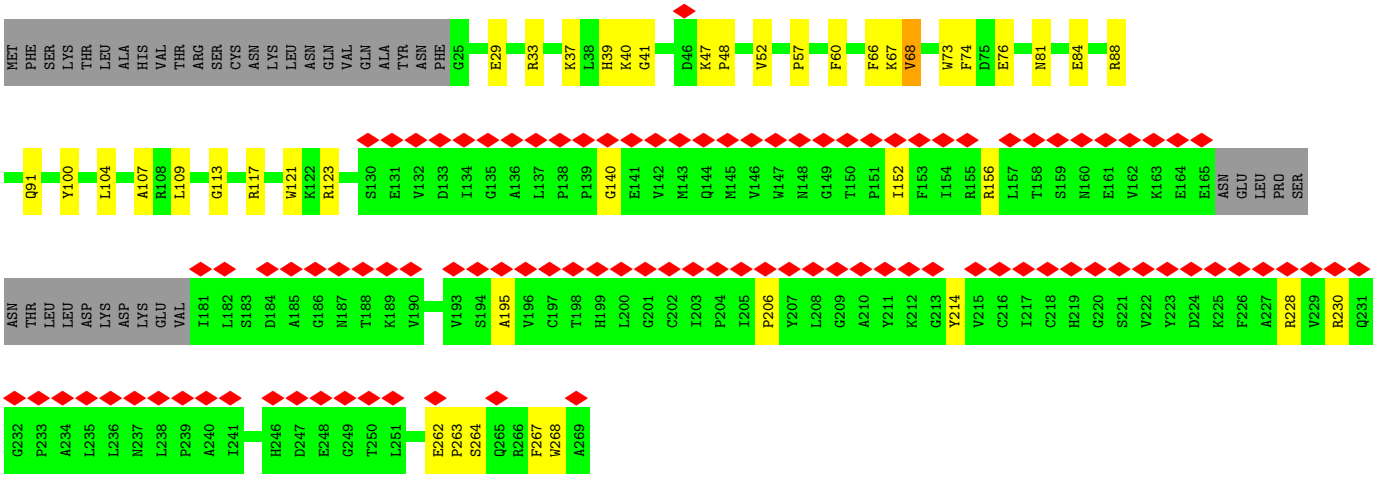
• Molecule 111: Cytochrome protein c1

Chain Qd:



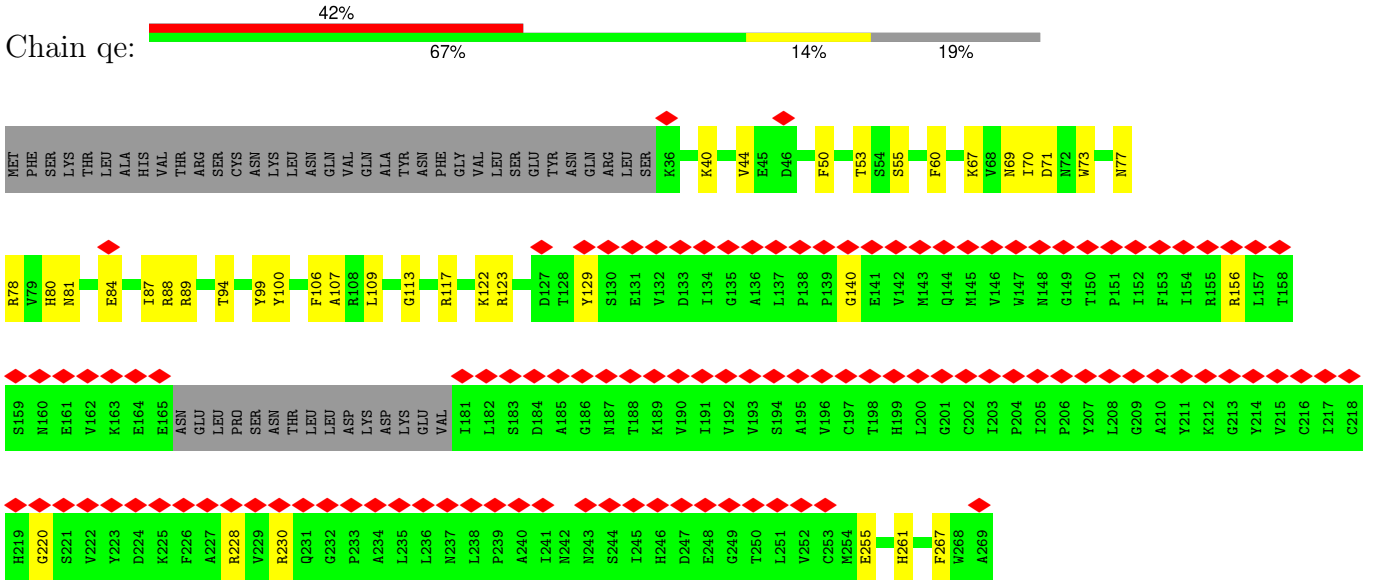
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain qE:



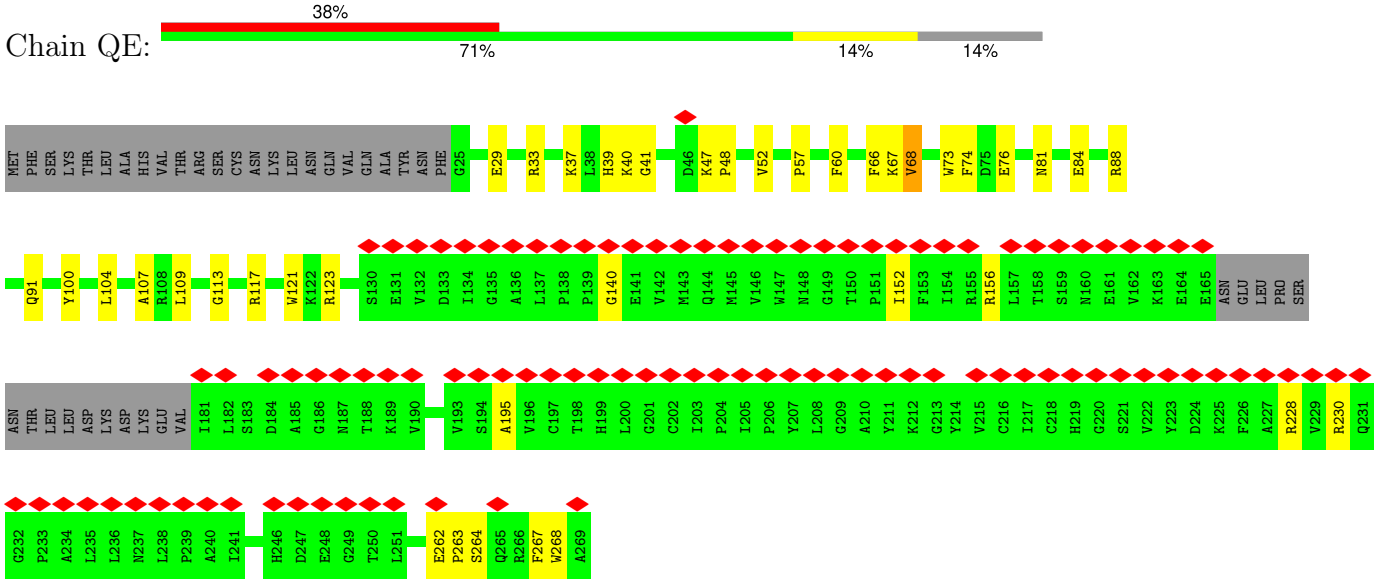
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain qe:



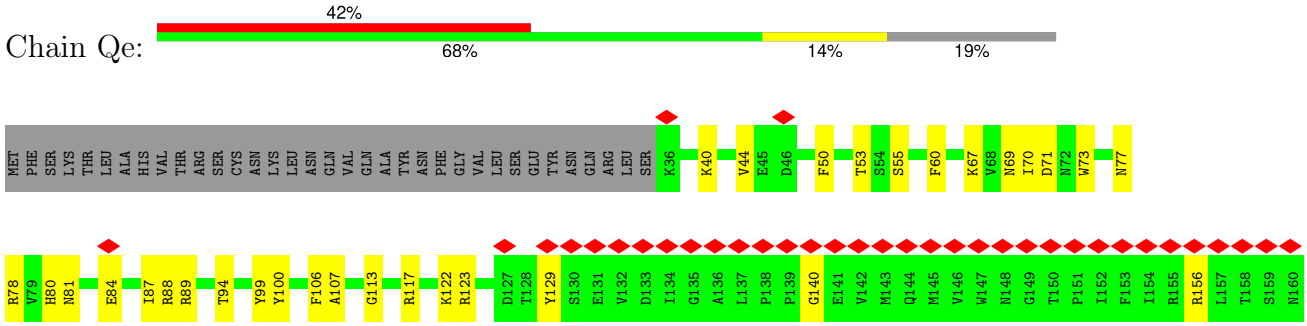
• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

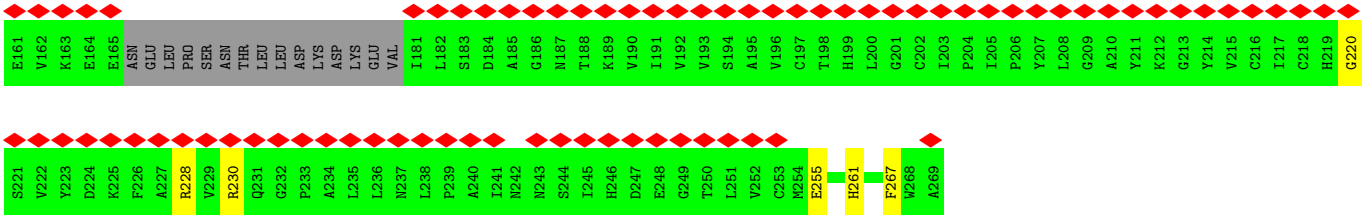
Chain QE:



• Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

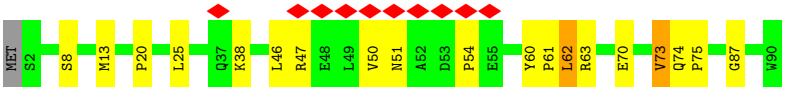
Chain Qe:





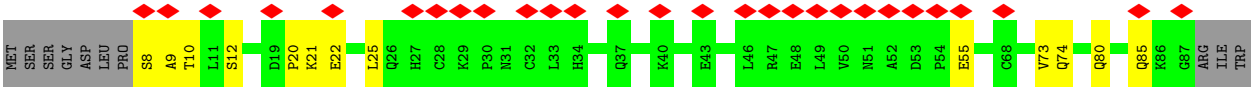
• Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain qF:



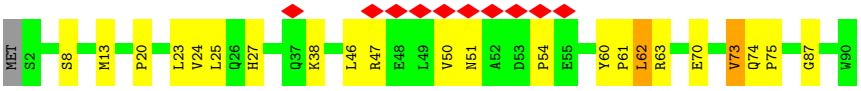
• Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain qf:



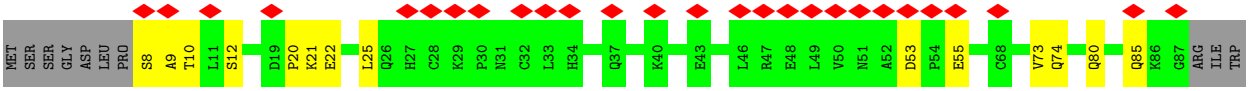
• Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain QF:



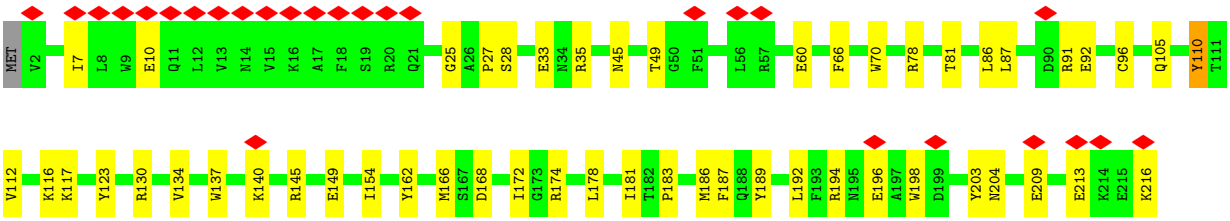
• Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

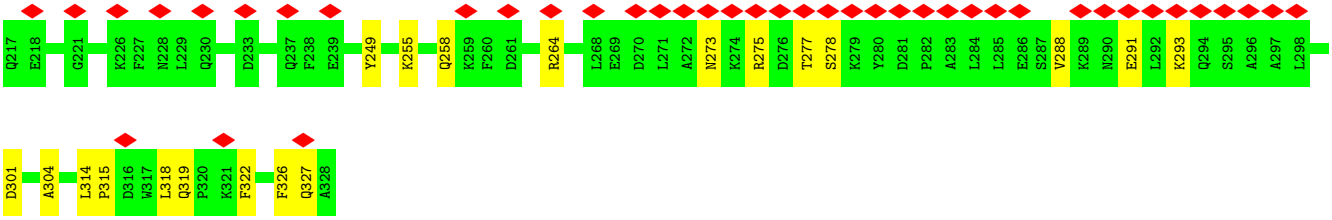
Chain Qf:



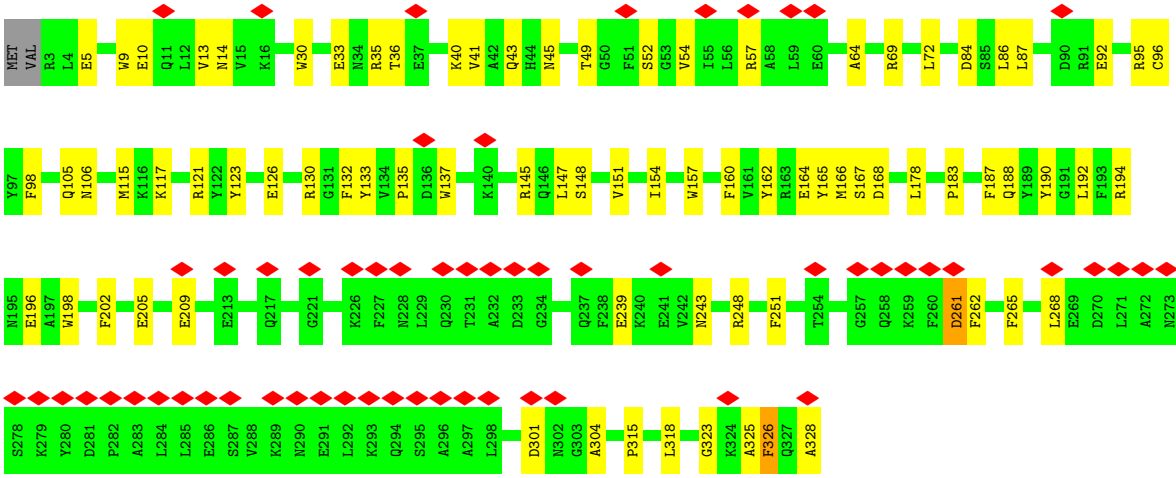
• Molecule 114: Sulphotransf domain-containing protein

Chain qG:

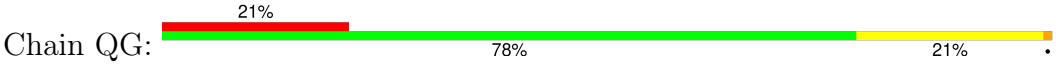


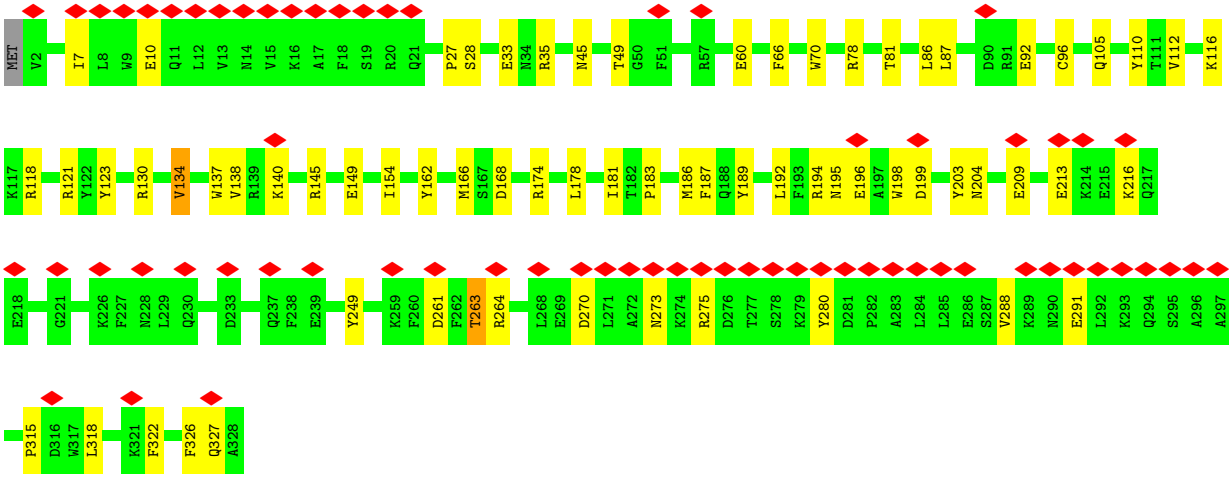


• Molecule 114: Sulphotransf domain-containing protein

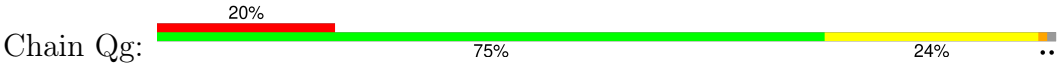


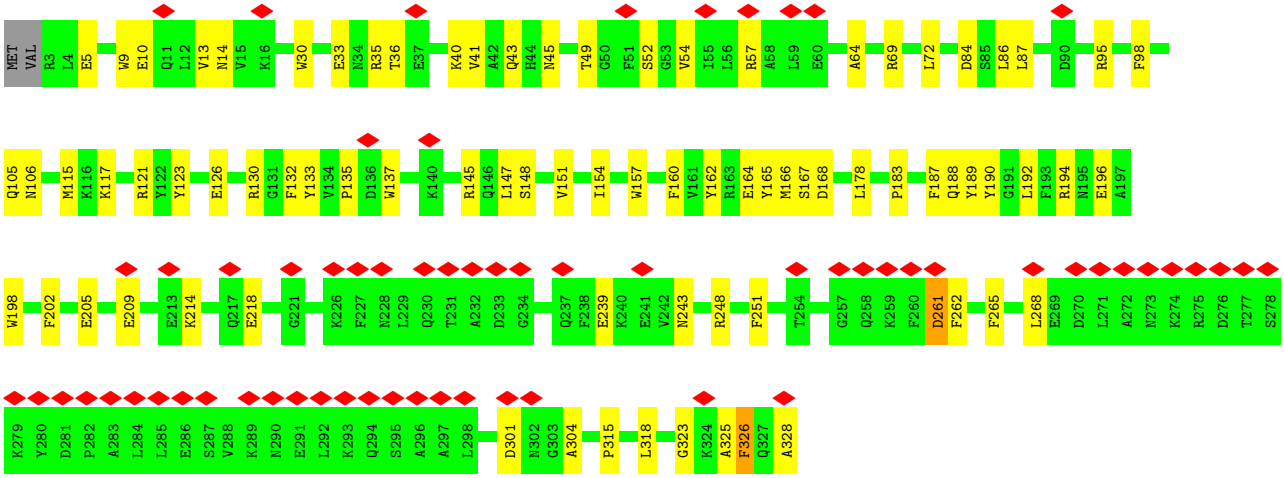
• Molecule 114: Sulphotransf domain-containing protein





• Molecule 114: Sulphotransf domain-containing protein



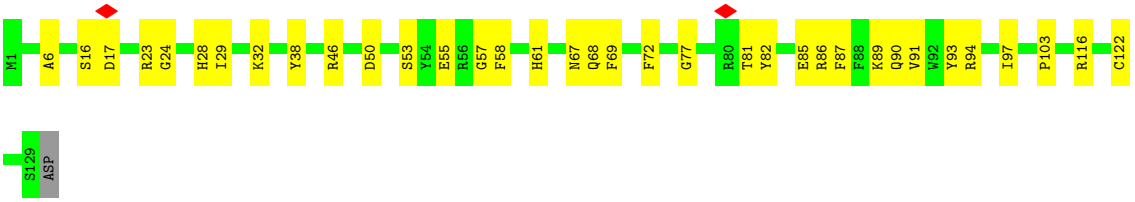


• Molecule 115: Transmembrane protein, putative

Chain qH:

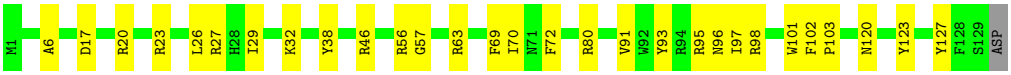
• Molecule 115: Transmembrane protein, putative

Chain qh:



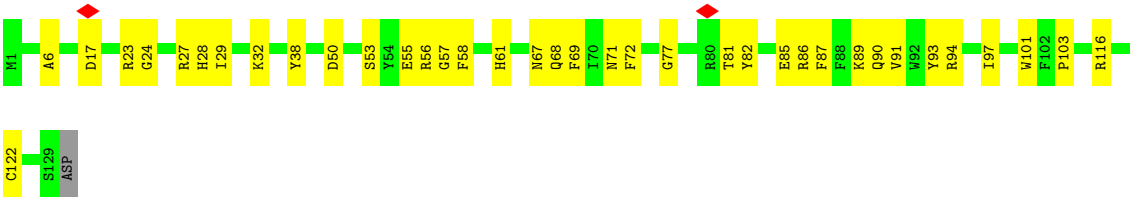
• Molecule 115: Transmembrane protein, putative

Chain QH:



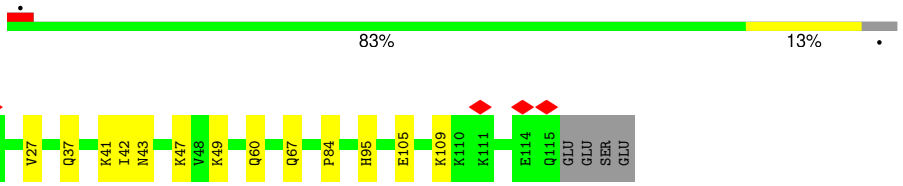
• Molecule 115: Transmembrane protein, putative

Chain Qh:



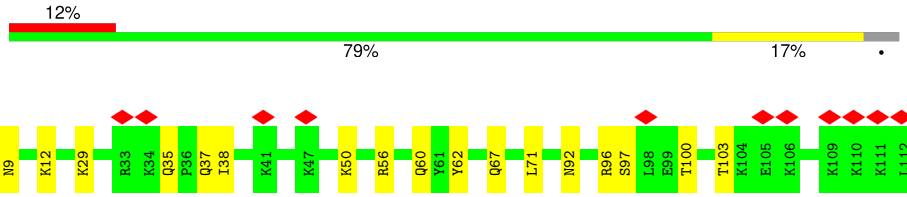
• Molecule 116: Transmembrane protein, putative

Chain qI:



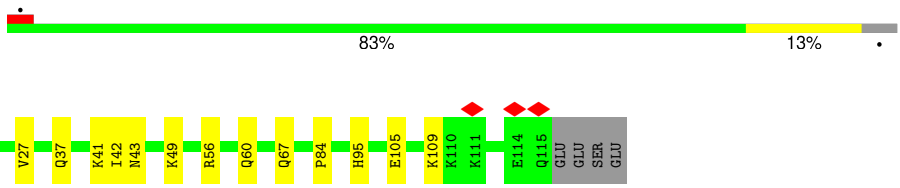
• Molecule 116: Transmembrane protein, putative

Chain qi:



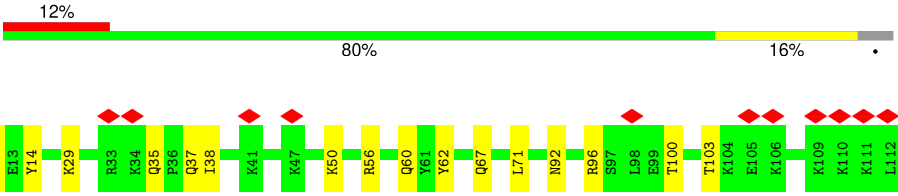
• Molecule 116: Transmembrane protein, putative

Chain QI:



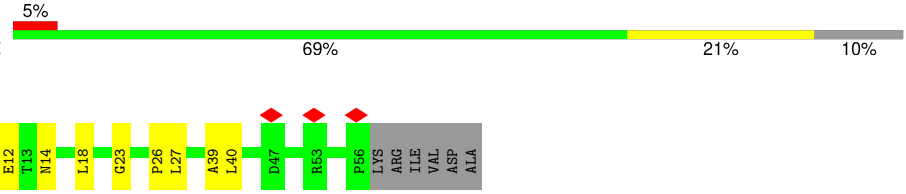
• Molecule 116: Transmembrane protein, putative

Chain Qi:



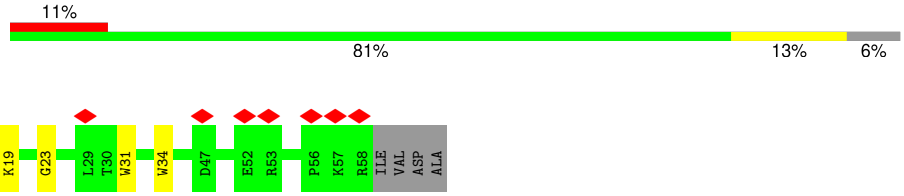
• Molecule 117: Transmembrane protein, putative

Chain qJ:



• Molecule 117: Transmembrane protein, putative

Chain qj:

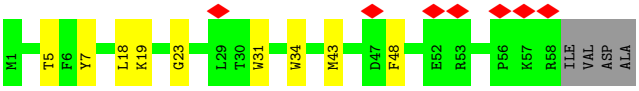


• Molecule 117: Transmembrane protein, putative

Chain QJ:

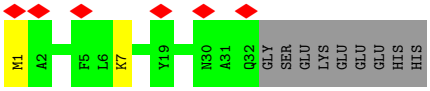
• Molecule 117: Transmembrane protein, putative

Chain Qj:



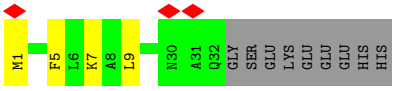
• Molecule 118: UQCRTT2

Chain qL:



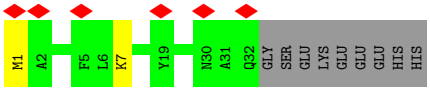
• Molecule 118: UQCRTT2

Chain ql:



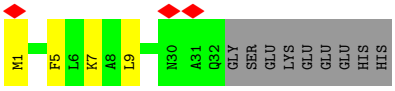
• Molecule 118: UQCRTT2

Chain QL:



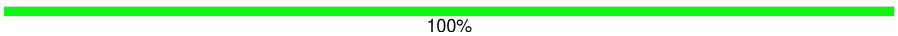
• Molecule 118: UQCRTT2

Chain Ql:



• Molecule 119: Unknown peptide

Chain qM:



There are no outlier residues recorded for this chain.

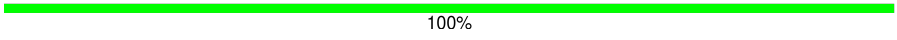
• Molecule 119: Unknown peptide

Chain qm:

There are no outlier residues recorded for this chain.

• Molecule 119: Unknown peptide

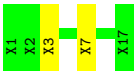
Chain Qm:



There are no outlier residues recorded for this chain.

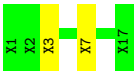
• Molecule 119: Unknown peptide

Chain u2:



• Molecule 119: Unknown peptide

Chain U2:



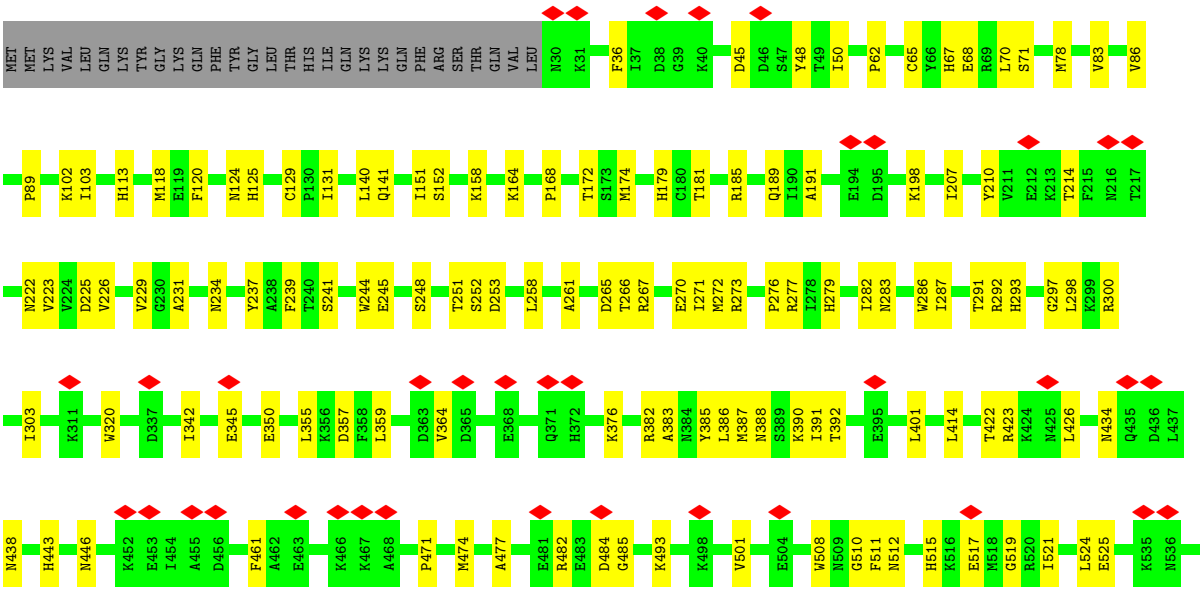
• Molecule 119: Unknown peptide

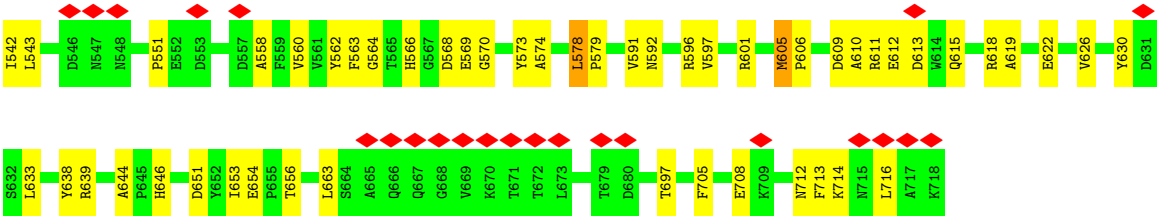
Chain QM:

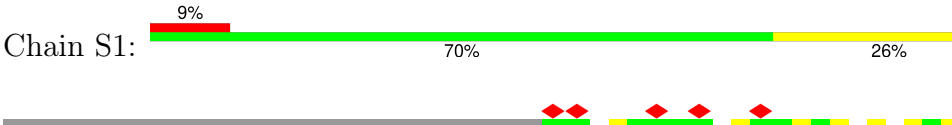
There are no outlier residues recorded for this chain.

• Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain s1:

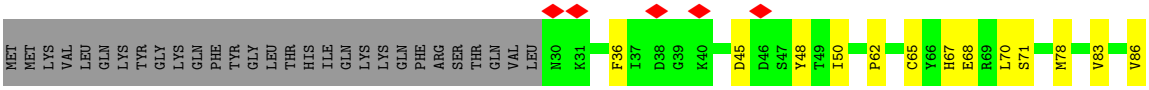


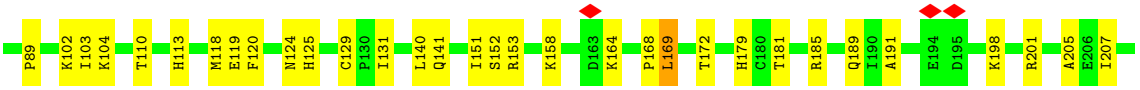


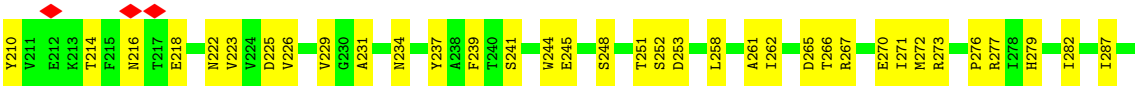


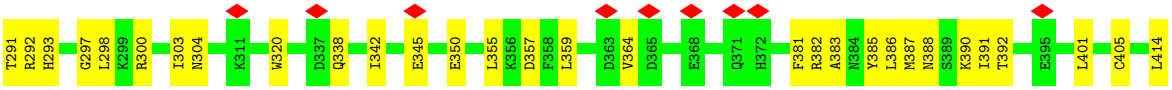
• Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

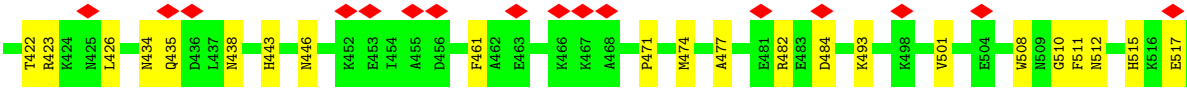
Chain S1:

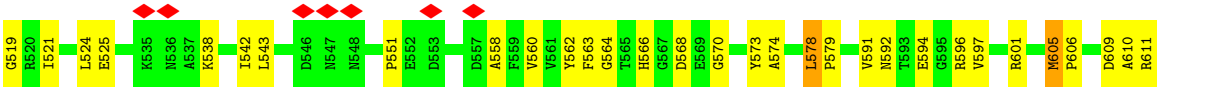


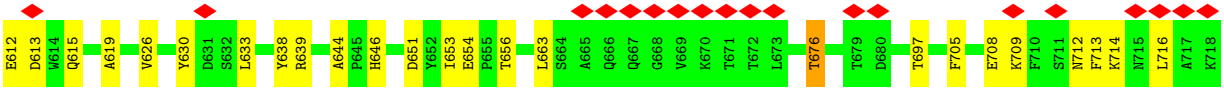


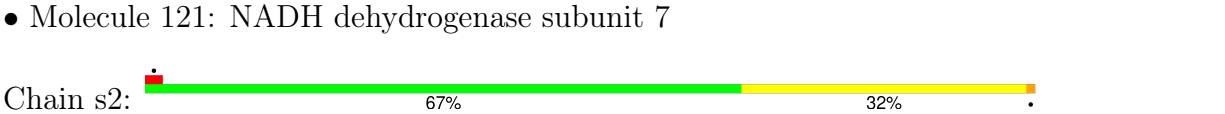


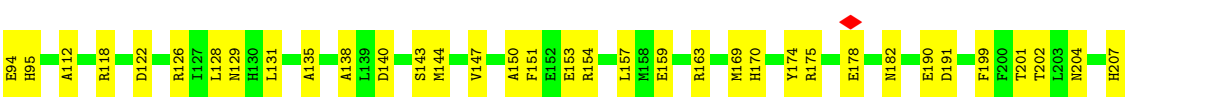






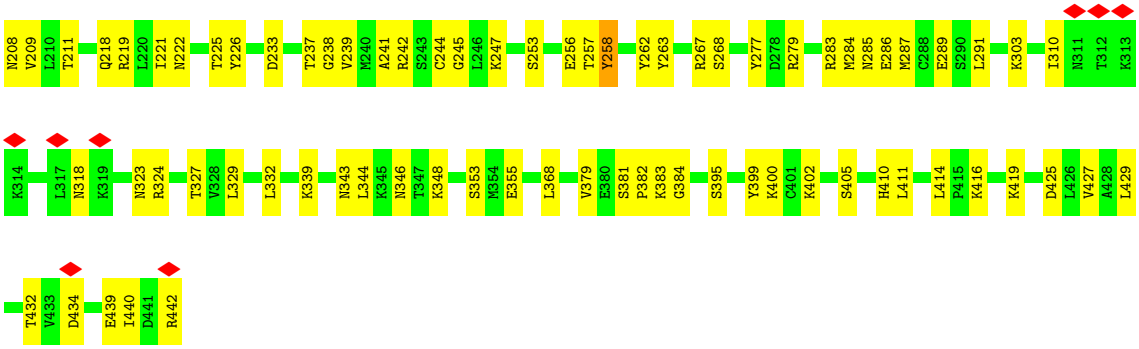






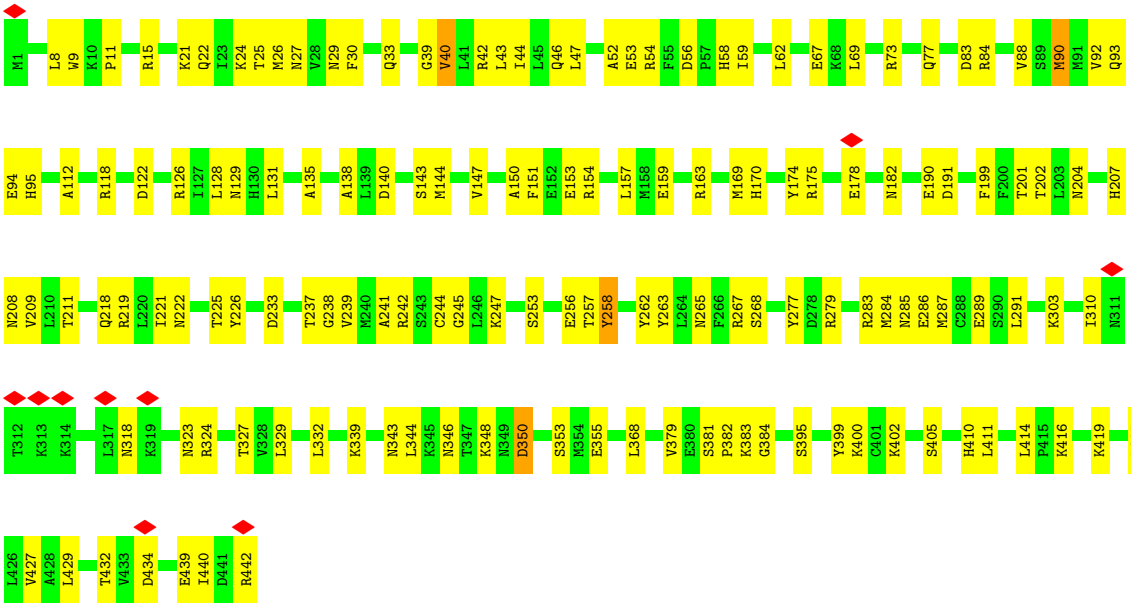
• Molecule 121: NADH dehydrogenase subunit 7

Chain s2:



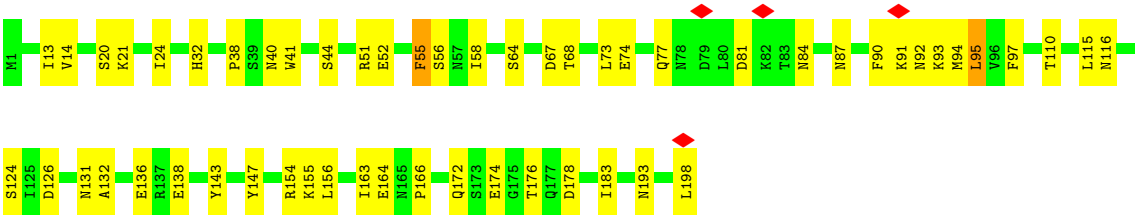
• Molecule 121: NADH dehydrogenase subunit 7

Chain S2:



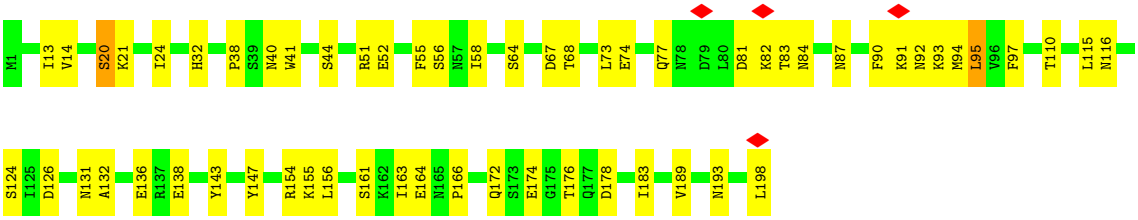
• Molecule 122: NADH dehydrogenase subunit 9

Chain s3:



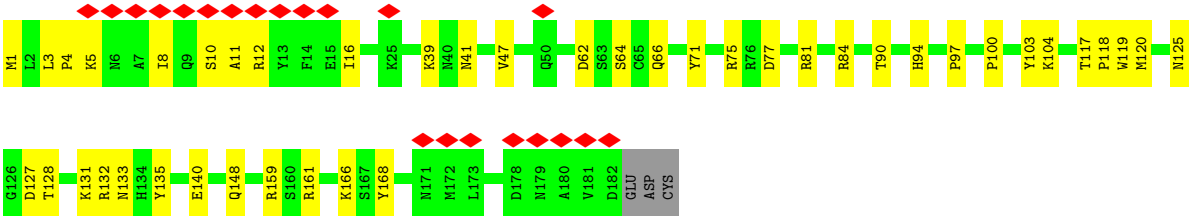
• Molecule 122: NADH dehydrogenase subunit 9

Chain S3:



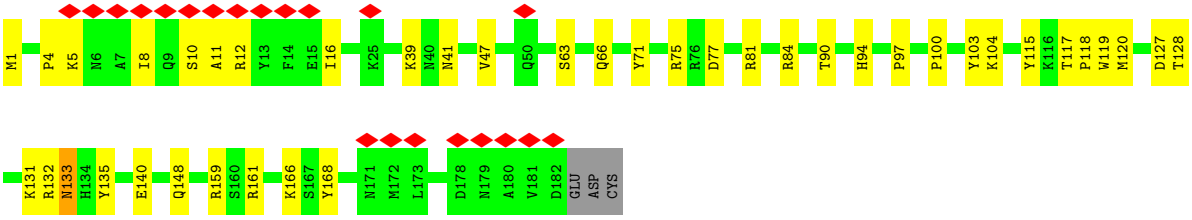
• Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain s4:



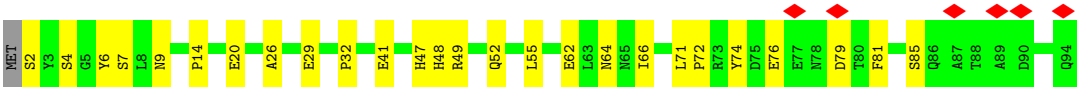
• Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:



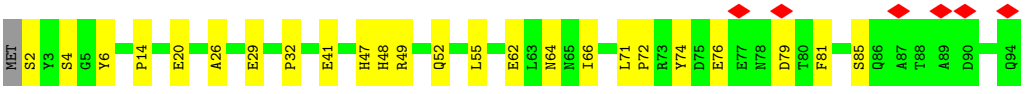
• Molecule 124: GRAM domain protein

Chain s5:



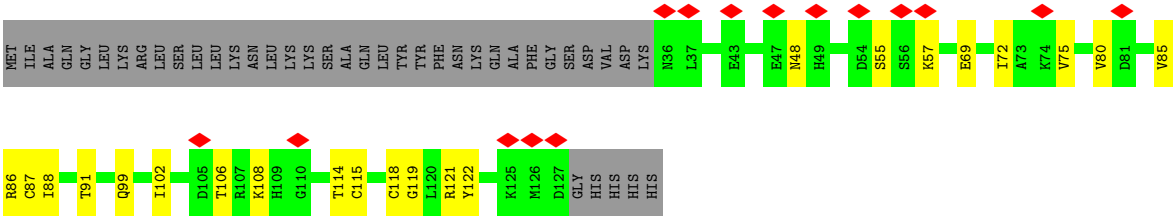
• Molecule 124: GRAM domain protein

Chain S5:



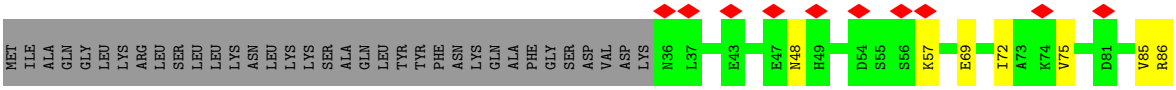
• Molecule 125: Zinc-finger protein

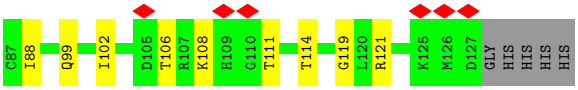
Chain s6:



• Molecule 125: Zinc-finger protein

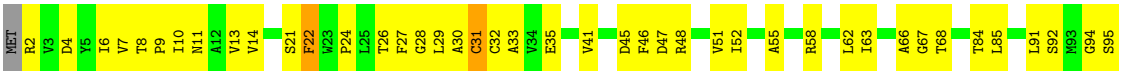
Chain S6:

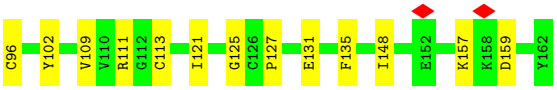




• Molecule 126: NADH dehydrogenase subunit 10

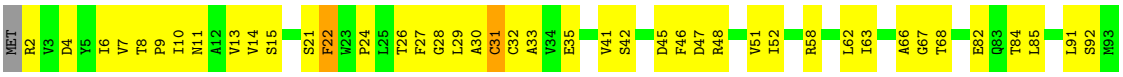
Chain s7:





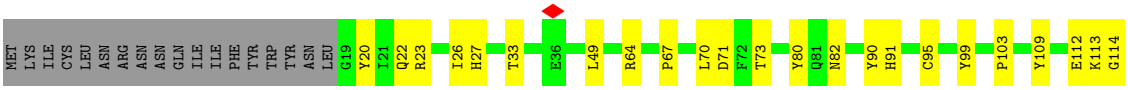
• Molecule 126: NADH dehydrogenase subunit 10

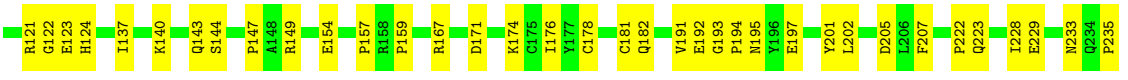
Chain S7:



• Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative

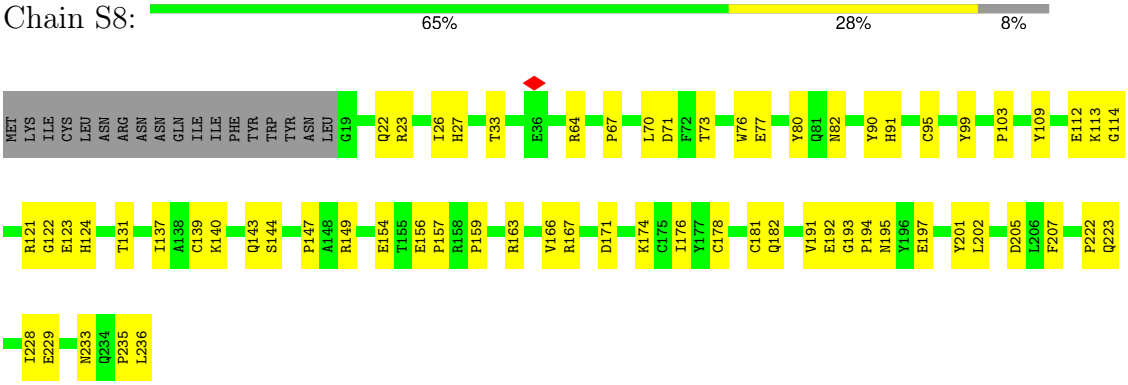
Chain s8:





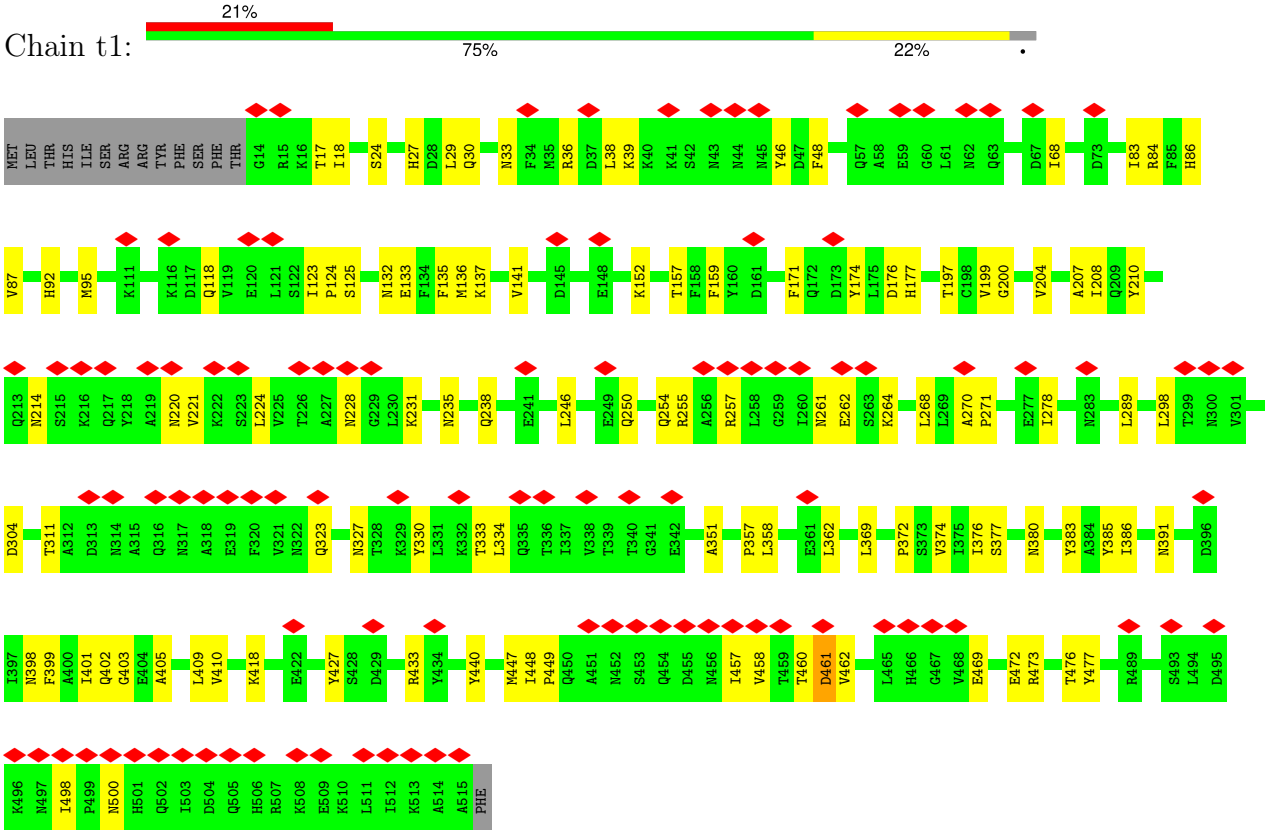
• Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative

Chain S8:



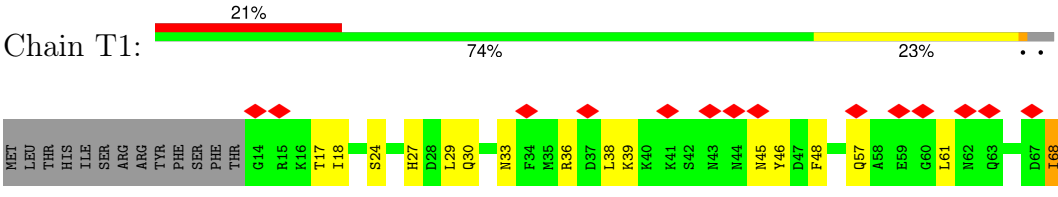
• Molecule 128: Lipid-A-disaccharide synthase

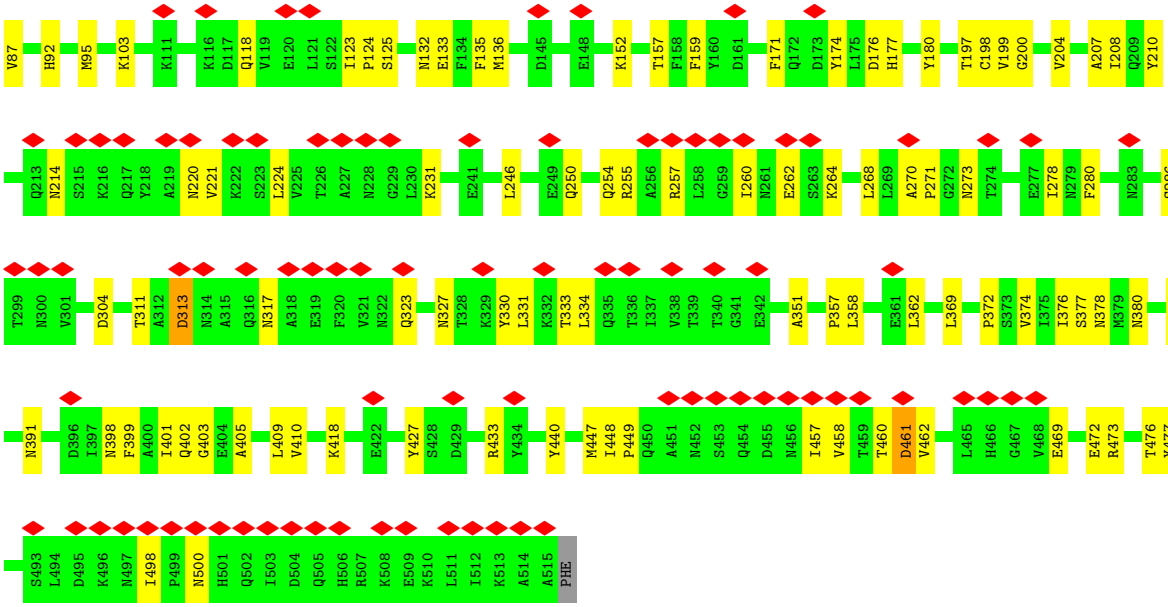
Chain t1:



• Molecule 128: Lipid-A-disaccharide synthase

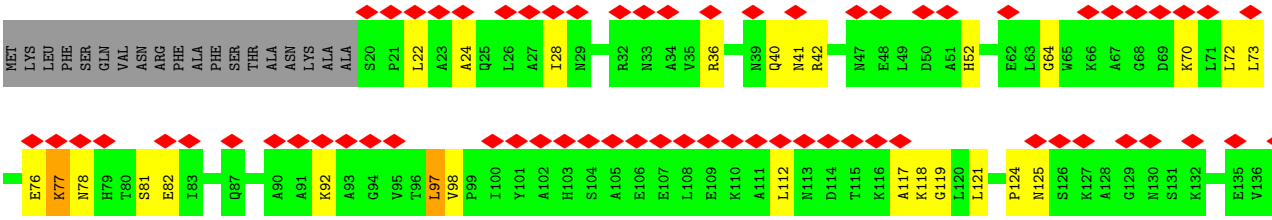
Chain T1:





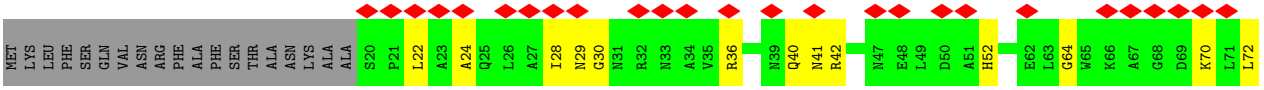
• Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

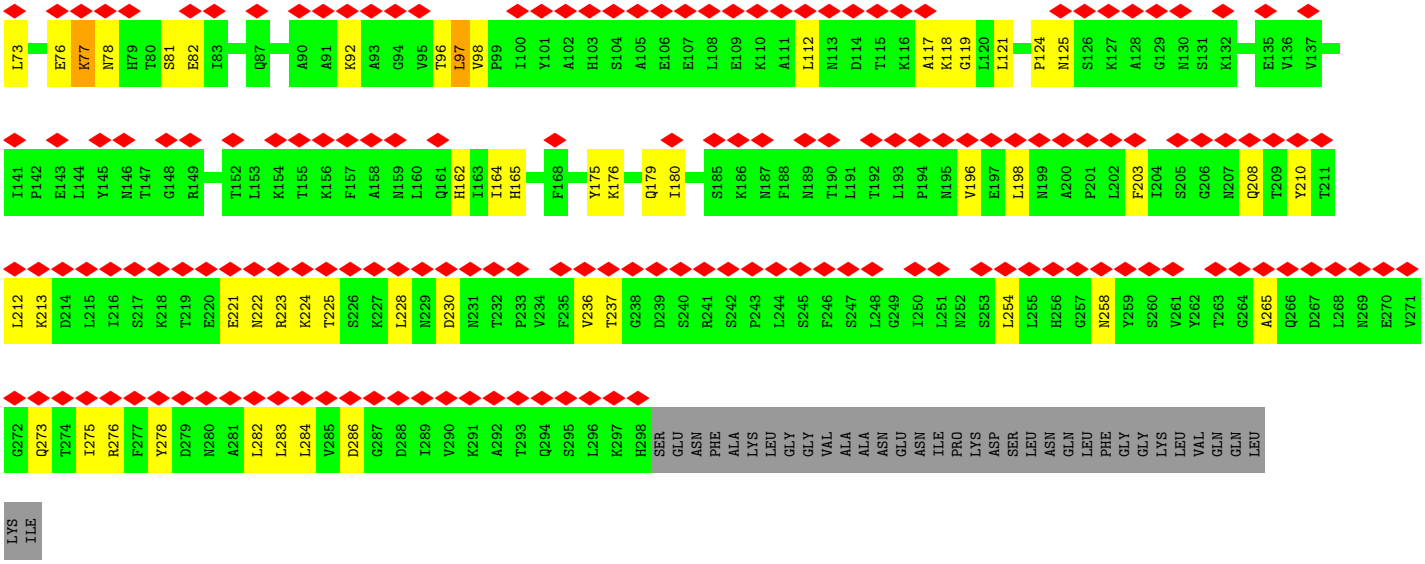
Chain t2:



• Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

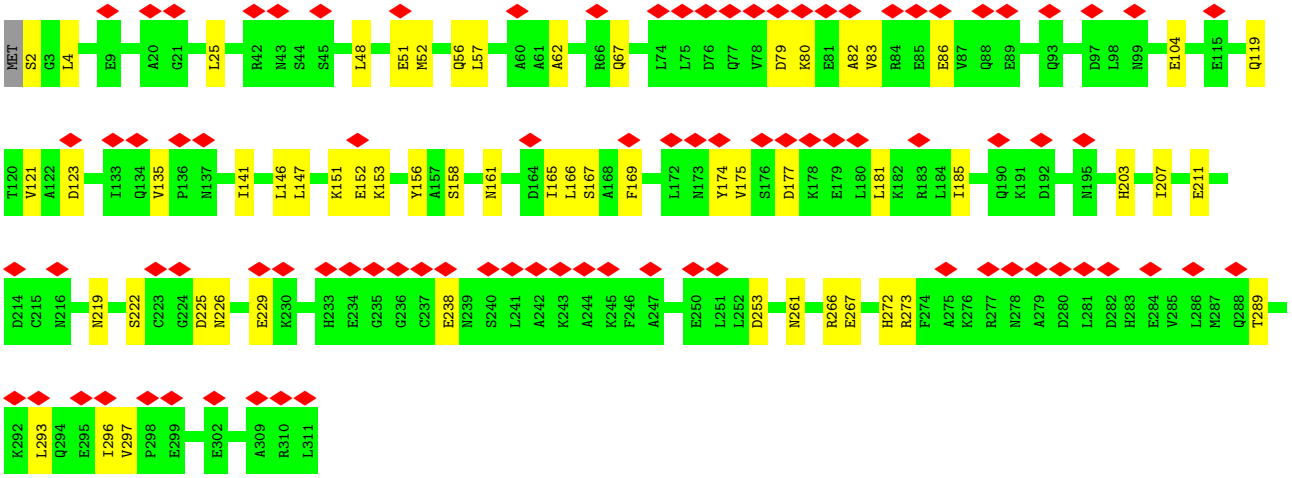
Chain T2:





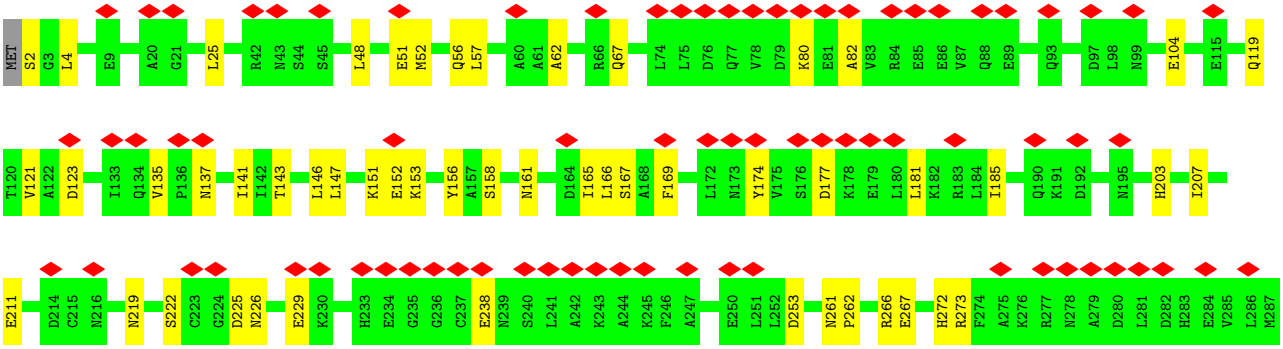
• Molecule 130: RNase III domain-containing protein

Chain t3:



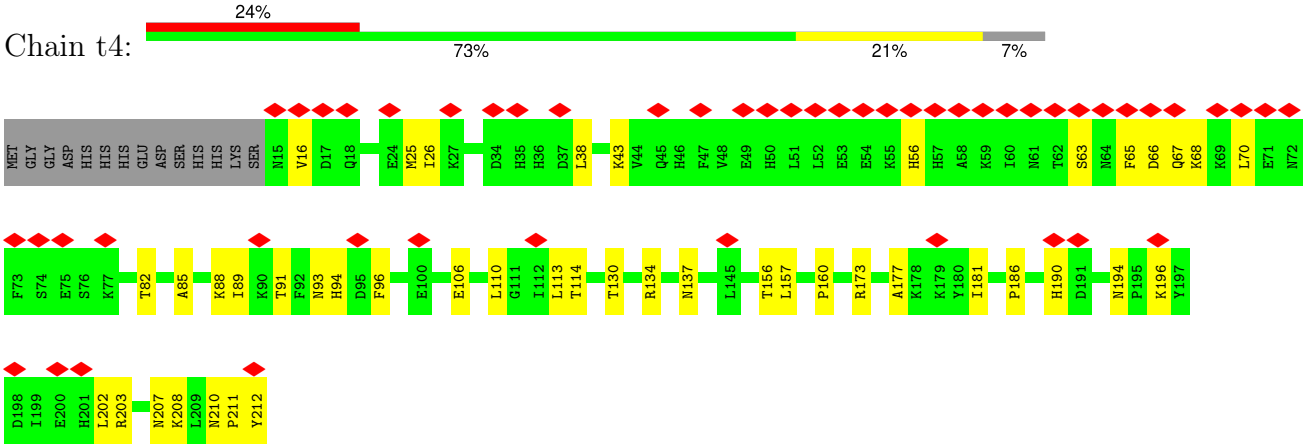
• Molecule 130: RNase III domain-containing protein

Chain T3:



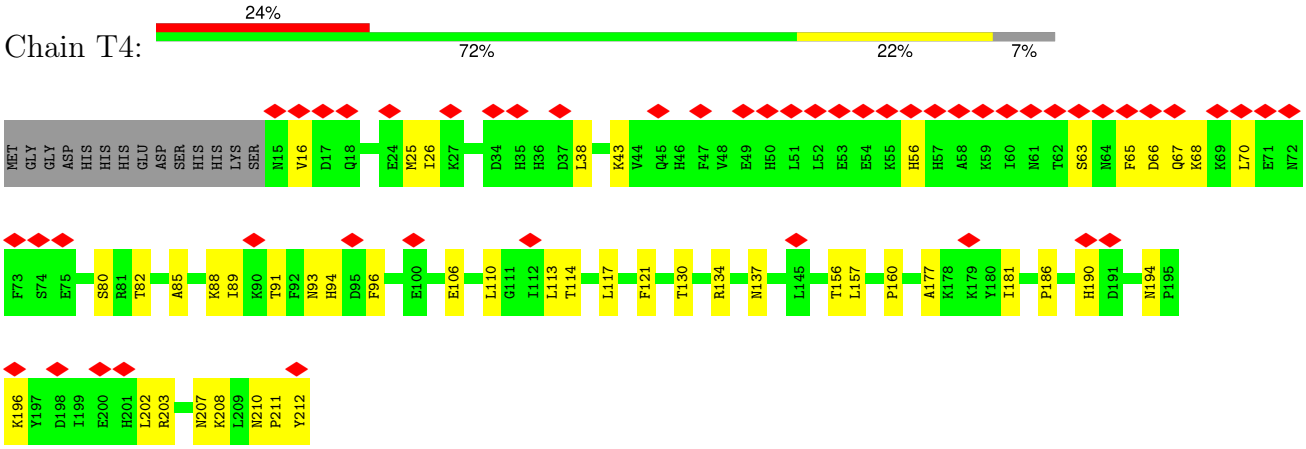
• Molecule 131: Transmembrane protein

Chain t4:



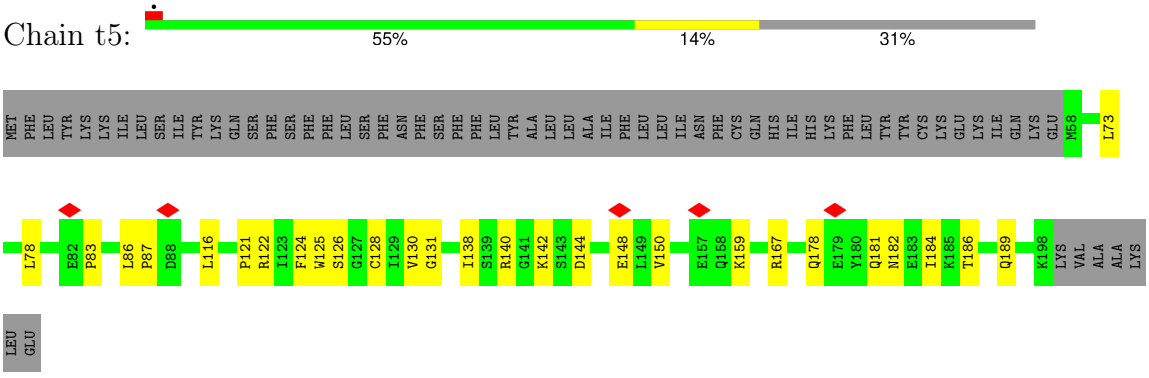
• Molecule 131: Transmembrane protein

Chain T4:



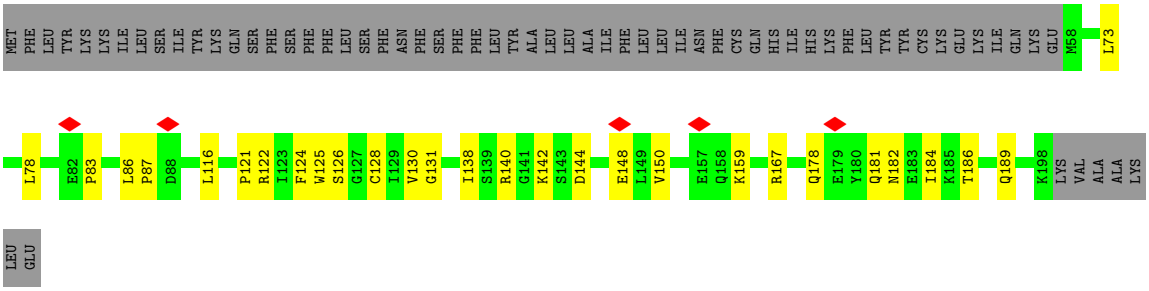
• Molecule 132: Transmembrane protein, putative

Chain t5:



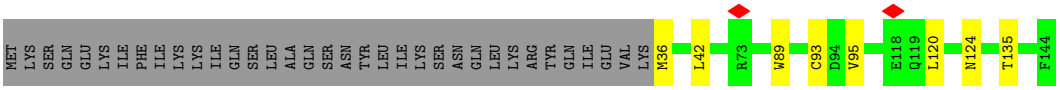
• Molecule 132: Transmembrane protein, putative

Chain T5:



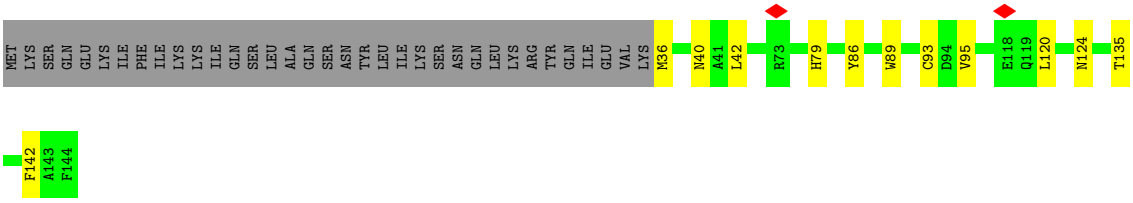
• Molecule 133: COX assembly mitochondrial protein

Chain t6:



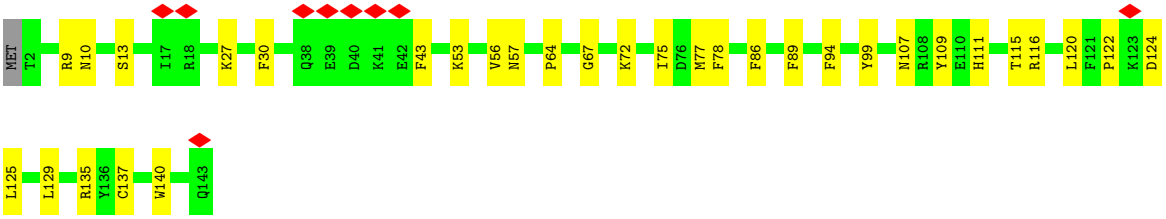
• Molecule 133: COX assembly mitochondrial protein

Chain T6:



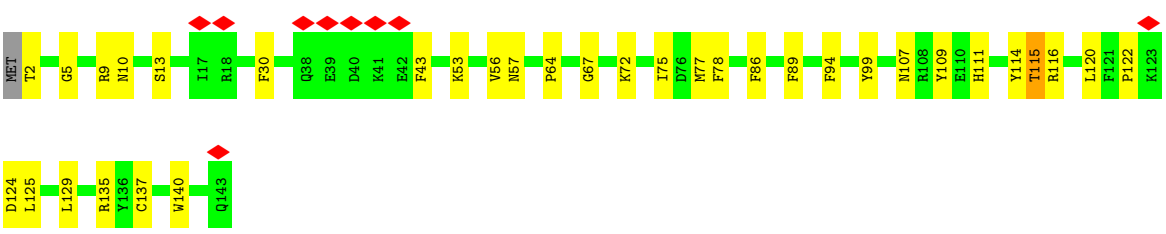
• Molecule 134: Transmembrane protein, putative

Chain t7:



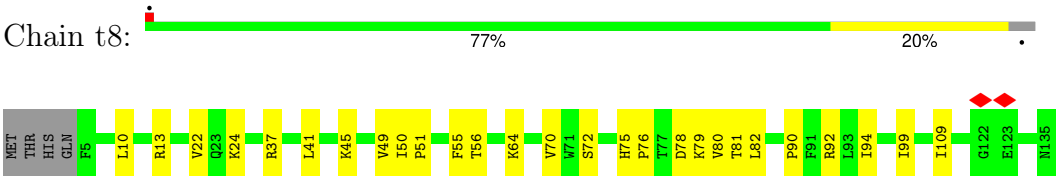
• Molecule 134: Transmembrane protein, putative

Chain T7:



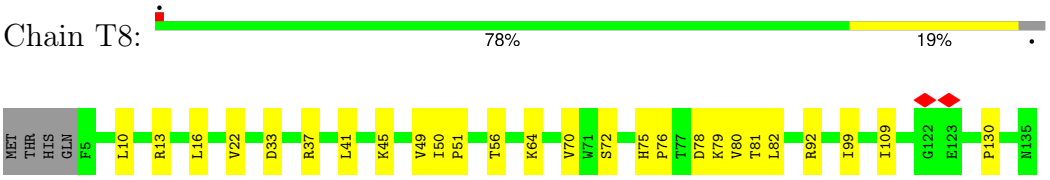
• Molecule 135: PH domain-containing protein

Chain t8:



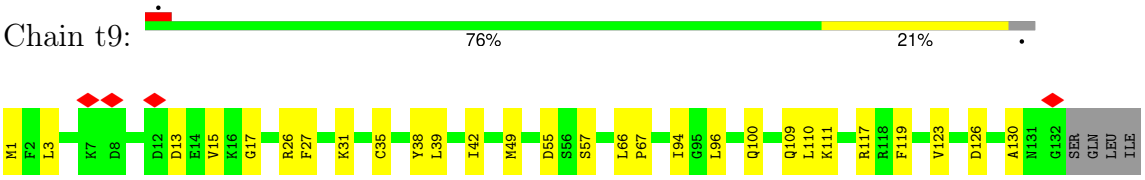
• Molecule 135: PH domain-containing protein

Chain T8:



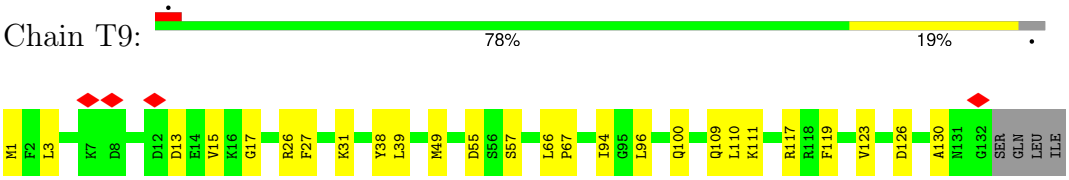
• Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain t9:



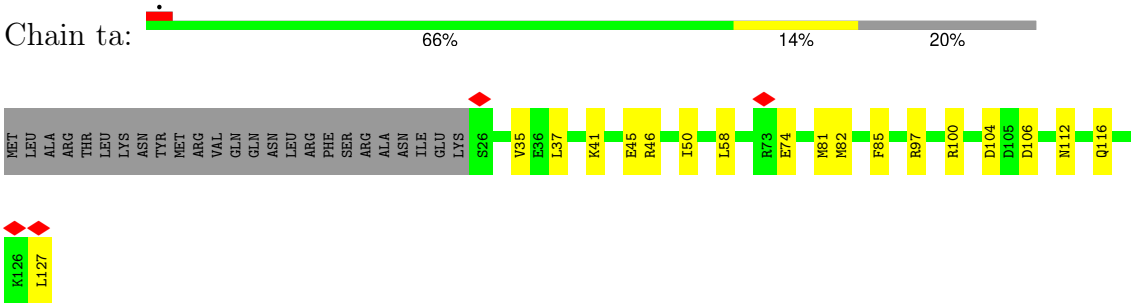
• Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain T9:



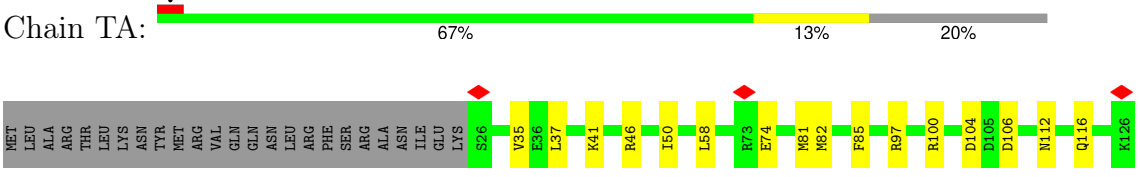
• Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain ta:



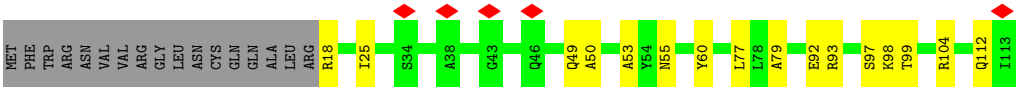
• Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain TA:



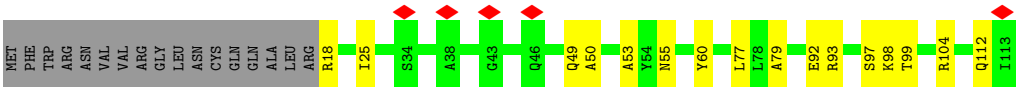
• Molecule 138: Transmembrane protein, putative

Chain tb:



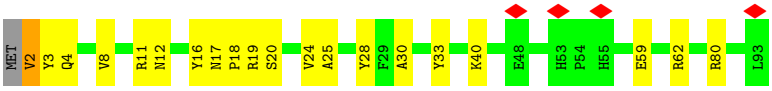
• Molecule 138: Transmembrane protein, putative

Chain TB:



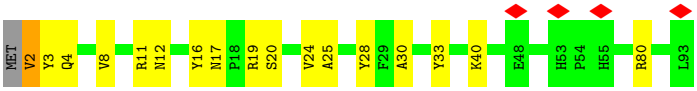
• Molecule 139: ATP synthase subunit e, mitochondrial

Chain tc:



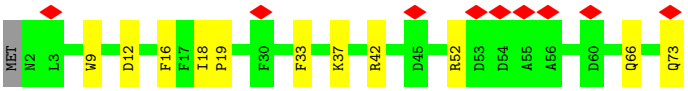
• Molecule 139: ATP synthase subunit e, mitochondrial

Chain TC:



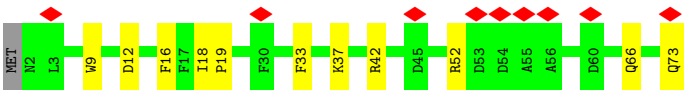
• Molecule 140: Transmembrane protein, putative

Chain td:



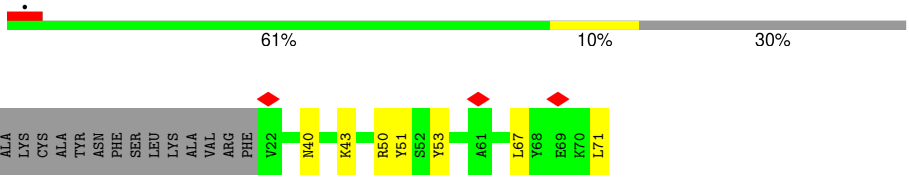
• Molecule 140: Transmembrane protein, putative

Chain TD:



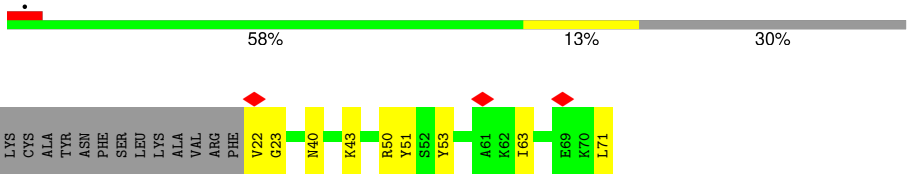
• Molecule 141: Transmembrane protein, putative

Chain te:



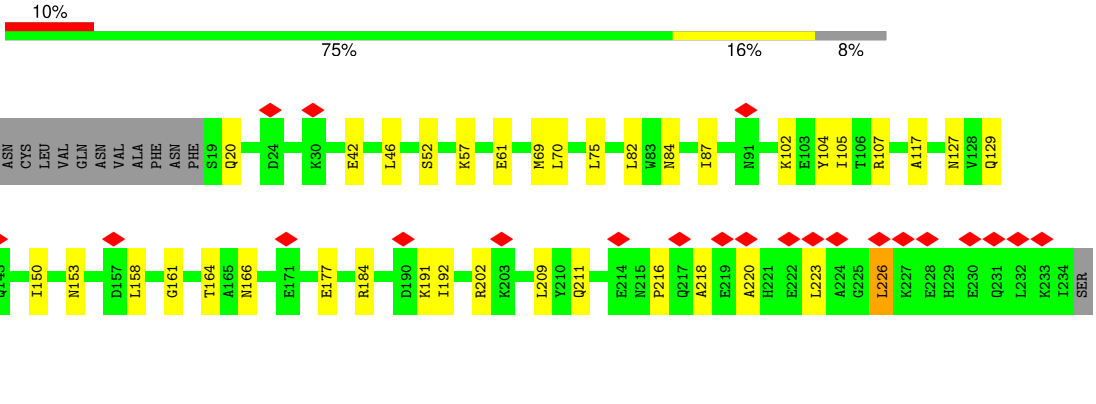
• Molecule 141: Transmembrane protein, putative

Chain TE:



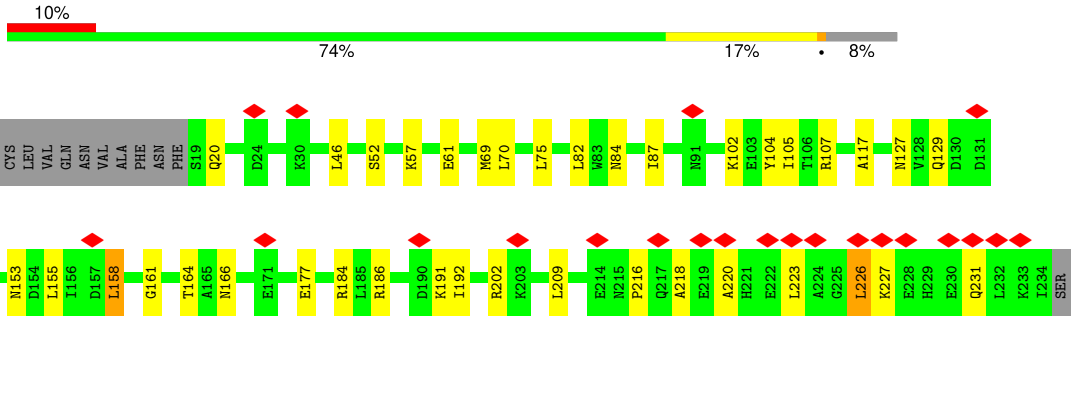
• Molecule 142: NDUTT15

Chain tf:



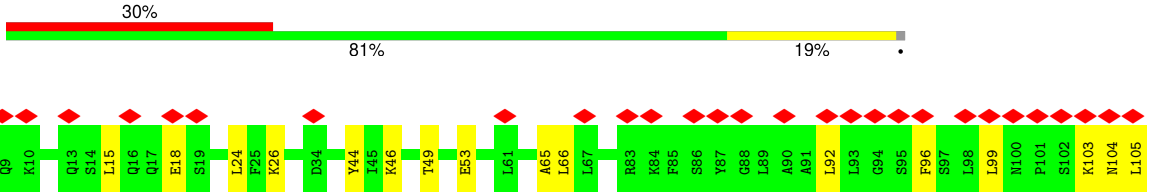
• Molecule 142: NDUTT15

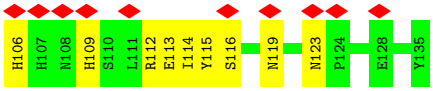
Chain TF:



• Molecule 143: NDUTT16

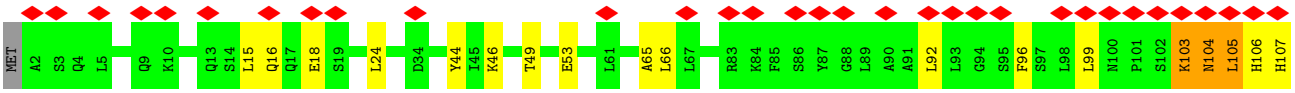
Chain tg:

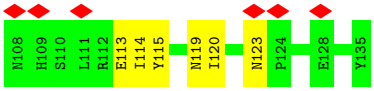




• Molecule 143: NDUTT16

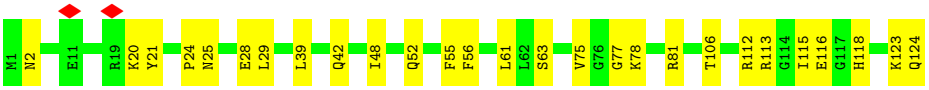
Chain TG:





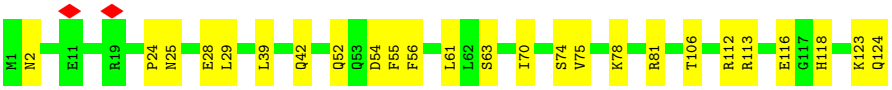
• Molecule 144: NDUTT17

Chain th:



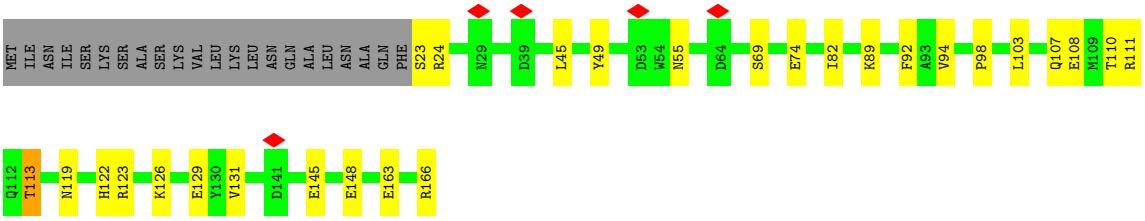
• Molecule 144: NDUTT17

Chain TH:



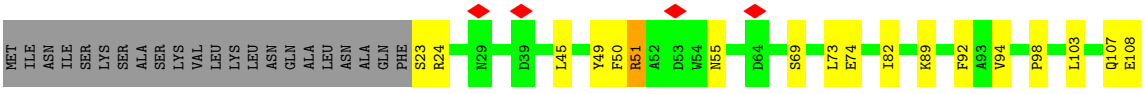
• Molecule 145: Thioredoxin

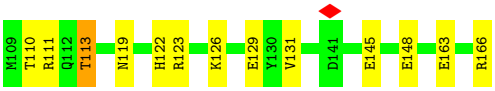
Chain tx:



• Molecule 145: Thioredoxin

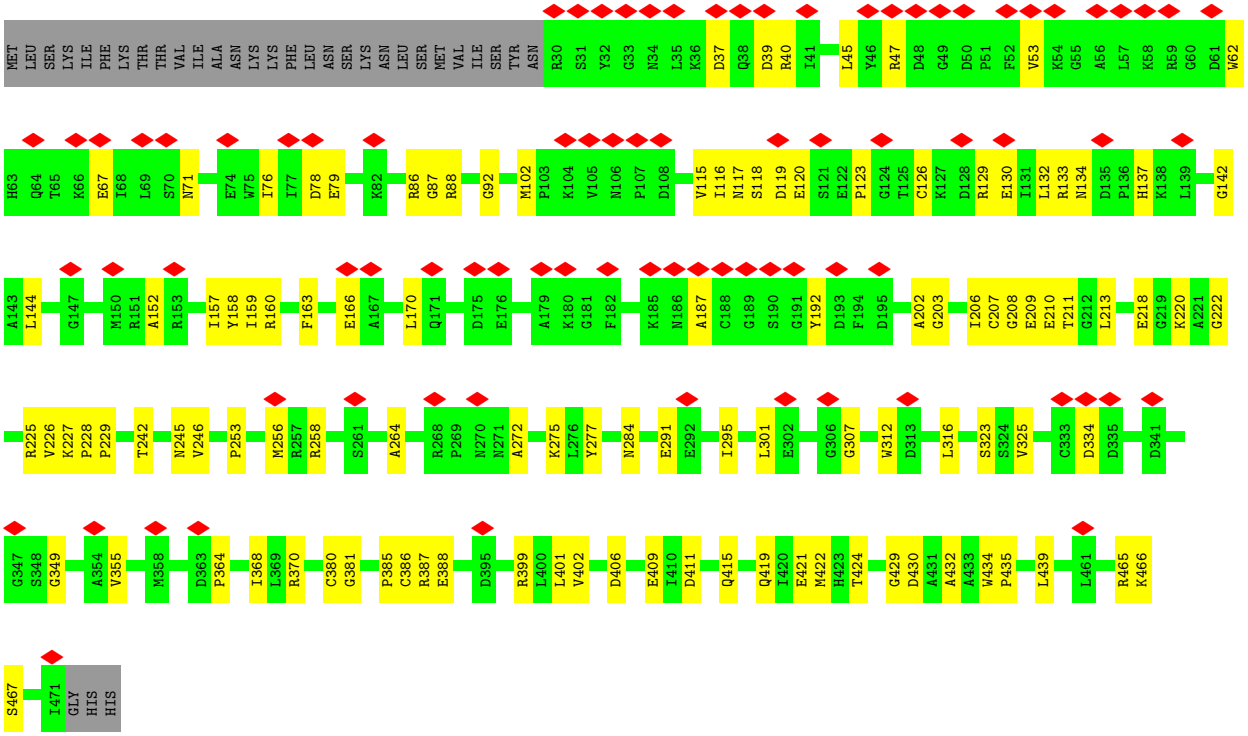
Chain TX:





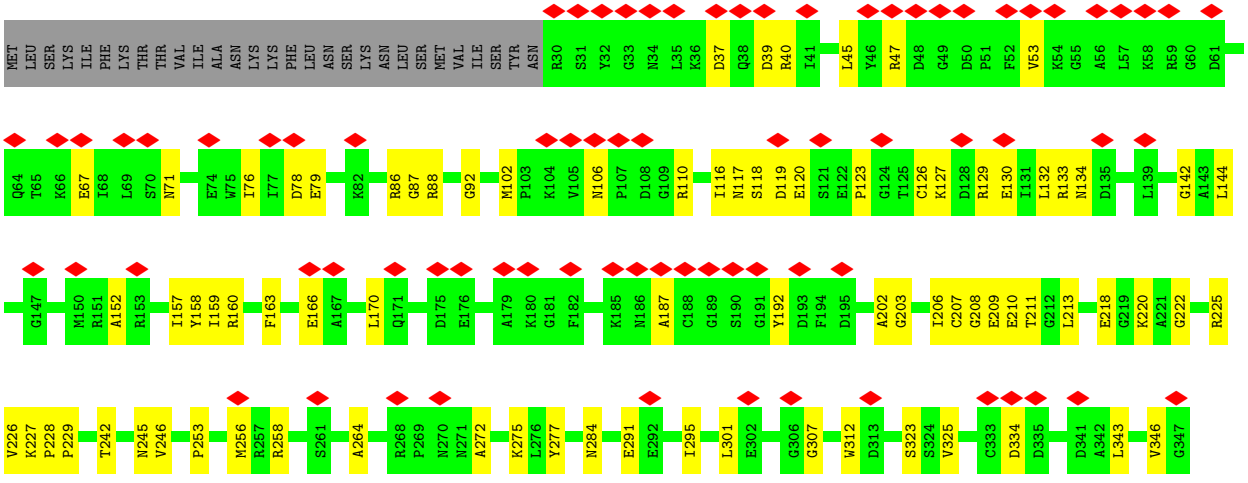
• Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

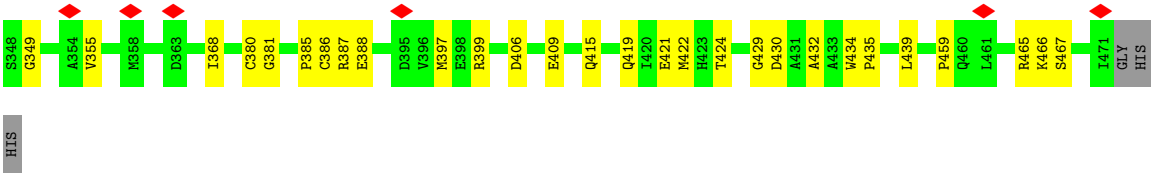
Chain v1:



• Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

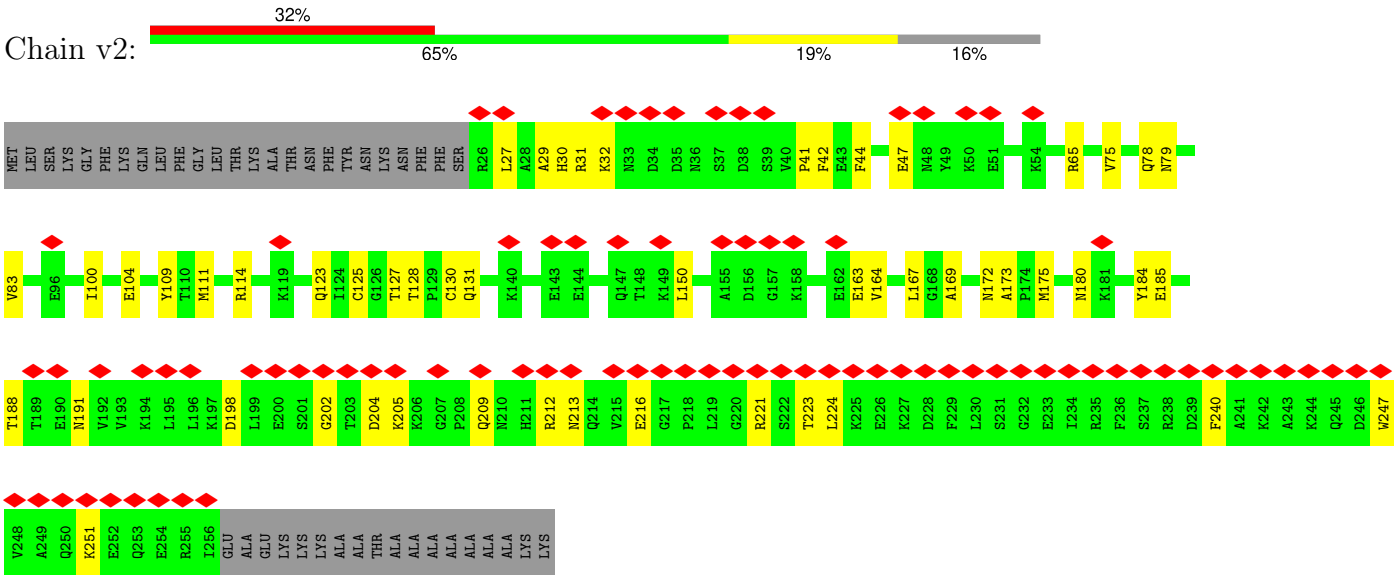
Chain V1:





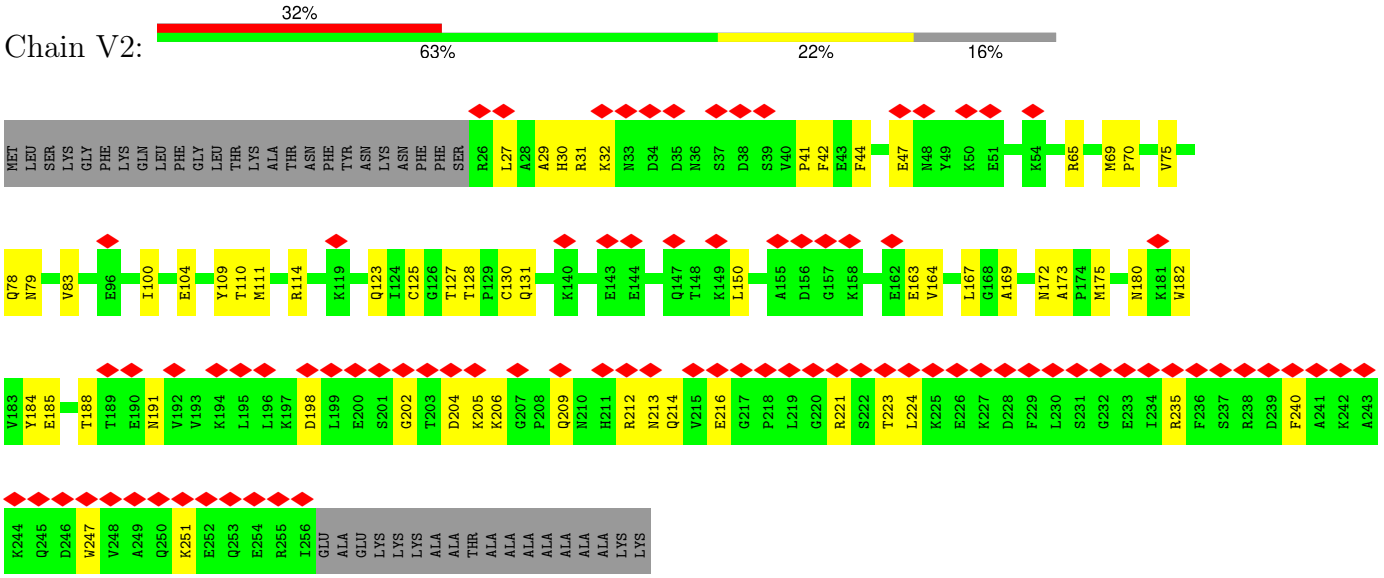
• Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit

Chain v2:



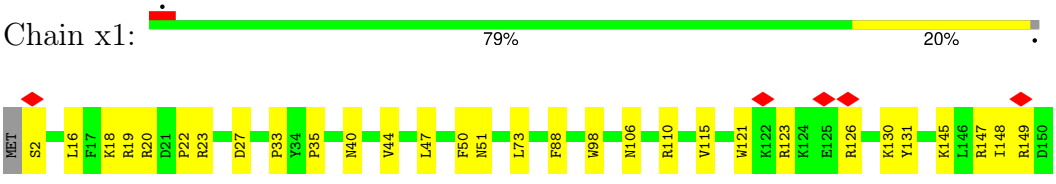
• Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit

Chain V2:



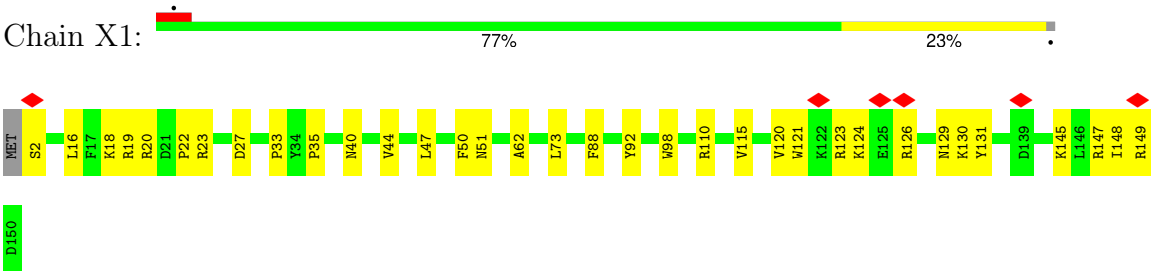
• Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

Chain x1:



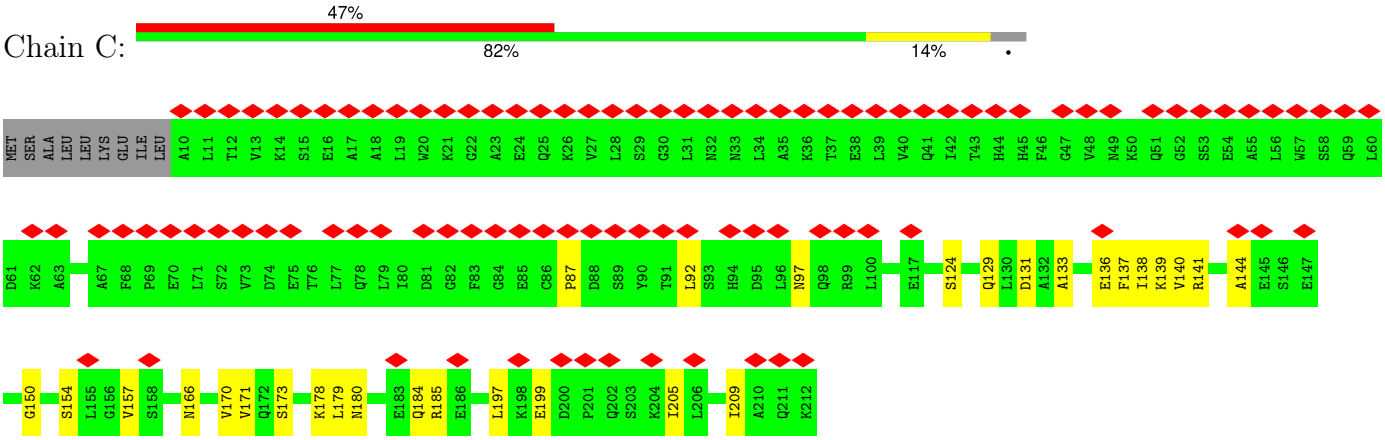
• Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

Chain X1:



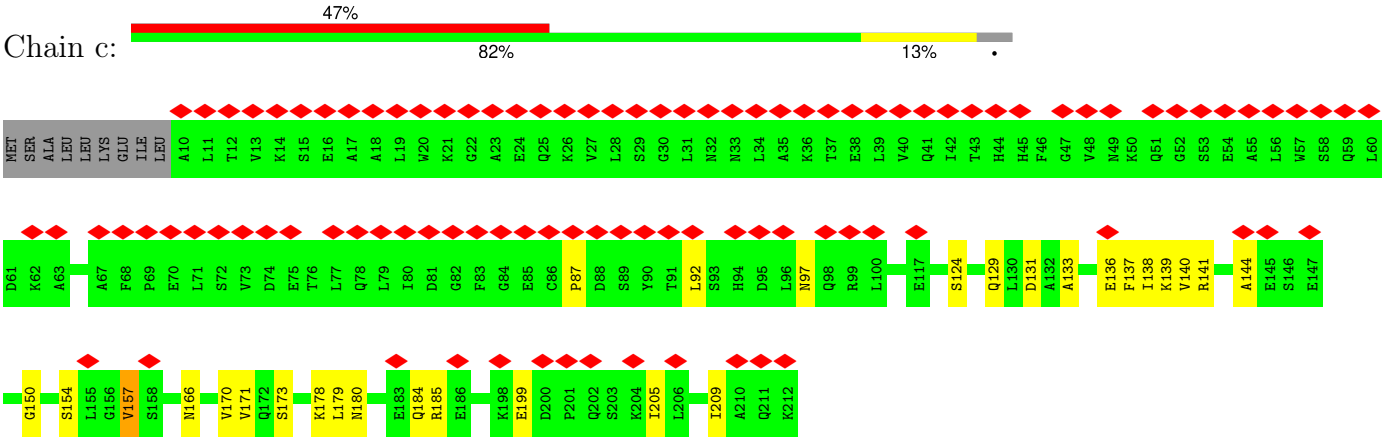
• Molecule 149: COXTT3

Chain C:



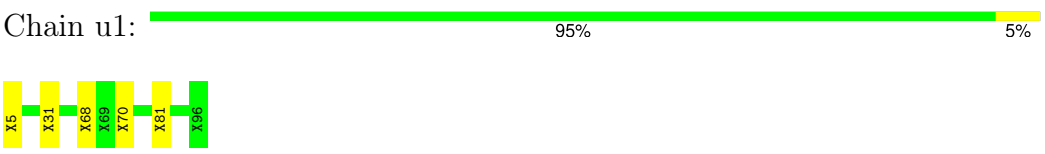
• Molecule 149: COXTT3

Chain c:



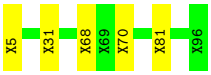
• Molecule 150: Unknown peptide

Chain u1:



• Molecule 150: Unknown peptide

Chain U1:


X5
X31
X68
X69
X70
X81
X96

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	97688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	140000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	60.050	Depositor
Minimum map value	-23.470	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.045	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	781.2, 781.2, 781.2	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FAD, PX2, HEM, SEP, PC1, ZMP, CDL, HEC, NDP, U10, ADP, P5S, ZN, HEA, CU, T7X, MG, FES, 3PE, F3S, TPO, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1T	0.11	0/546	0.19	0/735
1	1t	0.11	0/546	0.19	0/735
2	2E	0.10	0/2614	0.27	0/3553
2	2e	0.10	0/2614	0.27	0/3553
3	2F	0.12	0/1848	0.27	0/2500
3	2f	0.12	0/1848	0.27	0/2500
4	2G	0.12	0/1716	0.28	0/2317
4	2g	0.12	0/1716	0.28	0/2317
5	2H	0.11	0/812	0.24	0/1090
5	2h	0.11	0/812	0.24	0/1090
6	2I	0.12	0/930	0.24	0/1244
6	2i	0.12	0/930	0.25	0/1244
7	2J	0.12	0/866	0.24	0/1176
7	2j	0.12	0/866	0.24	0/1176
8	2K	0.15	0/821	0.30	0/1112
8	2k	0.15	0/821	0.30	0/1112
9	2L	0.12	0/738	0.25	0/990
9	2l	0.12	0/738	0.25	0/990
10	2M	0.11	0/660	0.25	0/895
10	2m	0.11	0/660	0.25	0/895
11	2N	0.12	0/521	0.33	0/708
11	2n	0.12	0/521	0.36	0/708
12	2O	0.12	0/367	0.23	0/496
12	2o	0.12	0/367	0.22	0/496
13	2T	0.09	0/574	0.22	0/772
13	2t	0.09	0/574	0.23	0/772
14	3T	0.10	0/662	0.21	0/888
14	3t	0.10	0/662	0.21	0/888
15	4A	0.09	0/836	0.22	0/1133
15	4a	0.09	0/836	0.21	0/1133
16	4T	0.10	0/491	0.21	0/662

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	4t	0.10	0/491	0.20	0/662
17	5T	0.10	0/514	0.23	0/693
17	5t	0.10	0/514	0.23	0/693
18	6A	0.13	0/1116	0.25	0/1512
18	6a	0.13	0/1116	0.25	0/1512
19	6B	0.11	0/1976	0.24	0/2673
19	6b	0.11	0/1976	0.24	0/2673
20	6C	0.20	0/926	0.33	0/1256
20	6c	0.20	0/926	0.33	0/1256
21	6L	0.10	0/649	0.26	0/871
21	6l	0.10	0/649	0.26	0/871
22	6T	0.09	0/573	0.22	0/770
22	6t	0.09	0/573	0.21	0/770
23	7A	0.10	0/1206	0.25	0/1631
23	7a	0.10	0/1206	0.24	0/1631
24	7C	0.09	0/1881	0.24	0/2558
24	7c	0.09	0/1881	0.24	0/2558
25	7L	0.11	0/1107	0.24	0/1505
25	7l	0.11	0/1107	0.24	0/1505
26	A	0.10	0/3874	0.25	0/5273
26	a	0.10	0/3874	0.26	0/5273
27	B	0.09	0/3453	0.24	0/4671
27	b	0.09	0/3453	0.24	0/4671
28	BP	0.11	0/2988	0.33	0/4052
28	bp	0.11	0/2988	0.33	0/4052
29	C1	0.12	0/5765	0.28	0/7819
29	c1	0.12	0/5765	0.28	0/7819
30	C2	0.12	0/5244	0.28	0/7107
30	c2	0.12	0/5244	0.28	0/7107
31	C3	0.12	0/5256	0.27	0/7142
31	c3	0.12	0/5256	0.27	0/7142
32	D	0.10	0/2430	0.26	0/3303
32	d	0.10	0/2430	0.26	0/3303
33	E	0.11	0/3266	0.30	2/4435 (0.0%)
33	e	0.10	0/3266	0.25	0/4435
34	F	0.10	0/2077	0.26	0/2824
34	f	0.10	0/2077	0.26	0/2824
35	FS	0.12	0/1562	0.28	0/2123
35	fs	0.12	0/1562	0.28	0/2123
36	G	0.10	0/2517	0.26	0/3433
36	g	0.10	0/2517	0.25	0/3433
37	H	0.11	0/2423	0.25	0/3279
37	h	0.11	0/2423	0.25	0/3279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	I	0.10	0/2001	0.25	0/2702
38	i	0.10	0/2001	0.25	0/2702
39	J	0.11	0/1621	0.25	0/2201
39	j	0.11	0/1621	0.26	0/2201
40	K	0.10	0/1755	0.25	0/2376
40	k	0.10	0/1755	0.24	0/2376
41	L	0.12	0/1718	0.24	0/2333
41	l	0.12	0/1718	0.24	0/2333
42	M	0.12	0/1941	0.26	0/2637
42	m	0.12	0/1941	0.26	0/2637
43	M1	0.12	0/2958	0.29	0/4013
43	m1	0.12	0/2958	0.29	0/4013
44	M2	0.11	0/2629	0.25	0/3564
44	m2	0.11	0/2629	0.25	0/3564
45	M3	0.10	0/2689	0.26	0/3657
45	m3	0.10	0/2689	0.25	0/3657
46	N	0.09	0/1770	0.24	0/2391
46	n	0.09	0/1770	0.23	0/2391
47	O	0.12	0/1098	0.23	0/1477
47	o	0.12	0/1098	0.23	0/1477
48	P	0.09	0/1436	0.23	0/1941
48	p	0.09	0/1436	0.23	0/1941
49	Q	0.12	0/1478	0.29	0/2005
49	q	0.12	0/1478	0.27	0/2005
50	R	0.10	0/1441	0.25	0/1952
50	r	0.10	0/1441	0.25	0/1952
51	S	0.12	0/1409	0.26	0/1900
51	s	0.12	0/1409	0.26	0/1900
52	SA	0.11	0/4722	0.28	0/6385
52	sa	0.11	0/4722	0.29	0/6385
53	SB	0.12	0/2315	0.28	0/3136
53	sb	0.12	0/2315	0.28	0/3136
54	SC	0.14	0/493	0.27	0/664
54	sc	0.14	0/493	0.27	0/664
55	SD	0.11	0/404	0.23	0/542
55	sd	0.11	0/404	0.22	0/542
56	T	0.11	0/1359	0.23	0/1842
56	t	0.11	0/1359	0.23	0/1842
57	U	0.12	0/1335	0.24	0/1794
57	u	0.12	0/1335	0.24	0/1794
58	V	0.10	0/1277	0.25	0/1735
58	v	0.11	0/1277	0.24	0/1735
59	VB	0.10	0/4712	0.24	0/6357

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
59	vb	0.10	0/4712	0.24	0/6357
60	W	0.10	0/1136	0.25	0/1545
60	w	0.10	0/1136	0.25	0/1545
61	X	0.12	0/1043	0.24	0/1413
61	x	0.11	0/1043	0.24	0/1413
62	Y	0.12	0/882	0.26	0/1192
62	y	0.12	0/882	0.27	0/1192
63	Y0	0.10	0/801	0.28	0/1087
63	y0	0.10	0/801	0.28	0/1087
64	Y5	0.10	0/1708	0.22	0/2306
64	y5	0.10	0/1708	0.22	0/2306
65	Y7	0.10	0/3012	0.22	0/4072
65	y7	0.10	0/3012	0.22	0/4072
66	Z	0.11	0/737	0.26	0/995
66	z	0.11	0/737	0.27	0/995
67	Z1	0.13	0/781	0.23	0/1053
67	z1	0.13	0/781	0.23	0/1053
68	1B	0.11	0/536	0.25	0/727
68	1b	0.11	0/536	0.24	0/727
69	2B	0.11	0/1520	0.26	0/2058
69	2b	0.11	0/1520	0.26	0/2058
70	4L	0.13	0/982	0.29	0/1335
70	4l	0.12	0/982	0.29	0/1335
71	5B	0.11	0/915	0.29	0/1224
71	5b	0.11	0/915	0.30	0/1224
72	A1	0.12	0/834	0.34	0/1132
72	a1	0.12	0/834	0.34	0/1132
73	A2	0.09	0/826	0.27	0/1116
73	a2	0.09	0/826	0.27	0/1116
74	A3	0.10	0/1115	0.23	0/1507
74	a3	0.09	0/1115	0.23	0/1507
75	A5	0.08	0/1336	0.20	0/1797
75	a5	0.08	0/1336	0.20	0/1797
76	A6	0.10	0/1459	0.24	0/1965
76	a6	0.10	0/1459	0.24	0/1965
77	A7	0.08	0/2408	0.23	0/3269
77	a7	0.08	0/2408	0.23	0/3269
78	A8	0.09	0/1099	0.23	0/1477
78	a8	0.09	0/1099	0.23	0/1477
79	A9	0.11	0/2807	0.26	0/3801
79	a9	0.11	0/2807	0.26	0/3801
80	AB	0.10	0/942	0.23	0/1272
80	ab	0.10	0/942	0.23	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
81	AC	0.10	0/822	0.23	0/1114
81	ac	0.10	0/822	0.23	0/1114
82	AL	0.08	0/1667	0.23	0/2256
82	al	0.09	0/1667	0.23	0/2256
83	AM	0.11	0/1379	0.26	0/1841
83	am	0.11	0/1379	0.26	0/1841
84	AN	0.09	0/1935	0.24	0/2616
84	an	0.09	0/1935	0.24	0/2616
85	B2	0.10	0/991	0.25	0/1333
85	b2	0.10	0/991	0.23	0/1333
86	B3	0.10	0/621	0.27	0/840
86	b3	0.10	0/621	0.26	0/840
87	B4	0.09	0/1015	0.21	0/1381
87	b4	0.09	0/1015	0.21	0/1381
88	B6	0.12	0/623	0.23	0/850
88	b6	0.12	0/623	0.23	0/850
89	B7	0.10	0/968	0.24	0/1307
89	b7	0.10	0/968	0.23	0/1307
90	B8	0.09	0/1494	0.25	0/2016
90	b8	0.09	0/1494	0.26	0/2016
91	B9	0.09	0/1644	0.24	0/2224
91	b9	0.09	0/1644	0.23	0/2224
92	BL	0.11	0/1489	0.24	0/2000
92	bl	0.11	0/1489	0.24	0/2000
93	BM	0.09	0/1351	0.23	0/1829
93	bm	0.09	0/1351	0.23	0/1829
94	C4	0.13	0/873	0.26	0/1175
94	c4	0.13	0/873	0.25	0/1175
95	FX	0.12	0/1186	0.33	0/1607
95	fx	0.12	0/1186	0.33	0/1607
96	G1	0.10	0/1810	0.26	0/2465
96	g1	0.10	0/1810	0.26	0/2465
97	G2	0.11	0/1793	0.27	0/2438
97	g2	0.10	0/1793	0.26	0/2438
98	G3	0.11	0/2865	0.25	0/3877
98	g3	0.10	0/2865	0.25	0/3877
99	J1	0.09	0/2219	0.21	0/2988
99	j1	0.09	0/2219	0.21	0/2988
100	N1	0.11	0/2376	0.27	0/3234
100	n1	0.11	0/2376	0.27	0/3234
101	N2	0.12	0/3173	0.27	0/4312
101	n2	0.12	0/3173	0.27	0/4312
102	N3	0.12	0/1051	0.24	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
102	n3	0.12	0/1051	0.24	0/1429
103	N4	0.13	0/4303	0.27	0/5844
103	n4	0.13	0/4303	0.27	0/5844
104	N5	0.12	0/6098	0.27	0/8297
104	n5	0.12	0/6098	0.27	0/8297
105	N6	0.11	0/2232	0.24	0/3035
105	n6	0.11	0/2232	0.24	0/3035
106	P1	0.10	0/1963	0.28	0/2658
106	p1	0.10	0/1963	0.28	0/2658
107	P2	0.10	0/1454	0.28	0/1970
107	p2	0.11	0/1454	0.28	0/1970
108	QA	0.10	0/3569	0.25	0/4835
108	Qa	0.09	0/3569	0.25	0/4835
108	qA	0.10	0/3569	0.25	0/4835
108	qa	0.09	0/3569	0.25	0/4835
109	QB	0.10	0/3921	0.26	0/5325
109	Qb	0.12	0/3921	0.28	0/5325
109	qB	0.11	0/3921	0.26	0/5325
109	qb	0.11	0/3921	0.28	0/5325
110	QC	0.12	0/3715	0.28	0/5046
110	Qc	0.12	0/3706	0.26	0/5035
110	qC	0.12	0/3715	0.27	0/5046
110	qc	0.12	0/3706	0.27	0/5035
111	QD	0.11	0/2580	0.27	0/3491
111	Qd	0.10	0/2580	0.25	0/3491
111	qD	0.11	0/2580	0.26	0/3491
111	qd	0.10	0/2580	0.25	0/3491
112	QE	0.11	0/1588	0.25	0/2162
112	Qe	0.11	0/1499	0.26	0/2042
112	qE	0.11	0/1588	0.25	0/2162
112	qe	0.11	0/1499	0.25	0/2042
113	QF	0.12	0/716	0.28	0/969
113	Qf	0.10	0/641	0.26	0/866
113	qF	0.11	0/716	0.29	0/969
113	qf	0.10	0/641	0.26	0/866
114	QG	0.10	0/2845	0.26	0/3839
114	Qg	0.09	0/2838	0.24	0/3829
114	qG	0.11	0/2845	0.26	0/3839
114	qg	0.09	0/2838	0.24	0/3829
115	QH	0.10	0/1133	0.28	0/1524
115	Qh	0.10	0/1133	0.27	0/1524
115	qH	0.10	0/1133	0.28	0/1524
115	qh	0.10	0/1133	0.27	0/1524

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
116	QI	0.09	0/1005	0.22	0/1365
116	Qi	0.11	0/1005	0.25	0/1365
116	qI	0.09	0/1005	0.22	0/1365
116	qi	0.10	0/1005	0.25	0/1365
117	QJ	0.10	0/502	0.22	0/687
117	Qj	0.09	0/522	0.22	0/712
117	qJ	0.10	0/502	0.22	0/687
117	qj	0.10	0/522	0.22	0/712
118	QL	0.07	0/273	0.19	0/371
118	Ql	0.09	0/273	0.20	0/371
118	qL	0.08	0/273	0.20	0/371
118	ql	0.09	0/273	0.19	0/371
120	S1	0.09	0/5518	0.25	0/7476
120	s1	0.09	0/5518	0.25	0/7476
121	S2	0.12	0/3680	0.27	0/4969
121	s2	0.12	0/3680	0.27	0/4969
122	S3	0.11	0/1718	0.29	0/2319
122	s3	0.11	0/1718	0.29	0/2319
123	S4	0.10	0/1543	0.27	0/2088
123	s4	0.10	0/1543	0.27	0/2088
124	S5	0.10	0/775	0.25	0/1048
124	s5	0.10	0/775	0.25	0/1048
125	S6	0.10	0/755	0.27	0/1022
125	s6	0.10	0/755	0.27	0/1022
126	S7	0.12	0/1311	0.29	0/1779
126	s7	0.11	0/1311	0.29	0/1779
127	S8	0.11	0/1867	0.27	0/2538
127	s8	0.11	0/1867	0.27	0/2538
128	T1	0.10	0/4153	0.25	0/5618
128	t1	0.10	0/4153	0.25	0/5618
129	T2	0.08	0/2224	0.23	0/3022
129	t2	0.08	0/2224	0.23	0/3022
130	T3	0.08	0/2527	0.22	0/3423
130	t3	0.08	0/2527	0.22	0/3423
131	T4	0.09	0/1689	0.23	0/2284
131	t4	0.09	0/1689	0.22	0/2284
132	T5	0.11	0/1163	0.25	0/1574
132	t5	0.11	0/1163	0.25	0/1574
133	T6	0.10	0/923	0.22	0/1239
133	t6	0.10	0/923	0.23	0/1239
134	T7	0.09	0/1223	0.21	0/1648
134	t7	0.09	0/1223	0.21	0/1648
135	T8	0.10	0/1112	0.23	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
135	t8	0.10	0/1112	0.23	0/1507
136	T9	0.10	0/1088	0.25	0/1458
136	t9	0.10	0/1088	0.26	0/1458
137	TA	0.10	0/877	0.23	0/1181
137	ta	0.10	0/877	0.24	0/1181
138	TB	0.09	0/825	0.19	0/1115
138	tb	0.09	0/825	0.19	0/1115
139	TC	0.09	0/811	0.21	0/1093
139	tc	0.09	0/811	0.21	0/1093
140	TD	0.08	0/634	0.20	0/855
140	td	0.08	0/634	0.20	0/855
141	TE	0.10	0/432	0.25	0/583
141	te	0.10	0/432	0.25	0/583
142	TF	0.08	0/1828	0.22	0/2472
142	tf	0.08	0/1828	0.22	0/2472
143	TG	0.09	0/1101	0.22	0/1486
143	tg	0.08	0/1101	0.22	0/1486
144	TH	0.10	0/1015	0.22	0/1366
144	th	0.09	0/1015	0.22	0/1366
145	TX	0.10	0/1235	0.23	0/1662
145	tx	0.10	0/1235	0.23	0/1662
146	V1	0.11	0/3485	0.27	0/4713
146	v1	0.10	0/3485	0.27	0/4713
147	V2	0.09	0/1895	0.26	0/2559
147	v2	0.09	0/1895	0.26	0/2559
148	X1	0.10	0/1261	0.24	0/1698
148	x1	0.10	0/1261	0.24	0/1698
149	C	0.09	0/1383	0.22	0/1880
149	c	0.09	0/1383	0.22	0/1880
All	All	0.11	0/556450	0.26	2/753536 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
146	V1	0	1
146	v1	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	E	281	HIS	CA-C-N	7.24	126.12	120.33
33	E	281	HIS	C-N-CA	7.24	126.12	120.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
146	V1	228	PRO	Peptide
146	v1	228	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1T	540	0	532	11	0
1	1t	540	0	532	11	0
2	2E	2560	0	2553	61	0
2	2e	2560	0	2553	60	0
3	2F	1803	0	1779	65	0
3	2f	1803	0	1779	63	0
4	2G	1671	0	1617	47	0
4	2g	1671	0	1617	49	0
5	2H	801	0	788	20	0
5	2h	801	0	788	23	0
6	2I	915	0	890	14	0
6	2i	915	0	890	13	0
7	2J	839	0	803	24	0
7	2j	839	0	803	24	0
8	2K	795	0	782	28	0
8	2k	795	0	782	30	0
9	2L	722	0	709	19	0
9	2l	722	0	709	18	0
10	2M	640	0	611	14	0
10	2m	640	0	611	16	0
11	2N	505	0	509	15	0
11	2n	505	0	509	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	2O	356	0	365	9	0
12	2o	356	0	365	7	0
13	2T	567	0	569	18	0
13	2t	567	0	569	20	0
14	3T	655	0	669	16	0
14	3t	655	0	669	13	0
15	4A	816	0	795	10	0
15	4a	816	0	795	13	0
16	4T	481	0	465	12	0
16	4t	481	0	465	12	0
17	5T	506	0	506	8	0
17	5t	506	0	506	8	0
18	6A	1083	0	1020	24	0
18	6a	1083	0	1020	21	0
19	6B	1912	0	1768	38	0
19	6b	1912	0	1768	41	0
20	6C	891	0	811	30	0
20	6c	891	0	811	29	0
21	6L	636	0	639	6	0
21	6l	636	0	639	6	0
22	6T	561	0	564	14	0
22	6t	561	0	564	13	0
23	7A	1166	0	1129	35	0
23	7a	1166	0	1129	33	0
24	7C	1825	0	1636	31	0
24	7c	1825	0	1636	30	0
25	7L	1078	0	1071	33	0
25	7l	1078	0	1071	33	0
26	A	3756	0	3557	62	0
26	a	3756	0	3557	59	0
27	B	3398	0	3463	50	0
27	b	3398	0	3463	52	0
28	BP	2920	0	2817	65	0
28	bp	2920	0	2817	65	0
29	C1	5576	0	5621	166	0
29	c1	5576	0	5621	173	0
30	C2	5094	0	5078	135	0
30	c2	5094	0	5078	142	0
31	C3	5084	0	5067	125	0
31	c3	5084	0	5067	130	0
32	D	2366	0	2290	34	0
32	d	2366	0	2290	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	E	3176	0	3108	76	0
33	e	3176	0	3108	75	0
34	F	2024	0	1958	55	0
34	f	2024	0	1958	56	0
35	FS	1509	0	1477	37	0
35	fs	1509	0	1477	38	0
36	G	2442	0	2290	70	0
36	g	2442	0	2290	72	0
37	H	2369	0	2319	49	0
37	h	2369	0	2319	54	0
38	I	1943	0	1865	48	0
38	i	1943	0	1865	45	0
39	J	1575	0	1567	26	0
39	j	1575	0	1567	25	0
40	K	1714	0	1678	37	0
40	k	1714	0	1678	34	0
41	L	1668	0	1643	34	0
41	l	1668	0	1643	33	0
42	M	1872	0	1760	74	0
42	m	1872	0	1760	74	0
43	M1	2863	0	2781	63	0
43	m1	2863	0	2781	65	0
44	M2	2558	0	2552	41	0
44	m2	2558	0	2552	45	0
45	M3	2620	0	2584	45	0
45	m3	2620	0	2584	43	0
46	N	1716	0	1648	45	0
46	n	1716	0	1648	44	0
47	O	1081	0	1053	17	0
47	o	1081	0	1053	18	0
48	P	1410	0	1391	27	0
48	p	1410	0	1391	27	0
49	Q	1434	0	1393	42	0
49	q	1434	0	1393	38	0
50	R	1407	0	1419	28	0
50	r	1407	0	1419	33	0
51	S	1388	0	1407	39	0
51	s	1388	0	1407	32	0
52	SA	4624	0	4573	124	0
52	sa	4624	0	4573	121	0
53	SB	2260	0	2233	60	0
53	sb	2260	0	2233	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	SC	481	0	475	18	0
54	sc	481	0	475	17	0
55	SD	393	0	413	13	0
55	sd	393	0	413	14	0
56	T	1315	0	1286	28	0
56	t	1315	0	1286	29	0
57	U	1304	0	1299	34	0
57	u	1304	0	1299	34	0
58	V	1234	0	1194	33	0
58	v	1234	0	1194	34	0
59	VB	4630	0	4406	120	0
59	vb	4630	0	4406	115	0
60	W	1096	0	1031	29	0
60	w	1096	0	1031	29	0
61	X	1012	0	1000	14	0
61	x	1012	0	1000	13	0
62	Y	859	0	812	23	0
62	y	859	0	812	26	0
63	Y0	775	0	798	23	0
63	y0	775	0	798	25	0
64	Y5	1659	0	1726	35	0
64	y5	1659	0	1726	35	0
65	Y7	2938	0	3010	69	0
65	y7	2938	0	3010	70	0
66	Z	717	0	694	19	0
66	z	717	0	694	21	0
67	Z1	766	0	747	9	0
67	z1	766	0	747	9	0
68	1B	516	0	528	24	0
68	1b	516	0	528	25	0
69	2B	1483	0	1554	43	0
69	2b	1483	0	1554	40	0
70	4L	957	0	987	34	0
70	4l	957	0	987	35	0
71	5B	888	0	917	30	0
71	5b	888	0	917	34	0
72	A1	806	0	801	22	0
72	a1	806	0	801	23	0
73	A2	811	0	800	26	0
73	a2	811	0	800	24	0
74	A3	1077	0	1004	27	0
74	a3	1077	0	1004	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	A5	1307	0	1317	25	0
75	a5	1307	0	1317	25	0
76	A6	1421	0	1382	39	0
76	a6	1421	0	1382	36	0
77	A7	2347	0	2249	50	0
77	a7	2347	0	2249	48	0
78	A8	1075	0	1024	22	0
78	a8	1075	0	1024	23	0
79	A9	2736	0	2665	49	0
79	a9	2736	0	2665	49	0
80	AB	926	0	902	12	0
80	ab	926	0	902	12	0
81	AC	806	0	784	15	0
81	ac	806	0	784	15	0
82	AL	1612	0	1511	40	0
82	al	1612	0	1511	39	0
83	AM	1349	0	1375	52	0
83	am	1349	0	1375	52	0
84	AN	1879	0	1818	27	0
84	an	1879	0	1818	28	0
85	B2	966	0	940	22	0
85	b2	966	0	940	20	0
86	B3	602	0	593	17	0
86	b3	602	0	593	16	0
87	B4	976	0	880	20	0
87	b4	976	0	880	21	0
88	B6	596	0	583	12	0
88	b6	596	0	583	15	0
89	B7	941	0	884	16	0
89	b7	941	0	884	17	0
90	B8	1456	0	1415	43	0
90	b8	1456	0	1415	44	0
91	B9	1596	0	1507	25	0
91	b9	1596	0	1507	25	0
92	BL	1461	0	1467	30	0
92	bl	1461	0	1467	36	0
93	BM	1321	0	1256	26	0
93	bm	1321	0	1256	27	0
94	C4	850	0	840	22	0
94	c4	850	0	840	18	0
95	FX	1162	0	1120	35	0
95	fx	1162	0	1120	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
96	G1	1773	0	1732	39	0
96	g1	1773	0	1732	39	0
97	G2	1762	0	1775	51	0
97	g2	1762	0	1775	45	0
98	G3	2804	0	2727	46	0
98	g3	2804	0	2727	47	0
99	J1	2170	0	2130	39	0
99	j1	2170	0	2130	40	0
100	N1	2305	0	2349	91	0
100	n1	2305	0	2349	93	0
101	N2	3073	0	3153	81	0
101	n2	3073	0	3153	77	0
102	N3	1017	0	1014	34	0
102	n3	1017	0	1014	34	0
103	N4	4170	0	4223	97	0
103	n4	4170	0	4223	104	0
104	N5	5908	0	5946	165	0
104	n5	5908	0	5946	165	0
105	N6	2168	0	2167	57	0
105	n6	2168	0	2167	63	0
106	P1	1908	0	1861	52	0
106	p1	1908	0	1861	51	0
107	P2	1414	0	1378	38	0
107	p2	1414	0	1378	40	0
108	QA	3517	0	3512	56	0
108	Qa	3517	0	3512	65	0
108	qA	3517	0	3512	57	0
108	qa	3517	0	3512	65	0
109	QB	3835	0	3734	63	0
109	Qb	3835	0	3734	89	0
109	qB	3835	0	3734	62	0
109	qb	3835	0	3734	84	0
110	QC	3589	0	3483	94	0
110	Qc	3580	0	3470	110	0
110	qC	3589	0	3483	99	0
110	qc	3580	0	3470	110	0
111	QD	2489	0	2343	54	0
111	Qd	2489	0	2343	65	0
111	qD	2489	0	2343	53	0
111	qd	2489	0	2343	63	0
112	QE	1559	0	1222	35	0
112	Qe	1471	0	1136	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
112	qE	1559	0	1222	36	0
112	qe	1471	0	1136	40	0
113	QF	702	0	700	21	0
113	Qf	630	0	633	12	0
113	qF	702	0	700	19	0
113	qf	630	0	633	11	0
114	QG	2767	0	2706	49	0
114	Qg	2760	0	2697	67	0
114	qG	2767	0	2706	54	0
114	qg	2760	0	2697	68	0
115	QH	1098	0	1040	28	0
115	Qh	1098	0	1040	36	0
115	qH	1098	0	1040	28	0
115	qh	1098	0	1040	35	0
116	QI	971	0	986	14	0
116	Qi	971	0	986	19	0
116	qI	971	0	986	13	0
116	qi	971	0	986	20	0
117	QJ	481	0	477	14	0
117	Qj	501	0	503	8	0
117	qJ	481	0	477	14	0
117	qj	501	0	503	9	0
118	QL	266	0	282	2	0
118	Ql	266	0	282	4	0
118	qL	266	0	282	2	0
118	ql	266	0	282	4	0
119	QM	85	0	19	0	0
119	Qm	85	0	19	0	0
119	U2	85	0	20	1	0
119	qM	85	0	19	0	0
119	qm	85	0	19	0	0
119	u2	85	0	20	1	0
120	S1	5410	0	5364	134	0
120	s1	5410	0	5364	125	0
121	S2	3598	0	3552	112	0
121	s2	3598	0	3552	110	0
122	S3	1681	0	1679	55	0
122	s3	1681	0	1679	51	0
123	S4	1500	0	1449	42	0
123	s4	1500	0	1449	39	0
124	S5	756	0	725	25	0
124	s5	756	0	725	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
125	S6	738	0	724	12	0
125	s6	738	0	724	16	0
126	S7	1278	0	1271	43	0
126	s7	1278	0	1271	42	0
127	S8	1812	0	1688	62	0
127	s8	1812	0	1688	59	0
128	T1	4059	0	4009	71	0
128	t1	4059	0	4009	67	0
129	T2	2180	0	2178	42	0
129	t2	2180	0	2178	40	0
130	T3	2479	0	2473	42	0
130	t3	2479	0	2473	42	0
131	T4	1644	0	1632	35	0
131	t4	1644	0	1632	33	0
132	T5	1138	0	1160	29	0
132	t5	1138	0	1160	28	0
133	T6	903	0	853	7	0
133	t6	903	0	853	4	0
134	T7	1187	0	1137	24	0
134	t7	1187	0	1137	22	0
135	T8	1084	0	1110	28	0
135	t8	1084	0	1110	28	0
136	T9	1066	0	1023	19	0
136	t9	1066	0	1023	20	0
137	TA	854	0	839	16	0
137	ta	854	0	839	18	0
138	TB	801	0	763	17	0
138	tb	801	0	763	17	0
139	TC	789	0	745	19	0
139	tc	789	0	745	21	0
140	TD	616	0	611	8	0
140	td	616	0	611	8	0
141	TE	420	0	427	8	0
141	te	420	0	427	7	0
142	TF	1789	0	1795	26	0
142	tf	1789	0	1795	25	0
143	TG	1081	0	1091	12	0
143	tg	1081	0	1091	12	0
144	TH	996	0	1023	20	0
144	th	996	0	1023	22	0
145	TX	1206	0	1155	24	0
145	tx	1206	0	1155	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
146	V1	3410	0	3357	71	0
146	v1	3410	0	3357	71	0
147	V2	1858	0	1842	43	0
147	v2	1858	0	1842	37	0
148	X1	1227	0	1208	26	0
148	x1	1227	0	1208	25	0
149	C	1368	0	1172	21	0
149	c	1368	0	1172	22	0
150	U1	460	0	95	4	0
150	u1	460	0	95	4	0
151	2E	43	0	31	1	0
151	2e	43	0	31	1	0
151	QD	43	0	30	1	0
151	Qd	43	0	30	0	0
151	qD	43	0	30	1	0
151	qd	43	0	30	0	0
152	2F	121	0	167	10	0
152	2G	50	0	77	3	0
152	2J	42	0	58	0	0
152	2f	121	0	167	10	0
152	2g	50	0	77	3	0
152	2j	42	0	58	0	0
152	5B	47	0	68	3	0
152	5b	47	0	68	3	0
152	6A	35	0	44	1	0
152	6C	33	0	40	0	0
152	6a	35	0	44	1	0
152	6c	33	0	40	0	0
152	7A	45	0	64	3	0
152	7C	43	0	63	5	0
152	7a	45	0	64	3	0
152	7c	43	0	63	5	0
152	A	82	0	112	6	0
152	AL	26	0	26	1	0
152	AM	39	0	52	4	0
152	AN	36	0	46	3	0
152	B9	34	0	42	3	0
152	C1	171	0	238	19	0
152	C2	36	0	46	1	0
152	C3	210	0	296	12	0
152	C4	41	0	56	4	0
152	D	35	0	44	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
152	F	38	0	50	2	0
152	FS	40	0	54	5	0
152	I	39	0	52	7	0
152	J	37	0	48	1	0
152	J1	40	0	54	3	0
152	M	116	0	157	6	0
152	M1	96	0	146	10	0
152	M2	132	0	195	6	0
152	N	109	0	140	11	0
152	N1	36	0	46	2	0
152	N3	31	0	36	1	0
152	N5	198	0	304	21	0
152	N6	54	0	88	7	0
152	P1	40	0	54	1	0
152	QB	44	0	65	4	0
152	QC	124	0	173	6	0
152	QE	63	0	74	6	0
152	QG	32	0	38	0	0
152	QI	73	0	97	11	0
152	QJ	66	0	80	6	0
152	Qb	43	0	63	4	0
152	Qc	85	0	121	6	0
152	Qe	76	0	103	3	0
152	Qg	32	0	38	3	0
152	Qi	72	0	95	5	0
152	Qj	36	0	46	2	0
152	S8	30	0	34	2	0
152	T1	33	0	40	0	0
152	T4	102	0	161	5	0
152	TC	89	0	129	6	0
152	TE	32	0	38	1	0
152	V	84	0	119	3	0
152	W	126	0	177	11	0
152	a	82	0	112	6	0
152	al	26	0	26	1	0
152	am	39	0	52	4	0
152	an	36	0	46	3	0
152	b9	34	0	42	3	0
152	c1	171	0	238	17	0
152	c2	36	0	46	1	0
152	c3	210	0	296	13	0
152	c4	41	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
152	d	35	0	44	5	0
152	f	38	0	50	2	0
152	fs	40	0	54	5	0
152	i	39	0	52	7	0
152	j	37	0	48	1	0
152	j1	40	0	54	3	0
152	m	116	0	157	6	0
152	m1	96	0	146	10	0
152	m2	132	0	195	7	0
152	n	109	0	140	12	0
152	n1	36	0	46	2	0
152	n3	31	0	36	2	0
152	n5	198	0	304	21	0
152	n6	54	0	88	6	0
152	p1	40	0	54	1	0
152	qB	44	0	65	5	0
152	qC	124	0	173	7	0
152	qE	91	0	104	8	0
152	qG	32	0	38	0	0
152	qI	73	0	97	10	0
152	qJ	38	0	50	4	0
152	qb	43	0	63	2	0
152	qc	85	0	121	6	0
152	qe	76	0	103	4	0
152	qg	32	0	38	3	0
152	qi	72	0	95	5	0
152	qj	36	0	46	2	0
152	s8	30	0	34	2	0
152	t1	33	0	40	0	0
152	t4	102	0	161	4	0
152	tc	89	0	129	9	0
152	te	32	0	38	1	0
152	v	84	0	119	4	0
152	w	126	0	177	11	0
153	2B	87	0	124	11	0
153	2G	207	0	255	13	0
153	2K	98	0	149	8	0
153	2M	96	0	145	8	0
153	2O	50	0	44	1	0
153	2b	87	0	124	10	0
153	2g	207	0	255	11	0
153	2k	98	0	149	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	2m	96	0	145	6	0
153	2o	50	0	44	1	0
153	5B	81	0	106	8	0
153	5b	81	0	106	7	0
153	6A	74	0	92	2	0
153	6C	157	0	205	16	0
153	6a	74	0	92	3	0
153	6c	157	0	205	15	0
153	7A	162	0	224	15	0
153	7C	136	0	166	8	0
153	7a	162	0	224	16	0
153	7c	136	0	166	8	0
153	A	145	0	184	11	0
153	A1	133	0	154	11	0
153	A9	163	0	217	10	0
153	AL	53	0	50	3	0
153	AM	56	0	56	6	0
153	AN	87	0	124	6	0
153	B	62	0	68	1	0
153	B3	140	0	171	6	0
153	B4	37	0	18	2	0
153	B8	69	0	82	5	0
153	BM	86	0	119	12	0
153	C	64	0	75	3	0
153	C1	302	0	389	34	0
153	C3	68	0	80	4	0
153	C4	98	0	149	4	0
153	E	195	0	228	17	0
153	F	100	0	156	10	0
153	FS	47	0	38	6	0
153	I	152	0	195	11	0
153	J	70	0	84	2	0
153	L	74	0	95	2	0
153	M	277	0	336	19	0
153	M1	214	0	266	16	0
153	M2	194	0	220	11	0
153	M3	118	0	124	5	0
153	N	84	0	118	7	0
153	N5	90	0	130	7	0
153	N6	90	0	130	7	0
153	P1	121	0	130	7	0
153	Q	135	0	161	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	QB	68	0	80	6	0
153	QC	120	0	128	9	0
153	QD	61	0	66	1	0
153	QG	86	0	122	1	0
153	QH	94	0	138	8	0
153	QI	71	0	86	5	0
153	Qb	68	0	80	3	0
153	Qc	167	0	166	3	0
153	Qg	100	0	156	9	0
153	Qi	71	0	86	5	0
153	R	65	0	74	4	0
153	SD	76	0	99	5	0
153	T	295	0	375	30	0
153	T1	55	0	54	4	0
153	T5	96	0	142	13	0
153	T7	73	0	93	8	0
153	TE	53	0	50	5	0
153	TH	84	0	115	5	0
153	U	60	0	64	4	0
153	U1	57	0	58	2	0
153	VB	297	0	382	26	0
153	W	84	0	118	7	0
153	Y5	70	0	84	1	0
153	Y7	65	0	74	2	0
153	Z	67	0	78	1	0
153	a	227	0	295	16	0
153	a1	67	0	78	9	0
153	a9	163	0	217	10	0
153	al	53	0	50	3	0
153	am	56	0	56	6	0
153	an	87	0	124	5	0
153	b	62	0	68	1	0
153	b3	140	0	171	5	0
153	b4	37	0	18	2	0
153	b8	69	0	82	5	0
153	bm	86	0	119	12	0
153	c	64	0	75	4	0
153	c1	302	0	389	32	0
153	c3	68	0	80	4	0
153	c4	98	0	149	5	0
153	e	195	0	228	17	0
153	f	100	0	156	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
153	fs	47	0	38	5	0
153	i	152	0	195	14	0
153	j	70	0	84	3	0
153	l	74	0	95	2	0
153	m	277	0	336	19	0
153	m1	214	0	266	15	0
153	m2	194	0	220	11	0
153	m3	118	0	124	5	0
153	n	84	0	118	7	0
153	n5	90	0	130	10	0
153	n6	90	0	130	7	0
153	p1	121	0	130	8	0
153	q	221	0	280	21	0
153	qB	68	0	80	6	0
153	qC	120	0	128	9	0
153	qD	61	0	66	1	0
153	qG	86	0	122	1	0
153	qH	94	0	138	8	0
153	qI	71	0	86	4	0
153	qb	68	0	80	3	0
153	qc	167	0	166	4	0
153	qg	100	0	156	8	0
153	qi	71	0	86	5	0
153	r	65	0	74	4	0
153	sd	76	0	99	5	0
153	t	295	0	375	31	0
153	t1	55	0	54	4	0
153	t5	96	0	142	12	0
153	t7	73	0	93	7	0
153	td	66	0	76	2	0
153	te	53	0	50	5	0
153	th	84	0	115	5	0
153	u	60	0	64	4	0
153	u1	57	0	58	2	0
153	vb	129	0	152	11	0
153	w	84	0	118	7	0
153	y5	70	0	84	1	0
153	y7	65	0	74	2	0
153	z	67	0	78	1	0
154	C1	120	0	108	19	0
154	c1	120	0	108	22	0
155	C1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
155	C2	2	0	0	0	0
155	c1	1	0	0	0	0
155	c2	2	0	0	0	0
156	C1	1	0	0	0	0
156	c1	1	0	0	0	0
157	FS	8	0	0	0	0
157	FX	4	0	0	0	0
157	QE	4	0	0	0	0
157	Qe	4	0	0	0	0
157	S1	4	0	0	0	0
157	SB	4	0	0	0	0
157	V2	4	0	0	0	0
157	fs	8	0	0	1	0
157	fx	4	0	0	0	0
157	qE	4	0	0	0	0
157	qe	4	0	0	0	0
157	s1	4	0	0	0	0
157	sb	4	0	0	0	0
157	v2	4	0	0	0	0
158	A3	89	0	126	10	0
158	AN	152	0	206	7	0
158	B4	48	0	73	6	0
158	BM	30	0	34	1	0
158	C4	51	0	82	3	0
158	G2	51	0	82	2	0
158	I	32	0	38	1	0
158	M2	31	0	36	2	0
158	M3	38	0	53	2	0
158	N4	36	0	46	0	0
158	N5	36	0	46	5	0
158	S8	41	0	59	0	0
158	SC	40	0	54	2	0
158	T4	25	0	24	1	0
158	T8	86	0	123	9	0
158	TA	26	0	26	1	0
158	VB	28	0	30	0	0
158	W	34	0	42	4	0
158	Y5	28	0	30	1	0
158	a3	89	0	126	10	0
158	an	152	0	206	7	0
158	b4	48	0	73	5	0
158	bm	30	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
158	c4	51	0	82	3	0
158	g2	51	0	82	1	0
158	i	32	0	38	1	0
158	m2	31	0	36	2	0
158	m3	38	0	53	2	0
158	n4	36	0	46	1	0
158	n5	36	0	46	4	0
158	s8	41	0	59	0	0
158	sc	40	0	54	2	0
158	t4	25	0	24	0	0
158	t8	86	0	123	9	0
158	ta	26	0	26	1	0
158	vb	28	0	30	0	0
158	w	34	0	42	4	0
158	y5	28	0	30	1	0
159	M2	36	0	38	1	0
159	m2	36	0	38	1	0
160	Qh	36	0	52	4	0
160	R	33	0	43	2	0
160	Y5	21	0	16	1	0
160	qh	36	0	52	4	0
160	r	33	0	43	2	0
160	y5	21	0	16	1	0
161	SA	53	0	29	5	0
161	sa	53	0	29	5	0
162	S1	16	0	0	3	0
162	S7	8	0	0	2	0
162	S8	16	0	0	2	0
162	SB	8	0	0	0	0
162	V1	8	0	0	1	0
162	s1	16	0	0	3	0
162	s7	8	0	0	2	0
162	s8	16	0	0	3	0
162	sb	8	0	0	0	0
162	v1	8	0	0	1	0
163	SB	7	0	0	1	0
163	sb	7	0	0	1	0
164	B8	63	0	90	8	0
164	QC	29	0	33	2	0
164	Qc	55	0	68	6	0
164	SC	63	0	90	6	0
164	b8	63	0	90	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
164	qC	29	0	33	1	0
164	qc	55	0	68	5	0
164	sc	63	0	90	7	0
165	S6	1	0	0	0	0
165	VB	2	0	0	0	0
165	s6	1	0	0	0	0
165	vb	2	0	0	0	0
166	QC	86	0	60	9	0
166	Qc	86	0	60	12	0
166	Y5	43	0	30	0	0
166	qC	86	0	60	10	0
166	qc	86	0	60	13	0
166	y5	43	0	30	0	0
167	A9	48	0	26	1	0
167	a9	48	0	26	1	0
168	AB	37	0	47	12	0
168	ab	37	0	47	12	0
169	B6	55	0	0	0	0
169	b6	55	0	0	0	0
170	B9	27	0	12	0	0
170	b9	27	0	12	1	0
171	V1	31	0	19	2	0
171	v1	31	0	19	1	0
All	All	568568	0	562502	10494	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 9.

All (10494) 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)
33:e:192:SER:HG	42:M:2:SER:N	1.56	1.02
31:c3:258:TYR:HH	45:m3:2:ALA:N	1.70	0.89
28:bp:176:SER:HB2	28:bp:192:TYR:O	1.72	0.88
28:BP:176:SER:HB2	28:BP:192:TYR:O	1.75	0.87
42:m:2:SER:N	33:E:192:SER:HG	1.74	0.86
127:s8:124:HIS:HE1	162:s8:302:SF4:S4	2.01	0.84
31:C3:258:TYR:HH	45:M3:2:ALA:N	1.76	0.83
105:N6:126:LEU:HD22	153:N6:302:CDL:H741	1.60	0.83
127:S8:124:HIS:HE1	162:S8:302:SF4:S4	2.01	0.83
75:a5:170:ALA:HA	122:s3:91:LYS:HG3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
105:n6:126:LEU:HD22	153:n6:302:CDL:H741	1.60	0.82
52:SA:81:PHE:HB3	52:SA:84:ARG:HG3	1.62	0.82
52:sa:81:PHE:HB3	52:sa:84:ARG:HG3	1.62	0.81
75:A5:170:ALA:HA	122:S3:91:LYS:HG3	1.60	0.81
99:j1:154:TYR:O	99:j1:179:SER:N	2.15	0.80
111:qd:38:LYS:NZ	115:qh:122:CYS:SG	2.55	0.80
2:2E:10:ASN:HD22	2:2E:84:HIS:HA	1.47	0.80
99:J1:154:TYR:O	99:J1:179:SER:N	2.15	0.79
120:S1:592:ASN:HB3	120:S1:596:ARG:HB2	1.65	0.79
31:c3:138:LEU:HB3	31:c3:149:PHE:O	1.83	0.78
120:s1:592:ASN:HB3	120:s1:596:ARG:HB2	1.64	0.78
123:S4:4:PRO:HB2	123:S4:11:ALA:HB1	1.65	0.78
111:Qd:38:LYS:NZ	115:Qh:122:CYS:SG	2.55	0.78
128:t1:17:THR:HB	128:t1:124:PRO:HA	1.66	0.77
123:s4:4:PRO:HB2	123:s4:11:ALA:HB1	1.65	0.77
128:T1:17:THR:HB	128:T1:124:PRO:HA	1.66	0.77
72:A1:47:ARG:NH2	72:A1:56:GLU:OE2	2.18	0.77
2:2e:10:ASN:HD22	2:2e:84:HIS:HA	1.48	0.76
72:a1:47:ARG:NH2	72:a1:56:GLU:OE2	2.18	0.76
99:j1:47:LEU:HD13	99:j1:73:ILE:HD12	1.68	0.76
52:sa:226:SER:O	52:sa:230:GLY:N	2.19	0.76
96:g1:122:ILE:HD11	96:g1:199:ALA:HA	1.67	0.76
80:ab:86:GLN:HE21	80:ab:90:LYS:HE3	1.51	0.76
108:qA:125:ASN:ND2	114:qg:167:SER:O	2.19	0.76
80:AB:86:GLN:HE21	80:AB:90:LYS:HE3	1.51	0.76
37:h:82:LYS:NZ	104:N5:64:VAL:O	2.19	0.75
91:b9:152:PHE:HB2	97:g2:175:ALA:HB1	1.68	0.75
153:c1:712:CDL:H511	153:m1:404:CDL:H742	1.69	0.75
35:fs:149:ASN:HD22	36:g:259:THR:HG21	1.51	0.75
35:FS:149:ASN:HD22	36:G:259:THR:HG21	1.51	0.75
18:6a:52:HIS:O	18:6a:56:ASN:ND2	2.20	0.75
28:bp:417:ILE:HB	28:bp:438:ALA:HB3	1.69	0.75
126:S7:29:LEU:HB2	126:S7:67:GLY:HA3	1.69	0.75
100:n1:88:PHE:HB2	139:tc:11:ARG:HD3	1.67	0.75
91:B9:152:PHE:HB2	97:G2:175:ALA:HB1	1.67	0.75
20:6C:33:ALA:HA	20:6C:36:TRP:CD1	2.22	0.75
110:qc:88:VAL:HG22	166:qc:502:HEM:HBC2	1.68	0.75
96:G1:122:ILE:HD11	96:G1:199:ALA:HA	1.67	0.75
108:qA:422:LYS:HD2	114:qG:327:GLN:HB3	1.67	0.74
114:qG:183:PRO:HA	114:qG:186:MET:HG2	1.69	0.74
3:2F:203:HIS:HA	3:2F:212:ARG:HH21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
100:N1:88:PHE:HB2	139:TC:11:ARG:HD3	1.68	0.74
108:QA:125:ASN:ND2	114:Qg:167:SER:O	2.19	0.74
153:C1:712:CDL:H511	153:M1:404:CDL:H742	1.68	0.74
52:SA:226:SER:O	52:SA:230:GLY:N	2.20	0.74
24:7C:233:MET:HB2	43:M1:14:LEU:HD12	1.70	0.74
99:J1:47:LEU:HD13	99:J1:73:ILE:HD12	1.68	0.74
20:6c:33:ALA:HA	20:6c:36:TRP:CD1	2.22	0.74
18:6A:52:HIS:O	18:6A:56:ASN:ND2	2.20	0.74
121:S2:329:LEU:HB2	121:S2:332:LEU:HD23	1.70	0.74
82:al:37:ARG:NH1	127:s8:112:GLU:OE2	2.21	0.74
100:n1:109:MET:HG3	100:n1:183:PHE:HB2	1.70	0.74
104:N5:80:SER:O	104:N5:83:ASN:N	2.19	0.74
128:T1:264:LYS:NZ	128:T1:304:ASP:O	2.21	0.73
129:T2:70:LYS:HB2	129:T2:117:ALA:HA	1.70	0.73
13:2t:50:LYS:HG3	17:5t:35:SER:HA	1.71	0.73
53:sb:122:CYS:HB3	53:sb:127:CYS:SG	2.27	0.73
95:fx:49:ASN:O	95:fx:52:GLY:N	2.20	0.73
82:AL:37:ARG:NH1	127:S8:112:GLU:OE2	2.21	0.73
87:B4:56:TYR:HH	138:TB:18:ARG:N	1.85	0.73
110:Qc:88:VAL:HG22	166:Qc:502:HEM:HBC2	1.68	0.73
4:2g:102:TYR:OH	53:sb:234:ARG:NH2	2.20	0.73
104:n5:80:SER:O	104:n5:83:ASN:N	2.19	0.73
3:2f:203:HIS:HA	3:2f:212:ARG:HH21	1.53	0.73
28:BP:417:ILE:HB	28:BP:438:ALA:HB3	1.69	0.73
3:2f:140:GLN:HE22	152:2f:301:PC1:H133	1.53	0.73
29:c1:310:PHE:HE1	153:c1:709:CDL:H721	1.54	0.73
29:C1:41:LEU:HD11	153:C1:701:CDL:HA61	1.70	0.73
100:n1:76:ILE:HA	102:n3:27:ALA:HB1	1.70	0.73
29:C1:672:ARG:HH21	43:M1:298:ALA:HB3	1.54	0.73
24:7c:233:MET:HB2	43:m1:14:LEU:HD12	1.70	0.73
91:b9:154:GLU:O	138:tb:18:ARG:NH2	2.22	0.73
126:s7:29:LEU:HB2	126:s7:67:GLY:HA3	1.69	0.73
52:sa:90:ALA:HB3	52:sa:184:GLY:HA3	1.70	0.73
129:t2:70:LYS:HB2	129:t2:117:ALA:HA	1.70	0.73
52:SA:90:ALA:HB3	52:SA:184:GLY:HA3	1.70	0.73
95:FX:49:ASN:O	95:FX:52:GLY:N	2.20	0.73
108:QA:422:LYS:HD2	114:QG:327:GLN:HB3	1.69	0.73
104:n5:64:VAL:O	37:H:82:LYS:NZ	2.18	0.72
121:s2:329:LEU:HB2	121:s2:332:LEU:HD23	1.69	0.72
29:C1:508:LEU:HB3	154:C1:703:HEA:HMA	1.70	0.72
104:N5:497:VAL:HG21	104:N5:595:LEU:HD21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2f:155:LEU:HD11	3:2f:245:LEU:HB2	1.71	0.72
104:n5:497:VAL:HG21	104:n5:595:LEU:HD21	1.71	0.72
89:B7:83:GLU:OE2	90:B8:115:ASN:ND2	2.22	0.72
128:T1:123:ILE:HD11	128:T1:152:LYS:HD3	1.71	0.72
29:C1:310:PHE:HE1	153:C1:708:CDL:H721	1.54	0.72
29:c1:41:LEU:HD11	153:c1:701:CDL:HA61	1.70	0.72
114:QG:183:PRO:HA	114:QG:186:MET:HG2	1.69	0.72
37:h:295:LYS:HG2	104:N5:83:ASN:HD21	1.55	0.72
13:2T:50:LYS:HG3	17:5T:35:SER:HA	1.70	0.72
29:c1:672:ARG:HH21	43:m1:298:ALA:HB3	1.54	0.72
74:a3:28:ASP:O	74:a3:34:ASN:ND2	2.22	0.72
3:2F:140:GLN:HE22	152:2F:301:PC1:H133	1.53	0.72
3:2f:212:ARG:NH1	53:sb:36:CYS:SG	2.61	0.72
100:N1:76:ILE:HA	102:N3:27:ALA:HB1	1.72	0.72
153:E:403:CDL:H351	153:E:403:CDL:H111	1.73	0.71
89:b7:83:GLU:OE2	90:b8:115:ASN:ND2	2.23	0.71
104:n5:423:VAL:HG11	104:n5:526:GLY:HA3	1.71	0.71
104:N5:423:VAL:HG11	104:N5:526:GLY:HA3	1.71	0.71
110:QC:246:PHE:HB2	152:QC:505:PC1:H231	1.72	0.71
100:n1:261:ILE:HA	100:n1:266:GLY:HA2	1.73	0.71
110:qC:246:PHE:HB2	152:qC:505:PC1:H231	1.72	0.71
3:2F:155:LEU:HD11	3:2F:245:LEU:HB2	1.71	0.71
100:N1:109:MET:HG3	100:N1:183:PHE:HB2	1.70	0.71
120:S1:605:MET:HE2	120:S1:606:PRO:HD2	1.73	0.71
53:SB:122:CYS:HB3	53:SB:127:CYS:SG	2.30	0.71
107:P2:178:ASN:HD22	107:P2:181:ALA:H	1.38	0.71
146:V1:102:MET:SD	146:V1:242:THR:OG1	2.49	0.71
158:A3:201:3PE:H221	101:N2:32:ILE:HD13	1.73	0.71
128:t1:199:VAL:HB	128:t1:476:THR:HG23	1.73	0.71
38:I:170:ASN:HB3	38:I:173:ILE:HG12	1.73	0.71
79:A9:233:ARG:NH2	79:A9:314:LYS:O	2.24	0.71
29:c1:510:HIS:HD1	29:c1:513:LEU:H	1.39	0.71
128:t1:123:ILE:HD11	128:t1:152:LYS:HD3	1.71	0.71
82:AL:176:LYS:NZ	120:S1:558:ALA:O	2.23	0.70
110:Qc:203:MET:HE3	166:Qc:503:HEM:HAA1	1.73	0.70
109:qB:143:ARG:NH1	109:qB:216:GLN:O	2.24	0.70
110:Qc:278:PRO:HG3	110:Qc:286:MET:HG3	1.72	0.70
23:7A:92:LEU:HB3	23:7A:99:THR:HG21	1.73	0.70
38:i:109:ARG:HH21	152:i:304:PC1:H12	1.57	0.70
42:m:185:PRO:HG3	62:y:64:LEU:HD13	1.73	0.70
153:am:201:CDL:H731	153:t7:201:CDL:H172	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
131:t4:110:LEU:HD13	131:t4:114:THR:HG21	1.73	0.70
100:N1:261:ILE:HA	100:N1:266:GLY:HA2	1.73	0.70
158:a3:201:3PE:H221	101:n2:32:ILE:HD13	1.72	0.70
120:s1:605:MET:HE2	120:s1:606:PRO:HD2	1.73	0.70
40:K:115:LYS:HD3	40:K:150:PHE:HB3	1.73	0.70
128:T1:199:VAL:HB	128:T1:476:THR:HG23	1.74	0.70
81:ac:107:GLU:O	91:b9:1:MET:N	2.25	0.70
42:M:134:LEU:HD13	42:M:141:ARG:HD2	1.74	0.70
153:e:403:CDL:H351	153:e:403:CDL:H111	1.72	0.70
109:qb:405:TYR:OH	109:qb:407:ASN:ND2	2.24	0.70
146:v1:116:ILE:HD12	146:v1:157:ILE:HG12	1.73	0.70
109:QB:143:ARG:NH1	109:QB:216:GLN:O	2.24	0.70
145:TX:89:LYS:HG3	145:TX:94:VAL:HB	1.74	0.70
146:V1:116:ILE:HD12	146:V1:157:ILE:HG12	1.73	0.70
84:an:153:THR:HG21	84:an:165:GLY:HA3	1.74	0.70
112:QE:47:LYS:HB3	145:TX:74:GLU:HB3	1.74	0.70
56:T:94:ARG:NH2	153:T:203:CDL:OA4	2.25	0.70
91:B9:154:GLU:O	138:TB:18:ARG:NH2	2.22	0.70
152:c1:711:PC1:H272	153:q:203:CDL:H841	1.74	0.69
31:c3:504:LEU:HB2	152:c3:601:PC1:H3D1	1.74	0.69
153:t:203:CDL:H351	153:t:203:CDL:H172	1.74	0.69
103:n4:345:ILE:HG12	103:n4:363:PHE:HB3	1.74	0.69
153:AM:201:CDL:H731	153:T7:201:CDL:H172	1.71	0.69
37:h:169:ASN:HB3	37:h:247:GLU:HA	1.74	0.69
153:T:203:CDL:H351	153:T:203:CDL:H172	1.74	0.69
81:AC:107:GLU:O	91:B9:1:MET:N	2.25	0.69
103:N4:190:SER:HB3	103:N4:274:PRO:HD3	1.74	0.69
125:S6:72:ILE:HG12	125:S6:119:GLY:HA3	1.74	0.69
23:7a:92:LEU:HB3	23:7a:99:THR:HG21	1.73	0.69
103:n4:190:SER:HB3	103:n4:274:PRO:HD3	1.74	0.69
113:qF:54:PRO:HG2	112:qe:220:GLY:HA3	1.74	0.69
108:Qa:185:GLU:HG3	115:Qh:24:GLY:HA2	1.74	0.69
109:Qb:405:TYR:OH	109:Qb:407:ASN:ND2	2.25	0.69
34:f:239:GLN:NE2	34:f:347:ASN:O	2.26	0.69
40:k:115:LYS:HD3	40:k:150:PHE:HB3	1.73	0.69
110:qc:203:MET:HE3	166:qc:503:HEM:HAA1	1.73	0.69
146:v1:102:MET:SD	146:v1:242:THR:OG1	2.49	0.69
30:C2:541:ASN:ND2	30:C2:545:TYR:OH	2.24	0.69
74:A3:28:ASP:O	74:A3:34:ASN:ND2	2.23	0.69
110:Qc:366:ALA:HB1	152:Qc:509:PC1:H2A1	1.74	0.69
110:qc:366:ALA:HB1	152:qc:509:PC1:H2A1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
125:s6:72:ILE:HG12	125:s6:119:GLY:HA3	1.73	0.69
106:P1:125:PRO:HB2	152:P1:401:PC1:H392	1.73	0.69
30:c2:58:PHE:O	30:c2:59:ARG:NH1	2.26	0.69
38:i:170:ASN:HB3	38:i:173:ILE:HG12	1.72	0.69
59:VB:465:ARG:NH1	59:VB:519:GLU:OE1	2.24	0.69
121:s2:46:GLN:HB3	121:s2:54:ARG:HB2	1.73	0.69
29:C1:510:HIS:HD1	29:C1:513:LEU:H	1.40	0.69
29:c1:202:ILE:HD13	39:j:170:ILE:HG22	1.75	0.69
29:c1:437:VAL:HG11	29:c1:462:ILE:HD11	1.74	0.69
30:c2:391:LEU:HG	47:o:116:LEU:HD22	1.75	0.69
56:t:94:ARG:NH2	153:t:203:CDL:OA4	2.25	0.69
98:g3:297:PHE:O	98:g3:302:LYS:NZ	2.26	0.69
105:n6:39:GLN:NE2	139:tc:28:TYR:OH	2.26	0.69
110:qc:278:PRO:HG3	110:qc:286:MET:HG3	1.72	0.69
27:B:297:LYS:NZ	27:B:373:ASN:OD1	2.25	0.69
152:C1:711:PC1:H272	153:VB:703:CDL:H841	1.74	0.69
33:E:173:GLU:OE1	33:E:278:ASN:ND2	2.26	0.69
33:e:173:GLU:OE1	33:e:278:ASN:ND2	2.26	0.69
79:a9:233:ARG:NH2	79:a9:314:LYS:O	2.24	0.69
110:qC:184:LEU:HG	164:qc:501:U10:H252	1.74	0.69
112:qE:47:LYS:HB3	145:tx:74:GLU:HB3	1.73	0.69
68:1b:59:ILE:HG13	74:a3:81:ARG:HH12	1.58	0.69
98:g3:257:MET:HG3	101:n2:50:ILE:HD12	1.75	0.69
106:p1:125:PRO:HB2	152:p1:401:PC1:H392	1.73	0.69
108:qa:185:GLU:HG3	115:qh:24:GLY:HA2	1.75	0.69
11:2N:6:TRP:HA	54:SC:11:PHE:HB3	1.75	0.69
68:1B:59:ILE:HG13	74:A3:81:ARG:HH12	1.58	0.69
83:AM:52:LEU:HD21	153:T7:201:CDL:H332	1.75	0.69
11:2n:6:TRP:HA	54:sc:11:PHE:HB3	1.75	0.68
19:6b:121:GLN:HA	19:6b:124:TYR:HB2	1.74	0.68
42:m:134:LEU:HD13	42:m:141:ARG:HD2	1.74	0.68
153:q:202:CDL:H161	153:q:203:CDL:H182	1.74	0.68
104:n5:116:LEU:HD13	138:tb:93:ARG:HG3	1.75	0.68
104:n5:708:ILE:HG12	153:n5:806:CDL:H191	1.75	0.68
107:p2:178:ASN:HD22	107:p2:181:ALA:H	1.38	0.68
143:tg:44:TYR:HB2	143:tg:114:ILE:HG21	1.73	0.68
31:C3:504:LEU:HB2	152:C3:601:PC1:H3D1	1.74	0.68
113:QF:54:PRO:HG2	112:Qe:220:GLY:HA3	1.73	0.68
87:b4:56:TYR:HH	138:tb:18:ARG:N	1.91	0.68
104:n5:83:ASN:HD21	37:H:295:LYS:HG2	1.55	0.68
111:qD:69:SER:OG	111:qD:237:ASN:ND2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:F:239:GLN:NE2	34:F:347:ASN:O	2.26	0.68
40:k:55:TYR:O	46:n:117:GLN:NE2	2.26	0.68
51:s:160:SER:OG	34:F:304:ASN:ND2	2.26	0.68
3:2F:212:ARG:NH1	53:SB:36:CYS:SG	2.61	0.68
89:B7:102:ASP:O	90:B8:187:ARG:NH2	2.26	0.68
103:N4:345:ILE:HG12	103:N4:363:PHE:HB3	1.74	0.68
111:QD:134:ARG:HH12	111:QD:141:TYR:H	1.42	0.68
152:QI:201:PC1:H271	117:QJ:26:PRO:HG2	1.75	0.68
74:a3:109:ASN:ND2	101:n2:1:MET:SD	2.66	0.68
110:qc:116:TRP:CD2	166:qc:503:HEM:HBC1	2.29	0.68
114:qg:123:TYR:HA	114:qg:126:GLU:HB3	1.75	0.68
29:C1:437:VAL:HG11	29:C1:462:ILE:HD11	1.74	0.68
74:A3:109:ASN:ND2	101:N2:1:MET:SD	2.66	0.68
84:AN:153:THR:HG21	84:AN:165:GLY:HA3	1.74	0.68
2:2e:322:LEU:HD21	4:2g:11:PHE:HB2	1.76	0.68
29:c1:555:TYR:HB2	29:c1:621:MET:HE1	1.73	0.68
31:c3:266:LEU:HB3	31:c3:271:ILE:HG21	1.76	0.68
83:am:52:LEU:HD21	153:t7:201:CDL:H332	1.76	0.68
105:N6:39:GLN:NE2	139:TC:28:TYR:OH	2.26	0.68
120:S1:65:CYS:O	120:S1:185:ARG:NH2	2.24	0.68
68:1b:21:ARG:NH1	100:n1:43:GLU:OE2	2.27	0.68
76:a6:44:THR:O	76:a6:55:LYS:NZ	2.26	0.68
100:n1:283:ILE:HD12	134:t7:111:HIS:HA	1.76	0.68
110:Qc:116:TRP:CD2	166:Qc:503:HEM:HBC1	2.29	0.68
121:S2:46:GLN:HB3	121:S2:54:ARG:HB2	1.73	0.68
29:c1:454:MET:HE1	152:c1:706:PC1:H332	1.76	0.68
3:2F:135:TYR:O	9:2L:2:LYS:NZ	2.26	0.68
40:K:55:TYR:O	46:N:117:GLN:NE2	2.26	0.68
83:AM:143:ARG:NH1	105:N6:76:TYR:O	2.26	0.68
110:QC:184:LEU:HG	164:Qc:501:U10:H252	1.74	0.68
113:Qf:85:GLN:O	116:Qi:96:ARG:NH2	2.27	0.68
131:T4:110:LEU:HD13	131:T4:114:THR:HG21	1.73	0.68
31:c3:460:ILE:HG12	31:c3:492:ILE:HG21	1.75	0.68
152:qI:201:PC1:H271	117:qJ:26:PRO:HG2	1.74	0.68
30:C2:58:PHE:O	30:C2:59:ARG:NH1	2.26	0.68
42:M:185:PRO:HG3	62:Y:64:LEU:HD13	1.74	0.68
79:A9:193:ALA:O	79:A9:256:GLY:HA2	1.94	0.68
27:b:297:LYS:NZ	27:b:373:ASN:OD1	2.27	0.68
51:s:109:ILE:HG21	51:s:124:GLU:HG3	1.75	0.68
89:b7:102:ASP:O	90:b8:187:ARG:NH2	2.26	0.68
103:n4:400:THR:HG23	103:n4:478:ASP:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
106:p1:166:VAL:HG22	106:p1:173:ILE:HG22	1.75	0.68
29:C1:202:ILE:HD13	39:J:170:ILE:HG22	1.75	0.68
38:I:109:ARG:HH21	152:I:301:PC1:H12	1.57	0.68
3:2f:137:ARG:NH1	152:2f:301:PC1:O12	2.27	0.68
153:f:401:CDL:H842	152:fs:204:PC1:H282	1.75	0.68
120:S1:258:LEU:HD11	120:S1:414:LEU:HB2	1.76	0.68
51:s:146:SER:HA	37:H:41:ARG:HB2	1.74	0.67
83:am:143:ARG:NH1	105:n6:76:TYR:O	2.26	0.67
42:m:99:ASN:HB3	60:w:17:LEU:HD11	1.77	0.67
145:tx:89:LYS:HG3	145:tx:94:VAL:HB	1.75	0.67
19:6B:121:GLN:HA	19:6B:124:TYR:HB2	1.74	0.67
34:F:194:LYS:NZ	43:M1:231:GLU:O	2.25	0.67
41:L:137:LEU:O	41:L:148:ARG:NH1	2.27	0.67
42:M:107:TRP:NE1	152:W:204:PC1:O12	2.22	0.67
66:Z:59:SER:HA	66:Z:64:VAL:HG23	1.77	0.67
68:1B:21:ARG:NH1	100:N1:43:GLU:OE2	2.27	0.67
2:2e:33:ASP:O	2:2e:35:PHE:N	2.26	0.67
4:2g:97:ASN:HD21	8:2k:20:VAL:H	1.42	0.67
34:f:304:ASN:ND2	51:S:160:SER:OG	2.27	0.67
82:al:176:LYS:NZ	120:s1:558:ALA:O	2.23	0.67
86:b3:45:LYS:HG2	107:p2:121:GLU:HG2	1.76	0.67
111:qD:134:ARG:HH12	111:qD:141:TYR:H	1.42	0.67
29:C1:454:MET:HE1	152:C1:709:PC1:H332	1.76	0.67
153:A1:102:CDL:HA62	140:TD:12:ASP:HB3	1.76	0.67
110:Qc:93:ILE:HG12	152:Qc:509:PC1:H231	1.76	0.67
122:S3:84:ASN:HB2	122:S3:87:ASN:HD22	1.58	0.67
52:sa:210:ASP:HA	52:sa:267:LEU:HG	1.75	0.67
100:n1:37:ALA:HB1	100:n1:67:TYR:HB2	1.76	0.67
110:qc:93:ILE:HG12	152:qc:509:PC1:H231	1.76	0.67
122:s3:84:ASN:HB2	122:s3:87:ASN:HD22	1.58	0.67
128:t1:87:VAL:HG13	128:t1:95:MET:HG3	1.76	0.67
3:2F:137:ARG:NH1	152:2F:301:PC1:O12	2.27	0.67
51:S:109:ILE:HG21	51:S:124:GLU:HG3	1.75	0.67
106:P1:120:GLU:HG2	153:P1:403:CDL:H342	1.75	0.67
152:c1:704:PC1:H31	31:c3:292:PHE:HE2	1.58	0.67
79:a9:193:ALA:O	79:a9:256:GLY:HA2	1.95	0.67
104:n5:85:LEU:O	104:n5:89:PHE:HB2	1.94	0.67
105:n6:251:ILE:HD13	121:s2:247:LYS:HE3	1.75	0.67
2:2E:151:THR:HA	2:2E:212:ALA:HB3	1.76	0.67
27:B:253:ARG:HB3	27:B:255:GLN:HG3	1.76	0.67
153:F:402:CDL:H842	152:FS:201:PC1:H282	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B3:45:LYS:HG2	107:P2:121:GLU:HG2	1.76	0.67
101:N2:146:THR:HG22	101:N2:148:PHE:H	1.59	0.67
104:N5:85:LEU:O	104:N5:89:PHE:HB2	1.94	0.67
104:N5:116:LEU:HD13	138:TB:93:ARG:HG3	1.76	0.67
105:N6:251:ILE:HD13	121:S2:247:LYS:HE3	1.74	0.67
7:2j:49:ARG:NH1	153:sd:101:CDL:OA3	2.28	0.67
27:b:253:ARG:HB3	27:b:255:GLN:HG3	1.76	0.67
29:c1:115:PHE:O	29:c1:119:ALA:HB3	1.95	0.67
29:c1:398:ILE:HB	154:c1:708:HEA:HBC1	1.77	0.67
29:c1:401:THR:HG21	29:c1:535:ALA:HA	1.77	0.67
106:p1:120:GLU:HG2	153:p1:403:CDL:H342	1.76	0.67
153:qc:505:CDL:OB3	114:qg:130:ARG:NH1	2.27	0.67
152:C1:706:PC1:H31	31:C3:292:PHE:HE2	1.58	0.67
82:AL:160:SER:HB3	120:S1:270:GLU:HG2	1.77	0.67
120:s1:65:CYS:O	120:s1:185:ARG:NH2	2.24	0.67
29:C1:115:PHE:O	29:C1:119:ALA:HB3	1.95	0.67
37:H:169:ASN:HB3	37:H:247:GLU:HA	1.75	0.67
83:AM:52:LEU:HD22	153:AM:201:CDL:H312	1.76	0.67
100:N1:37:ALA:HB1	100:N1:67:TYR:HB2	1.75	0.67
114:Qg:123:TYR:HA	114:Qg:126:GLU:HB3	1.76	0.67
122:s3:138:GLU:HG3	122:s3:156:LEU:HD23	1.77	0.67
30:C2:391:LEU:HG	47:O:116:LEU:HD22	1.75	0.67
100:N1:183:PHE:HB3	100:N1:261:ILE:HG21	1.76	0.67
104:N5:708:ILE:HG12	153:N5:806:CDL:H191	1.75	0.67
113:QF:70:GLU:OE1	113:QF:74:GLN:NE2	2.28	0.67
129:T2:223:ARG:HG2	129:T2:228:LEU:HD23	1.77	0.67
41:l:137:LEU:O	41:l:148:ARG:NH1	2.28	0.67
59:VB:497:HIS:HD1	65:Y7:189:TYR:HH	1.40	0.67
76:A6:172:PHE:O	82:AL:161:ARG:NH1	2.27	0.67
107:P2:33:ASP:OD1	107:P2:92:ASN:ND2	2.28	0.67
130:T3:48:LEU:HB2	130:T3:104:GLU:HG3	1.77	0.67
2:2e:11:LYS:HB3	2:2e:158:ASP:HA	1.76	0.67
46:n:76:ILE:HG13	46:n:77:THR:HG23	1.77	0.67
66:z:59:SER:HA	66:z:64:VAL:HG23	1.77	0.67
82:al:160:SER:HB3	120:s1:270:GLU:HG2	1.77	0.67
95:fx:126:GLU:OE2	95:fx:142:ARG:NH1	2.28	0.67
106:p1:142:ILE:HD13	153:p1:403:CDL:H532	1.77	0.67
130:t3:80:LYS:HE3	130:t3:82:ALA:HB3	1.77	0.67
2:2E:11:LYS:HB3	2:2E:158:ASP:HA	1.77	0.67
2:2E:33:ASP:O	2:2E:35:PHE:N	2.26	0.67
103:N4:310:ILE:HG23	103:N4:347:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:a6:172:PHE:O	82:al:161:ARG:NH1	2.27	0.66
85:b2:22:LYS:NZ	107:p2:182:TRP:O	2.26	0.66
103:n4:310:ILE:HG23	103:n4:347:LEU:HD11	1.75	0.66
42:M:99:ASN:HB3	60:W:17:LEU:HD11	1.76	0.66
46:N:76:ILE:HG13	46:N:77:THR:HG23	1.77	0.66
90:B8:91:TRP:NE1	164:B8:301:U10:O2	2.26	0.66
110:Qc:323:ASN:OD1	110:Qc:406:ARG:NH2	2.28	0.66
127:S8:124:HIS:CD2	127:S8:181:CYS:SG	2.88	0.66
146:V1:129:ARG:HE	146:V1:133:ARG:HH21	1.41	0.66
30:c2:160:ASP:HA	30:c2:163:LEU:HB2	1.77	0.66
29:C1:398:ILE:HB	154:C1:703:HEA:HBC1	1.76	0.66
153:AN:302:CDL:H261	153:AN:302:CDL:H732	1.77	0.66
90:B8:65:VAL:HG13	90:B8:66:ILE:HG13	1.77	0.66
106:P1:142:ILE:HD13	153:P1:403:CDL:H532	1.77	0.66
37:h:41:ARG:HB2	51:S:146:SER:HA	1.76	0.66
59:vb:465:ARG:NH1	59:vb:519:GLU:OE1	2.24	0.66
120:s1:258:LEU:HD11	120:s1:414:LEU:HB2	1.76	0.66
2:2E:322:LEU:HD21	4:2G:11:PHE:HB2	1.76	0.66
5:2H:152:ARG:O	9:2L:19:LYS:NZ	2.28	0.66
29:C1:401:THR:HG21	29:C1:535:ALA:HA	1.77	0.66
31:C3:460:ILE:HG12	31:C3:492:ILE:HG21	1.75	0.66
70:4L:82:LYS:HE3	121:S2:22:GLN:HB2	1.76	0.66
2:2e:151:THR:HA	2:2e:212:ALA:HB3	1.77	0.66
77:a7:7:ARG:HH21	153:t7:201:CDL:HB22	1.60	0.66
90:b8:65:VAL:HG13	90:b8:66:ILE:HG13	1.77	0.66
121:s2:399:TYR:OH	122:s3:67:ASP:O	2.14	0.66
32:D:160:ASP:HB2	32:D:186:ARG:HE	1.59	0.66
52:SA:381:VAL:HG13	52:SA:386:GLU:HG3	1.77	0.66
69:2B:163:SER:OG	135:T8:79:LYS:O	2.14	0.66
94:C4:54:MET:HE3	148:X1:22:PRO:HG3	1.78	0.66
95:FX:126:GLU:OE2	95:FX:142:ARG:NH1	2.28	0.66
106:P1:166:VAL:HG22	106:P1:173:ILE:HG22	1.76	0.66
126:S7:7:VAL:O	126:S7:11:ASN:N	2.27	0.66
128:T1:87:VAL:HG13	128:T1:95:MET:HG3	1.76	0.66
32:d:160:ASP:HB2	32:d:186:ARG:HE	1.59	0.66
103:n4:287:LYS:NZ	103:n4:364:SER:O	2.28	0.66
104:n5:79:ASP:OD2	57:U:17:TYR:OH	2.12	0.66
120:s1:357:ASP:OD2	120:s1:630:TYR:OH	2.14	0.66
110:QC:116:TRP:CD2	166:QC:502:HEM:HBC1	2.30	0.66
1:1T:33:ASN:O	22:6T:39:GLN:NE2	2.29	0.66
146:V1:163:PHE:HB3	146:V1:166:GLU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
95:fx:49:ASN:HD21	95:fx:55:GLU:HG3	1.61	0.66
103:n4:287:LYS:HD2	103:n4:364:SER:HB2	1.78	0.66
127:s8:124:HIS:CD2	127:s8:181:CYS:SG	2.88	0.66
146:v1:129:ARG:HE	146:v1:133:ARG:HH21	1.41	0.66
30:C2:160:ASP:HA	30:C2:163:LEU:HB2	1.78	0.66
69:2B:176:ILE:HD11	101:N2:302:TYR:HB2	1.77	0.66
85:B2:22:LYS:NZ	107:P2:182:TRP:O	2.26	0.66
99:J1:278:LYS:HG2	124:S5:85:SER:HA	1.77	0.66
101:N2:27:PHE:O	101:N2:31:ASN:ND2	2.29	0.66
103:N4:400:THR:HG23	103:N4:478:ASP:HA	1.76	0.66
30:c2:114:THR:O	30:c2:132:ASN:ND2	2.29	0.66
34:f:240:SER:HB3	34:f:244:ASP:HB2	1.78	0.66
153:an:302:CDL:H602	153:an:302:CDL:H851	1.78	0.66
101:n2:27:PHE:O	101:n2:31:ASN:ND2	2.29	0.66
31:C3:138:LEU:HB3	31:C3:149:PHE:O	1.96	0.66
38:I:135:ILE:O	66:Z:17:ARG:NH1	2.29	0.66
44:M2:118:HIS:HB2	152:N:301:PC1:H12	1.77	0.66
125:S6:114:THR:HG22	125:S6:121:ARG:HG2	1.76	0.66
153:a1:101:CDL:HA62	140:td:12:ASP:HB3	1.76	0.66
90:b8:91:TRP:NE1	164:b8:301:U10:O2	2.26	0.66
95:fx:50:ARG:NH1	95:fx:162:GLN:OE1	2.27	0.66
129:t2:223:ARG:HG2	129:t2:228:LEU:HD23	1.77	0.66
52:SA:270:ARG:NH1	52:SA:559:ASN:OD1	2.29	0.66
153:Qc:505:CDL:OB3	114:Qg:130:ARG:NH1	2.27	0.66
121:S2:395:SER:HB3	122:S3:74:GLU:HG3	1.78	0.66
52:sa:589:ARG:NH2	52:sa:632:ALA:O	2.29	0.66
107:p2:33:ASP:OD1	107:p2:92:ASN:ND2	2.28	0.66
110:qC:116:TRP:CD2	166:qC:502:HEM:HBC1	2.30	0.66
108:qa:139:SER:OG	108:qa:154:ASN:ND2	2.29	0.66
114:qg:30:TRP:NE1	114:qg:196:GLU:OE1	2.27	0.66
4:2G:97:ASN:HD21	8:2K:20:VAL:H	1.43	0.66
20:6C:23:ARG:NH2	153:F:402:CDL:OA4	2.28	0.66
98:G3:257:MET:HG3	101:N2:50:ILE:HD12	1.76	0.66
114:Qg:30:TRP:NE1	114:Qg:196:GLU:OE1	2.28	0.66
130:T3:80:LYS:HE3	130:T3:82:ALA:HB3	1.77	0.66
5:2h:152:ARG:O	9:2l:19:LYS:NZ	2.28	0.65
30:c2:202:ARG:NH1	32:d:342:THR:OG1	2.29	0.65
153:m:303:CDL:H131	152:m:305:PC1:H32	1.78	0.65
83:am:52:LEU:HD22	153:am:201:CDL:H312	1.76	0.65
99:j1:278:LYS:HG2	124:s5:85:SER:HA	1.77	0.65
113:qf:85:GLN:O	116:qi:96:ARG:NH2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:E:402:CDL:HA31	153:E:402:CDL:HB4	1.78	0.65
153:Q:202:CDL:H161	153:VB:703:CDL:H182	1.76	0.65
3:2f:79:VAL:HG21	11:2n:56:ASP:HB2	1.79	0.65
44:m2:118:HIS:HB2	152:n:301:PC1:H12	1.76	0.65
100:n1:183:PHE:HB3	100:n1:261:ILE:HG21	1.76	0.65
101:n2:146:THR:HG22	101:n2:148:PHE:H	1.60	0.65
104:n5:289:LEU:HD22	104:n5:428:LEU:HD12	1.78	0.65
113:qF:70:GLU:OE1	113:qF:74:GLN:NE2	2.29	0.65
52:SA:589:ARG:NH2	52:SA:632:ALA:O	2.29	0.65
95:FX:49:ASN:HD21	95:FX:55:GLU:HG3	1.61	0.65
103:N4:287:LYS:HD2	103:N4:364:SER:HB2	1.78	0.65
3:2f:135:TYR:O	9:2l:2:LYS:NZ	2.26	0.65
23:7a:106:ASP:O	23:7a:129:ARG:NH2	2.30	0.65
69:2b:163:SER:OG	135:t8:79:LYS:O	2.14	0.65
117:qJ:14:ASN:HB3	152:qJ:101:PC1:H231	1.78	0.65
2:2E:159:SER:HA	2:2E:163:SER:HB3	1.79	0.65
152:C3:601:PC1:H3F1	153:VB:706:CDL:H801	1.77	0.65
153:AN:302:CDL:H851	153:AN:302:CDL:H602	1.78	0.65
89:B7:25:GLN:O	89:B7:43:LYS:NZ	2.28	0.65
94:c4:54:MET:HE3	148:x1:22:PRO:HG3	1.78	0.65
4:2G:138:ASN:OD1	4:2G:142:LYS:NZ	2.29	0.65
45:M3:189:LYS:H	45:M3:193:HIS:HD1	1.44	0.65
77:A7:93:TYR:HE1	77:A7:115:LYS:HD2	1.62	0.65
29:c1:155:ILE:HD13	29:c1:295:LEU:HD21	1.76	0.65
31:c3:39:ARG:NH1	31:c3:143:ASN:O	2.30	0.65
45:m3:189:LYS:H	45:m3:193:HIS:HD1	1.44	0.65
65:y7:234:LEU:HG	65:y7:235:VAL:HG13	1.79	0.65
121:s2:395:SER:HB3	122:s3:74:GLU:HG3	1.78	0.65
7:2J:49:ARG:NH1	153:SD:101:CDL:OA3	2.28	0.65
153:7A:201:CDL:HA22	65:Y7:358:ARG:HD2	1.78	0.65
29:C1:155:ILE:HD13	29:C1:295:LEU:HD21	1.76	0.65
31:C3:39:ARG:NH1	31:C3:143:ASN:O	2.29	0.65
93:BM:169:ASN:HD22	93:BM:172:GLU:HG3	1.60	0.65
104:N5:289:LEU:HD22	104:N5:428:LEU:HD12	1.78	0.65
108:Qa:138:GLY:HA3	108:Qa:154:ASN:O	1.97	0.65
123:S4:120:MET:O	127:S8:167:ARG:NH1	2.30	0.65
146:V1:227:LYS:HA	146:V1:229:PRO:HD2	1.79	0.65
89:b7:25:GLN:O	89:b7:43:LYS:NZ	2.29	0.65
142:tf:220:ALA:HA	142:tf:226:LEU:HD21	1.79	0.65
153:A:504:CDL:HB4	153:A:504:CDL:H121	1.78	0.65
34:F:240:SER:HB3	34:F:244:ASP:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N:40:LEU:HD12	46:N:198:MET:HE2	1.78	0.65
52:SA:210:ASP:HA	52:SA:267:LEU:HG	1.77	0.65
2:2e:159:SER:HA	2:2e:163:SER:HB3	1.78	0.65
43:m1:55:ALA:O	43:m1:59:ASN:ND2	2.28	0.65
153:t:204:CDL:H812	153:t:204:CDL:H772	1.78	0.65
59:vb:105:GLU:HG3	59:vb:106:GLU:HG3	1.77	0.65
62:y:71:GLU:OE2	62:y:90:GLN:NE2	2.29	0.65
153:c4:401:CDL:H571	153:c4:401:CDL:H761	1.78	0.65
130:t3:48:LEU:HB2	130:t3:104:GLU:HG3	1.77	0.65
153:6C:203:CDL:OB4	57:U:62:ARG:NH2	2.30	0.65
98:G3:297:PHE:O	98:G3:302:LYS:NZ	2.26	0.65
122:S3:138:GLU:HG3	122:S3:156:LEU:HD23	1.77	0.65
1:1t:33:ASN:O	22:6t:39:GLN:NE2	2.30	0.65
52:sa:333:ARG:NH2	52:sa:579:GLY:O	2.29	0.65
153:an:302:CDL:H261	153:an:302:CDL:H732	1.78	0.65
146:v1:227:LYS:HA	146:v1:229:PRO:HD2	1.79	0.65
3:2F:169:ILE:HD11	10:2M:70:LEU:HD22	1.79	0.65
7:2J:101:HIS:O	9:2L:60:GLN:NE2	2.30	0.65
43:M1:17:ASP:O	43:M1:339:ASN:ND2	2.30	0.65
103:N4:287:LYS:NZ	103:N4:364:SER:O	2.28	0.65
106:P1:190:ARG:HH11	130:T3:56:GLN:HE21	1.45	0.65
117:QJ:14:ASN:HB3	152:QJ:102:PC1:H231	1.78	0.65
120:S1:276:PRO:HG3	120:S1:287:ILE:HG12	1.79	0.65
3:2f:169:ILE:HD11	10:2m:70:LEU:HD22	1.79	0.65
152:7c:303:PC1:H342	152:m1:401:PC1:H3D1	1.78	0.65
29:c1:508:LEU:HB3	154:c1:708:HEA:HMA	1.77	0.65
46:n:40:LEU:HD12	46:n:198:MET:HE2	1.79	0.65
71:5b:16:GLN:O	104:n5:477:GLN:NE2	2.30	0.65
72:a1:8:THR:HG21	127:s8:103:PRO:HG3	1.79	0.65
106:p1:190:ARG:HH11	130:t3:56:GLN:HE21	1.45	0.65
110:qc:52:LEU:HD11	110:qc:81:PHE:HA	1.78	0.65
3:2F:79:VAL:HG21	11:2N:56:ASP:HB2	1.79	0.65
152:7C:303:PC1:H342	152:M1:401:PC1:H3D1	1.78	0.65
40:K:190:LYS:O	40:K:195:LYS:NZ	2.29	0.65
76:A6:44:THR:O	76:A6:55:LYS:NZ	2.26	0.65
120:S1:357:ASP:OD2	120:S1:630:TYR:OH	2.14	0.65
20:6c:48:ARG:NH1	25:7l:871:SER:OG	2.29	0.65
32:d:159:VAL:HB	32:d:185:MET:HA	1.78	0.65
38:i:22:ALA:HB3	38:i:41:ALA:HA	1.79	0.65
42:m:107:TRP:NE1	152:w:204:PC1:O12	2.22	0.65
52:sa:270:ARG:NH1	52:sa:559:ASN:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:5b:201:CDL:H562	90:b8:96:MET:HE2	1.78	0.65
123:s4:120:MET:O	127:s8:167:ARG:NH1	2.30	0.65
19:6B:77:ASP:OD2	30:C2:563:ARG:NH1	2.29	0.65
23:7A:59:GLU:HG3	23:7A:65:LYS:HD3	1.78	0.65
27:B:360:HIS:NE2	27:B:367:ASP:OD1	2.27	0.65
32:D:159:VAL:HB	32:D:185:MET:HA	1.77	0.65
52:SA:333:ARG:NH2	52:SA:579:GLY:O	2.29	0.65
52:SA:493:GLY:H	52:SA:539:LYS:HB3	1.61	0.65
71:5B:16:GLN:O	104:N5:477:GLN:NE2	2.30	0.65
153:5B:201:CDL:H562	90:B8:96:MET:HE2	1.78	0.65
77:A7:7:ARG:HH21	153:T7:201:CDL:HB22	1.60	0.65
95:FX:50:ARG:NH1	95:FX:162:GLN:OE1	2.27	0.65
36:g:150:ILE:O	36:g:166:GLN:NE2	2.30	0.64
57:u:17:TYR:OH	104:N5:79:ASP:OD2	2.12	0.64
121:s2:44:ILE:HB	121:s2:56:ASP:HB3	1.78	0.64
127:s8:122:GLY:HA3	127:s8:193:GLY:O	1.97	0.64
49:Q:77:ARG:NH2	153:Q:201:CDL:OA4	2.28	0.64
73:A2:12:LEU:HD11	73:A2:91:VAL:HG22	1.79	0.64
112:QE:74:PHE:O	115:QH:63:ARG:NH1	2.30	0.64
152:QI:201:PC1:H262	117:QJ:23:GLY:HA2	1.79	0.64
127:S8:122:GLY:HA3	127:S8:193:GLY:O	1.97	0.64
153:7a:201:CDL:HA22	65:y7:358:ARG:HD2	1.78	0.64
30:c2:541:ASN:ND2	30:c2:545:TYR:OH	2.24	0.64
33:e:19:GLY:HA2	59:vb:428:PRO:HG2	1.79	0.64
43:m1:17:ASP:O	43:m1:339:ASN:ND2	2.30	0.64
45:m3:90:ARG:NH1	45:m3:128:GLY:O	2.30	0.64
122:s3:81:ASP:O	122:s3:87:ASN:ND2	2.30	0.64
43:M1:55:ALA:O	43:M1:59:ASN:ND2	2.28	0.64
53:SB:248:ILE:HG23	53:SB:256:THR:HG23	1.80	0.64
62:Y:71:GLU:OE2	62:Y:90:GLN:NE2	2.29	0.64
18:6a:47:ILE:O	64:y5:174:ARG:NH2	2.31	0.64
153:6c:202:CDL:OB4	57:u:62:ARG:NH2	2.30	0.64
38:i:22:ALA:HB2	38:i:44:GLN:HB2	1.79	0.64
70:4l:82:LYS:HE3	121:s2:22:GLN:HB2	1.78	0.64
113:qF:63:ARG:NH2	115:qH:127:TYR:OH	2.30	0.64
129:t2:76:GLU:O	129:t2:78:ASN:N	2.29	0.64
130:t3:158:SER:OG	130:t3:161:ASN:ND2	2.30	0.64
153:M:305:CDL:H131	152:M:307:PC1:H32	1.78	0.64
153:C4:401:CDL:H571	153:C4:401:CDL:H761	1.80	0.64
129:T2:76:GLU:O	129:T2:78:ASN:N	2.30	0.64
152:c3:601:PC1:H3F1	153:vb:704:CDL:H801	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:m3:31:PHE:O	45:m3:45:LYS:NZ	2.30	0.64
69:2b:176:ILE:HD11	101:n2:302:TYR:HB2	1.78	0.64
75:a5:77:LYS:HZ1	137:ta:37:LEU:HA	1.63	0.64
103:n4:381:ILE:HD11	103:n4:407:ILE:HD11	1.80	0.64
108:qA:308:LEU:HD23	108:qA:360:LEU:HB3	1.79	0.64
110:qc:55:SER:HB3	112:qe:117:ARG:HH21	1.63	0.64
3:2F:207:LEU:O	3:2F:212:ARG:NH1	2.31	0.64
24:7C:49:ASP:OD1	29:C1:630:ARG:NH2	2.30	0.64
30:C2:202:ARG:NH1	32:D:342:THR:OG1	2.29	0.64
100:N1:100:ILE:HD13	100:N1:132:LEU:HB3	1.79	0.64
105:N6:66:ILE:HD13	105:N6:89:GLU:HB3	1.80	0.64
121:S2:399:TYR:OH	122:S3:67:ASP:O	2.14	0.64
122:S3:81:ASP:O	122:S3:87:ASN:ND2	2.31	0.64
7:2j:101:HIS:O	9:2l:60:GLN:NE2	2.30	0.64
23:7a:59:GLU:HG3	23:7a:65:LYS:HD3	1.78	0.64
153:a:504:CDL:HB4	153:a:504:CDL:H121	1.78	0.64
36:g:93:ARG:NH2	36:g:240:GLU:OE2	2.30	0.64
38:i:135:ILE:O	66:z:17:ARG:NH1	2.29	0.64
40:k:190:LYS:O	40:k:195:LYS:NZ	2.29	0.64
46:n:55:THR:OG1	46:n:57:LYS:NZ	2.31	0.64
68:1b:51:ASN:OD1	83:am:61:GLN:NE2	2.30	0.64
120:s1:276:PRO:HG3	120:s1:287:ILE:HG12	1.79	0.64
23:7A:106:ASP:O	23:7A:129:ARG:NH2	2.30	0.64
35:FS:164:ARG:O	35:FS:168:GLU:HG2	1.98	0.64
43:M1:123:GLN:HG2	43:M1:328:THR:HB	1.78	0.64
45:M3:31:PHE:O	45:M3:45:LYS:NZ	2.30	0.64
72:A1:8:THR:HG21	127:S8:103:PRO:HG3	1.79	0.64
4:2g:138:ASN:OD1	4:2g:142:LYS:NZ	2.30	0.64
52:sa:341:GLU:OE1	52:sa:343:ARG:NH1	2.31	0.64
52:sa:381:VAL:HG13	52:sa:386:GLU:HG3	1.78	0.64
114:qG:137:TRP:O	114:qG:140:LYS:HB3	1.97	0.64
152:qi:201:PC1:H222	117:qj:19:LYS:HG2	1.79	0.64
125:s6:114:THR:HG22	125:s6:121:ARG:HG2	1.78	0.64
18:6A:43:ARG:NH1	18:6A:62:GLU:OE1	2.31	0.64
30:C2:7:THR:O	30:C2:544:PHE:N	2.30	0.64
46:N:55:THR:OG1	46:N:57:LYS:NZ	2.31	0.64
59:VB:105:GLU:HG3	59:VB:106:GLU:HG3	1.79	0.64
65:Y7:234:LEU:HG	65:Y7:235:VAL:HG13	1.79	0.64
68:1B:51:ASN:OD1	83:AM:61:GLN:NE2	2.30	0.64
108:QA:138:GLY:HA3	108:QA:154:ASN:O	1.97	0.64
109:Qb:295:ARG:NH1	110:Qc:217:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
128:T1:92:HIS:HE2	153:T1:601:CDL:HA32	1.63	0.64
136:T9:110:LEU:HD11	144:TH:24:PRO:HG2	1.79	0.64
5:2h:97:GLU:HG3	5:2h:171:LYS:HD3	1.79	0.64
15:4a:122:SER:O	33:e:346:HIS:NE2	2.29	0.64
35:fs:164:ARG:O	35:fs:168:GLU:HG2	1.98	0.64
53:sb:106:LEU:HA	53:sb:109:LYS:HG2	1.79	0.64
130:t3:152:GLU:HG3	130:t3:153:LYS:HG3	1.79	0.64
20:6C:48:ARG:NH1	25:7L:871:SER:OG	2.29	0.64
36:G:93:ARG:NH2	36:G:240:GLU:OE2	2.30	0.64
45:M3:90:ARG:NH1	45:M3:128:GLY:O	2.30	0.64
71:5B:1:MET:HA	153:5B:201:CDL:HB32	1.80	0.64
108:Qa:139:SER:OG	108:Qa:154:ASN:ND2	2.30	0.64
122:S3:73:LEU:HD23	122:S3:77:GLN:HA	1.79	0.64
19:6b:77:ASP:OD2	30:c2:563:ARG:NH1	2.29	0.64
153:7a:201:CDL:HB31	26:a:237:ARG:HG3	1.80	0.64
153:c1:712:CDL:H232	30:c2:52:ILE:HA	1.80	0.64
52:sa:263:ASP:OD2	161:sa:701:FAD:N6A	2.31	0.64
73:a2:12:LEU:HD11	73:a2:91:VAL:HG22	1.80	0.64
112:qE:140:GLY:HA2	112:qE:156:ARG:O	1.98	0.64
146:v1:117:ASN:ND2	146:v1:208:GLY:O	2.24	0.64
18:6A:47:ILE:O	64:Y5:174:ARG:NH2	2.31	0.64
27:B:418:GLN:HB2	27:B:422:ILE:HG22	1.79	0.64
153:C1:712:CDL:H412	153:C1:712:CDL:H221	1.78	0.64
30:C2:114:THR:O	30:C2:132:ASN:ND2	2.30	0.64
44:M2:44:ARG:NH2	44:M2:67:GLU:OE1	2.31	0.64
110:Qc:55:SER:HB3	112:Qe:117:ARG:HH21	1.63	0.64
126:S7:92:SER:OG	126:S7:113:CYS:SG	2.55	0.64
143:TG:104:ASN:HD21	143:TG:107:HIS:HB2	1.61	0.64
146:V1:206:ILE:HG12	146:V1:380:CYS:HB3	1.79	0.64
8:2k:91:LYS:O	8:2k:92:ASN:ND2	2.31	0.64
24:7c:49:ASP:OD1	29:c1:630:ARG:NH2	2.31	0.64
33:e:278:ASN:HB2	33:e:281:HIS:HD2	1.63	0.64
100:n1:76:ILE:HD13	126:s7:14:VAL:HG13	1.80	0.64
111:qd:43:LEU:HD11	111:qd:169:PRO:HG2	1.80	0.64
120:s1:223:VAL:HA	120:s1:226:VAL:HG22	1.80	0.64
146:v1:163:PHE:HB3	146:v1:166:GLU:HB2	1.78	0.64
20:6C:77:GLU:OE2	25:7L:965:ARG:NH1	2.31	0.64
153:M:305:CDL:H711	158:W:203:3PE:H272	1.80	0.64
52:SA:341:GLU:OE1	52:SA:343:ARG:NH1	2.31	0.64
53:SB:106:LEU:HA	53:SB:109:LYS:HG2	1.78	0.64
153:T:204:CDL:H812	153:T:204:CDL:H772	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:AN:175:LEU:HD11	158:AN:301:3PE:H3A1	1.80	0.64
91:B9:59:PHE:O	91:B9:63:ASN:ND2	2.31	0.64
110:Qc:52:LEU:HD11	110:Qc:81:PHE:HA	1.79	0.64
111:Qd:43:LEU:HD11	111:Qd:169:PRO:HG2	1.80	0.64
121:S2:44:ILE:HB	121:S2:56:ASP:HB3	1.78	0.64
142:TF:220:ALA:HA	142:TF:226:LEU:HD21	1.79	0.64
16:4t:30:LEU:HD22	41:l:215:THR:HB	1.80	0.64
20:6c:77:GLU:OE2	25:7l:965:ARG:NH1	2.31	0.64
153:6c:202:CDL:H311	153:6c:202:CDL:H712	1.80	0.64
24:7c:103:GLN:HG3	29:c1:553:VAL:HG12	1.79	0.64
153:c1:712:CDL:H412	153:c1:712:CDL:H221	1.78	0.64
49:q:123:ALA:O	49:q:127:ASN:ND2	2.30	0.64
52:sa:209:ILE:O	52:sa:270:ARG:NH2	2.31	0.64
93:bm:166:ASN:HA	138:tb:98:LYS:HE2	1.80	0.64
152:qI:201:PC1:H262	117:qJ:23:GLY:HA2	1.79	0.64
109:qb:295:ARG:NH1	110:qc:217:GLU:OE1	2.30	0.64
114:qg:117:LYS:NZ	115:qh:55:GLU:OE2	2.31	0.64
131:t4:96:PHE:O	131:t4:207:ASN:ND2	2.29	0.64
52:SA:263:ASP:OD2	161:SA:701:FAD:N6A	2.30	0.64
103:N4:381:ILE:HD11	103:N4:407:ILE:HD11	1.80	0.64
103:N4:484:SER:HB3	153:T5:301:CDL:H822	1.80	0.64
108:QA:308:LEU:HD23	108:QA:360:LEU:HB3	1.79	0.64
115:QH:6:ALA:HB3	109:Qb:362:THR:HG21	1.80	0.64
3:2f:207:LEU:O	3:2f:212:ARG:NH1	2.31	0.63
23:7a:80:VAL:HG11	65:y7:350:LEU:HB2	1.80	0.63
27:b:418:GLN:HB2	27:b:422:ILE:HG22	1.79	0.63
53:sb:248:ILE:HG23	53:sb:256:THR:HG23	1.80	0.63
71:5b:39:TYR:OH	87:b4:33:TYR:O	2.16	0.63
77:a7:93:TYR:HE1	77:a7:115:LYS:HD2	1.61	0.63
106:p1:162:VAL:HG21	106:p1:178:ILE:HG13	1.80	0.63
115:qH:6:ALA:HB3	109:qb:362:THR:HG21	1.81	0.63
128:t1:92:HIS:HE2	153:t1:601:CDL:HA32	1.62	0.63
128:t1:270:ALA:HB3	128:t1:357:PRO:HA	1.81	0.63
11:2N:43:GLN:NE2	11:2N:44:ASN:OD1	2.31	0.63
153:6C:203:CDL:H712	153:6C:203:CDL:H311	1.80	0.63
153:7A:201:CDL:HB31	26:A:237:ARG:HG3	1.80	0.63
24:7C:103:GLN:HG3	29:C1:553:VAL:HG12	1.80	0.63
29:C1:416:ARG:NH1	29:C1:417:VAL:O	2.31	0.63
41:L:169:ASN:O	41:L:173:TYR:CB	2.46	0.63
100:N1:77:LYS:HE3	126:S7:85:LEU:HB2	1.80	0.63
112:QE:140:GLY:HA2	112:QE:156:ARG:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
117:QJ:7:TYR:OH	114:Qg:194:ARG:NH1	2.31	0.63
18:6a:43:ARG:NH1	18:6a:62:GLU:OE1	2.31	0.63
71:5b:1:MET:HE1	153:5b:201:CDL:H361	1.80	0.63
122:s3:73:LEU:HD23	122:s3:77:GLN:HA	1.80	0.63
8:2K:91:LYS:O	8:2K:92:ASN:ND2	2.31	0.63
25:7L:920:LEU:HD12	25:7L:938:TYR:HB2	1.80	0.63
69:2B:74:ALA:HB1	69:2B:112:MET:HG3	1.80	0.63
93:BM:60:ILE:HG22	93:BM:62:ASN:H	1.63	0.63
121:S2:318:ASN:O	121:S2:324:ARG:NE	2.31	0.63
130:T3:152:GLU:HG3	130:T3:153:LYS:HG3	1.79	0.63
37:h:112:LYS:HB3	9:2L:53:GLU:HG2	1.80	0.63
52:sa:428:GLY:HA2	52:sa:449:ILE:HG22	1.80	0.63
94:c4:54:MET:SD	148:x1:147:ARG:NH1	2.70	0.63
114:qg:239:GLU:O	114:qg:243:ASN:ND2	2.31	0.63
43:M1:135:ARG:NH1	152:M1:401:PC1:O12	2.31	0.63
158:B4:202:3PE:H2B1	116:QI:84:PRO:HA	1.80	0.63
152:Qb:602:PC1:H2H2	110:Qc:234:MET:HG2	1.80	0.63
27:b:360:HIS:NE2	27:b:367:ASP:OD1	2.26	0.63
152:c1:704:PC1:H271	152:c1:704:PC1:H351	1.79	0.63
41:l:210:ASN:ND2	45:m3:329:SER:O	2.31	0.63
43:m1:123:GLN:HG2	43:m1:328:THR:HB	1.78	0.63
52:sa:91:GLN:HG3	52:sa:294:LEU:HD23	1.81	0.63
90:b8:53:ASN:ND2	103:n4:325:TRP:O	2.28	0.63
1:1T:53:ALA:HB1	22:6T:59:LEU:HG	1.79	0.63
31:C3:517:TYR:H	153:T:204:CDL:H751	1.64	0.63
130:T3:158:SER:OG	130:T3:161:ASN:ND2	2.30	0.63
153:a:504:CDL:HB21	45:m3:17:ASN:HD21	1.63	0.63
42:m:25:ASN:HD21	42:m:30:GLU:HA	1.63	0.63
49:q:77:ARG:NH2	153:q:201:CDL:OA4	2.28	0.63
103:n4:484:SER:HB3	153:t5:301:CDL:H822	1.80	0.63
112:qE:74:PHE:O	115:qH:63:ARG:NH1	2.30	0.63
114:qg:105:GLN:O	116:qi:9:ASN:ND2	2.32	0.63
128:t1:255:ARG:NH1	128:t1:262:GLU:O	2.32	0.63
16:4T:30:LEU:HD22	41:L:215:THR:HB	1.80	0.63
153:A:504:CDL:HB21	45:M3:17:ASN:HD21	1.63	0.63
27:B:60:ILE:O	27:B:103:ASN:ND2	2.32	0.63
30:C2:594:GLU:O	30:C2:597:TYR:HB3	1.99	0.63
33:E:19:GLY:HA2	59:VB:428:PRO:HG2	1.80	0.63
41:L:210:ASN:ND2	45:M3:329:SER:O	2.32	0.63
153:T:202:CDL:H322	153:T:202:CDL:H141	1.81	0.63
69:2B:35:ILE:HG22	69:2B:36:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
114:QG:137:TRP:O	114:QG:140:LYS:HB3	1.98	0.63
110:Qc:38:THR:HG21	166:Qc:503:HEM:HAB	1.81	0.63
110:Qc:222:TRP:HA	110:Qc:226:ALA:HB3	1.79	0.63
9:2l:53:GLU:HG2	37:H:112:LYS:HB3	1.80	0.63
41:l:169:ASN:O	41:l:173:TYR:CB	2.46	0.63
42:m:4:SER:HB2	33:E:186:PRO:HB2	1.81	0.63
48:p:133:ARG:HG3	48:p:134:GLN:HG3	1.80	0.63
84:an:175:LEU:HD11	158:an:301:3PE:H3A1	1.79	0.63
20:6C:36:TRP:CE2	152:C2:701:PC1:H153	2.34	0.63
49:Q:130:LYS:HE3	49:Q:165:LEU:HD12	1.81	0.63
52:SA:209:ILE:O	52:SA:270:ARG:NH2	2.31	0.63
75:A5:174:ARG:HD3	123:S4:4:PRO:HA	1.80	0.63
94:C4:54:MET:SD	148:X1:147:ARG:NH1	2.70	0.63
110:QC:343:THR:O	114:QG:35:ARG:NH2	2.22	0.63
111:QD:69:SER:OG	111:QD:237:ASN:ND2	2.23	0.63
108:Qa:309:PHE:HB2	108:Qa:454:VAL:HG13	1.79	0.63
114:Qg:117:LYS:NZ	115:Qh:55:GLU:OE2	2.31	0.63
3:2f:82:ASN:ND2	11:2n:61:GLU:OE1	2.32	0.63
29:c1:676:ILE:O	29:c1:679:HIS:ND1	2.28	0.63
33:e:186:PRO:HB2	42:M:4:SER:HB2	1.81	0.63
63:y0:33:PHE:HB3	64:y5:171:LYS:HG3	1.80	0.63
75:a5:174:ARG:HD3	123:s4:4:PRO:HA	1.81	0.63
100:n1:100:ILE:HD13	100:n1:132:LEU:HB3	1.80	0.63
105:n6:66:ILE:HD13	105:n6:89:GLU:HB3	1.80	0.63
30:C2:10:SER:HA	30:C2:21:SER:HB3	1.81	0.63
1:1t:53:ALA:HB1	22:6t:59:LEU:HG	1.80	0.63
4:2g:122:HIS:HE1	153:2g:204:CDL:H521	1.64	0.63
30:c2:594:GLU:O	30:c2:597:TYR:HB3	1.98	0.63
50:r:13:LYS:NZ	66:z:90:GLN:OE1	2.29	0.63
91:b9:59:PHE:O	91:b9:63:ASN:ND2	2.31	0.63
106:p1:23:ASP:OD2	106:p1:25:ARG:NH1	2.32	0.63
126:s7:92:SER:OG	126:s7:113:CYS:SG	2.54	0.63
130:t3:51:GLU:HG3	130:t3:52:MET:HG3	1.81	0.63
36:G:150:ILE:O	36:G:166:GLN:NE2	2.30	0.63
70:4L:84:LEU:HD22	101:N2:190:LEU:HB2	1.81	0.63
75:A5:77:LYS:HZ1	137:TA:37:LEU:HA	1.64	0.63
104:N5:200:PHE:O	104:N5:269:TYR:OH	2.17	0.63
106:P1:162:VAL:HG21	106:P1:178:ILE:HG13	1.80	0.63
146:V1:119:ASP:HA	146:V1:160:ARG:HB3	1.81	0.63
37:h:176:GLU:OE2	58:v:127:ARG:NH2	2.32	0.63
153:m:303:CDL:H711	158:w:203:3PE:H272	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:a1:101:CDL:H511	153:a1:101:CDL:H121	1.81	0.63
110:qC:68:GLU:OE1	111:qD:90:LYS:NZ	2.27	0.63
117:qJ:7:TYR:OH	114:qg:194:ARG:NH1	2.32	0.63
136:t9:110:LEU:HD11	144:th:24:PRO:HG2	1.79	0.63
4:2G:129:HIS:HD2	4:2G:131:ILE:HG12	1.64	0.63
153:C1:712:CDL:H232	30:C2:52:ILE:HA	1.81	0.63
49:Q:80:HIS:NE2	153:VB:703:CDL:OA3	2.30	0.63
61:X:11:TRP:HZ3	61:X:19:ILE:HG13	1.64	0.63
153:2B:201:CDL:H511	153:2B:201:CDL:H161	1.81	0.63
71:5B:1:MET:HE1	153:5B:201:CDL:H361	1.80	0.63
71:5B:52:TYR:HA	71:5B:56:LYS:HB2	1.81	0.63
104:N5:367:LEU:O	104:N5:371:ASN:ND2	2.31	0.63
114:Qg:239:GLU:O	114:Qg:243:ASN:ND2	2.31	0.63
137:TA:112:ASN:O	137:TA:116:GLN:NE2	2.32	0.63
4:2g:129:HIS:HD2	4:2g:131:ILE:HG12	1.64	0.62
20:6c:36:TRP:CE2	152:c2:703:PC1:H153	2.34	0.62
53:sb:75:ARG:NH1	53:sb:90:TYR:OH	2.32	0.62
60:w:123:TYR:OH	60:w:124:LYS:NZ	2.32	0.62
71:5b:1:MET:HA	153:5b:201:CDL:HB32	1.81	0.62
101:n2:323:ILE:HD11	101:n2:353:LEU:HD11	1.80	0.62
108:qA:138:GLY:HA3	108:qA:154:ASN:O	1.97	0.62
109:qb:266:ALA:O	109:qb:269:THR:OG1	2.17	0.62
44:M2:3:TYR:HB3	46:N:182:VAL:HG21	1.80	0.62
60:W:123:TYR:OH	60:W:124:LYS:NZ	2.32	0.62
64:Y5:123:PHE:O	64:Y5:127:ASN:ND2	2.30	0.62
106:P1:23:ASP:OD2	106:P1:25:ARG:NH1	2.32	0.62
116:QI:67:GLN:HE22	152:QI:202:PC1:H32	1.64	0.62
130:T3:51:GLU:HG3	130:T3:52:MET:HG3	1.81	0.62
29:c1:416:ARG:NH1	29:c1:417:VAL:O	2.31	0.62
153:e:402:CDL:HA31	153:e:402:CDL:HB4	1.79	0.62
44:m2:3:TYR:HB3	46:n:182:VAL:HG21	1.80	0.62
82:al:159:ARG:HH12	127:s8:154:GLU:HB3	1.63	0.62
97:g2:200:GLU:O	97:g2:204:ASN:ND2	2.31	0.62
106:p1:99:ASN:ND2	130:t3:156:TYR:O	2.32	0.62
108:qA:70:THR:OG1	108:qA:259:HIS:NE2	2.29	0.62
120:s1:601:ARG:HD3	123:s4:84:ARG:HD3	1.81	0.62
128:t1:409:LEU:HD22	128:t1:418:LYS:HE3	1.81	0.62
131:t4:93:ASN:ND2	131:t4:203:ARG:O	2.32	0.62
29:C1:307:THR:HA	29:C1:310:PHE:CE2	2.35	0.62
57:U:130:GLU:OE1	57:U:139:ASN:ND2	2.30	0.62
63:Y0:33:PHE:HB3	64:Y5:171:LYS:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
97:G2:200:GLU:O	97:G2:204:ASN:ND2	2.31	0.62
101:N2:323:ILE:HD11	101:N2:353:LEU:HD11	1.81	0.62
113:QF:63:ARG:NH2	115:QH:127:TYR:OH	2.31	0.62
108:Qa:116:THR:O	108:Qa:175:ARG:NH2	2.32	0.62
152:Qi:201:PC1:H222	117:Qj:19:LYS:HG2	1.79	0.62
44:m2:44:ARG:NH2	44:m2:67:GLU:OE1	2.31	0.62
69:2b:74:ALA:HB1	69:2b:112:MET:HG3	1.80	0.62
104:n5:77:GLN:HG3	104:n5:83:ASN:HB3	1.80	0.62
104:n5:323:ILE:HA	104:n5:421:ALA:HB2	1.81	0.62
108:qa:138:GLY:HA3	108:qa:154:ASN:O	1.98	0.62
110:qc:222:TRP:HA	110:qc:226:ALA:HB3	1.79	0.62
131:t4:113:LEU:HD23	152:t4:303:PC1:H11	1.81	0.62
142:tf:117:ALA:HB2	142:tf:150:ILE:HD12	1.82	0.62
146:v1:206:ILE:HG12	146:v1:380:CYS:HB3	1.80	0.62
6:2I:59:ASN:OD1	6:2I:61:GLN:NE2	2.33	0.62
31:C3:266:LEU:HB3	31:C3:271:ILE:HG21	1.79	0.62
42:M:110:LEU:HD11	152:W:201:PC1:H3E2	1.82	0.62
53:SB:75:ARG:NH1	53:SB:90:TYR:OH	2.32	0.62
72:A1:61:LYS:NZ	83:AM:153:LYS:O	2.31	0.62
104:N5:58:LEU:O	104:N5:62:ASN:ND2	2.32	0.62
152:QC:505:PC1:H242	111:QD:257:TYR:HB3	1.82	0.62
114:Qg:105:GLN:O	116:Qi:9:ASN:ND2	2.32	0.62
114:Qg:315:PRO:HD2	114:Qg:318:LEU:HD12	1.81	0.62
21:6l:1:MET:HB3	58:v:136:PRO:HD3	1.81	0.62
30:c2:10:SER:HA	30:c2:21:SER:HB3	1.81	0.62
43:m1:5:LEU:HD12	44:m2:198:LEU:HB3	1.81	0.62
77:a7:42:ARG:NH1	127:s8:236:LEU:O	2.33	0.62
99:j1:153:ARG:HA	99:j1:180:HIS:O	1.99	0.62
45:M3:254:ARG:NH2	45:M3:277:THR:O	2.32	0.62
70:4L:11:ILE:HB	105:N6:46:PHE:HE2	1.65	0.62
71:5B:39:TYR:OH	87:B4:33:TYR:O	2.16	0.62
82:AL:159:ARG:HH12	127:S8:154:GLU:HB3	1.63	0.62
117:QJ:18:LEU:HB2	152:QJ:102:PC1:H222	1.80	0.62
113:Qf:25:LEU:HD23	113:Qf:73:VAL:HG21	1.81	0.62
131:T4:93:ASN:ND2	131:T4:203:ARG:O	2.32	0.62
108:qa:309:PHE:HB2	108:qa:454:VAL:HG13	1.81	0.62
123:s4:8:ILE:HG12	123:s4:10:SER:H	1.65	0.62
5:2H:97:GLU:HG3	5:2H:171:LYS:HD3	1.80	0.62
7:2J:49:ARG:NH2	7:2J:51:SER:OG	2.32	0.62
33:E:13:ASN:ND2	33:E:24:ALA:O	2.33	0.62
38:I:139:GLU:OE1	38:I:220:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B3:61:LEU:HA	153:B3:102:CDL:H161	1.82	0.62
107:P2:62:LYS:NZ	107:P2:158:ASN:OD1	2.32	0.62
144:TH:116:GLU:OE1	144:TH:118:HIS:NE2	2.32	0.62
7:2j:102:ARG:HG3	9:2l:59:GLU:HG3	1.80	0.62
104:n5:268:VAL:HG22	104:n5:523:LEU:HD21	1.82	0.62
13:2T:7:ILE:HD12	30:C2:227:ARG:HG3	1.80	0.62
29:C1:446:GLY:O	30:C2:531:ARG:NH2	2.33	0.62
36:G:267:LYS:NZ	36:G:268:GLU:OE2	2.33	0.62
153:M1:402:CDL:H322	153:M1:402:CDL:H512	1.82	0.62
54:SC:39:TYR:OH	54:SC:43:ARG:NH2	2.33	0.62
152:5B:202:PC1:H251	152:5B:202:PC1:H362	1.81	0.62
153:A1:102:CDL:H511	153:A1:102:CDL:H121	1.81	0.62
77:A7:42:ARG:NH1	127:S8:236:LEU:O	2.33	0.62
97:G2:144:ASP:OD1	135:T8:13:ARG:NH1	2.32	0.62
99:J1:153:ARG:HA	99:J1:180:HIS:O	2.00	0.62
121:S2:199:PHE:HA	121:S2:202:THR:HG22	1.81	0.62
2:2e:127:GLN:HB3	2:2e:130:LEU:HB2	1.82	0.62
18:6a:53:GLU:OE1	64:y5:170:TYR:OH	2.18	0.62
35:fs:80:VAL:HG12	35:fs:82:GLY:H	1.64	0.62
36:g:267:LYS:NZ	36:g:268:GLU:OE2	2.33	0.62
42:m:110:LEU:HD11	152:w:201:PC1:H3E2	1.82	0.62
53:sb:47:LEU:O	53:sb:51:ASN:N	2.32	0.62
56:t:122:LEU:HD12	153:t:202:CDL:H192	1.81	0.62
152:5b:202:PC1:H362	152:5b:202:PC1:H251	1.81	0.62
86:b3:61:LEU:HA	153:b3:102:CDL:H161	1.82	0.62
104:n5:200:PHE:O	104:n5:269:TYR:OH	2.17	0.62
107:p2:62:LYS:NZ	107:p2:158:ASN:OD1	2.32	0.62
110:qc:323:ASN:OD1	110:qc:406:ARG:NH2	2.28	0.62
153:A:504:CDL:H592	61:X:58:ILE:HD11	1.81	0.62
37:H:176:GLU:OE2	58:V:127:ARG:NH2	2.32	0.62
43:M1:5:LEU:HD12	44:M2:198:LEU:HB3	1.81	0.62
120:S1:597:VAL:O	120:S1:651:ASP:N	2.28	0.62
25:7l:920:LEU:HD12	25:7l:938:TYR:HB2	1.80	0.62
158:b4:202:3PE:H2B1	116:qI:84:PRO:HA	1.80	0.62
90:b8:71:ILE:HG21	91:b9:16:VAL:HG21	1.81	0.62
93:bm:60:ILE:HG22	93:bm:62:ASN:H	1.64	0.62
104:n5:367:LEU:O	104:n5:371:ASN:ND2	2.31	0.62
112:qE:52:VAL:HG22	116:qI:27:VAL:HG11	1.82	0.62
117:qJ:18:LEU:HB2	152:qJ:101:PC1:H222	1.80	0.62
108:qa:87:SER:HA	109:qb:423:LEU:HD22	1.82	0.62
3:2F:291:GLU:HG3	3:2F:292:GLN:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:428:GLY:HA2	52:SA:449:ILE:HG22	1.80	0.62
90:B8:71:ILE:HG21	91:B9:16:VAL:HG21	1.80	0.62
98:G3:267:GLN:NE2	121:S2:225:THR:O	2.30	0.62
110:QC:60:PRO:HG3	110:QC:178:ILE:HG13	1.81	0.62
6:2i:59:ASN:OD1	6:2i:61:GLN:NE2	2.33	0.62
33:e:103:ASN:ND2	33:e:142:ASP:OD1	2.29	0.62
70:4l:84:LEU:HD22	101:n2:190:LEU:HB2	1.80	0.62
108:qa:116:THR:O	108:qa:175:ARG:NH2	2.32	0.62
114:qg:315:PRO:HD2	114:qg:318:LEU:HD12	1.81	0.62
121:s2:405:SER:HB2	121:s2:439:GLU:HB3	1.82	0.62
26:A:465:ARG:NH2	59:VB:403:ASP:OD1	2.33	0.62
27:B:63:MET:O	27:B:103:ASN:ND2	2.33	0.62
101:N2:19:ASN:OD1	148:X1:98:TRP:NE1	2.27	0.62
114:Qg:45:ASN:O	114:Qg:49:THR:OG1	2.18	0.62
123:S4:8:ILE:HG12	123:S4:10:SER:H	1.64	0.62
30:c2:7:THR:O	30:c2:544:PHE:N	2.31	0.62
52:sa:59:ALA:HB2	52:sa:449:ILE:HB	1.82	0.62
54:sc:39:TYR:OH	54:sc:43:ARG:NH2	2.33	0.62
68:1b:58:PHE:HB3	83:am:69:ILE:HG21	1.80	0.62
72:a1:61:LYS:NZ	83:am:153:LYS:O	2.31	0.62
79:a9:193:ALA:O	79:a9:256:GLY:CA	2.48	0.62
94:c4:16:ARG:NH2	94:c4:29:THR:O	2.32	0.62
96:g1:63:ILE:HD12	96:g1:81:ARG:HG2	1.81	0.62
104:n5:58:LEU:O	104:n5:62:ASN:ND2	2.32	0.62
105:n6:139:SER:O	139:tc:40:LYS:NZ	2.33	0.62
109:qb:199:LEU:O	109:qb:203:ASN:ND2	2.33	0.62
126:s7:7:VAL:O	126:s7:11:ASN:N	2.28	0.62
146:v1:119:ASP:HA	146:v1:160:ARG:HB3	1.81	0.62
3:2F:82:ASN:ND2	11:2N:61:GLU:OE1	2.32	0.62
19:6B:139:ARG:NH2	42:M:138:GLU:OE1	2.33	0.62
152:C1:706:PC1:H271	152:C1:706:PC1:H351	1.79	0.62
33:E:103:ASN:ND2	33:E:142:ASP:OD1	2.29	0.62
42:M:25:ASN:HD21	42:M:30:GLU:HA	1.63	0.62
44:M2:197:SER:HA	153:M2:404:CDL:H131	1.81	0.62
108:QA:116:THR:O	108:QA:175:ARG:NH2	2.33	0.62
111:QD:288:GLU:OE1	111:QD:290:TYR:OH	2.17	0.62
108:Qa:407:LEU:HB3	109:Qb:85:LEU:HG	1.82	0.62
128:T1:409:LEU:HD22	128:T1:418:LYS:HE3	1.81	0.62
153:c1:709:CDL:H712	31:c3:315:ILE:HD12	1.82	0.61
50:r:67:THR:HG22	64:y5:33:MET:HE2	1.82	0.61
109:qB:513:VAL:HG11	115:qH:32:LYS:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qc:38:THR:HG21	166:qc:503:HEM:HAB	1.80	0.61
113:qf:25:LEU:HD23	113:qf:73:VAL:HG21	1.82	0.61
23:7A:80:VAL:HG11	65:Y7:350:LEU:HB2	1.80	0.61
87:B4:111:LEU:HB3	158:B4:202:3PE:H361	1.82	0.61
99:J1:244:ALA:HB2	152:J1:400:PC1:H232	1.82	0.61
100:N1:141:GLY:HA3	100:N1:153:SER:HB3	1.81	0.61
121:S2:405:SER:HB2	121:S2:439:GLU:HB3	1.82	0.61
13:2t:7:ILE:HD12	30:c2:227:ARG:HG3	1.81	0.61
20:6c:23:ARG:NH2	153:f:401:CDL:OA4	2.28	0.61
153:a:504:CDL:H592	61:x:58:ILE:HD11	1.81	0.61
30:c2:130:LEU:HD22	30:c2:409:ILE:HD13	1.83	0.61
37:h:95:PRO:HG3	3:2F:292:GLN:HB3	1.82	0.61
38:i:139:GLU:OE1	38:i:220:GLN:NE2	2.33	0.61
49:q:130:LYS:HE3	49:q:165:LEU:HD12	1.80	0.61
152:qC:505:PC1:H242	111:qD:257:TYR:HB3	1.82	0.61
110:qc:302:LEU:HD23	152:qc:509:PC1:H2H1	1.82	0.61
114:qg:188:GLN:NE2	114:qg:190:TYR:OH	2.33	0.61
129:t2:40:GLN:OE1	129:t2:42:ARG:NH1	2.33	0.61
56:T:122:LEU:HD12	153:T:202:CDL:H192	1.81	0.61
92:BL:137:LYS:HA	92:BL:140:LYS:HE3	1.81	0.61
108:QA:70:THR:OG1	108:QA:259:HIS:NE2	2.29	0.61
109:QB:513:VAL:HG11	115:QH:32:LYS:HD2	1.82	0.61
28:bp:400:LYS:HB3	28:bp:411:VAL:HB	1.82	0.61
99:j1:268:GLU:OE1	105:n6:1:MET:N	2.33	0.61
105:n6:159:TYR:O	105:n6:163:ASN:ND2	2.34	0.61
107:p2:118:VAL:O	107:p2:143:ILE:HB	2.00	0.61
108:qA:116:THR:O	108:qA:175:ARG:NH2	2.34	0.61
111:qd:287:TRP:H	112:qe:69:ASN:HD21	1.48	0.61
158:t8:601:3PE:H272	158:t8:601:3PE:H361	1.82	0.61
137:ta:112:ASN:O	137:ta:116:GLN:NE2	2.33	0.61
7:2J:44:GLN:HA	153:SD:101:CDL:H122	1.80	0.61
33:E:278:ASN:HB2	33:E:281:HIS:HD2	1.64	0.61
94:C4:86:ASP:OD1	94:C4:89:ARG:NH2	2.34	0.61
96:G1:63:ILE:HD12	96:G1:81:ARG:HG2	1.81	0.61
112:QE:52:VAL:HG22	116:QI:27:VAL:HG11	1.82	0.61
114:Qg:84:ASP:HA	114:Qg:115:MET:HE3	1.82	0.61
129:T2:40:GLN:OE1	129:T2:42:ARG:NH1	2.33	0.61
15:4a:77:ARG:NH1	15:4a:112:ASP:OD1	2.34	0.61
153:m1:402:CDL:H512	153:m1:402:CDL:H322	1.82	0.61
93:bm:169:ASN:HD22	93:bm:172:GLU:HG3	1.65	0.61
111:qd:93:ASP:OD2	112:qe:123:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:s2:318:ASN:O	121:s2:324:ARG:NE	2.32	0.61
7:2J:102:ARG:HG3	9:2L:59:GLU:HG3	1.80	0.61
26:A:237:ARG:NH2	40:K:48:ASP:OD2	2.33	0.61
50:R:67:THR:HG22	64:Y5:33:MET:HE2	1.82	0.61
53:SB:47:LEU:O	53:SB:51:ASN:N	2.31	0.61
96:G1:197:ASP:OD2	103:N4:142:TYR:OH	2.18	0.61
97:G2:3:LEU:HD22	158:T8:602:3PE:H221	1.82	0.61
114:Qg:188:GLN:NE2	114:Qg:190:TYR:OH	2.34	0.61
19:6b:139:ARG:NH2	42:m:138:GLU:OE1	2.33	0.61
29:c1:562:MET:HE3	153:c1:712:CDL:H641	1.82	0.61
71:5b:52:TYR:HA	71:5b:56:LYS:HB2	1.81	0.61
97:g2:144:ASP:OD1	135:t8:13:ARG:NH1	2.32	0.61
29:C1:532:SER:OG	154:C1:702:HEA:O11	2.17	0.61
29:C1:562:MET:HE3	153:C1:712:CDL:H641	1.82	0.61
104:N5:268:VAL:HG22	104:N5:523:LEU:HD21	1.82	0.61
104:N5:323:ILE:HA	104:N5:421:ALA:HB2	1.82	0.61
112:Qe:84:GLU:OE2	116:Qi:37:GLN:NE2	2.26	0.61
122:S3:178:ASP:OD1	126:S7:111:ARG:NH1	2.34	0.61
123:S4:104:LYS:HD2	123:S4:135:TYR:HB3	1.81	0.61
131:T4:113:LEU:HD23	152:T4:303:PC1:H11	1.82	0.61
158:T8:601:3PE:H272	158:T8:601:3PE:H361	1.82	0.61
41:l:52:ILE:HD12	41:l:55:LYS:HD2	1.82	0.61
44:m2:197:SER:HA	153:m2:404:CDL:H131	1.81	0.61
153:t:202:CDL:H141	153:t:202:CDL:H322	1.81	0.61
76:a6:19:ASN:ND2	76:a6:20:ASN:OD1	2.34	0.61
87:b4:111:LEU:HB3	158:b4:202:3PE:H361	1.83	0.61
92:bl:137:LYS:HA	92:bl:140:LYS:HE3	1.82	0.61
100:n1:77:LYS:HE3	126:s7:85:LEU:HB2	1.81	0.61
111:qD:179:SER:HB3	111:qD:213:LEU:HD12	1.83	0.61
56:T:56:ARG:NH2	153:T:204:CDL:OB4	2.29	0.61
128:T1:270:ALA:HB3	128:T1:357:PRO:HA	1.82	0.61
2:2e:153:LEU:HB2	2:2e:184:ILE:HD11	1.81	0.61
3:2f:291:GLU:HG3	3:2f:292:GLN:HG2	1.82	0.61
7:2j:49:ARG:NH2	7:2j:51:SER:OG	2.32	0.61
29:c1:637:LEU:HD22	36:g:199:LEU:HD13	1.83	0.61
57:u:130:GLU:OE1	57:u:139:ASN:ND2	2.30	0.61
153:2b:201:CDL:H511	153:2b:201:CDL:H161	1.81	0.61
70:4l:11:ILE:HB	105:n6:46:PHE:HE2	1.65	0.61
94:c4:86:ASP:OD1	94:c4:89:ARG:NH2	2.33	0.61
97:g2:3:LEU:HD22	158:t8:602:3PE:H221	1.83	0.61
100:n1:73:LYS:NZ	126:s7:21:SER:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
114:qg:84:ASP:HA	114:qg:115:MET:HE3	1.82	0.61
128:t1:214:ASN:O	128:t1:250:GLN:NE2	2.30	0.61
129:t2:221:GLU:HA	129:t2:224:LYS:HE2	1.82	0.61
152:C1:711:PC1:H292	153:VB:703:CDL:H831	1.82	0.61
100:N1:44:ARG:NH2	126:S7:47:ASP:OD1	2.34	0.61
111:QD:179:SER:HB3	111:QD:213:LEU:HD12	1.83	0.61
120:S1:422:THR:HA	120:S1:426:LEU:HB3	1.82	0.61
146:V1:37:ASP:OD1	146:V1:40:ARG:NH1	2.33	0.61
29:c1:258:LYS:HB2	29:c1:261:VAL:HG13	1.83	0.61
29:c1:307:THR:HA	29:c1:310:PHE:CE2	2.34	0.61
31:c3:517:TYR:H	153:t:204:CDL:H751	1.64	0.61
70:4l:85:ASN:ND2	76:a6:20:ASN:O	2.29	0.61
146:v1:37:ASP:OD1	146:v1:40:ARG:NH1	2.34	0.61
148:x1:18:LYS:NZ	148:x1:145:LYS:O	2.33	0.61
18:6A:53:GLU:OE1	64:Y5:170:TYR:OH	2.18	0.61
29:C1:518:HIS:O	30:C2:524:LYS:NZ	2.28	0.61
35:FS:80:VAL:HG12	35:FS:82:GLY:H	1.65	0.61
36:G:66:ARG:HE	59:VB:214:ASN:HD21	1.49	0.61
52:SA:226:SER:O	52:SA:230:GLY:CA	2.49	0.61
58:V:78:GLU:HB2	58:V:82:PHE:HB3	1.82	0.61
79:A9:193:ALA:O	79:A9:256:GLY:CA	2.48	0.61
106:P1:99:ASN:ND2	130:T3:156:TYR:O	2.31	0.61
108:Qa:420:THR:OG1	108:Qa:432:HIS:NE2	2.31	0.61
109:Qb:200:LEU:HD22	109:Qb:303:ASN:HB3	1.83	0.61
52:sa:112:ASP:OD2	52:sa:175:ARG:NH1	2.34	0.61
58:v:78:GLU:HB2	58:v:82:PHE:HB3	1.83	0.61
59:vb:118:LEU:HD22	59:vb:223:MET:HG3	1.82	0.61
82:al:57:ASP:HB2	82:al:63:TYR:HE1	1.65	0.61
95:fx:37:ARG:NH2	99:j1:116:SER:O	2.34	0.61
101:n2:146:THR:HB	101:n2:149:THR:HG22	1.83	0.61
105:n6:21:ILE:HG12	124:s5:64:ASN:HB3	1.83	0.61
113:qF:70:GLU:HA	113:qF:73:VAL:HG22	1.83	0.61
129:t2:124:PRO:HG3	129:t2:165:HIS:HB2	1.83	0.61
11:2N:3:ARG:HH21	53:SB:84:GLN:HB2	1.65	0.61
21:6L:1:MET:HB3	58:V:136:PRO:HD3	1.82	0.61
25:7L:894:ASP:OD1	30:C2:147:ARG:NH1	2.28	0.61
29:C1:676:ILE:O	29:C1:679:HIS:ND1	2.28	0.61
68:1B:58:PHE:HB3	83:AM:69:ILE:HG21	1.80	0.61
70:4L:85:ASN:ND2	76:A6:20:ASN:O	2.30	0.61
108:Qa:87:SER:HA	109:Qb:423:LEU:HD22	1.82	0.61
108:Qa:96:ASP:O	108:Qa:248:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:Qb:211:ASP:OD2	112:Qe:78:ARG:NH2	2.34	0.61
110:Qc:235:ILE:HG23	152:Qe:303:PC1:H2H2	1.82	0.61
120:S1:601:ARG:HD3	123:S4:84:ARG:HD3	1.82	0.61
128:T1:273:ASN:ND2	128:T1:313:ASP:OD2	2.34	0.61
142:TF:117:ALA:HB2	142:TF:150:ILE:HD12	1.82	0.61
146:V1:76:ILE:HG23	146:V1:256:MET:HE3	1.81	0.61
5:2h:90:LEU:HD22	9:2l:12:THR:HG21	1.83	0.61
33:e:13:ASN:ND2	33:e:24:ALA:O	2.34	0.61
41:l:134:LEU:O	41:l:152:GLN:NE2	2.33	0.61
59:vb:354:ARG:NH1	59:vb:386:GLU:OE1	2.34	0.61
61:x:11:TRP:HZ3	61:x:19:ILE:HG13	1.64	0.61
79:a9:215:GLU:HA	153:a9:402:CDL:H511	1.82	0.61
109:qB:55:PRO:HD2	109:qB:58:LEU:HD12	1.83	0.61
114:qg:45:ASN:O	114:qg:49:THR:OG1	2.18	0.61
120:s1:597:VAL:O	120:s1:651:ASP:N	2.28	0.61
121:s2:199:PHE:HA	121:s2:202:THR:HG22	1.82	0.61
129:t2:64:GLY:O	129:t2:118:LYS:NZ	2.34	0.61
27:B:56:GLU:OE1	27:B:96:ARG:NH2	2.34	0.61
28:BP:400:LYS:HB3	28:BP:411:VAL:HB	1.83	0.61
45:M3:98:GLN:NE2	45:M3:109:THR:O	2.34	0.61
73:A2:62:ILE:HA	73:A2:72:LYS:HA	1.83	0.61
82:AL:57:ASP:HB2	82:AL:63:TYR:HE1	1.65	0.61
108:Qa:145:ASP:OD1	108:Qa:148:THR:OG1	2.18	0.61
146:V1:117:ASN:ND2	146:V1:208:GLY:O	2.25	0.61
19:6b:145:LEU:O	30:c2:392:ARG:NH2	2.33	0.60
26:a:465:ARG:NH2	59:vb:403:ASP:OD1	2.33	0.60
65:y7:105:PHE:H	149:c:97:ASN:HD21	1.49	0.60
104:n5:276:PHE:HB3	104:n5:282:VAL:HG22	1.83	0.60
108:qa:407:LEU:HB3	109:qb:85:LEU:HG	1.83	0.60
110:qc:235:ILE:HG23	152:qe:303:PC1:H2H2	1.82	0.60
2:2E:127:GLN:HB3	2:2E:130:LEU:HB2	1.82	0.60
153:7A:201:CDL:H571	153:7A:201:CDL:H792	1.83	0.60
52:SA:59:ALA:HB2	52:SA:449:ILE:HB	1.82	0.60
59:VB:354:ARG:NH1	59:VB:386:GLU:OE1	2.34	0.60
66:Z:11:ARG:NE	66:Z:16:GLU:OE2	2.34	0.60
76:A6:19:ASN:ND2	76:A6:20:ASN:OD1	2.34	0.60
38:i:136:GLN:NE2	57:U:46:THR:O	2.30	0.60
41:l:82:LEU:HD22	41:l:102:LEU:HD13	1.82	0.60
144:th:116:GLU:OE1	144:th:118:HIS:NE2	2.32	0.60
52:SA:112:ASP:OD2	52:SA:175:ARG:NH1	2.34	0.60
52:SA:508:MET:SD	52:SA:564:SER:OG	2.59	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
108:QA:99:THR:HG21	108:QA:221:LEU:HA	1.83	0.60
111:QD:93:ASP:OD1	112:QE:123:ARG:NH2	2.33	0.60
48:p:101:GLN:HG2	48:p:134:GLN:HG2	1.84	0.60
153:q:203:CDL:H211	153:vb:704:CDL:H832	1.84	0.60
105:n6:237:ASP:OD2	105:n6:240:ASN:ND2	2.34	0.60
110:qC:258:GLU:HG3	110:qC:261:MET:HE2	1.84	0.60
14:3T:1:MET:HB2	30:C2:278:ASN:HB3	1.82	0.60
15:4A:125:ASP:HB2	35:FS:95:VAL:HB	1.83	0.60
29:C1:338:SER:HB3	29:C1:399:ILE:HG22	1.84	0.60
29:C1:645:ARG:NH1	36:G:234:GLU:OE2	2.34	0.60
31:C3:481:LEU:O	31:C3:485:ASN:ND2	2.30	0.60
33:E:349:ASN:O	59:VB:164:GLN:NE2	2.33	0.60
42:M:159:ILE:HD13	42:M:193:THR:HG23	1.81	0.60
48:P:56:PHE:HB3	48:P:59:PHE:HB2	1.83	0.60
59:VB:118:LEU:HD22	59:VB:223:MET:HG3	1.83	0.60
65:Y7:105:PHE:H	149:C:97:ASN:HD21	1.49	0.60
79:A9:205:GLN:NE2	102:N3:35:GLN:O	2.33	0.60
98:G3:265:ILE:HD13	121:S2:8:LEU:HD13	1.83	0.60
99:J1:268:GLU:OE1	105:N6:1:MET:N	2.33	0.60
104:N5:602:GLY:HA2	104:N5:605:TYR:CE2	2.37	0.60
111:Qd:287:TRP:H	112:Qe:69:ASN:HD21	1.49	0.60
153:T5:301:CDL:H812	153:T5:301:CDL:H761	1.83	0.60
14:3t:1:MET:HB2	30:c2:278:ASN:HB3	1.82	0.60
15:4a:47:LYS:NZ	36:g:282:MET:O	2.30	0.60
30:c2:65:PRO:HD2	36:g:100:THR:HA	1.83	0.60
31:c3:311:ARG:NE	152:c3:605:PC1:O14	2.33	0.60
34:f:227:LEU:HB2	34:f:320:ILE:HD11	1.83	0.60
42:m:159:ILE:HD13	42:m:193:THR:HG23	1.82	0.60
43:m1:135:ARG:NH1	152:m1:401:PC1:O12	2.31	0.60
52:sa:396:TYR:HD2	52:sa:398:MET:HG2	1.66	0.60
52:sa:540:THR:O	52:sa:543:ARG:NH1	2.32	0.60
153:2b:201:CDL:H871	135:t8:64:LYS:HA	1.84	0.60
108:qA:99:THR:HG21	108:qA:221:LEU:HA	1.83	0.60
111:qd:151:LYS:HG2	111:qd:158:TRP:HB2	1.84	0.60
123:s4:104:LYS:HD2	123:s4:135:TYR:HB3	1.81	0.60
146:v1:76:ILE:HG23	146:v1:256:MET:HE3	1.81	0.60
152:A:501:PC1:O32	31:C3:455:TRP:NE1	2.28	0.60
34:F:227:LEU:HB2	34:F:320:ILE:HD11	1.84	0.60
153:F:402:CDL:HB22	153:F:402:CDL:HB4	1.83	0.60
38:I:22:ALA:HB3	38:I:41:ALA:HA	1.84	0.60
59:VB:488:ILE:HD13	65:Y7:208:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:VB:703:CDL:H211	153:VB:706:CDL:H832	1.84	0.60
70:4L:114:ASN:OD1	95:FX:140:ASN:ND2	2.34	0.60
79:A9:215:GLU:HA	153:A9:402:CDL:H511	1.82	0.60
82:AL:13:THR:HG22	82:AL:15:LYS:H	1.67	0.60
91:B9:167:GLU:OE2	135:T8:37:ARG:NH1	2.34	0.60
104:N5:276:PHE:HB3	104:N5:282:VAL:HG22	1.84	0.60
110:Qc:70:GLU:HB3	110:Qc:77:THR:HG21	1.82	0.60
29:c1:293:ASP:OD1	29:c1:364:ARG:NE	2.35	0.60
29:c1:645:ARG:NH1	36:g:234:GLU:OE2	2.34	0.60
31:c3:386:LYS:NZ	59:vb:91:GLU:O	2.34	0.60
34:f:119:TYR:HB2	58:v:41:GLN:HG2	1.83	0.60
152:f:402:PC1:H352	152:fs:204:PC1:H332	1.83	0.60
109:qB:360:ASP:OD2	109:qB:384:ASN:ND2	2.34	0.60
111:qD:187:PRO:HD3	113:qF:62:LEU:HD13	1.83	0.60
112:qE:109:LEU:HD11	152:qE:303:PC1:H261	1.83	0.60
122:s3:178:ASP:OD1	126:s7:111:ARG:NH1	2.34	0.60
131:t4:63:SER:HA	131:t4:196:LYS:HE3	1.84	0.60
15:4A:77:ARG:NH1	15:4A:112:ASP:OD1	2.34	0.60
27:B:19:TRP:HE1	27:B:84:THR:HG22	1.66	0.60
41:L:169:ASN:O	41:L:173:TYR:HB3	2.02	0.60
52:SA:540:THR:O	52:SA:543:ARG:NH1	2.33	0.60
56:T:110:ASN:ND2	63:Y0:62:ASN:O	2.34	0.60
71:5B:19:PHE:HZ	104:N5:472:LEU:HD23	1.67	0.60
83:AM:49:LYS:NZ	153:AM:201:CDL:OB3	2.32	0.60
107:P2:44:THR:HG21	107:P2:62:LYS:HD2	1.83	0.60
110:QC:258:GLU:HG3	110:QC:261:MET:HE2	1.84	0.60
111:Qd:93:ASP:OD2	112:Qe:123:ARG:NH2	2.35	0.60
121:S2:33:GLN:NE2	126:S7:26:THR:O	2.34	0.60
131:T4:65:PHE:O	131:T4:196:LYS:NZ	2.34	0.60
3:2f:191:GLY:N	3:2f:223:GLU:OE1	2.23	0.60
29:c1:446:GLY:O	30:c2:531:ARG:NH2	2.34	0.60
152:c1:711:PC1:H292	153:q:203:CDL:H831	1.82	0.60
56:t:56:ARG:NH2	153:t:204:CDL:OB4	2.29	0.60
153:b3:102:CDL:H322	153:b3:102:CDL:H561	1.84	0.60
92:bl:57:LYS:NZ	92:bl:58:GLU:OE2	2.35	0.60
108:qA:380:ILE:HG21	108:qA:480:LEU:HB3	1.84	0.60
109:qb:211:ASP:OD2	112:qe:78:ARG:NH2	2.34	0.60
110:qc:321:GLN:NE2	114:qg:196:GLU:OE2	2.29	0.60
19:6B:220:PRO:HA	49:Q:37:PRO:HB2	1.84	0.60
29:C1:293:ASP:OD1	29:C1:364:ARG:NE	2.34	0.60
29:C1:637:LEU:HD22	36:G:199:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:C1:708:CDL:H712	31:C3:315:ILE:HD12	1.82	0.60
34:F:119:TYR:HB2	58:V:41:GLN:HG2	1.83	0.60
152:F:401:PC1:H352	152:FS:201:PC1:H332	1.82	0.60
111:QD:166:LYS:HZ3	111:QD:245:ARG:H	1.50	0.60
109:Qb:199:LEU:O	109:Qb:203:ASN:ND2	2.33	0.60
132:T5:178:GLN:O	132:T5:182:ASN:ND2	2.33	0.60
26:a:237:ARG:NH2	40:k:48:ASP:OD2	2.33	0.60
30:c2:431:TYR:O	30:c2:439:THR:OG1	2.19	0.60
56:t:110:ASN:ND2	63:y0:62:ASN:O	2.34	0.60
107:p2:44:THR:HG21	107:p2:62:LYS:HD2	1.83	0.60
111:qD:166:LYS:HZ3	111:qD:245:ARG:H	1.49	0.60
110:qc:102:LYS:HD2	166:qc:503:HEM:HBD2	1.84	0.60
114:qg:145:ARG:HD2	116:qi:2:VAL:HA	1.83	0.60
120:s1:124:ASN:HD22	146:v1:388:GLU:HG3	1.67	0.60
41:L:134:LEU:O	41:L:152:GLN:NE2	2.33	0.60
100:N1:76:ILE:HD13	126:S7:14:VAL:HG13	1.83	0.60
104:N5:723:TYR:OH	107:P2:128:ARG:NH1	2.35	0.60
105:N6:138:PHE:HZ	124:S5:48:HIS:HB3	1.67	0.60
105:N6:139:SER:O	139:TC:40:LYS:NZ	2.33	0.60
111:Qd:151:LYS:HG2	111:Qd:158:TRP:HB2	1.84	0.60
146:V1:120:GLU:O	146:V1:160:ARG:NH1	2.35	0.60
24:7c:94:MET:HG3	43:m1:267:PRO:HG2	1.84	0.60
33:e:321:ASP:OD1	33:e:324:ARG:NH2	2.35	0.60
74:a3:57:LEU:HB3	74:a3:60:VAL:HB	1.84	0.60
104:n5:602:GLY:HA2	104:n5:605:TYR:CE2	2.37	0.60
108:qa:145:ASP:OD1	108:qa:148:THR:OG1	2.18	0.60
126:s7:35:GLU:HG3	126:s7:127:PRO:HB2	1.84	0.60
126:s7:46:PHE:HB3	126:s7:51:VAL:HB	1.84	0.60
153:t5:301:CDL:H812	153:t5:301:CDL:H761	1.84	0.60
38:I:152:GLN:HG2	38:I:195:PRO:HG3	1.83	0.60
49:Q:123:ALA:O	49:Q:127:ASN:ND2	2.31	0.60
53:SB:75:ARG:NH2	53:SB:115:THR:OG1	2.34	0.60
76:A6:115:LEU:HD12	168:AB:201:ZMP:H5A	1.84	0.60
105:N6:237:ASP:OD2	105:N6:240:ASN:ND2	2.34	0.60
107:P2:118:VAL:O	107:P2:143:ILE:HB	2.01	0.60
110:QC:52:LEU:HD11	110:QC:81:PHE:HA	1.84	0.60
110:Qc:321:GLN:NE2	114:Qg:196:GLU:OE2	2.30	0.60
3:2f:292:GLN:HB3	37:H:95:PRO:HG3	1.83	0.60
153:2g:201:CDL:H342	7:2j:28:PRO:HB3	1.83	0.60
11:2n:3:ARG:HH21	53:sb:84:GLN:HB2	1.65	0.60
11:2n:43:GLN:NE2	11:2n:44:ASN:OD1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:7a:58:GLU:OE2	23:7a:75:TYR:OH	2.19	0.60
76:a6:96:ARG:NH2	123:s4:71:TYR:O	2.34	0.60
91:b9:167:GLU:OE2	135:t8:37:ARG:NH1	2.34	0.60
95:fx:107:CYS:HB2	95:fx:144:ALA:HB3	1.84	0.60
98:g3:267:GLN:NE2	121:s2:225:THR:O	2.29	0.60
99:j1:244:ALA:HB2	152:j1:400:PC1:H232	1.82	0.60
105:n6:138:PHE:HZ	124:s5:48:HIS:HB3	1.67	0.60
152:qB:602:PC1:H331	114:qg:187:PHE:HZ	1.67	0.60
116:qI:67:GLN:HE22	152:qI:202:PC1:H32	1.66	0.60
120:s1:422:THR:HA	120:s1:426:LEU:HB3	1.83	0.60
153:C1:701:CDL:O1	40:K:40:HIS:O	2.20	0.60
31:C3:311:ARG:NE	152:C3:605:PC1:O14	2.33	0.60
52:SA:396:TYR:HD2	52:SA:398:MET:HG2	1.66	0.60
74:A3:64:PHE:HB3	158:A3:201:3PE:H342	1.84	0.60
95:FX:107:CYS:HB2	95:FX:144:ALA:HB3	1.84	0.60
110:QC:46:LEU:HD11	110:QC:193:ALA:HB2	1.84	0.60
120:S1:223:VAL:HA	120:S1:226:VAL:HG22	1.82	0.60
33:e:349:ASN:O	59:vb:164:GLN:NE2	2.34	0.60
66:z:38:GLU:O	67:z1:69:ASN:ND2	2.35	0.60
74:a3:64:PHE:HB3	158:a3:201:3PE:H342	1.84	0.60
100:n1:147:LYS:HE2	121:s2:26:MET:HG3	1.84	0.60
109:qb:200:LEU:HD22	109:qb:303:ASN:HB3	1.83	0.60
5:2H:90:LEU:HD22	9:2L:12:THR:HG21	1.83	0.60
6:2I:75:PHE:O	6:2I:79:ASN:ND2	2.32	0.60
41:L:82:LEU:HD22	41:L:102:LEU:HD13	1.82	0.60
88:B6:83:ASN:ND2	104:N5:193:TYR:O	2.33	0.60
100:N1:73:LYS:NZ	126:S7:21:SER:O	2.35	0.60
105:N6:21:ILE:HG12	124:S5:64:ASN:HB3	1.83	0.60
128:T1:255:ARG:NH1	128:T1:262:GLU:O	2.35	0.60
2:2e:81:TYR:CE1	2:2e:97:ILE:HG22	2.37	0.59
7:2j:44:GLN:HA	153:sd:101:CDL:H122	1.84	0.59
34:f:176:ALA:O	57:u:81:ASN:ND2	2.30	0.59
37:h:183:ARG:HD3	37:h:273:TYR:HE2	1.67	0.59
73:a2:62:ILE:HA	73:a2:72:LYS:HA	1.83	0.59
103:n4:286:VAL:HB	103:n4:342:MET:HE2	1.84	0.59
104:n5:338:LYS:NZ	104:n5:417:ASP:OD2	2.34	0.59
109:qB:77:VAL:HG21	109:qB:256:SER:HA	1.84	0.59
111:qD:78:ALA:HB1	111:qD:112:PHE:HZ	1.66	0.59
110:qc:272:ARG:NH2	111:qd:39:GLY:O	2.35	0.59
112:qe:113:GLY:HA3	152:qe:303:PC1:H351	1.84	0.59
2:2E:81:TYR:CE1	2:2E:97:ILE:HG22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C1:258:LYS:HB2	29:C1:261:VAL:HG13	1.83	0.59
40:K:81:HIS:HA	40:K:84:LYS:HE2	1.83	0.59
76:A6:32:ARG:HH11	79:A9:361:GLU:HG3	1.67	0.59
95:FX:37:ARG:NH2	99:J1:116:SER:O	2.34	0.59
109:QB:55:PRO:HD2	109:QB:58:LEU:HD12	1.83	0.59
110:QC:344:PRO:O	110:QC:406:ARG:NH2	2.34	0.59
129:T2:221:GLU:HA	129:T2:224:LYS:HE2	1.83	0.59
28:bp:82:GLY:HA3	28:bp:129:ASN:HD21	1.67	0.59
30:c2:8:GLU:OE2	30:c2:486:ARG:NH2	2.35	0.59
153:m:303:CDL:H722	153:m:303:CDL:H521	1.84	0.59
45:m3:98:GLN:NE2	45:m3:109:THR:O	2.35	0.59
52:sa:226:SER:O	52:sa:230:GLY:CA	2.50	0.59
64:y5:123:PHE:O	64:y5:127:ASN:ND2	2.30	0.59
120:s1:164:LYS:O	120:s1:172:THR:OG1	2.20	0.59
146:v1:120:GLU:O	146:v1:160:ARG:NH1	2.35	0.59
30:C2:8:GLU:OE2	30:C2:486:ARG:NH2	2.35	0.59
30:C2:137:LEU:HD21	30:C2:602:TYR:HB3	1.83	0.59
57:U:99:ILE:HB	57:U:100:PRO:HD3	1.84	0.59
80:AB:59:GLU:OE2	145:TX:123:ARG:NH2	2.35	0.59
93:BM:141:LYS:NZ	93:BM:145:GLU:OE2	2.36	0.59
98:G3:282:PHE:O	98:G3:287:TYR:OH	2.21	0.59
114:Qg:162:TYR:HA	114:Qg:166:MET:HB2	1.84	0.59
122:S3:52:GLU:O	122:S3:56:SER:N	2.35	0.59
126:S7:35:GLU:HG3	126:S7:127:PRO:HB2	1.84	0.59
129:T2:124:PRO:HG3	129:T2:165:HIS:HB2	1.83	0.59
134:T7:111:HIS:O	134:T7:115:THR:OG1	2.09	0.59
19:6b:44:VAL:HG22	25:7l:970:LEU:HB3	1.84	0.59
25:7l:894:ASP:OD1	30:c2:147:ARG:NH1	2.28	0.59
27:b:56:GLU:OE1	27:b:96:ARG:NH2	2.33	0.59
36:g:66:ARG:HE	59:vb:214:ASN:HD21	1.48	0.59
37:h:257:GLU:O	37:h:284:GLN:NE2	2.36	0.59
57:u:49:LYS:O	57:u:54:ARG:NH1	2.35	0.59
70:4l:114:ASN:OD1	95:fx:140:ASN:ND2	2.34	0.59
76:a6:115:LEU:HD12	168:ab:201:ZMP:H5A	1.84	0.59
121:s2:283:ARG:NH2	121:s2:432:THR:O	2.35	0.59
34:F:136:ARG:NH2	34:F:322:LYS:O	2.35	0.59
38:I:142:ASN:ND2	38:I:218:GLU:O	2.36	0.59
42:M:99:ASN:OD1	60:W:21:ARG:NH1	2.35	0.59
153:M3:403:CDL:H712	152:N:303:PC1:H261	1.84	0.59
109:QB:360:ASP:OD2	109:QB:384:ASN:ND2	2.34	0.59
126:S7:46:PHE:HB3	126:S7:51:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
152:7a:202:PC1:O14	26:a:334:ASN:ND2	2.35	0.59
25:7l:922:GLU:O	30:c2:600:ARG:NH1	2.35	0.59
27:b:19:TRP:HE1	27:b:84:THR:HG22	1.66	0.59
38:i:152:GLN:HG2	38:i:195:PRO:HG3	1.83	0.59
42:m:99:ASN:OD1	60:w:21:ARG:NH1	2.35	0.59
49:q:80:HIS:NE2	153:q:203:CDL:OA3	2.28	0.59
82:al:13:THR:HG22	82:al:15:LYS:H	1.67	0.59
84:an:101:HIS:ND1	153:n6:302:CDL:OA4	2.33	0.59
108:qa:96:ASP:O	108:qa:248:ARG:NH2	2.34	0.59
11:2N:19:SER:O	11:2N:23:LYS:NZ	2.31	0.59
30:C2:65:PRO:HD2	36:G:100:THR:HA	1.83	0.59
30:C2:431:TYR:O	30:C2:439:THR:OG1	2.20	0.59
42:M:153:LEU:HA	42:M:156:VAL:HG22	1.84	0.59
43:M1:259:THR:HA	43:M1:262:MET:HE2	1.84	0.59
153:2B:201:CDL:H871	135:T8:64:LYS:HA	1.84	0.59
100:N1:169:LEU:O	100:N1:173:ASN:ND2	2.32	0.59
105:N6:159:TYR:O	105:N6:163:ASN:ND2	2.34	0.59
110:Qc:102:LYS:HD2	166:Qc:503:HEM:HBD2	1.83	0.59
153:m3:403:CDL:H712	152:n:303:PC1:H261	1.85	0.59
100:n1:44:ARG:NH2	126:s7:47:ASP:OD1	2.34	0.59
110:qC:46:LEU:HD11	110:qC:193:ALA:HB2	1.84	0.59
127:s8:113:LYS:NZ	127:s8:197:GLU:OE2	2.36	0.59
12:2O:27:THR:HG22	54:SC:40:ALA:HB2	1.83	0.59
13:2T:62:TYR:OH	17:5T:47:GLN:NE2	2.34	0.59
28:BP:260:ASN:HB2	28:BP:269:LEU:HD22	1.84	0.59
36:G:181:ASN:ND2	59:VB:186:GLN:OE1	2.35	0.59
153:M:305:CDL:H722	153:M:305:CDL:H521	1.85	0.59
57:U:49:LYS:O	57:U:54:ARG:NH1	2.35	0.59
100:N1:147:LYS:HE2	121:S2:26:MET:HG3	1.84	0.59
101:N2:299:LEU:HD23	101:N2:303:TYR:HB2	1.84	0.59
104:N5:608:ARG:HD2	152:N5:803:PC1:H32	1.85	0.59
112:QE:109:LEU:HD11	152:QE:303:PC1:H261	1.83	0.59
120:S1:164:LYS:O	120:S1:172:THR:OG1	2.19	0.59
121:S2:90:MET:SD	121:S2:90:MET:N	2.76	0.59
129:T2:64:GLY:O	129:T2:118:LYS:NZ	2.34	0.59
130:T3:80:LYS:HZ3	130:T3:238:GLU:HB3	1.66	0.59
29:c1:334:PHE:HB3	29:c1:403:GLY:HA2	1.83	0.59
34:f:263:LYS:O	58:v:68:ARG:NH1	2.35	0.59
45:m3:254:ARG:NH2	45:m3:277:THR:O	2.35	0.59
77:a7:57:PRO:HG3	121:s2:343:ASN:HB3	1.85	0.59
83:am:159:LYS:HD2	153:te:101:CDL:H512	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:b8:112:ILE:O	90:b8:174:ARG:NH2	2.34	0.59
100:n1:230:THR:HG23	126:s7:55:ALA:HB3	1.82	0.59
101:n2:240:THR:OG1	105:n6:137:TYR:OH	2.21	0.59
108:qA:79:ILE:HD12	108:qA:424:VAL:HG21	1.85	0.59
110:qC:60:PRO:HG3	110:qC:178:ILE:HG13	1.85	0.59
120:s1:191:ALA:O	120:s1:438:ASN:ND2	2.36	0.59
13:2T:8:GLN:NE2	30:C2:215:SER:OG	2.33	0.59
23:7A:58:GLU:OE2	23:7A:75:TYR:OH	2.19	0.59
28:BP:82:GLY:HA3	28:BP:129:ASN:HD21	1.67	0.59
72:A1:25:VAL:HG22	153:A1:102:CDL:H201	1.84	0.59
105:N6:50:ILE:HD11	153:N6:302:CDL:H752	1.84	0.59
111:QD:78:ALA:HB1	111:QD:112:PHE:HZ	1.66	0.59
147:V2:128:THR:HA	147:V2:131:GLN:HG2	1.83	0.59
6:2i:75:PHE:O	6:2i:79:ASN:ND2	2.31	0.59
12:2o:27:THR:HG22	54:sc:40:ALA:HB2	1.85	0.59
13:2t:62:TYR:OH	17:5t:47:GLN:NE2	2.34	0.59
74:a3:97:GLN:HB2	101:n2:2:LEU:HD11	1.85	0.59
81:ac:59:ARG:NH1	93:bm:59:LEU:O	2.36	0.59
98:g3:265:ILE:HD13	121:s2:8:LEU:HD13	1.84	0.59
104:n5:207:ILE:HD11	104:n5:293:MET:HE1	1.84	0.59
104:n5:565:LEU:O	104:n5:568:THR:OG1	2.18	0.59
110:qC:52:LEU:HD11	110:qC:81:PHE:HA	1.84	0.59
136:t9:39:LEU:HD21	136:t9:117:ARG:HB2	1.84	0.59
147:v2:128:THR:HA	147:v2:131:GLN:HG2	1.83	0.59
153:7C:301:CDL:H841	153:7C:301:CDL:H351	1.85	0.59
29:C1:334:PHE:HB3	29:C1:403:GLY:HA2	1.83	0.59
72:A1:91:LEU:HD23	105:N6:153:ASP:HB3	1.85	0.59
92:BL:57:LYS:NZ	92:BL:58:GLU:OE2	2.34	0.59
93:BM:166:ASN:HA	138:TB:98:LYS:HE2	1.84	0.59
107:P2:115:LEU:HD11	107:P2:144:TYR:HB3	1.85	0.59
109:QB:77:VAL:HG21	109:QB:256:SER:HA	1.84	0.59
110:Qc:272:ARG:NH2	111:Qd:39:GLY:O	2.35	0.59
110:Qc:345:LYS:O	110:Qc:347:HIS:ND1	2.34	0.59
25:7l:899:GLN:NE2	25:7l:940:ARG:O	2.32	0.59
31:c3:494:ILE:HG12	153:vb:704:CDL:H741	1.85	0.59
38:i:142:ASN:ND2	38:i:218:GLU:O	2.36	0.59
41:l:143:TYR:OH	150:u1:31:UNK:O	2.21	0.59
48:p:56:PHE:HB3	48:p:59:PHE:HB2	1.84	0.59
75:a5:174:ARG:HD2	123:s4:1:MET:HB2	1.85	0.59
80:ab:59:GLU:OE2	145:tx:123:ARG:NH2	2.35	0.59
112:qE:140:GLY:CA	112:qE:156:ARG:O	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
114:qg:10:GLU:OE1	114:qg:14:ASN:ND2	2.35	0.59
132:t5:167:ARG:HH11	144:th:124:GLN:HE21	1.50	0.59
141:te:50:ARG:NH1	141:te:71:LEU:OXT	2.35	0.59
153:6A:201:CDL:H731	153:6A:201:CDL:H512	1.84	0.59
20:6C:9:ARG:HB2	35:FS:81:ALA:HA	1.84	0.59
23:7A:28:TYR:HB2	59:VB:273:MET:HE1	1.85	0.59
31:C3:386:LYS:NZ	59:VB:91:GLU:O	2.36	0.59
40:K:216:GLN:O	40:K:222:ASN:ND2	2.36	0.59
48:P:133:ARG:HG3	48:P:134:GLN:HG3	1.84	0.59
76:A6:96:ARG:NH2	123:S4:71:TYR:O	2.35	0.59
83:AM:159:LYS:HD2	153:TE:101:CDL:H512	1.84	0.59
114:Qg:10:GLU:OE1	114:Qg:14:ASN:ND2	2.35	0.59
114:Qg:145:ARG:HD2	116:Qi:2:VAL:HA	1.83	0.59
131:T4:63:SER:HA	131:T4:196:LYS:HE3	1.84	0.59
43:m1:259:THR:HA	43:m1:262:MET:HE2	1.83	0.59
50:r:148:GLN:O	50:r:152:GLU:HG2	2.02	0.59
52:sa:493:GLY:H	52:sa:539:LYS:HB3	1.68	0.59
84:an:55:ARG:NH2	84:an:56:ASN:OD1	2.34	0.59
101:n2:19:ASN:OD1	148:x1:98:TRP:NE1	2.27	0.59
104:n5:723:TYR:OH	107:p2:128:ARG:NH1	2.36	0.59
121:s2:33:GLN:NE2	126:s7:26:THR:O	2.35	0.59
19:6B:145:LEU:O	30:C2:392:ARG:NH2	2.33	0.59
26:A:221:ARG:NH2	26:A:374:GLU:OE1	2.36	0.59
31:C3:106:VAL:HG21	45:M3:248:LEU:HG	1.85	0.59
45:M3:113:SER:HB2	153:VB:701:CDL:HB31	1.85	0.59
77:A7:57:PRO:HG3	121:S2:343:ASN:HB3	1.83	0.59
84:AN:133:ASN:ND2	158:AN:303:3PE:O14	2.32	0.59
97:G2:100:HIS:H	97:G2:128:ASN:HD22	1.49	0.59
104:N5:207:ILE:HD11	104:N5:293:MET:HE1	1.84	0.59
152:QB:602:PC1:H331	114:Qg:187:PHE:HZ	1.68	0.59
111:QD:65:TYR:OH	111:QD:240:ASN:OD1	2.21	0.59
142:TF:153:ASN:HD22	142:TF:191:LYS:HG3	1.68	0.59
31:c3:217:ASP:OD2	40:k:34:ARG:NH2	2.36	0.59
31:c3:481:LEU:O	31:c3:485:ASN:ND2	2.30	0.59
41:l:169:ASN:O	41:l:173:TYR:HB3	2.02	0.59
45:m3:223:PHE:O	45:m3:227:GLN:NE2	2.36	0.59
53:sb:275:ILE:HB	163:sb:403:F3S:S4	2.42	0.59
57:u:99:ILE:HB	57:u:100:PRO:HD3	1.84	0.59
76:a6:32:ARG:HH11	79:a9:361:GLU:HG3	1.67	0.59
104:n5:608:ARG:HD2	152:n5:803:PC1:H32	1.85	0.59
128:t1:264:LYS:NZ	128:t1:304:ASP:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
132:t5:178:GLN:O	132:t5:182:ASN:ND2	2.33	0.59
2:2E:32:ALA:HB1	2:2E:63:LEU:HD13	1.85	0.59
37:H:183:ARG:HD3	37:H:273:TYR:HE2	1.67	0.59
101:N2:146:THR:HB	101:N2:149:THR:HG22	1.83	0.59
146:V1:123:PRO:HG2	146:V1:323:SER:HB3	1.85	0.59
11:2n:19:SER:O	11:2n:23:LYS:NZ	2.32	0.58
15:4a:125:ASP:HB2	35:fs:95:VAL:HB	1.84	0.58
153:7a:201:CDL:H792	153:7a:201:CDL:H571	1.83	0.58
26:a:221:ARG:NH2	26:a:374:GLU:OE1	2.35	0.58
29:c1:338:SER:HB3	29:c1:399:ILE:HG22	1.84	0.58
153:c1:701:CDL:O1	40:k:40:HIS:O	2.20	0.58
38:i:85:THR:HG23	153:r:201:CDL:H541	1.84	0.58
43:m1:268:LYS:NZ	43:m1:274:CYS:SG	2.76	0.58
59:vb:162:THR:O	59:vb:173:HIS:N	2.25	0.58
79:a9:205:GLN:NE2	102:n3:35:GLN:O	2.34	0.58
153:al:301:CDL:OA3	100:n1:64:ARG:NH1	2.36	0.58
96:g1:197:ASP:OD2	103:n4:142:TYR:OH	2.18	0.58
142:tf:57:LYS:NZ	142:tf:61:GLU:OE2	2.36	0.58
81:AC:107:GLU:OE1	91:B9:1:MET:N	2.35	0.58
86:B3:13:ARG:H	106:P1:251:ASN:HD22	1.51	0.58
90:B8:53:ASN:ND2	103:N4:325:TRP:O	2.28	0.58
152:C4:403:PC1:H2B2	152:C4:403:PC1:H3A1	1.85	0.58
107:p2:115:LEU:HD11	107:p2:144:TYR:HB3	1.84	0.58
112:qe:84:GLU:OE2	116:qi:37:GLN:NE2	2.26	0.58
122:s3:52:GLU:O	122:s3:56:SER:N	2.35	0.58
20:6C:1:MET:N	20:6C:1:MET:SD	2.76	0.58
31:C3:494:ILE:HG12	153:VB:706:CDL:H741	1.85	0.58
51:S:117:ASP:HB3	51:S:120:LEU:HB2	1.86	0.58
64:Y5:135:LYS:HE2	158:Y5:202:3PE:H112	1.86	0.58
153:B3:102:CDL:H322	153:B3:102:CDL:H561	1.84	0.58
112:QE:140:GLY:CA	112:QE:156:ARG:O	2.51	0.58
112:Qe:113:GLY:HA3	152:Qe:303:PC1:H351	1.84	0.58
120:S1:471:PRO:HB2	120:S1:501:VAL:HG22	1.85	0.58
139:TC:17:ASN:ND2	139:TC:20:SER:OG	2.36	0.58
13:2t:59:ASN:HD21	30:c2:225:ILE:HA	1.67	0.58
23:7a:28:TYR:HB2	59:vb:273:MET:HE1	1.85	0.58
153:f:401:CDL:HB22	153:f:401:CDL:HB4	1.83	0.58
72:a1:25:VAL:HG22	153:a1:101:CDL:H201	1.84	0.58
77:a7:208:ARG:NH2	121:s2:323:ASN:O	2.36	0.58
94:c4:65:LYS:NZ	148:x1:27:ASP:OD2	2.35	0.58
101:n2:299:LEU:HD23	101:n2:303:TYR:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
105:n6:50:ILE:HD11	153:n6:302:CDL:H752	1.84	0.58
109:qB:167:ILE:O	109:qB:171:SER:OG	2.20	0.58
115:qH:93:TYR:HA	115:qH:97:ILE:HB	1.84	0.58
122:s3:124:SER:OG	122:s3:136:GLU:OE1	2.21	0.58
2:2E:5:VAL:HG21	2:2E:17:ILE:HD11	1.85	0.58
24:7C:94:MET:HG3	43:M1:267:PRO:HG2	1.84	0.58
41:L:143:TYR:OH	150:U1:31:UNK:O	2.21	0.58
74:A3:57:LEU:HB3	74:A3:60:VAL:HB	1.84	0.58
103:N4:286:VAL:HB	103:N4:342:MET:HE2	1.84	0.58
152:N5:804:PC1:H232	152:N5:804:PC1:H362	1.85	0.58
117:QJ:8:LYS:NZ	117:QJ:12:GLU:OE2	2.29	0.58
19:6b:220:PRO:HA	49:q:37:PRO:HB2	1.84	0.58
31:c3:314:ILE:HB	59:vb:230:VAL:HG11	1.86	0.58
40:k:81:HIS:HA	40:k:84:LYS:HE2	1.83	0.58
43:m1:173:ARG:O	43:m1:184:ARG:NH2	2.35	0.58
45:m3:113:SER:HB2	153:vb:701:CDL:HB31	1.85	0.58
153:q:202:CDL:H522	153:q:202:CDL:H721	1.85	0.58
88:b6:98:VAL:HG11	153:bm:301:CDL:H142	1.86	0.58
104:n5:281:LEU:HB3	104:n5:284:ARG:HB3	1.85	0.58
111:qD:288:GLU:OE1	111:qD:290:TYR:OH	2.17	0.58
24:7C:203:MET:O	24:7C:206:THR:OG1	2.19	0.58
34:F:176:ALA:O	57:U:81:ASN:ND2	2.31	0.58
43:M1:232:GLN:NE2	152:V:202:PC1:O12	2.37	0.58
50:R:148:GLN:O	50:R:152:GLU:HG2	2.02	0.58
75:A5:174:ARG:HD2	123:S4:1:MET:HB2	1.85	0.58
77:A7:208:ARG:NH2	121:S2:323:ASN:O	2.36	0.58
153:AL:301:CDL:OA3	100:N1:64:ARG:NH1	2.36	0.58
93:BM:131:ASP:HB3	93:BM:134:ASP:HB2	1.85	0.58
153:BM:301:CDL:H802	153:BM:301:CDL:H751	1.85	0.58
104:N5:281:LEU:HB3	104:N5:284:ARG:HB3	1.85	0.58
112:Qe:129:TYR:HD1	112:Qe:255:GLU:HB2	1.68	0.58
127:S8:113:LYS:NZ	127:S8:197:GLU:OE2	2.36	0.58
132:T5:167:ARG:HH11	144:TH:124:GLN:HE21	1.50	0.58
136:T9:39:LEU:HD21	136:T9:117:ARG:HB2	1.84	0.58
29:c1:140:ILE:HA	65:y7:318:CYS:SG	2.44	0.58
153:c1:712:CDL:H812	153:c1:712:CDL:H762	1.86	0.58
40:k:216:GLN:O	40:k:222:ASN:ND2	2.36	0.58
42:m:46:ARG:NE	153:m:304:CDL:OB4	2.31	0.58
43:m1:71:GLN:O	51:S:167:GLN:NE2	2.35	0.58
97:g2:100:HIS:H	97:g2:128:ASN:HD22	1.49	0.58
109:qB:136:ASN:ND2	109:qB:151:SER:OG	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
114:qg:162:TYR:HA	114:qg:166:MET:HB2	1.83	0.58
120:s1:714:LYS:HD2	120:s1:716:LEU:HD23	1.86	0.58
31:C3:314:ILE:HB	59:VB:230:VAL:HG11	1.85	0.58
37:H:257:GLU:O	37:H:284:GLN:NE2	2.36	0.58
153:M3:403:CDL:O1	46:N:56:TYR:O	2.18	0.58
80:AB:59:GLU:OE1	145:TX:119:ASN:ND2	2.36	0.58
81:AC:59:ARG:NH1	93:BM:59:LEU:O	2.36	0.58
103:N4:167:ASN:ND2	135:T8:81:THR:OG1	2.35	0.58
115:QH:93:TYR:HA	115:QH:97:ILE:HB	1.84	0.58
121:S2:383:LYS:NZ	121:S2:434:ASP:OD1	2.36	0.58
2:2e:32:ALA:HB1	2:2e:63:LEU:HD13	1.85	0.58
153:6a:201:CDL:H731	153:6a:201:CDL:H512	1.84	0.58
33:e:333:THR:OG1	33:e:334:GLU:N	2.36	0.58
42:m:153:LEU:HA	42:m:156:VAL:HG22	1.84	0.58
65:y7:402:ASN:O	65:y7:406:HIS:ND1	2.36	0.58
153:a1:101:CDL:OB4	100:n1:62:ARG:NE	2.29	0.58
80:ab:59:GLU:OE1	145:tx:119:ASN:ND2	2.36	0.58
90:b8:100:PHE:O	90:b8:104:ASN:ND2	2.34	0.58
101:n2:138:ILE:HG12	101:n2:291:ILE:HG21	1.86	0.58
114:qG:315:PRO:HD2	114:qG:318:LEU:HD12	1.86	0.58
110:qc:70:GLU:HB3	110:qc:77:THR:HG21	1.84	0.58
110:qc:147:ALA:O	110:qc:151:ASN:ND2	2.34	0.58
120:s1:471:PRO:HB2	120:s1:501:VAL:HG22	1.84	0.58
120:s1:612:GLU:OE2	120:s1:615:GLN:NE2	2.37	0.58
153:2G:201:CDL:H571	153:2G:201:CDL:H141	1.86	0.58
52:SA:65:PHE:HE1	52:SA:195:SER:HB2	1.69	0.58
101:N2:262:ILE:HD13	101:N2:352:ILE:HD11	1.85	0.58
104:N5:77:GLN:HG3	104:N5:83:ASN:HB3	1.85	0.58
104:N5:338:LYS:NZ	104:N5:417:ASP:OD2	2.34	0.58
107:P2:87:GLU:HB2	107:P2:96:SER:HB2	1.85	0.58
109:Qb:444:ARG:NH1	109:Qb:450:GLU:OE1	2.36	0.58
110:Qc:425:LYS:HD2	114:Qg:148:SER:HB2	1.85	0.58
120:S1:124:ASN:HD22	146:V1:388:GLU:HG3	1.67	0.58
36:g:215:PRO:HB3	59:vb:158:TYR:HB2	1.85	0.58
52:sa:276:GLU:N	52:sa:400:GLY:O	2.34	0.58
57:u:7:ARG:NH1	58:v:122:ASP:OD2	2.37	0.58
84:an:1:MET:HG2	101:n2:313:ILE:HG21	1.85	0.58
98:g3:282:PHE:O	98:g3:287:TYR:OH	2.21	0.58
100:n1:141:GLY:HA3	100:n1:153:SER:HB3	1.84	0.58
116:qI:105:GLU:HG2	116:qI:109:LYS:HE3	1.86	0.58
117:qJ:8:LYS:NZ	117:qJ:12:GLU:OE2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
127:s8:229:GLU:O	127:s8:233:ASN:ND2	2.34	0.58
142:tf:153:ASN:HD22	142:tf:191:LYS:HG3	1.68	0.58
147:v2:205:LYS:O	147:v2:209:GLN:NE2	2.36	0.58
29:C1:629:ARG:O	29:C1:630:ARG:NH1	2.36	0.58
34:F:263:LYS:O	58:V:68:ARG:NH1	2.35	0.58
38:I:85:THR:HG23	153:R:201:CDL:H541	1.84	0.58
108:QA:380:ILE:HG21	108:QA:480:LEU:HB3	1.84	0.58
120:S1:191:ALA:O	120:S1:438:ASN:ND2	2.36	0.58
28:bp:260:ASN:HB2	28:bp:269:LEU:HD22	1.84	0.58
31:c3:306:GLN:HG2	31:c3:310:LYS:HD2	1.86	0.58
51:s:47:THR:HG23	65:y7:191:ASN:HD22	1.68	0.58
71:5b:19:PHE:HZ	104:n5:472:LEU:HD23	1.67	0.58
77:a7:266:HIS:NE2	127:s8:229:GLU:OE2	2.31	0.58
104:n5:86:LYS:NZ	37:H:298:SER:HB2	2.19	0.58
110:qc:345:LYS:O	110:qc:347:HIS:ND1	2.33	0.58
110:qc:425:LYS:HD2	114:qg:148:SER:HB2	1.85	0.58
121:s2:346:ASN:O	146:v1:465:ARG:NH1	2.37	0.58
139:tc:17:ASN:ND2	139:tc:20:SER:OG	2.36	0.58
153:C1:701:CDL:H712	65:Y7:356:PHE:HE2	1.69	0.58
31:C3:217:ASP:OD2	40:K:34:ARG:NH2	2.36	0.58
35:FS:91:GLN:HB2	42:M:13:HIS:HB3	1.86	0.58
36:G:215:PRO:HB3	59:VB:158:TYR:HB2	1.85	0.58
45:M3:102:LYS:NZ	45:M3:261:PRO:O	2.35	0.58
45:M3:223:PHE:O	45:M3:227:GLN:NE2	2.36	0.58
51:S:47:THR:HG23	65:Y7:191:ASN:HD22	1.68	0.58
78:A8:236:LYS:HE3	83:AM:75:MET:HB3	1.86	0.58
128:T1:254:GLN:OE1	128:T1:257:ARG:NE	2.35	0.58
153:7c:301:CDL:H351	153:7c:301:CDL:H841	1.85	0.58
28:bp:400:LYS:NZ	28:bp:401:LEU:O	2.37	0.58
30:c2:137:LEU:HD21	30:c2:602:TYR:HB3	1.84	0.58
36:g:42:ARG:NH1	59:vb:260:ASP:OD2	2.34	0.58
36:g:181:ASN:ND2	59:vb:186:GLN:OE1	2.35	0.58
49:q:129:ILE:HG22	49:q:137:TRP:HB2	1.85	0.58
50:r:96:VAL:HG22	153:r:201:CDL:H741	1.86	0.58
105:n6:126:LEU:HD23	153:n6:302:CDL:H582	1.86	0.58
108:qA:79:ILE:HD11	108:qA:420:THR:HG22	1.86	0.58
110:qc:353:LEU:HD21	160:qh:201:PX2:H10	1.85	0.58
128:t1:254:GLN:OE1	128:t1:257:ARG:NE	2.35	0.58
25:7L:922:GLU:O	30:C2:600:ARG:NH1	2.36	0.58
43:M1:268:LYS:NZ	43:M1:274:CYS:SG	2.77	0.58
50:R:96:VAL:HG22	153:R:201:CDL:H741	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:U:7:ARG:NH1	58:V:122:ASP:OD2	2.36	0.58
153:A1:102:CDL:OB4	100:N1:62:ARG:NE	2.30	0.58
73:A2:78:ASN:ND2	73:A2:82:GLU:OE1	2.37	0.58
83:AM:140:PHE:CG	124:S5:52:GLN:HG2	2.39	0.58
108:Qa:326:ALA:O	108:Qa:330:ASN:ND2	2.37	0.58
142:TF:57:LYS:NZ	142:TF:61:GLU:OE2	2.36	0.58
2:2e:5:VAL:HG21	2:2e:17:ILE:HD11	1.86	0.58
3:2f:278:VAL:HG13	6:2i:44:LEU:HD12	1.85	0.58
26:a:334:ASN:OD1	65:y7:332:TRP:NE1	2.35	0.58
30:c2:509:SER:OG	30:c2:512:ILE:O	2.18	0.58
104:n5:79:ASP:HA	104:n5:84:LYS:HD3	1.86	0.58
109:qb:136:ASN:ND2	109:qb:151:SER:OG	2.37	0.58
112:qe:129:TYR:HD1	112:qe:255:GLU:HB2	1.68	0.58
125:s6:88:ILE:HG22	125:s6:99:GLN:HG2	1.86	0.58
4:2G:162:GLU:OE2	53:SB:262:ARG:NH2	2.35	0.58
19:6B:44:VAL:HG22	25:7L:970:LEU:HB3	1.84	0.58
153:C1:712:CDL:H812	153:C1:712:CDL:H762	1.86	0.58
56:T:120:LEU:HD12	153:T:203:CDL:H211	1.85	0.58
66:Z:38:GLU:O	67:Z1:69:ASN:ND2	2.35	0.58
69:2B:124:LYS:NZ	69:2B:126:ASN:OD1	2.37	0.58
71:5B:10:LYS:NZ	90:B8:86:GLN:OE1	2.37	0.58
74:A3:97:GLN:HB2	101:N2:2:LEU:HD11	1.85	0.58
94:C4:65:LYS:NZ	148:X1:27:ASP:OD2	2.35	0.58
109:QB:136:ASN:ND2	109:QB:151:SER:OG	2.36	0.58
112:QE:113:GLY:HA3	152:QE:303:PC1:H352	1.85	0.58
114:QG:194:ARG:NH1	117:Qj:7:TYR:OH	2.34	0.58
120:S1:297:GLY:O	120:S1:566:HIS:NE2	2.35	0.58
121:S2:346:ASN:O	146:V1:465:ARG:NH1	2.37	0.58
135:T8:109:ILE:HG23	144:TH:2:ASN:HD21	1.69	0.58
14:3t:39:ARG:HG3	14:3t:41:ASP:H	1.69	0.57
37:h:298:SER:HB2	104:N5:86:LYS:NZ	2.19	0.57
57:u:46:THR:O	38:I:136:GLN:NE2	2.31	0.57
59:vb:466:GLN:OE1	59:vb:547:ASN:ND2	2.36	0.57
71:5b:10:LYS:NZ	90:b8:86:GLN:OE1	2.37	0.57
79:a9:302:TYR:HB2	153:a9:403:CDL:HA61	1.86	0.57
93:bm:186:ASP:OD1	93:bm:189:ARG:NH1	2.37	0.57
106:p1:219:ASN:OD1	106:p1:236:ARG:NH2	2.37	0.57
112:qE:37:LYS:NZ	145:tx:129:GLU:O	2.30	0.57
112:qE:113:GLY:HA3	152:qE:303:PC1:H352	1.85	0.57
143:tg:15:LEU:HD23	143:tg:24:LEU:HD13	1.85	0.57
52:SA:93:GLY:HA2	52:SA:183:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:596:LYS:HD3	52:SA:614:TYR:HB3	1.85	0.57
76:A6:53:SER:HB2	168:AB:201:ZMP:H19	1.86	0.57
108:QA:139:SER:OG	108:QA:154:ASN:ND2	2.36	0.57
110:Qc:114:ALA:HB2	114:Qg:178:LEU:HD22	1.85	0.57
121:S2:283:ARG:NH2	121:S2:432:THR:O	2.35	0.57
150:U1:68:UNK:O	150:U1:70:UNK:N	2.37	0.57
20:6c:9:ARG:HB2	35:fs:81:ALA:HA	1.85	0.57
153:c1:701:CDL:H712	65:y7:356:PHE:HE2	1.69	0.57
40:k:207:VAL:HG21	41:l:149:LEU:HD11	1.86	0.57
130:t3:169:PHE:HB2	130:t3:174:TYR:HB3	1.85	0.57
13:2T:59:ASN:HD21	30:C2:225:ILE:HA	1.68	0.57
26:A:334:ASN:OD1	65:Y7:332:TRP:NE1	2.35	0.57
29:C1:140:ILE:HA	65:Y7:318:CYS:SG	2.44	0.57
33:E:257:ASP:OD1	33:E:281:HIS:ND1	2.29	0.57
73:A2:25:ARG:HD2	73:A2:76:ALA:HB1	1.86	0.57
77:A7:266:HIS:NE2	127:S8:229:GLU:OE2	2.31	0.57
84:AN:55:ARG:NH2	84:AN:56:ASN:OD1	2.34	0.57
110:Qc:232:GLY:HA3	111:Qd:271:LYS:HG3	1.86	0.57
120:S1:388:ASN:ND2	120:S1:511:PHE:O	2.35	0.57
10:2m:15:LEU:HD13	12:2o:5:ILE:HD12	1.86	0.57
43:m1:232:GLN:NE2	152:v:202:PC1:O12	2.36	0.57
52:sa:65:PHE:HE1	52:sa:195:SER:HB2	1.69	0.57
72:a1:91:LEU:HD23	105:n6:153:ASP:HB3	1.86	0.57
93:bm:131:ASP:HB3	93:bm:134:ASP:HB2	1.85	0.57
100:n1:44:ARG:HH12	126:s7:52:ILE:HD13	1.69	0.57
102:n3:43:TYR:OH	121:s2:33:GLN:OE1	2.17	0.57
106:p1:161:VAL:HG13	106:p1:175:VAL:HG13	1.85	0.57
112:qE:60:PHE:CZ	115:qH:57:GLY:HA2	2.40	0.57
121:s2:383:LYS:NZ	121:s2:434:ASP:OD1	2.36	0.57
3:2F:278:VAL:HG13	6:2I:44:LEU:HD12	1.85	0.57
23:7A:120:ARG:NH1	46:N:72:ASP:OD1	2.38	0.57
33:E:38:LEU:HD21	33:E:286:GLU:HG3	1.86	0.57
50:R:13:LYS:NZ	66:Z:90:GLN:OE1	2.29	0.57
160:R:202:PX2:H3	66:Z:29:LYS:HE2	1.86	0.57
79:A9:302:TYR:HB2	153:A9:403:CDL:HA61	1.85	0.57
106:P1:219:ASN:OD1	106:P1:236:ARG:NH2	2.37	0.57
112:QE:60:PHE:CZ	115:QH:57:GLY:HA2	2.40	0.57
116:QI:105:GLU:HG2	116:QI:109:LYS:HE3	1.86	0.57
114:Qg:183:PRO:HB2	153:Qg:402:CDL:H421	1.86	0.57
3:2f:210:SER:OG	153:2g:204:CDL:OA9	2.20	0.57
51:s:40:ILE:HD13	59:vb:541:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:t:120:LEU:HD12	153:t:203:CDL:H211	1.85	0.57
65:y7:277:VAL:HG13	65:y7:280:LEU:HD12	1.85	0.57
93:bm:141:LYS:NZ	93:bm:145:GLU:OE2	2.36	0.57
97:g2:129:HIS:HB2	97:g2:146:ASN:HD22	1.69	0.57
110:qC:231:LEU:HD22	152:qI:202:PC1:H2E1	1.85	0.57
122:s3:126:ASP:HA	122:s3:132:ALA:HB3	1.86	0.57
128:t1:457:ILE:HG23	128:t1:469:GLU:HG3	1.85	0.57
153:2G:201:CDL:H342	7:2J:28:PRO:HB3	1.84	0.57
15:4A:47:LYS:NZ	36:G:282:MET:O	2.30	0.57
33:E:333:THR:OG1	33:E:334:GLU:N	2.37	0.57
85:B2:111:LEU:HD22	131:T4:26:ILE:HG13	1.86	0.57
90:B8:100:PHE:O	90:B8:104:ASN:ND2	2.34	0.57
90:B8:112:ILE:O	90:B8:174:ARG:NH2	2.34	0.57
104:N5:366:ILE:HG21	104:N5:444:ARG:HD2	1.86	0.57
109:QB:289:PRO:HB3	109:QB:475:GLU:HB3	1.87	0.57
108:Qa:68:GLU:OE1	108:Qa:259:HIS:ND1	2.37	0.57
128:T1:457:ILE:HG23	128:T1:469:GLU:HG3	1.85	0.57
2:2e:93:LYS:O	2:2e:97:ILE:HG23	2.04	0.57
31:c3:138:LEU:CB	31:c3:149:PHE:O	2.53	0.57
33:e:38:LEU:HD21	33:e:286:GLU:HG3	1.86	0.57
34:f:136:ARG:NH2	34:f:322:LYS:O	2.37	0.57
52:sa:93:GLY:HA2	52:sa:183:THR:HG21	1.86	0.57
52:sa:148:SER:H	52:sa:179:ALA:HA	1.70	0.57
75:a5:103:GLU:OE1	77:a7:141:ARG:NH2	2.32	0.57
86:b3:13:ARG:H	106:p1:251:ASN:HD22	1.52	0.57
153:c4:401:CDL:H231	158:c4:402:3PE:H2H2	1.85	0.57
104:n5:168:ASN:OD1	104:n5:216:TYR:OH	2.14	0.57
105:n6:56:TYR:HB3	152:n6:301:PC1:H3I2	1.86	0.57
108:qa:326:ALA:O	108:qa:330:ASN:ND2	2.36	0.57
30:C2:405:VAL:HG21	47:O:83:MET:HE1	1.86	0.57
35:FS:42:ARG:NH2	35:FS:50:ILE:O	2.33	0.57
153:Q:202:CDL:H522	153:Q:202:CDL:H721	1.85	0.57
84:AN:101:HIS:ND1	153:N6:302:CDL:OA4	2.34	0.57
90:B8:88:ALA:HB1	153:B8:302:CDL:H532	1.87	0.57
93:BM:186:ASP:OD1	93:BM:189:ARG:NH1	2.37	0.57
100:N1:147:LYS:HE3	102:N3:55:ILE:HG22	1.87	0.57
105:N6:56:TYR:HB3	152:N6:301:PC1:H3I2	1.86	0.57
106:P1:161:VAL:HG13	106:P1:175:VAL:HG13	1.85	0.57
111:QD:117:ALA:O	111:Qd:122:LYS:NZ	2.31	0.57
131:T4:96:PHE:O	131:T4:207:ASN:ND2	2.29	0.57
146:V1:301:LEU:HD11	146:V1:355:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6a:120:LEU:HB3	19:6b:187:PHE:HE1	1.70	0.57
20:6c:1:MET:SD	20:6c:1:MET:N	2.76	0.57
31:c3:106:VAL:HG21	45:m3:248:LEU:HG	1.85	0.57
153:m3:403:CDL:O1	46:n:56:TYR:O	2.18	0.57
46:n:183:PRO:HG2	46:n:184:LEU:HD12	1.86	0.57
51:s:117:ASP:HB3	51:s:120:LEU:HB2	1.86	0.57
52:sa:596:LYS:HD3	52:sa:614:TYR:HB3	1.86	0.57
53:sb:75:ARG:NH2	53:sb:115:THR:OG1	2.34	0.57
64:y5:135:LYS:HE2	158:y5:202:3PE:H112	1.86	0.57
73:a2:15:LEU:HB2	73:a2:47:PHE:HE2	1.70	0.57
73:a2:78:ASN:ND2	73:a2:82:GLU:OE1	2.38	0.57
83:am:140:PHE:CG	124:s5:52:GLN:HG2	2.39	0.57
96:g1:210:ARG:NH2	96:g1:252:GLU:O	2.37	0.57
99:j1:308:ASP:OD2	105:n6:12:ASN:ND2	2.37	0.57
101:n2:276:LEU:O	101:n2:337:LYS:NZ	2.37	0.57
104:n5:366:ILE:HG21	104:n5:444:ARG:HD2	1.86	0.57
152:n5:804:PC1:H232	152:n5:804:PC1:H362	1.85	0.57
112:qE:104:LEU:HD21	152:qI:202:PC1:H341	1.85	0.57
129:t2:198:LEU:HB3	129:t2:213:LYS:HB2	1.87	0.57
130:t3:80:LYS:HZ3	130:t3:238:GLU:HB3	1.68	0.57
14:3T:39:ARG:HG3	14:3T:41:ASP:H	1.69	0.57
21:6L:42:PRO:O	21:6L:45:LEU:HB2	2.05	0.57
42:M:117:ILE:HD11	153:M:305:CDL:H841	1.86	0.57
46:N:183:PRO:HG2	46:N:184:LEU:HD12	1.86	0.57
53:SB:230:TRP:O	55:SD:17:ARG:NH2	2.37	0.57
71:5B:86:ILE:HG12	101:N2:254:ILE:HG21	1.86	0.57
91:B9:108:ASP:HB3	104:N5:540:ARG:HH12	1.69	0.57
111:QD:187:PRO:HG3	113:QF:62:LEU:HD13	1.87	0.57
122:S3:124:SER:OG	122:S3:136:GLU:OE1	2.21	0.57
128:T1:214:ASN:O	128:T1:250:GLN:NE2	2.30	0.57
4:2g:122:HIS:CE1	153:2g:204:CDL:H521	2.40	0.57
28:bp:198:SER:O	28:bp:201:ASN:ND2	2.38	0.57
34:f:140:PRO:HG3	34:f:144:ILE:HD11	1.87	0.57
53:sb:230:TRP:O	55:sd:17:ARG:NH2	2.38	0.57
73:a2:25:ARG:HD2	73:a2:76:ALA:HB1	1.87	0.57
90:b8:88:ALA:HB1	153:b8:302:CDL:H532	1.87	0.57
109:qb:444:ARG:NH1	109:qb:450:GLU:OE1	2.37	0.57
121:s2:30:PHE:HB3	121:s2:43:LEU:HB3	1.87	0.57
122:s3:32:HIS:NE2	122:s3:110:THR:OG1	2.27	0.57
135:t8:109:ILE:HG23	144:th:2:ASN:HD21	1.69	0.57
146:v1:301:LEU:HD11	146:v1:355:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2K:34:ARG:HH22	153:2K:101:CDL:H112	1.69	0.57
49:Q:75:LYS:NZ	153:Q:201:CDL:O1	2.38	0.57
88:B6:98:VAL:HG11	153:BM:301:CDL:H142	1.85	0.57
103:N4:243:THR:HG23	103:N4:304:ILE:HD12	1.85	0.57
110:QC:68:GLU:OE1	111:QD:90:LYS:NZ	2.26	0.57
115:QH:70:ILE:N	153:QI:203:CDL:OB4	2.38	0.57
109:Qb:136:ASN:ND2	109:Qb:151:SER:OG	2.37	0.57
1:1t:11:THR:HG23	22:6t:5:LEU:HD22	1.86	0.57
43:m1:306:TRP:NE1	153:m1:405:CDL:OA9	2.31	0.57
48:p:38:LYS:H	48:p:117:ASN:HD22	1.53	0.57
54:sc:54:ALA:HB3	54:sc:57:GLU:HB2	1.87	0.57
76:a6:53:SER:HB2	168:ab:201:ZMP:H19	1.87	0.57
85:b2:111:LEU:HD22	131:t4:26:ILE:HG13	1.86	0.57
96:g1:139:VAL:HB	96:g1:157:MET:HG2	1.85	0.57
133:t6:89:TRP:CD1	133:t6:93:CYS:HG	2.22	0.57
15:4A:68:VAL:HG21	33:E:11:LEU:HD23	1.87	0.57
33:E:321:ASP:OD1	33:E:324:ARG:NH2	2.35	0.57
36:G:42:ARG:NH1	59:VB:260:ASP:OD2	2.35	0.57
54:SC:54:ALA:HB3	54:SC:57:GLU:HB2	1.87	0.57
65:Y7:277:VAL:HG13	65:Y7:280:LEU:HD12	1.85	0.57
95:FX:92:GLU:OE2	103:N4:193:ARG:NH1	2.23	0.57
97:G2:129:HIS:HB2	97:G2:146:ASN:HD22	1.69	0.57
104:N5:79:ASP:HA	104:N5:84:LYS:HD3	1.87	0.57
108:QA:319:ILE:O	108:QA:323:ASN:ND2	2.38	0.57
153:QB:601:CDL:H351	152:QB:602:PC1:H2E1	1.86	0.57
117:QJ:1:MET:SD	117:QJ:1:MET:N	2.77	0.57
8:2k:34:ARG:HH22	153:2k:101:CDL:H112	1.69	0.57
9:2l:48:HIS:ND1	10:2m:57:GLN:OE1	2.38	0.57
27:b:345:ASN:O	27:b:349:ASN:ND2	2.33	0.57
29:c1:226:PHE:HA	46:n:195:ARG:HH21	1.70	0.57
40:k:131:SER:O	48:p:174:LYS:NZ	2.37	0.57
42:m:117:ILE:HD11	153:m:303:CDL:H841	1.87	0.57
78:a8:137:GLN:O	78:a8:144:LYS:NZ	2.38	0.57
78:a8:236:LYS:HE3	83:am:75:MET:HB3	1.86	0.57
84:an:150:GLN:HE22	158:an:306:3PE:H242	1.70	0.57
107:p2:87:GLU:HB2	107:p2:96:SER:HB2	1.85	0.57
110:qc:116:TRP:CE2	166:qc:503:HEM:HBC1	2.40	0.57
145:tx:103:LEU:HD23	145:tx:108:GLU:HA	1.87	0.57
9:2L:48:HIS:ND1	10:2M:57:GLN:OE1	2.37	0.57
11:2N:37:TYR:HH	12:2O:37:TYR:HH	1.52	0.57
48:P:38:LYS:H	48:P:117:ASN:HD22	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Q:129:ILE:HG22	49:Q:137:TRP:HB2	1.85	0.57
153:BM:301:CDL:H231	104:N5:294:ILE:HD11	1.86	0.57
101:N2:276:LEU:O	101:N2:337:LYS:NZ	2.37	0.57
106:P1:102:PHE:CE1	106:P1:105:HIS:HB2	2.40	0.57
121:S2:30:PHE:HB3	121:S2:43:LEU:HB3	1.87	0.57
130:T3:169:PHE:HB2	130:T3:174:TYR:HB3	1.85	0.57
132:T5:140:ARG:NE	138:TB:92:GLU:OE2	2.38	0.57
141:TE:50:ARG:NH1	141:TE:71:LEU:OXT	2.38	0.57
148:X1:2:SER:HB2	148:X1:148:ILE:HA	1.86	0.57
21:6l:42:PRO:O	21:6l:45:LEU:HB2	2.05	0.57
30:c2:268:TRP:HH2	30:c2:310:LEU:HD12	1.70	0.57
30:c2:356:GLU:O	31:c3:578:LYS:NZ	2.38	0.57
91:b9:108:ASP:HB3	104:n5:540:ARG:HH12	1.69	0.57
97:g2:148:THR:HB	97:g2:166:VAL:HG22	1.87	0.57
101:n2:262:ILE:HD13	101:n2:352:ILE:HD11	1.86	0.57
109:qb:487:LEU:HD23	109:qb:487:LEU:H	1.70	0.57
147:v2:221:ARG:HH21	147:v2:224:LEU:HB2	1.70	0.57
1:1T:11:THR:HG23	22:6T:5:LEU:HD22	1.86	0.57
2:2E:93:LYS:O	2:2E:97:ILE:HG23	2.04	0.57
5:2H:160:GLN:O	5:2H:164:ASN:ND2	2.32	0.57
153:A:502:CDL:H711	153:C3:604:CDL:HB62	1.87	0.57
31:C3:306:GLN:HG2	31:C3:310:LYS:HD2	1.86	0.57
50:R:16:ASN:O	50:R:44:GLN:NE2	2.38	0.57
52:SA:315:MET:HE3	52:SA:331:VAL:HG13	1.85	0.57
71:5B:34:ARG:HD2	152:B9:201:PC1:H132	1.87	0.57
75:A5:103:GLU:OE1	77:A7:141:ARG:NH2	2.32	0.57
98:G3:56:THR:OG1	98:G3:57:ASN:N	2.38	0.57
111:Qd:77:PHE:HA	111:Qd:81:CYS:HB2	1.87	0.57
120:S1:714:LYS:HD2	120:S1:716:LEU:HD23	1.86	0.57
125:S6:88:ILE:HG22	125:S6:99:GLN:HG2	1.86	0.57
158:TA:201:3PE:H322	158:TA:201:3PE:H271	1.87	0.57
26:a:456:TRP:HE1	59:vb:339:ASN:HD22	1.53	0.56
33:e:138:LYS:HB2	153:e:402:CDL:H581	1.86	0.56
38:i:173:ILE:HG22	47:o:187:LYS:HG2	1.87	0.56
43:m1:301:PHE:HA	43:m1:305:PHE:HB3	1.87	0.56
57:u:138:ARG:HH12	57:u:142:LEU:HD22	1.70	0.56
153:bm:301:CDL:H751	153:bm:301:CDL:H802	1.85	0.56
108:qA:139:SER:OG	108:qA:154:ASN:ND2	2.36	0.56
109:qB:410:GLU:OE1	109:qB:413:ARG:NH2	2.31	0.56
110:qC:116:TRP:HA	166:qC:502:HEM:HBC2	1.87	0.56
128:t1:231:LYS:HG2	128:t1:472:GLU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
146:v1:123:PRO:HG2	146:v1:323:SER:HB3	1.86	0.56
4:2G:36:GLU:HB2	4:2G:102:TYR:CE1	2.39	0.56
25:7L:879:SER:HB2	25:7L:882:MET:HB2	1.87	0.56
43:M1:301:PHE:HA	43:M1:305:PHE:HB3	1.86	0.56
59:VB:466:GLN:OE1	59:VB:547:ASN:ND2	2.36	0.56
65:Y7:402:ASN:O	65:Y7:406:HIS:ND1	2.36	0.56
69:2B:120:ARG:HB2	103:N4:200:LEU:HD11	1.87	0.56
72:A1:51:ARG:NH2	78:A8:236:LYS:O	2.36	0.56
90:B8:90:TRP:CE2	104:N5:472:LEU:HD21	2.40	0.56
109:QB:445:ARG:NH1	109:QB:446:VAL:O	2.38	0.56
111:Qd:293:ARG:NH2	114:Qg:301:ASP:OD1	2.38	0.56
120:S1:612:GLU:OE2	120:S1:615:GLN:NE2	2.37	0.56
131:T4:117:LEU:HD21	152:T4:303:PC1:H361	1.86	0.56
147:V2:221:ARG:HH21	147:V2:224:LEU:HB2	1.70	0.56
149:C:136:GLU:HA	149:C:139:LYS:HE2	1.87	0.56
23:7a:120:ARG:NH1	46:n:72:ASP:OD1	2.38	0.56
28:bp:383:LEU:O	31:c3:215:GLN:NE2	2.37	0.56
30:c2:405:VAL:HG21	47:o:83:MET:HE1	1.86	0.56
46:n:100:ARG:NH1	65:y7:373:GLU:OE1	2.39	0.56
49:q:75:LYS:NZ	153:q:201:CDL:O1	2.38	0.56
153:q:203:CDL:H181	153:vb:704:CDL:H322	1.87	0.56
66:z:11:ARG:NE	66:z:16:GLU:OE2	2.34	0.56
92:bl:67:LEU:HB3	92:bl:110:VAL:HG12	1.87	0.56
100:n1:147:LYS:HE3	102:n3:55:ILE:HG22	1.87	0.56
103:n4:387:THR:OG1	103:n4:392:GLU:OE1	2.20	0.56
153:qB:601:CDL:H351	152:qB:602:PC1:H2E1	1.86	0.56
110:qc:377:ARG:NH2	113:qf:55:GLU:OE2	2.38	0.56
120:s1:390:LYS:HE3	120:s1:653:ILE:HD12	1.86	0.56
121:s2:90:MET:N	121:s2:90:MET:SD	2.76	0.56
130:t3:225:ASP:OD2	130:t3:273:ARG:NH2	2.39	0.56
40:K:191:SER:OG	48:P:26:GLN:O	2.23	0.56
40:K:207:VAL:HG21	41:L:149:LEU:HD11	1.86	0.56
152:W:201:PC1:H3I1	158:W:203:3PE:H371	1.87	0.56
78:A8:137:GLN:O	78:A8:144:LYS:NZ	2.38	0.56
81:AC:110:ASP:OD2	91:B9:38:ARG:NH1	2.39	0.56
97:G2:20:ARG:HH21	98:G3:37:GLN:HE22	1.53	0.56
104:N5:565:LEU:O	104:N5:568:THR:OG1	2.19	0.56
105:N6:126:LEU:HD23	153:N6:302:CDL:H582	1.86	0.56
110:Qc:377:ARG:NH2	113:Qf:55:GLU:OE2	2.38	0.56
122:S3:32:HIS:NE2	122:S3:110:THR:OG1	2.28	0.56
150:u1:68:UNK:O	150:u1:70:UNK:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2e:35:PHE:O	2:2e:62:LYS:NZ	2.39	0.56
29:c1:334:PHE:HA	29:c1:337:ILE:HD12	1.87	0.56
34:f:194:LYS:NZ	43:m1:231:GLU:O	2.25	0.56
34:f:322:LYS:HD2	35:fs:4:ILE:HD11	1.86	0.56
153:m:304:CDL:H552	153:t:201:CDL:H551	1.87	0.56
44:m2:62:ASN:HD21	153:m2:401:CDL:H341	1.70	0.56
52:sa:315:MET:HE3	52:sa:331:VAL:HG13	1.86	0.56
71:5b:34:ARG:HD2	152:b9:201:PC1:H132	1.86	0.56
153:bm:301:CDL:H231	104:n5:294:ILE:HD11	1.86	0.56
106:p1:51:GLU:HG3	107:p2:136:LEU:HD13	1.87	0.56
106:p1:54:PHE:HB3	153:p1:402:CDL:H551	1.88	0.56
109:qB:445:ARG:NH1	109:qB:446:VAL:O	2.38	0.56
112:qE:73:TRP:HA	112:qE:76:GLU:HB2	1.88	0.56
111:qd:124:TYR:O	111:qd:127:GLN:NE2	2.38	0.56
121:s2:211:THR:O	121:s2:277:TYR:OH	2.23	0.56
132:t5:140:ARG:NE	138:tb:92:GLU:OE2	2.38	0.56
158:ta:201:3PE:H322	158:ta:201:3PE:H271	1.87	0.56
1:1T:33:ASN:ND2	1:1T:41:GLN:OE1	2.34	0.56
18:6A:120:LEU:HB3	19:6B:187:PHE:HE1	1.70	0.56
25:7L:919:LYS:HG3	25:7L:939:MET:HE1	1.87	0.56
26:A:456:TRP:HE1	59:VB:339:ASN:HD22	1.53	0.56
28:BP:400:LYS:NZ	28:BP:401:LEU:O	2.37	0.56
29:C1:226:PHE:HA	46:N:195:ARG:HH21	1.70	0.56
30:C2:268:TRP:HH2	30:C2:310:LEU:HD12	1.70	0.56
34:F:140:PRO:HG3	34:F:144:ILE:HD11	1.87	0.56
38:I:104:TYR:OH	152:I:301:PC1:O22	2.18	0.56
153:M:306:CDL:H552	153:T:201:CDL:H551	1.87	0.56
45:M3:2:ALA:HA	45:M3:6:ILE:HB	1.86	0.56
51:S:40:ILE:HD13	59:VB:541:ILE:HD13	1.87	0.56
52:SA:148:SER:H	52:SA:179:ALA:HA	1.70	0.56
65:Y7:138:LEU:O	65:Y7:142:ASN:ND2	2.28	0.56
73:A2:15:LEU:HB2	73:A2:47:PHE:HE2	1.69	0.56
78:A8:233:HIS:O	83:AM:78:ARG:NH1	2.39	0.56
84:AN:1:MET:HG2	101:N2:313:ILE:HG21	1.86	0.56
92:BL:148:LEU:HA	103:N4:83:LEU:HD11	1.87	0.56
96:G1:139:VAL:HB	96:G1:157:MET:HG2	1.85	0.56
101:N2:138:ILE:HG12	101:N2:291:ILE:HG21	1.86	0.56
108:QA:121:VAL:HG12	114:Qg:168:ASP:HB2	1.86	0.56
109:QB:167:ILE:O	109:QB:171:SER:OG	2.20	0.56
110:QC:116:TRP:HA	166:QC:502:HEM:HBC2	1.88	0.56
110:QC:231:LEU:HD22	152:QI:202:PC1:H2E1	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:QD:43:LEU:HD11	111:QD:169:PRO:HG2	1.87	0.56
126:S7:91:LEU:HG	126:S7:121:ILE:HG23	1.86	0.56
128:T1:231:LYS:HG2	128:T1:472:GLU:HA	1.87	0.56
128:T1:313:ASP:OD1	128:T1:313:ASP:N	2.38	0.56
138:TB:79:ALA:HB1	153:TH:200:CDL:H741	1.87	0.56
139:TC:12:ASN:ND2	152:TC:101:PC1:O12	2.39	0.56
153:2g:201:CDL:H571	153:2g:201:CDL:H141	1.86	0.56
33:e:115:ASP:O	33:e:124:LYS:NZ	2.39	0.56
42:m:74:LYS:NZ	60:w:5:TYR:O	2.35	0.56
78:a8:233:HIS:O	83:am:78:ARG:NH1	2.39	0.56
92:bl:71:ARG:NH1	92:bl:105:LEU:O	2.39	0.56
106:p1:80:ASP:OD1	130:t3:2:SER:N	2.39	0.56
108:qA:34:ASP:OD2	109:qB:469:ARG:NH1	2.39	0.56
108:qA:121:VAL:HG12	114:qg:168:ASP:HB2	1.86	0.56
110:qC:343:THR:O	114:qG:35:ARG:NH2	2.22	0.56
121:s2:42:ARG:HB3	121:s2:58:HIS:HB2	1.87	0.56
126:s7:91:LEU:HG	126:s7:121:ILE:HG23	1.86	0.56
10:2M:15:LEU:HD13	12:2O:5:ILE:HD12	1.86	0.56
46:N:100:ARG:NH1	65:Y7:373:GLU:OE1	2.39	0.56
109:Qb:266:ALA:O	109:Qb:269:THR:OG1	2.24	0.56
128:T1:29:LEU:O	128:T1:33:ASN:ND2	2.38	0.56
153:7c:301:CDL:H792	153:7c:301:CDL:H432	1.87	0.56
25:7l:879:SER:HB2	25:7l:882:MET:HB2	1.87	0.56
35:fs:91:GLN:HB2	42:m:13:HIS:HB3	1.85	0.56
83:am:49:LYS:NZ	153:am:201:CDL:OB3	2.32	0.56
114:qG:145:ARG:NH1	114:qG:149:GLU:OE1	2.39	0.56
30:C2:130:LEU:HD22	30:C2:409:ILE:HD13	1.87	0.56
38:I:173:ILE:HG22	47:O:187:LYS:HG2	1.86	0.56
102:N3:43:TYR:OH	121:S2:33:GLN:OE1	2.17	0.56
104:N5:730:ASP:OD1	131:T4:134:ARG:NH2	2.38	0.56
108:QA:420:THR:OG1	108:QA:432:HIS:NE2	2.37	0.56
110:Qc:116:TRP:CE2	166:Qc:503:HEM:HBC1	2.40	0.56
110:Qc:357:ILE:HD11	160:Qh:201:PX2:H17	1.86	0.56
120:S1:70:LEU:O	123:S4:166:LYS:NZ	2.36	0.56
121:S2:42:ARG:HB3	121:S2:58:HIS:HB2	1.88	0.56
122:S3:38:PRO:HG2	122:S3:41:TRP:HB2	1.87	0.56
148:X1:18:LYS:NZ	148:X1:145:LYS:O	2.34	0.56
19:6b:102:ARG:NH1	25:7l:901:GLU:OE2	2.39	0.56
20:6c:1:MET:HE2	35:fs:176:VAL:HG11	1.88	0.56
24:7c:203:MET:O	24:7c:206:THR:OG1	2.19	0.56
25:7l:952:GLU:OE1	60:w:84:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:134:LEU:HB2	42:m:138:GLU:HB2	1.88	0.56
69:2b:124:LYS:NZ	69:2b:126:ASN:OD1	2.38	0.56
111:qD:43:LEU:HD11	111:qD:169:PRO:HG2	1.87	0.56
114:qg:36:THR:HG22	114:qg:40:LYS:HE3	1.86	0.56
120:s1:638:TYR:HE1	123:s4:39:LYS:HD3	1.71	0.56
130:t3:203:HIS:HB2	130:t3:211:GLU:HG3	1.87	0.56
26:A:357:ASN:HD21	26:A:361:LYS:HE3	1.70	0.56
29:C1:331:LEU:HD21	59:VB:171:GLU:HG2	1.88	0.56
29:C1:334:PHE:HA	29:C1:337:ILE:HD12	1.86	0.56
30:C2:356:GLU:O	31:C3:578:LYS:NZ	2.39	0.56
42:M:188:PRO:O	42:M:191:MET:HB3	2.06	0.56
49:Q:8:TRP:HD1	49:Q:110:LEU:HD11	1.70	0.56
51:S:94:LEU:HD22	64:Y5:94:LEU:HD11	1.87	0.56
108:QA:34:ASP:OD2	109:QB:469:ARG:NH1	2.39	0.56
109:Qb:487:LEU:HD23	109:Qb:487:LEU:H	1.70	0.56
120:S1:638:TYR:HE1	123:S4:39:LYS:HD3	1.71	0.56
134:T7:53:LYS:O	134:T7:57:ASN:ND2	2.33	0.56
147:V2:27:LEU:O	147:V2:114:ARG:NH2	2.39	0.56
149:c:136:GLU:HA	149:c:139:LYS:HE2	1.87	0.56
2:2e:93:LYS:NZ	2:2e:120:ASN:O	2.31	0.56
42:m:188:PRO:O	42:m:191:MET:HB3	2.06	0.56
59:vb:488:ILE:HD13	65:y7:208:LEU:HD22	1.88	0.56
69:2b:120:ARG:HB2	103:n4:200:LEU:HD11	1.87	0.56
95:fx:109:VAL:HG12	95:fx:160:ILE:HG12	1.88	0.56
100:n1:148:TYR:OH	121:s2:29:ASN:O	2.22	0.56
111:qD:65:TYR:OH	111:qD:240:ASN:OD1	2.21	0.56
121:s2:163:ARG:NH1	121:s2:191:ASP:OD2	2.34	0.56
134:t7:53:LYS:O	134:t7:57:ASN:ND2	2.33	0.56
134:t7:122:PRO:HD2	134:t7:125:LEU:HD12	1.88	0.56
6:2I:64:ARG:HB2	132:T5:189:GLN:HB3	1.88	0.56
153:6C:203:CDL:H401	153:F:402:CDL:H252	1.87	0.56
154:C1:702:HEA:HBA2	154:C1:702:HEA:HMA	1.87	0.56
59:VB:565:TRP:NE1	59:VB:578:ASP:OD2	2.30	0.56
153:C4:401:CDL:H231	158:C4:402:3PE:H2H2	1.86	0.56
96:G1:210:ARG:NH2	96:G1:252:GLU:O	2.38	0.56
114:Qg:36:THR:HG22	114:Qg:40:LYS:HE3	1.86	0.56
121:S2:92:VAL:HG11	121:S2:381:SER:HA	1.88	0.56
122:S3:126:ASP:HA	122:S3:132:ALA:HB3	1.86	0.56
129:T2:198:LEU:HB3	129:T2:213:LYS:HB2	1.86	0.56
4:2g:36:GLU:OE1	53:sb:234:ARG:NH2	2.37	0.56
19:6b:121:GLN:NE2	42:m:186:ASP:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c2:112:LEU:N	30:c2:502:ASN:O	2.39	0.56
58:v:78:GLU:OE2	58:v:84:ASN:ND2	2.39	0.56
152:w:201:PC1:H3I1	158:w:203:3PE:H371	1.88	0.56
83:am:149:ASN:ND2	105:n6:164:ASN:OD1	2.38	0.56
92:bl:114:HIS:CD2	103:n4:435:GLU:HG3	2.41	0.56
101:n2:4:ARG:NH2	148:x1:40:ASN:O	2.38	0.56
106:p1:102:PHE:CE1	106:p1:105:HIS:HB2	2.41	0.56
108:qA:101:ASP:OD2	108:qA:248:ARG:NH2	2.35	0.56
108:qA:319:ILE:O	108:qA:323:ASN:ND2	2.37	0.56
109:qB:289:PRO:HB3	109:qB:475:GLU:HB3	1.87	0.56
110:qc:114:ALA:HB2	114:qg:178:LEU:HD22	1.85	0.56
110:qc:357:ILE:HG12	115:qh:103:PRO:HG3	1.88	0.56
3:2F:210:SER:OG	153:2G:204:CDL:OA9	2.24	0.56
11:2N:31:VAL:HG13	11:2N:32:VAL:HG13	1.88	0.56
152:7A:202:PC1:O14	26:A:334:ASN:ND2	2.35	0.56
28:BP:198:SER:O	28:BP:201:ASN:ND2	2.38	0.56
34:F:322:LYS:HD2	35:FS:4:ILE:HD11	1.86	0.56
36:G:55:GLN:HE22	59:VB:296:GLN:HE22	1.52	0.56
57:U:138:ARG:HH12	57:U:142:LEU:HD22	1.70	0.56
77:A7:84:THR:HG23	77:A7:120:PRO:HB2	1.88	0.56
79:A9:72:PRO:HA	79:A9:98:MET:HB2	1.88	0.56
80:AB:33:ARG:NH1	95:FX:127:GLU:OE1	2.38	0.56
97:G2:148:THR:HB	97:G2:166:VAL:HG22	1.87	0.56
100:N1:148:TYR:OH	121:S2:29:ASN:O	2.22	0.56
114:QG:145:ARG:NH1	114:QG:149:GLU:OE1	2.39	0.56
120:S1:218:GLU:OE2	120:S1:709:LYS:NZ	2.39	0.56
120:S1:606:PRO:HB2	120:S1:610:ALA:HB3	1.88	0.56
121:S2:211:THR:O	121:S2:277:TYR:OH	2.22	0.56
2:2e:322:LEU:HD11	4:2g:11:PHE:HD1	1.71	0.56
7:2j:13:VAL:HB	8:2k:28:VAL:HG21	1.88	0.56
29:c1:557:ARG:NH2	153:c1:712:CDL:OB4	2.39	0.56
45:m3:2:ALA:HA	45:m3:6:ILE:HB	1.86	0.56
49:q:8:TRP:HD1	49:q:110:LEU:HD11	1.71	0.56
51:s:94:LEU:HD22	64:y5:94:LEU:HD11	1.87	0.56
72:a1:42:LYS:HG2	72:a1:46:GLU:HB2	1.88	0.56
84:an:133:ASN:ND2	158:an:303:3PE:O14	2.32	0.56
92:bl:148:LEU:HA	103:n4:83:LEU:HD11	1.88	0.56
115:qH:70:ILE:N	153:qI:203:CDL:OB4	2.38	0.56
108:qa:68:GLU:OE1	108:qa:259:HIS:ND1	2.36	0.56
153:qb:601:CDL:OA4	116:qi:67:GLN:NE2	2.38	0.56
111:qd:293:ARG:NH2	114:qg:301:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
114:qg:183:PRO:HB2	153:qg:402:CDL:H421	1.86	0.56
122:s3:38:PRO:HG2	122:s3:41:TRP:HB2	1.87	0.56
13:2T:10:GLU:OE2	17:5T:15:ARG:NH1	2.39	0.56
19:6B:121:GLN:NE2	42:M:186:ASP:O	2.39	0.56
26:A:325:GLN:OE1	61:X:102:LYS:NZ	2.29	0.56
28:BP:139:GLY:HA2	28:BP:143:ALA:HB3	1.87	0.56
28:BP:383:LEU:O	31:C3:215:GLN:NE2	2.37	0.56
30:C2:112:LEU:N	30:C2:502:ASN:O	2.39	0.56
33:E:115:ASP:O	33:E:124:LYS:NZ	2.39	0.56
33:E:138:LYS:HB2	153:E:402:CDL:H581	1.88	0.56
152:5B:202:PC1:H262	103:N4:205:TRP:CE2	2.41	0.56
88:B6:116:VAL:HG21	92:BL:84:LEU:HB3	1.87	0.56
130:T3:203:HIS:HB2	130:T3:211:GLU:HG3	1.87	0.56
134:T7:122:PRO:HD2	134:T7:125:LEU:HD12	1.88	0.56
37:h:148:TYR:HB3	37:h:170:LEU:HB2	1.88	0.56
52:sa:127:GLN:HE22	52:sa:623:ASP:HB3	1.71	0.56
152:5b:202:PC1:H262	103:n4:205:TRP:CE2	2.41	0.56
90:b8:90:TRP:CE2	104:n5:472:LEU:HD21	2.41	0.56
98:g3:53:ILE:HB	98:g3:75:ILE:HG12	1.87	0.56
117:qJ:1:MET:SD	117:qJ:1:MET:N	2.77	0.56
114:qg:41:VAL:O	114:qg:45:ASN:ND2	2.33	0.56
132:t5:126:SER:OG	153:t5:301:CDL:OA4	2.20	0.56
137:ta:100:ARG:NH1	137:ta:104:ASP:OD2	2.39	0.56
18:6A:29:PHE:HB3	59:VB:377:GLU:HB2	1.87	0.56
31:C3:309:TRP:HB3	152:C3:602:PC1:H231	1.87	0.56
52:SA:196:LEU:HD13	53:SB:180:LYS:HA	1.88	0.56
56:T:23:THR:HG22	56:T:151:PRO:HG2	1.87	0.56
63:Y0:31:ARG:HA	63:Y0:34:LYS:HG3	1.87	0.56
63:Y0:42:ALA:HB1	63:Y0:53:LEU:HD11	1.87	0.56
98:G3:53:ILE:HB	98:G3:75:ILE:HG12	1.87	0.56
100:N1:11:ASN:HB3	153:TE:101:CDL:H572	1.87	0.56
100:N1:51:GLN:HE22	121:S2:144:MET:HE2	1.71	0.56
100:N1:104:PHE:HE1	100:N1:129:LEU:HB3	1.71	0.56
104:N5:174:LEU:HD22	104:N5:230:ILE:HG21	1.88	0.56
112:QE:104:LEU:HD21	152:QI:202:PC1:H341	1.88	0.56
114:QG:60:GLU:OE2	114:QG:249:TYR:OH	2.22	0.56
114:QG:162:TYR:HA	114:QG:166:MET:HB2	1.87	0.56
2:2e:104:SER:O	2:2e:108:GLY:N	2.36	0.55
153:6c:202:CDL:H401	153:f:401:CDL:H252	1.87	0.55
25:7l:919:LYS:HG3	25:7l:939:MET:HE1	1.88	0.55
153:a:505:CDL:H511	59:vb:85:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c3:161:GLU:OE1	48:p:58:ASN:ND2	2.39	0.55
35:fs:42:ARG:NH2	35:fs:50:ILE:O	2.33	0.55
36:g:55:GLN:HE22	59:vb:296:GLN:HE22	1.52	0.55
42:m:2:SER:N	33:E:192:SER:OG	2.38	0.55
153:q:202:CDL:HA61	153:t:203:CDL:H311	1.88	0.55
52:sa:159:ALA:HB1	52:sa:172:GLN:HE21	1.71	0.55
52:sa:308:ASN:HB2	52:sa:343:ARG:HB3	1.88	0.55
56:t:23:THR:HG22	56:t:151:PRO:HG2	1.87	0.55
64:y5:187:ARG:NH2	65:y7:270:SER:OG	2.38	0.55
96:g1:60:SER:OG	96:g1:75:TRP:O	2.24	0.55
100:n1:104:PHE:HE1	100:n1:129:LEU:HB3	1.71	0.55
114:qG:60:GLU:OE2	114:qG:249:TYR:OH	2.22	0.55
108:qa:84:THR:HB	109:qb:82:VAL:HG21	1.87	0.55
112:qe:140:GLY:CA	112:qe:156:ARG:O	2.54	0.55
120:s1:297:GLY:O	120:s1:566:HIS:NE2	2.35	0.55
139:tc:12:ASN:ND2	152:tc:101:PC1:O12	2.38	0.55
23:7A:76:ARG:NH1	153:7A:201:CDL:OA3	2.39	0.55
153:7C:301:CDL:H792	153:7C:301:CDL:H432	1.87	0.55
25:7L:899:GLN:NE2	25:7L:940:ARG:O	2.33	0.55
27:B:124:LYS:HD2	27:B:128:GLN:HE21	1.69	0.55
31:C3:161:GLU:OE1	48:P:58:ASN:ND2	2.39	0.55
34:F:284:LEU:HD21	34:F:321:VAL:HG11	1.88	0.55
43:M1:173:ARG:O	43:M1:184:ARG:NH2	2.36	0.55
56:T:99:PHE:O	63:Y0:36:ARG:NH2	2.36	0.55
69:2B:120:ARG:NH1	103:N4:197:GLN:OE1	2.38	0.55
72:A1:42:LYS:HG2	72:A1:46:GLU:HB2	1.88	0.55
92:BL:67:LEU:HB3	92:BL:110:VAL:HG12	1.87	0.55
92:BL:114:HIS:CD2	103:N4:435:GLU:HG3	2.41	0.55
104:N5:55:ASN:ND2	104:N5:145:ASN:OD1	2.40	0.55
104:N5:98:SER:OG	104:N5:140:LYS:NZ	2.35	0.55
106:P1:80:ASP:OD1	130:T3:2:SER:N	2.39	0.55
110:Qc:302:LEU:HD23	152:Qc:509:PC1:H2H1	1.87	0.55
112:Qe:140:GLY:CA	112:Qe:156:ARG:O	2.54	0.55
120:S1:390:LYS:HE3	120:S1:653:ILE:HD12	1.86	0.55
145:TX:45:LEU:HD21	145:TX:131:VAL:HG21	1.88	0.55
145:TX:103:LEU:HD23	145:TX:108:GLU:HA	1.87	0.55
19:6b:218:ASP:OD1	42:m:141:ARG:NH2	2.38	0.55
38:i:251:LEU:HD12	60:W:67:ARG:HH12	1.71	0.55
51:s:42:MET:SD	64:y5:132:ASN:ND2	2.79	0.55
69:2b:120:ARG:NH1	103:n4:197:GLN:OE1	2.38	0.55
71:5b:86:ILE:HG12	101:n2:254:ILE:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
158:a3:202:3PE:H3D1	105:n6:186:ILE:HB	1.88	0.55
87:b4:34:MET:HE1	91:b9:10:ASN:HD22	1.71	0.55
104:n5:737:LEU:HD23	131:t4:130:THR:HG23	1.89	0.55
109:qb:121:ARG:NH1	109:qb:129:GLU:OE1	2.39	0.55
109:qb:267:PHE:HA	109:qb:270:VAL:HG23	1.88	0.55
134:t7:72:LYS:HD2	134:t7:75:ILE:HD11	1.88	0.55
138:tb:79:ALA:HB1	153:th:200:CDL:H741	1.87	0.55
24:7C:116:TYR:OH	40:K:30:GLN:NE2	2.39	0.55
26:A:304:ILE:HD11	31:C3:403:TRP:HZ2	1.71	0.55
52:SA:94:ILE:HG22	52:SA:446:LEU:HB2	1.88	0.55
57:U:4:THR:HG23	57:U:7:ARG:HH12	1.71	0.55
100:N1:44:ARG:HH12	126:S7:52:ILE:HD13	1.70	0.55
100:N1:192:ILE:HG22	100:N1:193:ILE:HG23	1.88	0.55
106:P1:51:GLU:HG3	107:P2:136:LEU:HD13	1.88	0.55
109:QB:48:GLU:OE1	109:QB:415:ARG:NH2	2.38	0.55
114:QG:168:ASP:HB2	108:Qa:121:VAL:HG12	1.88	0.55
112:Qe:140:GLY:HA2	112:Qe:156:ARG:O	2.06	0.55
13:2t:8:GLN:NE2	30:c2:215:SER:OG	2.33	0.55
13:2t:10:GLU:OE2	17:5t:15:ARG:NH1	2.39	0.55
26:a:360:TRP:CH2	153:a:505:CDL:H522	2.41	0.55
28:bp:139:GLY:HA2	28:bp:143:ALA:HB3	1.89	0.55
29:c1:531:LEU:HD21	154:c1:708:HEA:HBC2	1.88	0.55
52:sa:94:ILE:HG22	52:sa:446:LEU:HB2	1.88	0.55
63:y0:31:ARG:HA	63:y0:34:LYS:HG3	1.87	0.55
98:g3:56:THR:OG1	98:g3:57:ASN:N	2.38	0.55
100:n1:11:ASN:HB3	153:te:101:CDL:H572	1.87	0.55
109:qB:48:GLU:OE1	109:qB:415:ARG:NH2	2.38	0.55
114:qG:162:TYR:HA	114:qG:166:MET:HB2	1.87	0.55
111:qd:77:PHE:HA	111:qd:81:CYS:HB2	1.88	0.55
120:s1:606:PRO:HB2	120:s1:610:ALA:HB3	1.88	0.55
121:s2:67:GLU:OE2	121:s2:442:ARG:NH1	2.39	0.55
121:s2:204:ASN:O	121:s2:208:ASN:ND2	2.32	0.55
2:2E:35:PHE:O	2:2E:62:LYS:NZ	2.39	0.55
19:6B:218:ASP:OD1	42:M:141:ARG:NH2	2.38	0.55
20:6C:1:MET:HE2	35:FS:176:VAL:HG11	1.88	0.55
44:M2:62:ASN:HD21	153:M2:401:CDL:H341	1.70	0.55
44:M2:119:ARG:HG2	152:N:301:PC1:H2	1.88	0.55
44:M2:237:PRO:HG2	153:M2:404:CDL:H231	1.89	0.55
52:SA:96:ALA:HB2	52:SA:137:VAL:HG21	1.87	0.55
52:SA:159:ALA:HB1	52:SA:172:GLN:HE21	1.71	0.55
52:SA:308:ASN:HB2	52:SA:343:ARG:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B3:61:LEU:HD12	153:P1:402:CDL:H131	1.89	0.55
108:QA:87:SER:HA	109:QB:423:LEU:HD22	1.88	0.55
110:QC:259:PHE:HA	111:QD:167:LEU:HB3	1.88	0.55
108:Qa:81:GLU:OE2	108:Qa:416:ARG:NH1	2.39	0.55
108:Qa:320:VAL:HA	108:Qa:323:ASN:HD22	1.71	0.55
110:Qc:28:HIS:HB3	110:Qc:207:TRP:HH2	1.72	0.55
6:2i:64:ARG:HB2	132:t5:189:GLN:HB3	1.88	0.55
154:c1:702:HEA:HBA2	154:c1:702:HEA:HMA	1.89	0.55
49:q:5:TYR:HE2	67:z1:85:ARG:HD2	1.72	0.55
79:a9:90:ALA:HB3	79:a9:95:SER:HB3	1.89	0.55
88:b6:116:VAL:HG21	92:bl:84:LEU:HB3	1.87	0.55
92:bl:78:VAL:HG21	92:bl:102:ILE:HD11	1.87	0.55
100:n1:169:LEU:O	100:n1:173:ASN:ND2	2.32	0.55
103:n4:167:ASN:ND2	135:t8:81:THR:OG1	2.34	0.55
112:qe:140:GLY:HA2	112:qe:156:ARG:O	2.06	0.55
127:s8:154:GLU:HB2	127:s8:167:ARG:HB3	1.88	0.55
42:M:46:ARG:NE	153:M:306:CDL:OB4	2.30	0.55
42:M:115:TYR:OH	42:M:154:GLU:OE1	2.17	0.55
51:S:42:MET:SD	64:Y5:132:ASN:ND2	2.79	0.55
51:S:80:VAL:O	65:Y7:188:LYS:NZ	2.40	0.55
52:SA:621:THR:HG23	52:SA:628:PRO:HG3	1.87	0.55
53:SB:36:CYS:O	53:SB:40:ILE:HG12	2.06	0.55
59:VB:162:THR:O	59:VB:173:HIS:N	2.25	0.55
153:VB:703:CDL:H181	153:VB:706:CDL:H322	1.88	0.55
82:AL:105:GLN:OE1	127:S8:223:GLN:NE2	2.36	0.55
96:G1:60:SER:OG	96:G1:75:TRP:O	2.24	0.55
100:N1:104:PHE:HD2	100:N1:250:PHE:HB3	1.72	0.55
101:N2:4:ARG:NH2	148:X1:40:ASN:O	2.39	0.55
110:QC:283:ARG:HH22	152:QC:507:PC1:H32	1.70	0.55
110:QC:284:PRO:HG3	110:QC:370:THR:HA	1.88	0.55
3:2f:84:LYS:O	3:2f:103:ARG:NH1	2.39	0.55
4:2g:120:ASN:ND2	4:2g:123:ASN:O	2.29	0.55
4:2g:162:GLU:OE2	53:sb:262:ARG:NH2	2.36	0.55
18:6a:29:PHE:HB3	59:vb:377:GLU:HB2	1.88	0.55
28:bp:140:GLN:NE2	28:bp:175:GLU:O	2.39	0.55
88:b6:105:SER:OG	104:n5:231:SER:O	2.25	0.55
92:bl:79:ARG:NE	104:n5:365:ASP:OD2	2.29	0.55
110:qC:283:ARG:HH22	152:qC:507:PC1:H32	1.70	0.55
109:qb:102:GLU:OE2	116:qi:29:LYS:NZ	2.40	0.55
121:s2:128:LEU:HG	121:s2:157:LEU:HD13	1.89	0.55
145:tx:45:LEU:HD21	145:tx:131:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2F:191:GLY:N	3:2F:223:GLU:OE1	2.23	0.55
19:6B:102:ARG:NH1	25:7L:901:GLU:OE2	2.40	0.55
29:C1:20:PHE:HB3	29:C1:23:LEU:HB3	1.88	0.55
31:C3:138:LEU:HB3	31:C3:149:PHE:HB3	1.89	0.55
64:Y5:85:ARG:NH1	149:C:144:ALA:O	2.40	0.55
73:A2:87:ILE:O	73:A2:91:VAL:HG23	2.07	0.55
97:G2:64:PHE:HD2	97:G2:82:VAL:HG13	1.72	0.55
111:Qd:179:SER:HB3	111:Qd:213:LEU:HD12	1.87	0.55
112:Qe:88:ARG:NH2	153:Qi:202:CDL:OB4	2.40	0.55
142:TF:105:ILE:O	142:TF:140:LYS:NZ	2.31	0.55
4:2g:36:GLU:HB2	4:2g:102:TYR:CE1	2.42	0.55
24:7c:116:TYR:OH	40:k:30:GLN:NE2	2.39	0.55
26:a:357:ASN:HD21	26:a:361:LYS:HE3	1.70	0.55
28:bp:332:ASN:ND2	40:k:31:ASN:OD1	2.39	0.55
29:c1:20:PHE:HB3	29:c1:23:LEU:HB3	1.88	0.55
29:c1:331:LEU:HD21	59:vb:171:GLU:HG2	1.87	0.55
34:f:284:LEU:HD21	34:f:321:VAL:HG11	1.87	0.55
52:sa:333:ARG:HE	52:sa:582:ALA:HB2	1.72	0.55
57:u:4:THR:HG23	57:u:7:ARG:HH12	1.71	0.55
63:y0:16:PRO:O	63:y0:20:ALA:N	2.40	0.55
81:ac:107:GLU:OE1	91:b9:1:MET:N	2.35	0.55
86:b3:48:THR:HG22	104:n5:545:TYR:CZ	2.41	0.55
86:b3:61:LEU:HD12	153:p1:402:CDL:H131	1.89	0.55
106:p1:145:TYR:HA	106:p1:149:PHE:HB2	1.89	0.55
3:2F:129:VAL:O	12:2O:24:TYR:OH	2.22	0.55
29:C1:587:PRO:HG2	29:C1:590:ILE:HD13	1.89	0.55
48:P:100:PRO:HG2	48:P:106:ALA:HB2	1.88	0.55
48:P:101:GLN:HG2	48:P:134:GLN:HG2	1.89	0.55
49:Q:5:TYR:HE2	67:Z1:85:ARG:HD2	1.71	0.55
52:SA:333:ARG:HE	52:SA:582:ALA:HB2	1.72	0.55
53:SB:149:ASP:OD2	53:SB:151:SER:OG	2.24	0.55
88:B6:105:SER:OG	104:N5:231:SER:O	2.24	0.55
152:C4:403:PC1:H351	97:G2:18:MET:HE1	1.87	0.55
106:P1:54:PHE:HB3	153:P1:402:CDL:H551	1.88	0.55
121:S2:128:LEU:HG	121:S2:157:LEU:HD13	1.89	0.55
121:S2:163:ARG:NH1	121:S2:191:ASP:OD2	2.34	0.55
121:S2:199:PHE:HD2	121:S2:291:LEU:HD11	1.72	0.55
147:V2:205:LYS:O	147:V2:209:GLN:NE2	2.38	0.55
153:7a:201:CDL:H241	46:n:132:GLY:HA3	1.88	0.55
29:c1:518:HIS:O	30:c2:524:LYS:NZ	2.28	0.55
31:c3:309:TRP:HB3	152:c3:602:PC1:H231	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:y5:30:LEU:HB3	66:z:64:VAL:HG11	1.89	0.55
80:ab:33:ARG:NH1	95:fx:127:GLU:OE1	2.39	0.55
96:g1:222:GLN:NE2	98:g3:44:ASP:O	2.40	0.55
100:n1:51:GLN:HE22	121:s2:144:MET:HE2	1.71	0.55
104:n5:576:LEU:HD11	104:n5:668:LEU:HD11	1.89	0.55
110:qC:259:PHE:HA	111:qD:167:LEU:HB3	1.89	0.55
112:qE:91:GLN:OE1	116:qI:43:ASN:ND2	2.40	0.55
110:qc:232:GLY:HA3	111:qd:271:LYS:HG3	1.87	0.55
111:qd:179:SER:HB3	111:qd:213:LEU:HD12	1.88	0.55
120:s1:388:ASN:ND2	120:s1:511:PHE:O	2.35	0.55
121:s2:92:VAL:HG11	121:s2:381:SER:HA	1.88	0.55
26:A:274:GLU:OE2	26:A:366:ARG:NH1	2.40	0.55
42:M:157:TYR:HE1	153:W:202:CDL:HB21	1.72	0.55
51:S:26:LEU:HD22	59:VB:482:LEU:HD11	1.87	0.55
59:VB:85:HIS:CE1	153:VB:705:CDL:H511	2.42	0.55
103:N4:270:HIS:CE1	103:N4:282:SER:HB3	2.42	0.55
109:Qb:102:GLU:OE2	116:Qi:29:LYS:NZ	2.40	0.55
120:S1:298:LEU:HD23	120:S1:566:HIS:HE1	1.72	0.55
2:2e:11:LYS:HD3	2:2e:43:ARG:HD2	1.88	0.55
15:4a:68:VAL:HG21	33:e:11:LEU:HD23	1.88	0.55
153:q:203:CDL:H152	153:vb:704:CDL:H111	1.89	0.55
51:s:80:VAL:O	65:y7:188:LYS:NZ	2.40	0.55
63:y0:42:ALA:HB1	63:y0:53:LEU:HD11	1.88	0.55
72:a1:43:ASP:OD2	140:td:42:ARG:NH1	2.40	0.55
75:a5:129:ASP:OD1	75:a5:130:SER:N	2.39	0.55
100:n1:160:MET:HA	100:n1:163:ILE:HB	1.89	0.55
104:n5:661:LEU:HD11	152:n5:804:PC1:H3C1	1.89	0.55
113:qF:25:LEU:HD23	113:qF:73:VAL:HG11	1.87	0.55
114:qg:133:TYR:OH	115:qh:94:ARG:NE	2.40	0.55
153:qi:202:CDL:HA4	153:qi:202:CDL:H512	1.89	0.55
128:t1:38:LEU:HD23	128:t1:48:PHE:HE1	1.71	0.55
4:2G:122:HIS:HE1	153:2G:204:CDL:H521	1.71	0.55
5:2H:109:GLY:O	5:2H:113:CYS:N	2.38	0.55
10:2M:17:GLN:HE21	10:2M:22:GLY:HA2	1.71	0.55
153:M1:402:CDL:HB4	153:M2:401:CDL:H322	1.89	0.55
153:Q:202:CDL:HA61	153:T:203:CDL:H311	1.89	0.55
62:Y:16:TYR:OH	62:Y:38:ASP:OD1	2.21	0.55
79:A9:90:ALA:HB3	79:A9:95:SER:HB3	1.89	0.55
82:AL:162:ALA:HB3	120:S1:300:ARG:HA	1.89	0.55
86:B3:48:THR:HG22	104:N5:545:TYR:CZ	2.41	0.55
96:G1:222:GLN:NE2	98:G3:44:ASP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:Qd:124:TYR:O	111:Qd:127:GLN:NE2	2.38	0.55
121:S2:67:GLU:OE2	121:S2:442:ARG:NH1	2.39	0.55
131:T4:82:THR:HG23	131:T4:177:ALA:HB1	1.89	0.55
134:T7:72:LYS:HD2	134:T7:75:ILE:HD11	1.88	0.55
7:2j:3:HIS:NE2	7:2j:5:CYS:SG	2.80	0.55
154:c1:702:HEA:HBA2	154:c1:702:HEA:CMA	2.37	0.55
31:c3:558:LYS:HG3	41:l:104:GLU:HG2	1.89	0.55
38:i:105:PHE:O	38:i:124:ASN:ND2	2.40	0.55
60:w:39:TYR:OH	152:w:201:PC1:O14	2.25	0.55
60:w:67:ARG:HH12	38:I:251:LEU:HD12	1.71	0.55
95:fx:92:GLU:OE2	103:n4:193:ARG:NH1	2.23	0.55
121:s2:153:GLU:HG3	121:s2:202:THR:HG21	1.88	0.55
122:s3:174:GLU:OE2	123:s4:131:LYS:NZ	2.32	0.55
24:7C:156:GLY:HA3	152:M1:401:PC1:H3A1	1.89	0.55
28:BP:332:ASN:ND2	40:K:31:ASN:OD1	2.39	0.55
41:L:210:ASN:HD21	45:M3:327:VAL:HB	1.72	0.55
52:SA:91:GLN:HG3	52:SA:294:LEU:HD23	1.89	0.55
59:VB:459:ASN:ND2	65:Y7:243:TYR:OH	2.32	0.55
70:4L:55:THR:O	70:4L:58:SER:OG	2.22	0.55
71:5B:31:MET:HG2	153:B4:201:CDL:H711	1.89	0.55
92:BL:79:ARG:NE	104:N5:365:ASP:OD2	2.28	0.55
98:G3:132:PRO:HD2	98:G3:149:MET:HB3	1.89	0.55
110:QC:132:LEU:HD13	110:QC:184:LEU:HB3	1.89	0.55
114:QG:213:GLU:HA	114:QG:216:LYS:HD3	1.89	0.55
109:Qb:497:ILE:O	109:Qb:500:SER:OG	2.23	0.55
130:T3:225:ASP:OD2	130:T3:273:ARG:NH2	2.39	0.55
149:C:131:ASP:OD2	149:C:141:ARG:NH2	2.39	0.55
153:a:502:CDL:H711	153:c3:604:CDL:HB62	1.88	0.55
29:c1:532:SER:OG	154:c1:702:HEA:O11	2.25	0.55
29:c1:587:PRO:HG2	29:c1:590:ILE:HD13	1.89	0.55
37:h:257:GLU:OE1	37:h:257:GLU:N	2.32	0.55
42:m:157:TYR:HE1	153:w:202:CDL:HB21	1.72	0.55
153:m:303:CDL:H742	158:w:203:3PE:H272	1.89	0.55
43:m1:51:GLU:HB3	43:m1:96:ARG:HB3	1.89	0.55
50:r:16:ASN:O	50:r:44:GLN:NE2	2.38	0.55
79:a9:354:VAL:HG11	99:j1:218:TRP:HZ3	1.72	0.55
83:am:42:ARG:NH2	134:t7:78:PHE:O	2.40	0.55
84:an:14:VAL:HG13	84:an:19:TYR:HB3	1.88	0.55
90:b8:57:TYR:H	103:n4:462:ASN:HD21	1.55	0.55
97:g2:64:PHE:HD2	97:g2:82:VAL:HG13	1.72	0.55
100:n1:224:ALA:HB1	100:n1:227:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qC:284:PRO:HG3	110:qC:370:THR:HA	1.88	0.55
108:qa:81:GLU:OE2	108:qa:416:ARG:NH1	2.39	0.55
133:t6:120:LEU:O	133:t6:124:ASN:ND2	2.35	0.55
146:v1:207:CYS:SG	146:v1:222:GLY:HA3	2.47	0.55
33:E:50:ILE:HD11	33:E:66:LEU:HD23	1.89	0.55
37:H:148:TYR:HB3	37:H:170:LEU:HB2	1.88	0.55
48:P:121:TYR:HB2	48:P:147:LEU:HD11	1.89	0.55
95:FX:109:VAL:HG12	95:FX:160:ILE:HG12	1.88	0.55
108:Qa:84:THR:HB	109:Qb:82:VAL:HG21	1.87	0.55
109:Qb:267:PHE:HA	109:Qb:270:VAL:HG23	1.89	0.55
126:S7:131:GLU:OE2	127:S8:114:GLY:N	2.35	0.55
2:2e:3:LEU:HD23	2:2e:29:ILE:HG23	1.90	0.54
2:2e:234:ASN:HD22	43:M1:169:LYS:HD3	1.71	0.54
6:2i:3:SER:OG	6:2i:6:ASN:OD1	2.25	0.54
20:6c:3:SER:N	153:6c:201:CDL:OB4	2.41	0.54
33:e:118:ILE:HG21	153:e:403:CDL:H312	1.88	0.54
59:vb:431:ASP:OD2	59:vb:438:LYS:NZ	2.40	0.54
59:vb:459:ASN:ND2	65:y7:243:TYR:OH	2.32	0.54
79:a9:72:PRO:HA	79:a9:98:MET:HB2	1.89	0.54
83:am:52:LEU:HB2	153:am:201:CDL:H332	1.89	0.54
158:b4:202:3PE:H382	158:b4:202:3PE:H2A1	1.88	0.54
88:b6:83:ASN:ND2	104:n5:193:TYR:O	2.33	0.54
96:g1:34:ILE:HD12	98:g3:46:LEU:HB3	1.88	0.54
98:g3:132:PRO:HD2	98:g3:149:MET:HB3	1.88	0.54
104:n5:498:SER:O	104:n5:501:THR:OG1	2.24	0.54
109:qb:311:PRO:HB3	109:qb:315:ASP:HB3	1.89	0.54
120:s1:298:LEU:HD23	120:s1:566:HIS:HE1	1.72	0.54
129:t2:228:LEU:HD13	129:t2:282:LEU:HD22	1.89	0.54
131:t4:38:LEU:O	131:t4:43:LYS:NZ	2.40	0.54
2:2E:93:LYS:NZ	2:2E:120:ASN:O	2.30	0.54
2:2E:322:LEU:HD11	4:2G:11:PHE:HD1	1.71	0.54
3:2F:84:LYS:O	3:2F:103:ARG:NH1	2.39	0.54
4:2G:102:TYR:OH	53:SB:234:ARG:NH1	2.38	0.54
39:J:184:THR:HG22	152:N:303:PC1:H131	1.89	0.54
42:M:134:LEU:HB2	42:M:138:GLU:HB2	1.88	0.54
153:M2:404:CDL:HB32	153:N:304:CDL:H642	1.89	0.54
52:SA:70:GLU:HB3	52:SA:461:LYS:HD3	1.89	0.54
73:A2:8:ILE:HG23	73:A2:12:LEU:HD12	1.90	0.54
77:A7:76:SER:OG	122:S3:21:LYS:NZ	2.37	0.54
88:B6:77:ASN:HD22	93:BM:123:PRO:HG3	1.72	0.54
104:N5:576:LEU:HD11	104:N5:668:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:Qb:121:ARG:NH1	109:Qb:129:GLU:OE1	2.40	0.54
128:T1:38:LEU:HD23	128:T1:48:PHE:HE1	1.71	0.54
4:2g:129:HIS:CD2	4:2g:131:ILE:HG12	2.43	0.54
26:a:274:GLU:OE2	26:a:366:ARG:NH1	2.40	0.54
44:m2:119:ARG:HG2	152:n:301:PC1:H2	1.88	0.54
44:m2:237:PRO:HG2	153:m2:404:CDL:H231	1.89	0.54
153:m2:404:CDL:HB32	153:n:304:CDL:H642	1.89	0.54
103:n4:270:HIS:CE1	103:n4:282:SER:HB3	2.42	0.54
104:n5:730:ASP:OD1	131:t4:134:ARG:NH2	2.39	0.54
110:qC:88:VAL:HG21	166:qC:501:HEM:HMD1	1.89	0.54
112:qE:84:GLU:OE2	116:qI:37:GLN:NE2	2.32	0.54
153:qc:504:CDL:H732	153:qc:504:CDL:H791	1.89	0.54
40:K:131:SER:O	48:P:174:LYS:NZ	2.37	0.54
43:M1:51:GLU:HB3	43:M1:96:ARG:HB3	1.89	0.54
53:SB:140:LEU:HD12	53:SB:143:ILE:HD11	1.89	0.54
75:A5:80:LYS:O	75:A5:84:ASN:ND2	2.34	0.54
92:BL:78:VAL:HG21	92:BL:102:ILE:HD11	1.87	0.54
112:QE:91:GLN:OE1	116:QI:43:ASN:ND2	2.40	0.54
131:T4:38:LEU:O	131:T4:43:LYS:NZ	2.40	0.54
132:T5:126:SER:HB3	153:T5:301:CDL:HA61	1.89	0.54
145:TX:110:THR:OG1	145:TX:123:ARG:NH1	2.40	0.54
146:V1:79:GLU:HB3	146:V1:256:MET:HE1	1.89	0.54
146:V1:207:CYS:SG	146:V1:222:GLY:HA3	2.47	0.54
146:V1:368:ILE:HG13	146:V1:439:LEU:HB2	1.88	0.54
1:1t:33:ASN:ND2	1:1t:41:GLN:OE1	2.34	0.54
4:2g:41:HIS:CD2	4:2g:45:ASN:HD22	2.25	0.54
153:2m:101:CDL:HA22	54:sc:29:ILE:HG13	1.89	0.54
18:6a:43:ARG:NH2	59:vb:328:ASP:OD1	2.37	0.54
24:7c:156:GLY:HA3	152:m1:401:PC1:H3A1	1.89	0.54
39:j:184:THR:HG22	152:n:303:PC1:H131	1.89	0.54
48:p:121:TYR:HB2	48:p:147:LEU:HD11	1.89	0.54
64:y5:85:ARG:NH1	149:c:144:ALA:O	2.41	0.54
69:2b:78:PRO:HG3	153:2b:201:CDL:H741	1.89	0.54
75:a5:80:LYS:O	75:a5:84:ASN:ND2	2.34	0.54
76:a6:37:MET:O	122:s3:154:ARG:NH1	2.40	0.54
83:am:50:ALA:HB2	127:s8:80:TYR:HB2	1.89	0.54
87:b4:45:GLU:HG3	95:fx:93:LYS:HB3	1.89	0.54
108:qA:380:ILE:HG22	108:qA:384:LYS:HE2	1.89	0.54
108:qa:320:VAL:HA	108:qa:323:ASN:HD22	1.71	0.54
128:t1:270:ALA:HB1	128:t1:362:LEU:HD13	1.89	0.54
132:t5:126:SER:HB3	153:t5:301:CDL:HA61	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2F:210:SER:HA	153:2G:204:CDL:H552	1.89	0.54
4:2G:129:HIS:CD2	4:2G:131:ILE:HG12	2.42	0.54
6:2I:3:SER:OG	6:2I:6:ASN:OD1	2.25	0.54
30:C2:541:ASN:HD21	30:C2:545:TYR:HH	1.54	0.54
45:M3:179:LEU:HD23	45:M3:257:VAL:HG12	1.89	0.54
49:Q:36:SER:OG	49:Q:121:ASP:OD2	2.24	0.54
69:2B:78:PRO:HG3	153:2B:201:CDL:H741	1.89	0.54
102:N3:68:LEU:HD23	105:N6:95:ILE:HD11	1.89	0.54
103:N4:387:THR:OG1	103:N4:392:GLU:OE1	2.20	0.54
104:N5:661:LEU:HD11	152:N5:804:PC1:H3C1	1.89	0.54
109:QB:343:THR:OG1	109:QB:346:ARG:NH1	2.36	0.54
110:QC:223:PHE:O	110:QC:227:LEU:CB	2.55	0.54
112:QE:48:PRO:HB3	112:QE:67:LYS:HD2	1.89	0.54
112:QE:73:TRP:HA	112:QE:76:GLU:HB2	1.89	0.54
114:QG:192:LEU:O	114:QG:198:TRP:NE1	2.33	0.54
111:Qd:255:VAL:HG12	111:Qd:259:MET:HE3	1.89	0.54
120:S1:342:ILE:HD12	120:S1:542:ILE:HG12	1.89	0.54
129:T2:228:LEU:HD13	129:T2:282:LEU:HD22	1.89	0.54
3:2f:181:PHE:O	54:sc:53:ALA:HB2	2.07	0.54
5:2h:87:LEU:O	10:2m:50:ARG:NH2	2.40	0.54
29:c1:629:ARG:O	29:c1:630:ARG:NH1	2.36	0.54
34:f:227:LEU:HD11	34:f:231:GLY:HA2	1.88	0.54
41:l:210:ASN:HD21	45:m3:327:VAL:HB	1.72	0.54
43:m1:169:LYS:HD3	2:2E:234:ASN:HD22	1.72	0.54
51:s:26:LEU:HD22	59:vb:482:LEU:HD11	1.88	0.54
79:a9:198:PRO:HG3	79:a9:261:LEU:HD12	1.89	0.54
110:qC:126:PHE:CD1	166:qC:501:HEM:HBC1	2.42	0.54
110:qC:223:PHE:O	110:qC:227:LEU:CB	2.55	0.54
114:qG:168:ASP:HB2	108:qa:121:VAL:HG12	1.89	0.54
129:t2:203:PHE:HB2	129:t2:210:TYR:HB2	1.90	0.54
145:tx:110:THR:OG1	145:tx:123:ARG:NH1	2.40	0.54
146:v1:71:ASN:HD21	147:v2:240:PHE:HB3	1.73	0.54
4:2G:41:HIS:CD2	4:2G:45:ASN:HD22	2.26	0.54
153:C1:701:CDL:OB4	65:Y7:357:SER:OG	2.21	0.54
33:E:194:LEU:HD22	153:E:401:CDL:H212	1.90	0.54
44:M2:34:ILE:HG12	152:M2:405:PC1:H2C1	1.90	0.54
152:N:301:PC1:H2B2	152:N:301:PC1:H371	1.89	0.54
51:S:8:PHE:CE2	59:VB:367:TYR:HB3	2.42	0.54
53:SB:275:ILE:HB	163:SB:403:F3S:S4	2.47	0.54
71:5B:86:ILE:HA	101:N2:254:ILE:HD13	1.89	0.54
82:AL:37:ARG:HH21	82:AL:41:TYR:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:AN:14:VAL:HG13	84:AN:19:TYR:HB3	1.88	0.54
91:B9:145:ARG:NH2	138:TB:55:ASN:OD1	2.40	0.54
98:G3:306:GLN:NE2	98:G3:311:TYR:OH	2.41	0.54
99:J1:308:ASP:OD2	105:N6:12:ASN:ND2	2.39	0.54
110:QC:126:PHE:CD1	166:QC:501:HEM:HBC1	2.42	0.54
115:QH:23:ARG:HB3	115:QH:29:ILE:HG12	1.90	0.54
134:T7:56:VAL:HG21	134:T7:109:TYR:HB2	1.90	0.54
153:C:301:CDL:H522	153:C:301:CDL:H141	1.90	0.54
2:2e:19:GLY:HA3	2:2e:193:ALA:HB1	1.90	0.54
20:6c:23:ARG:O	20:6c:27:LEU:HG	2.08	0.54
27:b:339:PHE:HE2	65:y7:438:ILE:HD11	1.73	0.54
33:e:208:ARG:NH2	63:y0:58:ILE:O	2.41	0.54
46:n:195:ARG:O	46:n:198:MET:HG2	2.07	0.54
48:p:100:PRO:HG2	48:p:106:ALA:HB2	1.89	0.54
52:sa:621:THR:HG23	52:sa:628:PRO:HG3	1.87	0.54
72:a1:47:ARG:HH12	78:a8:187:ASN:HD22	1.55	0.54
102:n3:68:LEU:HD23	105:n6:95:ILE:HD11	1.89	0.54
131:t4:65:PHE:O	131:t4:196:LYS:NZ	2.34	0.54
146:v1:79:GLU:HB3	146:v1:256:MET:HE1	1.89	0.54
147:v2:27:LEU:O	147:v2:114:ARG:NH2	2.39	0.54
6:2I:64:ARG:HE	132:T5:186:THR:HG23	1.73	0.54
33:E:118:ILE:HG21	153:E:403:CDL:H312	1.88	0.54
46:N:106:GLY:N	46:N:110:ILE:O	2.34	0.54
59:VB:161:CYS:SG	59:VB:193:GLN:NE2	2.80	0.54
90:B8:57:TYR:H	103:N4:462:ASN:HD21	1.55	0.54
106:P1:145:TYR:HA	106:P1:149:PHE:HB2	1.89	0.54
110:QC:49:GLY:O	110:QC:53:ALA:N	2.40	0.54
109:Qb:73:VAL:HG13	109:Qb:246:PHE:HB3	1.89	0.54
142:TF:161:GLY:O	142:TF:164:THR:OG1	2.24	0.54
32:d:113:VAL:HG11	45:m3:200:GLN:HB3	1.89	0.54
47:o:135:ASN:ND2	56:t:2:GLY:O	2.40	0.54
50:r:94:ARG:NH2	51:s:98:ASP:OD1	2.41	0.54
53:sb:230:TRP:HZ2	164:sc:102:U10:H111	1.72	0.54
59:vb:161:CYS:SG	59:vb:193:GLN:NE2	2.81	0.54
78:a8:123:ASP:HA	78:a8:126:ARG:HH21	1.73	0.54
82:al:105:GLN:OE1	127:s8:223:GLN:NE2	2.37	0.54
82:al:162:ALA:HB3	120:s1:300:ARG:HA	1.90	0.54
104:n5:55:ASN:ND2	104:n5:145:ASN:OD1	2.40	0.54
111:qD:117:ALA:O	111:qd:122:LYS:NZ	2.31	0.54
110:qc:207:TRP:NE1	166:qc:503:HEM:O2A	2.41	0.54
125:s6:75:VAL:O	125:s6:121:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2H:87:LEU:O	10:2M:50:ARG:NH2	2.41	0.54
26:A:360:TRP:CH2	153:VB:705:CDL:H522	2.41	0.54
31:C3:212:ARG:HH21	40:K:49:ILE:HA	1.72	0.54
32:D:113:VAL:HG11	45:M3:200:GLN:HB3	1.89	0.54
44:M2:7:ARG:NH1	44:M2:10:GLU:OE2	2.41	0.54
46:N:195:ARG:O	46:N:198:MET:HG2	2.07	0.54
47:O:135:ASN:ND2	56:T:2:GLY:O	2.41	0.54
50:R:94:ARG:NH2	51:S:98:ASP:OD1	2.41	0.54
153:VB:703:CDL:H152	153:VB:706:CDL:H111	1.89	0.54
72:A1:43:ASP:OD2	140:TD:42:ARG:NH1	2.40	0.54
84:AN:150:GLN:HE22	158:AN:306:3PE:H242	1.70	0.54
104:N5:737:LEU:HD23	131:T4:130:THR:HG23	1.89	0.54
108:QA:140:PHE:HD1	108:QA:153:ALA:HB2	1.72	0.54
110:QC:102:LYS:HD2	166:QC:502:HEM:HBD2	1.90	0.54
110:Qc:108:PHE:HB2	110:Qc:313:PRO:HA	1.90	0.54
111:Qd:78:ALA:HB1	111:Qd:112:PHE:HZ	1.73	0.54
153:Qg:402:CDL:H741	153:Qg:402:CDL:H311	1.90	0.54
121:S2:153:GLU:HG3	121:S2:202:THR:HG21	1.88	0.54
127:S8:154:GLU:HB2	127:S8:167:ARG:HB3	1.89	0.54
127:S8:229:GLU:O	127:S8:233:ASN:ND2	2.34	0.54
128:T1:270:ALA:HB1	128:T1:362:LEU:HD13	1.90	0.54
24:7c:50:ARG:NH2	43:m1:274:CYS:O	2.41	0.54
26:a:304:ILE:HD11	31:c3:403:TRP:HZ2	1.72	0.54
33:e:50:ILE:HD11	33:e:66:LEU:HD23	1.89	0.54
33:e:344:ILE:HD11	36:g:223:ASP:HA	1.89	0.54
153:m1:402:CDL:HB4	153:m2:401:CDL:H322	1.89	0.54
45:m3:179:LEU:HD23	45:m3:257:VAL:HG12	1.89	0.54
158:m3:402:3PE:H2D1	153:vb:701:CDL:H821	1.90	0.54
46:n:58:LYS:HD3	46:n:61:TYR:HA	1.90	0.54
52:sa:96:ALA:HB2	52:sa:137:VAL:HG21	1.89	0.54
52:sa:196:LEU:HD13	53:sb:180:LYS:HA	1.89	0.54
53:sb:140:LEU:HD12	53:sb:143:ILE:HD11	1.90	0.54
68:1b:53:CYS:HB3	74:a3:74:VAL:HG11	1.90	0.54
72:a1:51:ARG:NH2	78:a8:236:LYS:O	2.36	0.54
77:a7:42:ARG:NH1	127:s8:233:ASN:O	2.41	0.54
88:b6:77:ASN:HD22	93:bm:123:PRO:HG3	1.73	0.54
107:p2:72:GLU:OE1	107:p2:80:LYS:NZ	2.41	0.54
108:qA:87:SER:HA	109:qB:423:LEU:HD22	1.89	0.54
108:qA:119:LYS:HE3	108:qA:182:VAL:HG21	1.90	0.54
110:qC:102:LYS:HD2	166:qC:502:HEM:HBD2	1.90	0.54
114:qG:213:GLU:HA	114:qG:216:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
112:qe:88:ARG:NH2	153:qi:202:CDL:OB4	2.39	0.54
2:2E:3:LEU:HD23	2:2E:29:ILE:HG23	1.90	0.54
153:2M:101:CDL:HA22	54:SC:29:ILE:HG13	1.89	0.54
16:4T:29:VAL:H	16:4T:32:ASP:HB2	1.73	0.54
20:6C:3:SER:N	153:6C:202:CDL:OB4	2.41	0.54
29:C1:557:ARG:NH2	153:C1:712:CDL:OB4	2.40	0.54
56:T:123:GLY:HA3	153:T:203:CDL:H212	1.89	0.54
59:VB:431:ASP:OD2	59:VB:438:LYS:NZ	2.41	0.54
158:A3:202:3PE:H3D1	105:N6:186:ILE:HB	1.88	0.54
79:A9:158:ARG:NH2	79:A9:254:SER:OG	2.41	0.54
104:N5:95:TYR:HE1	104:N5:136:LEU:HA	1.72	0.54
106:P1:40:GLN:O	106:P1:44:HIS:N	2.39	0.54
130:T3:219:ASN:ND2	130:T3:222:SER:O	2.41	0.54
4:2g:102:TYR:HH	53:sb:234:ARG:HH22	1.52	0.54
10:2m:17:GLN:HE21	10:2m:22:GLY:HA2	1.72	0.54
11:2n:31:VAL:HG13	11:2n:32:VAL:HG13	1.90	0.54
37:h:290:TYR:HE2	104:N5:69:HIS:CE1	2.25	0.54
43:m1:256:TRP:O	43:m1:259:THR:OG1	2.18	0.54
49:q:36:SER:OG	49:q:121:ASP:OD2	2.24	0.54
103:n4:159:VAL:HG11	103:n4:284:PHE:HZ	1.72	0.54
106:p1:205:GLN:HG3	106:p1:206:GLU:HG3	1.90	0.54
115:qH:101:TRP:HE1	153:qH:201:CDL:CA5	2.21	0.54
109:qb:326:ARG:NE	109:qb:421:GLU:OE1	2.41	0.54
2:2E:11:LYS:HD3	2:2E:43:ARG:HD2	1.88	0.54
2:2E:19:GLY:HA3	2:2E:193:ALA:HB1	1.89	0.54
33:E:54:ASN:ND2	33:E:146:PRO:O	2.41	0.54
52:SA:127:GLN:HE22	52:SA:623:ASP:HB3	1.72	0.54
68:1B:53:CYS:HB3	74:A3:74:VAL:HG11	1.90	0.54
158:A3:202:3PE:H242	158:A3:202:3PE:H322	1.90	0.54
78:A8:123:ASP:HA	78:A8:126:ARG:HH21	1.73	0.54
158:B4:202:3PE:H382	158:B4:202:3PE:H2A1	1.89	0.54
153:BM:301:CDL:H812	103:N4:68:ILE:HG12	1.90	0.54
96:G1:34:ILE:HD12	98:G3:46:LEU:HB3	1.88	0.54
99:J1:303:LEU:HD13	124:S5:72:PRO:HD3	1.90	0.54
108:QA:101:ASP:OD2	108:QA:248:ARG:NH2	2.35	0.54
108:QA:380:ILE:HG22	108:QA:384:LYS:HE2	1.89	0.54
109:Qb:311:PRO:HB3	109:Qb:315:ASP:HB3	1.89	0.54
128:T1:323:GLN:O	128:T1:327:ASN:ND2	2.41	0.54
133:T6:89:TRP:CD1	133:T6:93:CYS:HG	2.26	0.54
152:c1:706:PC1:H291	31:c3:326:VAL:HG13	1.90	0.54
31:c3:40:ASN:HA	31:c3:43:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:m2:34:ILE:HG12	152:m2:405:PC1:H2C1	1.89	0.54
46:n:110:ILE:HG23	46:n:115:GLN:HB2	1.90	0.54
52:sa:284:HIS:HB2	52:sa:395:HIS:HB2	1.88	0.54
54:sc:27:LEU:HA	54:sc:30:VAL:HG12	1.89	0.54
56:t:86:ARG:HG3	64:y5:156:ILE:HG12	1.90	0.54
56:t:123:GLY:HA3	153:t:203:CDL:H212	1.90	0.54
77:a7:80:VAL:HG21	122:s3:13:ILE:HA	1.89	0.54
81:ac:110:ASP:OD2	91:b9:38:ARG:NH1	2.39	0.54
83:am:109:ASP:O	83:am:113:ASN:ND2	2.35	0.54
104:n5:174:LEU:HD22	104:n5:230:ILE:HG21	1.88	0.54
110:qc:28:HIS:HB3	110:qc:207:TRP:HH2	1.72	0.54
146:v1:368:ILE:HG13	146:v1:439:LEU:HB2	1.88	0.54
8:2K:86:ARG:HH12	10:2M:52:GLN:HG3	1.73	0.54
24:7C:50:ARG:NH2	43:M1:274:CYS:O	2.41	0.54
33:E:344:ILE:HD11	36:G:223:ASP:HA	1.89	0.54
34:F:227:LEU:HD11	34:F:231:GLY:HA2	1.90	0.54
54:SC:27:LEU:HA	54:SC:30:VAL:HG12	1.90	0.54
63:Y0:16:PRO:O	63:Y0:20:ALA:N	2.40	0.54
64:Y5:30:LEU:HB3	66:Z:64:VAL:HG11	1.88	0.54
83:AM:50:ALA:HB2	127:S8:80:TYR:HB2	1.89	0.54
99:J1:127:LYS:O	99:J1:130:THR:OG1	2.26	0.54
105:N6:222:ASP:N	105:N6:226:ASP:OD2	2.39	0.54
114:QG:273:ASN:HB3	114:QG:275:ARG:HE	1.73	0.54
153:2g:204:CDL:OB4	55:sd:14:ILE:N	2.40	0.54
153:m:304:CDL:HA61	63:y0:59:PHE:HB2	1.89	0.54
44:m2:7:ARG:NH1	44:m2:10:GLU:OE2	2.41	0.54
52:sa:574:ARG:NH1	52:sa:576:GLU:OE2	2.38	0.54
71:5b:86:ILE:HA	101:n2:254:ILE:HD13	1.90	0.54
73:a2:87:ILE:O	73:a2:91:VAL:HG23	2.07	0.54
82:al:57:ASP:OD1	82:al:58:GLU:N	2.41	0.54
152:c4:403:PC1:H2B2	152:c4:403:PC1:H3A1	1.89	0.54
98:g3:306:GLN:NE2	98:g3:311:TYR:OH	2.41	0.54
100:n1:104:PHE:HD2	100:n1:250:PHE:HB3	1.72	0.54
108:qA:140:PHE:HD1	108:qA:153:ALA:HB2	1.73	0.54
109:qb:43:LEU:HD22	109:qb:48:GLU:HA	1.90	0.54
109:qb:381:PHE:HE1	109:qb:395:SER:HB3	1.73	0.54
128:t1:29:LEU:O	128:t1:33:ASN:ND2	2.38	0.54
153:2G:204:CDL:OB4	55:SD:14:ILE:N	2.41	0.54
28:BP:214:CYS:O	28:BP:263:THR:OG1	2.26	0.54
29:C1:540:PHE:CE1	154:C1:702:HEA:H253	2.43	0.54
47:O:65:ASN:ND2	47:O:67:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:AL:131:LEU:O	82:AL:134:THR:OG1	2.22	0.54
110:QC:88:VAL:HG21	166:QC:501:HEM:HMD1	1.89	0.54
153:Qc:504:CDL:H732	153:Qc:504:CDL:H791	1.89	0.54
153:c:301:CDL:H522	153:c:301:CDL:H141	1.89	0.54
8:2k:80:ILE:HB	10:2m:61:ARG:HH12	1.71	0.53
20:6c:92:GLU:OE2	21:6l:66:ARG:NH2	2.38	0.53
29:c1:310:PHE:HA	29:c1:343:LEU:HD22	1.91	0.53
29:c1:592:ASP:CG	30:c2:487:ARG:HH12	2.16	0.53
30:c2:360:LEU:HD11	30:c2:391:LEU:HD22	1.90	0.53
31:c3:212:ARG:HH21	40:k:49:ILE:HA	1.72	0.53
33:e:201:LEU:O	153:e:401:CDL:O1	2.27	0.53
34:f:222:ILE:HD11	34:f:303:ILE:HB	1.89	0.53
52:sa:214:ASP:OD1	52:sa:215:GLU:N	2.41	0.53
56:t:99:PHE:O	63:y0:36:ARG:NH2	2.37	0.53
71:5b:93:THR:HG21	101:n2:250:LEU:HD21	1.89	0.53
77:a7:84:THR:HG23	77:a7:120:PRO:HB2	1.88	0.53
79:a9:158:ARG:NH2	79:a9:254:SER:OG	2.42	0.53
158:b4:202:3PE:H292	158:b4:202:3PE:H362	1.90	0.53
97:g2:26:LEU:HG	158:g2:301:3PE:H231	1.90	0.53
100:n1:192:ILE:HG22	100:n1:193:ILE:HG23	1.88	0.53
4:2G:119:SER:HB3	152:2G:202:PC1:H31	1.90	0.53
153:2M:101:CDL:H511	55:SD:4:GLU:HB2	1.90	0.53
153:7A:201:CDL:H241	46:N:132:GLY:HA3	1.88	0.53
27:B:54:LEU:HD11	27:B:113:LEU:HD11	1.91	0.53
27:B:345:ASN:O	27:B:349:ASN:ND2	2.34	0.53
33:E:354:ARG:NH2	36:G:232:GLU:OE2	2.40	0.53
53:SB:230:TRP:HZ2	164:SC:102:U10:H111	1.73	0.53
61:X:117:HIS:ND1	61:X:118:CYS:O	2.39	0.53
83:AM:52:LEU:HB2	153:AM:201:CDL:H332	1.89	0.53
85:B2:67:PRO:HG3	152:T4:301:PC1:H112	1.90	0.53
87:B4:34:MET:HE1	91:B9:10:ASN:HD22	1.73	0.53
95:FX:166:SER:N	95:FX:170:ASP:OD2	2.41	0.53
97:G2:15:ILE:HA	97:G2:18:MET:HE3	1.90	0.53
98:G3:265:ILE:HD11	105:N6:234:ARG:HA	1.90	0.53
110:QC:345:LYS:O	110:QC:347:HIS:ND1	2.41	0.53
113:QF:70:GLU:HA	113:QF:73:VAL:HG22	1.90	0.53
114:QG:315:PRO:HD2	114:QG:318:LEU:HD12	1.90	0.53
113:Qf:21:LYS:NZ	113:Qf:74:GLN:OE1	2.41	0.53
82:al:37:ARG:HH21	82:al:41:TYR:HB3	1.72	0.53
99:j1:303:LEU:HD13	124:s5:72:PRO:HD3	1.90	0.53
104:n5:98:SER:OG	104:n5:140:LYS:NZ	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qC:132:LEU:HD13	110:qC:184:LEU:HB3	1.89	0.53
110:qC:344:PRO:O	110:qC:406:ARG:NH2	2.34	0.53
108:qa:31:ILE:O	116:qi:62:TYR:OH	2.24	0.53
121:s2:199:PHE:HD2	121:s2:291:LEU:HD11	1.73	0.53
3:2F:181:PHE:O	54:SC:53:ALA:HB2	2.08	0.53
5:2H:163:PHE:HB2	5:2H:191:TYR:CZ	2.43	0.53
28:BP:193:GLY:O	28:BP:215:GLY:N	2.41	0.53
39:J:103:LEU:HD13	39:J:136:VAL:HG21	1.91	0.53
68:1B:56:THR:HB	74:A3:92:ILE:HD11	1.91	0.53
70:4L:59:ILE:HG22	70:4L:63:ILE:HG13	1.91	0.53
75:A5:48:ASN:HB3	75:A5:51:LYS:HB3	1.90	0.53
90:B8:62:PRO:O	91:B9:9:LYS:NZ	2.30	0.53
97:G2:3:LEU:HD21	135:T8:49:VAL:HG21	1.91	0.53
103:N4:101:ASN:ND2	103:N4:107:ASN:OD1	2.42	0.53
103:N4:399:ILE:HG13	103:N4:475:LEU:HD13	1.91	0.53
109:QB:386:ILE:HD13	115:QH:38:TYR:HE1	1.73	0.53
109:Qb:381:PHE:HE1	109:Qb:395:SER:HB3	1.73	0.53
110:Qc:344:PRO:O	110:Qc:406:ARG:NH2	2.41	0.53
146:V1:71:ASN:HD21	147:V2:240:PHE:HB3	1.73	0.53
3:2f:100:LYS:NZ	131:t4:211:PRO:O	2.40	0.53
19:6b:95:PRO:O	21:6l:41:ARG:NH2	2.41	0.53
25:7l:870:ILE:HD11	50:R:173:ILE:HG22	1.90	0.53
29:c1:237:MET:HG2	46:n:164:ILE:HD11	1.90	0.53
37:h:34:ALA:O	37:h:38:GLN:HG2	2.08	0.53
42:m:118:HIS:HD2	152:w:201:PC1:H341	1.73	0.53
43:m1:280:TYR:O	43:m1:283:ALA:HB3	2.09	0.53
153:m1:404:CDL:H211	153:m1:404:CDL:H251	1.90	0.53
44:m2:294:TRP:NE1	153:m2:403:CDL:OA7	2.40	0.53
152:n:301:PC1:H371	152:n:301:PC1:H2B2	1.89	0.53
50:r:173:ILE:HG22	25:7L:870:ILE:HD11	1.90	0.53
71:5b:31:MET:HG2	153:b4:201:CDL:H711	1.89	0.53
77:a7:129:ILE:HG23	122:s3:24:ILE:HD13	1.91	0.53
153:bm:301:CDL:H812	103:n4:68:ILE:HG12	1.90	0.53
98:g3:265:ILE:HD11	105:n6:234:ARG:HA	1.89	0.53
103:n4:102:ASN:HB2	144:th:52:GLN:HE21	1.74	0.53
110:qC:49:GLY:O	110:qC:53:ALA:N	2.41	0.53
110:qc:108:PHE:HB2	110:qc:313:PRO:HA	1.90	0.53
111:qd:255:VAL:HG12	111:qd:259:MET:HE3	1.89	0.53
128:t1:17:THR:O	128:t1:125:SER:N	2.42	0.53
142:tf:161:GLY:O	142:tf:164:THR:OG1	2.24	0.53
3:2F:152:LYS:NZ	54:SC:57:GLU:OE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4A:78:ASP:OD1	15:4A:82:TYR:N	2.40	0.53
23:7A:41:ALA:HB3	59:VB:266:LEU:HB3	1.90	0.53
24:7C:163:HIS:NE2	152:7C:303:PC1:O14	2.22	0.53
29:C1:530:MET:HG2	154:C1:703:HEA:C2C	2.38	0.53
31:C3:40:ASN:HA	31:C3:43:ASN:HD21	1.73	0.53
34:F:299:GLN:NE2	58:V:77:PHE:O	2.34	0.53
40:K:30:GLN:N	40:K:46:TYR:OH	2.40	0.53
52:SA:239:TYR:HE2	52:SA:464:LEU:HB2	1.73	0.53
87:B4:45:GLU:HG3	95:FX:93:LYS:HB3	1.89	0.53
112:QE:84:GLU:OE2	116:QI:37:GLN:NE2	2.32	0.53
153:Qi:202:CDL:HA4	153:Qi:202:CDL:H512	1.89	0.53
126:S7:109:VAL:HG12	126:S7:111:ARG:H	1.72	0.53
6:2i:64:ARG:HE	132:t5:186:THR:HG23	1.73	0.53
23:7a:41:ALA:HB3	59:vb:266:LEU:HB3	1.89	0.53
27:b:63:MET:O	27:b:103:ASN:ND2	2.41	0.53
33:e:54:ASN:ND2	33:e:146:PRO:O	2.41	0.53
37:h:82:LYS:HE2	104:N5:67:ILE:HG13	1.90	0.53
52:sa:70:GLU:HB3	52:sa:461:LYS:HD3	1.89	0.53
65:y7:169:LEU:HG	65:y7:171:ASP:H	1.72	0.53
71:5b:30:GLU:HB2	90:b8:66:ILE:HD12	1.90	0.53
76:a6:160:LEU:HD11	120:s1:619:ALA:HA	1.91	0.53
84:an:106:GLN:O	84:an:110:THR:OG1	2.20	0.53
97:g2:3:LEU:HD21	135:t8:49:VAL:HG21	1.90	0.53
110:qC:338:ARG:NH2	114:qG:33:GLU:OE2	2.42	0.53
111:qD:93:ASP:OD1	112:qE:123:ARG:NH2	2.34	0.53
109:qb:492:HIS:CD2	109:qb:494:ASN:HB3	2.44	0.53
113:qf:21:LYS:NZ	113:qf:74:GLN:OE1	2.41	0.53
153:qg:402:CDL:H741	153:qg:402:CDL:H311	1.90	0.53
120:s1:342:ILE:HD12	120:s1:542:ILE:HG12	1.89	0.53
134:t7:56:VAL:HG21	134:t7:109:TYR:HB2	1.90	0.53
147:v2:223:THR:HG22	147:v2:224:LEU:HG	1.91	0.53
31:C3:558:LYS:HG3	41:L:104:GLU:HG2	1.89	0.53
34:F:222:ILE:HD11	34:F:303:ILE:HB	1.89	0.53
36:G:193:VAL:HG13	59:VB:179:LEU:HD22	1.91	0.53
43:M1:280:TYR:O	43:M1:283:ALA:HB3	2.09	0.53
52:SA:214:ASP:OD1	52:SA:215:GLU:N	2.41	0.53
85:B2:111:LEU:HD21	131:T4:25:MET:HE3	1.89	0.53
111:Qd:46:GLU:HB3	111:Qd:50:HIS:HB3	1.90	0.53
142:TF:127:ASN:OD1	142:TF:129:GLN:NE2	2.42	0.53
29:c1:76:ARG:HB3	29:c1:605:THR:HG23	1.91	0.53
29:c1:344:ARG:NH1	153:c1:709:CDL:OB4	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c2:197:PRO:HD2	45:m3:39:GLY:HA2	1.90	0.53
47:o:65:ASN:ND2	47:o:67:GLU:OE1	2.41	0.53
79:a9:60:ALA:HB2	122:s3:183:ILE:HD12	1.90	0.53
85:b2:111:LEU:HD21	131:t4:25:MET:HE3	1.89	0.53
91:b9:133:PHE:O	138:tb:60:TYR:OH	2.22	0.53
109:qB:497:ILE:O	109:qB:500:SER:OG	2.19	0.53
114:qG:78:ARG:NH2	114:qG:123:TYR:OH	2.41	0.53
115:qH:23:ARG:HB3	115:qH:29:ILE:HG12	1.90	0.53
109:qb:169:GLN:OE1	109:qb:269:THR:OG1	2.21	0.53
111:qd:43:LEU:HB3	111:qd:203:ASP:HA	1.91	0.53
120:s1:245:GLU:OE2	127:s8:140:LYS:NZ	2.32	0.53
128:t1:377:SER:HB3	128:t1:410:VAL:HG22	1.91	0.53
147:v2:169:ALA:HB3	147:v2:175:MET:HE3	1.90	0.53
3:2F:100:LYS:NZ	131:T4:211:PRO:O	2.40	0.53
3:2F:295:SER:HB2	6:2I:76:GLN:HE21	1.74	0.53
19:6B:95:PRO:O	21:6L:41:ARG:NH2	2.41	0.53
29:C1:76:ARG:HB3	29:C1:605:THR:HG23	1.91	0.53
29:C1:344:ARG:NH1	153:C1:708:CDL:OB4	2.42	0.53
34:F:269:ASP:OD1	34:F:269:ASP:N	2.40	0.53
36:G:162:PHE:HA	36:G:181:ASN:HA	1.89	0.53
42:M:190:ALA:O	62:Y:1:MET:N	2.42	0.53
153:M:305:CDL:H742	158:W:203:3PE:H272	1.89	0.53
153:M1:404:CDL:H211	153:M1:404:CDL:H251	1.90	0.53
60:W:39:TYR:OH	152:W:201:PC1:O14	2.25	0.53
79:A9:198:PRO:HG3	79:A9:261:LEU:HD12	1.91	0.53
97:G2:26:LEU:HG	158:G2:301:3PE:H231	1.90	0.53
103:N4:102:ASN:HB2	144:TH:52:GLN:HE21	1.73	0.53
104:N5:419:MET:SD	104:N5:430:HIS:NE2	2.81	0.53
108:QA:119:LYS:HE3	108:QA:182:VAL:HG21	1.89	0.53
128:T1:220:ASN:ND2	128:T1:461:ASP:O	2.41	0.53
5:2h:163:PHE:HB2	5:2h:191:TYR:CZ	2.43	0.53
26:a:95:LEU:HD11	59:vb:207:GLU:HB2	1.90	0.53
30:c2:508:ASN:OD1	30:c2:509:SER:N	2.41	0.53
33:e:354:ARG:NH2	36:g:232:GLU:OE2	2.40	0.53
36:g:162:PHE:HA	36:g:181:ASN:HA	1.90	0.53
39:j:103:LEU:HD13	39:j:136:VAL:HG21	1.91	0.53
52:sa:251:TYR:CG	52:sa:394:VAL:HG21	2.44	0.53
59:vb:227:ASP:OD1	59:vb:227:ASP:N	2.38	0.53
73:a2:8:ILE:HG23	73:a2:12:LEU:HD12	1.90	0.53
75:a5:48:ASN:HB3	75:a5:51:LYS:HB3	1.90	0.53
107:p2:146:ASN:O	107:p2:150:ASN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qC:274:LEU:HD11	110:qC:377:ARG:HD2	1.91	0.53
112:qE:48:PRO:HB3	112:qE:67:LYS:HD2	1.89	0.53
108:qa:453:LYS:O	108:qa:456:THR:OG1	2.26	0.53
130:t3:219:ASN:ND2	130:t3:222:SER:O	2.42	0.53
147:v2:167:LEU:HD12	147:v2:175:MET:HE1	1.89	0.53
20:6C:23:ARG:O	20:6C:27:LEU:HG	2.08	0.53
152:D:501:PC1:H251	152:D:501:PC1:H371	1.91	0.53
38:I:31:GLY:O	50:R:151:LYS:HG2	2.09	0.53
42:M:72:TYR:OH	42:M:91:ARG:NH1	2.42	0.53
153:M:306:CDL:HA61	63:Y0:59:PHE:HB2	1.89	0.53
152:W:204:PC1:H252	152:W:204:PC1:H362	1.91	0.53
108:Qa:31:ILE:HG22	152:Qi:201:PC1:H331	1.91	0.53
109:Qb:492:HIS:CD2	109:Qb:494:ASN:HB3	2.44	0.53
110:Qc:418:PHE:HZ	114:Qg:86:LEU:HD13	1.74	0.53
3:2f:295:SER:HB2	6:2i:76:GLN:HE21	1.74	0.53
5:2h:160:GLN:O	5:2h:164:ASN:ND2	2.32	0.53
29:c1:540:PHE:CE1	154:c1:702:HEA:H253	2.44	0.53
39:j:177:ASP:OD1	39:j:178:ALA:N	2.41	0.53
65:y7:138:LEU:O	65:y7:142:ASN:ND2	2.28	0.53
77:a7:230:ASN:HB3	77:a7:261:GLN:H	1.74	0.53
153:al:301:CDL:H712	153:t1:601:CDL:H752	1.90	0.53
108:qa:31:ILE:HG22	152:qi:201:PC1:H331	1.90	0.53
152:qb:602:PC1:H2C1	112:qe:107:ALA:HB2	1.91	0.53
120:s1:359:LEU:HB3	120:s1:364:VAL:HB	1.90	0.53
128:t1:323:GLN:O	128:t1:327:ASN:ND2	2.41	0.53
130:t3:166:LEU:HD23	130:t3:169:PHE:CZ	2.44	0.53
145:tx:55:ASN:ND2	145:tx:98:PRO:HD3	2.24	0.53
27:B:339:PHE:HE2	65:Y7:438:ILE:HD11	1.73	0.53
153:C1:708:CDL:H752	31:C3:318:VAL:HG12	1.91	0.53
52:SA:251:TYR:CG	52:SA:394:VAL:HG21	2.44	0.53
56:T:86:ARG:HG3	64:Y5:156:ILE:HG12	1.90	0.53
76:A6:37:MET:O	122:S3:154:ARG:NH1	2.41	0.53
78:A8:118:SER:OG	83:AM:89:ALA:HA	2.09	0.53
78:A8:183:LYS:HG3	78:A8:225:PHE:HB2	1.91	0.53
125:S6:75:VAL:O	125:S6:121:ARG:NH2	2.42	0.53
23:7a:76:ARG:NH1	153:7a:201:CDL:OA3	2.39	0.53
53:sb:214:GLU:OE1	53:sb:214:GLU:N	2.41	0.53
99:j1:29:LEU:HD12	99:j1:80:LEU:HD12	1.91	0.53
103:n4:7:ILE:HG23	103:n4:77:TYR:CZ	2.44	0.53
110:qC:329:VAL:HG23	110:qC:333:SER:HB3	1.91	0.53
152:qC:507:PC1:H382	153:qH:201:CDL:H651	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
108:qa:420:THR:OG1	108:qa:432:HIS:NE2	2.31	0.53
110:qc:46:LEU:HD11	110:qc:193:ALA:HB2	1.91	0.53
134:t7:137:CYS:HB2	134:t7:140:TRP:HD1	1.74	0.53
13:2T:10:GLU:HB3	30:C2:227:ARG:HH21	1.74	0.53
30:C2:389:PHE:HE1	47:O:144:PHE:HB2	1.73	0.53
34:F:202:ILE:HG12	152:V:202:PC1:H261	1.91	0.53
57:U:37:LYS:HA	57:U:41:VAL:HB	1.91	0.53
71:5B:30:GLU:OE1	90:B8:68:TYR:OH	2.20	0.53
153:A1:102:CDL:H162	140:TD:16:PHE:HA	1.90	0.53
98:G3:262:GLU:HA	98:G3:265:ILE:HG23	1.91	0.53
102:N3:71:TYR:OH	102:N3:110:ASP:OD2	2.26	0.53
152:QC:507:PC1:H382	153:QH:201:CDL:H651	1.89	0.53
109:Qb:326:ARG:NE	109:Qb:421:GLU:OE1	2.41	0.53
153:Qb:601:CDL:OA4	116:Qi:67:GLN:NE2	2.38	0.53
110:Qc:147:ALA:O	110:Qc:151:ASN:ND2	2.35	0.53
114:Qg:192:LEU:O	114:Qg:198:TRP:NE1	2.41	0.53
146:V1:78:ASP:OD2	147:V2:247:TRP:NE1	2.42	0.53
9:2l:16:ARG:NH1	9:2l:59:GLU:OE2	2.42	0.53
30:c2:389:PHE:HE1	47:o:144:PHE:HB2	1.73	0.53
37:h:79:ARG:HH21	104:N5:60:PHE:HB2	1.74	0.53
37:h:267:SER:HB3	57:u:5:THR:HG23	1.91	0.53
44:m2:281:GLY:N	152:m2:402:PC1:O14	2.41	0.53
52:sa:609:LYS:NZ	52:sa:610:THR:O	2.41	0.53
60:w:35:LEU:HD13	153:w:202:CDL:H111	1.91	0.53
65:y7:168:ILE:HD13	149:c:185:ARG:HD3	1.91	0.53
158:a3:202:3PE:H242	158:a3:202:3PE:H322	1.90	0.53
78:a8:166:MET:HA	78:a8:202:GLN:HE22	1.74	0.53
153:a9:403:CDL:OB4	126:s7:2:ARG:N	2.42	0.53
95:fx:132:ARG:NH2	101:n2:332:ASP:OD2	2.41	0.53
99:j1:69:LYS:O	99:j1:73:ILE:HG12	2.09	0.53
100:n1:163:ILE:HG12	100:n1:212:LEU:HG	1.90	0.53
101:n2:113:THR:HG23	101:n2:279:LEU:HD11	1.91	0.53
102:n3:71:TYR:OH	102:n3:110:ASP:OD2	2.26	0.53
103:n4:101:ASN:ND2	103:n4:107:ASN:OD1	2.42	0.53
104:n5:60:PHE:HB2	37:H:79:ARG:HH21	1.74	0.53
111:qd:78:ALA:HB1	111:qd:112:PHE:HZ	1.73	0.53
30:C2:360:LEU:HD11	30:C2:391:LEU:HD22	1.91	0.53
42:M:74:LYS:NZ	60:W:5:TYR:O	2.34	0.53
42:M:86:THR:H	59:VB:216:HIS:CE1	2.27	0.53
43:M1:76:ALA:HB1	152:M1:403:PC1:H271	1.91	0.53
152:N:301:PC1:H362	152:N:301:PC1:H292	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:62:ARG:HH11	52:SA:65:PHE:HD2	1.57	0.53
65:Y7:168:ILE:HD13	149:C:185:ARG:HD3	1.91	0.53
82:AL:57:ASP:OD1	82:AL:58:GLU:N	2.41	0.53
92:BL:71:ARG:NH1	92:BL:105:LEU:O	2.38	0.53
92:BL:83:ILE:HD12	132:T5:150:VAL:HG21	1.90	0.53
104:N5:498:SER:O	104:N5:501:THR:OG1	2.24	0.53
111:Qd:43:LEU:HB3	111:Qd:203:ASP:HA	1.91	0.53
115:Qh:101:TRP:HE1	160:Qh:201:PX2:C4	2.22	0.53
134:T7:10:ASN:HB3	134:T7:13:SER:HB3	1.90	0.53
149:c:131:ASP:OD2	149:c:141:ARG:NH2	2.39	0.53
2:2e:48:LYS:NZ	2:2e:60:GLU:OE2	2.42	0.53
16:4t:29:VAL:H	16:4t:32:ASP:HB2	1.73	0.53
17:5t:19:ASP:OD2	30:c2:227:ARG:NH2	2.26	0.53
25:7l:873:PRO:HB3	57:u:55:ASP:HB3	1.91	0.53
33:e:33:ASN:ND2	33:e:230:ASP:OD1	2.42	0.53
34:f:269:ASP:OD1	34:f:269:ASP:N	2.40	0.53
50:r:62:SER:HA	50:r:66:SER:HB3	1.91	0.53
52:sa:95:ASN:ND2	52:sa:442:GLY:O	2.41	0.53
52:sa:528:LEU:HD12	52:sa:531:ILE:HD12	1.91	0.53
57:u:37:LYS:HA	57:u:41:VAL:HB	1.91	0.53
70:4l:59:ILE:HG22	70:4l:63:ILE:HG13	1.90	0.53
77:a7:29:ARG:HB2	77:a7:32:TYR:HB3	1.91	0.53
101:n2:34:LEU:HD13	101:n2:52:ILE:HD13	1.91	0.53
104:n5:338:LYS:HB2	158:n5:802:3PE:H12	1.91	0.53
107:p2:89:HIS:NE2	107:p2:96:SER:OG	2.42	0.53
107:p2:123:TYR:HB2	107:p2:143:ILE:HG21	1.90	0.53
110:qC:223:PHE:O	110:qC:227:LEU:HB3	2.09	0.53
114:qG:194:ARG:NH1	117:qj:7:TYR:OH	2.34	0.53
126:s7:109:VAL:HG12	126:s7:111:ARG:H	1.73	0.53
131:t4:82:THR:HG23	131:t4:177:ALA:HB1	1.90	0.53
132:t5:131:GLY:HA3	153:t5:301:CDL:H631	1.90	0.53
32:D:220:ASN:HB2	32:D:228:LEU:HD12	1.91	0.53
33:E:33:ASN:ND2	33:E:230:ASP:OD1	2.42	0.53
50:R:62:SER:HA	50:R:66:SER:HB3	1.91	0.53
64:Y5:138:LYS:HB2	160:Y5:204:PX2:H2	1.91	0.53
153:AL:301:CDL:H712	153:T1:601:CDL:H752	1.89	0.53
99:J1:69:LYS:O	99:J1:73:ILE:HG12	2.09	0.53
106:P1:205:GLN:HG3	106:P1:206:GLU:HG3	1.90	0.53
27:b:324:LYS:HZ2	153:b:501:CDL:H1O1	1.54	0.52
28:bp:365:ASN:ND2	28:bp:406:ASP:OD1	2.41	0.52
30:c2:63:MET:HE1	58:v:88:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c3:501:TYR:CD1	31:c3:502:PRO:HD3	2.44	0.52
52:sa:296:THR:HG22	52:sa:371:ILE:HG21	1.91	0.52
152:w:204:PC1:H252	152:w:204:PC1:H362	1.91	0.52
91:b9:145:ARG:NH2	138:tb:55:ASN:OD1	2.41	0.52
104:n5:95:TYR:HE1	104:n5:136:LEU:HA	1.73	0.52
108:qA:96:ASP:OD1	108:qA:425:ARG:NH1	2.41	0.52
110:qC:224:ASP:OD1	112:qE:100:TYR:OH	2.25	0.52
153:qH:201:CDL:H142	153:qH:201:CDL:H322	1.91	0.52
128:t1:220:ASN:ND2	128:t1:461:ASP:O	2.42	0.52
13:2T:6:LYS:NZ	30:C2:249:LEU:O	2.41	0.52
13:2T:8:GLN:HA	30:C2:218:ILE:HG21	1.92	0.52
14:3T:8:ASP:OD1	14:3T:8:ASP:N	2.41	0.52
153:7A:201:CDL:OA4	65:Y7:358:ARG:NH1	2.41	0.52
26:A:408:VAL:O	26:A:414:GLN:NE2	2.42	0.52
29:C1:310:PHE:HA	29:C1:343:LEU:HD22	1.91	0.52
31:C3:192:LEU:HD11	153:C3:604:CDL:H202	1.91	0.52
46:N:58:LYS:HD3	46:N:61:TYR:HA	1.90	0.52
46:N:110:ILE:HG23	46:N:115:GLN:HB2	1.90	0.52
59:VB:408:LEU:HD22	59:VB:448:ALA:HB2	1.91	0.52
90:B8:135:ARG:NH2	92:BL:100:ASP:O	2.42	0.52
102:N3:38:THR:OG1	126:S7:82:GLU:OE1	2.25	0.52
107:P2:56:ASN:HB2	107:P2:59:ALA:HB3	1.91	0.52
114:QG:112:VAL:HG22	114:QG:116:LYS:HE2	1.91	0.52
115:QH:101:TRP:HE1	153:QH:201:CDL:CA5	2.21	0.52
108:Qa:334:LEU:O	108:Qa:338:LEU:N	2.42	0.52
108:Qa:453:LYS:O	108:Qa:456:THR:OG1	2.27	0.52
129:T2:22:LEU:HB3	129:T2:254:LEU:HD13	1.91	0.52
147:V2:167:LEU:HB2	147:V2:175:MET:HE1	1.91	0.52
3:2f:129:VAL:O	12:2o:24:TYR:OH	2.23	0.52
6:2i:87:ALA:O	37:H:106:ASN:ND2	2.42	0.52
15:4a:78:ASP:OD1	15:4a:82:TYR:N	2.40	0.52
26:a:287:TYR:OH	153:a:502:CDL:OB9	2.28	0.52
27:b:124:LYS:HD2	27:b:128:GLN:HE21	1.73	0.52
29:c1:291:SER:O	29:c1:295:LEU:HG	2.09	0.52
46:n:65:TRP:O	46:n:68:PHE:HB3	2.09	0.52
68:1b:56:THR:HB	74:a3:92:ILE:HD11	1.91	0.52
105:n6:214:GLN:HG2	121:s2:11:PRO:HG2	1.91	0.52
112:qE:39:HIS:O	112:qE:41:GLY:N	2.40	0.52
110:qc:135:VAL:HG21	110:qc:181:LEU:HD13	1.92	0.52
111:qd:309:ARG:NH1	111:qd:312:GLN:OE1	2.43	0.52
160:qh:201:PX2:H16	160:qh:201:PX2:H51	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
134:t7:10:ASN:HB3	134:t7:13:SER:HB3	1.91	0.52
29:C1:237:MET:HG2	46:N:164:ILE:HD11	1.90	0.52
33:E:208:ARG:NH2	63:Y0:58:ILE:O	2.41	0.52
43:M1:256:TRP:O	43:M1:259:THR:OG1	2.18	0.52
65:Y7:169:LEU:HG	65:Y7:171:ASP:H	1.72	0.52
106:P1:185:TYR:OH	130:T3:266:ARG:NH2	2.40	0.52
130:T3:166:LEU:HD23	130:T3:169:PHE:CZ	2.44	0.52
147:V2:169:ALA:HB3	147:V2:175:MET:HE3	1.90	0.52
27:b:54:LEU:HD11	27:b:113:LEU:HD11	1.91	0.52
33:e:48:TYR:HB2	33:e:274:VAL:HG22	1.91	0.52
34:f:202:ILE:HG12	152:v:202:PC1:H261	1.91	0.52
53:sb:36:CYS:O	53:sb:40:ILE:HG12	2.09	0.52
59:vb:114:GLU:OE2	59:vb:218:TYR:OH	2.25	0.52
71:5b:25:PHE:HE2	104:n5:410:GLY:HA2	1.74	0.52
78:a8:118:SER:OG	83:am:89:ALA:HA	2.09	0.52
94:c4:21:LYS:HZ1	103:n4:39:SER:HG	1.56	0.52
109:qB:386:ILE:HD13	115:qH:38:TYR:HE1	1.73	0.52
110:qC:329:VAL:O	118:qL:7:LYS:NZ	2.33	0.52
120:s1:67:HIS:HB3	120:s1:70:LEU:HB2	1.91	0.52
26:A:287:TYR:OH	153:A:502:CDL:OB9	2.27	0.52
153:A:504:CDL:H581	153:A:504:CDL:H621	1.92	0.52
33:E:48:TYR:HB2	33:E:274:VAL:HG22	1.91	0.52
37:H:267:SER:HB3	57:U:5:THR:HG23	1.91	0.52
42:M:118:HIS:HD2	152:W:201:PC1:H341	1.73	0.52
46:N:65:TRP:O	46:N:68:PHE:HB3	2.09	0.52
79:A9:60:ALA:HB2	122:S3:183:ILE:HD12	1.90	0.52
79:A9:354:VAL:HG11	99:J1:218:TRP:HZ3	1.73	0.52
158:B4:202:3PE:H362	158:B4:202:3PE:H292	1.90	0.52
101:N2:127:TYR:O	101:N2:130:SER:OG	2.26	0.52
103:N4:7:ILE:HG23	103:N4:77:TYR:CZ	2.44	0.52
107:P2:146:ASN:O	107:P2:150:ASN:N	2.41	0.52
109:Qb:43:LEU:HD22	109:Qb:48:GLU:HA	1.90	0.52
120:S1:67:HIS:HB3	120:S1:70:LEU:HB2	1.91	0.52
121:S2:94:GLU:HB3	121:S2:174:TYR:HB2	1.91	0.52
128:T1:377:SER:HB3	128:T1:410:VAL:HG22	1.91	0.52
134:T7:137:CYS:HB2	134:T7:140:TRP:HD1	1.75	0.52
135:T8:99:ILE:HD13	148:X1:130:LYS:HB3	1.91	0.52
2:2e:318:TRP:HE1	151:2e:401:HEC:HBB2	1.75	0.52
29:c1:517:MET:HE1	29:c1:583:PHE:HA	1.92	0.52
36:g:193:VAL:HG13	59:vb:179:LEU:HD22	1.92	0.52
52:sa:62:ARG:HH11	52:sa:65:PHE:HD2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:a8:183:LYS:HG3	78:a8:225:PHE:HB2	1.92	0.52
82:al:15:LYS:HG3	82:al:50:TYR:HB3	1.91	0.52
92:bl:83:ILE:HD12	132:t5:150:VAL:HG21	1.90	0.52
95:fx:166:SER:N	95:fx:170:ASP:OD2	2.42	0.52
96:g1:74:VAL:HG22	96:g1:95:ILE:HD12	1.92	0.52
107:p2:56:ASN:HB2	107:p2:59:ALA:HB3	1.91	0.52
114:qg:95:ARG:NH1	115:qh:50:ASP:O	2.42	0.52
115:qh:23:ARG:HB3	115:qh:29:ILE:HG12	1.92	0.52
121:s2:131:LEU:HD11	121:s2:199:PHE:HE1	1.74	0.52
135:t8:99:ILE:HD13	148:x1:130:LYS:HB3	1.92	0.52
13:2T:33:ASP:OD1	16:4T:42:ARG:NH2	2.33	0.52
43:M1:243:GLY:HA3	153:M1:404:CDL:H671	1.92	0.52
71:5B:30:GLU:HB2	90:B8:66:ILE:HD12	1.91	0.52
74:A3:116:ARG:HG3	137:TA:127:LEU:HD23	1.91	0.52
78:A8:166:MET:HA	78:A8:202:GLN:HE22	1.73	0.52
96:G1:74:VAL:HG22	96:G1:95:ILE:HD12	1.92	0.52
98:G3:278:LEU:HB2	98:G3:281:GLU:HG2	1.92	0.52
106:P1:56:LEU:HD23	107:P2:68:PRO:HB3	1.91	0.52
110:QC:274:LEU:HD11	110:QC:377:ARG:HD2	1.90	0.52
110:Qc:207:TRP:NE1	166:Qc:503:HEM:O2A	2.41	0.52
120:S1:609:ASP:O	120:S1:611:ARG:NH1	2.43	0.52
13:2t:10:GLU:HB3	30:c2:227:ARG:HH21	1.74	0.52
19:6b:53:PHE:O	19:6b:57:TYR:HB3	2.09	0.52
30:c2:417:ARG:NH1	30:c2:559:HIS:O	2.42	0.52
74:a3:79:TRP:CH2	148:x1:44:VAL:HG11	2.45	0.52
75:a5:57:THR:HG23	75:a5:58:LYS:HG3	1.92	0.52
87:b4:91:TRP:O	87:b4:99:ASN:ND2	2.35	0.52
95:fx:139:GLU:O	99:j1:98:TYR:OH	2.27	0.52
98:g3:262:GLU:HA	98:g3:265:ILE:HG23	1.92	0.52
98:g3:278:LEU:HB2	98:g3:281:GLU:HG2	1.92	0.52
100:n1:232:TYR:OH	100:n1:248:GLU:OE2	2.23	0.52
108:qA:203:PHE:HE2	108:qA:306:ALA:HB2	1.74	0.52
110:qC:112:GLN:NE2	110:qC:206:ASP:OD2	2.34	0.52
111:qd:308:SER:N	115:qh:50:ASP:OD2	2.42	0.52
125:s6:106:THR:OG1	125:s6:108:LYS:O	2.28	0.52
127:s8:22:GLN:NE2	142:tf:20:GLN:OE1	2.43	0.52
19:6B:53:PHE:O	19:6B:57:TYR:HB3	2.09	0.52
25:7L:893:LEU:HD11	30:C2:143:ILE:HB	1.92	0.52
29:C1:46:TYR:OH	153:C1:701:CDL:OA3	2.22	0.52
42:M:184:HIS:HD2	42:M:186:ASP:H	1.57	0.52
44:M2:111:LYS:NZ	46:N:22:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N:78:PHE:HA	46:N:151:LYS:HG2	1.92	0.52
52:SA:451:VAL:HG23	52:SA:452:PHE:HD1	1.75	0.52
84:AN:2:GLU:OE2	84:AN:188:LYS:NZ	2.36	0.52
85:B2:102:LEU:HD21	131:T4:88:LYS:HD2	1.91	0.52
86:B3:41:ARG:NH2	91:B9:48:TYR:OH	2.43	0.52
95:FX:27:HIS:HD2	95:FX:29:HIS:H	1.57	0.52
95:FX:66:LEU:HD22	95:FX:145:CYS:HB3	1.92	0.52
104:N5:702:ILE:HG12	106:P1:136:PHE:HE1	1.75	0.52
110:QC:338:ARG:NH2	114:QG:33:GLU:OE2	2.42	0.52
113:QF:38:LYS:NZ	115:QH:123:TYR:OH	2.43	0.52
114:QG:78:ARG:NH2	114:QG:123:TYR:OH	2.42	0.52
109:Qb:71:ASN:OD1	109:Qb:71:ASN:N	2.42	0.52
120:S1:245:GLU:OE2	127:S8:140:LYS:NZ	2.32	0.52
121:S2:135:ALA:HB1	121:S2:147:VAL:HA	1.91	0.52
128:T1:17:THR:O	128:T1:125:SER:N	2.41	0.52
128:T1:36:ARG:HA	128:T1:39:LYS:HZ2	1.74	0.52
132:T5:131:GLY:HA3	153:T5:301:CDL:H631	1.91	0.52
13:2t:41:GLU:OE2	13:2t:45:ARG:NH2	2.43	0.52
153:a:504:CDL:H621	153:a:504:CDL:H581	1.92	0.52
28:bp:193:GLY:O	28:bp:215:GLY:N	2.42	0.52
29:c1:530:MET:HG2	154:c1:708:HEA:C2C	2.40	0.52
31:c3:508:PHE:HB2	152:c3:603:PC1:H321	1.92	0.52
37:h:106:ASN:ND2	6:2I:87:ALA:O	2.42	0.52
37:h:151:PRO:HG3	37:h:233:THR:HG22	1.92	0.52
53:sb:149:ASP:OD2	53:sb:151:SER:OG	2.24	0.52
90:b8:62:PRO:O	91:b9:9:LYS:NZ	2.30	0.52
90:b8:135:ARG:NH2	92:bl:100:ASP:O	2.42	0.52
94:c4:38:MET:HE1	152:c4:403:PC1:H2A2	1.92	0.52
104:n5:419:MET:SD	104:n5:430:HIS:NE2	2.81	0.52
104:n5:419:MET:HE3	104:n5:481:LYS:HE2	1.91	0.52
104:n5:702:ILE:HG12	106:p1:136:PHE:HE1	1.75	0.52
109:qB:96:THR:HG21	109:qB:218:THR:HA	1.90	0.52
112:qe:67:LYS:HG2	114:qg:137:TRP:HZ3	1.75	0.52
120:s1:477:ALA:HB2	120:s1:515:HIS:HA	1.91	0.52
142:tf:127:ASN:OD1	142:tf:129:GLN:NE2	2.42	0.52
145:tx:23:SER:N	145:tx:69:SER:O	2.43	0.52
9:2L:16:ARG:NH1	9:2L:59:GLU:OE2	2.43	0.52
18:6A:1:MET:HG3	153:E:402:CDL:H122	1.91	0.52
18:6A:43:ARG:NH2	59:VB:328:ASP:OD1	2.37	0.52
27:B:29:ARG:NH1	27:B:126:ALA:HA	2.24	0.52
30:C2:209:TYR:HB2	32:D:171:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:574:ARG:NH1	52:SA:576:GLU:OE2	2.38	0.52
77:A7:29:ARG:HB2	77:A7:32:TYR:HB3	1.90	0.52
77:A7:230:ASN:HB3	77:A7:261:GLN:H	1.74	0.52
86:B3:64:GLY:HA3	153:B3:102:CDL:H192	1.92	0.52
99:J1:29:LEU:HD12	99:J1:80:LEU:HD12	1.90	0.52
104:N5:467:ALA:HA	104:N5:490:SER:HA	1.92	0.52
105:N6:24:ILE:O	105:N6:28:THR:OG1	2.24	0.52
109:QB:410:GLU:OE1	109:QB:413:ARG:NH2	2.32	0.52
109:QB:497:ILE:O	109:QB:500:SER:OG	2.19	0.52
109:Qb:71:ASN:ND2	109:Qb:270:VAL:O	2.42	0.52
142:TF:70:LEU:HD21	142:TF:75:LEU:HD13	1.90	0.52
147:V2:184:TYR:OH	147:V2:204:ASP:OD2	2.23	0.52
153:2m:101:CDL:H511	55:sd:4:GLU:HB2	1.91	0.52
13:2t:6:LYS:NZ	30:c2:249:LEU:O	2.41	0.52
34:f:214:TYR:HD1	51:S:161:GLU:HB3	1.75	0.52
36:g:275:ALA:O	36:g:279:GLU:HG2	2.10	0.52
43:m1:76:ALA:HB1	152:m1:403:PC1:H271	1.91	0.52
48:p:110:ASP:O	48:p:115:GLY:N	2.42	0.52
49:q:63:PRO:HG3	153:q:201:CDL:H172	1.92	0.52
52:sa:579:GLY:HA2	52:sa:634:ARG:HH12	1.75	0.52
62:y:4:THR:HG22	62:y:5:ALA:H	1.75	0.52
73:a2:51:VAL:O	73:a2:52:ARG:NH1	2.39	0.52
152:c4:403:PC1:H342	97:g2:11:THR:HG23	1.91	0.52
103:n4:285:LEU:O	103:n4:288:THR:OG1	2.20	0.52
104:n5:69:HIS:CE1	37:H:290:TYR:HE2	2.28	0.52
104:n5:235:TRP:H	104:n5:245:SER:HA	1.75	0.52
106:p1:105:HIS:ND1	106:p1:106:SER:O	2.39	0.52
109:qb:73:VAL:HG13	109:qb:246:PHE:HB3	1.92	0.52
110:qc:33:LEU:HD22	110:qc:230:GLU:HG2	1.92	0.52
121:s2:135:ALA:HB1	121:s2:147:VAL:HA	1.91	0.52
121:s2:253:SER:HB2	121:s2:256:GLU:HB2	1.91	0.52
147:v2:167:LEU:HB2	147:v2:175:MET:HE1	1.92	0.52
7:2J:3:HIS:NE2	7:2J:5:CYS:SG	2.81	0.52
14:3T:72:LYS:HE3	22:6T:41:LEU:HD22	1.92	0.52
25:7L:952:GLU:OE1	60:W:84:LYS:NZ	2.38	0.52
29:C1:291:SER:O	29:C1:295:LEU:HG	2.09	0.52
29:C1:657:GLN:NE2	36:G:105:TYR:OH	2.43	0.52
31:C3:508:PHE:HB2	152:C3:603:PC1:H321	1.92	0.52
40:K:119:LEU:HD21	40:K:150:PHE:HD2	1.75	0.52
43:M1:255:PRO:O	43:M1:259:THR:HG23	2.10	0.52
153:VB:703:CDL:H142	153:VB:703:CDL:H351	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:5B:25:PHE:HE2	104:N5:410:GLY:HA2	1.74	0.52
84:AN:114:LEU:HD11	153:QH:201:CDL:HB62	1.92	0.52
107:P2:72:GLU:OE1	107:P2:80:LYS:NZ	2.41	0.52
111:QD:259:MET:HB3	152:QE:303:PC1:H242	1.92	0.52
111:Qd:40:TYR:HB3	111:Qd:43:LEU:HD21	1.91	0.52
121:S2:204:ASN:O	121:S2:208:ASN:ND2	2.32	0.52
129:T2:164:ILE:HG12	129:T2:180:ILE:HG13	1.92	0.52
147:V2:27:LEU:HG	147:V2:29:ALA:H	1.75	0.52
147:V2:167:LEU:HD12	147:V2:175:MET:HE1	1.90	0.52
28:bp:214:CYS:O	28:bp:263:THR:OG1	2.28	0.52
153:c1:709:CDL:H752	31:c3:318:VAL:HG12	1.91	0.52
32:d:238:ASN:HB3	32:d:346:GLU:HA	1.92	0.52
52:sa:239:TYR:HE2	52:sa:464:LEU:HB2	1.74	0.52
153:a1:101:CDL:H162	140:td:16:PHE:HA	1.90	0.52
86:b3:64:GLY:HA3	153:b3:102:CDL:H192	1.92	0.52
95:fx:66:LEU:HD22	95:fx:145:CYS:HB3	1.91	0.52
96:g1:220:TYR:OH	97:g2:27:ASP:OD2	2.17	0.52
110:qC:60:PRO:HB3	110:qC:265:ILE:HD11	1.91	0.52
110:qC:345:LYS:O	110:qC:347:HIS:ND1	2.41	0.52
110:qc:418:PHE:HZ	114:qg:86:LEU:HD13	1.73	0.52
111:qd:40:TYR:HB3	111:qd:43:LEU:HD21	1.92	0.52
128:t1:36:ARG:HA	128:t1:39:LYS:HZ2	1.75	0.52
147:v2:27:LEU:HG	147:v2:29:ALA:H	1.75	0.52
2:2E:218:PHE:HB2	2:2E:223:ILE:HG13	1.92	0.52
11:2N:28:TYR:HA	11:2N:31:VAL:HG12	1.92	0.52
26:A:95:LEU:HD11	59:VB:207:GLU:HB2	1.91	0.52
29:C1:385:LEU:HD23	152:C1:709:PC1:H262	1.92	0.52
30:C2:507:THR:OG1	30:C2:527:CYS:SG	2.61	0.52
31:C3:501:TYR:CD1	31:C3:502:PRO:HD3	2.44	0.52
153:SD:101:CDL:H362	153:SD:101:CDL:H161	1.92	0.52
76:A6:160:LEU:HD11	120:S1:619:ALA:HA	1.91	0.52
77:A7:42:ARG:NH1	127:S8:233:ASN:O	2.41	0.52
87:B4:91:TRP:O	87:B4:99:ASN:ND2	2.35	0.52
94:C4:38:MET:HE1	152:C4:403:PC1:H2A2	1.90	0.52
96:G1:203:LEU:O	96:G1:207:GLN:HG2	2.10	0.52
101:N2:113:THR:HG23	101:N2:279:LEU:HD11	1.92	0.52
103:N4:159:VAL:HG11	103:N4:284:PHE:HZ	1.73	0.52
108:QA:203:PHE:HE2	108:QA:306:ALA:HB2	1.74	0.52
110:Qc:46:LEU:HD11	110:Qc:193:ALA:HB2	1.91	0.52
114:Qg:41:VAL:O	114:Qg:45:ASN:ND2	2.33	0.52
114:Qg:54:VAL:HG22	114:Qg:57:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
120:S1:266:THR:HG22	120:S1:271:ILE:HA	1.92	0.52
129:T2:203:PHE:HB2	129:T2:210:TYR:HB2	1.90	0.52
153:7a:201:CDL:H801	46:n:126:GLY:HA2	1.92	0.52
153:7a:203:CDL:H121	153:7a:203:CDL:H342	1.92	0.52
29:c1:657:GLN:NE2	36:g:105:TYR:OH	2.43	0.52
31:c3:15:ILE:HD13	31:c3:133:VAL:HB	1.92	0.52
31:c3:192:LEU:HD11	153:c3:604:CDL:H202	1.91	0.52
31:c3:380:LYS:HA	59:vb:97:TYR:HB3	1.91	0.52
43:m1:255:PRO:O	43:m1:259:THR:HG23	2.10	0.52
152:n:301:PC1:H292	152:n:301:PC1:H362	1.91	0.52
51:s:43:LYS:HD2	59:vb:500:TYR:CG	2.45	0.52
62:y:64:LEU:HD12	62:y:92:VAL:HG11	1.92	0.52
74:a3:116:ARG:HG3	137:ta:127:LEU:HD23	1.92	0.52
76:a6:19:ASN:OD1	99:j1:215:ASN:ND2	2.42	0.52
95:fx:27:HIS:HD2	95:fx:29:HIS:H	1.57	0.52
99:j1:127:LYS:O	99:j1:130:THR:OG1	2.26	0.52
114:qG:273:ASN:HB3	114:qG:275:ARG:HH21	1.75	0.52
108:qa:173:GLU:O	108:qa:240:GLN:NE2	2.43	0.52
110:qc:208:LYS:NZ	166:qc:503:HEM:O2D	2.43	0.52
121:s2:140:ASP:HB3	121:s2:427:VAL:HG12	1.92	0.52
146:v1:78:ASP:OD2	147:v2:247:TRP:NE1	2.42	0.52
4:2G:197:PHE:HB3	52:SA:204:ILE:HD12	1.92	0.52
153:7A:203:CDL:H121	153:7A:203:CDL:H342	1.92	0.52
25:7L:873:PRO:HB3	57:U:55:ASP:HB3	1.91	0.52
152:C1:709:PC1:H291	31:C3:326:VAL:HG13	1.90	0.52
30:C2:197:PRO:HD2	45:M3:39:GLY:HA2	1.90	0.52
39:J:177:ASP:OD1	39:J:178:ALA:N	2.41	0.52
59:VB:487:ALA:O	59:VB:491:ASN:ND2	2.42	0.52
71:5B:90:PHE:HA	101:N2:250:LEU:HD21	1.90	0.52
152:5B:202:PC1:H2B1	103:N4:208:LEU:HD21	1.92	0.52
76:A6:19:ASN:OD1	99:J1:215:ASN:ND2	2.43	0.52
77:A7:129:ILE:HG23	122:S3:24:ILE:HD13	1.91	0.52
78:A8:228:VAL:HG13	100:N1:112:PRO:HD2	1.92	0.52
95:FX:132:ARG:NH2	101:N2:332:ASP:OD2	2.42	0.52
103:N4:155:PHE:CZ	103:N4:181:PRO:HB2	2.45	0.52
105:N6:214:GLN:HG2	121:S2:11:PRO:HG2	1.91	0.52
109:QB:96:THR:HG21	109:QB:218:THR:HA	1.91	0.52
111:Qd:309:ARG:NH1	111:Qd:312:GLN:OE1	2.43	0.52
128:T1:383:TYR:HD1	128:T1:386:ILE:HD11	1.75	0.52
3:2f:209:TYR:HB2	53:sb:40:ILE:HG21	1.92	0.52
4:2g:108:ILE:HG23	4:2g:132:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2k:80:ILE:HB	10:2m:61:ARG:NH1	2.24	0.52
14:3t:72:LYS:HE3	22:6t:41:LEU:HD22	1.92	0.52
153:6c:202:CDL:H192	34:f:182:ILE:HG21	1.91	0.52
24:7c:142:SER:O	24:7c:145:LEU:HB3	2.10	0.52
152:a:501:PC1:O32	31:c3:455:TRP:NE1	2.28	0.52
27:b:89:ARG:HH21	59:vb:581:GLU:CD	2.17	0.52
32:d:193:ARG:HB2	39:j:217:LEU:HB3	1.92	0.52
65:y7:359:ALA:HB1	65:y7:364:PHE:HB2	1.92	0.52
87:b4:60:LEU:HD11	93:bm:129:MET:HE1	1.92	0.52
101:n2:129:PHE:O	101:n2:133:ASN:ND2	2.41	0.52
103:n4:155:PHE:CZ	103:n4:181:PRO:HB2	2.45	0.52
114:qG:112:VAL:HG22	114:qG:116:LYS:HE2	1.91	0.52
129:t2:22:LEU:HB3	129:t2:254:LEU:HD13	1.90	0.52
13:2T:41:GLU:OE2	13:2T:45:ARG:NH2	2.43	0.52
24:7C:205:ASP:OD2	37:H:127:ARG:NH2	2.43	0.52
27:B:29:ARG:NH2	27:B:129:ALA:HB3	2.25	0.52
27:B:89:ARG:HH21	59:VB:581:GLU:CD	2.17	0.52
32:D:312:ARG:O	32:D:321:ASN:ND2	2.40	0.52
158:M3:402:3PE:H2D1	153:VB:701:CDL:H821	1.90	0.52
46:N:191:ASN:OD1	46:N:191:ASN:N	2.38	0.52
57:U:97:TRP:CG	153:U:201:CDL:H512	2.45	0.52
60:W:35:LEU:HD13	153:W:202:CDL:H111	1.91	0.52
83:AM:49:LYS:NZ	152:S8:301:PC1:O14	2.43	0.52
83:AM:163:LEU:HD13	100:N1:17:LEU:HD12	1.91	0.52
87:B4:37:PRO:HG2	152:B9:201:PC1:H241	1.92	0.52
104:N5:419:MET:HE3	104:N5:481:LYS:HE2	1.90	0.52
152:N6:301:PC1:H261	152:TC:101:PC1:H232	1.92	0.52
153:QC:504:CDL:HB4	153:QC:504:CDL:H121	1.91	0.52
110:Qc:33:LEU:HD22	110:Qc:230:GLU:HG2	1.92	0.52
121:S2:253:SER:HB2	121:S2:256:GLU:HB2	1.90	0.52
147:V2:223:THR:HG22	147:V2:224:LEU:HG	1.92	0.52
2:2e:92:SER:OG	2:2e:95:ASN:OD1	2.29	0.51
8:2k:86:ARG:HH12	10:2m:52:GLN:HG3	1.73	0.51
25:7l:893:LEU:HD11	30:c2:143:ILE:HB	1.93	0.51
30:c2:209:TYR:HB2	32:d:171:ARG:HD2	1.92	0.51
30:c2:477:GLY:HA3	37:h:181:TRP:CE2	2.45	0.51
30:c2:478:GLU:HG3	30:c2:479:LEU:HG	1.92	0.51
32:d:321:ASN:OD1	39:j:210:GLN:NE2	2.43	0.51
153:m2:404:CDL:H351	153:m2:404:CDL:H132	1.92	0.51
53:sb:266:ASP:OD1	53:sb:267:VAL:N	2.43	0.51
57:u:97:TRP:CG	153:u:201:CDL:H512	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:b2:102:LEU:HD21	131:t4:88:LYS:HD2	1.91	0.51
101:n2:260:LEU:HB3	101:n2:288:TYR:HE1	1.75	0.51
104:n5:559:MET:HE2	104:n5:609:LEU:HD23	1.91	0.51
153:qC:504:CDL:HB4	153:qC:504:CDL:H121	1.91	0.51
114:qg:192:LEU:O	114:qg:198:TRP:NE1	2.41	0.51
127:s8:176:ILE:HG12	162:s8:302:SF4:S1	2.51	0.51
142:tf:70:LEU:HD21	142:tf:75:LEU:HD13	1.90	0.51
3:2F:103:ARG:HH21	5:2H:126:THR:HG21	1.75	0.51
4:2G:55:PHE:HA	7:2J:34:HIS:CE1	2.45	0.51
25:7L:954:GLU:OE1	25:7L:957:ARG:NH1	2.43	0.51
29:C1:681:VAL:HG21	34:F:114:GLU:HG3	1.92	0.51
30:C2:417:ARG:NH1	30:C2:559:HIS:O	2.42	0.51
31:C3:380:LYS:HA	59:VB:97:TYR:HB3	1.91	0.51
35:FS:102:GLY:HA2	35:FS:140:LYS:HE3	1.92	0.51
43:M1:306:TRP:NE1	153:M1:405:CDL:OA9	2.32	0.51
52:SA:284:HIS:HB2	52:SA:395:HIS:HB2	1.91	0.51
52:SA:574:ARG:NH2	52:SA:596:LYS:O	2.44	0.51
58:V:78:GLU:OE2	58:V:84:ASN:ND2	2.39	0.51
77:A7:31:ARG:NE	121:S2:159:GLU:OE2	2.37	0.51
153:A9:403:CDL:OB4	126:S7:2:ARG:N	2.42	0.51
101:N2:34:LEU:HD13	101:N2:52:ILE:HD13	1.91	0.51
104:N5:338:LYS:HB2	158:N5:802:3PE:H12	1.92	0.51
110:QC:38:THR:HG21	166:QC:502:HEM:HAB	1.91	0.51
110:QC:60:PRO:HB3	110:QC:265:ILE:HD11	1.91	0.51
110:QC:329:VAL:HG23	110:QC:333:SER:HB3	1.91	0.51
135:T8:75:HIS:HB3	135:T8:82:LEU:HD11	1.93	0.51
145:TX:55:ASN:ND2	145:TX:98:PRO:HD3	2.24	0.51
4:2g:119:SER:HB3	152:2g:202:PC1:H31	1.91	0.51
5:2h:133:GLU:HB3	5:2h:136:LYS:HZ2	1.76	0.51
27:b:314:LEU:HD21	27:b:332:PRO:HD3	1.92	0.51
28:bp:141:ASN:HB2	28:bp:192:TYR:HB2	1.92	0.51
31:c3:516:TYR:OH	42:m:121:TYR:O	2.25	0.51
42:m:86:THR:H	59:vb:216:HIS:CE1	2.27	0.51
42:m:190:ALA:O	62:y:1:MET:N	2.42	0.51
153:sd:101:CDL:H362	153:sd:101:CDL:H161	1.92	0.51
57:u:10:ASP:OD1	57:u:121:ARG:NH2	2.44	0.51
59:vb:565:TRP:NE1	59:vb:578:ASP:OD2	2.30	0.51
70:4l:55:THR:O	70:4l:58:SER:OG	2.22	0.51
85:b2:67:PRO:HG3	152:t4:301:PC1:H112	1.90	0.51
96:g1:142:GLN:HG2	97:g2:137:VAL:HG11	1.92	0.51
109:qb:185:VAL:HG12	109:qb:225:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:qb:317:ASP:OD2	109:qb:469:ARG:NH2	2.37	0.51
124:s5:26:ALA:HA	124:s5:32:PRO:HB3	1.93	0.51
124:s5:74:TYR:OH	124:s5:79:ASP:OD1	2.24	0.51
129:t2:273:GLN:O	129:t2:276:ARG:HG2	2.10	0.51
130:t3:253:ASP:OD1	130:t3:273:ARG:NH1	2.43	0.51
135:t8:75:HIS:HB3	135:t8:82:LEU:HD11	1.92	0.51
140:td:66:GLN:OE1	140:td:73:GLN:NE2	2.43	0.51
29:C1:517:MET:HE1	29:C1:583:PHE:HA	1.92	0.51
52:SA:274:PRO:HG2	52:SA:402:PRO:HG3	1.91	0.51
59:VB:497:HIS:ND1	65:Y7:189:TYR:OH	2.31	0.51
72:A1:47:ARG:HH12	78:A8:187:ASN:HD22	1.56	0.51
103:N4:159:VAL:HG21	103:N4:284:PHE:CE2	2.45	0.51
107:P2:123:TYR:HB2	107:P2:143:ILE:HG21	1.90	0.51
114:Qg:133:TYR:OH	115:Qh:94:ARG:NE	2.41	0.51
120:S1:50:ILE:HG23	120:S1:103:ILE:HD13	1.92	0.51
120:S1:350:GLU:HG2	120:S1:633:LEU:HD11	1.93	0.51
120:S1:359:LEU:HB3	120:S1:364:VAL:HB	1.91	0.51
121:S2:233:ASP:O	122:S3:131:ASN:ND2	2.44	0.51
140:TD:66:GLN:OE1	140:TD:73:GLN:NE2	2.43	0.51
145:TX:23:SER:N	145:TX:69:SER:O	2.43	0.51
153:7a:201:CDL:OA4	65:y7:358:ARG:NH1	2.41	0.51
25:7l:954:GLU:OE1	25:7l:957:ARG:NH1	2.44	0.51
26:a:408:VAL:O	26:a:414:GLN:NE2	2.41	0.51
32:d:312:ARG:O	32:d:321:ASN:ND2	2.38	0.51
152:d:501:PC1:H251	152:d:501:PC1:H371	1.91	0.51
42:m:72:TYR:OH	42:m:91:ARG:NH1	2.41	0.51
52:sa:155:ILE:HG21	52:sa:177:ALA:HB1	1.92	0.51
59:vb:408:LEU:HD22	59:vb:448:ALA:HB2	1.90	0.51
60:w:55:THR:HG23	62:y:105:PHE:HE1	1.75	0.51
95:fx:76:GLY:O	95:fx:163:ASN:ND2	2.32	0.51
108:qA:172:LEU:HD12	108:qA:270:LEU:HD22	1.91	0.51
109:qB:343:THR:OG1	109:qB:346:ARG:NH1	2.36	0.51
109:qB:362:THR:HG21	115:qh:6:ALA:HB3	1.93	0.51
120:s1:350:GLU:HG2	120:s1:633:LEU:HD11	1.92	0.51
135:t8:49:VAL:HG22	158:t8:602:3PE:H271	1.92	0.51
20:6C:92:GLU:OE2	21:6L:66:ARG:NH2	2.38	0.51
23:7A:39:ARG:HD3	26:A:428:GLN:NE2	2.25	0.51
24:7C:142:SER:O	24:7C:145:LEU:HB3	2.10	0.51
31:C3:525:GLU:HB2	153:T:202:CDL:H721	1.92	0.51
153:F:402:CDL:H152	153:F:402:CDL:H332	1.93	0.51
42:M:143:ARG:HH22	42:M:186:ASP:CG	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Q:63:PRO:HG3	153:Q:201:CDL:H172	1.92	0.51
49:Q:118:ASN:OD1	67:Z1:10:ASN:ND2	2.43	0.51
62:Y:4:THR:HG22	62:Y:5:ALA:H	1.75	0.51
153:A1:102:CDL:H111	153:A1:102:CDL:HB62	1.93	0.51
74:A3:79:TRP:CH2	148:X1:44:VAL:HG11	2.45	0.51
106:P1:105:HIS:ND1	106:P1:106:SER:O	2.39	0.51
108:QA:417:LEU:O	108:QA:421:VAL:HG13	2.11	0.51
109:Qb:113:LEU:HA	109:Qb:116:ARG:HG2	1.92	0.51
110:Qc:79:ASP:N	110:Qc:79:ASP:OD1	2.43	0.51
112:Qe:67:LYS:HG2	114:Qg:137:TRP:HZ3	1.74	0.51
120:S1:676:THR:HG1	129:T2:175:TYR:HH	1.58	0.51
130:T3:253:ASP:OD1	130:T3:273:ARG:NH1	2.43	0.51
142:TF:104:TYR:HA	142:TF:107:ARG:HH11	1.75	0.51
143:TG:103:LYS:HD3	143:TG:105:LEU:HD23	1.92	0.51
3:2f:103:ARG:HH21	5:2h:126:THR:HG21	1.75	0.51
27:b:20:GLN:HB3	27:b:87:ARG:HH21	1.74	0.51
38:i:55:LEU:HG	38:i:98:PHE:HD1	1.75	0.51
43:m1:243:GLY:HA3	153:m1:404:CDL:H671	1.92	0.51
51:s:80:VAL:HG12	51:s:81:THR:HG23	1.93	0.51
57:u:96:PHE:HB2	153:u:201:CDL:HA4	1.92	0.51
84:an:114:LEU:HD11	153:qH:201:CDL:HB62	1.91	0.51
106:p1:56:LEU:HD23	107:p2:68:PRO:HB3	1.91	0.51
153:qC:504:CDL:OB7	115:qH:96:ASN:ND2	2.43	0.51
115:qH:17:ASP:O	111:qd:314:ARG:NH2	2.44	0.51
120:s1:609:ASP:O	120:s1:611:ARG:NH1	2.42	0.51
124:s5:74:TYR:HE2	124:s5:76:GLU:HG2	1.74	0.51
142:tf:104:TYR:HA	142:tf:107:ARG:HH11	1.74	0.51
2:2E:92:SER:OG	2:2E:95:ASN:OD1	2.29	0.51
13:2T:29:LEU:HD22	16:4T:16:VAL:HG12	1.93	0.51
152:A:503:PC1:H11	31:C3:403:TRP:CD1	2.46	0.51
27:B:20:GLN:HB3	27:B:87:ARG:HH21	1.75	0.51
29:C1:286:TYR:CE1	30:C2:511:ASP:HB2	2.46	0.51
36:G:275:ALA:O	36:G:279:GLU:HG2	2.10	0.51
37:H:257:GLU:OE1	37:H:257:GLU:N	2.31	0.51
51:S:43:LYS:HD2	59:VB:500:TYR:CG	2.45	0.51
153:VB:705:CDL:HB61	153:VB:705:CDL:H131	1.91	0.51
64:Y5:187:ARG:NH2	65:Y7:270:SER:OG	2.38	0.51
105:N6:234:ARG:NE	121:S2:419:LYS:O	2.39	0.51
106:P1:105:HIS:HE1	130:T3:207:ILE:HG13	1.76	0.51
110:QC:223:PHE:O	110:QC:227:LEU:HB3	2.09	0.51
153:QH:201:CDL:H142	153:QH:201:CDL:H322	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:Qc:135:VAL:HG21	110:Qc:181:LEU:HD13	1.92	0.51
110:Qc:208:LYS:NZ	166:Qc:503:HEM:O2D	2.42	0.51
114:Qg:95:ARG:NH1	115:Qh:50:ASP:O	2.42	0.51
121:S2:138:ALA:HB1	121:S2:143:SER:HB2	1.92	0.51
127:S8:64:ARG:NH2	137:TA:41:LYS:O	2.43	0.51
142:TF:177:GLU:HG2	142:TF:209:LEU:HD22	1.92	0.51
13:2t:8:GLN:HA	30:c2:218:ILE:HG21	1.93	0.51
23:7a:39:ARG:HD3	26:a:428:GLN:NE2	2.26	0.51
31:c3:164:ASN:OD1	31:c3:172:ARG:NH2	2.44	0.51
40:k:30:GLN:N	40:k:46:TYR:OH	2.40	0.51
42:m:24:LEU:HD12	153:m:302:CDL:H711	1.93	0.51
49:q:118:ASN:OD1	67:z1:10:ASN:ND2	2.43	0.51
52:sa:445:SER:O	52:sa:449:ILE:HG23	2.11	0.51
60:w:17:LEU:HD13	158:w:203:3PE:H11	1.93	0.51
68:1b:31:GLN:NE2	121:s2:218:GLN:O	2.42	0.51
95:fx:27:HIS:CD2	95:fx:29:HIS:H	2.28	0.51
98:g3:250:MET:HB3	98:g3:255:PHE:HB2	1.93	0.51
100:n1:239:PHE:HD2	139:tc:2:VAL:HG22	1.76	0.51
104:n5:566:PRO:HG2	153:n5:806:CDL:H221	1.93	0.51
104:n5:636:LYS:HB3	106:p1:32:ILE:HB	1.92	0.51
106:p1:105:HIS:HE1	130:t3:207:ILE:HG13	1.76	0.51
152:qE:304:PC1:H2	117:qJ:39:ALA:HB1	1.93	0.51
109:qb:42:ARG:NH2	109:qb:54:ILE:O	2.37	0.51
148:x1:2:SER:HB2	148:x1:148:ILE:HA	1.92	0.51
2:2E:48:LYS:NZ	2:2E:60:GLU:OE2	2.43	0.51
14:3T:73:VAL:HG11	22:6T:10:ALA:HA	1.93	0.51
16:4T:7:GLN:HG3	30:C2:255:SER:HB3	1.91	0.51
32:D:238:ASN:HB3	32:D:346:GLU:HA	1.92	0.51
42:M:111:VAL:HG12	153:W:202:CDL:H661	1.93	0.51
60:W:38:ARG:NH2	153:W:202:CDL:OA3	2.38	0.51
69:2B:64:TYR:HA	69:2B:67:ILE:HG12	1.92	0.51
79:A9:75:HIS:ND1	167:A9:401:NDP:O1X	2.38	0.51
152:C4:403:PC1:H342	97:G2:11:THR:HG23	1.93	0.51
120:S1:214:THR:OG1	120:S1:708:GLU:OE1	2.26	0.51
120:S1:493:LYS:HE3	120:S1:663:LEU:HA	1.93	0.51
126:S7:68:THR:HA	126:S7:96:CYS:HB3	1.92	0.51
4:2g:55:PHE:HA	7:2j:34:HIS:CE1	2.45	0.51
16:4t:7:GLN:HG3	30:c2:255:SER:HB3	1.91	0.51
153:7c:302:CDL:H342	29:c1:36:LEU:HD23	1.93	0.51
30:c2:57:ARG:HE	58:v:91:ASN:HB3	1.76	0.51
152:c3:605:PC1:H321	59:vb:237:TYR:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:119:LEU:HD21	40:k:150:PHE:HD2	1.76	0.51
45:m3:97:ALA:HB2	45:m3:253:THR:HG22	1.93	0.51
51:s:161:GLU:HB3	34:F:214:TYR:HD1	1.76	0.51
64:y5:19:PRO:HB2	64:y5:22:PHE:H	1.74	0.51
71:5b:43:PHE:O	71:5b:47:LYS:HB2	2.11	0.51
152:5b:202:PC1:H2B1	103:n4:208:LEU:HD21	1.93	0.51
158:a3:201:3PE:H252	101:n2:28:PHE:HB3	1.93	0.51
153:a9:402:CDL:H582	153:a9:402:CDL:H741	1.92	0.51
90:b8:157:LYS:HA	90:b8:161:ARG:HD2	1.93	0.51
153:b8:302:CDL:H111	153:b8:302:CDL:HB4	1.93	0.51
126:s7:131:GLU:OE2	127:s8:114:GLY:N	2.35	0.51
147:v2:198:ASP:O	147:v2:202:GLY:N	2.44	0.51
14:3T:39:ARG:NH2	14:3T:51:GLU:OE2	2.34	0.51
15:4A:62:PRO:HG2	36:G:317:ARG:HH21	1.76	0.51
28:BP:140:GLN:NE2	28:BP:175:GLU:O	2.43	0.51
30:C2:63:MET:HE1	58:V:88:PRO:HD3	1.91	0.51
33:E:201:LEU:O	153:E:401:CDL:O1	2.27	0.51
152:FS:201:PC1:H361	152:FS:201:PC1:H241	1.92	0.51
38:I:55:LEU:HG	38:I:98:PHE:HD1	1.75	0.51
38:I:105:PHE:O	38:I:124:ASN:ND2	2.41	0.51
53:SB:264:ALA:O	53:SB:303:ARG:NH2	2.44	0.51
62:Y:64:LEU:HD12	62:Y:92:VAL:HG11	1.92	0.51
64:Y5:188:ILE:HG22	64:Y5:190:TYR:H	1.76	0.51
75:A5:57:THR:HG23	75:A5:58:LYS:HG3	1.92	0.51
75:A5:157:ARG:NH2	98:G3:279:GLU:OE1	2.43	0.51
82:AL:15:LYS:HG3	82:AL:50:TYR:HB3	1.92	0.51
103:N4:428:TYR:OH	103:N4:505:PHE:O	2.24	0.51
104:N5:345:LEU:HD22	158:N5:802:3PE:H391	1.91	0.51
108:QA:96:ASP:OD1	108:QA:425:ARG:NH1	2.43	0.51
109:QB:73:VAL:HG22	109:QB:246:PHE:HB2	1.93	0.51
152:QB:602:PC1:H332	153:Qg:402:CDL:H472	1.93	0.51
110:Qc:332:VAL:HA	110:Qc:335:PHE:HD2	1.76	0.51
120:S1:383:ALA:HB2	120:S1:656:THR:HG21	1.93	0.51
28:bp:203:ASP:O	28:bp:207:ASN:N	2.41	0.51
33:e:177:VAL:O	33:e:180:SER:OG	2.26	0.51
36:g:88:THR:OG1	36:g:89:MET:N	2.44	0.51
153:q:203:CDL:H142	153:q:203:CDL:H351	1.92	0.51
51:s:8:PHE:CE2	59:vb:367:TYR:HB3	2.46	0.51
61:x:117:HIS:ND1	61:x:118:CYS:O	2.40	0.51
77:a7:31:ARG:NE	121:s2:159:GLU:OE2	2.36	0.51
78:a8:228:VAL:HG13	100:n1:112:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
96:g1:203:LEU:O	96:g1:207:GLN:HG2	2.10	0.51
100:n1:279:ASN:HB3	134:t7:107:ASN:ND2	2.26	0.51
113:qF:38:LYS:NZ	115:qH:123:TYR:OH	2.43	0.51
110:qc:36:PHE:CD1	110:qc:230:GLU:HB3	2.46	0.51
121:s2:151:PHE:HB3	126:s7:41:VAL:HG21	1.93	0.51
126:s7:159:ASP:OD1	128:t1:137:LYS:NZ	2.37	0.51
128:t1:399:PHE:O	128:t1:402:GLN:NE2	2.44	0.51
136:t9:94:ILE:HG22	136:t9:126:ASP:HB3	1.91	0.51
4:2G:19:LEU:HD13	4:2G:53:LEU:HA	1.93	0.51
7:2J:25:ASN:HA	7:2J:30:LYS:HB2	1.93	0.51
30:C2:477:GLY:HA3	37:H:181:TRP:CE2	2.45	0.51
33:E:129:SER:HB3	33:E:190:PRO:HB3	1.93	0.51
46:N:86:ILE:HD12	153:N:304:CDL:H231	1.93	0.51
59:VB:113:HIS:NE2	59:VB:125:ASP:OD1	2.44	0.51
71:5B:43:PHE:O	71:5B:47:LYS:HB2	2.11	0.51
87:B4:60:LEU:HD11	93:BM:129:MET:HE1	1.93	0.51
101:N2:260:LEU:HB3	101:N2:288:TYR:HE1	1.76	0.51
110:QC:207:TRP:NE1	166:QC:502:HEM:O2A	2.32	0.51
152:Qb:602:PC1:H2C1	112:Qe:107:ALA:HB2	1.93	0.51
120:S1:525:GLU:HG3	120:S1:591:VAL:HG21	1.93	0.51
126:S7:32:CYS:HB3	126:S7:66:ALA:HB1	1.93	0.51
3:2f:137:ARG:HD3	152:2f:301:PC1:H341	1.93	0.51
18:6a:1:MET:HG3	153:e:402:CDL:H122	1.91	0.51
26:a:477:ILE:HG21	36:g:51:VAL:HG21	1.93	0.51
27:b:29:ARG:NH2	27:b:129:ALA:HB3	2.25	0.51
29:c1:92:LEU:HD11	29:c1:267:ARG:HA	1.93	0.51
33:e:194:LEU:HD22	153:e:401:CDL:H212	1.92	0.51
38:i:31:GLY:O	50:r:151:LYS:HG2	2.11	0.51
44:m2:32:TYR:CD2	44:m2:82:PHE:HB2	2.46	0.51
44:m2:273:GLU:OE1	44:m2:273:GLU:N	2.43	0.51
49:q:4:ASN:O	49:q:10:ASN:ND2	2.41	0.51
69:2b:64:TYR:HA	69:2b:67:ILE:HG12	1.92	0.51
103:n4:399:ILE:HG13	103:n4:475:LEU:HD13	1.91	0.51
109:qb:386:ILE:HD13	115:qh:38:TYR:HE1	1.76	0.51
120:s1:151:ILE:HD12	121:s2:344:LEU:HD13	1.91	0.51
56:T:104:GLN:HB2	56:T:107:GLN:HB2	1.93	0.51
57:U:96:PHE:HB2	153:U:201:CDL:HA4	1.92	0.51
64:Y5:19:PRO:HB2	64:Y5:22:PHE:H	1.74	0.51
76:A6:38:GLU:O	122:S3:154:ARG:NH2	2.44	0.51
82:AL:191:SER:O	129:T2:125:ASN:ND2	2.44	0.51
83:AM:140:PHE:HD1	124:S5:49:ARG:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:B4:39:VAL:HG13	90:B8:44:LYS:HB3	1.93	0.51
99:J1:270:LEU:HD11	124:S5:66:ILE:HG23	1.93	0.51
100:N1:74:LEU:HG	100:N1:242:ALA:HB2	1.93	0.51
104:N5:636:LYS:HB3	106:P1:32:ILE:HB	1.93	0.51
121:S2:88:VAL:HG12	121:S2:129:ASN:HA	1.93	0.51
121:S2:131:LEU:HD11	121:S2:199:PHE:HE1	1.75	0.51
127:S8:22:GLN:NE2	142:TF:20:GLN:OE1	2.42	0.51
135:T8:49:VAL:HG22	158:T8:602:3PE:H271	1.93	0.51
5:2h:109:GLY:O	5:2h:113:CYS:N	2.38	0.51
14:3t:73:VAL:HG11	22:6t:10:ALA:HA	1.93	0.51
27:b:29:ARG:NH1	27:b:126:ALA:HA	2.25	0.51
29:c1:286:TYR:CE1	30:c2:511:ASP:HB2	2.46	0.51
29:c1:521:PHE:HA	29:c1:524:VAL:HB	1.93	0.51
30:c2:12:GLN:OE1	30:c2:546:TYR:OH	2.29	0.51
31:c3:106:VAL:HG13	45:m3:247:PRO:HG2	1.93	0.51
35:fs:145:ALA:HB3	35:fs:146:PRO:HD3	1.92	0.51
41:l:134:LEU:HG	41:l:136:VAL:HG23	1.93	0.51
52:sa:273:LEU:HD21	52:sa:421:VAL:HG21	1.92	0.51
59:vb:113:HIS:HE1	59:vb:128:VAL:HG21	1.75	0.51
67:z1:40:TYR:HB2	153:u1:101:CDL:H382	1.93	0.51
153:a1:101:CDL:HB62	153:a1:101:CDL:H111	1.93	0.51
73:a2:62:ILE:HG12	73:a2:72:LYS:HB3	1.93	0.51
79:a9:213:ILE:HD13	79:a9:349:VAL:HG11	1.93	0.51
87:b4:37:PRO:HG2	152:b9:201:PC1:H241	1.93	0.51
95:fx:78:VAL:HB	95:fx:106:SER:HB3	1.93	0.51
103:n4:397:LEU:HD21	152:n5:801:PC1:H221	1.93	0.51
111:qD:259:MET:HB3	152:qE:303:PC1:H242	1.93	0.51
113:qF:87:GLY:HA2	116:qI:95:HIS:CE1	2.46	0.51
109:qb:299:MET:HB2	109:qb:483:PRO:HD3	1.93	0.51
152:qb:602:PC1:H12	112:qe:100:TYR:CE2	2.46	0.51
121:s2:233:ASP:O	122:s3:131:ASN:ND2	2.43	0.51
122:s3:172:GLN:OE1	123:s4:132:ARG:NH1	2.43	0.51
127:s8:64:ARG:NH2	137:ta:41:LYS:O	2.44	0.51
3:2F:209:TYR:HB2	53:SB:40:ILE:HG21	1.92	0.51
8:2K:51:ASN:ND2	54:SC:44:TYR:OH	2.43	0.51
19:6B:198:ALA:HB2	30:C2:354:PRO:HD2	1.92	0.51
24:7C:120:SEP:O	26:A:246:ASN:ND2	2.44	0.51
29:C1:100:ALA:HB2	29:C1:155:ILE:HG12	1.92	0.51
31:C3:15:ILE:HD13	31:C3:133:VAL:HB	1.91	0.51
31:C3:162:LEU:HG	31:C3:166:LYS:HE3	1.93	0.51
35:FS:145:ALA:HB3	35:FS:146:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:H:151:PRO:HG3	37:H:233:THR:HG22	1.93	0.51
44:M2:32:TYR:CD2	44:M2:82:PHE:HB2	2.46	0.51
53:SB:138:HIS:O	53:SB:281:THR:OG1	2.28	0.51
59:VB:181:ARG:O	59:VB:186:GLN:NE2	2.44	0.51
153:B8:302:CDL:H111	153:B8:302:CDL:HB4	1.93	0.51
95:FX:27:HIS:CD2	95:FX:29:HIS:H	2.28	0.51
95:FX:139:GLU:O	99:J1:98:TYR:OH	2.27	0.51
115:QH:17:ASP:O	111:Qd:314:ARG:NH2	2.44	0.51
109:Qb:185:VAL:HG12	109:Qb:225:LEU:HD13	1.92	0.51
115:Qh:23:ARG:HB3	115:Qh:29:ILE:HG12	1.92	0.51
121:S2:140:ASP:HB3	121:S2:427:VAL:HG12	1.93	0.51
122:S3:87:ASN:O	122:S3:91:LYS:HG2	2.11	0.51
134:T7:124:ASP:OD1	134:T7:124:ASP:N	2.43	0.51
147:V2:130:CYS:HA	147:V2:173:ALA:HB1	1.93	0.51
4:2g:100:GLU:HB3	8:2k:22:LEU:HD21	1.93	0.51
15:4a:62:PRO:HG2	36:g:317:ARG:HH21	1.75	0.51
153:6c:202:CDL:H552	58:v:111:GLN:HB3	1.93	0.51
153:a:505:CDL:HB61	153:a:505:CDL:H131	1.91	0.51
34:f:106:LEU:HD12	43:m1:260:ARG:HG3	1.93	0.51
39:j:108:GLN:O	39:j:112:LYS:NZ	2.44	0.51
42:m:143:ARG:HH22	42:m:186:ASP:CG	2.19	0.51
42:m:184:HIS:HD2	42:m:186:ASP:H	1.59	0.51
43:m1:62:LEU:O	43:m1:65:THR:OG1	2.24	0.51
43:m1:258:VAL:O	43:m1:262:MET:HG3	2.11	0.51
50:r:76:THR:HG22	50:r:109:LEU:HB3	1.92	0.51
62:y:16:TYR:OH	62:y:38:ASP:OD1	2.21	0.51
70:4l:17:ILE:HG12	71:5b:83:LEU:HD11	1.93	0.51
99:j1:268:GLU:HA	152:te:102:PC1:H252	1.93	0.51
103:n4:159:VAL:HG21	103:n4:284:PHE:CE2	2.45	0.51
110:qC:152:LEU:HD22	110:qC:299:LEU:HD13	1.93	0.51
114:qG:45:ASN:O	114:qG:49:THR:OG1	2.29	0.51
108:qa:426:THR:OG1	114:qg:328:ALA:O	2.26	0.51
110:qc:41:THR:HG23	152:qc:506:PC1:H362	1.93	0.51
113:qf:22:GLU:O	113:qf:25:LEU:HB2	2.11	0.51
114:qg:54:VAL:HG22	114:qg:57:ARG:HH22	1.74	0.51
120:s1:50:ILE:HG23	120:s1:103:ILE:HD13	1.92	0.51
121:s2:94:GLU:HB3	121:s2:174:TYR:HB2	1.92	0.51
127:s8:23:ARG:NH2	127:s8:26:ILE:O	2.44	0.51
128:t1:358:LEU:HD23	128:t1:376:ILE:HG13	1.93	0.51
143:tg:66:LEU:HD13	143:tg:92:LEU:HD11	1.93	0.51
4:2G:108:ILE:HG23	4:2G:132:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:6C:203:CDL:H192	34:F:182:ILE:HG21	1.91	0.51
29:C1:386:PHE:O	29:C1:390:GLY:N	2.44	0.51
30:C2:5:LEU:HD21	30:C2:542:VAL:HG11	1.93	0.51
30:C2:57:ARG:HE	58:V:91:ASN:HB3	1.76	0.51
38:I:84:PHE:HB2	153:R:201:CDL:HA32	1.93	0.51
44:M2:273:GLU:OE1	44:M2:273:GLU:N	2.43	0.51
51:S:80:VAL:HG12	51:S:81:THR:HG23	1.93	0.51
59:VB:371:THR:O	59:VB:555:SER:HA	2.11	0.51
103:N4:285:LEU:O	103:N4:288:THR:OG1	2.20	0.51
104:N5:566:PRO:HG2	153:N5:806:CDL:H221	1.92	0.51
109:QB:199:LEU:HD21	112:QE:57:PRO:HA	1.93	0.51
109:QB:362:THR:HG21	115:Qh:6:ALA:HB3	1.93	0.51
111:Qd:308:SER:N	115:Qh:50:ASP:OD2	2.43	0.51
120:S1:151:ILE:HD12	121:S2:344:LEU:HD13	1.91	0.51
120:S1:477:ALA:HB2	120:S1:515:HIS:HA	1.91	0.51
128:T1:399:PHE:O	128:T1:402:GLN:NE2	2.43	0.51
145:TX:55:ASN:HD22	145:TX:98:PRO:HD3	1.75	0.51
152:2f:302:PC1:H232	158:sc:101:3PE:H291	1.93	0.50
19:6b:158:VAL:O	19:6b:161:GLN:NE2	2.45	0.50
23:7a:59:GLU:HG2	31:c3:294:LYS:HD3	1.93	0.50
29:c1:385:LEU:HD23	152:c1:706:PC1:H262	1.92	0.50
46:n:78:PHE:HA	46:n:151:LYS:HG2	1.92	0.50
51:s:44:ASP:OD2	51:s:48:GLN:NE2	2.44	0.50
52:sa:49:TYR:HD1	52:sa:73:LYS:HG2	1.76	0.50
52:sa:129:MET:HG3	52:sa:451:VAL:HG21	1.93	0.50
59:vb:426:LYS:O	63:y0:60:TYR:OH	2.22	0.50
76:a6:44:THR:OG1	99:j1:197:ASP:OD2	2.24	0.50
77:a7:164:TRP:CZ2	121:s2:268:SER:HB3	2.46	0.50
82:al:191:SER:O	129:t2:125:ASN:ND2	2.44	0.50
85:b2:59:ILE:HD13	153:n5:806:CDL:H262	1.93	0.50
100:n1:154:ILE:HG13	102:n3:57:ILE:HG21	1.93	0.50
102:n3:28:GLU:HA	102:n3:31:TYR:CE2	2.46	0.50
103:n4:159:VAL:HG21	103:n4:284:PHE:CZ	2.46	0.50
104:n5:181:LEU:HB2	104:n5:294:ILE:HG12	1.93	0.50
104:n5:709:ILE:HG21	152:n5:803:PC1:H2B1	1.93	0.50
152:n6:301:PC1:H261	152:tc:101:PC1:H232	1.93	0.50
108:qa:334:LEU:O	108:qa:338:LEU:N	2.42	0.50
110:qc:79:ASP:N	110:qc:79:ASP:OD1	2.43	0.50
120:s1:383:ALA:HB2	120:s1:656:THR:HG21	1.93	0.50
121:s2:169:MET:HE2	126:s7:127:PRO:HG3	1.94	0.50
2:2E:318:TRP:HE1	151:2E:401:HEC:HBB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2J:13:VAL:HG22	8:2K:28:VAL:HG21	1.93	0.50
23:7A:35:TYR:O	23:7A:39:ARG:NH1	2.44	0.50
153:7A:201:CDL:H801	46:N:126:GLY:HA2	1.92	0.50
152:C3:605:PC1:H321	59:VB:237:TYR:HB2	1.93	0.50
153:M2:404:CDL:H351	153:M2:404:CDL:H132	1.92	0.50
49:Q:118:ASN:H	67:Z1:10:ASN:HD21	1.59	0.50
50:R:76:THR:HG22	50:R:109:LEU:HB3	1.92	0.50
52:SA:129:MET:HG3	52:SA:451:VAL:HG21	1.94	0.50
60:W:55:THR:HG23	62:Y:105:PHE:HE1	1.75	0.50
68:1B:33:THR:HG21	102:N3:64:LEU:HD13	1.93	0.50
83:AM:168:ASN:OD1	83:AM:169:GLY:N	2.44	0.50
98:G3:294:LEU:HD12	98:G3:305:GLN:HB2	1.93	0.50
103:N4:397:LEU:HD21	152:N5:801:PC1:H221	1.93	0.50
104:N5:181:LEU:HB2	104:N5:294:ILE:HG12	1.93	0.50
104:N5:559:MET:HE2	104:N5:609:LEU:HD23	1.91	0.50
109:Qb:386:ILE:HD13	115:Qh:38:TYR:HE1	1.76	0.50
112:Qe:84:GLU:HB2	112:Qe:87:ILE:HB	1.93	0.50
122:S3:172:GLN:OE1	123:S4:132:ARG:NH1	2.44	0.50
129:T2:273:GLN:O	129:T2:276:ARG:HG2	2.10	0.50
146:V1:245:ASN:ND2	171:V1:501:FMN:O2	2.36	0.50
4:2g:197:PHE:HB3	52:sa:204:ILE:HD12	1.94	0.50
18:6a:109:GLU:HG3	31:c3:349:LYS:HZ3	1.76	0.50
24:7c:120:SEP:O	26:a:246:ASN:ND2	2.44	0.50
29:c1:349:ILE:HD13	29:c1:392:PRO:HB2	1.93	0.50
31:c3:162:LEU:HG	31:c3:166:LYS:HE3	1.93	0.50
153:e:403:CDL:H541	153:e:403:CDL:H731	1.93	0.50
153:m1:402:CDL:HB61	153:m2:401:CDL:HA4	1.93	0.50
50:r:52:VAL:HG13	143:tg:113:GLU:HG2	1.92	0.50
65:y7:124:ILE:HG21	65:y7:137:LEU:HD21	1.92	0.50
85:b2:107:ASN:HD22	131:t4:56:HIS:CD2	2.30	0.50
97:g2:174:PRO:HD2	97:g2:177:ARG:HG3	1.92	0.50
108:qa:252:CYS:SG	108:qa:421:VAL:HG11	2.51	0.50
110:qc:54:PHE:O	112:qe:117:ARG:NH2	2.44	0.50
110:qc:332:VAL:HA	110:qc:335:PHE:HD2	1.76	0.50
19:6B:158:VAL:O	19:6B:161:GLN:NE2	2.45	0.50
28:BP:178:THR:HB	28:BP:190:TRP:CE2	2.46	0.50
29:C1:92:LEU:HD11	29:C1:267:ARG:HA	1.93	0.50
29:C1:105:MET:HE1	154:C1:702:HEA:H162	1.93	0.50
32:D:321:ASN:OD1	39:J:210:GLN:NE2	2.43	0.50
59:VB:113:HIS:HE1	59:VB:128:VAL:HG21	1.75	0.50
68:1B:31:GLN:NE2	121:S2:218:GLN:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:4L:17:ILE:HG12	71:5B:83:LEU:HD11	1.91	0.50
85:B2:107:ASN:HD22	131:T4:56:HIS:CD2	2.29	0.50
89:B7:11:GLN:NE2	131:T4:212:TYR:O	2.37	0.50
90:B8:64:TYR:O	104:N5:334:LYS:NZ	2.34	0.50
98:G3:164:VAL:HB	98:G3:182:ILE:HG12	1.93	0.50
98:G3:250:MET:HB3	98:G3:255:PHE:HB2	1.93	0.50
104:N5:360:THR:HG21	104:N5:390:LEU:HD21	1.93	0.50
104:N5:533:ARG:NH2	104:N5:627:GLN:OE1	2.40	0.50
104:N5:557:VAL:O	104:N5:560:ILE:HG13	2.11	0.50
110:QC:224:ASP:OD1	112:QE:100:TYR:OH	2.25	0.50
116:QI:56:ARG:HA	116:QI:60:GLN:HB3	1.93	0.50
108:Qa:252:CYS:SG	108:Qa:421:VAL:HG11	2.51	0.50
109:Qb:299:MET:HB2	109:Qb:483:PRO:HD3	1.93	0.50
129:T2:76:GLU:HG3	129:T2:77:LYS:HG2	1.93	0.50
136:T9:94:ILE:HG22	136:T9:126:ASP:HB3	1.93	0.50
146:V1:144:LEU:HD11	146:V1:187:ALA:HB1	1.92	0.50
28:bp:237:ASP:OD1	28:bp:237:ASP:N	2.44	0.50
29:c1:92:LEU:HD22	29:c1:270:THR:HB	1.94	0.50
29:c1:100:ALA:HB2	29:c1:155:ILE:HG12	1.92	0.50
29:c1:386:PHE:O	29:c1:390:GLY:N	2.43	0.50
31:c3:138:LEU:HB3	31:c3:149:PHE:HB3	1.93	0.50
38:i:149:GLU:HG2	38:i:195:PRO:HB2	1.93	0.50
44:m2:111:LYS:NZ	46:n:22:GLU:OE2	2.42	0.50
49:q:166:ASP:OD1	49:q:167:TYR:N	2.45	0.50
52:sa:574:ARG:NH2	52:sa:596:LYS:O	2.44	0.50
64:y5:188:ILE:HG22	64:y5:190:TYR:H	1.76	0.50
70:4l:8:TRP:CE3	70:4l:11:ILE:HD11	2.46	0.50
106:p1:185:TYR:OH	130:t3:266:ARG:NH2	2.40	0.50
120:s1:131:ILE:HG23	127:s8:137:ILE:HD12	1.93	0.50
120:s1:266:THR:HG22	120:s1:271:ILE:HA	1.92	0.50
120:s1:493:LYS:HE3	120:s1:663:LEU:HA	1.92	0.50
120:s1:525:GLU:HG3	120:s1:591:VAL:HG21	1.94	0.50
122:s3:87:ASN:O	122:s3:91:LYS:HG2	2.11	0.50
142:tf:177:GLU:HG2	142:tf:209:LEU:HD22	1.93	0.50
146:v1:144:LEU:HD11	146:v1:187:ALA:HB1	1.93	0.50
146:v1:152:ALA:O	146:v1:192:TYR:OH	2.26	0.50
29:C1:514:ASN:ND2	154:C1:703:HEA:O1A	2.45	0.50
32:D:160:ASP:HB2	32:D:186:ARG:NE	2.27	0.50
51:S:44:ASP:OD2	51:S:48:GLN:NE2	2.44	0.50
52:SA:155:ILE:HG21	52:SA:177:ALA:HB1	1.93	0.50
70:4L:11:ILE:HB	105:N6:46:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:A2:79:ASN:N	73:A2:79:ASN:OD1	2.45	0.50
78:A8:119:GLN:NE2	83:AM:85:LEU:O	2.38	0.50
95:FX:45:ILE:HD12	95:FX:156:MET:HE2	1.92	0.50
97:G2:79:GLN:H	97:G2:100:HIS:CD2	2.29	0.50
103:N4:384:ARG:HH12	103:N4:483:GLU:CD	2.19	0.50
104:N5:709:ILE:HG21	152:N5:803:PC1:H2B1	1.93	0.50
113:QF:25:LEU:HD23	113:QF:73:VAL:HG11	1.94	0.50
114:QG:45:ASN:O	114:QG:49:THR:OG1	2.29	0.50
117:QJ:39:ALA:HB1	152:QJ:101:PC1:H2	1.93	0.50
108:Qa:31:ILE:O	116:Qi:62:TYR:OH	2.24	0.50
147:V2:198:ASP:O	147:V2:202:GLY:N	2.44	0.50
3:2f:215:LEU:HD11	152:2f:303:PC1:H231	1.92	0.50
28:bp:374:ASN:ND2	28:bp:396:LYS:O	2.44	0.50
153:c1:712:CDL:H141	30:c2:56:ALA:HB1	1.94	0.50
30:c2:98:ASN:O	30:c2:102:ARG:HG2	2.12	0.50
30:c2:202:ARG:NH1	32:d:338:ASP:OD1	2.45	0.50
31:c3:276:ILE:O	31:c3:280:MET:HG2	2.11	0.50
49:q:133:LYS:NZ	61:x:4:PHE:O	2.38	0.50
52:sa:451:VAL:HG23	52:sa:452:PHE:HD1	1.75	0.50
60:w:21:ARG:HA	60:w:24:TYR:CE2	2.47	0.50
68:1b:33:THR:HG21	102:n3:64:LEU:HD13	1.93	0.50
70:4l:34:GLU:O	70:4l:38:LEU:HG	2.12	0.50
70:4l:55:THR:OG1	124:s5:4:SER:OG	2.30	0.50
83:am:140:PHE:HD1	124:s5:49:ARG:HG2	1.76	0.50
84:an:4:ASN:HB3	84:an:8:LYS:HD3	1.92	0.50
104:n5:467:ALA:HA	104:n5:490:SER:HA	1.92	0.50
114:qG:7:ILE:HG22	114:qG:10:GLU:HG3	1.92	0.50
120:s1:241:SER:HA	127:s8:140:LYS:HZ1	1.77	0.50
121:s2:239:VAL:HG12	121:s2:279:ARG:HG2	1.94	0.50
126:s7:68:THR:HA	126:s7:96:CYS:HB3	1.92	0.50
127:s8:95:CYS:HA	127:s8:99:TYR:CD2	2.47	0.50
3:2F:117:THR:HG21	11:2N:55:TYR:HE2	1.76	0.50
30:C2:202:ARG:NH1	32:D:338:ASP:OD1	2.45	0.50
31:C3:106:VAL:HG13	45:M3:247:PRO:HG2	1.93	0.50
41:L:134:LEU:HG	41:L:136:VAL:HG23	1.93	0.50
67:Z1:40:TYR:HB2	153:U1:101:CDL:H382	1.92	0.50
83:AM:149:ASN:ND2	105:N6:164:ASN:OD1	2.37	0.50
94:C4:28:THR:CG2	97:G2:18:MET:HG3	2.42	0.50
103:N4:159:VAL:HG21	103:N4:284:PHE:CZ	2.46	0.50
104:N5:471:GLY:N	104:N5:490:SER:HB2	2.26	0.50
109:QB:165:GLY:O	109:QB:169:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
152:Qb:602:PC1:H12	112:Qe:100:TYR:CE2	2.46	0.50
110:Qc:41:THR:HG23	152:Qc:506:PC1:H362	1.93	0.50
113:Qf:22:GLU:O	113:Qf:25:LEU:HB2	2.11	0.50
127:S8:176:ILE:HG12	162:S8:302:SF4:S1	2.51	0.50
129:T2:119:GLY:HA2	129:T2:162:HIS:O	2.12	0.50
136:T9:3:LEU:HD13	136:T9:15:VAL:HG21	1.94	0.50
3:2f:113:ILE:HG23	3:2f:146:LEU:HD11	1.94	0.50
25:7l:907:TRP:CG	25:7l:908:PRO:HD3	2.47	0.50
30:c2:5:LEU:HD21	30:c2:542:VAL:HG11	1.93	0.50
33:e:38:LEU:HB3	33:e:289:TRP:CD1	2.47	0.50
35:fs:102:GLY:HA2	35:fs:140:LYS:HE3	1.92	0.50
42:m:10:ASN:HD21	42:m:22:LYS:HG2	1.76	0.50
42:m:111:VAL:HG12	153:w:202:CDL:H661	1.93	0.50
152:m:301:PC1:H221	152:w:201:PC1:H332	1.93	0.50
43:m1:186:PRO:HB2	152:m2:405:PC1:H322	1.94	0.50
79:a9:45:ALA:HA	79:a9:118:VAL:O	2.11	0.50
83:am:49:LYS:NZ	152:s8:301:PC1:O14	2.44	0.50
83:am:163:LEU:HD13	100:n1:17:LEU:HD12	1.92	0.50
99:j1:281:VAL:HG21	124:s5:85:SER:HB2	1.94	0.50
152:j1:400:PC1:H391	139:tc:25:ALA:HB1	1.93	0.50
104:n5:153:LEU:O	104:n5:156:THR:OG1	2.30	0.50
104:n5:345:LEU:HD22	158:n5:802:3PE:H391	1.94	0.50
104:n5:557:VAL:O	104:n5:560:ILE:HG13	2.11	0.50
105:n6:24:ILE:O	105:n6:28:THR:OG1	2.23	0.50
105:n6:241:GLN:NE2	121:s2:221:ILE:O	2.44	0.50
107:p2:48:ASN:OD1	107:p2:49:GLY:N	2.45	0.50
109:qB:185:VAL:HG12	109:qB:225:LEU:HD13	1.93	0.50
109:qB:199:LEU:HD21	112:qE:57:PRO:HA	1.93	0.50
115:qH:69:PHE:HB2	115:qH:72:PHE:HB2	1.93	0.50
111:qd:46:GLU:HB3	111:qd:50:HIS:HB3	1.93	0.50
114:qg:192:LEU:HD21	152:qg:401:PC1:H282	1.94	0.50
142:tf:105:ILE:O	142:tf:140:LYS:NZ	2.32	0.50
145:tx:55:ASN:HD22	145:tx:98:PRO:HD3	1.76	0.50
2:2E:249:LEU:HD11	2:2E:271:ASN:HB3	1.94	0.50
26:A:66:SER:O	26:A:72:SER:OG	2.27	0.50
27:B:267:ILE:O	27:B:271:ASN:ND2	2.37	0.50
27:B:314:LEU:HD21	27:B:332:PRO:HD3	1.92	0.50
44:M2:281:GLY:N	152:M2:402:PC1:O14	2.40	0.50
51:S:85:ASP:OD2	149:C:124:SER:OG	2.27	0.50
65:Y7:359:ALA:HB1	65:Y7:364:PHE:HB2	1.93	0.50
100:N1:154:ILE:HG13	102:N3:57:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:QC:152:LEU:HD22	110:QC:299:LEU:HD13	1.93	0.50
153:QC:504:CDL:OB7	115:QH:96:ASN:ND2	2.44	0.50
109:Qb:42:ARG:NH2	109:Qb:54:ILE:O	2.37	0.50
146:V1:67:GLU:O	146:V1:71:ASN:ND2	2.45	0.50
147:V2:213:ASN:HB3	147:V2:216:GLU:HB3	1.93	0.50
1:1t:63:ILE:HG23	30:c2:317:LEU:HD11	1.94	0.50
8:2k:51:ASN:ND2	54:sc:44:TYR:OH	2.43	0.50
27:b:196:TYR:HE2	27:b:204:TYR:HB2	1.77	0.50
30:c2:213:ASN:O	30:c2:216:SER:OG	2.30	0.50
30:c2:461:TYR:OH	37:h:190:GLU:OE2	2.29	0.50
152:fs:204:PC1:H361	152:fs:204:PC1:H241	1.92	0.50
42:m:98:LEU:O	60:w:21:ARG:NH2	2.44	0.50
59:vb:181:ARG:O	59:vb:186:GLN:NE2	2.44	0.50
153:2b:201:CDL:H121	153:2b:201:CDL:H332	1.94	0.50
76:a6:38:GLU:O	122:s3:154:ARG:NH2	2.44	0.50
82:al:138:HIS:NE2	127:s8:207:PHE:O	2.37	0.50
93:bm:89:PRO:HD2	106:p1:24:ILE:HD11	1.94	0.50
111:qD:77:PHE:O	111:qD:82:GLY:N	2.43	0.50
110:qc:326:LYS:HA	110:qc:341:ILE:O	2.12	0.50
112:qe:53:THR:HG22	112:qe:55:SER:H	1.77	0.50
112:qe:70:ILE:HD11	114:qg:121:ARG:HD2	1.94	0.50
115:qh:69:PHE:HB2	115:qh:72:PHE:HB2	1.93	0.50
121:s2:88:VAL:HG12	121:s2:129:ASN:HA	1.93	0.50
122:s3:198:LEU:HD22	127:s8:149:ARG:HB3	1.93	0.50
129:t2:76:GLU:HG3	129:t2:77:LYS:HG2	1.93	0.50
133:t6:36:MET:HG3	133:t6:42:LEU:HD13	1.93	0.50
26:A:418:GLY:H	26:A:435:LYS:HG3	1.77	0.50
36:G:88:THR:OG1	36:G:89:MET:N	2.44	0.50
37:H:133:GLY:O	37:H:219:ASN:ND2	2.44	0.50
52:SA:445:SER:O	52:SA:449:ILE:HG23	2.11	0.50
53:SB:266:ASP:OD1	53:SB:267:VAL:N	2.44	0.50
72:A1:94:TYR:HB3	83:AM:143:ARG:HG2	1.94	0.50
92:BL:135:GLN:NE2	103:N4:86:PHE:O	2.34	0.50
100:N1:232:TYR:OH	100:N1:248:GLU:OE2	2.22	0.50
100:N1:239:PHE:HD2	139:TC:2:VAL:HG22	1.76	0.50
108:QA:297:LEU:HD21	108:Qa:209:LYS:HD2	1.93	0.50
153:QB:601:CDL:H111	152:QB:602:PC1:H271	1.93	0.50
110:QC:329:VAL:O	118:QL:7:LYS:NZ	2.33	0.50
3:2f:117:THR:HG21	11:2n:55:TYR:HE2	1.76	0.50
19:6b:198:ALA:HB2	30:c2:354:PRO:HD2	1.93	0.50
32:d:160:ASP:HB2	32:d:186:ARG:NE	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:m3:102:LYS:NZ	45:m3:261:PRO:O	2.36	0.50
52:sa:549:THR:HA	52:sa:552:ILE:HD12	1.93	0.50
53:sb:216:VAL:HG23	53:sb:218:CYS:HB3	1.93	0.50
65:y7:165:LYS:HE2	149:c:129:GLN:HB3	1.93	0.50
84:an:97:ASN:O	139:tc:19:ARG:NH2	2.45	0.50
90:b8:93:MET:HG2	152:n5:803:PC1:H3C2	1.94	0.50
95:fx:45:ILE:HD12	95:fx:156:MET:HE2	1.91	0.50
103:n4:27:ILE:HD11	158:t8:601:3PE:H351	1.94	0.50
103:n4:492:PHE:HB2	153:th:200:CDL:H412	1.93	0.50
109:qB:74:ARG:HH21	109:qB:440:THR:HA	1.77	0.50
110:qC:38:THR:HG21	166:qC:502:HEM:HAB	1.92	0.50
111:qD:56:TRP:NE1	111:qD:173:ASN:OD1	2.40	0.50
109:qb:71:ASN:ND2	109:qb:268:GLY:HA2	2.27	0.50
120:s1:562:TYR:CE2	120:s1:564:GLY:HA3	2.47	0.50
123:s4:97:PRO:HG2	123:s4:100:PRO:HA	1.94	0.50
153:6C:203:CDL:H552	58:V:111:GLN:HB3	1.92	0.50
29:C1:531:LEU:HD21	154:C1:703:HEA:HBC2	1.93	0.50
30:C2:12:GLN:OE1	30:C2:546:TYR:OH	2.29	0.50
34:F:106:LEU:HD12	43:M1:260:ARG:HG3	1.93	0.50
43:M1:186:PRO:HB2	152:M2:405:PC1:H322	1.93	0.50
45:M3:151:SER:HB3	45:M3:162:VAL:HG21	1.94	0.50
51:S:65:PRO:O	51:S:69:ARG:HB2	2.12	0.50
52:SA:95:ASN:ND2	52:SA:442:GLY:O	2.43	0.50
65:Y7:124:ILE:HG21	65:Y7:137:LEU:HD21	1.93	0.50
65:Y7:386:ILE:O	65:Y7:390:LYS:HB2	2.12	0.50
70:4L:69:LEU:HD11	105:N6:195:GLY:HA3	1.94	0.50
75:A5:129:ASP:OD1	75:A5:130:SER:N	2.39	0.50
76:A6:44:THR:OG1	99:J1:197:ASP:OD2	2.24	0.50
77:A7:208:ARG:HH21	121:S2:324:ARG:HA	1.76	0.50
84:AN:4:ASN:HB3	84:AN:8:LYS:HD3	1.92	0.50
93:BM:89:PRO:HD2	106:P1:24:ILE:HD11	1.94	0.50
100:N1:159:LEU:HD11	100:N1:221:LEU:HB2	1.93	0.50
101:N2:71:VAL:O	101:N2:75:ILE:HG12	2.12	0.50
102:N3:28:GLU:HA	102:N3:31:TYR:CE2	2.47	0.50
103:N4:492:PHE:HB2	153:TH:200:CDL:H412	1.94	0.50
104:N5:309:PHE:HD1	104:N5:350:LEU:HD23	1.77	0.50
110:Qc:36:PHE:CD1	110:Qc:230:GLU:HB3	2.46	0.50
110:Qc:54:PHE:O	112:Qe:117:ARG:NH2	2.43	0.50
114:Qg:192:LEU:HD21	152:Qg:401:PC1:H282	1.93	0.50
115:Qh:69:PHE:HB2	115:Qh:72:PHE:HB2	1.93	0.50
2:2e:248:PRO:HB3	2:2e:264:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7c:205:ASP:OD2	37:h:127:ARG:NH2	2.43	0.50
152:a:503:PC1:H11	31:c3:403:TRP:CD1	2.46	0.50
28:bp:178:THR:HB	28:bp:190:TRP:CE2	2.47	0.50
29:c1:384:HIS:NE2	152:c1:706:PC1:H12	2.27	0.50
33:e:341:TYR:HB2	63:y0:46:LEU:HD13	1.94	0.50
34:f:299:GLN:NE2	58:v:77:PHE:O	2.33	0.50
38:i:103:TYR:O	38:i:107:SER:OG	2.23	0.50
152:m:307:PC1:H251	152:m:307:PC1:H362	1.94	0.50
69:2b:20:ILE:HD12	69:2b:87:LEU:HB3	1.92	0.50
86:b3:41:ARG:NH2	91:b9:48:TYR:OH	2.44	0.50
90:b8:52:THR:HG23	103:n4:328:THR:HG23	1.94	0.50
90:b8:90:TRP:CD2	104:n5:472:LEU:HD21	2.47	0.50
98:g3:164:VAL:HB	98:g3:182:ILE:HG12	1.93	0.50
98:g3:263:GLU:HG3	105:n6:236:GLN:HA	1.94	0.50
104:n5:471:GLY:N	104:n5:490:SER:HB2	2.26	0.50
152:n5:805:PC1:H361	152:n5:805:PC1:H2C1	1.93	0.50
106:p1:173:ILE:HD13	106:p1:194:LEU:HD21	1.94	0.50
108:qA:120:THR:HG21	108:qA:169:ASP:HB3	1.94	0.50
109:qB:230:ASP:OD1	109:qB:230:ASP:N	2.45	0.50
115:qH:102:PHE:HB3	115:qH:103:PRO:HD3	1.93	0.50
110:qc:344:PRO:O	110:qc:406:ARG:NH2	2.42	0.50
127:s8:123:GLU:OE1	127:s8:195:ASN:ND2	2.45	0.50
129:t2:164:ILE:HG12	129:t2:180:ILE:HG13	1.92	0.50
132:t5:130:VAL:HG11	153:t5:301:CDL:H341	1.93	0.50
146:v1:291:GLU:HG2	146:v1:295:ILE:HD12	1.94	0.50
23:7A:13:TYR:OH	59:VB:268:ASP:OD1	2.22	0.50
153:7C:302:CDL:H342	29:C1:36:LEU:HD23	1.93	0.50
26:A:477:ILE:HG21	36:G:51:VAL:HG21	1.93	0.50
28:BP:136:PHE:HB3	28:BP:155:PRO:HA	1.93	0.50
29:C1:521:PHE:HA	29:C1:524:VAL:HB	1.93	0.50
29:C1:533:GLY:O	29:C1:537:THR:OG1	2.28	0.50
31:C3:290:VAL:HG22	31:C3:470:ARG:HE	1.77	0.50
33:E:9:ARG:H	33:E:235:ASN:HD22	1.60	0.50
43:M1:258:VAL:O	43:M1:262:MET:HG3	2.11	0.50
48:P:110:ASP:O	48:P:115:GLY:N	2.42	0.50
52:SA:49:TYR:HD1	52:SA:73:LYS:HG2	1.76	0.50
52:SA:579:GLY:HA2	52:SA:634:ARG:HH12	1.75	0.50
53:SB:230:TRP:NE1	164:SC:102:U10:O5	2.44	0.50
57:U:10:ASP:OD1	57:U:121:ARG:NH2	2.44	0.50
60:W:21:ARG:HA	60:W:24:TYR:CE2	2.47	0.50
65:Y7:165:LYS:HE2	149:C:129:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:4L:77:ILE:HD11	101:N2:162:PHE:HZ	1.77	0.50
77:A7:80:VAL:HG21	122:S3:13:ILE:HA	1.92	0.50
77:A7:209:ARG:NH2	121:S2:190:GLU:OE1	2.45	0.50
79:A9:213:ILE:HD13	79:A9:349:VAL:HG11	1.94	0.50
85:B2:59:ILE:HD13	153:N5:806:CDL:H262	1.94	0.50
90:B8:139:LEU:HB2	90:B8:141:LEU:HD13	1.94	0.50
90:B8:157:LYS:HA	90:B8:161:ARG:HD2	1.93	0.50
96:G1:65:GLU:OE2	99:J1:167:ARG:NH2	2.35	0.50
100:N1:279:ASN:HB3	134:T7:107:ASN:ND2	2.26	0.50
107:P2:48:ASN:OD1	107:P2:49:GLY:N	2.44	0.50
113:QF:87:GLY:HA2	116:QI:95:HIS:CE1	2.45	0.50
109:Qb:169:GLN:OE1	109:Qb:269:THR:OG1	2.24	0.50
112:Qe:53:THR:HG22	112:Qe:55:SER:H	1.77	0.50
114:Qg:157:TRP:HB2	116:Qi:6:LEU:HD11	1.93	0.50
124:S5:26:ALA:HA	124:S5:32:PRO:HB3	1.94	0.50
146:V1:86:ARG:O	146:V1:88:ARG:NH1	2.44	0.50
14:3t:30:LEU:HD22	22:6t:19:LYS:HG2	1.94	0.50
29:c1:681:VAL:HG21	34:f:114:GLU:HG3	1.93	0.50
33:e:77:VAL:HG21	33:e:157:ILE:HD11	1.94	0.50
33:e:87:ALA:O	33:e:154:LYS:NZ	2.44	0.50
42:m:194:SER:HA	62:y:1:MET:HE3	1.94	0.50
43:m1:261:GLU:OE1	43:m1:303:LYS:NZ	2.44	0.50
46:n:86:ILE:HD12	153:n:304:CDL:H231	1.93	0.50
49:q:118:ASN:H	67:z1:10:ASN:HD21	1.60	0.50
53:sb:230:TRP:NE1	164:sc:102:U10:O5	2.42	0.50
56:t:56:ARG:HD2	153:t:204:CDL:H341	1.94	0.50
69:2b:55:GLU:O	69:2b:128:SER:OG	2.26	0.50
75:a5:157:ARG:NH2	98:g3:279:GLU:OE1	2.43	0.50
79:a9:356:THR:HB	79:a9:359:ASN:HD22	1.77	0.50
83:am:168:ASN:OD1	83:am:169:GLY:N	2.44	0.50
99:j1:270:LEU:HD11	124:s5:66:ILE:HG23	1.93	0.50
102:n3:42:PHE:HE2	102:n3:52:GLU:HG3	1.76	0.50
108:qA:295:ARG:HH12	108:qA:471:LEU:HB2	1.77	0.50
109:qB:311:PRO:HG3	109:qB:470:TRP:CZ2	2.47	0.50
109:qb:113:LEU:HA	109:qb:116:ARG:HG2	1.93	0.50
109:qb:143:ARG:NH2	109:qb:202:GLU:OE1	2.45	0.50
109:qb:207:THR:OG1	109:qb:290:SER:OG	2.22	0.50
112:qe:84:GLU:HB2	112:qe:87:ILE:HB	1.94	0.50
125:s6:48:ASN:ND2	127:s8:159:PRO:O	2.31	0.50
128:t1:261:ASN:HB3	128:t1:264:LYS:HG3	1.94	0.50
136:t9:94:ILE:HD12	136:t9:130:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2F:215:LEU:HD11	152:2F:303:PC1:H231	1.93	0.50
23:7A:88:TYR:OH	65:Y7:339:ASN:O	2.25	0.50
27:B:324:LYS:HZ2	153:B:501:CDL:H1O1	1.54	0.50
32:D:193:ARG:HB2	39:J:217:LEU:HB3	1.92	0.50
152:M:303:PC1:H221	152:W:201:PC1:H332	1.93	0.50
61:X:80:GLY:O	61:X:83:PRO:HD2	2.12	0.50
62:Y:26:TRP:NE1	62:Y:85:TYR:OH	2.34	0.50
69:2B:20:ILE:HD12	69:2B:87:LEU:HB3	1.92	0.50
69:2B:30:ILE:HD11	158:C4:402:3PE:H2D2	1.93	0.50
73:A2:62:ILE:HG12	73:A2:72:LYS:HB3	1.93	0.50
158:A3:201:3PE:H252	101:N2:28:PHE:HB3	1.93	0.50
77:A7:79:PRO:HD2	77:A7:90:ARG:HH22	1.76	0.50
78:A8:128:GLN:OE1	78:A8:128:GLN:N	2.42	0.50
97:G2:174:PRO:HD2	97:G2:177:ARG:HG3	1.92	0.50
98:G3:7:PHE:HB2	148:X1:88:PHE:CE2	2.47	0.50
99:J1:268:GLU:HA	152:TE:102:PC1:H252	1.93	0.50
152:J1:400:PC1:H391	139:TC:25:ALA:HB1	1.93	0.50
102:N3:42:PHE:HE2	102:N3:52:GLU:HG3	1.76	0.50
103:N4:27:ILE:HD11	158:T8:601:3PE:H351	1.94	0.50
103:N4:333:LEU:HD22	103:N4:459:SER:HB2	1.94	0.50
109:QB:76:ALA:O	109:QB:249:ALA:HA	2.12	0.50
114:QG:134:VAL:HG13	114:QG:138:VAL:HB	1.93	0.50
108:Qa:173:GLU:O	108:Qa:240:GLN:NE2	2.43	0.50
108:Qa:426:THR:OG1	114:Qg:328:ALA:O	2.26	0.50
110:Qc:169:THR:OG1	110:Qc:177:THR:OG1	2.29	0.50
112:Qe:228:ARG:O	112:Qe:230:ARG:N	2.45	0.50
132:T5:126:SER:HB3	138:TB:77:LEU:HD13	1.94	0.50
146:V1:325:VAL:HG13	146:V1:349:GLY:H	1.76	0.50
13:2t:29:LEU:HD22	16:4t:16:VAL:HG12	1.92	0.49
31:c3:280:MET:HG3	65:y7:320:TYR:CZ	2.47	0.49
31:c3:290:VAL:HG22	31:c3:470:ARG:HE	1.77	0.49
32:d:220:ASN:HB2	32:d:228:LEU:HD12	1.94	0.49
153:f:401:CDL:H152	153:f:401:CDL:H332	1.93	0.49
50:r:85:PRO:HG3	64:y5:74:SER:HB3	1.94	0.49
70:4l:77:ILE:HD11	101:n2:162:PHE:HZ	1.77	0.49
158:a3:201:3PE:H231	102:n3:112:LEU:HD11	1.93	0.49
78:a8:128:GLN:OE1	78:a8:128:GLN:N	2.42	0.49
87:b4:48:ASN:OD1	87:b4:49:TYR:N	2.42	0.49
90:b8:140:GLY:O	92:bl:126:LYS:NZ	2.34	0.49
95:fx:105:SER:HB2	95:fx:108:GLN:HE21	1.77	0.49
97:g2:20:ARG:HH21	98:g3:37:GLN:HE22	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
98:g3:294:LEU:HD12	98:g3:305:GLN:HB2	1.94	0.49
103:n4:333:LEU:HD22	103:n4:459:SER:HB2	1.94	0.49
108:qA:332:LEU:HD21	108:qA:397:THR:HB	1.94	0.49
153:qB:601:CDL:H111	152:qB:602:PC1:H271	1.93	0.49
108:qa:420:THR:HG23	108:qa:430:ILE:HD12	1.94	0.49
120:s1:189:GLN:O	120:s1:423:ARG:NH1	2.43	0.49
125:s6:88:ILE:HD13	146:v1:466:LYS:HD3	1.94	0.49
146:v1:159:ILE:HD11	146:v1:170:LEU:HD23	1.94	0.49
1:1T:63:ILE:HG23	30:C2:317:LEU:HD11	1.94	0.49
23:7A:55:SER:O	65:Y7:308:ARG:NH2	2.42	0.49
30:C2:98:ASN:O	30:C2:102:ARG:HG2	2.12	0.49
30:C2:478:GLU:HG3	30:C2:479:LEU:HG	1.92	0.49
33:E:38:LEU:HB3	33:E:289:TRP:CD1	2.47	0.49
38:I:26:THR:O	38:I:29:ALA:HB3	2.11	0.49
152:M1:403:PC1:H241	152:M1:403:PC1:H352	1.94	0.49
52:SA:80:LEU:HD21	52:SA:259:THR:HG21	1.94	0.49
70:4L:52:CYS:HB2	83:AM:144:TYR:CD1	2.47	0.49
83:AM:42:ARG:NH2	134:T7:78:PHE:O	2.41	0.49
84:AN:97:ASN:O	139:TC:19:ARG:NH2	2.45	0.49
91:B9:70:GLY:O	91:B9:74:ASN:ND2	2.30	0.49
91:B9:142:SER:HB2	91:B9:152:PHE:HZ	1.76	0.49
93:BM:105:TYR:HE2	158:BM:302:3PE:H341	1.76	0.49
95:FX:78:VAL:HB	95:FX:106:SER:HB3	1.94	0.49
104:N5:314:LEU:HD23	104:N5:317:LEU:HD21	1.94	0.49
104:N5:684:ASN:O	104:N5:687:SER:OG	2.27	0.49
152:N5:805:PC1:H361	152:N5:805:PC1:H2C1	1.93	0.49
110:Qc:375:TYR:O	110:Qc:379:TYR:HB2	2.12	0.49
127:S8:23:ARG:NH2	127:S8:26:ILE:O	2.45	0.49
130:T3:166:LEU:HD23	130:T3:169:PHE:HZ	1.77	0.49
131:T4:89:ILE:HG12	131:T4:202:LEU:HD11	1.94	0.49
26:a:66:SER:O	26:a:72:SER:OG	2.27	0.49
29:c1:533:GLY:O	29:c1:537:THR:OG1	2.29	0.49
34:f:175:GLU:CD	34:f:211:ARG:HE	2.19	0.49
37:h:298:SER:HB2	104:N5:86:LYS:HZ3	1.77	0.49
51:s:85:ASP:OD2	149:c:124:SER:OG	2.27	0.49
59:vb:151:THR:HG23	59:vb:199:ARG:HA	1.95	0.49
59:vb:371:THR:O	59:vb:555:SER:HA	2.11	0.49
100:n1:41:LEU:HD13	100:n1:66:GLN:HB3	1.93	0.49
104:n5:81:ILE:HD13	104:n5:84:LYS:HB2	1.94	0.49
110:qc:375:TYR:O	110:qc:379:TYR:HB2	2.12	0.49
147:v2:130:CYS:HA	147:v2:173:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2E:153:LEU:HD23	2:2E:186:PRO:HG3	1.94	0.49
13:2T:24:GLN:HE21	16:4T:16:VAL:HG22	1.77	0.49
29:C1:464:MET:HB2	29:C1:465:PRO:HD3	1.94	0.49
30:C2:461:TYR:OH	37:H:190:GLU:OE2	2.29	0.49
31:C3:276:ILE:O	31:C3:280:MET:HG2	2.11	0.49
31:C3:280:MET:HG3	65:Y7:320:TYR:CZ	2.47	0.49
45:M3:97:ALA:HB2	45:M3:253:THR:HG22	1.93	0.49
153:2B:201:CDL:H121	153:2B:201:CDL:H332	1.94	0.49
70:4L:8:TRP:CE3	70:4L:11:ILE:HD11	2.46	0.49
75:A5:82:SER:HB3	75:A5:106:VAL:HG13	1.94	0.49
79:A9:45:ALA:HA	79:A9:118:VAL:O	2.11	0.49
153:A9:402:CDL:H582	153:A9:402:CDL:H741	1.92	0.49
82:AL:138:HIS:NE2	127:S8:207:PHE:O	2.36	0.49
97:G2:102:THR:HG23	97:G2:130:VAL:HB	1.94	0.49
109:QB:74:ARG:HH21	109:QB:440:THR:HA	1.76	0.49
109:QB:185:VAL:HG12	109:QB:225:LEU:HD13	1.93	0.49
110:Qc:164:TYR:CZ	110:Qc:171:LYS:HE3	2.47	0.49
120:S1:562:TYR:CE2	120:S1:564:GLY:HA3	2.47	0.49
129:T2:36:ARG:NH2	129:T2:41:ASN:OD1	2.45	0.49
149:c:137:PHE:O	149:c:140:VAL:HG22	2.12	0.49
13:2t:24:GLN:HE21	16:4t:16:VAL:HG22	1.77	0.49
24:7c:152:ILE:HG23	152:m1:401:PC1:H271	1.94	0.49
25:7l:862:LEU:HD22	153:I:303:CDL:H562	1.94	0.49
26:a:249:ASP:O	36:g:34:ARG:NH1	2.37	0.49
47:o:69:MET:O	47:o:74:LYS:NZ	2.45	0.49
51:s:167:GLN:NE2	43:M1:71:GLN:O	2.35	0.49
52:sa:508:MET:SD	52:sa:564:SER:OG	2.61	0.49
53:sb:264:ALA:O	53:sb:303:ARG:NH2	2.45	0.49
65:y7:386:ILE:O	65:y7:390:LYS:HB2	2.12	0.49
66:z:5:PRO:O	66:z:8:LYS:HG2	2.12	0.49
79:a9:137:TYR:O	79:a9:141:HIS:HB3	2.13	0.49
87:b4:39:VAL:HG13	90:b8:44:LYS:HB3	1.93	0.49
96:g1:217:ASN:HD22	96:g1:218:SER:N	2.10	0.49
97:g2:102:THR:HG23	97:g2:130:VAL:HB	1.94	0.49
103:n4:32:PHE:CD1	103:n4:52:LEU:HD11	2.48	0.49
104:n5:86:LYS:NZ	37:H:295:LYS:O	2.41	0.49
105:n6:222:ASP:N	105:n6:226:ASP:OD2	2.39	0.49
114:qG:194:ARG:HH11	117:qj:7:TYR:HH	1.56	0.49
110:qc:164:TYR:CZ	110:qc:171:LYS:HE3	2.47	0.49
112:qe:140:GLY:N	112:qe:156:ARG:O	2.46	0.49
127:s8:90:TYR:HB2	152:s8:301:PC1:H2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
129:t2:223:ARG:NH2	129:t2:230:ASP:OD1	2.45	0.49
146:v1:385:PRO:HB2	146:v1:424:THR:HG22	1.94	0.49
147:v2:213:ASN:HB3	147:v2:216:GLU:HB3	1.94	0.49
148:x1:2:SER:N	148:x1:149:ARG:H	2.10	0.49
3:2F:113:ILE:HG23	3:2F:146:LEU:HD11	1.94	0.49
23:7A:39:ARG:HD3	26:A:428:GLN:HE22	1.78	0.49
23:7A:59:GLU:HG2	31:C3:294:LYS:HD3	1.94	0.49
53:SB:214:GLU:N	53:SB:214:GLU:OE1	2.42	0.49
65:Y7:428:PHE:HA	65:Y7:431:ILE:HB	1.93	0.49
66:Z:5:PRO:O	66:Z:8:LYS:HG2	2.12	0.49
70:4L:34:GLU:O	70:4L:38:LEU:HG	2.12	0.49
108:QA:120:THR:HG21	108:QA:169:ASP:HB3	1.94	0.49
109:QB:311:PRO:HG3	109:QB:470:TRP:CZ2	2.48	0.49
114:Qg:69:ARG:NH1	114:Qg:248:ARG:O	2.45	0.49
123:S4:97:PRO:HG2	123:S4:100:PRO:HA	1.94	0.49
125:S6:88:ILE:HD13	146:V1:466:LYS:HD3	1.94	0.49
125:S6:106:THR:OG1	125:S6:108:LYS:O	2.31	0.49
132:T5:130:VAL:HG11	153:T5:301:CDL:H341	1.93	0.49
146:V1:291:GLU:HG2	146:V1:295:ILE:HD12	1.93	0.49
5:2h:188:LEU:O	5:2h:192:LEU:HG	2.13	0.49
7:2j:25:ASN:HA	7:2j:30:LYS:HB2	1.94	0.49
14:3t:39:ARG:NH2	14:3t:51:GLU:OE2	2.34	0.49
23:7a:86:LEU:HD23	29:c1:150:ILE:HD11	1.95	0.49
23:7a:95:ASP:OD2	23:7a:98:LYS:NZ	2.35	0.49
26:a:230:ASN:O	26:a:233:GLU:HG2	2.12	0.49
28:bp:136:PHE:HB3	28:bp:155:PRO:HA	1.93	0.49
30:c2:83:CYS:HA	30:c2:86:PRO:HD2	1.94	0.49
32:d:300:ARG:NH1	32:d:370:GLU:O	2.45	0.49
32:d:378:ARG:HH12	152:d:501:PC1:H342	1.77	0.49
35:fs:84:PHE:HB3	153:E:403:CDL:HB32	1.95	0.49
38:i:84:PHE:HB2	153:r:201:CDL:HA32	1.94	0.49
98:g3:7:PHE:HB2	148:x1:88:PHE:CE2	2.47	0.49
104:n5:628:ALA:O	104:n5:638:TYR:OH	2.26	0.49
109:qB:199:LEU:O	109:qB:203:ASN:ND2	2.42	0.49
152:qE:304:PC1:H332	117:qJ:40:LEU:HA	1.94	0.49
120:s1:181:THR:N	162:s1:802:SF4:S4	2.85	0.49
146:v1:325:VAL:HG13	146:v1:349:GLY:H	1.78	0.49
2:2E:82:VAL:HG22	2:2E:115:VAL:HG23	1.94	0.49
26:A:276:THR:OG1	40:K:182:GLN:NE2	2.45	0.49
153:C1:708:CDL:H532	152:C3:605:PC1:H251	1.95	0.49
153:E:403:CDL:H541	153:E:403:CDL:H731	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:L:148:ARG:NH2	59:VB:567:PRO:O	2.28	0.49
42:M:24:LEU:HD12	153:M:304:CDL:H711	1.93	0.49
43:M1:246:THR:HG23	43:M1:312:MET:HE3	1.95	0.49
153:M1:402:CDL:HB61	153:M2:401:CDL:HA4	1.93	0.49
44:M2:244:ARG:NH1	44:M2:273:GLU:OE2	2.42	0.49
52:SA:124:ASP:OD1	52:SA:124:ASP:N	2.45	0.49
59:VB:294:GLU:OE1	64:Y5:182:ASN:ND2	2.39	0.49
59:VB:297:PHE:HE2	64:Y5:185:ILE:HD12	1.78	0.49
70:4L:55:THR:OG1	124:S5:4:SER:OG	2.31	0.49
90:B8:93:MET:HG2	152:N5:803:PC1:H3C2	1.93	0.49
99:J1:281:VAL:HG21	124:S5:85:SER:HB2	1.94	0.49
103:N4:32:PHE:CD1	103:N4:52:LEU:HD11	2.48	0.49
110:QC:61:MET:HE3	111:Qd:124:TYR:HD2	1.77	0.49
115:QH:69:PHE:HB2	115:QH:72:PHE:HB2	1.93	0.49
110:Qc:244:VAL:O	110:Qc:248:MET:HB2	2.12	0.49
110:Qc:357:ILE:HG12	115:Qh:103:PRO:HG3	1.93	0.49
143:TG:66:LEU:HD13	143:TG:92:LEU:HD11	1.93	0.49
2:2e:69:LEU:HD22	53:sb:312:LEU:HD11	1.94	0.49
11:2n:28:TYR:HA	11:2n:31:VAL:HG12	1.93	0.49
21:6l:43:GLU:O	21:6l:46:VAL:HG22	2.13	0.49
28:bp:397:LYS:HE3	28:bp:399:VAL:HG12	1.95	0.49
43:m1:107:ASP:CG	43:m1:151:SER:HB2	2.38	0.49
51:s:65:PRO:O	51:s:69:ARG:HB2	2.12	0.49
52:sa:80:LEU:HD21	52:sa:259:THR:HG21	1.95	0.49
52:sa:275:LEU:HD11	52:sa:566:GLN:HB3	1.95	0.49
70:4l:52:CYS:HB2	83:am:144:TYR:CD1	2.46	0.49
77:a7:208:ARG:HH21	121:s2:324:ARG:HA	1.77	0.49
153:bm:301:CDL:H531	153:t5:301:CDL:H432	1.95	0.49
104:n5:289:LEU:HD11	104:n5:424:PRO:HB2	1.93	0.49
109:qB:73:VAL:HG22	109:qB:246:PHE:HB2	1.94	0.49
2:2E:91:PRO:HG3	53:SB:312:LEU:HB3	1.95	0.49
2:2E:184:ILE:HD13	2:2E:223:ILE:HD12	1.95	0.49
5:2H:123:CYS:SG	5:2H:124:ARG:HG2	2.53	0.49
7:2J:13:VAL:HG11	8:2K:25:LYS:HA	1.93	0.49
24:7C:127:CYS:SG	24:7C:128:GLU:N	2.85	0.49
28:BP:365:ASN:ND2	28:BP:406:ASP:OD1	2.40	0.49
29:C1:50:HIS:CE1	29:C1:51:LYS:HG2	2.48	0.49
29:C1:92:LEU:HD22	29:C1:270:THR:HB	1.93	0.49
29:C1:181:TYR:OH	46:N:47:ASP:OD2	2.30	0.49
29:C1:378:ASP:OD1	29:C1:378:ASP:N	2.45	0.49
29:C1:384:HIS:NE2	152:C1:709:PC1:H12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:304:GLN:NE2	45:M3:70:GLU:OE2	2.39	0.49
34:F:175:GLU:CD	34:F:211:ARG:HE	2.19	0.49
34:F:178:ILE:HD11	34:F:207:ALA:HB3	1.94	0.49
44:M2:294:TRP:NE1	153:M2:403:CDL:OA7	2.40	0.49
52:SA:445:SER:HB2	161:SA:701:FAD:N1	2.28	0.49
53:SB:216:VAL:HG23	53:SB:218:CYS:HB3	1.93	0.49
56:T:56:ARG:HD2	153:T:204:CDL:H341	1.94	0.49
101:N2:129:PHE:O	101:N2:133:ASN:ND2	2.41	0.49
104:N5:153:LEU:O	104:N5:156:THR:OG1	2.30	0.49
104:N5:289:LEU:HD11	104:N5:424:PRO:HB2	1.93	0.49
110:QC:83:LEU:HD12	152:QC:505:PC1:H362	1.95	0.49
110:QC:98:HIS:CE1	110:QC:102:LYS:HE3	2.48	0.49
110:QC:232:GLY:HA3	111:QD:271:LYS:HG3	1.95	0.49
109:Qb:317:ASP:OD2	109:Qb:469:ARG:NH2	2.37	0.49
121:S2:73:ARG:NE	127:S8:147:PRO:O	2.39	0.49
121:S2:151:PHE:HB3	126:S7:41:VAL:HG21	1.93	0.49
121:S2:411:LEU:HD22	121:S2:440:ILE:HD13	1.94	0.49
123:S4:12:ARG:HG2	123:S4:140:GLU:HB3	1.95	0.49
129:T2:223:ARG:NH2	129:T2:230:ASP:OD1	2.46	0.49
23:7a:55:SER:O	65:y7:308:ARG:NH2	2.42	0.49
153:i:302:CDL:OA3	42:M:201:LYS:NZ	2.45	0.49
153:m:302:CDL:H161	152:m:305:PC1:H222	1.95	0.49
56:t:104:GLN:HB2	56:t:107:GLN:HB2	1.93	0.49
152:w:201:PC1:H3A2	152:w:201:PC1:H2A2	1.95	0.49
72:a1:94:TYR:HB3	83:am:143:ARG:HG2	1.94	0.49
79:a9:234:GLN:HG2	79:a9:263:GLY:H	1.77	0.49
106:p1:235:GLU:HG2	106:p1:237:GLN:H	1.76	0.49
107:p2:135:PRO:HG2	107:p2:138:LEU:HG	1.94	0.49
109:qB:165:GLY:O	109:qB:169:GLN:HG2	2.12	0.49
110:qc:304:TYR:HE1	153:qg:402:CDL:H541	1.77	0.49
122:s3:73:LEU:HB2	122:s3:90:PHE:HZ	1.78	0.49
128:t1:30:GLN:OE1	128:t1:477:TYR:OH	2.23	0.49
128:t1:383:TYR:HD1	128:t1:386:ILE:HD11	1.76	0.49
132:t5:126:SER:HB3	138:tb:77:LEU:HD13	1.95	0.49
136:t9:3:LEU:HD13	136:t9:15:VAL:HG21	1.94	0.49
143:tg:65:ALA:HB3	143:tg:96:PHE:HZ	1.77	0.49
146:v1:67:GLU:O	146:v1:71:ASN:ND2	2.45	0.49
152:2F:302:PC1:H232	158:SC:101:3PE:H291	1.93	0.49
14:3T:19:ASP:OD2	22:6T:11:THR:OG1	2.28	0.49
20:6C:71:ALA:O	20:6C:75:GLU:HG2	2.13	0.49
26:A:307:LYS:HD3	61:X:46:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BP:141:ASN:HB2	28:BP:192:TYR:HB2	1.95	0.49
31:C3:590:ASN:HA	31:C3:593:ILE:HG12	1.95	0.49
34:F:192:LEU:HB3	34:F:196:ALA:HB3	1.95	0.49
35:FS:26:ARG:NH1	36:G:252:GLU:OE1	2.46	0.49
42:M:51:ARG:NH2	153:M:305:CDL:OA6	2.46	0.49
44:M2:20:SER:O	44:M2:24:ASN:ND2	2.36	0.49
47:O:173:ARG:HD3	47:O:177:ARG:HH21	1.78	0.49
68:1B:49:VAL:HG13	102:N3:97:PHE:HE1	1.77	0.49
69:2B:23:LEU:HD11	69:2B:162:LEU:HD11	1.94	0.49
77:A7:164:TRP:CZ2	121:S2:268:SER:HB3	2.47	0.49
77:A7:183:ASP:OD1	121:S2:204:ASN:ND2	2.45	0.49
81:AC:38:PRO:HB2	81:AC:40:LYS:HG2	1.95	0.49
90:B8:90:TRP:CD2	104:N5:472:LEU:HD21	2.48	0.49
90:B8:146:GLU:OE1	90:B8:146:GLU:N	2.42	0.49
95:FX:105:SER:HB2	95:FX:108:GLN:HE21	1.77	0.49
96:G1:142:GLN:HG2	97:G2:137:VAL:HG11	1.93	0.49
107:P2:135:PRO:HG2	107:P2:138:LEU:HG	1.93	0.49
108:QA:295:ARG:HH12	108:QA:471:LEU:HB2	1.77	0.49
114:QG:7:ILE:HG22	114:QG:10:GLU:HG3	1.95	0.49
121:S2:169:MET:HE2	126:S7:127:PRO:HG3	1.94	0.49
133:T6:120:LEU:O	133:T6:124:ASN:ND2	2.35	0.49
26:a:418:GLY:H	26:a:435:LYS:HG3	1.77	0.49
29:c1:50:HIS:CE1	29:c1:51:LYS:HG2	2.48	0.49
35:fs:90:LEU:O	35:fs:131:SER:HA	2.13	0.49
37:h:32:LYS:O	37:h:36:GLN:HG2	2.13	0.49
37:h:99:LEU:O	37:h:104:SER:OG	2.31	0.49
153:m:306:CDL:H142	152:m:307:PC1:H241	1.94	0.49
152:m1:403:PC1:H241	152:m1:403:PC1:H352	1.93	0.49
50:r:89:THR:OG1	51:s:98:ASP:OD2	2.25	0.49
59:vb:419:ASP:OD2	59:vb:421:GLN:NE2	2.46	0.49
68:1b:28:ARG:NH1	121:s2:425:ASP:OD1	2.46	0.49
68:1b:49:VAL:HG13	102:n3:97:PHE:HE1	1.77	0.49
75:a5:82:SER:HB3	75:a5:106:VAL:HG13	1.94	0.49
92:bl:115:PHE:CE1	103:n4:432:GLY:HA3	2.48	0.49
96:g1:53:GLN:OE1	96:g1:207:GLN:NE2	2.39	0.49
101:n2:71:VAL:O	101:n2:75:ILE:HG12	2.12	0.49
153:qc:505:CDL:HB21	114:qg:130:ARG:HH12	1.77	0.49
113:qf:10:THR:OG1	113:qf:80:GLN:OE1	2.31	0.49
128:t1:224:LEU:HD11	128:t1:462:VAL:HG13	1.94	0.49
129:t2:119:GLY:HA2	129:t2:162:HIS:O	2.12	0.49
130:t3:203:HIS:ND1	130:t3:211:GLU:OE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6A:109:GLU:HG3	31:C3:349:LYS:HZ2	1.77	0.49
19:6B:157:GLN:HG2	30:C2:168:LEU:HD21	1.94	0.49
20:6C:18:ASP:HB3	29:C1:416:ARG:NH2	2.28	0.49
25:7L:913:ARG:HB2	25:7L:920:LEU:HD23	1.95	0.49
28:BP:203:ASP:O	28:BP:207:ASN:N	2.41	0.49
29:C1:432:TYR:OH	153:C1:708:CDL:OA7	2.23	0.49
153:C3:604:CDL:H192	46:N:124:PRO:HG2	1.94	0.49
42:M:122:ASN:HA	42:M:126:PRO:HG2	1.94	0.49
43:M1:107:ASP:CG	43:M1:151:SER:HB2	2.38	0.49
49:Q:53:GLY:O	49:Q:57:VAL:HG23	2.13	0.49
59:VB:151:THR:HG23	59:VB:199:ARG:HA	1.94	0.49
59:VB:419:ASP:OD2	59:VB:421:GLN:NE2	2.45	0.49
60:W:17:LEU:HD13	158:W:203:3PE:H11	1.94	0.49
64:Y5:36:ASN:HB3	64:Y5:39:VAL:HG12	1.95	0.49
69:2B:171:TYR:HA	94:C4:59:LEU:HD13	1.95	0.49
79:A9:222:PHE:HE2	152:TC:102:PC1:H11	1.78	0.49
101:N2:216:SER:O	124:S5:47:HIS:NE2	2.45	0.49
102:N3:50:ILE:HD11	121:S2:27:ASN:HB2	1.95	0.49
111:QD:87:MET:HG2	111:QD:162:PHE:HB2	1.95	0.49
108:Qa:420:THR:HG23	108:Qa:430:ILE:HD12	1.94	0.49
4:2g:153:TYR:HE2	8:2k:13:LYS:HG2	1.78	0.49
5:2h:123:CYS:SG	5:2h:124:ARG:HG2	2.53	0.49
8:2k:53:PRO:HG2	55:sd:41:ILE:HD11	1.95	0.49
13:2t:33:ASP:OD1	16:4t:42:ARG:NH2	2.33	0.49
29:c1:321:ALA:HB3	29:c1:326:ARG:HD2	1.94	0.49
38:i:122:TYR:OH	153:i:302:CDL:OB9	2.26	0.49
42:m:51:ARG:NH2	153:m:303:CDL:OA6	2.46	0.49
65:y7:163:ALA:O	65:y7:167:SER:OG	2.30	0.49
69:2b:113:TYR:HA	69:2b:116:ILE:HG12	1.94	0.49
71:5b:10:LYS:NZ	90:b8:82:GLU:OE2	2.36	0.49
76:a6:148:LEU:HD11	79:a9:251:LEU:HD21	1.95	0.49
77:a7:209:ARG:NH2	121:s2:190:GLU:OE1	2.45	0.49
79:a9:40:ILE:HD11	123:s4:117:THR:HA	1.94	0.49
79:a9:68:ASP:OD2	82:al:149:ARG:NH2	2.45	0.49
93:bm:105:TYR:HE2	158:bm:302:3PE:H341	1.77	0.49
97:g2:79:GLN:H	97:g2:100:HIS:CD2	2.29	0.49
98:g3:271:MET:HA	121:s2:416:LYS:HE3	1.94	0.49
101:n2:218:THR:HG23	101:n2:229:ILE:HG13	1.94	0.49
104:n5:203:ASN:HB3	104:n5:290:ASN:HD21	1.77	0.49
108:qA:417:LEU:O	108:qA:421:VAL:HG13	2.13	0.49
109:qB:207:THR:HB	109:qB:292:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
152:qE:301:PC1:H151	116:qI:41:LYS:H	1.77	0.49
110:qc:345:LYS:N	110:qc:411:GLU:OE1	2.33	0.49
112:qe:228:ARG:O	112:qe:230:ARG:N	2.45	0.49
114:qg:157:TRP:HB2	116:qi:6:LEU:HD11	1.94	0.49
114:qg:261:ASP:OD1	114:qg:261:ASP:N	2.44	0.49
121:s2:112:ALA:HB1	121:s2:118:ARG:HG3	1.95	0.49
4:2G:100:GLU:HB3	8:2K:22:LEU:HD21	1.93	0.49
30:C2:128:PHE:HB2	30:C2:411:LEU:HB3	1.94	0.49
38:I:57:THR:HB	153:I:302:CDL:H371	1.94	0.49
42:M:194:SER:HA	62:Y:1:MET:HE3	1.95	0.49
61:X:62:PHE:HE2	61:X:79:ILE:HG22	1.78	0.49
79:A9:40:ILE:HD11	123:S4:117:THR:HA	1.94	0.49
79:A9:137:TYR:O	79:A9:141:HIS:HB3	2.12	0.49
96:G1:147:LEU:HD12	96:G1:166:PRO:HD3	1.95	0.49
104:N5:203:ASN:HB3	104:N5:290:ASN:HD21	1.76	0.49
109:QB:311:PRO:HB3	109:QB:315:ASP:HB3	1.94	0.49
111:Qd:42:GLU:O	111:Qd:204:HIS:N	2.43	0.49
120:S1:525:GLU:OE1	120:S1:646:HIS:NE2	2.39	0.49
124:S5:74:TYR:OH	124:S5:79:ASP:OD1	2.31	0.49
127:S8:90:TYR:HB2	152:S8:301:PC1:H2	1.95	0.49
129:T2:237:THR:OG1	129:T2:286:ASP:N	2.45	0.49
133:T6:135:THR:HG23	135:T8:76:PRO:HB2	1.94	0.49
143:TG:65:ALA:HB3	143:TG:96:PHE:HZ	1.77	0.49
2:2e:153:LEU:HD23	2:2e:186:PRO:HG3	1.94	0.49
2:2e:279:THR:HG22	2:2e:281:HIS:H	1.78	0.49
5:2h:111:LYS:HD2	5:2h:192:LEU:HD13	1.95	0.49
31:c3:39:ARG:O	31:c3:43:ASN:ND2	2.46	0.49
153:c3:604:CDL:H192	46:n:124:PRO:HG2	1.94	0.49
33:e:257:ASP:OD1	33:e:281:HIS:ND1	2.29	0.49
40:k:191:SER:OG	48:p:26:GLN:O	2.22	0.49
41:l:174:THR:HG21	49:q:170:PRO:HA	1.95	0.49
153:t:204:CDL:HA61	153:t:204:CDL:HA22	1.95	0.49
69:2b:30:ILE:HD11	158:c4:402:3PE:H2D2	1.94	0.49
76:a6:67:ILE:HG22	76:a6:68:PRO:HD3	1.95	0.49
104:n5:360:THR:HG21	104:n5:390:LEU:HD21	1.94	0.49
104:n5:433:THR:OG1	104:n5:434:LEU:N	2.45	0.49
106:p1:40:GLN:O	106:p1:44:HIS:N	2.39	0.49
152:qB:602:PC1:H332	153:qg:402:CDL:H472	1.94	0.49
109:qb:74:ARG:HH21	109:qb:440:THR:HA	1.77	0.49
146:v1:245:ASN:ND2	171:v1:501:FMN:O2	2.36	0.49
23:7A:86:LEU:HD23	29:C1:150:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BP:423:PHE:HE1	28:BP:450:LEU:HD22	1.77	0.49
31:C3:164:ASN:OD1	31:C3:172:ARG:NH2	2.44	0.49
31:C3:516:TYR:OH	42:M:121:TYR:O	2.25	0.49
32:D:234:SER:O	32:D:336:ASN:ND2	2.37	0.49
32:D:378:ARG:HH12	152:D:501:PC1:H342	1.77	0.49
33:E:341:TYR:HB2	63:Y0:46:LEU:HD13	1.94	0.49
153:FS:204:CDL:HA22	153:FS:204:CDL:HA62	1.94	0.49
38:I:149:GLU:HG2	38:I:195:PRO:HB2	1.94	0.49
52:SA:315:MET:HG3	52:SA:324:ASP:HA	1.95	0.49
73:A2:21:GLN:NE2	120:S1:654:GLU:OE1	2.45	0.49
158:A3:201:3PE:H231	102:N3:112:LEU:HD11	1.93	0.49
92:BL:114:HIS:CG	103:N4:435:GLU:HG3	2.48	0.49
98:G3:263:GLU:HG3	105:N6:236:GLN:HA	1.94	0.49
99:J1:183:ASP:OD2	121:S2:15:ARG:NH1	2.42	0.49
108:QA:332:LEU:HD21	108:QA:397:THR:HB	1.94	0.49
109:QB:207:THR:HB	109:QB:292:MET:HE3	1.95	0.49
109:Qb:74:ARG:HH21	109:Qb:440:THR:HA	1.77	0.49
109:Qb:143:ARG:NH2	109:Qb:202:GLU:OE1	2.44	0.49
110:Qc:194:TYR:CE2	110:Qc:198:ILE:HD11	2.48	0.49
153:Qc:505:CDL:HB21	114:Qg:130:ARG:HH12	1.78	0.49
112:Qe:140:GLY:N	112:Qe:156:ARG:O	2.46	0.49
137:TA:100:ARG:NH1	137:TA:104:ASP:OD2	2.41	0.49
149:C:137:PHE:O	149:C:140:VAL:HG22	2.12	0.49
19:6b:104:ASN:HD21	30:c2:573:LEU:HD23	1.78	0.49
23:7a:35:TYR:O	23:7a:39:ARG:NH1	2.45	0.49
24:7c:78:ASN:OD1	36:g:132:LYS:NZ	2.46	0.49
34:f:178:ILE:HD11	34:f:207:ALA:HB3	1.94	0.49
36:g:158:THR:HG23	36:g:163:VAL:HA	1.95	0.49
37:h:295:LYS:O	104:N5:86:LYS:NZ	2.42	0.49
43:m1:199:PHE:HD1	153:m1:402:CDL:H521	1.78	0.49
59:vb:377:GLU:HA	59:vb:380:LYS:HZ2	1.77	0.49
69:2b:171:TYR:HA	94:c4:59:LEU:HD13	1.95	0.49
70:4l:25:ASN:O	70:4l:29:ILE:HG13	2.13	0.49
75:a5:98:TYR:HB2	122:s3:14:VAL:HG13	1.95	0.49
84:an:221:HIS:NE2	103:n4:225:ASN:O	2.46	0.49
89:b7:11:GLN:NE2	131:t4:212:TYR:O	2.38	0.49
91:b9:162:HIS:O	103:n4:53:LYS:NZ	2.35	0.49
104:n5:67:ILE:HG13	37:H:82:LYS:HE2	1.94	0.49
104:n5:251:ASP:H	104:n5:254:SER:HB3	1.78	0.49
110:qC:345:LYS:N	110:qC:411:GLU:OE1	2.26	0.49
128:t1:405:ALA:HB3	128:t1:440:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:7L:907:TRP:CG	25:7L:908:PRO:HD3	2.47	0.49
26:A:230:ASN:O	26:A:233:GLU:HG2	2.12	0.49
30:C2:83:CYS:HA	30:C2:86:PRO:HD2	1.94	0.49
37:H:99:LEU:O	37:H:104:SER:OG	2.30	0.49
40:K:82:LEU:O	40:K:86:TYR:N	2.28	0.49
153:M3:403:CDL:H731	153:M3:403:CDL:HA61	1.94	0.49
47:O:69:MET:O	47:O:74:LYS:NZ	2.45	0.49
51:S:78:TYR:OH	64:Y5:95:ILE:HG12	2.12	0.49
52:SA:62:ARG:NH1	52:SA:143:TYR:OH	2.45	0.49
83:AM:109:ASP:O	83:AM:113:ASN:ND2	2.35	0.49
96:G1:217:ASN:HD22	96:G1:218:SER:N	2.10	0.49
101:N2:76:THR:HB	148:X1:16:LEU:HB3	1.95	0.49
101:N2:218:THR:HG23	101:N2:229:ILE:HG13	1.95	0.49
101:N2:236:ILE:HD13	124:S5:41:GLU:HB2	1.94	0.49
104:N5:537:ASP:OD2	104:N5:539:LYS:NZ	2.35	0.49
106:P1:235:GLU:HG2	106:P1:237:GLN:H	1.76	0.49
110:Qc:326:LYS:HA	110:Qc:341:ILE:O	2.13	0.49
120:S1:387:MET:HE3	120:S1:474:MET:HE1	1.95	0.49
120:S1:510:GLY:O	120:S1:512:ASN:ND2	2.46	0.49
121:S2:400:LYS:HE3	121:S2:402:LYS:HB2	1.95	0.49
132:T5:126:SER:OG	153:T5:301:CDL:OA4	2.20	0.49
133:T6:36:MET:HG3	133:T6:42:LEU:HD13	1.93	0.49
135:T8:50:ILE:HB	135:T8:51:PRO:HD3	1.95	0.49
18:6a:15:ILE:HD11	59:vb:312:VAL:HG21	1.95	0.48
26:a:276:THR:OG1	40:k:182:GLN:NE2	2.46	0.48
29:c1:378:ASP:OD1	29:c1:378:ASP:N	2.45	0.48
153:c1:709:CDL:H532	152:c3:605:PC1:H251	1.95	0.48
33:e:189:ASP:N	33:e:189:ASP:OD1	2.45	0.48
38:i:45:ASN:O	38:i:49:ASN:HB2	2.13	0.48
153:i:302:CDL:H562	25:7L:862:LEU:HD22	1.93	0.48
57:u:21:TYR:O	57:u:25:GLU:HB2	2.13	0.48
64:y5:39:VAL:HG22	64:y5:46:LYS:HG3	1.95	0.48
69:2b:23:LEU:HD11	69:2b:162:LEU:HD11	1.94	0.48
90:b8:139:LEU:HB2	90:b8:141:LEU:HD13	1.95	0.48
92:bl:135:GLN:NE2	103:n4:86:PHE:O	2.34	0.48
153:bm:301:CDL:H251	153:bm:301:CDL:H212	1.94	0.48
153:n5:806:CDL:H561	153:n5:806:CDL:H781	1.94	0.48
108:qA:411:GLU:OE1	109:qB:428:SER:N	2.44	0.48
120:s1:510:GLY:O	120:s1:512:ASN:ND2	2.46	0.48
142:tf:102:LYS:HZ1	142:tf:132:ALA:HB3	1.78	0.48
3:2F:137:ARG:HD3	152:2F:301:PC1:H341	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E:77:VAL:HG21	33:E:157:ILE:HD11	1.94	0.48
153:M:304:CDL:H312	60:W:22:PRO:HB3	1.93	0.48
43:M1:62:LEU:O	43:M1:65:THR:OG1	2.24	0.48
46:N:79:PRO:HG3	153:N:304:CDL:H151	1.94	0.48
50:R:85:PRO:HG3	64:Y5:74:SER:HB3	1.94	0.48
57:U:21:TYR:O	57:U:25:GLU:HB2	2.13	0.48
65:Y7:168:ILE:HG21	149:C:171:VAL:HG11	1.94	0.48
72:A1:18:PRO:HB3	153:A1:102:CDL:HB61	1.95	0.48
77:A7:19:TRP:HA	121:S2:201:THR:HG21	1.95	0.48
77:A7:93:TYR:OH	77:A7:116:GLU:OE1	2.22	0.48
82:AL:6:TRP:NE1	82:AL:28:THR:O	2.44	0.48
103:N4:314:ILE:HG12	103:N4:444:LEU:HD12	1.94	0.48
105:N6:241:GLN:NE2	121:S2:221:ILE:O	2.44	0.48
109:Qb:473:ASP:OD2	116:Qi:60:GLN:NE2	2.36	0.48
110:Qc:49:GLY:O	110:Qc:53:ALA:N	2.45	0.48
122:S3:198:LEU:HD22	127:S8:149:ARG:HB3	1.93	0.48
127:S8:71:ASP:N	127:S8:71:ASP:OD1	2.45	0.48
130:T3:167:SER:HA	130:T3:289:THR:HG21	1.95	0.48
144:TH:78:LYS:NZ	153:TH:200:CDL:OA4	2.38	0.48
4:2g:19:LEU:HD13	4:2g:53:LEU:HA	1.94	0.48
19:6b:157:GLN:HG2	30:c2:168:LEU:HD21	1.94	0.48
23:7a:39:ARG:HD3	26:a:428:GLN:HE22	1.77	0.48
24:7c:155:PHE:HB3	152:m1:401:PC1:H2A1	1.95	0.48
26:a:364:VAL:HG13	26:a:378:VAL:HG13	1.93	0.48
153:a:504:CDL:H311	31:c3:259:TYR:HB2	1.95	0.48
35:fs:26:ARG:NH1	36:g:252:GLU:OE1	2.45	0.48
42:m:118:HIS:NE2	152:m:301:PC1:O12	2.46	0.48
42:m:201:LYS:NZ	153:I:303:CDL:OA3	2.45	0.48
153:m:302:CDL:H312	60:w:22:PRO:HB3	1.93	0.48
45:m3:151:SER:HB3	45:m3:162:VAL:HG21	1.94	0.48
51:s:78:TYR:OH	64:y5:95:ILE:HG12	2.12	0.48
52:sa:335:MET:HE2	52:sa:392:PRO:HD3	1.95	0.48
52:sa:445:SER:HB2	161:sa:701:FAD:N1	2.28	0.48
64:y5:36:ASN:HB3	64:y5:39:VAL:HG12	1.95	0.48
83:am:113:ASN:O	83:am:117:SER:OG	2.22	0.48
100:n1:131:ILE:HG21	105:n6:90:PHE:HB3	1.95	0.48
104:n5:251:ASP:OD2	104:n5:444:ARG:NH1	2.34	0.48
104:n5:309:PHE:HD1	104:n5:350:LEU:HD23	1.77	0.48
104:n5:565:LEU:HD11	153:n5:806:CDL:H642	1.95	0.48
152:n5:805:PC1:H252	106:p1:140:VAL:HB	1.95	0.48
110:qC:61:MET:HE3	111:qd:124:TYR:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qc:72:VAL:HG13	110:qc:73:GLU:HG2	1.95	0.48
110:qc:244:VAL:O	110:qc:248:MET:HB2	2.12	0.48
121:s2:138:ALA:HB1	121:s2:143:SER:HB2	1.93	0.48
129:t2:223:ARG:NH1	129:t2:258:ASN:OD1	2.46	0.48
130:t3:166:LEU:HD23	130:t3:169:PHE:HZ	1.77	0.48
2:2E:104:SER:O	2:2E:108:GLY:N	2.36	0.48
43:M1:261:GLU:OE1	43:M1:303:LYS:NZ	2.44	0.48
153:Q:202:CDL:H542	153:Q:202:CDL:H732	1.95	0.48
153:T:204:CDL:H622	153:T:204:CDL:H571	1.95	0.48
59:VB:231:LEU:HD22	153:VB:706:CDL:HB22	1.95	0.48
69:2B:10:ASN:HD21	94:C4:70:GLN:CD	2.21	0.48
69:2B:113:TYR:HA	69:2B:116:ILE:HG12	1.94	0.48
69:2B:136:TYR:HH	96:G1:42:SER:HG	1.58	0.48
73:A2:51:VAL:O	73:A2:52:ARG:NH1	2.39	0.48
79:A9:106:ASP:OD1	79:A9:145:LYS:NZ	2.45	0.48
96:G1:53:GLN:OE1	96:G1:207:GLN:NE2	2.40	0.48
97:G2:103:VAL:HG11	97:G2:211:ASN:HB3	1.95	0.48
105:N6:7:THR:HG21	105:N6:13:ILE:HA	1.94	0.48
106:P1:162:VAL:HG13	130:T3:207:ILE:HD12	1.95	0.48
111:QD:96:LEU:HD11	111:QD:102:GLN:HA	1.96	0.48
111:QD:168:ARG:NE	151:QD:401:HEC:O2A	2.44	0.48
111:QD:293:ARG:NH1	114:QG:304:ALA:O	2.46	0.48
109:Qb:99:GLU:O	109:Qb:281:ASN:ND2	2.45	0.48
116:Qi:100:THR:O	116:Qi:103:THR:OG1	2.23	0.48
121:S2:239:VAL:HG12	121:S2:279:ARG:HG2	1.95	0.48
2:2e:82:VAL:HG22	2:2e:115:VAL:HG23	1.95	0.48
5:2h:94:TYR:OH	9:2l:14:VAL:O	2.25	0.48
29:c1:231:LEU:HA	29:c1:237:MET:SD	2.53	0.48
34:f:192:LEU:HB3	34:f:196:ALA:HB3	1.95	0.48
37:h:133:GLY:O	37:h:219:ASN:ND2	2.46	0.48
38:i:57:THR:HB	153:i:301:CDL:H371	1.95	0.48
41:l:148:ARG:NH2	59:vb:567:PRO:O	2.29	0.48
45:m3:129:TYR:CE1	153:vb:701:CDL:H792	2.49	0.48
52:sa:62:ARG:NH1	52:sa:143:TYR:OH	2.47	0.48
59:vb:86:ILE:O	59:vb:90:ILE:HG13	2.14	0.48
63:y0:52:GLU:OE1	63:y0:54:LYS:NZ	2.45	0.48
66:z:55:VAL:O	66:z:59:SER:HB3	2.14	0.48
69:2b:120:ARG:NH2	95:fx:88:ASN:HD22	2.10	0.48
70:4l:11:ILE:HB	105:n6:46:PHE:CE2	2.46	0.48
92:bl:114:HIS:CG	103:n4:435:GLU:HG3	2.48	0.48
153:bm:301:CDL:H541	103:n4:499:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
94:c4:49:ASP:O	94:c4:52:ARG:HG2	2.13	0.48
106:p1:162:VAL:HG13	130:t3:207:ILE:HD12	1.95	0.48
109:qB:76:ALA:O	109:qB:249:ALA:HA	2.12	0.48
110:qC:207:TRP:NE1	166:qC:502:HEM:O2A	2.32	0.48
111:qD:71:ARG:NE	116:qI:105:GLU:OE1	2.46	0.48
111:qD:145:PHE:N	111:qD:149:GLN:OE1	2.42	0.48
110:qc:194:TYR:CE2	110:qc:198:ILE:HD11	2.48	0.48
126:s7:32:CYS:HB3	126:s7:66:ALA:HB1	1.94	0.48
127:s8:26:ILE:HG13	127:s8:27:HIS:HD2	1.79	0.48
19:6B:52:HIS:O	19:6B:56:ASN:ND2	2.38	0.48
153:7A:203:CDL:H521	31:C3:283:TYR:HA	1.95	0.48
152:7C:303:PC1:H31	44:M2:208:LYS:HD3	1.95	0.48
29:C1:231:LEU:HA	29:C1:237:MET:SD	2.53	0.48
152:C3:606:PC1:H151	153:T:204:CDL:HB21	1.95	0.48
41:L:78:ILE:HD11	41:L:173:TYR:HB2	1.95	0.48
153:M:301:CDL:H142	152:M:302:PC1:H241	1.94	0.48
52:SA:296:THR:HG22	52:SA:371:ILE:HG12	1.95	0.48
59:VB:201:ARG:NH2	59:VB:207:GLU:OE1	2.46	0.48
69:2B:120:ARG:NH2	95:FX:88:ASN:HD22	2.10	0.48
76:A6:67:ILE:HG22	76:A6:68:PRO:HD3	1.95	0.48
79:A9:128:GLN:HG2	79:A9:305:GLU:HA	1.95	0.48
79:A9:234:GLN:HG2	79:A9:263:GLY:H	1.79	0.48
83:AM:55:ALA:HB2	137:TA:82:MET:HG3	1.95	0.48
92:BL:115:PHE:CE1	103:N4:432:GLY:HA3	2.48	0.48
111:QD:77:PHE:O	111:QD:82:GLY:N	2.43	0.48
112:QE:37:LYS:NZ	145:TX:129:GLU:O	2.30	0.48
110:Qc:345:LYS:N	110:Qc:411:GLU:OE1	2.32	0.48
128:T1:358:LEU:HD23	128:T1:376:ILE:HG13	1.94	0.48
2:2e:91:PRO:HG3	53:sb:312:LEU:HB3	1.94	0.48
22:6t:62:LEU:O	22:6t:64:LYS:NZ	2.31	0.48
24:7c:118:TYR:HB2	24:7c:122:ASP:HB2	1.94	0.48
24:7c:127:CYS:SG	24:7c:128:GLU:N	2.86	0.48
27:b:364:LYS:HG2	27:b:468:GLU:HG2	1.95	0.48
29:c1:105:MET:HE1	154:c1:702:HEA:H162	1.94	0.48
29:c1:322:MET:HE2	36:g:215:PRO:HG2	1.96	0.48
33:e:9:ARG:H	33:e:235:ASN:HD22	1.61	0.48
38:i:104:TYR:HE1	152:i:304:PC1:H2	1.78	0.48
41:l:78:ILE:HD11	41:l:173:TYR:HB2	1.95	0.48
153:m3:403:CDL:H731	153:m3:403:CDL:HA61	1.94	0.48
46:n:79:PRO:HG3	153:n:304:CDL:H151	1.94	0.48
59:vb:113:HIS:NE2	59:vb:125:ASP:OD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:x:62:PHE:HE2	61:x:79:ILE:HG22	1.77	0.48
77:a7:183:ASP:OD1	121:s2:204:ASN:ND2	2.45	0.48
79:a9:222:PHE:HE2	152:tc:102:PC1:H11	1.77	0.48
152:am:202:PC1:H221	102:n3:3:ASP:HA	1.95	0.48
152:c4:403:PC1:H252	135:t8:55:PHE:HZ	1.78	0.48
97:g2:36:ASP:OD1	97:g2:37:ILE:N	2.47	0.48
101:n2:166:ILE:HD13	105:n6:202:LEU:HB2	1.95	0.48
110:qC:72:VAL:HG13	110:qC:73:GLU:HG2	1.94	0.48
109:qb:513:VAL:HG21	115:qh:32:LYS:HG2	1.96	0.48
110:qc:49:GLY:O	110:qc:53:ALA:N	2.46	0.48
120:s1:198:LYS:HG2	120:s1:207:ILE:HD12	1.95	0.48
120:s1:214:THR:OG1	120:s1:708:GLU:OE1	2.27	0.48
126:s7:95:SER:N	162:s7:201:SF4:S3	2.87	0.48
21:6L:43:GLU:O	21:6L:46:VAL:HG22	2.13	0.48
27:B:364:LYS:HG2	27:B:468:GLU:HG2	1.95	0.48
28:BP:138:TRP:CE2	28:BP:140:GLN:HB3	2.49	0.48
29:C1:262:THR:HG22	29:C1:265:SER:H	1.78	0.48
154:C1:702:HEA:HBA2	154:C1:702:HEA:CMA	2.42	0.48
30:C2:141:LYS:HG2	30:C2:604:TRP:CZ2	2.49	0.48
39:J:85:LEU:HB3	39:J:193:GLN:HE22	1.78	0.48
152:M:302:PC1:H251	152:M:302:PC1:H362	1.94	0.48
45:M3:129:TYR:CE1	153:VB:701:CDL:H792	2.48	0.48
49:Q:166:ASP:OD1	49:Q:167:TYR:N	2.45	0.48
69:2B:24:ASN:HB3	101:N2:351:PHE:CE1	2.49	0.48
158:A3:201:3PE:H2F1	102:N3:101:PHE:HE2	1.79	0.48
87:B4:68:ARG:NH2	103:N4:386:HIS:O	2.43	0.48
94:C4:49:ASP:O	94:C4:52:ARG:HG2	2.13	0.48
104:N5:476:PHE:CE1	152:N5:803:PC1:H321	2.49	0.48
106:P1:173:ILE:HD13	106:P1:194:LEU:HD21	1.94	0.48
107:P2:39:LEU:HD11	107:P2:88:PHE:HB2	1.95	0.48
110:QC:353:LEU:HD23	114:QG:66:PHE:HB3	1.96	0.48
109:Qb:169:GLN:HG2	109:Qb:270:VAL:HG22	1.96	0.48
112:Qe:70:ILE:HD11	114:Qg:121:ARG:HD2	1.94	0.48
121:S2:40:VAL:HG11	121:S2:62:LEU:HD13	1.95	0.48
123:S4:94:HIS:CD2	123:S4:97:PRO:HB3	2.48	0.48
126:S7:95:SER:N	162:S7:201:SF4:S3	2.86	0.48
128:T1:224:LEU:HD11	128:T1:462:VAL:HG13	1.95	0.48
128:T1:405:ALA:HB3	128:T1:440:TYR:CZ	2.49	0.48
129:T2:223:ARG:NH1	129:T2:258:ASN:OD1	2.47	0.48
61:x:80:GLY:O	61:x:83:PRO:HD2	2.12	0.48
65:y7:428:PHE:HA	65:y7:431:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:4l:69:LEU:HD11	105:n6:195:GLY:HA3	1.94	0.48
78:a8:119:GLN:NE2	83:am:85:LEU:O	2.37	0.48
86:b3:54:LEU:HD12	153:n5:806:CDL:H741	1.96	0.48
88:b6:90:PRO:HD3	132:t5:125:TRP:CZ2	2.49	0.48
104:n5:54:PHE:HE1	104:n5:94:LEU:HA	1.78	0.48
105:n6:7:THR:HG21	105:n6:13:ILE:HA	1.94	0.48
108:qa:311:SER:HA	108:qa:454:VAL:HG22	1.95	0.48
116:qi:38:ILE:O	153:qi:202:CDL:O1	2.32	0.48
116:qi:100:THR:O	116:qi:103:THR:OG1	2.23	0.48
120:s1:141:GLN:NE2	162:s1:801:SF4:S3	2.87	0.48
120:s1:265:ASP:HB2	120:s1:273:ARG:HG2	1.96	0.48
120:s1:387:MET:HE3	120:s1:474:MET:HE1	1.95	0.48
123:s4:12:ARG:HG2	123:s4:140:GLU:HB3	1.95	0.48
130:t3:167:SER:HA	130:t3:289:THR:HG21	1.95	0.48
27:B:196:TYR:HE2	27:B:204:TYR:HB2	1.78	0.48
36:G:107:TYR:HD2	58:V:79:ARG:HH21	1.62	0.48
152:I:301:PC1:H321	153:I:302:CDL:H461	1.95	0.48
47:O:124:HIS:CE1	47:O:128:THR:HG21	2.48	0.48
52:SA:329:ASP:OD2	52:SA:634:ARG:NH2	2.35	0.48
53:SB:34:SER:HA	93:BM:97:PRO:HG3	1.96	0.48
59:VB:114:GLU:OE2	59:VB:218:TYR:OH	2.25	0.48
70:4L:25:ASN:O	70:4L:29:ILE:HG13	2.13	0.48
75:A5:98:TYR:HB2	122:S3:14:VAL:HG13	1.95	0.48
79:A9:117:ASN:HA	79:A9:156:VAL:HA	1.95	0.48
83:AM:113:ASN:O	83:AM:117:SER:OG	2.22	0.48
153:AM:201:CDL:H131	153:T7:201:CDL:H362	1.96	0.48
84:AN:72:ALA:HB2	84:AN:112:TYR:CG	2.49	0.48
95:FX:76:GLY:O	95:FX:163:ASN:ND2	2.32	0.48
96:G1:72:THR:OG1	96:G1:91:ASN:O	2.26	0.48
96:G1:216:TYR:HB2	97:G2:24:LEU:HD13	1.96	0.48
100:N1:41:LEU:HD13	100:N1:66:GLN:HB3	1.94	0.48
108:QA:252:CYS:SG	108:QA:421:VAL:HG11	2.53	0.48
111:QD:71:ARG:NE	116:QI:105:GLU:OE1	2.46	0.48
115:QH:102:PHE:HB3	115:QH:103:PRO:HD3	1.93	0.48
121:S2:355:GLU:OE1	121:S2:355:GLU:N	2.47	0.48
129:T2:275:ILE:HD11	129:T2:283:LEU:HD13	1.95	0.48
145:TX:49:TYR:HE1	145:TX:98:PRO:HB3	1.79	0.48
149:C:173:SER:HB3	149:C:179:LEU:HD21	1.96	0.48
2:2e:283:GLU:HG2	2:2e:284:LEU:H	1.79	0.48
20:6c:71:ALA:O	20:6c:75:GLU:HG2	2.13	0.48
31:c3:590:ASN:HA	31:c3:593:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:e:403:CDL:HB32	35:FS:84:PHE:HB3	1.94	0.48
36:g:113:GLU:HA	36:g:116:MET:HE2	1.95	0.48
43:m1:246:THR:HG23	43:m1:312:MET:HE3	1.95	0.48
52:sa:418:ASP:N	52:sa:418:ASP:OD1	2.47	0.48
59:vb:231:LEU:HD22	153:vb:704:CDL:HB22	1.94	0.48
69:2b:149:ILE:HG23	153:2b:201:CDL:H311	1.94	0.48
70:4l:10:LEU:HD11	105:n6:130:LEU:HD22	1.95	0.48
73:a2:52:ARG:HD2	120:s1:646:HIS:HE1	1.79	0.48
101:n2:192:VAL:HG22	101:n2:272:ILE:HA	1.96	0.48
101:n2:236:ILE:HD13	124:s5:41:GLU:HB2	1.95	0.48
101:n2:289:PHE:CE2	101:n2:344:THR:HG23	2.49	0.48
103:n4:4:LEU:HD22	144:th:39:LEU:HD13	1.96	0.48
104:n5:476:PHE:CE1	152:n5:803:PC1:H321	2.49	0.48
111:qD:87:MET:HG2	111:qD:162:PHE:HB2	1.95	0.48
108:qa:322:PHE:HE2	108:qa:454:VAL:HG21	1.79	0.48
109:qb:212:HIS:CE1	109:qb:281:ASN:HB3	2.49	0.48
114:qg:198:TRP:CD2	152:qg:401:PC1:H231	2.48	0.48
121:s2:169:MET:O	121:s2:170:HIS:ND1	2.47	0.48
129:t2:92:LYS:HA	129:t2:196:VAL:HG22	1.95	0.48
131:t4:89:ILE:HG12	131:t4:202:LEU:HD11	1.95	0.48
146:v1:86:ARG:O	146:v1:88:ARG:NH1	2.47	0.48
4:2G:53:LEU:HG	4:2G:88:PHE:CE2	2.48	0.48
5:2H:188:LEU:O	5:2H:192:LEU:HG	2.12	0.48
8:2K:53:PRO:HG2	55:SD:41:ILE:HD11	1.95	0.48
18:6A:15:ILE:HD11	59:VB:312:VAL:HG21	1.95	0.48
29:C1:349:ILE:HD13	29:C1:392:PRO:HB2	1.94	0.48
30:C2:213:ASN:O	30:C2:216:SER:OG	2.30	0.48
35:FS:90:LEU:O	35:FS:131:SER:HA	2.14	0.48
52:SA:274:PRO:HB3	52:SA:601:TRP:CE2	2.48	0.48
52:SA:504:MET:HG3	52:SA:561:LEU:HD23	1.96	0.48
153:T:204:CDL:HA22	153:T:204:CDL:HA61	1.95	0.48
59:VB:377:GLU:HA	59:VB:380:LYS:HZ2	1.78	0.48
74:A3:102:THR:HA	101:N2:2:LEU:HD13	1.95	0.48
80:AB:60:LYS:HA	80:AB:132:LEU:HD21	1.95	0.48
153:BM:301:CDL:H251	153:BM:301:CDL:H212	1.94	0.48
153:BM:301:CDL:H741	103:N4:497:PHE:HD1	1.79	0.48
104:N5:604:PHE:HZ	104:N5:710:LEU:HD22	1.79	0.48
152:N5:805:PC1:H252	106:P1:140:VAL:HB	1.95	0.48
153:N5:806:CDL:H561	153:N5:806:CDL:H781	1.95	0.48
111:QD:56:TRP:NE1	111:QD:173:ASN:OD1	2.40	0.48
110:Qc:329:VAL:O	118:Ql:7:LYS:NZ	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
129:T2:92:LYS:HA	129:T2:196:VAL:HG22	1.96	0.48
144:TH:24:PRO:HD2	144:TH:29:LEU:HD21	1.95	0.48
146:V1:159:ILE:HD11	146:V1:170:LEU:HD23	1.94	0.48
146:V1:385:PRO:HB2	146:V1:424:THR:HG22	1.95	0.48
3:2f:152:LYS:NZ	54:sc:57:GLU:OE1	2.37	0.48
4:2g:61:GLU:OE1	4:2g:89:ASN:ND2	2.45	0.48
25:7l:913:ARG:HB2	25:7l:920:LEU:HD23	1.95	0.48
152:c3:606:PC1:H151	153:t:204:CDL:HB21	1.95	0.48
153:i:301:CDL:H461	152:i:304:PC1:H321	1.94	0.48
43:m1:56:LEU:HD21	43:m1:80:MET:HE1	1.95	0.48
62:y:60:TRP:CE2	62:y:64:LEU:HD11	2.49	0.48
72:a1:41:PRO:HA	83:am:168:ASN:HA	1.95	0.48
79:a9:117:ASN:HA	79:a9:156:VAL:HA	1.95	0.48
92:bl:166:ARG:NH2	136:t9:13:ASP:OD2	2.38	0.48
97:g2:162:GLU:HG2	135:t8:22:VAL:HG11	1.95	0.48
103:n4:110:LYS:NZ	135:t8:72:SER:O	2.39	0.48
103:n4:384:ARG:HH12	103:n4:483:GLU:CD	2.20	0.48
104:n5:537:ASP:OD2	104:n5:539:LYS:NZ	2.35	0.48
110:qC:83:LEU:HD12	152:qC:505:PC1:H362	1.95	0.48
110:qC:169:THR:HG1	110:qC:177:THR:HG1	1.56	0.48
110:qC:232:GLY:HA3	111:qD:271:LYS:HG3	1.95	0.48
110:qC:238:ILE:HD12	152:qI:202:PC1:H2I1	1.96	0.48
114:qG:192:LEU:O	114:qG:198:TRP:NE1	2.32	0.48
109:qb:90:VAL:HG23	109:qb:164:LEU:HD13	1.96	0.48
109:qb:141:VAL:HG22	109:qb:146:THR:HG23	1.96	0.48
121:s2:411:LEU:HD22	121:s2:440:ILE:HD13	1.94	0.48
128:t1:177:HIS:HE2	128:t1:197:THR:HG1	1.60	0.48
133:t6:135:THR:HG23	135:t8:76:PRO:HB2	1.96	0.48
135:t8:50:ILE:HB	135:t8:51:PRO:HD3	1.95	0.48
144:th:112:ARG:NE	144:th:116:GLU:OE2	2.43	0.48
2:2E:69:LEU:HD22	53:SB:312:LEU:HD11	1.94	0.48
153:C1:712:CDL:H141	30:C2:56:ALA:HB1	1.95	0.48
38:I:40:VAL:HG12	38:I:44:GLN:HE21	1.79	0.48
45:M3:154:SER:HB2	45:M3:158:ASN:HB3	1.96	0.48
48:P:99:PHE:CG	48:P:100:PRO:HA	2.49	0.48
57:U:126:CYS:C	57:U:138:ARG:HD2	2.39	0.48
90:B8:52:THR:HG23	103:N4:328:THR:HG23	1.94	0.48
97:G2:162:GLU:HG2	135:T8:22:VAL:HG11	1.96	0.48
98:G3:271:MET:HA	121:S2:416:LYS:HE3	1.95	0.48
100:N1:163:ILE:HG12	100:N1:212:LEU:HG	1.95	0.48
104:N5:54:PHE:HD2	104:N5:146:LEU:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
112:QE:39:HIS:O	112:QE:41:GLY:N	2.41	0.48
113:QF:23:LEU:HG	113:QF:27:HIS:CE1	2.48	0.48
152:QJ:102:PC1:H142	110:Qc:3:TRP:CD2	2.49	0.48
128:T1:30:GLN:OE1	128:T1:477:TYR:OH	2.22	0.48
129:T2:82:GLU:OE1	129:T2:82:GLU:N	2.46	0.48
130:T3:147:LEU:HG	130:T3:151:LYS:HE2	1.95	0.48
136:T9:94:ILE:HD12	136:T9:130:ALA:HB2	1.94	0.48
20:6c:18:ASP:HB3	29:c1:416:ARG:NH2	2.28	0.48
28:bp:398:ILE:HD13	28:bp:412:THR:HG22	1.96	0.48
29:c1:464:MET:HB2	29:c1:465:PRO:HD3	1.95	0.48
29:c1:507:TRP:HZ2	30:c2:37:TRP:CD1	2.32	0.48
29:c1:574:ALA:HA	29:c1:604:SER:HA	1.94	0.48
29:c1:583:PHE:HE1	30:c2:34:GLN:HE22	1.60	0.48
31:c3:525:GLU:HB2	153:t:202:CDL:H721	1.95	0.48
153:f:401:CDL:H561	153:f:401:CDL:H361	1.96	0.48
44:m2:33:PRO:HG2	152:m2:405:PC1:H2B1	1.96	0.48
158:m3:402:3PE:H2A1	158:m3:402:3PE:H2E1	1.95	0.48
59:vb:151:THR:OG1	59:vb:154:THR:HB	2.14	0.48
59:vb:297:PHE:HE2	64:y5:185:ILE:HD12	1.78	0.48
74:a3:15:ASN:HB3	74:a3:18:ARG:HB2	1.96	0.48
80:ab:60:LYS:HA	80:ab:132:LEU:HD21	1.95	0.48
82:al:6:TRP:NE1	82:al:28:THR:O	2.44	0.48
84:an:72:ALA:HB2	84:an:112:TYR:CG	2.49	0.48
99:j1:299:ARG:O	99:j1:302:GLY:N	2.45	0.48
104:n5:314:LEU:HD23	104:n5:317:LEU:HD21	1.94	0.48
109:qB:499:ARG:NH2	109:qB:505:TYR:HB3	2.29	0.48
110:qC:353:LEU:HD23	114:qG:66:PHE:HB3	1.95	0.48
153:qI:203:CDL:HB31	153:qI:203:CDL:HA32	1.96	0.48
109:qb:96:THR:HG21	109:qb:218:THR:HA	1.96	0.48
110:qc:24:THR:HB	110:qc:219:GLU:HB2	1.96	0.48
129:t2:36:ARG:NH2	129:t2:41:ASN:OD1	2.46	0.48
5:2H:117:ARG:NH1	11:2N:56:ASP:OD1	2.46	0.48
14:3T:30:LEU:HD22	22:6T:19:LYS:HG2	1.95	0.48
27:B:284:ASP:OD1	27:B:284:ASP:N	2.46	0.48
29:C1:192:LEU:HD21	32:D:331:ILE:HD11	1.95	0.48
37:H:235:PHE:HB2	37:H:241:VAL:HG21	1.95	0.48
48:P:129:VAL:HB	48:P:133:ARG:HE	1.79	0.48
53:SB:277:MET:HG3	54:SC:19:PHE:CE1	2.49	0.48
153:T:204:CDL:H801	153:T:204:CDL:H841	1.96	0.48
73:A2:52:ARG:HD2	120:S1:646:HIS:HE1	1.79	0.48
74:A3:92:ILE:O	102:N3:90:THR:OG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:B8:135:ARG:HH12	92:BL:100:ASP:HB3	1.79	0.48
109:Qb:141:VAL:HG22	109:Qb:146:THR:HG23	1.96	0.48
110:Qc:264:ASP:OD2	111:Qd:89:TYR:OH	2.26	0.48
112:Qe:50:PHE:HZ	112:Qe:67:LYS:HE3	1.78	0.48
113:Qf:10:THR:OG1	113:Qf:80:GLN:OE1	2.31	0.48
114:Qg:198:TRP:CD2	152:Qg:401:PC1:H231	2.48	0.48
116:Qi:38:ILE:O	153:Qi:202:CDL:O1	2.32	0.48
123:S4:133:ASN:OD1	123:S4:133:ASN:N	2.36	0.48
127:S8:26:ILE:HG13	127:S8:27:HIS:HD2	1.79	0.48
127:S8:95:CYS:HA	127:S8:99:TYR:CD2	2.47	0.48
3:2f:295:SER:HB2	6:2i:76:GLN:HG3	1.96	0.48
5:2h:117:ARG:NH1	11:2n:56:ASP:OD1	2.46	0.48
7:2j:102:ARG:HD2	9:2l:16:ARG:HH22	1.78	0.48
19:6b:230:TYR:O	62:y:101:ARG:NE	2.41	0.48
28:bp:423:PHE:HE1	28:bp:450:LEU:HD22	1.78	0.48
29:c1:331:LEU:HB3	59:vb:175:LEU:HD22	1.96	0.48
30:c2:141:LYS:HG2	30:c2:604:TRP:CZ2	2.49	0.48
31:c3:552:SER:N	49:q:142:GLN:OE1	2.45	0.48
33:e:246:PRO:HG3	36:g:318:ILE:HB	1.96	0.48
35:fs:59:ILE:HG22	36:g:83:TYR:HB3	1.96	0.48
42:m:122:ASN:HA	42:m:126:PRO:HG2	1.94	0.48
44:m2:84:SER:HB2	44:m2:163:LEU:HD13	1.96	0.48
64:y5:164:TYR:HB3	64:y5:168:GLY:HA3	1.95	0.48
77:a7:19:TRP:HA	121:s2:201:THR:HG21	1.95	0.48
79:a9:267:TYR:HE1	98:g3:345:LYS:HG3	1.78	0.48
101:n2:28:PHE:CZ	102:n3:109:TYR:HB2	2.49	0.48
101:n2:216:SER:O	124:s5:47:HIS:NE2	2.46	0.48
102:n3:50:ILE:HD11	121:s2:27:ASN:HB2	1.95	0.48
108:qA:252:CYS:SG	108:qA:421:VAL:HG11	2.53	0.48
110:qC:98:HIS:CE1	110:qC:102:LYS:HE3	2.48	0.48
112:qE:107:ALA:HB2	152:qI:202:PC1:H2A1	1.96	0.48
110:qc:65:MET:HG2	111:qd:89:TYR:CD1	2.49	0.48
112:qe:122:LYS:HE2	112:qe:261:HIS:HB3	1.95	0.48
129:t2:82:GLU:OE1	129:t2:82:GLU:N	2.46	0.48
132:t5:86:LEU:HD21	138:tb:112:GLN:HG2	1.95	0.48
145:tx:82:ILE:HG21	145:tx:89:LYS:HD2	1.95	0.48
2:2E:30:VAL:HG22	2:2E:59:GLU:HB3	1.96	0.48
4:2G:12:LEU:HD23	4:2G:65:ILE:HG23	1.96	0.48
4:2G:153:TYR:HE2	8:2K:13:LYS:HG2	1.78	0.48
7:2J:50:VAL:HG11	7:2J:69:VAL:HG13	1.96	0.48
26:A:364:VAL:HG13	26:A:378:VAL:HG13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C1:583:PHE:HE1	30:C2:34:GLN:HE22	1.61	0.48
31:C3:383:LEU:HG	59:VB:93:THR:HG21	1.95	0.48
35:FS:118:VAL:HG22	36:G:233:TYR:HD1	1.79	0.48
44:M2:84:SER:HB2	44:M2:163:LEU:HD13	1.96	0.48
158:M3:402:3PE:H2A1	158:M3:402:3PE:H2E1	1.95	0.48
52:SA:288:ILE:HD12	52:SA:293:CYS:HB2	1.95	0.48
59:VB:151:THR:OG1	59:VB:154:THR:HB	2.14	0.48
59:VB:426:LYS:O	63:Y0:60:TYR:OH	2.24	0.48
68:1B:10:ILE:HD11	100:N1:257:MET:HG3	1.96	0.48
69:2B:149:ILE:HG23	153:2B:201:CDL:H311	1.94	0.48
82:AL:18:VAL:HG12	82:AL:50:TYR:HE1	1.79	0.48
92:BL:129:ASN:HB3	136:T9:17:GLY:HA3	1.96	0.48
98:G3:199:ARG:O	98:G3:203:GLN:HG2	2.14	0.48
103:N4:4:LEU:HD22	144:TH:39:LEU:HD13	1.96	0.48
114:QG:70:TRP:CH2	153:QH:201:CDL:H111	2.49	0.48
120:S1:131:ILE:HG23	127:S8:137:ILE:HD12	1.94	0.48
120:S1:265:ASP:HB2	120:S1:273:ARG:HG2	1.95	0.48
144:TH:54:ASP:OD2	144:TH:113:ARG:NH2	2.28	0.48
146:V1:202:ALA:HB3	147:V2:109:TYR:CD1	2.49	0.48
2:2e:30:VAL:HG22	2:2e:59:GLU:HB3	1.96	0.48
2:2e:249:LEU:HD11	2:2e:271:ASN:HB3	1.95	0.48
3:2f:95:LEU:HD21	5:2h:128:LEU:HD21	1.96	0.48
4:2g:53:LEU:HG	4:2g:88:PHE:CE2	2.49	0.48
27:b:284:ASP:OD1	27:b:284:ASP:N	2.46	0.48
35:fs:118:VAL:HG22	36:g:233:TYR:HD1	1.79	0.48
49:q:53:GLY:O	49:q:57:VAL:HG23	2.13	0.48
153:t:204:CDL:H571	153:t:204:CDL:H622	1.95	0.48
153:t:204:CDL:H801	153:t:204:CDL:H841	1.96	0.48
77:a7:55:ASP:HB3	121:s2:339:LYS:HE2	1.96	0.48
77:a7:79:PRO:HD2	77:a7:90:ARG:HH22	1.79	0.48
89:b7:118:TRP:CZ2	104:n5:698:ASN:HB3	2.48	0.48
153:bm:301:CDL:H741	103:n4:497:PHE:HD1	1.79	0.48
98:g3:199:ARG:O	98:g3:203:GLN:HG2	2.14	0.48
98:g3:241:ASP:OD1	101:n2:53:LYS:NZ	2.44	0.48
104:n5:604:PHE:HZ	104:n5:710:LEU:HD22	1.79	0.48
153:n5:806:CDL:H611	153:n5:806:CDL:H722	1.95	0.48
106:p1:110:GLY:HA3	130:t3:207:ILE:HD13	1.96	0.48
111:qD:293:ARG:NH1	114:qG:304:ALA:O	2.47	0.48
110:qc:98:HIS:CE1	110:qc:102:LYS:HE3	2.49	0.48
120:s1:70:LEU:O	123:s4:166:LYS:NZ	2.36	0.48
121:s2:400:LYS:HE3	121:s2:402:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2E:212:ALA:HA	2:2E:284:LEU:HG	1.96	0.48
2:2E:279:THR:HG22	2:2E:281:HIS:H	1.78	0.48
19:6B:216:PHE:HD1	56:T:143:LEU:HB3	1.79	0.48
24:7C:118:TYR:HB2	24:7C:122:ASP:HB2	1.95	0.48
24:7C:155:PHE:HB3	152:M1:401:PC1:H2A1	1.95	0.48
26:A:417:ASP:HA	26:A:435:LYS:O	2.14	0.48
29:C1:322:MET:HE2	36:G:215:PRO:HG2	1.95	0.48
29:C1:574:ALA:HA	29:C1:604:SER:HA	1.95	0.48
31:C3:381:TRP:O	59:VB:93:THR:OG1	2.31	0.48
32:D:300:ARG:NH1	32:D:370:GLU:O	2.45	0.48
33:E:189:ASP:OD1	33:E:189:ASP:N	2.46	0.48
38:I:110:TYR:HB3	50:R:173:ILE:HG21	1.96	0.48
42:M:10:ASN:HD21	42:M:22:LYS:HG2	1.78	0.48
43:M1:199:PHE:HD1	153:M1:402:CDL:H521	1.78	0.48
44:M2:156:TRP:HZ3	44:M2:256:ARG:HG3	1.79	0.48
158:M2:408:3PE:H31	153:N:304:CDL:HA62	1.96	0.48
158:M2:408:3PE:H332	153:N:304:CDL:H121	1.96	0.48
152:W:201:PC1:H3A2	152:W:201:PC1:H2A2	1.95	0.48
68:1B:28:ARG:NH1	121:S2:425:ASP:OD1	2.46	0.48
71:5B:50:ILE:O	71:5B:54:THR:OG1	2.24	0.48
79:A9:267:TYR:HE1	98:G3:345:LYS:HG3	1.77	0.48
83:AM:48:ARG:HH12	137:TA:74:GLU:HB3	1.79	0.48
88:B6:90:PRO:HD3	132:T5:125:TRP:CZ2	2.49	0.48
89:B7:118:TRP:CZ2	104:N5:698:ASN:HB3	2.48	0.48
101:N2:166:ILE:HD13	105:N6:202:LEU:HB2	1.95	0.48
152:N5:805:PC1:H391	153:P1:403:CDL:H361	1.96	0.48
110:QC:284:PRO:O	110:QC:287:ALA:HB3	2.14	0.48
111:QD:205:MET:HE1	113:QF:63:ARG:HB2	1.96	0.48
108:Qa:308:LEU:HD23	108:Qa:360:LEU:HB3	1.96	0.48
110:Qc:72:VAL:HG13	110:Qc:73:GLU:HG2	1.96	0.48
110:Qc:304:TYR:HE1	153:Qg:402:CDL:H541	1.78	0.48
111:Qd:288:GLU:OE1	111:Qd:290:TYR:OH	2.26	0.48
127:S8:71:ASP:OD2	127:S8:73:THR:OG1	2.25	0.48
149:c:92:LEU:HD12	149:c:92:LEU:H	1.79	0.48
149:c:173:SER:HB3	149:c:179:LEU:HD21	1.95	0.48
26:a:341:VAL:HG22	152:a:501:PC1:H2B2	1.95	0.47
29:c1:221:TYR:HE2	46:n:193:LEU:HD12	1.79	0.47
153:c1:712:CDL:H202	30:c2:56:ALA:HB2	1.95	0.47
30:c2:128:PHE:HB2	30:c2:411:LEU:HB3	1.97	0.47
30:c2:507:THR:OG1	30:c2:527:CYS:SG	2.61	0.47
33:e:129:SER:HB3	33:e:190:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:348:ASP:OD1	33:e:348:ASP:N	2.46	0.47
34:f:283:GLU:HG3	34:f:306:MET:HA	1.95	0.47
52:sa:590:ASP:HB3	52:sa:594:TRP:HB2	1.96	0.47
75:a5:86:LEU:HG	75:a5:106:VAL:HG11	1.96	0.47
90:b8:64:TYR:O	104:n5:334:LYS:NZ	2.34	0.47
90:b8:135:ARG:HH12	92:bl:100:ASP:HB3	1.79	0.47
108:qA:412:ARG:NH1	114:qG:322:PHE:O	2.40	0.47
110:qC:284:PRO:O	110:qC:287:ALA:HB3	2.14	0.47
110:qC:418:PHE:HZ	114:qG:86:LEU:HD13	1.79	0.47
108:qa:308:LEU:HD23	108:qa:360:LEU:HB3	1.95	0.47
113:qf:9:ALA:O	113:qf:12:SER:HB3	2.14	0.47
135:t8:78:ASP:OD1	135:t8:78:ASP:N	2.46	0.47
2:2E:283:GLU:HG2	2:2E:284:LEU:H	1.79	0.47
23:7A:128:ASP:OD1	23:7A:129:ARG:N	2.47	0.47
24:7C:78:ASN:OD1	36:G:132:LYS:NZ	2.46	0.47
26:A:105:MET:HE1	36:G:173:GLY:HA3	1.96	0.47
28:BP:397:LYS:HE3	28:BP:399:VAL:HG12	1.96	0.47
29:C1:342:THR:HB	29:C1:396:VAL:HG13	1.95	0.47
31:C3:39:ARG:O	31:C3:43:ASN:ND2	2.46	0.47
34:F:176:ALA:O	34:F:179:PRO:HD2	2.14	0.47
35:FS:59:ILE:HG22	36:G:83:TYR:HB3	1.96	0.47
36:G:113:GLU:HA	36:G:116:MET:HE2	1.95	0.47
153:M:304:CDL:H161	152:M:307:PC1:H222	1.95	0.47
46:N:169:ARG:NH2	152:N:301:PC1:O12	2.34	0.47
53:SB:212:LEU:HB3	53:SB:246:ARG:HB2	1.96	0.47
59:VB:86:ILE:O	59:VB:90:ILE:HG13	2.13	0.47
74:A3:15:ASN:HB3	74:A3:18:ARG:HB2	1.95	0.47
96:G1:109:THR:HG22	99:J1:118:ASP:HA	1.95	0.47
109:QB:199:LEU:O	109:QB:203:ASN:ND2	2.43	0.47
111:Qd:113:THR:HG23	111:Qd:131:GLU:HB2	1.96	0.47
146:V1:220:LYS:HG2	147:V2:65:ARG:HE	1.79	0.47
146:V1:312:TRP:NE1	146:V1:334:ASP:OD1	2.44	0.47
1:1t:71:TYR:HE2	30:c2:312:SER:HB2	1.80	0.47
7:2j:50:VAL:HG11	7:2j:69:VAL:HG13	1.96	0.47
15:4a:105:ASP:OD2	42:m:41:ARG:NH2	2.39	0.47
28:bp:263:THR:O	28:bp:268:SER:OG	2.32	0.47
29:c1:62:MET:HA	154:c1:702:HEA:H211	1.96	0.47
33:e:145:HIS:HB3	153:e:402:CDL:HB21	1.96	0.47
35:fs:118:VAL:O	36:g:93:ARG:NH1	2.42	0.47
42:m:198:ARG:HE	62:y:7:GLN:HE21	1.61	0.47
47:o:173:ARG:HD3	47:o:177:ARG:HH21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:sa:236:ARG:HB2	52:sa:473:LEU:HD21	1.96	0.47
52:sa:270:ARG:HG3	52:sa:605:VAL:HG21	1.97	0.47
52:sa:504:MET:HG3	52:sa:561:LEU:HD23	1.96	0.47
65:y7:168:ILE:HG21	149:c:171:VAL:HG11	1.95	0.47
87:b4:72:GLU:O	87:b4:76:VAL:HG23	2.14	0.47
100:n1:284:LEU:HD11	134:t7:27:LYS:HA	1.95	0.47
104:n5:73:THR:HG22	37:H:258:ARG:HH11	1.79	0.47
104:n5:112:LEU:HB3	104:n5:116:LEU:HD12	1.96	0.47
104:n5:684:ASN:O	104:n5:687:SER:OG	2.26	0.47
109:qB:363:ILE:HB	109:qB:382:TYR:HB3	1.96	0.47
111:qd:42:GLU:O	111:qd:204:HIS:N	2.42	0.47
134:t7:115:THR:OG1	137:ta:106:ASP:HB3	2.14	0.47
27:B:377:ILE:HD13	65:Y7:421:ILE:HG23	1.96	0.47
42:M:118:HIS:NE2	152:M:303:PC1:O12	2.46	0.47
52:SA:335:MET:HE2	52:SA:392:PRO:HD3	1.94	0.47
64:Y5:164:TYR:HB3	64:Y5:168:GLY:HA3	1.96	0.47
77:A7:98:GLN:HG3	77:A7:101:ASN:HD21	1.79	0.47
77:A7:252:ASP:OD1	77:A7:252:ASP:N	2.48	0.47
79:A9:356:THR:HB	79:A9:359:ASN:HD22	1.77	0.47
81:AC:110:ASP:OD1	81:AC:110:ASP:N	2.47	0.47
87:B4:144:ASP:OD2	103:N4:11:ARG:NH1	2.47	0.47
97:G2:177:ARG:NH1	138:TB:50:ALA:O	2.47	0.47
101:N2:28:PHE:CZ	102:N3:109:TYR:HB2	2.49	0.47
104:N5:54:PHE:HE1	104:N5:94:LEU:HA	1.78	0.47
109:QB:499:ARG:NH2	109:QB:505:TYR:HB3	2.29	0.47
110:QC:203:MET:HE2	166:QC:502:HEM:HAA2	1.96	0.47
152:QE:301:PC1:H151	116:QI:41:LYS:H	1.78	0.47
117:QJ:40:LEU:HA	152:QJ:101:PC1:H332	1.94	0.47
109:Qb:200:LEU:HD23	109:Qb:380:TYR:HD1	1.80	0.47
110:Qc:24:THR:HB	110:Qc:219:GLU:HB2	1.97	0.47
120:S1:141:GLN:NE2	162:S1:801:SF4:S3	2.87	0.47
120:S1:181:THR:N	162:S1:802:SF4:S4	2.86	0.47
120:S1:198:LYS:HG2	120:S1:207:ILE:HD12	1.95	0.47
149:C:92:LEU:HD12	149:C:92:LEU:H	1.78	0.47
20:6c:4:VAL:HG21	153:E:403:CDL:H552	1.97	0.47
29:c1:30:PHE:HE2	153:c1:703:CDL:H121	1.80	0.47
29:c1:126:HIS:HB3	29:c1:333:PRO:HD2	1.96	0.47
29:c1:568:SER:HB3	153:c1:712:CDL:H832	1.96	0.47
38:i:104:TYR:OH	152:i:304:PC1:O22	2.19	0.47
41:l:78:ILE:HG23	41:l:176:MET:HG3	1.96	0.47
158:m2:408:3PE:H332	153:n:304:CDL:H121	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:o:124:HIS:CE1	47:o:128:THR:HG21	2.48	0.47
53:sb:73:VAL:HB	53:sb:90:TYR:HE2	1.79	0.47
56:t:66:GLY:O	56:t:70:THR:OG1	2.28	0.47
62:y:26:TRP:NE1	62:y:85:TYR:OH	2.34	0.47
63:y0:41:ILE:HB	63:y0:56:LEU:HB2	1.96	0.47
77:a7:93:TYR:OH	77:a7:116:GLU:OE1	2.22	0.47
91:b9:142:SER:HB2	91:b9:152:PHE:HZ	1.79	0.47
102:n3:81:VAL:HB	105:n6:178:TYR:CZ	2.49	0.47
103:n4:275:SER:HB3	103:n4:379:ASP:HB2	1.97	0.47
114:qG:70:TRP:CH2	153:qH:201:CDL:H111	2.50	0.47
160:qh:201:PX2:H40	160:qh:201:PX2:H35	1.69	0.47
152:qi:203:PC1:H251	117:qj:34:TRP:HB2	1.96	0.47
121:s2:263:TYR:HB3	142:tf:52:SER:HB3	1.96	0.47
129:t2:237:THR:OG1	129:t2:286:ASP:N	2.47	0.47
130:t3:147:LEU:HG	130:t3:151:LYS:HE2	1.95	0.47
146:v1:399:ARG:NH2	146:v1:409:GLU:OE1	2.40	0.47
3:2F:95:LEU:HD21	5:2H:128:LEU:HD21	1.96	0.47
26:A:315:ALA:HB2	31:C3:407:TYR:CE2	2.50	0.47
153:A:504:CDL:H311	31:C3:259:TYR:HB2	1.95	0.47
29:C1:62:MET:HA	154:C1:702:HEA:H211	1.96	0.47
30:C2:112:LEU:HB2	30:C2:501:VAL:HG22	1.96	0.47
33:E:145:HIS:HB3	153:E:402:CDL:HB21	1.96	0.47
33:E:246:PRO:HG3	36:G:318:ILE:HB	1.96	0.47
52:SA:236:ARG:HB2	52:SA:473:LEU:HD21	1.96	0.47
62:Y:60:TRP:CE2	62:Y:64:LEU:HD11	2.49	0.47
69:2B:87:LEU:HD11	69:2B:166:ILE:HD11	1.97	0.47
77:A7:55:ASP:HB3	121:S2:339:LYS:HE2	1.96	0.47
152:AM:202:PC1:H221	102:N3:3:ASP:HA	1.95	0.47
86:B3:34:PHE:HA	86:B3:37:VAL:HG22	1.96	0.47
87:B4:72:GLU:O	87:B4:76:VAL:HG23	2.14	0.47
99:J1:160:VAL:HG11	99:J1:163:LYS:HD2	1.95	0.47
101:N2:152:PHE:HB3	105:N6:187:ILE:HG21	1.96	0.47
106:P1:110:GLY:HA3	130:T3:207:ILE:HD13	1.97	0.47
153:P1:403:CDL:HA62	153:P1:403:CDL:H141	1.97	0.47
112:QE:152:ILE:HA	112:QE:195:ALA:H	1.80	0.47
153:Qb:601:CDL:H721	110:Qc:20:PHE:HB2	1.96	0.47
110:Qc:270:ASP:OD1	110:Qc:270:ASP:N	2.47	0.47
112:Qe:122:LYS:HE2	112:Qe:261:HIS:HB3	1.96	0.47
120:S1:234:ASN:OD1	120:S1:293:HIS:NE2	2.42	0.47
121:S2:226:TYR:CE1	121:S2:244:CYS:HB3	2.49	0.47
121:S2:303:LYS:HA	142:TF:84:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
127:S8:171:ASP:HB3	127:S8:174:LYS:HB2	1.95	0.47
132:T5:86:LEU:HD21	138:TB:112:GLN:HG2	1.96	0.47
139:TC:2:VAL:HB	139:TC:4:GLN:HG2	1.96	0.47
145:TX:82:ILE:HG21	145:TX:89:LYS:HD2	1.96	0.47
26:a:315:ALA:HB2	31:c3:407:TYR:CE2	2.49	0.47
28:bp:214:CYS:SG	28:bp:215:GLY:N	2.88	0.47
29:c1:225:SER:HB2	46:n:199:ALA:HB2	1.97	0.47
153:c1:703:CDL:HA4	153:c1:703:CDL:H511	1.96	0.47
44:m2:224:LEU:HD11	44:m2:293:ALA:HB1	1.96	0.47
52:sa:329:ASP:OD2	52:sa:634:ARG:NH2	2.34	0.47
52:sa:621:THR:HG21	52:sa:626:VAL:HG11	1.97	0.47
59:vb:180:LEU:HG	59:vb:197:LEU:HB2	1.96	0.47
69:2b:50:LEU:HD21	101:n2:339:PHE:HB2	1.97	0.47
158:a3:201:3PE:H2F1	102:n3:101:PHE:HE2	1.78	0.47
77:a7:76:SER:OG	122:s3:21:LYS:NZ	2.39	0.47
79:a9:75:HIS:ND1	167:a9:401:NDP:O1X	2.38	0.47
85:b2:44:ASP:OD1	104:n5:646:ASN:ND2	2.47	0.47
99:j1:160:VAL:HG11	99:j1:163:LYS:HD2	1.95	0.47
103:n4:19:TYR:OH	103:n4:106:PRO:O	2.29	0.47
128:t1:380:ASN:ND2	128:t1:383:TYR:H	2.13	0.47
129:t2:275:ILE:HD11	129:t2:283:LEU:HD13	1.95	0.47
144:th:24:PRO:HD2	144:th:29:LEU:HD21	1.95	0.47
5:2H:111:LYS:HD2	5:2H:192:LEU:HD13	1.95	0.47
8:2K:49:ILE:HG23	55:SD:38:TYR:HB2	1.96	0.47
24:7C:152:ILE:HG23	152:M1:401:PC1:H271	1.96	0.47
29:C1:429:VAL:HB	42:M:105:ALA:HB1	1.96	0.47
29:C1:439:GLY:HA3	29:C1:455:TYR:CD2	2.50	0.47
29:C1:507:TRP:HZ2	30:C2:37:TRP:CD1	2.32	0.47
153:C1:707:CDL:HA4	153:C1:707:CDL:H511	1.97	0.47
38:I:104:TYR:HE1	152:I:301:PC1:H2	1.79	0.47
39:J:67:ILE:HD13	39:J:160:LEU:HD12	1.96	0.47
50:R:89:THR:OG1	51:S:98:ASP:OD2	2.25	0.47
53:SB:69:LYS:NZ	53:SB:149:ASP:O	2.35	0.47
72:A1:41:PRO:HA	83:AM:168:ASN:HA	1.95	0.47
86:B3:54:LEU:HD12	153:N5:806:CDL:H741	1.96	0.47
96:G1:220:TYR:OH	97:G2:27:ASP:OD2	2.17	0.47
101:N2:289:PHE:CE2	101:N2:344:THR:HG23	2.49	0.47
111:QD:246:VAL:HG12	111:QD:250:ARG:HD2	1.97	0.47
153:QI:203:CDL:HB31	153:QI:203:CDL:HA32	1.96	0.47
109:Qb:96:THR:HG21	109:Qb:218:THR:HA	1.96	0.47
109:Qb:513:VAL:HG21	115:Qh:32:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:Qd:79:ARG:HD2	111:Qd:218:VAL:HG13	1.96	0.47
121:S2:33:GLN:HG2	126:S7:27:PHE:HB2	1.96	0.47
121:S2:112:ALA:HB1	121:S2:118:ARG:HG3	1.95	0.47
121:S2:169:MET:O	121:S2:170:HIS:ND1	2.48	0.47
14:3t:8:ASP:OD1	14:3t:8:ASP:N	2.41	0.47
152:6a:202:PC1:H152	31:c3:360:ILE:HG23	1.96	0.47
19:6b:78:MET:HG3	30:c2:1:MET:HE3	1.97	0.47
24:7c:163:HIS:NE2	152:7c:303:PC1:O14	2.23	0.47
29:c1:75:ILE:CG2	154:c1:702:HEA:HMA	2.45	0.47
37:h:235:PHE:HB2	37:h:241:VAL:HG21	1.95	0.47
39:j:112:LYS:HA	39:j:117:GLN:HE21	1.78	0.47
44:m2:244:ARG:NH1	44:m2:273:GLU:OE2	2.42	0.47
48:p:39:VAL:HA	48:p:118:LEU:O	2.15	0.47
153:q:202:CDL:H542	153:q:202:CDL:H732	1.96	0.47
53:sb:116:LEU:HD11	53:sb:168:LEU:HD13	1.96	0.47
74:a3:57:LEU:HD21	102:n3:111:TRP:CE2	2.50	0.47
74:a3:92:ILE:O	102:n3:90:THR:OG1	2.27	0.47
97:g2:103:VAL:HG11	97:g2:211:ASN:HB3	1.96	0.47
98:g3:275:LEU:HB2	105:n6:225:LYS:HG2	1.96	0.47
101:n2:50:ILE:HG13	101:n2:51:ILE:HD12	1.95	0.47
152:n5:805:PC1:H391	153:p1:403:CDL:H361	1.95	0.47
106:p1:169:HIS:CD2	106:p1:170:LEU:HG	2.50	0.47
108:qA:297:LEU:HD21	108:qa:209:LYS:HD2	1.95	0.47
110:qC:1:MET:HG3	153:qb:601:CDL:H531	1.96	0.47
110:qC:203:MET:HE2	166:qC:502:HEM:HAA2	1.96	0.47
152:qJ:101:PC1:H142	110:qc:3:TRP:CD2	2.48	0.47
110:qc:264:ASP:OD2	111:qd:89:TYR:OH	2.25	0.47
114:qg:106:ASN:ND2	114:qg:165:TYR:OH	2.40	0.47
153:qg:402:CDL:H712	118:ql:9:LEU:HD21	1.96	0.47
126:s7:45:ASP:HB3	126:s7:48:ARG:HG3	1.95	0.47
128:t1:330:TYR:O	128:t1:333:THR:OG1	2.28	0.47
130:t3:166:LEU:HA	130:t3:169:PHE:CZ	2.50	0.47
144:th:61:LEU:HD13	144:th:106:THR:HB	1.97	0.47
1:1T:64:ARG:NE	30:C2:313:ASP:OD2	2.47	0.47
5:2H:133:GLU:HB3	5:2H:136:LYS:HZ2	1.79	0.47
7:2J:102:ARG:HD2	9:2L:16:ARG:HH22	1.79	0.47
29:C1:126:HIS:HB3	29:C1:333:PRO:HD2	1.96	0.47
152:C1:711:PC1:H11	152:C3:605:PC1:H262	1.97	0.47
153:F:402:CDL:H361	153:F:402:CDL:H561	1.96	0.47
52:SA:247:TYR:OH	52:SA:567:THR:OG1	2.26	0.47
52:SA:621:THR:HG21	52:SA:626:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:1B:41:ILE:HG13	100:N1:169:LEU:HD11	1.97	0.47
73:A2:78:ASN:HD22	73:A2:82:GLU:HB3	1.78	0.47
74:A3:57:LEU:HD21	102:N3:111:TRP:CE2	2.50	0.47
76:A6:88:ASN:ND2	76:A6:133:LEU:O	2.41	0.47
77:A7:183:ASP:HB3	77:A7:186:ALA:HB3	1.95	0.47
96:G1:128:THR:HG21	98:G3:149:MET:HB2	1.96	0.47
100:N1:115:SER:OG	100:N1:117:PHE:O	2.32	0.47
100:N1:138:MET:HA	100:N1:153:SER:HB2	1.97	0.47
101:N2:192:VAL:HG22	101:N2:272:ILE:HA	1.96	0.47
103:N4:269:THR:O	103:N4:273:ALA:N	2.41	0.47
104:N5:81:ILE:HD13	104:N5:84:LYS:HB2	1.94	0.47
110:QC:238:ILE:HD12	152:QI:202:PC1:H2I1	1.96	0.47
110:Qc:305:TYR:O	110:Qc:308:ILE:HG22	2.14	0.47
152:Qi:203:PC1:H251	117:Qj:34:TRP:HB2	1.96	0.47
126:S7:45:ASP:HB3	126:S7:48:ARG:HG3	1.95	0.47
127:S8:123:GLU:OE1	127:S8:195:ASN:ND2	2.45	0.47
128:T1:330:TYR:O	128:T1:333:THR:OG1	2.30	0.47
132:T5:167:ARG:NH2	138:TB:99:THR:O	2.30	0.47
152:7c:303:PC1:H31	44:m2:208:LYS:HD3	1.95	0.47
26:a:166:ASP:OD1	64:y5:190:TYR:OH	2.32	0.47
26:a:351:ILE:HD11	31:c3:465:VAL:HG13	1.97	0.47
28:bp:175:GLU:HB2	28:bp:246:ASP:HB2	1.95	0.47
29:c1:105:MET:HB3	154:c1:702:HEA:CAC	2.44	0.47
29:c1:581:LEU:HD21	29:c1:600:TRP:HB2	1.96	0.47
31:c3:383:LEU:HG	59:vb:93:THR:HG21	1.95	0.47
33:e:216:THR:O	33:e:220:VAL:HG22	2.15	0.47
51:s:43:LYS:HB2	59:vb:500:TYR:CZ	2.49	0.47
59:vb:201:ARG:NH2	59:vb:207:GLU:OE1	2.45	0.47
69:2b:24:ASN:HB3	101:n2:351:PHE:CE1	2.49	0.47
69:2b:87:LEU:HD11	69:2b:166:ILE:HD11	1.97	0.47
74:a3:102:THR:HA	101:n2:2:LEU:HD13	1.95	0.47
77:a7:183:ASP:HB3	77:a7:186:ALA:HB3	1.96	0.47
80:ab:72:SER:HB2	80:ab:79:LEU:HD11	1.95	0.47
81:ac:110:ASP:OD1	81:ac:110:ASP:N	2.47	0.47
153:bm:301:CDL:HA32	132:t5:138:ILE:HD13	1.96	0.47
101:n2:76:THR:HB	148:x1:16:LEU:HB3	1.96	0.47
104:n5:54:PHE:HD2	104:n5:146:LEU:HD22	1.79	0.47
104:n5:533:ARG:NH2	104:n5:627:GLN:OE1	2.40	0.47
107:p2:27:MET:HG2	107:p2:148:PHE:HZ	1.80	0.47
107:p2:39:LEU:HD11	107:p2:88:PHE:HB2	1.96	0.47
108:qa:150:TYR:CE2	108:qa:152:LYS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:qb:175:LYS:HA	109:qb:230:ASP:HB3	1.96	0.47
109:qb:295:ARG:HB3	115:qh:58:PHE:HB3	1.96	0.47
109:qb:499:ARG:NH2	109:qb:505:TYR:HB3	2.30	0.47
120:s1:385:TYR:O	120:s1:515:HIS:NE2	2.40	0.47
123:s4:94:HIS:CD2	123:s4:97:PRO:HB3	2.49	0.47
29:C1:221:TYR:HE2	46:N:193:LEU:HD12	1.79	0.47
37:H:32:LYS:O	37:H:36:GLN:HG2	2.14	0.47
42:M:198:ARG:HE	62:Y:7:GLN:HE21	1.61	0.47
153:M2:404:CDL:H342	153:M2:404:CDL:H111	1.97	0.47
63:Y0:41:ILE:HB	63:Y0:56:LEU:HB2	1.96	0.47
66:Z:55:VAL:O	66:Z:59:SER:HB3	2.14	0.47
85:B2:44:ASP:OD1	104:N5:646:ASN:ND2	2.47	0.47
153:BM:301:CDL:H531	153:T5:301:CDL:H432	1.96	0.47
102:N3:81:VAL:HB	105:N6:178:TYR:CZ	2.50	0.47
110:QC:72:VAL:HG13	110:QC:73:GLU:HG2	1.96	0.47
114:QG:81:THR:HG21	114:QG:145:ARG:HB3	1.96	0.47
114:QG:87:LEU:HA	114:QG:154:ILE:HG12	1.96	0.47
121:S2:263:TYR:HB3	142:TF:52:SER:HB3	1.97	0.47
141:TE:40:ASN:ND2	153:TE:101:CDL:OB4	2.48	0.47
146:V1:118:SER:HB2	146:V1:246:VAL:HG11	1.97	0.47
2:2e:125:GLU:HG2	7:2j:59:ALA:HB1	1.96	0.47
2:2e:148:GLU:O	2:2e:209:ARG:HA	2.15	0.47
3:2f:188:PRO:HD3	152:2f:302:PC1:H342	1.97	0.47
4:2g:178:ASP:HB2	54:sc:2:ARG:HG3	1.96	0.47
8:2k:41:VAL:HG13	153:2m:101:CDL:H632	1.97	0.47
18:6a:77:GLN:HG2	153:6a:201:CDL:HA22	1.96	0.47
18:6a:102:TYR:OH	31:c3:356:ARG:NH1	2.48	0.47
26:a:417:ASP:HA	26:a:435:LYS:O	2.14	0.47
29:c1:262:THR:HG22	29:c1:265:SER:H	1.79	0.47
29:c1:342:THR:HB	29:c1:396:VAL:HG13	1.96	0.47
32:d:311:ARG:HD2	32:d:373:LEU:HD22	1.96	0.47
33:e:12:ARG:HH22	59:vb:429:GLU:HG2	1.79	0.47
33:e:97:GLN:O	33:e:100:ASN:HB2	2.15	0.47
34:f:169:TYR:OH	51:S:169:LEU:O	2.26	0.47
153:fs:203:CDL:HA22	153:fs:203:CDL:HA62	1.95	0.47
37:h:258:ARG:HH11	104:N5:73:THR:HG22	1.79	0.47
39:j:62:GLU:HA	39:j:179:LEU:HD11	1.97	0.47
43:m1:293:SER:HA	43:m1:296:TYR:CE2	2.50	0.47
44:m2:156:TRP:HZ3	44:m2:256:ARG:HG3	1.80	0.47
44:m2:249:ASN:OD1	44:m2:250:ALA:N	2.48	0.47
158:m2:408:3PE:H31	153:n:304:CDL:HA62	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:n:60:MET:HG3	152:n:303:PC1:H342	1.97	0.47
46:n:106:GLY:N	46:n:110:ILE:O	2.34	0.47
48:p:31:LEU:O	48:p:175:HIS:NE2	2.41	0.47
48:p:120:LEU:HD21	48:p:165:LEU:HD11	1.97	0.47
52:sa:412:GLN:HB3	52:sa:601:TRP:HZ2	1.79	0.47
56:t:75:ILE:O	56:t:78:PHE:HB3	2.15	0.47
57:u:126:CYS:C	57:u:138:ARG:HD2	2.39	0.47
63:y0:33:PHE:O	64:y5:171:LYS:NZ	2.34	0.47
64:y5:138:LYS:HB2	160:y5:204:PX2:H2	1.97	0.47
65:y7:145:TYR:HB3	65:y7:157:LEU:HD21	1.97	0.47
68:1b:10:ILE:HD11	100:n1:257:MET:HG3	1.97	0.47
69:2b:10:ASN:HD21	94:c4:70:GLN:CD	2.21	0.47
71:5b:50:ILE:O	71:5b:54:THR:OG1	2.24	0.47
74:a3:77:ASP:CG	137:ta:97:ARG:HH12	2.22	0.47
79:a9:106:ASP:OD1	79:a9:145:LYS:NZ	2.45	0.47
79:a9:128:GLN:HG2	79:a9:305:GLU:HA	1.96	0.47
79:a9:210:ARG:NH2	79:a9:305:GLU:OE2	2.42	0.47
83:am:49:LYS:HE3	83:am:49:LYS:HB2	1.73	0.47
152:am:202:PC1:C21	105:n6:74:CYS:HB3	2.45	0.47
85:b2:41:SER:HB2	85:b2:44:ASP:HB2	1.96	0.47
96:g1:147:LEU:HD12	96:g1:166:PRO:HD3	1.95	0.47
100:n1:159:LEU:HD11	100:n1:221:LEU:HB2	1.97	0.47
101:n2:316:LEU:O	101:n2:320:ILE:HG12	2.15	0.47
104:n5:293:MET:O	104:n5:297:ILE:HG12	2.15	0.47
153:p1:403:CDL:H141	153:p1:403:CDL:HA62	1.97	0.47
107:p2:85:LYS:HB3	107:p2:98:ASP:HB2	1.97	0.47
114:qG:105:GLN:O	116:qI:9:ASN:ND2	2.48	0.47
109:qb:169:GLN:NE2	109:qb:266:ALA:O	2.46	0.47
153:qb:601:CDL:H721	110:qc:20:PHE:HB2	1.95	0.47
111:qd:229:PRO:HG2	113:qf:20:PRO:HD2	1.97	0.47
112:qe:80:HIS:CD2	116:qi:35:GLN:HB2	2.50	0.47
120:s1:241:SER:HB3	120:s1:272:MET:HE2	1.97	0.47
120:s1:303:ILE:HG22	120:s1:579:PRO:HB3	1.97	0.47
121:s2:226:TYR:CE1	121:s2:244:CYS:HB3	2.49	0.47
121:s2:303:LYS:HA	142:tf:84:ASN:HD21	1.80	0.47
121:s2:383:LYS:O	121:s2:410:HIS:NE2	2.45	0.47
127:s8:71:ASP:OD2	127:s8:73:THR:OG1	2.25	0.47
143:tg:119:ASN:O	143:tg:123:ASN:HB2	2.15	0.47
145:tx:49:TYR:HE1	145:tx:98:PRO:HB3	1.79	0.47
146:v1:202:ALA:HB3	147:v2:109:TYR:CD1	2.50	0.47
1:1T:71:TYR:HE2	30:C2:312:SER:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2E:34:VAL:H	2:2E:63:LEU:HB2	1.80	0.47
7:2J:23:PHE:HB3	153:2K:101:CDL:H172	1.96	0.47
18:6A:77:GLN:HG2	153:6A:201:CDL:HA22	1.97	0.47
27:B:291:PHE:HZ	27:B:450:PRO:HD2	1.80	0.47
29:C1:141:GLY:O	29:C1:145:GLN:HG2	2.15	0.47
30:C2:2:TRP:HE1	30:C2:571:HIS:CD2	2.33	0.47
30:C2:134:THR:HG21	30:C2:159:ALA:HB1	1.97	0.47
30:C2:568:PRO:HG2	30:C2:571:HIS:ND1	2.30	0.47
33:E:97:GLN:O	33:E:100:ASN:HB2	2.15	0.47
33:E:348:ASP:OD1	33:E:348:ASP:N	2.48	0.47
34:F:283:GLU:HG3	34:F:306:MET:HA	1.96	0.47
35:FS:4:ILE:O	35:FS:8:ALA:N	2.48	0.47
39:J:112:LYS:HA	39:J:117:GLN:HE21	1.79	0.47
41:L:174:THR:HG21	49:Q:170:PRO:HA	1.95	0.47
43:M1:293:SER:HA	43:M1:296:TYR:CE2	2.50	0.47
44:M2:33:PRO:HG2	152:M2:405:PC1:H2B1	1.96	0.47
44:M2:224:LEU:HD11	44:M2:293:ALA:HB1	1.97	0.47
44:M2:249:ASN:OD1	44:M2:250:ALA:N	2.48	0.47
49:Q:21:GLU:OE2	61:X:6:THR:OG1	2.29	0.47
51:S:43:LYS:HB2	59:VB:500:TYR:CZ	2.49	0.47
52:SA:299:CYS:SG	52:SA:371:ILE:HG21	2.54	0.47
53:SB:73:VAL:HB	53:SB:90:TYR:HE2	1.79	0.47
59:VB:180:LEU:HG	59:VB:197:LEU:HB2	1.96	0.47
59:VB:227:ASP:OD1	59:VB:227:ASP:N	2.38	0.47
60:W:53:ASP:HB2	60:W:58:TRP:NE1	2.30	0.47
63:Y0:52:GLU:OE1	63:Y0:54:LYS:NZ	2.45	0.47
65:Y7:163:ALA:O	65:Y7:167:SER:OG	2.30	0.47
70:4L:10:LEU:HD11	105:N6:130:LEU:HD22	1.96	0.47
80:AB:47:LEU:HD12	80:AB:48:PRO:HD2	1.97	0.47
85:B2:41:SER:HB2	85:B2:44:ASP:HB2	1.95	0.47
96:G1:157:MET:SD	96:G1:195:ASN:ND2	2.83	0.47
97:G2:18:MET:HB3	158:G2:301:3PE:H2G1	1.96	0.47
100:N1:15:LEU:HD11	153:TE:101:CDL:H581	1.97	0.47
101:N2:289:PHE:HE2	101:N2:344:THR:HG23	1.80	0.47
103:N4:275:SER:HB3	103:N4:379:ASP:HB2	1.96	0.47
104:N5:168:ASN:OD1	104:N5:216:TYR:OH	2.15	0.47
104:N5:293:MET:O	104:N5:297:ILE:HG12	2.15	0.47
107:P2:27:MET:HG2	107:P2:148:PHE:HZ	1.78	0.47
109:QB:230:ASP:OD1	109:QB:230:ASP:N	2.45	0.47
153:QB:601:CDL:OB9	110:QC:21:SER:OG	2.33	0.47
108:Qa:99:THR:HG21	108:Qa:221:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:Qb:416:ALA:O	109:Qb:420:ASN:ND2	2.32	0.47
110:Qc:65:MET:HG2	111:Qd:89:TYR:CD1	2.49	0.47
110:Qc:98:HIS:CE1	110:Qc:102:LYS:HE3	2.49	0.47
110:Qc:315:ILE:HD11	153:Qg:402:CDL:H131	1.97	0.47
111:Qd:98:LYS:HB2	112:Qe:267:PHE:CE2	2.50	0.47
113:Qf:9:ALA:O	113:Qf:12:SER:HB3	2.14	0.47
120:S1:293:HIS:HB3	120:S1:697:THR:HG21	1.97	0.47
128:T1:289:LEU:HD13	128:T1:334:LEU:HD22	1.97	0.47
134:T7:30:PHE:HZ	134:T7:129:LEU:HB2	1.78	0.47
146:V1:424:THR:HG21	146:V1:429:GLY:HA3	1.96	0.47
2:2e:111:ARG:NH2	2:2e:203:ASN:O	2.47	0.47
3:2f:119:HIS:CD2	12:2o:33:ASP:HA	2.50	0.47
3:2f:271:GLU:HG3	3:2f:272:ILE:HG13	1.96	0.47
8:2k:49:ILE:HG23	55:sd:38:TYR:HB2	1.96	0.47
9:2l:40:ASP:OD1	9:2l:41:ALA:N	2.48	0.47
29:c1:514:ASN:ND2	154:c1:708:HEA:O1A	2.47	0.47
30:c2:2:TRP:HE1	30:c2:571:HIS:CD2	2.33	0.47
38:i:110:TYR:HB3	50:r:173:ILE:HG21	1.96	0.47
153:q:202:CDL:H752	153:t:202:CDL:H181	1.97	0.47
57:u:38:LYS:O	66:Z:14:HIS:NE2	2.48	0.47
76:a6:88:ASN:ND2	76:a6:133:LEU:O	2.42	0.47
153:b3:102:CDL:H151	152:t4:303:PC1:H2H2	1.97	0.47
99:j1:32:ASP:OD1	99:j1:33:ARG:N	2.46	0.47
103:n4:243:THR:HG23	103:n4:304:ILE:HD13	1.97	0.47
103:n4:298:THR:HG23	103:n4:353:ASP:HB3	1.95	0.47
104:n5:86:LYS:HZ2	37:H:298:SER:HB2	1.80	0.47
110:qC:321:GLN:NE2	114:qG:196:GLU:OE2	2.48	0.47
109:qb:169:GLN:HG2	109:qb:270:VAL:HG22	1.97	0.47
109:qb:200:LEU:HD23	109:qb:380:TYR:HD1	1.79	0.47
110:qc:305:TYR:O	110:qc:308:ILE:HG22	2.14	0.47
111:qd:93:ASP:O	112:qe:123:ARG:NH1	2.45	0.47
120:s1:222:ASN:OD1	120:s1:292:ARG:NH2	2.47	0.47
120:s1:387:MET:HG2	120:s1:512:ASN:HB3	1.97	0.47
128:t1:207:ALA:HB1	128:t1:369:LEU:HD21	1.97	0.47
148:x1:73:LEU:HD21	148:x1:88:PHE:HB2	1.97	0.47
3:2F:119:HIS:ND1	3:2F:142:ASP:OD2	2.46	0.47
3:2F:188:PRO:HD3	152:2F:302:PC1:H342	1.97	0.47
19:6B:78:MET:HG3	30:C2:1:MET:HE3	1.96	0.47
20:6C:32:ALA:HA	20:6C:35:ILE:HG12	1.96	0.47
26:A:249:ASP:O	36:G:34:ARG:NH1	2.37	0.47
28:BP:398:ILE:HD13	28:BP:412:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:I:102:ASP:OD1	38:I:106:THR:OG1	2.32	0.47
39:J:76:LEU:HG	39:J:164:LEU:HD21	1.96	0.47
48:P:120:LEU:HD21	48:P:165:LEU:HD11	1.97	0.47
52:SA:590:ASP:HB3	52:SA:594:TRP:HB2	1.97	0.47
68:1B:18:ILE:HD13	100:N1:43:GLU:HA	1.97	0.47
71:5B:7:ILE:HD11	106:P1:207:ASN:HD22	1.79	0.47
72:A1:82:THR:HA	141:TE:43:LYS:HD2	1.97	0.47
82:AL:35:ALA:HB2	82:AL:79:GLU:HA	1.97	0.47
152:AM:202:PC1:C21	105:N6:74:CYS:HB3	2.45	0.47
85:B2:23:TYR:HB2	86:B3:43:ASN:ND2	2.30	0.47
87:B4:36:ASN:HA	152:B9:201:PC1:H361	1.97	0.47
97:G2:36:ASP:OD1	97:G2:37:ILE:N	2.48	0.47
103:N4:298:THR:HG23	103:N4:353:ASP:HB3	1.95	0.47
110:QC:1:MET:HG3	153:Qb:601:CDL:H531	1.97	0.47
114:QG:105:GLN:O	116:QI:9:ASN:ND2	2.48	0.47
108:Qa:150:TYR:CE2	108:Qa:152:LYS:HB3	2.49	0.47
120:S1:189:GLN:O	120:S1:423:ARG:NH1	2.43	0.47
120:S1:222:ASN:OD1	120:S1:292:ARG:NH2	2.47	0.47
122:S3:73:LEU:HB2	122:S3:90:PHE:HZ	1.79	0.47
128:T1:68:ILE:H	128:T1:68:ILE:HG13	1.55	0.47
146:V1:129:ARG:HB2	146:V1:163:PHE:CZ	2.50	0.47
2:2e:34:VAL:H	2:2e:63:LEU:HB2	1.80	0.47
2:2e:149:LEU:HD13	2:2e:210:TYR:HB2	1.97	0.47
4:2g:58:ARG:HE	4:2g:62:ASN:HD22	1.63	0.47
27:b:267:ILE:O	27:b:271:ASN:ND2	2.37	0.47
29:c1:143:TRP:O	65:y7:322:ASN:ND2	2.33	0.47
29:c1:192:LEU:HD21	32:d:331:ILE:HD11	1.95	0.47
153:c1:712:CDL:H242	30:c2:51:ILE:HG22	1.97	0.47
34:f:176:ALA:O	34:f:179:PRO:HD2	2.14	0.47
35:fs:127:ASN:ND2	36:g:270:TRP:O	2.46	0.47
38:i:42:TRP:CD1	38:i:232:LYS:HZ2	2.33	0.47
40:k:112:GLU:OE2	40:k:155:PHE:N	2.40	0.47
42:m:115:TYR:OH	42:m:154:GLU:OE1	2.17	0.47
53:sb:69:LYS:NZ	53:sb:149:ASP:O	2.36	0.47
57:u:109:TYR:CZ	104:N5:81:ILE:HB	2.50	0.47
59:vb:294:GLU:OE1	64:y5:182:ASN:ND2	2.39	0.47
71:5b:7:ILE:HD11	106:p1:207:ASN:HD22	1.78	0.47
153:5b:201:CDL:H381	152:n5:803:PC1:H262	1.97	0.47
73:a2:21:GLN:NE2	120:s1:654:GLU:OE1	2.46	0.47
82:al:18:VAL:HG12	82:al:50:TYR:HE1	1.80	0.47
153:am:201:CDL:H131	153:t7:201:CDL:H362	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:b2:23:TYR:HB2	86:b3:43:ASN:ND2	2.30	0.47
101:n2:73:TYR:HB2	148:x1:98:TRP:HZ3	1.80	0.47
104:n5:189:ILE:HG12	152:n5:801:PC1:H352	1.97	0.47
107:p2:27:MET:HG2	107:p2:148:PHE:CZ	2.50	0.47
112:qE:29:GLU:O	112:qE:33:ARG:HG2	2.15	0.47
108:qa:322:PHE:O	108:qa:326:ALA:N	2.43	0.47
120:s1:234:ASN:OD1	120:s1:293:HIS:NE2	2.42	0.47
120:s1:251:THR:OG1	120:s1:252:SER:N	2.48	0.47
146:v1:218:GLU:OE1	146:v1:220:LYS:NZ	2.47	0.47
2:2E:125:GLU:HG2	7:2J:59:ALA:HB1	1.96	0.47
3:2F:215:LEU:HD21	152:2F:303:PC1:H251	1.97	0.47
4:2G:97:ASN:ND2	8:2K:20:VAL:H	2.12	0.47
5:2H:122:LEU:HD21	11:2N:61:GLU:HA	1.97	0.47
17:5T:62:LYS:HG3	30:C2:239:ASN:HD22	1.79	0.47
22:6T:62:LEU:O	22:6T:64:LYS:NZ	2.31	0.47
26:A:58:LYS:HB2	26:A:92:HIS:CD2	2.50	0.47
36:G:158:THR:HG23	36:G:163:VAL:HA	1.96	0.47
43:M1:56:LEU:HD21	43:M1:80:MET:HE1	1.95	0.47
44:M2:232:SER:HA	44:M2:285:PHE:HE2	1.79	0.47
153:M2:403:CDL:H782	153:M2:403:CDL:H561	1.97	0.47
61:X:11:TRP:CZ3	61:X:19:ILE:HG13	2.48	0.47
62:Y:8:ASN:HD22	62:Y:10:TYR:HD2	1.63	0.47
76:A6:148:LEU:HD11	79:A9:251:LEU:HD21	1.96	0.47
93:BM:183:GLU:OE2	132:T5:159:LYS:NZ	2.47	0.47
100:N1:214:THR:HG22	100:N1:252:LEU:HA	1.97	0.47
104:N5:251:ASP:H	104:N5:254:SER:HB3	1.78	0.47
106:P1:102:PHE:HE1	106:P1:105:HIS:HB2	1.79	0.47
110:QC:418:PHE:HZ	114:QG:86:LEU:HD13	1.79	0.47
114:QG:273:ASN:HB3	114:QG:275:ARG:NE	2.30	0.47
117:QJ:1:MET:HG2	117:QJ:3:LEU:HG	1.97	0.47
108:Qa:203:PHE:HE2	108:Qa:306:ALA:HB2	1.80	0.47
120:S1:45:ASP:HB3	120:S1:48:TYR:CD1	2.50	0.47
120:S1:229:VAL:HG23	120:S1:231:ALA:H	1.80	0.47
120:S1:712:ASN:ND2	129:T2:82:GLU:OE2	2.48	0.47
128:T1:207:ALA:HB1	128:T1:369:LEU:HD21	1.97	0.47
2:2e:119:GLU:OE1	2:2e:160:THR:OG1	2.27	0.47
20:6c:32:ALA:HA	20:6c:35:ILE:HG12	1.96	0.47
23:7a:83:ALA:HB2	153:c1:701:CDL:H352	1.96	0.47
34:f:166:TYR:O	34:f:211:ARG:NH2	2.47	0.47
53:sb:60:LEU:HD22	53:sb:90:TYR:HD1	1.80	0.47
82:al:188:ASP:OD1	82:al:188:ASP:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:am:55:ALA:HB2	137:ta:82:MET:HG3	1.95	0.47
97:g2:130:VAL:HG22	97:g2:145:ASP:O	2.14	0.47
101:n2:152:PHE:HB3	105:n6:187:ILE:HG21	1.96	0.47
102:n3:42:PHE:CE2	102:n3:52:GLU:HG3	2.50	0.47
103:n4:91:LEU:HD11	136:t9:1:MET:HA	1.97	0.47
104:n5:288:PHE:CE1	152:n5:801:PC1:H252	2.50	0.47
104:n5:432:ALA:O	104:n5:433:THR:OG1	2.33	0.47
105:n6:8:SER:HA	105:n6:11:SER:O	2.14	0.47
110:qC:86:ARG:HD3	110:qC:86:ARG:HA	1.80	0.47
111:qD:168:ARG:NE	151:qD:401:HEC:O2A	2.45	0.47
114:qG:87:LEU:HA	114:qG:154:ILE:HG12	1.96	0.47
111:qd:98:LYS:HB2	112:qe:267:PHE:CE2	2.50	0.47
136:t9:119:PHE:O	136:t9:123:VAL:HG23	2.15	0.47
139:tc:2:VAL:HB	139:tc:4:GLN:HG2	1.96	0.47
3:2F:119:HIS:CD2	12:2O:33:ASP:HA	2.50	0.47
3:2F:295:SER:HB2	6:2I:76:GLN:HG3	1.96	0.47
4:2G:61:GLU:OE1	4:2G:89:ASN:ND2	2.45	0.47
26:A:166:ASP:OD1	64:Y5:190:TYR:OH	2.32	0.47
27:B:291:PHE:HE1	27:B:453:ASN:HD22	1.63	0.47
27:B:445:THR:HG21	65:Y7:420:LEU:HD23	1.97	0.47
28:BP:175:GLU:HB2	28:BP:246:ASP:HB2	1.96	0.47
29:C1:321:ALA:HB3	29:C1:326:ARG:HD2	1.96	0.47
30:C2:111:SER:HA	30:C2:502:ASN:CB	2.45	0.47
36:G:163:VAL:N	36:G:180:TRP:O	2.47	0.47
42:M:98:LEU:O	60:W:21:ARG:NH2	2.44	0.47
48:P:39:VAL:HA	48:P:118:LEU:O	2.15	0.47
59:VB:486:ILE:HD13	59:VB:599:ILE:HG21	1.96	0.47
70:4L:11:ILE:HA	70:4L:14:LEU:HB2	1.97	0.47
77:A7:209:ARG:NH1	77:A7:215:MET:HE1	2.30	0.47
79:A9:237:LEU:HG	79:A9:239:ASN:HD22	1.80	0.47
79:A9:291:HIS:CE1	79:A9:316:LYS:HD3	2.50	0.47
80:AB:72:SER:HB2	80:AB:79:LEU:HD11	1.96	0.47
86:B3:65:VAL:HA	86:B3:68:PHE:CD2	2.50	0.47
98:G3:186:SER:HB3	98:G3:187:PRO:HD3	1.97	0.47
101:N2:238:TYR:OH	124:S5:48:HIS:O	2.31	0.47
104:N5:432:ALA:O	104:N5:433:THR:OG1	2.33	0.47
108:QA:412:ARG:NE	108:QA:415:ASP:OD2	2.37	0.47
109:QB:199:LEU:HD23	109:QB:481:TRP:CH2	2.50	0.47
110:QC:36:PHE:CD2	110:QC:230:GLU:HB3	2.50	0.47
111:QD:145:PHE:N	111:QD:149:GLN:OE1	2.42	0.47
109:Qb:212:HIS:CE1	109:Qb:281:ASN:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:Qd:28:ARG:HB3	111:Qd:30:ASP:OD1	2.15	0.47
122:S3:73:LEU:HB2	122:S3:90:PHE:CZ	2.50	0.47
131:T4:67:GLN:NE2	131:T4:194:ASN:HB2	2.30	0.47
131:T4:68:LYS:O	131:T4:190:HIS:NE2	2.48	0.47
2:2e:197:GLN:O	2:2e:201:GLU:N	2.44	0.46
7:2j:47:ALA:HB1	153:sd:101:CDL:H311	1.97	0.46
18:6a:52:HIS:CD2	59:vb:412:ARG:HB3	2.50	0.46
26:a:54:TYR:CZ	26:a:173:LYS:HG3	2.50	0.46
26:a:105:MET:HE1	36:g:173:GLY:HA3	1.96	0.46
27:b:291:PHE:HE1	27:b:453:ASN:HD22	1.61	0.46
30:c2:122:TRP:CG	30:c2:556:TYR:HB2	2.50	0.46
30:c2:568:PRO:HG2	30:c2:571:HIS:ND1	2.30	0.46
31:c3:17:TRP:N	31:c3:54:GLY:O	2.47	0.46
39:j:67:ILE:HD13	39:j:160:LEU:HD12	1.96	0.46
43:m1:229:VAL:HG12	152:v:201:PC1:H12	1.97	0.46
153:m2:403:CDL:H782	153:m2:403:CDL:H561	1.97	0.46
50:r:77:GLY:HA3	160:r:202:PX2:H15	1.97	0.46
53:sb:277:MET:HG3	54:sc:19:PHE:CE1	2.50	0.46
72:a1:18:PRO:HB3	153:a1:101:CDL:HB61	1.96	0.46
82:al:35:ALA:HB2	82:al:79:GLU:HA	1.97	0.46
83:am:73:LYS:HG3	137:ta:100:ARG:HD3	1.97	0.46
87:b4:36:ASN:HA	152:b9:201:PC1:H361	1.97	0.46
92:bl:129:ASN:HB3	136:t9:17:GLY:HA3	1.96	0.46
96:g1:157:MET:SD	96:g1:195:ASN:ND2	2.82	0.46
96:g1:216:TYR:HB2	97:g2:24:LEU:HD13	1.97	0.46
100:n1:104:PHE:HD1	100:n1:129:LEU:HD13	1.80	0.46
153:qB:601:CDL:OB9	110:qC:21:SER:OG	2.32	0.46
110:qC:4:ASN:O	110:qc:14:LYS:NZ	2.40	0.46
112:qE:152:ILE:HA	112:qE:195:ALA:H	1.80	0.46
110:qc:68:GLU:HG3	111:qd:89:TYR:HB3	1.98	0.46
111:qd:28:ARG:HB3	111:qd:30:ASP:OD1	2.15	0.46
127:s8:71:ASP:N	127:s8:71:ASP:OD1	2.45	0.46
128:t1:86:HIS:ND1	153:t1:601:CDL:H112	2.30	0.46
3:2F:151:ARG:HH21	8:2K:91:LYS:NZ	2.13	0.46
3:2F:271:GLU:HG3	3:2F:272:ILE:HG13	1.96	0.46
4:2G:35:PHE:H	4:2G:163:GLU:HG2	1.80	0.46
14:3T:73:VAL:HA	14:3T:76:THR:HG22	1.97	0.46
18:6A:8:ARG:NE	33:E:139:ALA:O	2.48	0.46
30:C2:18:GLY:HA2	58:V:143:LYS:HG2	1.96	0.46
33:E:132:PHE:HB2	153:E:402:CDL:H311	1.97	0.46
33:E:216:THR:O	33:E:220:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:G:135:LEU:O	36:G:140:GLN:NE2	2.42	0.46
38:I:122:TYR:OH	153:I:303:CDL:OB9	2.26	0.46
53:SB:194:ASP:OD1	53:SB:195:ALA:N	2.46	0.46
69:2B:18:LEU:HD22	69:2B:176:ILE:HD12	1.97	0.46
73:A2:71:LYS:HE2	73:A2:93:GLN:HE22	1.80	0.46
76:A6:38:GLU:HG3	121:S2:54:ARG:HD3	1.97	0.46
76:A6:92:TYR:CE1	168:AB:201:ZMP:H6	2.50	0.46
83:AM:64:GLY:HA3	100:N1:198:ILE:HG12	1.96	0.46
153:BM:301:CDL:H541	103:N4:499:TYR:CZ	2.49	0.46
109:QB:363:ILE:HB	109:QB:382:TYR:HB3	1.96	0.46
108:Qa:322:PHE:HE2	108:Qa:454:VAL:HG21	1.80	0.46
109:Qb:175:LYS:HA	109:Qb:230:ASP:HB3	1.96	0.46
112:Qe:80:HIS:CD2	116:Qi:35:GLN:HB2	2.49	0.46
120:S1:387:MET:HG2	120:S1:512:ASN:HB3	1.97	0.46
121:S2:242:ARG:NH2	121:S2:286:GLU:OE2	2.47	0.46
122:S3:176:THR:HB	123:S4:75:ARG:HG3	1.96	0.46
128:T1:177:HIS:HE2	128:T1:197:THR:HG1	1.59	0.46
128:T1:380:ASN:ND2	128:T1:383:TYR:H	2.13	0.46
135:T8:41:LEU:HG	135:T8:45:LYS:HE3	1.97	0.46
153:7a:203:CDL:H521	31:c3:283:TYR:HA	1.96	0.46
27:b:445:THR:HG21	65:y7:420:LEU:HD23	1.97	0.46
30:c2:112:LEU:HB2	30:c2:501:VAL:HG22	1.96	0.46
30:c2:591:LYS:HG3	30:c2:595:THR:HB	1.97	0.46
41:l:194:ASP:OD2	41:l:200:TYR:OH	2.24	0.46
43:m1:306:TRP:CD2	153:m1:405:CDL:H132	2.50	0.46
53:sb:212:LEU:HB3	53:sb:246:ARG:HB2	1.96	0.46
59:vb:329:ARG:HG2	59:vb:332:ARG:HH12	1.80	0.46
60:w:38:ARG:NH2	153:w:202:CDL:OA3	2.38	0.46
79:a9:304:TRP:HZ2	153:a9:402:CDL:H552	1.80	0.46
87:b4:144:ASP:OD2	103:n4:11:ARG:NH1	2.48	0.46
152:n1:301:PC1:H12	153:td:101:CDL:HB4	1.97	0.46
101:n2:84:PHE:CE1	101:n2:91:LEU:HG	2.50	0.46
104:n5:69:HIS:NE2	37:H:290:TYR:HE2	2.13	0.46
105:n6:27:ILE:O	139:tc:33:TYR:OH	2.33	0.46
153:qB:601:CDL:H132	117:qJ:27:LEU:HD21	1.98	0.46
112:qE:84:GLU:OE1	116:qI:49:LYS:NZ	2.37	0.46
110:qc:214:ASP:OD1	110:qc:214:ASP:N	2.45	0.46
111:qd:79:ARG:HD2	111:qd:218:VAL:HG13	1.96	0.46
111:qd:113:THR:HG23	111:qd:131:GLU:HB2	1.97	0.46
122:s3:176:THR:HB	123:s4:75:ARG:HG3	1.96	0.46
135:t8:41:LEU:HG	135:t8:45:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
145:tx:145:GLU:HB2	145:tx:148:GLU:HG3	1.98	0.46
147:v2:184:TYR:OH	147:v2:204:ASP:OD2	2.23	0.46
3:2F:79:VAL:HG21	11:2N:57:SER:H	1.80	0.46
4:2G:36:GLU:HG2	4:2G:37:ASN:HD22	1.80	0.46
4:2G:178:ASP:HB2	54:SC:2:ARG:HG3	1.98	0.46
29:C1:504:THR:HG21	29:C1:579:PHE:CZ	2.51	0.46
29:C1:568:SER:HB3	153:C1:712:CDL:H832	1.96	0.46
32:D:311:ARG:HD2	32:D:373:LEU:HD22	1.96	0.46
38:I:42:TRP:CD1	38:I:232:LYS:HZ2	2.34	0.46
41:L:78:ILE:HG23	41:L:176:MET:HG3	1.96	0.46
153:Q:202:CDL:H752	153:T:202:CDL:H181	1.97	0.46
52:SA:302:GLU:HG3	52:SA:367:ARG:HH21	1.81	0.46
59:VB:547:ASN:O	65:Y7:240:ASN:ND2	2.49	0.46
70:4L:72:SER:HB2	102:N3:66:VAL:HB	1.97	0.46
72:A1:29:GLY:HA3	153:A1:101:CDL:H382	1.98	0.46
91:B9:134:GLY:HA2	91:B9:137:SER:O	2.15	0.46
94:C4:31:PRO:HG3	97:G2:18:MET:HG2	1.96	0.46
96:G1:136:ASP:N	96:G1:136:ASP:OD1	2.46	0.46
101:N2:73:TYR:HB2	148:X1:98:TRP:HZ3	1.80	0.46
103:N4:318:VAL:HG13	103:N4:447:VAL:HG11	1.98	0.46
105:N6:27:ILE:O	139:TC:33:TYR:OH	2.33	0.46
109:Qb:90:VAL:HG23	109:Qb:164:LEU:HD13	1.96	0.46
112:Qe:44:VAL:HA	112:Qe:71:ASP:HA	1.98	0.46
120:S1:303:ILE:HG22	120:S1:579:PRO:HB3	1.96	0.46
128:T1:86:HIS:ND1	153:T1:601:CDL:H112	2.30	0.46
146:V1:106:ASN:ND2	146:V1:110:ARG:O	2.28	0.46
1:1t:64:ARG:NE	30:c2:313:ASP:OD2	2.47	0.46
2:2e:92:SER:HA	7:2j:60:TYR:CZ	2.51	0.46
27:b:379:LYS:HB3	27:b:382:ILE:HD11	1.97	0.46
29:c1:504:THR:HG21	29:c1:579:PHE:CZ	2.50	0.46
30:c2:18:GLY:HA2	58:v:143:LYS:HG2	1.96	0.46
30:c2:76:LYS:HB3	152:w:204:PC1:H143	1.96	0.46
40:k:41:ASN:O	40:k:43:ASN:ND2	2.48	0.46
48:p:38:LYS:H	48:p:117:ASN:ND2	2.13	0.46
52:sa:94:ILE:HG21	52:sa:187:MET:HE1	1.96	0.46
52:sa:315:MET:HG3	52:sa:324:ASP:HA	1.96	0.46
73:a2:78:ASN:HD22	73:a2:82:GLU:HB3	1.78	0.46
82:al:177:LYS:NZ	120:s1:569:GLU:OE1	2.47	0.46
83:am:64:GLY:HA3	100:n1:198:ILE:HG12	1.96	0.46
86:b3:17:LYS:HB2	106:p1:245:LEU:HG	1.97	0.46
110:qC:283:ARG:HD2	110:qC:373:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:qb:484:SER:O	109:qb:488:ILE:HB	2.16	0.46
121:s2:355:GLU:OE1	121:s2:355:GLU:N	2.47	0.46
128:t1:401:ILE:HG13	128:t1:403:GLY:H	1.79	0.46
2:2E:149:LEU:HD13	2:2E:210:TYR:HB2	1.97	0.46
3:2F:124:GLN:HE22	9:2L:2:LYS:HB3	1.80	0.46
7:2J:47:ALA:HB1	153:SD:101:CDL:H311	1.97	0.46
20:6C:2:GLY:HA3	153:6C:202:CDL:HB22	1.98	0.46
153:7A:201:CDL:H631	153:7A:201:CDL:H672	1.97	0.46
26:A:351:ILE:HD11	31:C3:465:VAL:HG13	1.97	0.46
30:C2:76:LYS:HB3	152:W:204:PC1:H143	1.96	0.46
31:C3:365:SER:O	31:C3:368:ILE:HG12	2.15	0.46
33:E:104:ASP:OD2	64:Y5:114:TYR:N	2.49	0.46
40:K:41:ASN:O	40:K:43:ASN:ND2	2.48	0.46
41:L:102:LEU:HD21	41:L:106:ARG:HH21	1.81	0.46
50:R:52:VAL:HG13	143:TG:113:GLU:HG2	1.98	0.46
52:SA:94:ILE:HG21	52:SA:187:MET:HE1	1.97	0.46
56:T:75:ILE:O	56:T:78:PHE:HB3	2.15	0.46
59:VB:278:ALA:O	59:VB:282:LYS:HD3	2.15	0.46
59:VB:329:ARG:HG2	59:VB:332:ARG:HH12	1.80	0.46
70:4L:99:GLN:NE2	84:AN:84:SER:OG	2.48	0.46
78:A8:165:LYS:HE3	140:TD:52:ARG:HA	1.97	0.46
82:AL:133:ASN:HB2	127:S8:201:TYR:CD1	2.51	0.46
153:BM:301:CDL:HA32	132:T5:138:ILE:HD13	1.96	0.46
104:N5:62:ASN:OD1	104:N5:143:ASP:N	2.48	0.46
106:P1:169:HIS:CD2	106:P1:170:LEU:HG	2.50	0.46
111:Qd:177:ASN:HB3	111:Qd:201:TYR:CD1	2.51	0.46
120:S1:251:THR:OG1	120:S1:252:SER:N	2.48	0.46
130:T3:166:LEU:HA	130:T3:169:PHE:CZ	2.50	0.46
135:T8:78:ASP:OD1	135:T8:78:ASP:N	2.46	0.46
148:X1:73:LEU:HD21	148:X1:88:PHE:HB2	1.97	0.46
7:2j:23:PHE:HB3	153:2k:101:CDL:H172	1.97	0.46
10:2m:9:ASP:OD1	12:2o:12:ARG:NE	2.47	0.46
19:6b:125:GLN:N	42:m:146:ASP:OD2	2.38	0.46
153:7a:201:CDL:H412	46:n:65:TRP:HZ2	1.81	0.46
30:c2:111:SER:HA	30:c2:502:ASN:CB	2.45	0.46
44:m2:232:SER:HA	44:m2:285:PHE:HE2	1.79	0.46
52:sa:119:TRP:HZ3	52:sa:634:ARG:HB2	1.80	0.46
53:sb:34:SER:HA	93:bm:97:PRO:HG3	1.97	0.46
53:sb:201:GLN:O	53:sb:205:GLN:HB2	2.16	0.46
56:t:56:ARG:HH21	153:t:204:CDL:H1	1.81	0.46
62:y:8:ASN:HD22	62:y:10:TYR:HD2	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:y5:173:THR:O	64:y5:174:ARG:NH1	2.48	0.46
69:2b:18:LEU:HD22	69:2b:176:ILE:HD12	1.97	0.46
70:4l:11:ILE:HA	70:4l:14:LEU:HB2	1.97	0.46
81:ac:38:PRO:HB2	81:ac:40:LYS:HG2	1.97	0.46
82:al:189:ASP:N	82:al:189:ASP:OD1	2.48	0.46
93:bm:183:GLU:OE2	132:t5:159:LYS:NZ	2.47	0.46
96:g1:109:THR:HG22	99:j1:118:ASP:HA	1.96	0.46
100:n1:115:SER:OG	100:n1:117:PHE:O	2.34	0.46
100:n1:214:THR:HG22	100:n1:252:LEU:HA	1.97	0.46
110:qC:135:VAL:HA	110:qC:142:SER:HB3	1.98	0.46
111:qD:96:LEU:HD11	111:qD:102:GLN:HA	1.97	0.46
109:qb:393:PHE:O	109:qb:394:LEU:C	2.58	0.46
110:qc:126:PHE:CE1	166:qc:502:HEM:HBC1	2.50	0.46
114:qg:69:ARG:NH1	114:qg:248:ARG:O	2.46	0.46
4:2G:58:ARG:HE	4:2G:62:ASN:HD22	1.63	0.46
10:2M:12:LYS:HA	10:2M:15:LEU:HD12	1.98	0.46
152:6A:202:PC1:H152	31:C3:360:ILE:HG23	1.97	0.46
19:6B:170:TYR:OH	19:6B:171:ARG:NH1	2.48	0.46
28:BP:173:VAL:HG22	28:BP:178:THR:HG23	1.96	0.46
30:C2:122:TRP:CG	30:C2:556:TYR:HB2	2.50	0.46
39:J:130:CYS:SG	65:Y7:379:MET:HA	2.56	0.46
41:L:194:ASP:OD2	41:L:200:TYR:OH	2.25	0.46
69:2B:50:LEU:HD21	101:N2:339:PHE:HB2	1.97	0.46
69:2B:55:GLU:O	69:2B:128:SER:OG	2.26	0.46
153:5B:201:CDL:H381	152:N5:803:PC1:H262	1.97	0.46
79:A9:208:PHE:CZ	79:A9:272:VAL:HG11	2.51	0.46
82:AL:57:ASP:OD1	82:AL:95:PRO:HG3	2.16	0.46
82:AL:95:PRO:HA	82:AL:127:HIS:CG	2.51	0.46
83:AM:73:LYS:HG3	137:TA:100:ARG:HD3	1.97	0.46
100:N1:131:ILE:HG21	105:N6:90:PHE:HB3	1.96	0.46
104:N5:189:ILE:HG12	152:N5:801:PC1:H352	1.96	0.46
105:N6:8:SER:HA	105:N6:11:SER:O	2.14	0.46
107:P2:27:MET:HG2	107:P2:148:PHE:CZ	2.50	0.46
109:QB:311:PRO:HG3	109:QB:470:TRP:CE2	2.51	0.46
110:QC:55:SER:HB3	112:QE:117:ARG:HH21	1.80	0.46
109:Qb:97:ARG:O	109:Qb:281:ASN:ND2	2.49	0.46
109:Qb:169:GLN:NE2	109:Qb:266:ALA:O	2.44	0.46
110:Qc:102:LYS:HA	110:Qc:102:LYS:HD3	1.72	0.46
110:Qc:214:ASP:OD1	110:Qc:214:ASP:N	2.45	0.46
153:Qg:402:CDL:H712	118:Ql:9:LEU:HD21	1.96	0.46
136:T9:119:PHE:O	136:T9:123:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2g:36:GLU:HG2	4:2g:37:ASN:HD22	1.80	0.46
4:2g:58:ARG:NE	4:2g:62:ASN:HD22	2.14	0.46
14:3t:73:VAL:HA	14:3t:76:THR:HG22	1.97	0.46
26:a:152:ASP:O	26:a:155:ARG:HG2	2.16	0.46
153:a:504:CDL:HB22	45:m3:13:ALA:HB1	1.98	0.46
27:b:446:GLU:OE1	65:y7:412:TYR:OH	2.21	0.46
32:d:304:GLN:NE2	45:m3:70:GLU:OE2	2.39	0.46
48:p:99:PHE:CG	48:p:100:PRO:HA	2.51	0.46
48:p:129:VAL:HB	48:p:133:ARG:HE	1.80	0.46
52:sa:446:LEU:O	52:sa:449:ILE:HG12	2.15	0.46
53:sb:138:HIS:O	53:sb:281:THR:OG1	2.33	0.46
65:y7:148:PHE:CZ	149:c:138:ILE:HA	2.51	0.46
153:2b:201:CDL:H171	103:n4:25:PHE:HE2	1.81	0.46
71:5b:30:GLU:OE1	90:b8:68:TYR:OH	2.20	0.46
72:a1:54:LYS:NZ	83:am:149:ASN:O	2.47	0.46
79:a9:237:LEU:HG	79:a9:239:ASN:HD22	1.81	0.46
85:b2:121:SER:OG	90:b8:178:ASN:HB3	2.15	0.46
86:b3:34:PHE:HA	86:b3:37:VAL:HG22	1.97	0.46
164:b8:301:U10:H151	164:b8:301:U10:H171	1.70	0.46
96:g1:136:ASP:OD1	96:g1:136:ASP:N	2.48	0.46
103:n4:305:ASP:OD2	103:n4:307:SER:OG	2.31	0.46
104:n5:81:ILE:HB	57:U:109:TYR:CZ	2.50	0.46
109:qB:199:LEU:HD23	109:qB:481:TRP:CH2	2.50	0.46
110:qC:36:PHE:CD2	110:qC:230:GLU:HB3	2.51	0.46
153:qC:504:CDL:H532	115:qH:97:ILE:HD11	1.98	0.46
108:qa:203:PHE:HE2	108:qa:306:ALA:HB2	1.79	0.46
110:qc:234:MET:HE3	110:qc:238:ILE:HD11	1.96	0.46
110:qc:335:PHE:CD1	114:qg:52:SER:HB2	2.51	0.46
113:qf:22:GLU:HA	113:qf:25:LEU:HD12	1.97	0.46
120:s1:482:ARG:NH2	120:s1:484:ASP:OD1	2.41	0.46
121:s2:33:GLN:HG2	126:s7:27:PHE:HB2	1.96	0.46
128:t1:289:LEU:HD13	128:t1:334:LEU:HD22	1.97	0.46
130:t3:165:ILE:HG22	130:t3:169:PHE:CE2	2.50	0.46
146:v1:129:ARG:NH2	147:v2:185:GLU:OE2	2.48	0.46
146:v1:424:THR:HG21	146:v1:429:GLY:HA3	1.97	0.46
9:2L:37:ASN:HB3	9:2L:76:GLN:HB2	1.97	0.46
153:7C:301:CDL:H461	29:C1:63:VAL:HG11	1.97	0.46
26:A:341:VAL:HG22	152:A:501:PC1:H2B2	1.96	0.46
28:BP:214:CYS:SG	28:BP:215:GLY:N	2.88	0.46
29:C1:225:SER:HB2	46:N:199:ALA:HB2	1.96	0.46
36:G:45:PRO:O	59:VB:282:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:I:23:ARG:NH1	38:I:23:ARG:H	2.14	0.46
39:J:108:GLN:O	39:J:112:LYS:NZ	2.44	0.46
48:P:31:LEU:O	48:P:175:HIS:NE2	2.40	0.46
52:SA:119:TRP:HZ3	52:SA:634:ARG:HB2	1.80	0.46
52:SA:418:ASP:N	52:SA:418:ASP:OD1	2.47	0.46
52:SA:446:LEU:O	52:SA:449:ILE:HG12	2.15	0.46
53:SB:116:LEU:HD11	53:SB:168:LEU:HD13	1.97	0.46
58:V:86:HIS:HA	58:V:90:LEU:HD23	1.97	0.46
64:Y5:39:VAL:HG22	64:Y5:46:LYS:HG3	1.95	0.46
73:A2:65:TYR:OH	73:A2:90:LEU:O	2.21	0.46
73:A2:94:SER:OG	73:A2:98:ASN:ND2	2.48	0.46
74:A3:77:ASP:CG	137:TA:97:ARG:HH12	2.22	0.46
78:A8:196:ASN:HA	78:A8:199:VAL:HG22	1.97	0.46
79:A9:210:ARG:NH2	79:A9:305:GLU:OE2	2.42	0.46
92:BL:111:ARG:HB2	92:BL:117:ALA:HB2	1.98	0.46
101:N2:240:THR:OG1	105:N6:137:TYR:OH	2.21	0.46
101:N2:316:LEU:O	101:N2:320:ILE:HG12	2.15	0.46
102:N3:42:PHE:CE2	102:N3:52:GLU:HG3	2.50	0.46
104:N5:83:ASN:HA	104:N5:86:LYS:HE2	1.98	0.46
153:N5:806:CDL:H611	153:N5:806:CDL:H722	1.95	0.46
110:QC:112:GLN:NE2	110:QC:206:ASP:OD2	2.34	0.46
112:QE:107:ALA:HB2	152:QI:202:PC1:H2A1	1.96	0.46
108:Qa:402:LEU:HD11	114:Qg:326:PHE:HE1	1.81	0.46
109:Qb:130:LEU:HD11	109:Qb:137:LEU:HB2	1.97	0.46
109:Qb:393:PHE:O	109:Qb:394:LEU:C	2.58	0.46
110:Qc:335:PHE:CD1	114:Qg:52:SER:HB2	2.51	0.46
111:Qd:229:PRO:HG2	113:Qf:20:PRO:HD2	1.97	0.46
121:S2:238:GLY:HA3	121:S2:384:GLY:HA2	1.97	0.46
125:S6:106:THR:O	147:V2:31:ARG:NH1	2.49	0.46
127:S8:176:ILE:HG13	127:S8:178:CYS:HB3	1.97	0.46
128:T1:498:ILE:O	128:T1:500:ASN:ND2	2.49	0.46
148:X1:2:SER:N	148:X1:149:ARG:H	2.13	0.46
9:2l:37:ASN:HB3	9:2l:76:GLN:HB2	1.98	0.46
23:7a:128:ASP:OD1	23:7a:129:ARG:N	2.48	0.46
29:c1:141:GLY:O	29:c1:145:GLN:HG2	2.15	0.46
154:c1:708:HEA:H271	154:c1:708:HEA:H211	1.37	0.46
30:c2:335:THR:OG1	32:d:233:TYR:OH	2.23	0.46
30:c2:494:THR:OG1	30:c2:563:ARG:NH2	2.49	0.46
33:e:132:PHE:HB2	153:e:402:CDL:H311	1.98	0.46
153:e:403:CDL:H552	20:6C:4:VAL:HG21	1.97	0.46
38:i:151:GLU:HB3	38:i:155:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:76:LEU:HG	39:j:164:LEU:HD21	1.96	0.46
39:j:130:CYS:SG	65:y7:379:MET:HA	2.56	0.46
41:l:85:LEU:HD12	41:l:176:MET:HE1	1.98	0.46
44:m2:11:PRO:HB2	44:m2:16:VAL:HG13	1.98	0.46
153:m2:404:CDL:H342	153:m2:404:CDL:H111	1.96	0.46
45:m3:154:SER:HB2	45:m3:158:ASN:HB3	1.96	0.46
52:sa:65:PHE:HE2	52:sa:191:LEU:HD22	1.81	0.46
59:vb:350:ARG:NH1	59:vb:387:TPO:O2P	2.38	0.46
73:a2:71:LYS:HE2	73:a2:93:GLN:HE22	1.80	0.46
76:a6:170:THR:HG21	79:a9:30:LYS:HE3	1.97	0.46
78:a8:160:TYR:HB2	83:am:92:PHE:CD2	2.50	0.46
78:a8:196:ASN:HA	78:a8:199:VAL:HG22	1.97	0.46
79:a9:132:PHE:HD2	79:a9:174:PRO:HB3	1.81	0.46
83:am:48:ARG:HH12	137:ta:74:GLU:HB3	1.80	0.46
88:b6:105:SER:HB3	132:t5:142:LYS:HD3	1.98	0.46
98:g3:186:SER:HB3	98:g3:187:PRO:HD3	1.97	0.46
100:n1:161:LEU:HA	102:n3:68:LEU:HD22	1.97	0.46
100:n1:190:GLN:NE2	100:n1:261:ILE:O	2.43	0.46
101:n2:151:PHE:O	101:n2:154:ILE:HG13	2.15	0.46
101:n2:333:ILE:HD13	101:n2:342:TYR:HD2	1.81	0.46
106:p1:57:THR:HG22	107:p2:68:PRO:HG3	1.97	0.46
108:qA:110:LEU:O	108:qA:114:LYS:N	2.44	0.46
120:s1:45:ASP:HB3	120:s1:48:TYR:CD1	2.50	0.46
120:s1:712:ASN:ND2	129:t2:82:GLU:OE2	2.48	0.46
121:s2:40:VAL:HG11	121:s2:62:LEU:HD13	1.96	0.46
121:s2:69:LEU:HD22	121:s2:73:ARG:HH12	1.81	0.46
122:s3:93:LYS:NZ	123:s4:148:GLN:HE22	2.14	0.46
123:s4:77:ASP:OD1	123:s4:77:ASP:N	2.48	0.46
128:t1:398:ASN:OD1	128:t1:440:TYR:OH	2.28	0.46
128:t1:458:VAL:HG12	128:t1:460:THR:HG23	1.98	0.46
134:t7:116:ARG:NE	137:ta:106:ASP:OD1	2.48	0.46
136:t9:109:GLN:O	136:t9:111:LYS:N	2.48	0.46
144:th:78:LYS:NZ	153:th:200:CDL:OA4	2.38	0.46
2:2E:119:GLU:OE1	2:2E:160:THR:OG1	2.27	0.46
4:2G:40:GLU:C	4:2G:42:PHE:H	2.24	0.46
18:6A:46:TYR:OH	59:VB:321:GLU:OE2	2.29	0.46
19:6B:125:GLN:N	42:M:146:ASP:OD2	2.37	0.46
29:C1:143:TRP:O	65:Y7:322:ASN:ND2	2.33	0.46
30:C2:591:LYS:HG3	30:C2:595:THR:HB	1.98	0.46
36:G:223:ASP:N	36:G:223:ASP:OD1	2.46	0.46
38:I:95:TYR:HB2	158:I:304:3PE:H272	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:I:210:LYS:O	38:I:213:ILE:HG22	2.16	0.46
39:J:62:GLU:HA	39:J:179:LEU:HD11	1.97	0.46
59:VB:269:PRO:O	59:VB:273:MET:HG2	2.15	0.46
69:2B:33:MET:HA	101:N2:282:PHE:HE1	1.80	0.46
83:AM:127:MET:HG3	124:S5:55:LEU:HD13	1.98	0.46
87:B4:48:ASN:OD1	87:B4:49:TYR:N	2.42	0.46
94:C4:16:ARG:NH2	94:C4:29:THR:O	2.45	0.46
97:G2:130:VAL:HG22	97:G2:145:ASP:O	2.15	0.46
100:N1:250:PHE:HD1	100:N1:254:PHE:HE2	1.63	0.46
101:N2:50:ILE:HG13	101:N2:51:ILE:HD12	1.97	0.46
101:N2:84:PHE:CE1	101:N2:91:LEU:HG	2.50	0.46
104:N5:288:PHE:CE1	152:N5:801:PC1:H252	2.50	0.46
108:QA:254:ALA:HB2	108:QA:417:LEU:HD13	1.98	0.46
110:QC:79:ASP:OD1	110:QC:79:ASP:N	2.49	0.46
109:Qb:97:ARG:HD2	109:Qb:144:GLU:HG2	1.98	0.46
109:Qb:395:SER:HG	109:Qb:396:GLN:H	1.64	0.46
109:Qb:499:ARG:NH2	109:Qb:505:TYR:HB3	2.30	0.46
112:Qe:88:ARG:NE	115:Qh:68:GLN:O	2.46	0.46
113:Qf:53:ASP:OD1	113:Qf:53:ASP:N	2.48	0.46
120:S1:241:SER:HA	127:S8:140:LYS:HZ1	1.80	0.46
130:T3:165:ILE:HG22	130:T3:169:PHE:CE2	2.50	0.46
134:T7:115:THR:HB	137:TA:106:ASP:HB3	1.97	0.46
146:V1:218:GLU:OE1	146:V1:220:LYS:NZ	2.48	0.46
147:V2:100:ILE:O	147:V2:104:GLU:HG3	2.16	0.46
19:6b:216:PHE:HD1	56:t:143:LEU:HB3	1.79	0.46
26:a:76:VAL:HG22	26:a:195:LYS:HE2	1.98	0.46
29:c1:571:GLN:NE2	29:c1:611:THR:OG1	2.49	0.46
31:c3:190:LEU:HD12	40:k:149:VAL:HG11	1.98	0.46
70:4l:99:GLN:NE2	84:an:84:SER:OG	2.48	0.46
77:a7:193:GLN:NE2	77:a7:197:ASP:OD1	2.47	0.46
82:al:131:LEU:O	82:al:134:THR:OG1	2.22	0.46
96:g1:192:LEU:O	96:g1:196:ILE:HG13	2.15	0.46
109:qB:311:PRO:HG3	109:qB:470:TRP:CE2	2.51	0.46
117:qJ:1:MET:HG2	117:qJ:3:LEU:HG	1.97	0.46
109:qb:99:GLU:O	109:qb:281:ASN:ND2	2.46	0.46
115:qh:77:GLY:HA3	115:qh:81:THR:HB	1.97	0.46
131:t4:67:GLN:NE2	131:t4:194:ASN:HB2	2.30	0.46
132:t5:167:ARG:NH2	138:tb:99:THR:O	2.30	0.46
146:v1:129:ARG:HB2	146:v1:163:PHE:CZ	2.50	0.46
17:5T:19:ASP:OD2	30:C2:227:ARG:NH2	2.27	0.46
20:6C:26:LYS:HD2	153:6C:202:CDL:HB31	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7C:87:ILE:O	34:F:253:TYR:OH	2.30	0.46
26:A:296:CYS:O	26:A:301:PRO:HD3	2.16	0.46
29:C1:331:LEU:HB3	59:VB:175:LEU:HD22	1.96	0.46
29:C1:592:ASP:CG	30:C2:487:ARG:HH12	2.24	0.46
31:C3:568:SER:HB3	41:L:29:GLU:N	2.31	0.46
152:I:301:PC1:H382	153:I:302:CDL:H452	1.98	0.46
60:W:53:ASP:OD2	60:W:61:ARG:NH1	2.46	0.46
69:2B:160:LEU:HD11	153:2B:201:CDL:H771	1.97	0.46
153:A1:101:CDL:HB4	152:N1:301:PC1:H12	1.97	0.46
153:A1:102:CDL:H552	153:A1:102:CDL:H151	1.98	0.46
75:A5:86:LEU:HG	75:A5:106:VAL:HG11	1.96	0.46
76:A6:92:TYR:HE1	168:AB:201:ZMP:H6	1.80	0.46
78:A8:160:TYR:HB2	83:AM:92:PHE:CD2	2.50	0.46
82:AL:105:GLN:HE22	127:S8:194:PRO:HB3	1.80	0.46
100:N1:104:PHE:HD1	100:N1:129:LEU:HD13	1.79	0.46
101:N2:151:PHE:O	101:N2:154:ILE:HG13	2.15	0.46
104:N5:376:TYR:HB3	104:N5:390:LEU:HD23	1.98	0.46
110:QC:57:VAL:O	110:QC:59:GLU:N	2.45	0.46
111:QD:314:ARG:HD3	115:Qh:29:ILE:HB	1.98	0.46
108:Qa:95:LEU:HD21	108:Qa:172:LEU:HD21	1.97	0.46
109:Qb:295:ARG:HB3	115:Qh:58:PHE:HB3	1.96	0.46
110:Qc:68:GLU:HG3	111:Qd:89:TYR:HB3	1.98	0.46
121:S2:221:ILE:HG22	121:S2:222:ASN:HD22	1.81	0.46
130:T3:203:HIS:ND1	130:T3:211:GLU:OE2	2.38	0.46
131:T4:70:LEU:HD21	131:T4:190:HIS:HB2	1.98	0.46
158:T8:601:3PE:H262	144:TH:56:PHE:HE1	1.81	0.46
3:2f:79:VAL:HG21	11:2n:57:SER:H	1.81	0.46
3:2f:151:ARG:HH21	8:2k:91:LYS:NZ	2.14	0.46
11:2n:12:PHE:CE2	164:sc:102:U10:H1M2	2.50	0.46
29:c1:125:TYR:HD1	36:g:188:ILE:HB	1.81	0.46
29:c1:429:VAL:HB	42:m:105:ALA:HB1	1.97	0.46
29:c1:439:GLY:HA3	29:c1:455:TYR:CD2	2.51	0.46
30:c2:541:ASN:HD21	30:c2:545:TYR:HH	1.59	0.46
31:c3:207:ASN:ND2	31:c3:210:ASP:OD2	2.48	0.46
31:c3:568:SER:HB3	41:l:29:GLU:N	2.31	0.46
36:g:163:VAL:N	36:g:180:TRP:O	2.47	0.46
36:g:223:ASP:N	36:g:223:ASP:OD1	2.46	0.46
37:h:240:GLN:O	37:h:243:SER:OG	2.21	0.46
52:sa:94:ILE:HD12	52:sa:137:VAL:HG22	1.97	0.46
59:vb:500:TYR:O	59:vb:504:GLU:HG2	2.16	0.46
68:1b:41:ILE:HG13	100:n1:169:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:al:57:ASP:OD1	82:al:95:PRO:HG3	2.16	0.46
82:al:75:ARG:HG3	82:al:76:ARG:HG3	1.97	0.46
89:b7:118:TRP:CH2	104:n5:698:ASN:HB3	2.51	0.46
99:j1:183:ASP:OD2	121:s2:15:ARG:NH1	2.42	0.46
103:n4:31:ILE:HD11	158:t8:602:3PE:H291	1.97	0.46
103:n4:290:LEU:HD11	103:n4:342:MET:HE1	1.98	0.46
103:n4:418:PRO:HG3	104:n5:309:PHE:HD2	1.81	0.46
114:qG:81:THR:HG21	114:qG:145:ARG:HB3	1.97	0.46
109:qb:97:ARG:HD2	109:qb:144:GLU:HG2	1.97	0.46
120:s1:282:ILE:HA	120:s1:391:ILE:HD12	1.98	0.46
122:s3:132:ALA:O	122:s3:136:GLU:HB2	2.16	0.46
128:t1:498:ILE:O	128:t1:500:ASN:ND2	2.49	0.46
13:2T:28:VAL:HG12	13:2T:40:GLU:HB3	1.98	0.46
18:6A:52:HIS:CD2	59:VB:412:ARG:HB3	2.50	0.46
19:6B:64:ASP:HA	30:C2:456:LEU:HB2	1.98	0.46
23:7A:83:ALA:HB2	153:C1:701:CDL:H352	1.96	0.46
26:A:152:ASP:O	26:A:155:ARG:HG2	2.16	0.46
29:C1:30:PHE:HE2	153:C1:707:CDL:H121	1.80	0.46
30:C2:116:ARG:NH2	30:C2:129:GLU:OE1	2.48	0.46
31:C3:551:PRO:HB3	49:Q:142:GLN:HB2	1.97	0.46
38:I:151:GLU:HB3	38:I:155:ARG:HH21	1.80	0.46
40:K:91:LEU:HD21	40:K:107:LEU:HD13	1.96	0.46
43:M1:229:VAL:HG12	152:V:201:PC1:H12	1.98	0.46
49:Q:52:TYR:O	49:Q:55:SER:OG	2.24	0.46
70:4L:29:ILE:O	70:4L:33:SER:OG	2.33	0.46
77:A7:193:GLN:NE2	77:A7:197:ASP:OD1	2.47	0.46
79:A9:68:ASP:OD2	82:AL:149:ARG:NH2	2.45	0.46
86:B3:17:LYS:HB2	106:P1:245:LEU:HG	1.98	0.46
153:B3:102:CDL:H151	152:T4:303:PC1:H2H2	1.97	0.46
92:BL:143:LEU:HB3	93:BM:177:LEU:HD22	1.98	0.46
96:G1:72:THR:HG23	96:G1:93:VAL:HB	1.97	0.46
103:N4:454:ILE:HG21	158:N5:802:3PE:H252	1.98	0.46
105:N6:232:PHE:HA	121:S2:9:TRP:HA	1.98	0.46
106:P1:60:LEU:HD12	107:P2:68:PRO:HD3	1.98	0.46
109:QB:80:SER:HB2	109:QB:252:GLY:HA2	1.98	0.46
110:QC:321:GLN:NE2	114:QG:196:GLU:OE2	2.49	0.46
112:QE:29:GLU:O	112:QE:33:ARG:HG2	2.15	0.46
117:Qj:18:LEU:HD13	152:Qj:101:PC1:H321	1.98	0.46
129:T2:236:VAL:HG22	129:T2:284:LEU:HD22	1.98	0.46
4:2g:12:LEU:HD22	4:2g:63:TRP:HE3	1.81	0.46
4:2g:40:GLU:C	4:2g:42:PHE:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2i:32:ASN:HD22	9:2l:36:PHE:H	1.64	0.46
10:2m:12:LYS:HA	10:2m:15:LEU:HD12	1.98	0.46
17:5t:62:LYS:HG3	30:c2:239:ASN:HD22	1.79	0.46
20:6c:2:GLY:HA3	153:6c:201:CDL:HB22	1.98	0.46
29:c1:477:LEU:HD13	153:c1:712:CDL:H241	1.98	0.46
152:c1:711:PC1:H11	152:c3:605:PC1:H262	1.97	0.46
38:i:44:GLN:OE1	66:z:90:GLN:N	2.49	0.46
39:j:60:ASP:OD2	39:j:150:TYR:OH	2.25	0.46
39:j:85:LEU:HB3	39:j:193:GLN:HE22	1.79	0.46
44:m2:9:TRP:HE3	44:m2:308:LYS:HZ3	1.64	0.46
46:n:169:ARG:NH2	152:n:301:PC1:O12	2.35	0.46
49:q:93:VAL:HG13	153:q:201:CDL:H782	1.98	0.46
50:r:72:ILE:HD13	64:y5:29:PHE:HD1	1.80	0.46
52:sa:597:HIS:CD2	52:sa:617:VAL:HG22	2.51	0.46
53:sb:76:TYR:N	53:sb:167:ASP:OD1	2.38	0.46
66:z:14:HIS:NE2	57:U:38:LYS:O	2.48	0.46
152:am:202:PC1:H261	152:tc:101:PC1:H2G2	1.98	0.46
86:b3:65:VAL:HA	86:b3:68:PHE:CD2	2.50	0.46
96:g1:128:THR:HG21	98:g3:149:MET:HB2	1.97	0.46
97:g2:100:HIS:N	97:g2:128:ASN:HD22	2.13	0.46
99:j1:127:LYS:HB2	99:j1:130:THR:HG23	1.96	0.46
100:n1:138:MET:HA	100:n1:153:SER:HB2	1.98	0.46
101:n2:290:LEU:HB3	101:n2:291:ILE:HD12	1.97	0.46
108:qA:434:ASP:OD1	108:qA:434:ASP:N	2.48	0.46
111:qD:314:ARG:HD3	115:qh:29:ILE:HB	1.98	0.46
112:qe:78:ARG:HH21	112:qe:80:HIS:CD2	2.34	0.46
114:qg:209:GLU:OE1	118:ql:1:MET:N	2.49	0.46
127:s8:176:ILE:HG13	127:s8:178:CYS:HB3	1.97	0.46
141:te:40:ASN:ND2	153:te:101:CDL:OB4	2.48	0.46
146:v1:220:LYS:HG2	147:v2:65:ARG:HE	1.79	0.46
2:2E:92:SER:HA	7:2J:60:TYR:CZ	2.51	0.46
8:2K:41:VAL:HG13	153:2M:101:CDL:H632	1.97	0.46
9:2L:40:ASP:OD1	9:2L:41:ALA:N	2.49	0.46
20:6C:26:LYS:HG2	35:FS:168:GLU:HB3	1.98	0.46
27:B:379:LYS:HB3	27:B:382:ILE:HD11	1.98	0.46
29:C1:353:LEU:O	29:C1:357:VAL:HG22	2.16	0.46
29:C1:628:GLU:HG2	29:C1:630:ARG:HG2	1.97	0.46
31:C3:138:LEU:CB	31:C3:149:PHE:O	2.63	0.46
40:K:112:GLU:OE2	40:K:155:PHE:N	2.40	0.46
40:K:133:LEU:HD13	40:K:178:SER:HB2	1.97	0.46
49:Q:4:ASN:O	49:Q:10:ASN:ND2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SB:205:GLN:HB3	53:SB:251:SER:OG	2.15	0.46
54:SC:56:ASP:OD2	89:B7:49:ASN:ND2	2.49	0.46
164:SC:102:U10:H171	164:SC:102:U10:H151	1.74	0.46
56:T:56:ARG:HH21	153:T:204:CDL:H1	1.81	0.46
59:VB:162:THR:HB	59:VB:171:GLU:HB3	1.96	0.46
65:Y7:145:TYR:HB3	65:Y7:157:LEU:HD21	1.97	0.46
75:A5:174:ARG:NH1	123:S4:5:LYS:H	2.14	0.46
79:A9:132:PHE:HD2	79:A9:174:PRO:HB3	1.81	0.46
79:A9:304:TRP:HZ2	153:A9:402:CDL:H552	1.80	0.46
82:AL:75:ARG:HG3	82:AL:76:ARG:HG3	1.97	0.46
83:AM:141:ARG:HG2	105:N6:152:ILE:HG21	1.97	0.46
152:AM:202:PC1:H261	152:TC:101:PC1:H2G2	1.98	0.46
99:J1:200:ASN:HD22	99:J1:202:THR:HG23	1.80	0.46
103:N4:91:LEU:HD11	136:T9:1:MET:HA	1.97	0.46
104:N5:565:LEU:HD11	153:N5:806:CDL:H642	1.96	0.46
107:P2:69:PHE:CE2	107:P2:80:LYS:HE2	2.51	0.46
110:QC:135:VAL:HA	110:QC:142:SER:HB3	1.98	0.46
121:S2:209:VAL:HA	127:S8:91:HIS:HD1	1.81	0.46
4:2g:146:LEU:HB2	8:2k:20:VAL:HG11	1.97	0.46
153:2g:201:CDL:H151	153:2g:201:CDL:H591	1.98	0.46
19:6b:170:TYR:OH	19:6b:171:ARG:NH1	2.48	0.46
29:c1:621:MET:HG3	29:c1:622:MET:N	2.31	0.46
30:c2:134:THR:HG21	30:c2:159:ALA:HB1	1.98	0.46
31:c3:531:PHE:O	49:q:60:TYR:OH	2.29	0.46
36:g:107:TYR:HD2	58:v:79:ARG:HH21	1.62	0.46
40:k:91:LEU:HD21	40:k:107:LEU:HD13	1.97	0.46
59:vb:278:ALA:O	59:vb:282:LYS:HD3	2.16	0.46
60:w:53:ASP:OD2	60:w:61:ARG:NH1	2.46	0.46
68:1b:26:ARG:NE	100:n1:220:ASP:OD1	2.34	0.46
69:2b:43:ASN:N	69:2b:130:ILE:O	2.38	0.46
69:2b:160:LEU:HD11	153:2b:201:CDL:H771	1.98	0.46
77:a7:209:ARG:NH1	77:a7:215:MET:HE1	2.30	0.46
82:al:105:GLN:HE22	127:s8:194:PRO:HB3	1.80	0.46
83:am:167:ILE:HG21	100:n1:17:LEU:HD13	1.97	0.46
97:g2:177:ARG:NH1	138:tb:50:ALA:O	2.47	0.46
101:n2:289:PHE:HE2	101:n2:344:THR:HG23	1.80	0.46
103:n4:120:LEU:HD12	103:n4:120:LEU:HA	1.80	0.46
103:n4:318:VAL:HG13	103:n4:447:VAL:HG11	1.97	0.46
109:qB:112:ARG:O	109:qB:116:ARG:HG2	2.16	0.46
110:qc:57:VAL:O	110:qc:59:GLU:N	2.48	0.46
110:qc:246:PHE:HB2	152:qc:506:PC1:H231	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qc:270:ASP:N	110:qc:270:ASP:OD1	2.47	0.46
112:qe:50:PHE:HZ	112:qe:67:LYS:HE3	1.80	0.46
121:s2:39:GLY:HA3	126:s7:28:GLY:O	2.16	0.46
146:v1:118:SER:HB2	146:v1:246:VAL:HG11	1.97	0.46
147:v2:100:ILE:O	147:v2:104:GLU:HG3	2.16	0.46
152:2F:303:PC1:H11	8:2K:29:THR:HG23	1.98	0.46
4:2G:58:ARG:NE	4:2G:62:ASN:HD22	2.14	0.46
4:2G:161:ARG:O	4:2G:196:TYR:OH	2.33	0.46
26:A:76:VAL:HG22	26:A:195:LYS:HE2	1.98	0.46
29:C1:435:TYR:HB3	152:C1:710:PC1:H372	1.98	0.46
153:C1:712:CDL:H621	43:M1:207:PHE:HE1	1.81	0.46
30:C2:130:LEU:O	30:C2:133:PHE:HB3	2.15	0.46
33:E:87:ALA:O	33:E:154:LYS:NZ	2.44	0.46
40:K:163:PHE:HD2	40:K:164:ILE:HD12	1.80	0.46
59:VB:321:GLU:OE1	59:VB:412:ARG:NH2	2.48	0.46
65:Y7:148:PHE:CZ	149:C:138:ILE:HA	2.51	0.46
66:Z:75:ASN:OD1	66:Z:78:ARG:NH2	2.48	0.46
153:2B:201:CDL:H171	103:N4:25:PHE:HE2	1.81	0.46
153:5B:201:CDL:H421	152:N5:803:PC1:H352	1.98	0.46
83:AM:167:ILE:HG21	100:N1:17:LEU:HD13	1.97	0.46
90:B8:140:GLY:O	92:BL:126:LYS:NZ	2.33	0.46
104:N5:338:LYS:HD3	104:N5:414:TRP:HA	1.98	0.46
107:P2:85:LYS:HB3	107:P2:98:ASP:HB2	1.97	0.46
107:P2:181:ALA:O	107:P2:185:SER:OG	2.31	0.46
108:QA:266:VAL:HG13	108:QA:270:LEU:HD23	1.98	0.46
108:QA:434:ASP:OD1	108:QA:434:ASP:N	2.49	0.46
109:QB:121:ARG:NH1	109:QB:166:ASP:OD2	2.49	0.46
153:QB:601:CDL:H132	117:QJ:27:LEU:HD21	1.98	0.46
110:QC:22:VAL:HG21	115:QH:46:ARG:HG2	1.97	0.46
153:QC:503:CDL:H552	110:Qc:194:TYR:HD1	1.81	0.46
153:QC:503:CDL:H542	110:Qc:197:LEU:HD22	1.98	0.46
109:Qb:311:PRO:HG3	109:Qb:470:TRP:CZ2	2.51	0.46
109:Qb:311:PRO:HG3	109:Qb:470:TRP:CE2	2.51	0.46
109:Qb:462:LEU:HD23	109:Qb:465:ARG:HH21	1.81	0.46
110:Qc:114:ALA:HA	114:Qg:178:LEU:HD13	1.98	0.46
120:S1:568:ASP:OD1	120:S1:568:ASP:N	2.48	0.46
121:S2:69:LEU:HD22	121:S2:73:ARG:HH12	1.81	0.46
122:S3:84:ASN:HB2	122:S3:87:ASN:ND2	2.30	0.46
129:T2:222:ASN:HA	129:T2:225:THR:HG22	1.98	0.46
146:V1:210:GLU:HG3	146:V1:211:THR:H	1.81	0.46
146:V1:432:ALA:C	146:V1:435:PRO:HD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c1:88:LYS:NZ	43:m1:17:ASP:OD2	2.45	0.45
29:c1:435:TYR:HB3	152:c1:707:PC1:H372	1.98	0.45
29:c1:464:MET:HE1	30:c2:87:LEU:HA	1.98	0.45
31:c3:466:PHE:O	31:c3:470:ARG:HG2	2.16	0.45
31:c3:551:PRO:HB3	49:q:142:GLN:HB2	1.97	0.45
33:e:104:ASP:OD2	64:y5:114:TYR:N	2.49	0.45
36:g:45:PRO:O	59:vb:282:LYS:HE3	2.16	0.45
40:k:163:PHE:HD2	40:k:164:ILE:HD12	1.81	0.45
52:sa:124:ASP:OD1	52:sa:124:ASP:N	2.46	0.45
52:sa:284:HIS:CG	52:sa:294:LEU:HD11	2.51	0.45
52:sa:299:CYS:HB3	52:sa:356:LEU:HD21	1.98	0.45
73:a2:70:GLU:CD	120:s1:639:ARG:HH12	2.24	0.45
79:a9:291:HIS:CE1	79:a9:316:LYS:HD3	2.50	0.45
153:a9:403:CDL:H832	126:s7:13:VAL:HG11	1.98	0.45
82:al:133:ASN:HB2	127:s8:201:TYR:CD1	2.51	0.45
83:am:127:MET:HG3	124:s5:55:LEU:HD13	1.97	0.45
106:p1:60:LEU:HD12	107:p2:68:PRO:HD3	1.98	0.45
109:qB:48:GLU:HG3	117:qJ:2:TYR:HB2	1.98	0.45
153:qC:503:CDL:H552	110:qc:194:TYR:HD1	1.80	0.45
108:qa:96:ASP:O	108:qa:284:ARG:NH2	2.49	0.45
109:qb:295:ARG:NH2	115:qh:53:SER:OG	2.38	0.45
110:qc:315:ILE:HD11	153:qg:402:CDL:H131	1.97	0.45
110:qc:329:VAL:O	118:ql:7:LYS:NZ	2.38	0.45
110:qc:338:ARG:NH1	114:qg:33:GLU:OE1	2.49	0.45
152:qg:401:PC1:H221	118:ql:5:PHE:HB2	1.98	0.45
128:t1:24:SER:HB3	128:t1:27:HIS:ND1	2.31	0.45
128:t1:271:PRO:HB2	128:t1:278:ILE:HG12	1.98	0.45
139:tc:59:GLU:OE2	139:tc:62:ARG:NH2	2.35	0.45
4:2G:37:ASN:OD1	55:SD:21:LYS:N	2.50	0.45
153:A:504:CDL:HB22	45:M3:13:ALA:HB1	1.97	0.45
29:C1:125:TYR:HD1	36:G:188:ILE:HB	1.81	0.45
153:C1:712:CDL:H202	30:C2:56:ALA:HB2	1.96	0.45
30:C2:494:THR:OG1	30:C2:563:ARG:NH2	2.49	0.45
33:E:12:ARG:HH22	59:VB:429:GLU:HG2	1.80	0.45
38:I:21:ALA:HB3	38:I:45:ASN:HA	1.98	0.45
43:M1:306:TRP:CD2	153:M1:405:CDL:H132	2.50	0.45
52:SA:70:GLU:CD	52:SA:461:LYS:HB2	2.42	0.45
52:SA:94:ILE:HD12	52:SA:137:VAL:HG22	1.97	0.45
77:A7:78:ASP:HB2	77:A7:123:ASN:HB2	1.97	0.45
168:AB:201:ZMP:H25B	168:AB:201:ZMP:H22A	1.53	0.45
96:G1:192:LEU:O	96:G1:196:ILE:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
103:N4:31:ILE:HD11	158:T8:602:3PE:H291	1.97	0.45
103:N4:120:LEU:HD12	103:N4:120:LEU:HA	1.74	0.45
111:QD:47:VAL:HG21	111:QD:201:TYR:HE1	1.81	0.45
113:QF:8:SER:O	136:T9:26:ARG:NE	2.48	0.45
115:QH:101:TRP:NE1	153:QH:201:CDL:OA7	2.47	0.45
153:QI:203:CDL:H512	153:QI:203:CDL:HA4	1.99	0.45
109:Qb:292:MET:HE3	109:Qb:294:ILE:HD11	1.98	0.45
110:Qc:343:THR:O	114:Qg:35:ARG:NH2	2.28	0.45
120:S1:241:SER:HB3	120:S1:272:MET:HE2	1.97	0.45
121:S2:39:GLY:HA3	126:S7:28:GLY:O	2.16	0.45
128:T1:401:ILE:HG13	128:T1:403:GLY:H	1.80	0.45
130:T3:177:ASP:O	130:T3:181:LEU:HG	2.16	0.45
147:V2:75:VAL:HG11	147:V2:83:VAL:HG13	1.98	0.45
147:V2:150:LEU:HD21	147:V2:163:GLU:HB2	1.97	0.45
147:V2:175:MET:HB3	147:V2:185:GLU:HA	1.98	0.45
119:u2:3:UNK:O	119:u2:7:UNK:N	2.49	0.45
19:6b:124:TYR:N	42:m:146:ASP:OD2	2.49	0.45
20:6c:26:LYS:HD2	153:6c:201:CDL:HB31	1.98	0.45
29:c1:628:GLU:HG2	29:c1:630:ARG:HG2	1.98	0.45
30:c2:409:ILE:HG22	30:c2:584:MET:HG3	1.99	0.45
31:c3:365:SER:O	31:c3:368:ILE:HG12	2.15	0.45
33:e:64:LYS:NZ	33:e:159:GLU:OE2	2.33	0.45
42:m:202:TYR:HD1	38:I:112:SER:HB3	1.82	0.45
50:r:39:TYR:O	50:r:43:ASN:ND2	2.29	0.45
52:sa:160:PHE:CE2	52:sa:297:GLU:HB3	2.51	0.45
52:sa:593:ASN:O	52:sa:596:LYS:NZ	2.43	0.45
60:w:53:ASP:HB2	60:w:58:TRP:NE1	2.30	0.45
65:y7:114:PHE:CD1	149:c:199:GLU:HG3	2.51	0.45
71:5b:37:PHE:O	71:5b:41:SER:OG	2.15	0.45
78:a8:165:LYS:HE3	140:td:52:ARG:HA	1.97	0.45
96:g1:72:THR:HG23	96:g1:93:VAL:HB	1.97	0.45
99:j1:35:ALA:O	99:j1:86:ARG:NH2	2.41	0.45
100:n1:250:PHE:HD1	100:n1:254:PHE:HE2	1.63	0.45
102:n3:92:GLU:HG3	105:n6:178:TYR:HB3	1.99	0.45
109:qB:344:SER:HB3	109:qB:356:GLY:HA3	1.98	0.45
153:qB:601:CDL:H162	112:qE:104:LEU:HD22	1.98	0.45
110:qC:68:GLU:HG3	111:qD:89:TYR:HB3	1.97	0.45
153:qC:504:CDL:HB21	114:qG:130:ARG:HH12	1.81	0.45
111:qD:28:ARG:NH1	115:qH:120:ASN:OD1	2.49	0.45
111:qD:205:MET:HE1	113:qF:63:ARG:HB2	1.98	0.45
108:qa:402:LEU:HD11	114:qg:326:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:qd:115:HIS:CG	111:qd:116:PRO:HD2	2.51	0.45
112:qe:88:ARG:NE	115:qh:68:GLN:O	2.46	0.45
120:s1:71:SER:O	120:s1:185:ARG:NH1	2.42	0.45
121:s2:83:ASP:HB2	121:s2:84:ARG:HH11	1.81	0.45
121:s2:221:ILE:HG22	121:s2:222:ASN:HD22	1.81	0.45
127:s8:67:PRO:HG2	127:s8:70:LEU:HD23	1.98	0.45
129:t2:236:VAL:HG22	129:t2:284:LEU:HD22	1.98	0.45
146:v1:312:TRP:NE1	146:v1:334:ASP:OD1	2.43	0.45
2:2E:148:GLU:O	2:2E:209:ARG:HA	2.16	0.45
18:6A:81:ARG:NH1	153:Q:201:CDL:OB4	2.46	0.45
153:7A:201:CDL:H412	46:N:65:TRP:HZ2	1.81	0.45
24:7C:228:GLY:HA3	43:M1:330:VAL:HG21	1.99	0.45
25:7L:897:VAL:HG11	25:7L:902:VAL:HG21	1.98	0.45
26:A:354:SER:OG	31:C3:472:ASN:ND2	2.49	0.45
36:G:261:ARG:NH1	36:G:262:ASN:O	2.49	0.45
42:M:175:ARG:NH2	42:M:204:GLU:OE2	2.32	0.45
52:SA:162:GLY:HA3	52:SA:441:LEU:HD22	1.98	0.45
69:2B:119:LEU:O	103:N4:187:TYR:OH	2.28	0.45
76:A6:114:GLU:CD	122:S3:155:LYS:H	2.24	0.45
81:AC:63:ARG:NH2	93:BM:77:ASP:OD1	2.45	0.45
164:B8:301:U10:H222	164:B8:301:U10:H262	1.75	0.45
99:J1:127:LYS:HB2	99:J1:130:THR:HG23	1.97	0.45
104:N5:237:TYR:HA	104:N5:243:ARG:HA	1.98	0.45
109:QB:344:SER:HB3	109:QB:356:GLY:HA3	1.99	0.45
110:QC:103:ILE:HG23	110:QC:405:ARG:NH2	2.31	0.45
110:QC:352:ASN:HB3	110:QC:355:HIS:HB3	1.98	0.45
108:Qa:96:ASP:O	108:Qa:284:ARG:NH2	2.50	0.45
109:Qb:484:SER:O	109:Qb:488:ILE:HB	2.16	0.45
110:Qc:126:PHE:CE1	166:Qc:502:HEM:HBC1	2.51	0.45
148:X1:62:ALA:O	148:X1:92:TYR:OH	2.26	0.45
1:1t:52:HIS:HD1	16:4t:14:TYR:HH	1.64	0.45
2:2e:212:ALA:HA	2:2e:284:LEU:HG	1.97	0.45
3:2f:215:LEU:HD21	152:2f:303:PC1:H251	1.97	0.45
13:2t:28:VAL:HG12	13:2t:40:GLU:HB3	1.98	0.45
13:2t:48:ALA:HB2	16:4t:50:THR:HG23	1.99	0.45
26:a:58:LYS:HB2	26:a:92:HIS:CD2	2.50	0.45
28:bp:138:TRP:CE2	28:bp:140:GLN:HB3	2.50	0.45
28:bp:318:THR:HB	28:bp:327:LEU:HD22	1.98	0.45
31:c3:284:TRP:HB2	65:y7:317:TRP:HD1	1.81	0.45
33:e:78:GLN:HE21	33:e:256:LYS:NZ	2.15	0.45
33:e:185:GLU:HB2	33:e:251:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:208:TRP:CZ2	58:v:99:LEU:HD23	2.52	0.45
34:f:255:PHE:HD2	34:f:286:VAL:HG11	1.81	0.45
36:g:45:PRO:HG2	36:g:50:ILE:HD11	1.99	0.45
36:g:105:TYR:HB2	36:g:107:TYR:CZ	2.51	0.45
36:g:261:ARG:NH1	36:g:262:ASN:O	2.49	0.45
41:l:79:ASP:N	41:l:79:ASP:OD1	2.49	0.45
43:m1:118:LEU:HB3	43:m1:139:THR:CG2	2.47	0.45
43:m1:260:ARG:HA	43:m1:280:TYR:CD1	2.52	0.45
44:m2:2:ASN:OD1	44:m2:2:ASN:N	2.49	0.45
50:r:110:TYR:CZ	160:r:202:PX2:H4	2.51	0.45
65:y7:273:ALA:O	65:y7:278:LYS:NZ	2.44	0.45
67:z1:58:VAL:HG12	153:c:301:CDL:OB7	2.17	0.45
68:1b:18:ILE:HD13	100:n1:43:GLU:HA	1.97	0.45
69:2b:9:ILE:HG21	84:an:216:PHE:CE2	2.51	0.45
70:4l:65:GLY:HA2	102:n3:73:VAL:HG11	1.99	0.45
76:a6:92:TYR:CE1	168:ab:201:ZMP:H6	2.51	0.45
90:b8:129:LYS:HE3	90:b8:129:LYS:HB3	1.83	0.45
164:b8:301:U10:H421	164:b8:301:U10:H461	1.70	0.45
96:g1:161:ASN:HD22	97:g2:172:LEU:HB2	1.82	0.45
103:n4:15:GLU:HG3	103:n4:113:ILE:HD13	1.97	0.45
103:n4:16:PHE:HB3	144:th:55:PHE:CE2	2.52	0.45
104:n5:80:SER:O	104:n5:82:LEU:N	2.50	0.45
104:n5:389:ASN:HB2	104:n5:392:GLU:HB2	1.97	0.45
105:n6:232:PHE:HA	121:s2:9:TRP:HA	1.98	0.45
107:p2:134:ALA:HB1	107:p2:138:LEU:HD12	1.99	0.45
110:qC:135:VAL:HG21	110:qC:181:LEU:HD13	1.97	0.45
108:qa:95:LEU:HD21	108:qa:172:LEU:HD21	1.98	0.45
110:qc:114:ALA:HA	114:qg:178:LEU:HD13	1.97	0.45
110:qc:316:HIS:HD1	110:qc:402:SER:HB2	1.82	0.45
121:s2:209:VAL:HA	127:s8:91:HIS:HD1	1.80	0.45
131:t4:70:LEU:HD21	131:t4:190:HIS:HB2	1.98	0.45
158:t8:601:3PE:H262	144:th:56:PHE:HE1	1.81	0.45
147:v2:175:MET:HB3	147:v2:185:GLU:HA	1.98	0.45
1:1T:7:ASN:OD1	30:C2:271:ASN:ND2	2.30	0.45
153:2G:201:CDL:H591	153:2G:201:CDL:H151	1.99	0.45
153:6C:202:CDL:H751	35:FS:176:VAL:HG21	1.99	0.45
23:7A:95:ASP:OD2	23:7A:98:LYS:NZ	2.35	0.45
26:A:435:LYS:HE3	26:A:435:LYS:HB2	1.78	0.45
29:C1:581:LEU:HD21	29:C1:600:TRP:HB2	1.96	0.45
31:C3:466:PHE:O	31:C3:470:ARG:HG2	2.16	0.45
33:E:177:VAL:O	33:E:180:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:H:89:LYS:HD3	37:H:257:GLU:OE1	2.16	0.45
42:M:98:LEU:HD12	42:M:106:GLN:HB3	1.97	0.45
42:M:140:THR:HG22	62:Y:85:TYR:HE2	1.80	0.45
49:Q:19:SER:OG	49:Q:22:ASP:OD2	2.32	0.45
52:SA:284:HIS:CG	52:SA:294:LEU:HD11	2.51	0.45
55:SD:35:ILE:HD13	153:SD:101:CDL:H712	1.99	0.45
65:Y7:311:TYR:CE2	65:Y7:314:GLY:HA3	2.51	0.45
73:A2:70:GLU:CD	120:S1:639:ARG:HH12	2.24	0.45
76:A6:170:THR:HG21	79:A9:30:LYS:HE3	1.97	0.45
79:A9:127:LEU:HD23	79:A9:127:LEU:H	1.81	0.45
82:AL:189:ASP:OD1	82:AL:189:ASP:N	2.48	0.45
89:B7:57:MET:HE2	152:N5:804:PC1:H231	1.97	0.45
111:QD:95:LEU:HB2	111:QD:99:ALA:HB3	1.98	0.45
112:QE:66:PHE:HD2	112:QE:68:VAL:HG13	1.81	0.45
108:Qa:120:THR:O	108:Qa:125:ASN:HA	2.17	0.45
111:Qd:62:LEU:O	116:Qi:92:ASN:ND2	2.49	0.45
112:Qe:73:TRP:O	112:Qe:77:ASN:HB2	2.17	0.45
114:Qg:209:GLU:OE1	118:Ql:1:MET:N	2.49	0.45
120:S1:320:TRP:HZ3	120:S1:578:LEU:HG	1.81	0.45
120:S1:385:TYR:HB2	120:S1:524:LEU:HD13	1.97	0.45
127:S8:182:GLN:HB3	127:S8:191:VAL:HA	1.98	0.45
128:T1:458:VAL:HG12	128:T1:460:THR:HG23	1.98	0.45
146:V1:129:ARG:NH2	147:V2:185:GLU:OE2	2.48	0.45
147:V2:172:ASN:HB3	147:V2:185:GLU:HB3	1.99	0.45
2:2e:129:VAL:HG13	2:2e:130:LEU:HD12	1.97	0.45
4:2g:10:THR:HA	4:2g:13:LYS:HG2	1.98	0.45
18:6a:8:ARG:NH1	18:6a:8:ARG:HA	2.32	0.45
19:6b:181:GLN:O	19:6b:185:PHE:HB2	2.17	0.45
153:7a:201:CDL:H672	153:7a:201:CDL:H631	1.97	0.45
28:bp:173:VAL:HG22	28:bp:178:THR:HG23	1.97	0.45
30:c2:111:SER:HA	30:c2:502:ASN:HB3	1.97	0.45
152:d:501:PC1:H242	152:d:501:PC1:H282	1.99	0.45
153:e:401:CDL:H172	63:y0:78:LEU:HD13	1.99	0.45
34:f:342:ARG:O	36:g:249:ASN:ND2	2.49	0.45
42:m:94:GLN:HG2	60:w:7:ASN:HB3	1.99	0.45
42:m:98:LEU:HD12	42:m:106:GLN:HB3	1.97	0.45
45:m3:224:HIS:HA	45:m3:238:SER:HB3	1.97	0.45
59:vb:162:THR:HB	59:vb:171:GLU:HB3	1.98	0.45
59:vb:321:GLU:OE1	59:vb:412:ARG:NH2	2.48	0.45
59:vb:547:ASN:O	65:y7:240:ASN:ND2	2.49	0.45
72:a1:82:THR:HA	141:te:43:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
158:a3:201:3PE:H121	101:n2:32:ILE:HD11	1.99	0.45
75:a5:174:ARG:NH1	123:s4:5:LYS:H	2.14	0.45
79:a9:208:PHE:CZ	79:a9:272:VAL:HG11	2.51	0.45
80:ab:47:LEU:HD12	80:ab:48:PRO:HD2	1.97	0.45
87:b4:68:ARG:NH2	103:n4:386:HIS:O	2.44	0.45
95:fx:46:ASN:HB3	98:g3:301:PHE:CE2	2.52	0.45
103:n4:454:ILE:HG21	158:n5:802:3PE:H252	1.98	0.45
106:p1:25:ARG:NH2	106:p1:34:ASP:OD1	2.49	0.45
153:p1:402:CDL:H792	107:p2:71:LEU:HD21	1.99	0.45
109:qB:80:SER:HB2	109:qB:252:GLY:HA2	1.97	0.45
153:qC:503:CDL:OA4	114:qG:181:ILE:N	2.48	0.45
113:qF:8:SER:O	136:t9:26:ARG:NE	2.48	0.45
108:qa:99:THR:HG21	108:qa:221:LEU:HA	1.99	0.45
108:qa:120:THR:O	108:qa:125:ASN:HA	2.16	0.45
109:qb:350:LEU:HD12	109:qb:353:LYS:HD3	1.98	0.45
111:qd:318:TRP:CE2	114:qg:98:PHE:HB2	2.52	0.45
112:qe:73:TRP:O	112:qe:77:ASN:HB2	2.17	0.45
117:qj:18:LEU:HD13	152:qj:101:PC1:H321	1.97	0.45
120:s1:229:VAL:HG23	120:s1:231:ALA:H	1.80	0.45
120:s1:248:SER:OG	120:s1:265:ASP:OD2	2.33	0.45
120:s1:618:ARG:NH1	120:s1:622:GLU:OE1	2.35	0.45
121:s2:238:GLY:HA3	121:s2:384:GLY:HA2	1.98	0.45
122:s3:73:LEU:HB2	122:s3:90:PHE:CZ	2.50	0.45
26:A:54:TYR:CZ	26:A:173:LYS:HG3	2.51	0.45
27:B:89:ARG:HG2	59:VB:561:PRO:HB2	1.98	0.45
29:C1:88:LYS:NZ	43:M1:17:ASP:OD2	2.45	0.45
29:C1:132:VAL:HG21	29:C1:312:ASN:HD21	1.82	0.45
30:C2:197:PRO:HB3	30:C2:335:THR:HG21	1.99	0.45
31:C3:418:ASN:OD1	31:C3:420:ASN:ND2	2.50	0.45
33:E:131:LEU:O	33:E:135:ASN:ND2	2.31	0.45
36:G:159:ASN:N	36:G:159:ASN:OD1	2.50	0.45
39:J:103:LEU:HB3	39:J:104:PRO:HD3	1.98	0.45
42:M:83:PHE:O	59:VB:136:GLN:NE2	2.38	0.45
52:SA:65:PHE:HE2	52:SA:191:LEU:HD22	1.81	0.45
52:SA:270:ARG:HG3	52:SA:605:VAL:HG21	1.98	0.45
53:SB:306:ARG:NH1	53:SB:310:GLU:OE2	2.49	0.45
153:2B:201:CDL:H672	135:T8:80:VAL:HG21	1.98	0.45
73:A2:19:PHE:O	73:A2:53:GLU:HA	2.16	0.45
84:AN:106:GLN:O	84:AN:110:THR:OG1	2.21	0.45
101:N2:290:LEU:HB3	101:N2:291:ILE:HD12	1.97	0.45
103:N4:15:GLU:HG3	103:N4:113:ILE:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
104:N5:389:ASN:HB2	104:N5:392:GLU:HB2	1.97	0.45
104:N5:433:THR:OG1	104:N5:434:LEU:N	2.45	0.45
108:QA:80:THR:OG1	108:QA:259:HIS:ND1	2.34	0.45
110:QC:336:ILE:HD11	110:QC:341:ILE:HG22	1.98	0.45
115:Qh:77:GLY:HA3	115:Qh:81:THR:HB	1.97	0.45
116:Qi:71:LEU:HG	152:Qi:203:PC1:H272	1.98	0.45
120:S1:248:SER:OG	120:S1:265:ASP:OD2	2.34	0.45
122:S3:132:ALA:O	122:S3:136:GLU:HB2	2.16	0.45
128:T1:204:VAL:O	128:T1:208:ILE:HG12	2.17	0.45
143:TG:18:GLU:OE2	143:TG:115:TYR:OH	2.34	0.45
145:TX:145:GLU:HB2	145:TX:148:GLU:HG3	1.98	0.45
146:V1:118:SER:OG	146:V1:132:LEU:HD11	2.16	0.45
152:2f:303:PC1:H11	8:2k:29:THR:HG23	1.99	0.45
24:7c:52:TRP:CE2	24:7c:101:MET:HA	2.52	0.45
26:a:340:THR:HG21	152:a:501:PC1:H272	1.98	0.45
153:c1:712:CDL:H621	43:m1:207:PHE:HE1	1.81	0.45
36:g:159:ASN:N	36:g:159:ASN:OD1	2.49	0.45
39:j:103:LEU:HB3	39:j:104:PRO:HD3	1.98	0.45
50:r:8:TYR:HD1	50:r:8:TYR:HA	1.70	0.45
153:w:202:CDL:H561	153:w:202:CDL:H162	1.99	0.45
65:y7:350:LEU:O	65:y7:353:SER:OG	2.33	0.45
69:2b:99:LEU:HD23	84:an:179:PHE:HE2	1.81	0.45
78:a8:184:SER:HB3	78:a8:227:PHE:CZ	2.52	0.45
79:a9:127:LEU:HD23	79:a9:127:LEU:H	1.82	0.45
91:b9:134:GLY:HA2	91:b9:137:SER:O	2.16	0.45
91:b9:139:LYS:HE3	91:b9:143:GLU:HG2	1.99	0.45
92:bl:49:SER:HB3	136:t9:117:ARG:HD3	1.97	0.45
101:n2:221:THR:HA	101:n2:226:ILE:HD11	1.99	0.45
103:n4:314:ILE:HG12	103:n4:444:LEU:HD12	1.99	0.45
105:n6:175:LEU:O	105:n6:179:SER:HB2	2.17	0.45
111:qD:95:LEU:HB2	111:qD:99:ALA:HB3	1.98	0.45
109:qb:311:PRO:HG3	109:qb:470:TRP:CE2	2.52	0.45
110:qc:63:ILE:HD12	110:qc:138:CYS:SG	2.56	0.45
120:s1:261:ALA:HB1	120:s1:277:ARG:CZ	2.47	0.45
131:t4:68:LYS:O	131:t4:190:HIS:NE2	2.48	0.45
144:th:75:VAL:HG23	144:th:81:ARG:HG2	1.99	0.45
146:v1:45:LEU:O	146:v1:134:ASN:ND2	2.50	0.45
146:v1:432:ALA:C	146:v1:435:PRO:HD2	2.41	0.45
3:2F:218:LEU:HD12	153:2K:101:CDL:H842	1.98	0.45
4:2G:37:ASN:ND2	55:SD:21:LYS:HG3	2.31	0.45
26:A:340:THR:HG21	152:A:501:PC1:H272	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BP:352:PHE:HB3	28:BP:377:PHE:CZ	2.51	0.45
29:C1:524:VAL:HA	29:C1:527:PHE:CE2	2.51	0.45
30:C2:157:GLN:NE2	30:C2:370:GLU:OE2	2.50	0.45
31:C3:42:ILE:HD11	31:C3:134:ILE:HD11	1.98	0.45
31:C3:190:LEU:HB3	40:K:153:LEU:HD11	1.99	0.45
34:F:342:ARG:O	36:G:249:ASN:ND2	2.50	0.45
152:I:301:PC1:H332	153:I:302:CDL:H441	1.98	0.45
159:M2:406:P5S:H24A	159:M2:406:P5S:H21	1.73	0.45
47:O:123:ILE:HA	47:O:190:LEU:HD11	1.99	0.45
49:Q:81:SER:OG	59:VB:245:GLN:NE2	2.49	0.45
53:SB:60:LEU:HD22	53:SB:90:TYR:HD1	1.80	0.45
59:VB:253:VAL:HB	65:Y7:290:ILE:HD13	1.98	0.45
88:B6:105:SER:HB3	132:T5:142:LYS:HD3	1.99	0.45
164:B8:301:U10:H151	164:B8:301:U10:H171	1.70	0.45
97:G2:100:HIS:N	97:G2:128:ASN:HD22	2.13	0.45
101:N2:221:THR:HA	101:N2:226:ILE:HD11	1.99	0.45
101:N2:333:ILE:HD13	101:N2:342:TYR:HD2	1.81	0.45
103:N4:19:TYR:OH	103:N4:106:PRO:O	2.29	0.45
103:N4:290:LEU:HD11	103:N4:342:MET:HE1	1.98	0.45
104:N5:112:LEU:HB3	104:N5:116:LEU:HD12	1.97	0.45
109:QB:48:GLU:HG3	117:QJ:2:TYR:HB2	1.98	0.45
108:Qa:311:SER:HA	108:Qa:454:VAL:HG22	1.98	0.45
110:Qc:246:PHE:HB2	152:Qc:506:PC1:H231	1.98	0.45
111:Qd:57:PRO:HD3	111:Qd:233:TYR:OH	2.17	0.45
123:S4:77:ASP:OD1	123:S4:77:ASP:N	2.48	0.45
127:S8:67:PRO:HG2	127:S8:70:LEU:HD23	1.98	0.45
119:U2:3:UNK:O	119:U2:7:UNK:N	2.49	0.45
3:2f:267:ALA:HA	3:2f:270:LYS:HG2	1.99	0.45
5:2h:122:LEU:HD21	11:2n:61:GLU:HA	1.97	0.45
8:2k:30:ARG:NH1	55:sd:23:ASN:HD21	2.14	0.45
20:6c:40:TYR:CZ	20:6c:44:ILE:HD11	2.52	0.45
23:7a:126:ILE:HG23	46:n:51:TYR:HA	1.99	0.45
24:7c:77:GLN:HB2	24:7c:79:TYR:CE2	2.52	0.45
26:a:296:CYS:O	26:a:301:PRO:HD3	2.16	0.45
26:a:456:TRP:HE1	59:vb:339:ASN:ND2	2.14	0.45
31:c3:381:TRP:O	59:vb:93:THR:OG1	2.32	0.45
153:fs:203:CDL:OB2	33:E:119:ARG:NH2	2.50	0.45
36:g:104:ASP:HB2	58:v:78:GLU:HB3	1.98	0.45
37:h:290:TYR:HE2	104:N5:69:HIS:NE2	2.14	0.45
153:i:301:CDL:H381	153:i:301:CDL:H412	1.77	0.45
42:m:126:PRO:HB3	42:m:148:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m1:99:TYR:OH	43:m1:155:GLU:OE1	2.35	0.45
50:r:5:PHE:O	66:z:33:GLY:HA3	2.16	0.45
50:r:89:THR:HG23	51:s:94:LEU:HD23	1.99	0.45
53:sb:80:ASP:OD1	53:sb:80:ASP:N	2.49	0.45
59:vb:461:ARG:NH2	59:vb:520:SEP:O2P	2.50	0.45
66:z:75:ASN:OD1	66:z:78:ARG:NH2	2.47	0.45
72:a1:6:TYR:CE2	140:td:9:TRP:HB2	2.52	0.45
153:a1:101:CDL:H151	153:a1:101:CDL:H552	1.98	0.45
76:a6:38:GLU:HG3	121:s2:54:ARG:HD3	1.97	0.45
78:a8:133:GLU:O	78:a8:137:GLN:HG2	2.16	0.45
82:al:95:PRO:HA	82:al:127:HIS:CG	2.51	0.45
83:am:141:ARG:HG2	105:n6:152:ILE:HG21	1.98	0.45
90:b8:193:GLU:HG2	131:t4:16:VAL:HG21	1.97	0.45
104:n5:83:ASN:HA	104:n5:86:LYS:HE2	1.98	0.45
104:n5:376:TYR:HB3	104:n5:390:LEU:HD23	1.98	0.45
110:qC:55:SER:HB3	112:qE:117:ARG:HH21	1.81	0.45
110:qC:103:ILE:HG23	110:qC:405:ARG:NH2	2.31	0.45
153:qC:503:CDL:H542	110:qc:197:LEU:HD22	1.98	0.45
111:qd:139:HIS:HB2	111:qd:141:TYR:CE2	2.51	0.45
152:qi:201:PC1:H252	117:qj:23:GLY:HA2	1.99	0.45
120:s1:385:TYR:HB2	120:s1:524:LEU:HD13	1.97	0.45
120:s1:525:GLU:OE1	120:s1:646:HIS:NE2	2.39	0.45
127:s8:171:ASP:HB3	127:s8:174:LYS:HB2	1.97	0.45
127:s8:191:VAL:HG11	127:s8:228:ILE:HD11	1.98	0.45
129:t2:222:ASN:HA	129:t2:225:THR:HG22	1.98	0.45
146:v1:118:SER:OG	146:v1:132:LEU:HD11	2.16	0.45
147:v2:172:ASN:HB3	147:v2:185:GLU:HB3	1.98	0.45
4:2G:10:THR:HA	4:2G:13:LYS:HG2	1.98	0.45
6:2I:32:ASN:HD22	9:2L:36:PHE:H	1.65	0.45
13:2T:48:ALA:HB2	16:4T:50:THR:HG23	1.99	0.45
19:6B:124:TYR:N	42:M:146:ASP:OD2	2.49	0.45
20:6C:40:TYR:CZ	20:6C:44:ILE:HD11	2.52	0.45
24:7C:52:TRP:CE2	24:7C:101:MET:HA	2.52	0.45
28:BP:274:ASP:HB2	29:C1:19:TYR:HB2	1.99	0.45
29:C1:464:MET:HE1	30:C2:87:LEU:HA	1.98	0.45
29:C1:571:GLN:NE2	29:C1:611:THR:OG1	2.49	0.45
30:C2:187:GLY:HA2	30:C2:350:ILE:HD13	1.98	0.45
31:C3:207:ASN:ND2	31:C3:210:ASP:OD2	2.49	0.45
152:D:501:PC1:H242	152:D:501:PC1:H282	1.99	0.45
33:E:21:ALA:HB2	59:VB:308:ASN:HB3	1.98	0.45
38:I:44:GLN:OE1	66:Z:90:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:M2:210:TRP:HE1	44:M2:215:ASP:HB3	1.82	0.45
50:R:72:ILE:HD13	64:Y5:29:PHE:HD1	1.80	0.45
51:S:122:ARG:HE	51:S:144:PHE:HE2	1.64	0.45
52:SA:279:GLU:HA	52:SA:567:THR:HG23	1.98	0.45
53:SB:57:ASN:HD21	53:SB:72:LEU:HD21	1.81	0.45
55:SD:37:TYR:CZ	55:SD:41:ILE:HD13	2.52	0.45
58:V:147:ARG:HD3	58:V:147:ARG:HA	1.79	0.45
63:Y0:72:SER:O	63:Y0:76:LEU:HG	2.17	0.45
69:2B:9:ILE:HG21	84:AN:216:PHE:CE2	2.51	0.45
69:2B:99:LEU:HD23	84:AN:179:PHE:HE2	1.81	0.45
79:A9:127:LEU:HD11	79:A9:211:HIS:HE1	1.82	0.45
83:AM:73:LYS:HD3	83:AM:76:LYS:HD3	1.98	0.45
88:B6:108:LYS:HG2	88:B6:109:PRO:HD2	1.99	0.45
164:B8:301:U10:H421	164:B8:301:U10:H461	1.71	0.45
99:J1:32:ASP:OD1	99:J1:33:ARG:N	2.46	0.45
102:N3:92:GLU:HG3	105:N6:178:TYR:HB3	1.99	0.45
106:P1:57:THR:HG22	107:P2:68:PRO:HG3	1.98	0.45
108:QA:29:ASP:OD1	109:QB:465:ARG:NH2	2.50	0.45
110:QC:135:VAL:HG21	110:QC:181:LEU:HD13	1.98	0.45
153:QC:503:CDL:OA4	114:QG:181:ILE:N	2.48	0.45
108:Qa:406:VAL:HG22	114:Qg:325:ALA:HA	1.99	0.45
109:Qb:485:HIS:HD2	115:Qh:53:SER:HB3	1.82	0.45
113:Qf:22:GLU:HA	113:Qf:25:LEU:HD12	1.98	0.45
122:S3:92:ASN:HD22	122:S3:116:ASN:HD21	1.65	0.45
1:1t:4:GLU:HB2	30:c2:270:ASN:HB3	1.99	0.45
2:2e:94:LEU:O	2:2e:97:ILE:HG12	2.17	0.45
19:6b:52:HIS:O	19:6b:56:ASN:ND2	2.38	0.45
27:b:291:PHE:HZ	27:b:450:PRO:HD2	1.81	0.45
29:c1:75:ILE:HD11	29:c1:98:VAL:HA	1.99	0.45
29:c1:108:PHE:CE2	29:c1:152:LEU:HD12	2.52	0.45
32:d:252:LEU:HD21	39:j:219:ASP:HB2	1.99	0.45
153:e:403:CDL:HA4	153:FS:204:CDL:HB31	1.99	0.45
40:k:133:LEU:HD13	40:k:178:SER:HB2	1.98	0.45
42:m:106:GLN:NE2	153:m:303:CDL:H761	2.31	0.45
47:o:123:ILE:HA	47:o:190:LEU:HD11	1.99	0.45
48:p:72:ASP:HB3	48:p:105:GLN:HG2	1.98	0.45
49:q:136:ILE:HA	49:q:139:LYS:HE2	1.99	0.45
54:sc:56:ASP:OD2	89:b7:49:ASN:ND2	2.49	0.45
58:v:86:HIS:HA	58:v:90:LEU:HD23	1.97	0.45
72:a1:29:GLY:HA3	153:td:101:CDL:H382	1.97	0.45
79:a9:127:LEU:HD11	79:a9:211:HIS:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:am:21:HIS:HD2	127:s8:33:THR:HG22	1.82	0.45
91:b9:70:GLY:O	91:b9:74:ASN:ND2	2.30	0.45
97:g2:20:ARG:HE	98:g3:37:GLN:NE2	2.15	0.45
99:j1:200:ASN:HD22	99:j1:202:THR:HG23	1.80	0.45
100:n1:15:LEU:HD11	153:te:101:CDL:H581	1.98	0.45
100:n1:155:ARG:NH1	100:n1:227:GLU:OE1	2.38	0.45
104:n5:251:ASP:OD1	104:n5:444:ARG:NH2	2.38	0.45
106:p1:111:ASN:OD1	130:t3:207:ILE:HG12	2.17	0.45
107:p2:69:PHE:CE2	107:p2:80:LYS:HE2	2.51	0.45
120:s1:152:SER:HB3	121:s2:353:SER:HB2	1.99	0.45
3:2F:220:THR:O	3:2F:224:LEU:HG	2.17	0.45
8:2K:30:ARG:NH1	55:SD:23:ASN:HD21	2.14	0.45
152:7C:303:PC1:H2B1	44:M2:225:LEU:HD23	1.99	0.45
29:C1:75:ILE:HD11	29:C1:98:VAL:HA	1.99	0.45
29:C1:486:LEU:HD21	29:C1:560:GLY:HA3	1.98	0.45
31:C3:190:LEU:HD12	40:K:149:VAL:HG11	1.98	0.45
31:C3:284:TRP:HB2	65:Y7:317:TRP:HD1	1.81	0.45
31:C3:398:LEU:HD11	31:C3:489:PHE:CE1	2.52	0.45
34:F:208:TRP:CZ2	58:V:99:LEU:HD23	2.52	0.45
37:H:240:GLN:O	37:H:243:SER:OG	2.21	0.45
42:M:126:PRO:HB3	42:M:148:ILE:HD11	1.99	0.45
43:M1:118:LEU:HB3	43:M1:139:THR:CG2	2.47	0.45
45:M3:224:HIS:HA	45:M3:238:SER:HB3	1.97	0.45
49:Q:136:ILE:HA	49:Q:139:LYS:HE2	1.99	0.45
52:SA:160:PHE:CE2	52:SA:297:GLU:HB3	2.51	0.45
67:Z1:58:VAL:HG12	153:C:301:CDL:OB7	2.17	0.45
78:A8:133:GLU:O	78:A8:137:GLN:HG2	2.16	0.45
89:B7:118:TRP:CH2	104:N5:698:ASN:HB3	2.51	0.45
104:N5:548:LEU:HB3	104:N5:551:GLU:HB2	1.99	0.45
110:Qc:67:ARG:NH1	166:Qc:502:HEM:O1A	2.49	0.45
110:Qc:338:ARG:NH1	114:Qg:33:GLU:OE1	2.50	0.45
111:Qd:248:TYR:HB2	112:Qe:267:PHE:HE1	1.82	0.45
111:Qd:318:TRP:CE2	114:Qg:98:PHE:HB2	2.52	0.45
115:Qh:87:PHE:O	115:Qh:91:VAL:HB	2.17	0.45
121:S2:257:THR:HG21	121:S2:262:TYR:HB2	1.99	0.45
122:S3:93:LYS:NZ	123:S4:148:GLN:HE22	2.14	0.45
144:TH:61:LEU:HD13	144:TH:106:THR:HB	1.99	0.45
2:2e:154:THR:OG1	2:2e:158:ASP:OD2	2.29	0.45
3:2f:110:GLN:NE2	3:2f:114:ASP:OD1	2.50	0.45
3:2f:119:HIS:ND1	3:2f:142:ASP:OD2	2.46	0.45
3:2f:218:LEU:HD12	153:2k:101:CDL:H842	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6b:81:VAL:HG21	30:c2:1:MET:HB2	1.99	0.45
153:7c:301:CDL:H461	29:c1:63:VAL:HG11	1.97	0.45
27:b:281:LEU:HB2	27:b:289:LYS:O	2.17	0.45
28:bp:306:PHE:CZ	28:bp:362:VAL:HG13	2.52	0.45
28:bp:352:PHE:HB3	28:bp:377:PHE:CZ	2.51	0.45
152:c1:711:PC1:H262	59:vb:235:TYR:HA	1.98	0.45
30:c2:197:PRO:HB3	30:c2:335:THR:HG21	1.99	0.45
37:h:86:GLU:HG3	104:N5:67:ILE:HB	1.97	0.45
38:i:112:SER:HB3	42:M:202:TYR:HD1	1.82	0.45
42:m:83:PHE:O	59:vb:136:GLN:NE2	2.38	0.45
42:m:92:ASP:OD1	42:m:93:PHE:N	2.50	0.45
153:m1:404:CDL:H511	58:v:85:ILE:HG23	1.99	0.45
52:sa:569:LEU:HD13	52:sa:610:THR:HB	1.99	0.45
53:sb:306:ARG:NH1	53:sb:310:GLU:OE2	2.49	0.45
58:v:93:LYS:O	58:v:96:PRO:HD2	2.17	0.45
59:vb:269:PRO:O	59:vb:273:MET:HG2	2.15	0.45
73:a2:94:SER:OG	73:a2:98:ASN:ND2	2.49	0.45
79:a9:193:ALA:O	79:a9:256:GLY:N	2.50	0.45
94:c4:64:GLU:OE2	148:x1:130:LYS:NZ	2.35	0.45
109:qB:303:ASN:HD22	109:qB:380:TYR:HE1	1.65	0.45
110:qC:22:VAL:HG21	115:qH:46:ARG:HG2	1.98	0.45
111:qD:246:VAL:HG12	111:qD:250:ARG:HD2	1.98	0.45
113:qF:50:VAL:HG12	113:qF:51:ASN:HD22	1.82	0.45
109:qb:86:ALA:HB1	109:qb:254:VAL:HG13	1.99	0.45
111:qd:57:PRO:HD3	111:qd:233:TYR:OH	2.17	0.45
112:qe:44:VAL:HA	112:qe:71:ASP:HA	1.98	0.45
116:qi:71:LEU:HG	152:qi:203:PC1:H272	1.98	0.45
120:s1:298:LEU:HD23	120:s1:566:HIS:CE1	2.51	0.45
121:s2:257:THR:HG21	121:s2:262:TYR:HB2	1.99	0.45
127:s8:95:CYS:O	127:s8:99:TYR:HB2	2.17	0.45
128:t1:271:PRO:HB2	128:t1:278:ILE:HA	1.98	0.45
130:t3:62:ALA:HB2	130:t3:123:ASP:HB3	1.99	0.45
135:t8:56:THR:HG22	158:t8:601:3PE:H332	1.98	0.45
148:x1:19:ARG:NH2	148:x1:23:ARG:O	2.40	0.45
10:2M:16:LYS:HE3	10:2M:16:LYS:HB2	1.82	0.45
14:3T:70:TYR:OH	22:6T:11:THR:OG1	2.26	0.45
18:6A:8:ARG:NH1	18:6A:8:ARG:HA	2.32	0.45
19:6B:47:LYS:NZ	25:7L:970:LEU:O	2.50	0.45
19:6B:181:GLN:O	19:6B:185:PHE:HB2	2.17	0.45
19:6B:230:TYR:O	62:Y:101:ARG:NE	2.41	0.45
26:A:331:TRP:O	31:C3:264:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:58:SER:HB2	27:B:214:ARG:HH21	1.82	0.45
28:BP:374:ASN:ND2	28:BP:396:LYS:O	2.48	0.45
31:C3:520:TYR:HB2	56:T:45:LYS:HD3	1.99	0.45
42:M:92:ASP:OD1	42:M:93:PHE:N	2.50	0.45
153:M:305:CDL:H151	153:M:305:CDL:HB61	1.99	0.45
45:M3:206:ARG:NH2	45:M3:258:ALA:H	2.15	0.45
152:N:301:PC1:H292	152:N:301:PC1:H331	1.99	0.45
49:Q:118:ASN:H	67:Z1:10:ASN:ND2	2.14	0.45
50:R:89:THR:HG23	51:S:94:LEU:HD23	1.99	0.45
69:2B:58:SER:O	69:2B:127:LYS:NZ	2.49	0.45
72:A1:6:TYR:CE2	140:TD:9:TRP:HB2	2.52	0.45
84:AN:147:LEU:HD12	153:AN:302:CDL:H161	1.99	0.45
92:BL:85:THR:HB	92:BL:90:LEU:HD13	1.99	0.45
95:FX:46:ASN:HB3	98:G3:301:PHE:CE2	2.52	0.45
100:N1:224:ALA:HB1	100:N1:227:GLU:HB2	1.99	0.45
104:N5:117:PHE:HB2	144:TH:113:ARG:HG3	1.98	0.45
110:QC:123:PHE:O	110:QC:127:GLN:HG2	2.17	0.45
113:QF:50:VAL:HG12	113:QF:51:ASN:HD22	1.82	0.45
114:QG:28:SER:HA	108:Qa:124:THR:HG22	1.98	0.45
109:Qb:295:ARG:NH2	115:Qh:53:SER:OG	2.38	0.45
109:Qb:350:LEU:HD12	109:Qb:353:LYS:HD3	1.99	0.45
111:Qd:139:HIS:HB2	111:Qd:141:TYR:CE2	2.51	0.45
120:S1:261:ALA:HB1	120:S1:277:ARG:CZ	2.46	0.45
121:S2:267:ARG:O	121:S2:289:GLU:HG2	2.17	0.45
122:S3:94:MET:HB3	122:S3:115:LEU:HB2	1.99	0.45
126:S7:4:ASP:HA	126:S7:7:VAL:HG22	1.99	0.45
127:S8:191:VAL:HG11	127:S8:228:ILE:HD11	1.98	0.45
3:2f:124:GLN:HE22	9:2l:2:LYS:HB3	1.82	0.45
153:2g:201:CDL:H671	153:2k:101:CDL:H242	1.99	0.45
8:2k:80:ILE:HG22	10:2m:71:THR:HG22	1.99	0.45
14:3t:4:ARG:HH22	30:c2:275:LEU:HB3	1.82	0.45
14:3t:10:GLU:HG2	30:c2:247:LYS:HZ2	1.82	0.45
19:6b:64:ASP:HA	30:c2:456:LEU:HB2	1.98	0.45
19:6b:84:GLU:CD	30:c2:490:ARG:HH22	2.25	0.45
29:c1:46:TYR:OH	153:c1:701:CDL:OA3	2.22	0.45
29:c1:252:VAL:O	29:c1:255:ARG:NH1	2.45	0.45
29:c1:398:ILE:HG21	154:c1:708:HEA:HMC2	1.98	0.45
29:c1:645:ARG:NE	36:g:146:ILE:HD11	2.32	0.45
30:c2:187:GLY:HA2	30:c2:350:ILE:HD13	1.98	0.45
31:c3:515:PRO:HA	42:m:129:TRP:CE2	2.52	0.45
31:c3:545:ARG:NH1	49:q:104:THR:OG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:234:SER:O	32:d:336:ASN:ND2	2.37	0.45
36:g:135:LEU:O	36:g:140:GLN:NE2	2.42	0.45
36:g:213:ASP:OD1	36:g:213:ASP:N	2.46	0.45
41:l:102:LEU:HD21	41:l:106:ARG:HH21	1.81	0.45
42:m:140:THR:HG22	62:y:85:TYR:HE2	1.81	0.45
44:m2:20:SER:O	44:m2:24:ASN:ND2	2.36	0.45
44:m2:119:ARG:NE	153:n:304:CDL:OA7	2.50	0.45
52:sa:70:GLU:CD	52:sa:461:LYS:HB2	2.42	0.45
52:sa:162:GLY:HA3	52:sa:441:LEU:HD22	1.98	0.45
52:sa:288:ILE:HD12	52:sa:293:CYS:HB2	1.98	0.45
56:t:134:ASP:OD2	56:t:136:SER:OG	2.31	0.45
58:v:132:TRP:CH2	58:v:137:VAL:HG22	2.52	0.45
63:y0:72:SER:O	63:y0:76:LEU:HG	2.17	0.45
64:y5:96:GLU:OE2	67:z1:52:THR:OG1	2.27	0.45
71:5b:5:LYS:NZ	153:b8:302:CDL:OB4	2.46	0.45
81:ac:133:ASN:OD1	104:n5:627:GLN:NE2	2.31	0.45
84:an:53:GLU:HB2	152:an:304:PC1:H2	1.99	0.45
84:an:115:THR:HG21	158:an:301:3PE:H2G1	1.98	0.45
84:an:147:LEU:HD12	153:an:302:CDL:H161	1.99	0.45
92:bl:99:ALA:HB1	104:n5:375:LEU:HD21	1.99	0.45
99:j1:289:LEU:HG	99:j1:291:ILE:HG22	1.99	0.45
110:qC:33:LEU:HD13	110:qC:230:GLU:HA	1.99	0.45
114:qG:28:SER:HA	108:qa:124:THR:HG22	1.98	0.45
114:qG:189:TYR:CD1	114:qG:192:LEU:HB2	2.52	0.45
108:qa:406:VAL:HG22	114:qg:325:ALA:HA	1.99	0.45
109:qb:71:ASN:HD21	109:qb:268:GLY:HA2	1.82	0.45
109:qb:311:PRO:HG3	109:qb:470:TRP:CZ2	2.52	0.45
111:qd:175:ILE:H	111:qd:175:ILE:HD12	1.82	0.45
115:qh:87:PHE:O	115:qh:91:VAL:HB	2.17	0.45
120:s1:267:ARG:NH2	127:s8:143:GLN:OE1	2.50	0.45
127:s8:182:GLN:HB3	127:s8:191:VAL:HA	1.98	0.45
134:t7:124:ASP:OD1	134:t7:124:ASP:N	2.49	0.45
142:tf:153:ASN:HB3	142:tf:191:LYS:HZ2	1.82	0.45
18:6A:85:PHE:HA	153:Q:201:CDL:H552	1.99	0.45
23:7A:104:GLU:HG3	152:7A:202:PC1:H131	1.99	0.45
29:C1:91:SER:OG	29:C1:591:HIS:NE2	2.47	0.45
30:C2:111:SER:HA	30:C2:502:ASN:HB3	1.97	0.45
37:H:199:THR:HG22	37:H:201:GLY:H	1.82	0.45
41:L:79:ASP:N	41:L:79:ASP:OD1	2.49	0.45
41:L:85:LEU:HD12	41:L:176:MET:HE1	1.98	0.45
42:M:106:GLN:NE2	153:M:305:CDL:H761	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Q:46:LEU:HA	49:Q:110:LEU:HD13	1.98	0.45
51:S:9:LYS:O	51:S:13:GLN:HG2	2.17	0.45
52:SA:504:MET:HE3	52:SA:504:MET:HB3	1.89	0.45
57:U:2:SER:HB3	58:V:132:TRP:CE3	2.52	0.45
70:4L:20:VAL:HG21	71:5B:83:LEU:HB2	1.99	0.45
92:BL:99:ALA:HB1	104:N5:375:LEU:HD21	1.99	0.45
101:N2:147:LEU:HD13	101:N2:223:TRP:HH2	1.82	0.45
106:P1:111:ASN:OD1	130:T3:207:ILE:HG12	2.17	0.45
110:QC:283:ARG:HD2	110:QC:373:LEU:HB2	1.98	0.45
113:QF:13:MET:HE1	113:QF:23:LEU:HD22	1.99	0.45
114:QG:209:GLU:HB2	118:QL:1:MET:H3	1.82	0.45
117:QJ:2:TYR:OH	114:Qg:5:GLU:OE2	2.29	0.45
112:Qe:78:ARG:HH21	112:Qe:80:HIS:CD2	2.35	0.45
120:S1:267:ARG:NH2	127:S8:143:GLN:OE1	2.50	0.45
121:S2:237:THR:HA	121:S2:241:ALA:HB2	1.99	0.45
129:T2:81:SER:OG	129:T2:82:GLU:OE1	2.32	0.45
1:1t:7:ASN:OD1	30:c2:271:ASN:ND2	2.30	0.45
4:2g:41:HIS:HD2	4:2g:45:ASN:HD22	1.64	0.45
4:2g:97:ASN:ND2	8:2k:20:VAL:H	2.11	0.45
18:6a:109:GLU:HG2	31:c3:440:ARG:HH21	1.82	0.45
27:b:89:ARG:HG2	59:vb:561:PRO:HB2	1.97	0.45
28:bp:314:GLY:HA3	28:bp:356:LYS:HB3	1.99	0.45
153:c1:703:CDL:H782	153:c1:703:CDL:H312	1.98	0.45
33:e:8:HIS:HB2	33:e:239:LYS:HE2	1.98	0.45
33:e:21:ALA:HB2	59:vb:308:ASN:HB3	1.99	0.45
33:e:40:ASP:O	33:e:44:GLY:N	2.50	0.45
35:fs:4:ILE:O	35:fs:8:ALA:N	2.48	0.45
37:h:262:HIS:CE1	37:h:284:GLN:HG3	2.52	0.45
38:i:210:LYS:O	38:i:213:ILE:HG22	2.16	0.45
44:m2:1:MET:HE3	46:n:170:GLN:O	2.17	0.45
70:4l:72:SER:HB2	102:n3:66:VAL:HB	1.98	0.45
76:a6:92:TYR:HE1	168:ab:201:ZMP:H6	1.81	0.45
81:ac:58:ALA:HB2	81:ac:123:VAL:HG11	2.00	0.45
83:am:73:LYS:HD3	83:am:76:LYS:HD3	1.98	0.45
92:bl:69:GLU:OE2	92:bl:73:ARG:NE	2.46	0.45
100:n1:173:ASN:HB3	100:n1:199:PHE:HE2	1.82	0.45
101:n2:253:ILE:O	101:n2:257:ILE:HG12	2.16	0.45
102:n3:52:GLU:OE1	145:tx:166:ARG:NH2	2.50	0.45
104:n5:62:ASN:OD1	104:n5:143:ASP:N	2.50	0.45
104:n5:338:LYS:HD3	104:n5:414:TRP:HA	1.99	0.45
108:qA:29:ASP:OD1	109:qB:465:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qC:42:ILE:HG13	110:qC:91:LEU:HD21	1.99	0.45
113:qF:60:TYR:HB2	113:qF:61:PRO:HD3	1.99	0.45
153:qG:402:CDL:H122	153:qG:402:CDL:H732	1.99	0.45
108:qa:328:LEU:HD11	108:qa:394:GLU:HB3	1.98	0.45
109:qb:485:HIS:HD2	115:qh:53:SER:HB3	1.82	0.45
110:qc:67:ARG:NH1	166:qc:502:HEM:O1A	2.50	0.45
111:qd:62:LEU:O	116:qi:92:ASN:ND2	2.49	0.45
146:v1:210:GLU:HG3	146:v1:211:THR:H	1.81	0.45
3:2F:110:GLN:NE2	3:2F:114:ASP:OD1	2.50	0.45
4:2G:159:LYS:HD2	8:2K:10:MET:HE1	1.99	0.45
7:2J:53:ILE:HG13	10:2M:15:LEU:HB3	1.98	0.45
153:7A:203:CDL:H561	31:C3:279:ALA:HA	1.99	0.45
29:C1:593:TYR:CD2	29:C1:597:PHE:HB2	2.52	0.45
29:C1:645:ARG:NE	36:G:146:ILE:HD11	2.32	0.45
33:E:78:GLN:HE21	33:E:256:LYS:NZ	2.15	0.45
153:E:401:CDL:H172	63:Y0:78:LEU:HD13	1.99	0.45
35:FS:154:LYS:HD2	36:G:256:PRO:HD3	1.99	0.45
36:G:105:TYR:HB2	36:G:107:TYR:CZ	2.52	0.45
43:M1:260:ARG:HA	43:M1:280:TYR:CD1	2.52	0.45
44:M2:2:ASN:OD1	44:M2:2:ASN:N	2.49	0.45
44:M2:119:ARG:NE	153:N:304:CDL:OA7	2.50	0.45
49:Q:93:VAL:HG13	153:Q:201:CDL:H782	1.98	0.45
52:SA:569:LEU:HD12	52:SA:610:THR:HB	1.99	0.45
168:AB:201:ZMP:H1	168:AB:201:ZMP:H4A	1.67	0.45
90:B8:193:GLU:HG2	131:T4:16:VAL:HG21	1.99	0.45
103:N4:16:PHE:HB3	144:TH:55:PHE:CE2	2.51	0.45
104:N5:80:SER:O	104:N5:82:LEU:N	2.50	0.45
106:P1:25:ARG:NH2	106:P1:34:ASP:OD1	2.49	0.45
109:QB:303:ASN:HD22	109:QB:380:TYR:HE1	1.65	0.45
110:QC:68:GLU:HG3	111:QD:89:TYR:HB3	1.98	0.45
153:QC:504:CDL:H532	115:QH:97:ILE:HD11	1.99	0.45
109:Qb:207:THR:OG1	109:Qb:290:SER:OG	2.22	0.45
110:Qc:28:HIS:CD2	110:Qc:33:LEU:HD21	2.52	0.45
110:Qc:316:HIS:HD1	110:Qc:402:SER:HB2	1.82	0.45
111:Qd:286:ARG:HB3	115:Qh:61:HIS:HB2	1.99	0.45
120:S1:282:ILE:HA	120:S1:391:ILE:HD12	1.99	0.45
121:S2:348:LYS:HD2	121:S2:353:SER:HB3	1.98	0.45
153:T5:301:CDL:H321	153:T5:301:CDL:H122	1.99	0.45
134:T7:64:PRO:HG3	134:T7:99:TYR:HA	1.98	0.45
136:T9:49:MET:HE3	136:T9:67:PRO:HB2	1.99	0.45
136:T9:109:GLN:O	136:T9:111:LYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
146:V1:152:ALA:O	146:V1:192:TYR:OH	2.26	0.45
146:V1:209:GLU:O	146:V1:213:LEU:HB2	2.17	0.45
3:2f:206:ASN:HB2	53:sb:36:CYS:HB2	2.00	0.44
4:2g:35:PHE:H	4:2g:163:GLU:HG2	1.82	0.44
19:6b:37:PHE:HE1	25:7l:966:LYS:HD2	1.83	0.44
27:b:372:VAL:HG12	27:b:375:GLN:O	2.17	0.44
27:b:457:ARG:HA	27:b:457:ARG:HD3	1.77	0.44
28:bp:287:LYS:NZ	28:bp:291:GLU:OE2	2.46	0.44
29:c1:432:TYR:OH	153:c1:709:CDL:OA7	2.22	0.44
29:c1:593:TYR:CD2	29:c1:597:PHE:HB2	2.52	0.44
30:c2:157:GLN:NE2	30:c2:370:GLU:OE2	2.50	0.44
30:c2:341:GLU:OE1	47:o:97:SER:OG	2.23	0.44
31:c3:186:ASP:OD1	40:k:177:ARG:NH2	2.49	0.44
31:c3:520:TYR:HB2	56:t:45:LYS:HD3	1.98	0.44
153:e:403:CDL:H781	153:6C:202:CDL:H791	1.98	0.44
35:fs:154:LYS:HD2	36:g:256:PRO:HD3	1.99	0.44
38:i:95:TYR:HB2	158:i:303:3PE:H272	1.98	0.44
40:k:214:VAL:HG12	40:k:216:GLN:H	1.82	0.44
43:m1:91:LYS:HE3	43:m1:91:LYS:HB2	1.81	0.44
53:sb:57:ASN:HD21	53:sb:72:LEU:HD21	1.82	0.44
53:sb:166:LYS:HG2	53:sb:167:ASP:H	1.82	0.44
164:sc:102:U10:H171	164:sc:102:U10:H151	1.74	0.44
153:2b:201:CDL:H672	135:t8:80:VAL:HG21	1.98	0.44
73:a2:14:GLU:HG3	73:a2:48:PRO:HB2	1.99	0.44
73:a2:18:VAL:HA	73:a2:52:ARG:O	2.17	0.44
74:a3:57:LEU:HD22	74:a3:60:VAL:HG21	1.99	0.44
93:bm:58:ASN:O	93:bm:79:ASN:ND2	2.50	0.44
97:g2:100:HIS:CD2	135:t8:10:LEU:HD22	2.53	0.44
99:j1:299:ARG:HE	99:j1:305:VAL:HG21	1.81	0.44
100:n1:123:LEU:HD12	100:n1:181:PHE:HD1	1.82	0.44
100:n1:243:LEU:HD11	139:tc:2:VAL:N	2.32	0.44
104:n5:70:ASP:H	37:H:82:LYS:HZ1	1.65	0.44
104:n5:268:VAL:O	104:n5:272:THR:N	2.49	0.44
107:p2:118:VAL:HA	107:p2:119:PRO:HD3	1.84	0.44
109:qb:331:TYR:CD2	109:qb:355:LEU:HD13	2.52	0.44
120:s1:279:HIS:CD2	123:s4:159:ARG:HG3	2.52	0.44
121:s2:73:ARG:NE	127:s8:147:PRO:O	2.39	0.44
125:s6:106:THR:O	147:v2:31:ARG:NH1	2.50	0.44
129:t2:278:TYR:CZ	147:v2:41:PRO:HB3	2.52	0.44
145:tx:122:HIS:CE1	145:tx:126:LYS:HE3	2.52	0.44
147:v2:75:VAL:HG11	147:v2:83:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2E:129:VAL:HG13	2:2E:130:LEU:HD12	1.98	0.44
2:2E:197:GLN:O	2:2E:201:GLU:N	2.44	0.44
153:2G:201:CDL:H592	7:2J:35:TYR:HB3	1.99	0.44
19:6B:84:GLU:CD	30:C2:490:ARG:HH22	2.25	0.44
24:7C:77:GLN:HB2	24:7C:79:TYR:CE2	2.52	0.44
27:B:281:LEU:HB2	27:B:289:LYS:O	2.17	0.44
29:C1:272:ALA:HB1	29:C1:277:ILE:HG22	1.99	0.44
30:C2:201:LEU:HD13	45:M3:55:ASN:HB2	1.99	0.44
32:D:353:GLU:HG3	32:D:354:GLU:H	1.82	0.44
35:FS:127:ASN:ND2	36:G:270:TRP:O	2.46	0.44
44:M2:1:MET:HE3	46:N:170:GLN:O	2.17	0.44
45:M3:178:THR:O	45:M3:182:ASN:ND2	2.42	0.44
69:2B:53:PHE:HB3	69:2B:122:VAL:HG22	2.00	0.44
84:AN:53:GLU:HB2	152:AN:304:PC1:H2	1.99	0.44
84:AN:221:HIS:CE1	103:N4:226:THR:HB	2.52	0.44
86:B3:15:LEU:HD23	86:B3:15:LEU:HA	1.86	0.44
98:G3:154:SER:HB3	98:G3:173:GLU:HG2	1.99	0.44
153:QB:601:CDL:H162	112:QE:104:LEU:HD22	1.98	0.44
110:QC:116:TRP:CE2	166:QC:502:HEM:HBC1	2.53	0.44
114:QG:189:TYR:CD1	114:QG:192:LEU:HB2	2.52	0.44
115:QH:98:ARG:NE	153:QH:201:CDL:OA4	2.48	0.44
116:QI:60:GLN:HG3	152:QI:202:PC1:H151	1.99	0.44
117:QJ:18:LEU:HD22	152:QJ:102:PC1:H252	1.99	0.44
108:Qa:323:ASN:O	108:Qa:327:ALA:N	2.44	0.44
111:Qd:93:ASP:O	112:Qe:123:ARG:NH1	2.44	0.44
121:S2:383:LYS:O	121:S2:410:HIS:NE2	2.45	0.44
128:T1:24:SER:HB3	128:T1:27:HIS:ND1	2.31	0.44
144:TH:112:ARG:NE	144:TH:116:GLU:OE2	2.43	0.44
4:2g:105:LEU:HA	4:2g:105:LEU:HD23	1.85	0.44
7:2j:53:ILE:HG13	10:2m:15:LEU:HB3	1.98	0.44
28:bp:183:GLU:C	28:bp:185:GLY:H	2.26	0.44
28:bp:240:LYS:HG3	28:bp:254:GLN:HA	1.98	0.44
29:c1:353:LEU:O	29:c1:357:VAL:HG22	2.16	0.44
29:c1:524:VAL:HA	29:c1:527:PHE:CE2	2.52	0.44
31:c3:23:THR:O	31:c3:69:LYS:NZ	2.44	0.44
37:h:89:LYS:HD3	37:h:257:GLU:OE1	2.17	0.44
40:k:104:TRP:CE2	40:k:160:VAL:HG22	2.52	0.44
51:s:161:GLU:OE1	34:F:171:TYR:OH	2.31	0.44
52:sa:398:MET:HE2	52:sa:398:MET:HB3	1.75	0.44
56:t:34:LYS:NZ	153:t:204:CDL:OA4	2.50	0.44
56:t:138:ASN:HB3	153:t:202:CDL:H541	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:u:65:ARG:HA	57:u:69:GLN:HB3	1.99	0.44
59:vb:412:ARG:O	59:vb:418:TYR:OH	2.26	0.44
71:5b:32:PHE:CE1	71:5b:36:ILE:HG13	2.52	0.44
76:a6:114:GLU:CD	122:s3:155:LYS:H	2.24	0.44
84:an:2:GLU:OE2	84:an:188:LYS:NZ	2.36	0.44
85:b2:65:LEU:HB3	152:n5:804:PC1:H221	1.98	0.44
88:b6:87:MET:HG2	132:t5:124:PHE:CE2	2.53	0.44
91:b9:39:LEU:HD23	91:b9:76:MET:HE1	1.99	0.44
152:c4:403:PC1:H351	97:g2:18:MET:HE1	1.99	0.44
98:g3:154:SER:HB3	98:g3:173:GLU:HG2	1.99	0.44
100:n1:156:CYS:O	100:n1:160:MET:HG2	2.18	0.44
102:n3:2:GLY:HA3	102:n3:6:VAL:HG21	2.00	0.44
105:n6:159:TYR:HA	105:n6:162:PHE:CD2	2.52	0.44
106:p1:102:PHE:HE1	106:p1:105:HIS:HB2	1.79	0.44
110:qC:137:CYS:O	110:qC:142:SER:OG	2.32	0.44
110:qC:336:ILE:HD11	110:qC:341:ILE:HG22	1.98	0.44
112:qE:228:ARG:O	112:qE:230:ARG:N	2.50	0.44
109:qb:97:ARG:O	109:qb:281:ASN:ND2	2.48	0.44
114:qg:145:ARG:NH2	116:qi:4:GLY:O	2.50	0.44
120:s1:320:TRP:HZ3	120:s1:578:LEU:HG	1.80	0.44
122:s3:92:ASN:HD22	122:s3:116:ASN:HD21	1.65	0.44
141:te:53:TYR:HD1	141:te:71:LEU:HD23	1.82	0.44
147:v2:150:LEU:HD21	147:v2:163:GLU:HB2	1.98	0.44
3:2F:267:ALA:HA	3:2F:270:LYS:HG2	1.99	0.44
4:2G:146:LEU:HB2	8:2K:20:VAL:HG11	1.97	0.44
5:2H:94:TYR:OH	9:2L:14:VAL:O	2.26	0.44
24:7C:119:GLU:O	40:K:35:HIS:NE2	2.49	0.44
28:BP:318:THR:HB	28:BP:327:LEU:HD22	1.98	0.44
29:C1:56:ASN:HB3	29:C1:142:PHE:CZ	2.53	0.44
29:C1:415:ARG:NH1	29:C1:478:VAL:O	2.43	0.44
31:C3:457:PHE:O	31:C3:460:ILE:HG13	2.18	0.44
36:G:104:ASP:HB2	58:V:78:GLU:HB3	1.98	0.44
38:I:45:ASN:O	38:I:49:ASN:HB2	2.18	0.44
38:I:231:ASP:HB2	38:I:236:LEU:HD12	1.99	0.44
44:M2:11:PRO:HB2	44:M2:16:VAL:HG13	1.98	0.44
45:M3:104:GLN:HA	45:M3:108:ALA:O	2.17	0.44
49:Q:6:HIS:NE2	56:T:139:ASP:OD2	2.46	0.44
50:R:5:PHE:O	66:Z:33:GLY:HA3	2.17	0.44
50:R:39:TYR:O	50:R:43:ASN:ND2	2.29	0.44
50:R:77:GLY:HA3	160:R:202:PX2:H15	1.99	0.44
59:VB:461:ARG:NH2	59:VB:520:SEP:O2P	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:Y0:8:TYR:OH	63:Y0:31:ARG:NH1	2.42	0.44
158:A3:201:3PE:H121	101:N2:32:ILE:HD11	1.99	0.44
81:AC:86:ILE:HG13	81:AC:88:VAL:HG23	1.98	0.44
90:B8:121:LEU:HD22	90:B8:164:ILE:HG23	2.00	0.44
93:BM:64:SER:HB3	93:BM:67:ASP:HB2	1.99	0.44
98:G3:280:SER:HA	98:G3:283:TRP:NE1	2.33	0.44
100:N1:173:ASN:HB3	100:N1:199:PHE:HE2	1.82	0.44
153:P1:402:CDL:H792	107:P2:71:LEU:HD21	1.98	0.44
108:QA:412:ARG:NH1	114:QG:322:PHE:O	2.40	0.44
114:QG:288:VAL:HA	114:QG:291:GLU:HG2	1.98	0.44
111:Qd:115:HIS:CG	111:Qd:116:PRO:HD2	2.51	0.44
120:S1:638:TYR:CE1	123:S4:39:LYS:HD3	2.52	0.44
131:T4:156:THR:O	131:T4:160:PRO:HD3	2.17	0.44
135:T8:92:ARG:NE	148:X1:131:TYR:OH	2.50	0.44
146:V1:434:TRP:HB2	146:V1:435:PRO:HD3	1.99	0.44
153:2k:101:CDL:H561	153:2k:101:CDL:H532	1.79	0.44
23:7a:107:HIS:HB3	26:a:329:PHE:O	2.18	0.44
29:c1:132:VAL:HG21	29:c1:312:ASN:HD21	1.82	0.44
29:c1:218:LEU:HB2	29:c1:224:PHE:HZ	1.81	0.44
30:c2:524:LYS:HB2	30:c2:524:LYS:HE2	1.82	0.44
34:f:240:SER:O	34:f:243:GLY:N	2.49	0.44
38:i:21:ALA:HB3	38:i:45:ASN:HA	1.99	0.44
39:j:184:THR:HG21	153:j:301:CDL:HA61	1.99	0.44
42:m:200:HIS:HE1	42:m:202:TYR:CD2	2.35	0.44
153:m:303:CDL:H151	153:m:303:CDL:HB61	1.99	0.44
44:m2:210:TRP:HE1	44:m2:215:ASP:HB3	1.82	0.44
49:q:52:TYR:O	49:q:55:SER:OG	2.24	0.44
52:sa:86:HIS:NE2	161:sa:701:FAD:C9	2.77	0.44
52:sa:112:ASP:OD1	52:sa:164:SER:OG	2.30	0.44
52:sa:236:ARG:NH1	52:sa:471:LYS:O	2.49	0.44
55:sd:35:ILE:HD13	153:sd:101:CDL:H712	1.99	0.44
57:u:97:TRP:CG	57:u:98:PRO:HD3	2.53	0.44
59:vb:291:ARG:HG2	59:vb:295:LYS:HE2	1.99	0.44
71:5b:74:VAL:HG23	71:5b:77:LYS:H	1.82	0.44
168:ab:201:ZMP:H4A	168:ab:201:ZMP:H1	1.67	0.44
87:b4:96:LEU:HD22	116:qI:42:ILE:HD11	2.00	0.44
164:b8:301:U10:H251	164:b8:301:U10:H303	1.99	0.44
92:bl:137:LYS:HE3	92:bl:137:LYS:HB2	1.77	0.44
103:n4:269:THR:O	103:n4:273:ALA:N	2.41	0.44
104:n5:67:ILE:HB	37:H:86:GLU:HG3	1.99	0.44
108:qA:407:LEU:O	108:qA:411:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:qB:354:GLU:HB3	109:qB:510:TYR:OH	2.18	0.44
110:qC:123:PHE:O	110:qC:127:GLN:HG2	2.17	0.44
111:qD:147:GLN:HG3	111:qD:158:TRP:CD1	2.53	0.44
153:qI:203:CDL:H512	153:qI:203:CDL:HA4	1.99	0.44
108:qa:61:GLU:OE1	108:qa:61:GLU:N	2.51	0.44
109:qb:292:MET:HE3	109:qb:294:ILE:HD11	1.99	0.44
111:qd:248:TYR:HB2	112:qe:267:PHE:HE1	1.82	0.44
128:t1:92:HIS:NE2	153:t1:601:CDL:HA32	2.32	0.44
128:t1:401:ILE:HG13	128:t1:403:GLY:N	2.33	0.44
131:t4:207:ASN:ND2	131:t4:210:ASN:HB2	2.32	0.44
13:2T:3:ASP:O	13:2T:7:ILE:HG12	2.18	0.44
23:7A:107:HIS:HB3	26:A:329:PHE:O	2.18	0.44
29:C1:575:PHE:HD1	29:C1:578:LEU:HD12	1.83	0.44
154:C1:703:HEA:H211	154:C1:703:HEA:H271	1.37	0.44
30:C2:418:TYR:HH	30:C2:467:TYR:HH	1.59	0.44
31:C3:531:PHE:O	49:Q:60:TYR:OH	2.29	0.44
37:H:96:THR:HG23	37:H:121:THR:HG22	2.00	0.44
43:M1:167:PHE:O	43:M1:172:GLN:NE2	2.40	0.44
43:M1:300:PHE:N	153:M1:404:CDL:OB4	2.51	0.44
52:SA:236:ARG:NH1	52:SA:471:LYS:O	2.50	0.44
56:T:23:THR:HA	56:T:151:PRO:HB2	2.00	0.44
153:W:202:CDL:H561	153:W:202:CDL:H162	1.99	0.44
71:5B:32:PHE:CE1	71:5B:36:ILE:HG13	2.52	0.44
76:A6:21:TYR:OH	95:FX:134:SER:O	2.28	0.44
81:AC:58:ALA:HB2	81:AC:123:VAL:HG11	2.00	0.44
85:B2:81:PRO:HB2	85:B2:83:TYR:HE2	1.83	0.44
93:BM:58:ASN:O	93:BM:79:ASN:ND2	2.50	0.44
153:BM:301:CDL:H141	104:N5:182:PHE:HZ	1.82	0.44
99:J1:289:LEU:HG	99:J1:291:ILE:HG22	1.99	0.44
102:N3:52:GLU:OE1	145:TX:166:ARG:NH2	2.50	0.44
104:N5:166:PHE:HE2	132:T5:87:PRO:HG2	1.83	0.44
108:QA:407:LEU:O	108:QA:411:GLU:HG3	2.17	0.44
109:QB:112:ARG:O	109:QB:116:ARG:HG2	2.17	0.44
110:QC:327:ARG:NH1	110:QC:402:SER:OG	2.51	0.44
153:QC:504:CDL:HB21	114:QG:130:ARG:HH12	1.83	0.44
108:Qa:328:LEU:HD11	108:Qa:394:GLU:HB3	1.98	0.44
116:Qi:50:LYS:HE3	116:Qi:50:LYS:HB2	1.80	0.44
4:2g:37:ASN:ND2	55:sd:21:LYS:HG3	2.33	0.44
4:2g:159:LYS:HD2	8:2k:10:MET:HE1	1.98	0.44
19:6b:181:GLN:NE2	30:c2:506:ILE:O	2.51	0.44
24:7c:47:ILE:HG12	43:m1:282:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c1:218:LEU:HB2	29:c1:224:PHE:CZ	2.52	0.44
30:c2:201:LEU:HD13	45:m3:55:ASN:HB2	1.99	0.44
31:c3:190:LEU:HB3	40:k:153:LEU:HD11	1.99	0.44
35:fs:39:PRO:HD3	35:fs:54:PRO:HD3	2.00	0.44
45:m3:206:ARG:NH2	45:m3:258:ALA:H	2.15	0.44
152:n:301:PC1:H292	152:n:301:PC1:H331	1.99	0.44
50:r:87:ILE:HD12	64:y5:97:LEU:HD22	1.99	0.44
50:r:90:ARG:HE	51:s:95:LEU:HD11	1.82	0.44
53:sb:140:LEU:HG	53:sb:283:PRO:HG3	1.99	0.44
54:sc:25:ILE:O	54:sc:29:ILE:HG12	2.18	0.44
57:u:50:THR:HG21	57:u:132:TYR:CE1	2.52	0.44
59:vb:207:GLU:O	59:vb:210:TYR:HB3	2.18	0.44
59:vb:253:VAL:HB	65:y7:290:ILE:HD13	1.98	0.44
61:x:2:GLU:OE1	61:x:11:TRP:NE1	2.49	0.44
69:2b:33:MET:HA	101:n2:282:PHE:HE1	1.82	0.44
75:a5:92:ILE:O	75:a5:99:ARG:NH1	2.47	0.44
77:a7:255:ALA:HA	77:a7:258:LEU:HG	2.00	0.44
79:a9:61:ALA:HB2	79:a9:242:ALA:HB1	1.98	0.44
88:b6:108:LYS:HG2	88:b6:109:PRO:HD2	1.98	0.44
101:n2:147:LEU:HD13	101:n2:223:TRP:HH2	1.82	0.44
106:p1:170:LEU:HD23	130:t3:119:GLN:HG2	2.00	0.44
109:qB:121:ARG:NH1	109:qB:166:ASP:OD2	2.50	0.44
109:qB:311:PRO:HB3	109:qB:315:ASP:HB3	2.00	0.44
109:qB:323:PHE:O	109:qB:327:ILE:HG13	2.17	0.44
110:qC:116:TRP:CE2	166:qC:502:HEM:HBC1	2.52	0.44
108:qa:103:THR:C	108:qa:105:GLU:H	2.26	0.44
110:qc:132:LEU:HD13	110:qc:184:LEU:HB3	1.99	0.44
120:s1:179:HIS:CD2	120:s1:207:ILE:HD11	2.53	0.44
120:s1:568:ASP:OD1	120:s1:568:ASP:N	2.48	0.44
137:ta:50:ILE:HG22	137:ta:58:LEU:HD12	1.99	0.44
2:2E:140:ARG:NH2	2:2E:146:LEU:O	2.50	0.44
19:6B:81:VAL:HG21	30:C2:1:MET:HB2	1.98	0.44
26:A:37:LEU:HB3	26:A:41:ARG:NH1	2.33	0.44
29:C1:108:PHE:CE2	29:C1:152:LEU:HD12	2.52	0.44
29:C1:391:HIS:O	29:C1:394:VAL:HG22	2.17	0.44
29:C1:477:LEU:HD21	29:C1:492:MET:HE1	2.00	0.44
31:C3:397:LEU:O	31:C3:401:ILE:HG13	2.17	0.44
152:C3:601:PC1:H2D2	49:Q:94:LEU:HD23	1.99	0.44
152:C3:605:PC1:H282	153:VB:703:CDL:H821	2.00	0.44
33:E:55:SER:O	33:E:223:GLU:HG2	2.17	0.44
34:F:222:ILE:HA	34:F:238:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:F:255:PHE:HD2	34:F:286:VAL:HG11	1.82	0.44
40:K:25:ILE:HG22	40:K:26:TYR:CD2	2.52	0.44
153:M1:404:CDL:H511	58:V:85:ILE:HG23	1.99	0.44
52:SA:112:ASP:OD1	52:SA:164:SER:OG	2.31	0.44
52:SA:397:ASN:O	52:SA:399:GLY:N	2.50	0.44
153:T:204:CDL:H161	153:T:204:CDL:H201	2.00	0.44
59:VB:175:LEU:HD21	59:VB:177:PHE:HE1	1.82	0.44
68:1B:49:VAL:HG11	74:A3:67:ALA:HB1	1.99	0.44
70:4L:65:GLY:HA2	102:N3:73:VAL:HG11	1.99	0.44
77:A7:7:ARG:NE	153:T7:201:CDL:OB3	2.50	0.44
83:AM:115:LEU:HD22	124:S5:62:GLU:HB3	1.99	0.44
91:B9:162:HIS:O	103:N4:53:LYS:NZ	2.34	0.44
97:G2:178:LEU:HB2	138:TB:53:ALA:HA	2.00	0.44
98:G3:275:LEU:HB2	105:N6:225:LYS:HG2	1.97	0.44
100:N1:243:LEU:HD11	139:TC:2:VAL:N	2.32	0.44
101:N2:99:TYR:CE1	101:N2:103:ILE:HD11	2.53	0.44
101:N2:253:ILE:O	101:N2:257:ILE:HG12	2.18	0.44
105:N6:175:LEU:O	105:N6:179:SER:HB2	2.17	0.44
106:P1:170:LEU:HD23	130:T3:119:GLN:HG2	2.00	0.44
108:QA:395:LEU:HD22	108:QA:444:ALA:HB2	1.99	0.44
108:Qa:40:THR:OG1	109:Qb:457:SER:O	2.35	0.44
109:Qb:289:PRO:HD2	115:Qh:67:ASN:ND2	2.33	0.44
110:Qc:63:ILE:HD12	110:Qc:138:CYS:SG	2.57	0.44
111:Qd:177:ASN:HB3	111:Qd:201:TYR:CG	2.53	0.44
120:S1:225:ASP:OD2	120:S1:292:ARG:NH2	2.45	0.44
120:S1:446:ASN:ND2	129:T2:179:GLN:O	2.39	0.44
121:S2:83:ASP:HB2	121:S2:84:ARG:HH11	1.82	0.44
134:T7:77:MET:HG3	137:TA:81:MET:HE3	2.00	0.44
134:T7:116:ARG:NE	137:TA:106:ASP:OD1	2.51	0.44
4:2g:37:ASN:OD1	55:sd:21:LYS:N	2.49	0.44
10:2m:64:ASN:ND2	10:2m:68:ASN:O	2.50	0.44
18:6a:8:ARG:NE	33:e:139:ALA:O	2.47	0.44
25:7l:897:VAL:HG11	25:7l:902:VAL:HG21	1.99	0.44
28:bp:274:ASP:HB2	29:c1:19:TYR:HB2	1.99	0.44
29:c1:56:ASN:HB3	29:c1:142:PHE:CZ	2.52	0.44
29:c1:612:LEU:HD13	152:m1:401:PC1:H2F1	1.99	0.44
30:c2:116:ARG:NH2	30:c2:129:GLU:OE1	2.48	0.44
30:c2:130:LEU:O	30:c2:133:PHE:HB3	2.17	0.44
31:c3:457:PHE:O	31:c3:460:ILE:HG13	2.18	0.44
31:c3:517:TYR:OH	56:t:48:HIS:NE2	2.31	0.44
152:c3:601:PC1:H2D2	49:q:94:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:159:ASN:HD22	36:g:197:PRO:HA	1.83	0.44
153:i:301:CDL:H452	152:i:304:PC1:H382	1.99	0.44
43:m1:51:GLU:OE1	43:m1:96:ARG:NE	2.50	0.44
44:m2:196:ILE:HB	152:n:301:PC1:H332	1.98	0.44
49:q:46:LEU:HA	49:q:110:LEU:HD13	1.99	0.44
49:q:118:ASN:H	67:z1:10:ASN:ND2	2.15	0.44
51:s:122:ARG:HE	51:s:144:PHE:HE2	1.65	0.44
153:t:204:CDL:H161	153:t:204:CDL:H201	2.00	0.44
57:u:2:SER:HB3	58:v:132:TRP:CE3	2.52	0.44
69:2b:58:SER:O	69:2b:127:LYS:NZ	2.50	0.44
73:a2:19:PHE:O	73:a2:53:GLU:HA	2.17	0.44
76:a6:112:GLY:CA	168:ab:201:ZMP:H7	2.48	0.44
92:bl:85:THR:HB	92:bl:90:LEU:HD13	1.99	0.44
96:g1:185:ARG:NH2	96:g1:191:GLU:OE2	2.46	0.44
103:n4:71:PHE:CD1	103:n4:120:LEU:HD23	2.52	0.44
103:n4:440:ILE:HD12	103:n4:440:ILE:HA	1.86	0.44
112:qE:81:ASN:HD21	112:qE:88:ARG:HB2	1.82	0.44
109:qb:289:PRO:HD2	115:qh:67:ASN:ND2	2.33	0.44
111:qd:248:TYR:CE2	111:qd:249:LYS:HG3	2.53	0.44
115:qh:93:TYR:HA	115:qh:97:ILE:HB	2.00	0.44
128:t1:204:VAL:O	128:t1:208:ILE:HG12	2.17	0.44
145:tx:92:PHE:O	145:tx:111:ARG:NH2	2.50	0.44
147:v2:42:PHE:HE2	147:v2:79:ASN:HB2	1.82	0.44
1:1T:4:GLU:HB2	30:C2:270:ASN:HB3	1.99	0.44
26:A:139:SER:HB2	33:E:16:LEU:HG	1.99	0.44
26:A:308:THR:HB	61:X:47:PHE:HE1	1.82	0.44
28:BP:285:TYR:O	28:BP:288:HIS:HB3	2.17	0.44
29:C1:505:GLY:O	154:C1:703:HEA:HMB3	2.18	0.44
153:C1:707:CDL:H782	153:C1:707:CDL:H312	1.98	0.44
30:C2:341:GLU:OE1	47:O:97:SER:OG	2.23	0.44
31:C3:186:ASP:OD1	40:K:177:ARG:NH2	2.48	0.44
32:D:252:LEU:HD21	39:J:219:ASP:HB2	1.99	0.44
35:FS:39:PRO:HD3	35:FS:54:PRO:HD3	2.00	0.44
40:K:214:VAL:HG12	40:K:216:GLN:H	1.81	0.44
41:L:169:ASN:O	41:L:173:TYR:HB2	2.16	0.44
53:SB:61:THR:OG1	53:SB:62:SER:N	2.50	0.44
65:Y7:114:PHE:CD1	149:C:199:GLU:HG3	2.52	0.44
73:A2:18:VAL:HA	73:A2:52:ARG:O	2.18	0.44
74:A3:48:GLN:OE1	127:S8:70:LEU:N	2.47	0.44
75:A5:153:PRO:HA	122:S3:41:TRP:HZ3	1.83	0.44
77:A7:167:SER:O	77:A7:171:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
92:BL:69:GLU:OE2	92:BL:73:ARG:NE	2.46	0.44
153:C4:401:CDL:H311	153:C4:401:CDL:H522	1.99	0.44
97:G2:214:ILE:HG21	98:G3:96:LEU:HD21	2.00	0.44
100:N1:281:PHE:H	134:T7:107:ASN:ND2	2.15	0.44
103:N4:260:TRP:HB2	103:N4:316:GLY:HA2	2.00	0.44
104:N5:460:PRO:HG3	104:N5:585:TYR:CE1	2.53	0.44
109:QB:323:PHE:O	109:QB:327:ILE:HG13	2.17	0.44
111:QD:147:GLN:HG3	111:QD:158:TRP:CD1	2.52	0.44
113:QF:60:TYR:HB2	113:QF:61:PRO:HD3	1.99	0.44
120:S1:179:HIS:NE2	120:S1:205:ALA:O	2.46	0.44
120:S1:198:LYS:HE2	120:S1:198:LYS:HB3	1.85	0.44
123:S4:63:SER:O	123:S4:66:GLN:HB2	2.17	0.44
128:T1:313:ASP:CG	128:T1:317:ASN:HD22	2.26	0.44
132:T5:116:LEU:HB2	132:T5:122:ARG:HD3	2.00	0.44
2:2e:140:ARG:NH2	2:2e:146:LEU:O	2.50	0.44
14:3t:19:ASP:OD2	22:6t:11:THR:OG1	2.29	0.44
15:4a:54:GLY:HA2	15:4a:70:ILE:HD12	1.98	0.44
18:6a:85:PHE:HA	153:q:201:CDL:H552	1.99	0.44
20:6c:26:LYS:HG2	35:fs:168:GLU:HB3	1.98	0.44
153:6c:201:CDL:H751	35:fs:176:VAL:HG21	1.98	0.44
27:b:86:LYS:NZ	59:vb:581:GLU:OE1	2.50	0.44
29:c1:391:HIS:O	29:c1:394:VAL:HG22	2.17	0.44
37:h:38:GLN:NE2	51:S:145:ILE:HG21	2.33	0.44
37:h:96:THR:HG23	37:h:121:THR:HG22	1.99	0.44
42:m:175:ARG:NH2	42:m:204:GLU:OE2	2.32	0.44
153:m:302:CDL:H511	153:m:302:CDL:HB21	1.99	0.44
43:m1:62:LEU:HD11	58:v:48:PRO:HG2	2.00	0.44
158:sc:101:3PE:H372	158:sc:101:3PE:H241	2.00	0.44
55:sd:37:TYR:CZ	55:sd:41:ILE:HD13	2.52	0.44
59:vb:87:LYS:O	59:vb:91:GLU:HG3	2.18	0.44
70:4l:20:VAL:HG21	71:5b:83:LEU:HB2	1.99	0.44
153:5b:201:CDL:H421	152:n5:803:PC1:H352	1.98	0.44
79:a9:267:TYR:CD1	79:a9:275:MET:HE1	2.52	0.44
168:ab:201:ZMP:C14	168:ab:201:ZMP:H17	2.47	0.44
88:b6:122:VAL:HG21	132:t5:83:PRO:HD3	1.99	0.44
89:b7:57:MET:HE2	152:n5:804:PC1:H231	1.98	0.44
92:bl:139:ASN:O	92:bl:159:LYS:NZ	2.49	0.44
103:n4:488:LEU:HD13	153:th:200:CDL:H372	2.00	0.44
110:qc:28:HIS:CD2	110:qc:33:LEU:HD21	2.52	0.44
111:qd:177:ASN:HB3	111:qd:201:TYR:CD1	2.53	0.44
111:qd:267:ILE:HD11	112:qe:99:TYR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
120:s1:293:HIS:HB3	120:s1:697:THR:HG21	2.00	0.44
129:t2:81:SER:OG	129:t2:82:GLU:OE1	2.33	0.44
147:v2:123:GLN:NE2	147:v2:180:ASN:OD1	2.32	0.44
2:2E:35:PHE:HB2	2:2E:62:LYS:HG3	2.00	0.44
2:2E:39:TYR:O	2:2E:42:GLU:HG3	2.17	0.44
4:2G:40:GLU:O	4:2G:41:HIS:HB3	2.17	0.44
4:2G:41:HIS:HD2	4:2G:45:ASN:HD22	1.64	0.44
153:2K:101:CDL:H381	153:2K:101:CDL:HB21	2.00	0.44
11:2N:56:ASP:HB3	11:2N:59:VAL:HG23	2.00	0.44
16:4T:53:TYR:HA	16:4T:57:GLU:HB3	1.99	0.44
18:6A:120:LEU:HB3	19:6B:187:PHE:CE1	2.52	0.44
23:7A:126:ILE:HG23	46:N:51:TYR:HA	1.99	0.44
28:BP:314:GLY:HA3	28:BP:356:LYS:HB3	2.00	0.44
29:C1:119:ALA:HA	29:C1:123:ILE:HD13	2.00	0.44
30:C2:409:ILE:HG22	30:C2:584:MET:HG3	1.98	0.44
31:C3:258:TYR:OH	45:M3:2:ALA:N	2.44	0.44
33:E:336:ALA:HB3	36:G:73:PRO:HB2	2.00	0.44
34:F:231:GLY:HA3	34:F:326:ILE:O	2.18	0.44
34:F:266:ASP:OD1	34:F:267:ASN:N	2.51	0.44
36:G:45:PRO:HG2	36:G:50:ILE:HD11	1.99	0.44
42:M:94:GLN:HG2	60:W:7:ASN:HB3	1.99	0.44
43:M1:99:TYR:OH	43:M1:155:GLU:OE1	2.35	0.44
50:R:90:ARG:HE	51:S:95:LEU:HD11	1.82	0.44
58:V:116:ASN:OD1	58:V:119:ARG:NH2	2.39	0.44
61:X:2:GLU:OE1	61:X:11:TRP:NE1	2.48	0.44
69:2B:40:LEU:HA	69:2B:44:LEU:HD11	2.00	0.44
69:2B:55:GLU:HB3	69:2B:130:ILE:HG21	1.99	0.44
82:AL:2:GLY:HA2	100:N1:61:TYR:HB2	2.00	0.44
83:AM:165:ARG:HD2	83:AM:165:ARG:HA	1.80	0.44
84:AN:85:ILE:HG13	145:TX:107:GLN:NE2	2.32	0.44
85:B2:121:SER:OG	90:B8:178:ASN:HB3	2.18	0.44
88:B6:122:VAL:HG21	132:T5:83:PRO:HD3	2.00	0.44
97:G2:107:LYS:NZ	98:G3:110:LEU:O	2.48	0.44
100:N1:77:LYS:NZ	126:S7:85:LEU:O	2.51	0.44
100:N1:160:MET:HG2	105:N6:94:PHE:CE1	2.53	0.44
104:N5:72:TRP:CZ2	104:N5:76:PHE:HB3	2.53	0.44
104:N5:473:VAL:O	104:N5:477:GLN:HG2	2.18	0.44
108:QA:246:PRO:HA	108:QA:249:ILE:HD12	1.99	0.44
110:QC:15:LYS:O	110:QC:19:TYR:N	2.48	0.44
113:QF:74:GLN:HB2	113:QF:75:PRO:HD3	1.99	0.44
122:S3:68:THR:HG21	122:S3:95:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
122:S3:124:SER:HB2	122:S3:147:TYR:HB3	1.99	0.44
130:T3:261:ASN:O	130:T3:266:ARG:N	2.51	0.44
141:TE:53:TYR:HD1	141:TE:71:LEU:HD23	1.82	0.44
143:TG:44:TYR:HB2	143:TG:114:ILE:HG21	2.00	0.44
146:V1:415:GLN:O	146:V1:419:GLN:HG3	2.17	0.44
7:2j:16:LEU:HD13	8:2k:32:TRP:HE1	1.82	0.44
13:2t:3:ASP:O	13:2t:7:ILE:HG12	2.18	0.44
26:a:408:VAL:HG21	59:vb:339:ASN:HD21	1.83	0.44
28:bp:170:ASP:OD2	28:bp:239:TYR:OH	2.20	0.44
28:bp:285:TYR:O	28:bp:288:HIS:HB3	2.17	0.44
32:d:353:GLU:HG3	32:d:354:GLU:H	1.82	0.44
33:e:110:TYR:OH	33:e:147:PHE:O	2.27	0.44
34:f:346:HIS:HE1	36:g:253:ASP:HB3	1.83	0.44
45:m3:104:GLN:HA	45:m3:108:ALA:O	2.18	0.44
59:vb:156:PHE:CD1	59:vb:179:LEU:HD11	2.53	0.44
60:w:17:LEU:O	60:w:22:PRO:HD3	2.18	0.44
65:y7:311:TYR:CE2	65:y7:314:GLY:HA3	2.51	0.44
158:a3:202:3PE:H241	102:n3:90:THR:HG23	2.00	0.44
76:a6:50:VAL:HG13	98:g3:314:ALA:HB3	2.00	0.44
81:ac:86:ILE:HG13	81:ac:88:VAL:HG23	1.99	0.44
82:al:55:GLY:HA3	82:al:98:TRP:CH2	2.53	0.44
82:al:177:LYS:HD2	120:s1:573:TYR:CZ	2.53	0.44
83:am:73:LYS:O	83:am:77:ARG:HG3	2.17	0.44
92:bl:127:ILE:O	92:bl:131:VAL:HG23	2.18	0.44
94:c4:1:MET:O	135:t8:70:VAL:N	2.51	0.44
97:g2:202:LYS:HE2	97:g2:202:LYS:HB3	1.86	0.44
100:n1:281:PHE:H	134:t7:107:ASN:ND2	2.16	0.44
103:n4:341:GLU:O	103:n4:345:ILE:HG13	2.18	0.44
104:n5:237:TYR:HA	104:n5:243:ARG:HA	1.99	0.44
105:n6:234:ARG:NE	121:s2:419:LYS:O	2.40	0.44
107:p2:63:TYR:OH	107:p2:102:HIS:O	2.34	0.44
108:qA:91:MET:SD	108:qA:164:PHE:HB2	2.58	0.44
110:qC:109:GLU:HG2	114:qG:91:ARG:NE	2.32	0.44
110:qC:236:GLU:HB3	153:qD:402:CDL:H511	2.00	0.44
111:qD:47:VAL:HG21	111:qD:201:TYR:HE1	1.83	0.44
108:qa:252:CYS:HB2	108:qa:417:LEU:HD11	2.00	0.44
109:qb:130:LEU:HD11	109:qb:137:LEU:HB2	1.98	0.44
111:qd:145:PHE:N	111:qd:149:GLN:OE1	2.49	0.44
111:qd:286:ARG:HB3	115:qh:61:HIS:HB2	2.00	0.44
111:qd:288:GLU:OE1	111:qd:290:TYR:OH	2.26	0.44
120:s1:140:LEU:HD23	162:s1:801:SF4:S4	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
120:s1:482:ARG:HD2	129:t2:150:GLY:HA3	1.99	0.44
130:t3:177:ASP:O	130:t3:181:LEU:HG	2.16	0.44
131:t4:156:THR:O	131:t4:160:PRO:HD3	2.18	0.44
135:t8:92:ARG:NE	148:x1:131:TYR:OH	2.50	0.44
146:v1:158:TYR:CB	146:v1:213:LEU:HD21	2.48	0.44
146:v1:415:GLN:O	146:v1:419:GLN:HG3	2.18	0.44
148:x1:16:LEU:HD23	148:x1:115:VAL:HG11	2.00	0.44
27:B:253:ARG:HD3	27:B:253:ARG:HA	1.87	0.44
28:BP:240:LYS:HG3	28:BP:254:GLN:HA	1.98	0.44
33:E:40:ASP:O	33:E:44:GLY:N	2.50	0.44
37:H:262:HIS:CE1	37:H:284:GLN:HG3	2.52	0.44
39:J:95:THR:HG23	39:J:144:LEU:HD21	1.99	0.44
46:N:186:ALA:HB3	46:N:189:HIS:CD2	2.53	0.44
51:S:57:ALA:HB1	51:S:76:LYS:HD2	1.99	0.44
56:T:86:ARG:NH2	153:T:203:CDL:OB4	2.43	0.44
57:U:96:PHE:N	153:U:201:CDL:OA3	2.36	0.44
58:V:132:TRP:CH2	58:V:137:VAL:HG22	2.52	0.44
59:VB:500:TYR:O	59:VB:504:GLU:HG2	2.16	0.44
71:5B:4:ASN:HD21	153:5B:201:CDL:H392	1.83	0.44
71:5B:74:VAL:HG23	71:5B:77:LYS:H	1.82	0.44
77:A7:22:LEU:HD12	77:A7:23:PRO:HD2	2.00	0.44
78:A8:184:SER:HB3	78:A8:227:PHE:CZ	2.52	0.44
84:AN:115:THR:HG21	158:AN:301:3PE:H2G1	1.98	0.44
90:B8:74:VAL:HB	90:B8:78:LYS:HD3	1.99	0.44
93:BM:135:LEU:HD22	138:TB:25:ILE:HD13	1.99	0.44
97:G2:100:HIS:CD2	135:T8:10:LEU:HD22	2.53	0.44
101:N2:59:ILE:HG13	101:N2:125:ILE:HG23	1.99	0.44
101:N2:114:GLU:O	101:N2:117:ILE:HG22	2.17	0.44
102:N3:2:GLY:HA3	102:N3:6:VAL:HG21	1.99	0.44
104:N5:251:ASP:OD1	104:N5:444:ARG:NH2	2.38	0.44
104:N5:736:ILE:HG12	152:N5:805:PC1:H2B2	1.99	0.44
105:N6:93:VAL:O	105:N6:97:VAL:HG23	2.17	0.44
107:P2:134:ALA:HB1	107:P2:138:LEU:HD12	1.99	0.44
112:QE:121:TRP:NE1	112:QE:263:PRO:O	2.50	0.44
112:QE:268:TRP:CD1	152:QE:303:PC1:H152	2.52	0.44
108:Qa:61:GLU:OE1	108:Qa:61:GLU:N	2.51	0.44
108:Qa:79:ILE:O	108:Qa:252:CYS:HA	2.18	0.44
109:Qb:74:ARG:HE	109:Qb:439:VAL:HG12	1.83	0.44
112:Qe:81:ASN:O	112:Qe:81:ASN:ND2	2.51	0.44
152:Qg:401:PC1:H221	118:Ql:5:PHE:HB2	1.98	0.44
115:Qh:82:TYR:O	115:Qh:86:ARG:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
120:S1:179:HIS:CD2	120:S1:207:ILE:HD11	2.52	0.44
126:S7:63:ILE:HD11	126:S7:84:THR:HG21	1.99	0.44
128:T1:221:VAL:HG21	128:T1:246:LEU:HD21	1.99	0.44
131:T4:207:ASN:ND2	131:T4:210:ASN:HB2	2.32	0.44
136:T9:49:MET:HG3	136:T9:67:PRO:HG2	2.00	0.44
137:TA:50:ILE:HG22	137:TA:58:LEU:HD12	2.00	0.44
147:V2:42:PHE:HE2	147:V2:79:ASN:HB2	1.82	0.44
3:2f:220:THR:O	3:2f:224:LEU:HG	2.17	0.44
4:2g:40:GLU:O	4:2g:41:HIS:HB3	2.17	0.44
5:2h:86:ILE:HG22	8:2k:90:LEU:HG	1.99	0.44
153:6c:202:CDL:H641	34:f:201:LEU:HD22	1.99	0.44
26:a:37:LEU:HB3	26:a:41:ARG:NH1	2.33	0.44
28:bp:253:ASN:O	28:bp:256:GLY:N	2.51	0.44
29:c1:137:LEU:HD11	152:c1:704:PC1:H342	2.00	0.44
153:c1:701:CDL:H182	153:c1:701:CDL:H341	1.99	0.44
30:c2:71:TYR:HB3	59:vb:172:GLY:O	2.17	0.44
31:c3:398:LEU:HD11	31:c3:489:PHE:CE1	2.52	0.44
41:l:169:ASN:O	41:l:173:TYR:HB2	2.16	0.44
153:m:304:CDL:H312	153:m:304:CDL:HB32	2.00	0.44
51:s:57:ALA:HB1	51:s:76:LYS:HD2	1.99	0.44
56:t:23:THR:HA	56:t:151:PRO:HB2	2.00	0.44
61:x:11:TRP:CZ3	61:x:19:ILE:HG13	2.48	0.44
82:al:156:GLN:HE22	123:s4:118:PRO:HA	1.83	0.44
90:b8:74:VAL:HB	90:b8:78:LYS:HD3	1.99	0.44
93:bm:64:SER:HB3	93:bm:67:ASP:HB2	1.99	0.44
101:n2:114:GLU:O	101:n2:117:ILE:HG22	2.18	0.44
104:n5:188:LEU:HB3	152:n5:801:PC1:H332	2.00	0.44
108:qA:254:ALA:HB2	108:qA:417:LEU:HD13	1.98	0.44
109:qb:462:LEU:HD23	109:qb:465:ARG:HH21	1.82	0.44
134:t7:67:GLY:O	134:t7:94:PHE:HB3	2.18	0.44
143:tg:49:THR:O	143:tg:53:GLU:HG3	2.18	0.44
147:v2:212:ARG:HG3	147:v2:216:GLU:O	2.18	0.44
1:1T:52:HIS:HD1	16:4T:14:TYR:HH	1.65	0.44
3:2F:268:TYR:CG	8:2K:75:LEU:HD13	2.53	0.44
5:2H:86:ILE:HG22	8:2K:90:LEU:HG	1.99	0.44
5:2H:105:HIS:CD2	5:2H:152:ARG:HG2	2.53	0.44
27:B:291:PHE:HB3	27:B:357:LEU:HB3	2.00	0.44
153:C1:701:CDL:H182	153:C1:701:CDL:H341	2.00	0.44
33:E:8:HIS:HB2	33:E:239:LYS:HE2	1.98	0.44
33:E:185:GLU:HB2	33:E:251:ILE:HD11	1.98	0.44
34:F:166:TYR:O	34:F:211:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:F:194:LYS:HE2	43:M1:231:GLU:HB2	2.00	0.44
40:K:104:TRP:CE2	40:K:160:VAL:HG22	2.53	0.44
42:M:143:ARG:NH2	42:M:186:ASP:OD1	2.45	0.44
57:U:51:GLN:NE2	57:U:55:ASP:OD1	2.50	0.44
58:V:78:GLU:CD	58:V:84:ASN:HD21	2.24	0.44
59:VB:187:ARG:HA	59:VB:193:GLN:O	2.18	0.44
72:A1:54:LYS:NZ	83:AM:149:ASN:O	2.48	0.44
79:A9:267:TYR:CD1	79:A9:275:MET:HE1	2.52	0.44
83:AM:21:HIS:HD2	127:S8:33:THR:HG22	1.82	0.44
83:AM:73:LYS:O	83:AM:77:ARG:HG3	2.17	0.44
85:B2:65:LEU:HB3	152:N5:804:PC1:H221	1.99	0.44
97:G2:96:ILE:HD13	97:G2:110:ILE:HG22	2.00	0.44
100:N1:123:LEU:HD12	100:N1:181:PHE:HD1	1.82	0.44
103:N4:341:GLU:O	103:N4:345:ILE:HG13	2.18	0.44
152:N6:301:PC1:H2I3	152:TC:101:PC1:H2B1	2.00	0.44
110:QC:28:HIS:HB3	110:QC:207:TRP:HH2	1.81	0.44
110:QC:236:GLU:HB3	153:QD:402:CDL:H511	2.00	0.44
111:QD:28:ARG:NH1	115:QH:120:ASN:OD1	2.50	0.44
113:QF:13:MET:HE3	113:QF:20:PRO:HB3	1.99	0.44
108:Qa:166:MET:HE2	108:Qa:166:MET:HB3	1.93	0.44
110:Qc:64:PRO:O	110:Qc:68:GLU:HG2	2.18	0.44
110:Qc:98:HIS:O	110:Qc:102:LYS:HG2	2.18	0.44
110:Qc:116:TRP:O	166:Qc:503:HEM:HBC2	2.17	0.44
120:S1:279:HIS:CD2	123:S4:159:ARG:HG3	2.52	0.44
121:S2:21:LYS:HE2	121:S2:53:GLU:OE1	2.18	0.44
130:T3:67:GLN:HE22	130:T3:272:HIS:HE1	1.65	0.44
143:TG:46:LYS:HB2	144:TH:42:GLN:HG3	1.99	0.44
149:c:180:ASN:HB3	149:c:184:GLN:HB2	1.99	0.44
3:2f:158:ILE:HD13	3:2f:240:PHE:HE2	1.83	0.44
153:2g:201:CDL:H592	7:2j:35:TYR:HB3	1.99	0.44
153:6c:201:CDL:H791	153:E:403:CDL:H781	1.99	0.44
26:a:178:THR:HG22	26:a:183:GLU:HG2	2.00	0.44
152:a:501:PC1:H282	31:c3:406:PHE:CD1	2.53	0.44
29:c1:272:ALA:HB1	29:c1:277:ILE:HG22	1.99	0.44
29:c1:462:ILE:O	29:c1:465:PRO:HD2	2.18	0.44
153:c1:712:CDL:H162	30:c2:56:ALA:HA	2.00	0.44
153:c1:712:CDL:H592	43:m1:207:PHE:CE1	2.53	0.44
31:c3:267:PRO:O	31:c3:271:ILE:HG12	2.18	0.44
152:c3:605:PC1:H282	153:q:203:CDL:H821	2.00	0.44
33:e:55:SER:O	33:e:223:GLU:HG2	2.17	0.44
34:f:304:ASN:HD22	51:S:160:SER:HG	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:184:CYS:SG	36:g:191:LEU:HB2	2.58	0.44
37:h:280:SER:O	37:h:284:GLN:HG2	2.18	0.44
41:l:153:TYR:HB3	153:l:301:CDL:H211	2.00	0.44
49:q:109:ARG:HA	49:q:112:THR:HG22	2.00	0.44
52:sa:459:LEU:HA	52:sa:462:GLU:HG2	2.00	0.44
53:sb:194:ASP:OD1	53:sb:195:ALA:N	2.47	0.44
57:u:51:GLN:NE2	57:u:55:ASP:OD1	2.50	0.44
58:v:78:GLU:CD	58:v:84:ASN:HD21	2.23	0.44
69:2b:119:LEU:O	103:n4:187:TYR:OH	2.28	0.44
74:a3:20:VAL:HG22	96:g1:229:ASP:HB3	1.99	0.44
77:a7:22:LEU:HD12	77:a7:23:PRO:HD2	2.00	0.44
81:ac:63:ARG:NH2	93:bm:77:ASP:OD1	2.45	0.44
83:am:77:ARG:NH2	137:ta:104:ASP:OD1	2.47	0.44
84:an:85:ILE:HG13	145:tx:107:GLN:NE2	2.32	0.44
152:an:304:PC1:H332	110:qC:244:VAL:HG22	2.00	0.44
89:b7:118:TRP:NE1	90:b8:104:ASN:O	2.37	0.44
93:bm:135:LEU:HD22	138:tb:25:ILE:HD13	1.99	0.44
100:n1:262:VAL:HG23	100:n1:263:LEU:HG	2.00	0.44
101:n2:217:LEU:O	124:s5:48:HIS:NE2	2.47	0.44
104:n5:569:LEU:HD13	104:n5:660:ILE:HG21	2.00	0.44
152:n6:301:PC1:H282	139:tc:8:VAL:HG11	2.00	0.44
152:n6:301:PC1:H2I3	152:tc:101:PC1:H2B1	2.00	0.44
110:qC:200:GLY:O	110:qC:203:MET:HG3	2.18	0.44
111:qD:190:MET:HE1	111:qD:205:MET:HB2	2.00	0.44
115:qH:98:ARG:NE	153:qH:201:CDL:OA4	2.48	0.44
110:qc:116:TRP:O	166:qc:503:HEM:HBC2	2.17	0.44
127:s8:121:ARG:HB3	127:s8:192:GLU:OE1	2.18	0.44
128:t1:171:PHE:HA	128:t1:174:TYR:CD2	2.53	0.44
129:t2:77:LYS:HE2	129:t2:265:ALA:HB2	2.00	0.44
130:t3:67:GLN:HE22	130:t3:272:HIS:HE1	1.66	0.44
136:t9:49:MET:HG3	136:t9:67:PRO:HG2	2.00	0.44
2:2E:93:LYS:HE2	2:2E:93:LYS:HB3	1.90	0.44
14:3T:4:ARG:HH22	30:C2:275:LEU:HB3	1.82	0.44
18:6A:9:THR:HB	18:6A:14:ILE:HD11	1.99	0.44
20:6C:7:ARG:HH21	153:FS:204:CDL:HB4	1.83	0.44
153:7C:301:CDL:HA31	29:C1:36:LEU:HD11	2.00	0.44
29:C1:218:LEU:HB2	29:C1:224:PHE:CZ	2.53	0.44
153:C1:712:CDL:H592	43:M1:207:PHE:CE1	2.53	0.44
31:C3:17:TRP:N	31:C3:54:GLY:O	2.50	0.44
48:P:38:LYS:H	48:P:117:ASN:ND2	2.13	0.44
52:SA:597:HIS:CD2	52:SA:617:VAL:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:VB:495:ALA:HB3	59:VB:500:TYR:CZ	2.53	0.44
65:Y7:332:TRP:CZ2	153:Y7:501:CDL:H771	2.52	0.44
82:AL:86:GLN:HE22	100:N1:61:TYR:HD1	1.65	0.44
83:AM:111:LEU:HD13	124:S5:71:LEU:HD21	2.00	0.44
164:B8:301:U10:H251	164:B8:301:U10:H303	1.99	0.44
100:N1:282:ASN:HD22	134:T7:2:THR:HG21	1.83	0.44
100:N1:282:ASN:HD21	134:T7:5:GLY:HA2	1.83	0.44
104:N5:188:LEU:HB3	152:N5:801:PC1:H332	2.00	0.44
109:QB:235:ASN:O	109:QB:239:THR:HG22	2.18	0.44
110:QC:200:GLY:O	110:QC:203:MET:HG3	2.18	0.44
109:Qb:333:ALA:HB2	109:Qb:362:THR:HA	2.00	0.44
120:S1:169:LEU:HG	120:S1:293:HIS:CE1	2.51	0.44
120:S1:298:LEU:HD23	120:S1:566:HIS:CE1	2.51	0.44
120:S1:401:LEU:HD22	120:S1:461:PHE:HE2	1.82	0.44
123:S4:100:PRO:HB2	123:S4:103:TYR:HE1	1.83	0.44
135:T8:56:THR:HG22	158:T8:601:3PE:H332	1.98	0.44
145:TX:122:HIS:CE1	145:TX:126:LYS:HE3	2.52	0.44
146:V1:129:ARG:NH1	147:V2:169:ALA:HB2	2.33	0.44
146:V1:158:TYR:CB	146:V1:213:LEU:HD21	2.48	0.44
149:C:180:ASN:HB3	149:C:184:GLN:HB2	1.99	0.44
2:2e:9:ALA:HB3	2:2e:33:ASP:OD2	2.17	0.43
2:2e:35:PHE:HB2	2:2e:62:LYS:HG3	1.99	0.43
11:2n:56:ASP:HB3	11:2n:59:VAL:HG23	1.99	0.43
19:6b:144:ASP:O	19:6b:148:HIS:N	2.51	0.43
20:6c:10:TYR:OH	36:g:236:GLU:OE1	2.34	0.43
152:c1:711:PC1:H241	59:vb:237:TYR:HE1	1.83	0.43
31:c3:397:LEU:O	31:c3:401:ILE:HG13	2.17	0.43
35:fs:180:VAL:HG21	152:I:301:PC1:H241	2.00	0.43
38:i:22:ALA:HA	66:z:88:LYS:HB3	2.00	0.43
40:k:25:ILE:HG22	40:k:26:TYR:CD2	2.53	0.43
46:n:74:LYS:HD2	65:y7:341:GLY:HA3	2.00	0.43
46:n:186:ALA:HB3	46:n:189:HIS:CD2	2.53	0.43
51:s:46:VAL:HG21	65:y7:190:ILE:HD11	2.00	0.43
52:sa:79:LYS:NZ	52:sa:556:GLU:OE2	2.41	0.43
52:sa:301:GLY:HA2	52:sa:325:LEU:HD21	2.00	0.43
63:y0:67:TYR:O	63:y0:71:LYS:HG2	2.18	0.43
65:y7:244:LEU:HD21	65:y7:247:ILE:HD11	2.00	0.43
69:2b:45:SER:HB3	95:fx:172:MET:HE2	2.00	0.43
74:a3:107:TYR:HE2	124:s5:20:GLU:HG3	1.83	0.43
78:a8:228:VAL:HG22	100:n1:112:PRO:HG2	2.00	0.43
85:b2:23:TYR:CD2	86:b3:43:ASN:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:b8:121:LEU:HD22	90:b8:164:ILE:HG23	2.00	0.43
93:bm:155:ILE:HG21	153:t5:301:CDL:H402	1.99	0.43
153:bm:301:CDL:H731	103:n4:496:ILE:HG23	2.00	0.43
101:n2:9:GLU:HA	101:n2:84:PHE:HB2	2.00	0.43
101:n2:59:ILE:HG13	101:n2:125:ILE:HG23	2.00	0.43
103:n4:338:THR:HG23	103:n4:367:HIS:CE1	2.53	0.43
104:n5:75:ILE:HG23	104:n5:138:LEU:HD12	2.00	0.43
104:n5:460:PRO:HG3	104:n5:585:TYR:CE1	2.53	0.43
105:n6:185:PHE:O	105:n6:188:ILE:HG22	2.18	0.43
110:qC:55:SER:HB3	112:qE:117:ARG:NH2	2.33	0.43
110:qC:57:VAL:O	110:qC:59:GLU:N	2.45	0.43
110:qC:352:ASN:HB3	110:qC:355:HIS:HB3	1.98	0.43
111:qD:317:PHE:HB3	111:qD:318:TRP:CD2	2.53	0.43
109:qb:74:ARG:HE	109:qb:439:VAL:HG12	1.83	0.43
109:qb:435:ILE:HG12	109:qb:445:ARG:HD3	1.99	0.43
110:qc:102:LYS:HD3	110:qc:102:LYS:HA	1.72	0.43
114:qg:265:PHE:O	114:qg:268:LEU:HG	2.18	0.43
121:s2:267:ARG:O	121:s2:289:GLU:HG2	2.17	0.43
123:s4:12:ARG:HG3	123:s4:16:ILE:HD12	2.00	0.43
123:s4:100:PRO:HB2	123:s4:103:TYR:HE1	1.82	0.43
130:t3:261:ASN:O	130:t3:266:ARG:N	2.51	0.43
153:t5:301:CDL:H122	153:t5:301:CDL:H321	1.99	0.43
134:t7:64:PRO:HG3	134:t7:99:TYR:HA	1.98	0.43
147:v2:247:TRP:O	147:v2:251:LYS:HG2	2.18	0.43
2:2E:9:ALA:HB3	2:2E:33:ASP:OD2	2.18	0.43
2:2E:248:PRO:HB3	2:2E:264:LEU:HD23	2.00	0.43
10:2M:9:ASP:OD1	12:2O:12:ARG:NE	2.47	0.43
19:6B:144:ASP:O	19:6B:148:HIS:N	2.51	0.43
28:BP:190:TRP:HB3	28:BP:228:PRO:HA	1.99	0.43
28:BP:306:PHE:CZ	28:BP:362:VAL:HG13	2.52	0.43
28:BP:412:THR:O	28:BP:415:GLY:N	2.51	0.43
29:C1:477:LEU:HD13	153:C1:712:CDL:H241	1.99	0.43
154:C1:702:HEA:H211	154:C1:702:HEA:H271	1.40	0.43
152:C1:711:PC1:H241	59:VB:237:TYR:HE1	1.83	0.43
31:C3:515:PRO:HA	42:M:129:TRP:CE2	2.52	0.43
32:D:378:ARG:HH22	152:D:501:PC1:H342	1.82	0.43
34:F:346:HIS:HE1	36:G:253:ASP:HB3	1.83	0.43
42:M:38:VAL:HA	42:M:41:ARG:HG2	2.00	0.43
42:M:200:HIS:HE1	42:M:202:TYR:CD2	2.35	0.43
43:M1:262:MET:HG2	43:M1:266:TRP:CZ2	2.53	0.43
44:M2:196:ILE:HB	152:N:301:PC1:H332	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:R:123:PRO:HB2	66:Z:74:GLU:HA	1.99	0.43
52:SA:609:LYS:NZ	52:SA:610:THR:O	2.49	0.43
59:VB:156:PHE:CD1	59:VB:179:LEU:HD11	2.53	0.43
74:A3:107:TYR:HE2	124:S5:20:GLU:HG3	1.83	0.43
75:A5:65:TYR:HA	121:S2:245:GLY:HA3	2.00	0.43
87:B4:96:LEU:HD22	116:QI:42:ILE:HD11	2.00	0.43
101:N2:23:TYR:CE1	101:N2:66:LEU:HD12	2.53	0.43
101:N2:308:ASN:HA	101:N2:311:PHE:HB2	2.00	0.43
105:N6:159:TYR:HA	105:N6:162:PHE:CD2	2.52	0.43
108:QA:110:LEU:O	108:QA:114:LYS:N	2.43	0.43
114:QG:27:PRO:HA	114:QG:204:ASN:HA	1.99	0.43
108:Qa:186:LYS:NZ	109:Qb:339:GLN:O	2.39	0.43
109:Qb:73:VAL:HG11	109:Qb:267:PHE:HB3	2.00	0.43
109:Qb:435:ILE:HG12	109:Qb:445:ARG:HD3	1.99	0.43
120:S1:140:LEU:HD23	162:S1:801:SF4:S4	2.58	0.43
120:S1:471:PRO:O	120:S1:508:TRP:NE1	2.39	0.43
122:S3:174:GLU:OE2	123:S4:131:LYS:NZ	2.33	0.43
128:T1:171:PHE:HA	128:T1:174:TYR:CD2	2.53	0.43
129:T2:73:LEU:HD12	129:T2:97:LEU:HD21	1.99	0.43
131:T4:66:ASP:OD1	131:T4:66:ASP:N	2.51	0.43
134:T7:67:GLY:O	134:T7:94:PHE:HB3	2.18	0.43
139:TC:3:TYR:HE2	152:TC:102:PC1:H3E2	1.83	0.43
2:2e:39:TYR:O	2:2e:42:GLU:HG3	2.17	0.43
153:7a:203:CDL:H561	31:c3:279:ALA:HA	2.00	0.43
25:7l:933:ILE:O	25:7l:940:ARG:NH2	2.27	0.43
29:c1:119:ALA:HA	29:c1:123:ILE:HD13	2.00	0.43
29:c1:575:PHE:HD1	29:c1:578:LEU:HD12	1.83	0.43
31:c3:70:HIS:CD2	48:p:62:VAL:HA	2.53	0.43
33:e:383:LYS:HG3	33:e:384:HIS:CD2	2.53	0.43
37:h:265:ILE:HG22	37:h:271:GLU:HB2	2.00	0.43
40:k:185:ASP:HA	48:p:171:ASN:HB3	2.00	0.43
49:q:19:SER:OG	49:q:22:ASP:OD2	2.32	0.43
63:y0:27:TYR:O	63:y0:30:LEU:HG	2.18	0.43
65:y7:332:TRP:CZ2	153:y7:501:CDL:H771	2.53	0.43
66:z:58:LEU:O	66:z:61:ILE:HB	2.18	0.43
69:2b:171:TYR:HB2	94:c4:59:LEU:HB2	1.99	0.43
76:a6:10:THR:HB	76:a6:26:GLY:HA3	2.01	0.43
77:a7:98:GLN:HG3	77:a7:101:ASN:HD21	1.83	0.43
79:a9:288:HIS:HB3	99:j1:233:TYR:HA	2.00	0.43
87:b4:34:MET:HE1	91:b9:10:ASN:ND2	2.32	0.43
90:b8:59:GLN:NE2	103:n4:470:LYS:HE3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
94:c4:47:TYR:OH	158:c4:402:3PE:H11	2.18	0.43
104:n5:166:PHE:HE2	132:t5:87:PRO:HG2	1.83	0.43
104:n5:473:VAL:O	104:n5:477:GLN:HG2	2.18	0.43
110:qC:13:ILE:N	153:qc:504:CDL:OB4	2.40	0.43
112:qE:268:TRP:CD1	152:qE:303:PC1:H152	2.53	0.43
113:qF:74:GLN:HB2	113:qF:75:PRO:HD3	2.00	0.43
108:qa:378:HIS:O	108:qa:382:GLU:HG2	2.18	0.43
112:qe:40:LYS:HB3	115:qh:90:GLN:HE22	1.83	0.43
120:s1:118:MET:HA	120:s1:118:MET:HE3	2.00	0.43
120:s1:401:LEU:HD22	120:s1:461:PHE:HE2	1.82	0.43
121:s2:400:LYS:NZ	122:s3:143:TYR:OH	2.47	0.43
136:t9:49:MET:HE3	136:t9:67:PRO:HB2	1.99	0.43
139:tc:3:TYR:HE2	152:tc:102:PC1:H3E2	1.83	0.43
146:v1:209:GLU:O	146:v1:213:LEU:HB2	2.17	0.43
146:v1:406:ASP:H	146:v1:409:GLU:HG3	1.83	0.43
3:2F:175:ASN:O	3:2F:179:LEU:HG	2.18	0.43
5:2H:90:LEU:HB2	10:2M:51:ARG:NH1	2.33	0.43
153:2M:101:CDL:H781	153:2M:101:CDL:H742	2.01	0.43
19:6B:197:ALA:HA	30:C2:401:GLN:HG3	2.00	0.43
22:6T:13:ILE:HG12	22:6T:44:TYR:CE1	2.53	0.43
29:C1:125:TYR:CZ	36:G:208:ILE:HG21	2.54	0.43
152:C1:711:PC1:H262	59:VB:235:TYR:HA	1.99	0.43
153:C1:712:CDL:H242	30:C2:51:ILE:HG22	1.99	0.43
36:G:213:ASP:OD1	36:G:213:ASP:N	2.46	0.43
45:M3:187:LYS:HE3	45:M3:187:LYS:HB2	1.85	0.43
52:SA:91:GLN:HB3	52:SA:296:THR:HB	1.99	0.43
52:SA:371:ILE:HD12	52:SA:371:ILE:HA	1.85	0.43
57:U:50:THR:HG21	57:U:132:TYR:CE1	2.52	0.43
70:4L:15:ILE:HD13	70:4L:35:LEU:HG	2.00	0.43
74:A3:57:LEU:HD22	74:A3:60:VAL:HG21	1.99	0.43
76:A6:50:VAL:HG13	98:G3:314:ALA:HB3	2.00	0.43
77:A7:208:ARG:NH1	121:S2:327:THR:HG22	2.34	0.43
79:A9:61:ALA:HB2	79:A9:242:ALA:HB1	1.99	0.43
79:A9:219:TRP:HH2	153:A9:402:CDL:H591	1.83	0.43
81:AC:59:ARG:NH2	93:BM:80:ASP:HB3	2.33	0.43
87:B4:34:MET:HE1	91:B9:10:ASN:ND2	2.32	0.43
87:B4:110:TYR:HE2	158:B4:202:3PE:H11	1.83	0.43
88:B6:87:MET:HG2	132:T5:124:PHE:CE2	2.53	0.43
94:C4:24:MET:HB3	96:G1:53:GLN:NE2	2.33	0.43
95:FX:168:TYR:HB3	101:N2:337:LYS:HZ2	1.82	0.43
96:G1:83:ASP:HB2	98:G3:212:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
96:G1:239:THR:OG1	96:G1:240:ILE:N	2.51	0.43
152:J1:400:PC1:H2A1	105:N6:40:PHE:CZ	2.53	0.43
100:N1:44:ARG:HE	100:N1:56:PRO:HG3	1.82	0.43
100:N1:190:GLN:NE2	100:N1:261:ILE:O	2.43	0.43
104:N5:251:ASP:OD2	104:N5:444:ARG:NH1	2.34	0.43
104:N5:478:SER:HA	104:N5:538:PHE:CZ	2.54	0.43
104:N5:574:LYS:HE2	104:N5:599:ALA:HA	2.00	0.43
105:N6:175:LEU:O	105:N6:180:ILE:HG12	2.19	0.43
108:QA:91:MET:SD	108:QA:164:PHE:HB2	2.57	0.43
109:QB:342:ASN:HA	115:QH:27:ARG:HA	2.00	0.43
110:QC:84:HIS:O	110:QC:88:VAL:HG23	2.19	0.43
108:Qa:103:THR:C	108:Qa:105:GLU:H	2.26	0.43
108:Qa:115:ASN:HB3	108:Qa:186:LYS:HD3	2.00	0.43
108:Qa:380:ILE:HG23	108:Qa:481:LEU:HD23	2.00	0.43
110:Qc:57:VAL:O	110:Qc:59:GLU:N	2.48	0.43
110:Qc:132:LEU:HD13	110:Qc:184:LEU:HB3	2.00	0.43
111:Qd:145:PHE:N	111:Qd:149:GLN:OE1	2.49	0.43
115:Qh:85:GLU:O	115:Qh:89:LYS:HB3	2.18	0.43
120:S1:320:TRP:CZ3	120:S1:578:LEU:HG	2.53	0.43
120:S1:391:ILE:HG23	120:S1:414:LEU:HD13	2.00	0.43
121:S2:150:ALA:O	121:S2:154:ARG:HG3	2.18	0.43
126:S7:22:PHE:O	126:S7:51:VAL:HA	2.18	0.43
127:S8:202:LEU:HB2	127:S8:205:ASP:CG	2.43	0.43
128:T1:448:ILE:O	128:T1:473:ARG:NH1	2.52	0.43
129:T2:278:TYR:CZ	147:V2:41:PRO:HB3	2.52	0.43
130:T3:185:ILE:HD11	130:T3:293:LEU:HD13	2.01	0.43
132:T5:144:ASP:CG	138:TB:104:ARG:HH12	2.26	0.43
142:TF:192:ILE:HD11	142:TF:216:PRO:HG3	2.00	0.43
147:V2:247:TRP:O	147:V2:251:LYS:HG2	2.18	0.43
2:2e:93:LYS:HE2	2:2e:93:LYS:HB3	1.90	0.43
5:2h:90:LEU:HB2	10:2m:51:ARG:NH1	2.33	0.43
23:7a:73:LEU:HA	65:y7:354:PHE:HE1	1.84	0.43
23:7a:88:TYR:OH	65:y7:339:ASN:O	2.27	0.43
25:7l:863:PHE:HE2	35:fs:179:TRP:HZ3	1.66	0.43
29:c1:181:TYR:OH	46:n:47:ASP:OD2	2.30	0.43
29:c1:415:ARG:NH1	29:c1:478:VAL:O	2.43	0.43
29:c1:562:MET:HE3	153:c1:712:CDL:H612	2.00	0.43
30:c2:57:ARG:NE	58:v:91:ASN:HB3	2.33	0.43
30:c2:514:HIS:ND1	30:c2:560:MET:HE1	2.33	0.43
31:c3:418:ASN:OD1	31:c3:420:ASN:ND2	2.50	0.43
31:c3:463:PHE:HE2	152:c3:602:PC1:H292	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:119:ARG:NH2	153:FS:204:CDL:OB2	2.51	0.43
36:g:234:GLU:HA	36:g:237:TRP:HB2	1.99	0.43
39:j:228:HIS:HB3	39:j:231:LYS:O	2.19	0.43
52:sa:275:LEU:HA	52:sa:402:PRO:HD3	1.99	0.43
59:vb:234:PRO:HG3	153:vb:704:CDL:H551	2.00	0.43
60:w:33:TRP:CG	153:w:202:CDL:H462	2.54	0.43
76:a6:169:PRO:HB3	79:a9:40:ILE:O	2.18	0.43
77:a7:78:ASP:HB2	77:a7:123:ASN:HB2	1.99	0.43
168:ab:201:ZMP:H17	168:ab:201:ZMP:H14A	2.01	0.43
81:ac:59:ARG:NH2	93:bm:80:ASP:HB3	2.33	0.43
153:c4:401:CDL:H311	153:c4:401:CDL:H522	1.99	0.43
100:n1:44:ARG:HE	100:n1:56:PRO:HG3	1.82	0.43
100:n1:104:PHE:CE1	100:n1:129:LEU:HB3	2.53	0.43
101:n2:138:ILE:HG22	101:n2:139:PRO:HD3	2.00	0.43
101:n2:308:ASN:HA	101:n2:311:PHE:HB2	2.01	0.43
104:n5:283:GLU:CD	104:n5:283:GLU:H	2.27	0.43
108:qA:52:VAL:O	108:qA:56:ARG:NH1	2.49	0.43
108:qA:191:HIS:HB3	108:qA:225:ARG:HD2	2.00	0.43
112:qE:262:GLU:O	112:qE:264:SER:N	2.48	0.43
108:qa:79:ILE:O	108:qa:252:CYS:HA	2.18	0.43
111:qd:77:PHE:O	111:qd:82:GLY:N	2.42	0.43
112:qe:81:ASN:O	112:qe:81:ASN:ND2	2.51	0.43
120:s1:83:VAL:O	120:s1:86:VAL:HG12	2.18	0.43
121:s2:429:LEU:HA	121:s2:432:THR:HG22	1.99	0.43
122:s3:94:MET:HB3	122:s3:115:LEU:HB2	2.00	0.43
126:s7:30:ALA:O	126:s7:33:ALA:N	2.52	0.43
127:s8:202:LEU:HB2	127:s8:205:ASP:CG	2.43	0.43
129:t2:72:LEU:HD23	129:t2:98:VAL:HB	2.00	0.43
129:t2:73:LEU:HD12	129:t2:97:LEU:HD21	1.99	0.43
146:v1:434:TRP:HB2	146:v1:435:PRO:HD3	1.99	0.43
2:2E:94:LEU:O	2:2E:97:ILE:HG12	2.17	0.43
8:2K:43:GLY:HA3	153:2K:101:CDL:H781	2.01	0.43
19:6B:37:PHE:HE1	25:7L:966:LYS:HD2	1.83	0.43
25:7L:863:PHE:HE2	35:FS:179:TRP:HZ3	1.66	0.43
26:A:408:VAL:HG21	59:VB:339:ASN:HD21	1.83	0.43
28:BP:176:SER:O	28:BP:191:GLY:HA3	2.18	0.43
153:C1:712:CDL:H162	30:C2:56:ALA:HA	2.00	0.43
30:C2:7:THR:HG23	30:C2:544:PHE:HB2	1.99	0.43
30:C2:45:TRP:HD1	58:V:103:LEU:HD23	1.84	0.43
36:G:230:TRP:CG	59:VB:192:GLY:HA3	2.53	0.43
37:H:155:LYS:HB3	37:H:164:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:K:97:ASN:HA	40:K:100:LYS:HE2	2.01	0.43
42:M:157:TYR:CE1	153:W:202:CDL:HB21	2.53	0.43
50:R:122:GLU:HB3	66:Z:81:ARG:HH22	1.83	0.43
53:SB:106:LEU:HD12	53:SB:110:ASN:HD21	1.84	0.43
66:Z:58:LEU:O	66:Z:61:ILE:HB	2.18	0.43
68:1B:21:ARG:HH11	100:N1:216:ARG:NH2	2.16	0.43
69:2B:51:ASN:HB3	95:FX:103:PHE:CG	2.53	0.43
74:A3:20:VAL:HG22	96:G1:229:ASP:HB3	1.99	0.43
74:A3:81:ARG:NH2	74:A3:88:TYR:O	2.38	0.43
82:AL:55:GLY:HA3	82:AL:98:TRP:CH2	2.52	0.43
87:B4:52:VAL:HG22	87:B4:53:PRO:HD2	2.00	0.43
89:B7:117:ALA:HB1	106:P1:136:PHE:HB2	1.99	0.43
92:BL:166:ARG:NH2	136:T9:13:ASP:OD2	2.37	0.43
96:G1:118:GLY:N	96:G1:134:ILE:O	2.51	0.43
99:J1:149:ASP:HB3	99:J1:155:LYS:HD3	2.00	0.43
104:N5:694:TYR:O	104:N5:698:ASN:ND2	2.51	0.43
152:N5:803:PC1:H3F2	152:N5:803:PC1:H2C1	2.01	0.43
111:QD:119:GLN:HB2	111:QD:122:LYS:HB3	2.00	0.43
112:QE:262:GLU:O	112:QE:264:SER:N	2.49	0.43
152:QE:303:PC1:H2E2	152:QI:202:PC1:H2I2	2.01	0.43
153:QG:402:CDL:H732	153:QG:402:CDL:H122	1.99	0.43
108:Qa:329:LEU:HD13	108:Qa:363:LEU:HD21	2.00	0.43
109:Qb:359:PRO:HD2	109:Qb:387:PHE:CZ	2.54	0.43
120:S1:71:SER:O	120:S1:185:ARG:NH1	2.41	0.43
136:T9:96:LEU:O	136:T9:100:GLN:HG2	2.18	0.43
142:TF:153:ASN:HB3	142:TF:191:LYS:NZ	2.33	0.43
146:V1:45:LEU:O	146:V1:134:ASN:ND2	2.51	0.43
147:V2:235:ARG:HD3	147:V2:235:ARG:HA	1.78	0.43
2:2e:154:THR:HA	2:2e:187:VAL:O	2.18	0.43
2:2e:218:PHE:HB2	2:2e:223:ILE:HG12	2.00	0.43
3:2f:178:ASN:HB3	3:2f:186:LEU:HD21	2.00	0.43
18:6a:9:THR:HB	18:6a:14:ILE:HD11	1.99	0.43
19:6b:99:PRO:HB2	25:7l:921:LEU:HD11	2.01	0.43
26:a:325:GLN:OE1	61:x:102:LYS:NZ	2.29	0.43
27:b:460:LEU:HD12	27:b:463:ILE:HD11	2.01	0.43
28:bp:306:PHE:CE1	28:bp:326:GLN:HG3	2.53	0.43
28:bp:447:VAL:HA	28:bp:461:VAL:HG22	1.99	0.43
29:c1:50:HIS:CG	29:c1:124:PRO:HG2	2.53	0.43
153:e:403:CDL:H731	153:e:403:CDL:H571	2.01	0.43
34:f:222:ILE:HA	34:f:238:THR:HG22	2.00	0.43
153:fs:203:CDL:HB31	153:E:403:CDL:HA4	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:212:LYS:NZ	50:r:50:ASP:OD1	2.39	0.43
42:m:157:TYR:CE1	153:w:202:CDL:HB21	2.52	0.43
159:m2:406:P5S:H21	159:m2:406:P5S:H24A	1.73	0.43
48:p:18:LYS:HG3	48:p:24:TYR:CE2	2.53	0.43
52:sa:92:GLY:N	161:sa:701:FAD:O4	2.51	0.43
164:sc:102:U10:H222	164:sc:102:U10:H261	1.80	0.43
59:vb:495:ALA:HB3	59:vb:500:TYR:CZ	2.53	0.43
60:w:98:GLU:HB2	60:w:101:GLU:HG2	2.00	0.43
71:5b:32:PHE:HA	153:b4:201:CDL:H712	2.00	0.43
82:al:48:ASP:OD1	82:al:48:ASP:N	2.51	0.43
83:am:115:LEU:HD22	124:s5:62:GLU:HB3	2.00	0.43
93:bm:129:MET:HE2	103:n4:480:SER:HB3	2.00	0.43
96:g1:65:GLU:OE2	99:j1:167:ARG:NH2	2.35	0.43
98:g3:280:SER:HA	98:g3:283:TRP:NE1	2.33	0.43
100:n1:133:PHE:O	100:n1:137:ILE:HG12	2.19	0.43
101:n2:23:TYR:CE1	101:n2:66:LEU:HD12	2.53	0.43
103:n4:62:ILE:HD13	144:th:63:SER:HA	2.00	0.43
104:n5:733:SER:HB2	106:p1:116:TYR:HD1	1.83	0.43
105:n6:62:ILE:O	105:n6:66:ILE:HG13	2.18	0.43
108:qA:395:LEU:HD22	108:qA:444:ALA:HB2	1.98	0.43
113:qF:13:MET:HE3	113:qF:20:PRO:HB3	2.00	0.43
113:qF:38:LYS:HB3	113:qF:38:LYS:HE2	1.83	0.43
125:s6:86:ARG:NH1	146:v1:467:SER:OG	2.49	0.43
130:t3:185:ILE:HD11	130:t3:293:LEU:HD13	2.00	0.43
134:t7:77:MET:HG3	137:ta:81:MET:HE3	2.00	0.43
4:2G:122:HIS:CE1	153:2G:204:CDL:H521	2.53	0.43
153:2G:201:CDL:H671	153:2K:101:CDL:H242	1.99	0.43
16:4T:31:HIS:O	16:4T:35:ARG:HG3	2.18	0.43
19:6B:181:GLN:HG3	30:C2:508:ASN:HB2	2.01	0.43
22:6T:64:LYS:HE3	30:C2:296:SER:O	2.18	0.43
25:7L:860:MET:O	30:C2:92:ASN:HA	2.19	0.43
26:A:178:THR:HG22	26:A:183:GLU:HG2	2.00	0.43
27:B:210:VAL:HG13	27:B:214:ARG:HH11	1.83	0.43
27:B:403:PHE:O	27:B:409:LYS:HE3	2.19	0.43
28:BP:172:VAL:HG21	28:BP:242:ILE:HG13	2.01	0.43
29:C1:83:GLY:HA2	30:C2:487:ARG:NH2	2.33	0.43
29:C1:297:LEU:HB3	65:Y7:329:PHE:CZ	2.53	0.43
153:C1:708:CDL:H341	152:C1:711:PC1:H371	2.00	0.43
30:C2:71:TYR:HB3	59:VB:172:GLY:O	2.17	0.43
30:C2:242:ASP:OD1	30:C2:242:ASP:N	2.50	0.43
30:C2:335:THR:OG1	32:D:233:TYR:OH	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C3:70:HIS:CD2	48:P:62:VAL:HA	2.53	0.43
31:C3:91:PHE:CD2	45:M3:205:SER:HB2	2.54	0.43
31:C3:501:TYR:CG	31:C3:502:PRO:HD3	2.54	0.43
46:N:182:VAL:HB	46:N:185:SER:HB3	2.00	0.43
49:Q:109:ARG:HA	49:Q:112:THR:HG22	1.99	0.43
52:SA:225:MET:HG3	52:SA:485:LEU:HD11	2.00	0.43
53:SB:42:GLY:O	53:SB:46:GLY:N	2.52	0.43
53:SB:300:LYS:HE3	53:SB:300:LYS:HB2	1.80	0.43
158:SC:101:3PE:H372	158:SC:101:3PE:H241	2.00	0.43
59:VB:291:ARG:HG2	59:VB:295:LYS:HE2	1.99	0.43
80:AB:50:GLU:CD	80:AB:50:GLU:H	2.27	0.43
168:AB:201:ZMP:C14	168:AB:201:ZMP:H17	2.47	0.43
82:AL:188:ASP:OD1	82:AL:188:ASP:N	2.43	0.43
83:AM:167:ILE:HG13	100:N1:17:LEU:HB3	2.00	0.43
91:B9:133:PHE:O	138:TB:60:TYR:OH	2.22	0.43
91:B9:139:LYS:HE3	91:B9:143:GLU:HG2	2.00	0.43
94:C4:28:THR:HG22	97:G2:18:MET:HG3	2.00	0.43
94:C4:47:TYR:OH	158:C4:402:3PE:H11	2.18	0.43
96:G1:175:LEU:HB3	96:G1:185:ARG:O	2.18	0.43
102:N3:77:PHE:O	102:N3:80:PRO:HD2	2.19	0.43
105:N6:248:LEU:HD12	121:S2:285:ASN:ND2	2.34	0.43
108:QA:112:SER:O	108:QA:116:THR:OG1	2.32	0.43
113:QF:25:LEU:HD21	113:QF:70:GLU:OE2	2.19	0.43
112:Qe:40:LYS:HB3	115:Qh:90:GLN:HE22	1.82	0.43
114:Qg:135:PRO:HB2	114:Qg:137:TRP:CD1	2.54	0.43
120:S1:382:ARG:HB3	120:S1:386:LEU:HD12	2.00	0.43
121:S2:429:LEU:HA	121:S2:432:THR:HG22	1.99	0.43
125:S6:75:VAL:HG21	127:S8:131:THR:HB	2.01	0.43
127:S8:121:ARG:HB3	127:S8:192:GLU:OE1	2.18	0.43
128:T1:271:PRO:HB2	128:T1:278:ILE:HA	2.00	0.43
142:TF:102:LYS:HZ1	142:TF:132:ALA:HB3	1.84	0.43
2:2e:63:LEU:HD12	2:2e:63:LEU:HA	1.84	0.43
16:4t:31:HIS:O	16:4t:35:ARG:HG3	2.18	0.43
20:6c:7:ARG:HH21	153:fs:203:CDL:HB4	1.84	0.43
23:7a:104:GLU:HG3	152:7a:202:PC1:H131	1.99	0.43
24:7c:119:GLU:O	40:k:35:HIS:NE2	2.50	0.43
24:7c:228:GLY:HA3	43:m1:330:VAL:HG21	2.00	0.43
27:b:245:GLN:O	31:c3:131:TYR:OH	2.35	0.43
27:b:432:LEU:HB2	65:y7:409:ILE:HD13	2.00	0.43
28:bp:190:TRP:HB3	28:bp:228:PRO:HA	1.99	0.43
29:c1:524:VAL:HG13	29:c1:528:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:l:136:VAL:HA	59:vb:571:VAL:HG23	2.01	0.43
42:m:75:VAL:HG21	42:m:83:PHE:CD1	2.54	0.43
43:m1:262:MET:HG2	43:m1:266:TRP:CZ2	2.54	0.43
50:r:123:PRO:HB2	66:z:74:GLU:HA	1.99	0.43
71:5b:4:ASN:HD21	153:5b:201:CDL:H392	1.83	0.43
76:a6:108:ARG:O	168:ab:201:ZMP:H8A	2.19	0.43
82:al:3:LEU:HB3	153:al:301:CDL:HA31	2.01	0.43
82:al:13:THR:HG23	82:al:47:THR:HB	2.00	0.43
83:am:111:LEU:HD13	124:s5:71:LEU:HD21	1.99	0.43
85:b2:102:LEU:HD22	131:t4:91:THR:HG21	2.01	0.43
86:b3:41:ARG:NH1	104:n5:618:LYS:O	2.46	0.43
89:b7:117:ALA:HB1	106:p1:136:PHE:HB2	1.99	0.43
101:n2:99:TYR:CE1	101:n2:103:ILE:HD11	2.53	0.43
153:n6:302:CDL:H372	139:tc:30:ALA:HB1	2.01	0.43
111:qD:119:GLN:HB2	111:qD:122:LYS:HB3	2.01	0.43
114:qG:288:VAL:HA	114:qG:291:GLU:HG2	1.99	0.43
117:qJ:18:LEU:HD22	152:qJ:101:PC1:H252	1.99	0.43
108:qa:311:SER:O	108:qa:312:VAL:HG13	2.18	0.43
110:qc:64:PRO:O	110:qc:68:GLU:HG2	2.18	0.43
110:qc:343:THR:O	114:qg:35:ARG:NH2	2.28	0.43
114:qg:202:PHE:HB2	114:qg:205:GLU:HB2	2.00	0.43
115:qh:82:TYR:O	115:qh:86:ARG:HB3	2.18	0.43
120:s1:638:TYR:CE1	123:s4:39:LYS:HD3	2.52	0.43
126:s7:22:PHE:CZ	126:s7:62:LEU:HB2	2.54	0.43
3:2F:251:LYS:HG3	10:2M:74:GLN:HG3	2.00	0.43
15:4A:44:ILE:HG13	26:A:127:VAL:HG13	2.00	0.43
153:6C:203:CDL:H641	34:F:201:LEU:HD22	1.99	0.43
23:7A:58:GLU:HB3	23:7A:66:THR:HB	2.01	0.43
27:B:145:ARG:NH2	74:A3:9:PHE:HA	2.33	0.43
28:BP:117:VAL:HG22	28:BP:126:VAL:HG22	2.00	0.43
28:BP:170:ASP:OD2	28:BP:239:TYR:OH	2.20	0.43
29:C1:462:ILE:O	29:C1:465:PRO:HD2	2.18	0.43
31:C3:463:PHE:HE2	152:C3:602:PC1:H292	1.83	0.43
39:J:60:ASP:OD2	39:J:150:TYR:OH	2.24	0.43
39:J:184:THR:HG21	153:J:301:CDL:HA61	2.01	0.43
41:L:125:TYR:OH	153:L:301:CDL:OA3	2.26	0.43
153:M:306:CDL:H312	153:M:306:CDL:HB32	2.00	0.43
43:M1:62:LEU:HD11	58:V:48:PRO:HG2	2.00	0.43
52:SA:52:ILE:HD11	52:SA:77:ILE:HD12	2.01	0.43
52:SA:418:ASP:OD2	52:SA:615:ARG:NE	2.45	0.43
53:SB:140:LEU:HG	53:SB:283:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:W:13:ASN:O	60:W:17:LEU:HG	2.18	0.43
65:Y7:244:LEU:HD21	65:Y7:247:ILE:HD11	2.01	0.43
69:2B:50:LEU:HD23	69:2B:50:LEU:HA	1.91	0.43
69:2B:171:TYR:HB2	94:C4:59:LEU:HB2	1.99	0.43
73:A2:58:ASP:OD2	123:S4:41:ASN:ND2	2.51	0.43
77:A7:77:TYR:HB2	122:S3:20:SER:HB2	2.00	0.43
79:A9:165:ALA:HA	79:A9:197:ARG:HB3	2.00	0.43
82:AL:177:LYS:HD2	120:S1:573:TYR:CZ	2.53	0.43
85:B2:81:PRO:HB2	85:B2:83:TYR:CE2	2.54	0.43
90:B8:71:ILE:HG23	91:B9:13:TRP:HE3	1.84	0.43
93:BM:155:ILE:HG21	153:T5:301:CDL:H402	1.99	0.43
100:N1:150:PHE:O	100:N1:154:ILE:HG12	2.19	0.43
102:N3:48:LYS:HE2	102:N3:48:LYS:HB3	1.83	0.43
109:QB:354:GLU:HB3	109:QB:510:TYR:OH	2.18	0.43
110:QC:42:ILE:HG13	110:QC:91:LEU:HD21	1.99	0.43
112:QE:140:GLY:N	112:QE:156:ARG:O	2.51	0.43
114:QG:203:TYR:CZ	117:Qj:5:THR:HA	2.54	0.43
111:Qd:248:TYR:CE2	111:Qd:249:LYS:HG3	2.54	0.43
112:Qe:60:PHE:CE1	115:Qh:57:GLY:HA2	2.53	0.43
128:T1:271:PRO:HB2	128:T1:278:ILE:HG12	2.00	0.43
146:V1:39:ASP:HA	146:V1:258:ARG:HH12	1.82	0.43
5:2h:105:HIS:CD2	5:2h:152:ARG:HG2	2.53	0.43
6:2i:5:PHE:O	6:2i:9:GLU:HG3	2.19	0.43
8:2k:43:GLY:HA3	153:2k:101:CDL:H781	2.01	0.43
152:7c:303:PC1:H2B1	44:m2:225:LEU:HD23	2.00	0.43
27:b:88:TYR:O	27:b:91:SER:OG	2.34	0.43
27:b:210:VAL:HG13	27:b:214:ARG:HH11	1.84	0.43
28:bp:176:SER:O	28:bp:191:GLY:HA3	2.19	0.43
31:c3:523:GLY:O	153:t:202:CDL:H562	2.18	0.43
31:c3:576:TYR:CE2	31:c3:578:LYS:HB2	2.53	0.43
33:e:60:ALA:HA	33:e:152:GLU:HG3	2.00	0.43
34:f:266:ASP:OD1	34:f:267:ASN:N	2.51	0.43
36:g:230:TRP:CG	59:vb:192:GLY:HA3	2.53	0.43
37:h:114:ILE:HA	37:h:114:ILE:HD13	1.75	0.43
37:h:237:ASN:O	37:h:241:VAL:HG23	2.18	0.43
52:sa:284:HIS:O	52:sa:392:PRO:HA	2.18	0.43
56:t:56:ARG:NH2	153:t:204:CDL:H1	2.33	0.43
60:w:13:ASN:O	60:w:17:LEU:HG	2.18	0.43
68:1b:17:ALA:HB2	100:n1:210:PHE:CE2	2.54	0.43
69:2b:55:GLU:HB3	69:2b:130:ILE:HG21	1.99	0.43
69:2b:156:PHE:HB3	153:2b:201:CDL:H711	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:a3:32:SER:HB2	74:a3:45:ALA:HB2	2.00	0.43
74:a3:81:ARG:HD2	137:ta:97:ARG:NH1	2.34	0.43
77:a7:167:SER:O	77:a7:171:LYS:HG2	2.18	0.43
79:a9:234:GLN:HG2	79:a9:263:GLY:N	2.34	0.43
97:g2:96:ILE:HD13	97:g2:110:ILE:HG22	2.01	0.43
97:g2:214:ILE:HG21	98:g3:96:LEU:HD21	2.00	0.43
103:n4:399:ILE:HD13	103:n4:399:ILE:HA	1.87	0.43
104:n5:337:PHE:CD2	158:n5:802:3PE:H221	2.54	0.43
104:n5:731:SER:HA	104:n5:734:LYS:HG2	2.01	0.43
153:n5:806:CDL:H162	153:n5:806:CDL:H131	1.87	0.43
105:n6:58:ILE:O	105:n6:62:ILE:HG12	2.19	0.43
108:qA:314:TRP:CZ2	108:qA:354:HIS:HB2	2.54	0.43
110:qC:242:MET:HG3	152:qC:505:PC1:H321	2.01	0.43
108:qa:265:LEU:O	108:qa:268:THR:OG1	2.35	0.43
109:qb:476:LEU:HD13	109:qb:478:ILE:HD11	2.00	0.43
120:s1:253:ASP:OD2	120:s1:291:THR:OG1	2.24	0.43
121:s2:59:ILE:HD11	122:s3:156:LEU:HG	2.01	0.43
121:s2:237:THR:HA	121:s2:241:ALA:HB2	2.00	0.43
127:s8:194:PRO:HG3	127:s8:223:GLN:NE2	2.34	0.43
128:t1:221:VAL:HG21	128:t1:246:LEU:HD21	2.01	0.43
134:t7:89:PHE:CE1	153:t7:201:CDL:H562	2.54	0.43
143:tg:18:GLU:OE2	143:tg:115:TYR:OH	2.37	0.43
143:tg:46:LYS:HB2	144:th:42:GLN:HG3	2.00	0.43
146:v1:284:ASN:ND2	146:v1:307:GLY:O	2.50	0.43
24:7C:210:ASP:HB2	30:C2:473:ASN:HD21	1.83	0.43
152:A:501:PC1:H282	31:C3:406:PHE:CD1	2.53	0.43
28:BP:183:GLU:C	28:BP:185:GLY:H	2.25	0.43
28:BP:447:VAL:HA	28:BP:461:VAL:HG22	2.00	0.43
31:C3:153:ASN:O	31:C3:157:ASN:ND2	2.33	0.43
31:C3:277:LEU:HB3	65:Y7:324:ILE:HG12	2.01	0.43
33:E:383:LYS:HG3	33:E:384:HIS:CD2	2.52	0.43
34:F:168:LYS:HB3	34:F:171:TYR:HD2	1.84	0.43
38:I:113:ASN:HD21	38:I:239:LEU:HA	1.83	0.43
41:L:136:VAL:HA	59:VB:571:VAL:HG23	2.00	0.43
153:M:304:CDL:H511	153:M:304:CDL:HB21	1.99	0.43
44:M2:191:ALA:O	44:M2:195:ASN:ND2	2.32	0.43
50:R:8:TYR:HD1	50:R:8:TYR:HA	1.70	0.43
52:SA:92:GLY:N	161:SA:701:FAD:O4	2.51	0.43
52:SA:160:PHE:CE1	52:SA:176:THR:HG21	2.54	0.43
52:SA:398:MET:HE3	52:SA:440:ARG:HB2	2.00	0.43
56:T:56:ARG:NH2	153:T:204:CDL:H1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:U:65:ARG:HA	57:U:69:GLN:HB3	1.99	0.43
58:V:93:LYS:O	58:V:96:PRO:HD2	2.18	0.43
59:VB:550:PRO:HG3	59:VB:605:LEU:HD11	2.00	0.43
68:1B:21:ARG:HA	100:N1:217:ALA:HB3	2.00	0.43
68:1B:26:ARG:O	121:S2:219:ARG:NH1	2.47	0.43
70:4L:20:VAL:HG13	71:5B:79:PHE:HB3	1.99	0.43
153:A9:402:CDL:HA4	102:N3:21:TRP:CZ2	2.53	0.43
153:A9:403:CDL:H832	126:S7:13:VAL:HG11	2.00	0.43
83:AM:68:ILE:HD13	100:N1:198:ILE:HD11	2.01	0.43
85:B2:102:LEU:HD22	131:T4:91:THR:HG21	2.01	0.43
93:BM:129:MET:HE2	103:N4:480:SER:HB3	2.00	0.43
96:G1:59:ASN:HB2	97:G2:46:HIS:CD2	2.54	0.43
100:N1:32:ILE:HG13	100:N1:250:PHE:HE1	1.84	0.43
101:N2:138:ILE:HG22	101:N2:139:PRO:HD3	2.00	0.43
101:N2:296:PHE:CZ	101:N2:300:PHE:HE2	2.36	0.43
103:N4:423:PHE:HD2	104:N5:236:MET:HE1	1.83	0.43
104:N5:340:PHE:O	104:N5:344:LYS:HG2	2.17	0.43
152:N6:301:PC1:H282	139:TC:8:VAL:HG11	2.00	0.43
152:N6:301:PC1:H142	139:TC:16:TYR:CZ	2.54	0.43
109:QB:157:VAL:HG11	109:QB:254:VAL:HG23	2.01	0.43
110:QC:33:LEU:HD13	110:QC:230:GLU:HA	1.99	0.43
110:QC:137:CYS:O	110:QC:142:SER:OG	2.32	0.43
109:Qb:476:LEU:HD13	109:Qb:478:ILE:HD11	2.00	0.43
111:Qd:90:LYS:HE2	111:Qd:242:MET:O	2.19	0.43
120:S1:234:ASN:HB3	120:S1:237:TYR:HB3	2.01	0.43
121:S2:59:ILE:HD11	122:S3:156:LEU:HG	2.01	0.43
126:S7:22:PHE:CZ	126:S7:62:LEU:HB2	2.54	0.43
130:T3:62:ALA:HB2	130:T3:123:ASP:HB3	1.99	0.43
2:2e:322:LEU:HD13	153:2g:203:CDL:H322	2.01	0.43
3:2f:137:ARG:HE	152:2f:301:PC1:H361	1.83	0.43
9:2l:12:THR:OG1	9:2l:13:PRO:HD3	2.18	0.43
16:4t:53:TYR:HA	16:4t:57:GLU:HB3	1.99	0.43
17:5t:13:PHE:CD1	30:c2:249:LEU:HD22	2.53	0.43
22:6t:29:TYR:OH	22:6t:34:GLU:OE1	2.29	0.43
27:b:291:PHE:HB3	27:b:357:LEU:HB3	1.99	0.43
29:c1:387:TRP:O	29:c1:438:TRP:HB2	2.19	0.43
30:c2:7:THR:HG23	30:c2:544:PHE:HB2	2.00	0.43
31:c3:501:TYR:CG	31:c3:502:PRO:HD3	2.54	0.43
34:f:231:GLY:HA3	34:f:326:ILE:O	2.19	0.43
38:i:113:ASN:HD21	38:i:239:LEU:HA	1.83	0.43
43:m1:24:TRP:CZ2	153:m2:403:CDL:HB61	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m1:112:LEU:HB3	43:m1:324:LEU:HD23	1.99	0.43
45:m3:135:LEU:HD21	45:m3:191:ALA:HB2	2.00	0.43
50:r:147:ALA:O	50:r:151:LYS:HG3	2.19	0.43
52:sa:160:PHE:CE1	52:sa:176:THR:HG21	2.54	0.43
68:1b:49:VAL:HG11	74:a3:67:ALA:HB1	1.99	0.43
75:a5:65:TYR:HA	121:s2:245:GLY:HA3	2.00	0.43
75:a5:153:PRO:HA	122:s3:41:TRP:HZ3	1.83	0.43
79:a9:219:TRP:HH2	153:a9:402:CDL:H591	1.83	0.43
81:ac:62:ILE:HD12	93:bm:59:LEU:HD12	2.01	0.43
87:b4:110:TYR:HE2	158:b4:202:3PE:H11	1.84	0.43
87:b4:116:GLU:HG3	103:n4:437:SER:HB3	2.01	0.43
92:bl:54:PHE:HD2	103:n4:85:ILE:HG21	1.84	0.43
92:bl:143:LEU:HB3	93:bm:177:LEU:HD22	2.00	0.43
95:fx:154:ASN:ND2	95:fx:155:GLU:HG2	2.33	0.43
96:g1:59:ASN:HB2	97:g2:46:HIS:CD2	2.53	0.43
96:g1:118:GLY:N	96:g1:134:ILE:O	2.51	0.43
96:g1:242:TYR:HA	98:g3:235:THR:HG21	2.01	0.43
99:j1:149:ASP:HB3	99:j1:155:LYS:HD3	2.00	0.43
152:j1:400:PC1:H2A1	105:n6:40:PHE:CZ	2.53	0.43
100:n1:138:MET:HE2	105:n6:101:PHE:HE2	1.84	0.43
101:n2:296:PHE:CZ	101:n2:300:PHE:HE2	2.36	0.43
104:n5:72:TRP:CZ2	104:n5:76:PHE:HB3	2.54	0.43
104:n5:340:PHE:O	104:n5:344:LYS:HG2	2.17	0.43
152:n5:805:PC1:H132	106:p1:133:TYR:HD2	1.83	0.43
109:qB:342:ASN:HA	115:qH:27:ARG:HA	2.00	0.43
110:qC:28:HIS:HB3	110:qC:207:TRP:HH2	1.83	0.43
111:qD:115:HIS:CG	111:qD:116:PRO:HD2	2.54	0.43
114:qG:209:GLU:HB2	118:qL:1:MET:H3	1.84	0.43
108:qa:166:MET:HE2	108:qa:166:MET:HB3	1.93	0.43
120:s1:391:ILE:HG23	120:s1:414:LEU:HD13	2.00	0.43
128:t1:448:ILE:O	128:t1:473:ARG:NH1	2.51	0.43
3:2F:139:PHE:O	3:2F:143:ILE:HG12	2.19	0.43
17:5T:13:PHE:CD1	30:C2:249:LEU:HD22	2.53	0.43
19:6B:181:GLN:NE2	30:C2:506:ILE:O	2.51	0.43
20:6C:31:ILE:HG21	58:V:103:LEU:HD13	2.01	0.43
153:6C:203:CDL:H672	58:V:104:THR:HG22	2.01	0.43
26:A:161:GLU:OE1	26:A:161:GLU:N	2.42	0.43
152:A:503:PC1:H222	31:C3:400:TYR:HA	2.01	0.43
28:BP:141:ASN:HB2	28:BP:192:TYR:CB	2.49	0.43
28:BP:306:PHE:CE1	28:BP:326:GLN:HG3	2.53	0.43
28:BP:323:THR:H	28:BP:326:GLN:HE22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C1:380:ILE:HG22	29:C1:384:HIS:CD2	2.54	0.43
31:C3:270:LYS:HB3	153:Y7:501:CDL:H731	2.00	0.43
36:G:178:VAL:HG11	59:VB:187:ARG:HD2	2.01	0.43
37:H:280:SER:O	37:H:284:GLN:HG2	2.18	0.43
153:M1:402:CDL:H131	44:M2:65:PHE:CZ	2.54	0.43
46:N:60:MET:HG3	152:N:303:PC1:H342	2.01	0.43
46:N:74:LYS:HD2	65:Y7:341:GLY:HA3	1.99	0.43
52:SA:315:MET:HE1	52:SA:334:ALA:HB3	2.01	0.43
53:SB:166:LYS:HG2	53:SB:167:ASP:H	1.83	0.43
60:W:17:LEU:O	60:W:22:PRO:HD3	2.19	0.43
65:Y7:296:ASN:OD1	65:Y7:296:ASN:N	2.52	0.43
69:2B:156:PHE:HB3	153:2B:201:CDL:H711	1.99	0.43
77:A7:28:ARG:NH1	77:A7:29:ARG:O	2.52	0.43
91:B9:39:LEU:HD23	91:B9:76:MET:HE1	2.01	0.43
92:BL:58:GLU:O	92:BL:62:ILE:HG12	2.18	0.43
94:C4:48:PHE:CD1	153:C4:401:CDL:H812	2.54	0.43
97:G2:123:SER:OG	135:T8:33:ASP:OD1	2.32	0.43
103:N4:488:LEU:HD13	153:TH:200:CDL:H372	2.01	0.43
152:N5:805:PC1:H132	106:P1:133:TYR:HD2	1.83	0.43
105:N6:185:PHE:O	105:N6:188:ILE:HG22	2.18	0.43
153:N6:302:CDL:H372	139:TC:30:ALA:HB1	2.01	0.43
109:QB:345:ASP:HA	109:QB:353:LYS:HE2	2.01	0.43
110:QC:31:ASN:HD21	153:QC:504:CDL:H111	1.82	0.43
110:QC:210:GLU:OE1	115:QH:95:ARG:NH2	2.52	0.43
109:Qb:331:TYR:CD2	109:Qb:355:LEU:HD13	2.53	0.43
111:Qd:267:ILE:HD11	112:Qe:99:TYR:HA	2.00	0.43
114:Qg:147:LEU:O	114:Qg:151:VAL:HG23	2.19	0.43
114:Qg:265:PHE:O	114:Qg:268:LEU:HG	2.19	0.43
121:S2:350:ASP:OD1	121:S2:350:ASP:N	2.51	0.43
127:S8:95:CYS:O	127:S8:99:TYR:HB2	2.17	0.43
136:T9:55:ASP:OD2	136:T9:57:SER:OG	2.26	0.43
146:V1:399:ARG:NH2	146:V1:409:GLU:OE1	2.40	0.43
147:V2:212:ARG:HG3	147:V2:216:GLU:O	2.18	0.43
3:2f:139:PHE:O	3:2f:143:ILE:HG12	2.19	0.43
153:2o:101:CDL:HA32	153:2o:101:CDL:H512	2.00	0.43
15:4a:44:ILE:HG13	26:a:127:VAL:HG13	2.00	0.43
153:a:504:CDL:H401	31:c3:254:LEU:HB2	2.01	0.43
29:c1:487:PRO:HG3	29:c1:544:TYR:HB3	2.00	0.43
32:d:190:LYS:O	32:d:193:ARG:NH1	2.43	0.43
37:h:75:SER:O	37:h:79:ARG:HG3	2.19	0.43
37:h:82:LYS:NZ	104:N5:70:ASP:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:h:141:TYR:C	57:u:11:GLU:HG3	2.44	0.43
153:i:301:CDL:H441	152:i:304:PC1:H332	2.01	0.43
153:m:304:CDL:H152	63:y0:71:LYS:HB2	2.01	0.43
43:m1:263:VAL:HG21	43:m1:280:TYR:HA	2.01	0.43
46:n:169:ARG:HE	153:n:304:CDL:H712	1.84	0.43
47:o:103:PRO:O	47:o:105:GLN:NE2	2.52	0.43
51:s:9:LYS:O	51:s:13:GLN:HG2	2.18	0.43
53:sb:42:GLY:O	53:sb:46:GLY:N	2.52	0.43
53:sb:205:GLN:HB3	53:sb:251:SER:OG	2.18	0.43
53:sb:230:TRP:CZ2	164:sc:102:U10:H111	2.52	0.43
65:y7:424:LYS:HD2	65:y7:424:LYS:HA	1.83	0.43
66:z:4:ASP:HB3	66:z:7:LYS:HG2	2.01	0.43
77:a7:252:ASP:N	77:a7:252:ASP:OD1	2.47	0.43
96:g1:175:LEU:HB3	96:g1:185:ARG:O	2.19	0.43
100:n1:32:ILE:HG13	100:n1:250:PHE:HE1	1.84	0.43
103:n4:453:LEU:HD13	104:n5:344:LYS:HE2	2.01	0.43
104:n5:89:PHE:HE2	37:H:305:LEU:HD22	1.84	0.43
104:n5:736:ILE:HG12	152:n5:805:PC1:H2B2	2.00	0.43
106:p1:28:PHE:HB2	106:p1:31:GLU:HB2	2.01	0.43
107:p2:181:ALA:O	107:p2:185:SER:OG	2.31	0.43
108:qA:74:ASN:OD1	108:qA:74:ASN:N	2.43	0.43
108:qA:246:PRO:HA	108:qA:249:ILE:HD12	2.00	0.43
109:qB:350:LEU:O	109:qB:353:LYS:HB3	2.19	0.43
114:qG:27:PRO:HA	114:qG:204:ASN:HA	1.99	0.43
111:qd:264:GLY:O	111:qd:268:LEU:HG	2.19	0.43
120:s1:168:PRO:HD2	120:s1:705:PHE:CZ	2.54	0.43
120:s1:543:LEU:HD12	120:s1:563:PHE:HB2	2.01	0.43
126:s7:22:PHE:O	126:s7:51:VAL:HA	2.18	0.43
142:tf:153:ASN:HB3	142:tf:191:LYS:NZ	2.33	0.43
29:C1:50:HIS:CG	29:C1:124:PRO:HG2	2.54	0.43
29:C1:630:ARG:HD3	29:C1:630:ARG:HA	1.85	0.43
154:C1:703:HEA:H242	30:C2:41:PHE:CE2	2.54	0.43
31:C3:576:TYR:CE2	31:C3:578:LYS:HB2	2.53	0.43
153:E:403:CDL:H731	153:E:403:CDL:H571	2.00	0.43
35:FS:160:HIS:HE1	35:FS:170:TRP:CD1	2.37	0.43
36:G:234:GLU:HA	36:G:237:TRP:HB2	2.00	0.43
38:I:22:ALA:HB2	38:I:44:GLN:HB2	2.00	0.43
41:L:197:TYR:CE1	49:Q:165:LEU:HD21	2.54	0.43
42:M:163:GLU:HG3	42:M:200:HIS:CD2	2.53	0.43
153:M:306:CDL:H152	63:Y0:71:LYS:HB2	2.01	0.43
52:SA:50:ASP:HB2	52:SA:73:LYS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:119:TRP:HE1	52:SA:629:VAL:HG22	1.84	0.43
57:U:97:TRP:CG	57:U:98:PRO:HD3	2.53	0.43
64:Y5:91:THR:O	64:Y5:95:ILE:HG13	2.19	0.43
68:1B:17:ALA:HB2	100:N1:210:PHE:CE2	2.54	0.43
73:A2:19:PHE:HB3	73:A2:29:LEU:HD23	2.01	0.43
79:A9:234:GLN:HG2	79:A9:263:GLY:N	2.34	0.43
153:B3:102:CDL:OB3	107:P2:129:ARG:HG3	2.18	0.43
93:BM:105:TYR:CE1	104:N5:273:PHE:HB3	2.54	0.43
97:G2:191:ARG:HH12	138:TB:49:GLN:HG2	1.83	0.43
103:N4:321:SER:HB2	103:N4:447:VAL:HG12	2.01	0.43
103:N4:338:THR:HG23	103:N4:367:HIS:CE1	2.53	0.43
104:N5:75:ILE:HG23	104:N5:138:LEU:HD12	2.00	0.43
104:N5:268:VAL:O	104:N5:272:THR:N	2.49	0.43
104:N5:569:LEU:HD13	104:N5:660:ILE:HG21	2.01	0.43
110:QC:222:TRP:O	110:QC:223:PHE:C	2.62	0.43
108:Qa:252:CYS:HB2	108:Qa:417:LEU:HD11	2.00	0.43
108:Qa:311:SER:O	108:Qa:312:VAL:HG13	2.18	0.43
110:Qc:86:ARG:HD3	110:Qc:86:ARG:HA	1.79	0.43
110:Qc:184:LEU:HG	164:Qc:501:U10:C3	2.49	0.43
111:Qd:264:GLY:O	111:Qd:268:LEU:HG	2.19	0.43
114:Qg:160:PHE:CE1	114:Qg:164:GLU:HG3	2.54	0.43
120:S1:68:GLU:OE1	123:S4:161:ARG:NH1	2.52	0.43
125:S6:57:LYS:HD2	125:S6:69:GLU:HG2	2.01	0.43
127:S8:194:PRO:HG3	127:S8:223:GLN:NE2	2.34	0.43
128:T1:171:PHE:HA	128:T1:174:TYR:CE2	2.54	0.43
146:V1:406:ASP:H	146:V1:409:GLU:HG3	1.83	0.43
148:X1:16:LEU:HD23	148:X1:115:VAL:HG11	2.00	0.43
3:2f:251:LYS:HG3	10:2m:74:GLN:HG3	2.00	0.43
3:2f:268:TYR:CG	8:2k:75:LEU:HD13	2.54	0.43
22:6t:64:LYS:HE3	30:c2:296:SER:O	2.19	0.43
23:7a:14:TYR:OH	26:a:393:GLU:OE1	2.30	0.43
153:a:505:CDL:H662	31:c3:390:ILE:HG12	2.01	0.43
27:b:253:ARG:HD3	27:b:253:ARG:HA	1.87	0.43
29:c1:83:GLY:HA2	30:c2:487:ARG:NH2	2.34	0.43
29:c1:125:TYR:CZ	36:g:208:ILE:HG21	2.53	0.43
32:d:236:PHE:CZ	32:d:328:MET:HB3	2.54	0.43
33:e:4:ALA:HB1	36:g:294:TYR:HA	2.01	0.43
33:e:191:PHE:O	33:e:194:LEU:HB2	2.19	0.43
34:f:194:LYS:HE2	43:m1:231:GLU:HB2	2.00	0.43
34:f:261:ASP:N	34:f:261:ASP:OD1	2.46	0.43
34:f:313:HIS:ND1	35:fs:13:ARG:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:315:GLU:HG2	35:fs:11:TYR:HD2	1.84	0.43
36:g:178:VAL:HG11	59:vb:187:ARG:HD2	2.01	0.43
39:j:95:THR:HG23	39:j:144:LEU:HD21	1.99	0.43
42:m:163:GLU:HG3	42:m:200:HIS:CD2	2.53	0.43
43:m1:300:PHE:N	153:m1:404:CDL:OB4	2.51	0.43
153:m1:402:CDL:H131	44:m2:65:PHE:CZ	2.54	0.43
50:r:122:GLU:HB3	66:z:81:ARG:HH22	1.83	0.43
53:sb:58:PRO:HD2	53:sb:87:TYR:O	2.18	0.43
56:t:86:ARG:NH2	153:t:203:CDL:OB4	2.43	0.43
56:t:139:ASP:HA	153:t:202:CDL:H572	2.01	0.43
59:vb:487:ALA:O	59:vb:491:ASN:ND2	2.52	0.43
68:1b:21:ARG:HA	100:n1:217:ALA:HB3	2.00	0.43
74:a3:81:ARG:NH2	74:a3:88:TYR:O	2.38	0.43
77:a7:1:MET:HG3	77:a7:4:ALA:H	1.84	0.43
78:a8:179:GLU:O	78:a8:183:LYS:HG2	2.19	0.43
82:al:86:GLN:HE22	100:n1:61:TYR:HD1	1.65	0.43
99:j1:294:ILE:HD12	99:j1:306:ALA:HB1	2.00	0.43
101:n2:221:THR:H	124:s5:2:SER:HB3	1.84	0.43
102:n3:77:PHE:O	102:n3:80:PRO:HD2	2.19	0.43
104:n5:419:MET:O	104:n5:481:LYS:NZ	2.44	0.43
104:n5:548:LEU:HB3	104:n5:551:GLU:HB2	2.00	0.43
153:n5:806:CDL:HA32	107:p2:129:ARG:NH2	2.34	0.43
112:qE:140:GLY:N	112:qE:156:ARG:O	2.51	0.43
114:qG:277:THR:OG1	114:qG:278:SER:N	2.51	0.43
109:qb:333:ALA:HB2	109:qb:362:THR:HA	2.00	0.43
109:qb:359:PRO:HD2	109:qb:387:PHE:CZ	2.53	0.43
110:qc:184:LEU:HG	164:qc:501:U10:C3	2.49	0.43
115:qh:17:ASP:HB3	115:qh:29:ILE:HD13	2.00	0.43
120:s1:320:TRP:CZ3	120:s1:578:LEU:HG	2.53	0.43
120:s1:382:ARG:HB3	120:s1:386:LEU:HD12	2.00	0.43
121:s2:95:HIS:ND1	121:s2:122:ASP:OD2	2.43	0.43
128:t1:171:PHE:HA	128:t1:174:TYR:CE2	2.54	0.43
132:t5:116:LEU:HB2	132:t5:122:ARG:HD3	2.00	0.43
136:t9:96:LEU:O	136:t9:100:GLN:HG2	2.18	0.43
146:v1:39:ASP:HA	146:v1:258:ARG:HH12	1.84	0.43
26:A:72:SER:C	26:A:74:ASP:H	2.26	0.43
28:BP:205:PHE:HA	152:M2:407:PC1:H221	2.01	0.43
28:BP:254:GLN:C	28:BP:256:GLY:H	2.27	0.43
29:C1:216:ILE:HD13	46:N:192:ASP:HB3	2.00	0.43
30:C2:286:ASP:OD1	30:C2:286:ASP:N	2.49	0.43
31:C3:267:PRO:O	31:C3:271:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C3:552:SER:N	49:Q:142:GLN:OE1	2.45	0.43
36:G:96:PHE:HB2	36:G:237:TRP:CZ2	2.54	0.43
43:M1:24:TRP:CZ2	153:M2:403:CDL:HB61	2.54	0.43
48:P:67:LEU:O	48:P:75:GLN:NE2	2.52	0.43
53:SB:58:PRO:HD2	53:SB:87:TYR:O	2.19	0.43
164:SC:102:U10:O4	55:SD:12:TYR:OH	2.26	0.43
59:VB:87:LYS:O	59:VB:91:GLU:HG3	2.19	0.43
59:VB:207:GLU:O	59:VB:210:TYR:HB3	2.18	0.43
63:Y0:27:TYR:O	63:Y0:30:LEU:HG	2.19	0.43
168:AB:201:ZMP:H17	168:AB:201:ZMP:H14A	2.01	0.43
82:AL:156:GLN:HE22	123:S4:118:PRO:HA	1.83	0.43
85:B2:23:TYR:CD2	86:B3:43:ASN:HA	2.53	0.43
96:G1:161:ASN:HD22	97:G2:172:LEU:HB2	1.84	0.43
98:G3:170:VAL:HB	98:G3:186:SER:O	2.19	0.43
100:N1:262:VAL:HG23	100:N1:263:LEU:HG	2.00	0.43
101:N2:138:ILE:N	101:N2:139:PRO:HD2	2.34	0.43
101:N2:138:ILE:HG23	101:N2:291:ILE:HG12	2.01	0.43
103:N4:453:LEU:HD13	104:N5:344:LYS:HE2	2.01	0.43
104:N5:569:LEU:HA	104:N5:572:TYR:HD2	1.84	0.43
104:N5:733:SER:HB2	106:P1:116:TYR:HD1	1.83	0.43
105:N6:62:ILE:O	105:N6:66:ILE:HG13	2.17	0.43
108:QA:314:TRP:CZ2	108:QA:354:HIS:HB2	2.54	0.43
108:Qa:214:LEU:HD11	108:Qa:224:LEU:HD21	2.00	0.43
115:Qh:17:ASP:HB3	115:Qh:29:ILE:HD13	2.00	0.43
135:T8:49:VAL:HG13	158:T8:602:3PE:H2B2	2.01	0.43
143:TG:49:THR:O	143:TG:53:GLU:HG3	2.18	0.43
149:c:205:ILE:O	149:c:209:ILE:HG12	2.19	0.43
8:2k:30:ARG:HH22	153:2k:101:CDL:PA1	2.42	0.43
25:7l:896:ASN:HB2	60:w:102:ARG:HH12	1.84	0.43
27:b:145:ARG:NH2	74:a3:9:PHE:HA	2.34	0.43
29:c1:508:LEU:HB3	154:c1:708:HEA:CMA	2.45	0.43
32:d:195:PHE:HE1	39:j:217:LEU:HB2	1.84	0.43
33:e:336:ALA:HB3	36:g:73:PRO:HB2	2.01	0.43
34:f:212:MET:HG3	153:f:401:CDL:H511	2.00	0.43
37:h:199:THR:HG22	37:h:201:GLY:H	1.83	0.43
38:i:97:PHE:CE1	153:i:301:CDL:H352	2.54	0.43
45:m3:171:TYR:CD2	45:m3:208:TYR:HA	2.54	0.43
46:n:182:VAL:HB	46:n:185:SER:HB3	2.01	0.43
62:y:45:ASN:HD21	62:y:105:PHE:HA	1.84	0.43
63:y0:43:TYR:HE1	63:y0:56:LEU:HG	1.84	0.43
70:4l:20:VAL:HG13	71:5b:79:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:5b:100:ILE:HD13	158:an:301:3PE:H322	2.01	0.43
153:a9:402:CDL:HA4	102:n3:21:TRP:CZ2	2.53	0.43
84:an:221:HIS:CE1	103:n4:226:THR:HB	2.54	0.43
164:b8:301:U10:H161	164:b8:301:U10:H8	2.01	0.43
92:bl:58:GLU:O	92:bl:62:ILE:HG12	2.19	0.43
94:c4:48:PHE:CD1	153:c4:401:CDL:H812	2.54	0.43
101:n2:138:ILE:N	101:n2:139:PRO:HD2	2.34	0.43
103:n4:428:TYR:OH	103:n4:505:PHE:O	2.24	0.43
109:qB:235:ASN:O	109:qB:239:THR:HG22	2.19	0.43
110:qC:15:LYS:O	110:qC:19:TYR:N	2.48	0.43
110:qC:150:ALA:HB1	110:qC:171:LYS:HG2	2.00	0.43
114:qG:110:TYR:HD1	114:qG:110:TYR:HA	1.73	0.43
109:qb:71:ASN:ND2	109:qb:71:ASN:H	2.17	0.43
109:qb:430:ASP:OD1	109:qb:430:ASP:N	2.51	0.43
121:s2:150:ALA:O	121:s2:154:ARG:HG3	2.18	0.43
121:s2:182:ASN:HD21	127:s8:235:PRO:HB3	1.84	0.43
126:s7:4:ASP:HA	126:s7:7:VAL:HG22	2.00	0.43
3:2F:137:ARG:HE	152:2F:301:PC1:H361	1.83	0.43
10:2M:64:ASN:ND2	10:2M:68:ASN:O	2.49	0.43
153:2O:101:CDL:H512	153:2O:101:CDL:HA32	2.00	0.43
15:4A:54:GLY:HA2	15:4A:70:ILE:HD12	1.99	0.43
19:6B:10:LEU:HB2	19:6B:11:PRO:HD3	2.01	0.43
20:6C:53:ASN:HB2	58:V:137:VAL:HB	2.00	0.43
29:C1:530:MET:HG2	154:C1:703:HEA:C3C	2.49	0.43
31:C3:364:PRO:O	31:C3:368:ILE:HG23	2.19	0.43
31:C3:390:ILE:HG12	153:VB:705:CDL:H662	2.00	0.43
33:E:23:ARG:NH1	59:VB:419:ASP:OD1	2.52	0.43
34:F:212:MET:HG3	153:F:402:CDL:H511	2.00	0.43
36:G:159:ASN:HD22	36:G:197:PRO:HA	1.84	0.43
37:H:237:ASN:O	37:H:241:VAL:HG23	2.18	0.43
54:SC:25:ILE:O	54:SC:29:ILE:HG12	2.18	0.43
56:T:138:ASN:HB3	153:T:202:CDL:H541	2.01	0.43
57:U:97:TRP:CD1	153:U:201:CDL:H512	2.54	0.43
64:Y5:96:GLU:OE2	67:Z1:52:THR:OG1	2.26	0.43
76:A6:108:ARG:O	168:AB:201:ZMP:H8A	2.19	0.43
77:A7:255:ALA:HA	77:A7:258:LEU:HG	2.00	0.43
78:A8:179:GLU:O	78:A8:183:LYS:HG2	2.19	0.43
83:AM:172:LYS:HE2	141:TE:71:LEU:HD11	2.00	0.43
91:B9:127:LEU:HD21	103:N4:475:LEU:HD12	2.01	0.43
92:BL:127:ILE:O	92:BL:131:VAL:HG23	2.18	0.43
96:G1:242:TYR:HA	98:G3:235:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
108:QA:191:HIS:HB3	108:QA:225:ARG:HD2	2.01	0.43
111:QD:264:GLY:HA2	111:QD:267:ILE:HG22	2.01	0.43
114:QG:261:ASP:OD1	114:QG:263:THR:OG1	2.33	0.43
152:QI:202:PC1:H153	152:QI:202:PC1:H112	1.84	0.43
110:Qc:76:TYR:O	110:Qc:80:PHE:HD2	2.01	0.43
115:Qh:93:TYR:HA	115:Qh:97:ILE:HB	2.00	0.43
120:S1:62:PRO:HB2	120:S1:78:MET:HG3	2.01	0.43
120:S1:83:VAL:O	120:S1:86:VAL:HG12	2.19	0.43
120:S1:118:MET:HA	120:S1:118:MET:HE3	2.01	0.43
120:S1:387:MET:HB2	120:S1:594:GLU:HA	2.01	0.43
120:S1:482:ARG:NH2	120:S1:484:ASP:OD1	2.41	0.43
127:S8:139:CYS:HA	127:S8:163:ARG:HH21	1.84	0.43
129:T2:73:LEU:HD23	129:T2:73:LEU:HA	1.87	0.43
144:TH:25:ASN:HD21	144:TH:28:GLU:HG2	1.84	0.43
144:TH:75:VAL:HG23	144:TH:81:ARG:HG2	2.01	0.43
149:c:150:GLY:O	149:c:154:SER:OG	2.36	0.43
6:2i:32:ASN:ND2	9:2l:36:PHE:H	2.17	0.42
7:2j:102:ARG:HD2	9:2l:16:ARG:NH2	2.34	0.42
19:6b:46:GLU:OE2	58:v:131:TYR:OH	2.23	0.42
22:6t:13:ILE:HG12	22:6t:44:TYR:CE1	2.53	0.42
26:a:354:SER:OG	31:c3:472:ASN:ND2	2.50	0.42
27:b:58:SER:HB2	27:b:214:ARG:HH21	1.83	0.42
28:bp:141:ASN:HB2	28:bp:192:TYR:CB	2.49	0.42
29:c1:380:ILE:HG22	29:c1:384:HIS:CD2	2.54	0.42
30:c2:129:GLU:HG2	30:c2:132:ASN:ND2	2.34	0.42
33:e:193:GLN:O	33:e:197:GLY:N	2.52	0.42
41:l:134:LEU:HD12	41:l:135:PRO:HD2	2.01	0.42
46:n:67:ASP:O	46:n:71:ARG:N	2.51	0.42
46:n:186:ALA:HB3	46:n:189:HIS:HD2	1.84	0.42
59:vb:187:ARG:HA	59:vb:193:GLN:O	2.18	0.42
69:2b:51:ASN:HB3	95:fx:103:PHE:CG	2.54	0.42
70:4l:24:LYS:HA	70:4l:24:LYS:HD3	1.81	0.42
73:a2:58:ASP:OD2	123:s4:41:ASN:ND2	2.52	0.42
77:a7:93:TYR:CE1	77:a7:115:LYS:HD2	2.49	0.42
81:ac:58:ALA:HB1	81:ac:79:LEU:HD21	2.01	0.42
85:b2:23:TYR:HB2	86:b3:43:ASN:HD22	1.83	0.42
98:g3:170:VAL:HB	98:g3:186:SER:O	2.19	0.42
152:n5:803:PC1:H3F2	152:n5:803:PC1:H2C1	2.00	0.42
107:p2:120:TYR:HB2	107:p2:140:THR:HB	2.01	0.42
108:qA:79:ILE:O	108:qA:252:CYS:HA	2.19	0.42
110:qC:84:HIS:O	110:qC:88:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:qD:101:ARG:HB2	111:qD:104:GLU:HG2	2.01	0.42
113:qF:25:LEU:HD21	113:qF:70:GLU:OE2	2.19	0.42
117:qJ:2:TYR:OH	114:qg:5:GLU:OE2	2.29	0.42
108:qa:254:ALA:HB2	108:qa:417:LEU:HD13	2.01	0.42
108:qa:380:ILE:HG23	108:qa:481:LEU:HD23	2.00	0.42
112:qe:60:PHE:CE1	115:qh:57:GLY:HA2	2.54	0.42
114:qg:239:GLU:HG2	114:qg:262:PHE:CD1	2.54	0.42
120:s1:713:PHE:HB3	129:t2:52:HIS:CE1	2.54	0.42
121:s2:153:GLU:CD	121:s2:202:THR:HG21	2.44	0.42
121:s2:242:ARG:NH2	121:s2:286:GLU:OE2	2.47	0.42
122:s3:55:PHE:O	122:s3:58:ILE:HB	2.19	0.42
128:t1:372:PRO:HG3	128:t1:433:ARG:HA	2.01	0.42
130:t3:226:ASN:HB3	130:t3:229:GLU:HB3	2.01	0.42
146:v1:142:GLY:HA2	146:v1:253:PRO:HD3	2.01	0.42
146:v1:370:ARG:HA	146:v1:370:ARG:HD2	1.80	0.42
146:v1:424:THR:HB	162:v1:500:SF4:S2	2.59	0.42
3:2F:206:ASN:HB2	53:SB:36:CYS:HB2	2.01	0.42
21:6L:4:LYS:HE3	58:V:128:ASN:HB3	2.01	0.42
30:C2:518:ILE:HG21	30:C2:521:LEU:HD12	2.01	0.42
31:C3:517:TYR:OH	56:T:48:HIS:NE2	2.32	0.42
38:I:117:MET:HE3	153:I:303:CDL:HA21	2.01	0.42
38:I:126:TYR:O	38:I:130:ASN:ND2	2.42	0.42
39:J:228:HIS:HB3	39:J:231:LYS:O	2.19	0.42
43:M1:112:LEU:HB3	43:M1:324:LEU:HD23	2.00	0.42
45:M3:171:TYR:CD2	45:M3:208:TYR:HA	2.54	0.42
50:R:87:ILE:HD12	64:Y5:97:LEU:HD22	1.99	0.42
52:SA:459:LEU:HA	52:SA:462:GLU:HG2	2.01	0.42
59:VB:234:PRO:HG3	153:VB:706:CDL:H551	2.00	0.42
70:4L:24:LYS:HA	70:4L:24:LYS:HD3	1.82	0.42
74:A3:81:ARG:HD2	137:TA:97:ARG:NH1	2.34	0.42
76:A6:112:GLY:CA	168:AB:201:ZMP:H7	2.48	0.42
99:J1:48:ALA:O	99:J1:52:HIS:HB2	2.19	0.42
152:N1:301:PC1:H362	152:N1:301:PC1:H262	2.01	0.42
104:N5:296:MET:HG2	104:N5:433:THR:HA	2.01	0.42
104:N5:705:TRP:O	104:N5:709:ILE:HG12	2.19	0.42
110:QC:164:TYR:CZ	110:QC:171:LYS:HE3	2.54	0.42
108:Qa:330:ASN:ND2	108:Qa:350:ALA:HB3	2.34	0.42
108:Qa:378:HIS:O	108:Qa:382:GLU:HG2	2.18	0.42
109:Qb:80:SER:HB2	109:Qb:252:GLY:HA2	2.00	0.42
110:Qc:123:PHE:O	110:Qc:126:PHE:HB3	2.19	0.42
112:Qe:94:THR:HG21	153:Qi:202:CDL:H351	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
120:S1:89:PRO:HB3	120:S1:113:HIS:CD2	2.54	0.42
120:S1:253:ASP:OD2	120:S1:291:THR:OG1	2.23	0.42
120:S1:385:TYR:O	120:S1:515:HIS:NE2	2.40	0.42
121:S2:126:ARG:HA	121:S2:382:PRO:HG3	2.02	0.42
121:S2:400:LYS:NZ	122:S3:143:TYR:OH	2.46	0.42
126:S7:30:ALA:O	126:S7:33:ALA:N	2.51	0.42
128:T1:103:LYS:HE2	128:T1:103:LYS:HB3	1.84	0.42
128:T1:401:ILE:HG13	128:T1:403:GLY:N	2.34	0.42
129:T2:77:LYS:HE2	129:T2:265:ALA:HB2	2.00	0.42
136:T9:66:LEU:N	136:T9:67:PRO:HD2	2.34	0.42
145:TX:49:TYR:CZ	145:TX:51:ARG:HB3	2.54	0.42
146:V1:264:ALA:HA	146:V1:272:ALA:HB1	2.00	0.42
147:V2:32:LYS:HA	147:V2:32:LYS:HD2	1.86	0.42
3:2f:133:TRP:O	3:2f:137:ARG:NH2	2.50	0.42
3:2f:175:ASN:O	3:2f:179:LEU:HG	2.18	0.42
20:6c:53:ASN:HB2	58:v:137:VAL:HB	2.00	0.42
21:6l:4:LYS:HE3	58:v:128:ASN:HB3	2.01	0.42
25:7l:890:ASP:HB3	60:w:75:TYR:HB2	2.01	0.42
27:b:298:TYR:HB2	27:b:349:ASN:HD21	1.84	0.42
29:c1:81:HIS:CE1	29:c1:85:PRO:HB3	2.54	0.42
29:c1:477:LEU:HD21	29:c1:492:MET:HE1	2.00	0.42
29:c1:563:HIS:CD2	29:c1:618:PHE:HB2	2.54	0.42
30:c2:85:ILE:HB	30:c2:86:PRO:HD3	2.01	0.42
33:e:189:ASP:OD2	42:M:3:LEU:HB2	2.18	0.42
36:g:96:PHE:HZ	36:g:238:TRP:HD1	1.67	0.42
37:h:38:GLN:O	37:h:41:ARG:HB3	2.19	0.42
38:i:238:ARG:HA	38:i:250:LEU:HD21	2.02	0.42
152:i:304:PC1:H241	35:FS:180:VAL:HG21	2.00	0.42
40:k:82:LEU:O	40:k:86:TYR:N	2.28	0.42
41:l:29:GLU:HG2	41:l:30:MET:H	1.84	0.42
42:m:38:VAL:HA	42:m:41:ARG:HG2	2.00	0.42
43:m1:167:PHE:O	43:m1:172:GLN:NE2	2.40	0.42
44:m2:159:GLY:O	44:m2:169:LYS:NZ	2.45	0.42
52:sa:146:PRO:HD2	52:sa:186:ALA:HB1	2.02	0.42
153:t:204:CDL:H812	153:t:204:CDL:H732	2.01	0.42
59:vb:168:ASP:OD1	60:w:11:GLU:HB2	2.19	0.42
76:a6:79:LYS:HG2	76:a6:142:ASP:CG	2.44	0.42
80:ab:62:GLU:HG3	145:tx:113:THR:HB	2.01	0.42
83:am:156:LYS:HE3	83:am:161:VAL:HG22	2.01	0.42
153:bm:301:CDL:H141	104:n5:182:PHE:HZ	1.83	0.42
100:n1:187:VAL:HG11	100:n1:267:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
104:n5:694:TYR:O	104:n5:698:ASN:ND2	2.52	0.42
104:n5:705:TRP:O	104:n5:709:ILE:HG12	2.19	0.42
106:p1:190:ARG:NH1	130:t3:56:GLN:HE21	2.16	0.42
106:p1:224:LYS:HA	106:p1:230:GLU:O	2.19	0.42
106:p1:247:HIS:CG	106:p1:248:PRO:HD2	2.54	0.42
110:qC:102:LYS:HA	110:qC:102:LYS:HD3	1.74	0.42
109:qb:144:GLU:HG3	109:qb:214:PHE:HE1	1.85	0.42
124:s5:74:TYR:HB2	124:s5:81:PHE:CE2	2.54	0.42
126:s7:63:ILE:HD11	126:s7:84:THR:HG21	2.00	0.42
153:t5:301:CDL:H382	153:t5:301:CDL:H181	2.01	0.42
137:ta:46:ARG:O	137:ta:50:ILE:HG12	2.20	0.42
146:v1:129:ARG:NH1	147:v2:169:ALA:HB2	2.33	0.42
2:2E:63:LEU:HD21	2:2E:69:LEU:HD13	2.02	0.42
2:2E:81:TYR:CZ	2:2E:97:ILE:HG22	2.54	0.42
3:2F:209:TYR:CD1	53:SB:40:ILE:HG13	2.55	0.42
7:2J:29:PHE:HA	7:2J:32:THR:HG22	2.01	0.42
13:2T:57:PHE:CD2	17:5T:39:PHE:HB3	2.54	0.42
23:7A:73:LEU:HA	65:Y7:354:PHE:HE1	1.84	0.42
29:C1:20:PHE:HB3	29:C1:23:LEU:CB	2.49	0.42
29:C1:525:ALA:HB2	29:C1:578:LEU:HB2	2.01	0.42
29:C1:581:LEU:HD13	29:C1:601:HIS:CE1	2.54	0.42
30:C2:517:PHE:CE2	30:C2:519:PRO:HG3	2.54	0.42
31:C3:524:ARG:HG2	153:T:202:CDL:H571	2.01	0.42
32:D:311:ARG:HB2	32:D:322:TRP:HB3	2.02	0.42
33:E:185:GLU:OE2	33:E:187:ARG:NH1	2.50	0.42
34:F:175:GLU:HG2	153:F:402:CDL:H591	2.02	0.42
34:F:313:HIS:ND1	35:FS:13:ARG:HD2	2.34	0.42
38:I:39:GLN:OE1	38:I:232:LYS:HG3	2.19	0.42
39:J:80:ASP:OD2	39:J:167:ARG:NH2	2.51	0.42
40:K:173:GLU:OE2	48:P:9:HIS:NE2	2.53	0.42
42:M:75:VAL:HG21	42:M:83:PHE:CD1	2.54	0.42
44:M2:32:TYR:N	44:M2:33:PRO:HD2	2.34	0.42
45:M3:206:ARG:NH2	45:M3:256:GLN:O	2.44	0.42
49:Q:46:LEU:HD22	49:Q:114:ILE:HD12	2.01	0.42
49:Q:84:ARG:NE	153:VB:706:CDL:OB3	2.49	0.42
52:SA:283:PHE:O	52:SA:332:SER:OG	2.31	0.42
52:SA:397:ASN:ND2	52:SA:429:GLU:OE2	2.37	0.42
53:SB:109:LYS:HB3	53:SB:116:LEU:HD23	2.01	0.42
60:W:33:TRP:CG	153:W:202:CDL:H462	2.54	0.42
62:Y:52:GLU:O	62:Y:56:MET:HG3	2.19	0.42
69:2B:45:SER:HB3	95:FX:172:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:2B:100:LEU:HD11	101:N2:356:ILE:HG22	2.01	0.42
76:A6:79:LYS:HG2	76:A6:142:ASP:CG	2.44	0.42
77:A7:1:MET:HG3	77:A7:4:ALA:H	1.84	0.42
79:A9:193:ALA:O	79:A9:256:GLY:N	2.52	0.42
153:AN:302:CDL:H831	153:AN:302:CDL:H791	2.01	0.42
152:AN:304:PC1:H332	110:QC:244:VAL:HG22	2.00	0.42
95:FX:98:VAL:HG21	103:N4:197:GLN:HG2	2.01	0.42
97:G2:127:GLY:HA3	97:G2:145:ASP:H	1.84	0.42
105:N6:58:ILE:O	105:N6:62:ILE:HG12	2.19	0.42
110:QC:28:HIS:CD2	110:QC:33:LEU:HD21	2.54	0.42
110:QC:97:PHE:CZ	153:QC:504:CDL:H371	2.55	0.42
110:QC:242:MET:HG3	152:QC:505:PC1:H321	2.01	0.42
112:QE:81:ASN:HD21	112:QE:88:ARG:HB2	1.82	0.42
153:QI:203:CDL:H162	153:QI:203:CDL:H542	2.01	0.42
110:Qc:73:GLU:OE2	111:Qd:91:LYS:NZ	2.47	0.42
110:Qc:251:GLU:HB2	111:Qd:250:ARG:NH2	2.35	0.42
114:Qg:239:GLU:HG2	114:Qg:262:PHE:CD1	2.54	0.42
120:S1:551:PRO:HA	120:S1:573:TYR:HE2	1.84	0.42
125:S6:85:VAL:HG12	125:S6:102:ILE:HB	2.01	0.42
128:T1:210:TYR:OH	128:T1:254:GLN:NE2	2.52	0.42
130:T3:48:LEU:HB3	130:T3:57:LEU:HD21	2.00	0.42
131:T4:157:LEU:O	131:T4:160:PRO:HD2	2.19	0.42
132:T5:138:ILE:HD12	153:T5:301:CDL:H673	2.00	0.42
148:X1:19:ARG:NH2	148:X1:23:ARG:O	2.40	0.42
153:c:301:CDL:OB3	150:u1:5:UNK:N	2.51	0.42
3:2f:141:LYS:HE2	3:2f:141:LYS:HB2	1.87	0.42
153:6c:202:CDL:H672	58:v:104:THR:HG22	2.01	0.42
23:7a:58:GLU:HB3	23:7a:66:THR:HB	2.01	0.42
24:7c:188:ASP:O	24:7c:214:TYR:OH	2.36	0.42
153:7c:301:CDL:H431	29:c1:63:VAL:HG21	2.01	0.42
26:a:72:SER:C	26:a:74:ASP:H	2.27	0.42
27:b:253:ARG:NH2	48:p:88:ASP:O	2.41	0.42
29:c1:126:HIS:CG	29:c1:333:PRO:HG2	2.54	0.42
31:c3:153:ASN:O	31:c3:157:ASN:ND2	2.35	0.42
32:d:378:ARG:HH22	152:d:501:PC1:H342	1.82	0.42
37:h:197:VAL:HG11	37:h:282:VAL:HG11	2.01	0.42
38:i:35:GLU:O	38:i:39:GLN:HG2	2.19	0.42
41:l:197:TYR:CE1	49:q:165:LEU:HD21	2.54	0.42
42:m:7:GLY:O	33:E:186:PRO:HG3	2.20	0.42
52:sa:397:ASN:O	52:sa:399:GLY:N	2.52	0.42
57:u:96:PHE:N	153:u:201:CDL:OA3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:u:97:TRP:CD1	153:u:201:CDL:H512	2.53	0.42
65:y7:113:LYS:HD3	65:y7:113:LYS:HA	1.83	0.42
69:2b:23:LEU:HD22	69:2b:87:LEU:HD12	2.01	0.42
73:a2:19:PHE:HB3	73:a2:29:LEU:HD23	2.00	0.42
77:a7:208:ARG:NH1	121:s2:327:THR:HG22	2.34	0.42
80:ab:50:GLU:H	80:ab:50:GLU:CD	2.26	0.42
95:fx:98:VAL:HG21	103:n4:197:GLN:HG2	2.01	0.42
97:g2:191:ARG:HH12	138:tb:49:GLN:HG2	1.84	0.42
108:qA:297:LEU:H	108:qa:296:ASN:ND2	2.18	0.42
111:qD:316:TYR:HD1	114:qG:174:ARG:HD2	1.85	0.42
108:qa:115:ASN:HB3	108:qa:186:LYS:HD3	2.01	0.42
109:qb:492:HIS:HD2	111:qd:282:LEU:HD22	1.84	0.42
121:s2:284:MET:HA	121:s2:287:MET:HE3	2.02	0.42
121:s2:348:LYS:HD2	121:s2:353:SER:HB3	2.01	0.42
122:s3:124:SER:HB2	122:s3:147:TYR:HB3	2.01	0.42
136:t9:66:LEU:N	136:t9:67:PRO:HD2	2.34	0.42
143:tg:109:HIS:O	143:tg:113:GLU:HG3	2.20	0.42
147:v2:44:PHE:HA	147:v2:78:GLN:HE22	1.83	0.42
9:2L:12:THR:OG1	9:2L:13:PRO:HD3	2.18	0.42
22:6T:59:LEU:HD23	22:6T:59:LEU:HA	1.88	0.42
153:7C:302:CDL:H521	152:M2:402:PC1:H241	2.02	0.42
29:C1:137:LEU:HD11	152:C1:706:PC1:H342	2.00	0.42
29:C1:612:LEU:HD13	152:M1:401:PC1:H2F1	2.00	0.42
30:C2:57:ARG:NE	58:V:91:ASN:HB3	2.33	0.42
30:C2:511:ASP:OD1	30:C2:511:ASP:N	2.52	0.42
33:E:383:LYS:O	33:E:384:HIS:ND1	2.52	0.42
38:I:238:ARG:HA	38:I:250:LEU:HD21	2.01	0.42
42:M:195:THR:HG22	62:Y:7:GLN:HA	2.01	0.42
46:N:186:ALA:HB3	46:N:189:HIS:HD2	1.84	0.42
49:Q:78:ARG:O	49:Q:82:GLY:N	2.35	0.42
52:SA:566:GLN:NE2	52:SA:600:THR:HB	2.34	0.42
52:SA:569:LEU:HD23	52:SA:569:LEU:HA	1.79	0.42
53:SB:230:TRP:CZ2	164:SC:102:U10:H111	2.53	0.42
56:T:134:ASP:OD2	56:T:136:SER:OG	2.31	0.42
60:W:77:PRO:HB2	60:W:85:LYS:HB2	2.01	0.42
61:X:33:THR:HG23	61:X:106:ALA:HB1	2.01	0.42
63:Y0:67:TYR:O	63:Y0:71:LYS:HG2	2.18	0.42
75:A5:123:GLU:HG2	75:A5:131:ILE:HB	2.01	0.42
76:A6:111:LEU:HD13	122:S3:163:ILE:HG23	2.01	0.42
81:AC:50:TYR:CG	81:AC:54:PRO:HG3	2.55	0.42
82:AL:3:LEU:HB3	153:AL:301:CDL:HA31	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:AL:13:THR:HG23	82:AL:47:THR:HB	2.01	0.42
152:AL:302:PC1:H143	152:AL:302:PC1:H112	1.82	0.42
84:AN:90:MET:HB3	84:AN:104:ILE:HD11	2.01	0.42
85:B2:23:TYR:HB2	86:B3:43:ASN:HD22	1.84	0.42
164:B8:301:U10:H161	164:B8:301:U10:H121	1.92	0.42
153:BM:301:CDL:H731	103:N4:496:ILE:HG23	2.01	0.42
95:FX:154:ASN:ND2	95:FX:155:GLU:HG2	2.33	0.42
97:G2:34:GLU:HA	98:G3:15:MET:HG3	2.01	0.42
98:G3:172:PRO:HD3	98:G3:188:ALA:HB3	2.02	0.42
99:J1:299:ARG:HE	99:J1:305:VAL:HG21	1.83	0.42
100:N1:22:LEU:O	100:N1:26:ILE:HG12	2.20	0.42
100:N1:133:PHE:O	100:N1:137:ILE:HG12	2.19	0.42
104:N5:337:PHE:CD2	158:N5:802:3PE:H221	2.54	0.42
104:N5:719:TRP:HZ2	152:N5:803:PC1:H221	1.85	0.42
106:P1:46:LYS:HE2	106:P1:46:LYS:HB2	1.91	0.42
108:QA:297:LEU:H	108:Qa:296:ASN:ND2	2.17	0.42
110:QC:150:ALA:HB1	110:QC:171:LYS:HG2	2.00	0.42
111:QD:101:ARG:HB2	111:QD:104:GLU:HG2	2.02	0.42
111:QD:115:HIS:CG	111:QD:116:PRO:HD2	2.54	0.42
115:QH:20:ARG:O	111:Qd:314:ARG:NH2	2.51	0.42
108:Qa:119:LYS:NZ	108:Qa:126:GLU:OE1	2.36	0.42
111:Qd:161:ASP:OD2	111:Qd:163:SER:OG	2.21	0.42
114:Qg:202:PHE:HB2	114:Qg:205:GLU:HB2	2.00	0.42
152:Qi:201:PC1:H252	117:Qj:23:GLY:HA2	2.00	0.42
120:S1:119:GLU:OE2	120:S1:153:ARG:NE	2.46	0.42
123:S4:12:ARG:HA	123:S4:12:ARG:HD2	1.83	0.42
135:T8:130:PRO:O	136:T9:38:TYR:OH	2.35	0.42
137:TA:46:ARG:O	137:TA:50:ILE:HG12	2.19	0.42
142:TF:82:LEU:HD23	142:TF:87:ILE:HD12	2.02	0.42
149:C:197:LEU:HD23	149:C:197:LEU:HA	1.91	0.42
3:2f:209:TYR:CD1	53:sb:40:ILE:HG13	2.55	0.42
153:2k:101:CDL:H381	153:2k:101:CDL:HB21	2.00	0.42
15:4a:64:ARG:HH21	33:e:206:TRP:CD1	2.37	0.42
16:4t:23:ASP:OD1	16:4t:23:ASP:N	2.46	0.42
19:6b:47:LYS:NZ	25:7l:970:LEU:O	2.52	0.42
19:6b:174:TYR:OH	30:c2:167:GLN:NE2	2.53	0.42
24:7c:210:ASP:HB2	30:c2:473:ASN:HD21	1.84	0.42
152:7c:303:PC1:H352	44:m2:226:TRP:CZ3	2.54	0.42
29:c1:126:HIS:HB2	29:c1:336:THR:HG21	2.00	0.42
29:c1:525:ALA:HB2	29:c1:578:LEU:HB2	2.01	0.42
29:c1:639:LEU:HG	59:vb:189:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c2:45:TRP:HD1	58:v:103:LEU:HD23	1.83	0.42
31:c3:171:TYR:OH	45:m3:121:ASN:ND2	2.52	0.42
31:c3:364:PRO:O	31:c3:368:ILE:HG23	2.19	0.42
31:c3:506:PHE:O	31:c3:510:LYS:HG2	2.19	0.42
34:f:175:GLU:HG2	153:f:401:CDL:H591	2.02	0.42
37:h:82:LYS:HE3	104:N5:69:HIS:H	1.85	0.42
47:o:87:ASP:O	47:o:91:ARG:HG3	2.20	0.42
63:y0:12:SER:OG	63:y0:14:ASP:OD1	2.36	0.42
65:y7:296:ASN:OD1	65:y7:296:ASN:N	2.52	0.42
75:a5:184:ARG:HH21	120:s1:392:THR:HB	1.85	0.42
76:a6:111:LEU:HD13	122:s3:163:ILE:HG23	2.01	0.42
85:b2:77:MET:HG3	152:t4:301:PC1:H241	2.02	0.42
88:b6:87:MET:HE2	88:b6:87:MET:HB3	1.88	0.42
100:n1:9:PHE:CD2	100:n1:12:ILE:HD11	2.54	0.42
103:n4:260:TRP:HB2	103:n4:316:GLY:HA2	2.00	0.42
108:qA:112:SER:O	108:qA:116:THR:OG1	2.32	0.42
110:qC:79:ASP:OD1	110:qC:79:ASP:N	2.50	0.42
112:qE:66:PHE:HD2	112:qE:68:VAL:HG13	1.84	0.42
114:qG:264:ARG:HH21	114:qG:291:GLU:CD	2.28	0.42
164:qc:507:U10:H101	164:qc:507:U10:H152	2.01	0.42
114:qg:147:LEU:O	114:qg:151:VAL:HG23	2.19	0.42
120:s1:36:PHE:HB2	120:s1:102:LYS:HG2	2.01	0.42
120:s1:68:GLU:OE1	123:s4:161:ARG:NH1	2.52	0.42
121:s2:84:ARG:HG2	162:s7:201:SF4:S2	2.59	0.42
125:s6:85:VAL:HG12	125:s6:102:ILE:HB	2.01	0.42
130:t3:4:LEU:H	131:t4:137:ASN:ND2	2.17	0.42
146:v1:381:GLY:O	146:v1:387:ARG:NH1	2.52	0.42
148:x1:20:ARG:NH1	148:x1:33:PRO:HB3	2.35	0.42
2:2E:154:THR:HA	2:2E:187:VAL:O	2.20	0.42
3:2F:141:LYS:HE2	3:2F:141:LYS:HB2	1.86	0.42
4:2G:147:ILE:HG23	4:2G:157:GLN:HE21	1.84	0.42
24:7C:47:ILE:HG12	43:M1:282:LYS:HB3	1.99	0.42
24:7C:188:ASP:O	24:7C:214:TYR:OH	2.37	0.42
27:B:460:LEU:HD12	27:B:463:ILE:HD11	2.00	0.42
34:F:261:ASP:OD1	34:F:261:ASP:N	2.46	0.42
35:FS:27:ASP:OD2	36:G:83:TYR:OH	2.38	0.42
49:Q:77:ARG:HA	49:Q:77:ARG:HD3	1.88	0.42
51:S:46:VAL:HG21	65:Y7:190:ILE:HD11	2.00	0.42
64:Y5:173:THR:O	64:Y5:174:ARG:NH1	2.52	0.42
70:4L:23:PRO:HG3	105:N6:112:TYR:CD2	2.54	0.42
80:AB:86:GLN:HG2	80:AB:90:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:B3:44:THR:OG1	107:P2:122:ASP:OD1	2.34	0.42
111:QD:317:PHE:HB3	111:QD:318:TRP:CD2	2.54	0.42
109:Qb:430:ASP:OD1	109:Qb:430:ASP:N	2.51	0.42
114:Qg:30:TRP:CZ2	114:Qg:196:GLU:HB2	2.55	0.42
121:S2:84:ARG:HG2	162:S7:201:SF4:S2	2.59	0.42
134:T7:89:PHE:CE1	153:T7:201:CDL:H562	2.55	0.42
146:V1:424:THR:HB	162:V1:500:SF4:S2	2.59	0.42
4:2g:119:SER:HB3	152:2g:202:PC1:O22	2.19	0.42
24:7c:136:ARG:HB3	36:g:204:TYR:HB3	2.02	0.42
24:7c:151:PRO:HD3	29:c1:619:PHE:CG	2.55	0.42
152:a:503:PC1:H222	31:c3:400:TYR:HA	2.01	0.42
27:b:403:PHE:O	27:b:409:LYS:HE3	2.19	0.42
30:c2:517:PHE:CE2	30:c2:519:PRO:HG3	2.54	0.42
31:c3:145:SER:OG	31:c3:146:PHE:N	2.52	0.42
33:e:201:LEU:HD22	33:e:206:TRP:HB3	2.02	0.42
34:f:217:SER:HB2	51:S:160:SER:HB3	2.02	0.42
37:h:269:TYR:OH	57:u:7:ARG:NH2	2.52	0.42
42:m:191:MET:O	62:y:1:MET:HG3	2.19	0.42
43:m1:317:MET:HE2	43:m1:317:MET:HA	2.02	0.42
46:n:34:ASN:O	46:n:37:VAL:HG22	2.20	0.42
48:p:123:LYS:HE3	48:p:123:LYS:HB3	1.90	0.42
52:sa:225:MET:HG3	52:sa:485:LEU:HD11	2.01	0.42
53:sb:224:SER:OG	53:sb:281:THR:HG21	2.20	0.42
59:vb:123:PRO:HG2	59:vb:208:MET:O	2.20	0.42
59:vb:175:LEU:HD21	59:vb:177:PHE:HE1	1.83	0.42
70:4l:23:PRO:HG3	105:n6:112:TYR:CD2	2.54	0.42
153:a1:101:CDL:HB32	100:n1:64:ARG:NH2	2.35	0.42
83:am:167:ILE:HG13	100:n1:17:LEU:HB3	2.00	0.42
83:am:172:LYS:HE2	141:te:71:LEU:HD11	2.01	0.42
152:an:304:PC1:H361	110:qC:247:PHE:CD2	2.54	0.42
90:b8:89:TYR:CZ	153:b8:302:CDL:HB31	2.55	0.42
94:c4:24:MET:HB3	96:g1:53:GLN:NE2	2.34	0.42
100:n1:190:GLN:HG2	100:n1:195:LEU:HG	2.02	0.42
100:n1:239:PHE:HA	100:n1:242:ALA:HB3	2.01	0.42
104:n5:478:SER:HA	104:n5:538:PHE:CZ	2.54	0.42
108:qA:412:ARG:NE	108:qA:415:ASP:OD2	2.38	0.42
110:qC:113:GLU:HG2	114:qG:178:LEU:HD11	2.01	0.42
110:qC:210:GLU:OE1	115:qH:95:ARG:NH2	2.52	0.42
114:qG:203:TYR:CZ	117:qj:5:THR:HA	2.54	0.42
114:qG:314:LEU:O	114:qG:319:GLN:NE2	2.47	0.42
116:qi:56:ARG:HA	116:qi:60:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
120:s1:446:ASN:ND2	129:t2:179:GLN:O	2.38	0.42
128:t1:254:GLN:HB2	128:t1:351:ALA:HB2	2.01	0.42
135:t8:49:VAL:HG13	158:t8:602:3PE:H2B2	2.01	0.42
146:v1:203:GLY:H	147:v2:111:MET:HG2	1.84	0.42
1:1T:57:LYS:HD3	41:L:216:ILE:HD13	2.01	0.42
19:6B:174:TYR:OH	30:C2:167:GLN:NE2	2.52	0.42
153:A:504:CDL:H401	31:C3:254:LEU:HB2	2.01	0.42
27:B:432:LEU:HB2	65:Y7:409:ILE:HD13	2.00	0.42
29:C1:126:HIS:CG	29:C1:333:PRO:HG2	2.55	0.42
29:C1:387:TRP:O	29:C1:438:TRP:HB2	2.19	0.42
29:C1:562:MET:HE3	153:C1:712:CDL:H612	2.00	0.42
30:C2:514:HIS:ND1	30:C2:560:MET:HE1	2.33	0.42
33:E:110:TYR:OH	33:E:147:PHE:O	2.27	0.42
40:K:29:TYR:N	40:K:46:TYR:OH	2.53	0.42
43:M1:310:PRO:HA	153:M1:404:CDL:H221	2.01	0.42
47:O:87:ASP:O	47:O:91:ARG:HG3	2.20	0.42
50:R:123:PRO:HB3	66:Z:77:ILE:HB	2.01	0.42
52:SA:86:HIS:HB3	161:SA:701:FAD:O1A	2.19	0.42
63:Y0:43:TYR:HE1	63:Y0:56:LEU:HG	1.84	0.42
65:Y7:246:LYS:HD2	65:Y7:246:LYS:HA	1.85	0.42
69:2B:54:LYS:NZ	95:FX:84:GLY:O	2.52	0.42
71:5B:32:PHE:HA	153:B4:201:CDL:H712	2.00	0.42
74:A3:32:SER:HB2	74:A3:45:ALA:HB2	2.00	0.42
76:A6:10:THR:HB	76:A6:26:GLY:HA3	2.01	0.42
76:A6:169:PRO:HB3	79:A9:40:ILE:O	2.19	0.42
77:A7:63:HIS:CD2	120:S1:151:ILE:HG13	2.55	0.42
86:B3:41:ARG:NH1	104:N5:618:LYS:O	2.46	0.42
95:FX:126:GLU:HG3	95:FX:143:LEU:HD12	2.01	0.42
97:G2:132:ILE:HD13	97:G2:138:LEU:HD11	2.01	0.42
101:N2:9:GLU:HA	101:N2:84:PHE:HB2	2.00	0.42
103:N4:461:PHE:HB3	104:N5:333:LEU:HD11	2.02	0.42
110:QC:55:SER:HB3	112:QE:117:ARG:NH2	2.33	0.42
112:QE:228:ARG:O	112:QE:230:ARG:N	2.49	0.42
152:Qb:602:PC1:H2I1	110:Qc:238:ILE:HD12	2.01	0.42
110:Qc:307:PHE:HD2	153:Qg:402:CDL:H172	1.84	0.42
111:Qd:200:PRO:HA	111:Qd:205:MET:HG2	2.01	0.42
114:Qg:214:LYS:NZ	114:Qg:218:GLU:OE2	2.39	0.42
153:Qg:402:CDL:H761	153:Qg:402:CDL:H331	2.02	0.42
120:S1:36:PHE:HB2	120:S1:102:LYS:HG2	2.01	0.42
121:S2:258:TYR:CZ	121:S2:379:VAL:HG13	2.54	0.42
125:S6:86:ARG:NH1	146:V1:467:SER:OG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
128:T1:157:THR:O	128:T1:176:ASP:HB2	2.19	0.42
129:T2:72:LEU:HD23	129:T2:98:VAL:HB	2.01	0.42
2:2e:81:TYR:HE2	2:2e:96:LEU:HG	1.85	0.42
19:6b:197:ALA:HA	30:c2:401:GLN:HG3	2.00	0.42
20:6c:22:ALA:HA	153:6c:201:CDL:HA21	2.01	0.42
23:7a:13:TYR:OH	59:vb:268:ASP:OD1	2.22	0.42
25:7l:860:MET:O	30:c2:92:ASN:HA	2.19	0.42
26:a:161:GLU:OE1	26:a:161:GLU:N	2.42	0.42
29:c1:297:LEU:HB3	65:y7:329:PHE:CZ	2.53	0.42
29:c1:581:LEU:HD13	29:c1:601:HIS:CE1	2.55	0.42
31:c3:162:LEU:HD11	48:p:90:PHE:HB3	2.02	0.42
31:c3:266:LEU:HB2	31:c3:271:ILE:HD13	2.01	0.42
34:f:337:ASN:HD21	36:g:88:THR:HG21	1.84	0.42
35:fs:160:HIS:HE1	35:fs:170:TRP:CD1	2.37	0.42
37:h:155:LYS:HB3	37:h:164:GLU:HG2	2.01	0.42
37:h:305:LEU:HD22	104:N5:89:PHE:HE2	1.84	0.42
45:m3:279:TYR:CG	153:m3:401:CDL:H112	2.55	0.42
50:r:123:PRO:HB3	66:z:77:ILE:HB	2.01	0.42
57:u:113:VAL:HG22	104:N5:79:ASP:CG	2.44	0.42
60:w:21:ARG:HH21	152:w:204:PC1:P	2.43	0.42
77:a7:99:VAL:HG22	77:a7:100:ASN:H	1.84	0.42
80:ab:76:GLN:HE21	80:ab:93:LEU:HD23	1.85	0.42
81:ac:50:TYR:CG	81:ac:54:PRO:HG3	2.55	0.42
82:al:2:GLY:HA2	100:n1:61:TYR:HB2	2.00	0.42
84:an:177:TYR:HA	84:an:181:ASN:HB2	2.02	0.42
88:b6:127:ILE:O	92:bl:101:GLN:NE2	2.53	0.42
95:fx:126:GLU:HG3	95:fx:143:LEU:HD12	2.01	0.42
97:g2:97:ARG:HH11	97:g2:125:ASN:HD21	1.68	0.42
97:g2:132:ILE:HD13	97:g2:138:LEU:HD11	2.00	0.42
97:g2:178:LEU:HB2	138:tb:53:ALA:HA	2.00	0.42
99:j1:48:ALA:O	99:j1:52:HIS:HB2	2.19	0.42
100:n1:150:PHE:O	100:n1:154:ILE:HG12	2.19	0.42
109:qB:111:GLN:HE21	109:qB:139:VAL:HB	1.84	0.42
109:qB:472:TRP:O	109:qB:474:LYS:NZ	2.49	0.42
108:qa:40:THR:OG1	109:qb:457:SER:O	2.36	0.42
108:qa:329:LEU:HD13	108:qa:363:LEU:HD21	2.00	0.42
109:qb:388:GLY:HA2	109:qb:391:MET:HE2	2.01	0.42
110:qc:76:TYR:O	110:qc:80:PHE:HD2	2.02	0.42
115:qh:85:GLU:O	115:qh:89:LYS:HB3	2.18	0.42
120:s1:62:PRO:HB2	120:s1:78:MET:HG3	2.01	0.42
120:s1:89:PRO:HB3	120:s1:113:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
122:s3:68:THR:HG21	122:s3:95:LEU:HD21	2.01	0.42
123:s4:119:TRP:HD1	123:s4:120:MET:HG2	1.85	0.42
127:s8:171:ASP:OD2	127:s8:174:LYS:NZ	2.37	0.42
132:t5:73:LEU:HD22	132:t5:78:LEU:HD12	2.02	0.42
144:th:112:ARG:HD2	144:th:115:ILE:HD11	2.02	0.42
148:x1:47:LEU:O	148:x1:50:PHE:HB2	2.20	0.42
3:2F:158:ILE:HD13	3:2F:240:PHE:HE2	1.84	0.42
19:6B:99:PRO:HB2	25:7L:921:LEU:HD11	2.01	0.42
23:7A:21:ASP:O	23:7A:24:PHE:HB3	2.20	0.42
24:7C:103:GLN:HE21	29:C1:631:ALA:HA	1.84	0.42
28:BP:261:TRP:HB3	28:BP:280:PRO:HA	2.01	0.42
28:BP:263:THR:O	28:BP:268:SER:OG	2.34	0.42
29:C1:346:LEU:HD23	29:C1:349:ILE:HD11	2.02	0.42
29:C1:353:LEU:HD22	29:C1:389:PHE:CZ	2.55	0.42
29:C1:563:HIS:CD2	29:C1:618:PHE:HB2	2.54	0.42
152:C1:710:PC1:H143	42:M:127:TYR:CD2	2.54	0.42
33:E:201:LEU:HD22	33:E:206:TRP:HB3	2.02	0.42
36:G:96:PHE:HZ	36:G:238:TRP:HD1	1.68	0.42
36:G:184:CYS:SG	36:G:191:LEU:HB2	2.59	0.42
38:I:153:PHE:HZ	38:I:196:TRP:HZ3	1.68	0.42
38:I:213:ILE:HD12	38:I:213:ILE:HA	1.94	0.42
45:M3:135:LEU:HD21	45:M3:191:ALA:HB2	2.01	0.42
48:P:71:GLU:OE1	48:P:73:ASN:N	2.44	0.42
52:SA:346:GLY:HA3	52:SA:351:HIS:CE1	2.54	0.42
53:SB:72:LEU:HB2	53:SB:155:ILE:HG12	2.01	0.42
153:T:204:CDL:H812	153:T:204:CDL:H732	2.00	0.42
60:W:98:GLU:HB2	60:W:101:GLU:HG2	2.00	0.42
71:5B:50:ILE:HD11	103:N4:260:TRP:CD1	2.55	0.42
158:A3:202:3PE:H241	102:N3:90:THR:HG23	2.01	0.42
76:A6:100:ARG:H	123:S4:66:GLN:CD	2.28	0.42
77:A7:140:ASN:ND2	77:A7:143:SER:HB3	2.35	0.42
82:AL:48:ASP:OD1	82:AL:48:ASP:N	2.52	0.42
84:AN:177:TYR:HA	84:AN:181:ASN:HB2	2.02	0.42
94:C4:16:ARG:NH2	94:C4:30:SER:HB2	2.34	0.42
97:G2:163:ARG:O	97:G2:181:SER:OG	2.28	0.42
100:N1:161:LEU:HA	102:N3:68:LEU:HD22	2.01	0.42
104:N5:86:LYS:HG2	104:N5:87:ILE:N	2.35	0.42
111:QD:316:TYR:HD1	114:QG:174:ARG:HD2	1.85	0.42
110:Qc:407:PRO:HB2	110:Qc:409:ILE:HG22	2.02	0.42
114:Qg:106:ASN:ND2	114:Qg:165:TYR:OH	2.39	0.42
120:S1:713:PHE:HB3	129:T2:52:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
124:S5:29:GLU:OE1	139:TC:80:ARG:NH2	2.41	0.42
125:S6:48:ASN:ND2	127:S8:159:PRO:O	2.31	0.42
149:C:166:ASN:HB2	150:U1:81:UNK:HA	2.02	0.42
2:2e:63:LEU:HD21	2:2e:69:LEU:HD13	2.01	0.42
7:2j:29:PHE:HA	7:2j:32:THR:HG22	2.01	0.42
10:2m:16:LYS:HE3	10:2m:16:LYS:HB2	1.81	0.42
153:2m:101:CDL:H742	153:2m:101:CDL:H781	2.01	0.42
20:6c:31:ILE:HG21	58:v:103:LEU:HD13	2.01	0.42
26:a:139:SER:HB2	33:e:16:LEU:HG	2.01	0.42
26:a:366:ARG:HB3	26:a:379:THR:HB	2.01	0.42
29:c1:353:LEU:HD22	29:c1:389:PHE:CZ	2.55	0.42
29:c1:490:PHE:HB3	29:c1:541:SER:HB3	2.02	0.42
152:c1:711:PC1:H231	42:m:68:TRP:HZ2	1.85	0.42
31:c3:258:TYR:OH	45:m3:2:ALA:N	2.45	0.42
38:i:231:ASP:HB2	38:i:236:LEU:HD12	2.00	0.42
42:m:3:LEU:HB2	33:E:189:ASP:OD2	2.20	0.42
43:m1:310:PRO:HA	153:m1:404:CDL:H221	2.01	0.42
48:p:71:GLU:OE1	48:p:73:ASN:N	2.44	0.42
56:t:13:ARG:NH2	62:y:103:GLN:O	2.53	0.42
61:x:33:THR:HG23	61:x:106:ALA:HB1	2.01	0.42
62:y:52:GLU:O	62:y:56:MET:HG3	2.19	0.42
64:y5:91:THR:O	64:y5:95:ILE:HG13	2.19	0.42
68:1b:4:PHE:HD1	72:a1:28:LEU:HD21	1.84	0.42
68:1b:21:ARG:HH11	100:n1:216:ARG:NH2	2.16	0.42
68:1b:26:ARG:O	121:s2:219:ARG:NH1	2.47	0.42
69:2b:100:LEU:HD11	101:n2:356:ILE:HG22	2.01	0.42
153:5b:201:CDL:HA62	153:b8:302:CDL:H511	2.02	0.42
72:a1:17:THR:N	72:a1:18:PRO:HD2	2.35	0.42
77:a7:239:GLN:HG3	77:a7:240:VAL:N	2.35	0.42
79:a9:62:LEU:O	79:a9:67:SER:HB3	2.20	0.42
96:g1:72:THR:OG1	96:g1:91:ASN:O	2.26	0.42
100:n1:77:LYS:NZ	126:s7:85:LEU:O	2.53	0.42
104:n5:79:ASP:CG	57:U:113:VAL:HG22	2.44	0.42
104:n5:272:THR:HG23	104:n5:424:PRO:HG3	2.02	0.42
111:qD:188:PHE:CZ	113:qF:47:ARG:HG2	2.55	0.42
109:qb:80:SER:HB2	109:qb:252:GLY:HA2	2.01	0.42
114:qg:30:TRP:CZ2	114:qg:196:GLU:HB2	2.54	0.42
121:s2:126:ARG:HA	121:s2:382:PRO:HG3	2.02	0.42
123:s4:90:THR:HG21	123:s4:97:PRO:HG3	2.01	0.42
124:s5:7:SER:OG	124:s5:9:ASN:OD1	2.26	0.42
125:s6:57:LYS:HD2	125:s6:69:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
142:tf:184:ARG:NH1	142:tf:218:ALA:O	2.53	0.42
3:2F:141:LYS:NZ	3:2F:142:ASP:OD1	2.53	0.42
152:2G:202:PC1:H112	54:SC:6:TYR:OH	2.20	0.42
6:2I:32:ASN:ND2	9:2L:36:PHE:H	2.18	0.42
153:2M:101:CDL:HB22	54:SC:29:ILE:HG13	2.02	0.42
152:7C:303:PC1:H352	44:M2:226:TRP:CZ3	2.54	0.42
26:A:456:TRP:HE1	59:VB:339:ASN:ND2	2.15	0.42
153:A:504:CDL:H351	31:C3:258:TYR:CD2	2.54	0.42
27:B:250:VAL:HG21	31:C3:130:HIS:ND1	2.35	0.42
28:BP:307:SER:HB3	28:BP:319:PHE:CE2	2.55	0.42
29:C1:429:VAL:O	29:C1:433:MET:HG3	2.20	0.42
30:C2:497:LEU:O	30:C2:566:ALA:HA	2.20	0.42
31:C3:506:PHE:O	31:C3:510:LYS:HG2	2.19	0.42
32:D:190:LYS:O	32:D:193:ARG:NH1	2.42	0.42
35:FS:118:VAL:O	36:G:93:ARG:NH1	2.41	0.42
38:I:97:PHE:CE1	153:I:302:CDL:H352	2.54	0.42
48:P:123:LYS:HE3	48:P:123:LYS:HB3	1.90	0.42
52:SA:86:HIS:NE2	161:SA:701:FAD:C9	2.77	0.42
60:W:16:TRP:CE2	152:W:204:PC1:H121	2.55	0.42
72:A1:48:PHE:HB2	72:A1:51:ARG:HG2	2.02	0.42
73:A2:14:GLU:HG3	73:A2:48:PRO:HB2	2.01	0.42
85:B2:77:MET:HG3	152:T4:301:PC1:H241	2.02	0.42
96:G1:175:LEU:HB2	96:G1:187:LEU:HD21	2.02	0.42
100:N1:9:PHE:CD2	100:N1:12:ILE:HD11	2.55	0.42
100:N1:283:ILE:HG21	134:T7:114:TYR:HB2	2.01	0.42
101:N2:221:THR:H	124:S5:2:SER:HB3	1.84	0.42
101:N2:300:PHE:CZ	101:N2:315:LEU:HD21	2.55	0.42
103:N4:418:PRO:HG3	104:N5:309:PHE:HD2	1.84	0.42
104:N5:283:GLU:CD	104:N5:283:GLU:H	2.27	0.42
106:P1:224:LYS:HA	106:P1:230:GLU:O	2.19	0.42
107:P2:120:TYR:HB2	107:P2:140:THR:HB	2.02	0.42
108:QA:305:LEU:HD12	108:QA:375:ILE:HG22	2.02	0.42
110:QC:58:PRO:HD2	110:Qc:58:PRO:HD2	2.02	0.42
114:QG:70:TRP:CZ3	153:QH:201:CDL:H111	2.55	0.42
114:QG:118:ARG:O	114:QG:121:ARG:HG2	2.20	0.42
115:QH:91:VAL:O	115:QH:95:ARG:HB2	2.19	0.42
164:Qc:507:U10:H152	164:Qc:507:U10:H101	2.00	0.42
111:Qd:293:ARG:NH1	114:Qg:304:ALA:O	2.52	0.42
120:S1:543:LEU:HD11	120:S1:613:ASP:OD2	2.20	0.42
121:S2:310:ILE:HG12	142:TF:164:THR:HG22	2.01	0.42
128:T1:92:HIS:NE2	153:T1:601:CDL:HA32	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
129:T2:198:LEU:HA	129:T2:212:LEU:HB3	2.02	0.42
146:V1:87:GLY:O	146:V1:92:GLY:HA2	2.20	0.42
147:V2:44:PHE:HA	147:V2:78:GLN:HE22	1.83	0.42
148:X1:20:ARG:NH1	148:X1:33:PRO:HB3	2.35	0.42
2:2e:81:TYR:CZ	2:2e:97:ILE:HG22	2.54	0.42
7:2j:40:ASN:O	7:2j:44:GLN:HG2	2.20	0.42
153:6c:201:CDL:H341	29:c1:471:VAL:HG22	2.02	0.42
153:7c:301:CDL:HA31	29:c1:36:LEU:HD11	2.01	0.42
28:bp:254:GLN:C	28:bp:256:GLY:H	2.27	0.42
29:c1:505:GLY:O	154:c1:708:HEA:HMB3	2.19	0.42
29:c1:596:VAL:HG11	30:c2:482:VAL:HB	2.01	0.42
30:c2:209:TYR:HD1	30:c2:330:ILE:HG22	1.84	0.42
30:c2:590:ARG:NH2	30:c2:592:ARG:HH11	2.18	0.42
31:c3:345:ILE:HD11	61:x:120:LEU:HD23	2.02	0.42
34:f:168:LYS:HB3	34:f:171:TYR:HD2	1.84	0.42
34:f:171:TYR:OH	51:S:161:GLU:OE1	2.31	0.42
35:fs:27:ASP:OD2	36:g:83:TYR:OH	2.38	0.42
38:i:27:LEU:O	38:i:32:PHE:HB2	2.20	0.42
42:m:79:HIS:CE1	42:m:81:PHE:HB2	2.55	0.42
44:m2:1:MET:O	44:m2:4:SER:OG	2.31	0.42
53:sb:106:LEU:HD12	53:sb:110:ASN:HD21	1.84	0.42
70:4l:15:ILE:HD13	70:4l:35:LEU:HG	2.01	0.42
83:am:68:ILE:HD13	100:n1:198:ILE:HD11	2.01	0.42
153:an:302:CDL:H791	153:an:302:CDL:H831	2.01	0.42
92:bl:111:ARG:HB2	92:bl:117:ALA:HB2	2.01	0.42
96:g1:175:LEU:HB2	96:g1:187:LEU:HD21	2.01	0.42
96:g1:239:THR:OG1	96:g1:240:ILE:N	2.52	0.42
97:g2:107:LYS:NZ	98:g3:110:LEU:O	2.48	0.42
100:n1:138:MET:HE1	105:n6:98:VAL:HG22	2.02	0.42
103:n4:461:PHE:HB3	104:n5:333:LEU:HD11	2.02	0.42
152:n6:301:PC1:H142	139:tc:16:TYR:CZ	2.54	0.42
110:qC:327:ARG:NH1	110:qC:402:SER:OG	2.52	0.42
112:qE:121:TRP:NE1	112:qE:263:PRO:O	2.52	0.42
115:qH:91:VAL:O	115:qH:95:ARG:HB2	2.19	0.42
152:qI:202:PC1:H112	152:qI:202:PC1:H153	1.83	0.42
153:qI:203:CDL:H162	153:qI:203:CDL:H542	2.00	0.42
164:qc:501:U10:H71	164:qc:501:U10:H1M1	1.93	0.42
114:qg:9:TRP:CE2	114:qg:13:VAL:HG21	2.55	0.42
114:qg:160:PHE:CE1	114:qg:164:GLU:HG3	2.54	0.42
116:qi:97:SER:O	116:qi:100:THR:OG1	2.33	0.42
120:s1:471:PRO:O	120:s1:508:TRP:NE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
123:s4:168:TYR:HE2	146:v1:225:ARG:HB3	1.85	0.42
126:s7:8:THR:HB	126:s7:9:PRO:HD3	2.01	0.42
128:t1:200:GLY:HA3	128:t1:447:MET:O	2.20	0.42
136:t9:55:ASP:OD2	136:t9:57:SER:OG	2.27	0.42
2:2E:111:ARG:NH2	2:2E:203:ASN:O	2.49	0.42
3:2F:178:ASN:HB3	3:2F:186:LEU:HD21	2.01	0.42
15:4A:64:ARG:HH21	33:E:206:TRP:CD1	2.37	0.42
18:6A:120:LEU:HD23	18:6A:120:LEU:HA	1.80	0.42
20:6C:22:ALA:HA	153:6C:202:CDL:HA21	2.01	0.42
23:7A:72:TYR:CE1	153:C1:701:CDL:HB22	2.54	0.42
27:B:298:TYR:HB2	27:B:349:ASN:HD21	1.84	0.42
28:BP:137:GLY:N	28:BP:152:GLN:O	2.48	0.42
28:BP:384:ALA:HA	31:C3:215:GLN:NE2	2.35	0.42
29:C1:127:VAL:HG12	29:C1:321:ALA:HA	2.01	0.42
31:C3:495:MET:HE2	31:C3:495:MET:HB3	1.98	0.42
33:E:60:ALA:HA	33:E:152:GLU:HG3	2.00	0.42
34:F:337:ASN:ND2	36:G:88:THR:HG21	2.35	0.42
38:I:23:ARG:O	38:I:26:THR:N	2.51	0.42
42:M:191:MET:O	62:Y:1:MET:HG3	2.19	0.42
43:M1:317:MET:HE2	43:M1:317:MET:HA	2.02	0.42
44:M2:258:THR:O	44:M2:268:LYS:NZ	2.39	0.42
45:M3:125:PHE:O	45:M3:128:GLY:N	2.36	0.42
49:Q:19:SER:HB2	49:Q:102:TYR:O	2.20	0.42
53:SB:242:GLN:HE22	53:SB:286:LEU:HB3	1.85	0.42
59:VB:350:ARG:NH1	59:VB:387:TPO:O2P	2.39	0.42
63:Y0:33:PHE:O	64:Y5:171:LYS:NZ	2.34	0.42
68:1B:4:PHE:HD1	72:A1:28:LEU:HD21	1.85	0.42
69:2B:43:ASN:N	69:2B:130:ILE:O	2.38	0.42
70:4L:22:LYS:O	70:4L:24:LYS:NZ	2.46	0.42
75:A5:143:GLU:HB2	122:S3:51:ARG:HE	1.85	0.42
77:A7:179:TYR:HE2	77:A7:184:MET:HE3	1.85	0.42
77:A7:239:GLN:HG3	77:A7:240:VAL:N	2.35	0.42
78:A8:228:VAL:HG22	100:N1:112:PRO:HG2	2.00	0.42
83:AM:156:LYS:HE3	83:AM:161:VAL:HG22	2.00	0.42
152:AN:304:PC1:H361	110:QC:247:PHE:CD2	2.54	0.42
97:G2:20:ARG:HE	98:G3:37:GLN:NE2	2.17	0.42
98:G3:34:LEU:O	98:G3:38:GLN:HG2	2.20	0.42
98:G3:279:GLU:OE1	122:S3:44:SER:OG	2.37	0.42
100:N1:190:GLN:HG2	100:N1:195:LEU:HG	2.02	0.42
103:N4:62:ILE:HD13	144:TH:63:SER:HA	2.00	0.42
104:N5:145:ASN:HD22	104:N5:148:VAL:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
104:N5:731:SER:HA	104:N5:734:LYS:HG2	2.01	0.42
106:P1:124:LEU:HB3	106:P1:125:PRO:HD3	2.02	0.42
107:P2:66:LEU:HG	107:P2:137:PHE:HZ	1.85	0.42
109:QB:40:LYS:HB3	109:QB:43:LEU:HD12	2.01	0.42
110:QC:386:TYR:CZ	164:QC:506:U10:H212	2.55	0.42
111:QD:71:ARG:NH2	111:QD:104:GLU:OE1	2.39	0.42
111:QD:114:ILE:HB	111:QD:134:ARG:HG2	2.02	0.42
109:Qb:388:GLY:HA2	109:Qb:391:MET:HE2	2.01	0.42
164:Qc:507:U10:H171	164:Qc:507:U10:H13	1.86	0.42
111:Qd:215:ASP:OD1	111:Qd:215:ASP:N	2.52	0.42
126:S7:8:THR:HB	126:S7:9:PRO:HD3	2.01	0.42
153:T5:301:CDL:H382	153:T5:301:CDL:H181	2.01	0.42
136:T9:27:PHE:O	136:T9:31:LYS:HG2	2.19	0.42
2:2e:242:LEU:HD12	2:2e:243:GLU:HG3	2.02	0.42
8:2k:30:ARG:NH2	55:sd:20:LYS:HZ1	2.17	0.42
19:6b:86:TRP:HZ2	30:c2:470:ILE:HG13	1.85	0.42
23:7a:72:TYR:CE1	153:c1:701:CDL:HB22	2.55	0.42
23:7a:106:ASP:OD2	23:7a:110:LYS:HD2	2.20	0.42
26:a:386:THR:OG1	153:c3:604:CDL:OB2	2.37	0.42
28:bp:363:GLY:HA2	28:bp:453:SER:HB3	2.01	0.42
28:bp:412:THR:O	28:bp:415:GLY:N	2.51	0.42
152:c1:707:PC1:H143	42:m:127:TYR:CD2	2.54	0.42
154:c1:708:HEA:H242	30:c2:41:PHE:CE2	2.54	0.42
30:c2:497:LEU:O	30:c2:566:ALA:HA	2.19	0.42
36:g:288:TYR:O	36:g:290:LYS:HG3	2.20	0.42
42:m:39:GLN:HE21	42:m:43:TRP:NE1	2.17	0.42
42:m:195:THR:HG22	62:y:7:GLN:HA	2.01	0.42
44:m2:32:TYR:N	44:m2:33:PRO:HD2	2.34	0.42
47:o:119:LEU:HD23	47:o:119:LEU:HA	1.93	0.42
49:q:46:LEU:HD22	49:q:114:ILE:HD12	2.01	0.42
52:sa:52:ILE:HD11	52:sa:77:ILE:HD12	2.01	0.42
52:sa:86:HIS:HB3	161:sa:701:FAD:O1A	2.19	0.42
57:u:13:GLU:HB3	57:u:117:LYS:HG2	2.02	0.42
58:v:100:PHE:HA	58:v:104:THR:HB	2.01	0.42
59:vb:550:PRO:HG3	59:vb:605:LEU:HD11	2.00	0.42
62:y:58:LYS:HE2	62:y:58:LYS:HB3	1.86	0.42
71:5b:4:ASN:O	106:p1:207:ASN:ND2	2.45	0.42
71:5b:50:ILE:HD11	103:n4:260:TRP:CD1	2.55	0.42
73:a2:12:LEU:HD13	73:a2:15:LEU:HG	2.02	0.42
79:a9:220:TYR:OH	145:tx:163:GLU:HG2	2.20	0.42
82:al:23:GLU:HB3	82:al:27:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:b8:73:LEU:HD13	90:b8:79:GLY:HA2	2.02	0.42
93:bm:92:HIS:CE1	93:bm:111:TYR:HB3	2.55	0.42
93:bm:105:TYR:CE1	104:n5:273:PHE:HB3	2.54	0.42
97:g2:7:MET:HA	135:t8:50:ILE:HD11	2.02	0.42
97:g2:127:GLY:HA3	97:g2:145:ASP:H	1.84	0.42
100:n1:22:LEU:O	100:n1:26:ILE:HG12	2.20	0.42
100:n1:59:VAL:O	100:n1:63:GLY:HA2	2.20	0.42
109:qB:298:GLU:HG2	115:qH:56:ARG:HD2	2.01	0.42
110:qC:28:HIS:CD2	110:qC:33:LEU:HD21	2.54	0.42
110:qC:31:ASN:HD21	153:qC:504:CDL:H111	1.83	0.42
110:qC:58:PRO:HD2	110:qc:58:PRO:HD2	2.01	0.42
110:qC:65:MET:HG2	111:qD:89:TYR:CD1	2.55	0.42
114:qG:92:GLU:HA	114:qG:96:CYS:HB3	2.02	0.42
109:qb:473:ASP:OD2	116:qi:60:GLN:NE2	2.36	0.42
110:qc:98:HIS:O	110:qc:102:LYS:HG2	2.18	0.42
111:qd:90:LYS:HE2	111:qd:242:MET:O	2.19	0.42
111:qd:200:PRO:HA	111:qd:205:MET:HG2	2.01	0.42
111:qd:293:ARG:NH1	114:qg:304:ALA:O	2.53	0.42
111:qd:294:ASP:OD1	111:qd:294:ASP:N	2.53	0.42
114:qg:135:PRO:HB2	114:qg:137:TRP:CD1	2.54	0.42
120:s1:129:CYS:SG	120:s1:141:GLN:NE2	2.93	0.42
120:s1:355:LEU:HD22	120:s1:543:LEU:HD22	2.02	0.42
134:t7:43:PHE:HE1	134:t7:120:LEU:HB3	1.85	0.42
146:v1:421:GLU:HG2	146:v1:422:MET:HG3	2.02	0.42
4:2G:119:SER:HB3	152:2G:202:PC1:O22	2.20	0.42
6:2I:3:SER:O	6:2I:7:MET:HG2	2.20	0.42
6:2I:5:PHE:O	6:2I:9:GLU:HG3	2.18	0.42
10:2M:73:LYS:HE2	10:2M:73:LYS:HB3	1.89	0.42
14:3T:2:SER:O	22:6T:1:MET:N	2.40	0.42
16:4T:4:ASN:ND2	30:C2:250:PHE:HB3	2.35	0.42
23:7A:77:LEU:HD23	65:Y7:350:LEU:HD11	2.01	0.42
153:7A:201:CDL:H162	153:7A:201:CDL:H541	2.02	0.42
29:C1:218:LEU:HB2	29:C1:224:PHE:HZ	1.83	0.42
29:C1:315:ILE:HD11	31:C3:315:ILE:HG13	2.02	0.42
29:C1:398:ILE:HB	154:C1:703:HEA:CBC	2.48	0.42
29:C1:639:LEU:HG	59:VB:189:MET:HE1	2.01	0.42
30:C2:209:TYR:HD1	30:C2:330:ILE:HG22	1.84	0.42
31:C3:31:ASN:ND2	31:C3:69:LYS:O	2.52	0.42
31:C3:171:TYR:OH	45:M3:121:ASN:ND2	2.52	0.42
33:E:34:THR:HG23	33:E:51:GLY:O	2.19	0.42
38:I:102:ASP:O	38:I:106:THR:OG1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:K:185:ASP:HA	48:P:171:ASN:HB3	2.01	0.42
44:M2:205:LEU:HD23	44:M2:223:ALA:HA	2.02	0.42
45:M3:151:SER:O	45:M3:299:TRP:NE1	2.53	0.42
52:SA:284:HIS:O	52:SA:392:PRO:HA	2.19	0.42
52:SA:410:ILE:HG12	52:SA:420:ILE:HG12	2.02	0.42
53:SB:192:LYS:HE3	53:SB:193:PRO:HD2	2.00	0.42
59:VB:367:TYR:CE1	59:VB:562:LYS:HE2	2.55	0.42
75:A5:184:ARG:HH21	120:S1:392:THR:HB	1.85	0.42
76:A6:133:LEU:HD21	168:AB:201:ZMP:H25A	2.01	0.42
77:A7:99:VAL:HG22	77:A7:100:ASN:H	1.84	0.42
79:A9:288:HIS:HB3	99:J1:233:TYR:HA	2.00	0.42
80:AB:62:GLU:HG3	145:TX:113:THR:HB	2.02	0.42
80:AB:76:GLN:HE21	80:AB:93:LEU:HD23	1.85	0.42
94:C4:4:MET:HB2	135:T8:70:VAL:HG21	2.02	0.42
100:N1:109:MET:HE2	100:N1:122:ASN:HD21	1.84	0.42
100:N1:187:VAL:HG11	100:N1:267:TRP:CE2	2.54	0.42
104:N5:256:SER:HB3	104:N5:512:TYR:HE1	1.85	0.42
104:N5:271:TYR:CD2	104:N5:523:LEU:HD22	2.55	0.42
107:P2:33:ASP:CG	107:P2:89:HIS:HB3	2.45	0.42
107:P2:118:VAL:HA	107:P2:119:PRO:HD3	1.84	0.42
108:QA:307:LEU:O	108:QA:362:GLY:HA3	2.20	0.42
109:Qb:418:TYR:HB3	109:Qb:455:ILE:HD12	2.02	0.42
112:Qe:60:PHE:CZ	115:Qh:57:GLY:HA2	2.55	0.42
114:Qg:9:TRP:CE2	114:Qg:13:VAL:HG21	2.55	0.42
115:Qh:86:ARG:O	115:Qh:91:VAL:HG23	2.19	0.42
120:S1:338:GLN:O	120:S1:538:LYS:N	2.49	0.42
120:S1:543:LEU:HD12	120:S1:563:PHE:HB2	2.01	0.42
123:S4:90:THR:HG21	123:S4:97:PRO:HG3	2.01	0.42
123:S4:119:TRP:HD1	123:S4:120:MET:HG2	1.84	0.42
124:S5:74:TYR:HB2	124:S5:81:PHE:CE2	2.54	0.42
128:T1:200:GLY:HA3	128:T1:447:MET:O	2.20	0.42
130:T3:143:THR:HA	130:T3:147:LEU:HB2	2.02	0.42
130:T3:261:ASN:HB3	130:T3:267:GLU:HB3	2.01	0.42
146:V1:142:GLY:HA2	146:V1:253:PRO:HD3	2.01	0.42
146:V1:226:VAL:O	146:V1:229:PRO:HD2	2.19	0.42
148:X1:51:ASN:OD1	148:X1:110:ARG:NH2	2.53	0.42
149:c:166:ASN:HB2	150:u1:81:UNK:HA	2.01	0.42
3:2f:218:LEU:HB3	3:2f:219:PRO:HD3	2.02	0.42
16:4t:4:ASN:ND2	30:c2:250:PHE:HB3	2.35	0.42
18:6a:54:ALA:HB1	65:y7:281:SER:HB3	2.01	0.42
20:6c:54:PHE:CD2	42:m:170:ASP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:7l:905:PRO:HG2	25:7l:906:GLN:NE2	2.34	0.42
29:c1:28:LYS:HE2	29:c1:28:LYS:HB3	1.92	0.42
29:c1:325:LEU:HD23	29:c1:332:MET:HG2	2.02	0.42
154:c1:702:HEA:H211	154:c1:702:HEA:H271	1.40	0.42
30:c2:242:ASP:OD1	30:c2:242:ASP:N	2.50	0.42
30:c2:518:ILE:HG21	30:c2:521:LEU:HD12	2.01	0.42
31:c3:31:ASN:ND2	31:c3:69:LYS:O	2.53	0.42
31:c3:524:ARG:HG2	153:t:202:CDL:H571	2.02	0.42
33:e:34:THR:HG23	33:e:51:GLY:O	2.19	0.42
34:f:185:TRP:CZ2	58:v:112:ILE:HG23	2.55	0.42
35:fs:114:CYS:N	157:fs:201:FES:S2	2.93	0.42
35:fs:187:TYR:OH	153:I:303:CDL:OB4	2.34	0.42
39:j:182:TRP:HA	152:n:303:PC1:H132	2.02	0.42
52:sa:211:LEU:HD23	52:sa:222:VAL:HG12	2.01	0.42
52:sa:315:MET:HE1	52:sa:334:ALA:HB3	2.02	0.42
52:sa:398:MET:HE3	52:sa:440:ARG:HB2	2.02	0.42
53:sb:101:PHE:CE2	53:sb:134:CYS:HB3	2.55	0.42
53:sb:105:ILE:HD11	53:sb:156:ILE:HG21	2.01	0.42
55:sd:30:LEU:HD23	55:sd:30:LEU:HA	1.92	0.42
60:w:77:PRO:HB2	60:w:85:LYS:HB2	2.01	0.42
65:y7:115:ILE:HD12	65:y7:162:LEU:HD12	2.02	0.42
66:z:87:ASP:OD1	66:z:87:ASP:N	2.53	0.42
70:4l:81:TYR:CD2	70:4l:86:GLU:HB3	2.55	0.42
75:a5:123:GLU:HG2	75:a5:131:ILE:HB	2.01	0.42
75:a5:153:PRO:HA	122:s3:41:TRP:CZ3	2.55	0.42
76:a6:99:TYR:CD1	123:s4:66:GLN:HG3	2.54	0.42
77:a7:140:ASN:ND2	77:a7:143:SER:HB3	2.35	0.42
89:b7:87:HIS:H	89:b7:87:HIS:CD2	2.38	0.42
90:b8:28:TRP:HH2	93:bm:51:VAL:HG12	1.85	0.42
153:bm:301:CDL:H521	103:n4:499:TYR:CD1	2.55	0.42
97:g2:34:GLU:HA	98:g3:15:MET:HG3	2.00	0.42
97:g2:78:GLY:HA3	97:g2:100:HIS:HD2	1.85	0.42
101:n2:88:HIS:O	101:n2:149:THR:HG21	2.20	0.42
103:n4:321:SER:HB2	103:n4:447:VAL:HG12	2.01	0.42
103:n4:418:PRO:HA	103:n4:423:PHE:CG	2.55	0.42
104:n5:415:LEU:HB3	104:n5:416:PRO:HD3	2.02	0.42
104:n5:513:VAL:HG22	104:n5:660:ILE:HD13	2.02	0.42
108:qA:386:ILE:HG22	108:qA:451:VAL:HG11	2.02	0.42
109:qB:144:GLU:HG3	109:qB:214:PHE:HE1	1.85	0.42
111:qD:188:PHE:HD2	113:qF:46:LEU:HD23	1.84	0.42
108:qa:330:ASN:ND2	108:qa:350:ALA:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:qc:251:GLU:HB2	111:qd:250:ARG:NH2	2.34	0.42
110:qc:307:PHE:HD2	153:qg:402:CDL:H172	1.84	0.42
110:qc:336:ILE:HD11	110:qc:341:ILE:HG22	2.02	0.42
111:qd:215:ASP:OD1	111:qd:215:ASP:N	2.52	0.42
111:qd:273:PHE:CZ	153:qi:202:CDL:H732	2.55	0.42
114:qg:72:LEU:HD21	114:qg:251:PHE:HD2	1.85	0.42
115:qh:86:ARG:O	115:qh:91:VAL:HG23	2.19	0.42
120:s1:551:PRO:HA	120:s1:573:TYR:HE2	1.84	0.42
124:s5:29:GLU:OE1	139:tc:80:ARG:NH2	2.42	0.42
126:s7:58:ARG:HA	126:s7:85:LEU:HG	2.02	0.42
128:t1:84:ARG:HH12	128:t1:133:GLU:CD	2.28	0.42
132:t5:138:ILE:HD12	153:t5:301:CDL:H673	2.01	0.42
138:tb:97:SER:HA	144:th:123:LYS:HE3	2.02	0.42
139:tc:18:PRO:HD3	152:tc:102:PC1:H141	2.02	0.42
142:tf:166:ASN:HA	142:tf:202:ARG:HH12	1.85	0.42
146:v1:226:VAL:O	146:v1:229:PRO:HD2	2.19	0.42
2:2E:155:PHE:HB3	2:2E:162:VAL:HG21	2.01	0.42
2:2E:322:LEU:HD13	153:2G:203:CDL:H322	2.01	0.42
7:2J:102:ARG:HD2	9:2L:16:ARG:NH2	2.35	0.42
14:3T:10:GLU:HG2	30:C2:247:LYS:HZ2	1.84	0.42
18:6A:56:ASN:ND2	64:Y5:174:ARG:HH21	2.18	0.42
20:6C:54:PHE:CD2	42:M:170:ASP:HB2	2.55	0.42
23:7A:106:ASP:OD2	23:7A:110:LYS:HD2	2.20	0.42
24:7C:210:ASP:HB2	30:C2:473:ASN:ND2	2.35	0.42
26:A:60:HIS:NE2	26:A:86:ASP:OD1	2.52	0.42
28:BP:174:GLY:HA3	28:BP:177:TYR:CE2	2.55	0.42
32:D:178:TRP:HA	32:D:181:LYS:HD3	2.02	0.42
34:F:315:GLU:HG2	35:FS:11:TYR:HD2	1.84	0.42
37:H:141:TYR:C	57:U:11:GLU:HG3	2.45	0.42
43:M1:50:GLN:OE1	43:M1:311:GLY:N	2.47	0.42
43:M1:263:VAL:HG21	43:M1:280:TYR:HA	2.01	0.42
47:O:103:PRO:O	47:O:105:GLN:NE2	2.52	0.42
47:O:157:CYS:HB3	47:O:170:CYS:SG	2.60	0.42
52:SA:54:VAL:HG13	52:SA:208:VAL:HG21	2.00	0.42
53:SB:86:LYS:O	53:SB:88:VAL:HG23	2.19	0.42
56:T:139:ASP:HA	153:T:202:CDL:H572	2.02	0.42
59:VB:168:ASP:OD1	60:W:11:GLU:HB2	2.19	0.42
65:Y7:164:ASN:HB3	149:C:133:ALA:HB3	2.02	0.42
70:4L:81:TYR:CD2	70:4L:86:GLU:HB3	2.55	0.42
71:5B:10:LYS:NZ	90:B8:82:GLU:OE2	2.36	0.42
75:A5:178:LYS:HD3	123:S4:103:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:AC:53:ASN:HB3	81:AC:56:ASP:HB3	2.01	0.42
83:AM:59:LEU:HD12	137:TA:85:PHE:CE2	2.55	0.42
92:BL:54:PHE:HD2	103:N4:85:ILE:HG21	1.84	0.42
95:FX:93:LYS:HE2	95:FX:148:LEU:HD23	2.02	0.42
101:N2:113:THR:HG23	101:N2:279:LEU:HD21	2.02	0.42
105:N6:60:LEU:HD21	152:N6:301:PC1:H32	2.02	0.42
106:P1:247:HIS:CG	106:P1:248:PRO:HD2	2.54	0.42
110:QC:65:MET:HG2	111:QD:89:TYR:CD1	2.55	0.42
111:QD:150:ALA:HB1	111:QD:159:PRO:HD2	2.01	0.42
111:QD:289:MET:HG3	112:QE:68:VAL:HG11	2.02	0.42
110:Qc:242:MET:HE3	111:Qd:261:PHE:HD1	1.85	0.42
110:Qc:397:PHE:HA	110:Qc:401:ASN:HD22	1.85	0.42
111:Qd:284:SER:OG	112:Qe:77:ASN:ND2	2.42	0.42
120:S1:120:PHE:O	146:V1:388:GLU:HG2	2.20	0.42
120:S1:434:ASN:HB2	120:S1:443:HIS:CE1	2.55	0.42
120:S1:517:GLU:O	120:S1:521:ILE:HG13	2.20	0.42
121:S2:182:ASN:HD21	127:S8:235:PRO:HB3	1.84	0.42
145:TX:92:PHE:O	145:TX:111:ARG:NH2	2.50	0.42
2:2e:155:PHE:HB3	2:2e:162:VAL:HG21	2.01	0.41
3:2f:82:ASN:HB2	131:t4:208:LYS:HB2	2.01	0.41
13:2t:28:VAL:HG23	13:2t:29:LEU:HD12	2.02	0.41
153:7a:201:CDL:H162	153:7a:201:CDL:H541	2.02	0.41
24:7c:210:ASP:HB2	30:c2:473:ASN:ND2	2.35	0.41
153:a:505:CDL:H341	153:a:505:CDL:H381	2.02	0.41
27:b:113:LEU:O	27:b:117:LEU:N	2.50	0.41
28:bp:172:VAL:HG21	28:bp:242:ILE:HG13	2.01	0.41
28:bp:307:SER:HB3	28:bp:319:PHE:CE2	2.55	0.41
30:c2:197:PRO:HB2	32:d:335:PHE:CE1	2.55	0.41
30:c2:335:THR:OG1	32:d:217:GLU:OE1	2.26	0.41
30:c2:365:TYR:CZ	30:c2:390:ARG:HB2	2.54	0.41
31:c3:91:PHE:CD2	45:m3:205:SER:HB2	2.54	0.41
31:c3:353:PHE:O	31:c3:503:TRP:NE1	2.42	0.41
31:c3:356:ARG:NH1	152:c3:601:PC1:O11	2.52	0.41
33:e:34:THR:HG22	33:e:50:ILE:HG23	2.02	0.41
33:e:137:PHE:CZ	33:e:197:GLY:HA3	2.54	0.41
33:e:383:LYS:O	33:e:384:HIS:ND1	2.52	0.41
34:f:134:THR:HG22	34:f:136:ARG:H	1.84	0.41
35:fs:118:VAL:HG13	36:g:89:MET:SD	2.60	0.41
36:g:96:PHE:HB2	36:g:237:TRP:CZ2	2.54	0.41
41:l:37:ARG:O	41:l:39:LEU:N	2.52	0.41
45:m3:60:GLN:HB3	45:m3:64:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:n:29:PHE:HA	46:n:32:PHE:HB2	2.02	0.41
50:r:4:GLU:O	50:r:8:TYR:HB2	2.20	0.41
52:sa:346:GLY:HA3	52:sa:351:HIS:CE1	2.55	0.41
52:sa:532:TYR:OH	52:sa:605:VAL:O	2.26	0.41
55:sd:6:ILE:HG21	55:sd:24:ILE:HG21	2.02	0.41
59:vb:398:ILE:HG13	59:vb:552:TYR:HA	2.02	0.41
60:w:16:TRP:CE2	152:w:204:PC1:H121	2.55	0.41
65:y7:201:GLU:HB2	149:c:178:LYS:HG3	2.02	0.41
69:2b:53:PHE:HB3	69:2b:122:VAL:HG22	2.01	0.41
70:4l:29:ILE:O	70:4l:33:SER:OG	2.33	0.41
72:a1:48:PHE:HB2	72:a1:51:ARG:HG2	2.02	0.41
153:a9:403:CDL:H201	152:n3:201:PC1:H362	2.01	0.41
80:ab:86:GLN:HG2	80:ab:90:LYS:HB2	2.01	0.41
83:am:59:LEU:HD12	137:ta:85:PHE:CE2	2.55	0.41
84:an:90:MET:HB3	84:an:104:ILE:HD11	2.01	0.41
88:b6:109:PRO:HG3	104:n5:227:TYR:CE1	2.55	0.41
89:b7:102:ASP:HB3	90:b8:184:PHE:HE1	1.84	0.41
93:bm:113:ASP:OD1	93:bm:113:ASP:N	2.53	0.41
100:n1:109:MET:HE2	100:n1:122:ASN:HD21	1.84	0.41
104:n5:189:ILE:HG21	153:t5:301:CDL:H512	2.02	0.41
104:n5:719:TRP:HZ2	152:n5:803:PC1:H221	1.85	0.41
110:qC:222:TRP:O	110:qC:223:PHE:C	2.62	0.41
110:qC:386:TYR:CZ	164:qC:506:U10:H212	2.55	0.41
108:qa:214:LEU:HD11	108:qa:224:LEU:HD21	2.02	0.41
110:qc:83:LEU:O	110:qc:87:GLY:N	2.44	0.41
110:qc:407:PRO:HB2	110:qc:409:ILE:HG22	2.02	0.41
112:qe:94:THR:HG21	153:qi:202:CDL:H351	2.01	0.41
120:s1:434:ASN:HB2	120:s1:443:HIS:CE1	2.55	0.41
120:s1:517:GLU:O	120:s1:521:ILE:HG13	2.20	0.41
121:s2:258:TYR:CZ	121:s2:379:VAL:HG13	2.54	0.41
128:t1:83:ILE:HB	128:t1:86:HIS:HD2	1.84	0.41
128:t1:157:THR:O	128:t1:176:ASP:HB2	2.20	0.41
128:t1:449:PRO:HG2	128:t1:476:THR:HA	2.03	0.41
132:t5:144:ASP:CG	138:tb:104:ARG:HH12	2.27	0.41
158:t8:601:3PE:H3D2	158:t8:602:3PE:H2C2	2.02	0.41
145:tx:24:ARG:HD2	145:tx:24:ARG:HA	1.81	0.41
2:2E:242:LEU:HD12	2:2E:243:GLU:HG3	2.02	0.41
3:2F:82:ASN:HB2	131:T4:208:LYS:HB2	2.01	0.41
3:2F:94:PHE:HZ	3:2F:248:ARG:HG2	1.85	0.41
3:2F:133:TRP:O	3:2F:137:ARG:NH2	2.51	0.41
8:2K:30:ARG:HH22	153:2K:101:CDL:PA1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2K:34:ARG:HH22	153:2K:101:CDL:C11	2.32	0.41
153:2M:101:CDL:H562	153:2M:101:CDL:H531	1.87	0.41
15:4A:72:PHE:CE2	15:4A:114:GLU:HG2	2.55	0.41
18:6A:54:ALA:HB1	65:Y7:281:SER:HB3	2.02	0.41
23:7A:79:TRP:NE1	65:Y7:316:TYR:OH	2.52	0.41
24:7C:144:TYR:OH	153:7C:301:CDL:OB4	2.37	0.41
27:B:86:LYS:NZ	59:VB:581:GLU:OE1	2.50	0.41
27:B:88:TYR:CZ	27:B:94:GLY:HA2	2.55	0.41
27:B:252:GLU:HG3	27:B:253:ARG:H	1.85	0.41
27:B:457:ARG:HD3	27:B:457:ARG:HA	1.78	0.41
28:BP:366:THR:OG1	28:BP:403:ALA:HB1	2.20	0.41
29:C1:81:HIS:CE1	29:C1:85:PRO:HB3	2.54	0.41
29:C1:487:PRO:HG3	29:C1:544:TYR:HB3	2.02	0.41
32:D:236:PHE:CZ	32:D:328:MET:HB3	2.54	0.41
33:E:68:GLN:HE21	33:E:159:GLU:CD	2.28	0.41
33:E:94:LYS:HE3	33:E:94:LYS:HB2	1.88	0.41
33:E:130:TRP:HA	33:E:133:VAL:HG22	2.02	0.41
37:H:75:SER:O	37:H:79:ARG:HG3	2.19	0.41
42:M:71:THR:O	42:M:87:TYR:OH	2.22	0.41
43:M1:86:LEU:HB2	43:M1:89:TYR:HB3	2.02	0.41
50:R:4:GLU:O	50:R:8:TYR:HB2	2.19	0.41
52:SA:51:ALA:HB3	52:SA:67:LEU:HD13	2.02	0.41
153:T:204:CDL:H362	63:Y0:83:THR:HA	2.02	0.41
58:V:100:PHE:HA	58:V:104:THR:HB	2.01	0.41
70:4L:107:LYS:HE3	70:4L:107:LYS:HB2	1.84	0.41
72:A1:71:LYS:HG3	141:TE:51:TYR:CD2	2.55	0.41
76:A6:99:TYR:CD1	123:S4:66:GLN:HG3	2.55	0.41
77:A7:129:ILE:HG12	122:S3:24:ILE:HG12	2.01	0.41
79:A9:220:TYR:OH	145:TX:163:GLU:HG2	2.20	0.41
89:B7:87:HIS:CD2	89:B7:88:VAL:H	2.37	0.41
90:B8:28:TRP:HH2	93:BM:51:VAL:HG12	1.85	0.41
92:BL:41:PHE:CD2	92:BL:46:PRO:HG2	2.55	0.41
99:J1:33:ARG:HH12	99:J1:90:ASP:HA	1.84	0.41
99:J1:35:ALA:O	99:J1:86:ARG:NH2	2.41	0.41
110:QC:65:MET:HE2	110:QC:65:MET:HB3	1.96	0.41
111:QD:47:VAL:HG11	113:QF:70:GLU:HB2	2.02	0.41
111:QD:319:ALA:HB2	115:Qh:28:HIS:CD2	2.55	0.41
108:Qa:258:SER:HB3	108:Qa:261:GLU:HB3	2.02	0.41
109:Qb:86:ALA:HB1	109:Qb:254:VAL:HG13	2.02	0.41
109:Qb:173:PHE:CZ	109:Qb:237:VAL:HG21	2.55	0.41
121:S2:153:GLU:CD	121:S2:202:THR:HG21	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
121:S2:153:GLU:CG	121:S2:202:THR:HG21	2.50	0.41
121:S2:175:ARG:HB2	121:S2:178:GLU:O	2.20	0.41
127:S8:122:GLY:CA	127:S8:193:GLY:O	2.67	0.41
148:X1:47:LEU:O	148:X1:50:PHE:HB2	2.21	0.41
153:2m:101:CDL:H331	54:sc:32:LEU:HD11	2.02	0.41
19:6b:10:LEU:HB2	19:6b:11:PRO:HD3	2.01	0.41
24:7c:103:GLN:HE21	29:c1:631:ALA:HA	1.84	0.41
153:7c:302:CDL:H521	152:m2:402:PC1:H241	2.02	0.41
27:b:250:VAL:HG21	31:c3:130:HIS:ND1	2.35	0.41
29:c1:20:PHE:HB3	29:c1:23:LEU:CB	2.49	0.41
29:c1:105:MET:HB3	154:c1:702:HEA:C3C	2.50	0.41
29:c1:429:VAL:O	29:c1:433:MET:HG3	2.20	0.41
29:c1:654:ARG:HA	29:c1:654:ARG:HD2	1.88	0.41
31:c3:495:MET:HE2	31:c3:495:MET:HB3	1.98	0.41
33:e:23:ARG:NH1	59:vb:419:ASP:OD1	2.53	0.41
33:e:185:GLU:OE2	33:e:187:ARG:NH1	2.50	0.41
38:i:126:TYR:O	38:i:130:ASN:ND2	2.41	0.41
153:i:302:CDL:OB4	35:FS:187:TYR:OH	2.34	0.41
41:l:139:GLU:HB2	59:vb:568:ALA:HA	2.02	0.41
44:m2:205:LEU:HD23	44:m2:223:ALA:HA	2.02	0.41
62:y:69:LYS:HE3	62:y:69:LYS:HB2	1.87	0.41
68:1b:3:TYR:HB3	100:n1:110:TRP:HB3	2.02	0.41
68:1b:11:LEU:HB2	72:a1:23:TYR:CE2	2.55	0.41
73:a2:65:TYR:OH	73:a2:90:LEU:O	2.21	0.41
75:a5:105:LYS:NZ	122:s3:52:GLU:OE2	2.37	0.41
77:a7:179:TYR:HE2	77:a7:184:MET:HE3	1.85	0.41
80:ab:121:PHE:HD1	80:ab:121:PHE:HA	1.79	0.41
81:ac:53:ASN:HB3	81:ac:56:ASP:HB3	2.01	0.41
158:an:305:3PE:H381	115:qH:80:ARG:HB2	2.02	0.41
89:b7:20:GLU:HG2	132:t5:78:LEU:HD11	2.02	0.41
89:b7:61:ARG:NH2	131:t4:106:GLU:OE1	2.54	0.41
90:b8:146:GLU:OE1	90:b8:146:GLU:N	2.42	0.41
96:g1:83:ASP:HB2	98:g3:212:LEU:HD11	2.00	0.41
98:g3:172:PRO:HD3	98:g3:188:ALA:HB3	2.02	0.41
99:j1:33:ARG:HH12	99:j1:90:ASP:HA	1.85	0.41
100:n1:185:VAL:O	100:n1:188:ILE:HG12	2.20	0.41
103:n4:148:TYR:CE1	103:n4:184:LEU:HB3	2.55	0.41
105:n6:175:LEU:O	105:n6:180:ILE:HG12	2.19	0.41
106:p1:46:LYS:HE2	106:p1:46:LYS:HB2	1.91	0.41
111:qD:47:VAL:HG11	113:qF:70:GLU:HB2	2.02	0.41
152:qE:303:PC1:H2E2	152:qI:202:PC1:H2I2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
114:qG:25:GLY:N	114:qG:204:ASN:O	2.48	0.41
110:qc:357:ILE:HD11	160:qh:201:PX2:H17	2.02	0.41
112:qe:60:PHE:CZ	115:qh:57:GLY:HA2	2.55	0.41
122:s3:73:LEU:H	122:s3:90:PHE:HZ	1.68	0.41
130:t3:48:LEU:HB3	130:t3:57:LEU:HD21	2.00	0.41
2:2E:277:LYS:HE3	2:2E:277:LYS:HB2	1.93	0.41
7:2J:40:ASN:O	7:2J:44:GLN:HG2	2.20	0.41
14:3T:21:PHE:HA	17:5T:61:VAL:HG22	2.02	0.41
19:6B:50:LEU:HD21	20:6C:67:ARG:HB3	2.03	0.41
23:7A:59:GLU:OE2	23:7A:65:LYS:NZ	2.44	0.41
25:7L:897:VAL:HG12	25:7L:899:GLN:H	1.86	0.41
25:7L:903:ILE:HD12	25:7L:903:ILE:HA	1.86	0.41
26:A:366:ARG:HB3	26:A:379:THR:HB	2.01	0.41
27:B:113:LEU:O	27:B:117:LEU:N	2.50	0.41
27:B:398:VAL:HG21	65:Y7:408:VAL:HG13	2.02	0.41
30:C2:85:ILE:HB	30:C2:86:PRO:HD3	2.01	0.41
30:C2:197:PRO:HB2	32:D:335:PHE:CE1	2.55	0.41
31:C3:18:PHE:HE1	31:C3:134:ILE:HD12	1.85	0.41
31:C3:311:ARG:HA	31:C3:314:ILE:HG22	2.03	0.41
33:E:137:PHE:CZ	33:E:197:GLY:HA3	2.56	0.41
34:F:337:ASN:HD21	36:G:88:THR:HG21	1.85	0.41
42:M:39:GLN:HE21	42:M:43:TRP:NE1	2.17	0.41
43:M1:7:ASP:HA	44:M2:202:PHE:CE2	2.55	0.41
45:M3:60:GLN:HB3	45:M3:64:ARG:NH1	2.35	0.41
49:Q:63:PRO:HG2	153:Q:202:CDL:H431	2.02	0.41
50:R:106:CYS:HB2	50:R:107:PRO:HD3	2.02	0.41
51:S:47:THR:HG23	65:Y7:191:ASN:ND2	2.35	0.41
60:W:2:VAL:HG13	60:W:5:TYR:CE2	2.55	0.41
60:W:21:ARG:HH21	152:W:204:PC1:P	2.43	0.41
71:5B:100:ILE:HD13	158:AN:301:3PE:H322	2.02	0.41
82:AL:118:PHE:HB3	127:S8:222:PRO:HB3	2.02	0.41
158:AN:305:3PE:H381	115:QH:80:ARG:HB2	2.02	0.41
85:B2:109:HIS:CE1	131:T4:94:HIS:HE1	2.38	0.41
96:G1:89:ILE:HD13	96:G1:95:ILE:HD11	2.02	0.41
100:N1:239:PHE:HA	100:N1:242:ALA:HB3	2.01	0.41
103:N4:110:LYS:NZ	135:T8:72:SER:O	2.39	0.41
104:N5:64:VAL:O	104:N5:70:ASP:HB3	2.20	0.41
153:N6:302:CDL:H532	139:TC:24:VAL:HG22	2.02	0.41
108:QA:262:PHE:O	108:QA:266:VAL:HG23	2.20	0.41
109:QB:173:PHE:CZ	109:QB:237:VAL:HG21	2.55	0.41
109:QB:298:GLU:HG2	115:QH:56:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
110:QC:98:HIS:O	110:QC:102:LYS:HG2	2.21	0.41
110:QC:113:GLU:HG2	114:QG:178:LEU:HD11	2.01	0.41
111:QD:200:PRO:HA	111:QD:205:MET:HG2	2.03	0.41
114:QG:92:GLU:HA	114:QG:96:CYS:HB3	2.02	0.41
109:Qb:492:HIS:HD2	111:Qd:282:LEU:HD22	1.85	0.41
111:Qd:26:ILE:HD13	115:Qh:116:ARG:HH21	1.85	0.41
111:Qd:273:PHE:CZ	153:Qi:202:CDL:H732	2.55	0.41
120:S1:562:TYR:CE1	120:S1:570:GLY:HA3	2.55	0.41
122:S3:193:ASN:ND2	123:S4:128:THR:HG21	2.35	0.41
126:S7:24:PRO:HD3	126:S7:51:VAL:HG13	2.02	0.41
128:T1:45:ASN:O	128:T1:45:ASN:ND2	2.48	0.41
153:T5:301:CDL:H582	153:T5:301:CDL:H232	2.02	0.41
134:T7:86:PHE:HB2	153:T7:201:CDL:HB32	2.01	0.41
158:T8:601:3PE:H3D2	158:T8:602:3PE:H2C2	2.02	0.41
1:1t:57:LYS:HD3	41:l:216:ILE:HD13	2.01	0.41
5:2h:103:LEU:HD21	9:2l:7:ILE:HD13	2.02	0.41
7:2j:54:GLU:CD	12:2o:6:ARG:HD2	2.45	0.41
15:4a:105:ASP:O	42:m:49:TYR:OH	2.30	0.41
19:6b:181:GLN:HG3	30:c2:508:ASN:HB2	2.02	0.41
23:7a:50:ALA:HA	26:a:247:TYR:CZ	2.56	0.41
153:a:504:CDL:H351	31:c3:258:TYR:CD2	2.55	0.41
28:bp:174:GLY:HA3	28:bp:177:TYR:CE2	2.55	0.41
28:bp:189:SER:OG	28:bp:225:ARG:NH1	2.54	0.41
30:c2:513:VAL:HG12	30:c2:551:GLU:HG2	2.02	0.41
37:h:57:LYS:HE2	37:h:315:PHE:CD2	2.55	0.41
38:i:102:ASP:O	38:i:106:THR:OG1	2.37	0.41
153:j:301:CDL:H112	46:n:139:TYR:CZ	2.55	0.41
43:m1:51:GLU:HG3	43:m1:100:ALA:HB2	2.02	0.41
45:m3:246:TYR:N	45:m3:247:PRO:HD2	2.35	0.41
52:sa:351:HIS:HB2	52:sa:390:VAL:O	2.20	0.41
53:sb:109:LYS:HB3	53:sb:116:LEU:HD23	2.02	0.41
153:t:204:CDL:H362	63:y0:83:THR:HA	2.02	0.41
69:2b:40:LEU:HA	69:2b:44:LEU:HD11	2.01	0.41
95:fx:128:ARG:HH21	95:fx:129:ASN:HD21	1.69	0.41
101:n2:300:PHE:CZ	101:n2:315:LEU:HD21	2.55	0.41
104:n5:70:ASP:H	37:H:82:LYS:NZ	2.18	0.41
104:n5:560:ILE:HG22	104:n5:565:LEU:HD12	2.02	0.41
104:n5:570:GLY:HA2	104:n5:573:ILE:HG12	2.02	0.41
106:p1:124:LEU:HB3	106:p1:125:PRO:HD3	2.02	0.41
109:qB:157:VAL:HG11	109:qB:254:VAL:HG23	2.01	0.41
109:qB:173:PHE:CZ	109:qB:237:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
152:qB:602:PC1:H331	114:qg:187:PHE:CZ	2.52	0.41
114:qG:293:LYS:HE3	114:qG:293:LYS:HB3	1.95	0.41
108:qa:258:SER:HB3	108:qa:261:GLU:HB3	2.02	0.41
110:qc:257:TYR:HE2	152:qc:509:PC1:H121	1.86	0.41
110:qc:259:PHE:HA	111:qd:167:LEU:HB3	2.01	0.41
120:s1:283:ASN:ND2	120:s1:286:TRP:O	2.51	0.41
123:s4:62:ASP:OD1	123:s4:64:SER:OG	2.27	0.41
123:s4:81:ARG:HH22	123:s4:127:ASP:CG	2.28	0.41
132:t5:181:GLN:O	132:t5:184:ILE:HG22	2.20	0.41
135:t8:24:LYS:HE2	135:t8:24:LYS:HB3	1.93	0.41
136:t9:27:PHE:O	136:t9:31:LYS:HG2	2.19	0.41
7:2J:54:GLU:CD	12:2O:6:ARG:HD2	2.45	0.41
153:2M:101:CDL:H331	54:SC:32:LEU:HD11	2.02	0.41
29:C1:644:LYS:HD2	36:G:231:PHE:HB2	2.02	0.41
31:C3:145:SER:OG	31:C3:146:PHE:N	2.53	0.41
32:D:310:ARG:HG2	39:J:206:LEU:HB2	2.03	0.41
33:E:34:THR:HG22	33:E:50:ILE:HG23	2.02	0.41
37:H:269:TYR:OH	57:U:7:ARG:NH2	2.52	0.41
38:I:88:LEU:HD12	153:R:201:CDL:H511	2.02	0.41
41:L:29:GLU:HG2	41:L:30:MET:H	1.84	0.41
43:M1:51:GLU:OE1	43:M1:96:ARG:NE	2.50	0.41
153:M1:402:CDL:HA21	153:M1:402:CDL:HB31	2.02	0.41
45:M3:246:TYR:N	45:M3:247:PRO:HD2	2.35	0.41
46:N:34:ASN:O	46:N:37:VAL:HG22	2.20	0.41
46:N:169:ARG:HE	153:N:304:CDL:H712	1.84	0.41
51:S:90:PRO:HB2	64:Y5:94:LEU:HG	2.02	0.41
56:T:111:TRP:CD2	153:T:201:CDL:HB31	2.55	0.41
65:Y7:201:GLU:HB2	149:C:178:LYS:HG3	2.02	0.41
68:1B:39:HIS:NE2	127:S8:82:ASN:HB3	2.36	0.41
69:2B:159:ILE:HD13	153:2B:201:CDL:H673	2.02	0.41
72:A1:17:THR:N	72:A1:18:PRO:HD2	2.35	0.41
75:A5:144:LEU:HD13	122:S3:51:ARG:HB2	2.02	0.41
77:A7:93:TYR:CE1	77:A7:115:LYS:HD2	2.50	0.41
82:AL:101:TRP:CD1	82:AL:109:PHE:HB3	2.55	0.41
90:B8:89:TYR:CZ	153:B8:302:CDL:HB31	2.55	0.41
90:B8:145:GLY:HA2	92:BL:108:PRO:HG3	2.02	0.41
90:B8:198:LYS:HE3	90:B8:198:LYS:HB3	1.90	0.41
164:B8:301:U10:H161	164:B8:301:U10:H8	2.01	0.41
98:G3:58:LYS:HE3	98:G3:95:GLU:HA	2.02	0.41
101:N2:83:THR:HB	101:N2:87:SER:HA	2.01	0.41
101:N2:263:ALA:HB3	101:N2:349:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
103:N4:148:TYR:CE1	103:N4:184:LEU:HB3	2.55	0.41
104:N5:416:PRO:O	104:N5:419:MET:HG2	2.20	0.41
108:QA:79:ILE:O	108:QA:252:CYS:HA	2.19	0.41
108:QA:419:GLU:OE2	108:QA:435:TYR:OH	2.33	0.41
109:QB:495:ARG:NH2	152:QI:202:PC1:O22	2.54	0.41
110:QC:368:TYR:O	110:QC:371:SER:OG	2.32	0.41
111:QD:293:ARG:NH2	114:QG:301:ASP:OD1	2.52	0.41
114:QG:187:PHE:CG	152:Qj:101:PC1:H382	2.55	0.41
110:Qc:336:ILE:HD11	110:Qc:341:ILE:HG22	2.03	0.41
114:Qg:72:LEU:HD21	114:Qg:251:PHE:HD2	1.85	0.41
115:Qh:50:ASP:OD1	115:Qh:50:ASP:N	2.54	0.41
120:S1:104:LYS:O	120:S1:110:THR:OG1	2.34	0.41
126:S7:94:GLY:HA2	126:S7:125:GLY:O	2.21	0.41
129:T2:176:LYS:O	129:T2:180:ILE:HG12	2.21	0.41
131:T4:85:ALA:O	131:T4:89:ILE:HG13	2.20	0.41
142:TF:140:LYS:HD3	142:TF:140:LYS:HA	1.82	0.41
147:V2:188:THR:H	147:V2:191:ASN:HB2	1.86	0.41
148:X1:120:VAL:HB	148:X1:124:LYS:HZ2	1.85	0.41
15:4a:72:PHE:CE2	15:4a:114:GLU:HG2	2.55	0.41
153:6a:201:CDL:H711	59:vb:87:LYS:HD3	2.03	0.41
25:7l:913:ARG:HH21	25:7l:919:LYS:HD3	1.85	0.41
27:b:88:TYR:CZ	27:b:94:GLY:HA2	2.56	0.41
29:c1:387:TRP:CH2	154:c1:708:HEA:HBD1	2.55	0.41
31:c3:378:THR:O	31:c3:382:ASN:HB2	2.21	0.41
31:c3:446:ILE:HD12	31:c3:446:ILE:HA	1.92	0.41
31:c3:511:TYR:CZ	153:t:202:CDL:H801	2.55	0.41
32:d:311:ARG:HB2	32:d:322:TRP:HB3	2.01	0.41
33:e:186:PRO:HG3	42:M:7:GLY:O	2.20	0.41
34:f:337:ASN:ND2	36:g:88:THR:HG21	2.35	0.41
35:fs:86:TYR:HB3	35:fs:88:CYS:SG	2.60	0.41
153:fs:203:CDL:H321	153:E:403:CDL:H121	2.03	0.41
37:h:298:SER:HA	37:h:301:SER:HB2	2.03	0.41
40:k:173:GLU:OE2	48:p:9:HIS:NE2	2.53	0.41
41:l:72:PHE:O	41:l:75:GLN:HG2	2.20	0.41
42:m:191:MET:SD	62:y:30:ILE:HB	2.60	0.41
53:sb:75:ARG:NH1	53:sb:90:TYR:HH	2.18	0.41
61:x:30:ASN:OD1	61:x:30:ASN:N	2.52	0.41
66:z:12:ASP:OD1	57:U:133:TYR:OH	2.38	0.41
153:z:101:CDL:H151	153:z:101:CDL:H332	2.01	0.41
70:4l:54:ILE:HD13	124:s5:6:TYR:HB2	2.02	0.41
70:4l:88:LEU:HD11	105:n6:103:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:a6:56:THR:OG1	168:ab:201:ZMP:H14	2.20	0.41
77:a7:7:ARG:NE	153:t7:201:CDL:OB3	2.50	0.41
77:a7:126:ILE:HG22	77:a7:128:GLU:HG3	2.02	0.41
77:a7:129:ILE:HG12	122:s3:24:ILE:HG12	2.01	0.41
89:b7:87:HIS:CD2	89:b7:88:VAL:H	2.37	0.41
93:bm:134:ASP:O	144:th:77:GLY:N	2.46	0.41
95:fx:49:ASN:HD21	95:fx:55:GLU:CG	2.32	0.41
97:g2:108:VAL:HG22	97:g2:136:CYS:H	1.85	0.41
98:g3:262:GLU:OE1	121:s2:4:SER:OG	2.34	0.41
98:g3:262:GLU:HB3	105:n6:235:LYS:HD3	2.02	0.41
152:n1:301:PC1:H362	152:n1:301:PC1:H262	2.01	0.41
101:n2:138:ILE:HG23	101:n2:291:ILE:HG12	2.02	0.41
105:n6:248:LEU:HD12	121:s2:285:ASN:ND2	2.34	0.41
110:qC:97:PHE:CZ	153:qC:504:CDL:H371	2.54	0.41
111:qD:293:ARG:NH2	114:qG:301:ASP:OD1	2.53	0.41
115:qH:38:TYR:O	115:qh:16:SER:OG	2.38	0.41
108:qa:323:ASN:O	108:qa:327:ALA:N	2.44	0.41
109:qb:363:ILE:HB	109:qb:382:TYR:HB3	2.02	0.41
110:qc:232:GLY:HA3	111:qd:271:LYS:HE3	2.03	0.41
114:qg:40:LYS:O	114:qg:43:GLN:HG3	2.21	0.41
126:s7:6:ILE:O	126:s7:10:ILE:HG12	2.20	0.41
131:t4:85:ALA:O	131:t4:89:ILE:HG13	2.20	0.41
134:t7:30:PHE:HZ	134:t7:129:LEU:HB2	1.84	0.41
142:tf:46:LEU:HB2	142:tf:69:MET:HE2	2.02	0.41
4:2G:92:HIS:HA	4:2G:95:VAL:HG22	2.02	0.41
25:7L:905:PRO:HG2	25:7L:906:GLN:NE2	2.35	0.41
28:BP:287:LYS:NZ	28:BP:291:GLU:OE2	2.45	0.41
31:C3:212:ARG:HD2	40:K:51:MET:HE2	2.03	0.41
31:C3:284:TRP:HB2	65:Y7:317:TRP:CD1	2.56	0.41
31:C3:428:TYR:OH	32:D:226:LYS:NZ	2.52	0.41
37:H:298:SER:HA	37:H:301:SER:HB2	2.02	0.41
41:L:153:TYR:HB3	153:L:301:CDL:H211	2.02	0.41
42:M:79:HIS:CE1	42:M:81:PHE:HB2	2.55	0.41
53:SB:73:VAL:HG22	53:SB:156:ILE:HD12	2.02	0.41
164:SC:102:U10:H222	164:SC:102:U10:H261	1.80	0.41
59:VB:108:PHE:HA	65:Y7:294:ARG:HD3	2.03	0.41
59:VB:398:ILE:HG13	59:VB:552:TYR:HA	2.02	0.41
65:Y7:338:MET:HE3	65:Y7:340:PHE:HE1	1.86	0.41
153:Z:101:CDL:H151	153:Z:101:CDL:H332	2.01	0.41
153:A1:102:CDL:HB32	100:N1:64:ARG:NH2	2.35	0.41
76:A6:19:ASN:ND2	99:J1:211:ASN:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:A9:62:LEU:O	79:A9:67:SER:HB3	2.20	0.41
82:AL:55:GLY:HA3	82:AL:98:TRP:HH2	1.85	0.41
91:B9:22:TYR:OH	91:B9:94:GLU:OE2	2.33	0.41
99:J1:294:ILE:HD12	99:J1:306:ALA:HB1	2.01	0.41
101:N2:217:LEU:O	124:S5:48:HIS:NE2	2.47	0.41
101:N2:227:ASN:ND2	101:N2:303:TYR:O	2.29	0.41
102:N3:21:TRP:HA	139:TC:2:VAL:HG12	2.02	0.41
103:N4:83:LEU:O	103:N4:87:SER:N	2.52	0.41
104:N5:619:LYS:HE2	104:N5:619:LYS:HB2	1.83	0.41
106:P1:28:PHE:HB2	106:P1:31:GLU:HB2	2.01	0.41
109:QB:111:GLN:HE21	109:QB:139:VAL:HB	1.85	0.41
109:Qb:144:GLU:HG3	109:Qb:214:PHE:HE1	1.84	0.41
109:Qb:342:ASN:HA	115:Qh:27:ARG:HA	2.02	0.41
120:S1:644:ALA:HB1	120:S1:646:HIS:CE1	2.55	0.41
121:S2:47:LEU:HD23	121:S2:52:ALA:HA	2.02	0.41
126:S7:32:CYS:SG	126:S7:94:GLY:HA3	2.61	0.41
129:T2:29:ASN:OD1	129:T2:30:GLY:N	2.54	0.41
130:T3:226:ASN:HB3	130:T3:229:GLU:HB3	2.02	0.41
131:T4:117:LEU:HG	131:T4:121:PHE:CE2	2.55	0.41
138:TB:97:SER:HA	144:TH:123:LYS:HE3	2.01	0.41
142:TF:184:ARG:NH1	142:TF:218:ALA:O	2.53	0.41
143:TG:104:ASN:ND2	143:TG:107:HIS:HB2	2.33	0.41
146:V1:397:MET:HE3	146:V1:397:MET:HB3	1.95	0.41
3:2f:141:LYS:NZ	3:2f:142:ASP:OD1	2.53	0.41
4:2g:92:HIS:HA	4:2g:95:VAL:HG22	2.03	0.41
4:2g:102:TYR:CE2	4:2g:163:GLU:HG3	2.55	0.41
152:2g:202:PC1:H112	54:sc:6:TYR:OH	2.20	0.41
13:2t:57:PHE:CD2	17:5t:39:PHE:HB3	2.54	0.41
25:7l:938:TYR:OH	30:c2:600:ARG:O	2.37	0.41
28:bp:117:VAL:HG22	28:bp:126:VAL:HG22	2.02	0.41
28:bp:323:THR:H	28:bp:326:GLN:HE22	1.67	0.41
29:c1:276:PHE:HD2	29:c1:292:GLN:HE22	1.68	0.41
30:c2:355:GLY:HA3	31:c3:578:LYS:HD3	2.02	0.41
38:i:88:LEU:HD12	153:r:201:CDL:H511	2.02	0.41
153:m:306:CDL:HA61	33:E:126:LYS:HD2	2.02	0.41
43:m1:7:ASP:HA	44:m2:202:PHE:CE2	2.55	0.41
44:m2:71:THR:HG23	58:v:20:ASP:O	2.21	0.41
44:m2:81:GLY:O	44:m2:85:HIS:N	2.46	0.41
47:o:157:CYS:HB3	47:o:170:CYS:SG	2.60	0.41
49:q:63:PRO:HG2	153:q:202:CDL:H431	2.03	0.41
153:y5:201:CDL:H751	67:z1:59:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:y7:128:CYS:HB3	65:y7:133:ILE:HD11	2.03	0.41
65:y7:205:ILE:HD12	149:c:170:VAL:HG22	2.03	0.41
68:1b:39:HIS:NE2	127:s8:82:ASN:HB3	2.36	0.41
69:2b:159:ILE:HD13	153:2b:201:CDL:H673	2.02	0.41
70:4l:8:TRP:CZ3	70:4l:11:ILE:HD11	2.55	0.41
76:a6:19:ASN:ND2	99:j1:211:ASN:HB3	2.35	0.41
77:a7:28:ARG:NH1	77:a7:29:ARG:O	2.53	0.41
78:a8:174:PHE:CE2	78:a8:178:ARG:HD2	2.56	0.41
78:a8:195:ILE:O	78:a8:199:VAL:HG13	2.21	0.41
168:ab:201:ZMP:H22A	168:ab:201:ZMP:H25B	1.53	0.41
84:an:38:THR:OG1	105:n6:19:TYR:OH	2.36	0.41
98:g3:34:LEU:O	98:g3:38:GLN:HG2	2.20	0.41
98:g3:279:GLU:OE1	122:s3:44:SER:OG	2.38	0.41
99:j1:78:ALA:HB2	109:qB:278:PHE:HZ	1.86	0.41
103:n4:214:LEU:HA	103:n4:217:ILE:HG22	2.03	0.41
106:p1:48:PRO:HD2	107:p2:140:THR:HG21	2.03	0.41
107:p2:146:ASN:HB2	107:p2:153:TYR:CE2	2.56	0.41
108:qA:307:LEU:O	108:qA:362:GLY:HA3	2.20	0.41
108:qA:328:LEU:HG	108:qA:333:ARG:HG3	2.02	0.41
109:qB:384:ASN:OD1	109:qB:385:GLU:N	2.54	0.41
114:qG:187:PHE:CG	152:qj:101:PC1:H382	2.55	0.41
110:qc:98:HIS:HD2	166:qc:503:HEM:C1C	2.39	0.41
110:qc:378:PHE:O	110:qc:382:ILE:HG12	2.20	0.41
114:qg:5:GLU:OE1	114:qg:5:GLU:N	2.49	0.41
116:qi:71:LEU:HD13	117:qj:31:TRP:CE2	2.55	0.41
120:s1:234:ASN:HB3	120:s1:237:TYR:HB3	2.02	0.41
120:s1:525:GLU:HG3	120:s1:591:VAL:HG11	2.03	0.41
121:s2:175:ARG:HB2	121:s2:178:GLU:O	2.20	0.41
123:s4:125:ASN:OD1	123:s4:125:ASN:N	2.49	0.41
126:s7:32:CYS:SG	126:s7:94:GLY:HA3	2.61	0.41
128:t1:132:ASN:HB2	128:t1:135:PHE:HB3	2.03	0.41
134:t7:86:PHE:HB2	153:t7:201:CDL:HB32	2.01	0.41
142:tf:223:LEU:HD12	142:tf:226:LEU:HD23	2.02	0.41
147:v2:125:CYS:HA	147:v2:164:VAL:O	2.21	0.41
148:x1:51:ASN:OD1	148:x1:110:ARG:NH2	2.53	0.41
3:2F:186:LEU:HB2	3:2F:228:TRP:CH2	2.55	0.41
13:2T:28:VAL:HG23	13:2T:29:LEU:HD12	2.02	0.41
19:6B:86:TRP:HZ2	30:C2:470:ILE:HG13	1.85	0.41
20:6C:64:GLY:O	20:6C:68:ASN:ND2	2.46	0.41
23:7A:36:LEU:HD22	59:VB:105:GLU:HB3	2.02	0.41
153:7C:301:CDL:H431	29:C1:63:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BP:253:ASN:O	28:BP:256:GLY:N	2.52	0.41
29:C1:325:LEU:HD23	29:C1:332:MET:HG2	2.01	0.41
30:C2:355:GLY:HA3	31:C3:578:LYS:HD3	2.02	0.41
30:C2:365:TYR:CZ	30:C2:390:ARG:HB2	2.55	0.41
31:C3:162:LEU:HD11	48:P:90:PHE:HB3	2.02	0.41
31:C3:173:SER:HB3	48:P:35:ILE:HG21	2.03	0.41
31:C3:266:LEU:HB2	31:C3:271:ILE:HD13	2.02	0.41
31:C3:511:TYR:CZ	153:T:202:CDL:H801	2.56	0.41
39:J:57:HIS:CE1	46:N:48:HIS:HB3	2.56	0.41
39:J:96:TRP:HB3	152:J:302:PC1:H262	2.02	0.41
41:L:134:LEU:HD12	41:L:135:PRO:HD2	2.02	0.41
46:N:29:PHE:HA	46:N:32:PHE:HB2	2.02	0.41
48:P:72:ASP:HB3	48:P:105:GLN:HG3	2.01	0.41
52:SA:211:LEU:HD23	52:SA:222:VAL:HG12	2.01	0.41
53:SB:105:ILE:HG23	53:SB:116:LEU:HD21	2.03	0.41
56:T:21:LYS:HD3	56:T:157:VAL:HG11	2.01	0.41
59:VB:447:LEU:HD13	59:VB:455:PHE:CG	2.56	0.41
153:VB:705:CDL:H341	153:VB:705:CDL:H381	2.02	0.41
153:VB:706:CDL:H361	153:VB:706:CDL:H792	2.02	0.41
65:Y7:115:ILE:HD12	65:Y7:162:LEU:HD12	2.03	0.41
69:2B:23:LEU:HD22	69:2B:87:LEU:HD12	2.02	0.41
73:A2:12:LEU:HD13	73:A2:15:LEU:HG	2.02	0.41
74:A3:75:LEU:HD22	158:A3:202:3PE:H222	2.03	0.41
75:A5:92:ILE:O	75:A5:99:ARG:NH1	2.47	0.41
75:A5:153:PRO:HA	122:S3:41:TRP:CZ3	2.55	0.41
81:AC:62:ILE:HD12	93:BM:59:LEU:HD12	2.01	0.41
83:AM:44:ARG:HA	153:AM:201:CDL:HA22	2.02	0.41
96:G1:81:ARG:NH1	96:G1:83:ASP:OD2	2.49	0.41
97:G2:68:ASN:HD21	97:G2:85:TYR:HB3	1.85	0.41
98:G3:262:GLU:HB3	105:N6:235:LYS:HD3	2.02	0.41
100:N1:51:GLN:O	126:S7:42:SER:OG	2.32	0.41
100:N1:59:VAL:O	100:N1:63:GLY:HA2	2.20	0.41
100:N1:213:GLU:HG3	100:N1:255:PHE:CZ	2.56	0.41
104:N5:272:THR:HG23	104:N5:424:PRO:HG3	2.02	0.41
110:QC:33:LEU:HD22	110:QC:230:GLU:HG2	2.02	0.41
112:QE:39:HIS:CG	112:QE:40:LYS:H	2.38	0.41
112:QE:84:GLU:OE1	116:QI:49:LYS:NZ	2.38	0.41
110:Qc:413:TYR:OH	114:Qg:64:ALA:HA	2.21	0.41
111:Qd:175:ILE:H	111:Qd:175:ILE:HD12	1.86	0.41
111:Qd:183:HIS:CD2	113:Qf:21:LYS:HD3	2.55	0.41
114:Qg:192:LEU:HD12	114:Qg:198:TRP:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
153:Qg:402:CDL:H581	153:Qg:402:CDL:H722	2.03	0.41
116:Qi:71:LEU:HD13	117:Qj:31:TRP:CE2	2.55	0.41
120:S1:345:GLU:O	120:S1:519:GLY:N	2.54	0.41
121:S2:284:MET:HA	121:S2:287:MET:HE3	2.02	0.41
123:S4:12:ARG:HG3	123:S4:16:ILE:HD12	2.01	0.41
128:T1:372:PRO:HG3	128:T1:433:ARG:HA	2.02	0.41
130:T3:4:LEU:H	131:T4:137:ASN:ND2	2.17	0.41
130:T3:121:VAL:HA	130:T3:146:LEU:HD22	2.03	0.41
147:V2:123:GLN:NE2	147:V2:180:ASN:OD1	2.32	0.41
3:2f:82:ASN:O	3:2f:103:ARG:HD3	2.20	0.41
5:2h:108:LYS:HE3	5:2h:108:LYS:HB3	1.92	0.41
23:7a:80:VAL:HG21	65:y7:350:LEU:HB2	2.03	0.41
28:bp:205:PHE:HA	152:m2:407:PC1:H221	2.02	0.41
29:c1:529:ILE:HD11	29:c1:575:PHE:HB2	2.03	0.41
152:c1:711:PC1:H251	153:q:203:CDL:H762	2.02	0.41
30:c2:581:LEU:HD23	30:c2:581:LEU:HA	1.84	0.41
31:c3:284:TRP:HB2	65:y7:317:TRP:CD1	2.56	0.41
32:d:125:LEU:HB3	152:d:501:PC1:H151	2.03	0.41
33:e:126:LYS:HD2	153:M:301:CDL:HA61	2.02	0.41
153:f:401:CDL:H802	153:f:401:CDL:H831	1.93	0.41
153:f:401:CDL:H841	35:fs:170:TRP:HB3	2.02	0.41
153:i:301:CDL:OA3	35:FS:153:ARG:NH1	2.53	0.41
43:m1:57:VAL:HG22	152:m1:403:PC1:H371	2.02	0.41
45:m3:188:TYR:HB3	45:m3:194:CYS:HB2	2.03	0.41
52:sa:307:VAL:O	52:sa:352:ILE:HG23	2.19	0.41
52:sa:368:LEU:HB3	52:sa:371:ILE:HD11	2.03	0.41
68:1b:39:HIS:NE2	68:1b:43:ILE:HD11	2.35	0.41
74:a3:77:ASP:O	74:a3:81:ARG:HG3	2.20	0.41
75:a5:175:VAL:HG23	123:s4:3:LEU:HD13	2.02	0.41
76:a6:100:ARG:H	123:s4:66:GLN:CD	2.29	0.41
83:am:144:TYR:CE2	124:s5:14:PRO:HG3	2.56	0.41
90:b8:145:GLY:HA2	92:bl:108:PRO:HG3	2.01	0.41
96:g1:89:ILE:HD13	96:g1:95:ILE:HD11	2.02	0.41
101:n2:263:ALA:HB3	101:n2:349:ILE:HD11	2.02	0.41
103:n4:215:ILE:HD13	158:n4:601:3PE:H3A1	2.02	0.41
104:n5:271:TYR:CD2	104:n5:523:LEU:HD22	2.55	0.41
104:n5:296:MET:HG2	104:n5:433:THR:HA	2.01	0.41
109:qB:130:LEU:HD11	109:qB:137:LEU:HB2	2.03	0.41
109:qB:257:GLN:O	109:qB:261:GLN:HG2	2.20	0.41
110:qC:338:ARG:HH22	114:qG:33:GLU:CD	2.28	0.41
111:qD:150:ALA:HB1	111:qD:159:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:qD:264:GLY:HA2	111:qD:267:ILE:HG22	2.02	0.41
112:qE:39:HIS:CG	112:qE:40:LYS:H	2.38	0.41
109:qb:93:ARG:NH2	109:qb:372:SER:OG	2.54	0.41
110:qc:211:SER:OG	110:qc:349:VAL:HB	2.21	0.41
110:qc:242:MET:HE3	111:qd:261:PHE:HD1	1.86	0.41
120:s1:120:PHE:O	146:v1:388:GLU:HG2	2.20	0.41
120:s1:239:PHE:HD2	127:s8:157:PRO:HB3	1.85	0.41
120:s1:376:LYS:HD3	120:s1:485:GLY:HA3	2.03	0.41
121:s2:47:LEU:HD23	121:s2:52:ALA:HA	2.01	0.41
125:s6:115:CYS:HB3	125:s6:118:CYS:SG	2.61	0.41
126:s7:94:GLY:HA2	126:s7:125:GLY:O	2.21	0.41
130:t3:79:ASP:OD1	130:t3:80:LYS:N	2.54	0.41
140:td:18:ILE:HB	140:td:19:PRO:HD3	2.02	0.41
4:2G:105:LEU:HD23	4:2G:105:LEU:HA	1.85	0.41
9:2L:3:LEU:HD23	9:2L:3:LEU:HA	1.89	0.41
27:B:29:ARG:HH12	27:B:126:ALA:HA	1.85	0.41
28:BP:216:ALA:O	28:BP:261:TRP:NE1	2.53	0.41
29:C1:490:PHE:HB3	29:C1:541:SER:HB3	2.02	0.41
29:C1:563:HIS:CG	29:C1:618:PHE:HB2	2.56	0.41
29:C1:596:VAL:HG11	30:C2:482:VAL:HB	2.02	0.41
29:C1:623:PHE:CZ	29:C1:627:ILE:HD11	2.56	0.41
34:F:174:TYR:O	34:F:178:ILE:HG13	2.21	0.41
36:G:288:TYR:O	36:G:290:LYS:HG3	2.20	0.41
43:M1:57:VAL:HG22	152:M1:403:PC1:H371	2.02	0.41
44:M2:1:MET:O	44:M2:4:SER:OG	2.30	0.41
45:M3:77:ASP:HB3	45:M3:295:GLU:HB3	2.01	0.41
53:SB:101:PHE:CE2	53:SB:134:CYS:HB3	2.56	0.41
56:T:13:ARG:NH2	62:Y:103:GLN:O	2.53	0.41
64:Y5:14:ASN:OD1	64:Y5:15:LYS:N	2.53	0.41
65:Y7:421:ILE:O	65:Y7:423:LYS:N	2.52	0.41
66:Z:4:ASP:HB3	66:Z:7:LYS:HG2	2.01	0.41
68:1B:49:VAL:HG13	102:N3:97:PHE:CE1	2.55	0.41
153:5B:201:CDL:HA62	153:B8:302:CDL:H511	2.02	0.41
77:A7:236:ASN:HA	77:A7:239:GLN:HG2	2.03	0.41
78:A8:215:SER:HA	134:T7:135:ARG:HD3	2.03	0.41
81:AC:133:ASN:OD1	104:N5:627:GLN:NE2	2.31	0.41
84:AN:105:MET:HA	84:AN:105:MET:HE3	2.03	0.41
153:AN:302:CDL:H371	153:AN:302:CDL:H201	2.03	0.41
88:B6:109:PRO:HG3	104:N5:227:TYR:CE1	2.55	0.41
89:B7:87:HIS:CD2	89:B7:87:HIS:H	2.38	0.41
164:B8:301:U10:H121	164:B8:301:U10:H8	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
96:G1:54:SER:OG	96:G1:69:GLY:O	2.33	0.41
100:N1:160:MET:HA	100:N1:163:ILE:HB	2.02	0.41
101:N2:88:HIS:O	101:N2:149:THR:HG21	2.20	0.41
103:N4:424:ILE:HG12	104:N5:236:MET:HE2	2.02	0.41
104:N5:513:VAL:HG22	104:N5:660:ILE:HD13	2.02	0.41
109:QB:332:GLN:HG3	109:QB:335:LYS:HB2	2.01	0.41
109:QB:495:ARG:NH1	153:QB:601:CDL:OB4	2.52	0.41
111:QD:115:HIS:CD2	111:QD:116:PRO:HD2	2.55	0.41
108:Qa:238:LYS:HE2	108:Qa:238:LYS:HB3	1.86	0.41
108:Qa:409:ALA:HB2	114:Qg:323:GLY:C	2.45	0.41
114:Qg:40:LYS:O	114:Qg:43:GLN:HG3	2.21	0.41
126:S7:58:ARG:HA	126:S7:85:LEU:HG	2.02	0.41
130:T3:135:VAL:HG11	130:T3:141:ILE:HD12	2.02	0.41
132:T5:73:LEU:HD22	132:T5:78:LEU:HD12	2.02	0.41
134:T7:43:PHE:HE1	134:T7:120:LEU:HB3	1.86	0.41
140:TD:33:PHE:O	140:TD:37:LYS:HG2	2.20	0.41
143:TG:119:ASN:O	143:TG:123:ASN:HB2	2.21	0.41
4:2g:58:ARG:HB3	7:2j:34:HIS:CE1	2.56	0.41
4:2g:147:ILE:HG23	4:2g:157:GLN:HE21	1.85	0.41
8:2k:34:ARG:HH22	153:2k:101:CDL:C11	2.32	0.41
11:2n:28:TYR:O	11:2n:32:VAL:HG22	2.21	0.41
20:6c:33:ALA:HA	20:6c:36:TRP:NE1	2.35	0.41
23:7a:21:ASP:O	23:7a:24:PHE:HB3	2.19	0.41
23:7a:104:GLU:HG3	152:7a:202:PC1:H151	2.03	0.41
153:7a:201:CDL:H592	153:7a:201:CDL:H842	2.03	0.41
153:7a:203:CDL:HB62	31:c3:470:ARG:HH22	1.86	0.41
27:b:241:LEU:HD23	27:b:241:LEU:H	1.86	0.41
27:b:252:GLU:HG3	27:b:253:ARG:H	1.85	0.41
28:bp:303:ALA:HB3	28:bp:362:VAL:HG12	2.03	0.41
29:c1:61:SER:HB3	29:c1:113:ILE:HG13	2.03	0.41
29:c1:127:VAL:HG12	29:c1:321:ALA:HA	2.02	0.41
29:c1:630:ARG:HD3	29:c1:630:ARG:HA	1.86	0.41
31:c3:201:LEU:HD23	31:c3:201:LEU:HA	1.94	0.41
31:c3:270:LYS:HB3	153:y7:501:CDL:H731	2.01	0.41
31:c3:311:ARG:HA	31:c3:314:ILE:HG22	2.03	0.41
31:c3:358:PHE:CE2	31:c3:362:LEU:HD11	2.56	0.41
32:d:313:ASN:OD1	32:d:322:TRP:NE1	2.54	0.41
33:e:104:ASP:OD2	64:y5:113:LYS:HB3	2.21	0.41
35:fs:153:ARG:NH1	153:I:302:CDL:OA3	2.54	0.41
42:m:137:ASP:HB3	42:m:140:THR:OG1	2.21	0.41
44:m2:241:ILE:HD11	44:m2:278:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:m3:41:ASP:OD1	45:m3:41:ASP:N	2.52	0.41
48:p:61:HIS:HB2	48:p:95:TYR:CZ	2.56	0.41
49:q:19:SER:HB2	49:q:102:TYR:O	2.20	0.41
53:sb:242:GLN:HE22	53:sb:286:LEU:HB3	1.86	0.41
56:t:111:TRP:CD2	153:t:201:CDL:HB31	2.55	0.41
59:vb:108:PHE:HA	65:y7:294:ARG:HD3	2.02	0.41
62:y:27:ASN:ND2	62:y:82:ALA:O	2.54	0.41
63:y0:4:TRP:HB3	63:y0:6:PHE:CE1	2.55	0.41
75:a5:178:LYS:HD3	123:s4:103:TYR:CZ	2.55	0.41
76:a6:21:TYR:OH	95:fx:134:SER:O	2.28	0.41
90:b8:71:ILE:HG23	91:b9:13:TRP:HE3	1.84	0.41
99:j1:311:GLN:HE21	99:j1:311:GLN:HB3	1.66	0.41
103:n4:46:ASN:HD22	135:t8:41:LEU:HD13	1.86	0.41
104:n5:86:LYS:HG2	104:n5:87:ILE:N	2.35	0.41
105:n6:60:LEU:HD21	152:n6:301:PC1:H32	2.02	0.41
107:p2:118:VAL:HG21	107:p2:145:PHE:HB2	2.02	0.41
109:qB:40:LYS:HB3	109:qB:43:LEU:HD12	2.01	0.41
110:qC:98:HIS:O	110:qC:102:LYS:HG2	2.20	0.41
111:qD:98:LYS:HB2	112:qE:267:PHE:CE2	2.56	0.41
108:qa:139:SER:HG	108:qa:154:ASN:ND2	2.18	0.41
108:qa:169:ASP:O	108:qa:173:GLU:HB2	2.21	0.41
108:qa:417:LEU:O	108:qa:421:VAL:HG13	2.21	0.41
109:qb:504:TRP:HA	109:qb:507:ASN:ND2	2.36	0.41
110:qc:186:TYR:CD2	164:qc:501:U10:H162	2.55	0.41
110:qc:397:PHE:HA	110:qc:401:ASN:HD22	1.85	0.41
111:qd:28:ARG:HG2	115:qh:116:ARG:HH11	1.85	0.41
120:s1:644:ALA:HB1	120:s1:646:HIS:CE1	2.55	0.41
121:s2:1:MET:SD	121:s2:1:MET:N	2.78	0.41
121:s2:21:LYS:HE2	121:s2:53:GLU:OE1	2.19	0.41
121:s2:310:ILE:HG12	142:tf:164:THR:HG22	2.01	0.41
131:t4:157:LEU:O	131:t4:160:PRO:HD2	2.19	0.41
135:t8:90:PRO:O	135:t8:94:ILE:HG12	2.21	0.41
142:tf:192:ILE:HD11	142:tf:216:PRO:HG3	2.03	0.41
2:2E:19:GLY:O	2:2E:22:SER:OG	2.37	0.41
2:2E:81:TYR:HE2	2:2E:96:LEU:HG	1.84	0.41
2:2E:153:LEU:HD22	2:2E:184:ILE:HG21	2.02	0.41
4:2G:153:TYR:CE2	8:2K:13:LYS:HG2	2.56	0.41
14:3T:69:PHE:O	14:3T:73:VAL:HG23	2.21	0.41
18:6A:109:GLU:HG2	31:C3:440:ARG:HH21	1.85	0.41
22:6T:13:ILE:HG12	22:6T:44:TYR:CD1	2.56	0.41
153:7A:203:CDL:HA32	153:7A:203:CDL:OB4	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:7C:136:ARG:HB3	36:G:204:TYR:HB3	2.02	0.41
28:BP:363:GLY:HA2	28:BP:453:SER:HB3	2.02	0.41
28:BP:413:GLU:C	28:BP:415:GLY:H	2.29	0.41
29:C1:606:THR:HG21	43:M1:222:LYS:HD2	2.03	0.41
154:C1:703:HEA:HMB3	154:C1:703:HEA:HHB	1.87	0.41
31:C3:54:GLY:HA2	31:C3:60:ILE:HG13	2.03	0.41
31:C3:523:GLY:O	153:T:202:CDL:H562	2.19	0.41
34:F:185:TRP:CZ2	58:V:112:ILE:HG23	2.55	0.41
37:H:114:ILE:HD13	37:H:114:ILE:HA	1.76	0.41
45:M3:55:ASN:O	45:M3:59:LEU:HG	2.21	0.41
49:Q:126:ARG:NH1	49:Q:153:GLU:OE1	2.53	0.41
52:SA:220:ARG:NH2	52:SA:471:LYS:O	2.51	0.41
63:Y0:4:TRP:CZ3	63:Y0:53:LEU:HD21	2.55	0.41
73:A2:52:ARG:HD2	120:S1:646:HIS:CE1	2.56	0.41
76:A6:172:PHE:HB3	123:S4:115:TYR:HB2	2.03	0.41
78:A8:174:PHE:CE2	78:A8:178:ARG:HD2	2.56	0.41
80:AB:71:LEU:HB3	80:AB:79:LEU:HD21	2.03	0.41
89:B7:118:TRP:NE1	90:B8:104:ASN:O	2.37	0.41
103:N4:399:ILE:HD13	103:N4:399:ILE:HA	1.87	0.41
104:N5:189:ILE:HG21	153:T5:301:CDL:H512	2.01	0.41
152:N6:301:PC1:H153	152:N6:301:PC1:H111	1.89	0.41
106:P1:190:ARG:NH1	130:T3:56:GLN:HE21	2.15	0.41
108:QA:214:LEU:HD11	108:QA:224:LEU:HD21	2.02	0.41
108:QA:327:ALA:O	108:QA:331:ASN:ND2	2.48	0.41
109:QB:384:ASN:OD1	109:QB:385:GLU:N	2.54	0.41
110:QC:357:ILE:HG12	115:QH:103:PRO:HG3	2.03	0.41
111:QD:98:LYS:HB2	112:QE:267:PHE:CE2	2.56	0.41
111:QD:190:MET:HE1	111:QD:205:MET:HB2	2.03	0.41
113:Qf:8:SER:OG	113:Qf:9:ALA:N	2.54	0.41
117:Qj:43:MET:HE2	117:Qj:48:PHE:HE2	1.86	0.41
120:S1:201:ARG:HH12	147:V2:110:THR:HG23	1.86	0.41
120:S1:244:TRP:NE1	127:S8:144:SER:HB3	2.35	0.41
120:S1:355:LEU:HD22	120:S1:543:LEU:HD22	2.02	0.41
123:S4:63:SER:O	123:S4:66:GLN:CB	2.69	0.41
123:S4:81:ARG:HH22	123:S4:127:ASP:CG	2.28	0.41
127:S8:156:GLU:HB3	127:S8:166:VAL:HG11	2.03	0.41
153:TH:200:CDL:H741	153:TH:200:CDL:H712	1.91	0.41
146:V1:203:GLY:H	147:V2:111:MET:HG2	1.85	0.41
146:V1:275:LYS:HB3	146:V1:277:TYR:CE2	2.56	0.41
146:V1:343:LEU:HA	146:V1:346:VAL:HG22	2.03	0.41
146:V1:381:GLY:O	146:V1:387:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
148:X1:129:ASN:OD1	148:X1:129:ASN:N	2.54	0.41
153:U1:101:CDL:H521	153:U1:101:CDL:H341	2.02	0.41
152:2f:302:PC1:H222	54:sc:45:TYR:HE1	1.86	0.41
6:2i:3:SER:O	6:2i:7:MET:HG2	2.21	0.41
14:3t:2:SER:O	22:6t:1:MET:N	2.41	0.41
153:6c:202:CDL:H671	34:f:205:ASN:HD21	1.86	0.41
25:7l:906:GLN:O	25:7l:910:ILE:HG12	2.21	0.41
26:a:301:PRO:HB3	31:c3:403:TRP:CH2	2.56	0.41
153:a:504:CDL:H171	153:a:504:CDL:H751	2.02	0.41
28:bp:366:THR:OG1	28:bp:403:ALA:HB1	2.21	0.41
28:bp:384:ALA:HA	31:c3:215:GLN:NE2	2.35	0.41
28:bp:413:GLU:C	28:bp:415:GLY:H	2.29	0.41
29:c1:346:LEU:HD23	29:c1:349:ILE:HD11	2.03	0.41
154:c1:702:HEA:HMB1	154:c1:702:HEA:HHB	1.82	0.41
31:c3:277:LEU:HB3	65:y7:324:ILE:HG12	2.02	0.41
32:d:178:TRP:HA	32:d:181:LYS:HD3	2.02	0.41
43:m1:95:ASN:ND2	43:m1:161:TYR:OH	2.54	0.41
43:m1:153:PRO:HG3	152:m2:405:PC1:H3D2	2.02	0.41
49:q:81:SER:OG	59:vb:245:GLN:NE2	2.53	0.41
52:sa:54:VAL:HG13	52:sa:208:VAL:HG21	2.02	0.41
53:sb:105:ILE:HG23	53:sb:116:LEU:HD21	2.03	0.41
59:vb:497:HIS:ND1	65:y7:189:TYR:OH	2.31	0.41
63:y0:4:TRP:CZ3	63:y0:53:LEU:HD21	2.55	0.41
75:a5:144:LEU:HD13	122:s3:51:ARG:HB2	2.02	0.41
77:a7:229:ASP:HB3	125:s6:91:THR:HA	2.03	0.41
82:al:55:GLY:HA3	82:al:98:TRP:HH2	1.85	0.41
82:al:118:PHE:HB3	127:s8:222:PRO:HB3	2.02	0.41
84:an:154:ALA:HA	84:an:159:PRO:HA	2.03	0.41
89:b7:31:LYS:NZ	92:bl:88:SER:O	2.54	0.41
89:b7:80:GLN:O	89:b7:84:ASN:HB2	2.21	0.41
164:b8:301:U10:H161	164:b8:301:U10:H121	1.92	0.41
92:bl:75:ASN:ND2	104:n5:363:ASN:HB2	2.35	0.41
97:g2:216:LYS:HE2	97:g2:216:LYS:HB3	1.89	0.41
98:g3:58:LYS:HE3	98:g3:95:GLU:HA	2.03	0.41
153:n5:806:CDL:HA32	107:p2:129:ARG:HH22	1.85	0.41
106:p1:94:PRO:O	106:p1:163:ARG:NH2	2.50	0.41
108:qA:305:LEU:HD12	108:qA:375:ILE:HG22	2.02	0.41
109:qB:65:ARG:O	109:qB:76:ALA:HA	2.21	0.41
111:qD:115:HIS:CD2	111:qD:116:PRO:HD2	2.55	0.41
110:qc:116:TRP:CG	166:qc:503:HEM:HBC1	2.55	0.41
111:qd:69:SER:OG	111:qd:237:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
111:qd:297:TYR:CE1	116:qi:12:LYS:HA	2.56	0.41
112:qe:106:PHE:CD1	152:qe:303:PC1:H2F2	2.56	0.41
122:s3:84:ASN:HB2	122:s3:87:ASN:ND2	2.30	0.41
122:s3:193:ASN:ND2	123:s4:128:THR:HG21	2.35	0.41
124:s5:74:TYR:CE2	124:s5:76:GLU:HG2	2.55	0.41
126:s7:135:PHE:HB2	127:s8:109:TYR:OH	2.21	0.41
128:t1:136:MET:HE2	128:t1:159:PHE:CD2	2.56	0.41
129:t2:176:LYS:O	129:t2:180:ILE:HG12	2.20	0.41
142:tf:82:LEU:HD23	142:tf:87:ILE:HD12	2.02	0.41
146:v1:126:CYS:O	146:v1:130:GLU:HG2	2.21	0.41
146:v1:316:LEU:HD21	146:v1:364:PRO:HG3	2.02	0.41
3:2F:245:LEU:O	3:2F:249:VAL:HG23	2.21	0.41
4:2G:58:ARG:HB3	7:2J:34:HIS:CE1	2.56	0.41
4:2G:120:ASN:ND2	4:2G:123:ASN:O	2.28	0.41
12:2O:32:LEU:HD23	54:SC:43:ARG:HH22	1.86	0.41
25:7L:933:ILE:O	25:7L:940:ARG:NH2	2.27	0.41
29:C1:126:HIS:HB2	29:C1:336:THR:HG21	2.01	0.41
29:C1:134:TYR:HB2	29:C1:137:LEU:HB2	2.03	0.41
152:C1:711:PC1:H221	153:VB:703:CDL:H822	2.03	0.41
152:C1:711:PC1:H251	153:VB:703:CDL:H762	2.02	0.41
152:C1:711:PC1:H231	42:M:68:TRP:HZ2	1.85	0.41
152:C1:711:PC1:H242	153:VB:703:CDL:H822	2.02	0.41
31:C3:345:ILE:HD11	61:X:120:LEU:HD23	2.02	0.41
33:E:4:ALA:HB1	36:G:294:TYR:HA	2.02	0.41
34:F:189:PRO:HG2	34:F:190:LEU:HD12	2.03	0.41
39:J:182:TRP:HA	152:N:303:PC1:H132	2.02	0.41
153:J:301:CDL:H112	46:N:139:TYR:CZ	2.56	0.41
43:M1:51:GLU:HG3	43:M1:100:ALA:HB2	2.02	0.41
45:M3:279:TYR:CG	153:M3:401:CDL:H112	2.55	0.41
50:R:27:LEU:HB2	66:Z:72:TYR:OH	2.21	0.41
52:SA:532:TYR:OH	52:SA:605:VAL:O	2.26	0.41
53:SB:105:ILE:HD11	53:SB:156:ILE:HG21	2.01	0.41
69:2B:35:ILE:HG12	69:2B:69:SER:HB2	2.01	0.41
70:4L:8:TRP:CZ3	70:4L:11:ILE:HD11	2.55	0.41
73:A2:30:ARG:HG2	75:A5:193:ILE:HD12	2.03	0.41
77:A7:11:ILE:HG21	153:T7:201:CDL:H151	2.03	0.41
152:AM:202:PC1:H351	153:TE:101:CDL:H312	2.03	0.41
158:AN:306:3PE:H111	87:B4:90:TRP:HZ2	1.86	0.41
153:B3:102:CDL:H731	158:T4:302:3PE:H2	2.02	0.41
89:B7:80:GLN:O	89:B7:84:ASN:HB2	2.21	0.41
94:C4:1:MET:O	135:T8:70:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
100:N1:208:ILE:HG23	100:N1:219:PHE:CZ	2.56	0.41
101:N2:260:LEU:HD12	101:N2:262:ILE:HD11	2.03	0.41
103:N4:323:LYS:O	103:N4:327:GLN:HG2	2.21	0.41
107:P2:89:HIS:NE2	107:P2:96:SER:OG	2.42	0.41
110:QC:213:MET:HE3	110:QC:215:GLY:HA2	2.02	0.41
113:QF:20:PRO:O	113:QF:24:VAL:HG23	2.21	0.41
114:QG:189:TYR:HD1	114:QG:192:LEU:HB2	1.85	0.41
108:Qa:435:TYR:HD1	108:Qa:435:TYR:HA	1.76	0.41
109:Qb:363:ILE:HB	109:Qb:382:TYR:HB3	2.02	0.41
110:Qc:135:VAL:HA	110:Qc:142:SER:HB3	2.03	0.41
110:Qc:211:SER:OG	110:Qc:349:VAL:HB	2.20	0.41
110:Qc:259:PHE:HA	111:Qd:167:LEU:HB3	2.01	0.41
110:Qc:345:LYS:HB2	114:Qg:35:ARG:NH2	2.35	0.41
111:Qd:299:ASN:HD22	111:Qd:303:TYR:HE2	1.68	0.41
121:S2:24:LYS:NZ	121:S2:25:THR:O	2.54	0.41
149:C:205:ILE:O	149:C:209:ILE:HG12	2.20	0.41
3:2f:94:PHE:HZ	3:2f:248:ARG:HG2	1.85	0.41
3:2f:209:TYR:CZ	53:sb:37:LEU:HD13	2.56	0.41
4:2g:172:TYR:CD1	4:2g:198:LYS:HE3	2.55	0.41
153:2m:101:CDL:HB22	54:sc:29:ILE:HG13	2.02	0.41
13:2t:30:LYS:NZ	13:2t:40:GLU:OE2	2.42	0.41
22:6t:13:ILE:HG12	22:6t:44:TYR:CD1	2.56	0.41
24:7c:102:ARG:NH1	24:7c:103:GLN:O	2.54	0.41
25:7l:897:VAL:HG12	25:7l:899:GLN:H	1.85	0.41
25:7l:903:ILE:HD12	25:7l:903:ILE:HA	1.85	0.41
26:a:102:ASN:HB3	26:a:164:TRP:O	2.21	0.41
26:a:334:ASN:O	26:a:336:LEU:N	2.51	0.41
27:b:29:ARG:HG2	27:b:185:ILE:HD13	2.03	0.41
28:bp:240:LYS:N	28:bp:252:VAL:O	2.53	0.41
29:c1:134:TYR:CB	29:c1:137:LEU:HB2	2.50	0.41
29:c1:342:THR:HG22	29:c1:396:VAL:HA	2.03	0.41
29:c1:606:THR:HG21	43:m1:222:LYS:HD2	2.03	0.41
29:c1:644:LYS:HD2	36:g:231:PHE:HB2	2.02	0.41
152:c1:711:PC1:H242	153:q:203:CDL:H822	2.02	0.41
31:c3:173:SER:HB3	48:p:35:ILE:HG21	2.03	0.41
31:c3:265:LEU:HD13	46:n:54:ASP:HB3	2.03	0.41
31:c3:366:VAL:HG11	49:q:92:VAL:HG21	2.02	0.41
32:d:176:ASN:OD1	32:d:301:ARG:NH2	2.53	0.41
32:d:220:ASN:ND2	32:d:226:LYS:O	2.53	0.41
33:e:31:PHE:CD1	33:e:62:ARG:HG3	2.56	0.41
34:f:335:THR:O	35:fs:33:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:222:PHE:HB2	60:w:5:TYR:CE2	2.56	0.41
39:j:57:HIS:CE1	46:n:48:HIS:HB3	2.56	0.41
39:j:96:TRP:HB3	152:j:302:PC1:H262	2.03	0.41
40:k:97:ASN:HA	40:k:100:LYS:HE2	2.02	0.41
41:l:125:TYR:OH	153:l:301:CDL:OA3	2.26	0.41
43:m1:86:LEU:HB2	43:m1:89:TYR:HB3	2.02	0.41
45:m3:77:ASP:HB3	45:m3:295:GLU:HB3	2.01	0.41
45:m3:178:THR:O	45:m3:182:ASN:ND2	2.42	0.41
47:o:79:ALA:O	47:o:83:MET:HG2	2.21	0.41
50:r:106:CYS:HB2	50:r:107:PRO:HD3	2.02	0.41
52:sa:220:ARG:HH22	52:sa:471:LYS:C	2.28	0.41
53:sb:86:LYS:O	53:sb:88:VAL:HG23	2.21	0.41
53:sb:192:LYS:HE3	53:sb:193:PRO:HD2	2.02	0.41
164:sc:102:U10:O4	55:sd:12:TYR:OH	2.28	0.41
59:vb:367:TYR:CE1	59:vb:562:LYS:HE2	2.56	0.41
59:vb:398:ILE:O	59:vb:402:LEU:HG	2.21	0.41
59:vb:582:TYR:HA	59:vb:586:ILE:HD12	2.03	0.41
62:y:93:TYR:CZ	62:y:97:LEU:HD11	2.56	0.41
65:y7:164:ASN:HB3	149:c:133:ALA:HB3	2.03	0.41
71:5b:11:PHE:HD1	90:b8:86:GLN:HE21	1.68	0.41
72:a1:71:LYS:HD3	72:a1:71:LYS:HA	1.86	0.41
72:a1:71:LYS:HG3	141:te:51:TYR:CD2	2.56	0.41
73:a2:52:ARG:HD2	120:s1:646:HIS:CE1	2.56	0.41
76:a6:133:LEU:HD21	168:ab:201:ZMP:H25A	2.03	0.41
77:a7:208:ARG:HH11	121:s2:327:THR:HG22	1.86	0.41
79:a9:165:ALA:HA	79:a9:197:ARG:HB3	2.03	0.41
83:am:39:PHE:HB3	127:s8:49:LEU:HD11	2.03	0.41
84:an:52:TRP:CE3	84:an:55:ARG:HB2	2.56	0.41
86:b3:55:ARG:NH2	153:b3:102:CDL:HA22	2.36	0.41
87:b4:120:SER:O	87:b4:124:GLY:N	2.54	0.41
87:b4:147:GLN:HB3	103:n4:100:LEU:HD23	2.03	0.41
92:bl:41:PHE:CD2	92:bl:46:PRO:HG2	2.56	0.41
94:c4:97:VAL:HG22	139:tc:80:ARG:HG3	2.03	0.41
96:g1:137:GLU:OE1	96:g1:154:LYS:NZ	2.38	0.41
100:n1:79:ILE:HG21	100:n1:240:TYR:CE2	2.56	0.41
100:n1:213:GLU:HG3	100:n1:255:PHE:CZ	2.56	0.41
101:n2:113:THR:HG23	101:n2:279:LEU:HD21	2.02	0.41
101:n2:260:LEU:HD12	101:n2:262:ILE:HD11	2.03	0.41
102:n3:29:TYR:HD1	152:n3:201:PC1:H31	1.86	0.41
102:n3:48:LYS:HB3	102:n3:48:LYS:HE2	1.83	0.41
103:n4:100:LEU:HB2	144:th:48:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
103:n4:382:TYR:CD1	103:n4:388:ARG:HG3	2.56	0.41
104:n5:117:PHE:CD1	144:th:113:ARG:HD2	2.55	0.41
104:n5:173:ILE:HB	104:n5:217:TYR:HD2	1.86	0.41
104:n5:256:SER:HB3	104:n5:512:TYR:HE1	1.85	0.41
104:n5:497:VAL:O	104:n5:501:THR:HG23	2.21	0.41
153:n6:302:CDL:H532	139:tc:24:VAL:HG22	2.02	0.41
108:qA:177:THR:HA	108:qA:233:SER:HB2	2.03	0.41
108:qA:262:PHE:O	108:qA:266:VAL:HG23	2.21	0.41
109:qB:349:SER:HB3	109:qB:352:HIS:HB2	2.03	0.41
109:qB:495:ARG:NH1	153:qB:601:CDL:OB4	2.52	0.41
110:qC:164:TYR:CZ	110:qC:171:LYS:HE3	2.55	0.41
112:qE:206:PRO:HA	112:qE:214:TYR:H	1.86	0.41
115:qH:101:TRP:NE1	153:qH:201:CDL:OA7	2.47	0.41
152:qI:201:PC1:H152	152:qI:201:PC1:H111	1.86	0.41
109:qb:390:GLN:O	109:qb:391:MET:C	2.63	0.41
110:qc:413:TYR:OH	114:qg:64:ALA:HA	2.20	0.41
111:qd:183:HIS:CD2	113:qf:21:LYS:HD3	2.56	0.41
112:qe:44:VAL:HG11	114:qg:132:PHE:CE1	2.56	0.41
114:qg:92:GLU:HA	114:qg:96:CYS:HB3	2.03	0.41
120:s1:125:HIS:O	120:s1:158:LYS:NZ	2.54	0.41
120:s1:164:LYS:HZ3	120:s1:174:MET:HG3	1.86	0.41
120:s1:210:TYR:CE2	147:v2:30:HIS:HB2	2.56	0.41
120:s1:225:ASP:OD2	120:s1:292:ARG:NH2	2.44	0.41
120:s1:345:GLU:O	120:s1:519:GLY:N	2.54	0.41
120:s1:543:LEU:HD11	120:s1:613:ASP:OD2	2.20	0.41
127:s8:178:CYS:N	162:s8:302:SF4:S4	2.93	0.41
128:t1:18:ILE:HG12	128:t1:46:TYR:HB3	2.02	0.41
128:t1:210:TYR:OH	128:t1:254:GLN:NE2	2.53	0.41
129:t2:121:LEU:HA	129:t2:164:ILE:O	2.21	0.41
129:t2:286:ASP:HA	129:t2:291:LYS:HG3	2.03	0.41
130:t3:83:VAL:HA	130:t3:86:GLU:HG2	2.03	0.41
140:td:33:PHE:O	140:td:37:LYS:HG2	2.20	0.41
143:tg:26:LYS:HG2	143:tg:44:TYR:HE2	1.85	0.41
143:tg:112:ARG:O	143:tg:116:SER:OG	2.29	0.41
146:v1:47:ARG:NH2	146:v1:133:ARG:O	2.40	0.41
146:v1:87:GLY:O	146:v1:92:GLY:HA2	2.20	0.41
148:x1:35:PRO:HA	148:x1:121:TRP:CZ2	2.55	0.41
148:x1:106:ASN:ND2	148:x1:110:ARG:HE	2.19	0.41
3:2F:210:SER:OG	153:2G:204:CDL:HA62	2.21	0.41
3:2F:287:THR:O	3:2F:291:GLU:HG2	2.21	0.41
4:2G:104:GLU:HG3	8:2K:26:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2L:18:ASP:HB3	9:2L:21:LEU:HG	2.03	0.41
14:3T:37:LEU:HD21	14:3T:55:LEU:HD11	2.02	0.41
20:6C:26:LYS:HA	20:6C:29:PHE:CD2	2.56	0.41
20:6C:33:ALA:HA	20:6C:36:TRP:NE1	2.35	0.41
153:6C:203:CDL:H671	34:F:205:ASN:HD21	1.86	0.41
23:7A:50:ALA:HA	26:A:247:TYR:CZ	2.55	0.41
25:7L:906:GLN:O	25:7L:910:ILE:HG12	2.21	0.41
25:7L:980:ASP:N	25:7L:980:ASP:OD1	2.54	0.41
26:A:298:TYR:CZ	31:C3:252:LEU:HD13	2.56	0.41
26:A:334:ASN:O	26:A:336:LEU:N	2.52	0.41
27:B:238:THR:HA	27:B:239:PRO:HD3	1.97	0.41
28:BP:139:GLY:HA2	28:BP:144:LEU:HD13	2.01	0.41
28:BP:240:LYS:N	28:BP:252:VAL:O	2.53	0.41
29:C1:147:CYS:SG	29:C1:148:GLY:N	2.94	0.41
30:C2:45:TRP:CD1	58:V:103:LEU:HD23	2.56	0.41
30:C2:364:LYS:HD2	47:O:140:GLN:HG2	2.03	0.41
31:C3:265:LEU:HD13	46:N:54:ASP:HB3	2.03	0.41
31:C3:470:ARG:HD3	31:C3:470:ARG:HA	1.78	0.41
32:D:176:ASN:OD1	32:D:301:ARG:NH2	2.53	0.41
32:D:195:PHE:HE1	39:J:217:LEU:HB2	1.85	0.41
32:D:313:ASN:OD1	32:D:322:TRP:NE1	2.54	0.41
33:E:31:PHE:CD1	33:E:62:ARG:HG3	2.56	0.41
33:E:193:GLN:O	33:E:197:GLY:N	2.54	0.41
34:F:240:SER:HB2	34:F:246:PHE:HE2	1.86	0.41
34:F:335:THR:O	35:FS:33:PRO:HA	2.21	0.41
153:F:402:CDL:H121	153:F:402:CDL:H512	2.02	0.41
35:FS:118:VAL:HG13	36:G:89:MET:SD	2.60	0.41
36:G:222:PHE:HB2	60:W:5:TYR:CE2	2.56	0.41
37:H:197:VAL:HG11	37:H:282:VAL:HG11	2.03	0.41
37:H:227:ASP:OD1	37:H:227:ASP:N	2.54	0.41
38:I:35:GLU:O	38:I:39:GLN:HG2	2.20	0.41
40:K:61:THR:OG1	40:K:63:ASP:OD2	2.39	0.41
41:L:200:TYR:HB3	41:L:204:LEU:HB2	2.03	0.41
42:M:137:ASP:HB3	42:M:140:THR:OG1	2.21	0.41
42:M:185:PRO:HG2	62:Y:65:TYR:CE2	2.56	0.41
46:N:6:ALA:O	46:N:10:GLU:HG2	2.21	0.41
48:P:39:VAL:HG22	48:P:118:LEU:HB3	2.02	0.41
51:S:41:ASN:O	51:S:45:GLN:HG2	2.21	0.41
52:SA:146:PRO:HD2	52:SA:186:ALA:HB1	2.02	0.41
52:SA:209:ILE:HD11	52:SA:485:LEU:HD12	2.03	0.41
53:SB:86:LYS:O	53:SB:87:TYR:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SB:271:ASP:O	53:SB:273:GLN:NE2	2.54	0.41
59:VB:123:PRO:HG2	59:VB:208:MET:O	2.20	0.41
62:Y:45:ASN:HD21	62:Y:105:PHE:HA	1.85	0.41
63:Y0:4:TRP:HB3	63:Y0:6:PHE:CE1	2.55	0.41
64:Y5:101:LYS:HE2	64:Y5:101:LYS:HB3	1.88	0.41
153:Y5:201:CDL:H751	67:Z1:59:THR:HG23	2.03	0.41
68:1B:3:TYR:HB3	100:N1:110:TRP:HB3	2.03	0.41
71:5B:5:LYS:NZ	153:B8:302:CDL:OB4	2.48	0.41
153:5B:201:CDL:H751	106:P1:142:ILE:HG22	2.03	0.41
73:A2:37:TYR:CZ	120:S1:381:PHE:HE2	2.39	0.41
76:A6:127:THR:HB	122:S3:189:VAL:HG12	2.03	0.41
79:A9:252:GLN:HE21	79:A9:252:GLN:HB3	1.70	0.41
153:A9:403:CDL:H201	152:N3:201:PC1:H362	2.02	0.41
81:AC:58:ALA:HB1	81:AC:79:LEU:HD21	2.02	0.41
82:AL:23:GLU:HB3	82:AL:27:LYS:HB2	2.03	0.41
82:AL:163:PRO:HB3	120:S1:304:ASN:HD21	1.86	0.41
83:AM:47:GLY:N	127:S8:77:GLU:OE2	2.51	0.41
84:AN:154:ALA:HA	84:AN:159:PRO:HA	2.03	0.41
153:AN:302:CDL:H741	103:N4:247:PHE:CE1	2.56	0.41
94:C4:101:ASN:OD1	94:C4:101:ASN:N	2.54	0.41
96:G1:84:VAL:HA	99:J1:157:GLY:O	2.21	0.41
98:G3:23:ARG:HB3	98:G3:27:LYS:NZ	2.36	0.41
99:J1:78:ALA:HB2	109:QB:278:PHE:HZ	1.86	0.41
99:J1:289:LEU:HB3	99:J1:296:VAL:HB	2.03	0.41
100:N1:185:VAL:O	100:N1:188:ILE:HG12	2.20	0.41
101:N2:127:TYR:HA	101:N2:167:VAL:HG21	2.03	0.41
103:N4:477:MET:HE2	103:N4:477:MET:HB3	1.97	0.41
104:N5:77:GLN:HG3	104:N5:83:ASN:HD22	1.85	0.41
104:N5:334:LYS:HG3	158:N5:802:3PE:H121	2.03	0.41
108:QA:94:LEU:HB3	108:QA:250:PHE:HB2	2.03	0.41
108:QA:101:ASP:HB3	108:QA:243:ASN:OD1	2.21	0.41
111:QD:188:PHE:HD2	113:QF:46:LEU:HD23	1.85	0.41
111:QD:188:PHE:CZ	113:QF:47:ARG:HG2	2.55	0.41
111:QD:240:ASN:HA	111:QD:243:GLN:HG2	2.03	0.41
114:QG:264:ARG:HH21	114:QG:291:GLU:CD	2.28	0.41
114:QG:270:ASP:OD2	114:QG:280:TYR:OH	2.28	0.41
108:Qa:417:LEU:O	108:Qa:421:VAL:HG13	2.21	0.41
109:Qb:504:TRP:HA	109:Qb:507:ASN:ND2	2.36	0.41
110:Qc:83:LEU:O	110:Qc:87:GLY:N	2.44	0.41
110:Qc:186:TYR:CD2	164:Qc:501:U10:H162	2.56	0.41
110:Qc:378:PHE:O	110:Qc:382:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
160:Qh:201:PX2:H14	160:Qh:201:PX2:H43	2.03	0.41
120:S1:125:HIS:O	120:S1:158:LYS:NZ	2.54	0.41
120:S1:210:TYR:CE2	147:V2:30:HIS:HB2	2.56	0.41
120:S1:262:ILE:HG22	120:S1:287:ILE:HG21	2.03	0.41
120:S1:405:CYS:O	120:S1:435:GLN:NE2	2.54	0.41
120:S1:525:GLU:HG3	120:S1:591:VAL:HG11	2.03	0.41
122:S3:55:PHE:O	122:S3:58:ILE:HB	2.21	0.41
123:S4:168:TYR:HE2	146:V1:225:ARG:HB3	1.85	0.41
126:S7:123:VAL:HA	126:S7:124:PRO:HD3	1.87	0.41
128:T1:18:ILE:HG12	128:T1:46:TYR:HB3	2.03	0.41
128:T1:118:GLN:OE1	128:T1:124:PRO:HG3	2.21	0.41
128:T1:132:ASN:HB2	128:T1:135:PHE:HB3	2.03	0.41
128:T1:136:MET:HE3	128:T1:136:MET:HB3	1.99	0.41
128:T1:286:SER:HB3	128:T1:331:LEU:HB2	2.03	0.41
128:T1:383:TYR:CD1	128:T1:386:ILE:HD11	2.55	0.41
129:T2:24:ALA:O	129:T2:28:ILE:HG13	2.21	0.41
132:T5:178:GLN:HE21	132:T5:182:ASN:HD21	1.69	0.41
133:T6:79:HIS:HB3	133:T6:86:TYR:CD1	2.56	0.41
142:TF:186:ARG:HG2	146:V1:459:PRO:HB3	2.03	0.41
143:TG:15:LEU:HD23	143:TG:24:LEU:HD13	2.01	0.41
145:TX:23:SER:N	145:TX:73:LEU:HD23	2.36	0.41
171:V1:501:FMN:HM81	171:V1:501:FMN:HM73	1.92	0.41
147:V2:125:CYS:HA	147:V2:164:VAL:O	2.21	0.41
148:X1:123:ARG:HH21	148:X1:126:ARG:HH22	1.69	0.41
153:C:301:CDL:OB3	150:U1:5:UNK:N	2.54	0.41
149:c:157:VAL:O	153:c:301:CDL:HA31	2.21	0.41
3:2f:186:LEU:HB2	3:2f:228:TRP:CH2	2.55	0.41
3:2f:202:ALA:O	3:2f:212:ARG:NH2	2.54	0.41
3:2f:245:LEU:O	3:2f:249:VAL:HG23	2.21	0.41
8:2k:80:ILE:O	8:2k:80:ILE:HG13	2.20	0.41
11:2n:60:LYS:HE2	11:2n:60:LYS:HB3	1.89	0.41
19:6b:103:THR:HG21	20:6c:69:ARG:HG2	2.03	0.41
19:6b:110:LEU:HD22	42:m:180:ALA:O	2.21	0.41
27:b:127:TYR:CE2	27:b:214:ARG:HG2	2.56	0.41
28:bp:261:TRP:HB3	28:bp:280:PRO:HA	2.03	0.41
28:bp:268:SER:HB3	28:bp:305:HIS:CD2	2.56	0.41
29:c1:315:ILE:HD11	31:c3:315:ILE:HG13	2.02	0.41
33:e:130:TRP:HA	33:e:133:VAL:HG22	2.03	0.41
34:f:275:GLU:HG3	34:f:276:ASP:H	1.86	0.41
35:fs:170:TRP:CE2	152:fs:204:PC1:H252	2.56	0.41
43:m1:156:LEU:HD23	43:m1:156:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:m3:55:ASN:O	45:m3:59:LEU:HG	2.21	0.41
52:sa:51:ALA:HB3	52:sa:67:LEU:HD13	2.02	0.41
53:sb:192:LYS:HE3	53:sb:192:LYS:HB3	1.93	0.41
64:y5:101:LYS:HE2	64:y5:101:LYS:HB3	1.88	0.41
65:y7:108:LYS:HE3	65:y7:108:LYS:HB3	1.87	0.41
74:a3:75:LEU:HD22	158:a3:202:3PE:H222	2.03	0.41
77:a7:63:HIS:CD2	120:s1:151:ILE:HG13	2.55	0.41
79:a9:289:ILE:HD12	152:tc:102:PC1:H2B2	2.03	0.41
97:g2:41:GLU:HA	97:g2:42:PRO:HD3	1.92	0.41
101:n2:130:SER:O	101:n2:134:ILE:HG13	2.21	0.41
101:n2:260:LEU:HB2	101:n2:262:ILE:HG13	2.02	0.41
104:n5:173:ILE:HD11	104:n5:214:MET:HE2	2.03	0.41
104:n5:207:ILE:HG12	104:n5:266:VAL:HG22	2.03	0.41
104:n5:622:LYS:HG3	104:n5:626:LEU:HD13	2.03	0.41
153:p1:402:CDL:H561	153:p1:402:CDL:HA61	2.03	0.41
108:qA:214:LEU:HD11	108:qA:224:LEU:HD21	2.02	0.41
108:qA:331:ASN:HB2	108:qA:332:LEU:HD12	2.03	0.41
109:qB:324:PHE:CZ	109:qB:463:ILE:HG23	2.56	0.41
114:qG:70:TRP:CZ3	153:qH:201:CDL:H111	2.55	0.41
116:qI:47:LYS:HE2	116:qI:47:LYS:HB3	1.87	0.41
109:qb:173:PHE:CZ	109:qb:237:VAL:HG21	2.55	0.41
111:qd:299:ASN:HD22	111:qd:303:TYR:HE2	1.68	0.41
112:qe:109:LEU:HD11	152:qe:303:PC1:H242	2.03	0.41
114:qg:87:LEU:HA	114:qg:154:ILE:HG12	2.03	0.41
120:s1:244:TRP:NE1	127:s8:144:SER:HB3	2.36	0.41
127:s8:194:PRO:HG3	127:s8:223:GLN:CD	2.46	0.41
128:t1:136:MET:HE3	128:t1:136:MET:HB3	1.99	0.41
129:t2:283:LEU:HG	129:t2:285:VAL:HG22	2.03	0.41
130:t3:135:VAL:HG11	130:t3:141:ILE:HD12	2.02	0.41
131:t4:66:ASP:OD1	131:t4:66:ASP:N	2.51	0.41
144:th:20:LYS:HE3	144:th:21:TYR:CE2	2.56	0.41
146:v1:115:VAL:HG11	146:v1:213:LEU:HD22	2.02	0.41
146:v1:264:ALA:HA	146:v1:272:ALA:HB1	2.02	0.41
3:2F:82:ASN:O	3:2F:103:ARG:HD3	2.21	0.41
3:2F:209:TYR:CZ	53:SB:37:LEU:HD13	2.56	0.41
152:2F:302:PC1:H222	54:SC:45:TYR:HE1	1.86	0.41
8:2K:73:ASP:OD2	8:2K:76:ASN:HB2	2.21	0.41
16:4T:29:VAL:O	16:4T:33:GLU:HG3	2.21	0.41
23:7A:80:VAL:HG21	65:Y7:350:LEU:HB2	2.03	0.41
24:7C:102:ARG:NH1	24:7C:103:GLN:O	2.54	0.41
27:B:253:ARG:NH2	48:P:88:ASP:O	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BP:189:SER:OG	28:BP:225:ARG:NH1	2.53	0.41
28:BP:303:ALA:HB3	28:BP:362:VAL:HG12	2.02	0.41
29:C1:524:VAL:HG13	29:C1:528:HIS:CE1	2.56	0.41
34:F:201:LEU:HD23	34:F:201:LEU:HA	1.89	0.41
35:FS:155:MET:HE2	35:FS:155:MET:HB3	1.99	0.41
42:M:16:GLY:O	42:M:22:LYS:NZ	2.47	0.41
43:M1:95:ASN:ND2	43:M1:161:TYR:OH	2.54	0.41
51:S:8:PHE:CD2	59:VB:367:TYR:HB3	2.56	0.41
52:SA:249:ARG:HD3	52:SA:249:ARG:HA	1.91	0.41
57:U:26:LEU:HD23	57:U:26:LEU:HA	1.88	0.41
72:A1:71:LYS:HG3	141:TE:51:TYR:HD2	1.86	0.41
74:A3:77:ASP:O	74:A3:81:ARG:HG3	2.20	0.41
83:AM:119:HIS:HB2	83:AM:123:TYR:CD2	2.56	0.41
83:AM:144:TYR:CE2	124:S5:14:PRO:HG3	2.55	0.41
93:BM:92:HIS:CE1	93:BM:111:TYR:HB3	2.56	0.41
97:G2:97:ARG:HH11	97:G2:125:ASN:HD21	1.69	0.41
98:G3:286:ASN:HD21	99:J1:135:LYS:HE2	1.86	0.41
100:N1:104:PHE:CE1	100:N1:129:LEU:HB3	2.52	0.41
100:N1:230:THR:HG22	100:N1:231:GLY:H	1.86	0.41
103:N4:382:TYR:CD1	103:N4:388:ARG:HG3	2.56	0.41
103:N4:440:ILE:HD13	103:N4:440:ILE:HA	1.96	0.41
104:N5:77:GLN:NE2	104:N5:84:LYS:HD2	2.36	0.41
104:N5:480:THR:HG22	104:N5:609:LEU:HD11	2.02	0.41
104:N5:622:LYS:HG3	104:N5:626:LEU:HD13	2.03	0.41
108:QA:74:ASN:OD1	108:QA:74:ASN:N	2.43	0.41
109:QB:257:GLN:O	109:QB:261:GLN:HG2	2.21	0.41
109:QB:333:ALA:HB2	109:QB:362:THR:HA	2.03	0.41
110:QC:4:ASN:O	110:Qc:14:LYS:NZ	2.40	0.41
110:QC:273:PHE:HA	110:QC:276:VAL:HG13	2.03	0.41
111:QD:92:TYR:O	111:QD:105:LEU:HD21	2.21	0.41
108:Qa:90:ASP:OD1	108:Qa:154:ASN:HB3	2.21	0.41
108:Qa:254:ALA:HB2	108:Qa:417:LEU:HD13	2.02	0.41
110:Qc:42:ILE:HG13	110:Qc:91:LEU:HD21	2.03	0.41
112:Qe:44:VAL:HG11	114:Qg:132:PHE:CE1	2.56	0.41
112:Qe:106:PHE:CD1	152:Qe:303:PC1:H2F2	2.55	0.41
120:S1:129:CYS:SG	120:S1:141:GLN:NE2	2.93	0.41
120:S1:239:PHE:HD2	127:S8:157:PRO:HB3	1.86	0.41
122:S3:82:LYS:HG3	122:S3:83:THR:HG23	2.03	0.41
128:T1:83:ILE:HB	128:T1:86:HIS:HD2	1.84	0.41
128:T1:254:GLN:HB2	128:T1:351:ALA:HB2	2.03	0.41
131:T4:181:ILE:HG23	131:T4:186:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
146:V1:421:GLU:HG2	146:V1:422:MET:HG3	2.02	0.41
147:V2:69:MET:HB2	147:V2:70:PRO:HD3	2.03	0.41
147:V2:182:TRP:HB3	147:V2:206:LYS:HG3	2.03	0.41
2:2e:173:LYS:HE3	2:2e:173:LYS:HB3	1.91	0.40
4:2g:153:TYR:CE2	8:2k:13:LYS:HG2	2.55	0.40
18:6a:74:ASN:HB2	49:q:76:VAL:HG21	2.03	0.40
20:6c:26:LYS:HA	20:6c:29:PHE:CD2	2.56	0.40
23:7a:77:LEU:HD23	65:y7:350:LEU:HD11	2.01	0.40
27:b:398:VAL:HG21	65:y7:408:VAL:HG13	2.02	0.40
29:c1:134:TYR:HB2	29:c1:137:LEU:HB2	2.03	0.40
29:c1:178:LYS:HE2	29:c1:178:LYS:HB3	1.87	0.40
30:c2:312:SER:O	30:c2:316:GLN:HG2	2.21	0.40
31:c3:212:ARG:HD2	40:k:51:MET:HE2	2.03	0.40
153:e:403:CDL:H121	153:FS:204:CDL:H321	2.03	0.40
34:f:174:TYR:O	34:f:178:ILE:HG13	2.21	0.40
34:f:262:GLN:HG3	51:S:159:VAL:HG23	2.03	0.40
38:i:117:MET:HE3	153:i:302:CDL:HA21	2.02	0.40
153:i:301:CDL:H332	153:i:301:CDL:H732	2.04	0.40
42:m:185:PRO:HG2	62:y:65:TYR:CE2	2.56	0.40
53:sb:72:LEU:HB2	53:sb:155:ILE:HG12	2.03	0.40
56:t:21:LYS:HD3	56:t:157:VAL:HG11	2.01	0.40
58:v:117:TYR:HB2	152:v:202:PC1:H143	2.04	0.40
153:vb:704:CDL:H361	153:vb:704:CDL:H792	2.02	0.40
63:y0:64:TYR:CE1	63:y0:66:ASP:HB2	2.56	0.40
65:y7:168:ILE:HD11	149:c:133:ALA:HB2	2.03	0.40
69:2b:154:PHE:CD2	153:c4:401:CDL:H611	2.56	0.40
72:a1:66:LEU:HD12	141:te:67:LEU:HD21	2.02	0.40
73:a2:19:PHE:HB2	73:a2:26:SER:HB3	2.03	0.40
91:b9:127:LEU:HD21	103:n4:475:LEU:HD12	2.01	0.40
95:fx:93:LYS:HE2	95:fx:148:LEU:HD23	2.02	0.40
97:g2:68:ASN:HD21	97:g2:85:TYR:HB3	1.86	0.40
102:n3:21:TRP:HA	139:tc:2:VAL:HG12	2.02	0.40
104:n5:569:LEU:HA	104:n5:572:TYR:HD2	1.85	0.40
108:qA:209:LYS:HG2	108:qA:218:GLY:O	2.22	0.40
109:qB:178:VAL:HG21	109:qB:230:ASP:HA	2.03	0.40
110:qC:82:TRP:HE1	152:qC:505:PC1:H11	1.86	0.40
110:qC:98:HIS:HD2	166:qC:502:HEM:C1C	2.39	0.40
110:qC:223:PHE:O	110:qC:227:LEU:HB2	2.21	0.40
111:qD:289:MET:HG3	112:qE:68:VAL:HG11	2.03	0.40
109:qb:57:ALA:O	109:qb:448:ARG:NH2	2.54	0.40
110:qc:345:LYS:HB2	114:qg:35:ARG:NH2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
113:qf:8:SER:OG	113:qf:9:ALA:N	2.54	0.40
115:qh:50:ASP:OD1	115:qh:50:ASP:N	2.54	0.40
125:s6:55:SER:O	125:s6:57:LYS:NZ	2.53	0.40
129:t2:198:LEU:HA	129:t2:212:LEU:HB3	2.03	0.40
131:t4:181:ILE:HG23	131:t4:186:PRO:HG3	2.02	0.40
136:t9:31:LYS:O	136:t9:35:CYS:N	2.53	0.40
144:th:25:ASN:HD21	144:th:28:GLU:HG2	1.84	0.40
146:v1:411:ASP:OD1	146:v1:411:ASP:N	2.53	0.40
147:v2:32:LYS:HD2	147:v2:32:LYS:HA	1.86	0.40
4:2G:153:TYR:CD1	8:2K:15:PRO:HG3	2.56	0.40
24:7C:236:ILE:HG21	43:M1:11:ARG:HB2	2.03	0.40
26:A:380:ARG:NH2	26:A:431:LEU:HG	2.35	0.40
27:B:127:TYR:CE2	27:B:214:ARG:HG2	2.56	0.40
29:C1:540:PHE:O	29:C1:544:TYR:HD2	2.04	0.40
30:C2:312:SER:O	30:C2:316:GLN:HG2	2.21	0.40
30:C2:513:VAL:HG12	30:C2:551:GLU:HG2	2.03	0.40
31:C3:366:VAL:HG11	49:Q:92:VAL:HG21	2.02	0.40
31:C3:421:TRP:CE2	31:C3:432:LEU:HD13	2.55	0.40
33:E:191:PHE:O	33:E:194:LEU:HB2	2.21	0.40
153:F:402:CDL:H841	35:FS:170:TRP:HB3	2.02	0.40
39:J:141:LEU:O	39:J:145:ASN:ND2	2.37	0.40
42:M:191:MET:SD	62:Y:30:ILE:HB	2.61	0.40
52:SA:432:CYS:C	52:SA:434:SER:H	2.29	0.40
55:SD:6:ILE:HG21	55:SD:24:ILE:HG21	2.02	0.40
59:VB:582:TYR:HA	59:VB:586:ILE:HD12	2.03	0.40
62:Y:27:ASN:ND2	62:Y:82:ALA:O	2.53	0.40
70:4L:54:ILE:HD13	124:S5:6:TYR:HB2	2.02	0.40
76:A6:56:THR:OG1	168:AB:201:ZMP:H14	2.20	0.40
77:A7:279:LEU:HD11	82:AL:46:ARG:HD3	2.03	0.40
158:B4:202:3PE:H232	158:B4:202:3PE:H262	1.98	0.40
88:B6:94:LEU:HG	132:T5:128:CYS:SG	2.61	0.40
97:G2:163:ARG:NH2	135:T8:16:LEU:O	2.38	0.40
100:N1:53:ARG:HB3	126:S7:42:SER:HA	2.03	0.40
101:N2:73:TYR:HB2	148:X1:98:TRP:CZ3	2.57	0.40
103:N4:56:ASN:HD22	103:N4:149:ILE:HG13	1.86	0.40
104:N5:207:ILE:HG12	104:N5:266:VAL:HG22	2.03	0.40
109:QB:144:GLU:HG3	109:QB:214:PHE:HE1	1.85	0.40
109:QB:324:PHE:CZ	109:QB:463:ILE:HG23	2.56	0.40
110:QC:345:LYS:N	110:QC:411:GLU:OE1	2.26	0.40
115:QH:26:LEU:HD23	115:QH:26:LEU:HA	1.93	0.40
108:Qa:449:LYS:HD3	108:Qa:449:LYS:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
109:Qb:57:ALA:O	109:Qb:448:ARG:NH2	2.54	0.40
115:Qh:56:ARG:HB2	116:Qi:14:TYR:CZ	2.56	0.40
116:Qi:56:ARG:HA	116:Qi:60:GLN:HB3	2.03	0.40
120:S1:560:VAL:HB	120:S1:574:ALA:HA	2.03	0.40
122:S3:73:LEU:H	122:S3:90:PHE:HZ	1.68	0.40
128:T1:84:ARG:HH12	128:T1:133:GLU:CD	2.29	0.40
128:T1:136:MET:HE2	128:T1:159:PHE:CD2	2.56	0.40
128:T1:180:TYR:CZ	128:T1:198:CYS:HB2	2.56	0.40
129:T2:198:LEU:HD13	129:T2:212:LEU:HD23	2.03	0.40
140:TD:18:ILE:HB	140:TD:19:PRO:HD3	2.02	0.40
144:TH:70:ILE:O	144:TH:74:SER:OG	2.24	0.40
147:V2:47:GLU:H	147:V2:47:GLU:CD	2.29	0.40
3:2f:122:ARG:HD3	12:2o:34:TYR:CG	2.56	0.40
13:2t:51:ILE:HG12	17:5t:26:TYR:CZ	2.57	0.40
26:a:298:TYR:CZ	31:c3:252:LEU:HD13	2.56	0.40
26:a:380:ARG:NH2	26:a:431:LEU:HG	2.35	0.40
26:a:435:LYS:HB2	26:a:435:LYS:HE3	1.78	0.40
28:bp:169:LYS:N	28:bp:181:VAL:O	2.49	0.40
29:c1:137:LEU:HG	29:c1:308:ILE:HG23	2.03	0.40
30:c2:45:TRP:CD1	58:v:103:LEU:HD23	2.56	0.40
30:c2:286:ASP:OD1	30:c2:286:ASP:N	2.49	0.40
153:f:401:CDL:H402	153:f:401:CDL:H582	2.04	0.40
35:fs:22:GLU:OE1	35:fs:24:HIS:HE1	2.04	0.40
152:m1:403:PC1:H272	153:m1:405:CDL:H712	2.03	0.40
46:n:6:ALA:O	46:n:10:GLU:HG2	2.21	0.40
46:n:143:LYS:NZ	152:n:302:PC1:O14	2.51	0.40
47:o:139:ILE:HG12	47:o:193:TYR:CE1	2.57	0.40
50:r:27:LEU:HB2	66:z:72:TYR:OH	2.21	0.40
50:r:99:ILE:HA	64:y5:63:TYR:OH	2.22	0.40
52:sa:119:TRP:HE1	52:sa:629:VAL:HG22	1.85	0.40
64:y5:14:ASN:OD1	64:y5:15:LYS:N	2.54	0.40
75:a5:143:GLU:HB2	122:s3:51:ARG:HE	1.85	0.40
76:a6:104:LEU:HD23	123:s4:66:GLN:HG2	2.03	0.40
79:a9:31:PHE:CE2	79:a9:33:ASP:HB3	2.56	0.40
82:al:101:TRP:CD1	82:al:109:PHE:HB3	2.55	0.40
83:am:119:HIS:HB2	83:am:123:TYR:CD2	2.56	0.40
83:am:165:ARG:HD2	83:am:165:ARG:HA	1.79	0.40
152:am:202:PC1:H351	153:te:101:CDL:H312	2.03	0.40
158:an:306:3PE:H111	87:b4:90:TRP:HZ2	1.86	0.40
85:b2:87:ASP:OD1	85:b2:87:ASP:N	2.55	0.40
88:b6:79:ASN:HD21	88:b6:82:TRP:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
92:bl:174:PRO:HA	92:bl:175:PRO:HD3	1.98	0.40
101:n2:5:LEU:HG	101:n2:10:TYR:HE2	1.86	0.40
107:p2:66:LEU:HG	107:p2:137:PHE:HZ	1.86	0.40
110:qC:368:TYR:O	110:qC:371:SER:OG	2.32	0.40
111:qD:114:ILE:HB	111:qD:134:ARG:HG2	2.02	0.40
111:qD:134:ARG:NH2	111:qD:141:TYR:O	2.54	0.40
111:qD:319:ALA:HB2	115:qh:28:HIS:CD2	2.55	0.40
114:qG:189:TYR:HD1	114:qG:192:LEU:HB2	1.85	0.40
108:qa:308:LEU:HA	108:qa:362:GLY:HA3	2.03	0.40
108:qa:309:PHE:CE2	108:qa:459:PRO:HB3	2.56	0.40
109:qb:289:PRO:HB3	109:qb:475:GLU:HB3	2.02	0.40
110:qc:22:VAL:HG11	115:qh:46:ARG:HG2	2.03	0.40
110:qc:104:TYR:HB2	110:qc:359:PHE:CZ	2.57	0.40
110:qc:169:THR:OG1	110:qc:177:THR:OG1	2.29	0.40
121:s2:153:GLU:CG	121:s2:202:THR:HG21	2.50	0.40
121:s2:169:MET:HE1	126:s7:31:CYS:O	2.21	0.40
126:s7:24:PRO:HD3	126:s7:51:VAL:HG13	2.02	0.40
128:t1:235:ASN:HD22	128:t1:238:GLN:HG3	1.86	0.40
128:t1:383:TYR:CD1	128:t1:386:ILE:HD11	2.55	0.40
152:tc:101:PC1:H261	152:tc:101:PC1:H292	1.90	0.40
146:v1:62:TRP:HE1	146:v1:137:HIS:HB3	1.87	0.40
146:v1:275:LYS:HB3	146:v1:277:TYR:CE2	2.56	0.40
146:v1:401:LEU:HD12	146:v1:402:VAL:HG23	2.03	0.40
153:2M:101:CDL:H571	153:2M:101:CDL:H602	1.94	0.40
18:6A:74:ASN:HB2	49:Q:76:VAL:HG21	2.03	0.40
23:7A:104:GLU:HG3	152:7A:202:PC1:H151	2.03	0.40
26:A:192:PRO:HB2	26:A:207:VAL:HG21	2.04	0.40
26:A:301:PRO:HB3	31:C3:403:TRP:CH2	2.56	0.40
28:BP:268:SER:HB3	28:BP:305:HIS:CD2	2.56	0.40
29:C1:61:SER:HB3	29:C1:113:ILE:HG13	2.03	0.40
29:C1:342:THR:HG22	29:C1:396:VAL:HA	2.03	0.40
29:C1:540:PHE:HE1	154:C1:702:HEA:H253	1.85	0.40
153:C1:712:CDL:H251	30:C2:52:ILE:HG12	2.03	0.40
31:C3:79:ASP:O	31:C3:82:SER:OG	2.29	0.40
41:L:43:TYR:O	41:L:47:LEU:HG	2.21	0.40
41:L:72:PHE:O	41:L:75:GLN:HG2	2.21	0.40
46:N:192:ASP:OD1	46:N:192:ASP:N	2.53	0.40
68:1B:11:LEU:HB2	72:A1:23:TYR:CE2	2.55	0.40
79:A9:31:PHE:CE2	79:A9:33:ASP:HB3	2.56	0.40
153:A9:402:CDL:H371	153:A9:402:CDL:H341	1.95	0.40
85:B2:87:ASP:N	85:B2:87:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
89:B7:102:ASP:HB3	90:B8:184:PHE:HE1	1.86	0.40
92:BL:75:ASN:ND2	104:N5:363:ASN:HB2	2.36	0.40
92:BL:139:ASN:O	92:BL:159:LYS:NZ	2.49	0.40
95:FX:128:ARG:HH21	95:FX:129:ASN:HD21	1.69	0.40
97:G2:108:VAL:HG22	97:G2:136:CYS:H	1.85	0.40
101:N2:217:LEU:HA	124:S5:48:HIS:HE1	1.86	0.40
103:N4:46:ASN:HD22	135:T8:41:LEU:HD13	1.86	0.40
104:N5:415:LEU:HB3	104:N5:416:PRO:HD3	2.02	0.40
107:P2:119:PRO:HD2	107:P2:122:ASP:HB2	2.03	0.40
108:QA:258:SER:HB3	108:QA:261:GLU:HB3	2.03	0.40
110:QC:102:LYS:HA	110:QC:102:LYS:HD3	1.74	0.40
164:QC:506:U10:H1M1	164:QC:506:U10:H72	1.94	0.40
108:Qa:169:ASP:O	108:Qa:173:GLU:HB2	2.21	0.40
111:Qd:297:TYR:CE1	116:Qi:12:LYS:HA	2.57	0.40
114:Qg:87:LEU:HA	114:Qg:154:ILE:HG12	2.03	0.40
114:Qg:261:ASP:OD1	114:Qg:261:ASP:N	2.38	0.40
122:S3:64:SER:HB3	122:S3:97:PHE:CZ	2.56	0.40
128:T1:280:PHE:CD2	128:T1:378:ASN:HB3	2.56	0.40
129:T2:70:LYS:HD3	129:T2:96:THR:HB	2.02	0.40
142:TF:46:LEU:HB2	142:TF:69:MET:HE2	2.02	0.40
142:TF:227:LYS:O	142:TF:231:GLN:HG2	2.22	0.40
145:TX:50:PHE:HB3	145:TX:82:ILE:HD11	2.03	0.40
14:3t:69:PHE:O	14:3t:73:VAL:HG23	2.21	0.40
18:6a:120:LEU:HB3	19:6b:187:PHE:CE1	2.52	0.40
20:6c:54:PHE:HE2	42:m:167:LEU:HD13	1.87	0.40
24:7c:144:TYR:OH	153:7c:301:CDL:OB4	2.39	0.40
28:bp:190:TRP:HA	28:bp:225:ARG:HB2	2.03	0.40
28:bp:359:ASP:OD1	28:bp:360:PHE:N	2.54	0.40
29:c1:238:ILE:HD12	29:c1:238:ILE:HA	1.89	0.40
32:d:277:PHE:HB3	32:d:292:LEU:HD11	2.03	0.40
36:g:47:ASN:O	36:g:51:VAL:HG23	2.22	0.40
38:i:153:PHE:HZ	38:i:196:TRP:HZ3	1.68	0.40
39:j:61:GLU:HG2	39:j:62:GLU:N	2.36	0.40
39:j:96:TRP:CH2	153:j:301:CDL:H722	2.56	0.40
43:m1:118:LEU:HB3	43:m1:139:THR:HG23	2.03	0.40
153:m1:402:CDL:HB31	153:m1:402:CDL:HA21	2.02	0.40
44:m2:191:ALA:O	44:m2:195:ASN:ND2	2.33	0.40
47:o:132:LYS:HD3	47:o:132:LYS:HA	1.92	0.40
51:s:90:PRO:HB2	64:y5:94:LEU:HG	2.02	0.40
52:sa:226:SER:O	52:sa:230:GLY:HA2	2.22	0.40
57:u:111:GLN:HB3	57:u:112:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:vb:120:THR:HG22	63:y0:25:TRP:CE3	2.56	0.40
59:vb:447:LEU:HD13	59:vb:455:PHE:CG	2.56	0.40
70:4l:20:VAL:HB	71:5b:83:LEU:HD22	2.03	0.40
76:a6:109:ILE:HD13	76:a6:109:ILE:HA	1.93	0.40
78:a8:215:SER:HA	134:t7:135:ARG:HD3	2.03	0.40
79:a9:217:ASP:OD1	79:a9:282:ARG:NH1	2.53	0.40
85:b2:81:PRO:HB2	85:b2:83:TYR:CE2	2.57	0.40
88:b6:94:LEU:HG	132:t5:128:CYS:SG	2.61	0.40
91:b9:11:PHE:CZ	170:b9:202:ADP:H4'	2.57	0.40
92:bl:150:ASN:ND2	103:n4:84:ASN:OD1	2.53	0.40
98:g3:23:ARG:HB3	98:g3:27:LYS:NZ	2.37	0.40
100:n1:13:LEU:O	100:n1:16:PRO:HD2	2.22	0.40
104:n5:479:ASP:HB3	104:n5:482:LYS:HB2	2.04	0.40
111:qD:115:HIS:HB2	111:qD:131:GLU:HG2	2.04	0.40
108:qa:238:LYS:HE2	108:qa:238:LYS:HB3	1.85	0.40
108:qa:419:GLU:OE2	108:qa:435:TYR:OH	2.29	0.40
109:qb:381:PHE:CE1	109:qb:395:SER:HB3	2.55	0.40
109:qb:418:TYR:HB3	109:qb:455:ILE:HD12	2.02	0.40
110:qc:28:HIS:HB3	110:qc:207:TRP:CH2	2.54	0.40
110:qc:284:PRO:O	110:qc:287:ALA:HB3	2.21	0.40
125:s6:87:CYS:SG	125:s6:122:TYR:OH	2.75	0.40
127:s8:122:GLY:CA	127:s8:193:GLY:O	2.67	0.40
128:t1:118:GLN:OE1	128:t1:124:PRO:HG3	2.20	0.40
128:t1:228:ASN:OD1	128:t1:228:ASN:N	2.47	0.40
129:t2:24:ALA:O	129:t2:28:ILE:HG13	2.21	0.40
130:t3:261:ASN:HB3	130:t3:267:GLU:HB3	2.02	0.40
147:v2:188:THR:H	147:v2:191:ASN:HB2	1.86	0.40
148:x1:123:ARG:HH21	148:x1:126:ARG:HH22	1.69	0.40
3:2F:218:LEU:HB3	3:2F:219:PRO:HD3	2.02	0.40
8:2K:30:ARG:NH2	55:SD:20:LYS:HZ1	2.18	0.40
153:6C:202:CDL:H341	29:C1:471:VAL:HG22	2.02	0.40
25:7L:890:ASP:HB3	60:W:75:TYR:HB2	2.03	0.40
28:BP:252:VAL:HG22	28:BP:258:VAL:HG22	2.03	0.40
28:BP:359:ASP:OD1	28:BP:360:PHE:N	2.54	0.40
31:C3:23:THR:O	31:C3:69:LYS:NZ	2.43	0.40
33:E:34:THR:HG21	33:E:62:ARG:HH22	1.86	0.40
33:E:40:ASP:HB2	33:E:289:TRP:CZ2	2.57	0.40
152:F:401:PC1:H361	152:FS:201:PC1:H352	2.03	0.40
35:FS:170:TRP:CE2	152:FS:201:PC1:H252	2.56	0.40
36:G:244:GLN:HA	36:G:247:GLN:HB3	2.03	0.40
37:H:57:LYS:HD3	37:H:315:PHE:CG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
152:M1:403:PC1:H272	153:M1:405:CDL:H712	2.03	0.40
44:M2:9:TRP:CZ3	44:M2:11:PRO:HG3	2.57	0.40
52:SA:208:VAL:HG22	52:SA:224:CYS:SG	2.61	0.40
57:U:111:GLN:HB3	57:U:112:PRO:HD3	2.02	0.40
59:VB:398:ILE:O	59:VB:402:LEU:HG	2.20	0.40
59:VB:456:GLN:HG2	65:Y7:243:TYR:CD1	2.56	0.40
59:VB:587:ALA:HB3	59:VB:588:PRO:HD3	2.04	0.40
153:2B:201:CDL:H621	153:2B:201:CDL:H652	1.90	0.40
71:5B:11:PHE:HD1	90:B8:86:GLN:HE21	1.69	0.40
76:A6:104:LEU:HD23	123:S4:66:GLN:HG2	2.03	0.40
76:A6:109:ILE:HD13	76:A6:109:ILE:HA	1.92	0.40
83:AM:16:ARG:O	121:S2:265:ASN:HB2	2.21	0.40
83:AM:54:LEU:HD12	127:S8:76:TRP:HZ3	1.86	0.40
84:AN:50:HIS:HA	84:AN:55:ARG:NH2	2.37	0.40
90:B8:90:TRP:CH2	104:N5:472:LEU:HD11	2.56	0.40
95:FX:139:GLU:H	95:FX:139:GLU:CD	2.30	0.40
97:G2:78:GLY:HA3	97:G2:100:HIS:HD2	1.85	0.40
100:N1:25:ASN:HB3	100:N1:29:MET:HE3	2.03	0.40
102:N3:44:GLU:OE1	121:S2:29:ASN:ND2	2.55	0.40
104:N5:740:PHE:O	104:N5:744:ILE:HG12	2.22	0.40
108:QA:328:LEU:HG	108:QA:333:ARG:HG3	2.02	0.40
108:QA:386:ILE:HG22	108:QA:451:VAL:HG11	2.02	0.40
108:QA:411:GLU:OE1	109:QB:428:SER:N	2.45	0.40
109:QB:69:LEU:HD11	109:QB:75:LEU:HD11	2.03	0.40
109:QB:97:ARG:O	109:QB:281:ASN:ND2	2.49	0.40
114:QG:195:ASN:O	114:QG:199:ASP:N	2.54	0.40
109:Qb:93:ARG:NH2	109:Qb:372:SER:OG	2.54	0.40
109:Qb:390:GLN:O	109:Qb:391:MET:C	2.63	0.40
110:Qc:232:GLY:HA3	111:Qd:271:LYS:HE3	2.04	0.40
111:Qd:277:ALA:HB1	115:Qh:71:ASN:HA	2.03	0.40
122:S3:164:GLU:HG3	122:S3:166:PRO:HD3	2.04	0.40
126:S7:6:ILE:O	126:S7:10:ILE:HG12	2.21	0.40
127:S8:140:LYS:HD3	127:S8:143:GLN:HE22	1.87	0.40
127:S8:194:PRO:HG3	127:S8:223:GLN:CD	2.46	0.40
128:T1:57:GLN:HA	128:T1:61:LEU:HB2	2.03	0.40
141:TE:22:VAL:HB	141:TE:23:GLY:H	1.76	0.40
142:TF:166:ASN:HA	142:TF:202:ARG:HH12	1.86	0.40
146:V1:88:ARG:O	146:V1:127:LYS:NZ	2.55	0.40
146:V1:126:CYS:O	146:V1:130:GLU:HG2	2.21	0.40
147:V2:204:ASP:OD1	147:V2:204:ASP:N	2.54	0.40
149:C:150:GLY:O	149:C:154:SER:OG	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2g:56:TYR:OH	153:2g:203:CDL:OA4	2.33	0.40
4:2g:153:TYR:CD1	8:2k:15:PRO:HG3	2.56	0.40
153:7a:203:CDL:HA32	153:7a:203:CDL:OB4	2.21	0.40
27:b:145:ARG:HH21	74:a3:9:PHE:HA	1.86	0.40
29:c1:147:CYS:SG	29:c1:148:GLY:N	2.94	0.40
30:c2:207:ASN:HA	30:c2:210:LYS:HE3	2.03	0.40
30:c2:324:ARG:HD2	30:c2:324:ARG:HA	1.85	0.40
31:c3:421:TRP:CE2	31:c3:432:LEU:HD13	2.56	0.40
31:c3:428:TYR:OH	32:d:226:LYS:NZ	2.55	0.40
33:e:68:GLN:HE21	33:e:159:GLU:CD	2.28	0.40
36:g:299:GLN:HA	36:g:300:PRO:HD3	1.92	0.40
37:h:99:LEU:HB2	37:h:124:ILE:HA	2.04	0.40
38:i:23:ARG:HA	38:i:23:ARG:CZ	2.52	0.40
153:i:302:CDL:H711	25:7L:863:PHE:CG	2.56	0.40
44:m2:44:ARG:HD2	44:m2:59:ILE:HG21	2.04	0.40
44:m2:82:PHE:HA	44:m2:85:HIS:HB3	2.03	0.40
45:m3:125:PHE:O	45:m3:128:GLY:N	2.36	0.40
49:q:62:PHE:HB3	49:q:63:PRO:HD3	2.03	0.40
51:s:160:SER:HB3	34:F:217:SER:HB2	2.03	0.40
52:sa:50:ASP:HB2	52:sa:73:LYS:H	1.85	0.40
52:sa:165:LEU:O	52:sa:170:GLY:N	2.45	0.40
52:sa:209:ILE:HD11	52:sa:485:LEU:HD12	2.03	0.40
52:sa:322:ALA:HB2	52:sa:636:TYR:HB3	2.04	0.40
52:sa:377:ILE:HG21	53:sb:143:ILE:HG22	2.03	0.40
52:sa:533:GLU:HA	52:sa:536:LYS:HZ3	1.86	0.40
56:t:56:ARG:HG2	56:t:60:TRP:CD1	2.57	0.40
57:u:32:ARG:HH21	57:u:119:ASN:HD21	1.69	0.40
65:y7:338:MET:HE3	65:y7:340:PHE:HE1	1.85	0.40
68:1b:2:PRO:HB2	100:n1:267:TRP:HB2	2.04	0.40
69:2b:171:TYR:OH	148:x1:22:PRO:HB2	2.22	0.40
70:4l:2:LEU:H	105:n6:39:GLN:HE22	1.69	0.40
71:5b:45:GLY:O	71:5b:49:MET:HB2	2.22	0.40
77:a7:236:ASN:HA	77:a7:239:GLN:HG2	2.03	0.40
78:a8:126:ARG:HD3	78:a8:126:ARG:HA	1.91	0.40
85:b2:109:HIS:CE1	131:t4:94:HIS:HE1	2.39	0.40
90:b8:49:ILE:O	90:b8:52:THR:OG1	2.31	0.40
94:c4:4:MET:HB2	135:t8:70:VAL:HG21	2.03	0.40
96:g1:81:ARG:NH1	96:g1:83:ASP:OD2	2.48	0.40
96:g1:152:ILE:HG22	96:g1:156:ALA:HB3	2.03	0.40
98:g3:286:ASN:HD21	99:j1:135:LYS:HE2	1.86	0.40
100:n1:208:ILE:HG23	100:n1:219:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
102:n3:120:ALA:HB2	105:n6:233:ILE:HG13	2.04	0.40
103:n4:195:ALA:HA	103:n4:272:GLU:HB3	2.04	0.40
104:n5:171:PRO:HA	104:n5:217:TYR:CZ	2.57	0.40
104:n5:740:PHE:O	104:n5:744:ILE:HG12	2.21	0.40
105:n6:118:ASN:ND2	153:n6:302:CDL:OB8	2.55	0.40
107:p2:33:ASP:CG	107:p2:89:HIS:HB3	2.45	0.40
110:qC:33:LEU:HD22	110:qC:230:GLU:HG2	2.03	0.40
114:qG:172:ILE:HG22	117:qj:6:PHE:HB2	2.02	0.40
109:qb:473:ASP:OD1	112:qe:89:ARG:NH1	2.54	0.40
110:qc:123:PHE:O	110:qc:126:PHE:HB3	2.20	0.40
153:qg:402:CDL:H331	153:qg:402:CDL:H761	2.02	0.40
116:qi:50:LYS:HB2	116:qi:50:LYS:HE3	1.80	0.40
120:s1:562:TYR:CE1	120:s1:570:GLY:HA3	2.56	0.40
130:t3:121:VAL:HA	130:t3:146:LEU:HD22	2.03	0.40
130:t3:175:VAL:HG11	130:t3:296:ILE:HD13	2.03	0.40
136:t9:38:TYR:O	136:t9:42:ILE:HG13	2.22	0.40
137:ta:41:LYS:HD2	137:ta:45:GLU:HB3	2.03	0.40
142:tf:211:GLN:HB3	142:tf:223:LEU:HD22	2.04	0.40
153:th:200:CDL:H741	153:th:200:CDL:H712	1.91	0.40
147:v2:47:GLU:CD	147:v2:47:GLU:H	2.29	0.40
2:2E:62:LYS:HG2	2:2E:64:THR:HG23	2.03	0.40
2:2E:117:PRO:HA	2:2E:151:THR:HB	2.03	0.40
3:2F:122:ARG:HD3	12:2O:34:TYR:CG	2.56	0.40
3:2F:283:ASN:O	3:2F:287:THR:HG22	2.22	0.40
4:2G:122:HIS:ND1	153:2G:204:CDL:H542	2.37	0.40
5:2H:173:TYR:CE2	6:2I:1:MET:HG3	2.57	0.40
11:2N:28:TYR:O	11:2N:32:VAL:HG22	2.21	0.40
20:6C:54:PHE:HE2	42:M:167:LEU:HD13	1.87	0.40
153:7A:201:CDL:H792	26:A:235:LEU:HD21	2.04	0.40
25:7L:896:ASN:HB2	60:W:102:ARG:HH12	1.85	0.40
26:A:386:THR:OG1	153:C3:604:CDL:OB2	2.38	0.40
153:A:504:CDL:H171	153:A:504:CDL:H751	2.02	0.40
27:B:145:ARG:HH21	74:A3:9:PHE:HA	1.86	0.40
29:C1:559:PHE:HD1	29:C1:559:PHE:HA	1.79	0.40
30:C2:2:TRP:HE1	30:C2:571:HIS:HD2	1.69	0.40
32:D:117:VAL:HA	45:M3:204:TRP:HH2	1.87	0.40
35:FS:22:GLU:OE1	35:FS:24:HIS:HE1	2.04	0.40
38:I:196:TRP:HE1	38:I:222:LYS:HG2	1.87	0.40
40:K:217:ASN:ND2	41:L:140:TYR:OH	2.48	0.40
44:M2:44:ARG:HD2	44:M2:59:ILE:HG21	2.03	0.40
52:SA:155:ILE:HG13	53:SB:198:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SA:265:MET:HB3	52:SA:275:LEU:HD11	2.04	0.40
52:SA:299:CYS:HB3	52:SA:356:LEU:HD21	2.04	0.40
52:SA:406:LYS:O	52:SA:407:THR:OG1	2.35	0.40
52:SA:618:ILE:HG23	52:SA:620:HIS:CE1	2.57	0.40
64:Y5:39:VAL:HG23	64:Y5:45:LEU:HB3	2.04	0.40
65:Y7:205:ILE:HD12	149:C:170:VAL:HG22	2.03	0.40
68:1B:39:HIS:NE2	68:1B:43:ILE:HD11	2.35	0.40
75:A5:166:MET:HE2	122:S3:116:ASN:HB2	2.04	0.40
76:A6:115:LEU:HD22	122:S3:161:SER:HA	2.04	0.40
77:A7:82:GLU:OE2	77:A7:90:ARG:NH2	2.53	0.40
77:A7:126:ILE:HG22	77:A7:128:GLU:HG3	2.03	0.40
77:A7:208:ARG:HH11	121:S2:327:THR:HG22	1.86	0.40
89:B7:20:GLU:HG2	132:T5:78:LEU:HD11	2.03	0.40
89:B7:61:ARG:NH2	131:T4:106:GLU:OE1	2.54	0.40
90:B8:59:GLN:NE2	103:N4:470:LYS:HE3	2.35	0.40
90:B8:73:LEU:HD13	90:B8:79:GLY:HA2	2.03	0.40
91:B9:22:TYR:CE1	91:B9:35:LYS:HG2	2.57	0.40
93:BM:113:ASP:OD1	93:BM:113:ASP:N	2.53	0.40
153:BM:301:CDL:H521	103:N4:499:TYR:CD1	2.57	0.40
94:C4:97:VAL:HG22	139:TC:80:ARG:HG3	2.04	0.40
98:G3:279:GLU:HB3	98:G3:283:TRP:CH2	2.57	0.40
101:N2:260:LEU:HB2	101:N2:262:ILE:HG13	2.02	0.40
105:N6:118:ASN:ND2	153:N6:302:CDL:OB8	2.54	0.40
106:P1:48:PRO:HD2	107:P2:140:THR:HG21	2.03	0.40
153:QI:203:CDL:H521	153:QI:203:CDL:H552	1.86	0.40
108:Qa:322:PHE:O	108:Qa:326:ALA:N	2.45	0.40
109:Qb:473:ASP:OD1	112:Qe:89:ARG:NH1	2.54	0.40
109:Qb:487:LEU:O	109:Qb:491:SER:OG	2.39	0.40
110:Qc:3:TRP:CD1	110:Qc:3:TRP:H	2.38	0.40
164:Qc:507:U10:H71	164:Qc:507:U10:H111	1.91	0.40
120:S1:152:SER:HB3	121:S2:353:SER:HB2	2.02	0.40
121:S2:95:HIS:ND1	121:S2:122:ASP:OD2	2.43	0.40
121:S2:169:MET:HE1	126:S7:31:CYS:O	2.21	0.40
123:S4:117:THR:HA	123:S4:118:PRO:HD3	1.91	0.40
130:T3:137:ASN:OD1	130:T3:137:ASN:N	2.55	0.40
142:TF:223:LEU:HD12	142:TF:226:LEU:HD23	2.03	0.40
145:TX:24:ARG:HD2	145:TX:24:ARG:HA	1.80	0.40
148:X1:35:PRO:HA	148:X1:121:TRP:CZ2	2.56	0.40
153:u1:101:CDL:H341	153:u1:101:CDL:H521	2.02	0.40
2:2e:117:PRO:HA	2:2e:151:THR:HB	2.03	0.40
3:2f:287:THR:O	3:2f:291:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2h:123:CYS:SG	5:2h:124:ARG:N	2.95	0.40
5:2h:150:LYS:HE3	5:2h:150:LYS:HB3	1.90	0.40
26:a:163:ARG:HD2	36:g:71:ILE:HG21	2.03	0.40
26:a:307:LYS:HD3	61:x:46:TYR:CZ	2.56	0.40
28:bp:379:SER:HA	28:bp:384:ALA:HB3	2.03	0.40
153:c1:709:CDL:H742	31:c3:319:ILE:HG12	2.03	0.40
30:c2:372:ILE:HD12	62:y:68:TYR:HE2	1.87	0.40
32:d:190:LYS:HD3	32:d:211:PRO:HB2	2.04	0.40
33:e:94:LYS:HE3	33:e:94:LYS:HB2	1.89	0.40
152:f:402:PC1:H361	152:fs:204:PC1:H352	2.04	0.40
37:h:74:GLN:HB2	37:h:297:ALA:HB2	2.04	0.40
45:m3:279:TYR:CZ	153:m3:401:CDL:H131	2.56	0.40
50:r:49:LEU:O	50:r:54:ARG:NE	2.39	0.40
51:s:159:VAL:HG23	34:F:262:GLN:HG3	2.03	0.40
52:sa:118:ASP:HB2	52:sa:589:ARG:HH11	1.87	0.40
52:sa:432:CYS:C	52:sa:434:SER:H	2.29	0.40
57:u:97:TRP:CD1	57:u:98:PRO:HD3	2.56	0.40
59:vb:456:GLN:HG2	65:y7:243:TYR:CD1	2.57	0.40
60:w:2:VAL:HG13	60:w:5:TYR:CE2	2.55	0.40
70:4l:16:LEU:HD23	70:4l:16:LEU:HA	1.90	0.40
70:4l:114:ASN:CG	95:fx:113:ASN:HB2	2.47	0.40
77:a7:179:TYR:CD1	105:n6:246:PRO:HB2	2.57	0.40
153:a9:402:CDL:H371	153:a9:402:CDL:H341	1.95	0.40
152:al:302:PC1:H12	128:t1:385:TYR:HE1	1.87	0.40
83:am:44:ARG:HA	153:am:201:CDL:HA22	2.02	0.40
153:an:302:CDL:H201	153:an:302:CDL:H371	2.03	0.40
85:b2:84:ASP:OD1	131:t4:173:ARG:NH2	2.55	0.40
90:b8:90:TRP:CH2	104:n5:472:LEU:HD11	2.56	0.40
91:b9:80:LYS:HE3	91:b9:80:LYS:HB2	1.90	0.40
99:j1:289:LEU:HB3	99:j1:296:VAL:HB	2.02	0.40
100:n1:25:ASN:HB3	100:n1:29:MET:HE3	2.04	0.40
101:n2:83:THR:HB	101:n2:87:SER:HA	2.02	0.40
102:n3:115:VAL:HG21	105:n6:200:VAL:HG22	2.03	0.40
103:n4:56:ASN:HD22	103:n4:149:ILE:HG13	1.86	0.40
103:n4:126:ALA:HB2	103:n4:284:PHE:CE1	2.57	0.40
103:n4:142:TYR:O	103:n4:146:ILE:HG23	2.21	0.40
104:n5:193:TYR:CG	132:t5:121:PRO:HG3	2.57	0.40
104:n5:480:THR:HG22	104:n5:609:LEU:HD11	2.03	0.40
104:n5:556:PHE:HB2	104:n5:610:PHE:CE1	2.57	0.40
107:p2:51:GLN:O	107:p2:55:GLU:HG2	2.22	0.40
108:qA:101:ASP:HB3	108:qA:243:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
108:qA:203:PHE:CE2	108:qA:306:ALA:HB2	2.56	0.40
110:qC:357:ILE:HG12	115:qH:103:PRO:HG3	2.03	0.40
111:qD:296:VAL:HB	115:qH:56:ARG:HH12	1.86	0.40
114:qG:117:LYS:HD2	114:qG:117:LYS:HA	1.92	0.40
114:qG:255:LYS:O	114:qG:258:GLN:HG2	2.22	0.40
108:qa:409:ALA:HB2	114:qg:323:GLY:C	2.46	0.40
110:qc:135:VAL:HA	110:qc:142:SER:HB3	2.03	0.40
111:qd:26:ILE:HD13	115:qh:116:ARG:NH2	2.37	0.40
120:s1:560:VAL:HB	120:s1:574:ALA:HA	2.03	0.40
122:s3:64:SER:HB3	122:s3:97:PHE:CZ	2.56	0.40
122:s3:164:GLU:HG3	122:s3:166:PRO:HD3	2.04	0.40
125:s6:80:VAL:HG21	125:s6:85:VAL:HG21	2.03	0.40
126:s7:157:LYS:HD2	128:t1:141:VAL:HG22	2.04	0.40
127:s8:20:TYR:HB3	142:tf:42:GLU:HG2	2.03	0.40
20:6C:38:PRO:HB3	153:6C:203:CDL:H582	2.03	0.40
26:A:102:ASN:HB3	26:A:164:TRP:O	2.21	0.40
29:C1:134:TYR:CB	29:C1:137:LEU:HB2	2.50	0.40
32:D:190:LYS:HD3	32:D:211:PRO:HB2	2.03	0.40
153:FS:204:CDL:HA61	42:M:19:TRP:HE1	1.86	0.40
36:G:110:MET:HE2	36:G:114:GLU:HG2	2.03	0.40
41:L:139:GLU:HB2	59:VB:568:ALA:HA	2.02	0.40
153:M1:404:CDL:H121	153:M1:404:CDL:H602	2.03	0.40
45:M3:279:TYR:CZ	153:M3:401:CDL:H131	2.56	0.40
47:O:79:ALA:O	47:O:83:MET:HG2	2.21	0.40
47:O:139:ILE:HG12	47:O:193:TYR:CE1	2.57	0.40
49:Q:62:PHE:HB3	49:Q:63:PRO:HD3	2.03	0.40
51:S:78:TYR:CD1	51:S:93:VAL:HG21	2.57	0.40
52:SA:226:SER:O	52:SA:230:GLY:HA2	2.20	0.40
52:SA:398:MET:HE2	52:SA:398:MET:HB3	1.77	0.40
56:T:140:ASP:OD2	56:T:144:GLU:N	2.55	0.40
57:U:32:ARG:HH21	57:U:119:ASN:HD21	1.69	0.40
59:VB:507:SER:HB2	59:VB:541:ILE:HD11	2.03	0.40
59:VB:566:GLU:HG2	59:VB:568:ALA:H	1.85	0.40
61:X:26:ASP:HB3	61:X:29:VAL:HG23	2.04	0.40
62:Y:93:TYR:CZ	62:Y:97:LEU:HD11	2.56	0.40
70:4L:45:LEU:HD21	70:4L:60:SER:HB3	2.04	0.40
70:4L:114:ASN:HB3	95:FX:113:ASN:HB2	2.03	0.40
78:A8:195:ILE:O	78:A8:199:VAL:HG13	2.21	0.40
79:A9:217:ASP:OD1	79:A9:282:ARG:NH1	2.53	0.40
85:B2:45:LEU:HD23	106:P1:40:GLN:HG2	2.04	0.40
85:B2:89:ASN:HB3	131:T4:80:SER:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:B4:42:PRO:HA	87:B4:43:PRO:HD3	1.94	0.40
94:C4:72:ARG:HH11	133:T6:40:ASN:ND2	2.19	0.40
97:G2:7:MET:HA	135:T8:50:ILE:HD11	2.02	0.40
97:G2:157:GLU:CD	97:G2:157:GLU:H	2.29	0.40
100:N1:190:GLN:HB3	100:N1:265:GLY:HA2	2.04	0.40
103:N4:21:LEU:HD22	103:N4:153:THR:HG23	2.03	0.40
104:N5:193:TYR:CG	132:T5:121:PRO:HG3	2.57	0.40
104:N5:255:ILE:HD12	104:N5:255:ILE:HA	1.92	0.40
106:P1:247:HIS:O	106:P1:251:ASN:N	2.55	0.40
107:P2:146:ASN:HB2	107:P2:153:TYR:CE2	2.56	0.40
109:QB:350:LEU:O	109:QB:353:LYS:HB3	2.21	0.40
109:Qb:289:PRO:HB3	109:Qb:475:GLU:HB3	2.02	0.40
110:Qc:116:TRP:CG	166:Qc:503:HEM:HBC1	2.55	0.40
110:Qc:246:PHE:HB2	152:Qc:506:PC1:H262	2.04	0.40
110:Qc:353:LEU:HD21	160:Qh:201:PX2:H7	2.04	0.40
114:Qg:189:TYR:CD1	114:Qg:192:LEU:HB2	2.57	0.40
120:S1:168:PRO:HD2	120:S1:705:PHE:CZ	2.56	0.40
120:S1:216:ASN:OD1	120:S1:216:ASN:N	2.55	0.40
126:S7:135:PHE:HB2	127:S8:109:TYR:OH	2.21	0.40
128:T1:398:ASN:OD1	128:T1:440:TYR:OH	2.29	0.40
128:T1:449:PRO:HG2	128:T1:476:THR:HA	2.03	0.40
129:T2:121:LEU:HA	129:T2:164:ILE:O	2.21	0.40
130:T3:261:ASN:HB2	130:T3:262:PRO:HD3	2.02	0.40
132:T5:181:GLN:O	132:T5:184:ILE:HG22	2.20	0.40
133:T6:142:PHE:O	136:T9:117:ARG:HD3	2.21	0.40
142:TF:155:LEU:HD12	142:TF:158:LEU:HD23	2.03	0.40
146:V1:47:ARG:CZ	147:V2:214:GLN:HE22	2.35	0.40
146:V1:118:SER:OG	146:V1:118:SER:O	2.32	0.40
146:V1:284:ASN:ND2	146:V1:307:GLY:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1T	68/72 (94%)	68 (100%)	0	0	100	100
1	1t	68/72 (94%)	68 (100%)	0	0	100	100
2	2E	319/322 (99%)	300 (94%)	19 (6%)	0	100	100
2	2e	319/322 (99%)	300 (94%)	19 (6%)	0	100	100
3	2F	215/296 (73%)	206 (96%)	9 (4%)	0	100	100
3	2f	215/296 (73%)	206 (96%)	9 (4%)	0	100	100
4	2G	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
4	2g	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
5	2H	98/195 (50%)	92 (94%)	6 (6%)	0	100	100
5	2h	98/195 (50%)	92 (94%)	6 (6%)	0	100	100
6	2I	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
6	2i	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
7	2J	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
7	2j	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
8	2K	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
8	2k	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
9	2L	81/89 (91%)	80 (99%)	1 (1%)	0	100	100
9	2l	81/89 (91%)	80 (99%)	1 (1%)	0	100	100
10	2M	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
10	2m	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
11	2N	59/62 (95%)	52 (88%)	7 (12%)	0	100	100
11	2n	59/62 (95%)	52 (88%)	7 (12%)	0	100	100
12	2O	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
12	2o	40/46 (87%)	38 (95%)	2 (5%)	0	100	100
13	2T	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
13	2t	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
14	3T	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
14	3t	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
15	4A	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
15	4a	98/127 (77%)	97 (99%)	1 (1%)	0	100	100
16	4T	55/68 (81%)	54 (98%)	1 (2%)	0	100	100
16	4t	55/68 (81%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	5T	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
17	5t	60/81 (74%)	59 (98%)	1 (2%)	0	100	100
18	6A	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
18	6a	124/130 (95%)	119 (96%)	5 (4%)	0	100	100
19	6B	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
19	6b	220/230 (96%)	216 (98%)	4 (2%)	0	100	100
20	6C	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
20	6c	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
21	6L	75/88 (85%)	74 (99%)	1 (1%)	0	100	100
21	6l	75/88 (85%)	74 (99%)	1 (1%)	0	100	100
22	6T	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
22	6t	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
23	7A	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
23	7a	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
24	7C	208/236 (88%)	199 (96%)	9 (4%)	0	100	100
24	7c	208/236 (88%)	199 (96%)	9 (4%)	0	100	100
25	7L	129/990 (13%)	116 (90%)	13 (10%)	0	100	100
25	7l	129/990 (13%)	116 (90%)	13 (10%)	0	100	100
26	A	447/490 (91%)	429 (96%)	18 (4%)	0	100	100
26	a	447/490 (91%)	431 (96%)	16 (4%)	0	100	100
27	B	422/473 (89%)	411 (97%)	10 (2%)	1 (0%)	43	66
27	b	422/473 (89%)	408 (97%)	14 (3%)	0	100	100
28	BP	379/462 (82%)	348 (92%)	31 (8%)	0	100	100
28	bp	379/462 (82%)	349 (92%)	30 (8%)	0	100	100
29	C1	672/688 (98%)	648 (96%)	24 (4%)	0	100	100
29	c1	672/688 (98%)	648 (96%)	24 (4%)	0	100	100
30	C2	595/604 (98%)	572 (96%)	23 (4%)	0	100	100
30	c2	595/604 (98%)	573 (96%)	22 (4%)	0	100	100
31	C3	580/594 (98%)	557 (96%)	23 (4%)	0	100	100
31	c3	580/594 (98%)	558 (96%)	22 (4%)	0	100	100
32	D	287/402 (71%)	278 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	d	287/402 (71%)	279 (97%)	8 (3%)	0	100	100
33	E	382/385 (99%)	362 (95%)	20 (5%)	0	100	100
33	e	382/385 (99%)	365 (96%)	17 (4%)	0	100	100
34	F	241/348 (69%)	239 (99%)	2 (1%)	0	100	100
34	f	241/348 (69%)	239 (99%)	2 (1%)	0	100	100
35	FS	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
35	fs	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
36	G	291/318 (92%)	282 (97%)	9 (3%)	0	100	100
36	g	291/318 (92%)	282 (97%)	9 (3%)	0	100	100
37	H	296/318 (93%)	286 (97%)	10 (3%)	0	100	100
37	h	296/318 (93%)	289 (98%)	7 (2%)	0	100	100
38	I	229/252 (91%)	220 (96%)	9 (4%)	0	100	100
38	i	229/252 (91%)	222 (97%)	6 (3%)	1 (0%)	30	53
39	J	185/234 (79%)	183 (99%)	2 (1%)	0	100	100
39	j	185/234 (79%)	183 (99%)	2 (1%)	0	100	100
40	K	206/231 (89%)	198 (96%)	8 (4%)	0	100	100
40	k	206/231 (89%)	198 (96%)	8 (4%)	0	100	100
41	L	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
41	l	192/222 (86%)	186 (97%)	6 (3%)	0	100	100
42	M	217/220 (99%)	209 (96%)	8 (4%)	0	100	100
42	m	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
43	M1	344/346 (99%)	329 (96%)	15 (4%)	0	100	100
43	m1	344/346 (99%)	331 (96%)	13 (4%)	0	100	100
44	M2	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
44	m2	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
45	M3	327/330 (99%)	317 (97%)	10 (3%)	0	100	100
45	m3	327/330 (99%)	317 (97%)	10 (3%)	0	100	100
46	N	204/210 (97%)	199 (98%)	5 (2%)	0	100	100
46	n	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
47	O	127/193 (66%)	126 (99%)	1 (1%)	0	100	100
47	o	127/193 (66%)	126 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	P	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
48	p	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
49	Q	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
49	q	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
50	R	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
50	r	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
51	S	167/170 (98%)	163 (98%)	4 (2%)	0	100	100
51	s	167/170 (98%)	163 (98%)	4 (2%)	0	100	100
52	SA	597/636 (94%)	563 (94%)	34 (6%)	0	100	100
52	sa	597/636 (94%)	565 (95%)	32 (5%)	0	100	100
53	SB	277/312 (89%)	256 (92%)	21 (8%)	0	100	100
53	sb	277/312 (89%)	256 (92%)	21 (8%)	0	100	100
54	SC	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
54	sc	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
55	SD	42/44 (96%)	42 (100%)	0	0	100	100
55	sd	42/44 (96%)	42 (100%)	0	0	100	100
56	T	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
56	t	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
57	U	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
57	u	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
58	V	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
58	v	144/149 (97%)	138 (96%)	6 (4%)	0	100	100
59	VB	551/637 (86%)	542 (98%)	9 (2%)	0	100	100
59	vb	551/637 (86%)	542 (98%)	9 (2%)	0	100	100
60	W	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
60	w	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
61	X	120/122 (98%)	120 (100%)	0	0	100	100
61	x	120/122 (98%)	120 (100%)	0	0	100	100
62	Y	103/105 (98%)	103 (100%)	0	0	100	100
62	y	103/105 (98%)	103 (100%)	0	0	100	100
63	Y0	87/89 (98%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	y0	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
64	Y5	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
64	y5	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
65	Y7	339/453 (75%)	326 (96%)	13 (4%)	0	100	100
65	y7	339/453 (75%)	325 (96%)	14 (4%)	0	100	100
66	Z	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
66	z	85/90 (94%)	84 (99%)	1 (1%)	0	100	100
67	Z1	95/100 (95%)	95 (100%)	0	0	100	100
67	z1	95/100 (95%)	95 (100%)	0	0	100	100
68	1B	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
68	1b	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
69	2B	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
69	2b	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
70	4L	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
70	4l	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
71	5B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
71	5b	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
72	A1	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
72	a1	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
73	A2	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
73	a2	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
74	A3	127/135 (94%)	124 (98%)	3 (2%)	0	100	100
74	a3	127/135 (94%)	123 (97%)	4 (3%)	0	100	100
75	A5	153/206 (74%)	150 (98%)	3 (2%)	0	100	100
75	a5	153/206 (74%)	150 (98%)	3 (2%)	0	100	100
76	A6	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
76	a6	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
77	A7	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
77	a7	280/282 (99%)	274 (98%)	6 (2%)	0	100	100
78	A8	130/238 (55%)	130 (100%)	0	0	100	100
78	a8	130/238 (55%)	130 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	A9	338/362 (93%)	321 (95%)	17 (5%)	0	100	100
79	a9	338/362 (93%)	321 (95%)	17 (5%)	0	100	100
80	AB	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
80	ab	110/138 (80%)	109 (99%)	1 (1%)	0	100	100
81	AC	96/133 (72%)	93 (97%)	3 (3%)	0	100	100
81	ac	96/133 (72%)	93 (97%)	3 (3%)	0	100	100
82	AL	191/194 (98%)	181 (95%)	10 (5%)	0	100	100
82	al	191/194 (98%)	182 (95%)	9 (5%)	0	100	100
83	AM	158/175 (90%)	155 (98%)	3 (2%)	0	100	100
83	am	158/175 (90%)	155 (98%)	3 (2%)	0	100	100
84	AN	229/231 (99%)	223 (97%)	6 (3%)	0	100	100
84	an	229/231 (99%)	223 (97%)	6 (3%)	0	100	100
85	B2	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
85	b2	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
86	B3	67/83 (81%)	66 (98%)	1 (2%)	0	100	100
86	b3	67/83 (81%)	66 (98%)	1 (2%)	0	100	100
87	B4	113/147 (77%)	112 (99%)	1 (1%)	0	100	100
87	b4	113/147 (77%)	112 (99%)	1 (1%)	0	100	100
88	B6	68/129 (53%)	68 (100%)	0	0	100	100
88	b6	68/129 (53%)	68 (100%)	0	0	100	100
89	B7	114/120 (95%)	114 (100%)	0	0	100	100
89	b7	114/120 (95%)	114 (100%)	0	0	100	100
90	B8	173/207 (84%)	171 (99%)	2 (1%)	0	100	100
90	b8	173/207 (84%)	171 (99%)	2 (1%)	0	100	100
91	B9	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
91	b9	186/189 (98%)	180 (97%)	6 (3%)	0	100	100
92	BL	173/188 (92%)	167 (96%)	6 (4%)	0	100	100
92	bl	173/188 (92%)	167 (96%)	6 (4%)	0	100	100
93	BM	162/214 (76%)	156 (96%)	6 (4%)	0	100	100
93	bm	162/214 (76%)	156 (96%)	6 (4%)	0	100	100
94	C4	100/102 (98%)	98 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
94	c4	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
95	FX	144/172 (84%)	139 (96%)	5 (4%)	0	100	100
95	fx	144/172 (84%)	139 (96%)	5 (4%)	0	100	100
96	G1	227/257 (88%)	222 (98%)	5 (2%)	0	100	100
96	g1	227/257 (88%)	222 (98%)	5 (2%)	0	100	100
97	G2	228/233 (98%)	223 (98%)	5 (2%)	0	100	100
97	g2	228/233 (98%)	223 (98%)	5 (2%)	0	100	100
98	G3	344/346 (99%)	335 (97%)	9 (3%)	0	100	100
98	g3	344/346 (99%)	335 (97%)	9 (3%)	0	100	100
99	J1	259/317 (82%)	255 (98%)	4 (2%)	0	100	100
99	j1	259/317 (82%)	255 (98%)	4 (2%)	0	100	100
100	N1	281/284 (99%)	269 (96%)	11 (4%)	1 (0%)	30	53
100	n1	281/284 (99%)	268 (95%)	12 (4%)	1 (0%)	30	53
101	N2	358/360 (99%)	348 (97%)	10 (3%)	0	100	100
101	n2	358/360 (99%)	350 (98%)	8 (2%)	0	100	100
102	N3	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
102	n3	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
103	N4	503/505 (100%)	495 (98%)	8 (2%)	0	100	100
103	n4	503/505 (100%)	496 (99%)	7 (1%)	0	100	100
104	N5	707/750 (94%)	677 (96%)	30 (4%)	0	100	100
104	n5	707/750 (94%)	678 (96%)	29 (4%)	0	100	100
105	N6	253/255 (99%)	245 (97%)	8 (3%)	0	100	100
105	n6	253/255 (99%)	245 (97%)	8 (3%)	0	100	100
106	P1	228/251 (91%)	218 (96%)	10 (4%)	0	100	100
106	p1	228/251 (91%)	219 (96%)	9 (4%)	0	100	100
107	P2	165/189 (87%)	160 (97%)	5 (3%)	0	100	100
107	p2	165/189 (87%)	160 (97%)	5 (3%)	0	100	100
108	QA	450/482 (93%)	437 (97%)	13 (3%)	0	100	100
108	Qa	450/482 (93%)	434 (96%)	16 (4%)	0	100	100
108	qA	450/482 (93%)	438 (97%)	12 (3%)	0	100	100
108	qa	450/482 (93%)	433 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
109	QB	478/513 (93%)	463 (97%)	15 (3%)	0	100	100
109	Qb	478/513 (93%)	454 (95%)	24 (5%)	0	100	100
109	qB	478/513 (93%)	463 (97%)	15 (3%)	0	100	100
109	qb	478/513 (93%)	453 (95%)	25 (5%)	0	100	100
110	QC	424/426 (100%)	404 (95%)	20 (5%)	0	100	100
110	Qc	423/426 (99%)	405 (96%)	18 (4%)	0	100	100
110	qC	424/426 (100%)	405 (96%)	19 (4%)	0	100	100
110	qc	423/426 (99%)	405 (96%)	18 (4%)	0	100	100
111	QD	293/319 (92%)	279 (95%)	14 (5%)	0	100	100
111	Qd	293/319 (92%)	276 (94%)	17 (6%)	0	100	100
111	qD	293/319 (92%)	282 (96%)	11 (4%)	0	100	100
111	qd	293/319 (92%)	275 (94%)	18 (6%)	0	100	100
112	QE	226/269 (84%)	216 (96%)	10 (4%)	0	100	100
112	Qe	215/269 (80%)	204 (95%)	11 (5%)	0	100	100
112	qE	226/269 (84%)	216 (96%)	10 (4%)	0	100	100
112	qe	215/269 (80%)	205 (95%)	10 (5%)	0	100	100
113	QF	87/90 (97%)	87 (100%)	0	0	100	100
113	Qf	78/90 (87%)	76 (97%)	2 (3%)	0	100	100
113	qF	87/90 (97%)	87 (100%)	0	0	100	100
113	qf	78/90 (87%)	76 (97%)	2 (3%)	0	100	100
114	QG	325/328 (99%)	313 (96%)	12 (4%)	0	100	100
114	Qg	324/328 (99%)	316 (98%)	8 (2%)	0	100	100
114	qG	325/328 (99%)	312 (96%)	13 (4%)	0	100	100
114	qg	324/328 (99%)	316 (98%)	8 (2%)	0	100	100
115	QH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
115	Qh	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
115	qH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
115	qh	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
116	QI	112/119 (94%)	108 (96%)	4 (4%)	0	100	100
116	Qi	112/119 (94%)	111 (99%)	1 (1%)	0	100	100
116	qI	112/119 (94%)	108 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
116	qi	112/119 (94%)	110 (98%)	2 (2%)	0	100	100
117	QJ	54/62 (87%)	54 (100%)	0	0	100	100
117	Qj	56/62 (90%)	53 (95%)	3 (5%)	0	100	100
117	qJ	54/62 (87%)	54 (100%)	0	0	100	100
117	qj	56/62 (90%)	54 (96%)	2 (4%)	0	100	100
118	QL	30/41 (73%)	30 (100%)	0	0	100	100
118	Ql	30/41 (73%)	30 (100%)	0	0	100	100
118	qL	30/41 (73%)	30 (100%)	0	0	100	100
118	ql	30/41 (73%)	30 (100%)	0	0	100	100
120	S1	687/718 (96%)	661 (96%)	26 (4%)	0	100	100
120	s1	687/718 (96%)	662 (96%)	25 (4%)	0	100	100
121	S2	440/442 (100%)	424 (96%)	16 (4%)	0	100	100
121	s2	440/442 (100%)	423 (96%)	17 (4%)	0	100	100
122	S3	196/198 (99%)	193 (98%)	3 (2%)	0	100	100
122	s3	196/198 (99%)	193 (98%)	3 (2%)	0	100	100
123	S4	180/185 (97%)	172 (96%)	8 (4%)	0	100	100
123	s4	180/185 (97%)	172 (96%)	8 (4%)	0	100	100
124	S5	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
124	s5	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
125	S6	90/132 (68%)	84 (93%)	6 (7%)	0	100	100
125	s6	90/132 (68%)	85 (94%)	5 (6%)	0	100	100
126	S7	159/162 (98%)	152 (96%)	7 (4%)	0	100	100
126	s7	159/162 (98%)	151 (95%)	8 (5%)	0	100	100
127	S8	216/236 (92%)	214 (99%)	2 (1%)	0	100	100
127	s8	216/236 (92%)	214 (99%)	2 (1%)	0	100	100
128	T1	500/516 (97%)	482 (96%)	18 (4%)	0	100	100
128	t1	500/516 (97%)	481 (96%)	19 (4%)	0	100	100
129	T2	277/333 (83%)	268 (97%)	8 (3%)	1 (0%)	30	53
129	t2	277/333 (83%)	267 (96%)	9 (3%)	1 (0%)	30	53
130	T3	308/311 (99%)	304 (99%)	4 (1%)	0	100	100
130	t3	308/311 (99%)	304 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
131	T4	196/212 (92%)	194 (99%)	2 (1%)	0	100	100
131	t4	196/212 (92%)	194 (99%)	2 (1%)	0	100	100
132	T5	139/205 (68%)	136 (98%)	3 (2%)	0	100	100
132	t5	139/205 (68%)	136 (98%)	3 (2%)	0	100	100
133	T6	107/144 (74%)	103 (96%)	4 (4%)	0	100	100
133	t6	107/144 (74%)	103 (96%)	4 (4%)	0	100	100
134	T7	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
134	t7	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
135	T8	129/135 (96%)	128 (99%)	1 (1%)	0	100	100
135	t8	129/135 (96%)	128 (99%)	1 (1%)	0	100	100
136	T9	130/136 (96%)	128 (98%)	2 (2%)	0	100	100
136	t9	130/136 (96%)	128 (98%)	2 (2%)	0	100	100
137	TA	100/127 (79%)	96 (96%)	4 (4%)	0	100	100
137	ta	100/127 (79%)	95 (95%)	5 (5%)	0	100	100
138	TB	94/113 (83%)	94 (100%)	0	0	100	100
138	tb	94/113 (83%)	94 (100%)	0	0	100	100
139	TC	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
139	tc	90/93 (97%)	89 (99%)	1 (1%)	0	100	100
140	TD	70/73 (96%)	70 (100%)	0	0	100	100
140	td	70/73 (96%)	70 (100%)	0	0	100	100
141	TE	48/71 (68%)	43 (90%)	5 (10%)	0	100	100
141	te	48/71 (68%)	43 (90%)	5 (10%)	0	100	100
142	TF	214/236 (91%)	212 (99%)	2 (1%)	0	100	100
142	tf	214/236 (91%)	212 (99%)	2 (1%)	0	100	100
143	TG	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
143	tg	132/135 (98%)	132 (100%)	0	0	100	100
144	TH	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
144	th	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
145	TX	142/166 (86%)	141 (99%)	1 (1%)	0	100	100
145	tx	142/166 (86%)	141 (99%)	1 (1%)	0	100	100
146	V1	440/474 (93%)	424 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
146	v1	440/474 (93%)	424 (96%)	16 (4%)	0	100	100
147	V2	229/274 (84%)	219 (96%)	10 (4%)	0	100	100
147	v2	229/274 (84%)	220 (96%)	9 (4%)	0	100	100
148	X1	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
148	x1	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
149	C	201/212 (95%)	192 (96%)	8 (4%)	1 (0%)	24	49
149	c	201/212 (95%)	192 (96%)	8 (4%)	1 (0%)	24	49
All	All	65386/73196 (89%)	63252 (97%)	2126 (3%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
129	t2	77	LYS
129	T2	77	LYS
149	C	87	PRO
149	c	87	PRO
100	n1	229	VAL
27	B	238	THR
100	N1	229	VAL
38	i	23	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1T	61/63 (97%)	61 (100%)	0	100	100
1	1t	61/63 (97%)	61 (100%)	0	100	100
2	2E	286/287 (100%)	279 (98%)	7 (2%)	43	67
2	2e	286/287 (100%)	278 (97%)	8 (3%)	38	62
3	2F	193/268 (72%)	190 (98%)	3 (2%)	55	75
3	2f	193/268 (72%)	190 (98%)	3 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	2G	181/181 (100%)	178 (98%)	3 (2%)	53 73
4	2g	181/181 (100%)	179 (99%)	2 (1%)	65 80
5	2H	93/184 (50%)	93 (100%)	0	100 100
5	2h	93/184 (50%)	93 (100%)	0	100 100
6	2I	97/97 (100%)	95 (98%)	2 (2%)	47 69
6	2i	97/97 (100%)	94 (97%)	3 (3%)	35 59
7	2J	85/86 (99%)	85 (100%)	0	100 100
7	2j	85/86 (99%)	85 (100%)	0	100 100
8	2K	85/85 (100%)	85 (100%)	0	100 100
8	2k	85/85 (100%)	85 (100%)	0	100 100
9	2L	77/83 (93%)	75 (97%)	2 (3%)	40 65
9	2l	77/83 (93%)	76 (99%)	1 (1%)	61 78
10	2M	66/67 (98%)	65 (98%)	1 (2%)	57 76
10	2m	66/67 (98%)	65 (98%)	1 (2%)	57 76
11	2N	55/56 (98%)	53 (96%)	2 (4%)	31 56
11	2n	55/56 (98%)	54 (98%)	1 (2%)	51 72
12	2O	37/40 (92%)	37 (100%)	0	100 100
12	2o	37/40 (92%)	37 (100%)	0	100 100
13	2T	65/67 (97%)	65 (100%)	0	100 100
13	2t	65/67 (97%)	65 (100%)	0	100 100
14	3T	76/83 (92%)	74 (97%)	2 (3%)	40 65
14	3t	76/83 (92%)	74 (97%)	2 (3%)	40 65
15	4A	87/113 (77%)	87 (100%)	0	100 100
15	4a	87/113 (77%)	87 (100%)	0	100 100
16	4T	54/63 (86%)	54 (100%)	0	100 100
16	4t	54/63 (86%)	54 (100%)	0	100 100
17	5T	56/66 (85%)	56 (100%)	0	100 100
17	5t	56/66 (85%)	56 (100%)	0	100 100
18	6A	114/116 (98%)	114 (100%)	0	100 100
18	6a	114/116 (98%)	114 (100%)	0	100 100
19	6B	200/207 (97%)	200 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	6b	200/207 (97%)	200 (100%)	0	100 100
20	6C	86/88 (98%)	86 (100%)	0	100 100
20	6c	86/88 (98%)	86 (100%)	0	100 100
21	6L	72/81 (89%)	72 (100%)	0	100 100
21	6l	72/81 (89%)	72 (100%)	0	100 100
22	6T	62/63 (98%)	62 (100%)	0	100 100
22	6t	62/63 (98%)	62 (100%)	0	100 100
23	7A	120/120 (100%)	120 (100%)	0	100 100
23	7a	120/120 (100%)	120 (100%)	0	100 100
24	7C	198/218 (91%)	198 (100%)	0	100 100
24	7c	198/218 (91%)	198 (100%)	0	100 100
25	7L	122/943 (13%)	119 (98%)	3 (2%)	42 66
25	7l	122/943 (13%)	120 (98%)	2 (2%)	55 75
26	A	410/447 (92%)	410 (100%)	0	100 100
26	a	410/447 (92%)	410 (100%)	0	100 100
27	B	374/413 (91%)	371 (99%)	3 (1%)	73 85
27	b	374/413 (91%)	371 (99%)	3 (1%)	73 85
28	BP	308/386 (80%)	308 (100%)	0	100 100
28	bp	308/386 (80%)	308 (100%)	0	100 100
29	C1	599/613 (98%)	593 (99%)	6 (1%)	68 82
29	c1	599/613 (98%)	593 (99%)	6 (1%)	68 82
30	C2	565/569 (99%)	561 (99%)	4 (1%)	76 87
30	c2	565/569 (99%)	561 (99%)	4 (1%)	76 87
31	C3	553/565 (98%)	548 (99%)	5 (1%)	70 83
31	c3	553/565 (98%)	550 (100%)	3 (0%)	81 90
32	D	253/358 (71%)	251 (99%)	2 (1%)	73 85
32	d	253/358 (71%)	251 (99%)	2 (1%)	73 85
33	E	342/343 (100%)	341 (100%)	1 (0%)	86 92
33	e	342/343 (100%)	341 (100%)	1 (0%)	86 92
34	F	219/318 (69%)	217 (99%)	2 (1%)	70 83
34	f	219/318 (69%)	217 (99%)	2 (1%)	70 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	FS	164/164 (100%)	164 (100%)	0	100	100
35	fs	164/164 (100%)	164 (100%)	0	100	100
36	G	267/289 (92%)	265 (99%)	2 (1%)	76	87
36	g	267/289 (92%)	266 (100%)	1 (0%)	84	92
37	H	256/272 (94%)	248 (97%)	8 (3%)	35	59
37	h	256/272 (94%)	249 (97%)	7 (3%)	39	64
38	I	200/219 (91%)	199 (100%)	1 (0%)	81	90
38	i	200/219 (91%)	198 (99%)	2 (1%)	68	82
39	J	170/216 (79%)	169 (99%)	1 (1%)	78	89
39	j	170/216 (79%)	170 (100%)	0	100	100
40	K	191/213 (90%)	191 (100%)	0	100	100
40	k	191/213 (90%)	191 (100%)	0	100	100
41	L	181/206 (88%)	180 (99%)	1 (1%)	78	89
41	l	181/206 (88%)	180 (99%)	1 (1%)	78	89
42	M	198/199 (100%)	198 (100%)	0	100	100
42	m	198/199 (100%)	198 (100%)	0	100	100
43	M1	294/294 (100%)	294 (100%)	0	100	100
43	m1	294/294 (100%)	294 (100%)	0	100	100
44	M2	260/260 (100%)	260 (100%)	0	100	100
44	m2	260/260 (100%)	260 (100%)	0	100	100
45	M3	275/276 (100%)	275 (100%)	0	100	100
45	m3	275/276 (100%)	274 (100%)	1 (0%)	84	92
46	N	178/181 (98%)	174 (98%)	4 (2%)	45	69
46	n	178/181 (98%)	176 (99%)	2 (1%)	65	80
47	O	120/180 (67%)	120 (100%)	0	100	100
47	o	120/180 (67%)	120 (100%)	0	100	100
48	P	157/157 (100%)	156 (99%)	1 (1%)	78	89
48	p	157/157 (100%)	157 (100%)	0	100	100
49	Q	157/157 (100%)	157 (100%)	0	100	100
49	q	157/157 (100%)	156 (99%)	1 (1%)	78	89
50	R	156/157 (99%)	154 (99%)	2 (1%)	61	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	r	156/157 (99%)	154 (99%)	2 (1%)	61 78
51	S	153/154 (99%)	153 (100%)	0	100 100
51	s	153/154 (99%)	153 (100%)	0	100 100
52	SA	481/515 (93%)	470 (98%)	11 (2%)	44 67
52	sa	481/515 (93%)	471 (98%)	10 (2%)	47 69
53	SB	255/283 (90%)	245 (96%)	10 (4%)	28 54
53	sb	255/283 (90%)	247 (97%)	8 (3%)	35 59
54	SC	49/51 (96%)	46 (94%)	3 (6%)	17 40
54	sc	49/51 (96%)	46 (94%)	3 (6%)	17 40
55	SD	43/43 (100%)	43 (100%)	0	100 100
55	sd	43/43 (100%)	43 (100%)	0	100 100
56	T	137/139 (99%)	137 (100%)	0	100 100
56	t	137/139 (99%)	137 (100%)	0	100 100
57	U	137/138 (99%)	137 (100%)	0	100 100
57	u	137/138 (99%)	137 (100%)	0	100 100
58	V	133/135 (98%)	133 (100%)	0	100 100
58	v	133/135 (98%)	133 (100%)	0	100 100
59	VB	503/579 (87%)	498 (99%)	5 (1%)	68 82
59	vb	503/579 (87%)	500 (99%)	3 (1%)	78 89
60	W	112/113 (99%)	111 (99%)	1 (1%)	70 83
60	w	112/113 (99%)	111 (99%)	1 (1%)	70 83
61	X	105/105 (100%)	103 (98%)	2 (2%)	50 71
61	x	105/105 (100%)	104 (99%)	1 (1%)	68 82
62	Y	88/88 (100%)	88 (100%)	0	100 100
62	y	88/88 (100%)	88 (100%)	0	100 100
63	Y0	84/84 (100%)	84 (100%)	0	100 100
63	y0	84/84 (100%)	84 (100%)	0	100 100
64	Y5	185/185 (100%)	185 (100%)	0	100 100
64	y5	185/185 (100%)	185 (100%)	0	100 100
65	Y7	333/442 (75%)	332 (100%)	1 (0%)	86 92
65	y7	333/442 (75%)	332 (100%)	1 (0%)	86 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
66	Z	77/80 (96%)	76 (99%)	1 (1%)	61 78
66	z	77/80 (96%)	76 (99%)	1 (1%)	61 78
67	Z1	77/78 (99%)	77 (100%)	0	100 100
67	z1	77/78 (99%)	77 (100%)	0	100 100
68	1B	55/55 (100%)	55 (100%)	0	100 100
68	1b	55/55 (100%)	55 (100%)	0	100 100
69	2B	170/170 (100%)	169 (99%)	1 (1%)	78 89
69	2b	170/170 (100%)	169 (99%)	1 (1%)	78 89
70	4L	108/108 (100%)	106 (98%)	2 (2%)	50 71
70	4l	108/108 (100%)	106 (98%)	2 (2%)	50 71
71	5B	98/98 (100%)	98 (100%)	0	100 100
71	5b	98/98 (100%)	98 (100%)	0	100 100
72	A1	88/89 (99%)	88 (100%)	0	100 100
72	a1	88/89 (99%)	88 (100%)	0	100 100
73	A2	88/93 (95%)	88 (100%)	0	100 100
73	a2	88/93 (95%)	88 (100%)	0	100 100
74	A3	108/114 (95%)	108 (100%)	0	100 100
74	a3	108/114 (95%)	108 (100%)	0	100 100
75	A5	144/186 (77%)	144 (100%)	0	100 100
75	a5	144/186 (77%)	144 (100%)	0	100 100
76	A6	154/154 (100%)	154 (100%)	0	100 100
76	a6	154/154 (100%)	154 (100%)	0	100 100
77	A7	257/257 (100%)	255 (99%)	2 (1%)	73 85
77	a7	257/257 (100%)	256 (100%)	1 (0%)	84 92
78	A8	121/224 (54%)	121 (100%)	0	100 100
78	a8	121/224 (54%)	121 (100%)	0	100 100
79	A9	290/311 (93%)	290 (100%)	0	100 100
79	a9	290/311 (93%)	290 (100%)	0	100 100
80	AB	104/129 (81%)	103 (99%)	1 (1%)	68 82
80	ab	104/129 (81%)	103 (99%)	1 (1%)	68 82
81	AC	88/119 (74%)	87 (99%)	1 (1%)	65 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
81	ac	88/119 (74%)	87 (99%)	1 (1%)	65 80
82	AL	169/170 (99%)	167 (99%)	2 (1%)	63 79
82	al	169/170 (99%)	168 (99%)	1 (1%)	78 89
83	AM	142/156 (91%)	142 (100%)	0	100 100
83	am	142/156 (91%)	142 (100%)	0	100 100
84	AN	199/199 (100%)	199 (100%)	0	100 100
84	an	199/199 (100%)	199 (100%)	0	100 100
85	B2	103/109 (94%)	101 (98%)	2 (2%)	50 71
85	b2	103/109 (94%)	101 (98%)	2 (2%)	50 71
86	B3	64/74 (86%)	63 (98%)	1 (2%)	55 75
86	b3	64/74 (86%)	63 (98%)	1 (2%)	55 75
87	B4	102/128 (80%)	102 (100%)	0	100 100
87	b4	102/128 (80%)	102 (100%)	0	100 100
88	B6	64/117 (55%)	63 (98%)	1 (2%)	55 75
88	b6	64/117 (55%)	63 (98%)	1 (2%)	55 75
89	B7	97/99 (98%)	97 (100%)	0	100 100
89	b7	97/99 (98%)	97 (100%)	0	100 100
90	B8	156/180 (87%)	155 (99%)	1 (1%)	78 89
90	b8	156/180 (87%)	156 (100%)	0	100 100
91	B9	171/172 (99%)	171 (100%)	0	100 100
91	b9	171/172 (99%)	171 (100%)	0	100 100
92	BL	160/172 (93%)	160 (100%)	0	100 100
92	bl	160/172 (93%)	160 (100%)	0	100 100
93	BM	142/182 (78%)	141 (99%)	1 (1%)	76 87
93	bm	142/182 (78%)	141 (99%)	1 (1%)	76 87
94	C4	89/89 (100%)	88 (99%)	1 (1%)	65 80
94	c4	89/89 (100%)	89 (100%)	0	100 100
95	FX	130/152 (86%)	130 (100%)	0	100 100
95	fx	130/152 (86%)	130 (100%)	0	100 100
96	G1	195/218 (89%)	194 (100%)	1 (0%)	81 90
96	g1	195/218 (89%)	194 (100%)	1 (0%)	81 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
97	G2	195/197 (99%)	191 (98%)	4 (2%)	47	69
97	g2	195/197 (99%)	193 (99%)	2 (1%)	68	82
98	G3	309/309 (100%)	309 (100%)	0	100	100
98	g3	309/309 (100%)	309 (100%)	0	100	100
99	J1	222/270 (82%)	222 (100%)	0	100	100
99	j1	222/270 (82%)	222 (100%)	0	100	100
100	N1	249/250 (100%)	241 (97%)	8 (3%)	34	59
100	n1	249/250 (100%)	244 (98%)	5 (2%)	48	71
101	N2	346/346 (100%)	340 (98%)	6 (2%)	53	73
101	n2	346/346 (100%)	342 (99%)	4 (1%)	63	79
102	N3	111/112 (99%)	110 (99%)	1 (1%)	70	83
102	n3	111/112 (99%)	110 (99%)	1 (1%)	70	83
103	N4	463/463 (100%)	457 (99%)	6 (1%)	61	78
103	n4	463/463 (100%)	456 (98%)	7 (2%)	57	76
104	N5	653/694 (94%)	644 (99%)	9 (1%)	59	77
104	n5	653/694 (94%)	646 (99%)	7 (1%)	65	80
105	N6	244/244 (100%)	243 (100%)	1 (0%)	84	92
105	n6	244/244 (100%)	244 (100%)	0	100	100
106	P1	207/223 (93%)	206 (100%)	1 (0%)	81	90
106	p1	207/223 (93%)	206 (100%)	1 (0%)	81	90
107	P2	158/178 (89%)	156 (99%)	2 (1%)	61	78
107	p2	158/178 (89%)	158 (100%)	0	100	100
108	QA	385/409 (94%)	381 (99%)	4 (1%)	68	82
108	Qa	385/409 (94%)	380 (99%)	5 (1%)	61	78
108	qA	385/409 (94%)	383 (100%)	2 (0%)	81	90
108	qa	385/409 (94%)	380 (99%)	5 (1%)	61	78
109	QB	411/440 (93%)	406 (99%)	5 (1%)	63	79
109	Qb	411/440 (93%)	403 (98%)	8 (2%)	50	71
109	qB	411/440 (93%)	407 (99%)	4 (1%)	68	82
109	qb	411/440 (93%)	403 (98%)	8 (2%)	50	71
110	QC	386/386 (100%)	380 (98%)	6 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
110	Qc	385/386 (100%)	376 (98%)	9 (2%)	44 67
110	qC	386/386 (100%)	381 (99%)	5 (1%)	61 78
110	qc	385/386 (100%)	378 (98%)	7 (2%)	51 72
111	QD	255/274 (93%)	254 (100%)	1 (0%)	84 92
111	Qd	255/274 (93%)	254 (100%)	1 (0%)	84 92
111	qD	255/274 (93%)	254 (100%)	1 (0%)	84 92
111	qd	255/274 (93%)	254 (100%)	1 (0%)	84 92
112	QE	109/237 (46%)	108 (99%)	1 (1%)	70 83
112	Qe	99/237 (42%)	99 (100%)	0	100 100
112	qE	109/237 (46%)	108 (99%)	1 (1%)	70 83
112	qe	99/237 (42%)	99 (100%)	0	100 100
113	QF	80/81 (99%)	78 (98%)	2 (2%)	42 66
113	Qf	72/81 (89%)	72 (100%)	0	100 100
113	qF	80/81 (99%)	78 (98%)	2 (2%)	42 66
113	qf	72/81 (89%)	72 (100%)	0	100 100
114	QG	288/289 (100%)	284 (99%)	4 (1%)	59 77
114	Qg	287/289 (99%)	285 (99%)	2 (1%)	76 87
114	qG	288/289 (100%)	285 (99%)	3 (1%)	68 82
114	qg	287/289 (99%)	285 (99%)	2 (1%)	76 87
115	QH	117/118 (99%)	117 (100%)	0	100 100
115	Qh	117/118 (99%)	117 (100%)	0	100 100
115	qH	117/118 (99%)	117 (100%)	0	100 100
115	qh	117/118 (99%)	117 (100%)	0	100 100
116	QI	104/109 (95%)	103 (99%)	1 (1%)	68 82
116	Qi	104/109 (95%)	104 (100%)	0	100 100
116	qI	104/109 (95%)	102 (98%)	2 (2%)	50 71
116	qi	104/109 (95%)	104 (100%)	0	100 100
117	QJ	51/56 (91%)	51 (100%)	0	100 100
117	Qj	53/56 (95%)	53 (100%)	0	100 100
117	qJ	51/56 (91%)	51 (100%)	0	100 100
117	qj	53/56 (95%)	53 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
118	QL	28/36 (78%)	28 (100%)	0	100	100
118	Ql	28/36 (78%)	28 (100%)	0	100	100
118	qL	28/36 (78%)	28 (100%)	0	100	100
118	ql	28/36 (78%)	28 (100%)	0	100	100
120	S1	590/617 (96%)	585 (99%)	5 (1%)	73	85
120	s1	590/617 (96%)	587 (100%)	3 (0%)	81	90
121	S2	399/399 (100%)	390 (98%)	9 (2%)	44	67
121	s2	399/399 (100%)	391 (98%)	8 (2%)	48	71
122	S3	191/191 (100%)	188 (98%)	3 (2%)	55	75
122	s3	191/191 (100%)	187 (98%)	4 (2%)	47	69
123	S4	160/163 (98%)	158 (99%)	2 (1%)	61	78
123	s4	160/163 (98%)	158 (99%)	2 (1%)	61	78
124	S5	82/83 (99%)	81 (99%)	1 (1%)	63	79
124	s5	82/83 (99%)	82 (100%)	0	100	100
125	S6	82/116 (71%)	81 (99%)	1 (1%)	63	79
125	s6	82/116 (71%)	82 (100%)	0	100	100
126	S7	136/137 (99%)	132 (97%)	4 (3%)	37	61
126	s7	136/137 (99%)	132 (97%)	4 (3%)	37	61
127	S8	197/215 (92%)	197 (100%)	0	100	100
127	s8	197/215 (92%)	197 (100%)	0	100	100
128	T1	440/454 (97%)	430 (98%)	10 (2%)	44	67
128	t1	440/454 (97%)	432 (98%)	8 (2%)	51	72
129	T2	237/280 (85%)	234 (99%)	3 (1%)	61	78
129	t2	237/280 (85%)	234 (99%)	3 (1%)	61	78
130	T3	272/275 (99%)	270 (99%)	2 (1%)	76	87
130	t3	272/275 (99%)	270 (99%)	2 (1%)	76	87
131	T4	178/190 (94%)	178 (100%)	0	100	100
131	t4	178/190 (94%)	178 (100%)	0	100	100
132	T5	119/179 (66%)	118 (99%)	1 (1%)	73	85
132	t5	119/179 (66%)	118 (99%)	1 (1%)	73	85
133	T6	97/131 (74%)	96 (99%)	1 (1%)	68	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
133	t6	97/131 (74%)	96 (99%)	1 (1%)	68 82
134	T7	124/125 (99%)	122 (98%)	2 (2%)	55 75
134	t7	124/125 (99%)	123 (99%)	1 (1%)	73 85
135	T8	118/122 (97%)	118 (100%)	0	100 100
135	t8	118/122 (97%)	118 (100%)	0	100 100
136	T9	118/122 (97%)	118 (100%)	0	100 100
136	t9	118/122 (97%)	118 (100%)	0	100 100
137	TA	94/117 (80%)	93 (99%)	1 (1%)	65 80
137	ta	94/117 (80%)	93 (99%)	1 (1%)	65 80
138	TB	82/97 (84%)	82 (100%)	0	100 100
138	tb	82/97 (84%)	82 (100%)	0	100 100
139	TC	83/84 (99%)	82 (99%)	1 (1%)	63 79
139	tc	83/84 (99%)	82 (99%)	1 (1%)	63 79
140	TD	64/65 (98%)	64 (100%)	0	100 100
140	td	64/65 (98%)	64 (100%)	0	100 100
141	TE	45/63 (71%)	44 (98%)	1 (2%)	45 69
141	te	45/63 (71%)	45 (100%)	0	100 100
142	TF	195/212 (92%)	193 (99%)	2 (1%)	68 82
142	tf	195/212 (92%)	193 (99%)	2 (1%)	68 82
143	TG	121/122 (99%)	114 (94%)	7 (6%)	18 41
143	tg	121/122 (99%)	116 (96%)	5 (4%)	27 53
144	TH	108/108 (100%)	108 (100%)	0	100 100
144	th	108/108 (100%)	108 (100%)	0	100 100
145	TX	128/147 (87%)	126 (98%)	2 (2%)	55 75
145	tx	128/147 (87%)	127 (99%)	1 (1%)	73 85
146	V1	362/392 (92%)	359 (99%)	3 (1%)	73 85
146	v1	362/392 (92%)	359 (99%)	3 (1%)	73 85
147	V2	205/236 (87%)	204 (100%)	1 (0%)	81 90
147	v2	205/236 (87%)	204 (100%)	1 (0%)	81 90
148	X1	132/133 (99%)	132 (100%)	0	100 100
148	x1	132/133 (99%)	132 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
149	C	106/178 (60%)	105 (99%)	1 (1%)	70 83
149	c	106/178 (60%)	105 (99%)	1 (1%)	70 83
All	All	58230/65244 (89%)	57737 (99%)	493 (1%)	70 85

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2e	5	VAL
2	2e	115	VAL
2	2e	151	THR
2	2e	165	LEU
2	2e	183	ARG
2	2e	207	ASN
2	2e	215	THR
2	2e	246	ILE
3	2f	144	LEU
3	2f	181	PHE
3	2f	205	PHE
4	2g	65	ILE
4	2g	169	HIS
6	2i	42	GLN
6	2i	76	GLN
6	2i	81	ILE
9	2l	30	TYR
10	2m	37	TYR
11	2n	34	VAL
14	3t	58	CYS
14	3t	65	THR
25	7l	862	LEU
25	7l	926	VAL
27	b	149	TYR
27	b	241	LEU
27	b	421	VAL
29	c1	57	TYR
29	c1	336	THR
29	c1	394	VAL
29	c1	460	ILE
29	c1	486	LEU
29	c1	621	MET
30	c2	162	TYR
30	c2	224	PHE

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Mol	Chain	Res	Type
30	c2	298	PHE
30	c2	501	VAL
31	c3	55	THR
31	c3	152	ILE
31	c3	312	THR
32	d	166	VAL
32	d	368	THR
33	e	346	HIS
34	f	152	VAL
34	f	312	HIS
36	g	223	ASP
37	h	22	LYS
37	h	55	ARG
37	h	58	LEU
37	h	63	ILE
37	h	67	THR
37	h	114	ILE
37	h	162	VAL
38	i	23	ARG
38	i	24	VAL
41	l	164	THR
45	m3	34	GLN
46	n	56	TYR
46	n	181	ASP
49	q	83	TYR
50	r	8	TYR
50	r	111	TYR
52	sa	52	ILE
52	sa	54	VAL
52	sa	78	THR
52	sa	316	GLU
52	sa	352	ILE
52	sa	365	HIS
52	sa	371	ILE
52	sa	496	THR
52	sa	602	ILE
52	sa	629	VAL
53	sb	35	ILE
53	sb	47	LEU
53	sb	87	TYR
53	sb	122	CYS
53	sb	157	THR

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Mol	Chain	Res	Type
53	sb	161	HIS
53	sb	165	LEU
53	sb	231	HIS
54	sc	23	PHE
54	sc	26	ARG
54	sc	51	VAL
59	vb	166	ASN
59	vb	235	TYR
59	vb	565	TRP
60	w	103	TYR
61	x	65	PHE
65	y7	400	TYR
66	z	60	PHE
69	2b	66	LEU
70	4l	33	SER
70	4l	79	ILE
77	a7	101	ASN
80	ab	53	PHE
81	ac	64	LEU
82	al	96	VAL
85	b2	41	SER
85	b2	121	SER
86	b3	63	THR
88	b6	122	VAL
93	bm	83	HIS
96	g1	136	ASP
97	g2	122	VAL
97	g2	146	ASN
100	n1	81	VAL
100	n1	103	THR
100	n1	106	ILE
100	n1	166	PHE
100	n1	230	THR
101	n2	50	ILE
101	n2	138	ILE
101	n2	215	PHE
101	n2	221	THR
102	n3	24	THR
103	n4	120	LEU
103	n4	140	ARG
103	n4	224	THR
103	n4	346	TYR

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Mol	Chain	Res	Type
103	n4	399	ILE
103	n4	440	ILE
103	n4	479	LEU
104	n5	64	VAL
104	n5	67	ILE
104	n5	81	ILE
104	n5	86	LYS
104	n5	87	ILE
104	n5	156	THR
104	n5	236	MET
106	p1	174	SER
108	qA	79	ILE
108	qA	435	TYR
109	qB	88	VAL
109	qB	118	THR
109	qB	328	LEU
109	qB	455	ILE
110	qC	79	ASP
110	qC	86	ARG
110	qC	111	GLU
110	qC	202	ASP
110	qC	316	HIS
111	qD	95	LEU
112	qE	68	VAL
113	qF	62	LEU
113	qF	73	VAL
114	qG	110	TYR
114	qG	134	VAL
114	qG	326	PHE
116	qI	3	TYR
116	qI	60	GLN
108	qa	90	ASP
108	qa	177	THR
108	qa	202	LEU
108	qa	312	VAL
108	qa	454	VAL
109	qb	48	GLU
109	qb	71	ASN
109	qb	77	VAL
109	qb	172	VAL
109	qb	246	PHE
109	qb	279	VAL

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Mol	Chain	Res	Type
109	qb	417	LYS
109	qb	430	ASP
110	qc	71	ASP
110	qc	79	ASP
110	qc	86	ARG
110	qc	112	GLN
110	qc	154	ASP
110	qc	156	PHE
110	qc	316	HIS
111	qd	26	ILE
114	qg	261	ASP
114	qg	326	PHE
120	s1	578	LEU
120	s1	605	MET
120	s1	626	VAL
121	s2	40	VAL
121	s2	77	GLN
121	s2	90	MET
121	s2	93	GLN
121	s2	207	HIS
121	s2	258	TYR
121	s2	368	LEU
121	s2	414	LEU
122	s3	20	SER
122	s3	40	ASN
122	s3	55	PHE
122	s3	95	LEU
123	s4	47	VAL
123	s4	133	ASN
126	s7	22	PHE
126	s7	31	CYS
126	s7	102	TYR
126	s7	148	ILE
128	t1	68	ILE
128	t1	268	LEU
128	t1	298	LEU
128	t1	311	THR
128	t1	374	VAL
128	t1	391	ASN
128	t1	427	TYR
128	t1	461	ASP
129	t2	97	LEU

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Mol	Chain	Res	Type
129	t2	112	LEU
129	t2	208	GLN
130	t3	25	LEU
130	t3	297	VAL
132	t5	148	GLU
133	t6	95	VAL
134	t7	9	ARG
137	ta	35	VAL
139	tc	2	VAL
142	tf	158	LEU
142	tf	226	LEU
143	tg	99	LEU
143	tg	103	LYS
143	tg	104	ASN
143	tg	105	LEU
143	tg	106	HIS
145	tx	113	THR
146	v1	53	VAL
146	v1	386	CYS
146	v1	430	ASP
147	v2	127	THR
2	2E	5	VAL
2	2E	115	VAL
2	2E	151	THR
2	2E	165	LEU
2	2E	183	ARG
2	2E	215	THR
2	2E	246	ILE
3	2F	144	LEU
3	2F	181	PHE
3	2F	205	PHE
4	2G	65	ILE
4	2G	122	HIS
4	2G	169	HIS
6	2I	76	GLN
6	2I	81	ILE
9	2L	4	ASP
9	2L	30	TYR
10	2M	37	TYR
11	2N	34	VAL
11	2N	43	GLN
14	3T	58	CYS

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Mol	Chain	Res	Type
14	3T	65	THR
25	7L	862	LEU
25	7L	903	ILE
25	7L	926	VAL
27	B	103	ASN
27	B	149	TYR
27	B	421	VAL
29	C1	57	TYR
29	C1	183	GLN
29	C1	336	THR
29	C1	394	VAL
29	C1	460	ILE
29	C1	592	ASP
30	C2	131	LYS
30	C2	162	TYR
30	C2	298	PHE
30	C2	501	VAL
31	C3	55	THR
31	C3	121	LEU
31	C3	152	ILE
31	C3	272	ILE
31	C3	312	THR
32	D	166	VAL
32	D	368	THR
33	E	346	HIS
34	F	152	VAL
34	F	312	HIS
36	G	223	ASP
36	G	281	LEU
37	H	20	THR
37	H	24	LEU
37	H	41	ARG
37	H	55	ARG
37	H	63	ILE
37	H	67	THR
37	H	114	ILE
37	H	162	VAL
38	I	23	ARG
39	J	61	GLU
41	L	164	THR
46	N	56	TYR
46	N	181	ASP

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Mol	Chain	Res	Type
46	N	191	ASN
46	N	192	ASP
48	P	105	GLN
50	R	8	TYR
50	R	111	TYR
52	SA	52	ILE
52	SA	54	VAL
52	SA	78	THR
52	SA	316	GLU
52	SA	365	HIS
52	SA	371	ILE
52	SA	496	THR
52	SA	528	LEU
52	SA	602	ILE
52	SA	622	LEU
52	SA	629	VAL
53	SB	35	ILE
53	SB	47	LEU
53	SB	87	TYR
53	SB	122	CYS
53	SB	157	THR
53	SB	161	HIS
53	SB	165	LEU
53	SB	173	THR
53	SB	231	HIS
53	SB	234	ARG
54	SC	23	PHE
54	SC	26	ARG
54	SC	51	VAL
59	VB	165	MET
59	VB	166	ASN
59	VB	235	TYR
59	VB	486	ILE
59	VB	565	TRP
60	W	103	TYR
61	X	65	PHE
61	X	74	ILE
65	Y7	400	TYR
66	Z	60	PHE
69	2B	79	LEU
70	4L	33	SER
70	4L	79	ILE

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Mol	Chain	Res	Type
77	A7	101	ASN
77	A7	281	VAL
80	AB	53	PHE
81	AC	64	LEU
82	AL	96	VAL
82	AL	113	THR
85	B2	85	LEU
85	B2	121	SER
86	B3	63	THR
88	B6	122	VAL
90	B8	185	ILE
93	BM	83	HIS
94	C4	28	THR
96	G1	136	ASP
97	G2	81	THR
97	G2	113	VAL
97	G2	122	VAL
97	G2	146	ASN
100	N1	81	VAL
100	N1	91	VAL
100	N1	103	THR
100	N1	106	ILE
100	N1	160	MET
100	N1	166	PHE
100	N1	230	THR
100	N1	284	LEU
101	N2	50	ILE
101	N2	53	LYS
101	N2	138	ILE
101	N2	215	PHE
101	N2	221	THR
101	N2	250	LEU
102	N3	24	THR
103	N4	115	ILE
103	N4	120	LEU
103	N4	346	TYR
103	N4	399	ILE
103	N4	440	ILE
103	N4	479	LEU
104	N5	64	VAL
104	N5	67	ILE
104	N5	81	ILE

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Mol	Chain	Res	Type
104	N5	86	LYS
104	N5	87	ILE
104	N5	156	THR
104	N5	236	MET
104	N5	346	SER
104	N5	630	ARG
105	N6	75	LEU
106	P1	174	SER
107	P2	44	THR
107	P2	129	ARG
108	QA	79	ILE
108	QA	270	LEU
108	QA	272	GLN
108	QA	435	TYR
109	QB	88	VAL
109	QB	118	THR
109	QB	328	LEU
109	QB	332	GLN
109	QB	455	ILE
110	QC	79	ASP
110	QC	86	ARG
110	QC	108	PHE
110	QC	111	GLU
110	QC	202	ASP
110	QC	316	HIS
111	QD	95	LEU
112	QE	68	VAL
113	QF	62	LEU
113	QF	73	VAL
114	QG	110	TYR
114	QG	134	VAL
114	QG	263	THR
114	QG	326	PHE
116	QI	3	TYR
108	Qa	90	ASP
108	Qa	177	THR
108	Qa	202	LEU
108	Qa	312	VAL
108	Qa	454	VAL
109	Qb	48	GLU
109	Qb	71	ASN
109	Qb	77	VAL

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Mol	Chain	Res	Type
109	Qb	172	VAL
109	Qb	246	PHE
109	Qb	279	VAL
109	Qb	417	LYS
109	Qb	430	ASP
110	Qc	71	ASP
110	Qc	79	ASP
110	Qc	86	ARG
110	Qc	112	GLN
110	Qc	154	ASP
110	Qc	156	PHE
110	Qc	234	MET
110	Qc	316	HIS
110	Qc	332	VAL
111	Qd	26	ILE
114	Qg	261	ASP
114	Qg	326	PHE
120	S1	169	LEU
120	S1	578	LEU
120	S1	605	MET
120	S1	626	VAL
120	S1	676	THR
121	S2	40	VAL
121	S2	77	GLN
121	S2	90	MET
121	S2	93	GLN
121	S2	207	HIS
121	S2	258	TYR
121	S2	350	ASP
121	S2	368	LEU
121	S2	414	LEU
122	S3	20	SER
122	S3	40	ASN
122	S3	95	LEU
123	S4	47	VAL
123	S4	133	ASN
124	S5	76	GLU
125	S6	111	THR
126	S7	15	SER
126	S7	22	PHE
126	S7	31	CYS
126	S7	102	TYR

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Mol	Chain	Res	Type
128	T1	68	ILE
128	T1	260	ILE
128	T1	268	LEU
128	T1	298	LEU
128	T1	311	THR
128	T1	313	ASP
128	T1	374	VAL
128	T1	391	ASN
128	T1	427	TYR
128	T1	461	ASP
129	T2	97	LEU
129	T2	112	LEU
129	T2	208	GLN
130	T3	25	LEU
130	T3	297	VAL
132	T5	148	GLU
133	T6	95	VAL
134	T7	9	ARG
134	T7	115	THR
137	TA	35	VAL
139	TC	2	VAL
141	TE	63	ILE
142	TF	158	LEU
142	TF	226	LEU
143	TG	16	GLN
143	TG	99	LEU
143	TG	103	LYS
143	TG	104	ASN
143	TG	105	LEU
143	TG	106	HIS
143	TG	120	ILE
145	TX	51	ARG
145	TX	113	THR
146	V1	53	VAL
146	V1	386	CYS
146	V1	430	ASP
147	V2	127	THR
149	C	157	VAL
149	c	157	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1355) such sidechains are listed below:

Mol	Chain	Res	Type
1	1t	9	ASN
1	1t	59	HIS
2	2e	10	ASN
2	2e	78	HIS
2	2e	120	ASN
2	2e	182	HIS
2	2e	234	ASN
2	2e	252	ASN
2	2e	307	GLN
3	2f	124	GLN
3	2f	140	GLN
3	2f	292	GLN
4	2g	22	GLN
4	2g	24	GLN
4	2g	29	GLN
4	2g	41	HIS
4	2g	62	ASN
4	2g	96	GLN
4	2g	97	ASN
4	2g	99	HIS
4	2g	123	ASN
4	2g	157	GLN
4	2g	169	HIS
5	2h	91	GLN
5	2h	105	HIS
5	2h	110	ASN
5	2h	131	HIS
5	2h	149	GLN
5	2h	185	GLN
6	2i	32	ASN
6	2i	42	GLN
6	2i	59	ASN
6	2i	61	GLN
6	2i	62	GLN
7	2j	2	ASN
7	2j	34	HIS
7	2j	40	ASN
7	2j	92	GLN
7	2j	101	HIS
9	2l	56	GLN
9	2l	70	GLN
10	2m	17	GLN
12	2o	14	HIS

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Mol	Chain	Res	Type
13	2t	8	GLN
13	2t	24	GLN
13	2t	59	ASN
13	2t	65	ASN
14	3t	40	ASN
14	3t	60	ASN
17	5t	14	ASN
17	5t	40	GLN
17	5t	47	GLN
17	5t	51	GLN
18	6a	56	ASN
18	6a	67	HIS
18	6a	94	GLN
18	6a	113	GLN
19	6b	104	ASN
19	6b	114	GLN
19	6b	157	GLN
19	6b	161	GLN
20	6c	39	HIS
20	6c	72	HIS
23	7a	101	ASN
24	7c	95	HIS
24	7c	103	GLN
24	7c	114	HIS
24	7c	126	GLN
26	a	42	GLN
26	a	67	HIS
26	a	70	HIS
26	a	92	HIS
26	a	162	ASN
26	a	213	GLN
26	a	303	ASN
26	a	358	ASN
26	a	368	GLN
26	a	428	GLN
26	a	469	GLN
27	b	20	GLN
27	b	48	ASN
27	b	73	ASN
27	b	128	GLN
27	b	146	GLN
27	b	152	GLN

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Mol	Chain	Res	Type
27	b	212	GLN
27	b	251	GLN
27	b	257	GLN
27	b	401	ASN
27	b	415	GLN
27	b	418	GLN
27	b	425	HIS
27	b	438	GLN
28	bp	129	ASN
28	bp	229	GLN
28	bp	386	GLN
28	bp	436	ASN
29	c1	17	ASN
29	c1	81	HIS
29	c1	312	ASN
29	c1	327	HIS
29	c1	472	ASN
29	c1	526	HIS
29	c1	571	GLN
29	c1	657	GLN
29	c1	658	HIS
30	c2	4	ASN
30	c2	16	ASN
30	c2	34	GLN
30	c2	167	GLN
30	c2	208	GLN
30	c2	239	ASN
30	c2	309	GLN
30	c2	541	ASN
30	c2	559	HIS
31	c3	43	ASN
31	c3	104	ASN
31	c3	129	ASN
31	c3	153	ASN
31	c3	207	ASN
31	c3	223	ASN
31	c3	230	GLN
31	c3	306	GLN
31	c3	333	ASN
31	c3	420	ASN
31	c3	472	ASN
31	c3	569	GLN

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Mol	Chain	Res	Type
31	c3	574	ASN
31	c3	591	ASN
32	d	271	ASN
32	d	305	GLN
32	d	321	ASN
33	e	33	ASN
33	e	54	ASN
33	e	235	ASN
33	e	288	HIS
33	e	367	HIS
34	f	116	ASN
34	f	304	ASN
34	f	337	ASN
35	fs	24	HIS
35	fs	87	ASN
35	fs	105	GLN
35	fs	160	HIS
36	g	67	ASN
36	g	68	GLN
36	g	98	ASN
36	g	138	GLN
36	g	262	ASN
36	g	293	GLN
37	h	36	GLN
37	h	38	GLN
37	h	105	GLN
37	h	232	HIS
37	h	262	HIS
37	h	284	GLN
38	i	47	GLN
38	i	49	ASN
38	i	228	ASN
38	i	240	HIS
39	j	57	HIS
39	j	108	GLN
39	j	193	GLN
39	j	210	GLN
40	k	30	GLN
40	k	116	GLN
40	k	168	ASN
40	k	182	GLN
40	k	199	GLN

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Mol	Chain	Res	Type
40	k	216	GLN
40	k	217	ASN
40	k	230	ASN
41	l	36	ASN
41	l	169	ASN
41	l	170	GLN
41	l	178	HIS
42	m	10	ASN
42	m	13	HIS
42	m	25	ASN
42	m	39	GLN
42	m	62	HIS
42	m	79	HIS
42	m	94	GLN
42	m	184	HIS
43	m1	95	ASN
43	m1	208	GLN
44	m2	62	ASN
44	m2	80	GLN
44	m2	118	HIS
44	m2	143	ASN
44	m2	248	GLN
45	m3	17	ASN
45	m3	60	GLN
45	m3	117	GLN
45	m3	185	GLN
45	m3	197	GLN
45	m3	200	GLN
45	m3	313	GLN
46	n	23	HIS
46	n	101	GLN
46	n	120	HIS
46	n	208	HIS
47	o	65	ASN
47	o	105	GLN
47	o	179	ASN
48	p	36	ASN
48	p	44	ASN
48	p	60	ASN
48	p	75	GLN
48	p	87	ASN
48	p	91	GLN

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Mol	Chain	Res	Type
48	p	117	ASN
48	p	135	GLN
49	q	70	HIS
49	q	118	ASN
49	q	132	GLN
50	r	12	HIS
50	r	24	ASN
51	s	12	ASN
51	s	16	ASN
51	s	41	ASN
51	s	45	GLN
51	s	48	GLN
51	s	55	ASN
51	s	96	GLN
52	sa	127	GLN
52	sa	172	GLN
52	sa	185	HIS
52	sa	282	GLN
52	sa	284	HIS
52	sa	351	HIS
52	sa	366	GLN
52	sa	430	ASN
52	sa	439	ASN
52	sa	498	HIS
52	sa	526	GLN
52	sa	566	GLN
53	sb	57	ASN
53	sb	84	GLN
53	sb	110	ASN
53	sb	133	ASN
53	sb	138	HIS
53	sb	196	ASN
53	sb	242	GLN
53	sb	289	GLN
54	sc	15	ASN
55	sd	23	ASN
56	t	52	HIS
56	t	54	ASN
56	t	101	GLN
56	t	117	GLN
57	u	91	ASN
57	u	119	ASN

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Mol	Chain	Res	Type
58	v	31	GLN
59	vb	214	ASN
59	vb	216	HIS
59	vb	221	GLN
59	vb	240	HIS
59	vb	296	GLN
59	vb	339	ASN
59	vb	347	ASN
59	vb	485	ASN
59	vb	546	ASN
60	w	10	GLN
60	w	119	ASN
62	y	7	GLN
62	y	18	GLN
62	y	45	ASN
62	y	55	GLN
62	y	81	HIS
62	y	103	GLN
63	y0	49	ASN
64	y5	80	ASN
64	y5	133	ASN
64	y5	184	ASN
65	y7	118	ASN
65	y7	129	ASN
65	y7	191	ASN
65	y7	202	ASN
65	y7	309	GLN
65	y7	339	ASN
65	y7	376	ASN
65	y7	443	ASN
67	z1	9	ASN
67	z1	10	ASN
67	z1	74	GLN
68	1b	34	GLN
69	2b	10	ASN
69	2b	118	ASN
70	4l	25	ASN
70	4l	89	ASN
70	4l	94	ASN
70	4l	99	GLN
70	4l	100	ASN
71	5b	69	ASN

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Mol	Chain	Res	Type
73	a2	11	ASN
73	a2	24	GLN
73	a2	78	ASN
73	a2	85	ASN
73	a2	93	GLN
73	a2	98	ASN
74	a3	110	GLN
75	a5	87	HIS
75	a5	121	GLN
75	a5	164	ASN
76	a6	110	GLN
77	a7	21	GLN
77	a7	45	HIS
77	a7	63	HIS
77	a7	146	HIS
77	a7	236	ASN
77	a7	260	HIS
78	a8	187	ASN
78	a8	196	ASN
78	a8	197	GLN
79	a9	23	GLN
79	a9	28	GLN
79	a9	36	ASN
79	a9	38	GLN
79	a9	133	GLN
79	a9	139	ASN
79	a9	239	ASN
79	a9	252	GLN
79	a9	288	HIS
79	a9	325	HIS
79	a9	359	ASN
80	ab	28	GLN
80	ab	51	ASN
80	ab	81	ASN
80	ab	86	GLN
80	ab	87	ASN
80	ab	98	GLN
82	al	10	GLN
82	al	40	HIS
82	al	71	HIS
82	al	156	GLN
82	al	183	ASN

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Mol	Chain	Res	Type
83	am	97	ASN
83	am	119	HIS
83	am	174	ASN
84	an	12	HIS
84	an	29	HIS
84	an	106	GLN
84	an	129	ASN
84	an	150	GLN
84	an	158	ASN
84	an	181	ASN
84	an	208	GLN
85	b2	13	GLN
85	b2	36	HIS
85	b2	71	HIS
85	b2	109	HIS
86	b3	78	GLN
87	b4	40	GLN
87	b4	74	GLN
87	b4	114	GLN
88	b6	79	ASN
89	b7	13	HIS
89	b7	47	GLN
89	b7	78	HIS
89	b7	90	ASN
91	b9	10	ASN
91	b9	168	GLN
92	bl	43	ASN
92	bl	114	HIS
92	bl	165	GLN
93	bm	166	ASN
93	bm	169	ASN
94	c4	70	GLN
94	c4	100	ASN
95	fx	27	HIS
95	fx	29	HIS
95	fx	49	ASN
95	fx	129	ASN
95	fx	171	ASN
96	g1	47	HIS
96	g1	70	ASN
96	g1	202	GLN
96	g1	217	ASN

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Mol	Chain	Res	Type
97	g2	100	HIS
97	g2	125	ASN
97	g2	128	ASN
97	g2	139	GLN
97	g2	146	ASN
97	g2	152	ASN
98	g3	37	GLN
98	g3	52	ASN
98	g3	104	GLN
98	g3	108	GLN
98	g3	114	GLN
98	g3	119	ASN
98	g3	120	GLN
98	g3	133	ASN
98	g3	137	GLN
98	g3	158	ASN
98	g3	180	ASN
98	g3	205	HIS
98	g3	306	GLN
98	g3	323	ASN
99	j1	21	GLN
99	j1	93	ASN
99	j1	180	HIS
99	j1	212	HIS
99	j1	284	ASN
99	j1	287	GLN
99	j1	311	GLN
100	n1	57	HIS
101	n2	30	ASN
101	n2	31	ASN
101	n2	54	GLN
101	n2	55	ASN
101	n2	106	ASN
101	n2	122	ASN
101	n2	176	ASN
102	n3	8	HIS
102	n3	114	ASN
103	n4	46	ASN
103	n4	56	ASN
103	n4	270	HIS
103	n4	394	ASN
103	n4	462	ASN

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Mol	Chain	Res	Type
104	n5	55	ASN
104	n5	83	ASN
104	n5	101	HIS
104	n5	145	ASN
104	n5	324	ASN
104	n5	363	ASN
104	n5	527	ASN
104	n5	561	ASN
104	n5	575	HIS
104	n5	670	ASN
104	n5	698	ASN
105	n6	39	GLN
105	n6	118	ASN
105	n6	240	ASN
106	p1	44	HIS
106	p1	55	GLN
106	p1	58	ASN
106	p1	97	HIS
106	p1	99	ASN
106	p1	150	ASN
106	p1	169	HIS
106	p1	189	HIS
106	p1	205	GLN
106	p1	251	ASN
107	p2	91	GLN
107	p2	103	GLN
107	p2	178	ASN
108	qA	123	ASN
108	qA	125	ASN
108	qA	154	ASN
108	qA	227	ASN
108	qA	283	GLN
108	qA	413	GLN
108	qA	446	GLN
109	qB	71	ASN
109	qB	136	ASN
109	qB	196	GLN
109	qB	216	GLN
109	qB	303	ASN
109	qB	485	HIS
109	qB	492	HIS
110	qC	31	ASN

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Mol	Chain	Res	Type
110	qC	204	HIS
110	qC	209	ASN
110	qC	312	GLN
110	qC	321	GLN
110	qC	328	ASN
110	qC	380	ASN
110	qC	383	ASN
111	qD	147	GLN
111	qD	204	HIS
111	qD	307	ASN
111	qD	312	GLN
112	qE	31	ASN
112	qE	69	ASN
112	qE	80	HIS
113	qF	15	GLN
113	qF	16	GLN
113	qF	51	ASN
114	qG	11	GLN
115	qH	35	ASN
116	qI	26	GLN
116	qI	43	ASN
116	qI	58	ASN
116	qI	67	GLN
116	qI	115	GLN
118	qL	32	GLN
108	qa	154	ASN
108	qa	188	GLN
108	qa	227	ASN
108	qa	260	GLN
108	qa	283	GLN
108	qa	296	ASN
108	qa	404	ASN
108	qa	413	GLN
108	qa	467	GLN
109	qb	71	ASN
109	qb	125	GLN
109	qb	136	ASN
109	qb	170	ASN
109	qb	174	ASN
109	qb	177	GLN
109	qb	196	GLN
109	qb	224	ASN

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Mol	Chain	Res	Type
109	qb	226	HIS
109	qb	240	ASN
109	qb	257	GLN
109	qb	303	ASN
109	qb	332	GLN
109	qb	364	HIS
109	qb	407	ASN
109	qb	485	HIS
109	qb	492	HIS
110	qc	18	GLN
110	qc	31	ASN
110	qc	204	HIS
110	qc	312	GLN
110	qc	383	ASN
111	qd	147	GLN
111	qd	243	GLN
111	qd	299	ASN
112	qe	39	HIS
112	qe	69	ASN
112	qe	80	HIS
112	qe	91	GLN
113	qf	15	GLN
113	qf	16	GLN
113	qf	26	GLN
114	qg	11	GLN
114	qg	44	HIS
114	qg	230	GLN
114	qg	294	GLN
114	qg	319	GLN
115	qh	15	HIS
115	qh	35	ASN
115	qh	68	GLN
115	qh	90	GLN
116	qi	26	GLN
116	qi	58	ASN
116	qi	115	GLN
117	qj	14	ASN
118	ql	32	GLN
120	s1	124	ASN
120	s1	141	GLN
120	s1	263	GLN
120	s1	371	GLN

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Mol	Chain	Res	Type
120	s1	374	ASN
120	s1	438	ASN
120	s1	598	GLN
120	s1	666	GLN
120	s1	706	ASN
121	s2	19	ASN
121	s2	22	GLN
121	s2	177	ASN
121	s2	182	ASN
121	s2	222	ASN
121	s2	260	ASN
122	s3	2	GLN
122	s3	3	ASN
122	s3	40	ASN
122	s3	63	ASN
122	s3	87	ASN
122	s3	116	ASN
123	s4	91	ASN
123	s4	148	GLN
123	s4	171	ASN
124	s5	24	GLN
124	s5	52	GLN
124	s5	94	GLN
125	s6	70	GLN
125	s6	103	GLN
125	s6	109	HIS
125	s6	113	GLN
127	s8	22	GLN
127	s8	27	HIS
127	s8	40	HIS
127	s8	81	GLN
127	s8	108	ASN
127	s8	227	ASN
128	t1	45	ASN
128	t1	63	GLN
128	t1	104	GLN
128	t1	146	GLN
128	t1	166	ASN
128	t1	172	GLN
128	t1	273	ASN
128	t1	279	ASN
128	t1	327	ASN

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Mol	Chain	Res	Type
128	t1	392	ASN
128	t1	441	GLN
128	t1	450	GLN
128	t1	497	ASN
129	t2	25	GLN
129	t2	33	ASN
129	t2	39	ASN
129	t2	125	ASN
129	t2	138	ASN
129	t2	161	GLN
129	t2	162	HIS
129	t2	222	ASN
129	t2	294	GLN
130	t3	7	ASN
130	t3	56	GLN
130	t3	73	GLN
130	t3	95	HIS
130	t3	226	ASN
130	t3	249	HIS
130	t3	272	HIS
131	t4	15	ASN
131	t4	56	HIS
131	t4	78	GLN
131	t4	94	HIS
131	t4	161	ASN
131	t4	206	GLN
132	t5	76	GLN
132	t5	178	GLN
132	t5	181	GLN
132	t5	187	GLN
133	t6	40	ASN
133	t6	107	GLN
134	t7	3	ASN
134	t7	44	GLN
134	t7	107	ASN
134	t7	111	HIS
134	t7	143	GLN
135	t8	12	ASN
135	t8	15	ASN
135	t8	32	GLN
135	t8	110	GLN
136	t9	32	ASN

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Mol	Chain	Res	Type
136	t9	44	GLN
136	t9	109	GLN
136	t9	131	ASN
137	ta	48	GLN
138	tb	24	ASN
138	tb	35	HIS
138	tb	59	GLN
139	tc	17	ASN
139	tc	36	ASN
139	tc	55	HIS
139	tc	69	ASN
140	td	73	GLN
142	tf	20	GLN
142	tf	84	ASN
142	tf	95	ASN
142	tf	153	ASN
142	tf	217	GLN
142	tf	229	HIS
143	tg	6	GLN
143	tg	9	GLN
143	tg	16	GLN
143	tg	17	GLN
143	tg	79	ASN
144	th	2	ASN
144	th	25	ASN
144	th	52	GLN
144	th	119	ASN
144	th	124	GLN
145	tx	107	GLN
146	v1	71	ASN
146	v1	137	HIS
146	v1	414	GLN
146	v1	419	GLN
146	v1	458	HIS
146	v1	470	GLN
147	v2	48	ASN
147	v2	81	ASN
147	v2	245	GLN
148	x1	140	ASN
1	1T	9	ASN
2	2E	10	ASN
2	2E	99	HIS

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Mol	Chain	Res	Type
2	2E	120	ASN
2	2E	234	ASN
2	2E	252	ASN
2	2E	307	GLN
3	2F	124	GLN
3	2F	140	GLN
3	2F	292	GLN
4	2G	22	GLN
4	2G	24	GLN
4	2G	29	GLN
4	2G	45	ASN
4	2G	62	ASN
4	2G	96	GLN
4	2G	97	ASN
4	2G	99	HIS
4	2G	157	GLN
5	2H	91	GLN
5	2H	105	HIS
5	2H	110	ASN
5	2H	131	HIS
5	2H	149	GLN
5	2H	185	GLN
6	2I	32	ASN
6	2I	42	GLN
6	2I	59	ASN
6	2I	61	GLN
6	2I	62	GLN
7	2J	2	ASN
7	2J	34	HIS
7	2J	40	ASN
7	2J	44	GLN
7	2J	92	GLN
7	2J	101	HIS
9	2L	56	GLN
9	2L	70	GLN
10	2M	17	GLN
11	2N	43	GLN
12	2O	14	HIS
13	2T	8	GLN
13	2T	24	GLN
13	2T	59	ASN
13	2T	65	ASN

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Mol	Chain	Res	Type
14	3T	60	ASN
15	4A	124	HIS
17	5T	14	ASN
17	5T	40	GLN
17	5T	47	GLN
17	5T	51	GLN
18	6A	56	ASN
18	6A	94	GLN
18	6A	112	HIS
18	6A	113	GLN
19	6B	114	GLN
19	6B	157	GLN
19	6B	161	GLN
20	6C	72	HIS
23	7A	101	ASN
24	7C	95	HIS
24	7C	103	GLN
24	7C	114	HIS
24	7C	126	GLN
26	A	42	GLN
26	A	67	HIS
26	A	70	HIS
26	A	92	HIS
26	A	162	ASN
26	A	213	GLN
26	A	303	ASN
26	A	358	ASN
26	A	368	GLN
26	A	428	GLN
26	A	469	GLN
27	B	20	GLN
27	B	48	ASN
27	B	73	ASN
27	B	128	GLN
27	B	146	GLN
27	B	152	GLN
27	B	212	GLN
27	B	251	GLN
27	B	257	GLN
27	B	418	GLN
27	B	425	HIS
28	BP	129	ASN

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Mol	Chain	Res	Type
28	BP	229	GLN
28	BP	386	GLN
28	BP	436	ASN
29	C1	17	ASN
29	C1	50	HIS
29	C1	81	HIS
29	C1	312	ASN
29	C1	327	HIS
29	C1	472	ASN
29	C1	526	HIS
29	C1	571	GLN
29	C1	657	GLN
29	C1	658	HIS
30	C2	4	ASN
30	C2	16	ASN
30	C2	34	GLN
30	C2	157	GLN
30	C2	167	GLN
30	C2	208	GLN
30	C2	239	ASN
30	C2	293	ASN
30	C2	309	GLN
30	C2	541	ASN
30	C2	559	HIS
31	C3	43	ASN
31	C3	104	ASN
31	C3	129	ASN
31	C3	207	ASN
31	C3	223	ASN
31	C3	230	GLN
31	C3	297	GLN
31	C3	306	GLN
31	C3	333	ASN
31	C3	420	ASN
31	C3	472	ASN
31	C3	569	GLN
31	C3	574	ASN
31	C3	591	ASN
32	D	136	GLN
32	D	271	ASN
32	D	305	GLN
32	D	321	ASN

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Mol	Chain	Res	Type
33	E	33	ASN
33	E	54	ASN
33	E	235	ASN
33	E	288	HIS
33	E	346	HIS
33	E	367	HIS
34	F	116	ASN
34	F	304	ASN
34	F	337	ASN
35	FS	24	HIS
35	FS	105	GLN
35	FS	160	HIS
36	G	67	ASN
36	G	68	GLN
36	G	98	ASN
36	G	138	GLN
36	G	293	GLN
37	H	38	GLN
37	H	105	GLN
37	H	203	HIS
37	H	219	ASN
37	H	232	HIS
37	H	262	HIS
37	H	284	GLN
38	I	47	GLN
38	I	49	ASN
38	I	220	GLN
38	I	228	ASN
38	I	240	HIS
39	J	108	GLN
39	J	193	GLN
39	J	210	GLN
40	K	30	GLN
40	K	95	GLN
40	K	168	ASN
40	K	182	GLN
40	K	199	GLN
40	K	216	GLN
40	K	217	ASN
40	K	230	ASN
41	L	36	ASN
41	L	169	ASN

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Mol	Chain	Res	Type
41	L	170	GLN
41	L	178	HIS
42	M	10	ASN
42	M	13	HIS
42	M	25	ASN
42	M	39	GLN
42	M	62	HIS
42	M	79	HIS
42	M	94	GLN
42	M	184	HIS
42	M	200	HIS
43	M1	95	ASN
43	M1	208	GLN
43	M1	327	GLN
44	M2	62	ASN
44	M2	80	GLN
44	M2	118	HIS
44	M2	143	ASN
44	M2	248	GLN
45	M3	17	ASN
45	M3	60	GLN
45	M3	117	GLN
45	M3	185	GLN
45	M3	197	GLN
45	M3	200	GLN
45	M3	313	GLN
46	N	23	HIS
46	N	101	GLN
46	N	208	HIS
47	O	65	ASN
47	O	73	GLN
47	O	105	GLN
47	O	148	GLN
47	O	179	ASN
48	P	36	ASN
48	P	44	ASN
48	P	60	ASN
48	P	75	GLN
48	P	87	ASN
48	P	91	GLN
48	P	102	ASN
48	P	117	ASN

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Mol	Chain	Res	Type
48	P	135	GLN
49	Q	70	HIS
49	Q	118	ASN
49	Q	132	GLN
50	R	12	HIS
50	R	24	ASN
51	S	12	ASN
51	S	16	ASN
51	S	41	ASN
51	S	45	GLN
51	S	48	GLN
51	S	55	ASN
51	S	96	GLN
51	S	101	GLN
52	SA	91	GLN
52	SA	127	GLN
52	SA	172	GLN
52	SA	185	HIS
52	SA	282	GLN
52	SA	284	HIS
52	SA	351	HIS
52	SA	366	GLN
52	SA	430	ASN
52	SA	439	ASN
52	SA	498	HIS
52	SA	526	GLN
52	SA	566	GLN
52	SA	620	HIS
53	SB	57	ASN
53	SB	110	ASN
53	SB	133	ASN
53	SB	178	GLN
53	SB	196	ASN
53	SB	242	GLN
53	SB	289	GLN
55	SD	23	ASN
56	T	52	HIS
56	T	54	ASN
56	T	101	GLN
57	U	24	GLN
57	U	91	ASN
57	U	119	ASN

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Mol	Chain	Res	Type
58	V	31	GLN
59	VB	214	ASN
59	VB	216	HIS
59	VB	221	GLN
59	VB	240	HIS
59	VB	296	GLN
59	VB	339	ASN
59	VB	347	ASN
59	VB	485	ASN
59	VB	546	ASN
60	W	10	GLN
60	W	119	ASN
62	Y	7	GLN
62	Y	18	GLN
62	Y	45	ASN
62	Y	55	GLN
62	Y	81	HIS
62	Y	103	GLN
63	Y0	49	ASN
64	Y5	80	ASN
64	Y5	133	ASN
64	Y5	184	ASN
65	Y7	118	ASN
65	Y7	129	ASN
65	Y7	191	ASN
65	Y7	202	ASN
65	Y7	300	ASN
65	Y7	309	GLN
65	Y7	339	ASN
65	Y7	376	ASN
65	Y7	443	ASN
67	Z1	9	ASN
67	Z1	10	ASN
67	Z1	74	GLN
68	1B	34	GLN
69	2B	10	ASN
69	2B	118	ASN
70	4L	25	ASN
70	4L	89	ASN
70	4L	94	ASN
70	4L	99	GLN
70	4L	100	ASN

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Mol	Chain	Res	Type
71	5B	69	ASN
72	A1	68	HIS
73	A2	11	ASN
73	A2	24	GLN
73	A2	78	ASN
73	A2	93	GLN
73	A2	98	ASN
74	A3	53	ASN
74	A3	97	GLN
75	A5	87	HIS
75	A5	121	GLN
75	A5	164	ASN
76	A6	110	GLN
77	A7	21	GLN
77	A7	58	HIS
77	A7	63	HIS
77	A7	146	HIS
77	A7	236	ASN
77	A7	260	HIS
78	A8	187	ASN
78	A8	196	ASN
78	A8	197	GLN
79	A9	23	GLN
79	A9	28	GLN
79	A9	38	GLN
79	A9	133	GLN
79	A9	139	ASN
79	A9	239	ASN
79	A9	252	GLN
79	A9	288	HIS
79	A9	303	ASN
79	A9	325	HIS
79	A9	359	ASN
80	AB	28	GLN
80	AB	51	ASN
80	AB	81	ASN
80	AB	86	GLN
80	AB	87	ASN
80	AB	98	GLN
82	AL	10	GLN
82	AL	40	HIS
82	AL	71	HIS

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Mol	Chain	Res	Type
82	AL	156	GLN
82	AL	183	ASN
83	AM	97	ASN
83	AM	119	HIS
83	AM	174	ASN
84	AN	12	HIS
84	AN	29	HIS
84	AN	129	ASN
84	AN	150	GLN
84	AN	158	ASN
84	AN	208	GLN
85	B2	13	GLN
85	B2	36	HIS
85	B2	71	HIS
86	B3	78	GLN
87	B4	40	GLN
87	B4	114	GLN
88	B6	79	ASN
88	B6	119	GLN
89	B7	13	HIS
89	B7	25	GLN
89	B7	47	GLN
89	B7	85	ASN
89	B7	90	ASN
90	B8	109	GLN
91	B9	10	ASN
91	B9	168	GLN
92	BL	43	ASN
92	BL	114	HIS
92	BL	165	GLN
93	BM	163	GLN
93	BM	166	ASN
93	BM	169	ASN
94	C4	70	GLN
95	FX	27	HIS
95	FX	29	HIS
95	FX	49	ASN
95	FX	88	ASN
95	FX	129	ASN
95	FX	171	ASN
96	G1	47	HIS
96	G1	70	ASN

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Mol	Chain	Res	Type
96	G1	202	GLN
96	G1	217	ASN
97	G2	94	HIS
97	G2	100	HIS
97	G2	125	ASN
97	G2	128	ASN
97	G2	146	ASN
97	G2	152	ASN
98	G3	37	GLN
98	G3	52	ASN
98	G3	104	GLN
98	G3	108	GLN
98	G3	114	GLN
98	G3	119	ASN
98	G3	120	GLN
98	G3	133	ASN
98	G3	137	GLN
98	G3	158	ASN
98	G3	162	ASN
98	G3	176	GLN
98	G3	180	ASN
98	G3	323	ASN
99	J1	21	GLN
99	J1	93	ASN
99	J1	180	HIS
99	J1	212	HIS
99	J1	284	ASN
99	J1	287	GLN
99	J1	311	GLN
100	N1	57	HIS
100	N1	282	ASN
101	N2	30	ASN
101	N2	31	ASN
101	N2	54	GLN
101	N2	55	ASN
101	N2	106	ASN
101	N2	122	ASN
101	N2	176	ASN
101	N2	308	ASN
102	N3	8	HIS
102	N3	114	ASN
103	N4	46	ASN

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Mol	Chain	Res	Type
103	N4	56	ASN
103	N4	101	ASN
103	N4	107	ASN
103	N4	230	ASN
103	N4	270	HIS
103	N4	394	ASN
103	N4	462	ASN
104	N5	55	ASN
104	N5	83	ASN
104	N5	101	HIS
104	N5	145	ASN
104	N5	324	ASN
104	N5	363	ASN
104	N5	527	ASN
104	N5	561	ASN
104	N5	575	HIS
104	N5	670	ASN
104	N5	698	ASN
105	N6	39	GLN
105	N6	118	ASN
105	N6	240	ASN
106	P1	44	HIS
106	P1	55	GLN
106	P1	58	ASN
106	P1	97	HIS
106	P1	99	ASN
106	P1	150	ASN
106	P1	169	HIS
106	P1	189	HIS
106	P1	205	GLN
106	P1	251	ASN
107	P2	91	GLN
107	P2	103	GLN
107	P2	178	ASN
108	QA	123	ASN
108	QA	125	ASN
108	QA	154	ASN
108	QA	227	ASN
108	QA	230	ASN
108	QA	283	GLN
108	QA	413	GLN
108	QA	446	GLN

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Mol	Chain	Res	Type
109	QB	71	ASN
109	QB	125	GLN
109	QB	136	ASN
109	QB	196	GLN
109	QB	216	GLN
109	QB	303	ASN
109	QB	427	ASN
109	QB	485	HIS
109	QB	492	HIS
110	QC	31	ASN
110	QC	204	HIS
110	QC	209	ASN
110	QC	312	GLN
110	QC	321	GLN
110	QC	328	ASN
110	QC	380	ASN
110	QC	383	ASN
111	QD	80	ASN
111	QD	204	HIS
111	QD	212	GLN
111	QD	307	ASN
111	QD	312	GLN
112	QE	31	ASN
112	QE	69	ASN
112	QE	80	HIS
113	QF	15	GLN
113	QF	16	GLN
113	QF	51	ASN
114	QG	11	GLN
115	QH	35	ASN
115	QH	68	GLN
116	QI	26	GLN
116	QI	43	ASN
116	QI	58	ASN
116	QI	67	GLN
116	QI	115	GLN
118	QL	32	GLN
108	Qa	154	ASN
108	Qa	188	GLN
108	Qa	227	ASN
108	Qa	283	GLN
108	Qa	296	ASN

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Mol	Chain	Res	Type
108	Qa	404	ASN
108	Qa	413	GLN
108	Qa	467	GLN
109	Qb	125	GLN
109	Qb	136	ASN
109	Qb	170	ASN
109	Qb	174	ASN
109	Qb	177	GLN
109	Qb	196	GLN
109	Qb	224	ASN
109	Qb	226	HIS
109	Qb	257	GLN
109	Qb	303	ASN
109	Qb	332	GLN
109	Qb	364	HIS
109	Qb	407	ASN
109	Qb	485	HIS
109	Qb	492	HIS
110	Qc	18	GLN
110	Qc	31	ASN
110	Qc	204	HIS
110	Qc	312	GLN
110	Qc	383	ASN
111	Qd	147	GLN
111	Qd	243	GLN
111	Qd	299	ASN
112	Qe	39	HIS
112	Qe	69	ASN
112	Qe	80	HIS
113	Qf	15	GLN
113	Qf	16	GLN
113	Qf	26	GLN
114	Qg	11	GLN
114	Qg	44	HIS
114	Qg	230	GLN
114	Qg	294	GLN
114	Qg	319	GLN
115	Qh	15	HIS
115	Qh	35	ASN
115	Qh	68	GLN
115	Qh	90	GLN
116	Qi	26	GLN

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Mol	Chain	Res	Type
116	Qi	58	ASN
116	Qi	115	GLN
117	Qj	14	ASN
118	Ql	32	GLN
120	S1	124	ASN
120	S1	141	GLN
120	S1	263	GLN
120	S1	371	GLN
120	S1	374	ASN
120	S1	438	ASN
120	S1	598	GLN
120	S1	666	GLN
120	S1	706	ASN
121	S2	22	GLN
121	S2	177	ASN
121	S2	182	ASN
121	S2	222	ASN
121	S2	260	ASN
121	S2	346	ASN
122	S3	2	GLN
122	S3	3	ASN
122	S3	40	ASN
122	S3	57	ASN
122	S3	63	ASN
122	S3	87	ASN
122	S3	92	ASN
123	S4	91	ASN
123	S4	148	GLN
123	S4	171	ASN
124	S5	24	GLN
124	S5	52	GLN
124	S5	94	GLN
125	S6	70	GLN
125	S6	103	GLN
127	S8	27	HIS
127	S8	40	HIS
127	S8	81	GLN
127	S8	108	ASN
127	S8	227	ASN
128	T1	43	ASN
128	T1	45	ASN
128	T1	63	GLN

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Mol	Chain	Res	Type
128	T1	104	GLN
128	T1	146	GLN
128	T1	166	ASN
128	T1	172	GLN
128	T1	201	HIS
128	T1	239	HIS
128	T1	273	ASN
128	T1	279	ASN
128	T1	317	ASN
128	T1	327	ASN
128	T1	392	ASN
128	T1	441	GLN
128	T1	450	GLN
128	T1	497	ASN
129	T2	25	GLN
129	T2	33	ASN
129	T2	39	ASN
129	T2	125	ASN
129	T2	138	ASN
129	T2	161	GLN
129	T2	162	HIS
129	T2	222	ASN
129	T2	294	GLN
130	T3	7	ASN
130	T3	56	GLN
130	T3	73	GLN
130	T3	95	HIS
130	T3	226	ASN
130	T3	249	HIS
130	T3	272	HIS
131	T4	56	HIS
131	T4	78	GLN
131	T4	94	HIS
131	T4	161	ASN
131	T4	206	GLN
132	T5	76	GLN
132	T5	178	GLN
132	T5	181	GLN
132	T5	187	GLN
133	T6	40	ASN
133	T6	107	GLN
134	T7	3	ASN

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Mol	Chain	Res	Type
134	T7	44	GLN
134	T7	103	ASN
134	T7	107	ASN
134	T7	111	HIS
134	T7	143	GLN
135	T8	12	ASN
135	T8	15	ASN
135	T8	32	GLN
135	T8	110	GLN
136	T9	32	ASN
136	T9	131	ASN
137	TA	48	GLN
138	TB	24	ASN
138	TB	35	HIS
138	TB	59	GLN
139	TC	17	ASN
139	TC	36	ASN
139	TC	55	HIS
140	TD	73	GLN
142	TF	84	ASN
142	TF	95	ASN
142	TF	153	ASN
142	TF	217	GLN
142	TF	229	HIS
143	TG	6	GLN
143	TG	9	GLN
143	TG	16	GLN
143	TG	17	GLN
143	TG	79	ASN
144	TH	2	ASN
144	TH	25	ASN
144	TH	52	GLN
144	TH	119	ASN
144	TH	124	GLN
145	TX	107	GLN
146	V1	71	ASN
146	V1	137	HIS
146	V1	168	ASN
146	V1	414	GLN
146	V1	419	GLN
146	V1	458	HIS
146	V1	468	ASN

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Mol	Chain	Res	Type
146	V1	470	GLN
147	V2	48	ASN
147	V2	81	ASN
147	V2	245	GLN
149	C	97	ASN
149	C	172	GLN
149	C	184	GLN
149	c	97	ASN
149	c	172	GLN
149	c	184	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 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	$\#\|Z\| > 2$
24	SEP	7c	120	24	8,9,10	0.87	0	7,12,14	0.75	0
59	SEP	vb	520	59	8,9,10	0.89	0	7,12,14	0.84	0
59	TPO	vb	387	59	8,10,11	1.25	1 (12%)	10,14,16	1.13	0
24	SEP	7C	120	24	8,9,10	0.88	0	7,12,14	0.75	0
59	SEP	VB	520	59	8,9,10	0.89	0	7,12,14	0.83	0
59	TPO	VB	387	59	8,10,11	1.25	1 (12%)	10,14,16	1.13	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
24	SEP	7c	120	24	-	3/6/8/10	-
59	SEP	vb	520	59	-	3/6/8/10	-
59	TPO	vb	387	59	-	1/9/11/13	-
24	SEP	7C	120	24	-	3/6/8/10	-
59	SEP	VB	520	59	-	3/6/8/10	-
59	TPO	VB	387	59	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	VB	387	TPO	P-OG1	3.13	1.65	1.59
59	vb	387	TPO	P-OG1	3.12	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	7c	120	SEP	CB-OG-P-O1P
24	7c	120	SEP	CB-OG-P-O2P
24	7c	120	SEP	CB-OG-P-O3P
59	vb	387	TPO	O-C-CA-CB
59	vb	520	SEP	CB-OG-P-O1P
59	vb	520	SEP	CB-OG-P-O2P
59	vb	520	SEP	CB-OG-P-O3P
24	7C	120	SEP	CB-OG-P-O1P
24	7C	120	SEP	CB-OG-P-O2P
24	7C	120	SEP	CB-OG-P-O3P
59	VB	387	TPO	O-C-CA-CB
59	VB	520	SEP	CB-OG-P-O1P
59	VB	520	SEP	CB-OG-P-O2P
59	VB	520	SEP	CB-OG-P-O3P

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7c	120	SEP	1	0
59	vb	520	SEP	1	0
59	vb	387	TPO	1	0
24	7C	120	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	VB	520	SEP	1	0
59	VB	387	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 510 ligands modelled in this entry, 14 are monoatomic - leaving 496 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	$\#\|Z\| > 2$
153	CDL	p1	402	-	62,62,99	0.37	0	68,74,111	0.31	0
153	CDL	E	402	-	71,71,99	0.34	0	77,83,111	0.35	0
151	HEC	Qd	401	111	46,50,50	1.92	10 (21%)	58,82,82	1.85	8 (13%)
152	PC1	qc	506	-	37,37,53	0.34	0	43,45,61	0.33	0
153	CDL	C	301	-	63,63,99	0.37	0	69,75,111	0.44	0
158	3PE	AN	301	-	44,44,50	0.32	0	47,49,55	0.28	0
152	PC1	P1	401	-	39,39,53	0.33	0	45,47,61	0.33	0
153	CDL	qI	203	-	70,70,99	0.35	0	76,82,111	0.31	0
158	3PE	A3	201	-	44,44,50	0.33	0	47,49,55	0.56	1 (2%)
153	CDL	N5	806	-	89,89,99	0.31	0	95,101,111	0.28	0
153	CDL	N6	302	-	89,89,99	0.32	0	95,101,111	0.36	0
153	CDL	R	201	-	64,64,99	0.36	0	70,76,111	0.32	0
168	ZMP	ab	201	80	34,36,36	0.69	1 (2%)	41,45,45	0.75	0
152	PC1	qc	509	-	46,46,53	0.30	0	52,54,61	0.36	0
153	CDL	TE	101	-	52,52,99	0.39	0	58,64,111	0.33	0
153	CDL	2O	101	-	49,49,99	0.41	0	55,61,111	0.35	0
152	PC1	j	302	-	36,36,53	0.34	0	42,44,61	0.33	0
157	FES	FS	203	35	0,4,4	-	-	-		
160	PX2	y5	204	-	20,20,35	1.30	4 (20%)	23,25,40	1.31	2 (8%)
152	PC1	I	301	-	38,38,53	0.34	0	44,46,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	CDL	Qg	402	-	99,99,99	0.30	0	105,111,111	0.30	0
152	PC1	M1	401	-	53,53,53	0.29	0	59,61,61	0.30	0
160	PX2	r	202	-	32,32,35	1.03	4 (12%)	35,37,40	1.00	2 (5%)
152	PC1	qj	101	-	35,35,53	0.34	0	41,43,61	0.34	0
153	CDL	b3	101	-	57,57,99	0.37	0	63,69,111	0.32	0
153	CDL	u1	101	-	56,56,99	0.38	0	62,68,111	0.31	0
164	U10	qc	501	-	25,25,63	2.30	7 (28%)	24,29,79	1.92	8 (33%)
158	3PE	G2	301	-	50,50,50	0.30	0	53,55,55	0.29	0
158	3PE	S8	304	-	40,40,50	0.33	0	43,45,55	0.32	0
153	CDL	2b	201	-	86,86,99	0.31	0	92,98,111	0.36	0
158	3PE	g2	301	-	50,50,50	0.30	0	53,55,55	0.29	0
153	CDL	U1	101	-	56,56,99	0.38	0	62,68,111	0.31	0
158	3PE	y5	202	-	27,27,50	0.40	0	30,32,55	0.34	0
153	CDL	c1	712	-	94,94,99	0.31	0	100,106,111	0.32	0
152	PC1	B9	201	-	33,33,53	0.37	0	39,41,61	0.54	0
152	PC1	n5	805	-	53,53,53	0.28	0	59,61,61	0.33	0
152	PC1	M	303	-	44,44,53	0.31	0	50,52,61	0.39	0
152	PC1	TE	102	-	31,31,53	0.37	0	37,39,61	0.42	0
152	PC1	T4	301	-	47,47,53	0.31	0	53,55,61	0.38	0
157	FES	SB	401	53	0,4,4	-	-	-		
152	PC1	6a	202	-	34,34,53	0.36	0	40,42,61	0.36	0
153	CDL	7A	201	-	99,99,99	0.30	0	105,111,111	0.28	0
152	PC1	2F	302	-	41,41,53	0.33	0	47,49,61	0.43	0
153	CDL	qB	601	-	67,67,99	0.35	0	73,79,111	0.30	0
158	3PE	T8	602	-	38,38,50	0.33	0	41,43,55	0.36	0
152	PC1	M2	405	-	53,53,53	0.29	0	59,61,61	0.28	0
153	CDL	6C	203	-	81,81,99	0.32	0	87,93,111	0.30	0
152	PC1	qb	602	-	42,42,53	0.31	0	48,50,61	0.32	0
153	CDL	t5	301	-	95,95,99	0.30	0	101,107,111	0.32	0
160	PX2	R	202	-	32,32,35	1.02	4 (12%)	35,37,40	0.94	2 (5%)
152	PC1	t1	602	-	32,32,53	0.36	0	38,40,61	0.35	0
153	CDL	AL	301	-	52,52,99	0.39	0	58,64,111	0.33	0
152	PC1	c3	605	-	38,38,53	0.33	0	44,46,61	0.33	0
157	FES	FS	202	35	0,4,4	-	-	-		
158	3PE	I	304	-	31,31,50	0.37	0	34,36,55	0.33	0
157	FES	sb	401	53	0,4,4	-	-	-		
164	U10	b8	301	-	63,63,63	2.20	25 (39%)	78,79,79	1.70	23 (29%)
153	CDL	M2	403	-	65,65,99	0.36	0	71,77,111	0.30	0
166	HEM	QC	502	110	50,50,50	1.30	7 (14%)	67,82,82	1.60	12 (17%)
153	CDL	n6	302	-	89,89,99	0.32	0	95,101,111	0.36	0
152	PC1	W	201	-	48,48,53	0.30	0	54,56,61	0.30	0
152	PC1	N	303	-	35,35,53	0.34	0	41,43,61	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
152	PC1	N5	804	-	38,38,53	0.33	0	44,46,61	0.34	0
153	CDL	m	306	-	65,65,99	0.36	0	71,77,111	0.31	0
158	3PE	A3	202	-	43,43,50	0.32	0	46,48,55	0.30	0
169	T7X	B6	201	-	55,55,61	1.51	5 (9%)	64,67,73	1.10	4 (6%)
152	PC1	qG	401	-	31,31,53	0.37	0	37,39,61	0.42	0
153	CDL	Y7	501	-	64,64,99	0.36	0	70,76,111	0.37	0
158	3PE	vb	705	-	27,27,50	0.39	0	30,32,55	0.35	0
153	CDL	m2	403	-	65,65,99	0.36	0	71,77,111	0.30	0
153	CDL	T5	301	-	95,95,99	0.30	0	101,107,111	0.32	0
153	CDL	qH	201	-	93,93,99	0.31	0	99,105,111	0.26	0
151	HEC	qd	401	111	46,50,50	1.92	10 (21%)	58,82,82	1.85	8 (13%)
152	PC1	qi	201	-	29,29,53	0.39	0	35,37,61	0.43	0
153	CDL	qC	503	-	63,63,99	0.36	0	69,75,111	0.31	0
152	PC1	C3	605	-	38,38,53	0.33	0	44,46,61	0.33	0
161	FAD	SA	701	-	58,58,58	0.32	0	85,89,89	0.27	0
152	PC1	QE	303	-	38,38,53	0.34	0	44,46,61	0.34	0
153	CDL	Q	202	-	71,71,99	0.34	0	77,83,111	0.30	0
153	CDL	TH	200	-	83,83,99	0.32	0	89,95,111	0.28	0
158	3PE	a3	202	-	43,43,50	0.32	0	46,48,55	0.30	0
158	3PE	a3	201	-	44,44,50	0.33	0	47,49,55	0.56	1 (2%)
153	CDL	sd	101	-	75,75,99	0.34	0	81,87,111	0.31	0
158	3PE	c4	402	-	50,50,50	0.30	0	53,55,55	0.31	0
153	CDL	t	203	-	70,70,99	0.35	0	76,82,111	0.32	0
158	3PE	t8	602	-	38,38,50	0.33	0	41,43,55	0.36	0
153	CDL	i	302	-	74,74,99	0.34	0	80,86,111	0.29	0
152	PC1	N3	201	-	30,30,53	0.37	0	36,38,61	0.38	0
153	CDL	VB	705	-	81,81,99	0.32	0	87,93,111	0.29	0
153	CDL	B8	302	-	68,68,99	0.35	0	74,80,111	0.31	0
153	CDL	t	204	-	89,89,99	0.33	0	95,101,111	0.33	0
153	CDL	qc	504	-	63,63,99	0.37	0	69,75,111	0.34	0
162	SF4	v1	500	146	0,12,12	-	-	-		
157	FES	fs	202	35	0,4,4	-	-	-		
152	PC1	QC	507	-	49,49,53	0.30	0	55,57,61	0.31	0
153	CDL	q	203	-	85,85,99	0.32	0	91,97,111	0.31	0
152	PC1	m	305	-	34,34,53	0.35	0	40,42,61	0.35	0
170	ADP	B9	202	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
152	PC1	W	205	-	42,42,53	0.32	0	48,50,61	0.31	0
152	PC1	FS	201	-	39,39,53	0.33	0	45,47,61	0.28	0
152	PC1	Qi	203	-	41,41,53	0.33	0	47,49,61	0.37	0
153	CDL	6a	201	-	73,73,99	0.35	0	79,85,111	0.41	0
152	PC1	qE	304	-	27,27,53	0.39	0	33,35,61	0.46	0
153	CDL	A9	403	-	86,86,99	0.32	0	92,98,111	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	CDL	b4	201	-	36,36,99	0.43	0	42,48,111	0.40	0
153	CDL	E	401	-	59,59,99	0.37	0	65,71,111	0.34	0
157	FES	fx	201	95	0,4,4	-	-	-		
153	CDL	F	402	-	99,99,99	0.29	0	105,111,111	0.29	0
162	SF4	s8	302	127	0,12,12	-	-	-		
153	CDL	p1	403	-	57,57,99	0.39	0	63,69,111	0.40	0
169	T7X	b6	201	-	55,55,61	1.51	5 (9%)	64,67,73	1.10	4 (6%)
154	HEA	C1	703	29	67,67,67	2.29	26 (38%)	81,103,103	2.45	25 (30%)
152	PC1	J	302	-	36,36,53	0.34	0	42,44,61	0.33	0
153	CDL	VB	706	-	66,66,99	0.35	0	72,78,111	0.31	0
152	PC1	m1	403	-	41,41,53	0.33	0	47,49,61	0.39	0
152	PC1	7c	303	-	42,42,53	0.32	0	48,50,61	0.34	0
158	3PE	M2	408	-	30,30,50	0.38	0	33,35,55	0.37	0
153	CDL	7a	201	-	99,99,99	0.30	0	105,111,111	0.28	0
153	CDL	I	303	-	74,74,99	0.34	0	80,86,111	0.29	0
158	3PE	w	203	-	33,33,50	0.36	0	36,38,55	0.32	0
158	3PE	N4	601	-	35,35,50	0.35	0	38,40,55	0.37	0
153	CDL	qb	601	-	67,67,99	0.35	0	73,79,111	0.30	0
158	3PE	N5	802	-	35,35,50	0.36	0	38,40,55	0.32	0
153	CDL	m2	404	-	73,73,99	0.34	0	79,85,111	0.34	0
153	CDL	y5	201	-	69,69,99	0.35	0	75,81,111	0.31	0
153	CDL	VB	703	-	85,85,99	0.32	0	91,97,111	0.31	0
152	PC1	7A	202	-	44,44,53	0.31	0	50,52,61	0.33	0
153	CDL	e	401	-	59,59,99	0.37	0	65,71,111	0.34	0
170	ADP	b9	202	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
153	CDL	r	201	-	64,64,99	0.36	0	70,76,111	0.32	0
160	PX2	qh	201	-	35,35,35	1.00	4 (11%)	38,40,40	1.02	2 (5%)
153	CDL	T	202	-	74,74,99	0.34	0	80,86,111	0.35	0
153	CDL	QB	601	-	67,67,99	0.35	0	73,79,111	0.30	0
152	PC1	c1	704	-	48,48,53	0.30	0	54,56,61	0.28	0
152	PC1	c3	601	-	51,51,53	0.30	0	57,59,61	0.36	0
152	PC1	C1	706	-	48,48,53	0.30	0	54,56,61	0.28	0
153	CDL	C1	712	-	94,94,99	0.31	0	100,106,111	0.32	0
164	U10	SC	102	-	63,63,63	2.22	24 (38%)	78,79,79	1.65	20 (25%)
152	PC1	2f	302	-	41,41,53	0.33	0	47,49,61	0.43	0
152	PC1	b9	201	-	33,33,53	0.37	0	39,41,61	0.54	0
164	U10	B8	301	-	63,63,63	2.20	25 (39%)	78,79,79	1.70	23 (29%)
152	PC1	N5	805	-	53,53,53	0.28	0	59,61,61	0.33	0
162	SF4	s1	801	120	0,12,12	-	-	-		
152	PC1	p1	401	-	39,39,53	0.33	0	45,47,61	0.33	0
153	CDL	a	502	-	50,50,99	0.41	0	56,62,111	0.48	0
153	CDL	a9	403	-	86,86,99	0.32	0	92,98,111	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	CDL	c	301	-	63,63,99	0.37	0	69,75,111	0.44	0
153	CDL	fs	203	-	46,46,99	0.42	0	52,58,111	0.35	0
153	CDL	7C	302	-	50,50,99	0.40	0	56,62,111	0.35	0
153	CDL	i	301	-	76,76,99	0.33	0	82,88,111	0.31	0
152	PC1	m2	405	-	53,53,53	0.29	0	59,61,61	0.28	0
153	CDL	qG	402	-	85,85,99	0.32	0	91,97,111	0.28	0
152	PC1	7C	303	-	42,42,53	0.32	0	48,50,61	0.34	0
153	CDL	U	201	-	59,59,99	0.38	0	65,71,111	0.33	0
152	PC1	qC	505	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	W	202	-	83,83,99	0.32	0	89,95,111	0.33	0
153	CDL	b	501	-	61,61,99	0.37	0	67,73,111	0.32	0
162	SF4	S8	302	127	0,12,12	-	-	-		
153	CDL	c1	709	-	62,62,99	0.37	0	68,74,111	0.39	0
153	CDL	5b	201	-	80,80,99	0.33	0	86,92,111	0.33	0
153	CDL	2G	203	-	54,54,99	0.39	0	60,66,111	0.36	0
153	CDL	M	305	-	82,82,99	0.32	0	88,94,111	0.31	0
153	CDL	T	201	-	58,58,99	0.38	0	64,70,111	0.32	0
152	PC1	C3	603	-	30,30,53	0.37	0	36,38,61	0.35	0
152	PC1	Qe	301	-	32,32,53	0.36	0	38,40,61	0.36	0
153	CDL	t7	201	-	72,72,99	0.34	0	78,84,111	0.29	0
152	PC1	N1	301	-	35,35,53	0.35	0	41,43,61	0.35	0
153	CDL	2M	101	-	95,95,99	0.30	0	101,107,111	0.31	0
158	3PE	i	303	-	31,31,50	0.37	0	34,36,55	0.33	0
157	FES	Qe	302	-	0,4,4	-	-	-		
152	PC1	D	501	-	34,34,53	0.36	0	40,42,61	0.40	0
153	CDL	td	101	-	65,65,99	0.36	0	71,77,111	0.33	0
152	PC1	v	201	-	34,34,53	0.35	0	40,42,61	0.33	0
152	PC1	c3	606	-	48,48,53	0.31	0	54,56,61	0.37	0
166	HEM	Qc	502	110	50,50,50	1.29	7 (14%)	67,82,82	1.59	10 (14%)
153	CDL	m3	401	-	62,62,99	0.36	0	68,74,111	0.32	0
152	PC1	fs	204	-	39,39,53	0.33	0	45,47,61	0.28	0
153	CDL	C1	701	-	78,78,99	0.33	0	84,90,111	0.32	0
152	PC1	C1	710	-	37,37,53	0.34	0	43,45,61	0.33	0
161	FAD	sa	701	-	58,58,58	0.32	0	85,89,89	0.27	0
153	CDL	qc	508	-	46,46,99	0.42	0	52,58,111	0.42	0
153	CDL	QD	402	-	60,60,99	0.37	0	66,72,111	0.31	0
152	PC1	T4	303	-	53,53,53	0.30	0	59,61,61	0.37	0
153	CDL	m	303	-	82,82,99	0.32	0	88,94,111	0.31	0
158	3PE	n4	601	-	35,35,50	0.35	0	38,40,55	0.36	0
162	SF4	s7	201	126	0,12,12	-	-	-		
152	PC1	AL	302	-	25,25,53	0.40	0	31,33,61	0.39	0
152	PC1	QB	602	-	43,43,53	0.31	0	49,51,61	0.30	0
158	3PE	T8	601	-	46,46,50	0.33	0	49,51,55	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
158	3PE	t8	601	-	46,46,50	0.33	0	49,51,55	0.40	0
153	CDL	C3	604	-	67,67,99	0.35	0	73,79,111	0.31	0
152	PC1	Qe	303	-	42,42,53	0.32	0	48,50,61	0.45	0
152	PC1	6c	203	-	32,32,53	0.36	0	38,40,61	0.37	0
152	PC1	F	401	-	37,37,53	0.34	0	43,45,61	0.30	0
153	CDL	vb	701	-	61,61,99	0.36	0	67,73,111	0.32	0
152	PC1	c1	711	-	38,38,53	0.33	0	44,46,61	0.35	0
163	F3S	SB	403	53	0,9,9	-	-	-		
152	PC1	N5	803	-	52,52,53	0.29	0	58,60,61	0.31	0
153	CDL	VB	701	-	61,61,99	0.36	0	67,73,111	0.32	0
153	CDL	QH	201	-	93,93,99	0.31	0	99,105,111	0.26	0
153	CDL	c3	604	-	67,67,99	0.35	0	73,79,111	0.31	0
157	FES	fs	201	35	0,4,4	-	-	-		
162	SF4	S8	303	127	0,12,12	-	-	-		
158	3PE	ta	201	-	25,25,50	0.41	0	28,30,55	0.41	0
153	CDL	M	306	-	63,63,99	0.36	0	69,75,111	0.32	0
162	SF4	S1	801	120	0,12,12	-	-	-		
152	PC1	al	302	-	25,25,53	0.40	0	31,33,61	0.39	0
152	PC1	c4	403	-	40,40,53	0.32	0	46,48,61	0.31	0
158	3PE	BM	302	-	29,29,50	0.39	0	32,34,55	0.47	0
153	CDL	C1	708	-	62,62,99	0.37	0	68,74,111	0.39	0
166	HEM	qC	501	110	50,50,50	1.30	7 (14%)	67,82,82	1.59	10 (14%)
153	CDL	th	200	-	83,83,99	0.32	0	89,95,111	0.28	0
158	3PE	Y5	202	-	27,27,50	0.40	0	30,32,55	0.34	0
153	CDL	m1	405	-	56,56,99	0.38	0	62,68,111	0.38	0
152	PC1	a	503	-	40,40,53	0.34	0	46,48,61	0.37	0
162	SF4	s1	802	120	0,12,12	-	-	-		
152	PC1	qg	401	-	31,31,53	0.36	0	37,39,61	0.35	0
153	CDL	Y5	201	-	69,69,99	0.35	0	75,81,111	0.31	0
158	3PE	m3	402	-	37,37,50	0.34	0	40,42,55	0.31	0
153	CDL	7c	302	-	50,50,99	0.40	0	56,62,111	0.35	0
152	PC1	f	402	-	37,37,53	0.34	0	43,45,61	0.30	0
153	CDL	bm	301	-	85,85,99	0.32	0	91,97,111	0.31	0
152	PC1	c2	703	-	35,35,53	0.35	0	41,43,61	0.32	0
153	CDL	2o	101	-	49,49,99	0.41	0	55,61,111	0.35	0
152	PC1	c3	602	-	38,38,53	0.33	0	44,46,61	0.32	0
152	PC1	m1	401	-	53,53,53	0.29	0	59,61,61	0.30	0
152	PC1	N	302	-	31,31,53	0.36	0	37,39,61	0.33	0
153	CDL	qg	402	-	99,99,99	0.30	0	105,111,111	0.30	0
164	U10	QC	506	-	29,29,63	2.74	12 (41%)	36,38,79	1.62	8 (22%)
158	3PE	sc	101	-	39,39,50	0.33	0	42,44,55	0.31	0
152	PC1	v	202	-	48,48,53	0.31	0	54,56,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	CDL	A1	102	-	66,66,99	0.36	0	72,78,111	0.37	0
153	CDL	FS	204	-	46,46,99	0.42	0	52,58,111	0.35	0
152	PC1	an	304	-	35,35,53	0.35	0	41,43,61	0.34	0
158	3PE	VB	707	-	27,27,50	0.39	0	30,32,55	0.35	0
153	CDL	q	201	-	62,62,99	0.37	0	68,74,111	0.38	0
153	CDL	a	504	-	93,93,99	0.30	0	99,105,111	0.27	0
153	CDL	AM	201	-	55,55,99	0.39	0	61,67,111	0.33	0
153	CDL	a9	402	-	75,75,99	0.34	0	81,87,111	0.35	0
152	PC1	C3	606	-	48,48,53	0.31	0	54,56,61	0.37	0
152	PC1	QJ	101	-	27,27,53	0.39	0	33,35,61	0.45	0
152	PC1	Qi	201	-	29,29,53	0.39	0	35,37,61	0.43	0
158	3PE	C4	402	-	50,50,50	0.30	0	53,55,55	0.31	0
153	CDL	2G	204	-	62,62,99	0.36	0	68,74,111	0.32	0
152	PC1	qI	202	-	42,42,53	0.31	0	48,50,61	0.32	0
153	CDL	u	201	-	59,59,99	0.38	0	65,71,111	0.33	0
152	PC1	C3	602	-	38,38,53	0.33	0	44,46,61	0.32	0
153	CDL	M3	403	-	54,54,99	0.39	0	60,66,111	0.38	0
152	PC1	qE	303	-	38,38,53	0.33	0	44,46,61	0.34	0
153	CDL	Qi	202	-	70,70,99	0.35	0	76,82,111	0.35	0
153	CDL	B	501	-	61,61,99	0.37	0	67,73,111	0.32	0
153	CDL	Qb	601	-	67,67,99	0.35	0	73,79,111	0.30	0
152	PC1	7a	202	-	44,44,53	0.31	0	50,52,61	0.33	0
153	CDL	QG	402	-	85,85,99	0.32	0	91,97,111	0.28	0
162	SF4	sb	402	53	0,12,12	-	-	-		
153	CDL	am	201	-	55,55,99	0.39	0	61,67,111	0.33	0
167	NDP	a9	401	-	51,52,52	0.32	0	71,80,80	0.36	0
171	FMN	V1	501	-	33,33,33	0.20	0	48,50,50	0.36	0
153	CDL	m3	403	-	54,54,99	0.39	0	60,66,111	0.38	0
152	PC1	qB	602	-	43,43,53	0.32	0	49,51,61	0.30	0
152	PC1	2J	201	-	41,41,53	0.33	0	47,49,61	0.38	0
163	F3S	sb	403	53	0,9,9	-	-	-		
166	HEM	qC	502	110	50,50,50	1.30	7 (14%)	67,82,82	1.59	12 (17%)
153	CDL	2m	101	-	95,95,99	0.30	0	101,107,111	0.31	0
152	PC1	t4	303	-	53,53,53	0.30	0	59,61,61	0.37	0
152	PC1	C2	701	-	35,35,53	0.35	0	41,43,61	0.32	0
152	PC1	c3	603	-	30,30,53	0.37	0	36,38,61	0.35	0
153	CDL	Qc	508	-	46,46,99	0.42	0	52,58,111	0.42	0
153	CDL	a	505	-	81,81,99	0.32	0	87,93,111	0.29	0
162	SF4	S7	201	126	0,12,12	-	-	-		
153	CDL	Z	101	-	66,66,99	0.36	0	72,78,111	0.30	0
153	CDL	T7	201	-	72,72,99	0.34	0	78,84,111	0.29	0
153	CDL	b8	302	-	68,68,99	0.35	0	74,80,111	0.31	0
153	CDL	B4	201	-	36,36,99	0.43	0	42,48,111	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	CDL	f	401	-	99,99,99	0.29	0	105,111,111	0.29	0
153	CDL	B3	102	-	81,81,99	0.33	0	87,93,111	0.29	0
153	CDL	c1	703	-	64,64,99	0.36	0	70,76,111	0.31	0
152	PC1	qC	507	-	49,49,53	0.30	0	55,57,61	0.31	0
158	3PE	B4	202	-	47,47,50	0.31	0	50,52,55	0.29	0
152	PC1	m2	402	-	31,31,53	0.36	0	37,39,61	0.41	0
166	HEM	qc	503	110	50,50,50	1.30	7 (14%)	67,82,82	1.62	12 (17%)
153	CDL	m1	402	-	65,65,99	0.36	0	71,77,111	0.31	0
158	3PE	m2	408	-	30,30,50	0.38	0	33,35,55	0.37	0
164	U10	qC	506	-	29,29,63	2.74	12 (41%)	36,38,79	1.62	8 (22%)
152	PC1	N5	801	-	51,51,53	0.30	0	57,59,61	0.30	0
153	CDL	7c	301	-	84,84,99	0.32	0	90,96,111	0.33	0
152	PC1	qe	301	-	32,32,53	0.36	0	38,40,61	0.36	0
153	CDL	A	504	-	93,93,99	0.30	0	99,105,111	0.27	0
152	PC1	w	204	-	33,33,53	0.36	0	39,41,61	0.36	0
152	PC1	a	501	-	40,40,53	0.33	0	46,48,61	0.36	0
152	PC1	s8	301	-	29,29,53	0.38	0	35,37,61	0.36	0
153	CDL	M2	404	-	73,73,99	0.34	0	79,85,111	0.34	0
162	SF4	V1	500	146	0,12,12	-	-	-		
152	PC1	te	102	-	31,31,53	0.37	0	37,39,61	0.42	0
152	PC1	M2	402	-	31,31,53	0.36	0	37,39,61	0.41	0
153	CDL	I	302	-	76,76,99	0.33	0	82,88,111	0.31	0
157	FES	QE	302	-	0,4,4	-	-	-		
153	CDL	y7	501	-	64,64,99	0.36	0	70,76,111	0.37	0
160	PX2	Qh	201	-	35,35,35	1.00	4 (11%)	38,40,40	1.05	2 (5%)
154	HEA	c1	708	29	67,67,67	2.32	26 (38%)	81,103,103	2.64	34 (41%)
153	CDL	q	202	-	71,71,99	0.34	0	77,83,111	0.30	0
168	ZMP	AB	201	80	34,36,36	0.69	1 (2%)	41,45,45	0.76	0
152	PC1	2f	301	-	46,46,53	0.32	0	52,54,61	0.52	0
152	PC1	M2	407	-	45,45,53	0.31	0	51,53,61	0.39	0
152	PC1	S8	301	-	29,29,53	0.38	0	35,37,61	0.36	0
158	3PE	an	306	-	28,28,50	0.40	0	31,33,55	0.43	0
158	3PE	W	203	-	33,33,50	0.36	0	36,38,55	0.32	0
152	PC1	2g	202	-	49,49,53	0.31	0	55,57,61	0.41	0
153	CDL	vb	704	-	66,66,99	0.35	0	72,78,111	0.31	0
153	CDL	al	301	-	52,52,99	0.39	0	58,64,111	0.33	0
152	PC1	c1	706	-	44,44,53	0.32	0	50,52,61	0.44	0
152	PC1	QI	202	-	42,42,53	0.31	0	48,50,61	0.32	0
158	3PE	TA	201	-	25,25,50	0.41	0	28,30,55	0.41	0
158	3PE	bm	302	-	29,29,50	0.39	0	32,34,55	0.47	0
152	PC1	C4	403	-	40,40,53	0.33	0	46,48,61	0.32	0
152	PC1	Qb	602	-	42,42,53	0.31	0	48,50,61	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
157	FES	FX	201	95	0,4,4	-	-	-		
166	HEM	y5	203	-	50,50,50	1.28	6 (12%)	67,82,82	1.61	10 (14%)
153	CDL	n5	806	-	89,89,99	0.31	0	95,101,111	0.28	0
166	HEM	QC	501	110	50,50,50	1.30	7 (14%)	67,82,82	1.59	10 (14%)
152	PC1	A	503	-	40,40,53	0.34	0	46,48,61	0.37	0
152	PC1	qi	203	-	41,41,53	0.33	0	47,49,61	0.37	0
153	CDL	c4	401	-	97,97,99	0.30	0	103,109,111	0.31	0
153	CDL	t1	601	-	54,54,99	0.39	0	60,66,111	0.36	0
153	CDL	AN	302	-	86,86,99	0.32	0	92,98,111	0.29	0
152	PC1	Qc	509	-	46,46,53	0.30	0	52,54,61	0.36	0
153	CDL	Qc	505	-	55,55,99	0.38	0	61,67,111	0.36	0
152	PC1	J1	400	-	39,39,53	0.33	0	45,47,61	0.34	0
153	CDL	E	403	-	62,62,99	0.37	0	68,74,111	0.31	0
159	P5S	m2	406	-	34,35,53	1.38	4 (11%)	36,42,60	1.02	2 (5%)
153	CDL	m	304	-	63,63,99	0.36	0	69,75,111	0.32	0
153	CDL	T1	601	-	54,54,99	0.39	0	60,66,111	0.36	0
166	HEM	qc	502	110	50,50,50	1.29	7 (14%)	67,82,82	1.59	10 (14%)
164	U10	Qc	507	-	29,29,63	2.75	13 (44%)	36,38,79	1.57	8 (22%)
152	PC1	TC	101	-	41,41,53	0.32	0	47,49,61	0.30	0
153	CDL	7a	203	-	61,61,99	0.37	0	67,73,111	0.34	0
152	PC1	C3	601	-	51,51,53	0.30	0	57,59,61	0.36	0
152	PC1	n5	801	-	51,51,53	0.30	0	57,59,61	0.31	0
164	U10	Qc	501	-	25,25,63	2.29	7 (28%)	24,29,79	1.92	8 (33%)
152	PC1	qE	301	-	23,23,53	0.40	0	29,31,61	0.39	0
153	CDL	6A	201	-	73,73,99	0.35	0	79,85,111	0.41	0
157	FES	qE	302	-	0,4,4	-	-	-		
158	3PE	an	305	-	32,32,50	0.37	0	35,37,55	0.35	0
153	CDL	5B	201	-	80,80,99	0.33	0	86,92,111	0.33	0
153	CDL	2K	101	-	97,97,99	0.30	0	103,109,111	0.35	0
157	FES	V2	300	147	0,4,4	-	-	-		
153	CDL	m	302	-	63,63,99	0.36	0	69,75,111	0.32	0
158	3PE	n5	802	-	35,35,50	0.36	0	38,40,55	0.32	0
152	PC1	t4	301	-	47,47,53	0.31	0	53,55,61	0.38	0
159	P5S	M2	406	-	34,35,53	1.38	4 (11%)	36,42,60	1.02	2 (5%)
153	CDL	m2	401	-	53,53,99	0.39	0	59,65,111	0.40	0
157	FES	s1	803	120	0,4,4	-	-	-		
153	CDL	e	402	-	71,71,99	0.34	0	77,83,111	0.35	0
153	CDL	L	301	-	73,73,99	0.34	0	79,85,111	0.29	0
158	3PE	AN	303	-	44,44,50	0.32	0	47,49,55	0.29	0
152	PC1	6A	202	-	34,34,53	0.36	0	40,42,61	0.36	0
158	3PE	AN	305	-	32,32,50	0.37	0	35,37,55	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
152	PC1	AM	202	-	38,38,53	0.33	0	44,46,61	0.33	0
158	3PE	SC	101	-	39,39,50	0.33	0	42,44,55	0.31	0
153	CDL	T	203	-	70,70,99	0.35	0	76,82,111	0.32	0
152	PC1	T1	602	-	32,32,53	0.36	0	38,40,61	0.35	0
162	SF4	S1	802	120	0,12,12	-	-	-		
167	NDP	A9	401	-	51,52,52	0.32	0	71,80,80	0.36	0
162	SF4	SB	402	53	0,12,12	-	-	-		
152	PC1	qI	201	-	29,29,53	0.38	0	35,37,61	0.34	0
152	PC1	2f	303	-	31,31,53	0.37	0	37,39,61	0.33	0
152	PC1	tc	101	-	41,41,53	0.32	0	47,49,61	0.30	0
152	PC1	am	202	-	38,38,53	0.33	0	44,46,61	0.33	0
152	PC1	V	202	-	48,48,53	0.31	0	54,56,61	0.34	0
153	CDL	t	202	-	74,74,99	0.34	0	80,86,111	0.35	0
153	CDL	t	201	-	58,58,99	0.38	0	64,70,111	0.32	0
153	CDL	c1	701	-	78,78,99	0.33	0	84,90,111	0.32	0
158	3PE	t4	302	-	24,24,50	0.42	0	27,29,55	0.36	0
152	PC1	m	307	-	35,35,53	0.35	0	41,43,61	0.34	0
158	3PE	M3	402	-	37,37,50	0.34	0	40,42,55	0.31	0
152	PC1	N	301	-	40,40,53	0.33	0	46,48,61	0.30	0
157	FES	qe	302	-	0,4,4	-	-	-		
153	CDL	M1	404	-	90,90,99	0.31	0	96,102,111	0.28	0
152	PC1	m	301	-	44,44,53	0.31	0	50,52,61	0.39	0
152	PC1	n5	804	-	38,38,53	0.33	0	44,46,61	0.34	0
152	PC1	C1	709	-	44,44,53	0.32	0	50,52,61	0.44	0
152	PC1	2G	202	-	49,49,53	0.31	0	55,57,61	0.41	0
153	CDL	C1	707	-	64,64,99	0.36	0	70,76,111	0.31	0
153	CDL	j	301	-	69,69,99	0.35	0	75,81,111	0.29	0
153	CDL	w	202	-	83,83,99	0.32	0	89,95,111	0.33	0
152	PC1	5B	202	-	46,46,53	0.31	0	52,54,61	0.29	0
153	CDL	SD	101	-	75,75,99	0.34	0	81,87,111	0.31	0
152	PC1	2F	301	-	46,46,53	0.32	0	52,54,61	0.52	0
153	CDL	J	301	-	69,69,99	0.35	0	75,81,111	0.29	0
152	PC1	QC	508	-	35,35,53	0.35	0	41,43,61	0.35	0
152	PC1	c1	707	-	37,37,53	0.34	0	43,45,61	0.33	0
152	PC1	2F	303	-	31,31,53	0.37	0	37,39,61	0.33	0
152	PC1	Qc	506	-	37,37,53	0.34	0	43,45,61	0.33	0
152	PC1	AN	304	-	35,35,53	0.35	0	41,43,61	0.34	0
153	CDL	Qc	504	-	63,63,99	0.37	0	69,75,111	0.34	0
152	PC1	QJ	102	-	37,37,53	0.34	0	43,45,61	0.38	0
152	PC1	N6	301	-	53,53,53	0.28	0	59,61,61	0.31	0
158	3PE	AN	306	-	28,28,50	0.40	0	31,33,55	0.43	0
152	PC1	w	201	-	48,48,53	0.30	0	54,56,61	0.30	0
152	PC1	M1	403	-	41,41,53	0.33	0	47,49,61	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
152	PC1	Qj	101	-	35,35,53	0.34	0	41,43,61	0.34	0
153	CDL	P1	402	-	62,62,99	0.37	0	68,74,111	0.31	0
153	CDL	b3	102	-	81,81,99	0.33	0	87,93,111	0.30	0
158	3PE	an	303	-	44,44,50	0.32	0	47,49,55	0.29	0
152	PC1	6C	201	-	32,32,53	0.36	0	38,40,61	0.37	0
154	HEA	c1	702	29	67,67,67	2.32	25 (37%)	81,103,103	2.58	32 (39%)
152	PC1	n6	301	-	53,53,53	0.28	0	59,61,61	0.31	0
152	PC1	QE	301	-	23,23,53	0.40	0	29,31,61	0.39	0
153	CDL	an	302	-	86,86,99	0.32	0	92,98,111	0.29	0
153	CDL	M3	401	-	62,62,99	0.36	0	68,74,111	0.32	0
153	CDL	2B	201	-	86,86,99	0.31	0	92,98,111	0.36	0
166	HEM	Y5	203	-	50,50,50	1.28	6 (12%)	67,82,82	1.61	10 (14%)
152	PC1	n	301	-	40,40,53	0.33	0	46,48,61	0.30	0
152	PC1	d	501	-	34,34,53	0.36	0	40,42,61	0.40	0
153	CDL	2k	101	-	97,97,99	0.30	0	103,109,111	0.35	0
153	CDL	qc	505	-	55,55,99	0.38	0	61,67,111	0.36	0
153	CDL	6C	202	-	74,74,99	0.34	0	80,86,111	0.33	0
152	PC1	tc	102	-	46,46,53	0.31	0	52,54,61	0.32	0
153	CDL	l	301	-	73,73,99	0.34	0	79,85,111	0.29	0
153	CDL	7A	203	-	61,61,99	0.37	0	67,73,111	0.34	0
153	CDL	A1	101	-	65,65,99	0.36	0	71,77,111	0.33	0
152	PC1	qC	508	-	35,35,53	0.35	0	41,43,61	0.35	0
164	U10	qc	507	-	29,29,63	2.75	13 (44%)	36,38,79	1.57	8 (22%)
153	CDL	qD	402	-	60,60,99	0.37	0	66,72,111	0.31	0
153	CDL	qi	202	-	70,70,99	0.35	0	76,82,111	0.35	0
152	PC1	QI	201	-	29,29,53	0.38	0	35,37,61	0.34	0
152	PC1	A	501	-	40,40,53	0.33	0	46,48,61	0.37	0
152	PC1	n	303	-	35,35,53	0.34	0	41,43,61	0.34	0
153	CDL	7C	301	-	84,84,99	0.32	0	90,96,111	0.33	0
152	PC1	m2	407	-	45,45,53	0.31	0	51,53,61	0.39	0
152	PC1	QC	505	-	37,37,53	0.34	0	43,45,61	0.31	0
153	CDL	C4	401	-	97,97,99	0.30	0	103,109,111	0.31	0
153	CDL	A	502	-	50,50,99	0.41	0	56,62,111	0.48	0
158	3PE	T4	302	-	24,24,50	0.42	0	27,29,55	0.37	0
157	FES	S1	803	120	0,4,4	-	-	-		
153	CDL	6c	202	-	81,81,99	0.32	0	87,93,111	0.30	0
153	CDL	te	101	-	52,52,99	0.39	0	58,64,111	0.33	0
162	SF4	s8	303	127	0,12,12	-	-	-		
158	3PE	b4	202	-	47,47,50	0.31	0	50,52,55	0.29	0
152	PC1	M	307	-	34,34,53	0.35	0	40,42,61	0.35	0
153	CDL	M1	402	-	65,65,99	0.36	0	71,77,111	0.31	0
152	PC1	TC	102	-	46,46,53	0.31	0	52,54,61	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
166	HEM	Qc	503	110	50,50,50	1.30	7 (14%)	67,82,82	1.62	12 (17%)
152	PC1	V	201	-	34,34,53	0.35	0	40,42,61	0.33	0
153	CDL	2g	204	-	62,62,99	0.36	0	68,74,111	0.32	0
152	PC1	Qg	401	-	31,31,53	0.36	0	37,39,61	0.35	0
152	PC1	qJ	101	-	37,37,53	0.34	0	43,45,61	0.38	0
152	PC1	n1	301	-	35,35,53	0.35	0	41,43,61	0.35	0
153	CDL	z	101	-	66,66,99	0.36	0	72,78,111	0.30	0
153	CDL	2g	203	-	54,54,99	0.39	0	60,66,111	0.36	0
164	U10	sc	102	-	63,63,63	2.22	24 (38%)	78,79,79	1.64	20 (25%)
171	FMN	v1	501	-	33,33,33	0.20	0	48,50,50	0.36	0
153	CDL	n	304	-	83,83,99	0.32	0	89,95,111	0.32	0
153	CDL	QC	504	-	55,55,99	0.38	0	61,67,111	0.40	0
152	PC1	W	204	-	33,33,53	0.36	0	39,41,61	0.36	0
153	CDL	BM	301	-	85,85,99	0.32	0	91,97,111	0.31	0
153	CDL	a1	101	-	66,66,99	0.36	0	72,78,111	0.37	0
153	CDL	qC	504	-	55,55,99	0.38	0	61,67,111	0.40	0
152	PC1	i	304	-	38,38,53	0.34	0	44,46,61	0.34	0
153	CDL	6c	201	-	74,74,99	0.34	0	80,86,111	0.33	0
151	HEC	qD	401	111	46,50,50	1.92	9 (19%)	58,82,82	1.85	8 (13%)
157	FES	v2	300	147	0,4,4	-	-	-		
152	PC1	n5	803	-	52,52,53	0.29	0	58,60,61	0.31	0
152	PC1	5b	202	-	46,46,53	0.31	0	52,54,61	0.29	0
152	PC1	n3	201	-	30,30,53	0.37	0	36,38,61	0.38	0
152	PC1	2j	201	-	41,41,53	0.33	0	47,49,61	0.38	0
153	CDL	P1	403	-	57,57,99	0.39	0	63,69,111	0.40	0
153	CDL	M2	401	-	53,53,99	0.39	0	59,65,111	0.40	0
152	PC1	qe	303	-	42,42,53	0.32	0	48,50,61	0.45	0
152	PC1	w	205	-	42,42,53	0.32	0	48,50,61	0.31	0
153	CDL	M	304	-	63,63,99	0.36	0	69,75,111	0.32	0
153	CDL	A9	402	-	75,75,99	0.34	0	81,87,111	0.35	0
153	CDL	M	301	-	65,65,99	0.36	0	71,77,111	0.31	0
153	CDL	2G	201	-	88,88,99	0.31	0	94,100,111	0.28	0
154	HEA	C1	702	29	67,67,67	2.28	26 (38%)	81,103,103	2.48	29 (35%)
158	3PE	s8	304	-	40,40,50	0.33	0	43,45,55	0.32	0
153	CDL	e	403	-	62,62,99	0.37	0	68,74,111	0.31	0
153	CDL	M1	405	-	56,56,99	0.38	0	62,68,111	0.38	0
152	PC1	QG	401	-	31,31,53	0.37	0	37,39,61	0.42	0
153	CDL	T	204	-	89,89,99	0.33	0	95,101,111	0.33	0
153	CDL	Q	201	-	62,62,99	0.37	0	68,74,111	0.38	0
153	CDL	m1	404	-	90,90,99	0.31	0	96,102,111	0.28	0
160	PX2	Y5	204	-	20,20,35	1.30	4 (20%)	23,25,40	1.30	2 (8%)
152	PC1	j1	400	-	39,39,53	0.33	0	45,47,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
153	CDL	N	304	-	83,83,99	0.32	0	89,95,111	0.32	0
153	CDL	QC	503	-	63,63,99	0.36	0	69,75,111	0.31	0
151	HEC	QD	401	111	46,50,50	1.92	10 (21%)	58,82,82	1.84	8 (13%)
151	HEC	2e	401	2	46,50,50	1.92	9 (19%)	58,82,82	1.93	8 (13%)
152	PC1	M	302	-	35,35,53	0.35	0	41,43,61	0.34	0
153	CDL	QI	203	-	70,70,99	0.35	0	76,82,111	0.31	0
153	CDL	B3	101	-	57,57,99	0.37	0	63,69,111	0.32	0
153	CDL	2g	201	-	88,88,99	0.31	0	94,100,111	0.28	0
152	PC1	C1	711	-	38,38,53	0.33	0	44,46,61	0.35	0
152	PC1	n	302	-	31,31,53	0.36	0	37,39,61	0.33	0
151	HEC	2E	401	2	46,50,50	1.92	7 (15%)	58,82,82	1.85	8 (13%)
158	3PE	an	301	-	44,44,50	0.32	0	47,49,55	0.28	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
153	CDL	p1	402	-	-	19/73/73/110	-
153	CDL	E	402	-	-	20/82/82/110	-
151	HEC	Qd	401	111	-	8/14/54/54	-
152	PC1	qc	506	-	-	16/41/41/57	-
153	CDL	C	301	-	-	12/74/74/110	-
158	3PE	AN	301	-	-	4/48/48/54	-
152	PC1	P1	401	-	-	9/43/43/57	-
153	CDL	qI	203	-	-	17/81/81/110	-
158	3PE	A3	201	-	-	12/48/48/54	-
153	CDL	N5	806	-	-	20/100/100/110	-
153	CDL	N6	302	-	-	18/100/100/110	-
153	CDL	R	201	-	-	24/75/75/110	-
168	ZMP	ab	201	80	-	22/43/43/43	-
152	PC1	qc	509	-	-	11/50/50/57	-
153	CDL	TE	101	-	-	19/63/63/110	-
153	CDL	2O	101	-	-	18/60/60/110	-
152	PC1	j	302	-	-	4/40/40/57	-
157	FES	FS	203	35	-	-	0/1/1/1
160	PX2	y5	204	-	-	13/22/22/37	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	I	301	-	-	11/42/42/57	-
153	CDL	Qg	402	-	-	23/110/110/110	-
152	PC1	M1	401	-	-	14/57/57/57	-
160	PX2	r	202	-	-	23/34/34/37	-
152	PC1	qj	101	-	-	11/39/39/57	-
153	CDL	b3	101	-	-	13/68/68/110	-
153	CDL	u1	101	-	-	13/67/67/110	-
164	U10	qc	501	-	-	10/28/28/87	-
158	3PE	G2	301	-	-	13/54/54/54	-
158	3PE	S8	304	-	-	8/44/44/54	-
153	CDL	2b	201	-	-	16/97/97/110	-
158	3PE	g2	301	-	-	13/54/54/54	-
153	CDL	U1	101	-	-	13/67/67/110	-
158	3PE	y5	202	-	-	8/31/31/54	-
153	CDL	c1	712	-	-	16/105/105/110	-
152	PC1	B9	201	-	-	13/37/37/57	-
152	PC1	n5	805	-	-	15/57/57/57	-
152	PC1	M	303	-	-	15/48/48/57	-
152	PC1	TE	102	-	-	9/35/35/57	-
152	PC1	T4	301	-	-	18/51/51/57	-
157	FES	SB	401	53	-	-	0/1/1/1
152	PC1	6a	202	-	-	13/38/38/57	-
153	CDL	7A	201	-	-	14/110/110/110	-
152	PC1	2F	302	-	-	8/45/45/57	-
153	CDL	qB	601	-	-	10/78/78/110	-
158	3PE	T8	602	-	-	10/42/42/54	-
152	PC1	M2	405	-	-	8/57/57/57	-
153	CDL	6C	203	-	-	16/92/92/110	-
152	PC1	qb	602	-	-	6/46/46/57	-
153	CDL	t5	301	-	-	24/106/106/110	-
160	PX2	R	202	-	-	19/34/34/37	-
152	PC1	t1	602	-	-	12/36/36/57	-
153	CDL	AL	301	-	-	16/63/63/110	-
152	PC1	c3	605	-	-	3/42/42/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
157	FES	FS	202	35	-	-	0/1/1/1
158	3PE	I	304	-	-	8/35/35/54	-
157	FES	sb	401	53	-	-	0/1/1/1
164	U10	b8	301	-	-	13/63/87/87	0/1/1/1
153	CDL	M2	403	-	-	18/76/76/110	-
166	HEM	QC	502	110	-	8/14/54/54	-
153	CDL	n6	302	-	-	19/100/100/110	-
152	PC1	W	201	-	-	13/52/52/57	-
152	PC1	N	303	-	-	5/39/39/57	-
152	PC1	N5	804	-	-	11/42/42/57	-
153	CDL	m	306	-	-	15/76/76/110	-
158	3PE	A3	202	-	-	12/47/47/54	-
169	T7X	B6	201	-	-	24/50/74/80	0/1/1/1
152	PC1	qG	401	-	-	6/35/35/57	-
153	CDL	Y7	501	-	-	13/75/75/110	-
158	3PE	vb	705	-	-	10/31/31/54	-
153	CDL	m2	403	-	-	18/76/76/110	-
153	CDL	T5	301	-	-	24/106/106/110	-
153	CDL	qH	201	-	-	13/104/104/110	-
151	HEC	qd	401	111	-	8/14/54/54	-
152	PC1	qi	201	-	-	8/33/33/57	-
153	CDL	qC	503	-	-	7/74/74/110	-
152	PC1	C3	605	-	-	3/42/42/57	-
161	FAD	SA	701	-	-	10/34/50/50	0/6/6/6
152	PC1	QE	303	-	-	2/42/42/57	-
153	CDL	Q	202	-	-	19/82/82/110	-
153	CDL	TH	200	-	-	17/94/94/110	-
158	3PE	a3	202	-	-	12/47/47/54	-
158	3PE	a3	201	-	-	12/48/48/54	-
153	CDL	sd	101	-	-	16/86/86/110	-
158	3PE	c4	402	-	-	7/54/54/54	-
153	CDL	t	203	-	-	22/81/81/110	-
158	3PE	t8	602	-	-	10/42/42/54	-
153	CDL	i	302	-	-	13/85/85/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	N3	201	-	-	3/34/34/57	-
153	CDL	VB	705	-	-	17/92/92/110	-
153	CDL	B8	302	-	-	10/79/79/110	-
153	CDL	t	204	-	-	30/100/100/110	-
153	CDL	qc	504	-	-	21/74/74/110	-
162	SF4	v1	500	146	-	-	0/6/5/5
157	FES	fs	202	35	-	-	0/1/1/1
152	PC1	QC	507	-	-	12/53/53/57	-
153	CDL	q	203	-	-	15/96/96/110	-
152	PC1	m	305	-	-	10/38/38/57	-
170	ADP	B9	202	-	-	4/16/32/32	0/3/3/3
152	PC1	W	205	-	-	6/46/46/57	-
152	PC1	FS	201	-	-	5/43/43/57	-
152	PC1	Qi	203	-	-	14/45/45/57	-
153	CDL	6a	201	-	-	21/84/84/110	-
152	PC1	qE	304	-	-	10/31/31/57	-
153	CDL	A9	403	-	-	19/97/97/110	-
153	CDL	b4	201	-	-	9/44/44/110	-
153	CDL	E	401	-	-	15/70/70/110	-
157	FES	fx	201	95	-	-	0/1/1/1
153	CDL	F	402	-	-	17/110/110/110	-
162	SF4	s8	302	127	-	-	0/6/5/5
153	CDL	p1	403	-	-	14/68/68/110	-
169	T7X	b6	201	-	-	23/50/74/80	0/1/1/1
154	HEA	C1	703	29	-	15/36/76/76	-
152	PC1	J	302	-	-	4/40/40/57	-
153	CDL	VB	706	-	-	16/77/77/110	-
152	PC1	m1	403	-	-	7/45/45/57	-
152	PC1	7c	303	-	-	7/46/46/57	-
158	3PE	M2	408	-	-	9/34/34/54	-
153	CDL	7a	201	-	-	15/110/110/110	-
153	CDL	I	303	-	-	13/85/85/110	-
158	3PE	w	203	-	-	14/37/37/54	-
158	3PE	N4	601	-	-	7/39/39/54	-
153	CDL	qb	601	-	-	9/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
158	3PE	N5	802	-	-	8/39/39/54	-
153	CDL	m2	404	-	-	10/84/84/110	-
153	CDL	y5	201	-	-	12/80/80/110	-
153	CDL	VB	703	-	-	14/96/96/110	-
152	PC1	7A	202	-	-	12/48/48/57	-
153	CDL	e	401	-	-	15/70/70/110	-
170	ADP	b9	202	-	-	4/16/32/32	0/3/3/3
153	CDL	r	201	-	-	24/75/75/110	-
160	PX2	qh	201	-	-	17/37/37/37	-
153	CDL	T	202	-	-	12/85/85/110	-
153	CDL	QB	601	-	-	10/78/78/110	-
152	PC1	c1	704	-	-	14/52/52/57	-
152	PC1	c3	601	-	-	10/55/55/57	-
152	PC1	C1	706	-	-	14/52/52/57	-
153	CDL	C1	712	-	-	16/105/105/110	-
164	U10	SC	102	-	-	12/63/87/87	0/1/1/1
152	PC1	2f	302	-	-	8/45/45/57	-
152	PC1	b9	201	-	-	13/37/37/57	-
164	U10	B8	301	-	-	13/63/87/87	0/1/1/1
152	PC1	N5	805	-	-	16/57/57/57	-
162	SF4	s1	801	120	-	-	0/6/5/5
152	PC1	p1	401	-	-	9/43/43/57	-
153	CDL	a	502	-	-	13/61/61/110	-
153	CDL	a9	403	-	-	19/97/97/110	-
153	CDL	c	301	-	-	11/74/74/110	-
153	CDL	fs	203	-	-	10/57/57/110	-
153	CDL	7C	302	-	-	10/61/61/110	-
153	CDL	i	301	-	-	16/87/87/110	-
152	PC1	m2	405	-	-	8/57/57/57	-
153	CDL	qG	402	-	-	16/96/96/110	-
152	PC1	7C	303	-	-	7/46/46/57	-
153	CDL	U	201	-	-	11/70/70/110	-
152	PC1	qC	505	-	-	12/41/41/57	-
153	CDL	W	202	-	-	16/94/94/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	b	501	-	-	15/72/72/110	-
162	SF4	S8	302	127	-	-	0/6/5/5
153	CDL	c1	709	-	-	23/73/73/110	-
153	CDL	5b	201	-	-	16/91/91/110	-
153	CDL	2G	203	-	-	10/65/65/110	-
153	CDL	M	305	-	-	9/93/93/110	-
153	CDL	T	201	-	-	11/69/69/110	-
152	PC1	C3	603	-	-	6/34/34/57	-
152	PC1	Qe	301	-	-	5/36/36/57	-
153	CDL	t7	201	-	-	15/83/83/110	-
152	PC1	N1	301	-	-	9/39/39/57	-
153	CDL	2M	101	-	-	18/106/106/110	-
158	3PE	i	303	-	-	8/35/35/54	-
157	FES	Qe	302	-	-	-	0/1/1/1
152	PC1	D	501	-	-	15/38/38/57	-
153	CDL	td	101	-	-	17/76/76/110	-
152	PC1	v	201	-	-	4/38/38/57	-
152	PC1	c3	606	-	-	7/52/52/57	-
166	HEM	Qc	502	110	-	4/14/54/54	-
153	CDL	m3	401	-	-	7/73/73/110	-
152	PC1	fs	204	-	-	5/43/43/57	-
153	CDL	C1	701	-	-	22/89/89/110	-
152	PC1	C1	710	-	-	6/41/41/57	-
161	FAD	sa	701	-	-	10/34/50/50	0/6/6/6
153	CDL	qc	508	-	-	9/57/57/110	-
153	CDL	QD	402	-	-	16/71/71/110	-
152	PC1	T4	303	-	-	12/57/57/57	-
153	CDL	m	303	-	-	9/93/93/110	-
158	3PE	n4	601	-	-	8/39/39/54	-
162	SF4	s7	201	126	-	-	0/6/5/5
152	PC1	AL	302	-	-	2/29/29/57	-
152	PC1	QB	602	-	-	6/47/47/57	-
158	3PE	T8	601	-	-	12/50/50/54	-
158	3PE	t8	601	-	-	12/50/50/54	-
153	CDL	C3	604	-	-	5/78/78/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	Qe	303	-	-	13/46/46/57	-
152	PC1	6c	203	-	-	8/36/36/57	-
152	PC1	F	401	-	-	8/41/41/57	-
153	CDL	vb	701	-	-	14/72/72/110	-
152	PC1	c1	711	-	-	10/42/42/57	-
163	F3S	SB	403	53	-	-	0/3/3/3
152	PC1	N5	803	-	-	8/56/56/57	-
153	CDL	VB	701	-	-	13/72/72/110	-
153	CDL	QH	201	-	-	13/104/104/110	-
153	CDL	c3	604	-	-	6/78/78/110	-
157	FES	fs	201	35	-	-	0/1/1/1
162	SF4	S8	303	127	-	-	0/6/5/5
158	3PE	ta	201	-	-	10/29/29/54	-
153	CDL	M	306	-	-	11/74/74/110	-
162	SF4	S1	801	120	-	-	0/6/5/5
152	PC1	al	302	-	-	2/29/29/57	-
152	PC1	c4	403	-	-	5/44/44/57	-
158	3PE	BM	302	-	-	8/33/33/54	-
153	CDL	C1	708	-	-	24/73/73/110	-
166	HEM	qC	501	110	-	7/14/54/54	-
153	CDL	th	200	-	-	17/94/94/110	-
158	3PE	Y5	202	-	-	8/31/31/54	-
153	CDL	m1	405	-	-	14/67/67/110	-
152	PC1	a	503	-	-	8/44/44/57	-
162	SF4	s1	802	120	-	-	0/6/5/5
152	PC1	qg	401	-	-	6/35/35/57	-
153	CDL	Y5	201	-	-	14/80/80/110	-
158	3PE	m3	402	-	-	7/41/41/54	-
153	CDL	7c	302	-	-	10/61/61/110	-
152	PC1	f	402	-	-	8/41/41/57	-
153	CDL	bm	301	-	-	22/96/96/110	-
152	PC1	c2	703	-	-	10/39/39/57	-
153	CDL	2o	101	-	-	17/60/60/110	-
152	PC1	c3	602	-	-	13/42/42/57	-
152	PC1	m1	401	-	-	14/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	N	302	-	-	8/35/35/57	-
153	CDL	qg	402	-	-	23/110/110/110	-
164	U10	QC	506	-	-	4/23/47/87	0/1/1/1
158	3PE	sc	101	-	-	10/43/43/54	-
152	PC1	v	202	-	-	13/52/52/57	-
153	CDL	A1	102	-	-	14/77/77/110	-
153	CDL	FS	204	-	-	9/57/57/110	-
152	PC1	an	304	-	-	9/39/39/57	-
158	3PE	VB	707	-	-	10/31/31/54	-
153	CDL	q	201	-	-	11/73/73/110	-
153	CDL	a	504	-	-	15/104/104/110	-
153	CDL	AM	201	-	-	11/66/66/110	-
153	CDL	a9	402	-	-	14/86/86/110	-
152	PC1	C3	606	-	-	7/52/52/57	-
152	PC1	QJ	101	-	-	10/31/31/57	-
152	PC1	Qi	201	-	-	8/33/33/57	-
158	3PE	C4	402	-	-	7/54/54/54	-
153	CDL	2G	204	-	-	15/73/73/110	-
152	PC1	qI	202	-	-	6/46/46/57	-
153	CDL	u	201	-	-	11/70/70/110	-
152	PC1	C3	602	-	-	13/42/42/57	-
153	CDL	M3	403	-	-	12/65/65/110	-
152	PC1	qE	303	-	-	2/42/42/57	-
153	CDL	Qi	202	-	-	14/81/81/110	-
153	CDL	B	501	-	-	15/72/72/110	-
153	CDL	Qb	601	-	-	9/78/78/110	-
152	PC1	7a	202	-	-	12/48/48/57	-
153	CDL	QG	402	-	-	16/96/96/110	-
167	NDP	a9	401	-	-	7/34/77/77	0/5/5/5
153	CDL	am	201	-	-	11/66/66/110	-
171	FMN	V1	501	-	-	2/18/18/18	0/3/3/3
162	SF4	sb	402	53	-	-	0/6/5/5
153	CDL	m3	403	-	-	12/65/65/110	-
152	PC1	qB	602	-	-	6/47/47/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	2J	201	-	-	14/45/45/57	-
163	F3S	sb	403	53	-	-	0/3/3/3
166	HEM	qC	502	110	-	8/14/54/54	-
153	CDL	2m	101	-	-	18/106/106/110	-
152	PC1	t4	303	-	-	12/57/57/57	-
152	PC1	C2	701	-	-	10/39/39/57	-
152	PC1	c3	603	-	-	7/34/34/57	-
153	CDL	Qc	508	-	-	9/57/57/110	-
153	CDL	a	505	-	-	17/92/92/110	-
162	SF4	S7	201	126	-	-	0/6/5/5
153	CDL	Z	101	-	-	12/77/77/110	-
153	CDL	T7	201	-	-	15/83/83/110	-
153	CDL	b8	302	-	-	10/79/79/110	-
153	CDL	B4	201	-	-	9/44/44/110	-
153	CDL	f	401	-	-	16/110/110/110	-
153	CDL	B3	102	-	-	18/92/92/110	-
153	CDL	c1	703	-	-	8/75/75/110	-
152	PC1	qC	507	-	-	12/53/53/57	-
158	3PE	B4	202	-	-	10/51/51/54	-
152	PC1	m2	402	-	-	12/35/35/57	-
166	HEM	qc	503	110	-	9/14/54/54	-
153	CDL	m1	402	-	-	13/76/76/110	-
158	3PE	m2	408	-	-	9/34/34/54	-
164	U10	qC	506	-	-	4/23/47/87	0/1/1/1
152	PC1	N5	801	-	-	11/55/55/57	-
153	CDL	7c	301	-	-	23/95/95/110	-
152	PC1	qe	301	-	-	5/36/36/57	-
153	CDL	A	504	-	-	15/104/104/110	-
152	PC1	w	204	-	-	6/37/37/57	-
152	PC1	a	501	-	-	10/44/44/57	-
152	PC1	s8	301	-	-	9/33/33/57	-
153	CDL	M2	404	-	-	10/84/84/110	-
162	SF4	V1	500	146	-	-	0/6/5/5
152	PC1	te	102	-	-	10/35/35/57	-
152	PC1	M2	402	-	-	12/35/35/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	I	302	-	-	16/87/87/110	-
157	FES	QE	302	-	-	-	0/1/1/1
153	CDL	y7	501	-	-	12/75/75/110	-
160	PX2	Qh	201	-	-	20/37/37/37	-
154	HEA	c1	708	29	-	16/36/76/76	-
153	CDL	q	202	-	-	19/82/82/110	-
168	ZMP	AB	201	80	-	22/43/43/43	-
152	PC1	2f	301	-	-	21/50/50/57	-
152	PC1	M2	407	-	-	9/49/49/57	-
152	PC1	S8	301	-	-	9/33/33/57	-
158	3PE	an	306	-	-	5/32/32/54	-
158	3PE	W	203	-	-	12/37/37/54	-
152	PC1	2g	202	-	-	13/53/53/57	-
153	CDL	vb	704	-	-	16/77/77/110	-
153	CDL	al	301	-	-	15/63/63/110	-
152	PC1	c1	706	-	-	8/48/48/57	-
152	PC1	QI	202	-	-	6/46/46/57	-
158	3PE	TA	201	-	-	11/29/29/54	-
158	3PE	bm	302	-	-	8/33/33/54	-
152	PC1	C4	403	-	-	5/44/44/57	-
152	PC1	Qb	602	-	-	6/46/46/57	-
157	FES	FX	201	95	-	-	0/1/1/1
166	HEM	y5	203	-	-	8/14/54/54	-
153	CDL	n5	806	-	-	20/100/100/110	-
166	HEM	QC	501	110	-	7/14/54/54	-
152	PC1	A	503	-	-	8/44/44/57	-
152	PC1	qi	203	-	-	14/45/45/57	-
153	CDL	c4	401	-	-	22/108/108/110	-
153	CDL	t1	601	-	-	10/65/65/110	-
153	CDL	AN	302	-	-	15/97/97/110	-
152	PC1	Qc	509	-	-	11/50/50/57	-
153	CDL	Qc	505	-	-	16/66/66/110	-
152	PC1	J1	400	-	-	9/43/43/57	-
153	CDL	E	403	-	-	12/73/73/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
159	P5S	m2	406	-	-	30/41/41/59	-
153	CDL	m	304	-	-	11/74/74/110	-
153	CDL	T1	601	-	-	10/65/65/110	-
166	HEM	qc	502	110	-	4/14/54/54	-
164	U10	Qc	507	-	-	7/23/47/87	0/1/1/1
152	PC1	TC	101	-	-	7/45/45/57	-
153	CDL	7a	203	-	-	11/72/72/110	-
152	PC1	C3	601	-	-	10/55/55/57	-
152	PC1	n5	801	-	-	11/55/55/57	-
164	U10	Qc	501	-	-	10/28/28/87	-
152	PC1	qE	301	-	-	7/26/26/57	-
153	CDL	6A	201	-	-	20/84/84/110	-
157	FES	qE	302	-	-	-	0/1/1/1
158	3PE	an	305	-	-	4/36/36/54	-
153	CDL	5B	201	-	-	15/91/91/110	-
153	CDL	2K	101	-	-	32/108/108/110	-
157	FES	V2	300	147	-	-	0/1/1/1
153	CDL	m	302	-	-	11/74/74/110	-
158	3PE	n5	802	-	-	8/39/39/54	-
152	PC1	t4	301	-	-	18/51/51/57	-
159	P5S	M2	406	-	-	29/41/41/59	-
153	CDL	m2	401	-	-	15/64/64/110	-
157	FES	s1	803	120	-	-	0/1/1/1
153	CDL	e	402	-	-	20/82/82/110	-
153	CDL	L	301	-	-	22/84/84/110	-
158	3PE	AN	303	-	-	8/48/48/54	-
152	PC1	6A	202	-	-	13/38/38/57	-
158	3PE	AN	305	-	-	4/36/36/54	-
152	PC1	AM	202	-	-	8/42/42/57	-
158	3PE	SC	101	-	-	10/43/43/54	-
153	CDL	T	203	-	-	22/81/81/110	-
152	PC1	T1	602	-	-	12/36/36/57	-
162	SF4	S1	802	120	-	-	0/6/5/5
167	NDP	A9	401	-	-	7/34/77/77	0/5/5/5
162	SF4	SB	402	53	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	qI	201	-	-	5/33/33/57	-
152	PC1	2f	303	-	-	9/35/35/57	-
152	PC1	tc	101	-	-	7/45/45/57	-
152	PC1	am	202	-	-	8/42/42/57	-
152	PC1	V	202	-	-	13/52/52/57	-
153	CDL	t	202	-	-	12/85/85/110	-
153	CDL	t	201	-	-	12/69/69/110	-
153	CDL	c1	701	-	-	22/89/89/110	-
158	3PE	t4	302	-	-	4/28/28/54	-
152	PC1	m	307	-	-	11/39/39/57	-
158	3PE	M3	402	-	-	7/41/41/54	-
152	PC1	N	301	-	-	5/44/44/57	-
157	FES	qe	302	-	-	-	0/1/1/1
153	CDL	M1	404	-	-	17/101/101/110	-
152	PC1	m	301	-	-	15/48/48/57	-
152	PC1	n5	804	-	-	11/42/42/57	-
152	PC1	C1	709	-	-	8/48/48/57	-
152	PC1	2G	202	-	-	13/53/53/57	-
153	CDL	C1	707	-	-	8/75/75/110	-
153	CDL	j	301	-	-	15/80/80/110	-
153	CDL	w	202	-	-	16/94/94/110	-
152	PC1	5B	202	-	-	10/50/50/57	-
153	CDL	SD	101	-	-	16/86/86/110	-
152	PC1	2F	301	-	-	21/50/50/57	-
153	CDL	J	301	-	-	15/80/80/110	-
152	PC1	QC	508	-	-	9/39/39/57	-
152	PC1	c1	707	-	-	6/41/41/57	-
152	PC1	2F	303	-	-	9/35/35/57	-
152	PC1	Qc	506	-	-	16/41/41/57	-
152	PC1	AN	304	-	-	9/39/39/57	-
153	CDL	Qc	504	-	-	21/74/74/110	-
152	PC1	QJ	102	-	-	12/41/41/57	-
152	PC1	N6	301	-	-	12/57/57/57	-
158	3PE	AN	306	-	-	5/32/32/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
152	PC1	w	201	-	-	13/52/52/57	-
152	PC1	M1	403	-	-	7/45/45/57	-
152	PC1	Qj	101	-	-	11/39/39/57	-
153	CDL	P1	402	-	-	19/73/73/110	-
153	CDL	b3	102	-	-	20/92/92/110	-
158	3PE	an	303	-	-	7/48/48/54	-
152	PC1	6C	201	-	-	8/36/36/57	-
154	HEA	c1	702	29	-	12/36/76/76	-
152	PC1	n6	301	-	-	12/57/57/57	-
152	PC1	QE	301	-	-	7/26/26/57	-
153	CDL	an	302	-	-	15/97/97/110	-
153	CDL	M3	401	-	-	7/73/73/110	-
153	CDL	2B	201	-	-	16/97/97/110	-
166	HEM	Y5	203	-	-	8/14/54/54	-
152	PC1	n	301	-	-	5/44/44/57	-
152	PC1	d	501	-	-	15/38/38/57	-
153	CDL	2k	101	-	-	32/108/108/110	-
153	CDL	qc	505	-	-	16/66/66/110	-
153	CDL	6C	202	-	-	27/85/85/110	-
152	PC1	tc	102	-	-	14/50/50/57	-
153	CDL	l	301	-	-	22/84/84/110	-
153	CDL	7A	203	-	-	11/72/72/110	-
153	CDL	A1	101	-	-	17/76/76/110	-
152	PC1	qC	508	-	-	9/39/39/57	-
164	U10	qc	507	-	-	7/23/47/87	0/1/1/1
153	CDL	qD	402	-	-	16/71/71/110	-
153	CDL	qi	202	-	-	14/81/81/110	-
152	PC1	QI	201	-	-	4/33/33/57	-
152	PC1	A	501	-	-	10/44/44/57	-
152	PC1	n	303	-	-	6/39/39/57	-
153	CDL	7C	301	-	-	23/95/95/110	-
152	PC1	m2	407	-	-	9/49/49/57	-
152	PC1	QC	505	-	-	12/41/41/57	-
153	CDL	C4	401	-	-	22/108/108/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	A	502	-	-	13/61/61/110	-
158	3PE	T4	302	-	-	4/28/28/54	-
157	FES	S1	803	120	-	-	0/1/1/1
153	CDL	6c	202	-	-	16/92/92/110	-
153	CDL	te	101	-	-	20/63/63/110	-
162	SF4	s8	303	127	-	-	0/6/5/5
158	3PE	b4	202	-	-	11/51/51/54	-
152	PC1	M	307	-	-	10/38/38/57	-
153	CDL	M1	402	-	-	13/76/76/110	-
152	PC1	TC	102	-	-	14/50/50/57	-
166	HEM	Qc	503	110	-	9/14/54/54	-
152	PC1	V	201	-	-	4/38/38/57	-
153	CDL	2g	204	-	-	16/73/73/110	-
152	PC1	Qg	401	-	-	7/35/35/57	-
152	PC1	qJ	101	-	-	12/41/41/57	-
152	PC1	n1	301	-	-	9/39/39/57	-
153	CDL	z	101	-	-	12/77/77/110	-
153	CDL	2g	203	-	-	10/65/65/110	-
164	U10	sc	102	-	-	12/63/87/87	0/1/1/1
171	FMN	v1	501	-	-	2/18/18/18	0/3/3/3
153	CDL	n	304	-	-	33/94/94/110	-
153	CDL	QC	504	-	-	11/66/66/110	-
152	PC1	W	204	-	-	6/37/37/57	-
153	CDL	BM	301	-	-	22/96/96/110	-
153	CDL	a1	101	-	-	13/77/77/110	-
153	CDL	qC	504	-	-	11/66/66/110	-
152	PC1	i	304	-	-	11/42/42/57	-
153	CDL	6c	201	-	-	27/85/85/110	-
151	HEC	qD	401	111	-	6/14/54/54	-
157	FES	v2	300	147	-	-	0/1/1/1
152	PC1	n5	803	-	-	8/56/56/57	-
152	PC1	5b	202	-	-	10/50/50/57	-
152	PC1	n3	201	-	-	3/34/34/57	-
152	PC1	2j	201	-	-	14/45/45/57	-
153	CDL	P1	403	-	-	14/68/68/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
153	CDL	M2	401	-	-	15/64/64/110	-
152	PC1	qe	303	-	-	13/46/46/57	-
152	PC1	w	205	-	-	6/46/46/57	-
153	CDL	M	304	-	-	11/74/74/110	-
153	CDL	A9	402	-	-	15/86/86/110	-
153	CDL	M	301	-	-	15/76/76/110	-
153	CDL	2G	201	-	-	19/99/99/110	-
154	HEA	C1	702	29	-	12/36/76/76	-
158	3PE	s8	304	-	-	8/44/44/54	-
153	CDL	e	403	-	-	12/73/73/110	-
153	CDL	M1	405	-	-	15/67/67/110	-
152	PC1	QG	401	-	-	6/35/35/57	-
153	CDL	T	204	-	-	30/100/100/110	-
153	CDL	Q	201	-	-	11/73/73/110	-
153	CDL	m1	404	-	-	17/101/101/110	-
160	PX2	Y5	204	-	-	13/22/22/37	-
152	PC1	j1	400	-	-	9/43/43/57	-
153	CDL	N	304	-	-	33/94/94/110	-
153	CDL	QC	503	-	-	7/74/74/110	-
151	HEC	QD	401	111	-	6/14/54/54	-
151	HEC	2e	401	2	-	9/14/54/54	-
152	PC1	M	302	-	-	11/39/39/57	-
153	CDL	QI	203	-	-	17/81/81/110	-
153	CDL	B3	101	-	-	13/68/68/110	-
153	CDL	2g	201	-	-	19/99/99/110	-
152	PC1	C1	711	-	-	10/42/42/57	-
152	PC1	n	302	-	-	8/35/35/57	-
151	HEC	2E	401	2	-	9/14/54/54	-
158	3PE	an	301	-	-	3/48/48/54	-

All (440) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	sc	102	U10	C6-C1	10.50	1.54	1.35
164	SC	102	U10	C6-C1	10.49	1.54	1.35
164	qc	507	U10	C6-C1	10.36	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	Qc	507	U10	C6-C1	10.36	1.53	1.35
164	qC	506	U10	C6-C1	10.30	1.53	1.35
164	QC	506	U10	C6-C1	10.30	1.53	1.35
164	b8	301	U10	C6-C1	10.25	1.53	1.35
164	B8	301	U10	C6-C1	10.25	1.53	1.35
164	Qc	501	U10	C6-C1	8.99	1.53	1.33
164	qc	501	U10	C6-C1	8.99	1.53	1.33
151	2e	401	HEC	CAC-C3C	7.27	1.58	1.35
151	2E	401	HEC	CAC-C3C	7.23	1.58	1.35
151	Qd	401	HEC	CAC-C3C	7.17	1.58	1.35
151	qd	401	HEC	CAC-C3C	7.17	1.58	1.35
151	QD	401	HEC	CAC-C3C	7.15	1.58	1.35
151	qD	401	HEC	CAC-C3C	7.15	1.58	1.35
151	2e	401	HEC	CAB-C3B	6.73	1.56	1.35
151	qd	401	HEC	CAB-C3B	6.73	1.56	1.35
151	Qd	401	HEC	CAB-C3B	6.73	1.56	1.35
151	QD	401	HEC	CAB-C3B	6.71	1.56	1.35
151	qD	401	HEC	CAB-C3B	6.70	1.56	1.35
151	2E	401	HEC	CAB-C3B	6.49	1.56	1.35
154	C1	703	HEA	C4B-NB	-5.99	1.29	1.40
154	C1	703	HEA	FE-ND	5.51	2.11	1.94
154	c1	708	HEA	FE-ND	5.46	2.11	1.94
154	C1	702	HEA	FE-ND	5.46	2.11	1.94
154	c1	702	HEA	C3B-C2B	5.43	1.47	1.34
154	C1	702	HEA	C3B-C2B	5.29	1.46	1.34
154	c1	708	HEA	C3B-C2B	5.28	1.46	1.34
169	B6	201	T7X	P1-O1	5.02	1.74	1.59
169	b6	201	T7X	P1-O1	5.02	1.74	1.59
154	c1	702	HEA	FE-ND	4.93	2.10	1.94
164	qc	507	U10	C4-C3	4.90	1.54	1.36
164	Qc	507	U10	C4-C3	4.90	1.54	1.36
164	QC	506	U10	C4-C3	4.88	1.53	1.36
164	qC	506	U10	C4-C3	4.87	1.53	1.36
154	C1	703	HEA	C3D-C2D	4.79	1.47	1.36
164	B8	301	U10	C4-C3	4.77	1.53	1.36
164	b8	301	U10	C4-C3	4.76	1.53	1.36
154	c1	702	HEA	FE-NB	4.74	2.09	1.94
170	b9	202	ADP	C5-C4	4.69	1.47	1.39
170	B9	202	ADP	C5-C4	4.69	1.47	1.39
154	c1	708	HEA	C11-C3B	-4.69	1.45	1.51
154	C1	703	HEA	FE-NC	4.69	2.10	1.95
164	sc	102	U10	C4-C3	4.68	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	SC	102	U10	C4-C3	4.68	1.53	1.36
154	c1	702	HEA	FE-NC	4.59	2.10	1.95
154	c1	702	HEA	C3A-C2A	4.57	1.47	1.37
154	c1	702	HEA	C11-C3B	-4.57	1.45	1.51
154	c1	708	HEA	FE-NC	4.38	2.09	1.95
154	c1	708	HEA	FE-NB	4.36	2.08	1.94
154	C1	702	HEA	FE-NC	4.32	2.09	1.95
154	C1	703	HEA	C3B-C2B	4.29	1.44	1.34
154	C1	703	HEA	C11-C3B	-4.26	1.46	1.51
154	c1	708	HEA	C3A-C2A	4.24	1.46	1.37
154	C1	703	HEA	CHC-C4B	4.18	1.46	1.38
154	c1	708	HEA	CHA-C1A	4.17	1.46	1.38
154	C1	702	HEA	C3A-C2A	4.16	1.46	1.37
154	C1	702	HEA	C3D-C2D	4.13	1.45	1.36
154	c1	702	HEA	C3D-C2D	4.08	1.45	1.36
154	C1	703	HEA	FE-NB	4.03	2.07	1.94
154	C1	702	HEA	C1D-ND	-4.01	1.33	1.40
169	B6	201	T7X	O16-C10	3.99	1.45	1.34
169	b6	201	T7X	O16-C10	3.98	1.45	1.34
154	c1	708	HEA	C1D-ND	-3.94	1.33	1.40
154	C1	702	HEA	FE-NB	3.93	2.07	1.94
154	C1	702	HEA	CHC-C4B	3.91	1.46	1.38
154	c1	702	HEA	C4B-NB	-3.87	1.33	1.40
154	C1	702	HEA	C4B-NB	-3.86	1.33	1.40
154	C1	703	HEA	C3A-C2A	3.81	1.45	1.37
154	c1	702	HEA	C1D-ND	-3.81	1.33	1.40
154	C1	703	HEA	C1B-NB	-3.78	1.31	1.38
154	c1	708	HEA	C3D-C2D	3.74	1.44	1.36
154	c1	702	HEA	CHC-C4B	3.70	1.45	1.38
154	c1	708	HEA	C4B-NB	-3.69	1.33	1.40
154	C1	703	HEA	CHC-C1C	3.67	1.47	1.39
154	c1	708	HEA	CHC-C4B	3.64	1.45	1.38
154	c1	702	HEA	CHA-C1A	3.64	1.45	1.38
154	C1	702	HEA	C11-C3B	-3.62	1.47	1.51
166	qC	502	HEM	C4D-ND	-3.61	1.34	1.40
166	QC	502	HEM	C4D-ND	-3.61	1.34	1.40
166	qC	501	HEM	C4D-ND	-3.59	1.34	1.40
166	QC	501	HEM	C4D-ND	-3.59	1.34	1.40
154	c1	702	HEA	CHD-C1D	3.56	1.45	1.38
166	qc	503	HEM	C4D-ND	-3.55	1.34	1.40
166	Qc	503	HEM	C4D-ND	-3.55	1.34	1.40
154	C1	702	HEA	C4A-NA	3.51	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
169	b6	201	T7X	O18-C11	3.51	1.43	1.33
169	B6	201	T7X	O18-C11	3.51	1.43	1.33
166	qc	502	HEM	C4D-ND	-3.51	1.34	1.40
151	2E	401	HEC	CBC-CAC	-3.51	1.36	1.49
166	Qc	502	HEM	C4D-ND	-3.51	1.34	1.40
154	c1	708	HEA	C4C-NC	-3.49	1.33	1.39
166	Y5	203	HEM	C4D-ND	-3.48	1.34	1.40
166	y5	203	HEM	C4D-ND	-3.48	1.34	1.40
154	C1	702	HEA	C4C-NC	-3.43	1.33	1.39
151	qD	401	HEC	CBC-CAC	-3.42	1.36	1.49
151	2e	401	HEC	CBC-CAC	-3.42	1.36	1.49
151	Qd	401	HEC	CBC-CAC	-3.42	1.36	1.49
151	qd	401	HEC	CBC-CAC	-3.42	1.36	1.49
151	QD	401	HEC	CBC-CAC	-3.40	1.36	1.49
154	c1	708	HEA	CHD-C4C	3.40	1.47	1.39
154	c1	708	HEA	CHB-C1B	3.38	1.46	1.39
154	C1	703	HEA	CHD-C1D	3.37	1.45	1.38
154	C1	702	HEA	CHD-C4C	3.34	1.46	1.39
154	C1	702	HEA	CHA-C1A	3.28	1.44	1.38
154	c1	702	HEA	C1C-NC	-3.27	1.33	1.39
154	c1	702	HEA	CHD-C4C	3.27	1.46	1.39
169	b6	201	T7X	P1-O13	3.25	1.72	1.59
169	B6	201	T7X	P1-O13	3.25	1.72	1.59
154	c1	702	HEA	C1A-NA	3.23	1.45	1.39
154	C1	703	HEA	C4C-NC	-3.23	1.33	1.39
154	C1	703	HEA	CHA-C1A	3.22	1.44	1.38
159	m2	406	P5S	O19-C17	3.19	1.42	1.33
159	M2	406	P5S	O19-C17	3.19	1.42	1.33
154	c1	708	HEA	C4B-C3B	3.17	1.50	1.44
154	C1	702	HEA	CHD-C1D	3.16	1.44	1.38
154	C1	702	HEA	C1C-NC	-3.11	1.33	1.39
166	qc	503	HEM	C1B-NB	-3.10	1.34	1.40
166	Qc	503	HEM	C1B-NB	-3.09	1.34	1.40
166	qc	502	HEM	C1B-NB	-3.07	1.34	1.40
166	Qc	502	HEM	C1B-NB	-3.07	1.34	1.40
154	c1	702	HEA	CHA-C4D	3.05	1.46	1.39
154	C1	702	HEA	CHC-C1C	3.05	1.46	1.39
166	qC	502	HEM	C1B-NB	-3.04	1.35	1.40
166	QC	502	HEM	C1B-NB	-3.04	1.35	1.40
154	C1	703	HEA	CHA-C4D	3.03	1.46	1.39
154	c1	708	HEA	CHA-C4D	3.02	1.46	1.39
166	qC	501	HEM	C1B-NB	-3.02	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
166	QC	501	HEM	C1B-NB	-3.02	1.35	1.40
154	C1	702	HEA	C1B-NB	-3.01	1.32	1.38
164	SC	102	U10	C41-C39	3.01	1.57	1.51
164	sc	102	U10	C41-C39	3.00	1.57	1.51
154	c1	702	HEA	C4C-NC	-2.99	1.34	1.39
164	B8	301	U10	C41-C39	2.98	1.57	1.51
164	b8	301	U10	C41-C39	2.98	1.57	1.51
166	y5	203	HEM	C1B-NB	-2.95	1.35	1.40
166	Y5	203	HEM	C1B-NB	-2.95	1.35	1.40
154	C1	702	HEA	CHA-C4D	2.95	1.45	1.39
164	sc	102	U10	C7-C8	2.94	1.55	1.50
154	c1	702	HEA	C1B-NB	-2.92	1.33	1.38
164	SC	102	U10	C7-C8	2.92	1.55	1.50
169	B6	201	T7X	C12-C10	2.86	1.59	1.50
169	b6	201	T7X	C12-C10	2.86	1.59	1.50
164	SC	102	U10	C26-C24	2.85	1.57	1.51
154	c1	708	HEA	C4A-NA	2.85	1.45	1.39
164	sc	102	U10	C26-C24	2.85	1.57	1.51
154	c1	702	HEA	CHB-C4A	2.85	1.44	1.38
154	c1	708	HEA	CHD-C1D	2.83	1.44	1.38
166	qC	502	HEM	C1C-C2C	-2.83	1.39	1.45
154	C1	702	HEA	C4D-ND	-2.83	1.33	1.38
166	QC	502	HEM	C1C-C2C	-2.82	1.39	1.45
164	b8	301	U10	C26-C24	2.82	1.57	1.51
164	QC	506	U10	C7-C8	2.82	1.55	1.50
164	B8	301	U10	C26-C24	2.82	1.57	1.51
164	qC	506	U10	C7-C8	2.82	1.55	1.50
166	qc	503	HEM	C1C-C2C	-2.80	1.39	1.45
166	Qc	503	HEM	C1C-C2C	-2.80	1.39	1.45
154	C1	702	HEA	C1A-NA	2.79	1.44	1.39
154	c1	708	HEA	C4D-ND	-2.78	1.33	1.38
154	c1	702	HEA	CHC-C1C	2.77	1.45	1.39
164	sc	102	U10	C31-C29	2.76	1.57	1.51
164	SC	102	U10	C31-C29	2.76	1.57	1.51
166	qc	503	HEM	C1D-ND	-2.74	1.33	1.38
160	qh	201	PX2	O7-C2	-2.74	1.40	1.46
160	Y5	204	PX2	O7-C2	-2.74	1.40	1.46
166	QC	502	HEM	C1D-ND	-2.74	1.33	1.38
166	Qc	503	HEM	C1D-ND	-2.74	1.33	1.38
166	qC	502	HEM	C1D-ND	-2.73	1.33	1.38
164	Qc	507	U10	C7-C8	2.73	1.54	1.50
164	qc	507	U10	C7-C8	2.73	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	b8	301	U10	C7-C8	2.72	1.54	1.50
164	B8	301	U10	C7-C8	2.72	1.54	1.50
159	m2	406	P5S	O37-C38	2.71	1.41	1.34
159	M2	406	P5S	O37-C38	2.71	1.41	1.34
160	Qh	201	PX2	O7-C2	-2.71	1.40	1.46
160	y5	204	PX2	O7-C2	-2.71	1.40	1.46
154	C1	702	HEA	CHB-C1B	2.69	1.45	1.39
164	SC	102	U10	C21-C19	2.68	1.56	1.51
170	b9	202	ADP	C5-C6	2.67	1.48	1.41
170	B9	202	ADP	C5-C6	2.67	1.48	1.41
164	sc	102	U10	C21-C19	2.67	1.56	1.51
164	b8	301	U10	C31-C29	2.67	1.56	1.51
164	B8	301	U10	C31-C29	2.66	1.56	1.51
166	Qc	502	HEM	C1D-ND	-2.66	1.33	1.38
166	qc	502	HEM	C1D-ND	-2.66	1.33	1.38
159	m2	406	P5S	O37-C2	-2.65	1.40	1.46
159	M2	406	P5S	O37-C2	-2.65	1.40	1.46
154	c1	702	HEA	C4A-NA	2.65	1.44	1.39
164	b8	301	U10	C21-C19	2.64	1.56	1.51
164	B8	301	U10	C21-C19	2.64	1.56	1.51
154	C1	703	HEA	O2D-CGD	-2.63	1.22	1.30
151	2E	401	HEC	CMD-C2D	2.63	1.56	1.50
154	c1	708	HEA	CHB-C4A	2.62	1.43	1.38
166	qC	501	HEM	C1D-ND	-2.62	1.33	1.38
166	QC	501	HEM	C1D-ND	-2.62	1.33	1.38
166	y5	203	HEM	C1D-ND	-2.60	1.33	1.38
166	Y5	203	HEM	C1D-ND	-2.60	1.33	1.38
166	qC	501	HEM	C1C-C2C	-2.60	1.40	1.45
166	QC	501	HEM	C1C-C2C	-2.60	1.40	1.45
164	sc	102	U10	C46-C44	2.55	1.56	1.51
164	SC	102	U10	C46-C44	2.55	1.56	1.51
154	C1	703	HEA	C1C-NC	-2.54	1.34	1.39
154	C1	703	HEA	CHB-C1B	2.54	1.45	1.39
164	sc	102	U10	C7-C6	2.54	1.56	1.51
164	qc	501	U10	C21-C19	2.53	1.56	1.51
164	sc	102	U10	O5-C5	-2.53	1.17	1.23
164	SC	102	U10	C7-C6	2.53	1.56	1.51
168	AB	201	ZMP	C9-C10	-2.53	1.48	1.50
164	Qc	501	U10	C21-C19	2.52	1.56	1.51
164	SC	102	U10	O5-C5	-2.52	1.17	1.23
168	ab	201	ZMP	C9-C10	-2.52	1.48	1.50
154	c1	708	HEA	C1C-NC	-2.51	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
154	c1	702	HEA	C4D-ND	-2.51	1.33	1.38
154	c1	702	HEA	O2D-CGD	-2.50	1.22	1.30
154	C1	702	HEA	O2D-CGD	-2.50	1.22	1.30
164	b8	301	U10	O5-C5	-2.50	1.17	1.23
164	B8	301	U10	O5-C5	-2.49	1.17	1.23
166	QC	502	HEM	FE-NB	2.49	2.02	1.94
164	sc	102	U10	C36-C34	2.49	1.56	1.51
166	qC	502	HEM	FE-NB	2.49	2.02	1.94
166	qc	503	HEM	FE-NB	2.49	2.02	1.94
164	SC	102	U10	C36-C34	2.49	1.56	1.51
166	Qc	503	HEM	FE-NB	2.49	2.02	1.94
166	Qc	502	HEM	C1C-C2C	-2.49	1.40	1.45
154	C1	702	HEA	O2A-CGA	-2.49	1.22	1.30
154	C1	703	HEA	C4A-NA	2.48	1.44	1.39
166	qc	502	HEM	C1C-C2C	-2.48	1.40	1.45
154	c1	708	HEA	O2A-CGA	-2.48	1.22	1.30
166	Y5	203	HEM	FE-NB	2.48	2.02	1.94
166	y5	203	HEM	FE-NB	2.48	2.02	1.94
164	qC	506	U10	C7-C6	2.47	1.56	1.51
164	QC	506	U10	C7-C6	2.47	1.56	1.51
164	B8	301	U10	C46-C44	2.47	1.56	1.51
166	Y5	203	HEM	C1C-C2C	-2.47	1.40	1.45
164	b8	301	U10	C36-C34	2.47	1.56	1.51
164	b8	301	U10	C46-C44	2.46	1.56	1.51
154	C1	703	HEA	CHB-C4A	2.46	1.43	1.38
164	B8	301	U10	C36-C34	2.46	1.56	1.51
166	y5	203	HEM	C1C-C2C	-2.46	1.40	1.45
154	c1	702	HEA	CHB-C1B	2.45	1.44	1.39
164	SC	102	U10	O3-C3M	-2.43	1.39	1.45
164	qc	507	U10	O5-C5	-2.43	1.17	1.23
160	R	202	PX2	O7-C2	-2.42	1.40	1.46
164	Qc	507	U10	O5-C5	-2.42	1.18	1.23
164	sc	102	U10	O3-C3M	-2.42	1.39	1.45
164	qC	506	U10	O5-C5	-2.42	1.18	1.23
154	c1	702	HEA	O2A-CGA	-2.42	1.22	1.30
166	QC	501	HEM	FE-NB	2.41	2.02	1.94
154	c1	708	HEA	C1A-NA	2.41	1.44	1.39
164	QC	506	U10	O5-C5	-2.41	1.18	1.23
154	C1	703	HEA	CHD-C4C	2.41	1.44	1.39
164	qC	506	U10	C6-C5	2.41	1.53	1.46
166	qC	501	HEM	FE-NB	2.41	2.02	1.94
154	c1	708	HEA	O2D-CGD	-2.41	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	QC	506	U10	C6-C5	2.41	1.53	1.46
164	Qc	507	U10	C11-C9	2.41	1.56	1.51
160	r	202	PX2	O7-C2	-2.41	1.40	1.46
164	qc	507	U10	C11-C9	2.41	1.56	1.51
154	c1	708	HEA	C1B-NB	-2.39	1.34	1.38
166	Qc	502	HEM	FE-NB	2.39	2.02	1.94
166	qc	502	HEM	FE-NB	2.39	2.02	1.94
164	b8	301	U10	C51-C49	2.38	1.56	1.51
164	B8	301	U10	C51-C49	2.38	1.56	1.51
164	B8	301	U10	C27-C28	2.38	1.57	1.50
164	b8	301	U10	C27-C28	2.37	1.57	1.50
164	SC	102	U10	C51-C49	2.37	1.56	1.51
164	sc	102	U10	C51-C49	2.37	1.56	1.51
160	Y5	204	PX2	O5-C4	2.37	1.40	1.33
164	B8	301	U10	C11-C9	2.36	1.56	1.51
164	QC	506	U10	C11-C9	2.36	1.56	1.51
164	qC	506	U10	C11-C9	2.36	1.56	1.51
164	b8	301	U10	C11-C9	2.36	1.56	1.51
160	R	202	PX2	O5-C4	2.36	1.40	1.33
164	sc	102	U10	C27-C28	2.36	1.57	1.50
164	SC	102	U10	C27-C28	2.36	1.57	1.50
160	y5	204	PX2	O5-C4	2.36	1.40	1.33
160	qh	201	PX2	O5-C4	2.35	1.40	1.33
160	r	202	PX2	O5-C4	2.35	1.40	1.33
164	B8	301	U10	O2-C2	-2.34	1.18	1.23
154	c1	708	HEA	CHC-C1C	2.34	1.44	1.39
164	Qc	507	U10	C7-C6	2.34	1.55	1.51
164	qc	507	U10	C7-C6	2.34	1.55	1.51
164	b8	301	U10	O2-C2	-2.33	1.18	1.23
160	Qh	201	PX2	O5-C4	2.32	1.40	1.33
164	qc	501	U10	C22-C23	2.31	1.57	1.50
154	C1	702	HEA	CHB-C4A	2.31	1.42	1.38
164	Qc	501	U10	C22-C23	2.31	1.57	1.50
151	Qd	401	HEC	CBB-CAB	-2.31	1.41	1.49
164	qc	507	U10	C6-C5	2.31	1.53	1.46
164	Qc	507	U10	C6-C5	2.31	1.53	1.46
151	qd	401	HEC	CBB-CAB	-2.31	1.41	1.49
164	sc	102	U10	C6-C5	2.31	1.53	1.46
164	b8	301	U10	O3-C3M	-2.30	1.40	1.45
151	qD	401	HEC	CBB-CAB	-2.30	1.41	1.49
164	B8	301	U10	O3-C3M	-2.30	1.40	1.45
164	B8	301	U10	C6-C5	2.30	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
170	b9	202	ADP	C5-N7	-2.30	1.34	1.39
170	B9	202	ADP	C5-N7	-2.30	1.34	1.39
164	b8	301	U10	C6-C5	2.30	1.53	1.46
164	SC	102	U10	C6-C5	2.29	1.52	1.46
151	QD	401	HEC	CBB-CAB	-2.29	1.41	1.49
164	qc	507	U10	C16-C14	2.28	1.56	1.51
164	sc	102	U10	C22-C23	2.28	1.57	1.50
164	SC	102	U10	C22-C23	2.28	1.57	1.50
164	Qc	507	U10	C16-C14	2.28	1.56	1.51
164	sc	102	U10	O2-C2	-2.27	1.18	1.23
164	b8	301	U10	C16-C14	2.27	1.56	1.51
164	SC	102	U10	C16-C14	2.26	1.56	1.51
164	sc	102	U10	C16-C14	2.26	1.56	1.51
164	SC	102	U10	O2-C2	-2.26	1.18	1.23
151	2E	401	HEC	CBB-CAB	-2.26	1.41	1.49
164	B8	301	U10	C16-C14	2.26	1.56	1.51
164	b8	301	U10	C22-C23	2.26	1.57	1.50
151	2e	401	HEC	CBB-CAB	-2.26	1.41	1.49
164	qc	501	U10	C11-C9	2.26	1.56	1.51
164	Qc	501	U10	C11-C9	2.26	1.55	1.51
164	B8	301	U10	C22-C23	2.26	1.57	1.50
164	qC	506	U10	O3-C3M	-2.26	1.40	1.45
159	m2	406	P5S	P12-O16	2.26	1.68	1.59
164	QC	506	U10	O3-C3M	-2.25	1.40	1.45
154	C1	703	HEA	O2A-CGA	-2.25	1.23	1.30
160	R	202	PX2	O7-C16	2.25	1.40	1.34
159	M2	406	P5S	P12-O16	2.25	1.68	1.59
170	b9	202	ADP	C8-N7	2.25	1.36	1.31
160	r	202	PX2	O7-C16	2.25	1.40	1.34
164	qc	507	U10	O3-C3M	-2.24	1.40	1.45
164	Qc	507	U10	O3-C3M	-2.24	1.40	1.45
170	B9	202	ADP	C8-N7	2.24	1.36	1.31
164	B8	301	U10	C7-C6	2.24	1.55	1.51
164	b8	301	U10	C7-C6	2.24	1.55	1.51
164	SC	102	U10	C42-C43	2.23	1.57	1.50
164	sc	102	U10	C42-C43	2.22	1.57	1.50
151	qD	401	HEC	CMD-C2D	2.22	1.55	1.50
151	Qd	401	HEC	CMD-C2D	2.22	1.55	1.50
151	qd	401	HEC	CMD-C2D	2.22	1.55	1.50
151	2e	401	HEC	CMD-C2D	2.22	1.55	1.50
151	QD	401	HEC	CMD-C2D	2.22	1.55	1.50
164	SC	102	U10	C11-C9	2.21	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
160	Qh	201	PX2	O5-C3	-2.21	1.40	1.45
164	QC	506	U10	O2-C2	-2.21	1.18	1.23
151	2E	401	HEC	C3B-C2B	-2.21	1.33	1.41
164	qC	506	U10	O2-C2	-2.20	1.18	1.23
164	b8	301	U10	C42-C43	2.20	1.57	1.50
166	y5	203	HEM	FE-ND	2.20	2.01	1.94
164	B8	301	U10	C42-C43	2.20	1.57	1.50
166	Y5	203	HEM	FE-ND	2.20	2.01	1.94
151	QD	401	HEC	C3D-C2D	-2.19	1.33	1.38
151	qD	401	HEC	C3D-C2D	-2.19	1.33	1.38
164	qC	506	U10	C16-C14	2.19	1.55	1.51
164	Qc	507	U10	O2-C2	-2.19	1.18	1.23
164	sc	102	U10	C11-C9	2.19	1.55	1.51
164	qc	507	U10	O2-C2	-2.19	1.18	1.23
164	QC	506	U10	C16-C14	2.18	1.55	1.51
160	R	202	PX2	O5-C3	-2.17	1.40	1.45
164	Qc	507	U10	O4-C4M	-2.17	1.40	1.45
160	r	202	PX2	O5-C3	-2.17	1.40	1.45
164	qc	507	U10	O4-C4M	-2.17	1.40	1.45
160	y5	204	PX2	O5-C3	-2.17	1.40	1.45
151	Qd	401	HEC	C3D-C2D	-2.17	1.33	1.38
151	qd	401	HEC	C3D-C2D	-2.17	1.33	1.38
166	QC	501	HEM	FE-ND	2.16	2.01	1.94
166	qc	502	HEM	FE-ND	2.16	2.01	1.94
166	qC	501	HEM	FE-ND	2.16	2.01	1.94
154	C1	703	HEA	CMC-C2C	-2.16	1.46	1.50
160	Y5	204	PX2	O5-C3	-2.16	1.40	1.45
154	C1	703	HEA	C1A-NA	2.16	1.43	1.39
166	Qc	502	HEM	FE-ND	2.16	2.01	1.94
154	C1	703	HEA	C4B-C3B	2.15	1.48	1.44
164	SC	102	U10	C17-C18	2.14	1.57	1.50
164	sc	102	U10	C17-C18	2.14	1.56	1.50
160	y5	204	PX2	O7-C16	2.13	1.40	1.34
164	qc	507	U10	C17-C18	2.12	1.56	1.50
164	Qc	507	U10	C17-C18	2.12	1.56	1.50
164	QC	506	U10	C12-C13	2.12	1.56	1.50
164	qC	506	U10	C12-C13	2.12	1.56	1.50
164	b8	301	U10	O4-C4M	-2.12	1.40	1.45
160	qh	201	PX2	O5-C3	-2.12	1.40	1.45
164	B8	301	U10	O4-C4M	-2.12	1.40	1.45
151	Qd	401	HEC	C3C-C2C	-2.11	1.34	1.41
166	QC	501	HEM	C4B-NB	-2.11	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	B8	301	U10	C32-C33	2.11	1.56	1.50
164	b8	301	U10	C32-C33	2.11	1.56	1.50
151	qd	401	HEC	C3C-C2C	-2.11	1.34	1.41
166	qC	501	HEM	C4B-NB	-2.11	1.34	1.38
164	B8	301	U10	C12-C13	2.11	1.56	1.50
160	Qh	201	PX2	O7-C16	2.11	1.40	1.34
151	Qd	401	HEC	CMA-C3A	2.11	1.55	1.50
151	qd	401	HEC	CMA-C3A	2.11	1.55	1.50
164	b8	301	U10	C12-C13	2.11	1.56	1.50
164	qc	507	U10	C12-C13	2.11	1.56	1.50
164	Qc	507	U10	C12-C13	2.11	1.56	1.50
151	qD	401	HEC	C3C-C2C	-2.11	1.34	1.41
164	sc	102	U10	C32-C33	2.10	1.56	1.50
164	SC	102	U10	C32-C33	2.10	1.56	1.50
154	C1	703	HEA	C1D-ND	-2.10	1.36	1.40
166	Qc	502	HEM	C4B-NB	-2.10	1.34	1.38
164	qC	506	U10	C17-C18	2.10	1.56	1.50
164	QC	506	U10	C17-C18	2.10	1.56	1.50
160	Y5	204	PX2	O7-C16	2.10	1.40	1.34
164	B8	301	U10	C17-C18	2.10	1.56	1.50
166	qc	502	HEM	C4B-NB	-2.09	1.34	1.38
164	b8	301	U10	C17-C18	2.09	1.56	1.50
151	QD	401	HEC	C3C-C2C	-2.09	1.34	1.41
160	qh	201	PX2	O7-C16	2.09	1.40	1.34
151	2e	401	HEC	C3C-C2C	-2.08	1.34	1.41
151	2e	401	HEC	C3B-C2B	-2.08	1.34	1.41
151	2E	401	HEC	C3C-C2C	-2.07	1.34	1.41
151	qd	401	HEC	CMB-C2B	2.07	1.55	1.50
151	2e	401	HEC	C3D-C2D	-2.06	1.33	1.38
164	qc	501	U10	C16-C14	2.06	1.55	1.51
164	Qc	501	U10	C16-C14	2.06	1.55	1.51
151	Qd	401	HEC	CMB-C2B	2.06	1.55	1.50
164	SC	102	U10	C12-C13	2.06	1.56	1.50
166	qC	502	HEM	C4B-NB	-2.05	1.34	1.38
151	QD	401	HEC	CMB-C2B	2.05	1.55	1.50
164	sc	102	U10	C12-C13	2.05	1.56	1.50
166	QC	502	HEM	C4B-NB	-2.05	1.34	1.38
151	qD	401	HEC	CMB-C2B	2.04	1.55	1.50
164	B8	301	U10	C37-C38	2.04	1.56	1.50
154	C1	702	HEA	C1C-C2C	2.03	1.47	1.43
164	b8	301	U10	C37-C38	2.03	1.56	1.50
151	QD	401	HEC	C3B-C2B	-2.03	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
164	qc	501	U10	C12-C13	2.03	1.56	1.50
164	Qc	501	U10	C12-C13	2.03	1.56	1.50
151	qD	401	HEC	C3B-C2B	-2.03	1.34	1.41
166	QC	502	HEM	FE-ND	2.03	2.01	1.94
166	qC	502	HEM	FE-ND	2.03	2.01	1.94
151	2e	401	HEC	CMB-C2B	2.02	1.54	1.50
164	SC	102	U10	C37-C38	2.02	1.56	1.50
164	sc	102	U10	C37-C38	2.02	1.56	1.50
166	Qc	503	HEM	FE-ND	2.02	2.01	1.94
151	Qd	401	HEC	C3B-C2B	-2.02	1.34	1.41
166	qc	503	HEM	FE-ND	2.01	2.01	1.94
166	qc	503	HEM	C4B-NB	-2.01	1.34	1.38
151	qd	401	HEC	C3B-C2B	-2.01	1.34	1.41
166	Qc	503	HEM	C4B-NB	-2.01	1.34	1.38
164	qc	501	U10	C26-C24	2.01	1.57	1.51
164	Qc	501	U10	C26-C24	2.01	1.57	1.51
151	QD	401	HEC	CMA-C3A	2.00	1.54	1.50

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
151	2e	401	HEC	CBB-CAB-C3B	-9.14	109.17	127.43
151	2E	401	HEC	CBB-CAB-C3B	-8.91	109.62	127.43
151	qd	401	HEC	CBB-CAB-C3B	-8.86	109.72	127.43
151	Qd	401	HEC	CBB-CAB-C3B	-8.84	109.76	127.43
151	qD	401	HEC	CBB-CAB-C3B	-8.73	109.98	127.43
151	QD	401	HEC	CBB-CAB-C3B	-8.66	110.12	127.43
154	c1	708	HEA	C3C-C2C-C1C	-7.18	98.71	107.17
151	qD	401	HEC	CBC-CAC-C3C	-7.00	113.44	127.43
151	2e	401	HEC	CBC-CAC-C3C	-6.97	113.50	127.43
151	QD	401	HEC	CBC-CAC-C3C	-6.93	113.57	127.43
151	Qd	401	HEC	CBC-CAC-C3C	-6.85	113.74	127.43
151	qd	401	HEC	CBC-CAC-C3C	-6.82	113.80	127.43
154	C1	702	HEA	C3C-C4C-NC	6.69	115.44	109.80
151	2E	401	HEC	CBC-CAC-C3C	-6.68	114.08	127.43
154	c1	702	HEA	CAD-CBD-CGD	-6.67	95.98	113.67
154	c1	702	HEA	C3C-C2C-C1C	-6.62	99.37	107.17
154	C1	703	HEA	C3C-C4C-NC	6.53	115.30	109.80
154	C1	703	HEA	C2B-C1B-NB	6.44	117.34	109.90
154	c1	708	HEA	CAD-CBD-CGD	-6.42	96.63	113.67
154	C1	703	HEA	CAA-CBA-CGA	-6.29	96.99	113.67
154	C1	703	HEA	C13-C12-C11	-6.22	104.46	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
154	c1	708	HEA	C2B-C1B-NB	6.12	116.98	109.90
154	C1	702	HEA	CAD-CBD-CGD	-6.08	97.54	113.67
154	c1	708	HEA	C13-C12-C11	-6.08	104.68	114.39
154	c1	702	HEA	C3D-C4D-ND	6.06	116.20	110.35
154	c1	702	HEA	C2D-C1D-ND	5.96	116.69	109.84
154	C1	703	HEA	CAD-CBD-CGD	-5.85	98.14	113.67
170	b9	202	ADP	C5-C4-N3	-5.77	118.77	126.72
170	B9	202	ADP	C5-C4-N3	-5.77	118.77	126.72
154	C1	702	HEA	C3B-C4B-NB	5.66	116.35	109.84
154	C1	702	HEA	C2B-C1B-NB	5.61	116.39	109.90
154	c1	708	HEA	CHB-C1B-C2B	-5.53	116.30	125.03
154	C1	703	HEA	CHB-C1B-C2B	-5.50	116.34	125.03
154	c1	708	HEA	C3C-C4C-NC	5.47	114.41	109.80
154	c1	702	HEA	C3C-C4C-NC	5.47	114.41	109.80
154	C1	702	HEA	C3C-C2C-C1C	-5.27	100.96	107.17
154	c1	702	HEA	C1D-C2D-C3D	-5.24	101.47	106.98
154	C1	702	HEA	CHB-C1B-C2B	-5.22	116.79	125.03
154	c1	708	HEA	C2C-C1C-NC	5.08	118.29	110.14
154	c1	708	HEA	CAA-CBA-CGA	-5.02	100.35	113.67
166	y5	203	HEM	CHC-C4B-NB	4.82	129.60	124.42
166	Y5	203	HEM	CHC-C4B-NB	4.81	129.60	124.42
154	c1	708	HEA	C3B-C4B-NB	4.74	115.29	109.84
154	C1	702	HEA	C1D-C2D-C3D	-4.72	102.02	106.98
170	b9	202	ADP	N3-C4-N9	4.67	135.12	127.17
154	c1	702	HEA	C2B-C1B-NB	4.67	115.30	109.90
170	B9	202	ADP	N3-C4-N9	4.67	135.10	127.17
154	C1	702	HEA	C2D-C1D-ND	4.62	115.15	109.84
154	c1	702	HEA	CAA-CBA-CGA	-4.62	101.42	113.67
154	c1	702	HEA	C2C-C1C-NC	4.54	117.41	110.14
154	c1	702	HEA	CHA-C4D-C3D	-4.48	118.24	124.77
166	qC	501	HEM	CHC-C4B-NB	4.48	129.24	124.42
166	QC	501	HEM	CHC-C4B-NB	4.47	129.24	124.42
154	C1	703	HEA	C1B-C2B-C3B	-4.46	101.63	106.80
166	qC	502	HEM	CHC-C4B-NB	4.46	129.22	124.42
166	QC	502	HEM	CHC-C4B-NB	4.46	129.22	124.42
166	qC	501	HEM	CHD-C4C-NC	4.45	129.30	124.45
154	c1	702	HEA	CHB-C1B-C2B	-4.44	118.02	125.03
166	QC	501	HEM	CHD-C4C-NC	4.43	129.28	124.45
166	qc	502	HEM	CHC-C4B-NB	4.43	129.19	124.42
154	C1	702	HEA	CAA-CBA-CGA	-4.43	101.92	113.67
166	Qc	502	HEM	CHC-C4B-NB	4.42	129.18	124.42
166	Qc	503	HEM	CHC-C4B-NB	4.41	129.17	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	qc	503	HEM	CHC-C4B-NB	4.40	129.16	124.42
166	y5	203	HEM	CHD-C4C-NC	4.39	129.23	124.45
166	Y5	203	HEM	CHD-C4C-NC	4.37	129.21	124.45
166	qc	502	HEM	CHD-C4C-NC	4.28	129.12	124.45
166	Qc	502	HEM	CHD-C4C-NC	4.28	129.12	124.45
169	b6	201	T7X	O16-C10-C12	4.24	120.65	111.48
169	B6	201	T7X	O16-C10-C12	4.24	120.65	111.48
154	c1	708	HEA	C3D-C4D-ND	4.20	114.41	110.35
154	c1	702	HEA	C13-C12-C11	-4.19	107.69	114.39
154	C1	703	HEA	C2D-C1D-ND	4.17	114.64	109.84
166	Qc	503	HEM	CHD-C4C-NC	4.17	128.99	124.45
154	C1	703	HEA	C3B-C4B-NB	4.15	114.61	109.84
166	qc	503	HEM	CHD-C4C-NC	4.14	128.97	124.45
154	c1	708	HEA	C2D-C1D-ND	4.08	114.53	109.84
160	Qh	201	PX2	O7-C16-C17	4.07	120.29	111.48
160	y5	204	PX2	O7-C16-C17	4.05	120.24	111.48
154	C1	703	HEA	C3D-C4D-ND	4.03	114.25	110.35
154	C1	702	HEA	C4B-C3B-C2B	-4.03	100.66	107.44
160	Y5	204	PX2	O7-C16-C17	4.00	120.13	111.48
166	QC	502	HEM	CHD-C4C-NC	3.93	128.73	124.45
166	Y5	203	HEM	CHB-C1B-NB	3.89	129.18	124.37
154	C1	703	HEA	C1D-C2D-C3D	-3.89	102.89	106.98
166	y5	203	HEM	CHB-C1B-NB	3.88	129.17	124.37
164	Qc	501	U10	C12-C13-C14	-3.88	118.75	127.62
166	qC	502	HEM	CHD-C4C-NC	3.88	128.68	124.45
160	qh	201	PX2	O7-C16-C17	3.87	119.86	111.48
154	C1	702	HEA	C3D-C4D-ND	3.87	114.09	110.35
164	qc	501	U10	C12-C13-C14	-3.85	118.81	127.62
166	qc	503	HEM	CHB-C1B-NB	3.82	129.09	124.37
166	Qc	503	HEM	CHB-C1B-NB	3.81	129.08	124.37
154	c1	708	HEA	C1D-C2D-C3D	-3.80	102.98	106.98
166	Qc	502	HEM	CHB-C1B-NB	3.75	129.00	124.37
166	qc	502	HEM	CHB-C1B-NB	3.73	128.99	124.37
159	m2	406	P5S	O37-C38-C39	3.70	119.50	111.48
159	M2	406	P5S	O37-C38-C39	3.70	119.50	111.48
166	qC	501	HEM	CHB-C1B-NB	3.69	128.93	124.37
166	QC	501	HEM	CHB-C1B-NB	3.68	128.92	124.37
160	r	202	PX2	O7-C16-C17	3.67	119.43	111.48
166	QC	502	HEM	CHB-C1B-NB	3.66	128.90	124.37
166	qC	502	HEM	CHB-C1B-NB	3.65	128.88	124.37
154	c1	708	HEA	C1B-C2B-C3B	-3.65	102.57	106.80
170	b9	202	ADP	C2-N3-C4	3.64	120.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
170	B9	202	ADP	C2-N3-C4	3.64	120.71	111.83
154	C1	703	HEA	C4C-C3C-C2C	-3.60	102.82	107.30
154	C1	702	HEA	C2C-C1C-NC	3.59	115.89	110.14
154	c1	702	HEA	C3B-C4B-NB	3.56	113.93	109.84
154	c1	708	HEA	CMB-C2B-C3B	3.55	137.14	130.28
164	qc	507	U10	C7-C8-C9	-3.53	120.75	126.83
164	Qc	507	U10	C7-C8-C9	-3.53	120.75	126.83
164	qC	506	U10	C12-C13-C14	-3.53	119.55	127.62
164	QC	506	U10	C12-C13-C14	-3.52	119.56	127.62
154	C1	702	HEA	C13-C12-C11	-3.49	108.81	114.39
169	B6	201	T7X	C20-C19-C18	3.48	152.97	123.57
169	b6	201	T7X	C20-C19-C18	3.48	152.96	123.57
169	B6	201	T7X	C17-C16-C15	3.46	152.80	123.57
169	b6	201	T7X	C17-C16-C15	3.46	152.79	123.57
164	SC	102	U10	C37-C38-C39	-3.44	119.75	127.62
164	sc	102	U10	C37-C38-C39	-3.44	119.75	127.62
166	qc	503	HEM	C4D-ND-C1D	3.42	109.26	105.21
166	Qc	503	HEM	C4D-ND-C1D	3.42	109.25	105.21
154	C1	703	HEA	C3C-C2C-C1C	-3.41	103.15	107.17
164	Qc	501	U10	C1M-C1-C2	3.41	120.14	116.13
164	qc	501	U10	C1M-C1-C2	3.40	120.13	116.13
164	B8	301	U10	C27-C28-C29	-3.38	119.89	127.62
164	b8	301	U10	C27-C28-C29	-3.38	119.89	127.62
170	B9	202	ADP	C4-C5-N7	-3.34	106.77	110.58
164	B8	301	U10	C42-C43-C44	-3.33	120.00	127.62
170	b9	202	ADP	C4-C5-N7	-3.33	106.78	110.58
164	b8	301	U10	C42-C43-C44	-3.32	120.02	127.62
154	c1	702	HEA	OMA-CMA-C3A	-3.28	118.22	125.62
166	qC	502	HEM	C4D-ND-C1D	3.26	109.07	105.21
166	QC	502	HEM	C4D-ND-C1D	3.25	109.06	105.21
164	b8	301	U10	C17-C18-C19	-3.25	120.18	127.62
164	B8	301	U10	C17-C18-C19	-3.25	120.19	127.62
154	c1	702	HEA	CMC-C2C-C1C	3.24	130.36	125.42
164	Qc	501	U10	C17-C18-C19	-3.24	120.21	127.62
164	qc	507	U10	C20-C19-C21	3.24	119.94	116.13
164	qc	501	U10	C17-C18-C19	-3.23	120.22	127.62
164	Qc	507	U10	C20-C19-C21	3.23	119.93	116.13
154	c1	708	HEA	C4B-C3B-C2B	-3.23	102.01	107.44
154	C1	702	HEA	C13-C14-C15	-3.21	120.27	127.62
164	sc	102	U10	C47-C48-C49	-3.21	120.28	127.62
164	SC	102	U10	C47-C48-C49	-3.21	120.28	127.62
154	c1	702	HEA	C4B-C3B-C2B	-3.20	102.06	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
170	b9	202	ADP	N3-C2-N1	-3.17	123.78	128.58
170	B9	202	ADP	N3-C2-N1	-3.16	123.80	128.58
164	qc	507	U10	C12-C13-C14	-3.16	120.39	127.62
164	Qc	507	U10	C12-C13-C14	-3.16	120.39	127.62
164	QC	506	U10	C17-C18-C19	-3.14	120.44	127.62
164	B8	301	U10	C10-C9-C11	3.14	120.67	115.23
164	b8	301	U10	C10-C9-C11	3.13	120.67	115.23
164	sc	102	U10	C15-C14-C16	3.13	120.67	115.23
164	qC	506	U10	C17-C18-C19	-3.13	120.45	127.62
164	SC	102	U10	C15-C14-C16	3.11	120.62	115.23
154	C1	703	HEA	C13-C14-C15	-3.09	120.55	127.62
164	QC	506	U10	C20-C19-C21	3.09	119.76	116.13
164	qC	506	U10	C20-C19-C21	3.09	119.76	116.13
151	2e	401	HEC	CBD-CAD-C3D	3.09	121.06	112.53
164	qC	506	U10	C7-C6-C1	-3.08	119.60	124.89
164	QC	506	U10	C7-C6-C1	-3.08	119.61	124.89
164	SC	102	U10	C27-C28-C29	-3.07	120.59	127.62
164	SC	102	U10	C12-C13-C14	-3.07	120.60	127.62
164	B8	301	U10	C37-C38-C39	-3.07	120.60	127.62
164	sc	102	U10	C27-C28-C29	-3.07	120.60	127.62
164	sc	102	U10	C12-C13-C14	-3.07	120.60	127.62
164	b8	301	U10	C37-C38-C39	-3.07	120.60	127.62
164	QC	506	U10	C7-C8-C9	-3.06	121.56	126.83
164	B8	301	U10	C22-C23-C24	-3.05	120.64	127.62
164	qC	506	U10	C7-C8-C9	-3.05	121.57	126.83
164	b8	301	U10	C22-C23-C24	-3.05	120.64	127.62
160	R	202	PX2	O7-C16-C17	3.04	118.06	111.48
164	sc	102	U10	C32-C33-C34	-3.04	120.67	127.62
164	SC	102	U10	C32-C33-C34	-3.04	120.67	127.62
154	c1	708	HEA	CMB-C2B-C1B	-3.04	120.29	125.03
154	C1	703	HEA	C26-C15-C16	3.03	120.49	115.23
166	qC	501	HEM	CHA-C4D-ND	3.02	128.10	124.37
164	b8	301	U10	C32-C33-C34	-3.02	120.72	127.62
164	B8	301	U10	C32-C33-C34	-3.02	120.72	127.62
166	QC	501	HEM	CHA-C4D-ND	3.01	128.09	124.37
164	SC	102	U10	C22-C23-C24	-2.98	120.81	127.62
154	c1	702	HEA	CMB-C2B-C1B	-2.97	120.40	125.03
154	c1	708	HEA	CHA-C4D-C3D	-2.97	120.45	124.77
154	c1	702	HEA	C13-C14-C15	-2.97	120.84	127.62
164	sc	102	U10	C22-C23-C24	-2.97	120.84	127.62
166	Y5	203	HEM	CHA-C4D-ND	2.94	128.00	124.37
166	y5	203	HEM	CHA-C4D-ND	2.93	128.00	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
151	2E	401	HEC	O1D-CGD-CBD	-2.93	113.80	123.09
164	B8	301	U10	C47-C48-C49	-2.93	120.92	127.62
164	b8	301	U10	C47-C48-C49	-2.93	120.92	127.62
154	C1	703	HEA	C4B-C3B-C2B	-2.93	102.52	107.44
154	c1	708	HEA	C27-C19-C20	2.92	120.30	115.23
166	qc	502	HEM	CHA-C4D-ND	2.92	127.98	124.37
166	Qc	502	HEM	CHA-C4D-ND	2.92	127.98	124.37
166	QC	501	HEM	C4D-ND-C1D	2.92	108.66	105.21
154	c1	708	HEA	C26-C15-C16	2.91	120.28	115.23
166	qC	501	HEM	C4D-ND-C1D	2.91	108.65	105.21
164	qc	501	U10	C20-C19-C21	2.91	120.28	115.23
154	c1	708	HEA	CMC-C2C-C3C	2.91	133.39	126.55
164	b8	301	U10	C35-C34-C36	2.91	120.27	115.23
164	B8	301	U10	C35-C34-C36	2.90	120.27	115.23
164	Qc	501	U10	C20-C19-C21	2.90	120.27	115.23
164	Qc	507	U10	C17-C18-C19	-2.89	121.00	127.62
164	B8	301	U10	C12-C13-C14	-2.89	121.01	127.62
164	qc	507	U10	C17-C18-C19	-2.89	121.01	127.62
164	b8	301	U10	C12-C13-C14	-2.89	121.02	127.62
166	Qc	502	HEM	C4D-ND-C1D	2.88	108.61	105.21
166	qc	502	HEM	C4D-ND-C1D	2.87	108.61	105.21
154	c1	708	HEA	C17-C18-C19	-2.87	121.05	127.62
166	y5	203	HEM	C4D-ND-C1D	2.87	108.61	105.21
154	c1	708	HEA	CHA-C1A-NA	2.87	127.58	124.45
166	Y5	203	HEM	C4D-ND-C1D	2.86	108.60	105.21
151	2e	401	HEC	O1D-CGD-CBD	-2.85	114.05	123.09
154	c1	702	HEA	CMB-C2B-C3B	2.84	135.76	130.28
166	qC	502	HEM	CHA-C4D-ND	2.83	127.86	124.37
164	qc	507	U10	C1M-C1-C6	-2.82	119.81	124.45
164	Qc	507	U10	C1M-C1-C6	-2.82	119.81	124.45
164	qC	506	U10	C10-C9-C11	2.82	120.12	115.23
166	QC	502	HEM	CHA-C4D-ND	2.82	127.85	124.37
164	SC	102	U10	C45-C44-C46	2.82	120.12	115.23
164	QC	506	U10	C10-C9-C11	2.82	120.12	115.23
151	2E	401	HEC	CBD-CAD-C3D	2.81	120.31	112.53
154	C1	703	HEA	C27-C19-C20	2.81	120.11	115.23
166	qc	502	HEM	C1B-NB-C4B	2.81	108.53	105.21
164	sc	102	U10	C45-C44-C46	2.81	120.10	115.23
164	QC	506	U10	C1M-C1-C6	-2.81	119.83	124.45
164	B8	301	U10	C7-C6-C1	-2.81	120.08	124.89
164	qC	506	U10	C1M-C1-C6	-2.80	119.84	124.45
164	b8	301	U10	C7-C6-C1	-2.80	120.08	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
164	sc	102	U10	C30-C29-C31	2.80	120.09	115.23
166	Qc	502	HEM	C1B-NB-C4B	2.80	108.53	105.21
160	qh	201	PX2	O5-C4-C5	2.80	120.38	111.83
164	SC	102	U10	C30-C29-C31	2.80	120.09	115.23
164	b8	301	U10	C45-C44-C46	2.80	120.09	115.23
154	c1	702	HEA	C17-C18-C19	-2.79	121.23	127.62
164	B8	301	U10	C45-C44-C46	2.79	120.07	115.23
164	sc	102	U10	C25-C24-C26	2.79	120.07	115.23
164	SC	102	U10	C25-C24-C26	2.78	120.06	115.23
164	B8	301	U10	C50-C49-C51	2.78	120.05	115.23
164	b8	301	U10	C50-C49-C51	2.78	120.05	115.23
160	y5	204	PX2	O5-C4-C5	2.77	120.28	111.83
166	qC	501	HEM	CHA-C1A-NA	2.77	128.88	123.86
154	C1	703	HEA	CMB-C2B-C3B	2.77	135.63	130.28
166	QC	501	HEM	CHA-C1A-NA	2.77	128.88	123.86
164	SC	102	U10	C17-C18-C19	-2.77	121.29	127.62
154	C1	703	HEA	C17-C18-C19	-2.76	121.30	127.62
151	Qd	401	HEC	O1D-CGD-CBD	-2.76	114.33	123.09
151	qd	401	HEC	O1D-CGD-CBD	-2.76	114.33	123.09
166	Y5	203	HEM	CHD-C1D-ND	2.76	127.39	124.42
166	y5	203	HEM	CHD-C1D-ND	2.76	127.39	124.42
164	sc	102	U10	C50-C49-C51	2.76	120.02	115.23
154	C1	702	HEA	C27-C19-C20	2.76	120.02	115.23
164	SC	102	U10	C50-C49-C51	2.76	120.02	115.23
164	sc	102	U10	C40-C39-C41	2.76	120.01	115.23
164	SC	102	U10	C40-C39-C41	2.75	120.01	115.23
166	qc	502	HEM	CHA-C1A-NA	2.75	128.85	123.86
166	Qc	502	HEM	CHA-C1A-NA	2.75	128.85	123.86
151	qD	401	HEC	O1D-CGD-CBD	-2.75	114.38	123.09
166	QC	502	HEM	CHA-C1A-NA	2.75	128.84	123.86
164	sc	102	U10	C17-C18-C19	-2.74	121.34	127.62
151	QD	401	HEC	O1D-CGD-CBD	-2.74	114.39	123.09
154	C1	702	HEA	CMB-C2B-C1B	-2.74	120.75	125.03
159	M2	406	P5S	O19-C17-C20	2.74	120.20	111.83
159	m2	406	P5S	O19-C17-C20	2.74	120.20	111.83
154	c1	702	HEA	C27-C19-C20	2.74	119.99	115.23
166	qC	502	HEM	CHA-C1A-NA	2.74	128.83	123.86
164	sc	102	U10	C42-C43-C44	-2.74	121.36	127.62
166	qC	501	HEM	C1B-NB-C4B	2.74	108.45	105.21
164	SC	102	U10	C42-C43-C44	-2.73	121.37	127.62
166	QC	501	HEM	C1B-NB-C4B	2.73	108.44	105.21
154	C1	702	HEA	CMB-C2B-C3B	2.73	135.55	130.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	y5	203	HEM	CHA-C1A-NA	2.72	128.80	123.86
166	Y5	203	HEM	CHA-C1A-NA	2.72	128.80	123.86
160	Y5	204	PX2	O5-C4-C5	2.72	120.13	111.83
154	C1	702	HEA	C17-C18-C19	-2.72	121.40	127.62
170	b9	202	ADP	C4-N9-C8	2.71	108.58	105.74
164	Qc	507	U10	C10-C9-C11	2.71	119.93	115.23
164	qc	507	U10	C10-C9-C11	2.70	119.92	115.23
160	r	202	PX2	O5-C4-C5	2.70	120.07	111.83
160	Qh	201	PX2	O5-C4-C5	2.70	120.06	111.83
170	B9	202	ADP	C4-N9-C8	2.70	108.57	105.74
166	qc	503	HEM	CHA-C4D-ND	2.69	127.70	124.37
164	sc	102	U10	C35-C34-C36	2.69	119.89	115.23
164	SC	102	U10	C35-C34-C36	2.69	119.89	115.23
166	Qc	503	HEM	CHA-C4D-ND	2.68	127.68	124.37
154	C1	703	HEA	C2C-C1C-NC	2.67	114.43	110.14
164	qc	501	U10	C25-C24-C26	2.67	119.27	116.13
164	Qc	501	U10	C25-C24-C26	2.67	119.27	116.13
154	C1	702	HEA	C1B-C2B-C3B	-2.67	103.70	106.80
164	SC	102	U10	C20-C19-C21	2.66	119.85	115.23
164	b8	301	U10	C25-C24-C26	2.66	119.85	115.23
166	y5	203	HEM	C1B-NB-C4B	2.66	108.36	105.21
166	Y5	203	HEM	C1B-NB-C4B	2.66	108.36	105.21
164	sc	102	U10	C20-C19-C21	2.66	119.84	115.23
164	B8	301	U10	C25-C24-C26	2.66	119.84	115.23
160	R	202	PX2	O5-C4-C5	2.65	119.92	111.83
169	B6	201	T7X	O18-C11-C31	2.65	119.92	111.83
169	b6	201	T7X	O18-C11-C31	2.65	119.91	111.83
164	B8	301	U10	C20-C19-C21	2.64	119.80	115.23
154	c1	708	HEA	C13-C14-C15	-2.63	121.60	127.62
164	b8	301	U10	C20-C19-C21	2.63	119.80	115.23
164	Qc	507	U10	C7-C6-C1	-2.61	120.42	124.89
164	qc	507	U10	C7-C6-C1	-2.61	120.42	124.89
164	b8	301	U10	C40-C39-C41	2.59	119.73	115.23
164	B8	301	U10	C40-C39-C41	2.59	119.73	115.23
164	qc	501	U10	C10-C9-C11	2.58	119.71	115.23
154	c1	702	HEA	C4D-C3D-C2D	-2.57	103.16	106.89
164	Qc	501	U10	C10-C9-C11	2.55	119.66	115.23
154	c1	702	HEA	C1B-C2B-C3B	-2.55	103.84	106.80
154	C1	702	HEA	C4C-C3C-C2C	-2.54	104.14	107.30
164	Qc	501	U10	C22-C23-C24	-2.54	121.81	127.62
154	C1	702	HEA	CHA-C4D-C3D	-2.54	121.07	124.77
166	QC	502	HEM	C1B-NB-C4B	2.53	108.20	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	qC	502	HEM	C1B-NB-C4B	2.52	108.20	105.21
164	B8	301	U10	C30-C29-C31	2.52	119.61	115.23
164	qc	501	U10	C22-C23-C24	-2.52	121.85	127.62
151	2e	401	HEC	CMD-C2D-C1D	-2.52	121.58	125.42
164	b8	301	U10	C30-C29-C31	2.52	119.60	115.23
166	qc	503	HEM	C1B-NB-C4B	2.51	108.19	105.21
164	B8	301	U10	C7-C8-C9	-2.51	122.52	126.83
164	b8	301	U10	C1M-C1-C6	-2.50	120.33	124.45
166	Qc	503	HEM	C1B-NB-C4B	2.50	108.17	105.21
164	B8	301	U10	C1M-C1-C6	-2.50	120.34	124.45
154	c1	702	HEA	C26-C15-C16	2.50	119.57	115.23
154	c1	708	HEA	O1D-CGD-CBD	-2.49	115.19	123.09
164	B8	301	U10	C15-C14-C16	2.49	119.55	115.23
164	b8	301	U10	C7-C8-C9	-2.49	122.55	126.83
164	b8	301	U10	C15-C14-C16	2.49	119.55	115.23
166	Qc	503	HEM	CHA-C1A-NA	2.48	128.37	123.86
164	SC	102	U10	C7-C8-C9	-2.48	122.55	126.83
166	qc	503	HEM	CHA-C1A-NA	2.48	128.36	123.86
164	sc	102	U10	C7-C8-C9	-2.48	122.56	126.83
166	Qc	503	HEM	C1C-CHC-C4B	-2.48	120.76	126.02
151	Qd	401	HEC	CHC-C4B-NB	2.47	127.14	124.45
164	Qc	501	U10	C15-C14-C16	2.47	119.51	115.23
166	qc	503	HEM	C1C-CHC-C4B	-2.47	120.78	126.02
170	B9	202	ADP	C5-N7-C8	2.46	107.32	103.45
164	qc	501	U10	C15-C14-C16	2.46	119.50	115.23
166	Qc	502	HEM	CHD-C1D-ND	2.46	127.07	124.42
170	b9	202	ADP	C5-N7-C8	2.45	107.31	103.45
166	qc	502	HEM	CHD-C1D-ND	2.45	127.06	124.42
154	c1	702	HEA	CHC-C4B-NB	-2.45	121.34	124.37
166	qc	503	HEM	CHD-C1D-ND	2.44	127.05	124.42
151	qd	401	HEC	CHC-C4B-NB	2.44	127.11	124.45
151	2e	401	HEC	CHC-C4B-NB	2.44	127.11	124.45
166	Qc	503	HEM	CHD-C1D-ND	2.43	127.04	124.42
154	c1	708	HEA	CHC-C4B-NB	-2.42	121.37	124.37
151	Qd	401	HEC	CBD-CAD-C3D	2.42	119.21	112.53
151	qd	401	HEC	CBD-CAD-C3D	2.42	119.21	112.53
170	B9	202	ADP	C3'-C2'-C1'	2.41	106.02	101.46
170	b9	202	ADP	C3'-C2'-C1'	2.41	106.02	101.46
164	Qc	507	U10	C15-C14-C16	2.40	119.39	115.23
164	qc	507	U10	C15-C14-C16	2.40	119.39	115.23
154	C1	702	HEA	OMA-CMA-C3A	-2.39	120.23	125.62
154	C1	703	HEA	CMC-C2C-C3C	2.39	132.16	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
151	qD	401	HEC	CBD-CAD-C3D	2.38	119.12	112.53
166	qc	503	HEM	C2A-C1A-NA	-2.38	107.51	110.15
154	C1	702	HEA	C26-C15-C16	2.38	119.36	115.23
166	Qc	503	HEM	C2A-C1A-NA	-2.38	107.51	110.15
166	qc	503	HEM	CHB-C1B-C2B	-2.37	120.23	126.95
151	2e	401	HEC	O1A-CGA-CBA	-2.36	115.59	123.09
166	Qc	503	HEM	CHB-C1B-C2B	-2.36	120.23	126.95
166	QC	501	HEM	CHD-C1D-ND	2.36	126.96	124.42
166	qC	501	HEM	CHD-C1D-ND	2.35	126.95	124.42
151	QD	401	HEC	CBD-CAD-C3D	2.35	119.02	112.53
164	QC	506	U10	C15-C14-C16	2.35	119.30	115.23
164	qC	506	U10	C15-C14-C16	2.34	119.30	115.23
151	QD	401	HEC	CHC-C4B-NB	2.34	127.00	124.45
151	qD	401	HEC	O1A-CGA-CBA	-2.33	115.69	123.09
151	qD	401	HEC	CHC-C4B-NB	2.33	126.99	124.45
154	c1	702	HEA	C1D-ND-C4D	-2.33	102.45	105.21
151	QD	401	HEC	O1A-CGA-CBA	-2.32	115.75	123.09
166	qC	502	HEM	C1C-CHC-C4B	-2.30	121.12	126.02
166	QC	502	HEM	C1C-CHC-C4B	-2.30	121.12	126.02
151	2E	401	HEC	CHC-C4B-NB	2.30	126.96	124.45
154	c1	702	HEA	CHD-C1D-C2D	-2.30	120.41	126.95
154	c1	702	HEA	CHC-C1C-C2C	-2.30	120.75	127.43
164	SC	102	U10	C56-C54-C55	2.29	119.86	114.59
164	sc	102	U10	C56-C54-C55	2.29	119.86	114.59
166	QC	502	HEM	C4A-CHB-C1B	-2.29	120.87	126.25
166	qC	502	HEM	C4A-CHB-C1B	-2.29	120.87	126.25
164	B8	301	U10	C56-C54-C55	2.28	119.84	114.59
164	b8	301	U10	C56-C54-C55	2.28	119.84	114.59
166	Y5	203	HEM	CHB-C1B-C2B	-2.28	120.47	126.95
166	y5	203	HEM	CHB-C1B-C2B	-2.28	120.48	126.95
166	QC	502	HEM	CHB-C1B-C2B	-2.27	120.50	126.95
151	qd	401	HEC	O1A-CGA-CBA	-2.26	115.91	123.09
151	Qd	401	HEC	O1A-CGA-CBA	-2.26	115.91	123.09
166	qC	502	HEM	CHB-C1B-C2B	-2.26	120.52	126.95
154	c1	708	HEA	C4C-NC-C1C	-2.26	102.14	105.82
166	Qc	502	HEM	CHB-C1B-C2B	-2.25	120.55	126.95
154	C1	702	HEA	C27-C19-C18	-2.25	117.86	123.63
164	SC	102	U10	C10-C9-C11	2.24	119.12	115.23
151	2E	401	HEC	O1A-CGA-CBA	-2.24	115.98	123.09
166	qc	502	HEM	CHB-C1B-C2B	-2.24	120.58	126.95
166	qC	502	HEM	CHD-C1D-ND	2.23	126.83	124.42
166	QC	502	HEM	CHD-C1D-ND	2.23	126.82	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
166	qc	503	HEM	C4A-CHB-C1B	-2.22	121.02	126.25
166	Qc	503	HEM	C4A-CHB-C1B	-2.22	121.03	126.25
166	qC	501	HEM	CHB-C1B-C2B	-2.22	120.65	126.95
151	2E	401	HEC	O2A-CGA-O1A	2.21	129.03	123.33
166	y5	203	HEM	C1C-CHC-C4B	-2.21	121.32	126.02
166	QC	501	HEM	CHB-C1B-C2B	-2.21	120.67	126.95
154	c1	708	HEA	OMA-CMA-C3A	-2.21	120.64	125.62
166	qC	501	HEM	C1C-CHC-C4B	-2.21	121.33	126.02
166	Y5	203	HEM	C1C-CHC-C4B	-2.21	121.33	126.02
154	c1	702	HEA	C27-C19-C18	-2.21	117.96	123.63
166	QC	501	HEM	C1C-CHC-C4B	-2.20	121.34	126.02
164	sc	102	U10	C52-C53-C54	-2.20	120.31	127.64
164	SC	102	U10	C52-C53-C54	-2.20	120.32	127.64
164	b8	301	U10	C8-C7-C6	-2.19	106.68	112.08
151	qd	401	HEC	CMD-C2D-C1D	-2.19	122.08	125.42
154	c1	708	HEA	C4D-C3D-C2D	-2.19	103.70	106.89
151	qD	401	HEC	O2A-CGA-O1A	2.19	128.96	123.33
158	a3	201	3PE	O31-C3-C2	-2.19	102.09	108.40
164	B8	301	U10	C8-C7-C6	-2.19	106.69	112.08
158	A3	201	3PE	O31-C3-C2	-2.19	102.09	108.40
166	qc	502	HEM	C1C-CHC-C4B	-2.18	121.38	126.02
154	C1	702	HEA	CMD-C2D-C1D	2.18	128.44	125.03
154	C1	703	HEA	C3A-C2A-C1A	-2.18	104.98	107.05
166	qC	502	HEM	C2A-C1A-NA	-2.18	107.73	110.15
151	Qd	401	HEC	CMD-C2D-C1D	-2.18	122.10	125.42
166	QC	502	HEM	C2A-C1A-NA	-2.18	107.73	110.15
154	c1	702	HEA	CAD-C3D-C2D	2.18	131.95	127.87
154	C1	702	HEA	CMC-C2C-C3C	2.17	131.66	126.55
166	Qc	502	HEM	C1C-CHC-C4B	-2.17	121.40	126.02
151	QD	401	HEC	O2A-CGA-O1A	2.17	128.91	123.33
151	QD	401	HEC	CMD-C2D-C1D	-2.17	122.12	125.42
151	2e	401	HEC	O2A-CGA-O1A	2.16	128.89	123.33
151	qD	401	HEC	CMD-C2D-C1D	-2.16	122.13	125.42
154	C1	702	HEA	CHC-C4B-NB	-2.16	121.70	124.37
154	c1	708	HEA	CHB-C1B-NB	2.13	126.72	124.42
154	c1	702	HEA	CMD-C2D-C1D	2.13	128.37	125.03
154	C1	702	HEA	CHB-C1B-NB	2.13	126.72	124.42
154	C1	703	HEA	CMD-C2D-C1D	2.13	128.37	125.03
164	sc	102	U10	C10-C9-C11	2.12	118.91	115.23
164	B8	301	U10	C52-C53-C54	-2.11	120.62	127.64
164	b8	301	U10	C52-C53-C54	-2.11	120.62	127.64
154	c1	708	HEA	C27-C19-C18	-2.10	118.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
154	c1	702	HEA	CHB-C1B-NB	2.10	126.68	124.42
154	C1	702	HEA	C3A-C2A-C1A	-2.09	105.07	107.05
151	Qd	401	HEC	O2A-CGA-O1A	2.08	128.69	123.33
151	qd	401	HEC	O2A-CGA-O1A	2.08	128.69	123.33
151	2E	401	HEC	CMD-C2D-C1D	-2.07	122.26	125.42
154	c1	708	HEA	CMD-C2D-C1D	2.06	128.26	125.03
154	C1	703	HEA	CHA-C4D-C3D	-2.05	121.78	124.77
154	c1	708	HEA	CHC-C1C-C2C	-2.05	121.49	127.43
154	C1	703	HEA	C27-C19-C18	-2.03	118.42	123.63
154	c1	708	HEA	CHC-C1C-NC	-2.01	120.22	123.86
154	c1	708	HEA	O1A-CGA-CBA	-2.00	116.74	123.09

There are no chirality outliers.

All (5653) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
152	2f	301	PC1	C11-O13-P-O14
152	2f	301	PC1	C1-O11-P-O12
152	2f	301	PC1	C1-O11-P-O14
152	2f	301	PC1	C1-O11-P-O13
152	2f	302	PC1	C11-O13-P-O12
152	2f	302	PC1	C11-O13-P-O11
152	2f	302	PC1	C1-O11-P-O12
152	2f	303	PC1	C11-O13-P-O12
152	2g	202	PC1	C11-O13-P-O11
152	2j	201	PC1	C11-O13-P-O11
152	2j	201	PC1	C1-O11-P-O12
152	2j	201	PC1	C1-O11-P-O14
152	2j	201	PC1	C1-O11-P-O13
152	2j	201	PC1	O13-C11-C12-N
152	6a	202	PC1	C1-O11-P-O12
152	6a	202	PC1	C1-O11-P-O14
152	6a	202	PC1	C1-O11-P-O13
152	6c	203	PC1	C1-O11-P-O12
152	6c	203	PC1	C1-O11-P-O14
152	6c	203	PC1	C1-O11-P-O13
152	7a	202	PC1	C1-O11-P-O12
152	7a	202	PC1	C1-O11-P-O14
152	7a	202	PC1	C1-O11-P-O13
152	7c	303	PC1	C11-O13-P-O12
152	7c	303	PC1	C11-O13-P-O11
152	7c	303	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
152	a	501	PC1	C11-O13-P-O12
152	a	501	PC1	C11-O13-P-O14
152	a	501	PC1	C11-O13-P-O11
152	c1	704	PC1	C11-O13-P-O12
152	c1	704	PC1	C11-O13-P-O11
152	c1	704	PC1	C1-O11-P-O12
152	c1	706	PC1	C11-O13-P-O12
152	c1	706	PC1	C11-O13-P-O11
152	c1	706	PC1	C1-O11-P-O14
152	c1	706	PC1	C1-O11-P-O13
152	c1	707	PC1	C11-O13-P-O11
152	c1	711	PC1	C11-O13-P-O14
152	c3	601	PC1	C1-O11-P-O14
152	c3	601	PC1	C1-O11-P-O13
152	c3	601	PC1	C2-C1-O11-P
152	c3	602	PC1	C1-O11-P-O12
152	c3	602	PC1	C1-O11-P-O14
152	c3	602	PC1	C1-O11-P-O13
152	c3	602	PC1	O21-C2-C3-O31
152	c3	603	PC1	C11-O13-P-O12
152	c3	606	PC1	C1-O11-P-O14
152	c3	606	PC1	C1-O11-P-O13
152	d	501	PC1	C11-O13-P-O14
152	d	501	PC1	C11-O13-P-O11
152	d	501	PC1	C1-O11-P-O12
152	f	402	PC1	C11-O13-P-O14
152	f	402	PC1	C11-O13-P-O11
152	f	402	PC1	C1-O11-P-O14
152	f	402	PC1	C1-O11-P-O13
152	i	304	PC1	C11-O13-P-O11
152	i	304	PC1	C1-O11-P-O12
152	i	304	PC1	C1-O11-P-O14
152	i	304	PC1	C1-O11-P-O13
152	j	302	PC1	C1-O11-P-O14
152	j	302	PC1	C1-O11-P-O13
152	m	301	PC1	C11-O13-P-O12
152	m	301	PC1	C11-O13-P-O11
152	m	301	PC1	C1-O11-P-O12
152	m	301	PC1	C1-O11-P-O13
152	m	305	PC1	C11-O13-P-O12
152	m	305	PC1	C11-O13-P-O11
152	m	305	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
152	m	305	PC1	C1-O11-P-O14
152	m	305	PC1	C1-O11-P-O13
152	m	305	PC1	O13-C11-C12-N
152	m	307	PC1	C11-O13-P-O12
152	m	307	PC1	C11-O13-P-O14
152	m	307	PC1	C11-O13-P-O11
152	m	307	PC1	C1-O11-P-O12
152	m	307	PC1	C1-O11-P-O14
152	m1	401	PC1	C11-O13-P-O12
152	m1	401	PC1	C11-O13-P-O14
152	m1	401	PC1	C11-O13-P-O11
152	m1	403	PC1	C1-O11-P-O12
152	m1	403	PC1	C1-O11-P-O14
152	m1	403	PC1	C1-O11-P-O13
152	m2	402	PC1	C11-O13-P-O12
152	m2	402	PC1	C11-O13-P-O11
152	m2	402	PC1	C1-O11-P-O14
152	m2	402	PC1	C1-O11-P-O13
152	m2	402	PC1	O13-C11-C12-N
152	m2	405	PC1	C11-O13-P-O12
152	m2	405	PC1	C11-O13-P-O14
152	m2	405	PC1	C11-O13-P-O11
152	m2	407	PC1	C11-O13-P-O12
152	m2	407	PC1	C11-O13-P-O14
152	m2	407	PC1	C11-O13-P-O11
152	m2	407	PC1	C1-O11-P-O14
152	n	302	PC1	C11-O13-P-O12
152	n	302	PC1	C11-O13-P-O11
152	n	302	PC1	C1-O11-P-O13
152	v	201	PC1	C11-O13-P-O11
152	v	202	PC1	C11-O13-P-O11
152	v	202	PC1	C1-O11-P-O14
152	w	201	PC1	C11-O13-P-O12
152	w	201	PC1	C11-O13-P-O14
152	w	201	PC1	C11-O13-P-O11
152	w	201	PC1	C1-O11-P-O14
152	w	204	PC1	C11-O13-P-O11
152	w	204	PC1	C1-O11-P-O12
152	w	204	PC1	C1-O11-P-O14
152	w	204	PC1	C1-O11-P-O13
152	w	205	PC1	C11-O13-P-O12
152	w	205	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
152	w	205	PC1	C11-O13-P-O11
152	5b	202	PC1	C11-O13-P-O12
152	5b	202	PC1	C11-O13-P-O14
152	5b	202	PC1	C11-O13-P-O11
152	5b	202	PC1	C1-O11-P-O13
152	am	202	PC1	C11-O13-P-O12
152	am	202	PC1	C11-O13-P-O14
152	am	202	PC1	C11-O13-P-O11
152	am	202	PC1	C1-O11-P-O12
152	am	202	PC1	C1-O11-P-O14
152	am	202	PC1	C1-O11-P-O13
152	an	304	PC1	C11-O13-P-O11
152	an	304	PC1	C1-O11-P-O12
152	an	304	PC1	C1-O11-P-O14
152	an	304	PC1	C1-O11-P-O13
152	b9	201	PC1	C11-O13-P-O12
152	b9	201	PC1	C11-O13-P-O11
152	b9	201	PC1	C1-O11-P-O14
152	b9	201	PC1	C1-O11-P-O13
152	c4	403	PC1	C11-O13-P-O12
152	c4	403	PC1	C11-O13-P-O11
152	j1	400	PC1	C11-O13-P-O11
152	j1	400	PC1	C1-O11-P-O12
152	j1	400	PC1	C1-O11-P-O14
152	j1	400	PC1	C1-O11-P-O13
152	n1	301	PC1	C1-O11-P-O12
152	n1	301	PC1	C1-O11-P-O14
152	n1	301	PC1	C1-O11-P-O13
152	n5	801	PC1	C11-O13-P-O14
152	n5	801	PC1	C11-O13-P-O11
152	n5	803	PC1	C1-O11-P-O13
152	n5	804	PC1	C11-O13-P-O12
152	n5	804	PC1	C11-O13-P-O14
152	n5	804	PC1	C11-O13-P-O11
152	n5	804	PC1	C1-O11-P-O12
152	n5	804	PC1	C1-O11-P-O13
152	n5	805	PC1	C11-O13-P-O12
152	n5	805	PC1	C1-O11-P-O12
152	n5	805	PC1	O21-C2-C3-O31
152	n6	301	PC1	C11-O13-P-O12
152	n6	301	PC1	C11-O13-P-O11
152	p1	401	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
152	p1	401	PC1	C1-O11-P-O14
152	p1	401	PC1	C1-O11-P-O13
152	qB	602	PC1	C11-O13-P-O12
152	qB	602	PC1	C11-O13-P-O11
152	qC	505	PC1	C11-O13-P-O12
152	qC	505	PC1	C11-O13-P-O11
152	qC	505	PC1	C1-O11-P-O12
152	qC	505	PC1	C1-O11-P-O14
152	qC	505	PC1	C1-O11-P-O13
152	qC	507	PC1	C1-O11-P-O12
152	qC	507	PC1	C1-O11-P-O13
152	qC	508	PC1	C1-O11-P-O14
152	qC	508	PC1	C1-O11-P-O13
152	qE	301	PC1	C11-O13-P-O14
152	qE	301	PC1	C11-O13-P-O11
152	qE	301	PC1	C1-O11-P-O13
152	qE	303	PC1	C1-O11-P-O14
152	qE	304	PC1	C1-O11-P-O12
152	qE	304	PC1	C1-O11-P-O14
152	qE	304	PC1	C1-O11-P-O13
152	qG	401	PC1	C11-O13-P-O12
152	qG	401	PC1	C11-O13-P-O14
152	qG	401	PC1	C11-O13-P-O11
152	qI	201	PC1	C11-O13-P-O12
152	qI	201	PC1	C11-O13-P-O14
152	qI	201	PC1	C11-O13-P-O11
152	qJ	101	PC1	C11-O13-P-O12
152	qJ	101	PC1	C1-O11-P-O12
152	qJ	101	PC1	C1-O11-P-O14
152	qJ	101	PC1	C1-O11-P-O13
152	qJ	101	PC1	O13-C11-C12-N
152	qb	602	PC1	C11-O13-P-O11
152	qc	506	PC1	C11-O13-P-O12
152	qc	506	PC1	C11-O13-P-O14
152	qc	506	PC1	C11-O13-P-O11
152	qc	506	PC1	C1-O11-P-O12
152	qc	506	PC1	C1-O11-P-O14
152	qc	509	PC1	C1-O11-P-O14
152	qc	509	PC1	C1-O11-P-O13
152	qe	303	PC1	C11-O13-P-O14
152	qe	303	PC1	C11-O13-P-O11
152	qe	303	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
152	qe	303	PC1	C1-O11-P-O13
152	qg	401	PC1	C11-O13-P-O12
152	qg	401	PC1	C11-O13-P-O11
152	qi	201	PC1	C1-O11-P-O12
152	qi	201	PC1	C1-O11-P-O14
152	qi	201	PC1	C1-O11-P-O13
152	qi	203	PC1	C1-O11-P-O13
152	qj	101	PC1	C11-O13-P-O12
152	qj	101	PC1	C11-O13-P-O11
152	qj	101	PC1	O11-C1-C2-O21
152	s8	301	PC1	C1-O11-P-O12
152	s8	301	PC1	C1-O11-P-O13
152	t1	602	PC1	C11-O13-P-O12
152	t1	602	PC1	C11-O13-P-O14
152	t1	602	PC1	C11-O13-P-O11
152	t1	602	PC1	C1-O11-P-O13
152	t4	301	PC1	C11-O13-P-O12
152	t4	301	PC1	C11-O13-P-O14
152	t4	301	PC1	C1-O11-P-O12
152	t4	301	PC1	C1-O11-P-O14
152	t4	301	PC1	C1-O11-P-O13
152	t4	303	PC1	C11-O13-P-O12
152	t4	303	PC1	C11-O13-P-O14
152	t4	303	PC1	C11-O13-P-O11
152	t4	303	PC1	C1-O11-P-O13
152	tc	102	PC1	C11-O13-P-O14
152	tc	102	PC1	C11-O13-P-O11
152	tc	102	PC1	C1-O11-P-O12
152	tc	102	PC1	C1-O11-P-O13
152	te	102	PC1	C11-O13-P-O12
152	te	102	PC1	C11-O13-P-O11
152	te	102	PC1	C1-O11-P-O14
152	2F	301	PC1	C11-O13-P-O14
152	2F	301	PC1	C1-O11-P-O12
152	2F	301	PC1	C1-O11-P-O14
152	2F	301	PC1	C1-O11-P-O13
152	2F	302	PC1	C11-O13-P-O12
152	2F	302	PC1	C11-O13-P-O11
152	2F	302	PC1	C1-O11-P-O12
152	2F	303	PC1	C11-O13-P-O12
152	2G	202	PC1	C11-O13-P-O11
152	2J	201	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
152	2J	201	PC1	C1-O11-P-O12
152	2J	201	PC1	C1-O11-P-O14
152	2J	201	PC1	C1-O11-P-O13
152	2J	201	PC1	O13-C11-C12-N
152	6A	202	PC1	C1-O11-P-O12
152	6A	202	PC1	C1-O11-P-O14
152	6A	202	PC1	C1-O11-P-O13
152	6C	201	PC1	C1-O11-P-O12
152	6C	201	PC1	C1-O11-P-O14
152	6C	201	PC1	C1-O11-P-O13
152	7A	202	PC1	C1-O11-P-O12
152	7A	202	PC1	C1-O11-P-O14
152	7A	202	PC1	C1-O11-P-O13
152	7C	303	PC1	C11-O13-P-O12
152	7C	303	PC1	C11-O13-P-O11
152	7C	303	PC1	C1-O11-P-O14
152	A	501	PC1	C11-O13-P-O12
152	A	501	PC1	C11-O13-P-O14
152	A	501	PC1	C11-O13-P-O11
152	C1	706	PC1	C11-O13-P-O12
152	C1	706	PC1	C11-O13-P-O11
152	C1	706	PC1	C1-O11-P-O12
152	C1	709	PC1	C11-O13-P-O12
152	C1	709	PC1	C11-O13-P-O11
152	C1	709	PC1	C1-O11-P-O14
152	C1	709	PC1	C1-O11-P-O13
152	C1	710	PC1	C11-O13-P-O11
152	C1	711	PC1	C11-O13-P-O14
152	C3	601	PC1	C1-O11-P-O14
152	C3	601	PC1	C1-O11-P-O13
152	C3	601	PC1	C2-C1-O11-P
152	C3	602	PC1	C1-O11-P-O12
152	C3	602	PC1	C1-O11-P-O14
152	C3	602	PC1	C1-O11-P-O13
152	C3	602	PC1	O21-C2-C3-O31
152	C3	603	PC1	C11-O13-P-O12
152	C3	606	PC1	C1-O11-P-O14
152	C3	606	PC1	C1-O11-P-O13
152	D	501	PC1	C11-O13-P-O14
152	D	501	PC1	C11-O13-P-O11
152	D	501	PC1	C1-O11-P-O12
152	F	401	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
152	F	401	PC1	C11-O13-P-O11
152	F	401	PC1	C1-O11-P-O14
152	F	401	PC1	C1-O11-P-O13
152	I	301	PC1	C11-O13-P-O11
152	I	301	PC1	C1-O11-P-O12
152	I	301	PC1	C1-O11-P-O14
152	I	301	PC1	C1-O11-P-O13
152	J	302	PC1	C1-O11-P-O14
152	J	302	PC1	C1-O11-P-O13
152	M	302	PC1	C11-O13-P-O12
152	M	302	PC1	C11-O13-P-O14
152	M	302	PC1	C11-O13-P-O11
152	M	302	PC1	C1-O11-P-O12
152	M	302	PC1	C1-O11-P-O14
152	M	303	PC1	C11-O13-P-O12
152	M	303	PC1	C11-O13-P-O11
152	M	303	PC1	C1-O11-P-O12
152	M	303	PC1	C1-O11-P-O13
152	M	307	PC1	C11-O13-P-O12
152	M	307	PC1	C11-O13-P-O11
152	M	307	PC1	C1-O11-P-O12
152	M	307	PC1	C1-O11-P-O14
152	M	307	PC1	C1-O11-P-O13
152	M	307	PC1	O13-C11-C12-N
152	M1	401	PC1	C11-O13-P-O12
152	M1	401	PC1	C11-O13-P-O14
152	M1	401	PC1	C11-O13-P-O11
152	M1	403	PC1	C1-O11-P-O12
152	M1	403	PC1	C1-O11-P-O14
152	M1	403	PC1	C1-O11-P-O13
152	M2	402	PC1	C11-O13-P-O12
152	M2	402	PC1	C11-O13-P-O11
152	M2	402	PC1	C1-O11-P-O14
152	M2	402	PC1	C1-O11-P-O13
152	M2	402	PC1	O13-C11-C12-N
152	M2	405	PC1	C11-O13-P-O12
152	M2	405	PC1	C11-O13-P-O14
152	M2	405	PC1	C11-O13-P-O11
152	M2	407	PC1	C11-O13-P-O12
152	M2	407	PC1	C11-O13-P-O14
152	M2	407	PC1	C11-O13-P-O11
152	M2	407	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
152	N	302	PC1	C11-O13-P-O12
152	N	302	PC1	C11-O13-P-O11
152	N	302	PC1	C1-O11-P-O13
152	V	201	PC1	C11-O13-P-O11
152	V	202	PC1	C11-O13-P-O11
152	V	202	PC1	C1-O11-P-O14
152	W	201	PC1	C11-O13-P-O12
152	W	201	PC1	C11-O13-P-O14
152	W	201	PC1	C11-O13-P-O11
152	W	201	PC1	C1-O11-P-O14
152	W	204	PC1	C11-O13-P-O11
152	W	204	PC1	C1-O11-P-O12
152	W	204	PC1	C1-O11-P-O14
152	W	204	PC1	C1-O11-P-O13
152	W	205	PC1	C11-O13-P-O12
152	W	205	PC1	C11-O13-P-O14
152	W	205	PC1	C11-O13-P-O11
152	5B	202	PC1	C11-O13-P-O12
152	5B	202	PC1	C11-O13-P-O14
152	5B	202	PC1	C11-O13-P-O11
152	5B	202	PC1	C1-O11-P-O13
152	AM	202	PC1	C11-O13-P-O12
152	AM	202	PC1	C11-O13-P-O14
152	AM	202	PC1	C11-O13-P-O11
152	AM	202	PC1	C1-O11-P-O12
152	AM	202	PC1	C1-O11-P-O14
152	AM	202	PC1	C1-O11-P-O13
152	AN	304	PC1	C11-O13-P-O11
152	AN	304	PC1	C1-O11-P-O12
152	AN	304	PC1	C1-O11-P-O14
152	AN	304	PC1	C1-O11-P-O13
152	B9	201	PC1	C11-O13-P-O12
152	B9	201	PC1	C11-O13-P-O11
152	B9	201	PC1	C1-O11-P-O14
152	B9	201	PC1	C1-O11-P-O13
152	C4	403	PC1	C11-O13-P-O12
152	C4	403	PC1	C11-O13-P-O11
152	J1	400	PC1	C11-O13-P-O11
152	J1	400	PC1	C1-O11-P-O12
152	J1	400	PC1	C1-O11-P-O14
152	J1	400	PC1	C1-O11-P-O13
152	N1	301	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
152	N1	301	PC1	C1-O11-P-O14
152	N1	301	PC1	C1-O11-P-O13
152	N5	801	PC1	C11-O13-P-O14
152	N5	801	PC1	C11-O13-P-O11
152	N5	803	PC1	C1-O11-P-O13
152	N5	804	PC1	C11-O13-P-O12
152	N5	804	PC1	C11-O13-P-O14
152	N5	804	PC1	C11-O13-P-O11
152	N5	804	PC1	C1-O11-P-O12
152	N5	804	PC1	C1-O11-P-O13
152	N5	805	PC1	C11-O13-P-O12
152	N5	805	PC1	C1-O11-P-O12
152	N5	805	PC1	C1-O11-P-O13
152	N5	805	PC1	O21-C2-C3-O31
152	N6	301	PC1	C11-O13-P-O12
152	N6	301	PC1	C11-O13-P-O11
152	P1	401	PC1	C1-O11-P-O12
152	P1	401	PC1	C1-O11-P-O14
152	P1	401	PC1	C1-O11-P-O13
152	QB	602	PC1	C11-O13-P-O12
152	QB	602	PC1	C11-O13-P-O11
152	QC	505	PC1	C11-O13-P-O12
152	QC	505	PC1	C11-O13-P-O11
152	QC	505	PC1	C1-O11-P-O12
152	QC	505	PC1	C1-O11-P-O14
152	QC	505	PC1	C1-O11-P-O13
152	QC	507	PC1	C1-O11-P-O12
152	QC	507	PC1	C1-O11-P-O13
152	QC	508	PC1	C1-O11-P-O14
152	QC	508	PC1	C1-O11-P-O13
152	QE	301	PC1	C11-O13-P-O14
152	QE	301	PC1	C11-O13-P-O11
152	QE	301	PC1	C1-O11-P-O13
152	QE	303	PC1	C1-O11-P-O14
152	QG	401	PC1	C11-O13-P-O12
152	QG	401	PC1	C11-O13-P-O14
152	QG	401	PC1	C11-O13-P-O11
152	QI	201	PC1	C11-O13-P-O12
152	QI	201	PC1	C11-O13-P-O14
152	QI	201	PC1	C11-O13-P-O11
152	QI	201	PC1	C1-O11-P-O14
152	QJ	101	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
152	QJ	101	PC1	C1-O11-P-O14
152	QJ	101	PC1	C1-O11-P-O13
152	QJ	102	PC1	C11-O13-P-O12
152	QJ	102	PC1	C1-O11-P-O12
152	QJ	102	PC1	C1-O11-P-O14
152	QJ	102	PC1	C1-O11-P-O13
152	QJ	102	PC1	O13-C11-C12-N
152	Qb	602	PC1	C11-O13-P-O11
152	Qc	506	PC1	C11-O13-P-O12
152	Qc	506	PC1	C11-O13-P-O14
152	Qc	506	PC1	C11-O13-P-O11
152	Qc	506	PC1	C1-O11-P-O12
152	Qc	506	PC1	C1-O11-P-O14
152	Qc	509	PC1	C1-O11-P-O14
152	Qc	509	PC1	C1-O11-P-O13
152	Qe	303	PC1	C11-O13-P-O14
152	Qe	303	PC1	C11-O13-P-O11
152	Qe	303	PC1	C1-O11-P-O12
152	Qe	303	PC1	C1-O11-P-O13
152	Qg	401	PC1	C11-O13-P-O12
152	Qg	401	PC1	C11-O13-P-O11
152	Qi	201	PC1	C1-O11-P-O12
152	Qi	201	PC1	C1-O11-P-O14
152	Qi	201	PC1	C1-O11-P-O13
152	Qi	203	PC1	C1-O11-P-O13
152	Qj	101	PC1	C11-O13-P-O12
152	Qj	101	PC1	C11-O13-P-O11
152	Qj	101	PC1	O11-C1-C2-O21
152	S8	301	PC1	C1-O11-P-O12
152	S8	301	PC1	C1-O11-P-O13
152	T1	602	PC1	C11-O13-P-O12
152	T1	602	PC1	C11-O13-P-O14
152	T1	602	PC1	C11-O13-P-O11
152	T1	602	PC1	C1-O11-P-O13
152	T4	301	PC1	C11-O13-P-O12
152	T4	301	PC1	C11-O13-P-O14
152	T4	301	PC1	C1-O11-P-O12
152	T4	301	PC1	C1-O11-P-O14
152	T4	301	PC1	C1-O11-P-O13
152	T4	303	PC1	C11-O13-P-O12
152	T4	303	PC1	C11-O13-P-O14
152	T4	303	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
152	T4	303	PC1	C1-O11-P-O13
152	TC	102	PC1	C11-O13-P-O14
152	TC	102	PC1	C11-O13-P-O11
152	TC	102	PC1	C1-O11-P-O12
152	TC	102	PC1	C1-O11-P-O13
152	TE	102	PC1	C11-O13-P-O12
152	TE	102	PC1	C11-O13-P-O11
152	TE	102	PC1	C1-O11-P-O14
153	2g	201	CDL	CB2-OB2-PB2-OB3
153	2g	201	CDL	CB2-OB2-PB2-OB4
153	2g	201	CDL	CB2-OB2-PB2-OB5
153	2g	201	CDL	CB3-OB5-PB2-OB3
153	2g	203	CDL	CA2-OA2-PA1-OA4
153	2g	203	CDL	CA2-OA2-PA1-OA5
153	2g	203	CDL	CA3-OA5-PA1-OA2
153	2g	203	CDL	CA3-OA5-PA1-OA4
153	2g	204	CDL	CA2-OA2-PA1-OA3
153	2g	204	CDL	CA2-OA2-PA1-OA4
153	2g	204	CDL	CA2-OA2-PA1-OA5
153	2g	204	CDL	CA3-OA5-PA1-OA4
153	2g	204	CDL	CB3-OB5-PB2-OB2
153	2g	204	CDL	CB3-OB5-PB2-OB3
153	2g	204	CDL	CB3-OB5-PB2-OB4
153	2k	101	CDL	CA3-OA5-PA1-OA2
153	2k	101	CDL	CA3-OA5-PA1-OA4
153	2k	101	CDL	CB2-OB2-PB2-OB3
153	2k	101	CDL	CB2-OB2-PB2-OB4
153	2k	101	CDL	CB2-OB2-PB2-OB5
153	2k	101	CDL	CB3-OB5-PB2-OB2
153	2k	101	CDL	CB3-OB5-PB2-OB3
153	2k	101	CDL	CB3-OB5-PB2-OB4
153	2m	101	CDL	CA3-OA5-PA1-OA2
153	2m	101	CDL	CA3-OA5-PA1-OA3
153	2m	101	CDL	CA3-OA5-PA1-OA4
153	2m	101	CDL	CB2-OB2-PB2-OB3
153	2m	101	CDL	CB2-OB2-PB2-OB4
153	2m	101	CDL	CB2-OB2-PB2-OB5
153	2o	101	CDL	CA2-OA2-PA1-OA4
153	2o	101	CDL	CA3-OA5-PA1-OA2
153	2o	101	CDL	CA3-OA5-PA1-OA3
153	2o	101	CDL	CA3-OA5-PA1-OA4
153	2o	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
153	6a	201	CDL	CA2-OA2-PA1-OA3
153	6a	201	CDL	CA2-OA2-PA1-OA5
153	6a	201	CDL	CA3-OA5-PA1-OA3
153	6a	201	CDL	CA3-OA5-PA1-OA4
153	6a	201	CDL	CB3-OB5-PB2-OB2
153	6c	201	CDL	CB2-OB2-PB2-OB3
153	6c	201	CDL	CB3-OB5-PB2-OB3
153	6c	201	CDL	CB3-OB5-PB2-OB4
153	6c	201	CDL	OB5-CB3-CB4-OB6
153	6c	202	CDL	CA2-OA2-PA1-OA3
153	6c	202	CDL	CA2-OA2-PA1-OA5
153	6c	202	CDL	CA3-OA5-PA1-OA2
153	6c	202	CDL	CB3-OB5-PB2-OB2
153	6c	202	CDL	CB3-OB5-PB2-OB3
153	7a	201	CDL	CA2-OA2-PA1-OA4
153	7a	201	CDL	CA3-OA5-PA1-OA2
153	7a	201	CDL	CA3-OA5-PA1-OA3
153	7a	201	CDL	CB2-OB2-PB2-OB3
153	7a	201	CDL	CB2-OB2-PB2-OB5
153	7a	203	CDL	CA2-OA2-PA1-OA3
153	7a	203	CDL	CA2-OA2-PA1-OA5
153	7a	203	CDL	CB3-OB5-PB2-OB3
153	7c	301	CDL	CA3-OA5-PA1-OA2
153	7c	301	CDL	CB3-OB5-PB2-OB2
153	7c	301	CDL	CB3-OB5-PB2-OB4
153	7c	302	CDL	CA3-OA5-PA1-OA2
153	7c	302	CDL	CA3-OA5-PA1-OA3
153	7c	302	CDL	CB2-OB2-PB2-OB3
153	7c	302	CDL	CB2-OB2-PB2-OB5
153	a	502	CDL	CA2-OA2-PA1-OA3
153	a	502	CDL	CA2-OA2-PA1-OA5
153	a	502	CDL	CA3-OA5-PA1-OA2
153	a	502	CDL	CB2-OB2-PB2-OB4
153	a	504	CDL	CA2-OA2-PA1-OA3
153	a	504	CDL	CA2-OA2-PA1-OA4
153	a	504	CDL	CA3-OA5-PA1-OA3
153	a	504	CDL	CB3-OB5-PB2-OB3
153	a	505	CDL	CB2-C1-CA2-OA2
153	b	501	CDL	CA2-OA2-PA1-OA3
153	b	501	CDL	CA2-OA2-PA1-OA4
153	b	501	CDL	CA2-OA2-PA1-OA5
153	b	501	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
153	b	501	CDL	CA3-OA5-PA1-OA3
153	b	501	CDL	CA3-OA5-PA1-OA4
153	c1	701	CDL	CA2-OA2-PA1-OA3
153	c1	701	CDL	CA2-OA2-PA1-OA4
153	c1	701	CDL	CA2-OA2-PA1-OA5
153	c1	701	CDL	CA3-OA5-PA1-OA2
153	c1	701	CDL	CB2-OB2-PB2-OB3
153	c1	701	CDL	CB2-OB2-PB2-OB4
153	c1	701	CDL	CB2-OB2-PB2-OB5
153	c1	701	CDL	CB3-OB5-PB2-OB3
153	c1	703	CDL	CA3-OA5-PA1-OA2
153	c1	703	CDL	CA3-OA5-PA1-OA3
153	c1	703	CDL	CB3-OB5-PB2-OB2
153	c1	703	CDL	CB3-OB5-PB2-OB3
153	c1	703	CDL	CB3-OB5-PB2-OB4
153	c1	709	CDL	C1-CA2-OA2-PA1
153	c1	709	CDL	CA2-OA2-PA1-OA4
153	c1	709	CDL	CA2-OA2-PA1-OA5
153	c1	709	CDL	CB2-OB2-PB2-OB3
153	c1	709	CDL	CB2-OB2-PB2-OB4
153	c1	709	CDL	CB2-OB2-PB2-OB5
153	c1	709	CDL	CB3-OB5-PB2-OB3
153	c1	712	CDL	CB2-OB2-PB2-OB3
153	c3	604	CDL	CA2-OA2-PA1-OA3
153	c3	604	CDL	CA2-OA2-PA1-OA4
153	c3	604	CDL	CA2-OA2-PA1-OA5
153	e	401	CDL	CA3-OA5-PA1-OA2
153	e	401	CDL	CA3-OA5-PA1-OA3
153	e	401	CDL	CA3-OA5-PA1-OA4
153	e	401	CDL	CB2-OB2-PB2-OB3
153	e	401	CDL	CB2-OB2-PB2-OB4
153	e	401	CDL	CB3-OB5-PB2-OB3
153	e	402	CDL	CA2-OA2-PA1-OA3
153	e	402	CDL	CB2-OB2-PB2-OB4
153	e	402	CDL	CB2-OB2-PB2-OB5
153	e	403	CDL	CB2-OB2-PB2-OB3
153	e	403	CDL	CB2-OB2-PB2-OB4
153	e	403	CDL	CB2-OB2-PB2-OB5
153	e	403	CDL	CB3-OB5-PB2-OB2
153	e	403	CDL	CB3-OB5-PB2-OB4
153	f	401	CDL	CB3-OB5-PB2-OB2
153	f	401	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
153	f	401	CDL	CB3-OB5-PB2-OB4
153	fs	203	CDL	CB3-OB5-PB2-OB2
153	fs	203	CDL	CB3-OB5-PB2-OB3
153	fs	203	CDL	CB3-OB5-PB2-OB4
153	i	301	CDL	CA2-OA2-PA1-OA4
153	i	301	CDL	CA2-OA2-PA1-OA5
153	i	301	CDL	CA3-OA5-PA1-OA3
153	i	302	CDL	CA3-OA5-PA1-OA2
153	i	302	CDL	CA3-OA5-PA1-OA3
153	i	302	CDL	CB2-OB2-PB2-OB3
153	i	302	CDL	OB5-CB3-CB4-OB6
153	j	301	CDL	CA2-OA2-PA1-OA3
153	j	301	CDL	CA2-OA2-PA1-OA5
153	j	301	CDL	CA3-OA5-PA1-OA2
153	j	301	CDL	CA3-OA5-PA1-OA4
153	j	301	CDL	CB3-OB5-PB2-OB2
153	j	301	CDL	CB3-OB5-PB2-OB3
153	j	301	CDL	CB3-OB5-PB2-OB4
153	l	301	CDL	CA3-OA5-PA1-OA2
153	l	301	CDL	CA3-OA5-PA1-OA4
153	l	301	CDL	CB2-OB2-PB2-OB3
153	l	301	CDL	CB2-OB2-PB2-OB4
153	l	301	CDL	CB3-OB5-PB2-OB2
153	l	301	CDL	CB3-OB5-PB2-OB3
153	l	301	CDL	CB3-OB5-PB2-OB4
153	m	302	CDL	CA3-OA5-PA1-OA4
153	m	302	CDL	CB2-OB2-PB2-OB3
153	m	302	CDL	CB2-OB2-PB2-OB4
153	m	302	CDL	CB2-OB2-PB2-OB5
153	m	303	CDL	CA2-OA2-PA1-OA3
153	m	304	CDL	CA2-OA2-PA1-OA4
153	m	304	CDL	CA2-OA2-PA1-OA5
153	m	304	CDL	CA4-CA3-OA5-PA1
153	m	304	CDL	CB3-OB5-PB2-OB2
153	m	304	CDL	CB3-OB5-PB2-OB3
153	m	304	CDL	CB3-OB5-PB2-OB4
153	m	306	CDL	CA2-OA2-PA1-OA3
153	m	306	CDL	CA2-OA2-PA1-OA4
153	m	306	CDL	CA2-OA2-PA1-OA5
153	m	306	CDL	CA3-OA5-PA1-OA2
153	m	306	CDL	CA3-OA5-PA1-OA3
153	m	306	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
153	m	306	CDL	CB2-OB2-PB2-OB4
153	m	306	CDL	CB2-OB2-PB2-OB5
153	m1	404	CDL	CA2-OA2-PA1-OA4
153	m1	404	CDL	CA2-OA2-PA1-OA5
153	m1	404	CDL	CB2-OB2-PB2-OB3
153	m1	404	CDL	CB2-OB2-PB2-OB4
153	m1	404	CDL	CB2-OB2-PB2-OB5
153	m1	404	CDL	CB3-OB5-PB2-OB3
153	m1	404	CDL	CB3-OB5-PB2-OB4
153	m1	405	CDL	CA2-OA2-PA1-OA3
153	m1	405	CDL	CA2-OA2-PA1-OA5
153	m1	405	CDL	CA3-OA5-PA1-OA2
153	m1	405	CDL	CA3-OA5-PA1-OA3
153	m1	405	CDL	CB2-OB2-PB2-OB4
153	m1	405	CDL	CB2-OB2-PB2-OB5
153	m1	405	CDL	CB3-OB5-PB2-OB3
153	m2	401	CDL	CB2-OB2-PB2-OB3
153	m2	401	CDL	CB2-OB2-PB2-OB5
153	m2	403	CDL	CA3-OA5-PA1-OA2
153	m2	403	CDL	CA3-OA5-PA1-OA4
153	m2	403	CDL	CB2-OB2-PB2-OB3
153	m2	403	CDL	CB2-OB2-PB2-OB4
153	m2	403	CDL	CB2-OB2-PB2-OB5
153	m2	403	CDL	CB3-OB5-PB2-OB2
153	m2	403	CDL	CB3-OB5-PB2-OB3
153	m2	403	CDL	CB3-OB5-PB2-OB4
153	m2	404	CDL	CA3-OA5-PA1-OA2
153	m2	404	CDL	CA3-OA5-PA1-OA4
153	m3	401	CDL	CA2-OA2-PA1-OA3
153	m3	403	CDL	CA3-OA5-PA1-OA2
153	m3	403	CDL	CA3-OA5-PA1-OA4
153	m3	403	CDL	CB3-OB5-PB2-OB2
153	m3	403	CDL	CB3-OB5-PB2-OB4
153	n	304	CDL	CA2-OA2-PA1-OA4
153	n	304	CDL	CA2-OA2-PA1-OA5
153	n	304	CDL	CA3-OA5-PA1-OA4
153	n	304	CDL	CB2-OB2-PB2-OB3
153	n	304	CDL	CB2-OB2-PB2-OB4
153	n	304	CDL	CB2-OB2-PB2-OB5
153	n	304	CDL	CB3-OB5-PB2-OB2
153	n	304	CDL	CB3-OB5-PB2-OB3
153	n	304	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
153	q	201	CDL	CB2-OB2-PB2-OB3
153	q	201	CDL	CB2-OB2-PB2-OB4
153	q	201	CDL	CB2-OB2-PB2-OB5
153	q	201	CDL	CB3-OB5-PB2-OB2
153	q	202	CDL	CB2-OB2-PB2-OB5
153	q	202	CDL	CB3-OB5-PB2-OB2
153	q	202	CDL	CB3-OB5-PB2-OB4
153	q	202	CDL	CB4-CB3-OB5-PB2
153	q	203	CDL	CA2-OA2-PA1-OA3
153	q	203	CDL	CA2-OA2-PA1-OA4
153	q	203	CDL	CA2-OA2-PA1-OA5
153	q	203	CDL	CA3-OA5-PA1-OA2
153	q	203	CDL	CA3-OA5-PA1-OA3
153	q	203	CDL	CA3-OA5-PA1-OA4
153	r	201	CDL	CA2-OA2-PA1-OA5
153	r	201	CDL	CA3-OA5-PA1-OA2
153	r	201	CDL	CA3-OA5-PA1-OA3
153	r	201	CDL	CA3-OA5-PA1-OA4
153	r	201	CDL	CB2-OB2-PB2-OB3
153	r	201	CDL	CB3-OB5-PB2-OB2
153	r	201	CDL	CB3-OB5-PB2-OB4
153	r	201	CDL	CB4-CB3-OB5-PB2
153	sd	101	CDL	CA2-OA2-PA1-OA3
153	sd	101	CDL	CB2-OB2-PB2-OB4
153	sd	101	CDL	CB2-OB2-PB2-OB5
153	sd	101	CDL	CB3-OB5-PB2-OB2
153	sd	101	CDL	CB3-OB5-PB2-OB4
153	t	201	CDL	CA3-OA5-PA1-OA3
153	t	201	CDL	CB3-OB5-PB2-OB2
153	t	201	CDL	CB3-OB5-PB2-OB3
153	t	201	CDL	CB3-OB5-PB2-OB4
153	t	201	CDL	OB5-CB3-CB4-OB6
153	t	202	CDL	CA2-OA2-PA1-OA4
153	t	203	CDL	O1-C1-CB2-OB2
153	t	203	CDL	CA2-OA2-PA1-OA5
153	t	203	CDL	CB3-OB5-PB2-OB2
153	t	203	CDL	CB3-OB5-PB2-OB3
153	t	204	CDL	CA3-OA5-PA1-OA2
153	t	204	CDL	CA3-OA5-PA1-OA3
153	t	204	CDL	CB3-OB5-PB2-OB2
153	t	204	CDL	CB3-OB5-PB2-OB4
153	t	204	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
153	u	201	CDL	CA2-OA2-PA1-OA3
153	u	201	CDL	CA2-OA2-PA1-OA5
153	u	201	CDL	CA3-OA5-PA1-OA2
153	u	201	CDL	CA3-OA5-PA1-OA3
153	u	201	CDL	CA3-OA5-PA1-OA4
153	u	201	CDL	CB3-OB5-PB2-OB2
153	vb	701	CDL	CA2-OA2-PA1-OA3
153	vb	701	CDL	CA2-OA2-PA1-OA5
153	vb	701	CDL	CA3-OA5-PA1-OA2
153	vb	701	CDL	OA6-CA4-CA6-OA8
153	vb	704	CDL	CA2-OA2-PA1-OA3
153	vb	704	CDL	CA2-OA2-PA1-OA4
153	vb	704	CDL	CA2-OA2-PA1-OA5
153	vb	704	CDL	CA3-OA5-PA1-OA4
153	vb	704	CDL	CB2-OB2-PB2-OB3
153	vb	704	CDL	CB2-OB2-PB2-OB4
153	vb	704	CDL	CB2-OB2-PB2-OB5
153	w	202	CDL	CA3-OA5-PA1-OA2
153	w	202	CDL	CB3-OB5-PB2-OB2
153	w	202	CDL	CB3-OB5-PB2-OB3
153	y5	201	CDL	CA3-OA5-PA1-OA4
153	y7	501	CDL	CA2-OA2-PA1-OA3
153	y7	501	CDL	CA2-OA2-PA1-OA4
153	y7	501	CDL	CA2-OA2-PA1-OA5
153	y7	501	CDL	CA3-OA5-PA1-OA3
153	y7	501	CDL	CB2-OB2-PB2-OB5
153	z	101	CDL	CA2-OA2-PA1-OA3
153	z	101	CDL	CA2-OA2-PA1-OA5
153	z	101	CDL	CB3-OB5-PB2-OB2
153	z	101	CDL	CB3-OB5-PB2-OB4
153	2b	201	CDL	CB2-OB2-PB2-OB4
153	2b	201	CDL	CB2-OB2-PB2-OB5
153	2b	201	CDL	CB3-OB5-PB2-OB2
153	2b	201	CDL	CB3-OB5-PB2-OB4
153	5b	201	CDL	CA2-OA2-PA1-OA3
153	5b	201	CDL	CA2-OA2-PA1-OA5
153	5b	201	CDL	CB2-OB2-PB2-OB4
153	5b	201	CDL	CB3-OB5-PB2-OB3
153	a1	101	CDL	CA2-OA2-PA1-OA3
153	a1	101	CDL	CA2-OA2-PA1-OA5
153	a1	101	CDL	CA3-OA5-PA1-OA2
153	a1	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	a1	101	CDL	CA3-OA5-PA1-OA4
153	a1	101	CDL	CB3-OB5-PB2-OB3
153	a9	402	CDL	CA2-OA2-PA1-OA4
153	a9	402	CDL	CA3-OA5-PA1-OA3
153	a9	402	CDL	CB3-OB5-PB2-OB3
153	a9	403	CDL	CA2-OA2-PA1-OA3
153	a9	403	CDL	CA2-OA2-PA1-OA4
153	a9	403	CDL	CA2-OA2-PA1-OA5
153	a9	403	CDL	CA3-OA5-PA1-OA2
153	a9	403	CDL	CA3-OA5-PA1-OA3
153	a9	403	CDL	CA3-OA5-PA1-OA4
153	a9	403	CDL	CB2-OB2-PB2-OB3
153	a9	403	CDL	CB3-OB5-PB2-OB4
153	al	301	CDL	CA2-OA2-PA1-OA5
153	al	301	CDL	CA3-OA5-PA1-OA2
153	al	301	CDL	CA3-OA5-PA1-OA4
153	al	301	CDL	CB2-OB2-PB2-OB3
153	al	301	CDL	CB2-OB2-PB2-OB4
153	al	301	CDL	CB3-OB5-PB2-OB2
153	al	301	CDL	CB3-OB5-PB2-OB3
153	am	201	CDL	CA2-OA2-PA1-OA3
153	am	201	CDL	CA2-OA2-PA1-OA4
153	am	201	CDL	CA2-OA2-PA1-OA5
153	am	201	CDL	CB2-OB2-PB2-OB3
153	am	201	CDL	CB2-OB2-PB2-OB4
153	am	201	CDL	CB2-OB2-PB2-OB5
153	an	302	CDL	C1-CA2-OA2-PA1
153	an	302	CDL	CB2-OB2-PB2-OB4
153	an	302	CDL	CB2-OB2-PB2-OB5
153	an	302	CDL	CB3-OB5-PB2-OB3
153	b3	101	CDL	CA3-OA5-PA1-OA2
153	b3	101	CDL	CB2-OB2-PB2-OB3
153	b3	101	CDL	CB2-OB2-PB2-OB4
153	b3	101	CDL	CB2-OB2-PB2-OB5
153	b3	102	CDL	CA2-OA2-PA1-OA3
153	b3	102	CDL	CA2-OA2-PA1-OA4
153	b3	102	CDL	CA2-OA2-PA1-OA5
153	b3	102	CDL	CA3-OA5-PA1-OA2
153	b3	102	CDL	CB3-OB5-PB2-OB2
153	b4	201	CDL	CA2-OA2-PA1-OA3
153	b4	201	CDL	CA2-OA2-PA1-OA5
153	b8	302	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
153	b8	302	CDL	CB3-OB5-PB2-OB3
153	bm	301	CDL	CA2-OA2-PA1-OA3
153	bm	301	CDL	CA2-OA2-PA1-OA5
153	bm	301	CDL	CB3-OB5-PB2-OB2
153	bm	301	CDL	CB3-OB5-PB2-OB4
153	c4	401	CDL	CA2-OA2-PA1-OA3
153	c4	401	CDL	CA2-OA2-PA1-OA4
153	c4	401	CDL	CA2-OA2-PA1-OA5
153	c4	401	CDL	CA3-OA5-PA1-OA3
153	c4	401	CDL	CB2-OB2-PB2-OB5
153	n5	806	CDL	CA2-OA2-PA1-OA3
153	n5	806	CDL	CA2-OA2-PA1-OA5
153	n5	806	CDL	CA3-OA5-PA1-OA2
153	n5	806	CDL	CA3-OA5-PA1-OA3
153	n5	806	CDL	CB2-OB2-PB2-OB3
153	n6	302	CDL	CA2-OA2-PA1-OA3
153	n6	302	CDL	CA2-OA2-PA1-OA4
153	n6	302	CDL	CA2-OA2-PA1-OA5
153	n6	302	CDL	CA3-OA5-PA1-OA3
153	n6	302	CDL	CB2-OB2-PB2-OB4
153	n6	302	CDL	CB2-OB2-PB2-OB5
153	p1	402	CDL	CA2-OA2-PA1-OA3
153	p1	402	CDL	CA3-OA5-PA1-OA2
153	p1	402	CDL	CB2-OB2-PB2-OB3
153	p1	402	CDL	CB2-OB2-PB2-OB5
153	p1	402	CDL	CB3-OB5-PB2-OB2
153	p1	402	CDL	CB3-OB5-PB2-OB3
153	p1	402	CDL	CB3-OB5-PB2-OB4
153	p1	403	CDL	CA2-OA2-PA1-OA3
153	p1	403	CDL	CA2-OA2-PA1-OA4
153	p1	403	CDL	CA2-OA2-PA1-OA5
153	p1	403	CDL	CA3-OA5-PA1-OA2
153	p1	403	CDL	CA3-OA5-PA1-OA4
153	qB	601	CDL	CA2-OA2-PA1-OA3
153	qB	601	CDL	CA2-OA2-PA1-OA4
153	qB	601	CDL	CA2-OA2-PA1-OA5
153	qB	601	CDL	CB3-OB5-PB2-OB2
153	qC	503	CDL	CA3-OA5-PA1-OA2
153	qC	504	CDL	CA3-OA5-PA1-OA2
153	qC	504	CDL	CA3-OA5-PA1-OA3
153	qC	504	CDL	CB2-OB2-PB2-OB4
153	qC	504	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
153	qC	504	CDL	CB3-OB5-PB2-OB2
153	qC	504	CDL	CB3-OB5-PB2-OB4
153	qD	402	CDL	CA2-OA2-PA1-OA4
153	qD	402	CDL	CA2-OA2-PA1-OA5
153	qD	402	CDL	CA3-OA5-PA1-OA3
153	qD	402	CDL	CB2-OB2-PB2-OB3
153	qD	402	CDL	CB2-OB2-PB2-OB4
153	qD	402	CDL	CB3-OB5-PB2-OB3
153	qG	402	CDL	CA2-OA2-PA1-OA3
153	qG	402	CDL	CA2-OA2-PA1-OA4
153	qG	402	CDL	CA2-OA2-PA1-OA5
153	qG	402	CDL	CA3-OA5-PA1-OA3
153	qG	402	CDL	CA3-OA5-PA1-OA4
153	qG	402	CDL	CB2-OB2-PB2-OB3
153	qH	201	CDL	O1-C1-CB2-OB2
153	qH	201	CDL	CA2-OA2-PA1-OA3
153	qH	201	CDL	CA2-OA2-PA1-OA5
153	qH	201	CDL	CB2-OB2-PB2-OB3
153	qH	201	CDL	CB2-OB2-PB2-OB5
153	qH	201	CDL	CB3-OB5-PB2-OB2
153	qH	201	CDL	CB3-OB5-PB2-OB3
153	qI	203	CDL	CA2-OA2-PA1-OA4
153	qI	203	CDL	CA2-OA2-PA1-OA5
153	qI	203	CDL	CA3-OA5-PA1-OA4
153	qI	203	CDL	CB2-OB2-PB2-OB4
153	qI	203	CDL	CB2-OB2-PB2-OB5
153	qI	203	CDL	CB3-OB5-PB2-OB2
153	qI	203	CDL	CB3-OB5-PB2-OB3
153	qc	504	CDL	CA2-OA2-PA1-OA3
153	qc	504	CDL	CA2-OA2-PA1-OA5
153	qc	504	CDL	CA3-OA5-PA1-OA2
153	qc	504	CDL	CA3-OA5-PA1-OA3
153	qc	504	CDL	CA3-OA5-PA1-OA4
153	qc	504	CDL	CB2-OB2-PB2-OB5
153	qc	504	CDL	CB3-OB5-PB2-OB2
153	qc	504	CDL	CB3-OB5-PB2-OB3
153	qc	504	CDL	CB3-OB5-PB2-OB4
153	qc	505	CDL	CA2-OA2-PA1-OA3
153	qc	505	CDL	CA2-OA2-PA1-OA5
153	qc	505	CDL	CA3-OA5-PA1-OA2
153	qc	505	CDL	CA3-OA5-PA1-OA3
153	qc	505	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
153	qc	505	CDL	CB2-OB2-PB2-OB4
153	qc	505	CDL	CB2-OB2-PB2-OB5
153	qc	505	CDL	CB3-OB5-PB2-OB2
153	qc	505	CDL	CB3-OB5-PB2-OB3
153	qc	505	CDL	CB3-OB5-PB2-OB4
153	qc	508	CDL	CA2-OA2-PA1-OA3
153	qg	402	CDL	CA2-OA2-PA1-OA4
153	qg	402	CDL	CA3-OA5-PA1-OA2
153	qg	402	CDL	CA3-OA5-PA1-OA4
153	qg	402	CDL	CB3-OB5-PB2-OB2
153	qi	202	CDL	CA3-OA5-PA1-OA2
153	qi	202	CDL	CA3-OA5-PA1-OA3
153	qi	202	CDL	CA3-OA5-PA1-OA4
153	qi	202	CDL	CB2-OB2-PB2-OB5
153	t1	601	CDL	CA3-OA5-PA1-OA3
153	t1	601	CDL	CB3-OB5-PB2-OB2
153	t1	601	CDL	CB3-OB5-PB2-OB3
153	t1	601	CDL	CB3-OB5-PB2-OB4
153	t5	301	CDL	CA2-OA2-PA1-OA3
153	t5	301	CDL	CA2-OA2-PA1-OA4
153	t5	301	CDL	CA2-OA2-PA1-OA5
153	t5	301	CDL	CA3-OA5-PA1-OA2
153	t5	301	CDL	CA3-OA5-PA1-OA3
153	t5	301	CDL	CB2-OB2-PB2-OB3
153	t5	301	CDL	CB2-OB2-PB2-OB5
153	t5	301	CDL	CB3-OB5-PB2-OB3
153	t7	201	CDL	CA2-OA2-PA1-OA4
153	t7	201	CDL	CA2-OA2-PA1-OA5
153	t7	201	CDL	CA3-OA5-PA1-OA2
153	t7	201	CDL	CB2-OB2-PB2-OB3
153	t7	201	CDL	CB2-OB2-PB2-OB4
153	t7	201	CDL	CB2-OB2-PB2-OB5
153	td	101	CDL	CA2-OA2-PA1-OA4
153	td	101	CDL	CB2-OB2-PB2-OB3
153	td	101	CDL	CB3-OB5-PB2-OB2
153	td	101	CDL	CB3-OB5-PB2-OB3
153	td	101	CDL	CB3-OB5-PB2-OB4
153	te	101	CDL	CA2-OA2-PA1-OA5
153	te	101	CDL	CB2-OB2-PB2-OB3
153	te	101	CDL	CB2-OB2-PB2-OB4
153	te	101	CDL	CB3-OB5-PB2-OB2
153	te	101	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
153	te	101	CDL	CB3-OB5-PB2-OB4
153	th	200	CDL	CA2-OA2-PA1-OA4
153	th	200	CDL	CA3-OA5-PA1-OA2
153	th	200	CDL	CA3-OA5-PA1-OA3
153	th	200	CDL	OA6-CA4-CA6-OA8
153	th	200	CDL	CB2-OB2-PB2-OB4
153	th	200	CDL	CB2-OB2-PB2-OB5
153	th	200	CDL	CB3-OB5-PB2-OB2
153	2G	201	CDL	CB2-OB2-PB2-OB3
153	2G	201	CDL	CB2-OB2-PB2-OB4
153	2G	201	CDL	CB2-OB2-PB2-OB5
153	2G	201	CDL	CB3-OB5-PB2-OB3
153	2G	203	CDL	CA2-OA2-PA1-OA4
153	2G	203	CDL	CA2-OA2-PA1-OA5
153	2G	203	CDL	CA3-OA5-PA1-OA2
153	2G	203	CDL	CA3-OA5-PA1-OA4
153	2G	204	CDL	CA2-OA2-PA1-OA3
153	2G	204	CDL	CA2-OA2-PA1-OA4
153	2G	204	CDL	CA2-OA2-PA1-OA5
153	2G	204	CDL	CA3-OA5-PA1-OA4
153	2G	204	CDL	CB3-OB5-PB2-OB2
153	2G	204	CDL	CB3-OB5-PB2-OB4
153	2K	101	CDL	CA3-OA5-PA1-OA2
153	2K	101	CDL	CA3-OA5-PA1-OA4
153	2K	101	CDL	CB2-OB2-PB2-OB3
153	2K	101	CDL	CB2-OB2-PB2-OB4
153	2K	101	CDL	CB2-OB2-PB2-OB5
153	2K	101	CDL	CB3-OB5-PB2-OB2
153	2K	101	CDL	CB3-OB5-PB2-OB3
153	2K	101	CDL	CB3-OB5-PB2-OB4
153	2M	101	CDL	CA3-OA5-PA1-OA2
153	2M	101	CDL	CA3-OA5-PA1-OA3
153	2M	101	CDL	CA3-OA5-PA1-OA4
153	2M	101	CDL	CB2-OB2-PB2-OB3
153	2M	101	CDL	CB2-OB2-PB2-OB4
153	2M	101	CDL	CB2-OB2-PB2-OB5
153	2O	101	CDL	CA2-OA2-PA1-OA4
153	2O	101	CDL	CA3-OA5-PA1-OA2
153	2O	101	CDL	CA3-OA5-PA1-OA3
153	2O	101	CDL	CA3-OA5-PA1-OA4
153	2O	101	CDL	CB2-OB2-PB2-OB5
153	6A	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	6A	201	CDL	CA2-OA2-PA1-OA5
153	6A	201	CDL	CA3-OA5-PA1-OA3
153	6A	201	CDL	CA3-OA5-PA1-OA4
153	6A	201	CDL	CB3-OB5-PB2-OB2
153	6C	202	CDL	CB2-OB2-PB2-OB3
153	6C	202	CDL	CB3-OB5-PB2-OB3
153	6C	202	CDL	CB3-OB5-PB2-OB4
153	6C	202	CDL	OB5-CB3-CB4-OB6
153	6C	203	CDL	CA2-OA2-PA1-OA3
153	6C	203	CDL	CA2-OA2-PA1-OA5
153	6C	203	CDL	CA3-OA5-PA1-OA2
153	6C	203	CDL	CB3-OB5-PB2-OB2
153	7A	201	CDL	CA2-OA2-PA1-OA4
153	7A	201	CDL	CA3-OA5-PA1-OA2
153	7A	201	CDL	CA3-OA5-PA1-OA3
153	7A	201	CDL	CB2-OB2-PB2-OB3
153	7A	201	CDL	CB2-OB2-PB2-OB5
153	7A	203	CDL	CA2-OA2-PA1-OA3
153	7A	203	CDL	CA2-OA2-PA1-OA5
153	7A	203	CDL	CB3-OB5-PB2-OB2
153	7A	203	CDL	CB3-OB5-PB2-OB3
153	7C	301	CDL	CA3-OA5-PA1-OA2
153	7C	301	CDL	CB3-OB5-PB2-OB2
153	7C	301	CDL	CB3-OB5-PB2-OB4
153	7C	302	CDL	CA3-OA5-PA1-OA2
153	7C	302	CDL	CA3-OA5-PA1-OA3
153	7C	302	CDL	CB2-OB2-PB2-OB3
153	7C	302	CDL	CB2-OB2-PB2-OB5
153	A	502	CDL	CA2-OA2-PA1-OA3
153	A	502	CDL	CA2-OA2-PA1-OA5
153	A	502	CDL	CA3-OA5-PA1-OA2
153	A	502	CDL	CB2-OB2-PB2-OB4
153	A	504	CDL	CA2-OA2-PA1-OA3
153	A	504	CDL	CA2-OA2-PA1-OA4
153	A	504	CDL	CA3-OA5-PA1-OA3
153	A	504	CDL	CB3-OB5-PB2-OB3
153	B	501	CDL	CA2-OA2-PA1-OA3
153	B	501	CDL	CA2-OA2-PA1-OA4
153	B	501	CDL	CA2-OA2-PA1-OA5
153	B	501	CDL	CA3-OA5-PA1-OA2
153	B	501	CDL	CA3-OA5-PA1-OA3
153	B	501	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
153	C1	701	CDL	CA2-OA2-PA1-OA3
153	C1	701	CDL	CA2-OA2-PA1-OA4
153	C1	701	CDL	CA2-OA2-PA1-OA5
153	C1	701	CDL	CA3-OA5-PA1-OA2
153	C1	701	CDL	CB2-OB2-PB2-OB3
153	C1	701	CDL	CB2-OB2-PB2-OB4
153	C1	701	CDL	CB2-OB2-PB2-OB5
153	C1	701	CDL	CB3-OB5-PB2-OB3
153	C1	707	CDL	CA3-OA5-PA1-OA2
153	C1	707	CDL	CA3-OA5-PA1-OA3
153	C1	707	CDL	CB3-OB5-PB2-OB2
153	C1	707	CDL	CB3-OB5-PB2-OB3
153	C1	707	CDL	CB3-OB5-PB2-OB4
153	C1	708	CDL	C1-CA2-OA2-PA1
153	C1	708	CDL	CA2-OA2-PA1-OA4
153	C1	708	CDL	CA2-OA2-PA1-OA5
153	C1	708	CDL	CB2-OB2-PB2-OB3
153	C1	708	CDL	CB2-OB2-PB2-OB4
153	C1	708	CDL	CB2-OB2-PB2-OB5
153	C1	708	CDL	CB3-OB5-PB2-OB3
153	C1	712	CDL	CB2-OB2-PB2-OB3
153	C3	604	CDL	CA2-OA2-PA1-OA3
153	C3	604	CDL	CA2-OA2-PA1-OA4
153	C3	604	CDL	CA2-OA2-PA1-OA5
153	E	401	CDL	CA3-OA5-PA1-OA2
153	E	401	CDL	CA3-OA5-PA1-OA3
153	E	401	CDL	CA3-OA5-PA1-OA4
153	E	401	CDL	CB2-OB2-PB2-OB3
153	E	401	CDL	CB2-OB2-PB2-OB4
153	E	401	CDL	CB3-OB5-PB2-OB3
153	E	402	CDL	CA2-OA2-PA1-OA3
153	E	402	CDL	CB2-OB2-PB2-OB4
153	E	402	CDL	CB2-OB2-PB2-OB5
153	E	403	CDL	CB2-OB2-PB2-OB3
153	E	403	CDL	CB2-OB2-PB2-OB4
153	E	403	CDL	CB2-OB2-PB2-OB5
153	E	403	CDL	CB3-OB5-PB2-OB4
153	F	402	CDL	CB3-OB5-PB2-OB2
153	F	402	CDL	CB3-OB5-PB2-OB3
153	F	402	CDL	CB3-OB5-PB2-OB4
153	FS	204	CDL	CB3-OB5-PB2-OB2
153	FS	204	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
153	FS	204	CDL	CB3-OB5-PB2-OB4
153	I	302	CDL	CA2-OA2-PA1-OA4
153	I	302	CDL	CA2-OA2-PA1-OA5
153	I	302	CDL	CA3-OA5-PA1-OA3
153	I	303	CDL	CA3-OA5-PA1-OA2
153	I	303	CDL	CA3-OA5-PA1-OA3
153	I	303	CDL	CB2-OB2-PB2-OB3
153	I	303	CDL	OB5-CB3-CB4-OB6
153	J	301	CDL	CA2-OA2-PA1-OA3
153	J	301	CDL	CA2-OA2-PA1-OA5
153	J	301	CDL	CA3-OA5-PA1-OA2
153	J	301	CDL	CA3-OA5-PA1-OA4
153	J	301	CDL	CB3-OB5-PB2-OB2
153	J	301	CDL	CB3-OB5-PB2-OB3
153	J	301	CDL	CB3-OB5-PB2-OB4
153	L	301	CDL	CA3-OA5-PA1-OA2
153	L	301	CDL	CA3-OA5-PA1-OA4
153	L	301	CDL	CB2-OB2-PB2-OB3
153	L	301	CDL	CB2-OB2-PB2-OB4
153	L	301	CDL	CB3-OB5-PB2-OB2
153	L	301	CDL	CB3-OB5-PB2-OB3
153	L	301	CDL	CB3-OB5-PB2-OB4
153	M	301	CDL	CA2-OA2-PA1-OA3
153	M	301	CDL	CA2-OA2-PA1-OA4
153	M	301	CDL	CA2-OA2-PA1-OA5
153	M	301	CDL	CA3-OA5-PA1-OA2
153	M	301	CDL	CA3-OA5-PA1-OA3
153	M	301	CDL	CA3-OA5-PA1-OA4
153	M	301	CDL	CB2-OB2-PB2-OB4
153	M	301	CDL	CB2-OB2-PB2-OB5
153	M	304	CDL	CA3-OA5-PA1-OA4
153	M	304	CDL	CB2-OB2-PB2-OB3
153	M	304	CDL	CB2-OB2-PB2-OB4
153	M	304	CDL	CB2-OB2-PB2-OB5
153	M	305	CDL	CA2-OA2-PA1-OA3
153	M	306	CDL	CA2-OA2-PA1-OA5
153	M	306	CDL	CA4-CA3-OA5-PA1
153	M	306	CDL	CB3-OB5-PB2-OB2
153	M	306	CDL	CB3-OB5-PB2-OB3
153	M	306	CDL	CB3-OB5-PB2-OB4
153	M1	404	CDL	CA2-OA2-PA1-OA4
153	M1	404	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
153	M1	404	CDL	CB2-OB2-PB2-OB3
153	M1	404	CDL	CB2-OB2-PB2-OB4
153	M1	404	CDL	CB2-OB2-PB2-OB5
153	M1	404	CDL	CB3-OB5-PB2-OB3
153	M1	404	CDL	CB3-OB5-PB2-OB4
153	M1	405	CDL	CA2-OA2-PA1-OA3
153	M1	405	CDL	CA2-OA2-PA1-OA5
153	M1	405	CDL	CA3-OA5-PA1-OA2
153	M1	405	CDL	CA3-OA5-PA1-OA3
153	M1	405	CDL	CB2-OB2-PB2-OB4
153	M1	405	CDL	CB2-OB2-PB2-OB5
153	M1	405	CDL	CB3-OB5-PB2-OB3
153	M2	401	CDL	CB2-OB2-PB2-OB3
153	M2	401	CDL	CB2-OB2-PB2-OB5
153	M2	403	CDL	CA3-OA5-PA1-OA2
153	M2	403	CDL	CA3-OA5-PA1-OA4
153	M2	403	CDL	CB2-OB2-PB2-OB3
153	M2	403	CDL	CB2-OB2-PB2-OB4
153	M2	403	CDL	CB2-OB2-PB2-OB5
153	M2	403	CDL	CB3-OB5-PB2-OB2
153	M2	403	CDL	CB3-OB5-PB2-OB3
153	M2	403	CDL	CB3-OB5-PB2-OB4
153	M2	404	CDL	CA3-OA5-PA1-OA2
153	M2	404	CDL	CA3-OA5-PA1-OA4
153	M3	401	CDL	CA2-OA2-PA1-OA3
153	M3	403	CDL	CA3-OA5-PA1-OA2
153	M3	403	CDL	CA3-OA5-PA1-OA4
153	M3	403	CDL	CB3-OB5-PB2-OB2
153	M3	403	CDL	CB3-OB5-PB2-OB4
153	N	304	CDL	CA2-OA2-PA1-OA4
153	N	304	CDL	CA2-OA2-PA1-OA5
153	N	304	CDL	CA3-OA5-PA1-OA4
153	N	304	CDL	CB2-OB2-PB2-OB3
153	N	304	CDL	CB2-OB2-PB2-OB4
153	N	304	CDL	CB2-OB2-PB2-OB5
153	N	304	CDL	CB3-OB5-PB2-OB2
153	N	304	CDL	CB3-OB5-PB2-OB3
153	N	304	CDL	CB3-OB5-PB2-OB4
153	Q	201	CDL	CB2-OB2-PB2-OB3
153	Q	201	CDL	CB2-OB2-PB2-OB4
153	Q	201	CDL	CB2-OB2-PB2-OB5
153	Q	201	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
153	Q	202	CDL	CB2-OB2-PB2-OB5
153	Q	202	CDL	CB3-OB5-PB2-OB2
153	Q	202	CDL	CB3-OB5-PB2-OB4
153	Q	202	CDL	CB4-CB3-OB5-PB2
153	R	201	CDL	CA2-OA2-PA1-OA5
153	R	201	CDL	CA3-OA5-PA1-OA2
153	R	201	CDL	CA3-OA5-PA1-OA3
153	R	201	CDL	CA3-OA5-PA1-OA4
153	R	201	CDL	CB2-OB2-PB2-OB3
153	R	201	CDL	CB3-OB5-PB2-OB2
153	R	201	CDL	CB3-OB5-PB2-OB4
153	R	201	CDL	CB4-CB3-OB5-PB2
153	SD	101	CDL	CA2-OA2-PA1-OA3
153	SD	101	CDL	CB2-OB2-PB2-OB4
153	SD	101	CDL	CB2-OB2-PB2-OB5
153	SD	101	CDL	CB3-OB5-PB2-OB2
153	SD	101	CDL	CB3-OB5-PB2-OB4
153	T	201	CDL	CA3-OA5-PA1-OA3
153	T	201	CDL	CB3-OB5-PB2-OB2
153	T	201	CDL	CB3-OB5-PB2-OB3
153	T	201	CDL	CB3-OB5-PB2-OB4
153	T	201	CDL	OB5-CB3-CB4-OB6
153	T	202	CDL	CA2-OA2-PA1-OA4
153	T	203	CDL	O1-C1-CB2-OB2
153	T	203	CDL	CA2-OA2-PA1-OA5
153	T	203	CDL	CB3-OB5-PB2-OB2
153	T	203	CDL	CB3-OB5-PB2-OB3
153	T	204	CDL	CA3-OA5-PA1-OA2
153	T	204	CDL	CA3-OA5-PA1-OA3
153	T	204	CDL	CB3-OB5-PB2-OB2
153	T	204	CDL	CB3-OB5-PB2-OB4
153	T	204	CDL	CB4-CB3-OB5-PB2
153	U	201	CDL	CA2-OA2-PA1-OA3
153	U	201	CDL	CA2-OA2-PA1-OA5
153	U	201	CDL	CA3-OA5-PA1-OA2
153	U	201	CDL	CA3-OA5-PA1-OA3
153	U	201	CDL	CA3-OA5-PA1-OA4
153	U	201	CDL	CB3-OB5-PB2-OB2
153	VB	701	CDL	CA2-OA2-PA1-OA3
153	VB	701	CDL	CA2-OA2-PA1-OA5
153	VB	701	CDL	CA3-OA5-PA1-OA2
153	VB	701	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
153	VB	701	CDL	CB3-OB5-PB2-OB3
153	VB	703	CDL	CA2-OA2-PA1-OA3
153	VB	703	CDL	CA2-OA2-PA1-OA4
153	VB	703	CDL	CA2-OA2-PA1-OA5
153	VB	703	CDL	CA3-OA5-PA1-OA2
153	VB	703	CDL	CA3-OA5-PA1-OA3
153	VB	703	CDL	CA3-OA5-PA1-OA4
153	VB	705	CDL	CB2-C1-CA2-OA2
153	VB	706	CDL	CA2-OA2-PA1-OA3
153	VB	706	CDL	CA2-OA2-PA1-OA4
153	VB	706	CDL	CA2-OA2-PA1-OA5
153	VB	706	CDL	CA3-OA5-PA1-OA4
153	VB	706	CDL	CB2-OB2-PB2-OB3
153	VB	706	CDL	CB2-OB2-PB2-OB4
153	VB	706	CDL	CB2-OB2-PB2-OB5
153	W	202	CDL	CA3-OA5-PA1-OA2
153	W	202	CDL	CB3-OB5-PB2-OB2
153	W	202	CDL	CB3-OB5-PB2-OB3
153	Y5	201	CDL	CA3-OA5-PA1-OA4
153	Y7	501	CDL	CA2-OA2-PA1-OA3
153	Y7	501	CDL	CA2-OA2-PA1-OA4
153	Y7	501	CDL	CA2-OA2-PA1-OA5
153	Y7	501	CDL	CA3-OA5-PA1-OA3
153	Y7	501	CDL	CB2-OB2-PB2-OB5
153	Z	101	CDL	CA2-OA2-PA1-OA3
153	Z	101	CDL	CA2-OA2-PA1-OA5
153	Z	101	CDL	CB3-OB5-PB2-OB2
153	Z	101	CDL	CB3-OB5-PB2-OB4
153	2B	201	CDL	CB2-OB2-PB2-OB4
153	2B	201	CDL	CB2-OB2-PB2-OB5
153	2B	201	CDL	CB3-OB5-PB2-OB2
153	2B	201	CDL	CB3-OB5-PB2-OB4
153	5B	201	CDL	CA2-OA2-PA1-OA3
153	5B	201	CDL	CA2-OA2-PA1-OA5
153	5B	201	CDL	CB2-OB2-PB2-OB4
153	5B	201	CDL	CB3-OB5-PB2-OB3
153	A1	101	CDL	CA2-OA2-PA1-OA4
153	A1	101	CDL	CB2-OB2-PB2-OB3
153	A1	101	CDL	CB3-OB5-PB2-OB2
153	A1	101	CDL	CB3-OB5-PB2-OB3
153	A1	101	CDL	CB3-OB5-PB2-OB4
153	A1	102	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	A1	102	CDL	CA2-OA2-PA1-OA5
153	A1	102	CDL	CA3-OA5-PA1-OA2
153	A1	102	CDL	CA3-OA5-PA1-OA3
153	A1	102	CDL	CA3-OA5-PA1-OA4
153	A1	102	CDL	CB3-OB5-PB2-OB3
153	A9	402	CDL	CA2-OA2-PA1-OA4
153	A9	402	CDL	CA3-OA5-PA1-OA3
153	A9	402	CDL	CB3-OB5-PB2-OB3
153	A9	403	CDL	CA2-OA2-PA1-OA3
153	A9	403	CDL	CA2-OA2-PA1-OA4
153	A9	403	CDL	CA2-OA2-PA1-OA5
153	A9	403	CDL	CA3-OA5-PA1-OA2
153	A9	403	CDL	CA3-OA5-PA1-OA3
153	A9	403	CDL	CA3-OA5-PA1-OA4
153	A9	403	CDL	CB2-OB2-PB2-OB3
153	A9	403	CDL	CB3-OB5-PB2-OB4
153	AL	301	CDL	CA2-OA2-PA1-OA5
153	AL	301	CDL	CA3-OA5-PA1-OA2
153	AL	301	CDL	CA3-OA5-PA1-OA4
153	AL	301	CDL	CB2-OB2-PB2-OB3
153	AL	301	CDL	CB2-OB2-PB2-OB4
153	AL	301	CDL	CB3-OB5-PB2-OB2
153	AL	301	CDL	CB3-OB5-PB2-OB3
153	AM	201	CDL	CA2-OA2-PA1-OA3
153	AM	201	CDL	CA2-OA2-PA1-OA4
153	AM	201	CDL	CA2-OA2-PA1-OA5
153	AM	201	CDL	CB2-OB2-PB2-OB3
153	AM	201	CDL	CB2-OB2-PB2-OB4
153	AM	201	CDL	CB2-OB2-PB2-OB5
153	AN	302	CDL	C1-CA2-OA2-PA1
153	AN	302	CDL	CB2-OB2-PB2-OB4
153	AN	302	CDL	CB2-OB2-PB2-OB5
153	AN	302	CDL	CB3-OB5-PB2-OB3
153	B3	101	CDL	CA3-OA5-PA1-OA2
153	B3	101	CDL	CB2-OB2-PB2-OB3
153	B3	101	CDL	CB2-OB2-PB2-OB4
153	B3	101	CDL	CB2-OB2-PB2-OB5
153	B3	102	CDL	O1-C1-CA2-OA2
153	B3	102	CDL	CA2-OA2-PA1-OA3
153	B3	102	CDL	CA2-OA2-PA1-OA4
153	B3	102	CDL	CA2-OA2-PA1-OA5
153	B3	102	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
153	B4	201	CDL	CA2-OA2-PA1-OA3
153	B4	201	CDL	CA2-OA2-PA1-OA5
153	B8	302	CDL	CB3-OB5-PB2-OB2
153	B8	302	CDL	CB3-OB5-PB2-OB3
153	BM	301	CDL	CA2-OA2-PA1-OA3
153	BM	301	CDL	CA2-OA2-PA1-OA5
153	BM	301	CDL	CB3-OB5-PB2-OB2
153	BM	301	CDL	CB3-OB5-PB2-OB4
153	C4	401	CDL	CA2-OA2-PA1-OA3
153	C4	401	CDL	CA2-OA2-PA1-OA4
153	C4	401	CDL	CA2-OA2-PA1-OA5
153	C4	401	CDL	CA3-OA5-PA1-OA3
153	C4	401	CDL	CB2-OB2-PB2-OB5
153	N5	806	CDL	CA2-OA2-PA1-OA3
153	N5	806	CDL	CA2-OA2-PA1-OA5
153	N5	806	CDL	CA3-OA5-PA1-OA2
153	N5	806	CDL	CA3-OA5-PA1-OA3
153	N5	806	CDL	CB2-OB2-PB2-OB3
153	N6	302	CDL	CA2-OA2-PA1-OA3
153	N6	302	CDL	CA2-OA2-PA1-OA4
153	N6	302	CDL	CA2-OA2-PA1-OA5
153	N6	302	CDL	CA3-OA5-PA1-OA3
153	N6	302	CDL	CB2-OB2-PB2-OB4
153	N6	302	CDL	CB2-OB2-PB2-OB5
153	P1	402	CDL	CA2-OA2-PA1-OA3
153	P1	402	CDL	CA3-OA5-PA1-OA2
153	P1	402	CDL	CB2-OB2-PB2-OB3
153	P1	402	CDL	CB2-OB2-PB2-OB5
153	P1	402	CDL	CB3-OB5-PB2-OB2
153	P1	402	CDL	CB3-OB5-PB2-OB3
153	P1	402	CDL	CB3-OB5-PB2-OB4
153	P1	403	CDL	CA2-OA2-PA1-OA3
153	P1	403	CDL	CA2-OA2-PA1-OA4
153	P1	403	CDL	CA2-OA2-PA1-OA5
153	P1	403	CDL	CA3-OA5-PA1-OA2
153	P1	403	CDL	CA3-OA5-PA1-OA4
153	QB	601	CDL	CA2-OA2-PA1-OA3
153	QB	601	CDL	CA2-OA2-PA1-OA4
153	QB	601	CDL	CA2-OA2-PA1-OA5
153	QB	601	CDL	CB3-OB5-PB2-OB2
153	QC	503	CDL	CA3-OA5-PA1-OA2
153	QC	504	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
153	QC	504	CDL	CA3-OA5-PA1-OA3
153	QC	504	CDL	CB2-OB2-PB2-OB4
153	QC	504	CDL	CB2-OB2-PB2-OB5
153	QC	504	CDL	CB3-OB5-PB2-OB2
153	QC	504	CDL	CB3-OB5-PB2-OB4
153	QD	402	CDL	CA2-OA2-PA1-OA4
153	QD	402	CDL	CA2-OA2-PA1-OA5
153	QD	402	CDL	CA3-OA5-PA1-OA3
153	QD	402	CDL	CB2-OB2-PB2-OB3
153	QD	402	CDL	CB2-OB2-PB2-OB4
153	QD	402	CDL	CB3-OB5-PB2-OB3
153	QG	402	CDL	CA2-OA2-PA1-OA3
153	QG	402	CDL	CA2-OA2-PA1-OA4
153	QG	402	CDL	CA2-OA2-PA1-OA5
153	QG	402	CDL	CA3-OA5-PA1-OA3
153	QG	402	CDL	CA3-OA5-PA1-OA4
153	QG	402	CDL	CB2-OB2-PB2-OB3
153	QH	201	CDL	O1-C1-CB2-OB2
153	QH	201	CDL	CA2-OA2-PA1-OA3
153	QH	201	CDL	CA2-OA2-PA1-OA5
153	QH	201	CDL	CB2-OB2-PB2-OB3
153	QH	201	CDL	CB2-OB2-PB2-OB5
153	QH	201	CDL	CB3-OB5-PB2-OB3
153	QI	203	CDL	CA2-OA2-PA1-OA4
153	QI	203	CDL	CA2-OA2-PA1-OA5
153	QI	203	CDL	CA3-OA5-PA1-OA4
153	QI	203	CDL	CB2-OB2-PB2-OB4
153	QI	203	CDL	CB2-OB2-PB2-OB5
153	QI	203	CDL	CB3-OB5-PB2-OB3
153	Qc	504	CDL	CA2-OA2-PA1-OA3
153	Qc	504	CDL	CA2-OA2-PA1-OA5
153	Qc	504	CDL	CA3-OA5-PA1-OA2
153	Qc	504	CDL	CA3-OA5-PA1-OA3
153	Qc	504	CDL	CA3-OA5-PA1-OA4
153	Qc	504	CDL	CB2-OB2-PB2-OB5
153	Qc	504	CDL	CB3-OB5-PB2-OB2
153	Qc	504	CDL	CB3-OB5-PB2-OB3
153	Qc	504	CDL	CB3-OB5-PB2-OB4
153	Qc	505	CDL	CA2-OA2-PA1-OA3
153	Qc	505	CDL	CA2-OA2-PA1-OA5
153	Qc	505	CDL	CA3-OA5-PA1-OA2
153	Qc	505	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	Qc	505	CDL	CB2-OB2-PB2-OB3
153	Qc	505	CDL	CB2-OB2-PB2-OB4
153	Qc	505	CDL	CB2-OB2-PB2-OB5
153	Qc	505	CDL	CB3-OB5-PB2-OB2
153	Qc	505	CDL	CB3-OB5-PB2-OB3
153	Qc	505	CDL	CB3-OB5-PB2-OB4
153	Qc	508	CDL	CA2-OA2-PA1-OA3
153	Qg	402	CDL	CA2-OA2-PA1-OA4
153	Qg	402	CDL	CA3-OA5-PA1-OA2
153	Qg	402	CDL	CA3-OA5-PA1-OA4
153	Qg	402	CDL	CB3-OB5-PB2-OB2
153	Qi	202	CDL	CA3-OA5-PA1-OA2
153	Qi	202	CDL	CA3-OA5-PA1-OA3
153	Qi	202	CDL	CA3-OA5-PA1-OA4
153	Qi	202	CDL	CB2-OB2-PB2-OB5
153	T1	601	CDL	CA3-OA5-PA1-OA3
153	T1	601	CDL	CB3-OB5-PB2-OB2
153	T1	601	CDL	CB3-OB5-PB2-OB3
153	T1	601	CDL	CB3-OB5-PB2-OB4
153	T5	301	CDL	CA2-OA2-PA1-OA3
153	T5	301	CDL	CA2-OA2-PA1-OA4
153	T5	301	CDL	CA2-OA2-PA1-OA5
153	T5	301	CDL	CA3-OA5-PA1-OA2
153	T5	301	CDL	CA3-OA5-PA1-OA3
153	T5	301	CDL	CB2-OB2-PB2-OB3
153	T5	301	CDL	CB2-OB2-PB2-OB5
153	T5	301	CDL	CB3-OB5-PB2-OB3
153	T7	201	CDL	CA2-OA2-PA1-OA4
153	T7	201	CDL	CA2-OA2-PA1-OA5
153	T7	201	CDL	CA3-OA5-PA1-OA2
153	T7	201	CDL	CB2-OB2-PB2-OB3
153	T7	201	CDL	CB2-OB2-PB2-OB4
153	T7	201	CDL	CB2-OB2-PB2-OB5
153	TE	101	CDL	CA2-OA2-PA1-OA5
153	TE	101	CDL	CB2-OB2-PB2-OB3
153	TE	101	CDL	CB2-OB2-PB2-OB4
153	TE	101	CDL	CB3-OB5-PB2-OB2
153	TE	101	CDL	CB3-OB5-PB2-OB4
153	TH	200	CDL	CA2-OA2-PA1-OA4
153	TH	200	CDL	CA3-OA5-PA1-OA2
153	TH	200	CDL	CA3-OA5-PA1-OA3
153	TH	200	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
153	TH	200	CDL	CB2-OB2-PB2-OB4
153	TH	200	CDL	CB2-OB2-PB2-OB5
153	TH	200	CDL	CB3-OB5-PB2-OB2
153	C	301	CDL	CB3-OB5-PB2-OB3
153	C	301	CDL	CB3-OB5-PB2-OB4
153	c	301	CDL	CB3-OB5-PB2-OB3
153	c	301	CDL	CB3-OB5-PB2-OB4
153	u1	101	CDL	CA2-OA2-PA1-OA4
153	u1	101	CDL	CA2-OA2-PA1-OA5
153	u1	101	CDL	CA3-OA5-PA1-OA2
153	u1	101	CDL	CB3-OB5-PB2-OB2
153	u1	101	CDL	CB3-OB5-PB2-OB3
153	U1	101	CDL	CA2-OA2-PA1-OA4
153	U1	101	CDL	CA2-OA2-PA1-OA5
153	U1	101	CDL	CA3-OA5-PA1-OA2
153	U1	101	CDL	CB3-OB5-PB2-OB2
153	U1	101	CDL	CB3-OB5-PB2-OB3
154	c1	702	HEA	C1A-C2A-CAA-CBA
154	c1	702	HEA	C3A-C2A-CAA-CBA
154	c1	702	HEA	C2A-C3A-CMA-OMA
154	c1	702	HEA	C4A-C3A-CMA-OMA
154	c1	702	HEA	C21-C22-C23-C24
154	c1	708	HEA	C2A-C3A-CMA-OMA
154	c1	708	HEA	C4A-C3A-CMA-OMA
154	C1	702	HEA	C1A-C2A-CAA-CBA
154	C1	702	HEA	C3A-C2A-CAA-CBA
154	C1	702	HEA	C2A-C3A-CMA-OMA
154	C1	702	HEA	C4A-C3A-CMA-OMA
154	C1	702	HEA	C21-C22-C23-C24
154	C1	703	HEA	C2A-C3A-CMA-OMA
154	C1	703	HEA	C4A-C3A-CMA-OMA
158	i	303	3PE	C1-O11-P-O12
158	i	303	3PE	O13-C11-C12-N
158	m2	408	3PE	C1-O11-P-O12
158	m2	408	3PE	C1-O11-P-O14
158	m2	408	3PE	C11-O13-P-O11
158	m2	408	3PE	C11-O13-P-O14
158	m3	402	3PE	O13-C11-C12-N
158	sc	101	3PE	C1-O11-P-O12
158	sc	101	3PE	C1-O11-P-O13
158	sc	101	3PE	C1-O11-P-O14
158	sc	101	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
158	sc	101	3PE	C11-O13-P-O12
158	sc	101	3PE	C11-O13-P-O14
158	sc	101	3PE	O13-C11-C12-N
158	vb	705	3PE	C1-O11-P-O12
158	vb	705	3PE	C1-O11-P-O13
158	w	203	3PE	C1-O11-P-O12
158	w	203	3PE	O13-C11-C12-N
158	y5	202	3PE	C1-O11-P-O13
158	y5	202	3PE	C11-O13-P-O11
158	y5	202	3PE	O13-C11-C12-N
158	a3	201	3PE	C11-O13-P-O11
158	a3	201	3PE	C11-O13-P-O12
158	a3	202	3PE	C11-O13-P-O11
158	a3	202	3PE	C11-O13-P-O12
158	a3	202	3PE	C11-O13-P-O14
158	a3	202	3PE	O13-C11-C12-N
158	an	303	3PE	O13-C11-C12-N
158	an	305	3PE	C11-O13-P-O11
158	an	306	3PE	C1-O11-P-O12
158	an	306	3PE	C1-O11-P-O14
158	b4	202	3PE	C1-O11-P-O13
158	b4	202	3PE	C11-O13-P-O11
158	b4	202	3PE	C11-O13-P-O14
158	bm	302	3PE	C11-O13-P-O11
158	bm	302	3PE	C11-O13-P-O12
158	bm	302	3PE	O13-C11-C12-N
158	c4	402	3PE	C11-O13-P-O11
158	c4	402	3PE	C11-O13-P-O12
158	c4	402	3PE	C12-C11-O13-P
158	g2	301	3PE	C1-O11-P-O14
158	g2	301	3PE	O13-C11-C12-N
158	n4	601	3PE	C1-O11-P-O13
158	n4	601	3PE	C11-O13-P-O14
158	n5	802	3PE	C11-O13-P-O11
158	n5	802	3PE	C11-O13-P-O12
158	n5	802	3PE	C11-O13-P-O14
158	s8	304	3PE	C1-O11-P-O13
158	s8	304	3PE	C1-O11-P-O14
158	s8	304	3PE	C11-O13-P-O11
158	s8	304	3PE	O13-C11-C12-N
158	s8	304	3PE	O21-C2-C3-O31
158	t4	302	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
158	t4	302	3PE	C11-O13-P-O12
158	t4	302	3PE	C11-O13-P-O14
158	t4	302	3PE	O13-C11-C12-N
158	t8	601	3PE	C1-O11-P-O12
158	t8	601	3PE	C1-O11-P-O13
158	t8	601	3PE	O13-C11-C12-N
158	t8	602	3PE	C11-O13-P-O11
158	t8	602	3PE	C11-O13-P-O12
158	t8	602	3PE	O13-C11-C12-N
158	t8	602	3PE	O21-C2-C3-O31
158	ta	201	3PE	C1-O11-P-O12
158	ta	201	3PE	C1-O11-P-O13
158	ta	201	3PE	C1-O11-P-O14
158	ta	201	3PE	C11-O13-P-O14
158	ta	201	3PE	O13-C11-C12-N
158	I	304	3PE	C1-O11-P-O12
158	I	304	3PE	O13-C11-C12-N
158	M2	408	3PE	C1-O11-P-O12
158	M2	408	3PE	C1-O11-P-O14
158	M2	408	3PE	C11-O13-P-O11
158	M2	408	3PE	C11-O13-P-O14
158	M3	402	3PE	O13-C11-C12-N
158	SC	101	3PE	C1-O11-P-O12
158	SC	101	3PE	C1-O11-P-O13
158	SC	101	3PE	C1-O11-P-O14
158	SC	101	3PE	C11-O13-P-O11
158	SC	101	3PE	C11-O13-P-O12
158	SC	101	3PE	C11-O13-P-O14
158	VB	707	3PE	C1-O11-P-O12
158	VB	707	3PE	C1-O11-P-O13
158	W	203	3PE	C1-O11-P-O12
158	W	203	3PE	O13-C11-C12-N
158	Y5	202	3PE	C1-O11-P-O13
158	Y5	202	3PE	C11-O13-P-O11
158	Y5	202	3PE	O13-C11-C12-N
158	A3	201	3PE	C11-O13-P-O11
158	A3	201	3PE	C11-O13-P-O12
158	A3	202	3PE	C11-O13-P-O11
158	A3	202	3PE	C11-O13-P-O12
158	A3	202	3PE	C11-O13-P-O14
158	A3	202	3PE	O13-C11-C12-N
158	AN	303	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
158	AN	305	3PE	C11-O13-P-O11
158	AN	305	3PE	C11-O13-P-O12
158	AN	306	3PE	C1-O11-P-O12
158	AN	306	3PE	C1-O11-P-O14
158	B4	202	3PE	C1-O11-P-O13
158	B4	202	3PE	C11-O13-P-O11
158	B4	202	3PE	C11-O13-P-O14
158	BM	302	3PE	C11-O13-P-O11
158	BM	302	3PE	C11-O13-P-O12
158	BM	302	3PE	O13-C11-C12-N
158	C4	402	3PE	C11-O13-P-O11
158	C4	402	3PE	C11-O13-P-O12
158	C4	402	3PE	C12-C11-O13-P
158	G2	301	3PE	C1-O11-P-O14
158	G2	301	3PE	O13-C11-C12-N
158	N4	601	3PE	C1-O11-P-O13
158	N4	601	3PE	C11-O13-P-O14
158	N5	802	3PE	C11-O13-P-O11
158	N5	802	3PE	C11-O13-P-O12
158	N5	802	3PE	C11-O13-P-O14
158	S8	304	3PE	C1-O11-P-O13
158	S8	304	3PE	C1-O11-P-O14
158	S8	304	3PE	C11-O13-P-O11
158	S8	304	3PE	O13-C11-C12-N
158	S8	304	3PE	O21-C2-C3-O31
158	T4	302	3PE	C11-O13-P-O11
158	T4	302	3PE	C11-O13-P-O12
158	T4	302	3PE	C11-O13-P-O14
158	T4	302	3PE	O13-C11-C12-N
158	T8	601	3PE	C1-O11-P-O12
158	T8	601	3PE	C1-O11-P-O13
158	T8	601	3PE	O13-C11-C12-N
158	T8	602	3PE	C11-O13-P-O11
158	T8	602	3PE	C11-O13-P-O12
158	T8	602	3PE	O13-C11-C12-N
158	T8	602	3PE	O21-C2-C3-O31
158	TA	201	3PE	C1-O11-P-O12
158	TA	201	3PE	C1-O11-P-O13
158	TA	201	3PE	C1-O11-P-O14
158	TA	201	3PE	C11-O13-P-O11
158	TA	201	3PE	C11-O13-P-O14
158	TA	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
159	m2	406	P5S	O-C-CA-CB
159	m2	406	P5S	OXT-C-CA-CB
159	m2	406	P5S	O19-C1-C2-O37
159	m2	406	P5S	C-CA-CB-OG
159	m2	406	P5S	N-CA-CB-OG
159	m2	406	P5S	CA-CB-OG-P12
159	m2	406	P5S	CB-OG-P12-O16
159	m2	406	P5S	C3-O16-P12-OG
159	m2	406	P5S	C3-O16-P12-O13
159	m2	406	P5S	C3-O16-P12-O15
159	M2	406	P5S	O-C-CA-CB
159	M2	406	P5S	OXT-C-CA-CB
159	M2	406	P5S	O19-C1-C2-O37
159	M2	406	P5S	C-CA-CB-OG
159	M2	406	P5S	N-CA-CB-OG
159	M2	406	P5S	CA-CB-OG-P12
159	M2	406	P5S	CB-OG-P12-O16
159	M2	406	P5S	C3-O16-P12-OG
159	M2	406	P5S	C3-O16-P12-O13
159	M2	406	P5S	C3-O16-P12-O15
160	r	202	PX2	C1-O4-P1-O1
160	r	202	PX2	C1-O4-P1-O3
160	y5	204	PX2	C1-O4-P1-O1
160	y5	204	PX2	C1-O4-P1-O2
160	y5	204	PX2	C1-O4-P1-O3
160	y5	204	PX2	O8-C16-O7-C2
160	y5	204	PX2	C17-C16-O7-C2
160	qh	201	PX2	C1-O4-P1-O1
160	qh	201	PX2	C1-O4-P1-O2
160	qh	201	PX2	C1-O4-P1-O3
160	R	202	PX2	C1-O4-P1-O1
160	R	202	PX2	C1-O4-P1-O2
160	R	202	PX2	C1-O4-P1-O3
160	Y5	204	PX2	C1-O4-P1-O1
160	Y5	204	PX2	C1-O4-P1-O2
160	Y5	204	PX2	C1-O4-P1-O3
160	Y5	204	PX2	C17-C16-O7-C2
160	Qh	201	PX2	C1-O4-P1-O1
160	Qh	201	PX2	C1-O4-P1-O2
160	Qh	201	PX2	C1-O4-P1-O3
160	Qh	201	PX2	O8-C16-O7-C2
160	Qh	201	PX2	C17-C16-O7-C2

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Mol	Chain	Res	Type	Atoms
161	sa	701	FAD	C5B-O5B-PA-O2A
161	sa	701	FAD	C2'-C3'-C4'-O4'
161	sa	701	FAD	O3'-C3'-C4'-O4'
161	SA	701	FAD	C5B-O5B-PA-O2A
161	SA	701	FAD	C2'-C3'-C4'-O4'
161	SA	701	FAD	O3'-C3'-C4'-O4'
164	sc	102	U10	C9-C11-C12-C13
164	sc	102	U10	C19-C21-C22-C23
164	sc	102	U10	C33-C34-C36-C37
164	sc	102	U10	C35-C34-C36-C37
164	qc	501	U10	C12-C11-C9-C8
164	qc	501	U10	C12-C11-C9-C10
164	qc	501	U10	C23-C24-C26-C27
164	qc	507	U10	C18-C19-C21-C22
164	qc	507	U10	C20-C19-C21-C22
164	SC	102	U10	C9-C11-C12-C13
164	SC	102	U10	C19-C21-C22-C23
164	SC	102	U10	C33-C34-C36-C37
164	SC	102	U10	C35-C34-C36-C37
164	Qc	501	U10	C12-C11-C9-C10
164	Qc	501	U10	C23-C24-C26-C27
164	Qc	507	U10	C18-C19-C21-C22
164	Qc	507	U10	C20-C19-C21-C22
166	y5	203	HEM	C2B-C3B-CAB-CBB
166	qC	501	HEM	C2C-C3C-CAC-CBC
166	qc	503	HEM	C2C-C3C-CAC-CBC
166	Y5	203	HEM	C2B-C3B-CAB-CBB
166	QC	501	HEM	C2C-C3C-CAC-CBC
166	Qc	503	HEM	C2C-C3C-CAC-CBC
168	ab	201	ZMP	C16-C17-C18-C21
168	ab	201	ZMP	C16-C17-C18-C19
168	ab	201	ZMP	C16-C17-C18-C20
168	ab	201	ZMP	C17-C16-N2-C15
168	ab	201	ZMP	C12-C11-S1-C10
168	ab	201	ZMP	C7-C8-C9-C10
168	AB	201	ZMP	C16-C17-C18-C21
168	AB	201	ZMP	C16-C17-C18-C19
168	AB	201	ZMP	C16-C17-C18-C20
168	AB	201	ZMP	C17-C16-N2-C15
168	AB	201	ZMP	C12-C11-S1-C10
168	AB	201	ZMP	C7-C8-C9-C10
169	b6	201	T7X	C7-O13-P1-O11

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Mol	Chain	Res	Type	Atoms
169	b6	201	T7X	C12-C10-O16-C8
169	b6	201	T7X	O17-C10-O16-C8
169	b6	201	T7X	C16-C17-C18-C19
169	B6	201	T7X	C7-O13-P1-O11
169	B6	201	T7X	C12-C10-O16-C8
169	B6	201	T7X	O17-C10-O16-C8
169	B6	201	T7X	C16-C17-C18-C19
170	b9	202	ADP	O4'-C4'-C5'-O5'
170	B9	202	ADP	O4'-C4'-C5'-O5'
154	c1	702	HEA	C21-C22-C23-C25
154	C1	702	HEA	C21-C22-C23-C25
160	Y5	204	PX2	O8-C16-O7-C2
164	sc	102	U10	C12-C11-C9-C10
164	sc	102	U10	C15-C14-C16-C17
164	b8	301	U10	C15-C14-C16-C17
164	SC	102	U10	C12-C11-C9-C10
164	SC	102	U10	C15-C14-C16-C17
164	B8	301	U10	C15-C14-C16-C17
164	sc	102	U10	C13-C14-C16-C17
164	b8	301	U10	C13-C14-C16-C17
164	SC	102	U10	C13-C14-C16-C17
164	B8	301	U10	C13-C14-C16-C17
164	Qc	501	U10	C12-C11-C9-C8
168	ab	201	ZMP	C14-C13-N1-C12
168	AB	201	ZMP	C14-C13-N1-C12
153	6c	201	CDL	O1-C1-CA2-OA2
153	a	505	CDL	O1-C1-CA2-OA2
153	b3	102	CDL	O1-C1-CA2-OA2
153	qg	402	CDL	O1-C1-CB2-OB2
153	6C	202	CDL	O1-C1-CA2-OA2
153	VB	705	CDL	O1-C1-CA2-OA2
153	Qg	402	CDL	O1-C1-CB2-OB2
168	ab	201	ZMP	O3-C16-N2-C15
168	AB	201	ZMP	O3-C16-N2-C15
154	c1	702	HEA	C27-C19-C20-C21
154	c1	708	HEA	C27-C19-C20-C21
154	C1	702	HEA	C27-C19-C20-C21
154	C1	703	HEA	C27-C19-C20-C21
164	b8	301	U10	C35-C34-C36-C37
164	B8	301	U10	C35-C34-C36-C37
154	c1	708	HEA	C18-C19-C20-C21
154	C1	703	HEA	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
164	b8	301	U10	C33-C34-C36-C37
164	B8	301	U10	C33-C34-C36-C37
161	sa	701	FAD	O3'-C3'-C4'-C5'
161	SA	701	FAD	O3'-C3'-C4'-C5'
154	c1	702	HEA	C15-C16-C17-C18
154	c1	702	HEA	C19-C20-C21-C22
154	c1	708	HEA	C15-C16-C17-C18
154	c1	708	HEA	C19-C20-C21-C22
154	C1	702	HEA	C15-C16-C17-C18
154	C1	702	HEA	C19-C20-C21-C22
154	C1	703	HEA	C15-C16-C17-C18
154	C1	703	HEA	C19-C20-C21-C22
164	b8	301	U10	C9-C11-C12-C13
164	b8	301	U10	C19-C21-C22-C23
164	b8	301	U10	C24-C26-C27-C28
164	b8	301	U10	C29-C31-C32-C33
164	b8	301	U10	C44-C46-C47-C48
164	b8	301	U10	C49-C51-C52-C53
164	qc	501	U10	C14-C16-C17-C18
164	qc	501	U10	C19-C21-C22-C23
164	qc	507	U10	C9-C11-C12-C13
164	B8	301	U10	C9-C11-C12-C13
164	B8	301	U10	C19-C21-C22-C23
164	B8	301	U10	C24-C26-C27-C28
164	B8	301	U10	C29-C31-C32-C33
164	B8	301	U10	C44-C46-C47-C48
164	B8	301	U10	C49-C51-C52-C53
164	Qc	501	U10	C14-C16-C17-C18
164	Qc	501	U10	C19-C21-C22-C23
164	Qc	507	U10	C9-C11-C12-C13
161	sa	701	FAD	C2'-C3'-C4'-C5'
161	SA	701	FAD	C2'-C3'-C4'-C5'
152	qi	203	PC1	C2-C1-O11-P
152	Qi	203	PC1	C2-C1-O11-P
153	qD	402	CDL	CA4-CA3-OA5-PA1
153	QD	402	CDL	CA4-CA3-OA5-PA1
166	qC	501	HEM	C3D-CAD-CBD-CGD
166	qC	502	HEM	C3D-CAD-CBD-CGD
166	QC	501	HEM	C3D-CAD-CBD-CGD
166	QC	502	HEM	C3D-CAD-CBD-CGD
159	m2	406	P5S	C41-C42-C43-C44
159	M2	406	P5S	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
168	ab	201	ZMP	O2-C13-N1-C12
168	AB	201	ZMP	O2-C13-N1-C12
159	m2	406	P5S	C23-C24-C25-C26
159	M2	406	P5S	C23-C24-C25-C26
153	2g	201	CDL	CA2-C1-CB2-OB2
153	6c	201	CDL	CB2-C1-CA2-OA2
153	t	203	CDL	CA2-C1-CB2-OB2
153	qg	402	CDL	CA2-C1-CB2-OB2
153	2G	201	CDL	CA2-C1-CB2-OB2
153	6C	202	CDL	CB2-C1-CA2-OA2
153	T	203	CDL	CA2-C1-CB2-OB2
153	Qg	402	CDL	CA2-C1-CB2-OB2
160	r	202	PX2	C5-C4-O5-C3
160	Qh	201	PX2	C5-C4-O5-C3
152	2f	303	PC1	C11-C12-N-C15
152	7a	202	PC1	C11-C12-N-C15
152	c2	703	PC1	C11-C12-N-C13
152	c3	603	PC1	C11-C12-N-C13
152	c3	605	PC1	C11-C12-N-C13
152	fs	204	PC1	C11-C12-N-C13
152	n	301	PC1	C11-C12-N-C15
152	5b	202	PC1	C11-C12-N-C13
152	qB	602	PC1	C11-C12-N-C15
152	qb	602	PC1	C11-C12-N-C15
152	qj	101	PC1	C11-C12-N-C15
152	2F	303	PC1	C11-C12-N-C15
152	7A	202	PC1	C11-C12-N-C15
152	C2	701	PC1	C11-C12-N-C13
152	C3	603	PC1	C11-C12-N-C13
152	C3	605	PC1	C11-C12-N-C13
152	FS	201	PC1	C11-C12-N-C13
152	N	301	PC1	C11-C12-N-C15
152	5B	202	PC1	C11-C12-N-C13
152	QB	602	PC1	C11-C12-N-C15
152	QC	508	PC1	C11-C12-N-C13
152	Qb	602	PC1	C11-C12-N-C15
152	Qj	101	PC1	C11-C12-N-C15
154	c1	702	HEA	C18-C19-C20-C21
154	C1	702	HEA	C18-C19-C20-C21
164	sc	102	U10	C12-C11-C9-C8
164	SC	102	U10	C12-C11-C9-C8
153	c1	712	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
153	C1	712	CDL	CB5-C51-C52-C53
153	2g	201	CDL	O1-C1-CB2-OB2
153	b3	101	CDL	O1-C1-CB2-OB2
153	2G	201	CDL	O1-C1-CB2-OB2
160	Qh	201	PX2	O6-C4-O5-C3
153	C1	708	CDL	CA7-C31-C32-C33
160	r	202	PX2	O6-C4-O5-C3
153	a	505	CDL	OB5-CB3-CB4-OB6
153	al	301	CDL	OB5-CB3-CB4-OB6
153	VB	705	CDL	OB5-CB3-CB4-OB6
153	AL	301	CDL	OB5-CB3-CB4-OB6
153	t7	201	CDL	CB7-C71-C72-C73
153	FS	204	CDL	CB7-C71-C72-C73
153	T7	201	CDL	CB7-C71-C72-C73
159	m2	406	P5S	C17-C20-C21-C22
159	M2	406	P5S	C17-C20-C21-C22
161	sa	701	FAD	O4B-C4B-C5B-O5B
161	sa	701	FAD	C3B-C4B-C5B-O5B
161	SA	701	FAD	O4B-C4B-C5B-O5B
161	SA	701	FAD	C3B-C4B-C5B-O5B
170	b9	202	ADP	C3'-C4'-C5'-O5'
170	B9	202	ADP	C3'-C4'-C5'-O5'
164	Qc	501	U10	C15-C14-C16-C17
152	n	303	PC1	C31-C32-C33-C34
152	w	204	PC1	C31-C32-C33-C34
152	qC	507	PC1	C21-C22-C23-C24
152	W	204	PC1	C31-C32-C33-C34
152	QC	507	PC1	C21-C22-C23-C24
152	c2	703	PC1	C11-C12-N-C14
152	c3	603	PC1	C11-C12-N-C15
152	fs	204	PC1	C11-C12-N-C14
152	m2	402	PC1	C11-C12-N-C15
152	n	301	PC1	C11-C12-N-C14
152	w	205	PC1	C11-C12-N-C13
152	an	304	PC1	C11-C12-N-C14
152	j1	400	PC1	C11-C12-N-C15
152	qB	602	PC1	C11-C12-N-C13
152	qC	508	PC1	C11-C12-N-C13
152	qj	101	PC1	C11-C12-N-C13
152	C2	701	PC1	C11-C12-N-C14
152	C3	603	PC1	C11-C12-N-C15
152	FS	201	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
152	M2	402	PC1	C11-C12-N-C15
152	N	301	PC1	C11-C12-N-C14
152	W	205	PC1	C11-C12-N-C13
152	AN	304	PC1	C11-C12-N-C14
152	J1	400	PC1	C11-C12-N-C15
152	QB	602	PC1	C11-C12-N-C13
152	Qj	101	PC1	C11-C12-N-C13
152	qI	202	PC1	C31-C32-C33-C34
152	N	303	PC1	C31-C32-C33-C34
152	QI	202	PC1	C31-C32-C33-C34
153	2g	201	CDL	CA5-C11-C12-C13
153	7c	301	CDL	CA5-C11-C12-C13
153	fs	203	CDL	CB7-C71-C72-C73
153	n6	302	CDL	CA5-C11-C12-C13
153	te	101	CDL	CB5-C51-C52-C53
153	2G	201	CDL	CA5-C11-C12-C13
153	7C	301	CDL	CA5-C11-C12-C13
153	2B	201	CDL	CB7-C71-C72-C73
153	N6	302	CDL	CA5-C11-C12-C13
153	TE	101	CDL	CB5-C51-C52-C53
160	R	202	PX2	C16-C17-C18-C19
152	6c	203	PC1	C21-C22-C23-C24
152	c3	602	PC1	C21-C22-C23-C24
152	t4	303	PC1	C21-C22-C23-C24
152	6C	201	PC1	C21-C22-C23-C24
152	C3	602	PC1	C21-C22-C23-C24
152	T4	303	PC1	C21-C22-C23-C24
153	7a	203	CDL	CA7-C31-C32-C33
153	c1	709	CDL	CA7-C31-C32-C33
153	t	204	CDL	CA5-C11-C12-C13
153	2b	201	CDL	CB7-C71-C72-C73
153	7A	203	CDL	CA7-C31-C32-C33
153	T	204	CDL	CA5-C11-C12-C13
169	b6	201	T7X	C10-C12-C13-C14
169	B6	201	T7X	C10-C12-C13-C14
160	Qh	201	PX2	C7-C8-C9-C10
153	e	402	CDL	O1-C1-CA2-OA2
153	E	402	CDL	O1-C1-CA2-OA2
153	B3	101	CDL	O1-C1-CB2-OB2
153	e	403	CDL	CB7-C71-C72-C73
153	qc	505	CDL	CA7-C31-C32-C33
153	E	403	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
153	Qc	505	CDL	CA7-C31-C32-C33
160	qh	201	PX2	C16-C17-C18-C19
160	Y5	204	PX2	C16-C17-C18-C19
160	Qh	201	PX2	C16-C17-C18-C19
154	c1	702	HEA	C17-C18-C19-C27
154	C1	702	HEA	C17-C18-C19-C27
160	y5	204	PX2	C16-C17-C18-C19
160	R	202	PX2	C4-C5-C6-C7
160	qh	201	PX2	C5-C4-O5-C3
160	R	202	PX2	C5-C4-O5-C3
153	th	200	CDL	CA5-C11-C12-C13
153	TH	200	CDL	CA5-C11-C12-C13
153	qb	601	CDL	CB5-C51-C52-C53
153	Qb	601	CDL	CB5-C51-C52-C53
153	qH	201	CDL	CA2-C1-CB2-OB2
153	QH	201	CDL	CA2-C1-CB2-OB2
152	qC	507	PC1	C33-C34-C35-C36
152	QC	507	PC1	C33-C34-C35-C36
160	Qh	201	PX2	C11-C12-C13-C14
152	2f	303	PC1	C11-C12-N-C13
152	6a	202	PC1	C11-C12-N-C13
152	6a	202	PC1	C11-C12-N-C14
152	6a	202	PC1	C11-C12-N-C15
152	7a	202	PC1	C11-C12-N-C13
152	7a	202	PC1	C11-C12-N-C14
152	c3	602	PC1	C11-C12-N-C15
152	c3	605	PC1	C11-C12-N-C14
152	m	307	PC1	C11-C12-N-C13
152	w	205	PC1	C11-C12-N-C14
152	n6	301	PC1	C11-C12-N-C15
152	qC	507	PC1	C11-C12-N-C13
152	qC	508	PC1	C11-C12-N-C15
152	qb	602	PC1	C11-C12-N-C13
152	qe	303	PC1	C11-C12-N-C14
152	qi	201	PC1	C11-C12-N-C14
152	2F	303	PC1	C11-C12-N-C13
152	6A	202	PC1	C11-C12-N-C13
152	6A	202	PC1	C11-C12-N-C14
152	7A	202	PC1	C11-C12-N-C13
152	C3	602	PC1	C11-C12-N-C15
152	C3	605	PC1	C11-C12-N-C14
152	M	302	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
152	W	205	PC1	C11-C12-N-C14
152	N6	301	PC1	C11-C12-N-C15
152	QC	507	PC1	C11-C12-N-C13
152	QC	508	PC1	C11-C12-N-C15
152	Qb	602	PC1	C11-C12-N-C13
152	Qe	303	PC1	C11-C12-N-C14
152	Qi	201	PC1	C11-C12-N-C14
153	qH	201	CDL	C12-C13-C14-C15
153	y5	201	CDL	CB7-C71-C72-C73
153	Y5	201	CDL	CB7-C71-C72-C73
164	qc	501	U10	C15-C14-C16-C17
153	QH	201	CDL	C12-C13-C14-C15
160	r	202	PX2	C17-C16-O7-C2
160	r	202	PX2	O8-C16-O7-C2
152	n3	201	PC1	C31-C32-C33-C34
153	m2	404	CDL	O1-C1-CB2-OB2
153	M2	404	CDL	O1-C1-CB2-OB2
152	7c	303	PC1	C31-C32-C33-C34
152	7C	303	PC1	C31-C32-C33-C34
152	N3	201	PC1	C31-C32-C33-C34
151	2e	401	HEC	C4D-C3D-CAD-CBD
151	2E	401	HEC	C4D-C3D-CAD-CBD
153	7a	203	CDL	CB4-CB3-OB5-PB2
153	m1	405	CDL	C1-CA2-OA2-PA1
153	b3	101	CDL	C1-CB2-OB2-PB2
153	7A	203	CDL	CB4-CB3-OB5-PB2
153	M1	405	CDL	C1-CA2-OA2-PA1
153	B3	101	CDL	C1-CB2-OB2-PB2
158	ta	201	3PE	C2-C1-O11-P
158	TA	201	3PE	C2-C1-O11-P
153	td	101	CDL	C14-C15-C16-C17
153	A1	101	CDL	C14-C15-C16-C17
168	ab	201	ZMP	C4-C5-C6-C7
168	AB	201	ZMP	C4-C5-C6-C7
152	qC	507	PC1	C38-C39-C3A-C3B
152	QC	507	PC1	C38-C39-C3A-C3B
152	c2	703	PC1	C11-C12-N-C15
152	5b	202	PC1	C11-C12-N-C14
152	5b	202	PC1	C11-C12-N-C15
152	n5	801	PC1	C11-C12-N-C13
152	qC	507	PC1	C11-C12-N-C14
152	qC	507	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
152	6A	202	PC1	C11-C12-N-C15
152	7A	202	PC1	C11-C12-N-C14
152	C2	701	PC1	C11-C12-N-C15
152	M2	402	PC1	C11-C12-N-C14
152	5B	202	PC1	C11-C12-N-C14
152	5B	202	PC1	C11-C12-N-C15
152	N5	801	PC1	C11-C12-N-C13
152	QC	507	PC1	C11-C12-N-C14
152	QC	507	PC1	C11-C12-N-C15
153	vb	701	CDL	CA5-C11-C12-C13
153	VB	701	CDL	CA5-C11-C12-C13
160	R	202	PX2	O6-C4-O5-C3
152	c1	711	PC1	C33-C34-C35-C36
153	m	302	CDL	C31-C32-C33-C34
153	c4	401	CDL	C78-C79-C80-C81
153	C4	401	CDL	C78-C79-C80-C81
152	C1	711	PC1	C33-C34-C35-C36
152	Qi	203	PC1	C24-C25-C26-C27
153	M	304	CDL	C31-C32-C33-C34
152	t4	303	PC1	C37-C38-C39-C3A
152	qi	203	PC1	C24-C25-C26-C27
152	T4	303	PC1	C37-C38-C39-C3A
153	e	402	CDL	C57-C58-C59-C60
153	N	304	CDL	C74-C75-C76-C77
153	VB	703	CDL	C13-C14-C15-C16
169	B6	201	T7X	C39-C40-C41-C42
153	n	304	CDL	C74-C75-C76-C77
153	q	203	CDL	C13-C14-C15-C16
160	qh	201	PX2	C21-C22-C23-C24
169	b6	201	T7X	C39-C40-C41-C42
152	i	304	PC1	C21-C22-C23-C24
152	I	301	PC1	C21-C22-C23-C24
153	a	505	CDL	CB7-C71-C72-C73
153	n	304	CDL	CA5-C11-C12-C13
153	an	302	CDL	CB5-C51-C52-C53
153	VB	705	CDL	CB7-C71-C72-C73
153	AN	302	CDL	CB5-C51-C52-C53
152	c1	704	PC1	C3B-C3C-C3D-C3E
152	C1	706	PC1	C3B-C3C-C3D-C3E
153	w	202	CDL	C62-C63-C64-C65
153	W	202	CDL	C62-C63-C64-C65
158	m3	402	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
158	a3	201	3PE	C34-C35-C36-C37
158	M3	402	3PE	C27-C28-C29-C2A
158	A3	201	3PE	C34-C35-C36-C37
153	C1	701	CDL	CA5-C11-C12-C13
153	N	304	CDL	CA5-C11-C12-C13
153	E	402	CDL	C57-C58-C59-C60
160	Qh	201	PX2	C21-C22-C23-C24
160	qh	201	PX2	O6-C4-O5-C3
152	c3	606	PC1	C22-C23-C24-C25
153	c1	701	CDL	CA5-C11-C12-C13
152	M2	405	PC1	C22-C23-C24-C25
153	m1	404	CDL	C54-C55-C56-C57
153	M1	404	CDL	C54-C55-C56-C57
153	P1	402	CDL	C53-C54-C55-C56
153	Qc	504	CDL	C54-C55-C56-C57
159	m2	406	P5S	C21-C22-C23-C24
159	M2	406	P5S	C21-C22-C23-C24
169	B6	201	T7X	C34-C35-C36-C37
152	C3	606	PC1	C22-C23-C24-C25
153	w	202	CDL	C58-C59-C60-C61
153	W	202	CDL	C58-C59-C60-C61
160	qh	201	PX2	C11-C12-C13-C14
169	b6	201	T7X	C34-C35-C36-C37
153	2G	203	CDL	CB3-CB4-CB6-OB8
153	B3	102	CDL	CA3-CA4-CA6-OA8
152	m2	405	PC1	C22-C23-C24-C25
153	p1	402	CDL	C53-C54-C55-C56
153	qc	504	CDL	C54-C55-C56-C57
153	td	101	CDL	C17-C18-C19-C20
153	a9	402	CDL	C77-C78-C79-C80
153	a9	403	CDL	C18-C19-C20-C21
153	A1	101	CDL	C17-C18-C19-C20
153	A9	402	CDL	C77-C78-C79-C80
153	A9	403	CDL	C18-C19-C20-C21
158	AN	303	3PE	C32-C33-C34-C35
160	r	202	PX2	C21-C22-C23-C24
158	an	303	3PE	C32-C33-C34-C35
158	g2	301	3PE	C2E-C2F-C2G-C2H
152	M	302	PC1	C22-C23-C24-C25
153	7c	301	CDL	C78-C79-C80-C81
153	7C	301	CDL	C78-C79-C80-C81
152	2f	303	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
152	a	503	PC1	C11-C12-N-C15
152	c3	602	PC1	C11-C12-N-C13
152	c3	603	PC1	C11-C12-N-C14
152	c3	605	PC1	C11-C12-N-C15
152	fs	204	PC1	C11-C12-N-C15
152	m	307	PC1	C11-C12-N-C14
152	m1	401	PC1	C11-C12-N-C15
152	m2	402	PC1	C11-C12-N-C14
152	n	301	PC1	C11-C12-N-C13
152	w	201	PC1	C11-C12-N-C13
152	an	304	PC1	C11-C12-N-C15
152	j1	400	PC1	C11-C12-N-C13
152	j1	400	PC1	C11-C12-N-C14
152	qB	602	PC1	C11-C12-N-C14
152	qC	505	PC1	C11-C12-N-C14
152	qe	303	PC1	C11-C12-N-C13
152	qi	201	PC1	C11-C12-N-C15
152	qj	101	PC1	C11-C12-N-C14
152	2F	303	PC1	C11-C12-N-C14
152	A	503	PC1	C11-C12-N-C15
152	C3	602	PC1	C11-C12-N-C13
152	C3	603	PC1	C11-C12-N-C14
152	C3	605	PC1	C11-C12-N-C15
152	FS	201	PC1	C11-C12-N-C15
152	M	302	PC1	C11-C12-N-C14
152	M1	401	PC1	C11-C12-N-C15
152	N	301	PC1	C11-C12-N-C13
152	W	201	PC1	C11-C12-N-C13
152	AN	304	PC1	C11-C12-N-C13
152	AN	304	PC1	C11-C12-N-C15
152	J1	400	PC1	C11-C12-N-C13
152	J1	400	PC1	C11-C12-N-C14
152	QB	602	PC1	C11-C12-N-C14
152	QC	505	PC1	C11-C12-N-C14
152	Qe	303	PC1	C11-C12-N-C13
152	Qi	201	PC1	C11-C12-N-C15
152	Qj	101	PC1	C11-C12-N-C14
152	m	307	PC1	C22-C23-C24-C25
158	G2	301	3PE	C2E-C2F-C2G-C2H
160	R	202	PX2	C5-C6-C7-C8
168	AB	201	ZMP	C3-C4-C5-C6
152	n6	301	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
152	N6	301	PC1	C38-C39-C3A-C3B
153	m2	403	CDL	C11-C12-C13-C14
153	M2	403	CDL	C11-C12-C13-C14
153	N5	806	CDL	C61-C62-C63-C64
168	ab	201	ZMP	C3-C4-C5-C6
160	y5	204	PX2	C5-C4-O5-C3
152	qi	203	PC1	C23-C24-C25-C26
152	Qi	203	PC1	C23-C24-C25-C26
153	n5	806	CDL	C61-C62-C63-C64
160	Qh	201	PX2	C5-C6-C7-C8
151	2E	401	HEC	C3D-CAD-CBD-CGD
153	c1	703	CDL	C53-C54-C55-C56
153	C1	707	CDL	C53-C54-C55-C56
152	tc	101	PC1	C25-C26-C27-C28
153	2k	101	CDL	C56-C57-C58-C59
152	p1	401	PC1	C32-C33-C34-C35
152	TC	101	PC1	C25-C26-C27-C28
153	2K	101	CDL	C56-C57-C58-C59
160	r	202	PX2	C5-C6-C7-C8
164	Qc	501	U10	C13-C14-C16-C17
152	qc	509	PC1	C37-C38-C39-C3A
152	P1	401	PC1	C32-C33-C34-C35
153	t5	301	CDL	C15-C16-C17-C18
153	T5	301	CDL	C15-C16-C17-C18
152	Qc	509	PC1	C37-C38-C39-C3A
153	N5	806	CDL	C57-C58-C59-C60
153	f	401	CDL	C39-C40-C41-C42
153	n5	806	CDL	C57-C58-C59-C60
153	t5	301	CDL	C38-C39-C40-C41
153	F	402	CDL	C39-C40-C41-C42
153	Q	202	CDL	C11-C12-C13-C14
153	T5	301	CDL	C38-C39-C40-C41
158	m3	402	3PE	C21-C22-C23-C24
153	C1	712	CDL	C76-C77-C78-C79
152	qc	506	PC1	C34-C35-C36-C37
153	qC	503	CDL	C75-C76-C77-C78
153	QC	503	CDL	C75-C76-C77-C78
159	m2	406	P5S	C39-C38-O37-C2
159	M2	406	P5S	C39-C38-O37-C2
160	R	202	PX2	C17-C16-O7-C2
159	m2	406	P5S	C38-C39-C40-C41
159	M2	406	P5S	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
168	ab	201	ZMP	C22-C23-C24-C25
168	AB	201	ZMP	C22-C23-C24-C25
160	R	202	PX2	O8-C16-O7-C2
153	c1	712	CDL	C76-C77-C78-C79
153	c3	604	CDL	C54-C55-C56-C57
153	q	202	CDL	C11-C12-C13-C14
153	C3	604	CDL	C54-C55-C56-C57
152	Qc	506	PC1	C34-C35-C36-C37
153	B3	102	CDL	C14-C15-C16-C17
152	2f	301	PC1	C31-C32-C33-C34
152	2F	301	PC1	C31-C32-C33-C34
153	p1	402	CDL	CA5-C11-C12-C13
153	P1	402	CDL	CA5-C11-C12-C13
158	M3	402	3PE	C21-C22-C23-C24
153	b3	102	CDL	C14-C15-C16-C17
153	te	101	CDL	C52-C53-C54-C55
153	2K	101	CDL	C74-C75-C76-C77
153	m	303	CDL	C54-C55-C56-C57
166	y5	203	HEM	C2C-C3C-CAC-CBC
166	qC	502	HEM	C2B-C3B-CAB-CBB
166	qc	502	HEM	C2C-C3C-CAC-CBC
166	qc	503	HEM	C2B-C3B-CAB-CBB
166	Y5	203	HEM	C2C-C3C-CAC-CBC
166	QC	502	HEM	C2B-C3B-CAB-CBB
166	QC	502	HEM	C2C-C3C-CAC-CBC
166	Qc	502	HEM	C2C-C3C-CAC-CBC
166	Qc	503	HEM	C2B-C3B-CAB-CBB
152	a	501	PC1	C11-C12-N-C13
152	c1	707	PC1	C11-C12-N-C14
152	c3	602	PC1	C11-C12-N-C14
152	m	307	PC1	C11-C12-N-C15
152	m2	402	PC1	C11-C12-N-C13
152	n	302	PC1	C11-C12-N-C14
152	w	201	PC1	C11-C12-N-C15
152	w	205	PC1	C11-C12-N-C15
152	an	304	PC1	C11-C12-N-C13
152	n5	801	PC1	C11-C12-N-C15
152	n6	301	PC1	C11-C12-N-C13
152	n6	301	PC1	C11-C12-N-C14
152	qC	508	PC1	C11-C12-N-C14
152	qb	602	PC1	C11-C12-N-C14
152	qe	301	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
152	qe	303	PC1	C11-C12-N-C15
152	qi	201	PC1	C11-C12-N-C13
152	t1	602	PC1	C11-C12-N-C13
152	2G	202	PC1	C11-C12-N-C13
152	A	501	PC1	C11-C12-N-C13
152	C1	710	PC1	C11-C12-N-C14
152	C3	602	PC1	C11-C12-N-C14
152	M	302	PC1	C11-C12-N-C15
152	M2	402	PC1	C11-C12-N-C13
152	N	302	PC1	C11-C12-N-C14
152	W	201	PC1	C11-C12-N-C15
152	W	205	PC1	C11-C12-N-C15
152	N5	801	PC1	C11-C12-N-C15
152	N6	301	PC1	C11-C12-N-C13
152	N6	301	PC1	C11-C12-N-C14
152	QC	505	PC1	C11-C12-N-C15
152	QC	508	PC1	C11-C12-N-C14
152	Qb	602	PC1	C11-C12-N-C14
152	Qe	301	PC1	C11-C12-N-C14
152	Qe	303	PC1	C11-C12-N-C15
152	Qi	201	PC1	C11-C12-N-C13
152	T1	602	PC1	C11-C12-N-C13
153	2k	101	CDL	C74-C75-C76-C77
152	6a	202	PC1	C24-C25-C26-C27
152	6A	202	PC1	C24-C25-C26-C27
152	m1	401	PC1	C24-C25-C26-C27
152	M1	401	PC1	C24-C25-C26-C27
153	m	302	CDL	C52-C53-C54-C55
153	C1	701	CDL	C73-C74-C75-C76
153	M	304	CDL	C52-C53-C54-C55
153	c1	701	CDL	C73-C74-C75-C76
159	M2	406	P5S	O47-C38-O37-C2
153	n5	806	CDL	OB5-CB3-CB4-OB6
153	qi	202	CDL	OB5-CB3-CB4-OB6
153	N5	806	CDL	OB5-CB3-CB4-OB6
153	Qi	202	CDL	OB5-CB3-CB4-OB6
158	c4	402	3PE	O11-C1-C2-O21
158	C4	402	3PE	O11-C1-C2-O21
153	M	305	CDL	C54-C55-C56-C57
164	sc	102	U10	C49-C51-C52-C53
164	SC	102	U10	C49-C51-C52-C53
166	y5	203	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
166	y5	203	HEM	C4C-C3C-CAC-CBC
166	qC	501	HEM	C4C-C3C-CAC-CBC
166	Y5	203	HEM	C4B-C3B-CAB-CBB
166	QC	501	HEM	C4C-C3C-CAC-CBC
168	ab	201	ZMP	C6-C7-C8-C9
168	AB	201	ZMP	C6-C7-C8-C9
160	y5	204	PX2	O6-C4-O5-C3
153	i	302	CDL	C36-C37-C38-C39
153	I	303	CDL	C36-C37-C38-C39
153	N5	806	CDL	C18-C19-C20-C21
153	6c	202	CDL	CB5-C51-C52-C53
153	2b	201	CDL	CB5-C51-C52-C53
153	n5	806	CDL	CA7-C31-C32-C33
153	2M	101	CDL	CA5-C11-C12-C13
153	2B	201	CDL	CB5-C51-C52-C53
158	a3	202	3PE	C31-C32-C33-C34
158	A3	202	3PE	C31-C32-C33-C34
152	c2	703	PC1	O21-C2-C3-O31
152	m2	407	PC1	O21-C2-C3-O31
152	C2	701	PC1	O21-C2-C3-O31
152	M2	407	PC1	O21-C2-C3-O31
153	a	502	CDL	OB6-CB4-CB6-OB8
153	m	306	CDL	OB6-CB4-CB6-OB8
153	2G	204	CDL	OA6-CA4-CA6-OA8
153	A	502	CDL	OB6-CB4-CB6-OB8
153	M	301	CDL	OB6-CB4-CB6-OB8
158	a3	202	3PE	O21-C2-C3-O31
158	g2	301	3PE	O21-C2-C3-O31
158	A3	202	3PE	O21-C2-C3-O31
158	G2	301	3PE	O21-C2-C3-O31
160	qh	201	PX2	O7-C2-C3-O5
169	b6	201	T7X	C12-C13-C14-C15
152	w	204	PC1	C33-C34-C35-C36
152	W	204	PC1	C33-C34-C35-C36
153	n5	806	CDL	C18-C19-C20-C21
169	B6	201	T7X	C31-C32-C33-C34
153	2M	101	CDL	C71-C72-C73-C74
152	qB	602	PC1	C24-C25-C26-C27
153	2m	101	CDL	C71-C72-C73-C74
153	c4	401	CDL	C34-C35-C36-C37
153	TE	101	CDL	C52-C53-C54-C55
152	d	501	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
152	m	301	PC1	C2-C1-O11-P
152	D	501	PC1	C2-C1-O11-P
152	M	303	PC1	C2-C1-O11-P
153	qB	601	CDL	CA4-CA3-OA5-PA1
153	QB	601	CDL	CA4-CA3-OA5-PA1
152	QB	602	PC1	C24-C25-C26-C27
153	C4	401	CDL	C34-C35-C36-C37
169	b6	201	T7X	C31-C32-C33-C34
153	t5	301	CDL	C59-C60-C61-C62
166	y5	203	HEM	C3D-CAD-CBD-CGD
159	m2	406	P5S	O47-C38-O37-C2
153	a9	403	CDL	CA2-C1-CB2-OB2
153	A9	403	CDL	CA2-C1-CB2-OB2
153	B3	102	CDL	CB2-C1-CA2-OA2
153	r	201	CDL	O1-C1-CB2-OB2
153	b3	101	CDL	C11-C12-C13-C14
158	SC	101	3PE	C33-C34-C35-C36
153	m	306	CDL	C11-C12-C13-C14
153	b3	102	CDL	C76-C77-C78-C79
153	I	303	CDL	C54-C55-C56-C57
153	M	301	CDL	C11-C12-C13-C14
153	B3	101	CDL	C11-C12-C13-C14
153	B3	102	CDL	C72-C73-C74-C75
153	T5	301	CDL	C59-C60-C61-C62
158	sc	101	3PE	C33-C34-C35-C36
153	6c	201	CDL	CB5-C51-C52-C53
153	6C	203	CDL	CB5-C51-C52-C53
153	2k	101	CDL	C38-C39-C40-C41
153	i	302	CDL	C54-C55-C56-C57
153	b3	102	CDL	C72-C73-C74-C75
153	2K	101	CDL	C38-C39-C40-C41
153	B3	102	CDL	C76-C77-C78-C79
153	M1	404	CDL	C72-C73-C74-C75
152	a	503	PC1	C11-C12-N-C13
152	a	503	PC1	C11-C12-N-C14
152	w	201	PC1	C11-C12-N-C14
152	n5	801	PC1	C11-C12-N-C14
152	qC	505	PC1	C11-C12-N-C13
152	qC	505	PC1	C11-C12-N-C15
152	qJ	101	PC1	C11-C12-N-C15
152	W	201	PC1	C11-C12-N-C14
152	N5	801	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
152	QC	505	PC1	C11-C12-N-C13
168	ab	201	ZMP	O3-C16-C17-O4
168	AB	201	ZMP	O3-C16-C17-O4
153	m1	404	CDL	C72-C73-C74-C75
160	qh	201	PX2	C17-C18-C19-C20
169	B6	201	T7X	C12-C13-C14-C15
153	6a	201	CDL	C34-C35-C36-C37
153	6A	201	CDL	C34-C35-C36-C37
152	n5	805	PC1	O11-C1-C2-C3
152	N5	805	PC1	O11-C1-C2-C3
153	6c	201	CDL	OB5-CB3-CB4-CB6
153	7a	203	CDL	OB5-CB3-CB4-CB6
153	f	401	CDL	OB5-CB3-CB4-CB6
153	i	301	CDL	OB5-CB3-CB4-CB6
153	sd	101	CDL	OA5-CA3-CA4-CA6
153	t	201	CDL	OB5-CB3-CB4-CB6
153	vb	701	CDL	OB5-CB3-CB4-CB6
153	c4	401	CDL	OB5-CB3-CB4-CB6
153	n5	806	CDL	OB5-CB3-CB4-CB6
153	qB	601	CDL	OB5-CB3-CB4-CB6
153	qb	601	CDL	OB5-CB3-CB4-CB6
153	6C	202	CDL	OB5-CB3-CB4-CB6
153	7A	203	CDL	OB5-CB3-CB4-CB6
153	F	402	CDL	OB5-CB3-CB4-CB6
153	I	302	CDL	OB5-CB3-CB4-CB6
153	N	304	CDL	OA5-CA3-CA4-CA6
153	SD	101	CDL	OA5-CA3-CA4-CA6
153	SD	101	CDL	OB5-CB3-CB4-CB6
153	T	201	CDL	OB5-CB3-CB4-CB6
153	VB	701	CDL	OB5-CB3-CB4-CB6
153	C4	401	CDL	OB5-CB3-CB4-CB6
153	N5	806	CDL	OB5-CB3-CB4-CB6
153	QB	601	CDL	OB5-CB3-CB4-CB6
153	Qb	601	CDL	OB5-CB3-CB4-CB6
153	u1	101	CDL	OB5-CB3-CB4-CB6
153	U1	101	CDL	OB5-CB3-CB4-CB6
158	c4	402	3PE	O11-C1-C2-C3
158	ta	201	3PE	O11-C1-C2-C3
158	C4	402	3PE	O11-C1-C2-C3
158	TA	201	3PE	O11-C1-C2-C3
153	AM	201	CDL	C34-C35-C36-C37
158	t8	601	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
153	6C	202	CDL	CB5-C51-C52-C53
153	u	201	CDL	C13-C14-C15-C16
153	am	201	CDL	C34-C35-C36-C37
153	U	201	CDL	C13-C14-C15-C16
158	T8	601	3PE	C22-C23-C24-C25
153	2m	101	CDL	CA5-C11-C12-C13
153	6c	201	CDL	C15-C16-C17-C18
153	7a	201	CDL	C62-C63-C64-C65
153	6C	202	CDL	C15-C16-C17-C18
153	7A	201	CDL	C62-C63-C64-C65
169	b6	201	T7X	C38-C39-C40-C41
169	B6	201	T7X	C38-C39-C40-C41
153	t	204	CDL	C59-C60-C61-C62
153	a9	402	CDL	C33-C34-C35-C36
153	n6	302	CDL	C51-C52-C53-C54
153	T	204	CDL	C59-C60-C61-C62
153	A9	402	CDL	C33-C34-C35-C36
153	N6	302	CDL	C51-C52-C53-C54
153	bm	301	CDL	C13-C14-C15-C16
158	b4	202	3PE	C24-C25-C26-C27
158	B4	202	3PE	C24-C25-C26-C27
153	c4	401	CDL	CA7-C31-C32-C33
153	C4	401	CDL	CA7-C31-C32-C33
152	2j	201	PC1	C1-C2-C3-O31
152	c3	602	PC1	C1-C2-C3-O31
152	s8	301	PC1	C1-C2-C3-O31
152	t1	602	PC1	C1-C2-C3-O31
152	tc	102	PC1	C1-C2-C3-O31
152	2J	201	PC1	C1-C2-C3-O31
152	S8	301	PC1	C1-C2-C3-O31
152	T1	602	PC1	C1-C2-C3-O31
152	TC	102	PC1	C1-C2-C3-O31
153	2g	203	CDL	CB3-CB4-CB6-OB8
153	2g	204	CDL	CA3-CA4-CA6-OA8
153	6c	201	CDL	CA3-CA4-CA6-OA8
153	7c	302	CDL	CA3-CA4-CA6-OA8
153	b	501	CDL	CB3-CB4-CB6-OB8
153	a9	402	CDL	CB3-CB4-CB6-OB8
153	b3	102	CDL	CA3-CA4-CA6-OA8
153	bm	301	CDL	CA3-CA4-CA6-OA8
153	qc	504	CDL	CB3-CB4-CB6-OB8
153	th	200	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
153	2G	204	CDL	CA3-CA4-CA6-OA8
153	6C	202	CDL	CA3-CA4-CA6-OA8
153	7C	301	CDL	CA3-CA4-CA6-OA8
153	B	501	CDL	CB3-CB4-CB6-OB8
153	A9	402	CDL	CB3-CB4-CB6-OB8
153	BM	301	CDL	CA3-CA4-CA6-OA8
153	Qc	504	CDL	CB3-CB4-CB6-OB8
153	TH	200	CDL	CA3-CA4-CA6-OA8
158	g2	301	3PE	C1-C2-C3-O31
158	s8	304	3PE	C1-C2-C3-O31
158	t8	602	3PE	C1-C2-C3-O31
158	G2	301	3PE	C1-C2-C3-O31
158	S8	304	3PE	C1-C2-C3-O31
158	T8	602	3PE	C1-C2-C3-O31
159	m2	406	P5S	O19-C1-C2-C3
159	M2	406	P5S	O19-C1-C2-C3
160	Y5	204	PX2	C1-C2-C3-O5
152	5B	202	PC1	C36-C37-C38-C39
153	an	302	CDL	C80-C81-C82-C83
153	AN	302	CDL	C80-C81-C82-C83
158	c4	402	3PE	C33-C34-C35-C36
158	C4	402	3PE	C33-C34-C35-C36
152	5b	202	PC1	C36-C37-C38-C39
152	5b	202	PC1	C38-C39-C3A-C3B
153	R	201	CDL	O1-C1-CB2-OB2
152	t4	303	PC1	C27-C28-C29-C2A
152	5B	202	PC1	C38-C39-C3A-C3B
153	q	203	CDL	C52-C53-C54-C55
153	BM	301	CDL	C13-C14-C15-C16
169	b6	201	T7X	C36-C37-C38-C39
169	B6	201	T7X	C36-C37-C38-C39
160	Y5	204	PX2	C5-C4-O5-C3
152	T4	303	PC1	C27-C28-C29-C2A
153	bm	301	CDL	C77-C78-C79-C80
153	E	401	CDL	C13-C14-C15-C16
153	VB	703	CDL	C52-C53-C54-C55
153	BM	301	CDL	C77-C78-C79-C80
153	t	202	CDL	C14-C15-C16-C17
153	E	403	CDL	C52-C53-C54-C55
153	T	202	CDL	C14-C15-C16-C17
152	a	501	PC1	C11-C12-N-C14
152	c1	707	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
152	m1	401	PC1	C11-C12-N-C14
152	n	302	PC1	C11-C12-N-C13
152	b9	201	PC1	C11-C12-N-C13
152	qe	301	PC1	C11-C12-N-C15
152	t1	602	PC1	C11-C12-N-C15
152	A	501	PC1	C11-C12-N-C14
152	A	503	PC1	C11-C12-N-C13
152	M1	401	PC1	C11-C12-N-C14
152	N	302	PC1	C11-C12-N-C13
152	B9	201	PC1	C11-C12-N-C13
152	Qe	301	PC1	C11-C12-N-C15
152	T1	602	PC1	C11-C12-N-C15
153	2g	201	CDL	C18-C19-C20-C21
153	b8	302	CDL	C55-C56-C57-C58
153	2G	201	CDL	C18-C19-C20-C21
153	B8	302	CDL	C55-C56-C57-C58
153	t	203	CDL	CB5-C51-C52-C53
153	y5	201	CDL	CA7-C31-C32-C33
153	T	203	CDL	CB5-C51-C52-C53
164	qc	501	U10	C13-C14-C16-C17
160	r	202	PX2	C23-C24-C25-C26
153	i	301	CDL	CB4-CB3-OB5-PB2
153	a9	402	CDL	CB4-CB3-OB5-PB2
153	I	302	CDL	CB4-CB3-OB5-PB2
153	A9	402	CDL	CB4-CB3-OB5-PB2
153	e	403	CDL	C52-C53-C54-C55
153	Y5	201	CDL	CA7-C31-C32-C33
158	an	301	3PE	C22-C23-C24-C25
158	AN	301	3PE	C22-C23-C24-C25
151	2e	401	HEC	C3D-CAD-CBD-CGD
166	Y5	203	HEM	C3D-CAD-CBD-CGD
160	r	202	PX2	C1-O4-P1-O2
153	m1	404	CDL	C74-C75-C76-C77
153	M1	404	CDL	C74-C75-C76-C77
153	C1	712	CDL	CB7-C71-C72-C73
153	e	401	CDL	C13-C14-C15-C16
152	tc	101	PC1	C28-C29-C2A-C2B
153	c1	712	CDL	CB7-C71-C72-C73
153	2k	101	CDL	C57-C58-C59-C60
152	2g	202	PC1	O11-C1-C2-O21
152	t4	301	PC1	O11-C1-C2-O21
152	2G	202	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
152	T4	301	PC1	O11-C1-C2-O21
153	6c	201	CDL	OA5-CA3-CA4-OA6
153	c1	701	CDL	OB5-CB3-CB4-OB6
153	e	402	CDL	OB5-CB3-CB4-OB6
153	m1	402	CDL	OB5-CB3-CB4-OB6
153	n6	302	CDL	OB5-CB3-CB4-OB6
153	qC	503	CDL	OB5-CB3-CB4-OB6
153	qg	402	CDL	OB5-CB3-CB4-OB6
153	6C	202	CDL	OA5-CA3-CA4-OA6
153	C1	701	CDL	OB5-CB3-CB4-OB6
153	C1	712	CDL	OB5-CB3-CB4-OB6
153	E	402	CDL	OB5-CB3-CB4-OB6
153	M1	402	CDL	OB5-CB3-CB4-OB6
153	N6	302	CDL	OB5-CB3-CB4-OB6
153	Qg	402	CDL	OB5-CB3-CB4-OB6
158	bm	302	3PE	O11-C1-C2-O21
158	BM	302	3PE	O11-C1-C2-O21
153	2K	101	CDL	C57-C58-C59-C60
152	t4	303	PC1	C25-C26-C27-C28
152	T4	303	PC1	C25-C26-C27-C28
153	qi	202	CDL	C56-C57-C58-C59
154	C1	703	HEA	O11-C11-C12-C13
153	Qi	202	CDL	C56-C57-C58-C59
152	6a	202	PC1	C26-C27-C28-C29
152	6A	202	PC1	C26-C27-C28-C29
152	TC	101	PC1	C28-C29-C2A-C2B
153	w	202	CDL	C55-C56-C57-C58
153	W	202	CDL	C55-C56-C57-C58
153	BM	301	CDL	C40-C41-C42-C43
160	qh	201	PX2	C22-C23-C24-C25
153	2b	201	CDL	C16-C17-C18-C19
153	T	202	CDL	C75-C76-C77-C78
153	2B	201	CDL	C16-C17-C18-C19
168	ab	201	ZMP	C1-C22-C23-C24
168	AB	201	ZMP	C1-C22-C23-C24
152	m1	403	PC1	O21-C2-C3-O31
152	M1	403	PC1	O21-C2-C3-O31
153	2g	203	CDL	OB6-CB4-CB6-OB8
153	2g	204	CDL	OA6-CA4-CA6-OA8
153	2k	101	CDL	OA6-CA4-CA6-OA8
153	7c	302	CDL	OA6-CA4-CA6-OA8
153	m	303	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
153	b3	102	CDL	OA6-CA4-CA6-OA8
153	2G	203	CDL	OB6-CB4-CB6-OB8
153	2K	101	CDL	OA6-CA4-CA6-OA8
153	7C	302	CDL	OA6-CA4-CA6-OA8
153	M	305	CDL	OA6-CA4-CA6-OA8
153	B3	102	CDL	OA6-CA4-CA6-OA8
160	r	202	PX2	O7-C2-C3-O5
160	R	202	PX2	C24-C25-C26-C27
153	2m	101	CDL	O1-C1-CA2-OA2
153	2b	201	CDL	C79-C80-C81-C82
153	c4	401	CDL	C81-C82-C83-C84
153	t1	601	CDL	C72-C73-C74-C75
153	C4	401	CDL	C81-C82-C83-C84
153	t5	301	CDL	C78-C79-C80-C81
153	2B	201	CDL	C79-C80-C81-C82
153	T5	301	CDL	C78-C79-C80-C81
158	c4	402	3PE	C2B-C2C-C2D-C2E
152	2g	202	PC1	C11-C12-N-C13
152	A	503	PC1	C11-C12-N-C14
152	C1	710	PC1	C11-C12-N-C13
152	QJ	102	PC1	C11-C12-N-C15
152	d	501	PC1	O21-C21-C22-C23
152	D	501	PC1	O21-C21-C22-C23
153	6a	201	CDL	C32-C31-CA7-OA8
153	6A	201	CDL	C32-C31-CA7-OA8
153	Q	202	CDL	C12-C11-CA5-OA6
158	N4	601	3PE	C25-C26-C27-C28
160	qh	201	PX2	C6-C7-C8-C9
154	c1	708	HEA	C3B-C11-C12-C13
154	C1	703	HEA	C3B-C11-C12-C13
153	t	202	CDL	C75-C76-C77-C78
158	C4	402	3PE	C2B-C2C-C2D-C2E
153	bm	301	CDL	C40-C41-C42-C43
160	Y5	204	PX2	C17-C18-C19-C20
164	qc	507	U10	C13-C14-C16-C17
164	Qc	507	U10	C13-C14-C16-C17
153	T1	601	CDL	C72-C73-C74-C75
153	l	301	CDL	C55-C56-C57-C58
153	L	301	CDL	C55-C56-C57-C58
158	n4	601	3PE	C25-C26-C27-C28
153	b3	102	CDL	C62-C63-C64-C65
153	B3	102	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
152	m1	403	PC1	C2-C1-O11-P
152	qE	304	PC1	C2-C1-O11-P
152	tc	102	PC1	C2-C1-O11-P
152	M1	403	PC1	C2-C1-O11-P
152	QJ	101	PC1	C2-C1-O11-P
152	TC	102	PC1	C2-C1-O11-P
153	7c	301	CDL	C1-CB2-OB2-PB2
153	m2	401	CDL	CB4-CB3-OB5-PB2
153	m3	403	CDL	CA4-CA3-OA5-PA1
153	q	201	CDL	C1-CA2-OA2-PA1
153	t	202	CDL	CA4-CA3-OA5-PA1
153	y5	201	CDL	CA4-CA3-OA5-PA1
153	b3	101	CDL	CA4-CA3-OA5-PA1
153	qc	508	CDL	C1-CA2-OA2-PA1
153	7C	301	CDL	C1-CB2-OB2-PB2
153	M2	401	CDL	CB4-CB3-OB5-PB2
153	M3	403	CDL	CA4-CA3-OA5-PA1
153	Q	201	CDL	C1-CA2-OA2-PA1
153	T	202	CDL	CA4-CA3-OA5-PA1
153	Y5	201	CDL	CA4-CA3-OA5-PA1
153	B3	101	CDL	CA4-CA3-OA5-PA1
153	Qc	508	CDL	C1-CA2-OA2-PA1
168	ab	201	ZMP	S1-C11-C12-N1
168	AB	201	ZMP	S1-C11-C12-N1
152	n	301	PC1	C22-C23-C24-C25
153	m2	403	CDL	C52-C53-C54-C55
153	7C	302	CDL	C31-C32-C33-C34
153	M2	403	CDL	C52-C53-C54-C55
153	m2	401	CDL	C32-C31-CA7-OA8
153	q	202	CDL	C12-C11-CA5-OA6
153	te	101	CDL	C32-C31-CA7-OA8
153	M2	401	CDL	C32-C31-CA7-OA8
152	N	301	PC1	C22-C23-C24-C25
153	QB	601	CDL	C12-C13-C14-C15
153	Qb	601	CDL	C71-C72-C73-C74
151	2e	401	HEC	C2A-CAA-CBA-CGA
151	2E	401	HEC	C2A-CAA-CBA-CGA
153	7c	302	CDL	C31-C32-C33-C34
153	qI	203	CDL	C12-C13-C14-C15
153	qb	601	CDL	C71-C72-C73-C74
160	Qh	201	PX2	C10-C11-C12-C13
153	w	202	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
152	m	301	PC1	O11-C1-C2-C3
152	v	201	PC1	O11-C1-C2-C3
152	w	201	PC1	O11-C1-C2-C3
152	M	303	PC1	O11-C1-C2-C3
152	V	201	PC1	O11-C1-C2-C3
152	W	201	PC1	O11-C1-C2-C3
153	2g	203	CDL	OB5-CB3-CB4-CB6
153	2o	101	CDL	OB5-CB3-CB4-CB6
153	6c	201	CDL	OA5-CA3-CA4-CA6
153	6c	202	CDL	OB5-CB3-CB4-CB6
153	a	504	CDL	OB5-CB3-CB4-CB6
153	a	505	CDL	OB5-CB3-CB4-CB6
153	i	302	CDL	OB5-CB3-CB4-CB6
153	j	301	CDL	OB5-CB3-CB4-CB6
153	m2	401	CDL	OB5-CB3-CB4-CB6
153	n	304	CDL	OA5-CA3-CA4-CA6
153	n	304	CDL	OB5-CB3-CB4-CB6
153	q	202	CDL	OB5-CB3-CB4-CB6
153	r	201	CDL	OB5-CB3-CB4-CB6
153	sd	101	CDL	OB5-CB3-CB4-CB6
153	t	204	CDL	OB5-CB3-CB4-CB6
153	u	201	CDL	OB5-CB3-CB4-CB6
153	al	301	CDL	OB5-CB3-CB4-CB6
153	b3	101	CDL	OA5-CA3-CA4-CA6
153	qD	402	CDL	OB5-CB3-CB4-CB6
153	qG	402	CDL	OB5-CB3-CB4-CB6
153	qi	202	CDL	OB5-CB3-CB4-CB6
153	t5	301	CDL	OB5-CB3-CB4-CB6
153	2G	203	CDL	OB5-CB3-CB4-CB6
153	2G	204	CDL	OB5-CB3-CB4-CB6
153	2O	101	CDL	OB5-CB3-CB4-CB6
153	6C	203	CDL	OB5-CB3-CB4-CB6
153	A	504	CDL	OB5-CB3-CB4-CB6
153	I	303	CDL	OB5-CB3-CB4-CB6
153	J	301	CDL	OB5-CB3-CB4-CB6
153	M2	401	CDL	OB5-CB3-CB4-CB6
153	N	304	CDL	OB5-CB3-CB4-CB6
153	Q	202	CDL	OB5-CB3-CB4-CB6
153	R	201	CDL	OB5-CB3-CB4-CB6
153	T	204	CDL	OB5-CB3-CB4-CB6
153	U	201	CDL	OB5-CB3-CB4-CB6
153	VB	705	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
153	AL	301	CDL	OB5-CB3-CB4-CB6
153	B3	101	CDL	OA5-CA3-CA4-CA6
153	QD	402	CDL	OB5-CB3-CB4-CB6
153	QG	402	CDL	OB5-CB3-CB4-CB6
153	Qi	202	CDL	OB5-CB3-CB4-CB6
153	T5	301	CDL	OB5-CB3-CB4-CB6
160	r	202	PX2	O4-C1-C2-C3
152	b9	201	PC1	C11-C12-N-C14
152	2G	202	PC1	C11-C12-N-C14
152	M1	401	PC1	C11-C12-N-C13
152	B9	201	PC1	C11-C12-N-C14
153	a9	403	CDL	O1-C1-CB2-OB2
153	2M	101	CDL	O1-C1-CA2-OA2
153	a	504	CDL	CA5-C11-C12-C13
153	m	302	CDL	CB5-C51-C52-C53
153	A	504	CDL	CA5-C11-C12-C13
153	M	304	CDL	CB5-C51-C52-C53
153	W	202	CDL	CA7-C31-C32-C33
160	y5	204	PX2	C17-C18-C19-C20
169	B6	201	T7X	C44-C45-C46-C47
153	qB	601	CDL	C12-C13-C14-C15
153	QI	203	CDL	C12-C13-C14-C15
160	Y5	204	PX2	O6-C4-O5-C3
169	b6	201	T7X	C44-C45-C46-C47
164	qc	507	U10	C15-C14-C16-C17
164	Qc	507	U10	C15-C14-C16-C17
158	M3	402	3PE	C2A-C2B-C2C-C2D
152	n	303	PC1	O31-C31-C32-C33
153	TE	101	CDL	C32-C31-CA7-OA8
153	sd	101	CDL	C71-C72-C73-C74
152	7a	202	PC1	C22-C23-C24-C25
158	m3	402	3PE	C2A-C2B-C2C-C2D
152	7A	202	PC1	C22-C23-C24-C25
152	te	102	PC1	C32-C33-C34-C35
160	qh	201	PX2	C10-C11-C12-C13
153	qG	402	CDL	C21-C22-C23-C24
160	r	202	PX2	C24-C25-C26-C27
153	t	202	CDL	C56-C57-C58-C59
160	Qh	201	PX2	C19-C20-C21-C22
152	c2	703	PC1	C1-C2-C3-O31
152	qC	508	PC1	C1-C2-C3-O31
152	qc	506	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
152	C2	701	PC1	C1-C2-C3-O31
152	C3	602	PC1	C1-C2-C3-O31
152	QC	508	PC1	C1-C2-C3-O31
152	Qc	506	PC1	C1-C2-C3-O31
153	a	502	CDL	CB3-CB4-CB6-OB8
153	m	303	CDL	CA3-CA4-CA6-OA8
153	m	306	CDL	CB3-CB4-CB6-OB8
153	m1	402	CDL	CA3-CA4-CA6-OA8
153	m2	403	CDL	CA3-CA4-CA6-OA8
153	sd	101	CDL	CB3-CB4-CB6-OB8
153	t	201	CDL	CB3-CB4-CB6-OB8
153	t	204	CDL	CA3-CA4-CA6-OA8
153	b4	201	CDL	CB3-CB4-CB6-OB8
153	7C	302	CDL	CA3-CA4-CA6-OA8
153	A	502	CDL	CB3-CB4-CB6-OB8
153	M	301	CDL	CB3-CB4-CB6-OB8
153	M	305	CDL	CA3-CA4-CA6-OA8
153	M1	402	CDL	CA3-CA4-CA6-OA8
153	M2	403	CDL	CA3-CA4-CA6-OA8
153	SD	101	CDL	CB3-CB4-CB6-OB8
153	T	201	CDL	CB3-CB4-CB6-OB8
153	T	204	CDL	CA3-CA4-CA6-OA8
153	B4	201	CDL	CB3-CB4-CB6-OB8
158	a3	202	3PE	C1-C2-C3-O31
158	an	301	3PE	C1-C2-C3-O31
158	A3	202	3PE	C1-C2-C3-O31
158	AN	301	3PE	C1-C2-C3-O31
160	qh	201	PX2	C1-C2-C3-O5
168	ab	201	ZMP	N2-C16-C17-O4
168	AB	201	ZMP	N2-C16-C17-O4
152	am	202	PC1	C38-C39-C3A-C3B
152	AM	202	PC1	C38-C39-C3A-C3B
153	a	505	CDL	C64-C65-C66-C67
153	VB	705	CDL	C64-C65-C66-C67
152	b9	201	PC1	C34-C35-C36-C37
153	2g	201	CDL	C16-C17-C18-C19
153	2G	201	CDL	C16-C17-C18-C19
158	a3	202	3PE	C21-C22-C23-C24
158	g2	301	3PE	C21-C22-C23-C24
158	A3	202	3PE	C21-C22-C23-C24
169	b6	201	T7X	C33-C34-C35-C36
169	B6	201	T7X	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
153	QG	402	CDL	C21-C22-C23-C24
158	B4	202	3PE	C3A-C3B-C3C-C3D
153	P1	402	CDL	C74-C75-C76-C77
153	E	402	CDL	CB5-C51-C52-C53
158	G2	301	3PE	C21-C22-C23-C24
152	qC	505	PC1	C22-C23-C24-C25
152	QC	505	PC1	C22-C23-C24-C25
152	TE	102	PC1	C32-C33-C34-C35
153	p1	402	CDL	C74-C75-C76-C77
153	SD	101	CDL	C71-C72-C73-C74
152	B9	201	PC1	C34-C35-C36-C37
152	b9	201	PC1	C36-C37-C38-C39
153	m1	402	CDL	C54-C55-C56-C57
153	vb	701	CDL	C73-C74-C75-C76
153	M1	402	CDL	C54-C55-C56-C57
152	n5	805	PC1	O11-C1-C2-O21
152	qc	509	PC1	O11-C1-C2-O21
152	N5	805	PC1	O11-C1-C2-O21
152	Qc	509	PC1	O11-C1-C2-O21
153	2g	204	CDL	OB5-CB3-CB4-OB6
153	2o	101	CDL	OB5-CB3-CB4-OB6
153	c1	709	CDL	OA5-CA3-CA4-OA6
153	c1	712	CDL	OB5-CB3-CB4-OB6
153	fs	203	CDL	OA5-CA3-CA4-OA6
153	n	304	CDL	OA5-CA3-CA4-OA6
153	t	204	CDL	OB5-CB3-CB4-OB6
153	u	201	CDL	OB5-CB3-CB4-OB6
153	b3	102	CDL	OB5-CB3-CB4-OB6
153	p1	402	CDL	OB5-CB3-CB4-OB6
153	2O	101	CDL	OB5-CB3-CB4-OB6
153	C1	708	CDL	OA5-CA3-CA4-OA6
153	FS	204	CDL	OA5-CA3-CA4-OA6
153	N	304	CDL	OA5-CA3-CA4-OA6
153	SD	101	CDL	OB5-CB3-CB4-OB6
153	T	204	CDL	OB5-CB3-CB4-OB6
153	U	201	CDL	OB5-CB3-CB4-OB6
153	P1	402	CDL	OB5-CB3-CB4-OB6
153	QC	503	CDL	OB5-CB3-CB4-OB6
153	C	301	CDL	OB5-CB3-CB4-OB6
153	c	301	CDL	OB5-CB3-CB4-OB6
153	u1	101	CDL	OB5-CB3-CB4-OB6
153	U1	101	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
152	B9	201	PC1	C36-C37-C38-C39
152	M2	407	PC1	C38-C39-C3A-C3B
158	b4	202	3PE	C3A-C3B-C3C-C3D
152	m2	407	PC1	C38-C39-C3A-C3B
153	VB	701	CDL	C73-C74-C75-C76
153	A9	403	CDL	O1-C1-CB2-OB2
152	6c	203	PC1	C2-C1-O11-P
152	a	503	PC1	C2-C1-O11-P
152	n5	804	PC1	C2-C1-O11-P
152	6C	201	PC1	C2-C1-O11-P
152	A	503	PC1	C2-C1-O11-P
152	N5	804	PC1	C2-C1-O11-P
153	2o	101	CDL	CB4-CB3-OB5-PB2
153	fs	203	CDL	CA4-CA3-OA5-PA1
153	t	204	CDL	CA4-CA3-OA5-PA1
153	t	204	CDL	C1-CB2-OB2-PB2
153	p1	403	CDL	CB4-CB3-OB5-PB2
153	2O	101	CDL	CB4-CB3-OB5-PB2
153	FS	204	CDL	CA4-CA3-OA5-PA1
153	T	204	CDL	CA4-CA3-OA5-PA1
153	T	204	CDL	C1-CB2-OB2-PB2
153	P1	403	CDL	CB4-CB3-OB5-PB2
153	u1	101	CDL	CA4-CA3-OA5-PA1
153	U1	101	CDL	CA4-CA3-OA5-PA1
158	bm	302	3PE	C2-C1-O11-P
158	BM	302	3PE	C2-C1-O11-P
153	7a	201	CDL	C64-C65-C66-C67
153	7A	201	CDL	C64-C65-C66-C67
153	td	101	CDL	C72-C71-CB7-OB8
153	A1	101	CDL	C72-C71-CB7-OB8
152	qC	508	PC1	O21-C2-C3-O31
152	QC	508	PC1	O21-C2-C3-O31
153	7c	301	CDL	OA6-CA4-CA6-OA8
153	m1	402	CDL	OA6-CA4-CA6-OA8
153	n	304	CDL	OB6-CB4-CB6-OB8
153	b4	201	CDL	OB6-CB4-CB6-OB8
153	bm	301	CDL	OA6-CA4-CA6-OA8
153	n5	806	CDL	OB6-CB4-CB6-OB8
153	qc	504	CDL	OB6-CB4-CB6-OB8
153	M1	402	CDL	OA6-CA4-CA6-OA8
153	N	304	CDL	OB6-CB4-CB6-OB8
153	B4	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
153	BM	301	CDL	OA6-CA4-CA6-OA8
153	N5	806	CDL	OB6-CB4-CB6-OB8
153	Qc	504	CDL	OB6-CB4-CB6-OB8
158	vb	705	3PE	O21-C2-C3-O31
158	w	203	3PE	O21-C2-C3-O31
158	a3	201	3PE	O21-C2-C3-O31
158	n5	802	3PE	O21-C2-C3-O31
158	VB	707	3PE	O21-C2-C3-O31
158	W	203	3PE	O21-C2-C3-O31
158	A3	201	3PE	O21-C2-C3-O31
158	N5	802	3PE	O21-C2-C3-O31
169	b6	201	T7X	C41-C42-C43-C44
169	b6	201	T7X	C19-C20-C21-C22
169	B6	201	T7X	C19-C20-C21-C22
153	T	202	CDL	C56-C57-C58-C59
153	t5	301	CDL	C76-C77-C78-C79
153	T5	301	CDL	C76-C77-C78-C79
153	6c	201	CDL	CA7-C31-C32-C33
164	b8	301	U10	C12-C11-C9-C10
164	B8	301	U10	C12-C11-C9-C10
164	b8	301	U10	C12-C11-C9-C8
164	B8	301	U10	C12-C11-C9-C8
153	P1	403	CDL	C34-C35-C36-C37
159	M2	406	P5S	C39-C40-C41-C42
169	B6	201	T7X	C41-C42-C43-C44
152	2F	301	PC1	C2C-C2D-C2E-C2F
159	m2	406	P5S	C39-C40-C41-C42
153	al	301	CDL	CB7-C71-C72-C73
153	6C	202	CDL	CA7-C31-C32-C33
153	AL	301	CDL	CB7-C71-C72-C73
153	p1	403	CDL	C34-C35-C36-C37
152	2f	301	PC1	C2C-C2D-C2E-C2F
160	r	202	PX2	C17-C18-C19-C20
160	R	202	PX2	C17-C18-C19-C20
161	sa	701	FAD	PA-O3P-P-O5'
161	SA	701	FAD	PA-O3P-P-O5'
158	ta	201	3PE	C21-C22-C23-C24
158	TA	201	3PE	C21-C22-C23-C24
152	m	301	PC1	C11-C12-N-C13
152	m	305	PC1	C11-C12-N-C15
152	m1	401	PC1	C11-C12-N-C13
152	m2	405	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
152	n	302	PC1	C11-C12-N-C15
152	qE	304	PC1	C11-C12-N-C13
152	M	303	PC1	C11-C12-N-C13
152	M	307	PC1	C11-C12-N-C15
152	M2	405	PC1	C11-C12-N-C14
152	N	302	PC1	C11-C12-N-C15
152	QJ	101	PC1	C11-C12-N-C13
152	qC	505	PC1	C34-C35-C36-C37
169	b6	201	T7X	C21-C22-C23-C24
169	B6	201	T7X	C21-C22-C23-C24
153	6a	201	CDL	C36-C37-C38-C39
153	p1	403	CDL	C73-C74-C75-C76
153	6A	201	CDL	C36-C37-C38-C39
153	P1	403	CDL	C73-C74-C75-C76
153	y5	201	CDL	C12-C11-CA5-OA6
153	Y5	201	CDL	C12-C11-CA5-OA6
153	N5	806	CDL	CA7-C31-C32-C33
153	c1	709	CDL	CB2-C1-CA2-OA2
153	e	402	CDL	CB2-C1-CA2-OA2
153	an	302	CDL	CB2-C1-CA2-OA2
153	C1	708	CDL	CB2-C1-CA2-OA2
153	AN	302	CDL	CB2-C1-CA2-OA2
153	C	301	CDL	CA2-C1-CB2-OB2
152	QC	505	PC1	C34-C35-C36-C37
152	2g	202	PC1	O11-C1-C2-C3
152	qc	509	PC1	O11-C1-C2-C3
152	qj	101	PC1	O11-C1-C2-C3
152	tc	102	PC1	O11-C1-C2-C3
152	2G	202	PC1	O11-C1-C2-C3
152	QC	507	PC1	O11-C1-C2-C3
152	Qc	509	PC1	O11-C1-C2-C3
152	Qj	101	PC1	O11-C1-C2-C3
153	2g	204	CDL	OB5-CB3-CB4-CB6
153	c1	701	CDL	OB5-CB3-CB4-CB6
153	m1	404	CDL	OB5-CB3-CB4-CB6
153	a1	101	CDL	OB5-CB3-CB4-CB6
153	a9	403	CDL	OB5-CB3-CB4-CB6
153	b3	102	CDL	OB5-CB3-CB4-CB6
153	p1	402	CDL	OB5-CB3-CB4-CB6
153	qD	402	CDL	OA5-CA3-CA4-CA6
153	6C	202	CDL	OA5-CA3-CA4-CA6
153	C1	701	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
153	M1	404	CDL	OB5-CB3-CB4-CB6
153	B8	302	CDL	OB5-CB3-CB4-CB6
153	P1	402	CDL	OB5-CB3-CB4-CB6
153	QD	402	CDL	OA5-CA3-CA4-CA6
158	n5	802	3PE	O11-C1-C2-C3
158	N5	802	3PE	O11-C1-C2-C3
153	2k	101	CDL	C54-C55-C56-C57
153	6a	201	CDL	CB4-CB3-OB5-PB2
153	l	301	CDL	C1-CA2-OA2-PA1
153	m2	404	CDL	CB4-CB3-OB5-PB2
153	6A	201	CDL	CB4-CB3-OB5-PB2
153	2K	101	CDL	C54-C55-C56-C57
153	m1	405	CDL	CA5-C11-C12-C13
153	bm	301	CDL	CA7-C31-C32-C33
153	M1	405	CDL	CA5-C11-C12-C13
152	TC	102	PC1	C35-C36-C37-C38
153	b3	102	CDL	C55-C56-C57-C58
153	T	204	CDL	C57-C58-C59-C60
153	t	204	CDL	C57-C58-C59-C60
153	R	201	CDL	C51-C52-C53-C54
160	qh	201	PX2	C7-C8-C9-C10
153	r	201	CDL	C51-C52-C53-C54
153	td	101	CDL	C16-C17-C18-C19
153	A1	101	CDL	C16-C17-C18-C19
153	B3	102	CDL	C55-C56-C57-C58
153	q	202	CDL	C72-C71-CB7-OB8
153	Q	202	CDL	C72-C71-CB7-OB8
166	qC	501	HEM	C2B-C3B-CAB-CBB
166	qC	502	HEM	C2C-C3C-CAC-CBC
166	QC	501	HEM	C2B-C3B-CAB-CBB
152	tc	102	PC1	C35-C36-C37-C38
153	c1	701	CDL	C15-C16-C17-C18
152	a	501	PC1	C11-C12-N-C15
152	m	301	PC1	C11-C12-N-C15
152	m	305	PC1	C11-C12-N-C14
152	m2	405	PC1	C11-C12-N-C15
152	qJ	101	PC1	C11-C12-N-C14
152	t1	602	PC1	C11-C12-N-C14
152	M	303	PC1	C11-C12-N-C15
152	QJ	102	PC1	C11-C12-N-C14
152	T1	602	PC1	C11-C12-N-C14
160	r	202	PX2	C1-C2-O7-C16

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Mol	Chain	Res	Type	Atoms
153	C1	701	CDL	C15-C16-C17-C18
152	V	202	PC1	C24-C25-C26-C27
152	v	202	PC1	C24-C25-C26-C27
153	m2	404	CDL	C75-C76-C77-C78
153	c1	701	CDL	C14-C15-C16-C17
153	M2	404	CDL	C75-C76-C77-C78
153	I	302	CDL	C38-C39-C40-C41
152	n5	801	PC1	C26-C27-C28-C29
153	i	301	CDL	C38-C39-C40-C41
152	2j	201	PC1	O11-C1-C2-O21
152	v	201	PC1	O11-C1-C2-O21
152	w	201	PC1	O11-C1-C2-O21
152	qJ	101	PC1	O11-C1-C2-O21
152	tc	102	PC1	O11-C1-C2-O21
152	2J	201	PC1	O11-C1-C2-O21
152	V	201	PC1	O11-C1-C2-O21
152	W	201	PC1	O11-C1-C2-O21
152	QJ	102	PC1	O11-C1-C2-O21
152	TC	102	PC1	O11-C1-C2-O21
153	2g	203	CDL	OB5-CB3-CB4-OB6
153	6c	202	CDL	OB5-CB3-CB4-OB6
153	c1	701	CDL	OA5-CA3-CA4-OA6
153	j	301	CDL	OB5-CB3-CB4-OB6
153	m	306	CDL	OB5-CB3-CB4-OB6
153	m1	404	CDL	OB5-CB3-CB4-OB6
153	m3	403	CDL	OB5-CB3-CB4-OB6
153	q	202	CDL	OB5-CB3-CB4-OB6
153	q	203	CDL	OB5-CB3-CB4-OB6
153	r	201	CDL	OB5-CB3-CB4-OB6
153	sd	101	CDL	OA5-CA3-CA4-OA6
153	sd	101	CDL	OB5-CB3-CB4-OB6
153	a1	101	CDL	OB5-CB3-CB4-OB6
153	b3	101	CDL	OA5-CA3-CA4-OA6
153	b8	302	CDL	OB5-CB3-CB4-OB6
153	p1	403	CDL	OB5-CB3-CB4-OB6
153	qG	402	CDL	OB5-CB3-CB4-OB6
153	qI	203	CDL	OB5-CB3-CB4-OB6
153	qc	508	CDL	OB5-CB3-CB4-OB6
153	2G	203	CDL	OB5-CB3-CB4-OB6
153	C1	701	CDL	OA5-CA3-CA4-OA6
153	J	301	CDL	OB5-CB3-CB4-OB6
153	M	301	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
153	M1	404	CDL	OB5-CB3-CB4-OB6
153	M3	403	CDL	OB5-CB3-CB4-OB6
153	Q	202	CDL	OB5-CB3-CB4-OB6
153	R	201	CDL	OB5-CB3-CB4-OB6
153	SD	101	CDL	OA5-CA3-CA4-OA6
153	VB	703	CDL	OB5-CB3-CB4-OB6
153	Y7	501	CDL	OB5-CB3-CB4-OB6
153	A1	102	CDL	OB5-CB3-CB4-OB6
153	B3	101	CDL	OA5-CA3-CA4-OA6
153	B8	302	CDL	OB5-CB3-CB4-OB6
153	P1	403	CDL	OB5-CB3-CB4-OB6
153	QG	402	CDL	OB5-CB3-CB4-OB6
153	Qc	508	CDL	OB5-CB3-CB4-OB6
158	n5	802	3PE	O11-C1-C2-O21
158	N5	802	3PE	O11-C1-C2-O21
159	m2	406	P5S	O37-C2-C3-O16
159	M2	406	P5S	O37-C2-C3-O16
153	C1	701	CDL	C14-C15-C16-C17
158	T8	602	3PE	C2A-C2B-C2C-C2D
169	b6	201	T7X	C32-C33-C34-C35
158	t8	602	3PE	C2A-C2B-C2C-C2D
152	m2	407	PC1	C1-C2-C3-O31
152	n5	805	PC1	C1-C2-C3-O31
152	M2	407	PC1	C1-C2-C3-O31
152	N5	805	PC1	C1-C2-C3-O31
153	2k	101	CDL	CA3-CA4-CA6-OA8
153	7c	301	CDL	CA3-CA4-CA6-OA8
153	q	202	CDL	CB3-CB4-CB6-OB8
153	vb	701	CDL	CA3-CA4-CA6-OA8
153	n5	806	CDL	CB3-CB4-CB6-OB8
153	2K	101	CDL	CA3-CA4-CA6-OA8
153	Q	202	CDL	CB3-CB4-CB6-OB8
153	VB	701	CDL	CA3-CA4-CA6-OA8
153	Z	101	CDL	CB3-CB4-CB6-OB8
153	N5	806	CDL	CB3-CB4-CB6-OB8
158	w	203	3PE	C1-C2-C3-O31
158	W	203	3PE	C1-C2-C3-O31
160	r	202	PX2	C1-C2-C3-O5
152	qC	508	PC1	C31-C32-C33-C34
152	QC	508	PC1	C31-C32-C33-C34
166	qC	502	HEM	C4C-C3C-CAC-CBC
166	qc	503	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
166	Y5	203	HEM	C4C-C3C-CAC-CBC
166	QC	502	HEM	C4C-C3C-CAC-CBC
166	Qc	503	HEM	C4C-C3C-CAC-CBC
152	N5	801	PC1	C26-C27-C28-C29
154	c1	708	HEA	O11-C11-C12-C13
153	an	302	CDL	C78-C79-C80-C81
153	AN	302	CDL	C78-C79-C80-C81
169	B6	201	T7X	C32-C33-C34-C35
152	2f	301	PC1	C12-C11-O13-P
152	c1	706	PC1	C12-C11-O13-P
152	d	501	PC1	C12-C11-O13-P
152	j	302	PC1	C12-C11-O13-P
152	v	202	PC1	C12-C11-O13-P
152	n5	805	PC1	C12-C11-O13-P
152	qc	506	PC1	C12-C11-O13-P
152	t4	301	PC1	C12-C11-O13-P
152	2F	301	PC1	C12-C11-O13-P
152	C1	709	PC1	C12-C11-O13-P
152	D	501	PC1	C12-C11-O13-P
152	J	302	PC1	C12-C11-O13-P
152	V	202	PC1	C12-C11-O13-P
152	N5	805	PC1	C12-C11-O13-P
152	Qc	506	PC1	C12-C11-O13-P
152	T4	301	PC1	C12-C11-O13-P
158	y5	202	3PE	C12-C11-O13-P
158	Y5	202	3PE	C12-C11-O13-P
153	6C	203	CDL	C62-C63-C64-C65
153	e	403	CDL	C76-C77-C78-C79
152	qc	506	PC1	O21-C2-C3-O31
152	s8	301	PC1	O21-C2-C3-O31
152	t4	303	PC1	O21-C2-C3-O31
152	Qc	506	PC1	O21-C2-C3-O31
152	S8	301	PC1	O21-C2-C3-O31
153	m2	403	CDL	OA6-CA4-CA6-OA8
153	m3	401	CDL	OA6-CA4-CA6-OA8
153	q	202	CDL	OB6-CB4-CB6-OB8
153	t	201	CDL	OB6-CB4-CB6-OB8
153	t	204	CDL	OA6-CA4-CA6-OA8
153	z	101	CDL	OB6-CB4-CB6-OB8
153	7C	301	CDL	OA6-CA4-CA6-OA8
153	L	301	CDL	OB6-CB4-CB6-OB8
153	M2	403	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
153	M3	401	CDL	OA6-CA4-CA6-OA8
153	Q	202	CDL	OB6-CB4-CB6-OB8
153	T	201	CDL	OB6-CB4-CB6-OB8
153	T	204	CDL	OA6-CA4-CA6-OA8
153	Z	101	CDL	OB6-CB4-CB6-OB8
160	Y5	204	PX2	O7-C2-C3-O5
153	7C	301	CDL	C38-C39-C40-C41
153	E	403	CDL	C76-C77-C78-C79
152	M1	401	PC1	C25-C26-C27-C28
153	6c	202	CDL	C62-C63-C64-C65
153	7c	301	CDL	C38-C39-C40-C41
152	2g	202	PC1	C11-C12-N-C14
152	c1	707	PC1	C11-C12-N-C15
152	f	402	PC1	C11-C12-N-C13
152	f	402	PC1	C11-C12-N-C14
152	qE	304	PC1	C11-C12-N-C14
152	s8	301	PC1	C11-C12-N-C13
152	C1	710	PC1	C11-C12-N-C15
152	F	401	PC1	C11-C12-N-C13
152	F	401	PC1	C11-C12-N-C14
152	M	307	PC1	C11-C12-N-C14
152	M2	405	PC1	C11-C12-N-C15
152	QJ	101	PC1	C11-C12-N-C14
152	S8	301	PC1	C11-C12-N-C13
152	m1	401	PC1	C25-C26-C27-C28
167	a9	401	NDP	C2D-C1D-N1N-C6N
153	m2	401	CDL	CA5-C11-C12-C13
153	M2	401	CDL	CA5-C11-C12-C13
152	T4	301	PC1	C35-C36-C37-C38
152	t4	301	PC1	C35-C36-C37-C38
153	VB	706	CDL	C74-C75-C76-C77
152	qC	507	PC1	C2-C1-O11-P
152	QC	507	PC1	C2-C1-O11-P
153	e	402	CDL	C1-CA2-OA2-PA1
153	t	203	CDL	C1-CB2-OB2-PB2
153	qc	505	CDL	C1-CA2-OA2-PA1
153	L	301	CDL	C1-CA2-OA2-PA1
153	M2	404	CDL	CB4-CB3-OB5-PB2
153	T	203	CDL	C1-CB2-OB2-PB2
153	Qc	505	CDL	C1-CA2-OA2-PA1
152	tc	102	PC1	C34-C35-C36-C37
152	Qb	602	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
152	TC	102	PC1	C34-C35-C36-C37
153	vb	704	CDL	C74-C75-C76-C77
153	T	204	CDL	C19-C20-C21-C22
158	W	203	3PE	C35-C36-C37-C38
152	2f	301	PC1	O13-C11-C12-N
152	2f	302	PC1	O13-C11-C12-N
152	2g	202	PC1	O13-C11-C12-N
152	6a	202	PC1	O13-C11-C12-N
152	6c	203	PC1	O13-C11-C12-N
152	7a	202	PC1	O13-C11-C12-N
152	7c	303	PC1	O13-C11-C12-N
152	c1	706	PC1	O13-C11-C12-N
152	c1	711	PC1	O13-C11-C12-N
152	c3	606	PC1	O13-C11-C12-N
152	d	501	PC1	O13-C11-C12-N
152	i	304	PC1	O13-C11-C12-N
152	m2	407	PC1	O13-C11-C12-N
152	n	303	PC1	O13-C11-C12-N
152	v	202	PC1	O13-C11-C12-N
152	am	202	PC1	O13-C11-C12-N
152	n3	201	PC1	O13-C11-C12-N
152	n5	803	PC1	O13-C11-C12-N
152	n5	804	PC1	O13-C11-C12-N
152	p1	401	PC1	O13-C11-C12-N
152	qE	301	PC1	O13-C11-C12-N
152	qE	303	PC1	O13-C11-C12-N
152	qc	506	PC1	O13-C11-C12-N
152	qc	509	PC1	O13-C11-C12-N
152	qg	401	PC1	O13-C11-C12-N
152	t4	301	PC1	O13-C11-C12-N
152	tc	102	PC1	O13-C11-C12-N
152	te	102	PC1	O13-C11-C12-N
152	2F	301	PC1	O13-C11-C12-N
152	2F	302	PC1	O13-C11-C12-N
152	2G	202	PC1	O13-C11-C12-N
152	6A	202	PC1	O13-C11-C12-N
152	6C	201	PC1	O13-C11-C12-N
152	7A	202	PC1	O13-C11-C12-N
152	7C	303	PC1	O13-C11-C12-N
152	C1	709	PC1	O13-C11-C12-N
152	C1	711	PC1	O13-C11-C12-N
152	C3	606	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
152	D	501	PC1	O13-C11-C12-N
152	I	301	PC1	O13-C11-C12-N
152	M2	407	PC1	O13-C11-C12-N
152	N	303	PC1	O13-C11-C12-N
152	V	202	PC1	O13-C11-C12-N
152	AM	202	PC1	O13-C11-C12-N
152	N3	201	PC1	O13-C11-C12-N
152	N5	803	PC1	O13-C11-C12-N
152	N5	804	PC1	O13-C11-C12-N
152	P1	401	PC1	O13-C11-C12-N
152	QE	301	PC1	O13-C11-C12-N
152	QE	303	PC1	O13-C11-C12-N
152	Qc	506	PC1	O13-C11-C12-N
152	Qc	509	PC1	O13-C11-C12-N
152	Qg	401	PC1	O13-C11-C12-N
152	T4	301	PC1	O13-C11-C12-N
152	TC	102	PC1	O13-C11-C12-N
152	TE	102	PC1	O13-C11-C12-N
153	t	204	CDL	C19-C20-C21-C22
152	t4	301	PC1	O31-C31-C32-C33
152	2f	301	PC1	C25-C26-C27-C28
152	qe	303	PC1	C22-C23-C24-C25
152	2F	301	PC1	C25-C26-C27-C28
153	m2	404	CDL	CA2-C1-CB2-OB2
153	E	402	CDL	CB2-C1-CA2-OA2
153	M2	404	CDL	CA2-C1-CB2-OB2
152	Qe	303	PC1	C22-C23-C24-C25
160	qh	201	PX2	C19-C20-C21-C22
158	w	203	3PE	C35-C36-C37-C38
153	BM	301	CDL	CA7-C31-C32-C33
153	BM	301	CDL	C15-C16-C17-C18
152	c2	703	PC1	C24-C25-C26-C27
152	W	201	PC1	C33-C34-C35-C36
152	w	201	PC1	C33-C34-C35-C36
153	l	301	CDL	C16-C17-C18-C19
152	qe	301	PC1	C11-C12-N-C13
152	qi	203	PC1	C11-C12-N-C13
152	A	501	PC1	C11-C12-N-C15
152	Qe	301	PC1	C11-C12-N-C13
152	Qi	203	PC1	C11-C12-N-C13
152	S8	301	PC1	C11-C12-N-C14
152	TC	101	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
152	c3	602	PC1	C25-C26-C27-C28
152	C3	602	PC1	C25-C26-C27-C28
153	6C	202	CDL	C12-C13-C14-C15
160	Qh	201	PX2	C17-C18-C19-C20
152	C3	601	PC1	O31-C31-C32-C33
152	T4	301	PC1	O31-C31-C32-C33
153	L	301	CDL	C16-C17-C18-C19
153	Qg	402	CDL	C83-C84-C85-C86
152	qb	602	PC1	C26-C27-C28-C29
152	C2	701	PC1	C24-C25-C26-C27
153	qg	402	CDL	C83-C84-C85-C86
152	n	303	PC1	C33-C34-C35-C36
167	a9	401	NDP	C2D-C1D-N1N-C2N
167	A9	401	NDP	C2D-C1D-N1N-C6N
152	n1	301	PC1	O11-C1-C2-C3
152	qC	507	PC1	O11-C1-C2-C3
152	qJ	101	PC1	O11-C1-C2-C3
152	N1	301	PC1	O11-C1-C2-C3
152	QJ	102	PC1	O11-C1-C2-C3
152	TC	102	PC1	O11-C1-C2-C3
153	fs	203	CDL	OA5-CA3-CA4-CA6
153	m3	403	CDL	OB5-CB3-CB4-CB6
153	q	203	CDL	OB5-CB3-CB4-CB6
153	t	203	CDL	OB5-CB3-CB4-CB6
153	y7	501	CDL	OB5-CB3-CB4-CB6
153	b8	302	CDL	OB5-CB3-CB4-CB6
153	qC	503	CDL	OB5-CB3-CB4-CB6
153	qI	203	CDL	OB5-CB3-CB4-CB6
153	FS	204	CDL	OA5-CA3-CA4-CA6
153	M3	403	CDL	OB5-CB3-CB4-CB6
153	T	203	CDL	OB5-CB3-CB4-CB6
153	VB	703	CDL	OB5-CB3-CB4-CB6
153	Y7	501	CDL	OB5-CB3-CB4-CB6
153	A1	102	CDL	OB5-CB3-CB4-CB6
153	A9	403	CDL	OB5-CB3-CB4-CB6
153	B3	102	CDL	OB5-CB3-CB4-CB6
153	QC	503	CDL	OB5-CB3-CB4-CB6
153	C	301	CDL	OB5-CB3-CB4-CB6
153	c	301	CDL	OB5-CB3-CB4-CB6
158	bm	302	3PE	O11-C1-C2-C3
158	BM	302	3PE	O11-C1-C2-C3
159	m2	406	P5S	C1-C2-C3-O16

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Mol	Chain	Res	Type	Atoms
159	M2	406	P5S	C1-C2-C3-O16
152	a	503	PC1	C27-C28-C29-C2A
152	A	503	PC1	C27-C28-C29-C2A
153	bm	301	CDL	C15-C16-C17-C18
164	qC	506	U10	C18-C19-C21-C22
164	QC	506	U10	C18-C19-C21-C22
168	ab	201	ZMP	C19-C18-C21-O5
168	AB	201	ZMP	C19-C18-C21-O5
171	v1	501	FMN	N10-C1'-C2'-O2'
171	V1	501	FMN	N10-C1'-C2'-O2'
153	6c	201	CDL	C12-C13-C14-C15
153	5B	201	CDL	C38-C39-C40-C41
153	A9	402	CDL	C31-C32-C33-C34
153	n6	302	CDL	O1-C1-CA2-OA2
152	qg	401	PC1	C23-C24-C25-C26
153	a9	402	CDL	C31-C32-C33-C34
153	N6	302	CDL	C58-C59-C60-C61
153	5b	201	CDL	C38-C39-C40-C41
152	N6	301	PC1	C31-C32-C33-C34
152	p1	401	PC1	C2-C1-O11-P
152	qg	401	PC1	C2-C1-O11-P
152	P1	401	PC1	C2-C1-O11-P
152	Qg	401	PC1	C2-C1-O11-P
153	7c	302	CDL	CB4-CB3-OB5-PB2
153	a	505	CDL	C1-CA2-OA2-PA1
153	c1	701	CDL	C1-CA2-OA2-PA1
153	c1	709	CDL	CA4-CA3-OA5-PA1
153	j	301	CDL	C1-CA2-OA2-PA1
153	m2	403	CDL	C1-CA2-OA2-PA1
153	n	304	CDL	C1-CB2-OB2-PB2
153	b3	101	CDL	C1-CA2-OA2-PA1
153	n5	806	CDL	C1-CB2-OB2-PB2
153	qC	503	CDL	C1-CA2-OA2-PA1
153	qG	402	CDL	C1-CB2-OB2-PB2
153	7C	302	CDL	CB4-CB3-OB5-PB2
153	E	402	CDL	C1-CA2-OA2-PA1
153	M2	403	CDL	C1-CA2-OA2-PA1
153	N	304	CDL	C1-CB2-OB2-PB2
153	VB	705	CDL	C1-CA2-OA2-PA1
153	B3	101	CDL	C1-CA2-OA2-PA1
153	N5	806	CDL	C1-CB2-OB2-PB2
153	QC	503	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
153	QG	402	CDL	C1-CB2-OB2-PB2
153	n6	302	CDL	C58-C59-C60-C61
151	2e	401	HEC	C4B-C3B-CAB-CBB
151	2e	401	HEC	C4C-C3C-CAC-CBC
151	qD	401	HEC	C4B-C3B-CAB-CBB
151	qd	401	HEC	C4B-C3B-CAB-CBB
151	2E	401	HEC	C4B-C3B-CAB-CBB
151	2E	401	HEC	C4C-C3C-CAC-CBC
151	QD	401	HEC	C4B-C3B-CAB-CBB
151	Qd	401	HEC	C4B-C3B-CAB-CBB
152	Qg	401	PC1	C23-C24-C25-C26
153	I	302	CDL	C31-C32-C33-C34
152	c3	601	PC1	O31-C31-C32-C33
152	2f	301	PC1	O11-C1-C2-O21
152	m	301	PC1	O11-C1-C2-O21
152	qC	507	PC1	O11-C1-C2-O21
152	2F	301	PC1	O11-C1-C2-O21
152	M	303	PC1	O11-C1-C2-O21
152	QC	507	PC1	O11-C1-C2-O21
153	7a	201	CDL	OB5-CB3-CB4-OB6
153	7a	203	CDL	OB5-CB3-CB4-OB6
153	a	504	CDL	OB5-CB3-CB4-OB6
153	f	401	CDL	OB5-CB3-CB4-OB6
153	m2	401	CDL	OB5-CB3-CB4-OB6
153	m2	403	CDL	OB5-CB3-CB4-OB6
153	n	304	CDL	OB5-CB3-CB4-OB6
153	t	203	CDL	OB5-CB3-CB4-OB6
153	vb	701	CDL	OB5-CB3-CB4-OB6
153	y7	501	CDL	OB5-CB3-CB4-OB6
153	a9	403	CDL	OB5-CB3-CB4-OB6
153	c4	401	CDL	OB5-CB3-CB4-OB6
153	qB	601	CDL	OB5-CB3-CB4-OB6
153	qD	402	CDL	OA5-CA3-CA4-OA6
153	qD	402	CDL	OB5-CB3-CB4-OB6
153	qb	601	CDL	OB5-CB3-CB4-OB6
153	t5	301	CDL	OB5-CB3-CB4-OB6
153	2G	204	CDL	OB5-CB3-CB4-OB6
153	6C	203	CDL	OB5-CB3-CB4-OB6
153	7A	201	CDL	OB5-CB3-CB4-OB6
153	7A	203	CDL	OB5-CB3-CB4-OB6
153	A	504	CDL	OB5-CB3-CB4-OB6
153	F	402	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
153	M2	401	CDL	OB5-CB3-CB4-OB6
153	M2	403	CDL	OB5-CB3-CB4-OB6
153	N	304	CDL	OB5-CB3-CB4-OB6
153	T	203	CDL	OB5-CB3-CB4-OB6
153	VB	701	CDL	OB5-CB3-CB4-OB6
153	A1	102	CDL	OA5-CA3-CA4-OA6
153	A9	403	CDL	OB5-CB3-CB4-OB6
153	B3	102	CDL	OB5-CB3-CB4-OB6
153	C4	401	CDL	OB5-CB3-CB4-OB6
153	QB	601	CDL	OB5-CB3-CB4-OB6
153	QD	402	CDL	OA5-CA3-CA4-OA6
153	QD	402	CDL	OB5-CB3-CB4-OB6
153	T5	301	CDL	OB5-CB3-CB4-OB6
158	a3	201	3PE	O11-C1-C2-O21
158	A3	201	3PE	O11-C1-C2-O21
152	TC	101	PC1	C26-C27-C28-C29
152	c1	711	PC1	C11-C12-N-C15
152	qi	203	PC1	C11-C12-N-C14
152	s8	301	PC1	C11-C12-N-C14
152	tc	101	PC1	C11-C12-N-C13
152	C1	711	PC1	C11-C12-N-C15
152	C3	601	PC1	C11-C12-N-C13
152	Qi	203	PC1	C11-C12-N-C14
152	n6	301	PC1	C31-C32-C33-C34
153	t7	201	CDL	CA5-C11-C12-C13
152	tc	101	PC1	C26-C27-C28-C29
153	n	304	CDL	C55-C56-C57-C58
153	N	304	CDL	C55-C56-C57-C58
152	2j	201	PC1	O21-C2-C3-O31
152	i	304	PC1	O21-C2-C3-O31
152	qe	301	PC1	O21-C2-C3-O31
152	I	301	PC1	O21-C2-C3-O31
152	T4	303	PC1	O21-C2-C3-O31
153	6c	201	CDL	OA6-CA4-CA6-OA8
153	l	301	CDL	OB6-CB4-CB6-OB8
153	sd	101	CDL	OB6-CB4-CB6-OB8
153	6C	202	CDL	OA6-CA4-CA6-OA8
153	SD	101	CDL	OB6-CB4-CB6-OB8
158	an	301	3PE	O21-C2-C3-O31
158	AN	301	3PE	O21-C2-C3-O31
153	c4	401	CDL	C57-C58-C59-C60
152	qe	301	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
152	Qe	301	PC1	C1-C2-C3-O31
153	a	504	CDL	CB3-CB4-CB6-OB8
153	l	301	CDL	CB3-CB4-CB6-OB8
153	m1	402	CDL	CB3-CB4-CB6-OB8
153	n	304	CDL	CB3-CB4-CB6-OB8
153	z	101	CDL	CB3-CB4-CB6-OB8
153	A	504	CDL	CB3-CB4-CB6-OB8
153	L	301	CDL	CB3-CB4-CB6-OB8
153	M1	402	CDL	CB3-CB4-CB6-OB8
153	N	304	CDL	CB3-CB4-CB6-OB8
158	a3	201	3PE	C1-C2-C3-O31
158	A3	201	3PE	C1-C2-C3-O31
159	m2	406	P5S	C20-C21-C22-C23
159	M2	406	P5S	C20-C21-C22-C23
152	d	501	PC1	O31-C31-C32-C33
152	D	501	PC1	O31-C31-C32-C33
153	2o	101	CDL	C12-C13-C14-C15
153	2O	101	CDL	C12-C13-C14-C15
168	ab	201	ZMP	C2-C3-C4-C5
153	T7	201	CDL	CA5-C11-C12-C13
153	i	301	CDL	C31-C32-C33-C34
153	C4	401	CDL	C57-C58-C59-C60
164	qc	507	U10	C2-C3-O3-C3M
164	Qc	507	U10	C2-C3-O3-C3M
153	B	501	CDL	C51-C52-C53-C54
168	AB	201	ZMP	C2-C3-C4-C5
151	2e	401	HEC	C2C-C3C-CAC-CBC
151	qD	401	HEC	C2B-C3B-CAB-CBB
151	qd	401	HEC	C2B-C3B-CAB-CBB
151	qd	401	HEC	C2C-C3C-CAC-CBC
151	2E	401	HEC	C2C-C3C-CAC-CBC
151	QD	401	HEC	C2B-C3B-CAB-CBB
151	Qd	401	HEC	C2B-C3B-CAB-CBB
151	Qd	401	HEC	C2C-C3C-CAC-CBC
152	2f	301	PC1	C11-O13-P-O12
152	2f	301	PC1	C11-O13-P-O11
152	2f	301	PC1	C11-C12-N-C15
152	2f	302	PC1	C1-O11-P-O14
152	2f	302	PC1	C1-O11-P-O13
152	2f	303	PC1	C11-O13-P-O14
152	2f	303	PC1	C11-O13-P-O11
152	2g	202	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
152	2j	201	PC1	C11-O13-P-O14
152	7c	303	PC1	C1-O11-P-O13
152	c1	704	PC1	C11-O13-P-O14
152	c1	704	PC1	C1-O11-P-O14
152	c1	704	PC1	C1-O11-P-O13
152	c1	707	PC1	C11-O13-P-O14
152	c2	703	PC1	C1-O11-P-O14
152	c3	601	PC1	C1-O11-P-O12
152	c3	603	PC1	C11-O13-P-O14
152	c3	603	PC1	C11-O13-P-O11
152	d	501	PC1	C1-O11-P-O14
152	d	501	PC1	C1-O11-P-O13
152	f	402	PC1	C1-O11-P-O12
152	i	304	PC1	C11-O13-P-O14
152	m	301	PC1	C11-O13-P-O14
152	m	305	PC1	C11-O13-P-O14
152	m	307	PC1	C1-O11-P-O13
152	m1	401	PC1	C1-O11-P-O12
152	m1	401	PC1	C1-O11-P-O14
152	m1	401	PC1	C1-O11-P-O13
152	m2	402	PC1	C11-O13-P-O14
152	m2	402	PC1	C1-O11-P-O12
152	n	302	PC1	C1-O11-P-O14
152	n	303	PC1	C11-O13-P-O14
152	v	201	PC1	C11-O13-P-O14
152	v	202	PC1	C11-O13-P-O14
152	v	202	PC1	C1-O11-P-O12
152	v	202	PC1	C1-O11-P-O13
152	an	304	PC1	C11-O13-P-O14
152	b9	201	PC1	C11-O13-P-O14
152	b9	201	PC1	C11-C12-N-C15
152	j1	400	PC1	C11-O13-P-O14
152	n3	201	PC1	C11-O13-P-O14
152	n5	801	PC1	C11-O13-P-O12
152	n5	803	PC1	C11-O13-P-O12
152	n5	803	PC1	C11-O13-P-O14
152	n5	803	PC1	C11-O13-P-O11
152	n5	803	PC1	C1-O11-P-O14
152	n5	804	PC1	C1-O11-P-O14
152	n5	805	PC1	C11-O13-P-O14
152	n5	805	PC1	C11-O13-P-O11
152	n5	805	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
152	n6	301	PC1	C1-O11-P-O14
152	qC	508	PC1	C1-O11-P-O12
152	qE	301	PC1	C1-O11-P-O14
152	qI	201	PC1	C1-O11-P-O14
152	qJ	101	PC1	C11-C12-N-C13
152	qc	506	PC1	C1-O11-P-O13
152	qc	509	PC1	C1-O11-P-O12
152	qe	303	PC1	C11-O13-P-O12
152	qi	203	PC1	C1-O11-P-O14
152	s8	301	PC1	C11-O13-P-O14
152	t1	602	PC1	C1-O11-P-O14
152	t4	301	PC1	C11-O13-P-O11
152	t4	303	PC1	C1-O11-P-O14
152	tc	102	PC1	C11-O13-P-O12
152	te	102	PC1	C1-O11-P-O13
152	2F	301	PC1	C11-O13-P-O12
152	2F	301	PC1	C11-O13-P-O11
152	2F	301	PC1	C11-C12-N-C15
152	2F	302	PC1	C1-O11-P-O14
152	2F	302	PC1	C1-O11-P-O13
152	2F	303	PC1	C11-O13-P-O14
152	2F	303	PC1	C11-O13-P-O11
152	2G	202	PC1	C11-O13-P-O14
152	2G	202	PC1	C11-C12-N-C15
152	2J	201	PC1	C11-O13-P-O14
152	7C	303	PC1	C1-O11-P-O13
152	C1	706	PC1	C11-O13-P-O14
152	C1	706	PC1	C1-O11-P-O14
152	C1	706	PC1	C1-O11-P-O13
152	C1	710	PC1	C11-O13-P-O14
152	C2	701	PC1	C1-O11-P-O14
152	C3	601	PC1	C1-O11-P-O12
152	C3	603	PC1	C11-O13-P-O14
152	D	501	PC1	C1-O11-P-O14
152	D	501	PC1	C1-O11-P-O13
152	F	401	PC1	C1-O11-P-O12
152	I	301	PC1	C11-O13-P-O14
152	M	302	PC1	C1-O11-P-O13
152	M	303	PC1	C11-O13-P-O14
152	M	307	PC1	C11-O13-P-O14
152	M1	401	PC1	C1-O11-P-O12
152	M1	401	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
152	M1	401	PC1	C1-O11-P-O13
152	M2	402	PC1	C11-O13-P-O14
152	M2	402	PC1	C1-O11-P-O12
152	N	302	PC1	C1-O11-P-O14
152	N	303	PC1	C11-O13-P-O14
152	V	201	PC1	C11-O13-P-O14
152	V	202	PC1	C11-O13-P-O14
152	V	202	PC1	C1-O11-P-O12
152	V	202	PC1	C1-O11-P-O13
152	AN	304	PC1	C11-O13-P-O14
152	B9	201	PC1	C11-O13-P-O14
152	B9	201	PC1	C11-C12-N-C15
152	J1	400	PC1	C11-O13-P-O14
152	N3	201	PC1	C11-O13-P-O14
152	N5	801	PC1	C11-O13-P-O12
152	N5	803	PC1	C11-O13-P-O12
152	N5	803	PC1	C11-O13-P-O14
152	N5	803	PC1	C11-O13-P-O11
152	N5	803	PC1	C1-O11-P-O14
152	N5	804	PC1	C1-O11-P-O14
152	N5	805	PC1	C11-O13-P-O14
152	N5	805	PC1	C11-O13-P-O11
152	N6	301	PC1	C1-O11-P-O14
152	QC	508	PC1	C1-O11-P-O12
152	QE	301	PC1	C1-O11-P-O14
152	QJ	102	PC1	C11-C12-N-C13
152	Qc	506	PC1	C1-O11-P-O13
152	Qc	509	PC1	C1-O11-P-O12
152	Qe	303	PC1	C11-O13-P-O12
152	Qi	203	PC1	C1-O11-P-O14
152	S8	301	PC1	C11-O13-P-O14
152	T1	602	PC1	C1-O11-P-O14
152	T4	301	PC1	C11-O13-P-O11
152	T4	301	PC1	C11-C12-N-C14
152	T4	303	PC1	C1-O11-P-O14
152	TC	101	PC1	C11-C12-N-C14
152	TC	102	PC1	C11-O13-P-O12
153	2g	201	CDL	CB3-OB5-PB2-OB2
153	2g	201	CDL	CB3-OB5-PB2-OB4
153	2g	204	CDL	CA3-OA5-PA1-OA2
153	2g	204	CDL	CA3-OA5-PA1-OA3
153	2g	204	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
153	2k	101	CDL	CA2-OA2-PA1-OA3
153	2k	101	CDL	CA3-OA5-PA1-OA3
153	2o	101	CDL	CB2-OB2-PB2-OB3
153	2o	101	CDL	CB3-OB5-PB2-OB2
153	6a	201	CDL	CA2-OA2-PA1-OA4
153	6a	201	CDL	CA3-OA5-PA1-OA2
153	6a	201	CDL	CB3-OB5-PB2-OB3
153	6c	201	CDL	CB2-OB2-PB2-OB5
153	6c	201	CDL	CB3-OB5-PB2-OB2
153	6c	202	CDL	CA3-OA5-PA1-OA3
153	7a	201	CDL	CA3-OA5-PA1-OA4
153	7a	201	CDL	CB2-OB2-PB2-OB4
153	7a	203	CDL	CA2-OA2-PA1-OA4
153	7a	203	CDL	CB2-OB2-PB2-OB3
153	7a	203	CDL	CB3-OB5-PB2-OB2
153	7c	301	CDL	CA3-OA5-PA1-OA3
153	7c	301	CDL	CB2-OB2-PB2-OB3
153	7c	301	CDL	CB2-OB2-PB2-OB4
153	7c	301	CDL	CB2-OB2-PB2-OB5
153	7c	301	CDL	CB3-OB5-PB2-OB3
153	7c	302	CDL	CB2-OB2-PB2-OB4
153	a	502	CDL	CA2-OA2-PA1-OA4
153	a	502	CDL	CB2-OB2-PB2-OB5
153	a	502	CDL	CB3-OB5-PB2-OB3
153	a	504	CDL	CA2-OA2-PA1-OA5
153	a	504	CDL	CB3-OB5-PB2-OB2
153	b	501	CDL	CB3-OB5-PB2-OB3
153	c1	701	CDL	CA3-OA5-PA1-OA3
153	c1	701	CDL	CB3-OB5-PB2-OB2
153	c1	703	CDL	CA3-OA5-PA1-OA4
153	c1	709	CDL	CB3-OB5-PB2-OB2
153	c1	709	CDL	CB3-OB5-PB2-OB4
153	e	401	CDL	CB2-OB2-PB2-OB5
153	e	401	CDL	CB3-OB5-PB2-OB2
153	e	401	CDL	CB3-OB5-PB2-OB4
153	e	402	CDL	CA3-OA5-PA1-OA3
153	e	403	CDL	CB3-OB5-PB2-OB3
153	fs	203	CDL	CA3-OA5-PA1-OA3
153	i	301	CDL	CA3-OA5-PA1-OA2
153	i	301	CDL	CA3-OA5-PA1-OA4
153	i	301	CDL	CB3-OB5-PB2-OB4
153	i	302	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	i	302	CDL	CA3-OA5-PA1-OA4
153	i	302	CDL	CB2-OB2-PB2-OB4
153	i	302	CDL	CB2-OB2-PB2-OB5
153	j	301	CDL	CA2-OA2-PA1-OA4
153	l	301	CDL	CB2-OB2-PB2-OB5
153	m	302	CDL	CA3-OA5-PA1-OA2
153	m	302	CDL	CA3-OA5-PA1-OA3
153	m	302	CDL	CB3-OB5-PB2-OB3
153	m	303	CDL	CA2-OA2-PA1-OA4
153	m	303	CDL	CA2-OA2-PA1-OA5
153	m	303	CDL	CB3-OB5-PB2-OB3
153	m	304	CDL	CA2-OA2-PA1-OA3
153	m	304	CDL	CB2-OB2-PB2-OB5
153	m	306	CDL	CB2-OB2-PB2-OB3
153	m1	402	CDL	CA3-OA5-PA1-OA3
153	m1	404	CDL	CB3-OB5-PB2-OB2
153	m1	405	CDL	CB2-OB2-PB2-OB3
153	m1	405	CDL	CB3-OB5-PB2-OB2
153	m1	405	CDL	CB3-OB5-PB2-OB4
153	m2	401	CDL	CA2-OA2-PA1-OA3
153	m2	401	CDL	CB3-OB5-PB2-OB2
153	m2	401	CDL	CB3-OB5-PB2-OB3
153	m2	401	CDL	CB3-OB5-PB2-OB4
153	m2	403	CDL	CA3-OA5-PA1-OA3
153	m3	403	CDL	CB3-OB5-PB2-OB3
153	n	304	CDL	CA3-OA5-PA1-OA2
153	n	304	CDL	CA3-OA5-PA1-OA3
153	q	201	CDL	CB3-OB5-PB2-OB3
153	q	202	CDL	CB2-OB2-PB2-OB3
153	r	201	CDL	CB2-OB2-PB2-OB4
153	r	201	CDL	CB2-OB2-PB2-OB5
153	sd	101	CDL	CB2-OB2-PB2-OB3
153	sd	101	CDL	CB3-OB5-PB2-OB3
153	t	201	CDL	CA3-OA5-PA1-OA2
153	t	201	CDL	CA3-OA5-PA1-OA4
153	t	203	CDL	CA2-OA2-PA1-OA3
153	t	203	CDL	CA3-OA5-PA1-OA2
153	t	203	CDL	CA3-OA5-PA1-OA3
153	t	203	CDL	CA3-OA5-PA1-OA4
153	t	203	CDL	CB3-OB5-PB2-OB4
153	u	201	CDL	CB3-OB5-PB2-OB3
153	vb	701	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
153	vb	701	CDL	CB3-OB5-PB2-OB3
153	vb	704	CDL	CA3-OA5-PA1-OA2
153	vb	704	CDL	CA3-OA5-PA1-OA3
153	w	202	CDL	CA3-OA5-PA1-OA3
153	w	202	CDL	CB3-OB5-PB2-OB4
153	y7	501	CDL	CB2-OB2-PB2-OB3
153	z	101	CDL	CA2-OA2-PA1-OA4
153	z	101	CDL	CB3-OB5-PB2-OB3
153	5b	201	CDL	CA2-OA2-PA1-OA4
153	5b	201	CDL	CB2-OB2-PB2-OB5
153	5b	201	CDL	CB3-OB5-PB2-OB2
153	5b	201	CDL	CB3-OB5-PB2-OB4
153	a1	101	CDL	CB2-OB2-PB2-OB5
153	a9	402	CDL	CA3-OA5-PA1-OA2
153	a9	403	CDL	CB2-OB2-PB2-OB5
153	a9	403	CDL	CB3-OB5-PB2-OB2
153	a9	403	CDL	CB3-OB5-PB2-OB3
153	al	301	CDL	CA2-OA2-PA1-OA3
153	al	301	CDL	CB2-OB2-PB2-OB5
153	al	301	CDL	CB3-OB5-PB2-OB4
153	an	302	CDL	CA3-OA5-PA1-OA3
153	b3	101	CDL	CA3-OA5-PA1-OA3
153	b3	101	CDL	CB3-OB5-PB2-OB2
153	b3	102	CDL	CB3-OB5-PB2-OB3
153	b4	201	CDL	CA2-OA2-PA1-OA4
153	b8	302	CDL	CA2-OA2-PA1-OA3
153	b8	302	CDL	CB3-OB5-PB2-OB4
153	bm	301	CDL	CA2-OA2-PA1-OA4
153	c4	401	CDL	CB2-OB2-PB2-OB3
153	n5	806	CDL	CA3-OA5-PA1-OA4
153	n5	806	CDL	CB2-OB2-PB2-OB4
153	n5	806	CDL	CB2-OB2-PB2-OB5
153	n6	302	CDL	CA3-OA5-PA1-OA2
153	n6	302	CDL	CA3-OA5-PA1-OA4
153	p1	402	CDL	CA2-OA2-PA1-OA4
153	p1	402	CDL	CA2-OA2-PA1-OA5
153	p1	402	CDL	CA3-OA5-PA1-OA3
153	p1	402	CDL	CA3-OA5-PA1-OA4
153	p1	403	CDL	CA3-OA5-PA1-OA3
153	qB	601	CDL	CB3-OB5-PB2-OB3
153	qC	503	CDL	CA3-OA5-PA1-OA3
153	qC	504	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	qC	504	CDL	CA3-OA5-PA1-OA4
153	qD	402	CDL	CA3-OA5-PA1-OA2
153	qD	402	CDL	CA3-OA5-PA1-OA4
153	qD	402	CDL	CB2-OB2-PB2-OB5
153	qG	402	CDL	CA3-OA5-PA1-OA2
153	qH	201	CDL	CA2-OA2-PA1-OA4
153	qH	201	CDL	CB3-OB5-PB2-OB4
153	qI	203	CDL	CA3-OA5-PA1-OA2
153	qI	203	CDL	CA3-OA5-PA1-OA3
153	qc	504	CDL	CA2-OA2-PA1-OA4
153	qc	504	CDL	CB2-OB2-PB2-OB3
153	qc	504	CDL	CB2-OB2-PB2-OB4
153	qc	505	CDL	CA3-OA5-PA1-OA4
153	qg	402	CDL	CA2-OA2-PA1-OA3
153	qg	402	CDL	CA2-OA2-PA1-OA5
153	qg	402	CDL	CB2-OB2-PB2-OB3
153	qg	402	CDL	CB2-OB2-PB2-OB4
153	qg	402	CDL	CB2-OB2-PB2-OB5
153	qg	402	CDL	CB3-OB5-PB2-OB3
153	qi	202	CDL	CB2-OB2-PB2-OB3
153	t1	601	CDL	CA3-OA5-PA1-OA2
153	t5	301	CDL	CA3-OA5-PA1-OA4
153	t7	201	CDL	CA2-OA2-PA1-OA3
153	t7	201	CDL	CA3-OA5-PA1-OA3
153	td	101	CDL	CA2-OA2-PA1-OA5
153	td	101	CDL	CB2-OB2-PB2-OB4
153	td	101	CDL	CB2-OB2-PB2-OB5
153	te	101	CDL	CA2-OA2-PA1-OA3
153	te	101	CDL	CA3-OA5-PA1-OA3
153	te	101	CDL	CB2-OB2-PB2-OB5
153	th	200	CDL	CA2-OA2-PA1-OA3
153	th	200	CDL	CA2-OA2-PA1-OA5
153	th	200	CDL	CA3-OA5-PA1-OA4
153	th	200	CDL	CB2-OB2-PB2-OB3
153	th	200	CDL	CB3-OB5-PB2-OB3
153	2G	201	CDL	CB3-OB5-PB2-OB2
153	2G	201	CDL	CB3-OB5-PB2-OB4
153	2G	204	CDL	CA3-OA5-PA1-OA2
153	2G	204	CDL	CA3-OA5-PA1-OA3
153	2G	204	CDL	CB2-OB2-PB2-OB3
153	2K	101	CDL	CA2-OA2-PA1-OA3
153	2K	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	2O	101	CDL	CB2-OB2-PB2-OB3
153	2O	101	CDL	CB3-OB5-PB2-OB2
153	6A	201	CDL	CA2-OA2-PA1-OA4
153	6A	201	CDL	CA3-OA5-PA1-OA2
153	6A	201	CDL	CB3-OB5-PB2-OB3
153	6C	202	CDL	CB2-OB2-PB2-OB5
153	6C	202	CDL	CB3-OB5-PB2-OB2
153	6C	203	CDL	CA3-OA5-PA1-OA3
153	6C	203	CDL	CB3-OB5-PB2-OB3
153	7A	201	CDL	CA3-OA5-PA1-OA4
153	7A	201	CDL	CB2-OB2-PB2-OB4
153	7A	203	CDL	CA2-OA2-PA1-OA4
153	7A	203	CDL	CB2-OB2-PB2-OB3
153	7C	301	CDL	CA3-OA5-PA1-OA3
153	7C	301	CDL	CB2-OB2-PB2-OB3
153	7C	301	CDL	CB2-OB2-PB2-OB4
153	7C	301	CDL	CB2-OB2-PB2-OB5
153	7C	301	CDL	CB3-OB5-PB2-OB3
153	7C	302	CDL	CB2-OB2-PB2-OB4
153	A	502	CDL	CA2-OA2-PA1-OA4
153	A	502	CDL	CB2-OB2-PB2-OB5
153	A	502	CDL	CB3-OB5-PB2-OB3
153	A	504	CDL	CA2-OA2-PA1-OA5
153	A	504	CDL	CB3-OB5-PB2-OB2
153	B	501	CDL	CB3-OB5-PB2-OB3
153	C1	701	CDL	CA3-OA5-PA1-OA3
153	C1	701	CDL	CB3-OB5-PB2-OB2
153	C1	707	CDL	CA3-OA5-PA1-OA4
153	C1	708	CDL	CB3-OB5-PB2-OB2
153	C1	708	CDL	CB3-OB5-PB2-OB4
153	E	401	CDL	CB2-OB2-PB2-OB5
153	E	401	CDL	CB3-OB5-PB2-OB2
153	E	401	CDL	CB3-OB5-PB2-OB4
153	E	402	CDL	CA3-OA5-PA1-OA3
153	E	403	CDL	CB3-OB5-PB2-OB2
153	E	403	CDL	CB3-OB5-PB2-OB3
153	FS	204	CDL	CA3-OA5-PA1-OA3
153	I	302	CDL	CA3-OA5-PA1-OA2
153	I	302	CDL	CA3-OA5-PA1-OA4
153	I	302	CDL	CB3-OB5-PB2-OB4
153	I	303	CDL	CA2-OA2-PA1-OA3
153	I	303	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
153	I	303	CDL	CB2-OB2-PB2-OB4
153	I	303	CDL	CB2-OB2-PB2-OB5
153	J	301	CDL	CA2-OA2-PA1-OA4
153	L	301	CDL	CB2-OB2-PB2-OB5
153	M	301	CDL	CB2-OB2-PB2-OB3
153	M	304	CDL	CA3-OA5-PA1-OA2
153	M	304	CDL	CA3-OA5-PA1-OA3
153	M	304	CDL	CB3-OB5-PB2-OB3
153	M	305	CDL	CA2-OA2-PA1-OA4
153	M	305	CDL	CA2-OA2-PA1-OA5
153	M	305	CDL	CB3-OB5-PB2-OB3
153	M	306	CDL	CA2-OA2-PA1-OA3
153	M	306	CDL	CA2-OA2-PA1-OA4
153	M	306	CDL	CB2-OB2-PB2-OB5
153	M1	402	CDL	CA3-OA5-PA1-OA3
153	M1	404	CDL	CB3-OB5-PB2-OB2
153	M1	405	CDL	CA3-OA5-PA1-OA4
153	M1	405	CDL	CB2-OB2-PB2-OB3
153	M1	405	CDL	CB3-OB5-PB2-OB2
153	M1	405	CDL	CB3-OB5-PB2-OB4
153	M2	401	CDL	CA2-OA2-PA1-OA3
153	M2	401	CDL	CB3-OB5-PB2-OB2
153	M2	401	CDL	CB3-OB5-PB2-OB3
153	M2	401	CDL	CB3-OB5-PB2-OB4
153	M2	403	CDL	CA3-OA5-PA1-OA3
153	M3	403	CDL	CB3-OB5-PB2-OB3
153	N	304	CDL	CA3-OA5-PA1-OA2
153	N	304	CDL	CA3-OA5-PA1-OA3
153	Q	201	CDL	CB3-OB5-PB2-OB3
153	Q	202	CDL	CB2-OB2-PB2-OB3
153	R	201	CDL	CB2-OB2-PB2-OB4
153	R	201	CDL	CB2-OB2-PB2-OB5
153	SD	101	CDL	CB2-OB2-PB2-OB3
153	SD	101	CDL	CB3-OB5-PB2-OB3
153	T	201	CDL	CA3-OA5-PA1-OA2
153	T	201	CDL	CA3-OA5-PA1-OA4
153	T	203	CDL	CA2-OA2-PA1-OA3
153	T	203	CDL	CA3-OA5-PA1-OA2
153	T	203	CDL	CA3-OA5-PA1-OA3
153	T	203	CDL	CA3-OA5-PA1-OA4
153	T	203	CDL	CB3-OB5-PB2-OB4
153	U	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
153	VB	701	CDL	CA2-OA2-PA1-OA4
153	VB	706	CDL	CA3-OA5-PA1-OA2
153	VB	706	CDL	CA3-OA5-PA1-OA3
153	W	202	CDL	CA3-OA5-PA1-OA3
153	W	202	CDL	CB3-OB5-PB2-OB4
153	Y5	201	CDL	CA3-OA5-PA1-OA2
153	Y5	201	CDL	CA3-OA5-PA1-OA3
153	Y7	501	CDL	CB2-OB2-PB2-OB3
153	Z	101	CDL	CA2-OA2-PA1-OA4
153	Z	101	CDL	CB3-OB5-PB2-OB3
153	5B	201	CDL	CA2-OA2-PA1-OA4
153	5B	201	CDL	CB2-OB2-PB2-OB5
153	5B	201	CDL	CB3-OB5-PB2-OB2
153	A1	101	CDL	CA2-OA2-PA1-OA5
153	A1	101	CDL	CB2-OB2-PB2-OB4
153	A1	101	CDL	CB2-OB2-PB2-OB5
153	A1	102	CDL	CB2-OB2-PB2-OB5
153	A9	402	CDL	CA3-OA5-PA1-OA2
153	A9	402	CDL	CA3-OA5-PA1-OA4
153	A9	403	CDL	CB2-OB2-PB2-OB4
153	A9	403	CDL	CB3-OB5-PB2-OB2
153	A9	403	CDL	CB3-OB5-PB2-OB3
153	AL	301	CDL	CA2-OA2-PA1-OA3
153	AL	301	CDL	CB2-OB2-PB2-OB5
153	AL	301	CDL	CB3-OB5-PB2-OB4
153	AN	302	CDL	CA3-OA5-PA1-OA3
153	B3	101	CDL	CA3-OA5-PA1-OA3
153	B3	101	CDL	CB3-OB5-PB2-OB2
153	B4	201	CDL	CA2-OA2-PA1-OA4
153	B8	302	CDL	CA2-OA2-PA1-OA3
153	B8	302	CDL	CB3-OB5-PB2-OB4
153	BM	301	CDL	CA2-OA2-PA1-OA4
153	C4	401	CDL	CB2-OB2-PB2-OB3
153	N5	806	CDL	CA3-OA5-PA1-OA4
153	N5	806	CDL	CB2-OB2-PB2-OB4
153	N5	806	CDL	CB2-OB2-PB2-OB5
153	N6	302	CDL	CA3-OA5-PA1-OA2
153	N6	302	CDL	CA3-OA5-PA1-OA4
153	P1	402	CDL	CA2-OA2-PA1-OA4
153	P1	402	CDL	CA2-OA2-PA1-OA5
153	P1	402	CDL	CA3-OA5-PA1-OA3
153	P1	402	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
153	P1	403	CDL	CA3-OA5-PA1-OA3
153	QB	601	CDL	CB3-OB5-PB2-OB3
153	QC	503	CDL	CA3-OA5-PA1-OA3
153	QC	504	CDL	CA2-OA2-PA1-OA3
153	QC	504	CDL	CA3-OA5-PA1-OA4
153	QD	402	CDL	CA3-OA5-PA1-OA2
153	QD	402	CDL	CA3-OA5-PA1-OA4
153	QD	402	CDL	CB2-OB2-PB2-OB5
153	QG	402	CDL	CA3-OA5-PA1-OA2
153	QH	201	CDL	CA2-OA2-PA1-OA4
153	QH	201	CDL	CB3-OB5-PB2-OB2
153	QH	201	CDL	CB3-OB5-PB2-OB4
153	QI	203	CDL	CA3-OA5-PA1-OA2
153	QI	203	CDL	CA3-OA5-PA1-OA3
153	QI	203	CDL	CB3-OB5-PB2-OB2
153	Qc	504	CDL	CA2-OA2-PA1-OA4
153	Qc	504	CDL	CB2-OB2-PB2-OB3
153	Qc	504	CDL	CB2-OB2-PB2-OB4
153	Qc	505	CDL	CA3-OA5-PA1-OA4
153	Qg	402	CDL	CA2-OA2-PA1-OA3
153	Qg	402	CDL	CA2-OA2-PA1-OA5
153	Qg	402	CDL	CB2-OB2-PB2-OB3
153	Qg	402	CDL	CB2-OB2-PB2-OB4
153	Qg	402	CDL	CB2-OB2-PB2-OB5
153	Qg	402	CDL	CB3-OB5-PB2-OB3
153	Qi	202	CDL	CB2-OB2-PB2-OB3
153	T1	601	CDL	CA3-OA5-PA1-OA2
153	T5	301	CDL	CA3-OA5-PA1-OA4
153	T7	201	CDL	CA2-OA2-PA1-OA3
153	T7	201	CDL	CA3-OA5-PA1-OA3
153	TE	101	CDL	CA2-OA2-PA1-OA3
153	TE	101	CDL	CA3-OA5-PA1-OA3
153	TE	101	CDL	CB2-OB2-PB2-OB5
153	TE	101	CDL	CB3-OB5-PB2-OB3
153	TH	200	CDL	CA2-OA2-PA1-OA3
153	TH	200	CDL	CA2-OA2-PA1-OA5
153	TH	200	CDL	CA3-OA5-PA1-OA4
153	TH	200	CDL	CB2-OB2-PB2-OB3
153	TH	200	CDL	CB3-OB5-PB2-OB3
153	C	301	CDL	CB3-OB5-PB2-OB2
153	c	301	CDL	CB3-OB5-PB2-OB2
153	u1	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
153	u1	101	CDL	CA3-OA5-PA1-OA3
153	u1	101	CDL	CB2-OB2-PB2-OB3
153	u1	101	CDL	CB2-OB2-PB2-OB4
153	u1	101	CDL	CB2-OB2-PB2-OB5
153	U1	101	CDL	CA2-OA2-PA1-OA3
153	U1	101	CDL	CA3-OA5-PA1-OA3
153	U1	101	CDL	CB2-OB2-PB2-OB3
153	U1	101	CDL	CB2-OB2-PB2-OB4
153	U1	101	CDL	CB2-OB2-PB2-OB5
154	c1	708	HEA	C11-C12-C13-C14
158	i	303	3PE	C1-O11-P-O13
158	i	303	3PE	C1-O11-P-O14
158	m2	408	3PE	C1-O11-P-O13
158	m2	408	3PE	C11-O13-P-O12
158	m2	408	3PE	O13-C11-C12-N
158	vb	705	3PE	C1-O11-P-O14
158	vb	705	3PE	C11-O13-P-O11
158	vb	705	3PE	C11-O13-P-O12
158	vb	705	3PE	C11-O13-P-O14
158	w	203	3PE	C1-O11-P-O13
158	w	203	3PE	C1-O11-P-O14
158	y5	202	3PE	C1-O11-P-O14
158	y5	202	3PE	C11-O13-P-O14
158	an	305	3PE	C11-O13-P-O12
158	an	305	3PE	C11-O13-P-O14
158	an	306	3PE	C1-O11-P-O13
158	an	306	3PE	O13-C11-C12-N
158	b4	202	3PE	C1-O11-P-O14
158	g2	301	3PE	C1-O11-P-O13
158	n4	601	3PE	C1-O11-P-O14
158	n5	802	3PE	C1-O11-P-O14
158	s8	304	3PE	C1-O11-P-O12
158	s8	304	3PE	C11-O13-P-O14
158	t8	602	3PE	C11-O13-P-O14
158	ta	201	3PE	C11-O13-P-O11
158	I	304	3PE	C1-O11-P-O13
158	I	304	3PE	C1-O11-P-O14
158	M2	408	3PE	C1-O11-P-O13
158	M2	408	3PE	C11-O13-P-O12
158	M2	408	3PE	O13-C11-C12-N
158	SC	101	3PE	O13-C11-C12-N
158	VB	707	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
158	VB	707	3PE	C11-O13-P-O11
158	VB	707	3PE	C11-O13-P-O12
158	VB	707	3PE	C11-O13-P-O14
158	Y5	202	3PE	C1-O11-P-O14
158	Y5	202	3PE	C11-O13-P-O14
158	AN	305	3PE	C11-O13-P-O14
158	AN	306	3PE	C1-O11-P-O13
158	AN	306	3PE	O13-C11-C12-N
158	B4	202	3PE	C1-O11-P-O14
158	G2	301	3PE	C1-O11-P-O13
158	N4	601	3PE	C1-O11-P-O14
158	N5	802	3PE	C1-O11-P-O14
158	S8	304	3PE	C1-O11-P-O12
158	S8	304	3PE	C11-O13-P-O14
158	T8	602	3PE	C11-O13-P-O14
159	m2	406	P5S	CB-OG-P12-O13
159	M2	406	P5S	CB-OG-P12-O13
161	sa	701	FAD	C5B-O5B-PA-O1A
161	sa	701	FAD	C5B-O5B-PA-O3P
161	SA	701	FAD	C5B-O5B-PA-O1A
161	SA	701	FAD	C5B-O5B-PA-O3P
168	ab	201	ZMP	O4-C17-C18-C21
168	AB	201	ZMP	O4-C17-C18-C21
153	W	202	CDL	CB5-C51-C52-C53
164	Qc	501	U10	C20-C19-C21-C22
153	vb	704	CDL	C12-C11-CA5-OA6
153	VB	706	CDL	C12-C11-CA5-OA6
153	6c	201	CDL	C32-C31-CA7-OA8
158	AN	306	3PE	C22-C23-C24-C25
152	T4	301	PC1	C28-C29-C2A-C2B
153	e	402	CDL	CB5-C51-C52-C53
152	m2	407	PC1	C2-C1-O11-P
152	w	201	PC1	C2-C1-O11-P
152	an	304	PC1	C2-C1-O11-P
152	n1	301	PC1	C2-C1-O11-P
152	tc	101	PC1	C2-C1-O11-P
152	M2	407	PC1	C2-C1-O11-P
152	W	201	PC1	C2-C1-O11-P
152	AN	304	PC1	C2-C1-O11-P
152	N1	301	PC1	C2-C1-O11-P
152	TC	101	PC1	C2-C1-O11-P
153	2g	203	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
153	2k	101	CDL	CA4-CA3-OA5-PA1
153	2k	101	CDL	CB4-CB3-OB5-PB2
153	a	502	CDL	CA4-CA3-OA5-PA1
153	c1	709	CDL	CB4-CB3-OB5-PB2
153	e	403	CDL	CB4-CB3-OB5-PB2
153	f	401	CDL	CB4-CB3-OB5-PB2
153	l	301	CDL	CA4-CA3-OA5-PA1
153	m	302	CDL	C1-CA2-OA2-PA1
153	m	304	CDL	C1-CB2-OB2-PB2
153	m2	403	CDL	C1-CB2-OB2-PB2
153	m3	403	CDL	C1-CB2-OB2-PB2
153	r	201	CDL	C1-CA2-OA2-PA1
153	t	203	CDL	CA4-CA3-OA5-PA1
153	vb	701	CDL	CB4-CB3-OB5-PB2
153	w	202	CDL	CA4-CA3-OA5-PA1
153	y7	501	CDL	CB4-CB3-OB5-PB2
153	a9	403	CDL	C1-CA2-OA2-PA1
153	an	302	CDL	CA4-CA3-OA5-PA1
153	an	302	CDL	CB4-CB3-OB5-PB2
153	p1	402	CDL	C1-CA2-OA2-PA1
153	p1	403	CDL	C1-CB2-OB2-PB2
153	qc	504	CDL	C1-CA2-OA2-PA1
153	qg	402	CDL	CA4-CA3-OA5-PA1
153	qg	402	CDL	C1-CB2-OB2-PB2
153	t1	601	CDL	CB4-CB3-OB5-PB2
153	t7	201	CDL	C1-CA2-OA2-PA1
153	2K	101	CDL	CA4-CA3-OA5-PA1
153	2K	101	CDL	CB4-CB3-OB5-PB2
153	A	502	CDL	CA4-CA3-OA5-PA1
153	C1	701	CDL	C1-CA2-OA2-PA1
153	C1	708	CDL	CA4-CA3-OA5-PA1
153	C1	708	CDL	CB4-CB3-OB5-PB2
153	E	403	CDL	CB4-CB3-OB5-PB2
153	F	402	CDL	CB4-CB3-OB5-PB2
153	J	301	CDL	C1-CA2-OA2-PA1
153	L	301	CDL	CA4-CA3-OA5-PA1
153	M	304	CDL	C1-CA2-OA2-PA1
153	M	306	CDL	C1-CB2-OB2-PB2
153	M2	403	CDL	C1-CB2-OB2-PB2
153	M3	403	CDL	C1-CB2-OB2-PB2
153	R	201	CDL	C1-CA2-OA2-PA1
153	T	203	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
153	VB	701	CDL	CB4-CB3-OB5-PB2
153	W	202	CDL	CA4-CA3-OA5-PA1
153	Y7	501	CDL	CB4-CB3-OB5-PB2
153	A9	403	CDL	C1-CA2-OA2-PA1
153	AN	302	CDL	CA4-CA3-OA5-PA1
153	AN	302	CDL	CB4-CB3-OB5-PB2
153	P1	402	CDL	C1-CA2-OA2-PA1
153	P1	403	CDL	C1-CB2-OB2-PB2
153	Qc	504	CDL	C1-CA2-OA2-PA1
153	Qg	402	CDL	CA4-CA3-OA5-PA1
153	Qg	402	CDL	C1-CB2-OB2-PB2
153	T1	601	CDL	CB4-CB3-OB5-PB2
153	T7	201	CDL	C1-CA2-OA2-PA1
158	y5	202	3PE	C2-C1-O11-P
158	Y5	202	3PE	C2-C1-O11-P
159	m2	406	P5S	C2-C3-O16-P12
159	M2	406	P5S	C2-C3-O16-P12
152	t4	301	PC1	C28-C29-C2A-C2B
158	an	306	3PE	C22-C23-C24-C25
168	AB	201	ZMP	C1-C2-C3-C4
153	w	202	CDL	CB5-C51-C52-C53
153	6C	202	CDL	C32-C31-CA7-OA8
168	ab	201	ZMP	C1-C2-C3-C4
153	M	305	CDL	C81-C82-C83-C84
153	b	501	CDL	C51-C52-C53-C54
153	A	504	CDL	C32-C33-C34-C35
152	A	501	PC1	C31-C32-C33-C34
153	a	504	CDL	C32-C33-C34-C35
153	m	303	CDL	C81-C82-C83-C84
167	A9	401	NDP	C2D-C1D-N1N-C2N
169	B6	201	T7X	C35-C36-C37-C38
152	2f	301	PC1	C1-C2-O21-C21
152	2f	302	PC1	C3-C2-O21-C21
152	b9	201	PC1	C1-C2-O21-C21
152	2F	301	PC1	C1-C2-O21-C21
152	2F	302	PC1	C3-C2-O21-C21
152	B9	201	PC1	C1-C2-O21-C21
153	a	502	CDL	CA3-CA4-OA6-CA5
153	A	502	CDL	CA3-CA4-OA6-CA5
160	R	202	PX2	C3-C2-O7-C16
169	b6	201	T7X	C35-C36-C37-C38
153	2o	101	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
164	sc	102	U10	C39-C41-C42-C43
164	SC	102	U10	C39-C41-C42-C43
152	a	501	PC1	C31-C32-C33-C34
152	n5	801	PC1	C21-C22-C23-C24
152	N5	801	PC1	C21-C22-C23-C24
153	A	504	CDL	C59-C60-C61-C62
152	2g	202	PC1	C11-C12-N-C15
152	c1	711	PC1	C11-C12-N-C13
152	m	301	PC1	C11-C12-N-C14
152	m2	405	PC1	C11-C12-N-C13
152	tc	101	PC1	C11-C12-N-C14
152	C1	711	PC1	C11-C12-N-C13
152	C3	601	PC1	C11-C12-N-C15
152	M	303	PC1	C11-C12-N-C14
152	2j	201	PC1	O11-C1-C2-C3
152	qi	203	PC1	O11-C1-C2-C3
152	t4	301	PC1	O11-C1-C2-C3
152	Qi	203	PC1	O11-C1-C2-C3
152	T4	301	PC1	O11-C1-C2-C3
153	c1	701	CDL	OA5-CA3-CA4-CA6
153	e	401	CDL	OB5-CB3-CB4-CB6
153	e	402	CDL	OB5-CB3-CB4-CB6
153	m	306	CDL	OB5-CB3-CB4-CB6
153	m1	402	CDL	OB5-CB3-CB4-CB6
153	z	101	CDL	OB5-CB3-CB4-CB6
153	p1	403	CDL	OB5-CB3-CB4-CB6
153	qg	402	CDL	OB5-CB3-CB4-CB6
153	C1	701	CDL	OA5-CA3-CA4-CA6
153	E	401	CDL	OB5-CB3-CB4-CB6
153	E	402	CDL	OB5-CB3-CB4-CB6
153	M	301	CDL	OB5-CB3-CB4-CB6
153	M1	402	CDL	OB5-CB3-CB4-CB6
153	Z	101	CDL	OB5-CB3-CB4-CB6
153	P1	403	CDL	OB5-CB3-CB4-CB6
153	QI	203	CDL	OB5-CB3-CB4-CB6
153	Qg	402	CDL	OB5-CB3-CB4-CB6
153	a	504	CDL	C59-C60-C61-C62
153	u	201	CDL	C53-C54-C55-C56
153	U	201	CDL	C53-C54-C55-C56
153	F	402	CDL	C16-C17-C18-C19
153	f	401	CDL	C16-C17-C18-C19
153	q	201	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
153	Q	201	CDL	CB5-C51-C52-C53
151	2e	401	HEC	C2D-C3D-CAD-CBD
151	2E	401	HEC	C2D-C3D-CAD-CBD
153	c	301	CDL	CA2-C1-CB2-OB2
152	n1	301	PC1	O11-C1-C2-O21
152	n5	804	PC1	O11-C1-C2-O21
152	N1	301	PC1	O11-C1-C2-O21
152	N5	804	PC1	O11-C1-C2-O21
153	i	301	CDL	OB5-CB3-CB4-OB6
153	a1	101	CDL	OA5-CA3-CA4-OA6
153	I	302	CDL	OB5-CB3-CB4-OB6
153	Z	101	CDL	OB5-CB3-CB4-OB6
153	QI	203	CDL	OB5-CB3-CB4-OB6
153	Qb	601	CDL	OB5-CB3-CB4-OB6
158	ta	201	3PE	O11-C1-C2-O21
158	TA	201	3PE	O11-C1-C2-O21
160	r	202	PX2	O4-C1-C2-O7
152	n5	801	PC1	C27-C28-C29-C2A
168	ab	201	ZMP	C2-C1-C22-C23
167	a9	401	NDP	O4D-C1D-N1N-C6N
164	qc	501	U10	C20-C19-C21-C22
153	a9	403	CDL	C32-C31-CA7-OA8
153	T	201	CDL	C12-C11-CA5-OA6
152	N5	801	PC1	C27-C28-C29-C2A
164	qC	506	U10	C2-C3-O3-C3M
164	qc	507	U10	C5-C4-O4-C4M
164	QC	506	U10	C2-C3-O3-C3M
164	Qc	507	U10	C5-C4-O4-C4M
153	Qg	402	CDL	CA7-C31-C32-C33
153	c3	604	CDL	CB4-CB3-OB5-PB2
153	b8	302	CDL	CA4-CA3-OA5-PA1
153	td	101	CDL	CA4-CA3-OA5-PA1
153	2G	203	CDL	C1-CB2-OB2-PB2
153	C3	604	CDL	CB4-CB3-OB5-PB2
153	A1	101	CDL	CA4-CA3-OA5-PA1
153	B8	302	CDL	CA4-CA3-OA5-PA1
152	t1	602	PC1	O21-C2-C3-O31
152	tc	102	PC1	O21-C2-C3-O31
152	2J	201	PC1	O21-C2-C3-O31
152	Qe	301	PC1	O21-C2-C3-O31
152	T1	602	PC1	O21-C2-C3-O31
152	TC	102	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
153	b	501	CDL	OB6-CB4-CB6-OB8
153	m1	402	CDL	OB6-CB4-CB6-OB8
153	A	504	CDL	OB6-CB4-CB6-OB8
153	B	501	CDL	OB6-CB4-CB6-OB8
153	M1	402	CDL	OB6-CB4-CB6-OB8
152	c3	603	PC1	O21-C21-C22-C23
152	qg	401	PC1	O21-C21-C22-C23
153	t	201	CDL	C12-C11-CA5-OA6
153	qi	202	CDL	C32-C31-CA7-OA8
153	2O	101	CDL	C72-C71-CB7-OB8
153	M2	401	CDL	C12-C11-CA5-OA6
153	A9	403	CDL	C32-C31-CA7-OA8
153	6a	201	CDL	O1-C1-CB2-OB2
153	6A	201	CDL	O1-C1-CB2-OB2
153	M	306	CDL	O1-C1-CB2-OB2
153	N6	302	CDL	C12-C13-C14-C15
152	7c	303	PC1	C32-C33-C34-C35
152	7C	303	PC1	C32-C33-C34-C35
153	n6	302	CDL	C12-C13-C14-C15
152	M2	405	PC1	C11-C12-N-C13
152	N	303	PC1	O31-C31-C32-C33
152	Qg	401	PC1	O21-C21-C22-C23
153	f	401	CDL	C32-C31-CA7-OA8
153	m2	401	CDL	C12-C11-CA5-OA6
153	F	402	CDL	C32-C31-CA7-OA8
153	Qi	202	CDL	C32-C31-CA7-OA8
153	BM	301	CDL	C76-C77-C78-C79
168	AB	201	ZMP	C2-C1-C22-C23
152	c1	704	PC1	C2A-C2B-C2C-C2D
153	t	204	CDL	C17-C18-C19-C20
152	C3	603	PC1	O21-C21-C22-C23
153	t1	601	CDL	C72-C71-CB7-OB8
152	i	304	PC1	C1-C2-C3-O31
152	m1	403	PC1	C1-C2-C3-O31
152	I	301	PC1	C1-C2-C3-O31
152	M1	403	PC1	C1-C2-C3-O31
153	2g	201	CDL	CB3-CB4-CB6-OB8
152	C1	706	PC1	C2A-C2B-C2C-C2D
153	l	301	CDL	C12-C13-C14-C15
153	6c	201	CDL	CA5-C11-C12-C13
158	w	203	3PE	C21-C22-C23-C24
158	W	203	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
153	T	204	CDL	C17-C18-C19-C20
153	a	505	CDL	C34-C35-C36-C37
153	VB	705	CDL	C34-C35-C36-C37
153	a	505	CDL	C32-C31-CA7-OA8
153	m	304	CDL	C52-C51-CB5-OB6
153	b8	302	CDL	C72-C71-CB7-OB8
153	M	306	CDL	C52-C51-CB5-OB6
153	T1	601	CDL	C72-C71-CB7-OB8
160	r	202	PX2	C4-C5-C6-C7
158	an	303	3PE	C27-C28-C29-C2A
158	AN	303	3PE	C27-C28-C29-C2A
153	c1	712	CDL	C72-C73-C74-C75
154	c1	708	HEA	C2D-C3D-CAD-CBD
153	6C	202	CDL	CA5-C11-C12-C13
153	VB	706	CDL	C12-C11-CA5-OA7
153	B8	302	CDL	C72-C71-CB7-OB8
158	a3	201	3PE	O21-C21-C22-C23
158	A3	201	3PE	O21-C21-C22-C23
153	n5	806	CDL	C31-C32-C33-C34
153	L	301	CDL	C12-C13-C14-C15
153	a	505	CDL	C14-C15-C16-C17
153	N5	806	CDL	C31-C32-C33-C34
153	VB	705	CDL	C14-C15-C16-C17
153	qg	402	CDL	CA7-C31-C32-C33
153	VB	705	CDL	C32-C31-CA7-OA8
152	qE	304	PC1	C11-C12-N-C15
152	t4	301	PC1	C11-C12-N-C14
152	QJ	101	PC1	C11-C12-N-C15
164	qC	506	U10	C4-C3-O3-C3M
164	QC	506	U10	C4-C3-O3-C3M
153	e	402	CDL	C51-C52-C53-C54
153	bm	301	CDL	C22-C23-C24-C25
153	Qi	202	CDL	CB7-C71-C72-C73
153	C1	712	CDL	C72-C73-C74-C75
153	6a	201	CDL	C32-C31-CA7-OA9
153	6A	201	CDL	C32-C31-CA7-OA9
153	b3	102	CDL	CB2-C1-CA2-OA2
159	m2	406	P5S	OXT-C-CA-N
153	z	101	CDL	C31-C32-C33-C34
153	qi	202	CDL	CB7-C71-C72-C73
152	N5	805	PC1	C35-C36-C37-C38
153	bm	301	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
169	B6	201	T7X	C31-C11-O18-C9
153	a	505	CDL	CA4-CA3-OA5-PA1
153	l	301	CDL	CB4-CB3-OB5-PB2
153	m2	404	CDL	CA4-CA3-OA5-PA1
153	am	201	CDL	C1-CA2-OA2-PA1
153	th	200	CDL	CB4-CB3-OB5-PB2
153	F	402	CDL	C1-CB2-OB2-PB2
153	L	301	CDL	CB4-CB3-OB5-PB2
153	M2	404	CDL	CA4-CA3-OA5-PA1
153	VB	705	CDL	CA4-CA3-OA5-PA1
153	TH	200	CDL	CB4-CB3-OB5-PB2
158	t8	601	3PE	C2-C1-O11-P
158	T8	601	3PE	C2-C1-O11-P
152	n5	805	PC1	C35-C36-C37-C38
153	BM	301	CDL	C22-C23-C24-C25
152	N6	301	PC1	C26-C27-C28-C29
153	Z	101	CDL	C31-C32-C33-C34
166	qc	503	HEM	C3D-CAD-CBD-CGD
166	Qc	503	HEM	C3D-CAD-CBD-CGD
169	b6	201	T7X	C31-C11-O18-C9
169	B6	201	T7X	O19-C11-O18-C9
153	n	304	CDL	C72-C71-CB7-OB8
153	N	304	CDL	C72-C71-CB7-OB8
153	a	504	CDL	OA5-CA3-CA4-OA6
153	z	101	CDL	OB5-CB3-CB4-OB6
153	A	504	CDL	OA5-CA3-CA4-OA6
153	qc	504	CDL	C33-C34-C35-C36
152	2J	201	PC1	O11-C1-C2-C3
153	Qc	504	CDL	C78-C79-C80-C81
158	an	305	3PE	C33-C34-C35-C36
169	b6	201	T7X	O19-C11-O18-C9
166	qC	502	HEM	C4B-C3B-CAB-CBB
166	qc	502	HEM	C4C-C3C-CAC-CBC
166	qc	503	HEM	C4B-C3B-CAB-CBB
166	QC	502	HEM	C4B-C3B-CAB-CBB
166	Qc	502	HEM	C4C-C3C-CAC-CBC
166	Qc	503	HEM	C4B-C3B-CAB-CBB
152	n6	301	PC1	C26-C27-C28-C29
153	E	402	CDL	C51-C52-C53-C54
160	r	202	PX2	O7-C16-C17-C18
160	qh	201	PX2	C20-C21-C22-C23
153	Qc	504	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
158	AN	305	3PE	C33-C34-C35-C36
159	m2	406	P5S	C42-C43-C44-C45
159	M2	406	P5S	C42-C43-C44-C45
152	TC	102	PC1	C3B-C3C-C3D-C3E
153	qc	504	CDL	C78-C79-C80-C81
152	2F	301	PC1	C11-C12-N-C14
152	S8	301	PC1	C11-C12-N-C15
153	m	304	CDL	O1-C1-CB2-OB2
153	N6	302	CDL	O1-C1-CA2-OA2
152	tc	102	PC1	C3B-C3C-C3D-C3E
159	M2	406	P5S	C40-C41-C42-C43
153	6C	203	CDL	C74-C75-C76-C77
160	Qh	201	PX2	C24-C25-C26-C27
159	m2	406	P5S	C40-C41-C42-C43
153	t7	201	CDL	CB5-C51-C52-C53
153	Qc	504	CDL	C73-C74-C75-C76
153	qc	504	CDL	C73-C74-C75-C76
152	c1	711	PC1	O21-C2-C3-O31
152	qG	401	PC1	O21-C2-C3-O31
152	QG	401	PC1	O21-C2-C3-O31
153	m1	404	CDL	OB6-CB4-CB6-OB8
153	te	101	CDL	OB6-CB4-CB6-OB8
153	M1	404	CDL	OB6-CB4-CB6-OB8
153	B3	102	CDL	OB6-CB4-CB6-OB8
153	TE	101	CDL	OB6-CB4-CB6-OB8
153	bm	301	CDL	C20-C21-C22-C23
153	BM	301	CDL	C20-C21-C22-C23
153	7a	201	CDL	C37-C38-C39-C40
158	t8	602	3PE	C28-C29-C2A-C2B
153	7A	201	CDL	C37-C38-C39-C40
160	R	202	PX2	C19-C20-C21-C22
153	vb	704	CDL	C12-C11-CA5-OA7
152	M1	403	PC1	C2A-C2B-C2C-C2D
153	6c	202	CDL	C74-C75-C76-C77
158	t8	602	3PE	C24-C25-C26-C27
158	T8	602	3PE	C24-C25-C26-C27
153	2G	204	CDL	C51-C52-C53-C54
152	m1	403	PC1	C2A-C2B-C2C-C2D
153	M1	402	CDL	C13-C14-C15-C16
158	T8	602	3PE	C28-C29-C2A-C2B
153	M2	401	CDL	C32-C31-CA7-OA9
153	e	401	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
152	2F	301	PC1	C32-C33-C34-C35
153	m1	402	CDL	C13-C14-C15-C16
167	a9	401	NDP	O4D-C1D-N1N-C2N
167	A9	401	NDP	O4D-C1D-N1N-C6N
153	2m	101	CDL	C20-C21-C22-C23
153	C1	707	CDL	C71-C72-C73-C74
152	2f	301	PC1	C32-C33-C34-C35
152	J1	400	PC1	C32-C33-C34-C35
153	c1	703	CDL	C71-C72-C73-C74
152	qc	509	PC1	C2-C1-O11-P
152	Qc	509	PC1	C2-C1-O11-P
152	S8	301	PC1	C2-C1-O11-P
153	7c	302	CDL	C1-CA2-OA2-PA1
153	f	401	CDL	C1-CB2-OB2-PB2
153	5b	201	CDL	CA4-CA3-OA5-PA1
153	7C	302	CDL	C1-CA2-OA2-PA1
153	5B	201	CDL	CA4-CA3-OA5-PA1
153	AL	301	CDL	C1-CA2-OA2-PA1
153	AM	201	CDL	C1-CA2-OA2-PA1
154	C1	703	HEA	CAD-CBD-CGD-O1D
152	N5	805	PC1	C36-C37-C38-C39
153	6C	202	CDL	C73-C74-C75-C76
152	j1	400	PC1	C32-C33-C34-C35
153	6a	201	CDL	C71-C72-C73-C74
153	c1	712	CDL	C53-C54-C55-C56
153	Qc	504	CDL	C71-C72-C73-C74
152	N5	805	PC1	C28-C29-C2A-C2B
153	n	304	CDL	C51-C52-C53-C54
153	N	304	CDL	C51-C52-C53-C54
152	c3	601	PC1	C11-C12-N-C13
152	f	402	PC1	C11-C12-N-C15
152	m	305	PC1	C11-C12-N-C13
152	qi	203	PC1	C11-C12-N-C15
152	s8	301	PC1	C11-C12-N-C15
152	F	401	PC1	C11-C12-N-C15
152	M	307	PC1	C11-C12-N-C13
152	Qi	203	PC1	C11-C12-N-C15
152	n5	805	PC1	C28-C29-C2A-C2B
153	6c	201	CDL	C73-C74-C75-C76
153	2M	101	CDL	C20-C21-C22-C23
158	w	203	3PE	C38-C39-C3A-C3B
159	M2	406	P5S	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
152	d	501	PC1	O22-C21-C22-C23
152	D	501	PC1	O22-C21-C22-C23
153	m2	401	CDL	C32-C31-CA7-OA9
153	A9	403	CDL	C51-C52-C53-C54
152	W	201	PC1	C3C-C3D-C3E-C3F
153	a9	403	CDL	C51-C52-C53-C54
153	C1	712	CDL	C53-C54-C55-C56
154	C1	703	HEA	CAA-CBA-CGA-O1A
153	6A	201	CDL	C71-C72-C73-C74
158	T8	602	3PE	C27-C28-C29-C2A
153	m1	404	CDL	CB3-CB4-CB6-OB8
153	2G	201	CDL	CB3-CB4-CB6-OB8
153	M1	404	CDL	CB3-CB4-CB6-OB8
152	n5	805	PC1	C36-C37-C38-C39
153	qc	504	CDL	C71-C72-C73-C74
153	Y5	201	CDL	C71-C72-C73-C74
153	Q	202	CDL	C12-C11-CA5-OA7
152	w	201	PC1	C3C-C3D-C3E-C3F
153	y5	201	CDL	C71-C72-C73-C74
166	qc	503	HEM	CAA-CBA-CGA-O1A
158	W	203	3PE	C38-C39-C3A-C3B
158	i	303	3PE	C25-C26-C27-C28
158	t8	602	3PE	C27-C28-C29-C2A
158	I	304	3PE	C25-C26-C27-C28
153	q	202	CDL	C12-C11-CA5-OA7
153	7c	301	CDL	C39-C40-C41-C42
153	i	301	CDL	C39-C40-C41-C42
152	V	202	PC1	C36-C37-C38-C39
153	7C	301	CDL	C39-C40-C41-C42
153	C4	401	CDL	C74-C75-C76-C77
160	y5	204	PX2	O5-C4-C5-C6
152	2g	202	PC1	C1-C2-O21-C21
152	c1	706	PC1	C3-C2-O21-C21
152	c3	601	PC1	C1-C2-O21-C21
152	m	301	PC1	C3-C2-O21-C21
152	qE	304	PC1	C3-C2-O21-C21
152	qe	303	PC1	C3-C2-O21-C21
152	t4	301	PC1	C1-C2-O21-C21
152	te	102	PC1	C1-C2-O21-C21
152	2G	202	PC1	C1-C2-O21-C21
152	A	501	PC1	C3-C2-O21-C21
152	C1	709	PC1	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
152	C3	601	PC1	C1-C2-O21-C21
152	M	303	PC1	C3-C2-O21-C21
152	QJ	101	PC1	C3-C2-O21-C21
152	Qe	303	PC1	C3-C2-O21-C21
152	T4	301	PC1	C1-C2-O21-C21
152	TE	102	PC1	C1-C2-O21-C21
153	2k	101	CDL	CA3-CA4-OA6-CA5
153	6a	201	CDL	CA6-CA4-OA6-CA5
153	c1	709	CDL	CA3-CA4-OA6-CA5
153	e	402	CDL	CB6-CB4-OB6-CB5
153	m1	405	CDL	CB3-CB4-OB6-CB5
153	m2	404	CDL	CB3-CB4-OB6-CB5
153	m3	403	CDL	CB3-CB4-OB6-CB5
153	q	201	CDL	CB6-CB4-OB6-CB5
153	y7	501	CDL	CA6-CA4-OA6-CA5
153	5b	201	CDL	CA3-CA4-OA6-CA5
153	a1	101	CDL	CA3-CA4-OA6-CA5
153	a9	402	CDL	CB3-CB4-OB6-CB5
153	qi	202	CDL	CA6-CA4-OA6-CA5
153	2K	101	CDL	CA3-CA4-OA6-CA5
153	6A	201	CDL	CA6-CA4-OA6-CA5
153	C1	708	CDL	CA3-CA4-OA6-CA5
153	E	402	CDL	CB6-CB4-OB6-CB5
153	M1	405	CDL	CB3-CB4-OB6-CB5
153	M2	404	CDL	CB3-CB4-OB6-CB5
153	M3	403	CDL	CB3-CB4-OB6-CB5
153	Q	201	CDL	CB6-CB4-OB6-CB5
153	Y7	501	CDL	CA6-CA4-OA6-CA5
153	5B	201	CDL	CA3-CA4-OA6-CA5
153	A1	102	CDL	CA3-CA4-OA6-CA5
153	A9	402	CDL	CB3-CB4-OB6-CB5
153	Qi	202	CDL	CA6-CA4-OA6-CA5
153	C	301	CDL	CA3-CA4-OA6-CA5
153	c	301	CDL	CA3-CA4-OA6-CA5
158	a3	201	3PE	C1-C2-O21-C21
158	bm	302	3PE	C3-C2-O21-C21
158	t8	601	3PE	C3-C2-O21-C21
158	A3	201	3PE	C1-C2-O21-C21
158	BM	302	3PE	C3-C2-O21-C21
158	T8	601	3PE	C3-C2-O21-C21
153	sd	101	CDL	C14-C15-C16-C17
152	v	202	PC1	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
153	bm	301	CDL	C33-C34-C35-C36
153	c4	401	CDL	C74-C75-C76-C77
153	I	302	CDL	C39-C40-C41-C42
151	qD	401	HEC	CAA-CBA-CGA-O1A
151	QD	401	HEC	CAA-CBA-CGA-O1A
166	qc	503	HEM	CAA-CBA-CGA-O2A
166	Qc	503	HEM	CAA-CBA-CGA-O1A
166	Qc	503	HEM	CAA-CBA-CGA-O2A
153	E	401	CDL	C16-C17-C18-C19
152	te	102	PC1	C23-C24-C25-C26
154	c1	708	HEA	CAA-CBA-CGA-O2A
153	QI	203	CDL	C52-C53-C54-C55
153	te	101	CDL	C32-C31-CA7-OA9
152	2f	301	PC1	C11-C12-N-C14
152	tc	101	PC1	C11-C12-N-C15
152	C3	601	PC1	C11-C12-N-C14
152	TC	101	PC1	C11-C12-N-C15
153	6c	201	CDL	C35-C36-C37-C38
153	i	301	CDL	C12-C13-C14-C15
153	qI	203	CDL	C52-C53-C54-C55
153	6C	202	CDL	C35-C36-C37-C38
151	Qd	401	HEC	CAA-CBA-CGA-O1A
154	c1	708	HEA	CAD-CBD-CGD-O1D
154	C1	703	HEA	CAA-CBA-CGA-O2A
152	v	202	PC1	C21-C22-C23-C24
152	V	202	PC1	C21-C22-C23-C24
153	I	302	CDL	C12-C13-C14-C15
153	2o	101	CDL	OA5-CA3-CA4-OA6
153	c1	709	CDL	OB5-CB3-CB4-OB6
153	C1	708	CDL	OB5-CB3-CB4-OB6
153	E	401	CDL	OB5-CB3-CB4-OB6
153	n	304	CDL	C53-C54-C55-C56
152	2F	303	PC1	O31-C31-C32-C33
153	c1	709	CDL	C12-C11-CA5-OA6
153	b4	201	CDL	C72-C71-CB7-OB8
153	C1	708	CDL	C12-C11-CA5-OA6
153	B4	201	CDL	C72-C71-CB7-OB8
153	N	304	CDL	C53-C54-C55-C56
151	qd	401	HEC	CAA-CBA-CGA-O1A
153	c1	712	CDL	C12-C13-C14-C15
158	M2	408	3PE	C32-C33-C34-C35
158	m2	408	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
152	s8	301	PC1	C2-C1-O11-P
153	2g	201	CDL	C1-CB2-OB2-PB2
153	6c	201	CDL	C1-CA2-OA2-PA1
153	6c	201	CDL	CA4-CA3-OA5-PA1
153	6c	201	CDL	C1-CB2-OB2-PB2
153	b	501	CDL	C1-CA2-OA2-PA1
153	m	303	CDL	CB4-CB3-OB5-PB2
153	m	306	CDL	C1-CB2-OB2-PB2
153	n	304	CDL	CA4-CA3-OA5-PA1
153	t	203	CDL	CB4-CB3-OB5-PB2
153	al	301	CDL	C1-CA2-OA2-PA1
153	b4	201	CDL	C1-CA2-OA2-PA1
153	t5	301	CDL	C1-CB2-OB2-PB2
153	6C	202	CDL	C1-CA2-OA2-PA1
153	6C	202	CDL	C1-CB2-OB2-PB2
153	M	305	CDL	CB4-CB3-OB5-PB2
153	N	304	CDL	CA4-CA3-OA5-PA1
153	T	203	CDL	CB4-CB3-OB5-PB2
153	QC	504	CDL	C1-CA2-OA2-PA1
153	T5	301	CDL	C1-CB2-OB2-PB2
166	qc	503	HEM	CAD-CBD-CGD-O1D
164	sc	102	U10	C20-C19-C21-C22
153	7a	201	CDL	OB5-CB3-CB4-CB6
153	c1	712	CDL	OB5-CB3-CB4-CB6
153	t	202	CDL	OA5-CA3-CA4-CA6
153	vb	704	CDL	OB5-CB3-CB4-CB6
153	7A	201	CDL	OB5-CB3-CB4-CB6
153	T	202	CDL	OA5-CA3-CA4-CA6
152	TE	102	PC1	C23-C24-C25-C26
153	C1	712	CDL	C12-C13-C14-C15
151	QD	401	HEC	CAA-CBA-CGA-O2A
166	qC	502	HEM	CAA-CBA-CGA-O1A
166	QC	502	HEM	CAA-CBA-CGA-O1A
166	Qc	503	HEM	CAD-CBD-CGD-O1D
153	2g	204	CDL	C52-C53-C54-C55
153	qC	503	CDL	C74-C75-C76-C77
153	QC	503	CDL	C74-C75-C76-C77
153	t	202	CDL	C13-C14-C15-C16
153	QI	203	CDL	C56-C57-C58-C59
152	D	501	PC1	C24-C25-C26-C27
153	7A	201	CDL	CB5-C51-C52-C53
152	C1	711	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
153	2g	201	CDL	OB6-CB4-CB6-OB8
153	a	504	CDL	OB6-CB4-CB6-OB8
153	b3	102	CDL	OB6-CB4-CB6-OB8
153	2G	201	CDL	OB6-CB4-CB6-OB8
166	qC	501	HEM	CAD-CBD-CGD-O1D
166	qC	502	HEM	CAA-CBA-CGA-O2A
166	QC	501	HEM	CAD-CBD-CGD-O2D
166	QC	502	HEM	CAA-CBA-CGA-O2A
152	d	501	PC1	C24-C25-C26-C27
153	6c	202	CDL	C32-C33-C34-C35
153	T	202	CDL	C13-C14-C15-C16
153	BM	301	CDL	C75-C76-C77-C78
153	qI	203	CDL	C56-C57-C58-C59
160	R	202	PX2	C21-C22-C23-C24
167	A9	401	NDP	O4D-C1D-N1N-C2N
153	n	304	CDL	CB5-C51-C52-C53
153	t	204	CDL	CB5-C51-C52-C53
153	N	304	CDL	CB5-C51-C52-C53
153	qB	601	CDL	C72-C71-CB7-OB8
153	QB	601	CDL	C72-C71-CB7-OB8
154	c1	708	HEA	C4D-C3D-CAD-CBD
151	qD	401	HEC	CAA-CBA-CGA-O2A
166	qC	501	HEM	CAD-CBD-CGD-O2D
166	QC	501	HEM	CAD-CBD-CGD-O1D
153	bm	301	CDL	C75-C76-C77-C78
153	6C	203	CDL	C32-C33-C34-C35
158	g2	301	3PE	C33-C34-C35-C36
152	qc	506	PC1	C33-C34-C35-C36
153	t	203	CDL	C20-C21-C22-C23
153	T	203	CDL	C20-C21-C22-C23
153	Qg	402	CDL	C33-C34-C35-C36
158	G2	301	3PE	C33-C34-C35-C36
152	c1	711	PC1	C11-C12-N-C14
152	C1	711	PC1	C11-C12-N-C14
153	T	204	CDL	CB5-C51-C52-C53
153	N6	302	CDL	C73-C74-C75-C76
164	SC	102	U10	C20-C19-C21-C22
167	a9	401	NDP	C2B-O2B-P2B-O1X
167	A9	401	NDP	C2B-O2B-P2B-O1X
153	A9	402	CDL	C73-C74-C75-C76
152	C4	403	PC1	O21-C21-C22-C23
153	SD	101	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
153	t5	301	CDL	C56-C57-C58-C59
169	b6	201	T7X	C13-C14-C15-C16
151	qd	401	HEC	CAA-CBA-CGA-O2A
154	c1	708	HEA	CAA-CBA-CGA-O1A
154	c1	708	HEA	CAD-CBD-CGD-O2D
154	C1	703	HEA	CAD-CBD-CGD-O2D
153	a9	402	CDL	C73-C74-C75-C76
152	c4	403	PC1	O21-C21-C22-C23
152	m1	401	PC1	C31-C32-C33-C34
153	Y5	201	CDL	CA5-C11-C12-C13
153	qg	402	CDL	C33-C34-C35-C36
153	T5	301	CDL	C56-C57-C58-C59
153	qi	202	CDL	C53-C54-C55-C56
153	BM	301	CDL	C33-C34-C35-C36
151	Qd	401	HEC	CAA-CBA-CGA-O2A
153	n6	302	CDL	C73-C74-C75-C76
153	C1	712	CDL	C77-C78-C79-C80
153	Qi	202	CDL	C53-C54-C55-C56
167	a9	401	NDP	PN-O3-PA-O1A
167	a9	401	NDP	PN-O3-PA-O2A
167	A9	401	NDP	PN-O3-PA-O1A
167	A9	401	NDP	PN-O3-PA-O2A
170	b9	202	ADP	PB-O3A-PA-O1A
170	B9	202	ADP	PB-O3A-PA-O1A
153	2M	101	CDL	C74-C75-C76-C77
158	b4	202	3PE	C23-C24-C25-C26
158	A3	202	3PE	C32-C33-C34-C35
152	M1	401	PC1	C31-C32-C33-C34
152	Qc	506	PC1	C33-C34-C35-C36
158	a3	202	3PE	C32-C33-C34-C35
158	B4	202	3PE	C23-C24-C25-C26
153	c1	712	CDL	C77-C78-C79-C80
169	B6	201	T7X	C13-C14-C15-C16
153	a	505	CDL	CB4-CB3-OB5-PB2
153	b	501	CDL	CB4-CB3-OB5-PB2
153	c1	709	CDL	C1-CB2-OB2-PB2
153	e	403	CDL	C1-CA2-OA2-PA1
153	q	202	CDL	CA4-CA3-OA5-PA1
153	r	201	CDL	C1-CB2-OB2-PB2
153	vb	701	CDL	C1-CA2-OA2-PA1
153	p1	402	CDL	CA4-CA3-OA5-PA1
153	qC	504	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
153	qD	402	CDL	CB4-CB3-OB5-PB2
153	qG	402	CDL	C1-CA2-OA2-PA1
153	t1	601	CDL	C1-CA2-OA2-PA1
153	2G	201	CDL	C1-CB2-OB2-PB2
153	6C	202	CDL	CA4-CA3-OA5-PA1
153	B	501	CDL	C1-CA2-OA2-PA1
153	B	501	CDL	CB4-CB3-OB5-PB2
153	C1	708	CDL	C1-CB2-OB2-PB2
153	E	403	CDL	C1-CA2-OA2-PA1
153	M	301	CDL	C1-CB2-OB2-PB2
153	Q	202	CDL	CA4-CA3-OA5-PA1
153	R	201	CDL	C1-CB2-OB2-PB2
153	VB	701	CDL	C1-CA2-OA2-PA1
153	VB	705	CDL	CB4-CB3-OB5-PB2
153	B4	201	CDL	C1-CA2-OA2-PA1
153	P1	402	CDL	CA4-CA3-OA5-PA1
153	QD	402	CDL	CB4-CB3-OB5-PB2
153	QG	402	CDL	C1-CA2-OA2-PA1
153	T1	601	CDL	C1-CA2-OA2-PA1
153	C	301	CDL	C1-CA2-OA2-PA1
153	C	301	CDL	CA4-CA3-OA5-PA1
153	c	301	CDL	C1-CA2-OA2-PA1
153	c	301	CDL	CA4-CA3-OA5-PA1
171	v1	501	FMN	C4'-C5'-O5'-P
171	V1	501	FMN	C4'-C5'-O5'-P
158	T8	601	3PE	C36-C37-C38-C39
152	c1	706	PC1	O21-C21-C22-C23
152	C1	709	PC1	O21-C21-C22-C23
153	P1	402	CDL	C52-C53-C54-C55
158	t8	601	3PE	C36-C37-C38-C39
153	7a	201	CDL	CB5-C51-C52-C53
153	f	401	CDL	C81-C82-C83-C84
153	m1	404	CDL	C22-C23-C24-C25
153	p1	402	CDL	C52-C53-C54-C55
153	qc	504	CDL	C75-C76-C77-C78
153	t5	301	CDL	C37-C38-C39-C40
153	M1	404	CDL	C22-C23-C24-C25
169	B6	201	T7X	C43-C44-C45-C46
152	5B	202	PC1	C28-C29-C2A-C2B
152	N6	301	PC1	C28-C29-C2A-C2B
153	T5	301	CDL	C37-C38-C39-C40
153	y5	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
153	F	402	CDL	C81-C82-C83-C84
152	c1	711	PC1	C1-C2-C3-O31
152	C1	711	PC1	C1-C2-C3-O31
153	a	505	CDL	CB3-CB4-CB6-OB8
153	m1	405	CDL	CB3-CB4-CB6-OB8
153	M1	405	CDL	CB3-CB4-CB6-OB8
153	VB	705	CDL	CB3-CB4-CB6-OB8
164	qC	506	U10	C14-C16-C17-C18
164	QC	506	U10	C14-C16-C17-C18
152	C3	602	PC1	C22-C23-C24-C25
153	Qc	504	CDL	C75-C76-C77-C78
151	2e	401	HEC	CAA-CBA-CGA-O2A
152	5b	202	PC1	C28-C29-C2A-C2B
153	7C	301	CDL	C53-C54-C55-C56
152	c3	602	PC1	C22-C23-C24-C25
153	bm	301	CDL	C73-C74-C75-C76
152	c1	704	PC1	C26-C27-C28-C29
153	7c	301	CDL	C53-C54-C55-C56
152	N6	301	PC1	C35-C36-C37-C38
152	C1	706	PC1	C26-C27-C28-C29
152	c3	601	PC1	O11-C1-C2-O21
152	C3	601	PC1	O11-C1-C2-O21
153	e	401	CDL	OB5-CB3-CB4-OB6
153	vb	704	CDL	OB5-CB3-CB4-OB6
153	qc	508	CDL	OA5-CA3-CA4-OA6
153	te	101	CDL	OB5-CB3-CB4-OB6
153	2O	101	CDL	OA5-CA3-CA4-OA6
153	Qc	508	CDL	OA5-CA3-CA4-OA6
153	TE	101	CDL	OB5-CB3-CB4-OB6
158	SC	101	3PE	O11-C1-C2-O21
152	m1	401	PC1	C2D-C2E-C2F-C2G
169	b6	201	T7X	C43-C44-C45-C46
152	n	303	PC1	O32-C31-C32-C33
153	c1	712	CDL	C52-C51-CB5-OB6
153	C1	712	CDL	C52-C51-CB5-OB6
153	B8	302	CDL	C12-C11-CA5-OA6
152	n6	301	PC1	C28-C29-C2A-C2B
152	n6	301	PC1	C35-C36-C37-C38
153	l	301	CDL	C71-C72-C73-C74
153	7C	301	CDL	C77-C78-C79-C80
153	BM	301	CDL	C73-C74-C75-C76
151	2E	401	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
152	N5	801	PC1	C35-C36-C37-C38
153	7c	301	CDL	C77-C78-C79-C80
153	2m	101	CDL	C75-C76-C77-C78
153	qc	508	CDL	C71-C72-C73-C74
158	G2	301	3PE	C3C-C3D-C3E-C3F
153	TE	101	CDL	C32-C31-CA7-OA9
152	n5	801	PC1	C35-C36-C37-C38
158	g2	301	3PE	C3C-C3D-C3E-C3F
152	M1	401	PC1	C2D-C2E-C2F-C2G
152	i	304	PC1	C11-C12-N-C14
152	T4	301	PC1	C11-C12-N-C15
154	C1	703	HEA	C11-C12-C13-C14
153	b8	302	CDL	C12-C11-CA5-OA6
153	2M	101	CDL	C12-C11-CA5-OA6
158	y5	202	3PE	O21-C21-C22-C23
158	Y5	202	3PE	O21-C21-C22-C23
158	A3	201	3PE	C22-C23-C24-C25
159	m2	406	P5S	C25-C26-C27-C28
152	Qb	602	PC1	C24-C25-C26-C27
158	a3	201	3PE	C22-C23-C24-C25
153	c1	709	CDL	OB5-CB3-CB4-CB6
153	r	201	CDL	OA5-CA3-CA4-CA6
153	bm	301	CDL	OA5-CA3-CA4-CA6
153	n6	302	CDL	OB5-CB3-CB4-CB6
153	C1	708	CDL	OB5-CB3-CB4-CB6
153	C1	712	CDL	OB5-CB3-CB4-CB6
153	R	201	CDL	OA5-CA3-CA4-CA6
153	VB	706	CDL	OB5-CB3-CB4-CB6
153	BM	301	CDL	OA5-CA3-CA4-CA6
153	N6	302	CDL	OB5-CB3-CB4-CB6
153	C1	712	CDL	C51-C52-C53-C54
153	L	301	CDL	C71-C72-C73-C74
153	Qc	508	CDL	C71-C72-C73-C74
152	n1	301	PC1	O21-C2-C3-O31
152	N1	301	PC1	O21-C2-C3-O31
153	r	201	CDL	OB6-CB4-CB6-OB8
153	am	201	CDL	OB6-CB4-CB6-OB8
153	E	402	CDL	OB6-CB4-CB6-OB8
153	R	201	CDL	OB6-CB4-CB6-OB8
153	AM	201	CDL	OB6-CB4-CB6-OB8
152	2f	303	PC1	O31-C31-C32-C33
152	6A	202	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
166	qc	503	HEM	CAD-CBD-CGD-O2D
159	m2	406	P5S	O37-C38-C39-C40
159	M2	406	P5S	O37-C38-C39-C40
160	R	202	PX2	O7-C16-C17-C18
153	2k	101	CDL	C55-C56-C57-C58
153	6C	203	CDL	C53-C54-C55-C56
159	M2	406	P5S	C25-C26-C27-C28
153	6c	202	CDL	C53-C54-C55-C56
153	N6	302	CDL	C13-C14-C15-C16
153	m1	402	CDL	C1-CA2-OA2-PA1
153	c4	401	CDL	C1-CB2-OB2-PB2
153	I	302	CDL	C1-CB2-OB2-PB2
153	M1	402	CDL	C1-CA2-OA2-PA1
153	C4	401	CDL	C1-CB2-OB2-PB2
160	r	202	PX2	C2-C1-O4-P1
153	n6	302	CDL	C13-C14-C15-C16
153	2K	101	CDL	C55-C56-C57-C58
153	L	301	CDL	C54-C55-C56-C57
158	B4	202	3PE	C26-C27-C28-C29
152	m1	401	PC1	C29-C2A-C2B-C2C
152	M1	401	PC1	C29-C2A-C2B-C2C
152	6a	202	PC1	C31-C32-C33-C34
153	T7	201	CDL	CB5-C51-C52-C53
153	2k	101	CDL	C53-C54-C55-C56
153	2K	101	CDL	C53-C54-C55-C56
158	b4	202	3PE	C26-C27-C28-C29
153	Qg	402	CDL	C56-C57-C58-C59
153	an	302	CDL	O1-C1-CA2-OA2
153	AN	302	CDL	O1-C1-CA2-OA2
153	qg	402	CDL	C56-C57-C58-C59
166	Qc	503	HEM	CAD-CBD-CGD-O2D
154	C1	703	HEA	C2D-C3D-CAD-CBD
153	c1	709	CDL	C12-C11-CA5-OA7
153	b4	201	CDL	C72-C71-CB7-OB9
153	C1	708	CDL	C12-C11-CA5-OA7
153	B4	201	CDL	C72-C71-CB7-OB9
153	l	301	CDL	C54-C55-C56-C57
166	y5	203	HEM	C2A-CAA-CBA-CGA
166	Y5	203	HEM	C2A-CAA-CBA-CGA
152	qb	602	PC1	C24-C25-C26-C27
153	2b	201	CDL	C62-C63-C64-C65
152	C1	711	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
153	2m	101	CDL	C12-C11-CA5-OA6
153	m2	403	CDL	C72-C71-CB7-OB8
153	VB	705	CDL	CA5-C11-C12-C13
153	Y5	201	CDL	C12-C11-CA5-OA7
153	A1	101	CDL	C72-C71-CB7-OB9
153	2G	201	CDL	C11-C12-C13-C14
153	C1	712	CDL	C16-C17-C18-C19
153	2B	201	CDL	C62-C63-C64-C65
152	qC	507	PC1	C29-C2A-C2B-C2C
153	TH	200	CDL	C77-C78-C79-C80
158	g2	301	3PE	C2D-C2E-C2F-C2G
152	C2	701	PC1	C23-C24-C25-C26
152	c1	711	PC1	O21-C21-C22-C23
153	7a	203	CDL	C32-C31-CA7-OA8
153	7A	203	CDL	C32-C31-CA7-OA8
164	qc	501	U10	C18-C19-C21-C22
164	Qc	501	U10	C18-C19-C21-C22
166	qc	502	HEM	C2B-C3B-CAB-CBB
166	Qc	502	HEM	C2B-C3B-CAB-CBB
152	2j	201	PC1	C11-C12-N-C15
152	2J	201	PC1	C11-C12-N-C15
152	I	301	PC1	C11-C12-N-C14
153	Y5	201	CDL	C33-C34-C35-C36
153	y5	201	CDL	C12-C11-CA5-OA7
158	AN	303	3PE	C29-C2A-C2B-C2C
153	FS	204	CDL	C12-C11-CA5-OA6
153	M2	403	CDL	C72-C71-CB7-OB8
153	2g	201	CDL	C11-C12-C13-C14
153	m1	402	CDL	C53-C54-C55-C56
153	a	505	CDL	CA5-C11-C12-C13
152	a	501	PC1	C3-C2-O21-C21
152	a	503	PC1	C3-C2-O21-C21
152	d	501	PC1	C3-C2-O21-C21
152	qG	401	PC1	C3-C2-O21-C21
152	qi	201	PC1	C1-C2-O21-C21
152	qi	203	PC1	C3-C2-O21-C21
152	A	503	PC1	C3-C2-O21-C21
152	D	501	PC1	C3-C2-O21-C21
152	QG	401	PC1	C3-C2-O21-C21
152	Qi	201	PC1	C1-C2-O21-C21
152	Qi	203	PC1	C3-C2-O21-C21
152	T4	303	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
153	2k	101	CDL	CB3-CB4-OB6-CB5
153	2m	101	CDL	CB3-CB4-OB6-CB5
153	7c	301	CDL	CB6-CB4-OB6-CB5
153	m2	401	CDL	CB6-CB4-OB6-CB5
153	n	304	CDL	CA3-CA4-OA6-CA5
153	t	202	CDL	CA6-CA4-OA6-CA5
153	t	204	CDL	CA6-CA4-OA6-CA5
153	w	202	CDL	CA6-CA4-OA6-CA5
153	2b	201	CDL	CA3-CA4-OA6-CA5
153	2b	201	CDL	CB3-CB4-OB6-CB5
153	c4	401	CDL	CA6-CA4-OA6-CA5
153	qc	508	CDL	CB6-CB4-OB6-CB5
153	qg	402	CDL	CA6-CA4-OA6-CA5
153	t5	301	CDL	CB3-CB4-OB6-CB5
153	2K	101	CDL	CB3-CB4-OB6-CB5
153	2M	101	CDL	CB3-CB4-OB6-CB5
153	7C	301	CDL	CB6-CB4-OB6-CB5
153	M2	401	CDL	CB6-CB4-OB6-CB5
153	N	304	CDL	CA3-CA4-OA6-CA5
153	T	202	CDL	CA6-CA4-OA6-CA5
153	T	204	CDL	CA6-CA4-OA6-CA5
153	W	202	CDL	CA6-CA4-OA6-CA5
153	2B	201	CDL	CA3-CA4-OA6-CA5
153	2B	201	CDL	CA6-CA4-OA6-CA5
153	2B	201	CDL	CB3-CB4-OB6-CB5
153	C4	401	CDL	CA6-CA4-OA6-CA5
153	Qc	508	CDL	CB6-CB4-OB6-CB5
153	Qg	402	CDL	CA6-CA4-OA6-CA5
153	T5	301	CDL	CB3-CB4-OB6-CB5
160	y5	204	PX2	C1-C2-O7-C16
160	y5	204	PX2	C3-C2-O7-C16
153	M1	402	CDL	C53-C54-C55-C56
153	BM	301	CDL	C21-C22-C23-C24
153	y5	201	CDL	C33-C34-C35-C36
160	Qh	201	PX2	C12-C13-C14-C15
153	td	101	CDL	C72-C71-CB7-OB9
152	c2	703	PC1	C23-C24-C25-C26
153	c1	709	CDL	C76-C77-C78-C79
158	an	303	3PE	C29-C2A-C2B-C2C
153	j	301	CDL	O1-C1-CA2-OA2
152	a	503	PC1	C24-C25-C26-C27
153	fs	203	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
152	2F	302	PC1	C2B-C2C-C2D-C2E
152	QC	507	PC1	C29-C2A-C2B-C2C
153	2m	101	CDL	C74-C75-C76-C77
153	c1	712	CDL	C51-C52-C53-C54
153	C1	708	CDL	C76-C77-C78-C79
153	c1	712	CDL	C16-C17-C18-C19
153	2o	101	CDL	CA4-CA3-OA5-PA1
153	i	301	CDL	C1-CB2-OB2-PB2
153	2O	101	CDL	CA4-CA3-OA5-PA1
152	C1	711	PC1	C22-C23-C24-C25
158	m2	408	3PE	C35-C36-C37-C38
153	r	201	CDL	OA5-CA3-CA4-OA6
153	t	202	CDL	OA5-CA3-CA4-OA6
153	b4	201	CDL	OB5-CB3-CB4-OB6
153	R	201	CDL	OA5-CA3-CA4-OA6
153	T	202	CDL	OA5-CA3-CA4-OA6
153	VB	706	CDL	OB5-CB3-CB4-OB6
153	B4	201	CDL	OB5-CB3-CB4-OB6
152	2f	302	PC1	C2B-C2C-C2D-C2E
152	qe	303	PC1	C26-C27-C28-C29
158	M2	408	3PE	C35-C36-C37-C38
152	2F	301	PC1	C11-C12-N-C13
151	2e	401	HEC	CAA-CBA-CGA-O1A
158	G2	301	3PE	C25-C26-C27-C28
152	m2	405	PC1	C1-C2-C3-O31
152	M2	405	PC1	C1-C2-C3-O31
153	p1	403	CDL	CA3-CA4-CA6-OA8
153	P1	403	CDL	CA3-CA4-CA6-OA8
158	vb	705	3PE	C1-C2-C3-O31
158	b4	202	3PE	C1-C2-C3-O31
158	B4	202	3PE	C1-C2-C3-O31
166	qC	501	HEM	C4B-C3B-CAB-CBB
166	qc	502	HEM	C4B-C3B-CAB-CBB
166	QC	501	HEM	C4B-C3B-CAB-CBB
166	Qc	502	HEM	C4B-C3B-CAB-CBB
152	c1	711	PC1	C22-C23-C24-C25
153	bm	301	CDL	C21-C22-C23-C24
153	7C	301	CDL	C12-C13-C14-C15
151	2E	401	HEC	CAA-CBA-CGA-O1A
153	l	301	CDL	CA5-C11-C12-C13
152	A	503	PC1	C24-C25-C26-C27
152	Qe	303	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
158	g2	301	3PE	C25-C26-C27-C28
152	qE	304	PC1	O21-C21-C22-C23
153	b3	102	CDL	C12-C11-CA5-OA6
152	t1	602	PC1	C12-C11-O13-P
152	te	102	PC1	C12-C11-O13-P
152	T1	602	PC1	C12-C11-O13-P
152	TE	102	PC1	C12-C11-O13-P
158	b4	202	3PE	C12-C11-O13-P
158	B4	202	3PE	C12-C11-O13-P
152	C1	706	PC1	C24-C25-C26-C27
152	c1	704	PC1	C24-C25-C26-C27
153	6C	202	CDL	C11-C12-C13-C14
153	6c	201	CDL	C11-C12-C13-C14
153	7c	301	CDL	C12-C13-C14-C15
153	C4	401	CDL	C62-C63-C64-C65
153	th	200	CDL	C77-C78-C79-C80
153	m3	401	CDL	C72-C71-CB7-OB8
153	M3	401	CDL	C52-C51-CB5-OB6
160	R	202	PX2	O5-C4-C5-C6
153	l	301	CDL	C11-C12-C13-C14
153	q	201	CDL	C55-C56-C57-C58
153	Q	201	CDL	C55-C56-C57-C58
153	2M	101	CDL	C75-C76-C77-C78
153	a	505	CDL	OB6-CB4-CB6-OB8
153	e	402	CDL	OB6-CB4-CB6-OB8
153	qG	402	CDL	OA6-CA4-CA6-OA8
153	VB	705	CDL	OB6-CB4-CB6-OB8
153	QG	402	CDL	OA6-CA4-CA6-OA8
152	2J	201	PC1	C22-C23-C24-C25
153	Y5	201	CDL	C37-C38-C39-C40
153	L	301	CDL	CA5-C11-C12-C13
153	L	301	CDL	C11-C12-C13-C14
153	Q	202	CDL	C41-C42-C43-C44
152	P1	401	PC1	O21-C21-C22-C23
153	c1	701	CDL	C32-C31-CA7-OA8
153	f	401	CDL	C52-C51-CB5-OB6
153	m3	401	CDL	C52-C51-CB5-OB6
153	w	202	CDL	C72-C71-CB7-OB8
153	C1	701	CDL	C32-C31-CA7-OA8
153	F	402	CDL	C52-C51-CB5-OB6
153	M3	401	CDL	C72-C71-CB7-OB8
153	W	202	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
153	TE	101	CDL	C12-C11-CA5-OA6
153	7a	201	CDL	C78-C79-C80-C81
153	q	202	CDL	C41-C42-C43-C44
158	g2	301	3PE	C34-C35-C36-C37
158	G2	301	3PE	C34-C35-C36-C37
153	t	204	CDL	OA5-CA3-CA4-CA6
153	qC	504	CDL	OB5-CB3-CB4-CB6
153	qc	508	CDL	OB5-CB3-CB4-CB6
153	te	101	CDL	OB5-CB3-CB4-CB6
153	QC	504	CDL	OB5-CB3-CB4-CB6
153	Qc	508	CDL	OB5-CB3-CB4-CB6
152	Qj	101	PC1	C23-C24-C25-C26
153	6c	201	CDL	C56-C57-C58-C59
153	t	204	CDL	CB7-C71-C72-C73
153	T	204	CDL	CB7-C71-C72-C73
152	2j	201	PC1	C22-C23-C24-C25
153	y5	201	CDL	C37-C38-C39-C40
153	7A	201	CDL	C78-C79-C80-C81
152	2f	301	PC1	C11-C12-N-C13
152	t4	301	PC1	C11-C12-N-C15
153	6C	202	CDL	C56-C57-C58-C59
154	c1	708	HEA	C17-C18-C19-C27
154	C1	703	HEA	C17-C18-C19-C27
152	m2	402	PC1	O31-C31-C32-C33
152	p1	401	PC1	O21-C21-C22-C23
152	QJ	101	PC1	O21-C21-C22-C23
153	te	101	CDL	C12-C11-CA5-OA6
153	Z	101	CDL	C52-C51-CB5-OB6
152	7a	202	PC1	C23-C24-C25-C26
153	6C	203	CDL	C55-C56-C57-C58
152	qj	101	PC1	C23-C24-C25-C26
153	2K	101	CDL	C13-C14-C15-C16
152	N5	801	PC1	C2C-C2D-C2E-C2F
153	7c	301	CDL	C43-C44-C45-C46
153	j	301	CDL	C16-C17-C18-C19
153	m1	402	CDL	C31-C32-C33-C34
153	7C	301	CDL	C43-C44-C45-C46
153	J	301	CDL	C16-C17-C18-C19
153	M1	402	CDL	C31-C32-C33-C34
153	2k	101	CDL	C13-C14-C15-C16
153	2k	101	CDL	C51-C52-C53-C54
153	t	204	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
153	qD	402	CDL	C72-C73-C74-C75
153	2K	101	CDL	C51-C52-C53-C54
153	QD	402	CDL	C72-C73-C74-C75
152	Qc	506	PC1	C31-C32-C33-C34
153	2o	101	CDL	C52-C51-CB5-OB6
153	2O	101	CDL	C52-C51-CB5-OB6
153	B	501	CDL	C13-C14-C15-C16
153	a	502	CDL	C52-C51-CB5-OB6
153	q	202	CDL	C52-C51-CB5-OB6
153	Q	202	CDL	C52-C51-CB5-OB6
158	sc	101	3PE	O31-C31-C32-C33
152	n5	803	PC1	C34-C35-C36-C37
152	qI	202	PC1	C2B-C2C-C2D-C2E
152	N5	803	PC1	C34-C35-C36-C37
153	b	501	CDL	C13-C14-C15-C16
153	t	204	CDL	C78-C79-C80-C81
152	al	302	PC1	C2-C1-O11-P
152	AL	302	PC1	C2-C1-O11-P
153	y7	501	CDL	C1-CB2-OB2-PB2
153	Y7	501	CDL	C1-CB2-OB2-PB2
153	A1	101	CDL	C1-CB2-OB2-PB2
152	N	303	PC1	C33-C34-C35-C36
153	T	204	CDL	C78-C79-C80-C81
152	7A	202	PC1	C23-C24-C25-C26
153	c4	401	CDL	C62-C63-C64-C65
153	t	204	CDL	C76-C77-C78-C79
158	a3	201	3PE	C32-C33-C34-C35
152	M2	402	PC1	O31-C31-C32-C33
153	qi	202	CDL	C52-C51-CB5-OB6
153	VB	703	CDL	C52-C51-CB5-OB6
153	B3	102	CDL	C12-C11-CA5-OA6
158	M3	402	3PE	O31-C31-C32-C33
158	SC	101	3PE	O31-C31-C32-C33
153	6c	202	CDL	C55-C56-C57-C58
153	a	504	CDL	C71-C72-C73-C74
170	b9	202	ADP	PB-O3A-PA-O2A
170	B9	202	ADP	PB-O3A-PA-O2A
158	a3	201	3PE	C32-C31-O31-C3
153	A	504	CDL	C71-C72-C73-C74
158	A3	201	3PE	C32-C33-C34-C35
152	n5	801	PC1	C2C-C2D-C2E-C2F
152	2J	201	PC1	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
152	qC	505	PC1	O31-C31-C32-C33
152	qj	101	PC1	O31-C31-C32-C33
152	Qj	101	PC1	O31-C31-C32-C33
153	2o	101	CDL	C32-C31-CA7-OA8
153	b	501	CDL	C32-C31-CA7-OA8
153	q	203	CDL	C52-C51-CB5-OB6
153	t	202	CDL	C12-C11-CA5-OA6
153	z	101	CDL	C52-C51-CB5-OB6
153	2O	101	CDL	C32-C31-CA7-OA8
153	A	502	CDL	C52-C51-CB5-OB6
153	B	501	CDL	C32-C31-CA7-OA8
153	T	202	CDL	C12-C11-CA5-OA6
153	Qi	202	CDL	C52-C51-CB5-OB6
152	c2	703	PC1	C32-C33-C34-C35
152	QI	202	PC1	C2B-C2C-C2D-C2E
153	J	301	CDL	O1-C1-CA2-OA2
153	N5	806	CDL	C77-C78-C79-C80
153	T	204	CDL	C81-C82-C83-C84
152	m	301	PC1	O21-C21-C22-C23
152	b9	201	PC1	O21-C21-C22-C23
152	7A	202	PC1	O21-C21-C22-C23
153	m2	404	CDL	C52-C51-CB5-OB6
153	5b	201	CDL	C72-C71-CB7-OB8
153	t7	201	CDL	C12-C11-CA5-OA6
153	2K	101	CDL	C52-C51-CB5-OB6
153	I	302	CDL	C12-C11-CA5-OA6
153	M2	404	CDL	C52-C51-CB5-OB6
153	Qg	402	CDL	C52-C51-CB5-OB6
158	m3	402	3PE	O31-C31-C32-C33
158	vb	705	3PE	O21-C21-C22-C23
158	VB	707	3PE	O21-C21-C22-C23
160	r	202	PX2	O5-C4-C5-C6
153	n5	806	CDL	C77-C78-C79-C80
153	qc	505	CDL	C31-C32-C33-C34
153	T	204	CDL	C11-C12-C13-C14
153	T	204	CDL	C76-C77-C78-C79
152	c3	601	PC1	C11-C12-N-C15
152	d	501	PC1	C11-C12-N-C14
152	D	501	PC1	C11-C12-N-C14
152	C2	701	PC1	C32-C33-C34-C35
152	2j	201	PC1	C31-C32-C33-C34
153	2g	204	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
153	QI	203	CDL	C16-C17-C18-C19
158	A3	201	3PE	C32-C31-O31-C3
152	7a	202	PC1	O21-C21-C22-C23
152	qJ	101	PC1	O21-C21-C22-C23
152	qc	509	PC1	O31-C31-C32-C33
152	M	303	PC1	O21-C21-C22-C23
152	B9	201	PC1	O21-C21-C22-C23
152	QC	505	PC1	O31-C31-C32-C33
152	QJ	102	PC1	O21-C21-C22-C23
152	Qc	509	PC1	O31-C31-C32-C33
153	2g	201	CDL	C12-C11-CA5-OA6
153	2k	101	CDL	C52-C51-CB5-OB6
153	i	301	CDL	C12-C11-CA5-OA6
153	2G	201	CDL	C12-C11-CA5-OA6
153	5B	201	CDL	C72-C71-CB7-OB8
153	T7	201	CDL	C12-C11-CA5-OA6
158	n4	601	3PE	O21-C21-C22-C23
158	I	304	3PE	O21-C21-C22-C23
158	N4	601	3PE	O21-C21-C22-C23
153	t	204	CDL	C11-C12-C13-C14
153	q	202	CDL	C72-C71-CB7-OB9
153	Q	202	CDL	C72-C71-CB7-OB9
153	q	203	CDL	CA7-C31-C32-C33
153	AN	302	CDL	C53-C54-C55-C56
152	c3	602	PC1	O21-C21-C22-C23
152	6C	201	PC1	O21-C21-C22-C23
152	C3	602	PC1	O21-C21-C22-C23
152	QE	301	PC1	O31-C31-C32-C33
153	qb	601	CDL	C72-C71-CB7-OB8
153	qg	402	CDL	C52-C51-CB5-OB6
153	I	303	CDL	C52-C51-CB5-OB6
153	Qb	601	CDL	C72-C71-CB7-OB8
158	i	303	3PE	O21-C21-C22-C23
158	t8	601	3PE	O21-C21-C22-C23
158	AN	303	3PE	O31-C31-C32-C33
158	T8	601	3PE	O21-C21-C22-C23
152	C1	706	PC1	C3A-C3B-C3C-C3D
153	Qc	505	CDL	C31-C32-C33-C34
153	c4	401	CDL	C55-C56-C57-C58
153	T	203	CDL	C22-C23-C24-C25
153	an	302	CDL	C53-C54-C55-C56
153	th	200	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
152	c1	704	PC1	C3A-C3B-C3C-C3D
153	t	203	CDL	C22-C23-C24-C25
152	c4	403	PC1	O31-C31-C32-C33
153	2k	101	CDL	C72-C71-CB7-OB8
153	t	204	CDL	C52-C51-CB5-OB6
153	2K	101	CDL	C72-C71-CB7-OB8
153	J	301	CDL	C72-C71-CB7-OB8
153	T	204	CDL	C52-C51-CB5-OB6
158	an	303	3PE	O31-C31-C32-C33
160	Y5	204	PX2	O5-C4-C5-C6
152	c1	704	PC1	C28-C29-C2A-C2B
152	n5	803	PC1	C3A-C3B-C3C-C3D
158	an	303	3PE	C25-C26-C27-C28
152	C1	706	PC1	C28-C29-C2A-C2B
152	N5	803	PC1	C3A-C3B-C3C-C3D
153	2m	101	CDL	C18-C19-C20-C21
153	6C	203	CDL	C34-C35-C36-C37
153	TH	200	CDL	C11-C12-C13-C14
153	6c	202	CDL	C34-C35-C36-C37
158	AN	303	3PE	C25-C26-C27-C28
153	td	101	CDL	C1-CB2-OB2-PB2
153	Qb	601	CDL	C1-CA2-OA2-PA1
152	qc	506	PC1	C31-C32-C33-C34
152	2f	303	PC1	O21-C21-C22-C23
152	qE	301	PC1	O31-C31-C32-C33
152	2F	303	PC1	O21-C21-C22-C23
152	N5	805	PC1	O31-C31-C32-C33
153	6a	201	CDL	C72-C71-CB7-OB8
153	qI	203	CDL	C12-C11-CA5-OA6
152	2f	301	PC1	C1-C2-C3-O31
152	n1	301	PC1	C1-C2-C3-O31
152	2F	301	PC1	C1-C2-C3-O31
153	m3	401	CDL	CA3-CA4-CA6-OA8
153	M3	401	CDL	CA3-CA4-CA6-OA8
158	n5	802	3PE	C1-C2-C3-O31
158	VB	707	3PE	C1-C2-C3-O31
158	N5	802	3PE	C1-C2-C3-O31
152	T4	301	PC1	C11-C12-N-C13
166	y5	203	HEM	CAA-CBA-CGA-O1A
166	Y5	203	HEM	CAA-CBA-CGA-O1A
152	c3	606	PC1	C25-C26-C27-C28
152	C3	606	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
158	W	203	3PE	C25-C26-C27-C28
152	2g	202	PC1	O31-C31-C32-C33
152	6a	202	PC1	O21-C21-C22-C23
152	6c	203	PC1	O21-C21-C22-C23
152	n5	804	PC1	O21-C21-C22-C23
152	qI	202	PC1	O31-C31-C32-C33
152	qi	203	PC1	O31-C31-C32-C33
152	2G	202	PC1	O31-C31-C32-C33
152	Qi	203	PC1	O31-C31-C32-C33
153	e	401	CDL	C72-C71-CB7-OB8
153	l	301	CDL	C72-C71-CB7-OB8
153	6A	201	CDL	C72-C71-CB7-OB8
153	E	401	CDL	C72-C71-CB7-OB8
153	E	402	CDL	C12-C11-CA5-OA6
153	N	304	CDL	C12-C11-CA5-OA6
153	2B	201	CDL	C12-C11-CA5-OA6
158	W	203	3PE	O21-C21-C22-C23
169	b6	201	T7X	O18-C11-C31-C32
152	7a	202	PC1	C26-C27-C28-C29
158	G2	301	3PE	C2D-C2E-C2F-C2G
152	c1	704	PC1	O21-C2-C3-O31
152	j	302	PC1	O21-C2-C3-O31
152	C1	706	PC1	O21-C2-C3-O31
152	J	302	PC1	O21-C2-C3-O31
153	r	201	CDL	OA6-CA4-CA6-OA8
153	n6	302	CDL	OA6-CA4-CA6-OA8
153	R	201	CDL	OA6-CA4-CA6-OA8
153	2M	101	CDL	C18-C19-C20-C21
152	7A	202	PC1	C26-C27-C28-C29
153	2g	201	CDL	C59-C60-C61-C62
153	A9	402	CDL	C34-C35-C36-C37
158	W	203	3PE	C33-C34-C35-C36
158	w	203	3PE	C25-C26-C27-C28
166	y5	203	HEM	CAA-CBA-CGA-O2A
166	Y5	203	HEM	CAA-CBA-CGA-O2A
152	qc	506	PC1	O21-C21-C22-C23
152	6A	202	PC1	O21-C21-C22-C23
152	QI	202	PC1	O31-C31-C32-C33
152	Qc	506	PC1	O21-C21-C22-C23
153	a	505	CDL	C12-C11-CA5-OA6
153	e	402	CDL	C12-C11-CA5-OA6
153	t	203	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
153	2b	201	CDL	C12-C11-CA5-OA6
153	qG	402	CDL	C52-C51-CB5-OB6
153	T	203	CDL	C32-C31-CA7-OA8
153	VB	705	CDL	C12-C11-CA5-OA6
153	AN	302	CDL	C52-C51-CB5-OB6
153	QG	402	CDL	C52-C51-CB5-OB6
153	QI	203	CDL	C12-C11-CA5-OA6
153	e	402	CDL	C61-C62-C63-C64
153	te	101	CDL	C54-C55-C56-C57
152	2F	301	PC1	C21-C22-C23-C24
153	qb	601	CDL	CA5-C11-C12-C13
152	Qe	303	PC1	C33-C34-C35-C36
153	t	203	CDL	C13-C14-C15-C16
153	a9	402	CDL	C34-C35-C36-C37
153	2G	201	CDL	C59-C60-C61-C62
152	2G	202	PC1	C36-C37-C38-C39
158	w	203	3PE	C33-C34-C35-C36
153	e	402	CDL	C31-C32-C33-C34
153	C4	401	CDL	C51-C52-C53-C54
152	2f	301	PC1	C21-C22-C23-C24
153	m2	403	CDL	OB5-CB3-CB4-CB6
153	M2	403	CDL	OB5-CB3-CB4-CB6
153	T	204	CDL	OA5-CA3-CA4-CA6
152	n5	805	PC1	O31-C31-C32-C33
152	M	302	PC1	O21-C21-C22-C23
152	C4	403	PC1	O31-C31-C32-C33
152	N5	804	PC1	O21-C21-C22-C23
153	i	302	CDL	C52-C51-CB5-OB6
153	n	304	CDL	C12-C11-CA5-OA6
153	an	302	CDL	C52-C51-CB5-OB6
153	t5	301	CDL	C12-C11-CA5-OA6
153	L	301	CDL	C72-C71-CB7-OB8
158	w	203	3PE	O21-C21-C22-C23
169	B6	201	T7X	O18-C11-C31-C32
153	E	402	CDL	C31-C32-C33-C34
153	E	402	CDL	C61-C62-C63-C64
153	T	203	CDL	C13-C14-C15-C16
152	2g	202	PC1	C36-C37-C38-C39
152	qi	203	PC1	C29-C2A-C2B-C2C
153	5b	201	CDL	C32-C33-C34-C35
153	VB	703	CDL	CA7-C31-C32-C33
152	Qi	203	PC1	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
164	b8	301	U10	C30-C29-C31-C32
152	qe	303	PC1	C33-C34-C35-C36
153	c4	401	CDL	C51-C52-C53-C54
160	R	202	PX2	C7-C8-C9-C10
152	m	307	PC1	O21-C21-C22-C23
153	j	301	CDL	C72-C71-CB7-OB8
153	r	201	CDL	C12-C11-CA5-OA6
153	T5	301	CDL	C12-C11-CA5-OA6
153	5B	201	CDL	C32-C33-C34-C35
160	r	202	PX2	C7-C8-C9-C10
153	Qb	601	CDL	CA5-C11-C12-C13
152	qj	101	PC1	C33-C34-C35-C36
152	Qj	101	PC1	C33-C34-C35-C36
153	2k	101	CDL	C35-C36-C37-C38
153	2G	204	CDL	C55-C56-C57-C58
152	a	501	PC1	C1-C2-O21-C21
152	c3	606	PC1	C1-C2-O21-C21
152	c3	606	PC1	C3-C2-O21-C21
152	d	501	PC1	C1-C2-O21-C21
152	m	301	PC1	C1-C2-O21-C21
152	qG	401	PC1	C1-C2-O21-C21
152	qi	201	PC1	C3-C2-O21-C21
152	qi	203	PC1	C1-C2-O21-C21
152	t4	301	PC1	C3-C2-O21-C21
152	t4	303	PC1	C1-C2-O21-C21
152	t4	303	PC1	C3-C2-O21-C21
152	te	102	PC1	C3-C2-O21-C21
152	A	501	PC1	C1-C2-O21-C21
152	C3	606	PC1	C1-C2-O21-C21
152	C3	606	PC1	C3-C2-O21-C21
152	D	501	PC1	C1-C2-O21-C21
152	M	303	PC1	C1-C2-O21-C21
152	QG	401	PC1	C1-C2-O21-C21
152	Qi	201	PC1	C3-C2-O21-C21
152	Qi	203	PC1	C1-C2-O21-C21
152	T4	301	PC1	C3-C2-O21-C21
152	T4	303	PC1	C3-C2-O21-C21
152	TE	102	PC1	C3-C2-O21-C21
153	2k	101	CDL	CA6-CA4-OA6-CA5
153	2k	101	CDL	CB6-CB4-OB6-CB5
153	2m	101	CDL	CB6-CB4-OB6-CB5
153	6a	201	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
153	6a	201	CDL	CB6-CB4-OB6-CB5
153	7c	301	CDL	CB3-CB4-OB6-CB5
153	c1	709	CDL	CA6-CA4-OA6-CA5
153	c1	712	CDL	CB3-CB4-OB6-CB5
153	c1	712	CDL	CB6-CB4-OB6-CB5
153	m2	401	CDL	CB3-CB4-OB6-CB5
153	m3	403	CDL	CB6-CB4-OB6-CB5
153	n	304	CDL	CA6-CA4-OA6-CA5
153	q	201	CDL	CB3-CB4-OB6-CB5
153	t	202	CDL	CA3-CA4-OA6-CA5
153	t	204	CDL	CA3-CA4-OA6-CA5
153	w	202	CDL	CA3-CA4-OA6-CA5
153	2b	201	CDL	CA6-CA4-OA6-CA5
153	qc	508	CDL	CB3-CB4-OB6-CB5
153	t5	301	CDL	CB6-CB4-OB6-CB5
153	2K	101	CDL	CA6-CA4-OA6-CA5
153	2K	101	CDL	CB6-CB4-OB6-CB5
153	2M	101	CDL	CB6-CB4-OB6-CB5
153	6A	201	CDL	CB3-CB4-OB6-CB5
153	6A	201	CDL	CB6-CB4-OB6-CB5
153	7C	301	CDL	CB3-CB4-OB6-CB5
153	C1	708	CDL	CA6-CA4-OA6-CA5
153	C1	712	CDL	CB3-CB4-OB6-CB5
153	C1	712	CDL	CB6-CB4-OB6-CB5
153	M2	401	CDL	CB3-CB4-OB6-CB5
153	M3	403	CDL	CB6-CB4-OB6-CB5
153	N	304	CDL	CA6-CA4-OA6-CA5
153	Q	201	CDL	CB3-CB4-OB6-CB5
153	T	202	CDL	CA3-CA4-OA6-CA5
153	T	204	CDL	CA3-CA4-OA6-CA5
153	W	202	CDL	CA3-CA4-OA6-CA5
153	Qc	508	CDL	CB3-CB4-OB6-CB5
153	T5	301	CDL	CB6-CB4-OB6-CB5
153	C	301	CDL	CA6-CA4-OA6-CA5
153	C	301	CDL	CB6-CB4-OB6-CB5
153	c	301	CDL	CA6-CA4-OA6-CA5
153	c	301	CDL	CB6-CB4-OB6-CB5
158	t8	601	3PE	C1-C2-O21-C21
158	T8	601	3PE	C1-C2-O21-C21
152	N5	805	PC1	C11-C12-N-C14
153	C	301	CDL	O1-C1-CB2-OB2
153	2m	101	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
152	fs	204	PC1	O21-C21-C22-C23
152	v	202	PC1	O31-C31-C32-C33
153	t	204	CDL	C72-C71-CB7-OB8
153	qc	505	CDL	C72-C71-CB7-OB8
153	T	204	CDL	C72-C71-CB7-OB8
153	Qc	505	CDL	C72-C71-CB7-OB8
160	Qh	201	PX2	O5-C4-C5-C6
152	a	501	PC1	C23-C24-C25-C26
153	n	304	CDL	C52-C53-C54-C55
153	t7	201	CDL	C22-C23-C24-C25
153	2K	101	CDL	C35-C36-C37-C38
153	QH	201	CDL	C31-C32-C33-C34
153	T7	201	CDL	C22-C23-C24-C25
158	a3	202	3PE	C27-C28-C29-C2A
153	2M	101	CDL	C58-C59-C60-C61
153	N	304	CDL	C52-C53-C54-C55
158	A3	202	3PE	C25-C26-C27-C28
153	q	203	CDL	C12-C13-C14-C15
153	y5	201	CDL	C35-C36-C37-C38
153	al	301	CDL	C72-C73-C74-C75
153	qH	201	CDL	C31-C32-C33-C34
153	qH	201	CDL	C56-C57-C58-C59
153	AL	301	CDL	C72-C73-C74-C75
153	QH	201	CDL	C56-C57-C58-C59
158	a3	202	3PE	C25-C26-C27-C28
152	al	302	PC1	O31-C31-C32-C33
152	AL	302	PC1	O31-C31-C32-C33
158	TA	201	3PE	O31-C31-C32-C33
153	N	304	CDL	C75-C76-C77-C78
153	5B	201	CDL	C14-C15-C16-C17
158	A3	202	3PE	C27-C28-C29-C2A
152	FS	201	PC1	O21-C21-C22-C23
152	N	302	PC1	O21-C21-C22-C23
153	r	201	CDL	C52-C51-CB5-OB6
152	qj	101	PC1	O32-C31-C32-C33
153	2k	101	CDL	C52-C51-CB5-OB7
153	2o	101	CDL	C32-C31-CA7-OA9
153	2K	101	CDL	C52-C51-CB5-OB7
153	5b	201	CDL	C14-C15-C16-C17
158	BM	302	3PE	C33-C34-C35-C36
164	sc	102	U10	C29-C31-C32-C33
164	SC	102	U10	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
152	A	501	PC1	C23-C24-C25-C26
153	n	304	CDL	C75-C76-C77-C78
153	Y5	201	CDL	C35-C36-C37-C38
158	n4	601	3PE	C26-C27-C28-C29
153	q	202	CDL	C1-CB2-OB2-PB2
153	qb	601	CDL	C1-CA2-OA2-PA1
153	Q	202	CDL	C1-CB2-OB2-PB2
153	N5	806	CDL	CB4-CB3-OB5-PB2
151	qD	401	HEC	C4C-C3C-CAC-CBC
151	qd	401	HEC	C4C-C3C-CAC-CBC
151	QD	401	HEC	C4C-C3C-CAC-CBC
151	Qd	401	HEC	C4C-C3C-CAC-CBC
152	QC	505	PC1	O32-C31-C32-C33
153	m3	401	CDL	C52-C51-CB5-OB7
153	VB	703	CDL	C52-C51-CB5-OB7
152	n	302	PC1	O21-C21-C22-C23
152	p1	401	PC1	O31-C31-C32-C33
152	V	202	PC1	O31-C31-C32-C33
152	P1	401	PC1	O31-C31-C32-C33
153	R	201	CDL	C12-C11-CA5-OA6
153	2G	201	CDL	C79-C80-C81-C82
152	qC	505	PC1	O32-C31-C32-C33
152	Qj	101	PC1	O32-C31-C32-C33
153	t7	201	CDL	C12-C11-CA5-OA7
153	2O	101	CDL	C32-C31-CA7-OA9
153	B	501	CDL	C32-C31-CA7-OA9
153	T7	201	CDL	C12-C11-CA5-OA7
152	2f	301	PC1	C2A-C2B-C2C-C2D
153	2g	201	CDL	C79-C80-C81-C82
153	R	201	CDL	C72-C73-C74-C75
153	TE	101	CDL	C54-C55-C56-C57
158	sc	101	3PE	O11-C1-C2-O21
152	w	201	PC1	C25-C26-C27-C28
153	6a	201	CDL	C17-C18-C19-C20
153	e	402	CDL	C12-C13-C14-C15
152	Qc	509	PC1	C31-C32-C33-C34
153	E	402	CDL	C12-C13-C14-C15
152	t1	602	PC1	O21-C21-C22-C23
152	T1	602	PC1	O21-C21-C22-C23
153	t1	601	CDL	C32-C31-CA7-OA8
153	A	502	CDL	C12-C11-CA5-OA6
153	F	402	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
153	VB	706	CDL	C72-C71-CB7-OB8
153	T1	601	CDL	C32-C31-CA7-OA8
158	a3	201	3PE	O31-C31-C32-C33
158	A3	201	3PE	O31-C31-C32-C33
152	2F	301	PC1	C2A-C2B-C2C-C2D
153	r	201	CDL	C72-C73-C74-C75
153	6C	203	CDL	C61-C62-C63-C64
153	C1	701	CDL	C11-C12-C13-C14
152	7a	202	PC1	O22-C21-C22-C23
152	qE	304	PC1	O22-C21-C22-C23
152	7A	202	PC1	O22-C21-C22-C23
153	b	501	CDL	C32-C31-CA7-OA9
153	m2	404	CDL	C52-C51-CB5-OB7
153	q	203	CDL	C52-C51-CB5-OB7
153	I	302	CDL	C12-C11-CA5-OA7
153	M2	404	CDL	C52-C51-CB5-OB7
158	an	303	3PE	O32-C31-C32-C33
158	AN	303	3PE	O32-C31-C32-C33
158	N4	601	3PE	O22-C21-C22-C23
153	6c	202	CDL	C61-C62-C63-C64
153	C4	401	CDL	C55-C56-C57-C58
153	C4	401	CDL	C79-C80-C81-C82
158	N4	601	3PE	C26-C27-C28-C29
153	qI	203	CDL	C16-C17-C18-C19
160	y5	204	PX2	C4-C5-C6-C7
152	W	201	PC1	C25-C26-C27-C28
153	c4	401	CDL	C79-C80-C81-C82
153	6A	201	CDL	C17-C18-C19-C20
153	VB	703	CDL	C12-C13-C14-C15
153	T5	301	CDL	C77-C78-C79-C80
158	bm	302	3PE	C33-C34-C35-C36
153	sd	101	CDL	C55-C56-C57-C58
153	W	202	CDL	C14-C15-C16-C17
152	2j	201	PC1	C11-C12-N-C13
152	c3	601	PC1	C11-C12-N-C14
152	i	304	PC1	C11-C12-N-C15
152	t4	301	PC1	C11-C12-N-C13
152	2J	201	PC1	C11-C12-N-C13
152	I	301	PC1	C11-C12-N-C15
153	a	502	CDL	C12-C11-CA5-OA6
153	fs	203	CDL	C72-C71-CB7-OB8
153	vb	704	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
153	2g	201	CDL	C12-C11-CA5-OA7
153	2k	101	CDL	C72-C71-CB7-OB9
153	w	202	CDL	C72-C71-CB7-OB9
153	5b	201	CDL	C72-C71-CB7-OB9
153	2G	201	CDL	C12-C11-CA5-OA7
153	2K	101	CDL	C72-C71-CB7-OB9
153	W	202	CDL	C72-C71-CB7-OB9
153	B3	102	CDL	C12-C11-CA5-OA7
158	n4	601	3PE	O22-C21-C22-C23
158	VB	707	3PE	O22-C21-C22-C23
152	qc	509	PC1	C31-C32-C33-C34
153	w	202	CDL	C14-C15-C16-C17
153	SD	101	CDL	C55-C56-C57-C58
153	2B	201	CDL	C31-C32-C33-C34
153	c1	709	CDL	O1-C1-CA2-OA2
153	C1	708	CDL	O1-C1-CA2-OA2
153	Y7	501	CDL	O1-C1-CA2-OA2
152	c1	704	PC1	C23-C24-C25-C26
152	N	301	PC1	C25-C26-C27-C28
153	E	403	CDL	C72-C73-C74-C75
164	B8	301	U10	C30-C29-C31-C32
152	qc	509	PC1	O32-C31-C32-C33
152	qi	203	PC1	O32-C31-C32-C33
152	6C	201	PC1	O22-C21-C22-C23
152	C4	403	PC1	O32-C31-C32-C33
152	Qc	509	PC1	O32-C31-C32-C33
152	Qi	203	PC1	O32-C31-C32-C33
153	c1	701	CDL	C32-C31-CA7-OA9
153	i	301	CDL	C12-C11-CA5-OA7
153	qb	601	CDL	C72-C71-CB7-OB9
153	te	101	CDL	C12-C11-CA5-OA7
153	C1	701	CDL	C32-C31-CA7-OA9
153	M3	401	CDL	C52-C51-CB5-OB7
153	TE	101	CDL	C12-C11-CA5-OA7
158	vb	705	3PE	O22-C21-C22-C23
153	2b	201	CDL	C31-C32-C33-C34
153	f	401	CDL	C72-C71-CB7-OB8
153	R	201	CDL	C52-C51-CB5-OB6
153	A1	102	CDL	C72-C71-CB7-OB8
164	qc	501	U10	C25-C24-C26-C27
164	Qc	501	U10	C25-C24-C26-C27
153	c1	701	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
153	t5	301	CDL	C77-C78-C79-C80
152	2f	303	PC1	O22-C21-C22-C23
152	6a	202	PC1	O22-C21-C22-C23
152	p1	401	PC1	O22-C21-C22-C23
153	q	202	CDL	C52-C51-CB5-OB7
153	an	302	CDL	C52-C51-CB5-OB7
153	Q	202	CDL	C52-C51-CB5-OB7
153	5B	201	CDL	C72-C71-CB7-OB9
153	Qb	601	CDL	C72-C71-CB7-OB9
160	R	202	PX2	O6-C4-C5-C6
160	Y5	204	PX2	O6-C4-C5-C6
158	i	303	3PE	C23-C24-C25-C26
158	I	304	3PE	C23-C24-C25-C26
152	n	301	PC1	C25-C26-C27-C28
153	y5	201	CDL	C53-C54-C55-C56
153	te	101	CDL	C57-C58-C59-C60
152	C2	701	PC1	O31-C31-C32-C33
151	qd	401	HEC	CAD-CBD-CGD-O2D
166	QC	502	HEM	CAD-CBD-CGD-O2D
152	v	202	PC1	C38-C39-C3A-C3B
153	e	403	CDL	C72-C73-C74-C75
153	qG	402	CDL	C33-C34-C35-C36
153	Y5	201	CDL	C53-C54-C55-C56
153	2O	101	CDL	C52-C51-CB5-OB7
152	m2	402	PC1	O32-C31-C32-C33
152	n5	804	PC1	O22-C21-C22-C23
152	qE	301	PC1	O32-C31-C32-C33
152	6A	202	PC1	O22-C21-C22-C23
152	M2	402	PC1	O32-C31-C32-C33
152	B9	201	PC1	O22-C21-C22-C23
152	P1	401	PC1	O22-C21-C22-C23
152	QE	301	PC1	O32-C31-C32-C33
152	QI	202	PC1	O32-C31-C32-C33
153	t	204	CDL	C52-C51-CB5-OB7
153	t	204	CDL	C72-C71-CB7-OB9
153	b3	102	CDL	C12-C11-CA5-OA7
153	qi	202	CDL	C52-C51-CB5-OB7
153	F	402	CDL	C52-C51-CB5-OB7
153	T	204	CDL	C52-C51-CB5-OB7
153	AN	302	CDL	C52-C51-CB5-OB7
153	Qi	202	CDL	C52-C51-CB5-OB7
160	Qh	201	PX2	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
153	P1	403	CDL	CA5-C11-C12-C13
158	w	203	3PE	C31-C32-C33-C34
158	W	203	3PE	C31-C32-C33-C34
158	a3	202	3PE	C29-C2A-C2B-C2C
153	a1	101	CDL	OB6-CB4-CB6-OB8
153	A1	102	CDL	OB6-CB4-CB6-OB8
158	b4	202	3PE	O21-C2-C3-O31
152	V	202	PC1	C38-C39-C3A-C3B
153	7C	301	CDL	C58-C59-C60-C61
153	F	402	CDL	C31-C32-C33-C34
152	C1	706	PC1	C23-C24-C25-C26
152	Qe	303	PC1	C24-C25-C26-C27
152	6c	203	PC1	O22-C21-C22-C23
152	c3	602	PC1	O22-C21-C22-C23
152	b9	201	PC1	O22-C21-C22-C23
152	n5	805	PC1	O32-C31-C32-C33
152	qI	202	PC1	O32-C31-C32-C33
152	C3	602	PC1	O22-C21-C22-C23
152	Qc	506	PC1	O22-C21-C22-C23
153	a	505	CDL	C12-C11-CA5-OA7
153	f	401	CDL	C52-C51-CB5-OB7
153	m3	401	CDL	C72-C71-CB7-OB9
153	M3	401	CDL	C72-C71-CB7-OB9
153	T	202	CDL	C12-C11-CA5-OA7
153	T	204	CDL	C72-C71-CB7-OB9
153	VB	705	CDL	C12-C11-CA5-OA7
153	2B	201	CDL	C12-C11-CA5-OA7
153	QG	402	CDL	C52-C51-CB5-OB7
153	Qg	402	CDL	C52-C51-CB5-OB7
158	I	304	3PE	O22-C21-C22-C23
158	M3	402	3PE	O32-C31-C32-C33
152	c2	703	PC1	O31-C31-C32-C33
153	a1	101	CDL	C72-C71-CB7-OB8
153	M1	402	CDL	C52-C51-CB5-OB6
158	M3	402	3PE	O21-C21-C22-C23
153	p1	403	CDL	CA5-C11-C12-C13
153	f	401	CDL	C31-C32-C33-C34
152	qe	303	PC1	C24-C25-C26-C27
153	7c	301	CDL	C58-C59-C60-C61
153	QG	402	CDL	C33-C34-C35-C36
158	A3	202	3PE	C29-C2A-C2B-C2C
158	T8	601	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
152	N1	301	PC1	C1-C2-C3-O31
153	e	402	CDL	CB3-CB4-CB6-OB8
153	am	201	CDL	CB3-CB4-CB6-OB8
153	E	402	CDL	CB3-CB4-CB6-OB8
153	A1	102	CDL	CB3-CB4-CB6-OB8
153	AM	201	CDL	CB3-CB4-CB6-OB8
151	Qd	401	HEC	CAD-CBD-CGD-O2D
153	BM	301	CDL	C78-C79-C80-C81
153	TE	101	CDL	C57-C58-C59-C60
158	t8	601	3PE	C37-C38-C39-C3A
152	c4	403	PC1	O32-C31-C32-C33
152	QJ	101	PC1	O22-C21-C22-C23
152	QJ	102	PC1	O22-C21-C22-C23
153	t	202	CDL	C12-C11-CA5-OA7
153	2b	201	CDL	C12-C11-CA5-OA7
153	qG	402	CDL	C52-C51-CB5-OB7
158	i	303	3PE	O22-C21-C22-C23
158	m3	402	3PE	O32-C31-C32-C33
158	t8	601	3PE	O22-C21-C22-C23
160	r	202	PX2	O6-C4-C5-C6
153	2m	101	CDL	C53-C54-C55-C56
153	2M	101	CDL	C53-C54-C55-C56
153	c3	604	CDL	C1-CB2-OB2-PB2
153	t	201	CDL	C1-CB2-OB2-PB2
153	n5	806	CDL	CB4-CB3-OB5-PB2
153	t5	301	CDL	CB4-CB3-OB5-PB2
153	Y7	501	CDL	CA4-CA3-OA5-PA1
153	T5	301	CDL	CB4-CB3-OB5-PB2
152	QI	202	PC1	O21-C21-C22-C23
153	m1	402	CDL	C52-C51-CB5-OB6
153	t	203	CDL	C72-C71-CB7-OB8
153	c4	401	CDL	C72-C71-CB7-OB8
153	td	101	CDL	C52-C51-CB5-OB6
153	A1	101	CDL	C52-C51-CB5-OB6
154	C1	702	HEA	CAD-CBD-CGD-O1D
152	2g	202	PC1	O32-C31-C32-C33
152	m	301	PC1	O22-C21-C22-C23
152	qJ	101	PC1	O22-C21-C22-C23
152	M	303	PC1	O22-C21-C22-C23
153	i	302	CDL	C52-C51-CB5-OB7
153	qI	203	CDL	C12-C11-CA5-OA7
153	qg	402	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
153	I	303	CDL	C52-C51-CB5-OB7
153	J	301	CDL	C72-C71-CB7-OB9
153	T	203	CDL	C32-C31-CA7-OA9
153	QI	203	CDL	C12-C11-CA5-OA7
158	w	203	3PE	O22-C21-C22-C23
158	T8	601	3PE	O22-C21-C22-C23
153	q	201	CDL	CA5-C11-C12-C13
152	c1	707	PC1	O31-C31-C32-C33
152	C1	710	PC1	O31-C31-C32-C33
153	m3	403	CDL	C12-C11-CA5-OA6
153	M3	403	CDL	C12-C11-CA5-OA6
153	N	304	CDL	C52-C51-CB5-OB6
153	T	204	CDL	C12-C11-CA5-OA6
154	c1	702	HEA	CAD-CBD-CGD-O1D
152	qc	506	PC1	O22-C21-C22-C23
152	N5	804	PC1	O22-C21-C22-C23
153	j	301	CDL	C72-C71-CB7-OB9
153	y7	501	CDL	O1-C1-CA2-OA2
152	a	503	PC1	C28-C29-C2A-C2B
151	qd	401	HEC	CAD-CBD-CGD-O1D
166	qC	502	HEM	CAD-CBD-CGD-O2D
153	qc	505	CDL	C33-C34-C35-C36
153	5B	201	CDL	C52-C53-C54-C55
152	2F	303	PC1	O22-C21-C22-C23
152	N5	805	PC1	O32-C31-C32-C33
153	e	401	CDL	C72-C71-CB7-OB9
153	t	203	CDL	C32-C31-CA7-OA9
153	E	401	CDL	C72-C71-CB7-OB9
158	W	203	3PE	O22-C21-C22-C23
152	N6	301	PC1	O31-C31-C32-C33
153	n	304	CDL	C52-C51-CB5-OB6
153	c4	401	CDL	C12-C11-CA5-OA6
153	C4	401	CDL	C12-C11-CA5-OA6
153	C4	401	CDL	C72-C71-CB7-OB8
158	g2	301	3PE	O21-C21-C22-C23
158	G2	301	3PE	O21-C21-C22-C23
159	m2	406	P5S	O-C-CA-N
153	c1	712	CDL	C78-C79-C80-C81
153	m1	404	CDL	C15-C16-C17-C18
153	M1	404	CDL	C15-C16-C17-C18
152	A	503	PC1	C28-C29-C2A-C2B
153	vb	701	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
152	2g	202	PC1	C34-C35-C36-C37
152	qc	506	PC1	C23-C24-C25-C26
153	e	402	CDL	C12-C11-CA5-OA7
153	l	301	CDL	C72-C71-CB7-OB9
152	2G	202	PC1	C34-C35-C36-C37
152	Qc	506	PC1	C23-C24-C25-C26
153	5b	201	CDL	C52-C53-C54-C55
153	a9	402	CDL	C55-C56-C57-C58
153	N6	302	CDL	C79-C80-C81-C82
153	Qb	601	CDL	C53-C54-C55-C56
152	n1	301	PC1	O31-C31-C32-C33
152	qI	201	PC1	O31-C31-C32-C33
152	qI	202	PC1	O21-C21-C22-C23
152	N1	301	PC1	O31-C31-C32-C33
152	Qg	401	PC1	O31-C31-C32-C33
153	2g	203	CDL	C12-C11-CA5-OA6
153	6c	201	CDL	C52-C51-CB5-OB6
153	7c	301	CDL	C12-C11-CA5-OA6
153	q	203	CDL	C32-C31-CA7-OA8
153	t	204	CDL	C12-C11-CA5-OA6
153	bm	301	CDL	C52-C51-CB5-OB6
153	qC	504	CDL	C72-C71-CB7-OB8
153	qc	508	CDL	C32-C31-CA7-OA8
153	td	101	CDL	C12-C11-CA5-OA6
153	2G	203	CDL	C12-C11-CA5-OA6
153	6C	202	CDL	C52-C51-CB5-OB6
153	T	203	CDL	C72-C71-CB7-OB8
153	2B	201	CDL	C72-C71-CB7-OB8
153	AL	301	CDL	C72-C71-CB7-OB8
153	AM	201	CDL	C72-C71-CB7-OB8
153	BM	301	CDL	C52-C51-CB5-OB6
153	Qc	508	CDL	C32-C31-CA7-OA8
158	n4	601	3PE	O31-C31-C32-C33
158	t8	601	3PE	O31-C31-C32-C33
158	T8	601	3PE	O31-C31-C32-C33
153	R	201	CDL	C57-C58-C59-C60
153	Qc	505	CDL	C33-C34-C35-C36
153	r	201	CDL	C57-C58-C59-C60
151	qD	401	HEC	CAD-CBD-CGD-O2D
151	QD	401	HEC	CAD-CBD-CGD-O2D
152	fs	204	PC1	O22-C21-C22-C23
152	2G	202	PC1	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
153	6a	201	CDL	C72-C71-CB7-OB9
153	n	304	CDL	C12-C11-CA5-OA7
153	bm	301	CDL	C52-C51-CB5-OB7
153	F	402	CDL	C72-C71-CB7-OB9
153	N	304	CDL	C12-C11-CA5-OA7
169	B6	201	T7X	O19-C11-C31-C32
153	A9	402	CDL	CA5-C11-C12-C13
153	VB	706	CDL	C73-C74-C75-C76
152	QI	202	PC1	C2D-C2E-C2F-C2G
153	vb	704	CDL	C73-C74-C75-C76
152	6A	202	PC1	C32-C33-C34-C35
153	7a	201	CDL	C16-C17-C18-C19
153	f	401	CDL	C72-C73-C74-C75
153	C1	712	CDL	C78-C79-C80-C81
153	F	402	CDL	C72-C73-C74-C75
152	2f	301	PC1	O21-C21-C22-C23
152	n6	301	PC1	O31-C31-C32-C33
152	2F	301	PC1	O21-C21-C22-C23
153	2b	201	CDL	C72-C71-CB7-OB8
153	a9	402	CDL	C52-C51-CB5-OB6
153	am	201	CDL	C72-C71-CB7-OB8
153	7C	301	CDL	C12-C11-CA5-OA6
153	A1	101	CDL	C12-C11-CA5-OA6
153	QC	504	CDL	C72-C71-CB7-OB8
158	m3	402	3PE	O21-C21-C22-C23
158	AN	301	3PE	O31-C31-C32-C33
158	AN	303	3PE	O21-C21-C22-C23
160	Qh	201	PX2	O7-C16-C17-C18
152	6a	202	PC1	C32-C33-C34-C35
153	A9	402	CDL	C55-C56-C57-C58
151	Qd	401	HEC	CAD-CBD-CGD-O1D
153	C1	708	CDL	CB7-C71-C72-C73
153	Q	201	CDL	CA5-C11-C12-C13
152	v	202	PC1	O32-C31-C32-C33
152	FS	201	PC1	O22-C21-C22-C23
152	V	202	PC1	O32-C31-C32-C33
153	E	402	CDL	C12-C11-CA5-OA7
153	L	301	CDL	C72-C71-CB7-OB9
152	qI	202	PC1	C2D-C2E-C2F-C2G
153	qb	601	CDL	C53-C54-C55-C56
153	n6	302	CDL	C79-C80-C81-C82

There are no ring outliers.

445 monomers are involved in 1712 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	p1	402	CDL	4	0
153	E	402	CDL	5	0
152	qc	506	PC1	2	0
153	C	301	CDL	3	0
158	AN	301	3PE	3	0
152	P1	401	PC1	1	0
153	qI	203	CDL	4	0
158	A3	201	3PE	6	0
153	N5	806	CDL	7	0
153	N6	302	CDL	7	0
153	R	201	CDL	4	0
168	ab	201	ZMP	12	0
152	qc	509	PC1	4	0
153	TE	101	CDL	5	0
153	2O	101	CDL	1	0
152	j	302	PC1	1	0
160	y5	204	PX2	1	0
152	I	301	PC1	7	0
153	Qg	402	CDL	9	0
152	M1	401	PC1	6	0
160	r	202	PX2	2	0
152	qj	101	PC1	2	0
153	u1	101	CDL	2	0
164	qc	501	U10	4	0
158	G2	301	3PE	2	0
153	2b	201	CDL	10	0
158	g2	301	3PE	1	0
153	U1	101	CDL	2	0
158	y5	202	3PE	1	0
153	c1	712	CDL	15	0
152	B9	201	PC1	3	0
152	n5	805	PC1	5	0
152	M	303	PC1	2	0
152	TE	102	PC1	1	0
152	T4	301	PC1	2	0
152	6a	202	PC1	1	0
153	7A	201	CDL	11	0
152	2F	302	PC1	3	0
153	qB	601	CDL	6	0
158	T8	602	3PE	5	0
152	M2	405	PC1	3	0
153	6C	203	CDL	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
152	qb	602	PC1	2	0
153	t5	301	CDL	12	0
160	R	202	PX2	2	0
153	AL	301	CDL	3	0
152	c3	605	PC1	5	0
158	I	304	3PE	1	0
164	b8	301	U10	6	0
153	M2	403	CDL	3	0
166	QC	502	HEM	7	0
153	n6	302	CDL	7	0
152	W	201	PC1	6	0
152	N	303	PC1	4	0
152	N5	804	PC1	4	0
153	m	306	CDL	2	0
158	A3	202	3PE	4	0
153	Y7	501	CDL	2	0
153	m2	403	CDL	3	0
153	T5	301	CDL	13	0
153	qH	201	CDL	8	0
152	qi	201	PC1	3	0
153	qC	503	CDL	3	0
152	C3	605	PC1	5	0
161	SA	701	FAD	5	0
152	QE	303	PC1	5	0
153	Q	202	CDL	6	0
153	TH	200	CDL	5	0
158	a3	202	3PE	4	0
158	a3	201	3PE	6	0
153	sd	101	CDL	5	0
158	c4	402	3PE	3	0
153	t	203	CDL	6	0
158	t8	602	3PE	5	0
153	i	302	CDL	6	0
152	N3	201	PC1	1	0
153	VB	705	CDL	5	0
153	B8	302	CDL	5	0
153	t	204	CDL	14	0
153	qc	504	CDL	2	0
162	v1	500	SF4	1	0
152	QC	507	PC1	2	0
153	q	203	CDL	11	0
152	m	305	PC1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
152	FS	201	PC1	5	0
152	Qi	203	PC1	2	0
153	6a	201	CDL	3	0
152	qE	304	PC1	2	0
153	A9	403	CDL	4	0
153	b4	201	CDL	2	0
153	E	401	CDL	3	0
153	F	402	CDL	10	0
162	s8	302	SF4	3	0
153	p1	403	CDL	4	0
154	C1	703	HEA	11	0
152	J	302	PC1	1	0
153	VB	706	CDL	9	0
152	m1	403	PC1	4	0
152	7c	303	PC1	5	0
158	M2	408	3PE	2	0
153	7a	201	CDL	11	0
153	I	303	CDL	5	0
158	w	203	3PE	4	0
153	qb	601	CDL	3	0
158	N5	802	3PE	5	0
153	m2	404	CDL	5	0
153	y5	201	CDL	1	0
153	VB	703	CDL	12	0
152	7A	202	PC1	3	0
153	e	401	CDL	3	0
170	b9	202	ADP	1	0
153	r	201	CDL	4	0
160	qh	201	PX2	4	0
153	T	202	CDL	9	0
153	QB	601	CDL	6	0
152	c1	704	PC1	3	0
152	c3	601	PC1	4	0
152	C1	706	PC1	3	0
153	C1	712	CDL	16	0
164	SC	102	U10	6	0
152	2f	302	PC1	3	0
152	b9	201	PC1	3	0
164	B8	301	U10	8	0
152	N5	805	PC1	5	0
162	s1	801	SF4	2	0
152	p1	401	PC1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	a	502	CDL	2	0
153	a9	403	CDL	4	0
153	c	301	CDL	4	0
153	fs	203	CDL	5	0
153	7C	302	CDL	2	0
153	i	301	CDL	8	0
152	m2	405	PC1	4	0
153	qG	402	CDL	1	0
152	7C	303	PC1	5	0
153	U	201	CDL	4	0
152	qC	505	PC1	5	0
153	W	202	CDL	7	0
153	b	501	CDL	1	0
162	S8	302	SF4	2	0
153	c1	709	CDL	7	0
153	5b	201	CDL	7	0
153	2G	203	CDL	1	0
153	M	305	CDL	8	0
153	T	201	CDL	2	0
152	C3	603	PC1	1	0
153	t7	201	CDL	7	0
152	N1	301	PC1	2	0
153	2M	101	CDL	8	0
158	i	303	3PE	1	0
152	D	501	PC1	4	0
153	td	101	CDL	2	0
152	v	201	PC1	1	0
152	c3	606	PC1	1	0
166	Qc	502	HEM	3	0
153	m3	401	CDL	2	0
152	fs	204	PC1	5	0
153	C1	701	CDL	8	0
152	C1	710	PC1	2	0
161	sa	701	FAD	5	0
153	QD	402	CDL	1	0
152	T4	303	PC1	3	0
153	m	303	CDL	8	0
158	n4	601	3PE	1	0
162	s7	201	SF4	2	0
152	AL	302	PC1	1	0
152	QB	602	PC1	4	0
158	T8	601	3PE	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
158	t8	601	3PE	5	0
153	C3	604	CDL	4	0
152	Qe	303	PC1	3	0
152	F	401	PC1	2	0
153	vb	701	CDL	3	0
152	c1	711	PC1	8	0
163	SB	403	F3S	1	0
152	N5	803	PC1	8	0
153	VB	701	CDL	3	0
153	QH	201	CDL	8	0
153	c3	604	CDL	4	0
157	fs	201	FES	1	0
158	ta	201	3PE	1	0
153	M	306	CDL	5	0
162	S1	801	SF4	2	0
152	al	302	PC1	1	0
152	c4	403	PC1	5	0
158	BM	302	3PE	1	0
153	C1	708	CDL	7	0
166	qC	501	HEM	2	0
153	th	200	CDL	5	0
158	Y5	202	3PE	1	0
153	m1	405	CDL	3	0
152	a	503	PC1	2	0
162	s1	802	SF4	1	0
152	qg	401	PC1	3	0
153	Y5	201	CDL	1	0
158	m3	402	3PE	2	0
153	7c	302	CDL	2	0
152	f	402	PC1	2	0
153	bm	301	CDL	12	0
152	c2	703	PC1	1	0
153	2o	101	CDL	1	0
152	c3	602	PC1	2	0
152	m1	401	PC1	6	0
153	qg	402	CDL	8	0
164	QC	506	U10	2	0
158	sc	101	3PE	2	0
152	v	202	PC1	3	0
153	A1	102	CDL	9	0
153	FS	204	CDL	6	0
152	an	304	PC1	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	q	201	CDL	5	0
153	a	504	CDL	9	0
153	AM	201	CDL	6	0
153	a9	402	CDL	6	0
152	C3	606	PC1	1	0
152	QJ	101	PC1	2	0
152	Qi	201	PC1	3	0
158	C4	402	3PE	3	0
153	2G	204	CDL	7	0
152	qI	202	PC1	7	0
153	u	201	CDL	4	0
152	C3	602	PC1	2	0
153	M3	403	CDL	3	0
152	qE	303	PC1	5	0
153	Qi	202	CDL	5	0
153	B	501	CDL	1	0
153	Qb	601	CDL	3	0
152	7a	202	PC1	3	0
153	QG	402	CDL	1	0
153	am	201	CDL	6	0
167	a9	401	NDP	1	0
171	V1	501	FMN	2	0
153	m3	403	CDL	3	0
152	qB	602	PC1	5	0
163	sb	403	F3S	1	0
166	qC	502	HEM	8	0
153	2m	101	CDL	6	0
152	t4	303	PC1	2	0
152	C2	701	PC1	1	0
152	c3	603	PC1	1	0
153	a	505	CDL	5	0
162	S7	201	SF4	2	0
153	Z	101	CDL	1	0
153	T7	201	CDL	8	0
153	b8	302	CDL	5	0
153	B4	201	CDL	2	0
153	f	401	CDL	11	0
153	B3	102	CDL	6	0
153	c1	703	CDL	3	0
152	qC	507	PC1	2	0
158	B4	202	3PE	6	0
152	m2	402	PC1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
166	qc	503	HEM	10	0
153	m1	402	CDL	6	0
158	m2	408	3PE	2	0
164	qC	506	U10	1	0
152	N5	801	PC1	4	0
153	7c	301	CDL	6	0
153	A	504	CDL	9	0
152	w	204	PC1	5	0
152	a	501	PC1	4	0
152	s8	301	PC1	2	0
153	M2	404	CDL	5	0
162	V1	500	SF4	1	0
152	te	102	PC1	1	0
152	M2	402	PC1	2	0
153	I	302	CDL	6	0
153	y7	501	CDL	2	0
160	Qh	201	PX2	4	0
154	c1	708	HEA	11	0
153	q	202	CDL	6	0
168	AB	201	ZMP	12	0
152	2f	301	PC1	4	0
152	M2	407	PC1	1	0
152	S8	301	PC1	2	0
158	an	306	3PE	2	0
158	W	203	3PE	4	0
152	2g	202	PC1	3	0
153	vb	704	CDL	8	0
153	al	301	CDL	3	0
152	c1	706	PC1	4	0
152	QI	202	PC1	9	0
158	TA	201	3PE	1	0
158	bm	302	3PE	1	0
152	C4	403	PC1	4	0
152	Qb	602	PC1	4	0
153	n5	806	CDL	10	0
166	QC	501	HEM	2	0
152	A	503	PC1	2	0
152	qi	203	PC1	2	0
153	c4	401	CDL	5	0
153	t1	601	CDL	4	0
153	AN	302	CDL	6	0
152	Qc	509	PC1	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	Qc	505	CDL	2	0
152	J1	400	PC1	3	0
153	E	403	CDL	9	0
159	m2	406	P5S	1	0
153	m	304	CDL	5	0
153	T1	601	CDL	4	0
166	qc	502	HEM	3	0
164	Qc	507	U10	3	0
152	TC	101	PC1	4	0
153	7a	203	CDL	5	0
152	C3	601	PC1	3	0
152	n5	801	PC1	4	0
164	Qc	501	U10	3	0
152	qE	301	PC1	1	0
153	6A	201	CDL	2	0
158	an	305	3PE	1	0
153	5B	201	CDL	8	0
153	2K	101	CDL	8	0
153	m	302	CDL	4	0
158	n5	802	3PE	4	0
152	t4	301	PC1	2	0
159	M2	406	P5S	1	0
153	m2	401	CDL	3	0
153	e	402	CDL	5	0
153	L	301	CDL	2	0
158	AN	303	3PE	1	0
152	6A	202	PC1	1	0
158	AN	305	3PE	1	0
152	AM	202	PC1	4	0
158	SC	101	3PE	2	0
153	T	203	CDL	6	0
162	S1	802	SF4	1	0
167	A9	401	NDP	1	0
152	qI	201	PC1	3	0
152	2f	303	PC1	3	0
152	tc	101	PC1	5	0
152	am	202	PC1	4	0
152	V	202	PC1	2	0
153	t	202	CDL	9	0
153	t	201	CDL	2	0
153	c1	701	CDL	7	0
152	m	307	PC1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
158	M3	402	3PE	2	0
152	N	301	PC1	7	0
153	M1	404	CDL	7	0
152	m	301	PC1	2	0
152	n5	804	PC1	4	0
152	C1	709	PC1	4	0
152	2G	202	PC1	3	0
153	C1	707	CDL	3	0
153	j	301	CDL	3	0
153	w	202	CDL	7	0
152	5B	202	PC1	3	0
153	SD	101	CDL	5	0
152	2F	301	PC1	4	0
153	J	301	CDL	2	0
152	c1	707	PC1	2	0
152	2F	303	PC1	3	0
152	Qc	506	PC1	3	0
152	AN	304	PC1	3	0
153	Qc	504	CDL	1	0
152	QJ	102	PC1	4	0
152	N6	301	PC1	7	0
158	AN	306	3PE	2	0
152	w	201	PC1	6	0
152	M1	403	PC1	4	0
152	Qj	101	PC1	2	0
153	P1	402	CDL	3	0
153	b3	102	CDL	5	0
158	an	303	3PE	1	0
154	c1	702	HEA	11	0
152	n6	301	PC1	6	0
152	QE	301	PC1	1	0
153	an	302	CDL	5	0
153	M3	401	CDL	2	0
153	2B	201	CDL	11	0
152	n	301	PC1	7	0
152	d	501	PC1	5	0
153	2k	101	CDL	9	0
153	qc	505	CDL	2	0
153	6C	202	CDL	7	0
152	tc	102	PC1	4	0
153	l	301	CDL	2	0
153	7A	203	CDL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	A1	101	CDL	2	0
164	qc	507	U10	1	0
153	qD	402	CDL	1	0
153	qi	202	CDL	5	0
152	QI	201	PC1	2	0
152	A	501	PC1	4	0
152	n	303	PC1	4	0
153	7C	301	CDL	6	0
152	m2	407	PC1	1	0
152	QC	505	PC1	4	0
153	C4	401	CDL	4	0
153	A	502	CDL	2	0
158	T4	302	3PE	1	0
153	6c	202	CDL	8	0
153	te	101	CDL	5	0
158	b4	202	3PE	5	0
152	M	307	PC1	2	0
153	M1	402	CDL	6	0
152	TC	102	PC1	2	0
166	Qc	503	HEM	9	0
152	V	201	PC1	1	0
153	2g	204	CDL	4	0
152	Qg	401	PC1	3	0
152	qJ	101	PC1	4	0
152	n1	301	PC1	2	0
153	z	101	CDL	1	0
153	2g	203	CDL	2	0
164	sc	102	U10	7	0
171	v1	501	FMN	1	0
153	n	304	CDL	7	0
153	QC	504	CDL	6	0
152	W	204	PC1	5	0
153	BM	301	CDL	12	0
153	a1	101	CDL	9	0
153	qC	504	CDL	6	0
152	i	304	PC1	7	0
153	6c	201	CDL	7	0
151	qD	401	HEC	1	0
152	n5	803	PC1	8	0
152	5b	202	PC1	3	0
152	n3	201	PC1	2	0
153	P1	403	CDL	4	0

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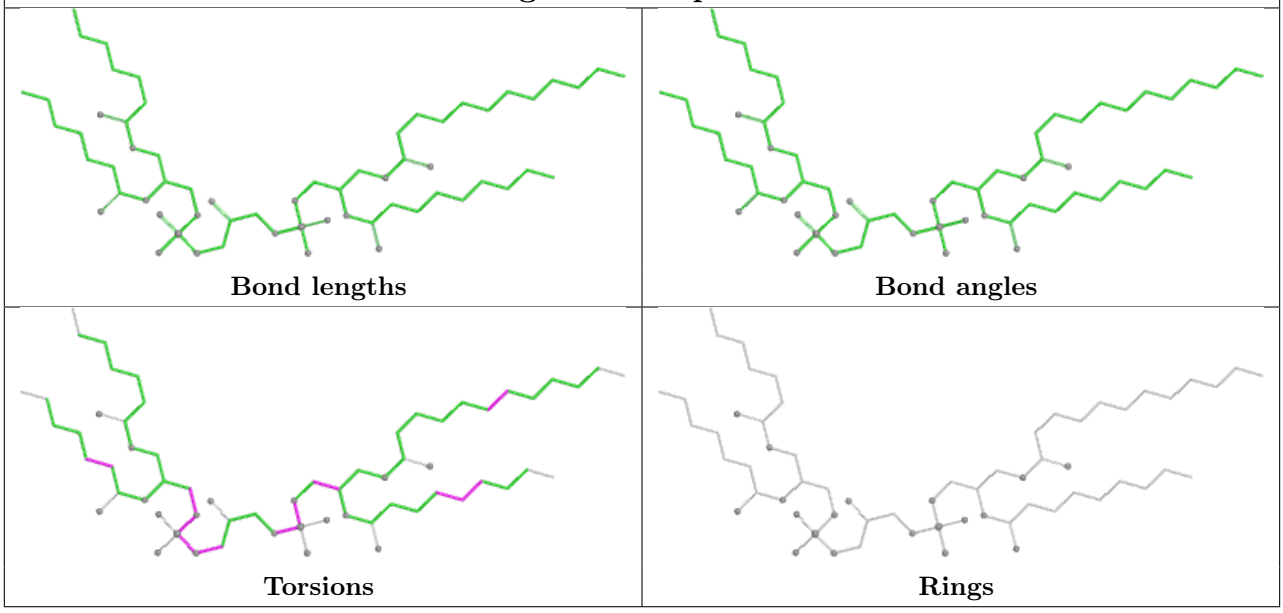
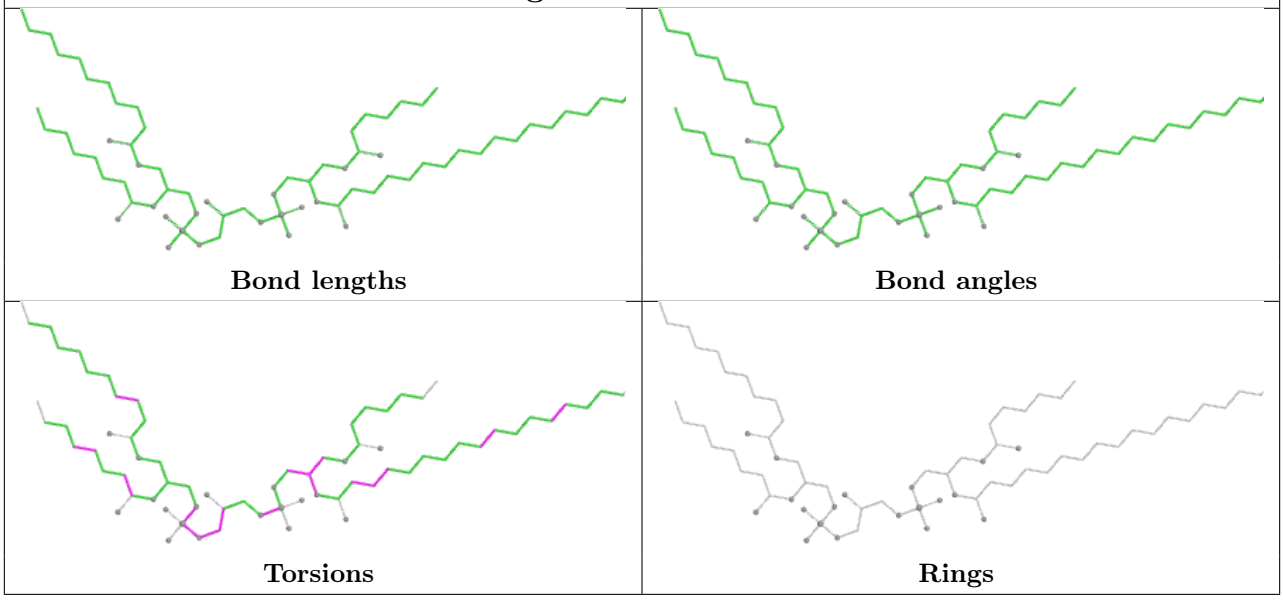
Mol	Chain	Res	Type	Clashes	Symm-Clashes
153	M2	401	CDL	3	0
152	qe	303	PC1	4	0
153	M	304	CDL	4	0
153	A9	402	CDL	6	0
153	M	301	CDL	2	0
153	2G	201	CDL	5	0
154	C1	702	HEA	8	0
153	e	403	CDL	9	0
153	M1	405	CDL	3	0
153	T	204	CDL	13	0
153	Q	201	CDL	6	0
153	m1	404	CDL	6	0
160	Y5	204	PX2	1	0
152	j1	400	PC1	3	0
153	N	304	CDL	7	0
153	QC	503	CDL	3	0
151	QD	401	HEC	1	0
151	2e	401	HEC	1	0
152	M	302	PC1	2	0
153	QI	203	CDL	5	0
153	2g	201	CDL	5	0
152	C1	711	PC1	10	0
152	n	302	PC1	1	0
151	2E	401	HEC	1	0
158	an	301	3PE	3	0

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

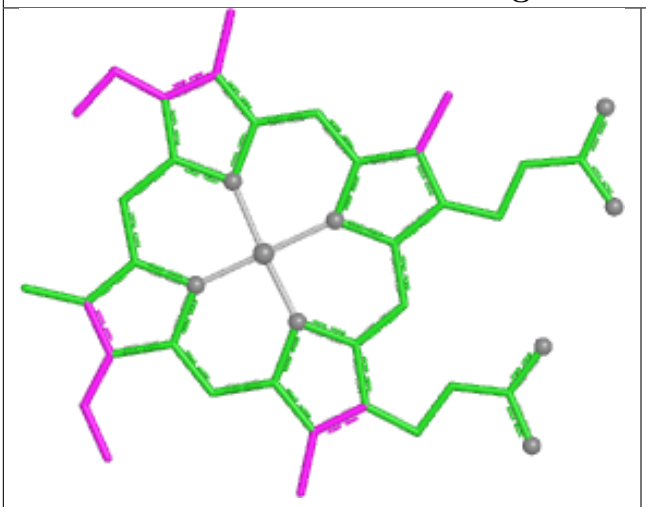
Ligand CDL p1 402



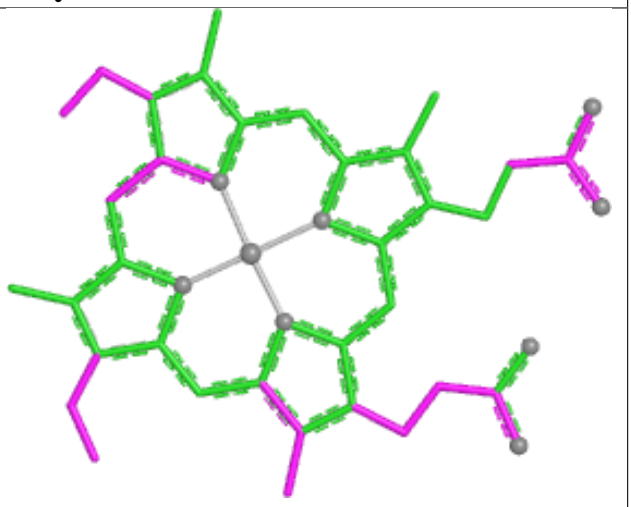
Ligand CDL E 402



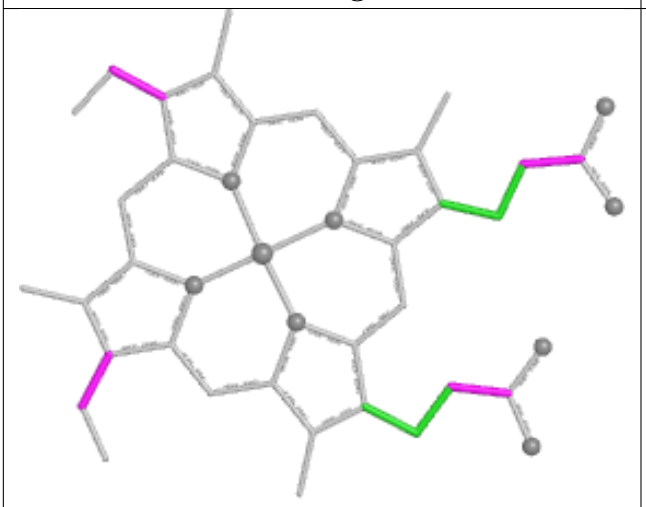
Ligand HEC Qd 401



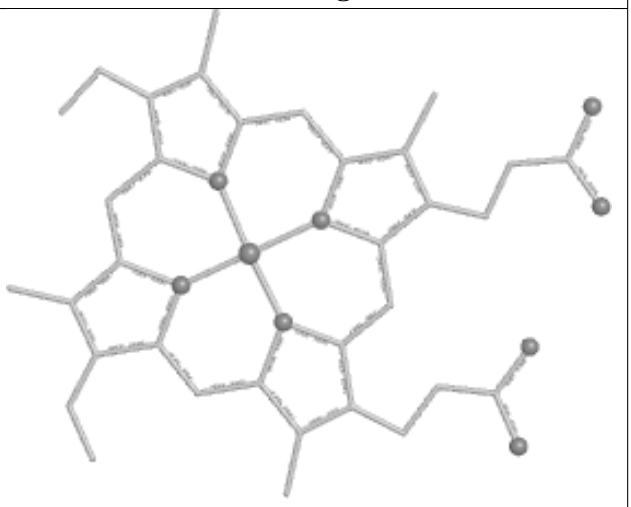
Bond lengths



Bond angles

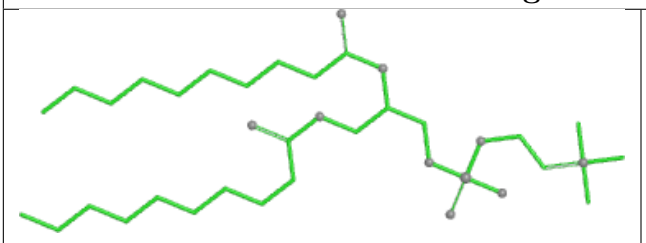


Torsions

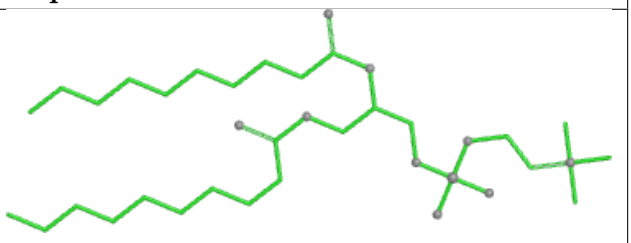


Rings

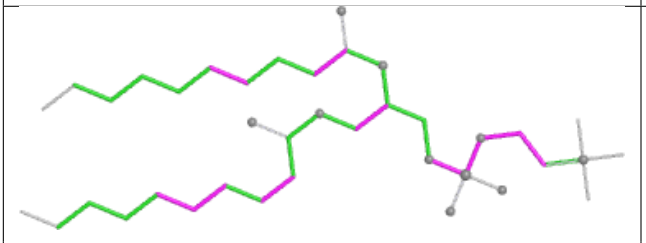
Ligand PC1 qc 506



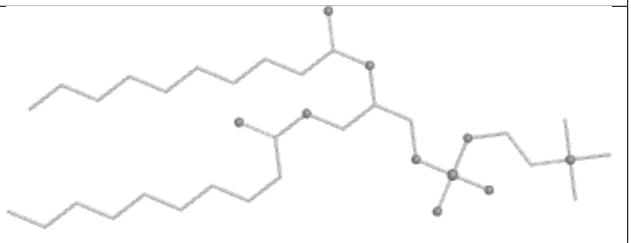
Bond lengths



Bond angles

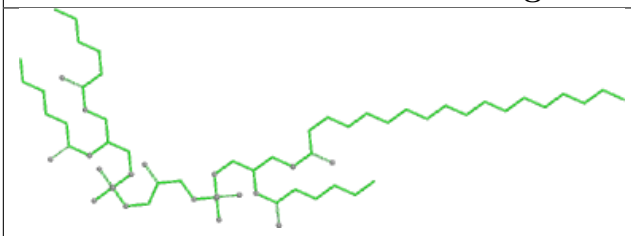


Torsions



Rings

Ligand CDL C 301



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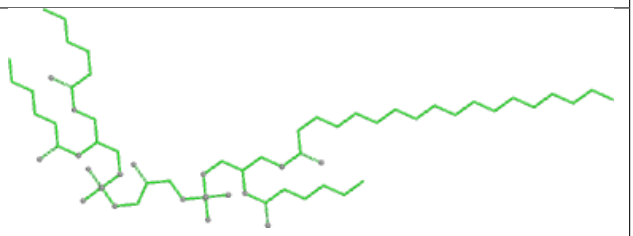

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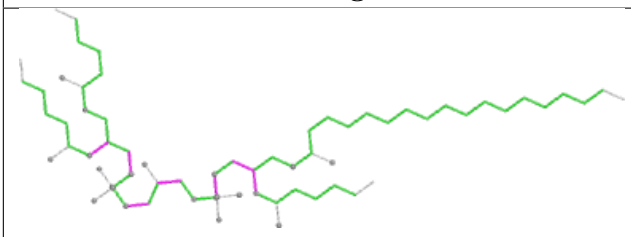

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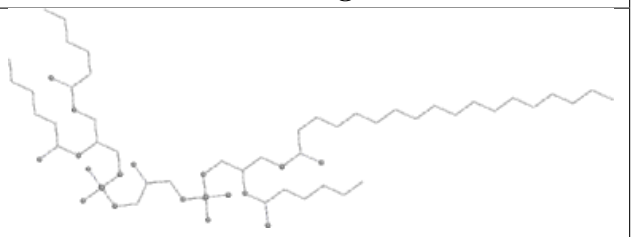
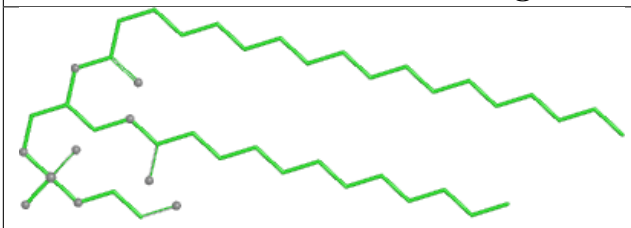


Rings

Ligand 3PE AN 301



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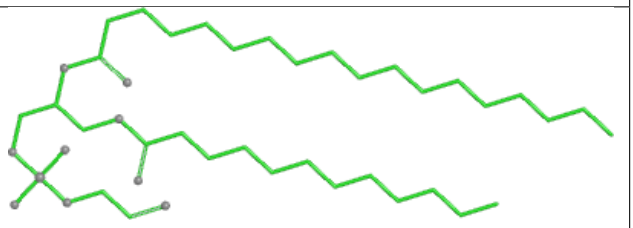

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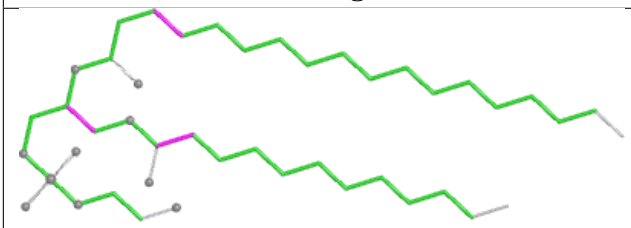

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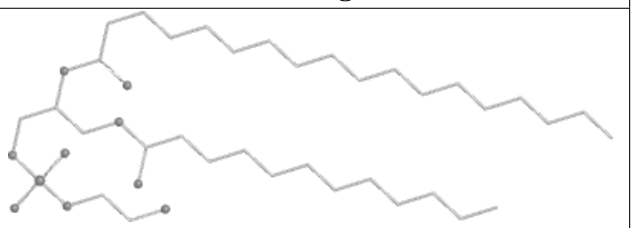
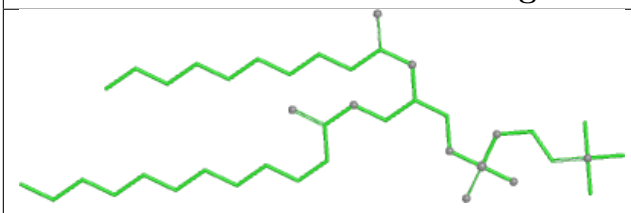


Rings

Ligand PC1 P1 401



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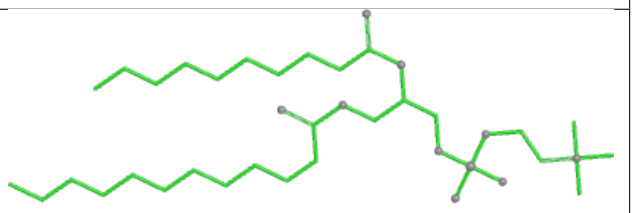

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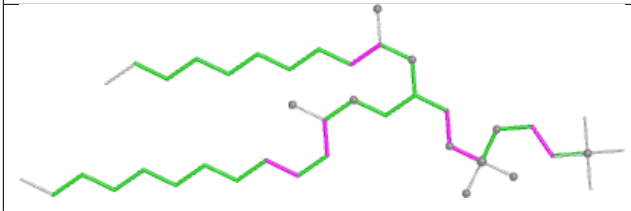

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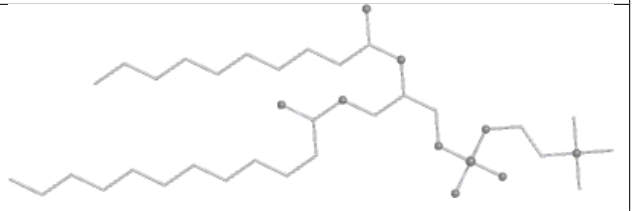
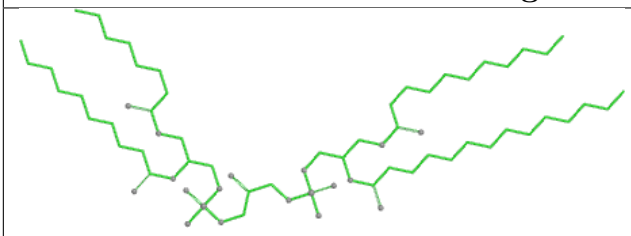


Rings

Ligand CDL qI 203



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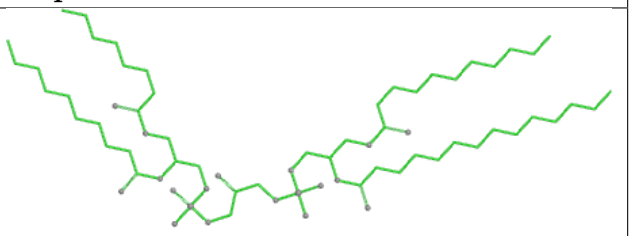

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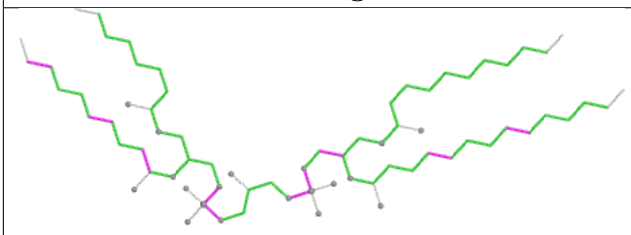

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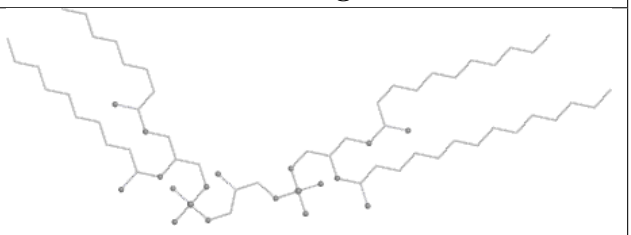
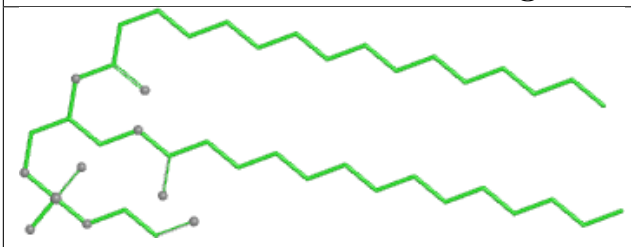


Rings

Ligand 3PE A3 201



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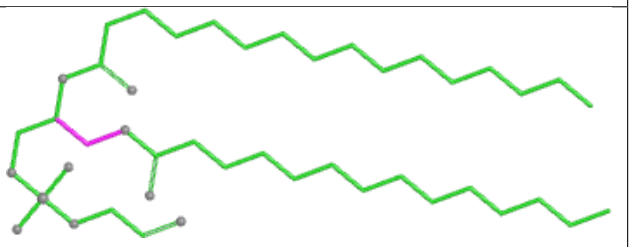

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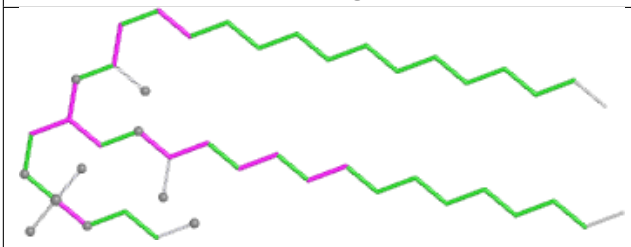

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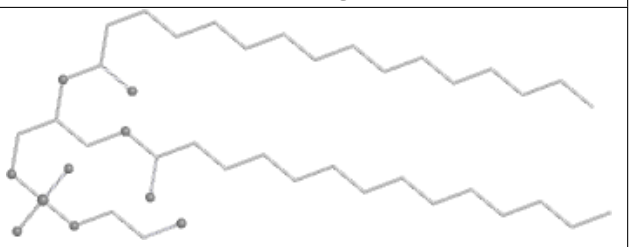
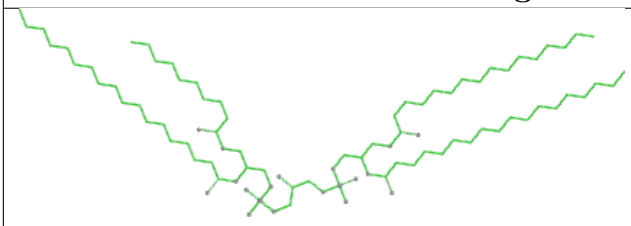


Rings

Ligand CDL N5 806



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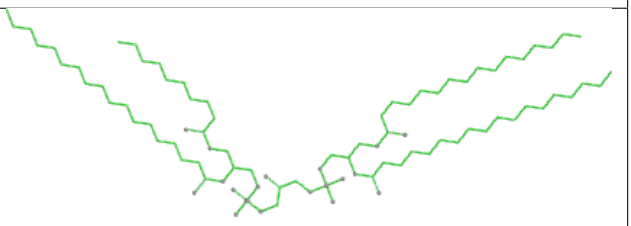
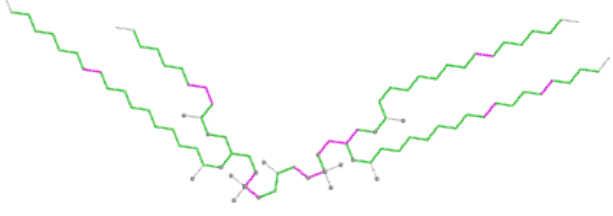


Bond angles



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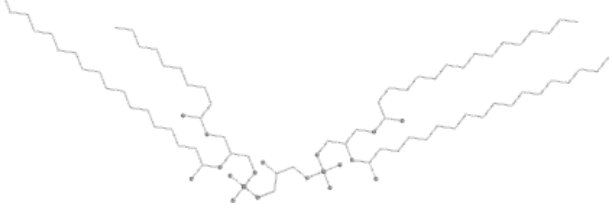
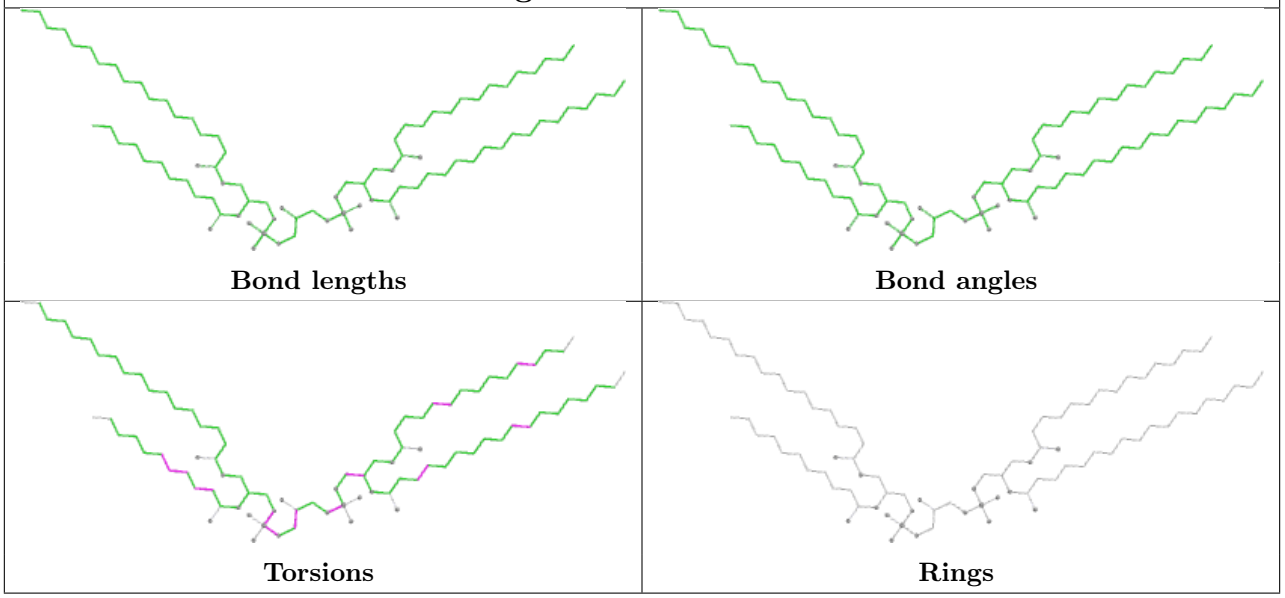
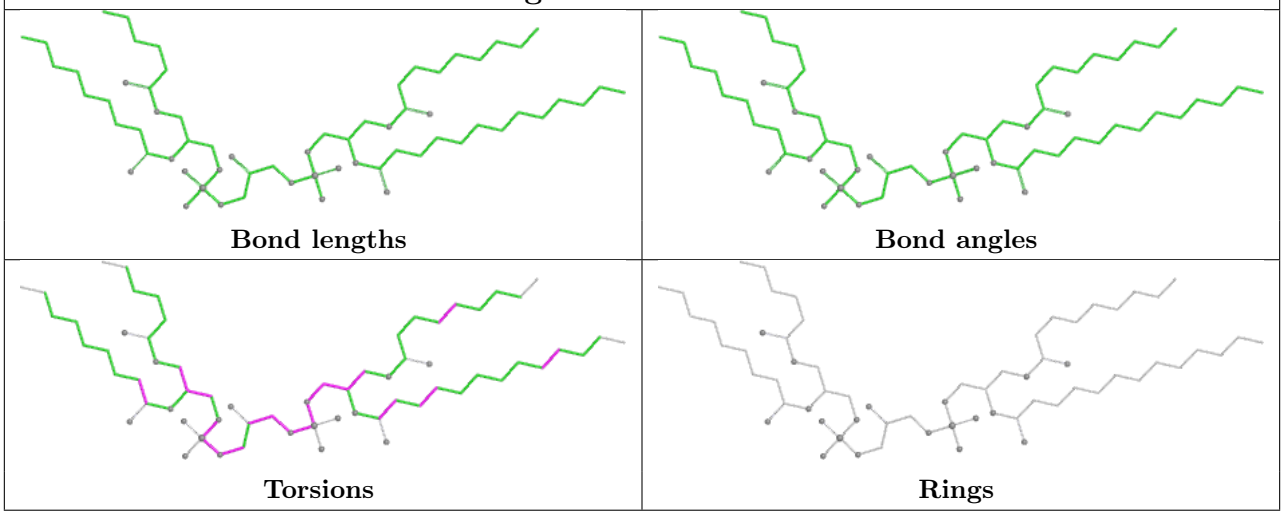


Rings

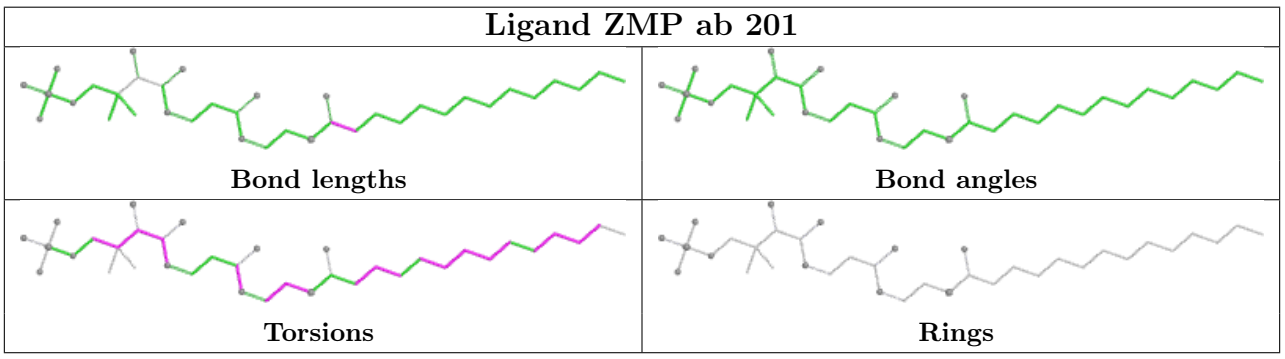
Ligand CDL N6 302



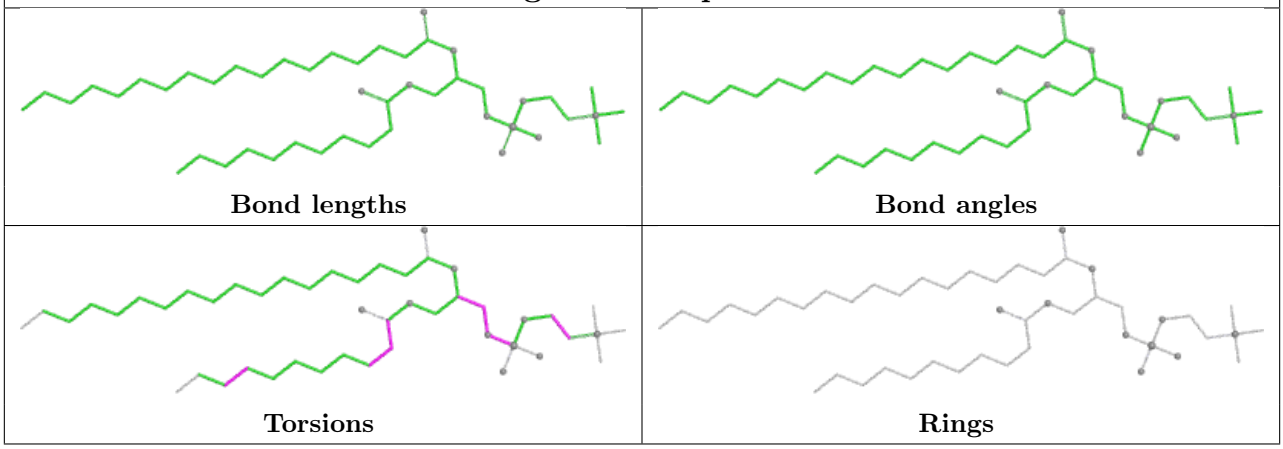
Ligand CDL R 201



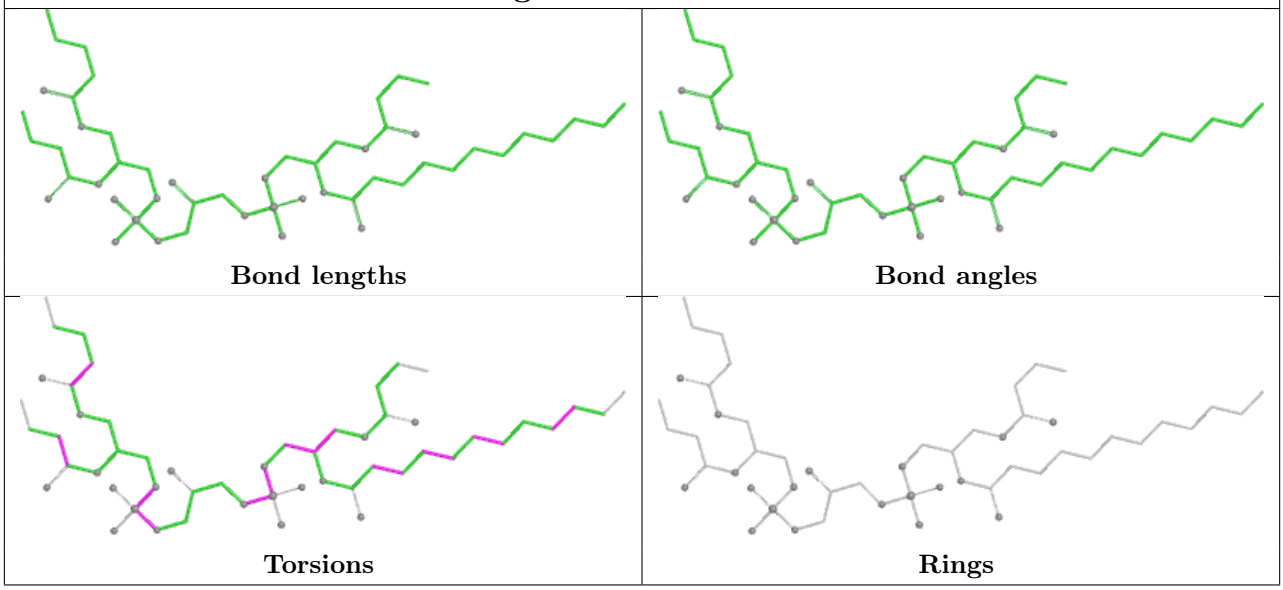
Ligand ZMP ab 201



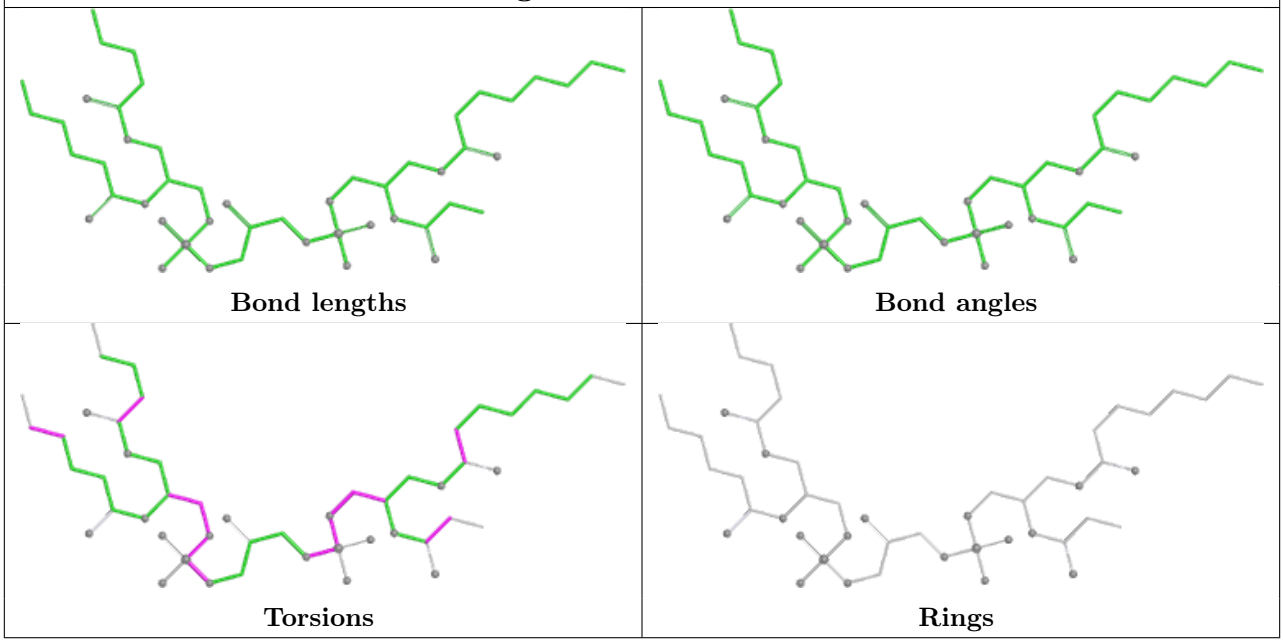
Ligand PC1 qc 509

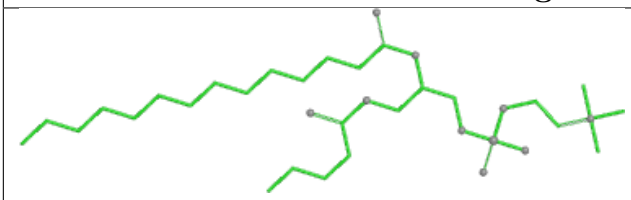
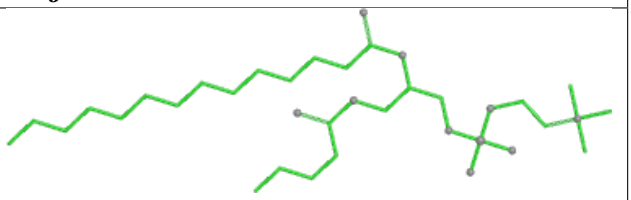
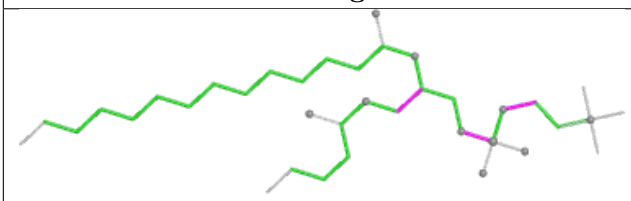
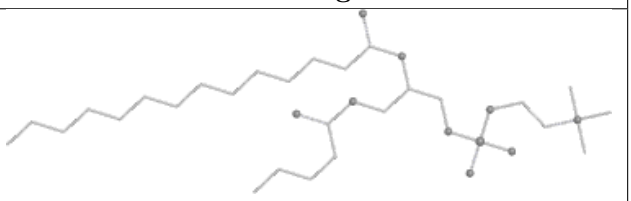


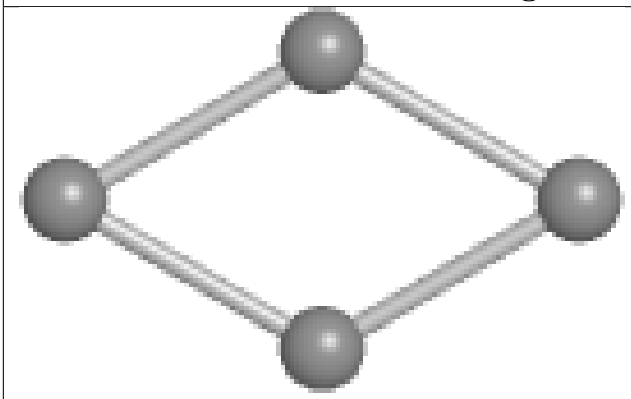
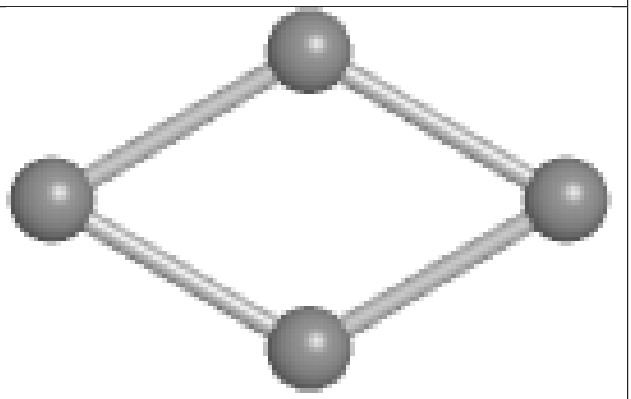
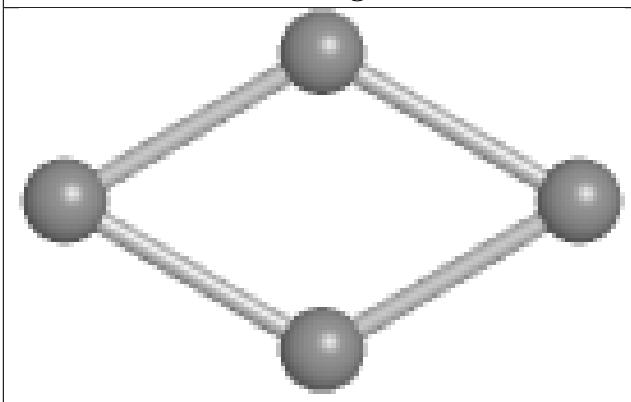
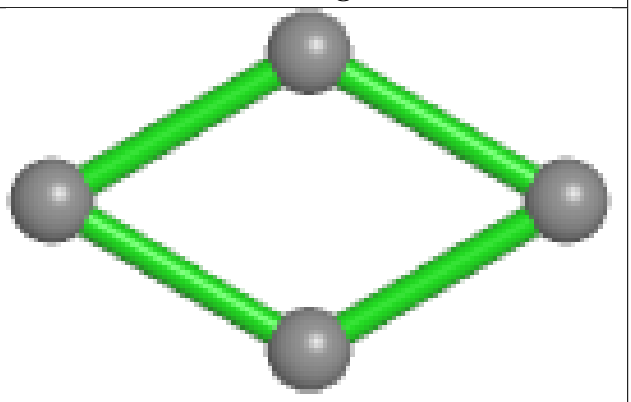
Ligand CDL TE 101



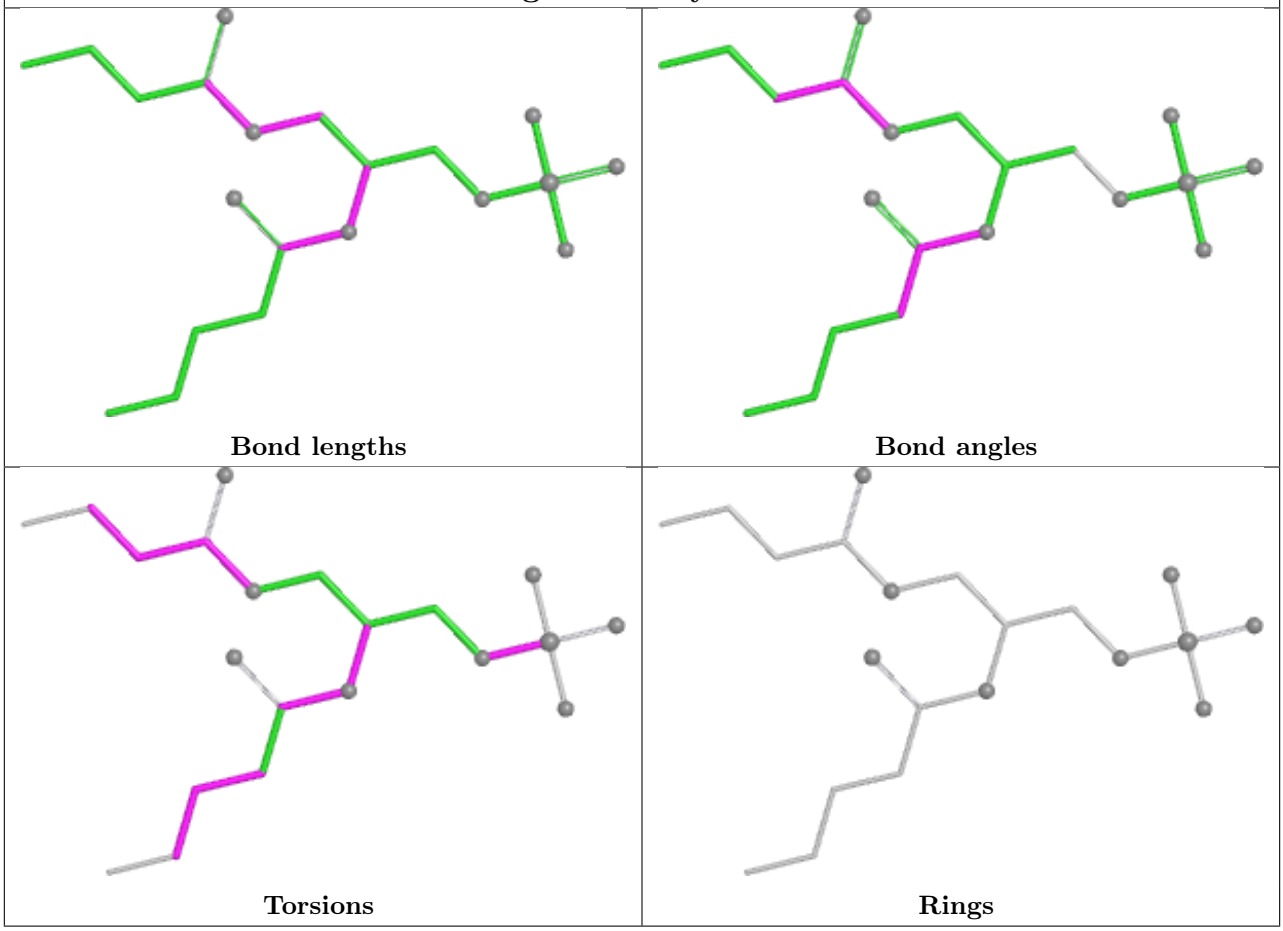
Ligand CDL 2O 101



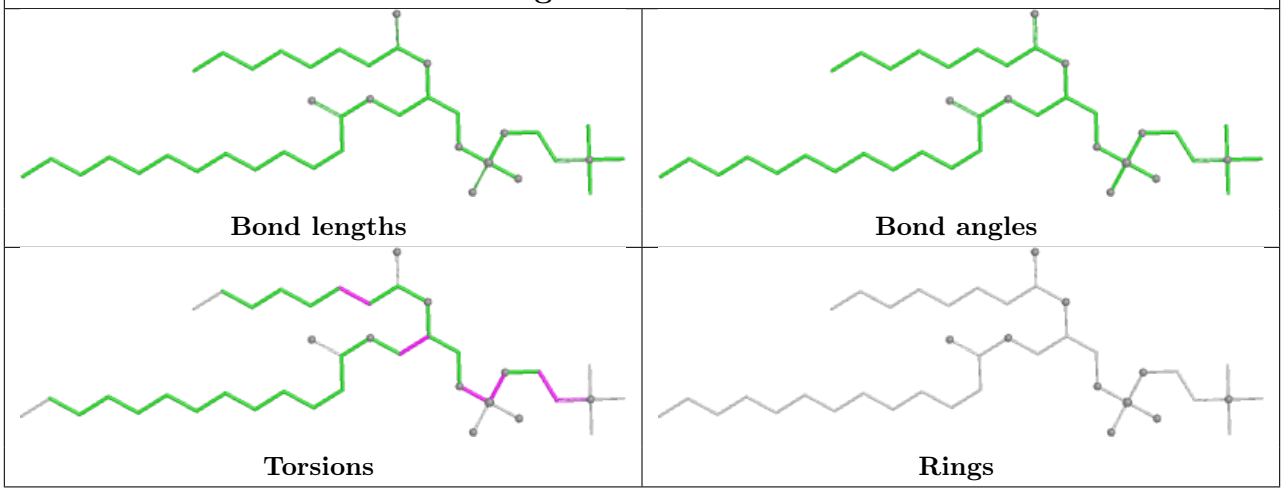
Ligand PC1 j 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FES FS 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

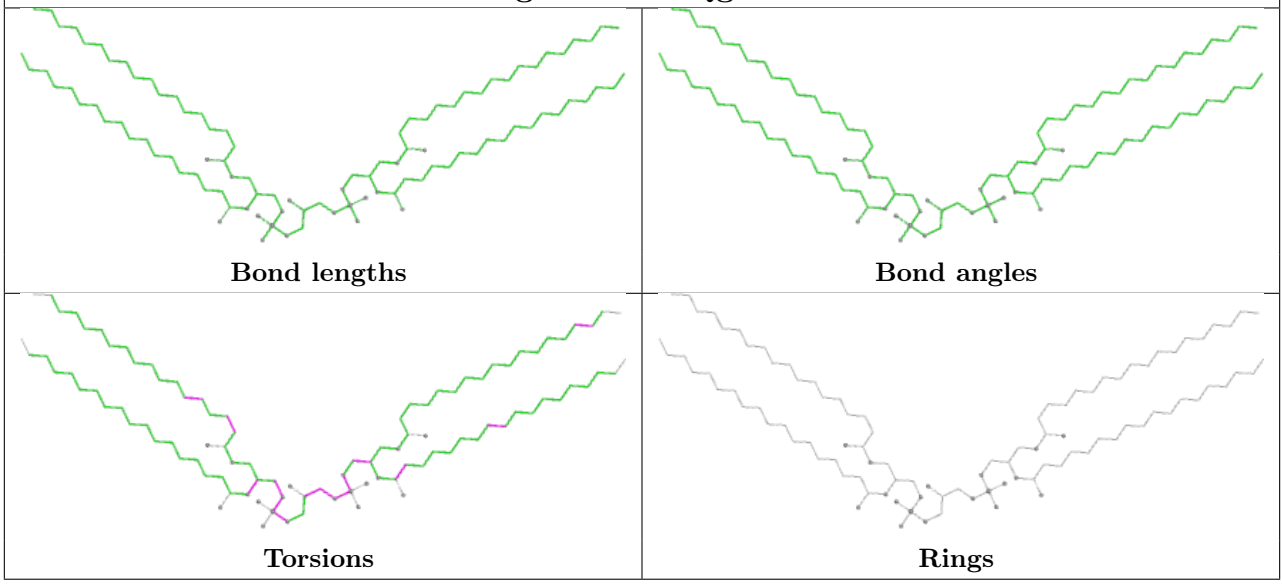
Ligand PX2 y5 204



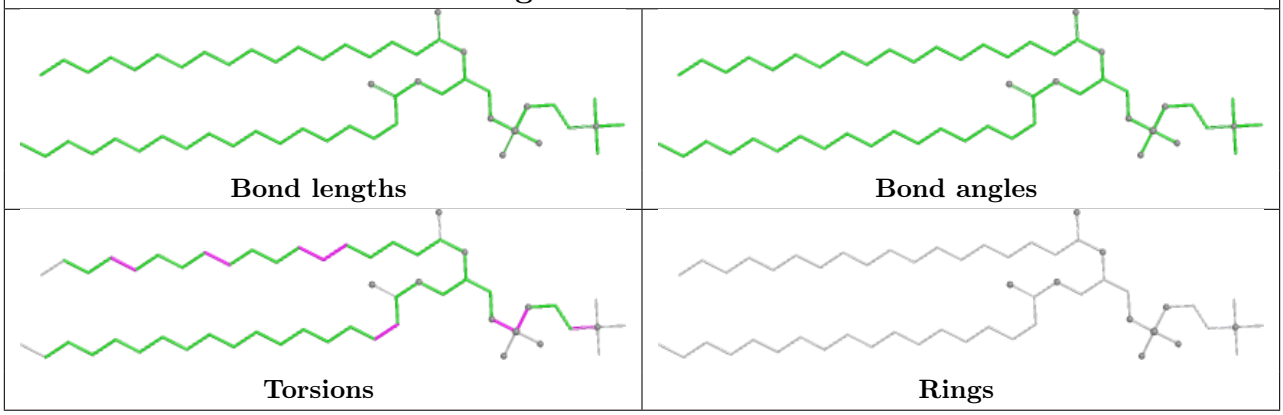
Ligand PC1 I 301



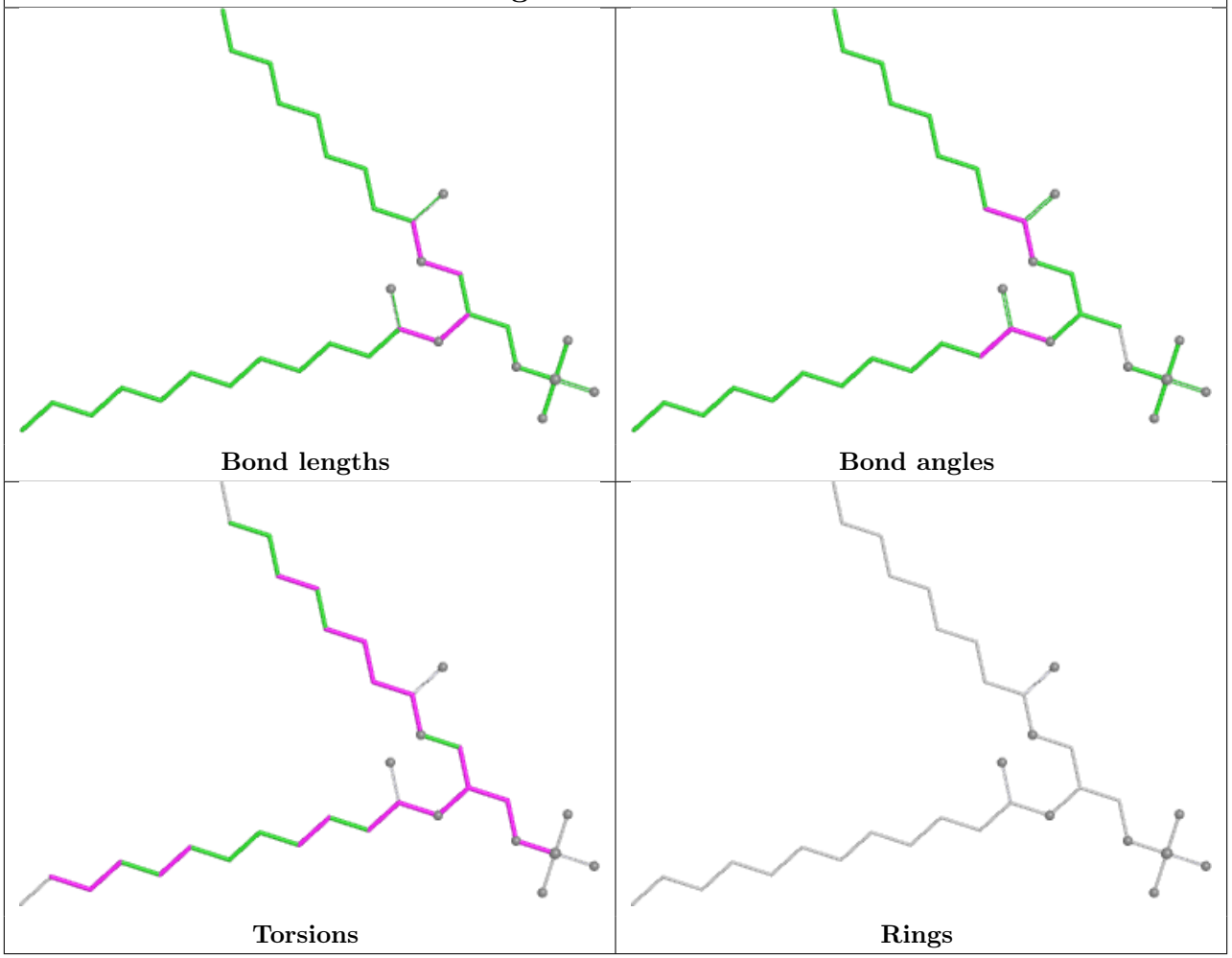
Ligand CDL Qg 402



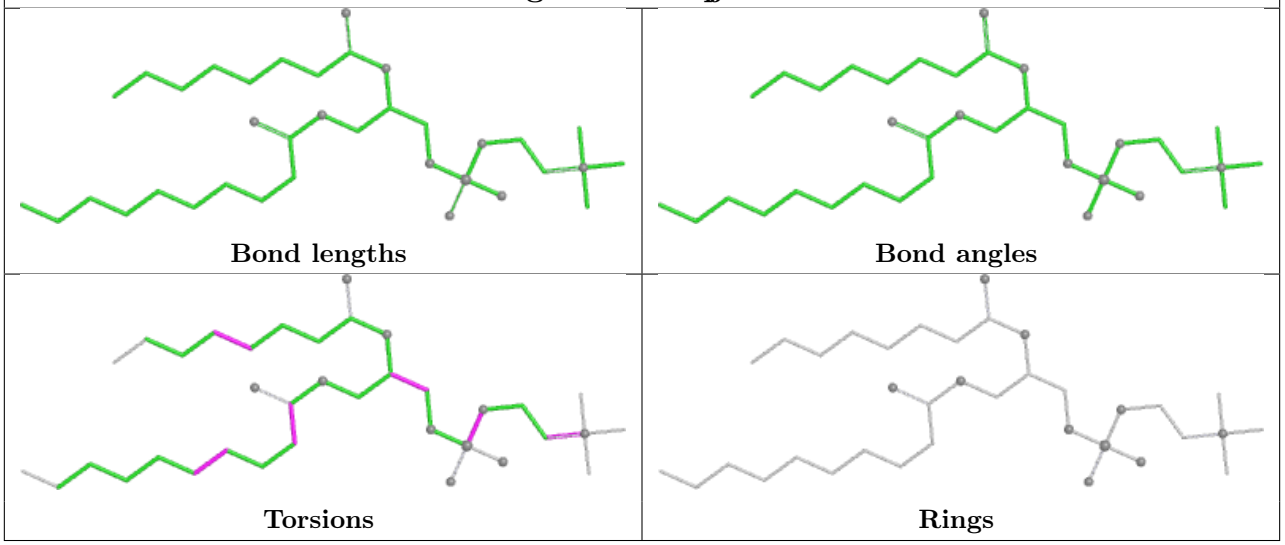
Ligand PC1 M1 401



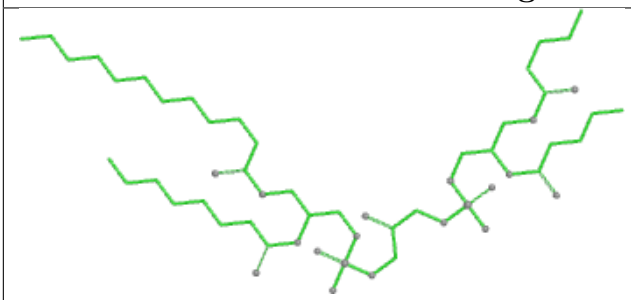
Ligand PX2 r 202



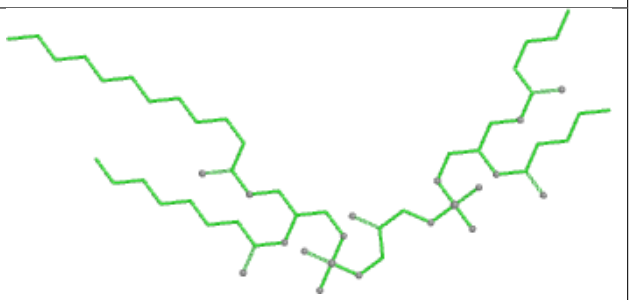
Ligand PC1 qj 101



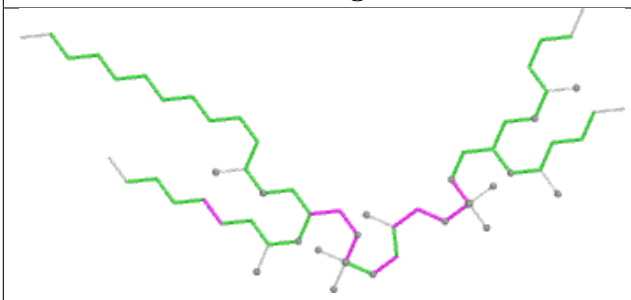
Ligand CDL b3 101



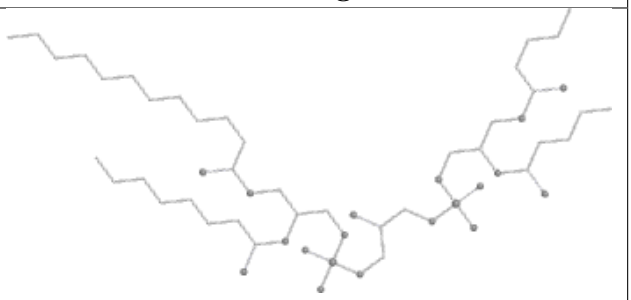
Bond lengths



Bond angles

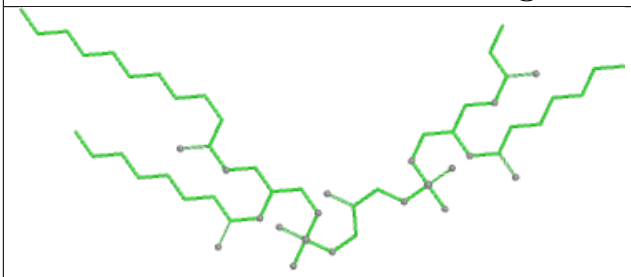


Torsions

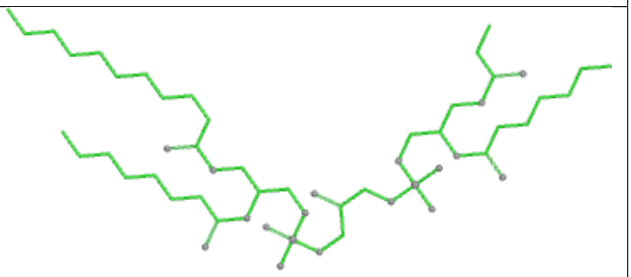


Rings

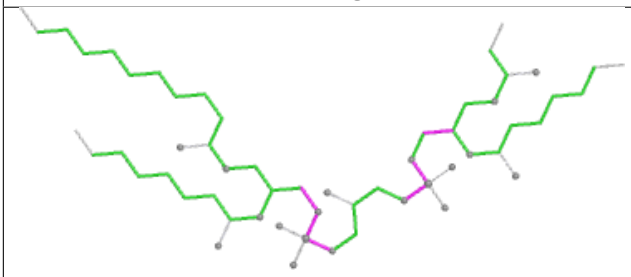
Ligand CDL u1 101



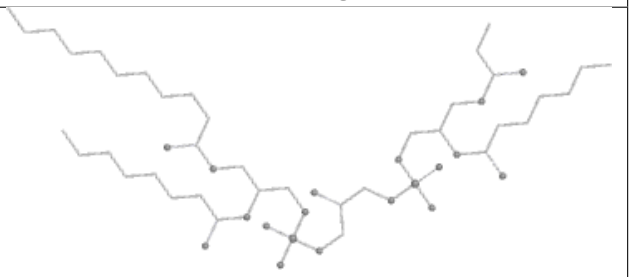
Bond lengths



Bond angles

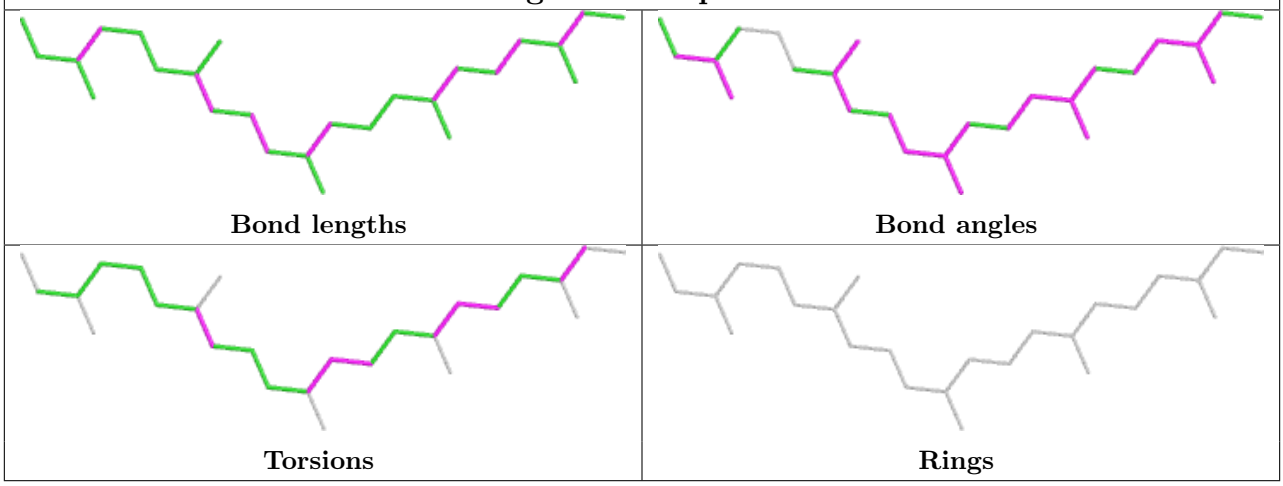


Torsions

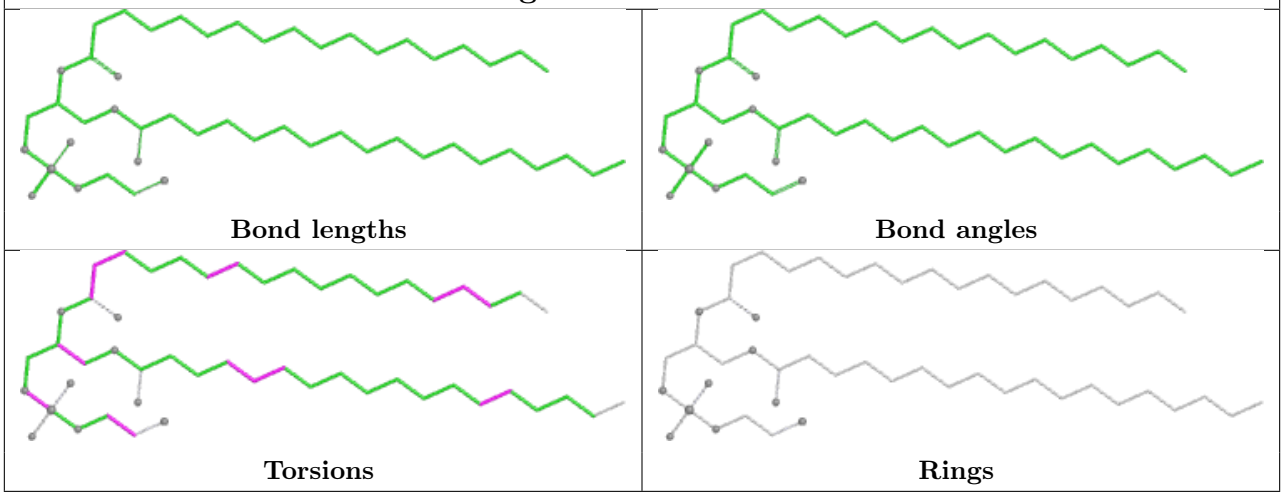


Rings

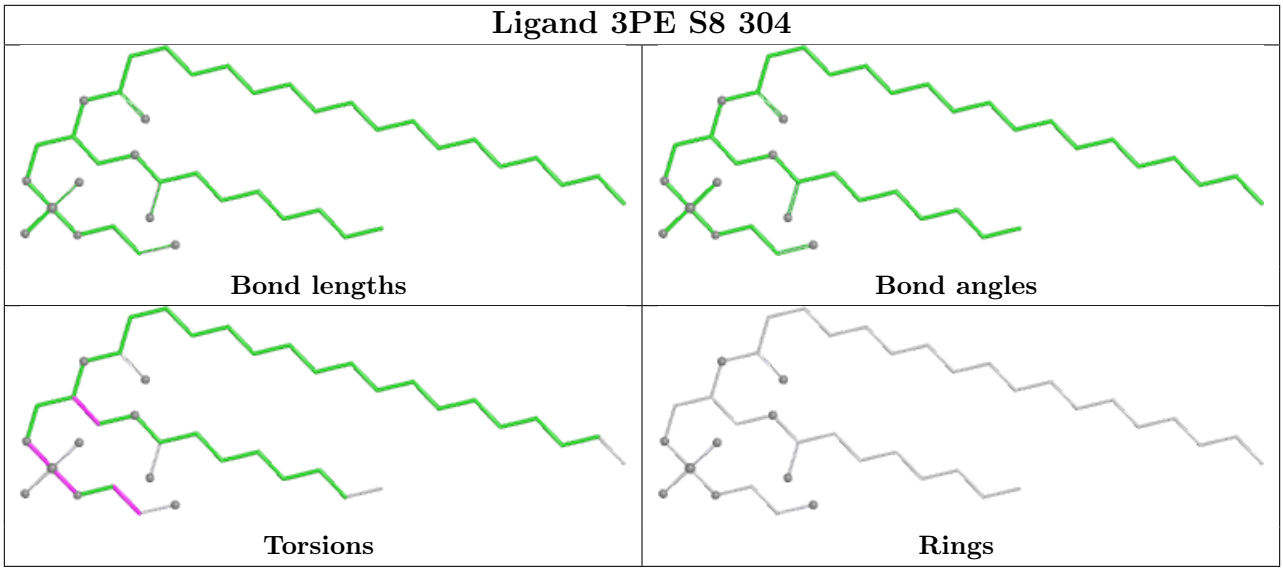
Ligand U10 qc 501



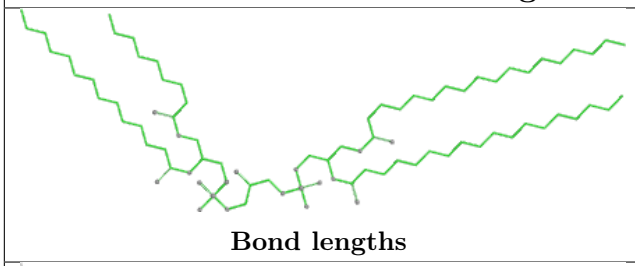
Ligand 3PE G2 301

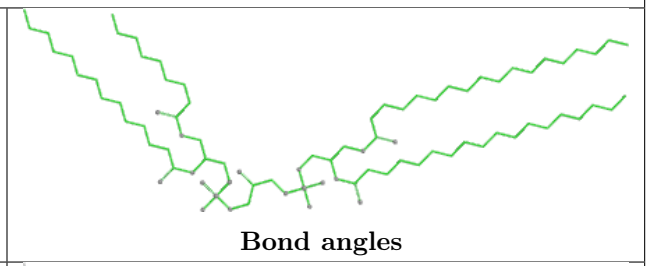


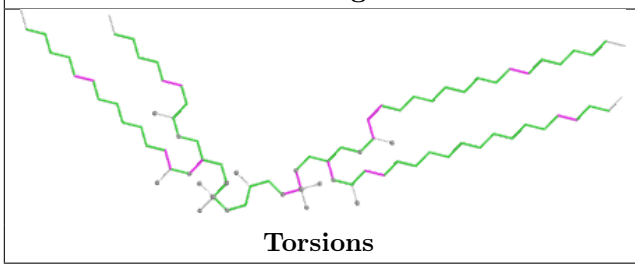
Ligand 3PE S8 304

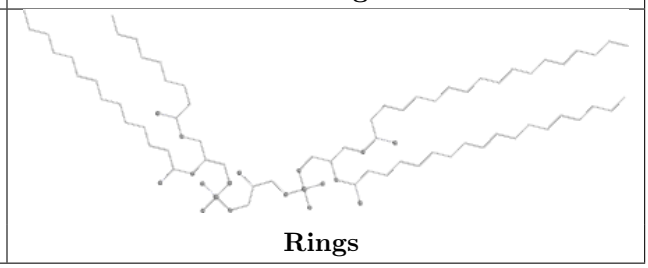


Ligand CDL 2b 201

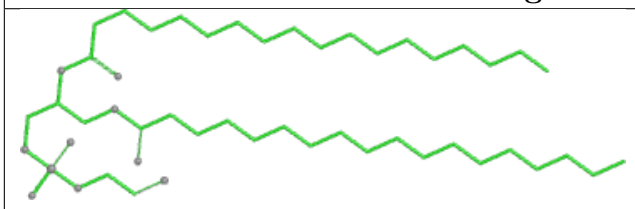

Bond lengths


Bond angles


Torsions


Rings

Ligand 3PE g2 301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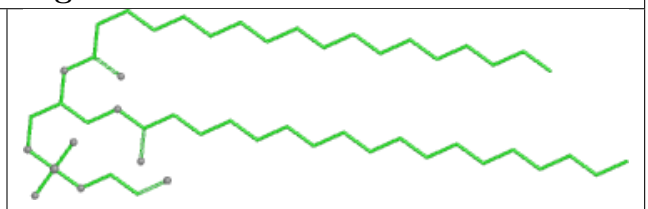
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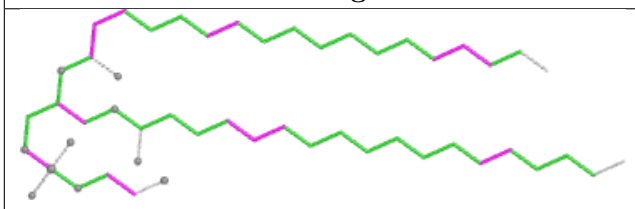
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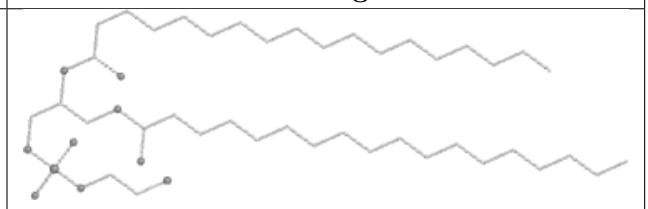
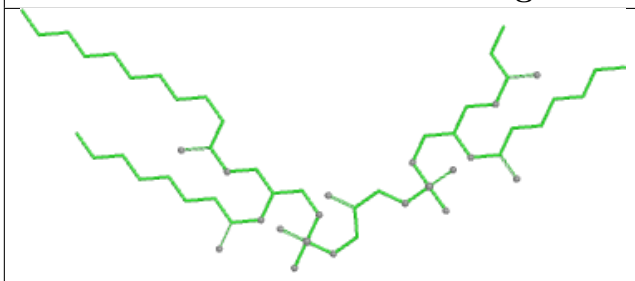

Rings

Ligand CDL U1 101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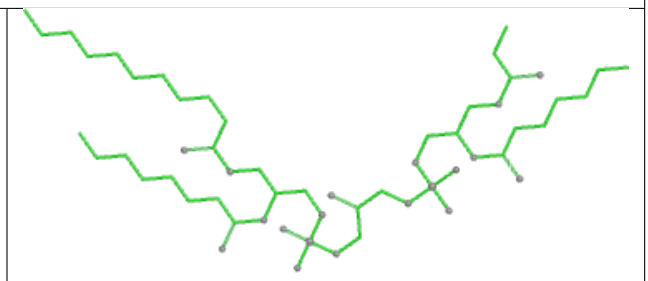
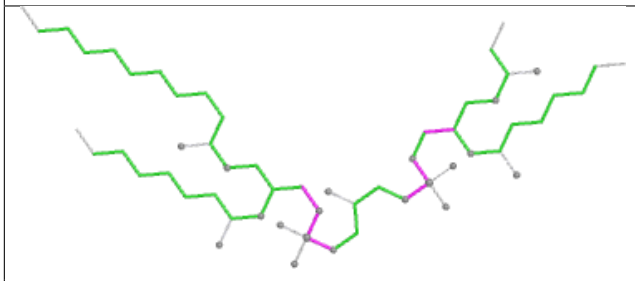

Bond angles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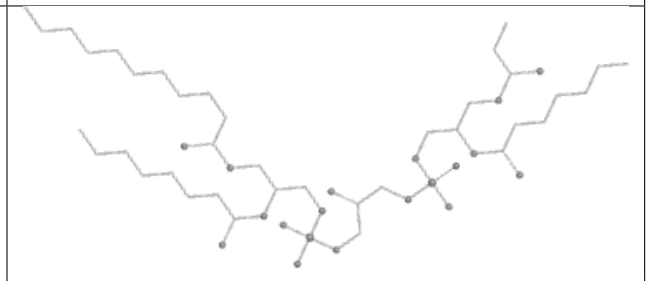
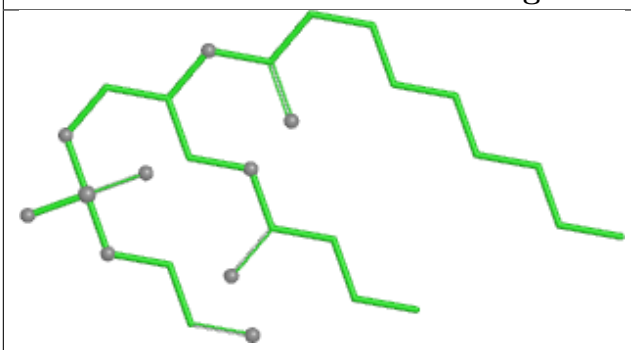

Rings

Ligand 3PE y5 202



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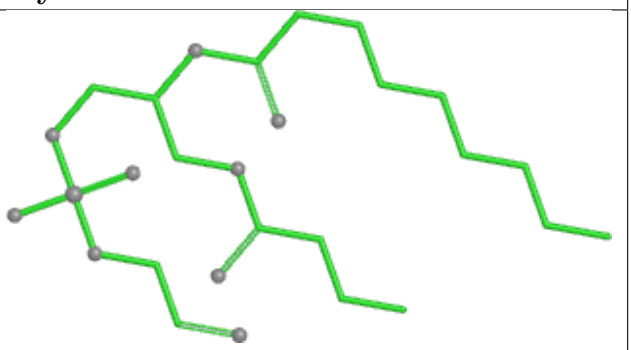
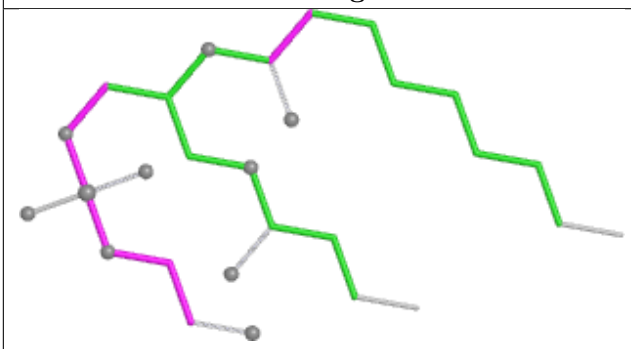


Bond angles



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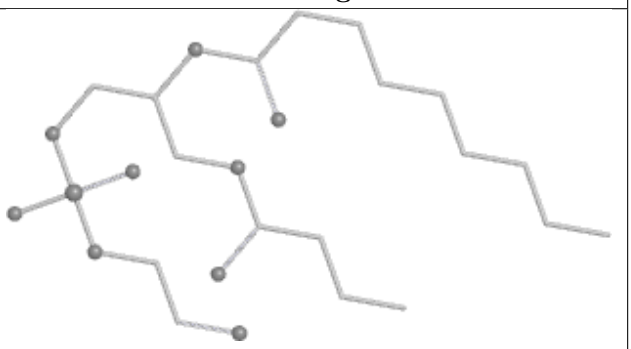
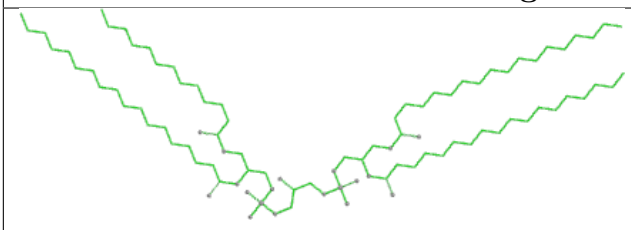
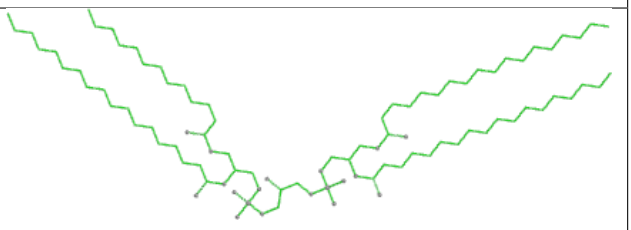


Rings

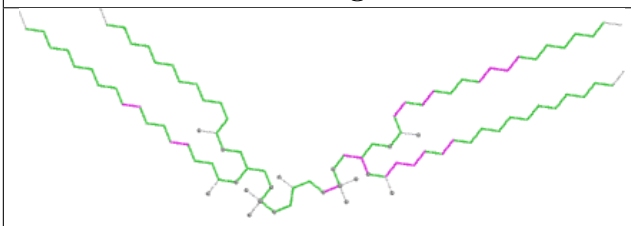
Ligand CDL c1 712



Bond lengths



Bond angles



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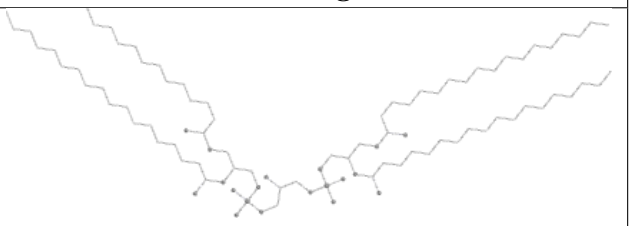
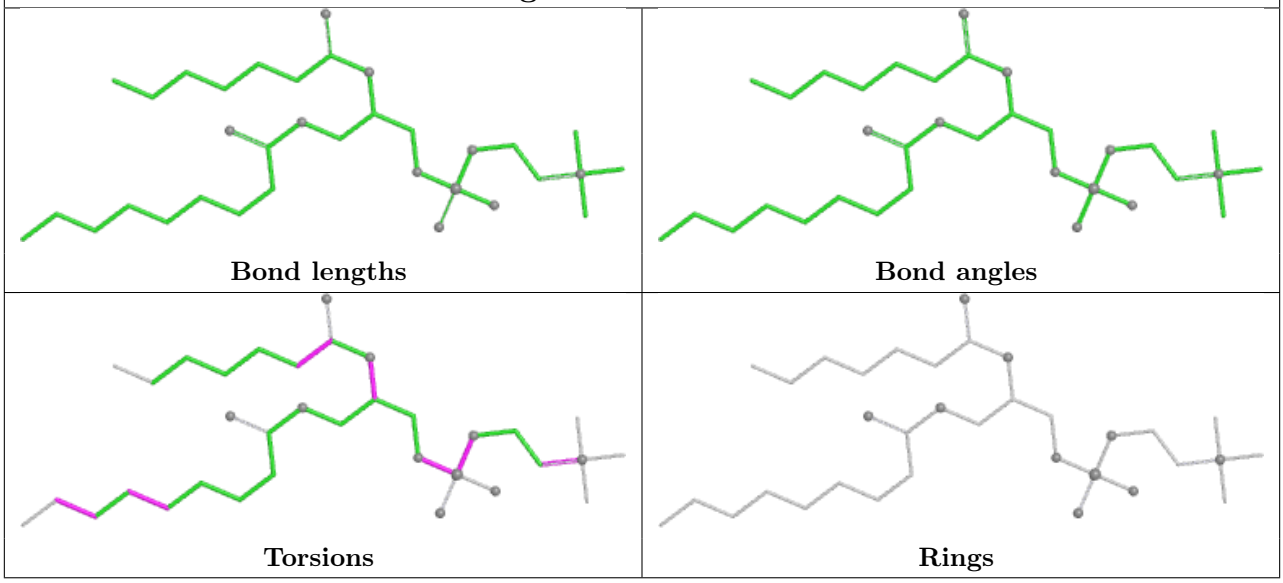
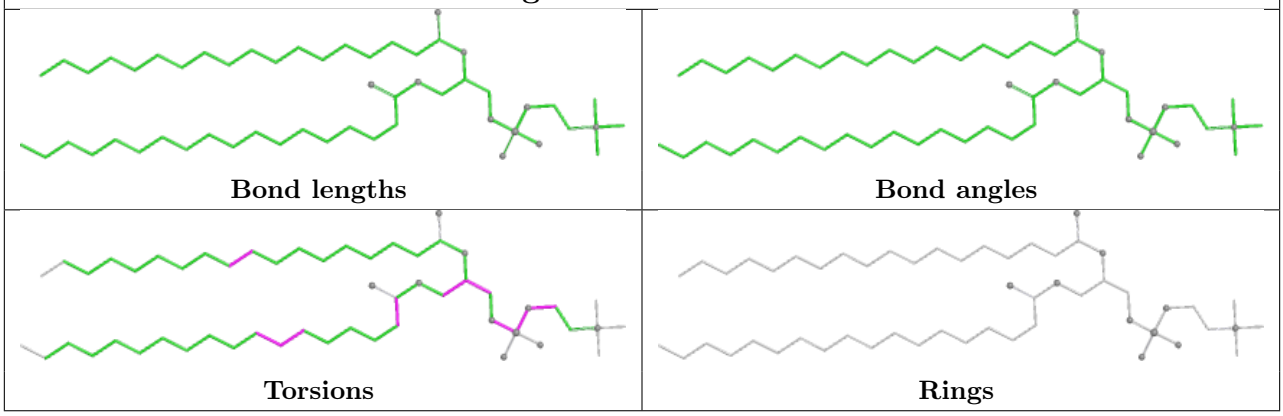


Rings

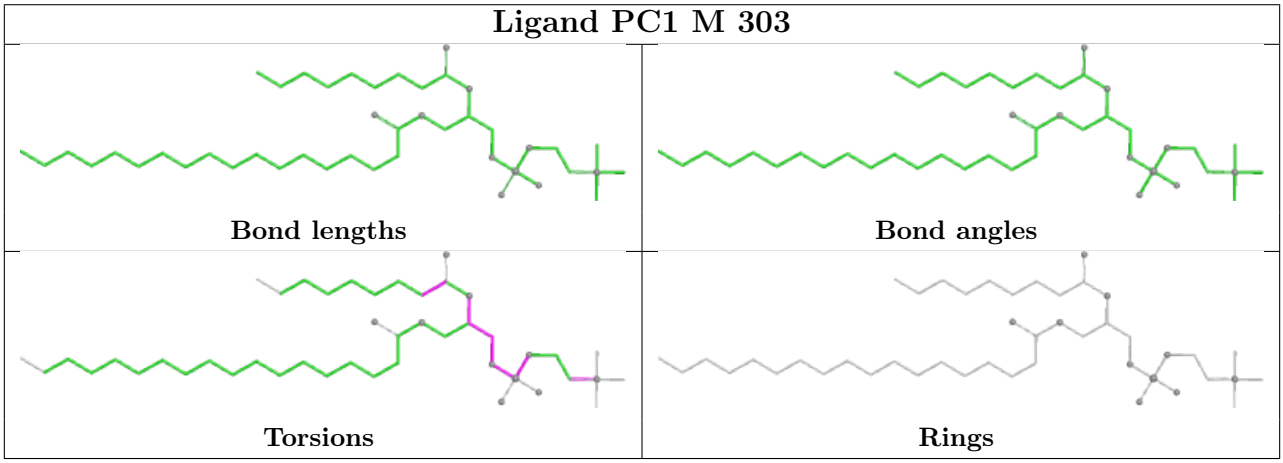
Ligand PC1 B9 201



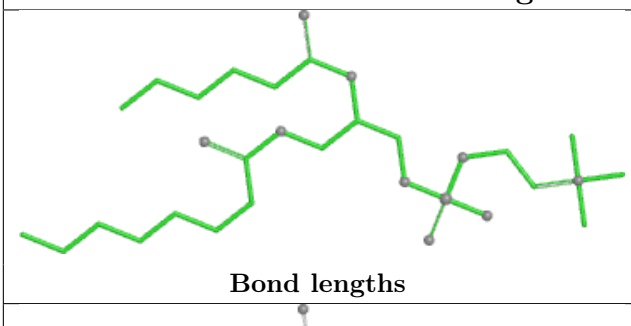
Ligand PC1 n5 805



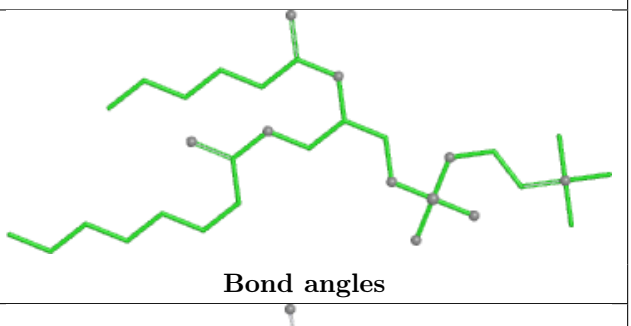
Ligand PC1 M 303



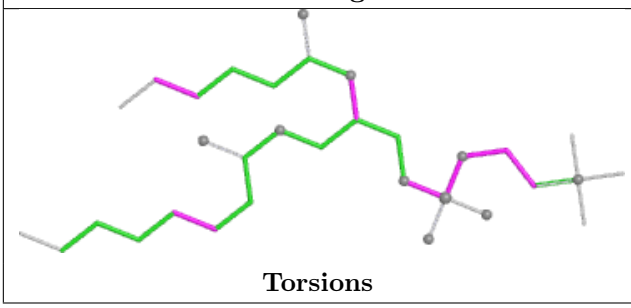
Ligand PC1 TE 102



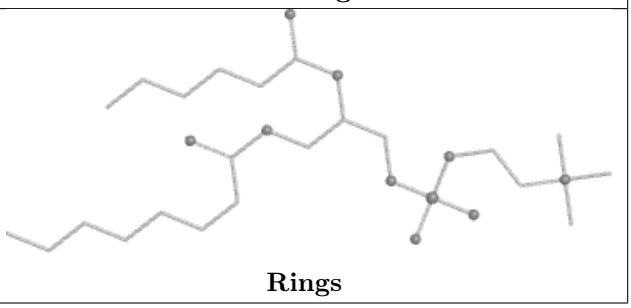
Bond lengths



Bond angles

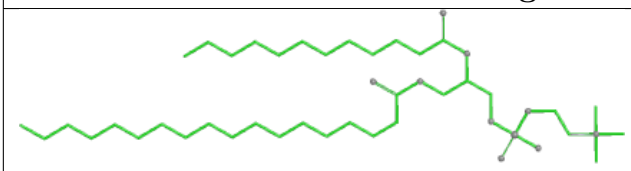


Torsions



Rings

Ligand PC1 T4 301



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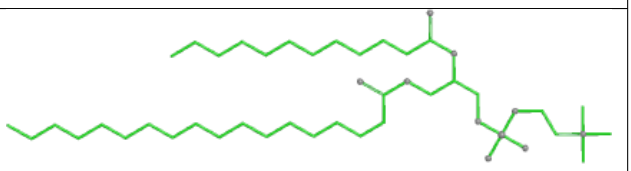
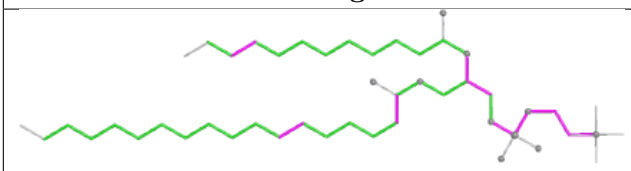
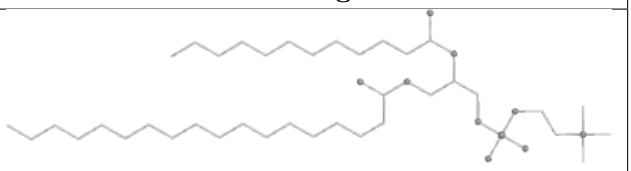


Bond angles

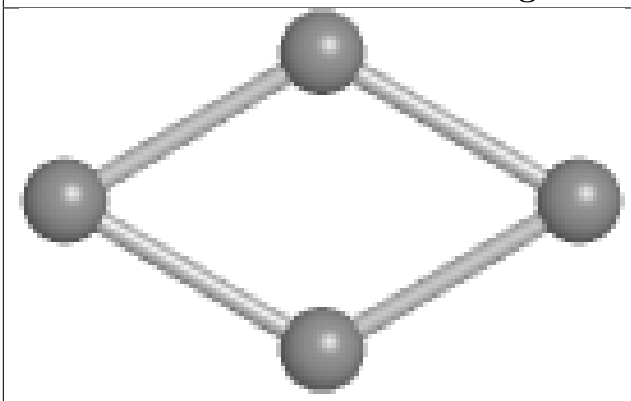


Torsions

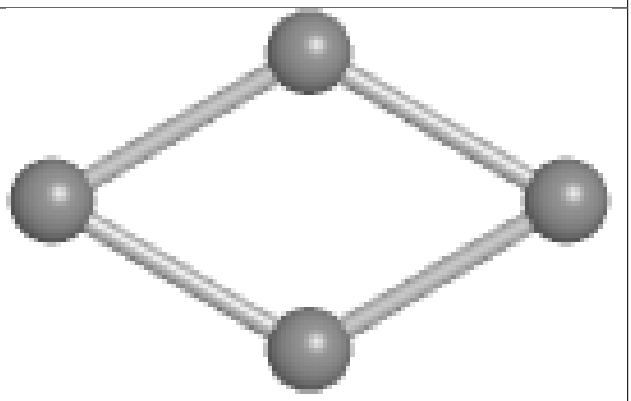


Rings

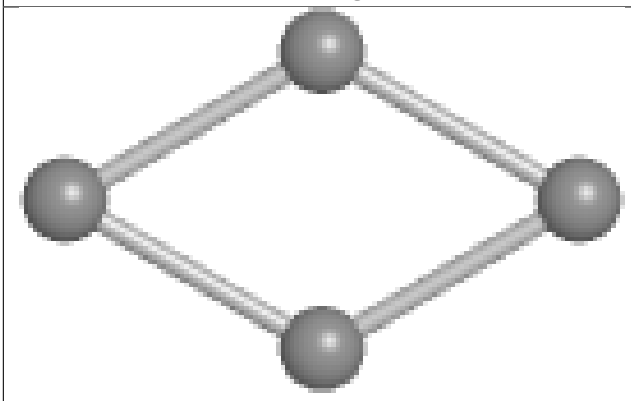
Ligand FES SB 401



Bond lengths



Bond angles



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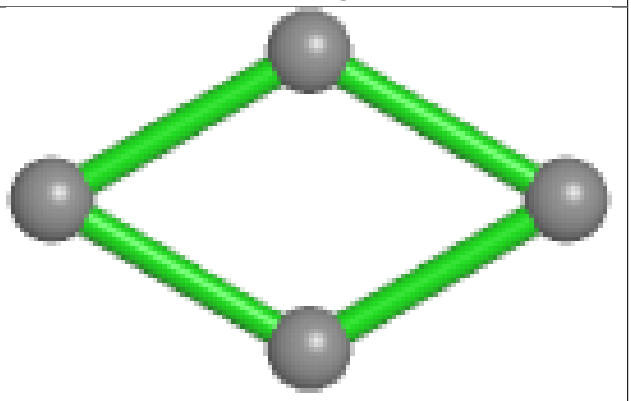
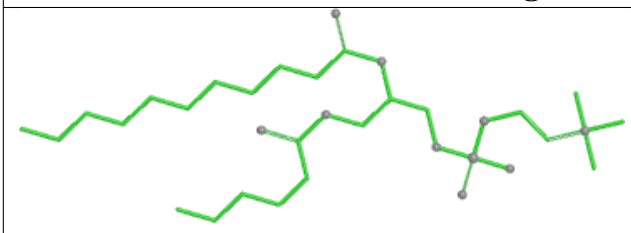
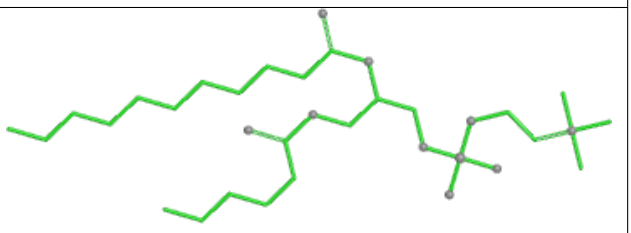


Rings

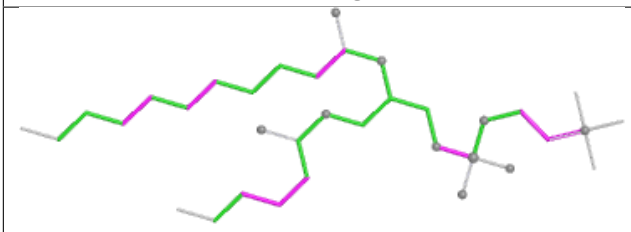
Ligand PC1 6a 202



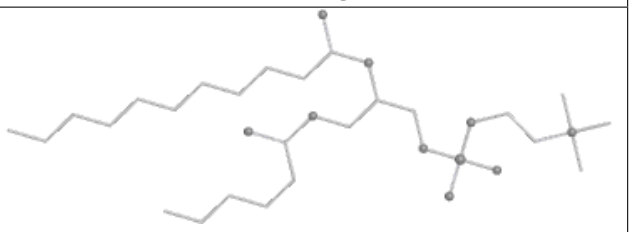
Bond lengths



Bond angles

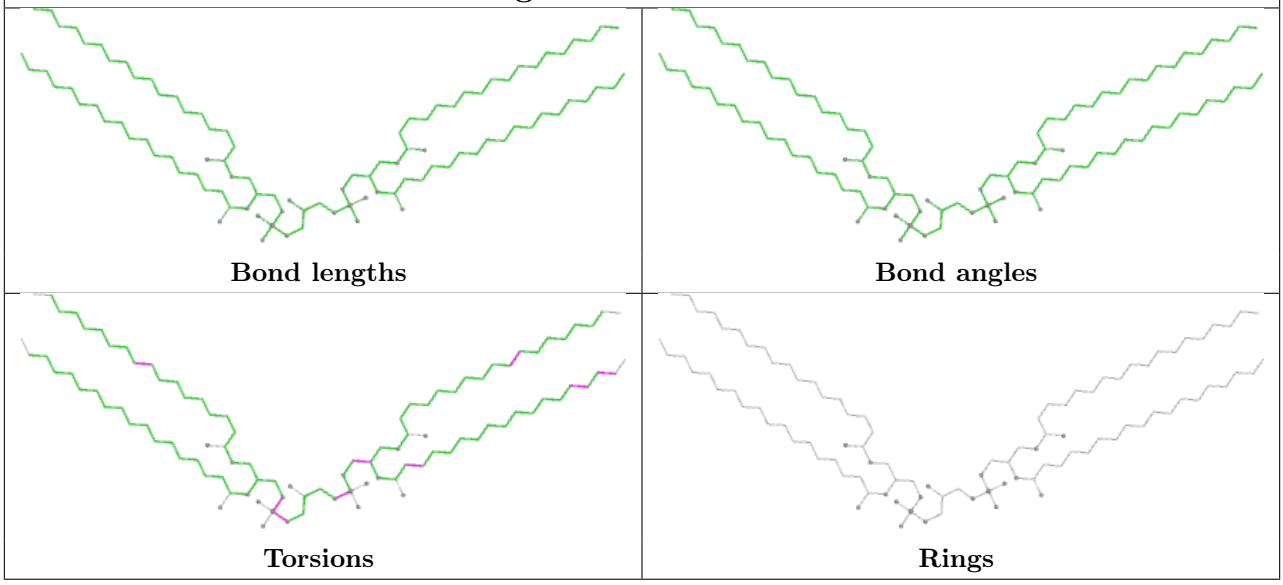


Torsions

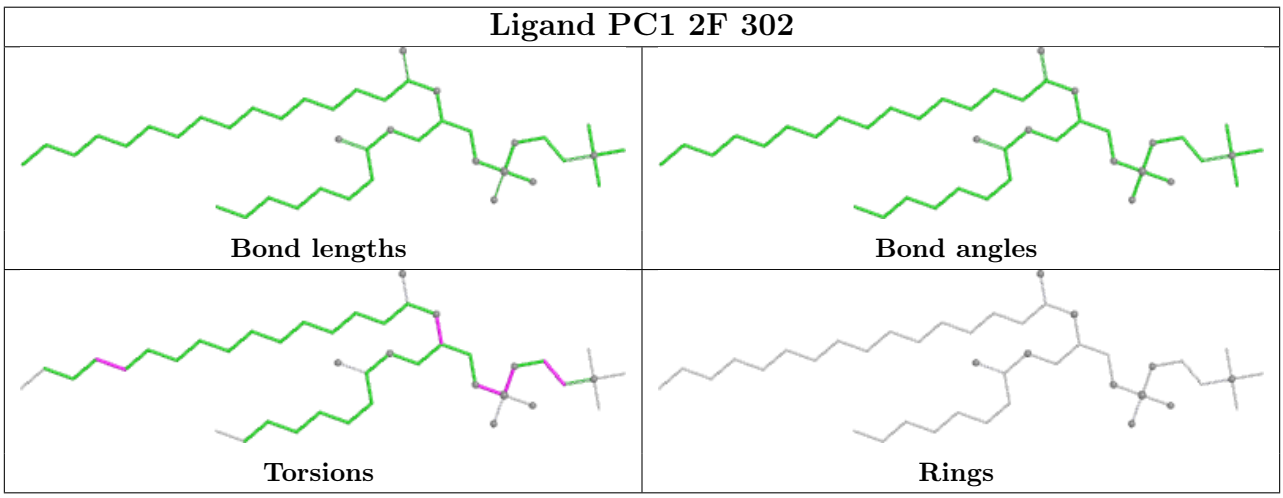


Rings

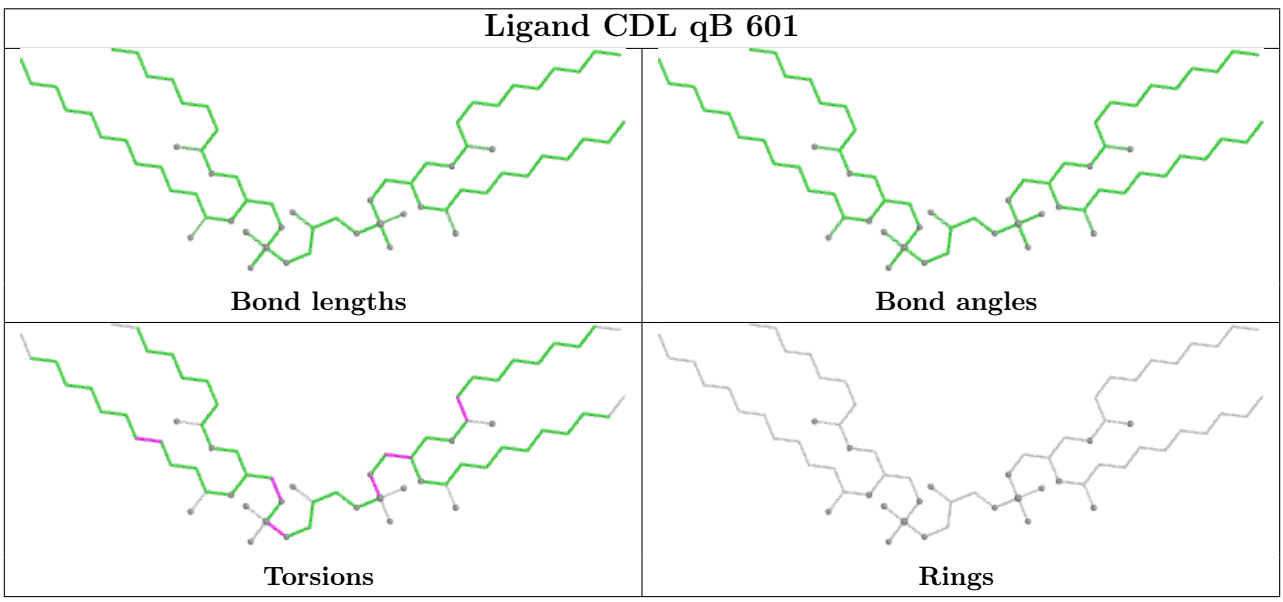
Ligand CDL 7A 201



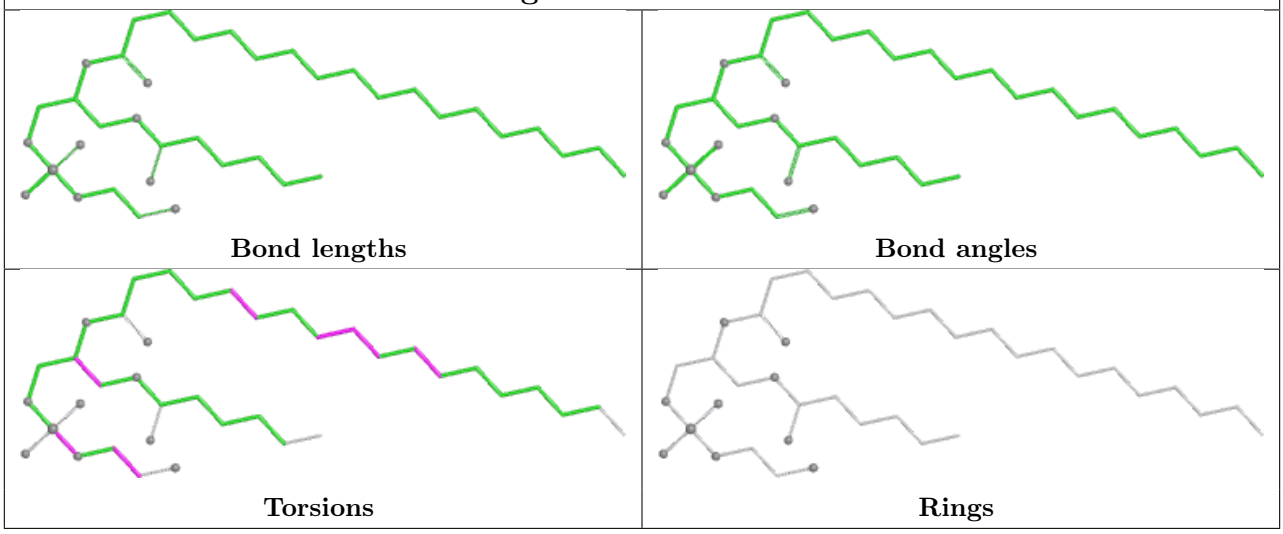
Ligand PC1 2F 302



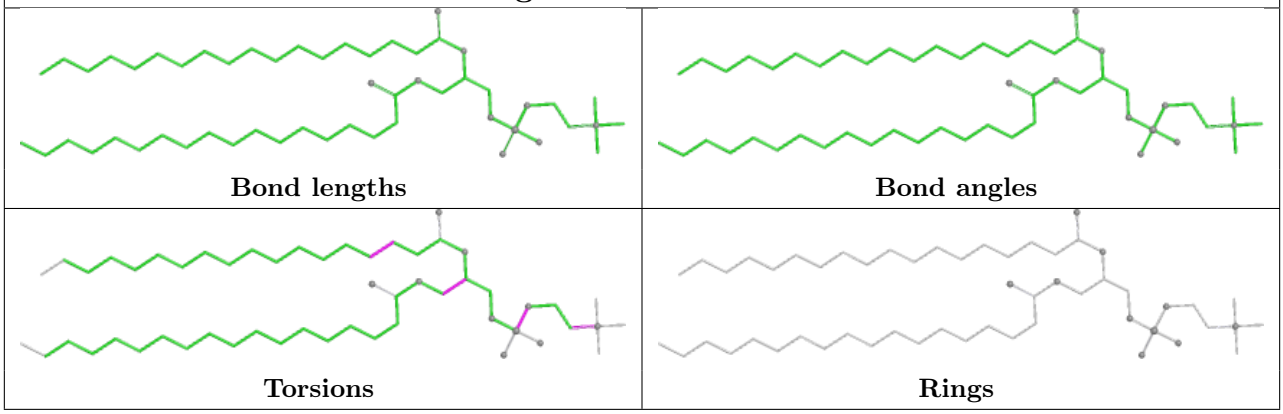
Ligand CDL qB 601



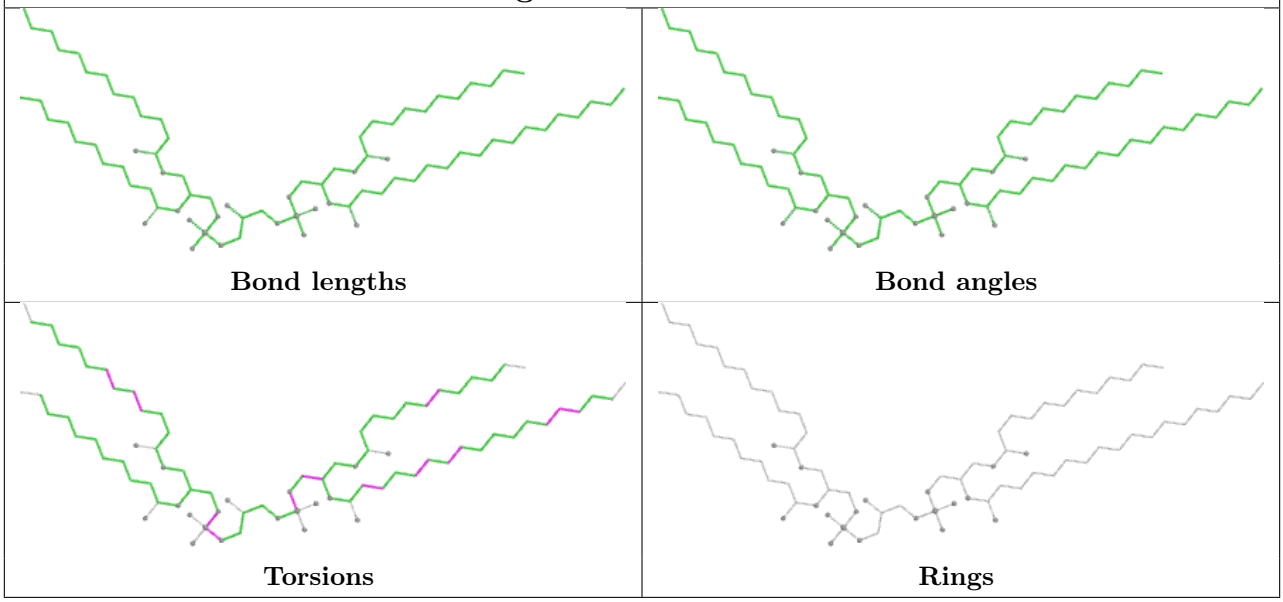
Ligand 3PE T8 602



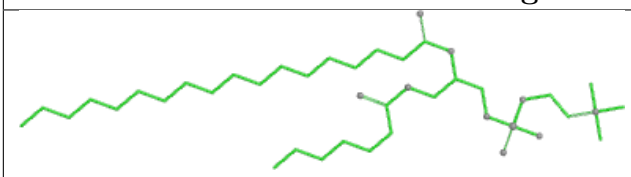
Ligand PC1 M2 405



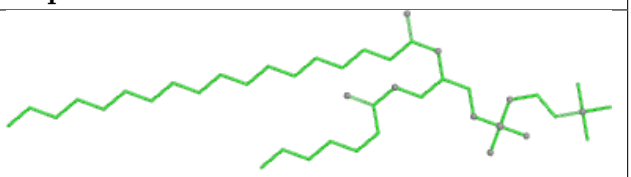
Ligand CDL 6C 203



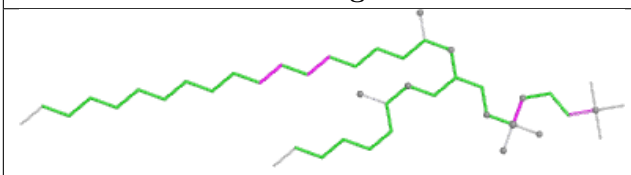
Ligand PC1 qb 602



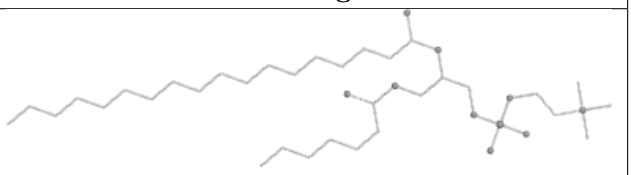
Bond lengths



Bond angles

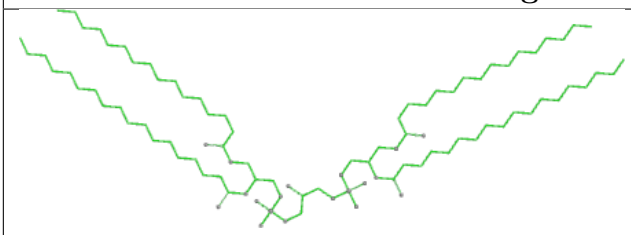


Torsions

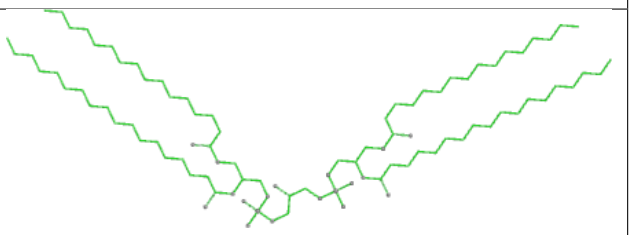


Rings

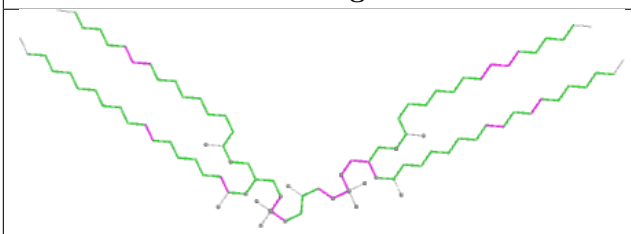
Ligand CDL t5 301



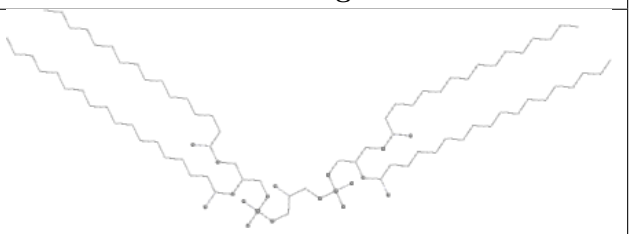
Bond lengths



Bond angles

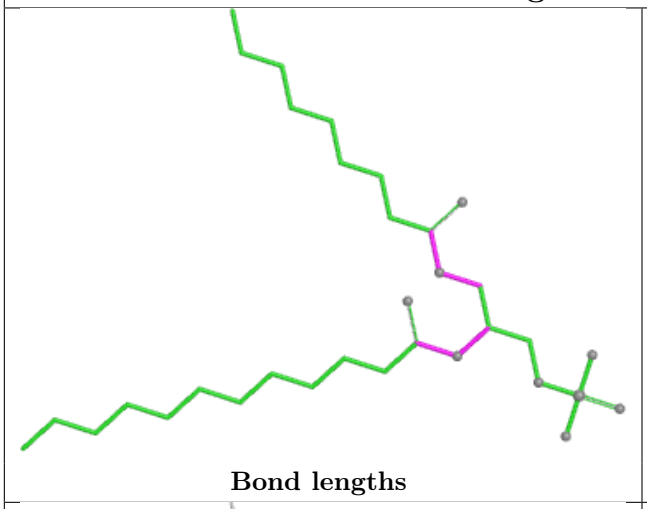


Torsions



Rings

Ligand PX2 R 202



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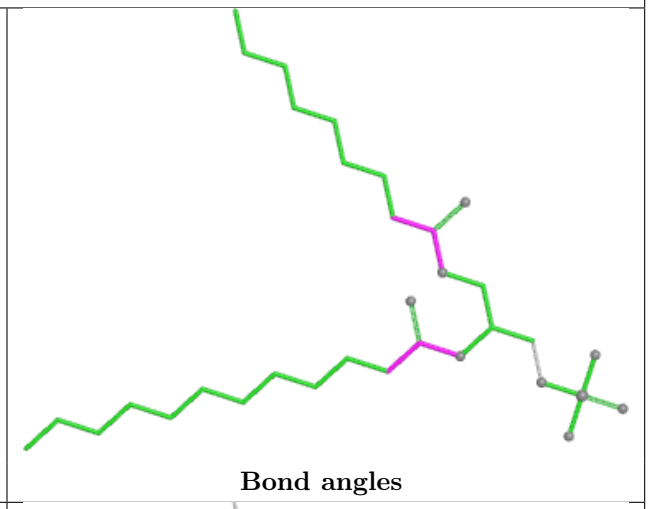
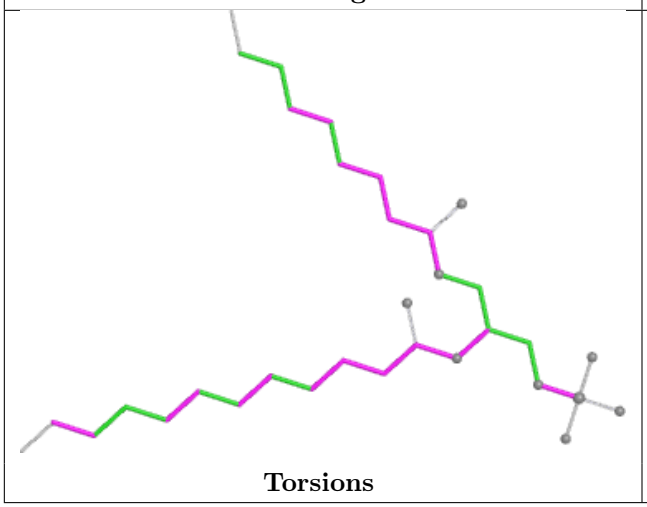
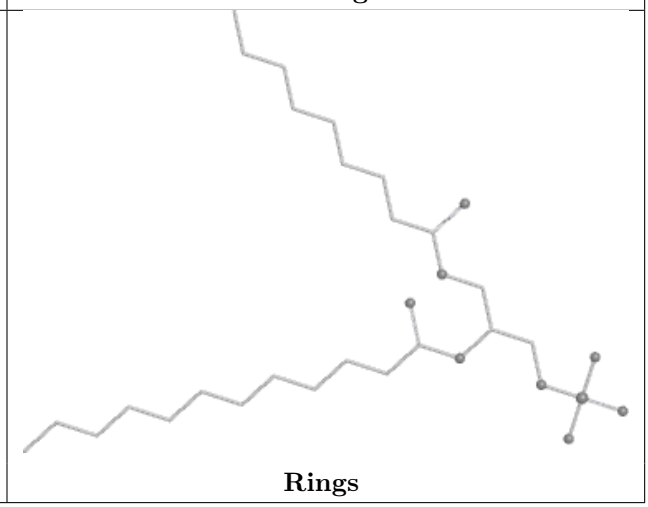


Bond angles

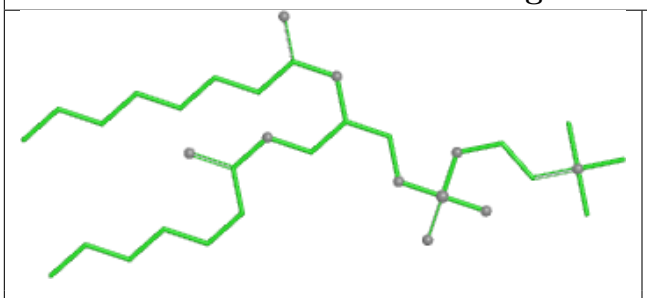


Torsions



Rings

Ligand PC1 t1 602



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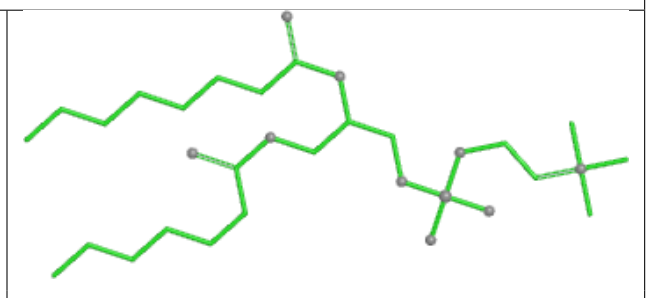
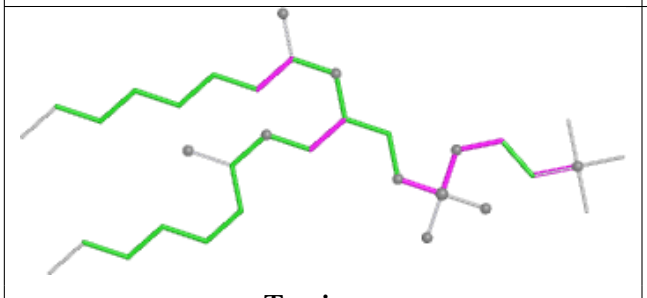
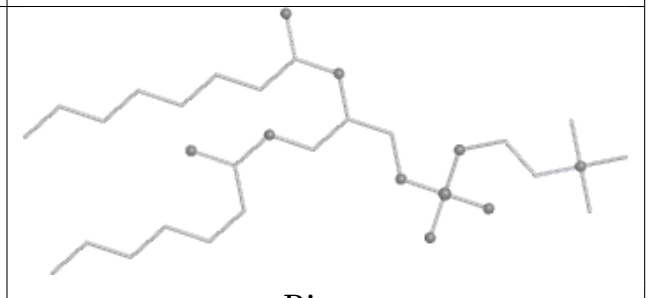


Bond angles

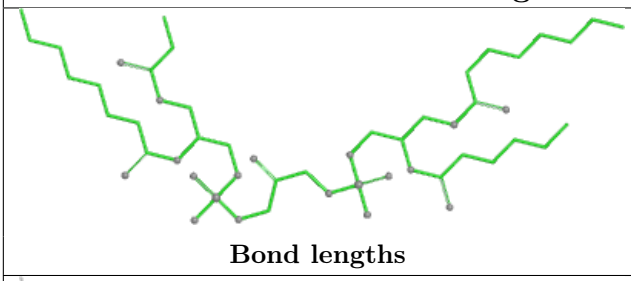


Torsions



Rings

Ligand CDL AL 301



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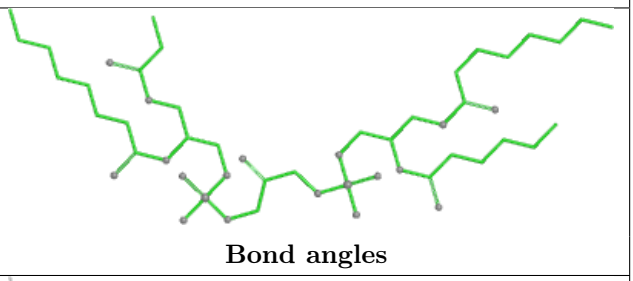
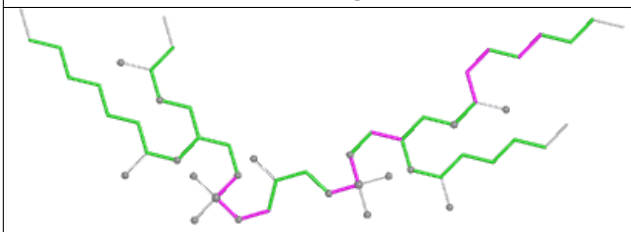


Bond angles



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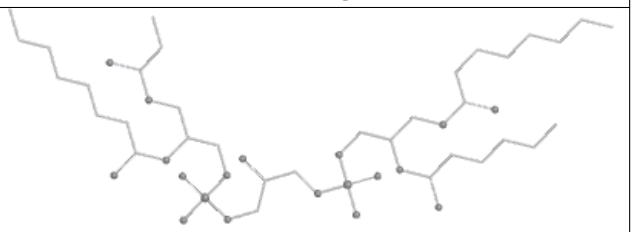
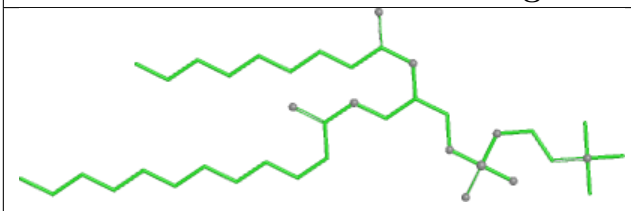


Rings

Ligand PC1 c3 605



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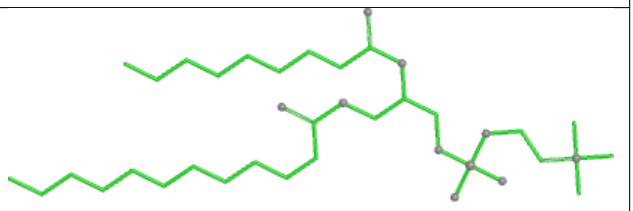
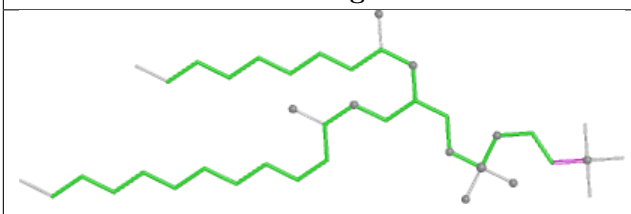


Bond angles



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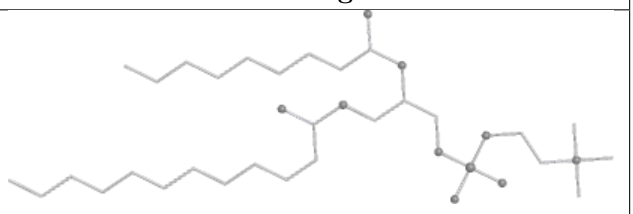
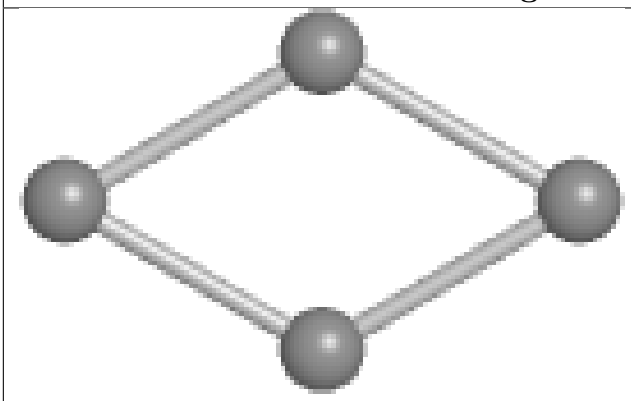


Rings

Ligand FES FS 202



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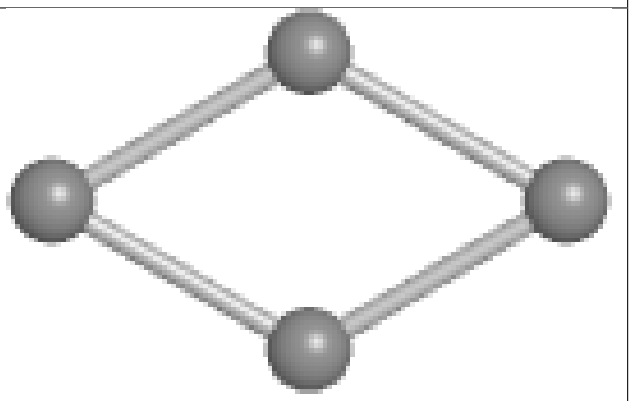
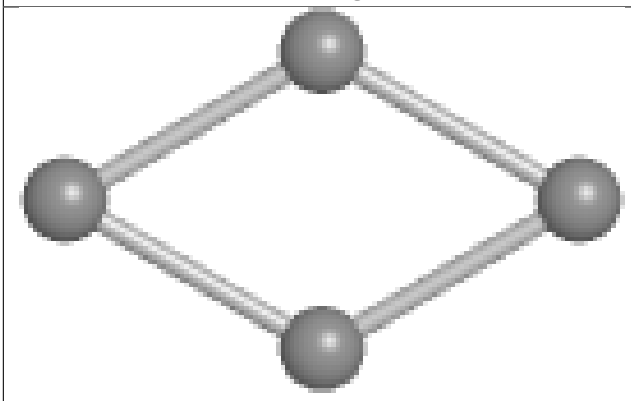


Bond angles



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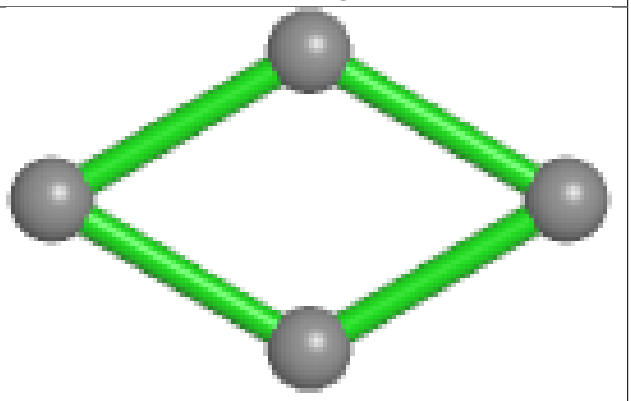
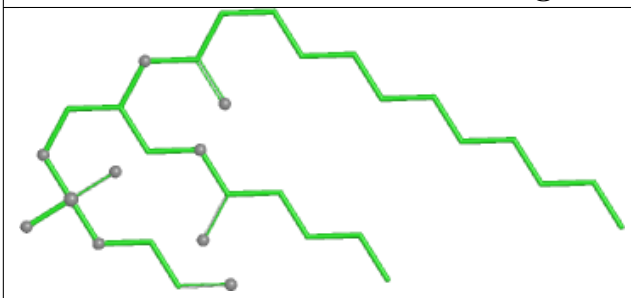


Rings

Ligand 3PE I 304



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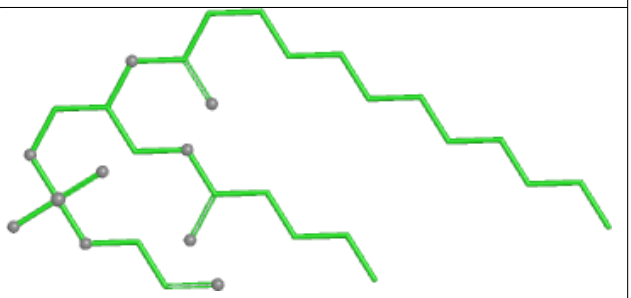
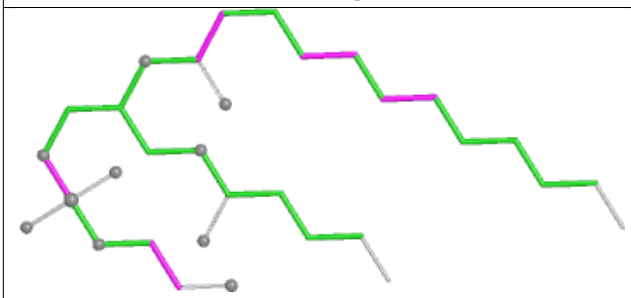


Bond angles



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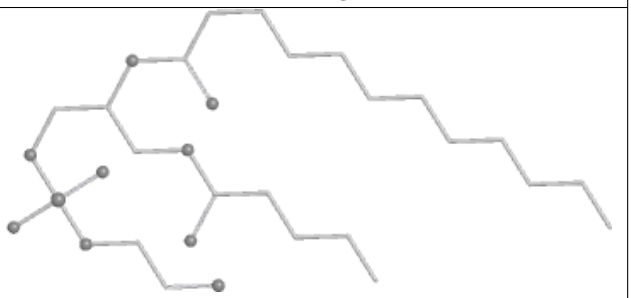
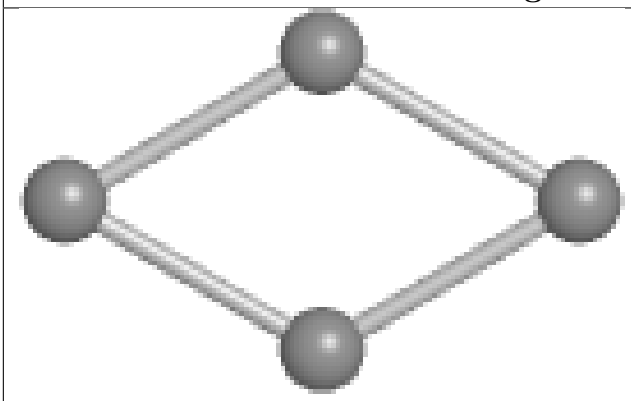


Rings

Ligand FES sb 401



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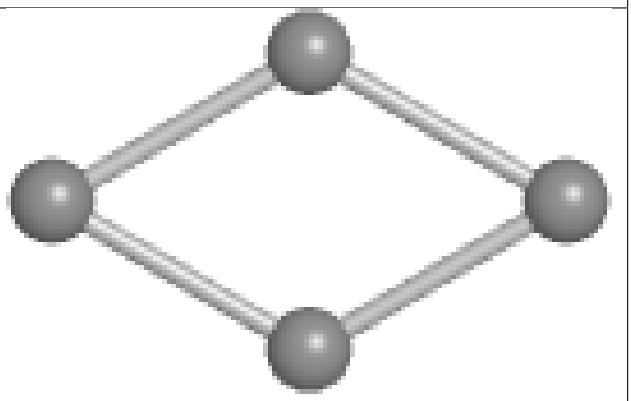
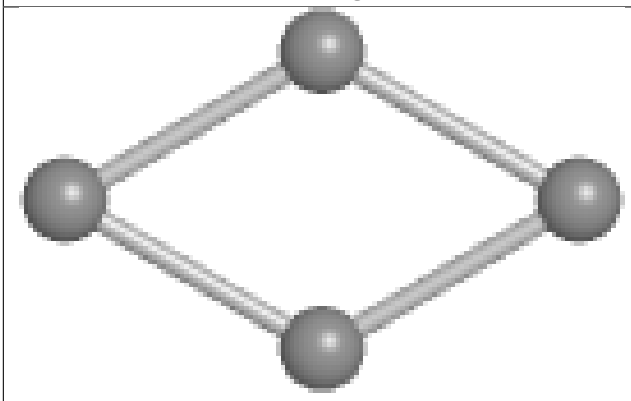


Bond angles



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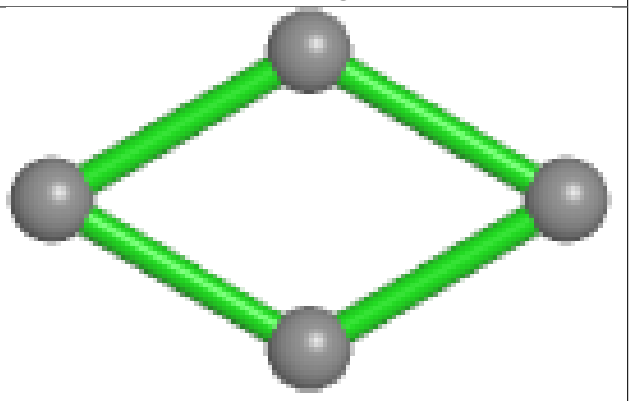
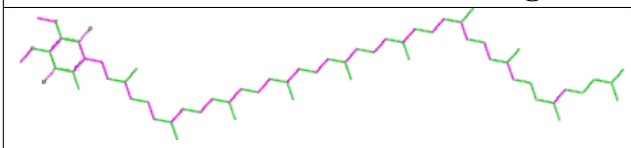


Rings

Ligand U10 b8 301



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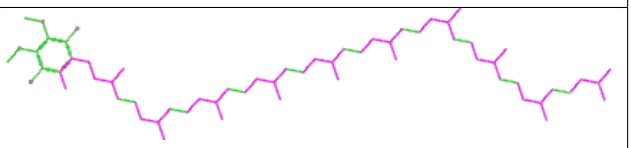
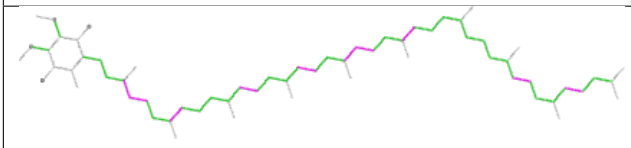
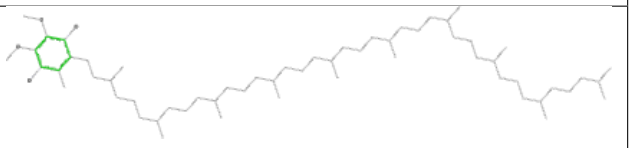


Bond angles

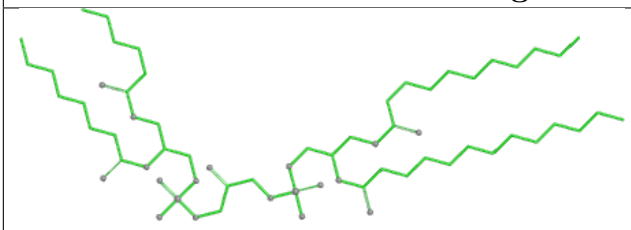


Torsions



Rings

Ligand CDL M2 403



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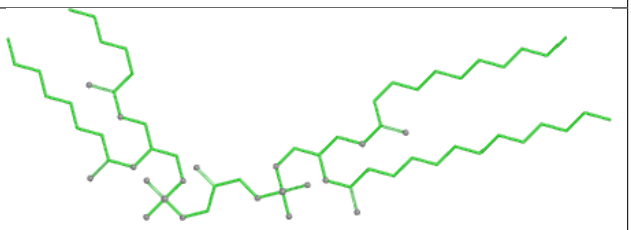
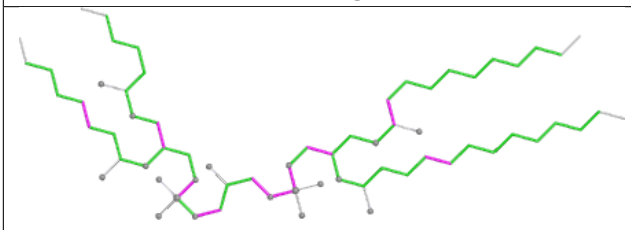
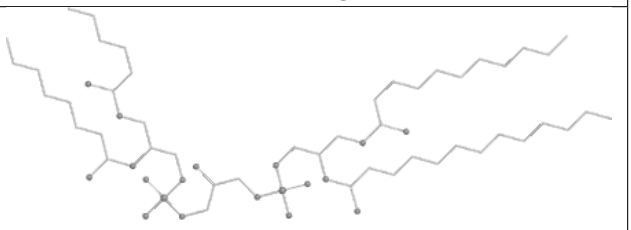


Bond angles

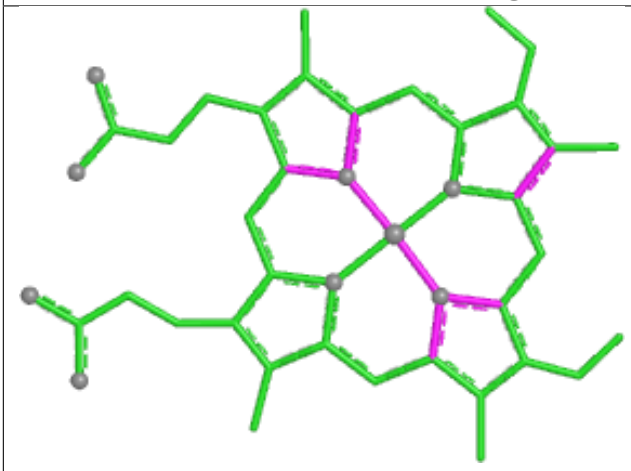


Torsions

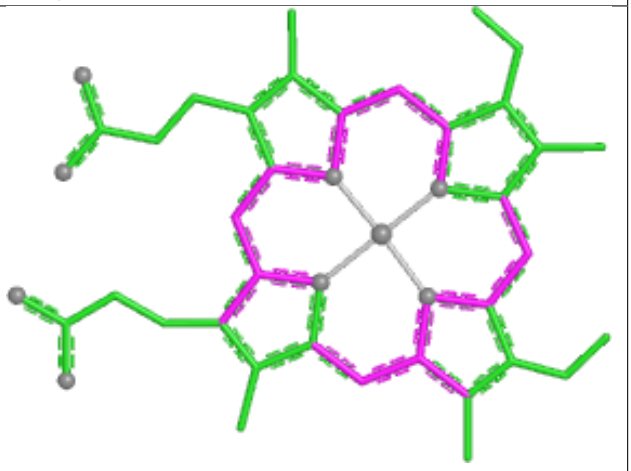


Rings

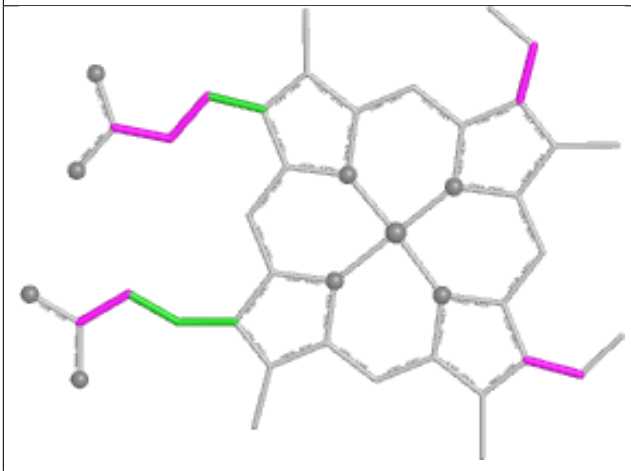
Ligand HEM QC 502



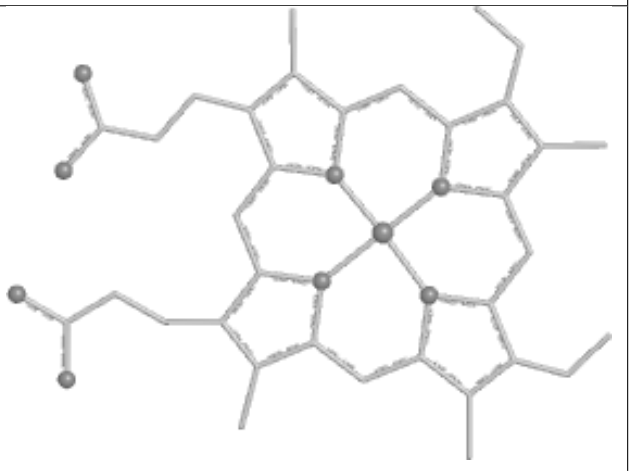
Bond lengths



Bond angles

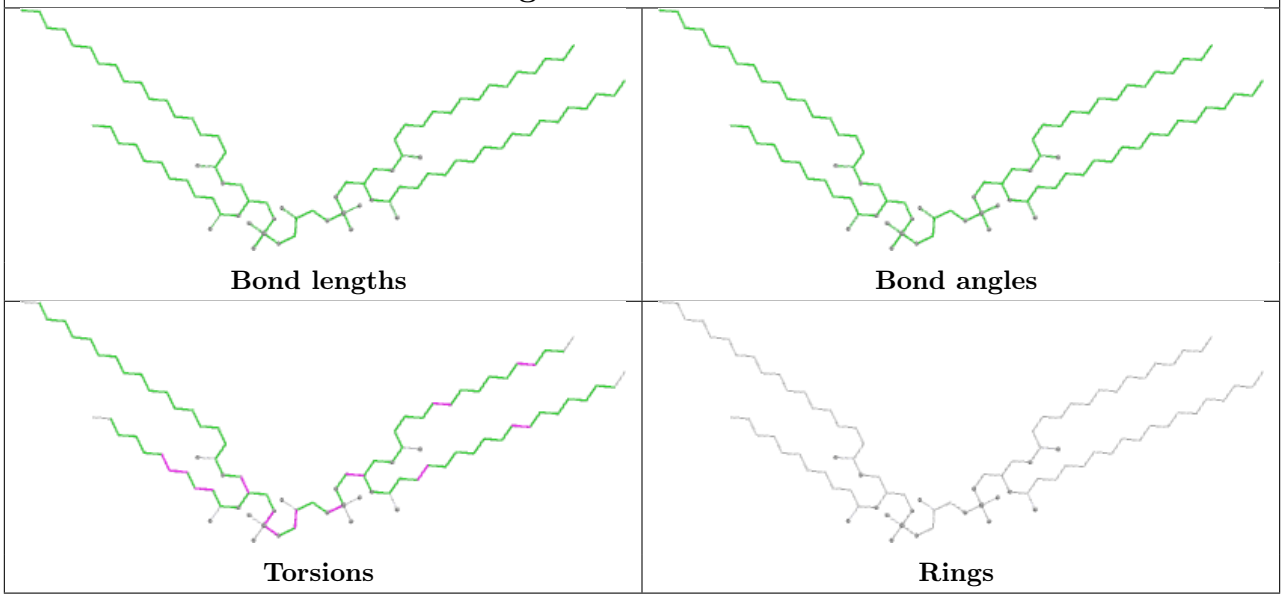


Torsions

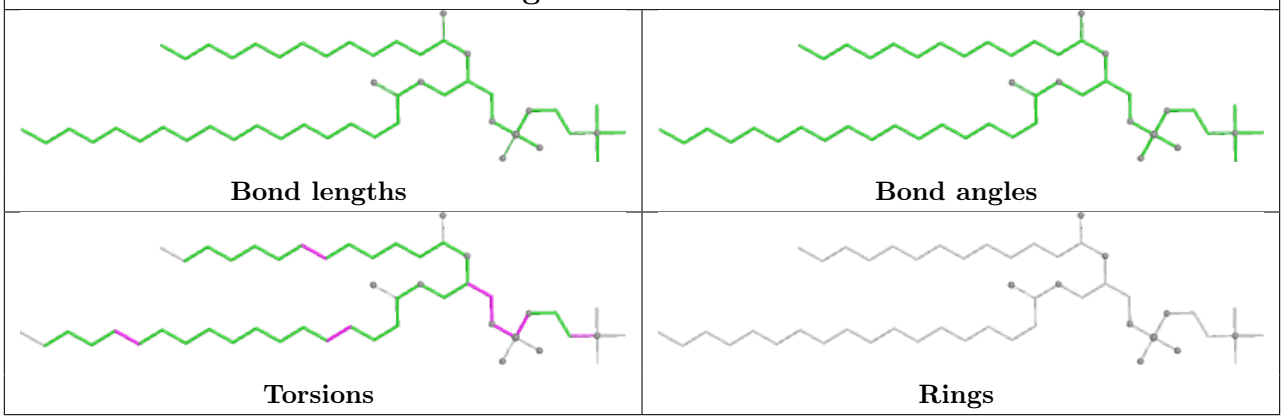


Rings

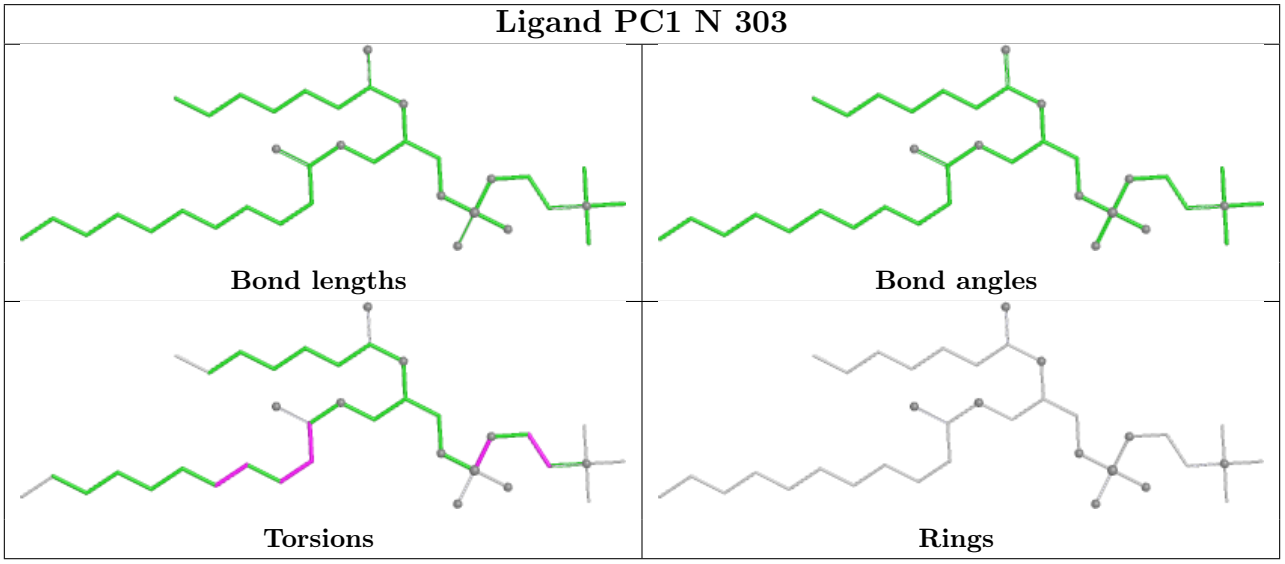
Ligand CDL n6 302



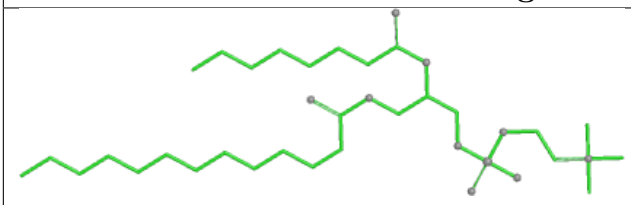
Ligand PC1 W 201



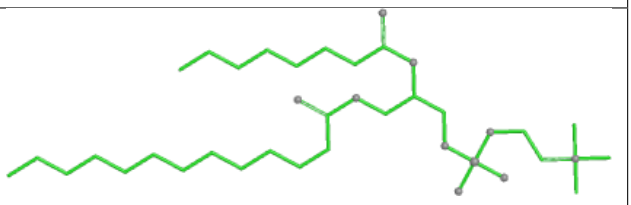
Ligand PC1 N 303



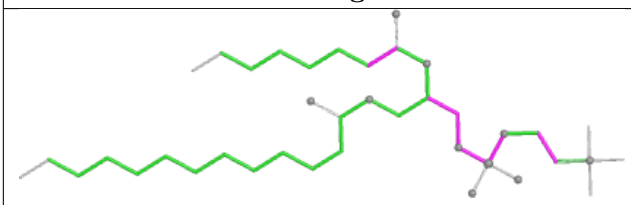
Ligand PC1 N5 804



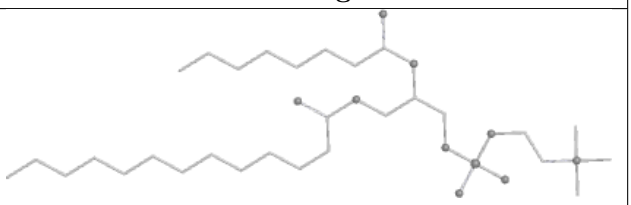
Bond lengths



Bond angles

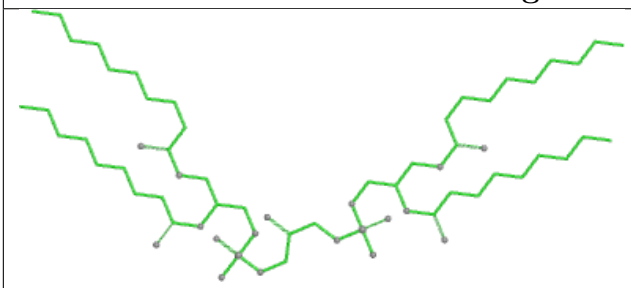


Torsions

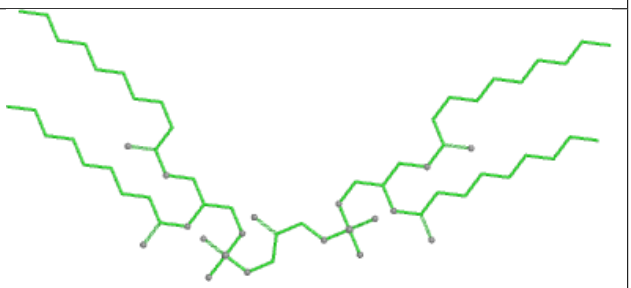


Rings

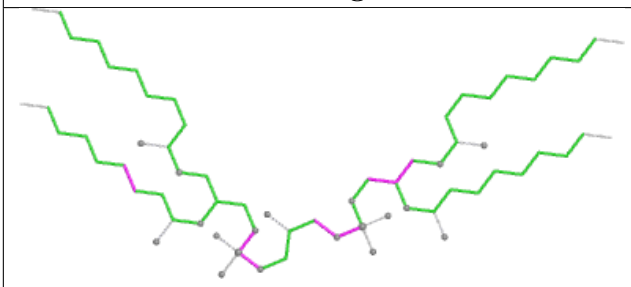
Ligand CDL m 306



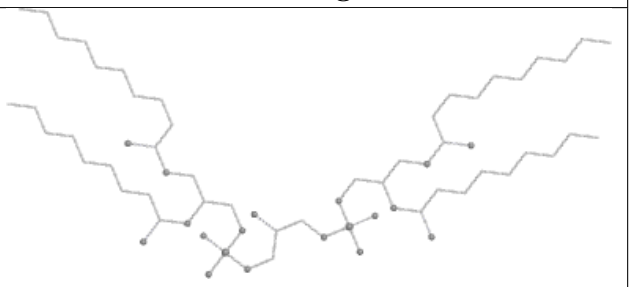
Bond lengths



Bond angles

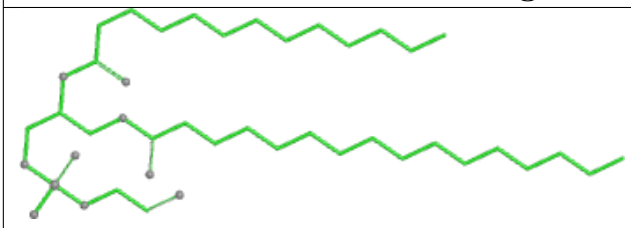


Torsions

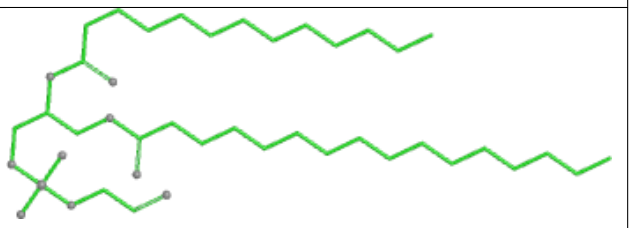


Rings

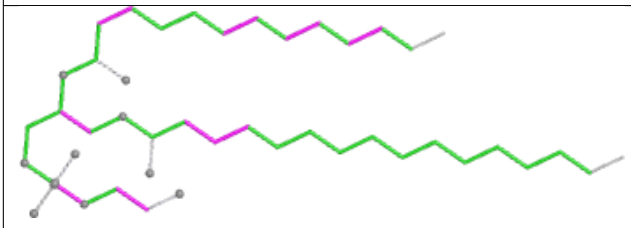
Ligand 3PE A3 202



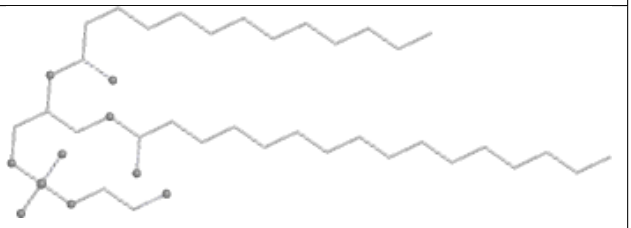
Bond lengths



Bond angles

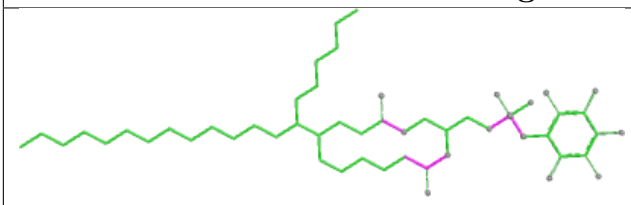


Torsions



Rings

Ligand T7X B6 201



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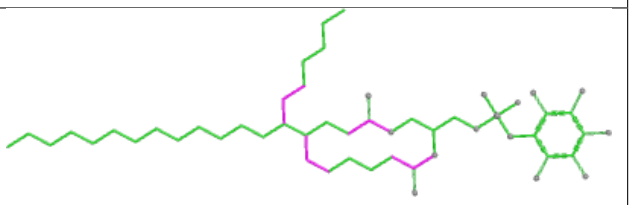

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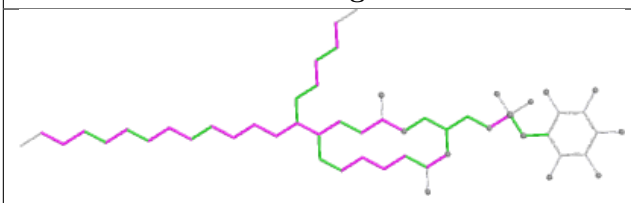

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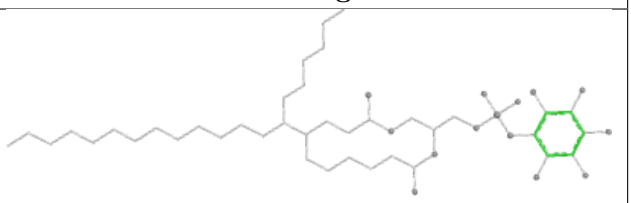
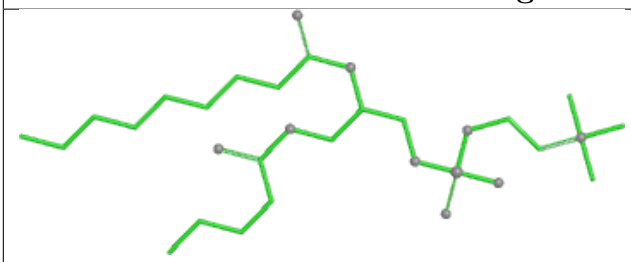


Rings

Ligand PC1 qG 401



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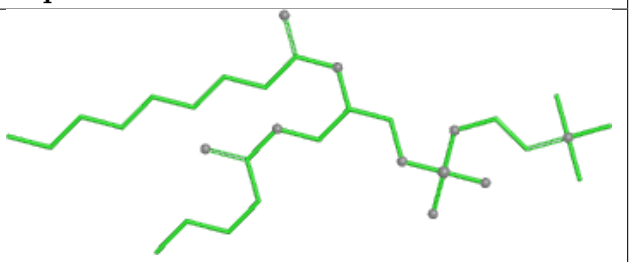

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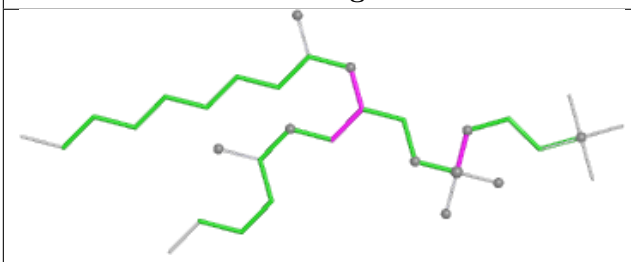

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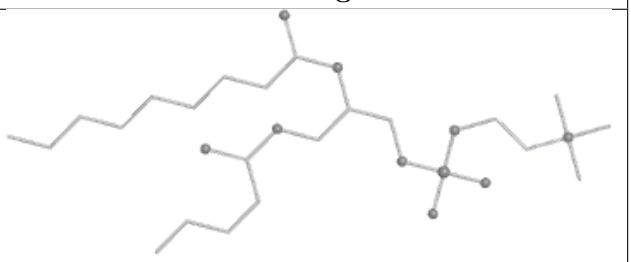
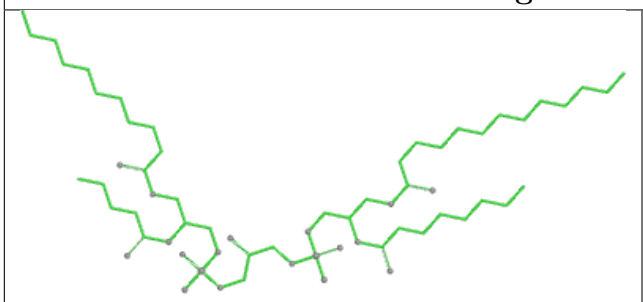


Rings

Ligand CDL Y7 501



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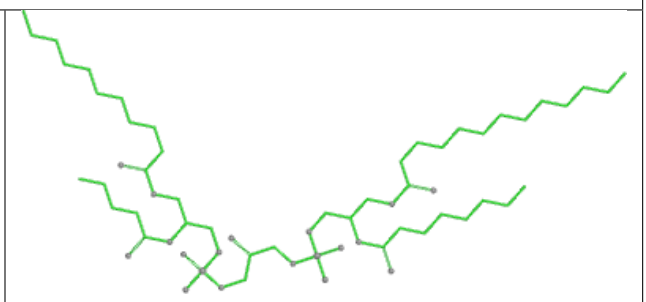

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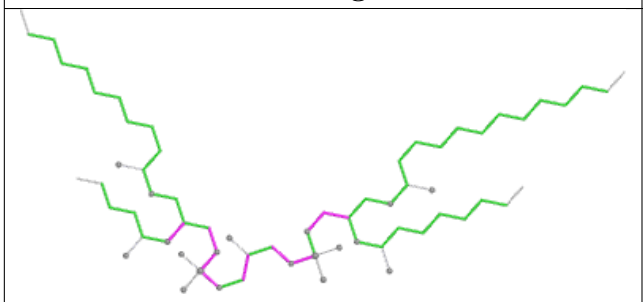

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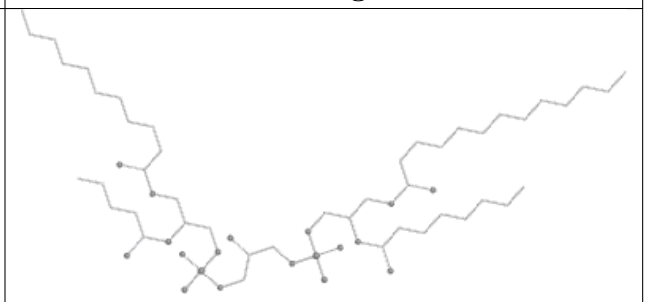
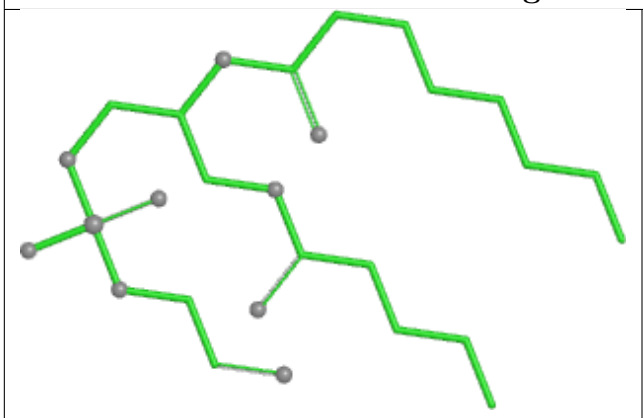


Rings

Ligand 3PE vb 705



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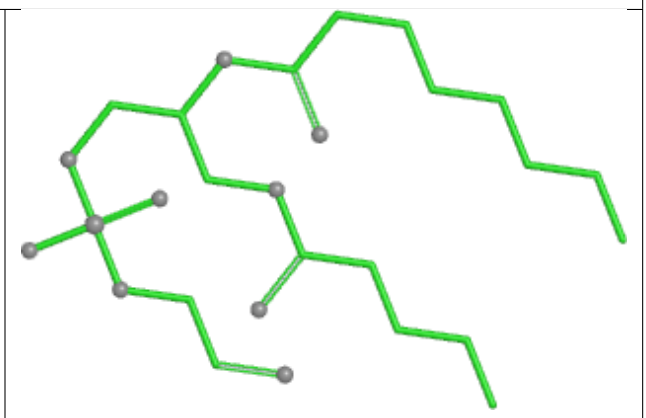

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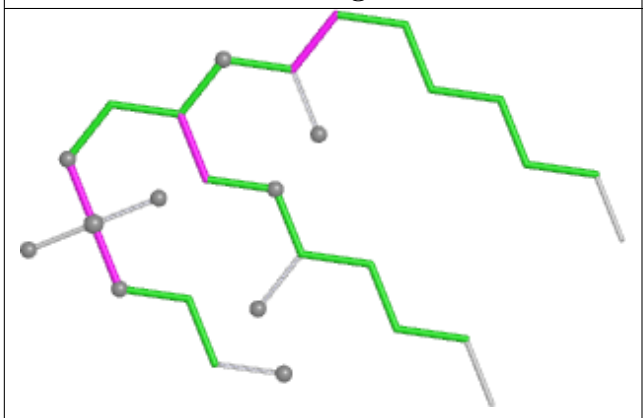

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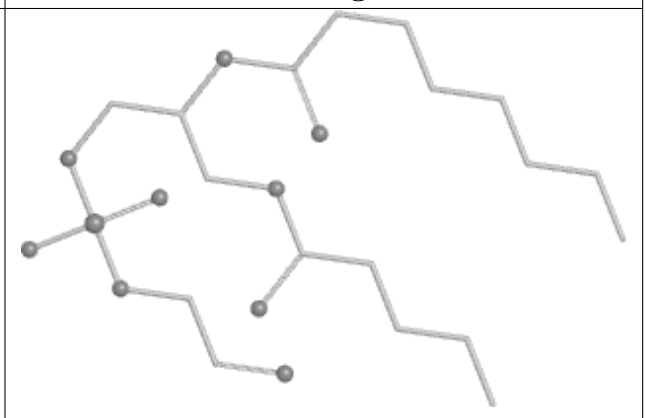
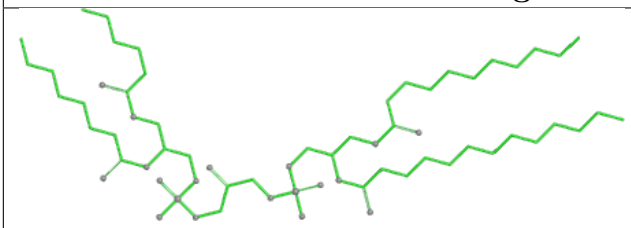


Rings

Ligand CDL m2 403



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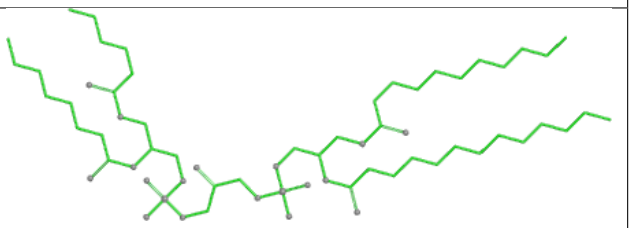

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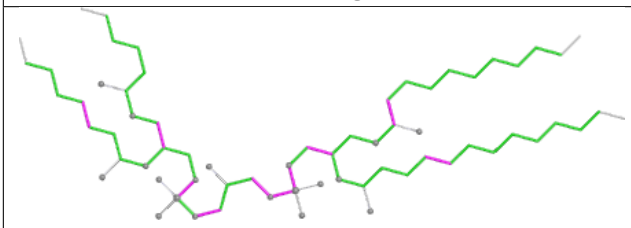

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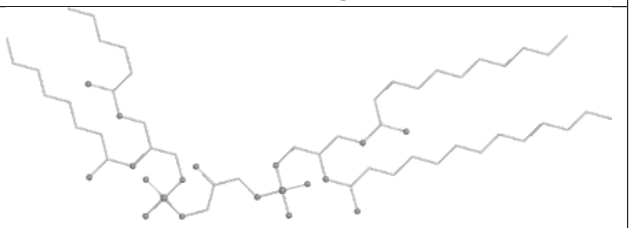
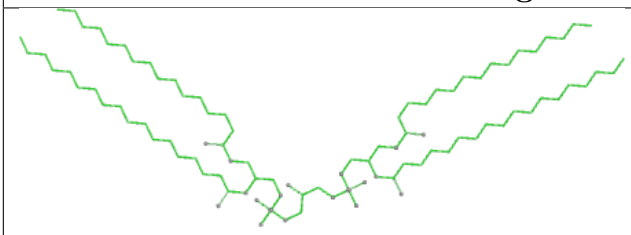


Rings

Ligand CDL T5 301



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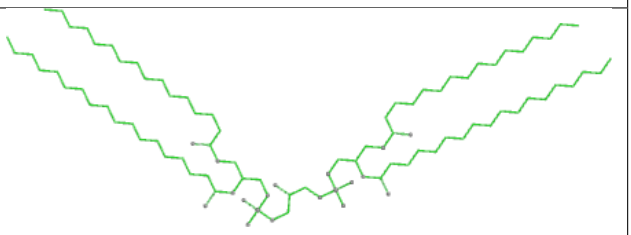
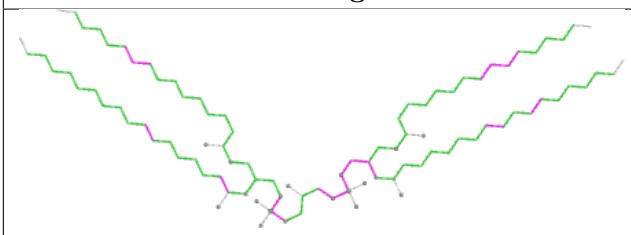


Bond angles



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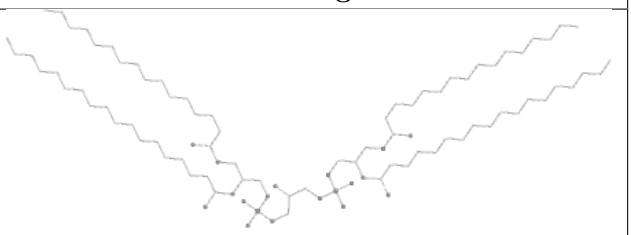
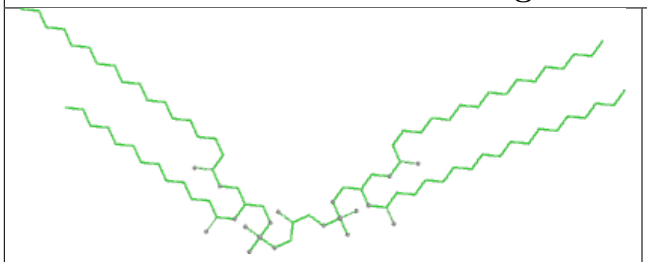


Rings

Ligand CDL qH 201



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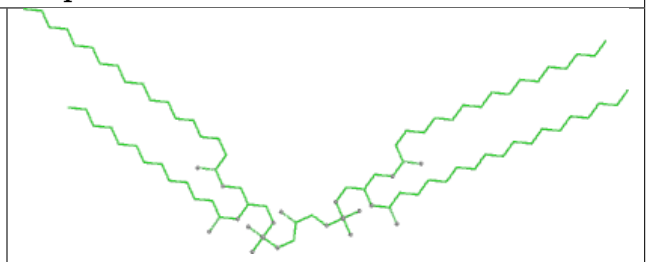

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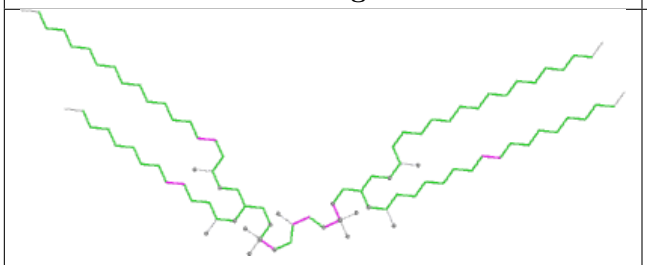

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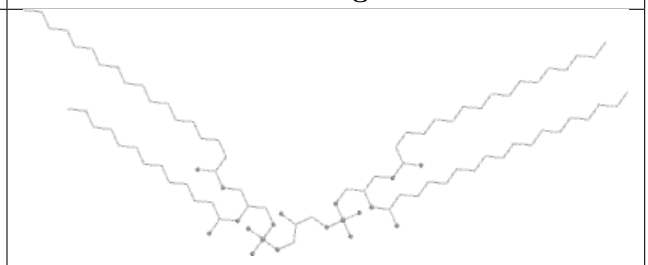
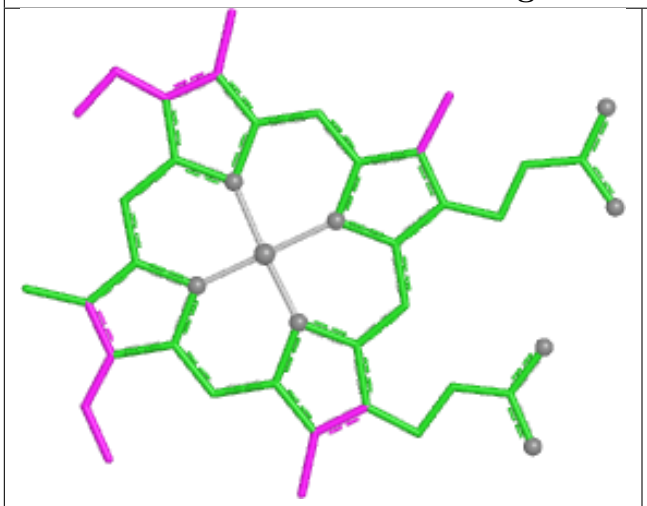


Rings

Ligand HEC qd 401



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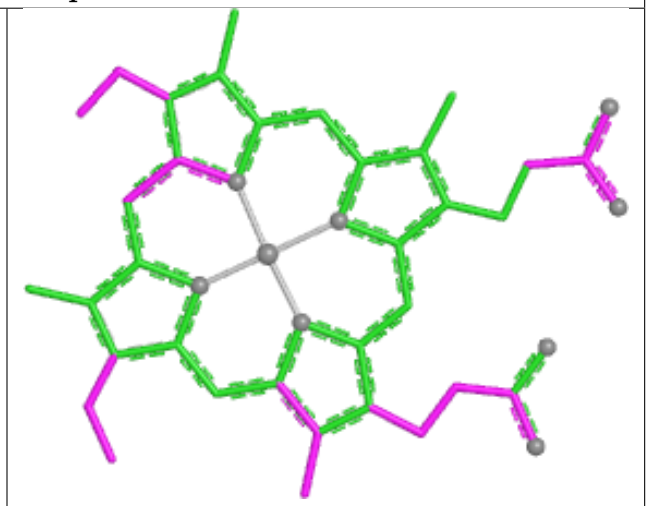
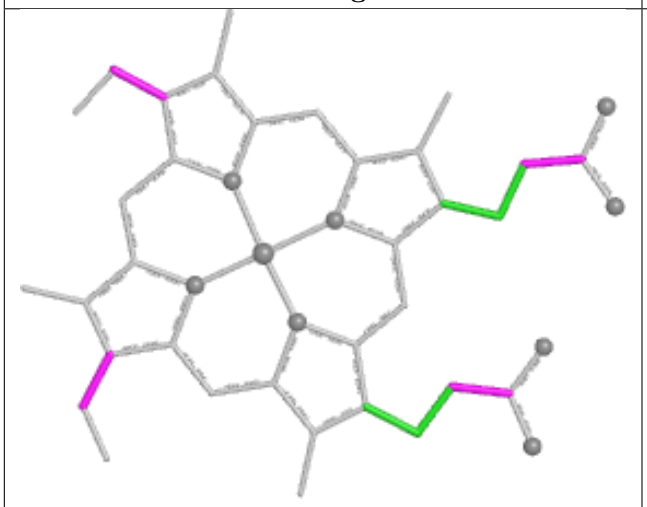


Bond angles



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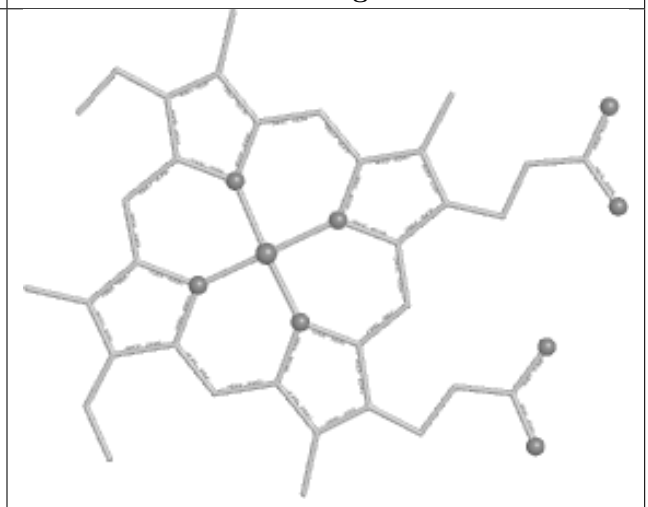
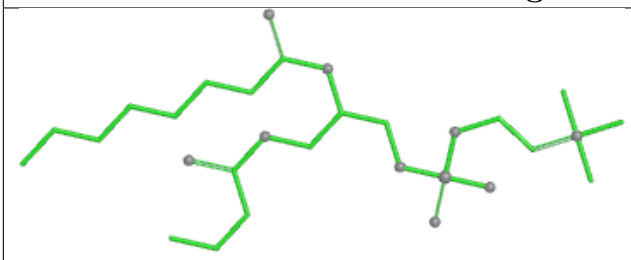


Rings

Ligand PC1 qi 201



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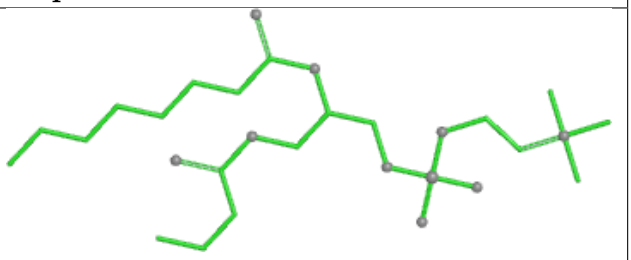

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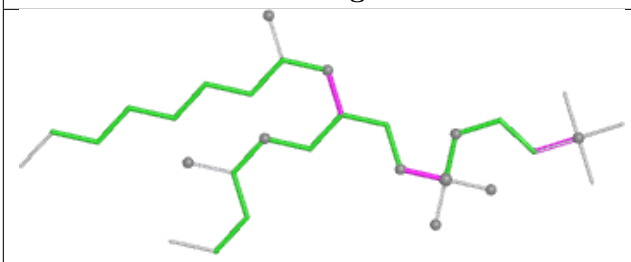

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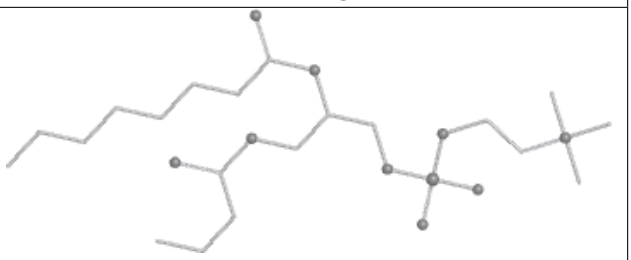
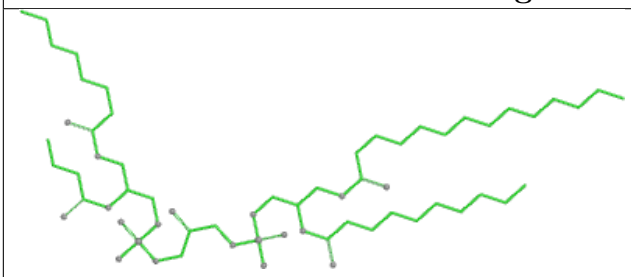


Rings

Ligand CDL qC 503



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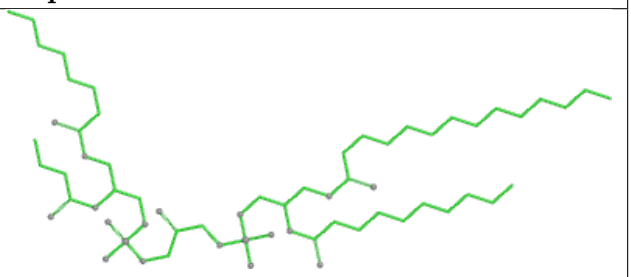
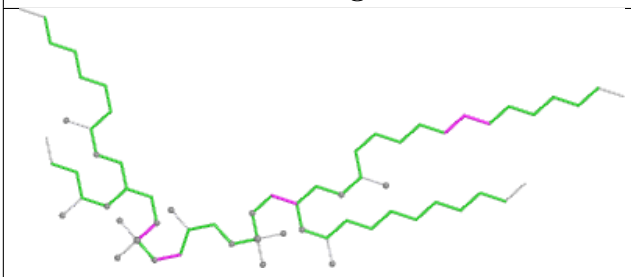


Bond angles



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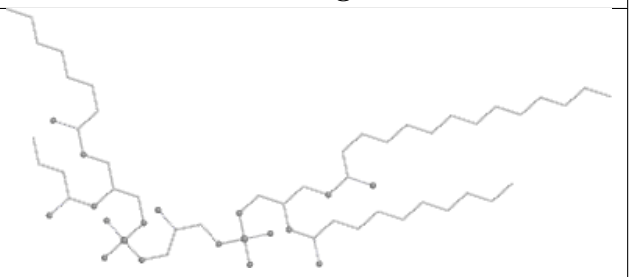
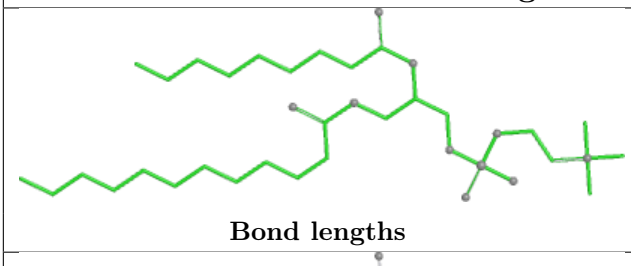


Rings

Ligand PC1 C3 605



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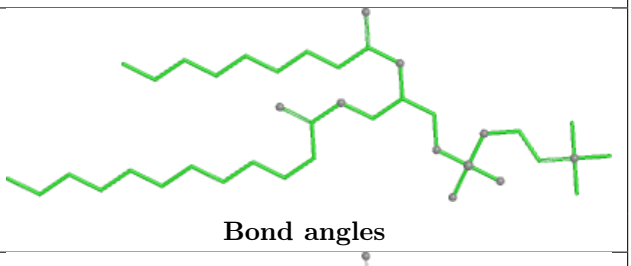
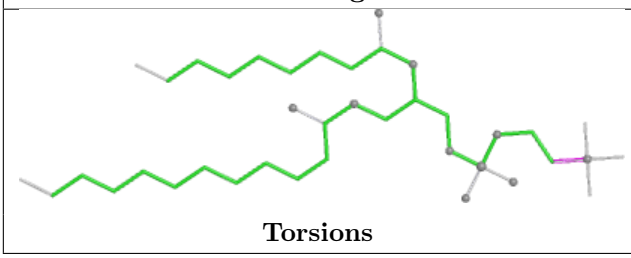
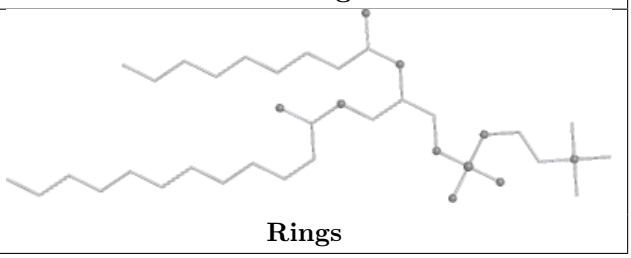


Bond angles

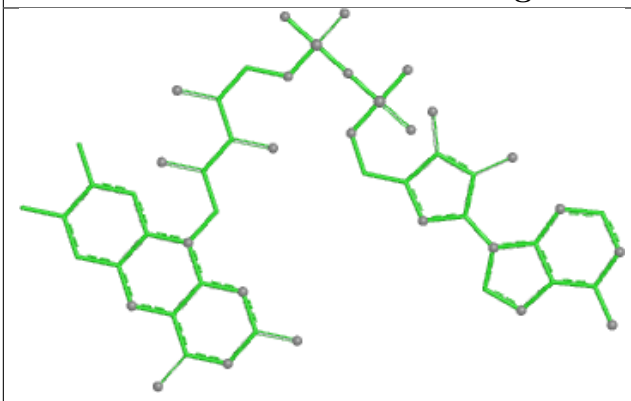


Torsions



Rings

Ligand FAD SA 701



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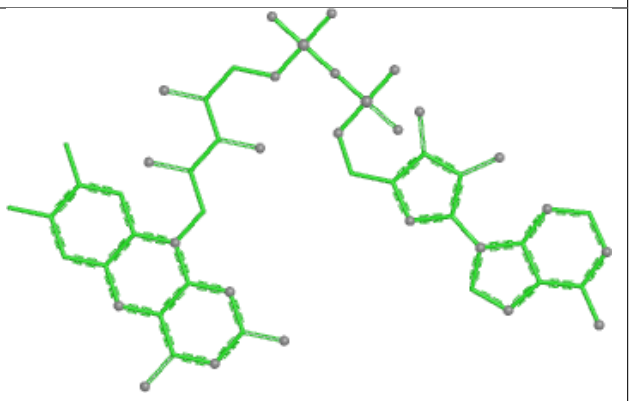
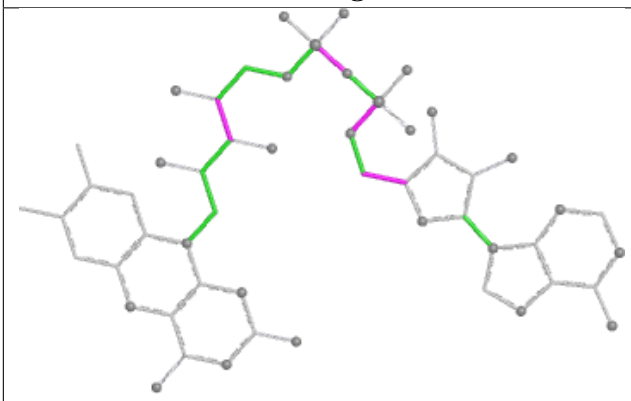


Bond angles



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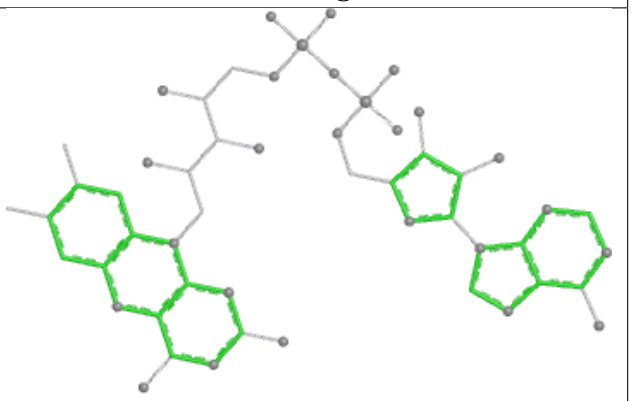
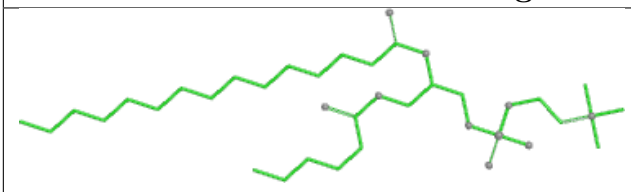


Rings

Ligand PC1 QE 303



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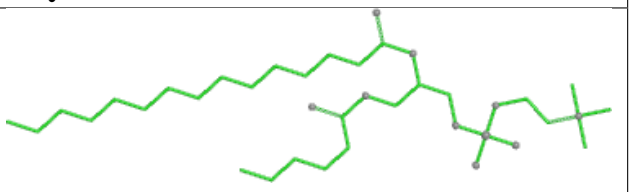
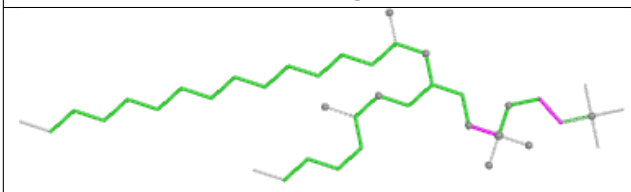
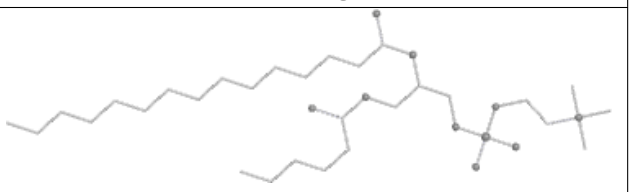


Bond angles

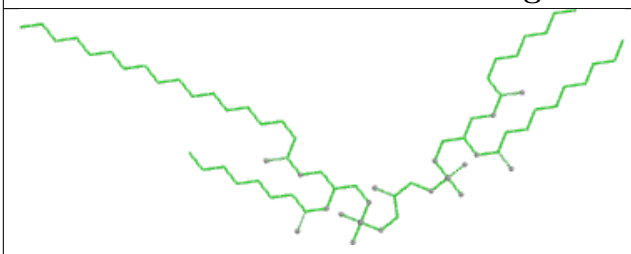


Torsions

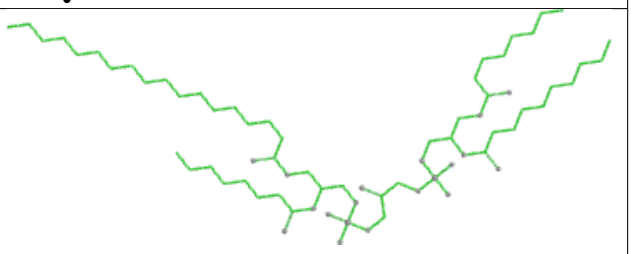


Rings

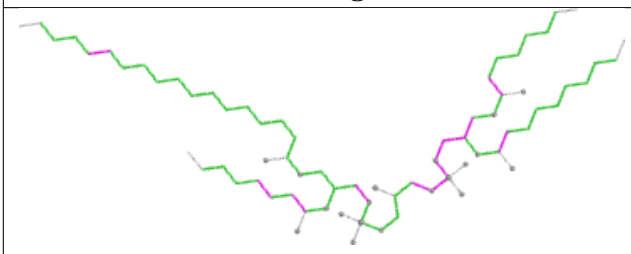
Ligand CDL Q 202



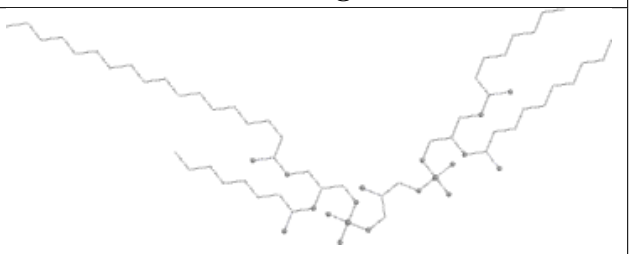
Bond lengths



Bond angles

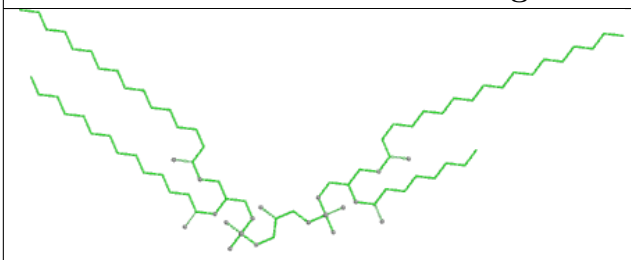


Torsions

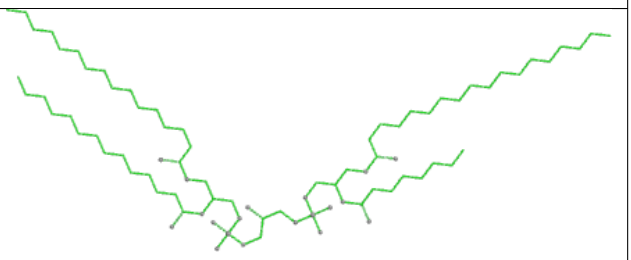


Rings

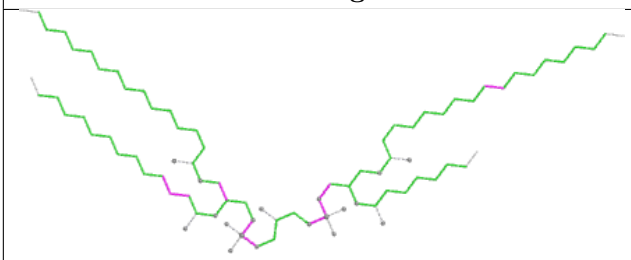
Ligand CDL TH 200



Bond lengths



Bond angles



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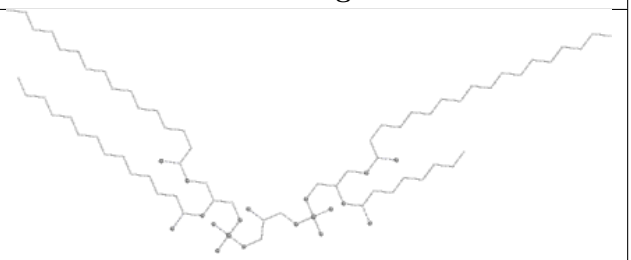
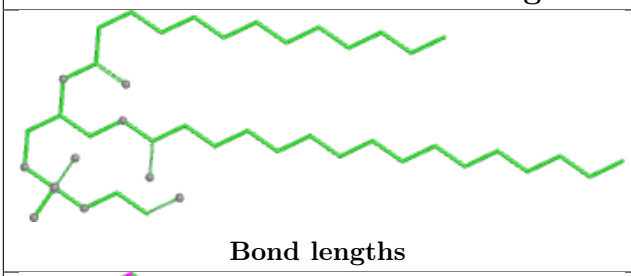


Rings

Ligand 3PE a3 202



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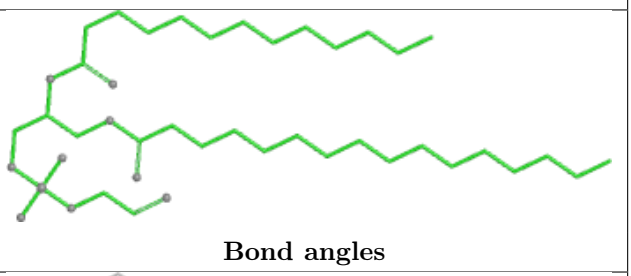

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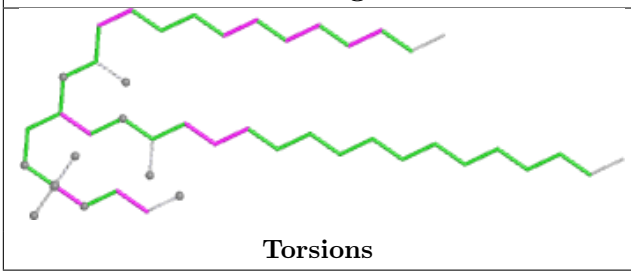

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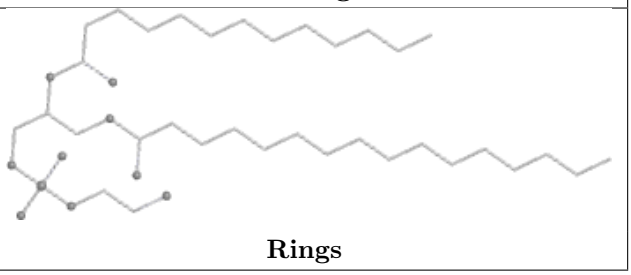
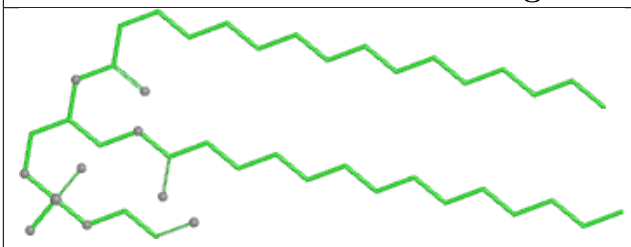


Rings

Ligand 3PE a3 201



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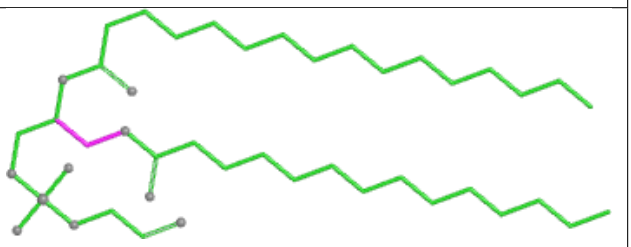
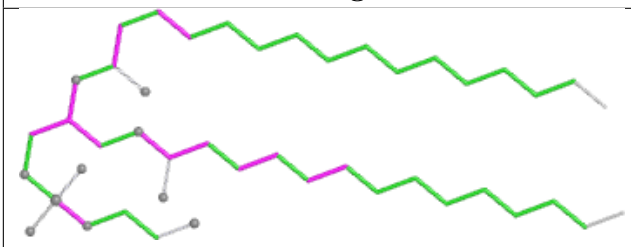


Bond angles



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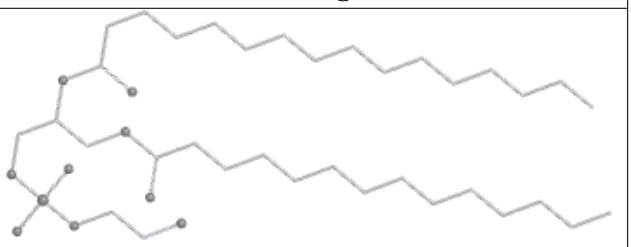
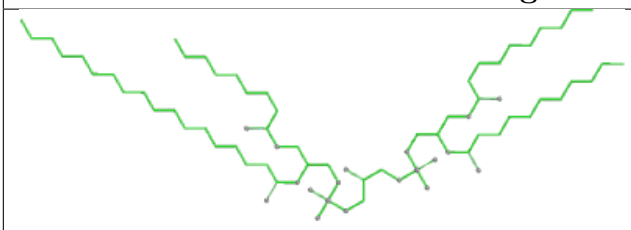


Rings

Ligand CDL sd 101



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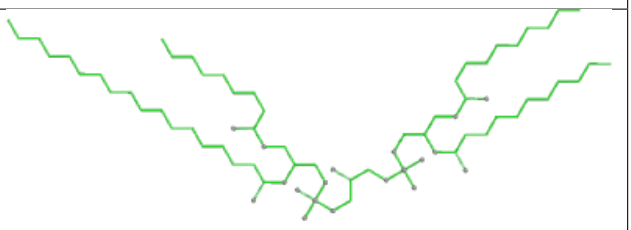
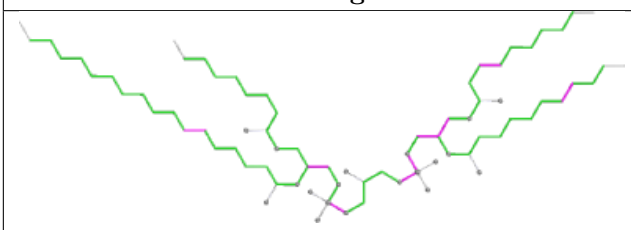


Bond angles



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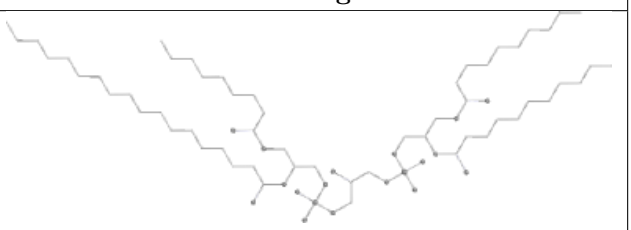
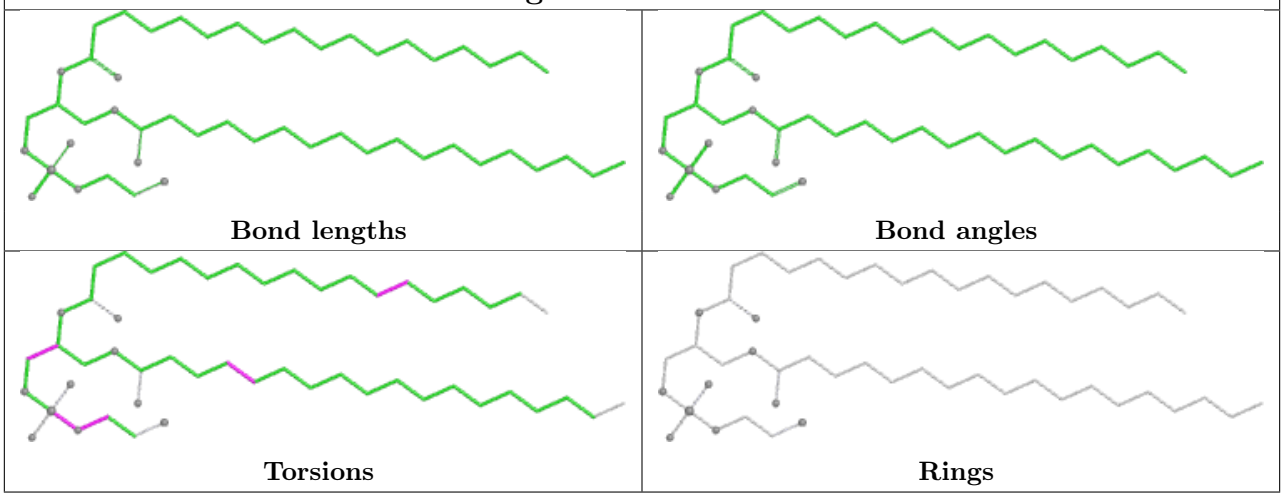
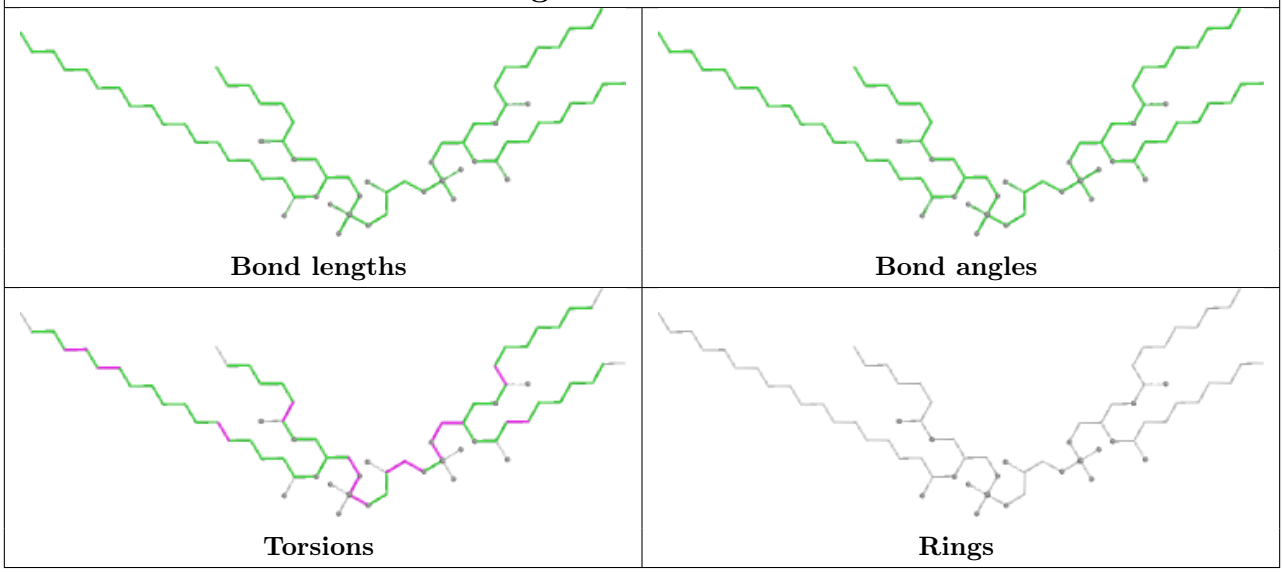


Rings

Ligand 3PE c4 402



Ligand CDL t 203



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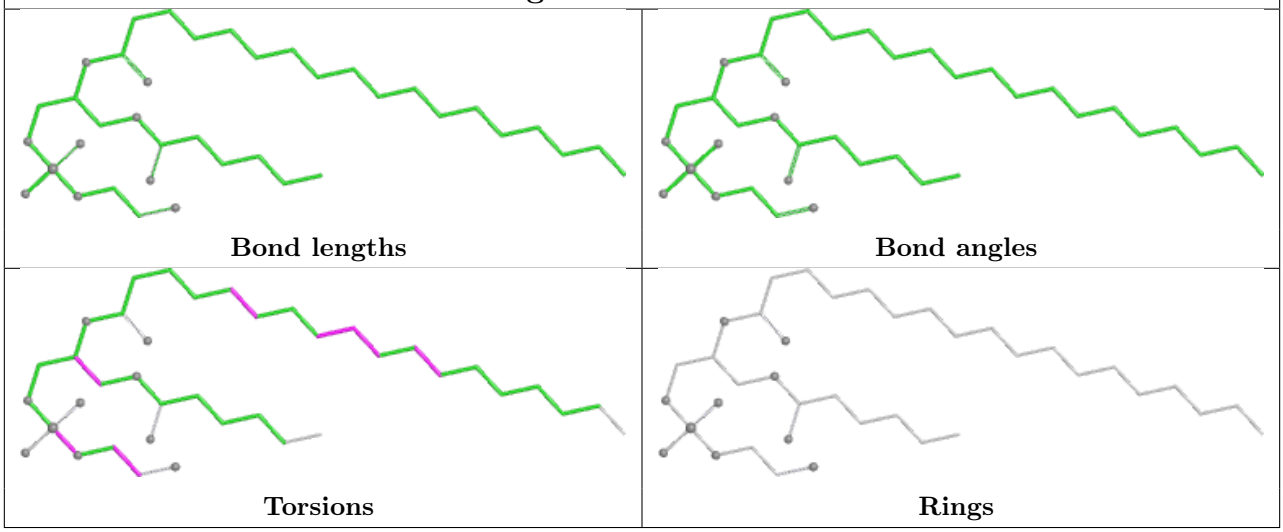
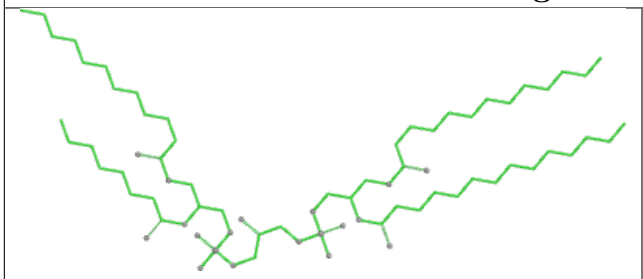
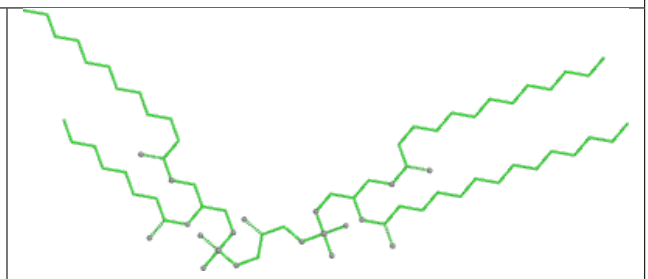


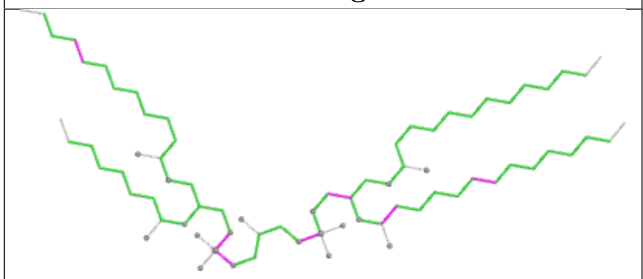
Ligand CDL i 302



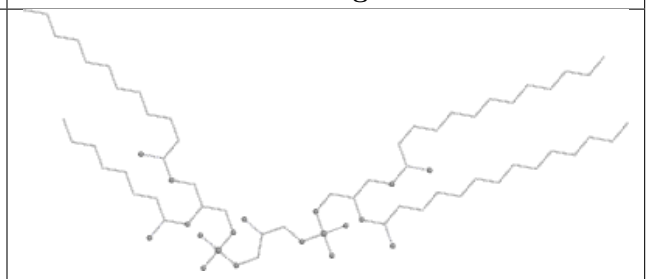
Bond lengths



Bond angles

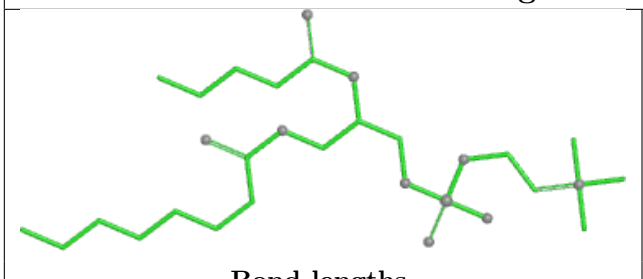


Torsions



Rings

Ligand PC1 N3 201



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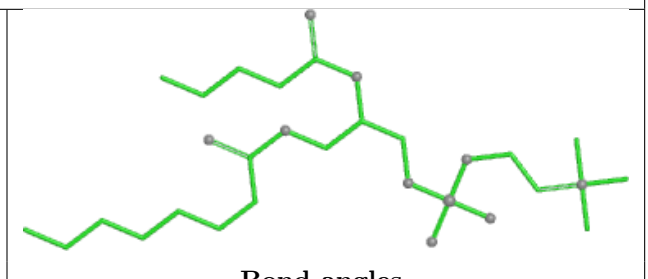
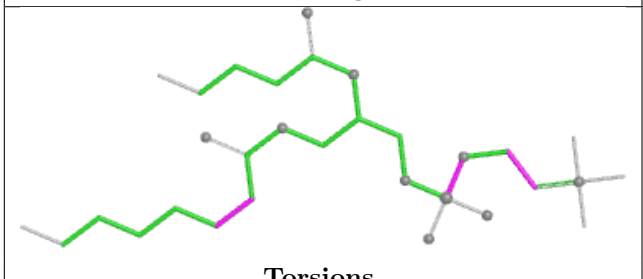


Bond angles



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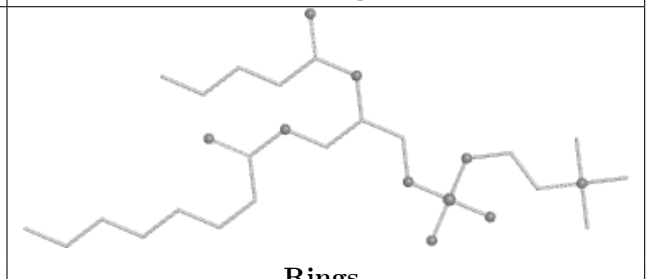
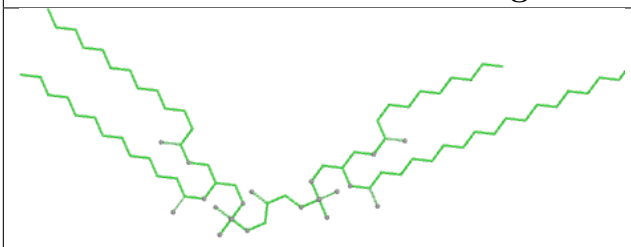


Rings

Ligand CDL VB 705



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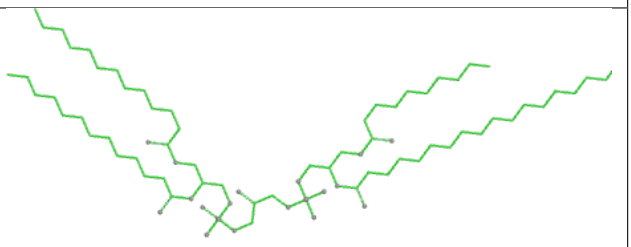
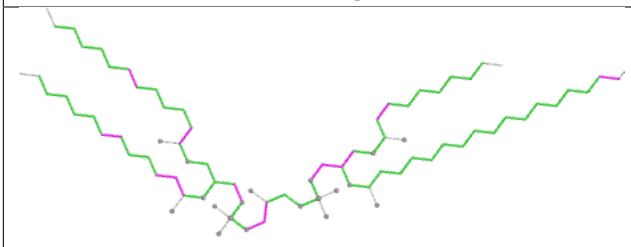


Bond angles



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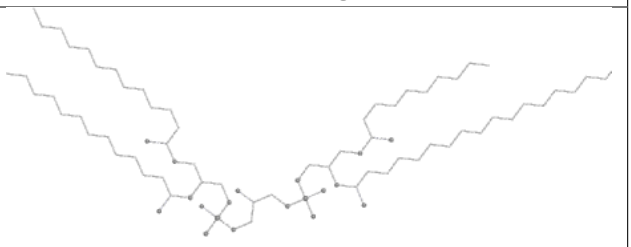
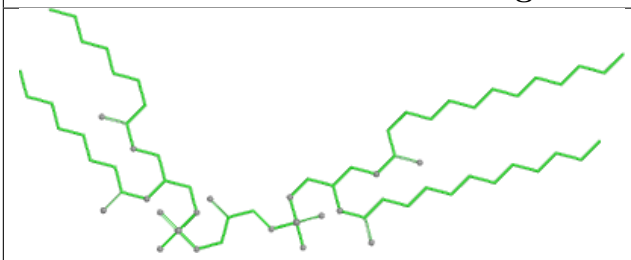


Rings

Ligand CDL B8 302



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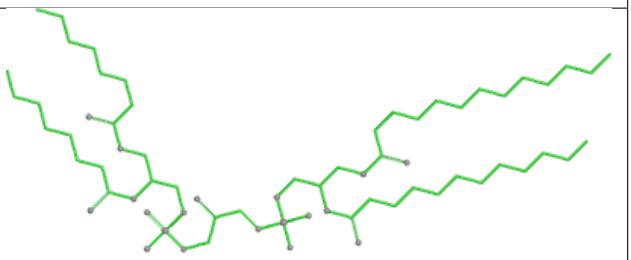
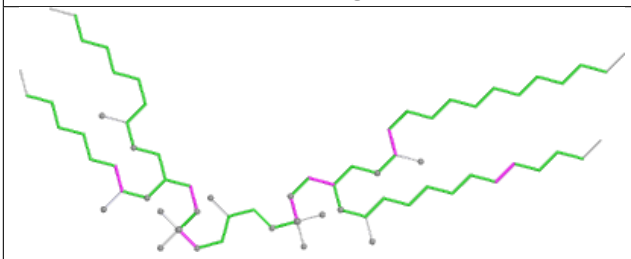


Bond angles



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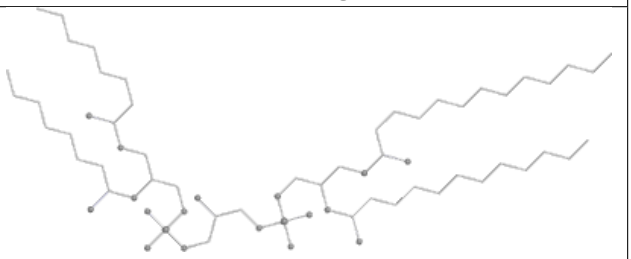
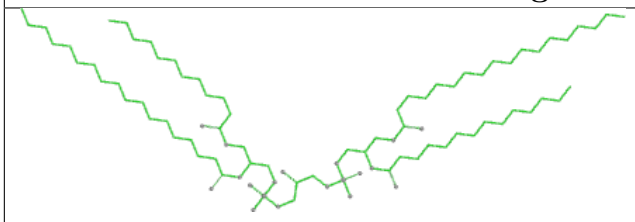


Rings

Ligand CDL t 204



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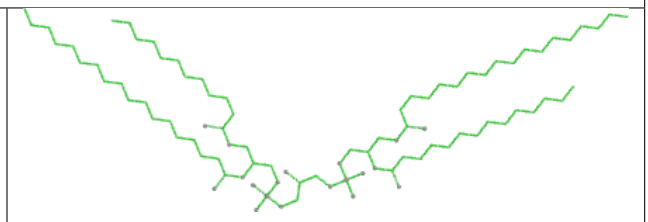
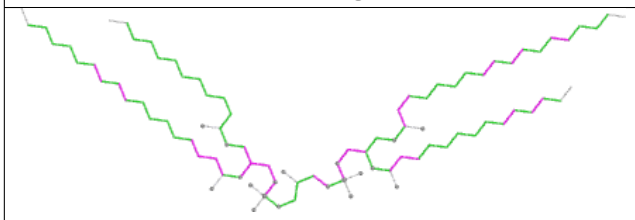


Bond angles



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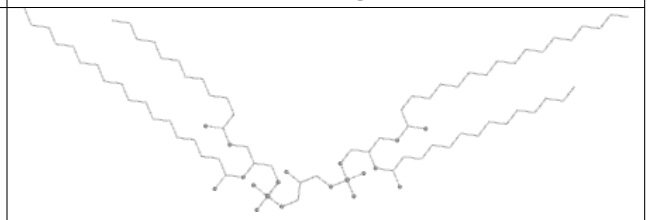
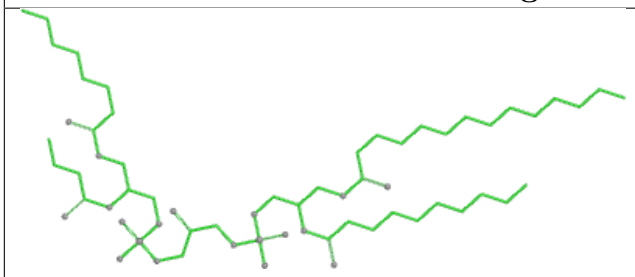


Rings

Ligand CDL qc 504



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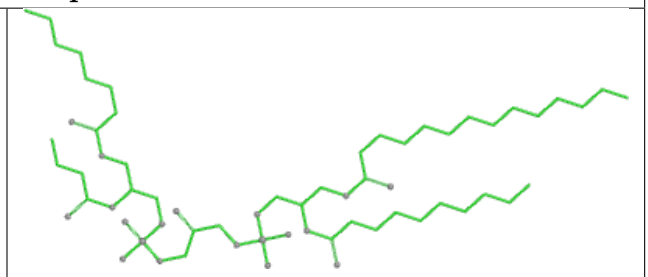
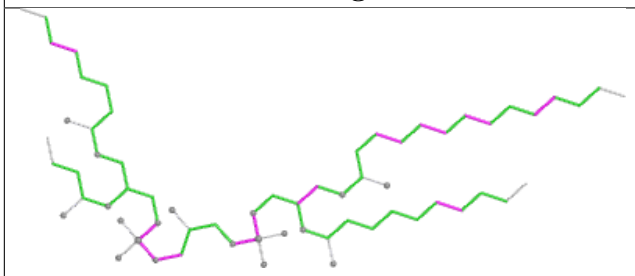
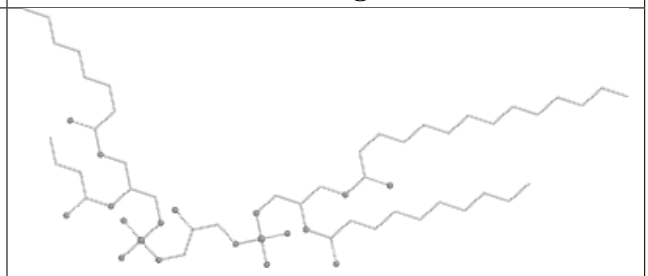


Bond angles

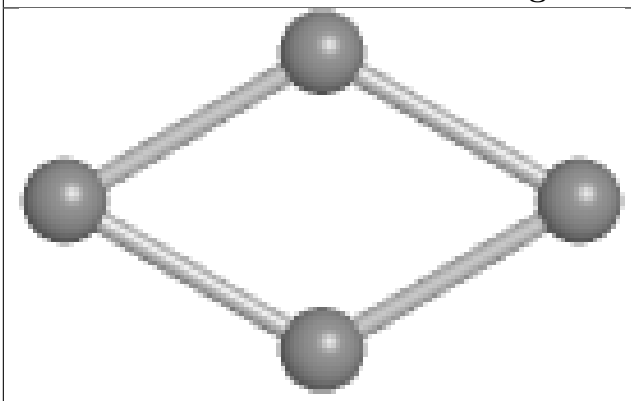


Torsions



Rings

Ligand FES fs 202



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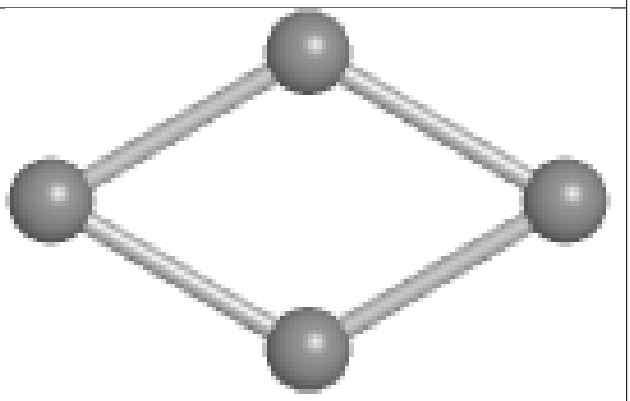
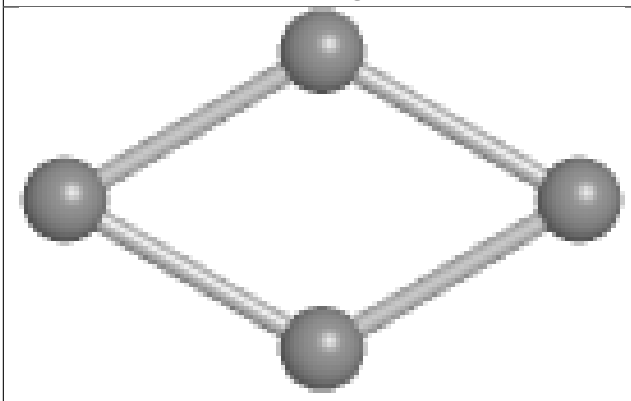
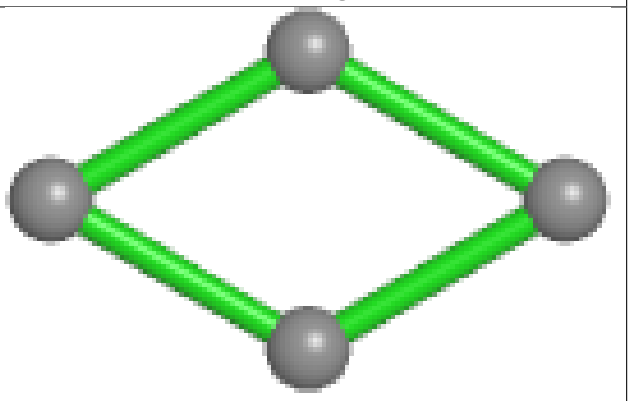


Bond angles

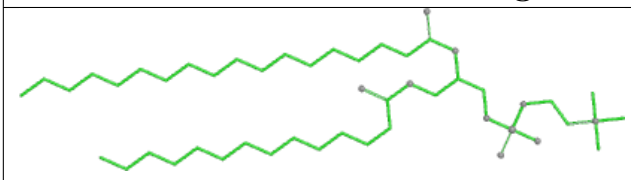


Torsions



Rings

Ligand PC1 QC 507



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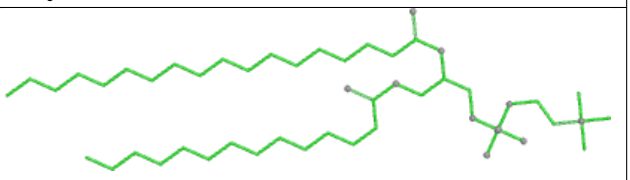
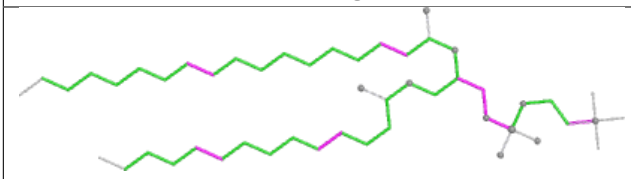
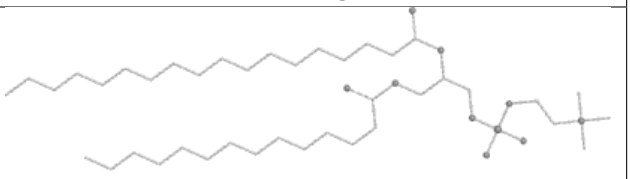


Bond angles

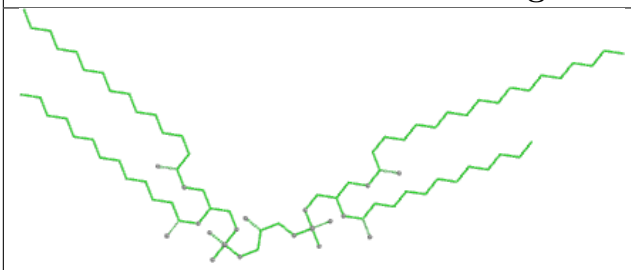


Torsions

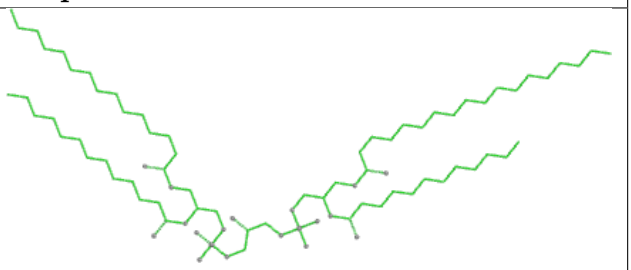


Rings

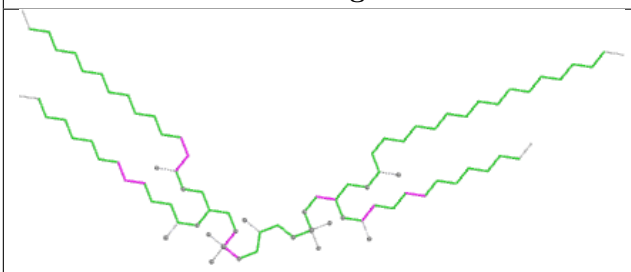
Ligand CDL q 203



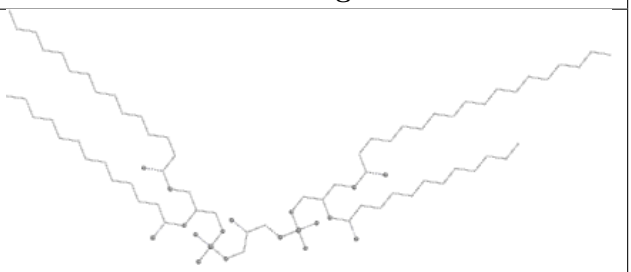
Bond lengths



Bond angles

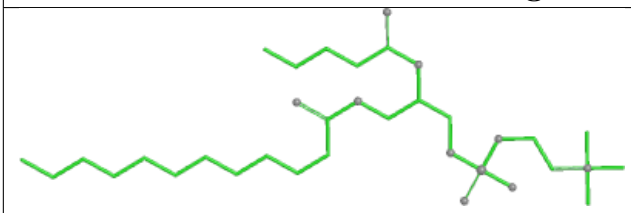


Torsions



Rings

Ligand PC1 m 305



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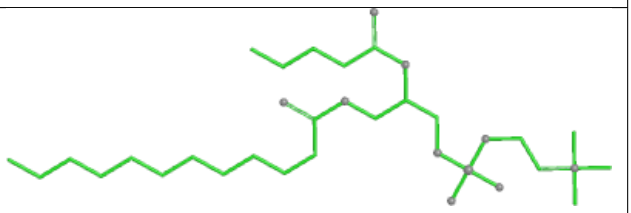
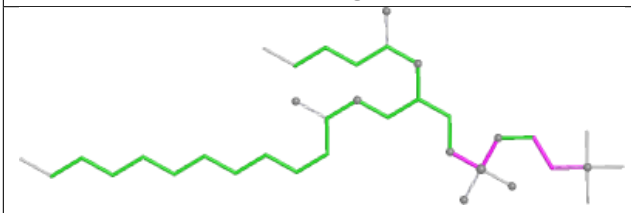


Bond angles



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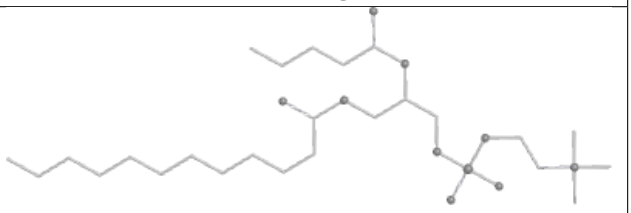
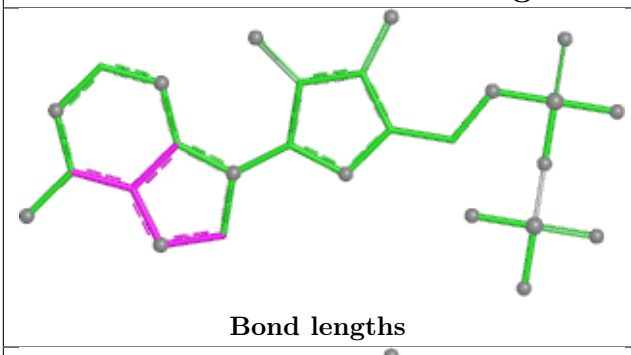


Rings

Ligand ADP B9 202



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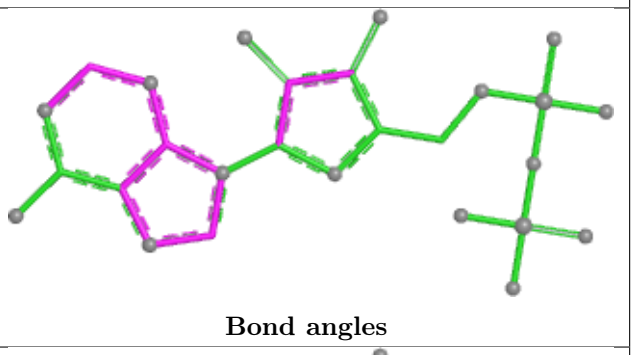
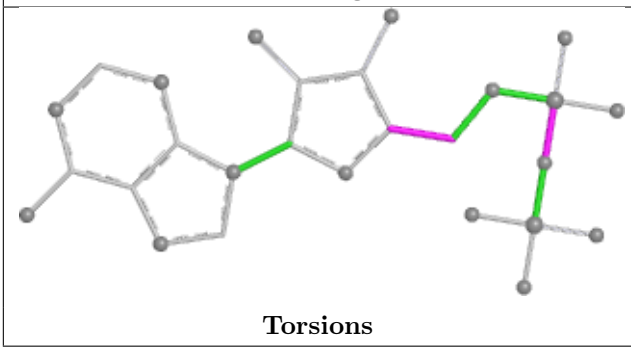


Bond angles



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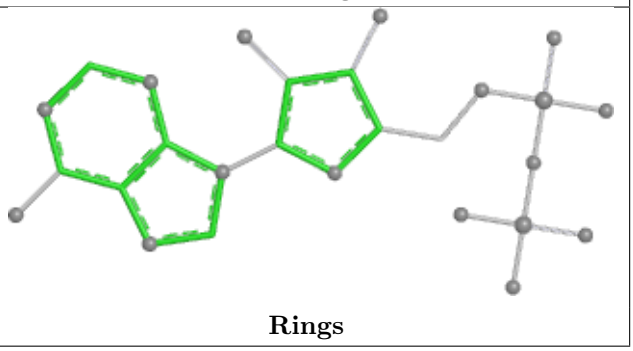
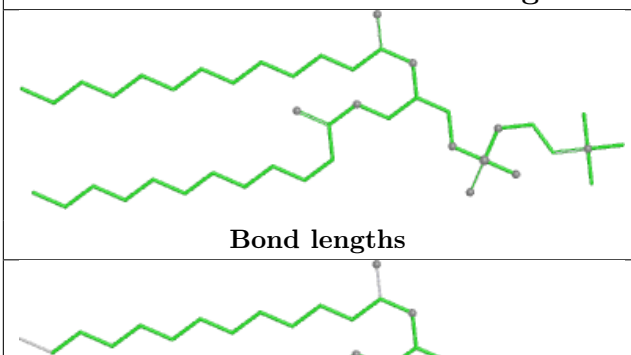


Rings

Ligand PC1 W 205



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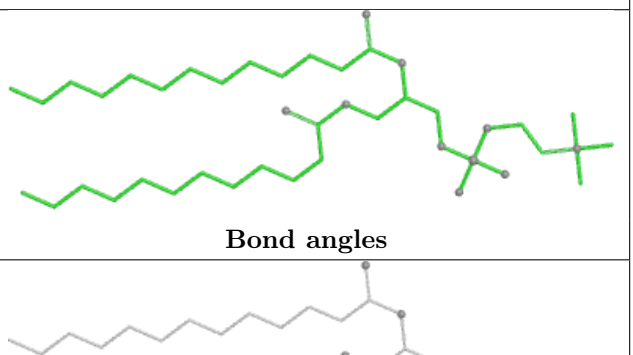
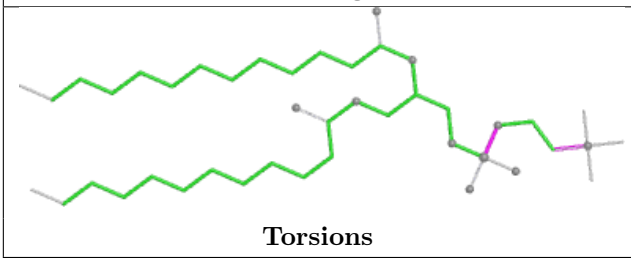


Bond angles



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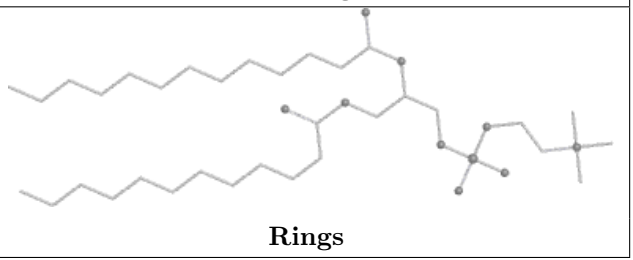
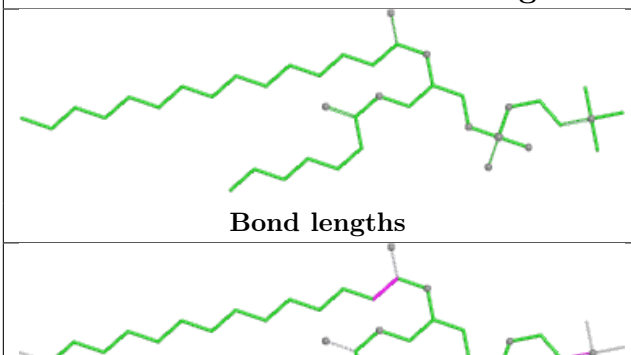


Rings

Ligand PC1 FS 201



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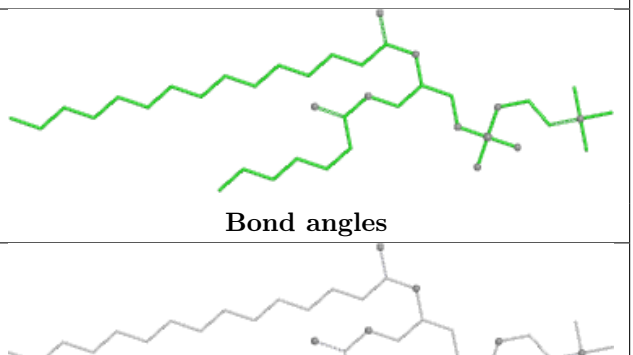
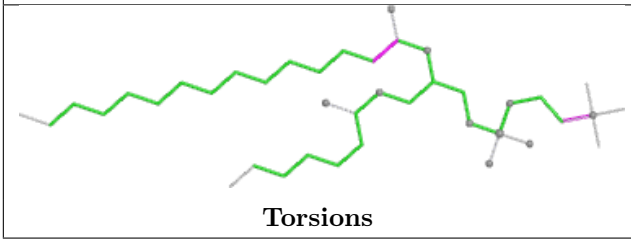


Bond angles



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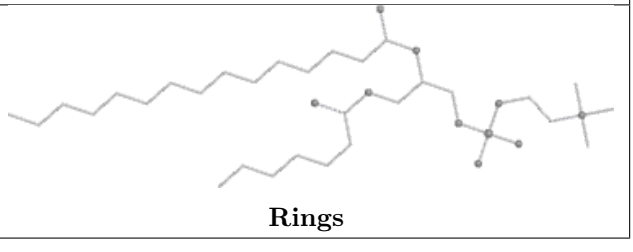
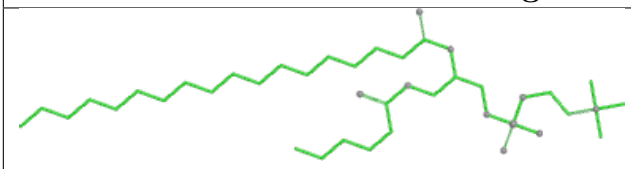
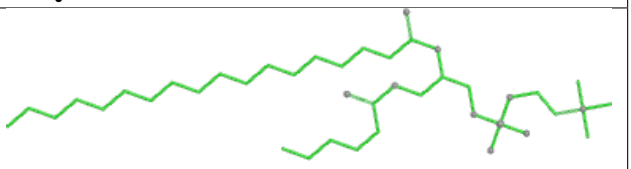


Rings

Ligand PC1 Qi 203


Bond lengths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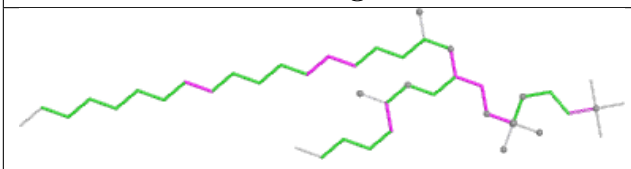
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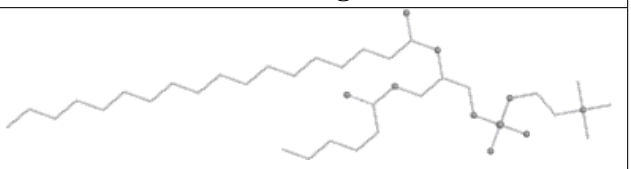
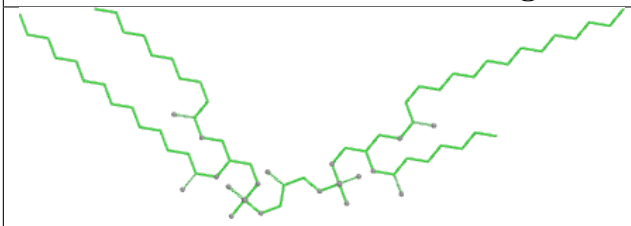

Rings

Ligand CDL 6a 201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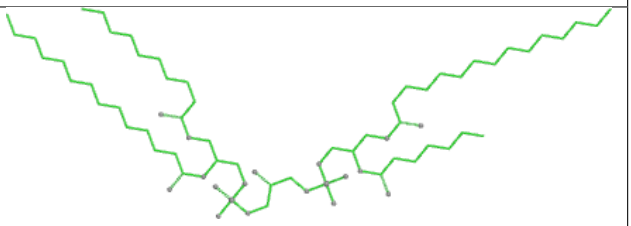
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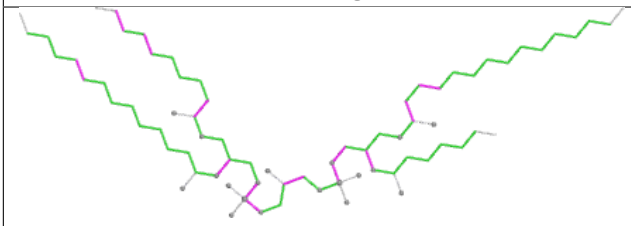
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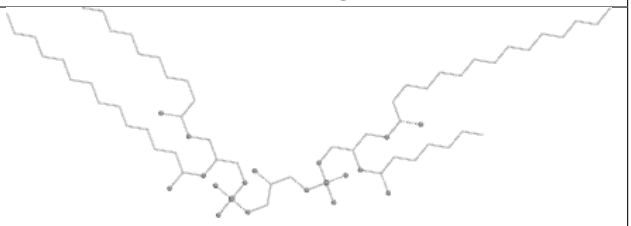
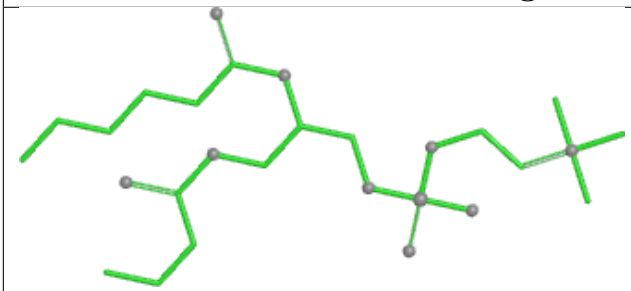

Rings

Ligand PC1 qE 304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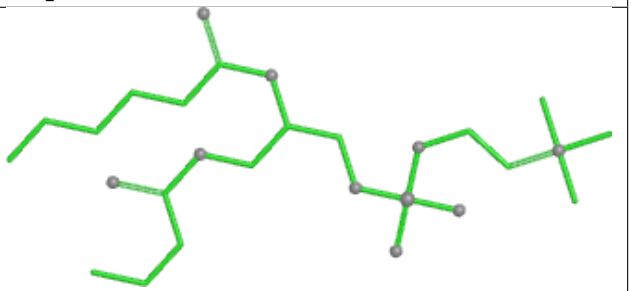
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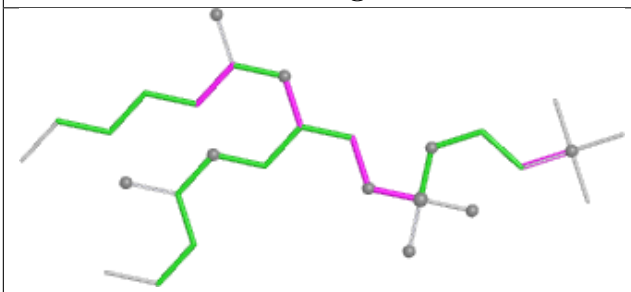
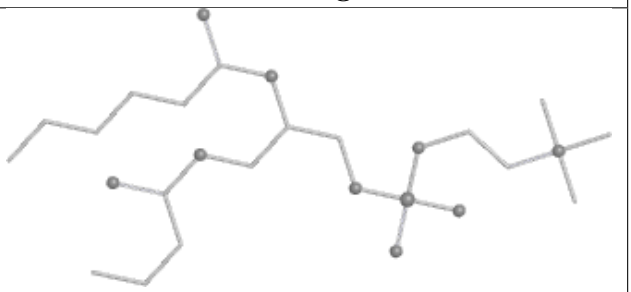
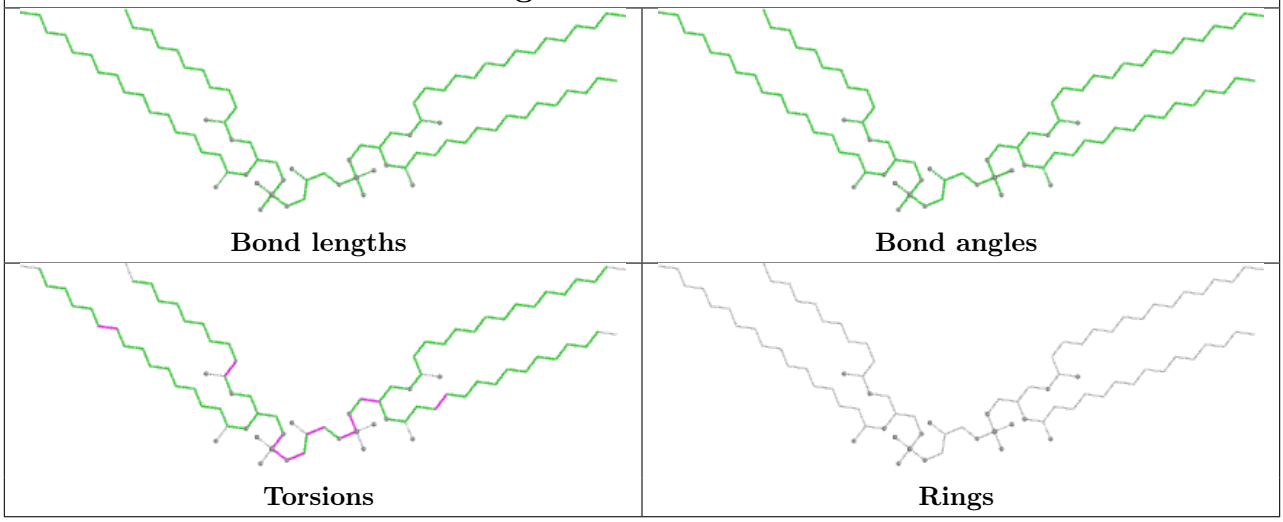
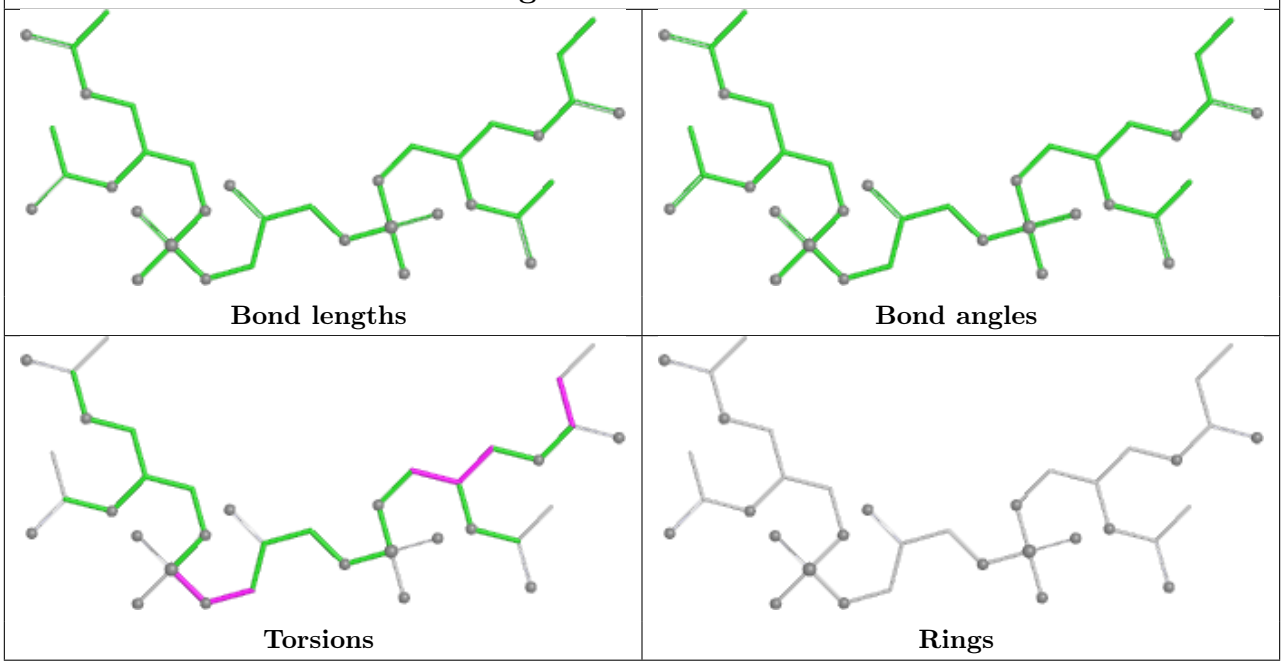

Torsions


Rings

Ligand CDL A9 403



Ligand CDL b4 201



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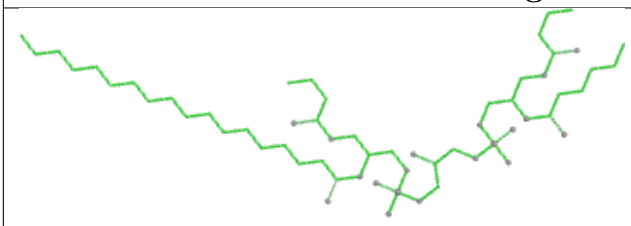
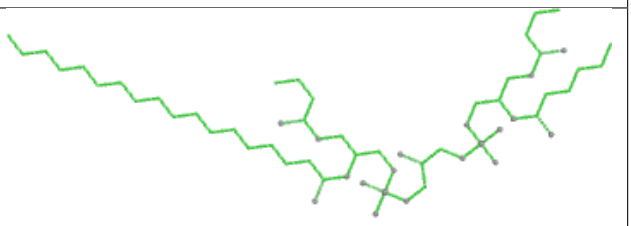
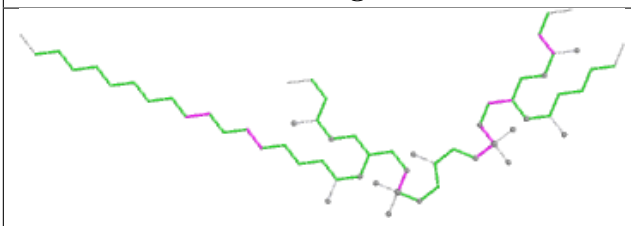


Bond lengths



Bond angles



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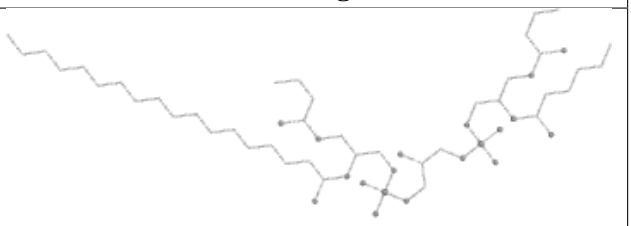
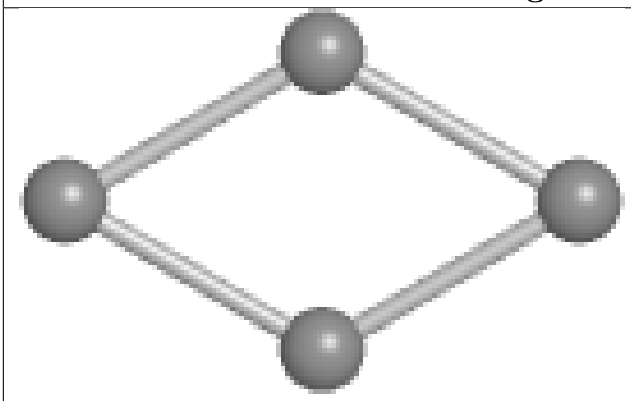


Rings

Ligand FES fx 201



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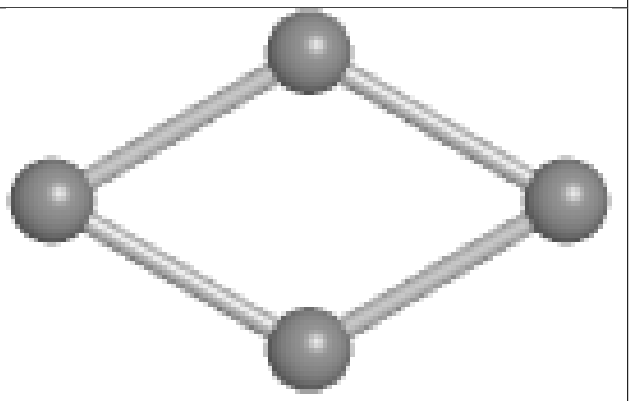
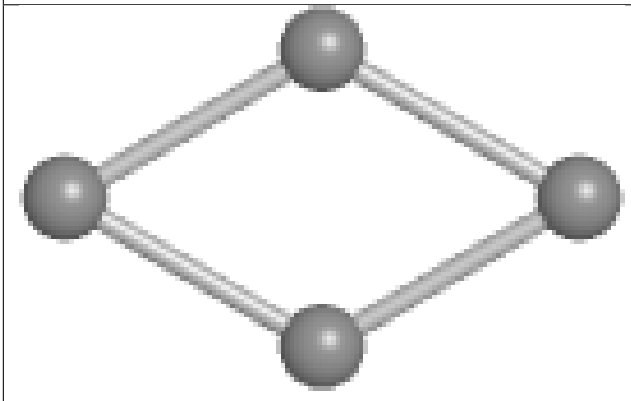


Bond angles



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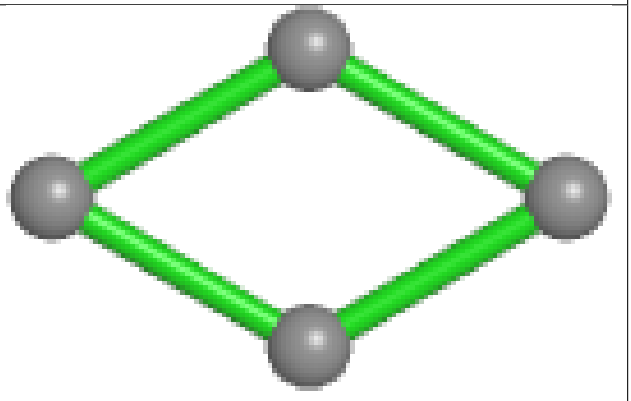
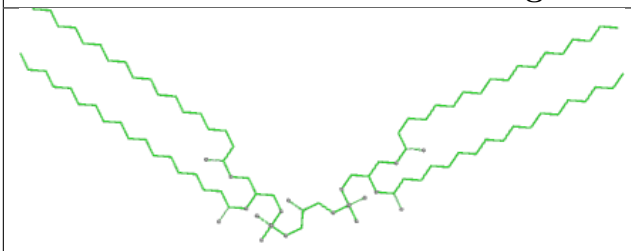


Rings

Ligand CDL F 402



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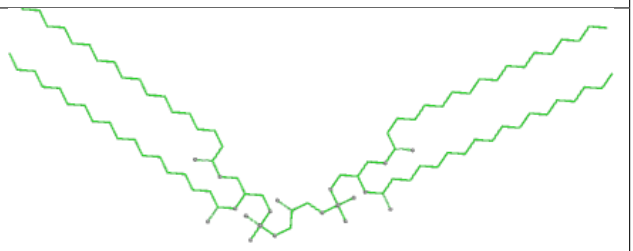
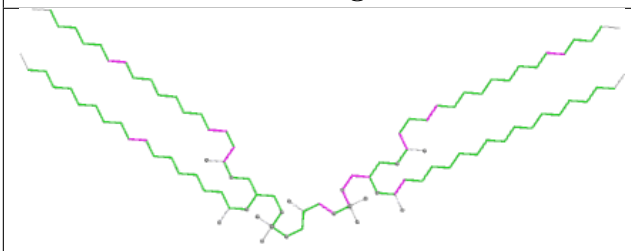


Bond angles



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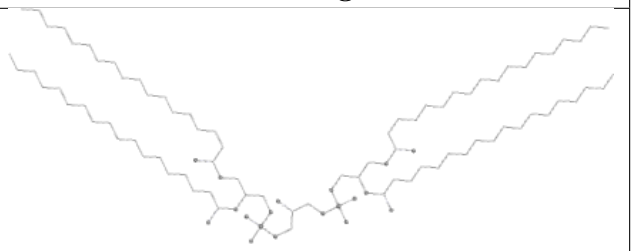
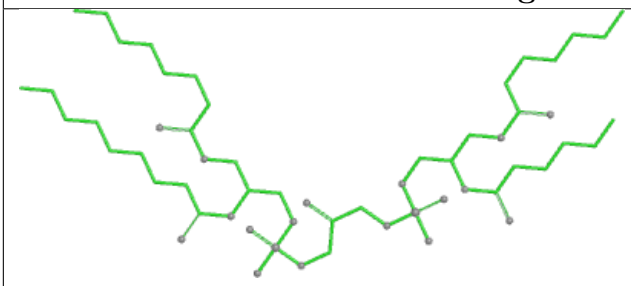


Rings

Ligand CDL p1 403



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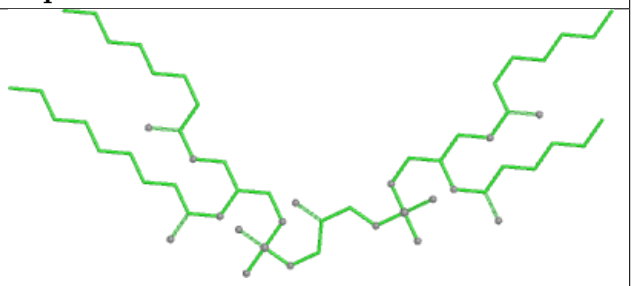
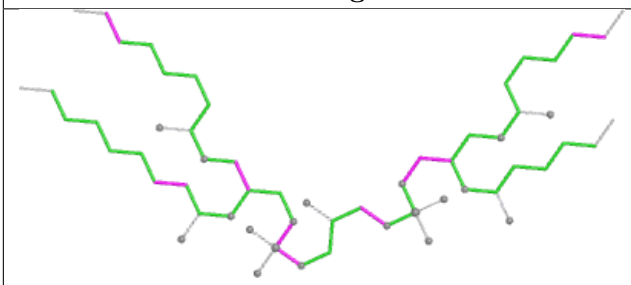


Bond angles



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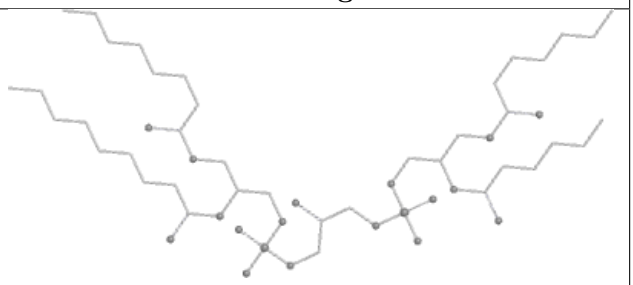
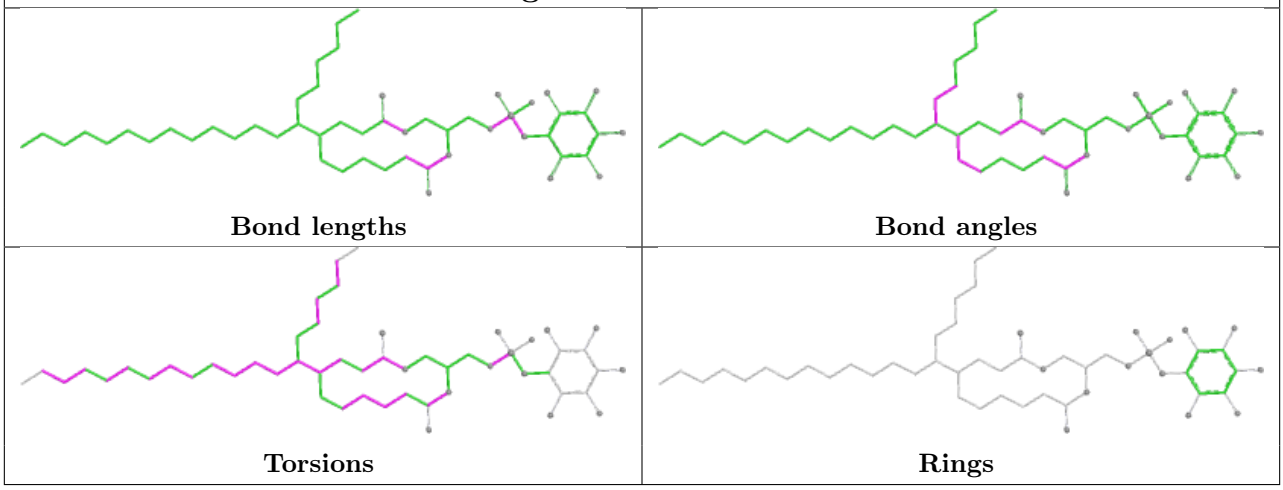
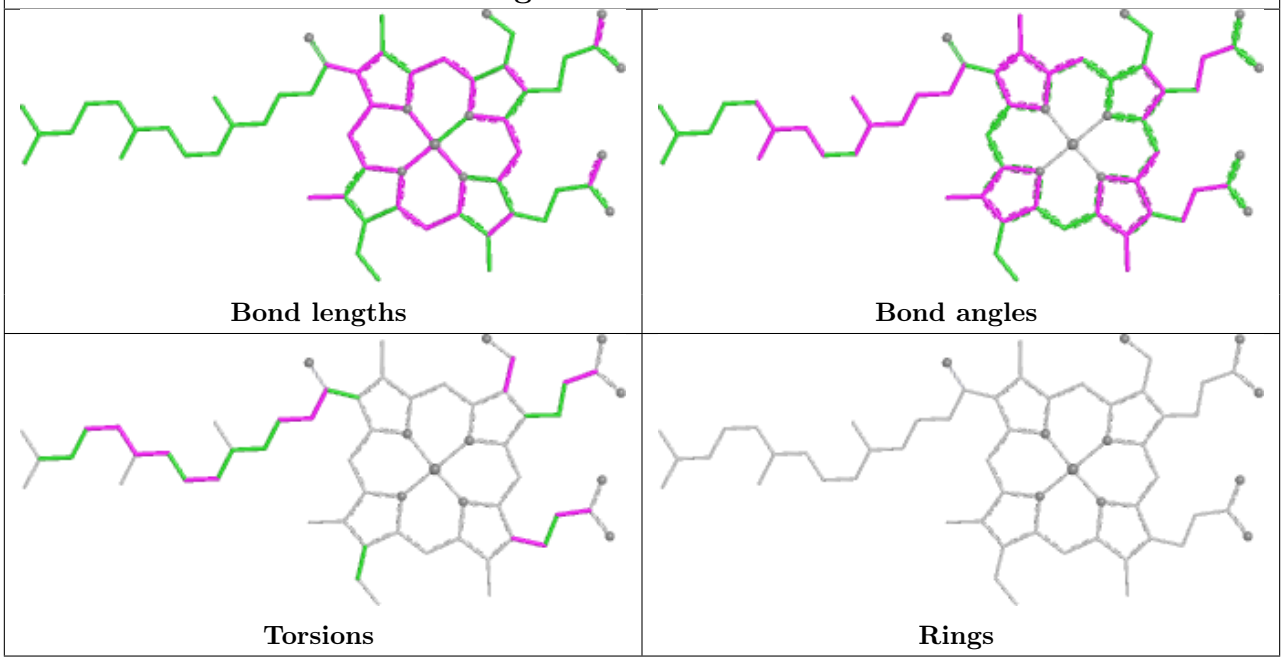


Rings

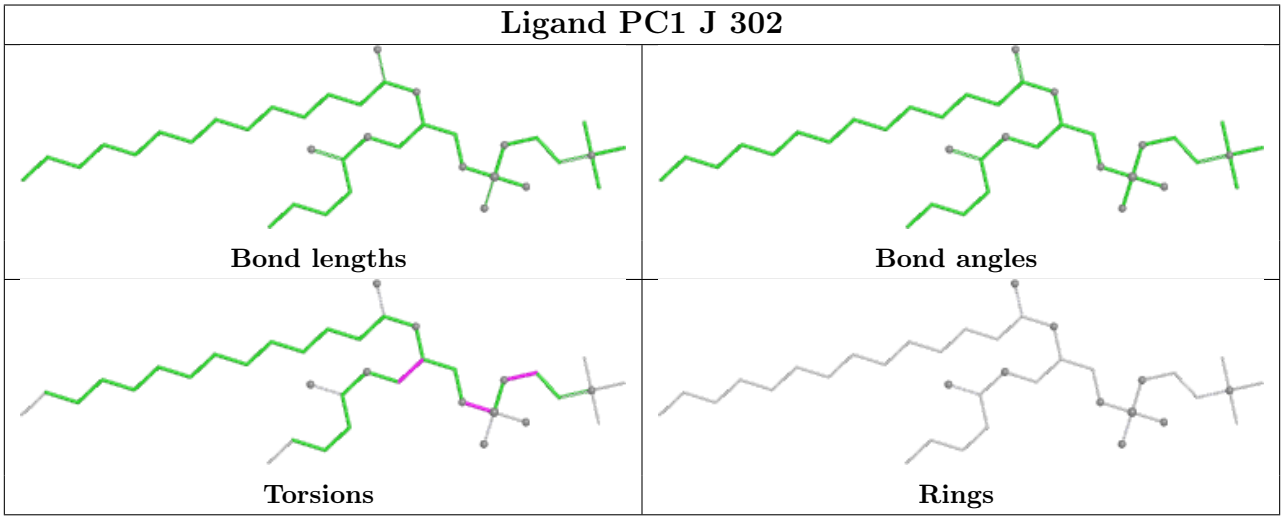
Ligand T7X b6 201



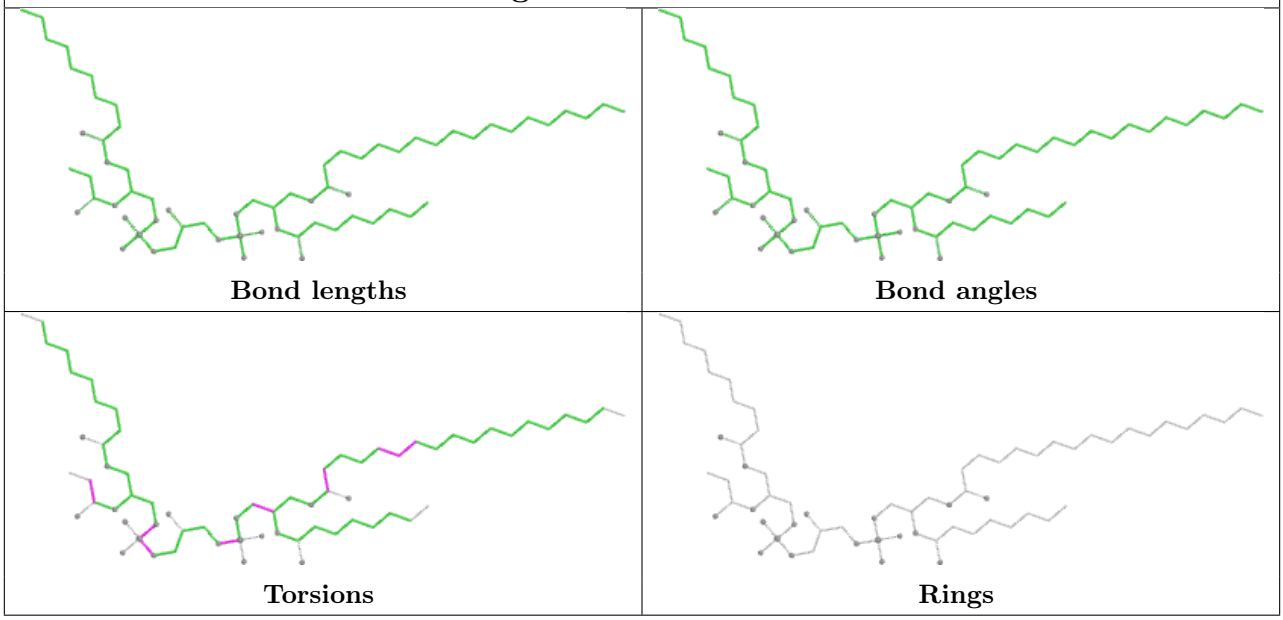
Ligand HEA C1 703



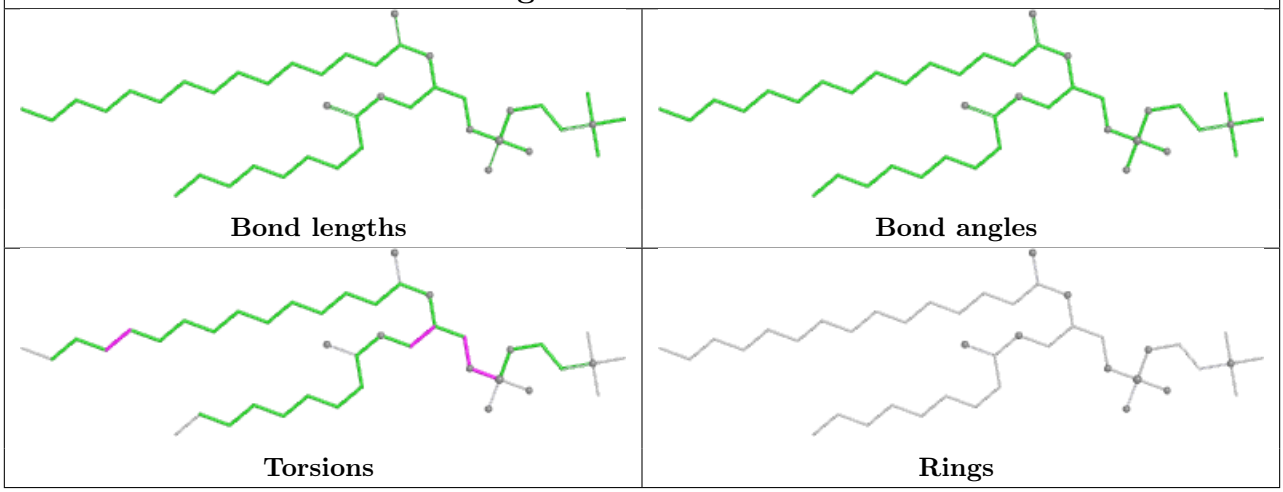
Ligand PC1 J 302



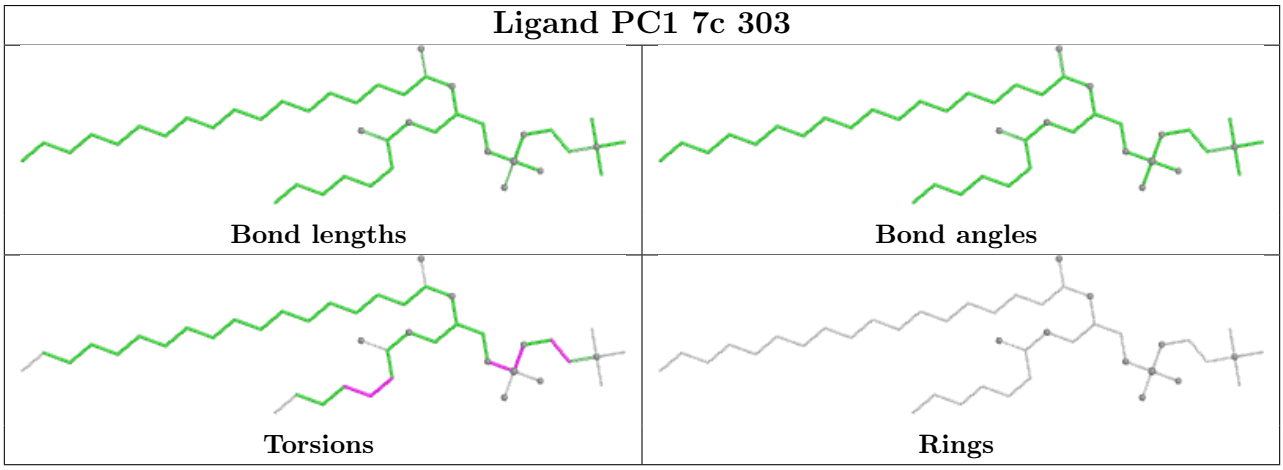
Ligand CDL VB 706



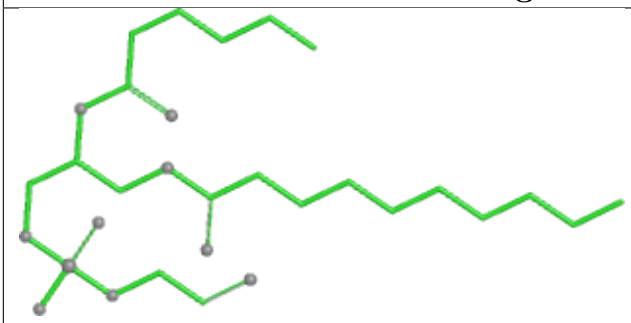
Ligand PC1 m1 403



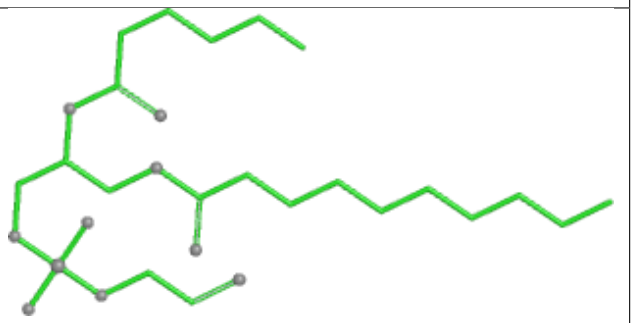
Ligand PC1 7c 303



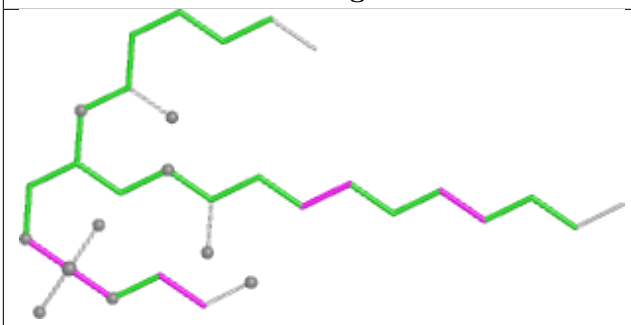
Ligand 3PE M2 408



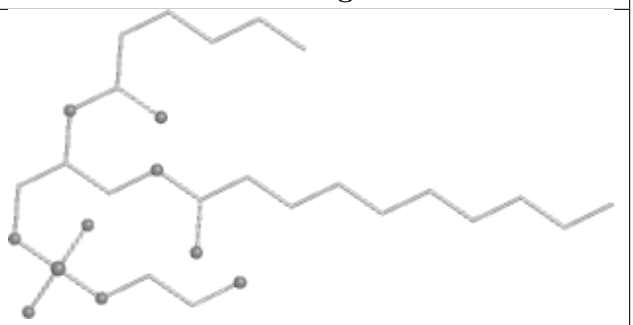
Bond lengths



Bond angles

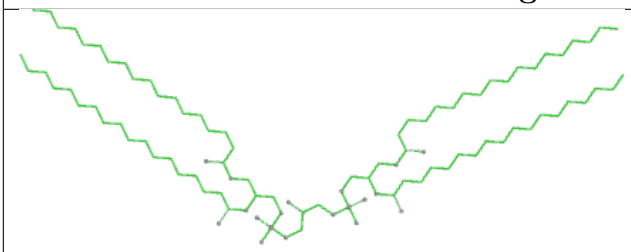


Torsions



Rings

Ligand CDL 7a 201



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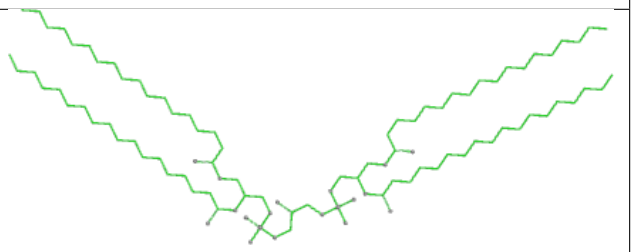
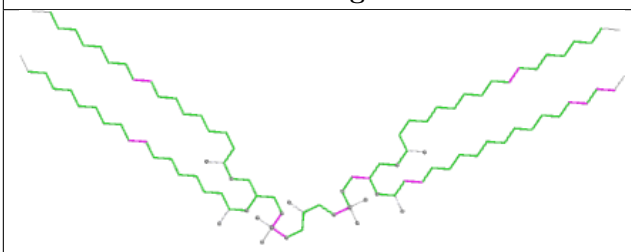
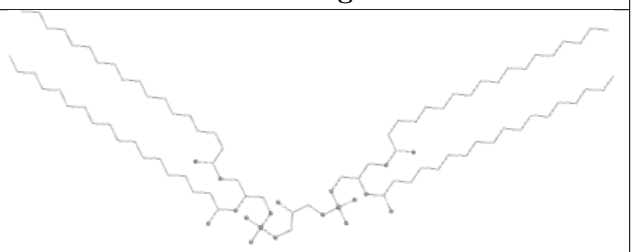


Bond angles

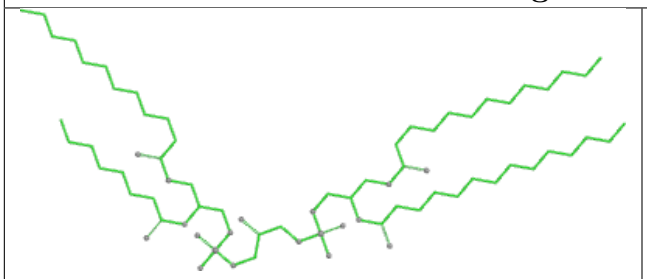


Torsions



Rings

Ligand CDL I 303



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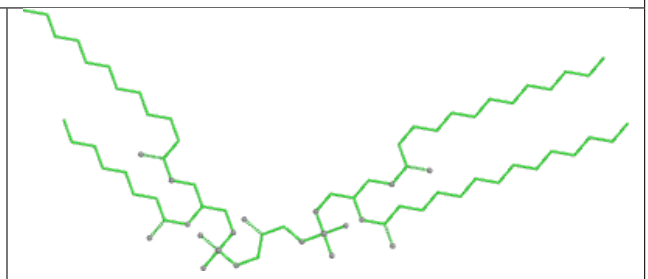
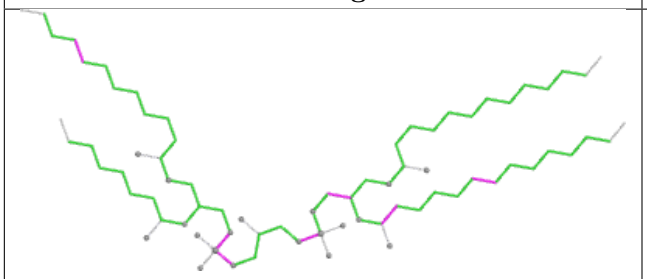
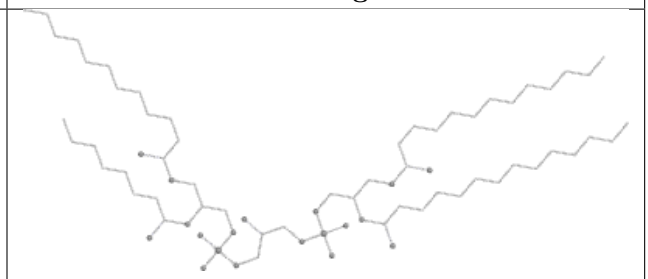


Bond angles

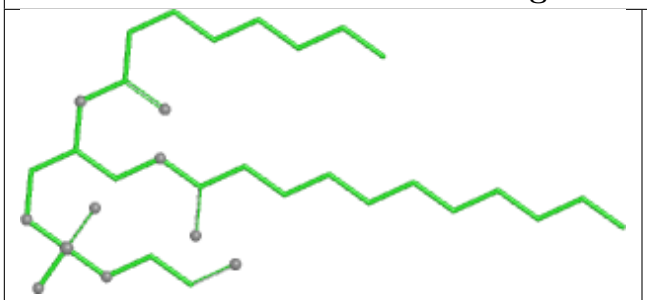


Torsions

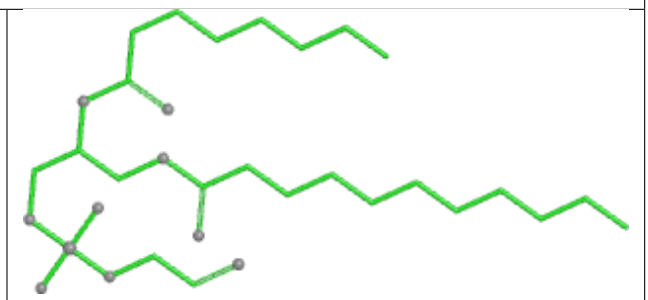


Rings

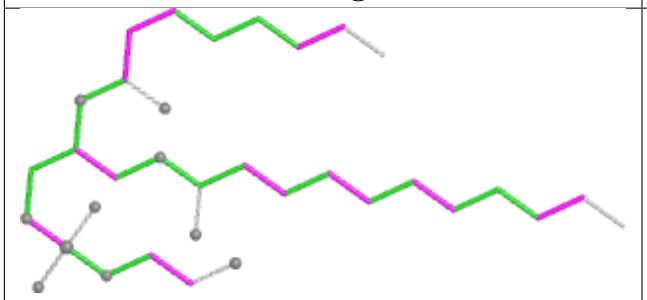
Ligand 3PE w 203



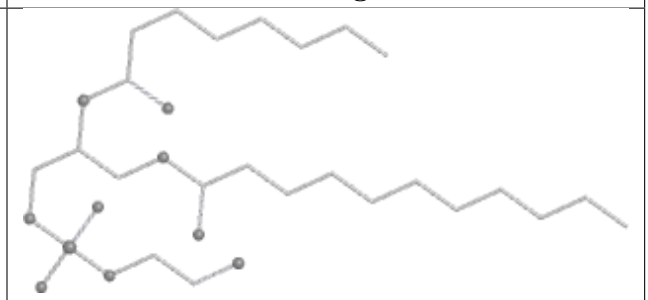
Bond lengths



Bond angles

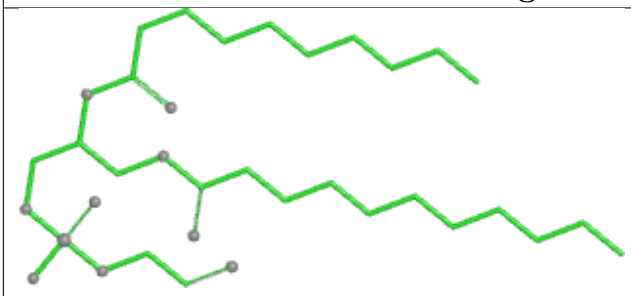


Torsions

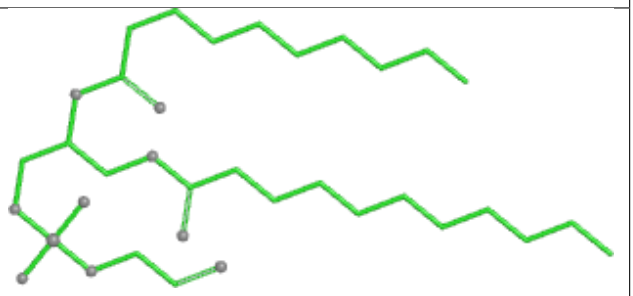


Rings

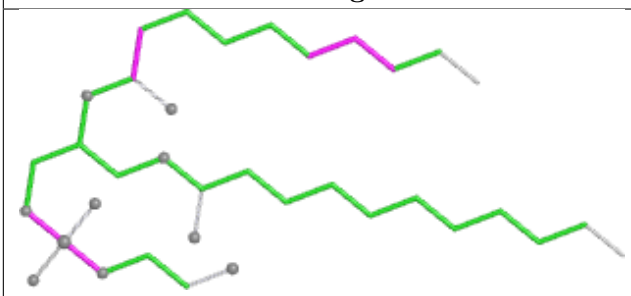
Ligand 3PE N4 601



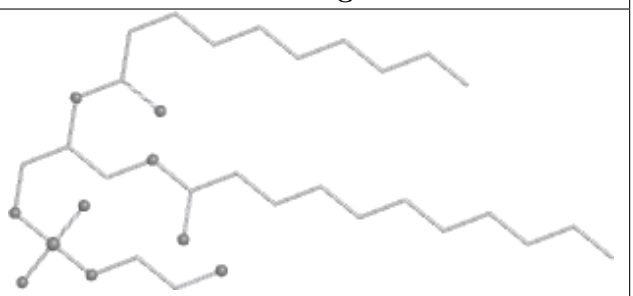
Bond lengths



Bond angles

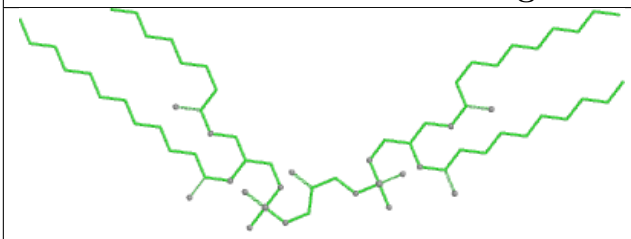


Torsions

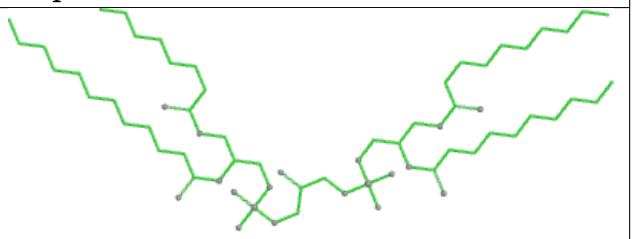


Rings

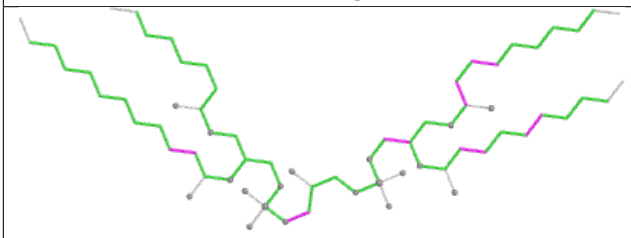
Ligand CDL qb 601



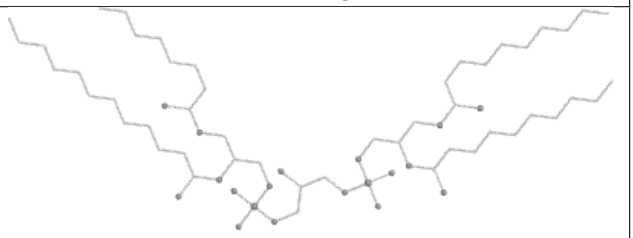
Bond lengths



Bond angles

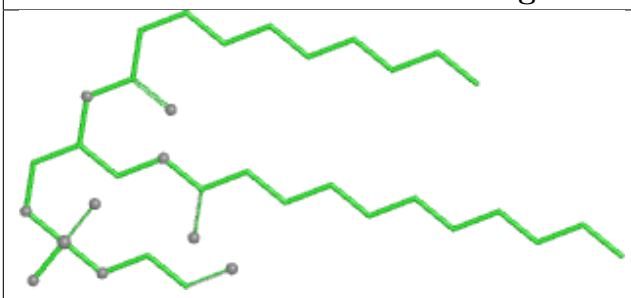


Torsions



Rings

Ligand 3PE N5 802



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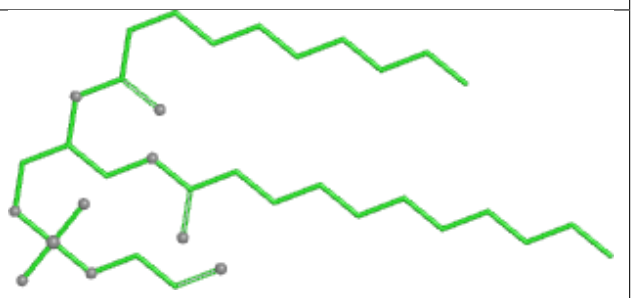
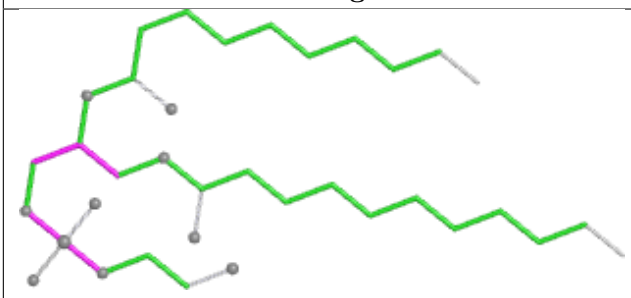
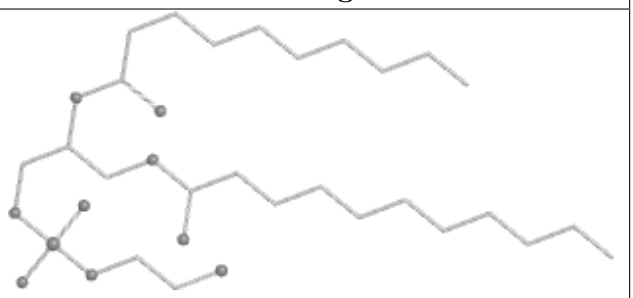


Bond angles

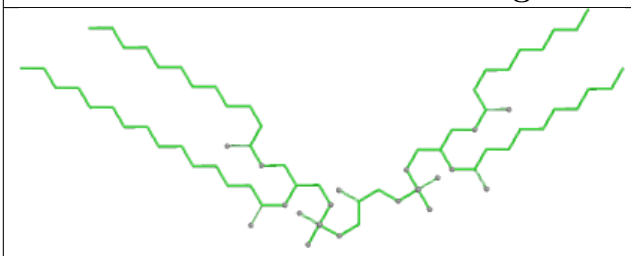


Torsions



Rings

Ligand CDL m2 404



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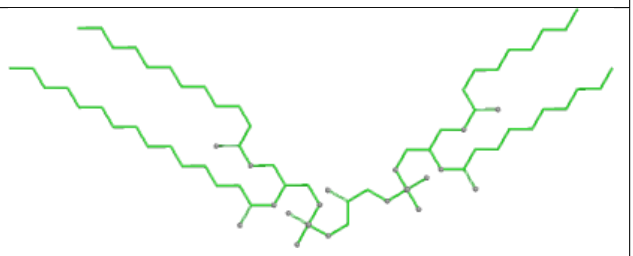
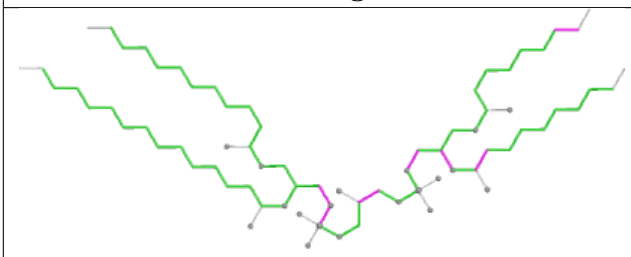


Bond angles



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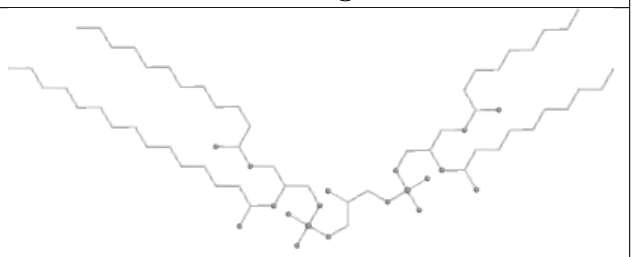
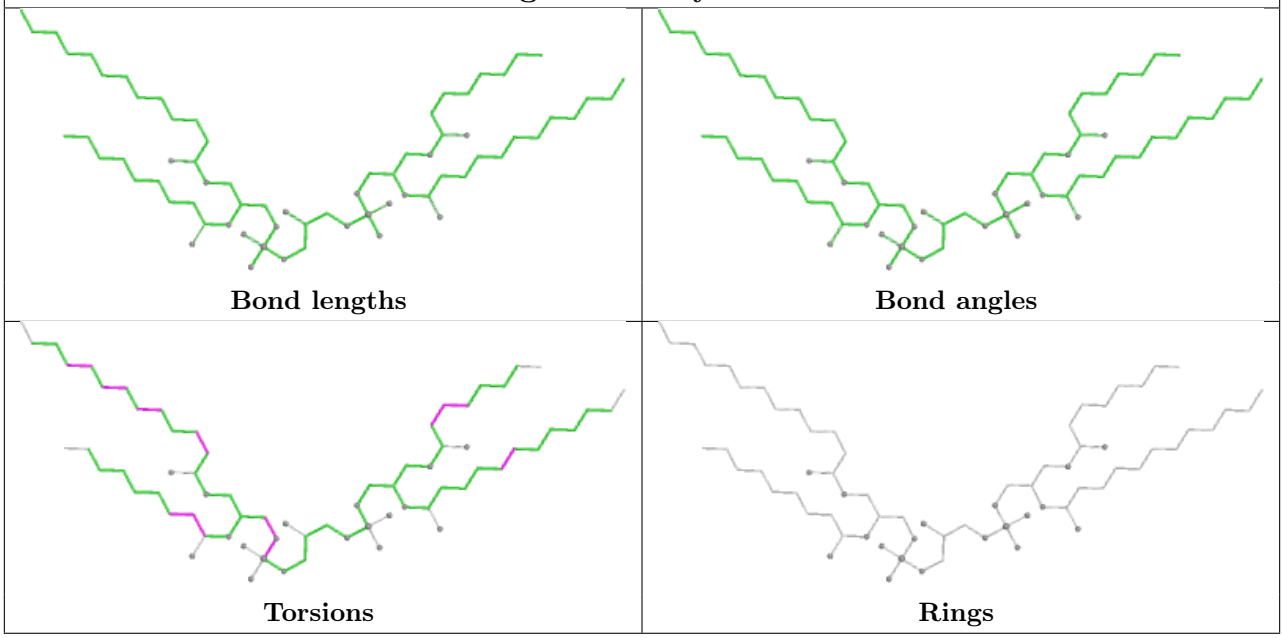
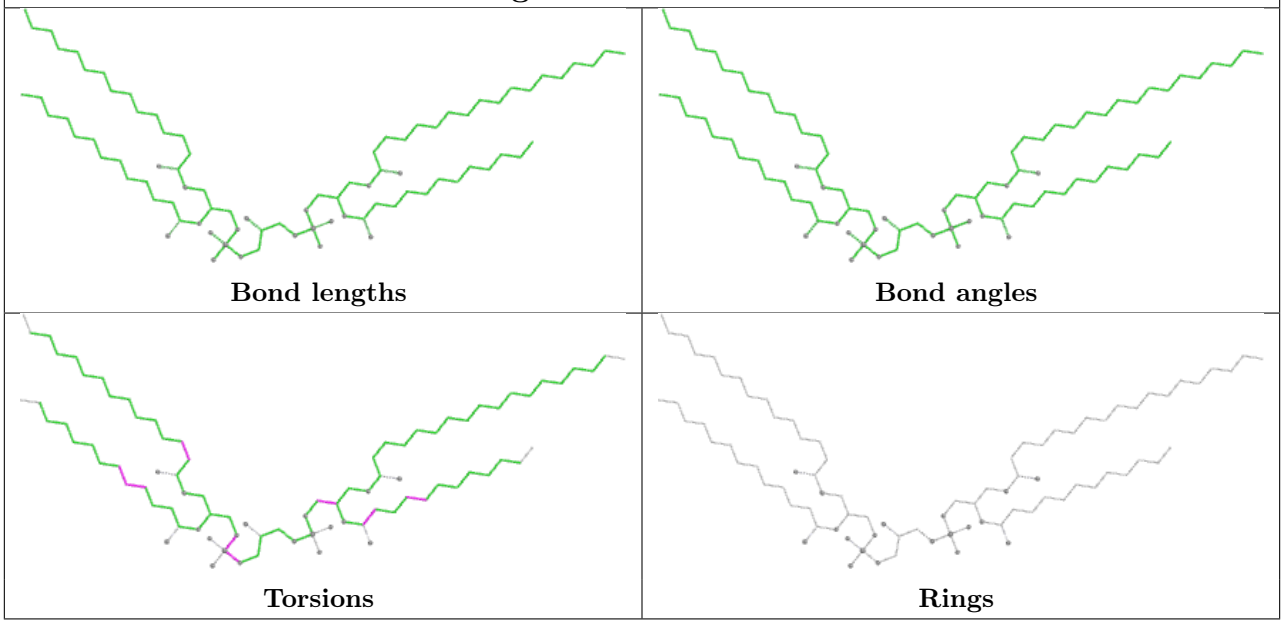


Rings

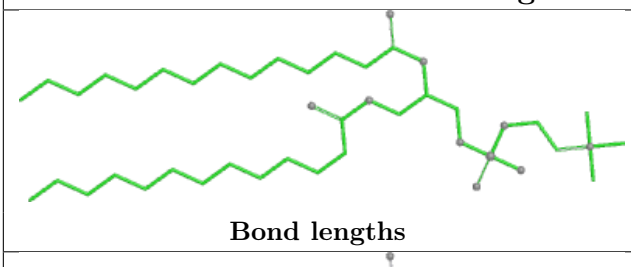
Ligand CDL y5 201



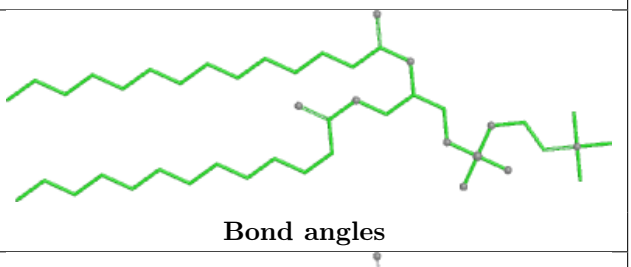
Ligand CDL VB 703



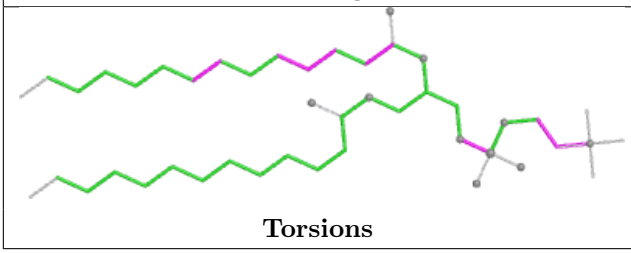
Ligand PC1 7A 202



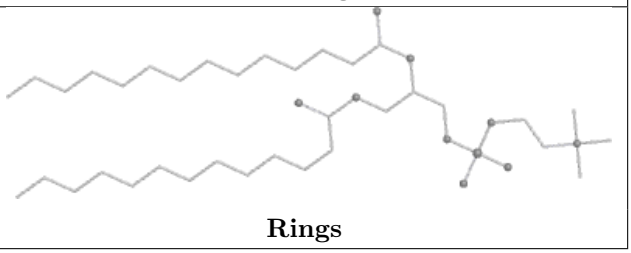
Bond lengths



Bond angles

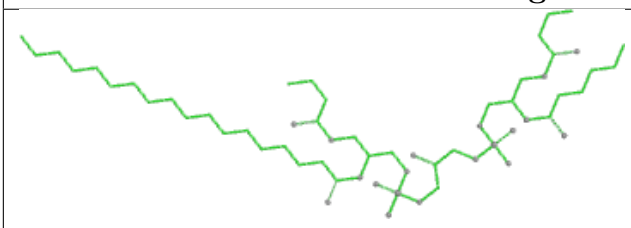


Torsions



Rings

Ligand CDL e 401



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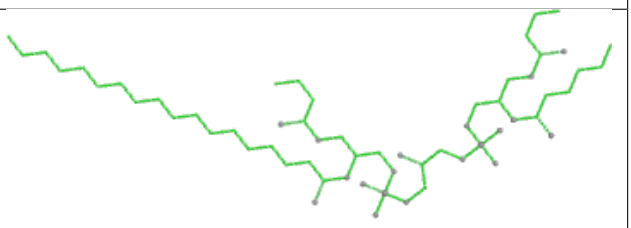
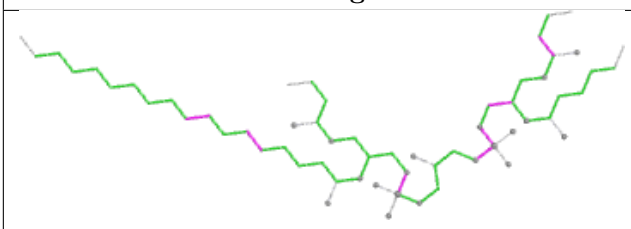


Bond angles



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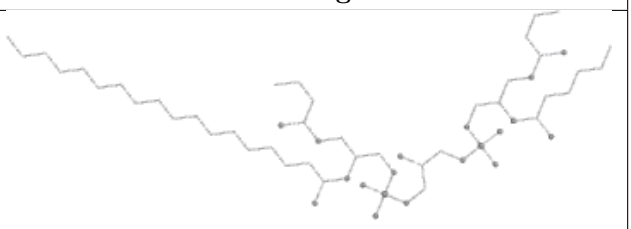
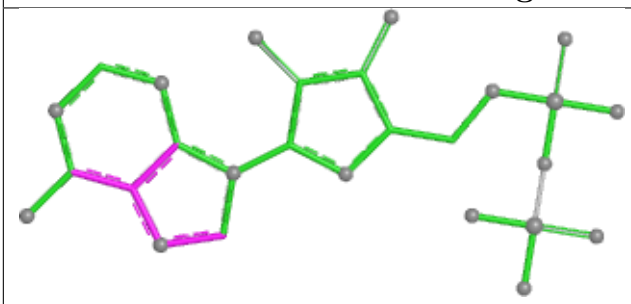


Rings

Ligand ADP b9 202



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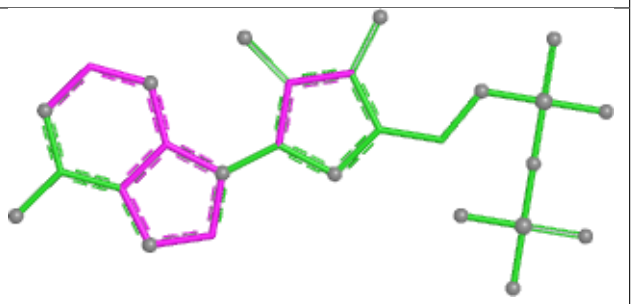
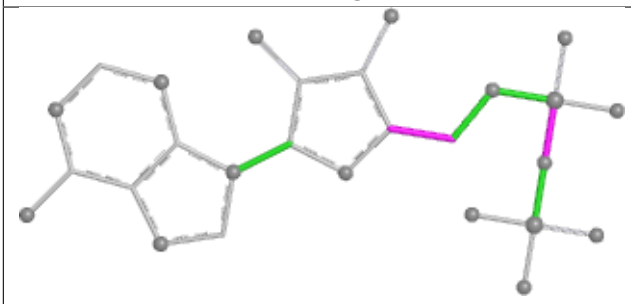


Bond angles



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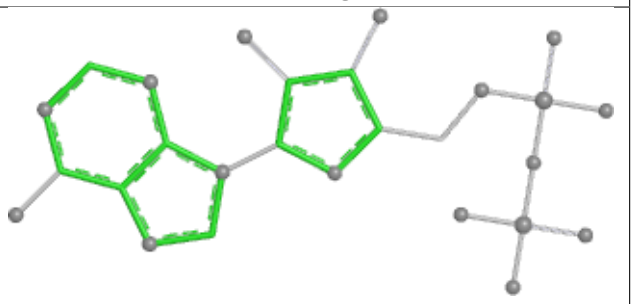
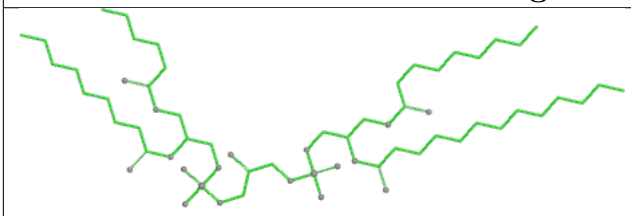


Rings

Ligand CDL r 201



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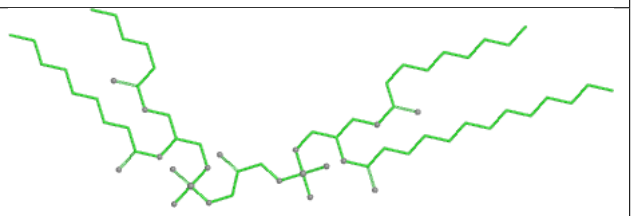
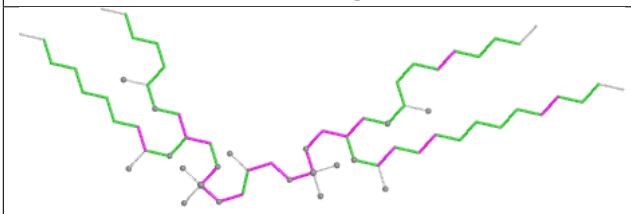
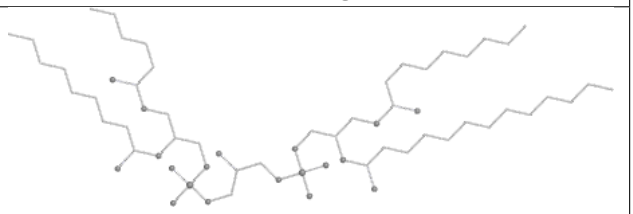


Bond angles

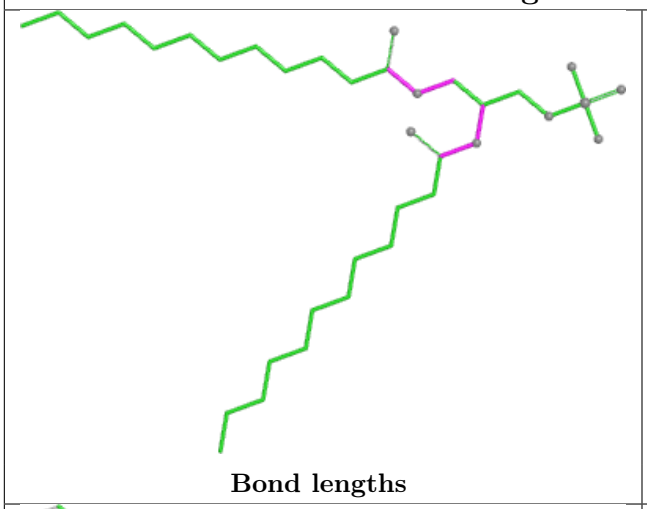


Torsions

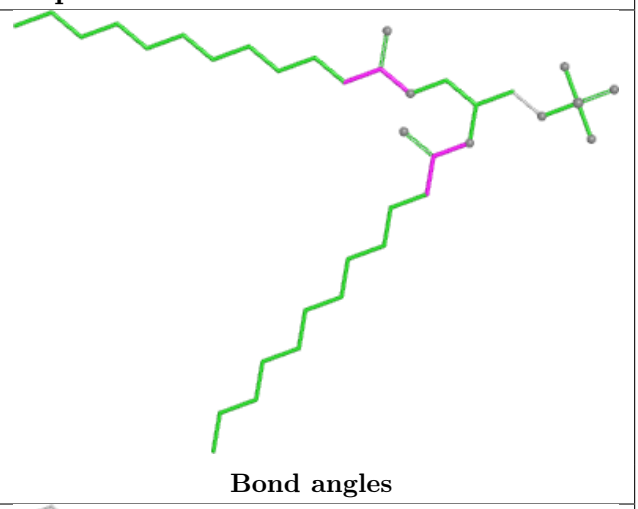


Rings

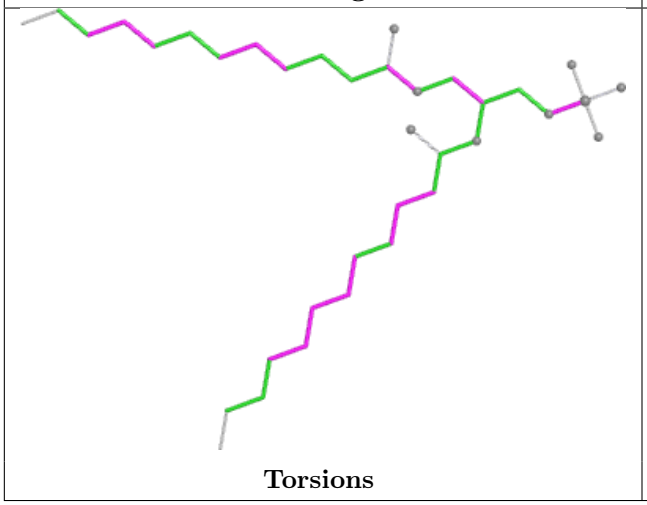
Ligand PX2 qh 201



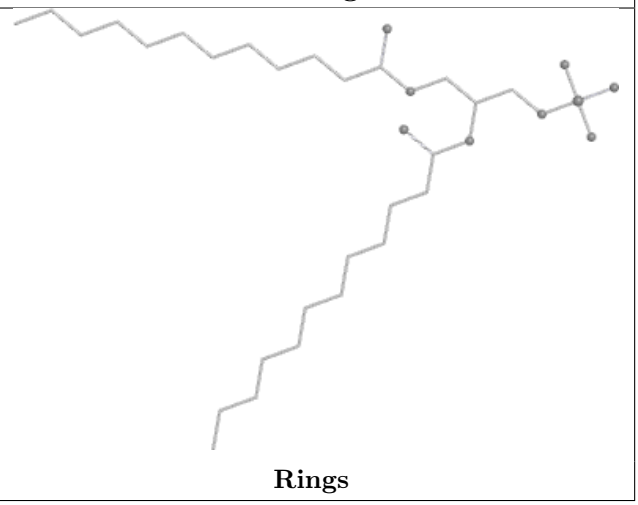
Bond lengths



Bond angles

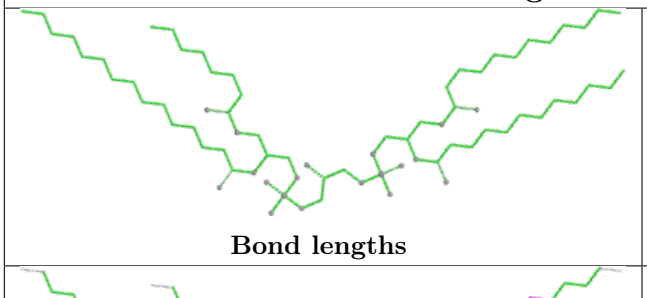


Torsions



Rings

Ligand CDL T 202



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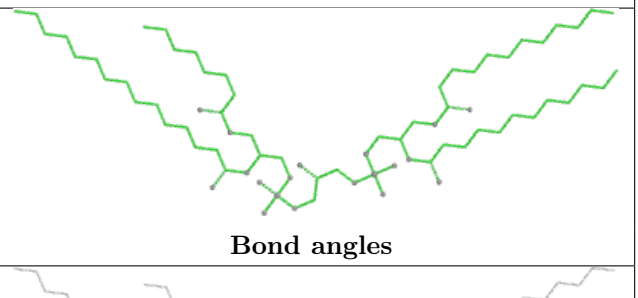
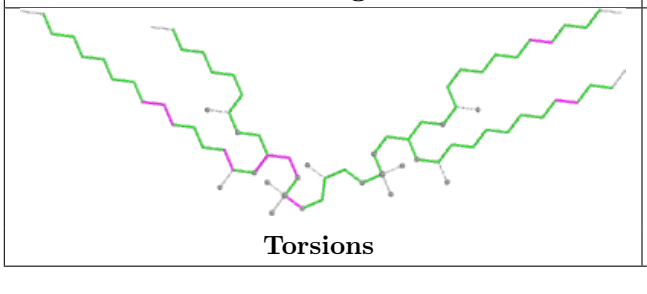
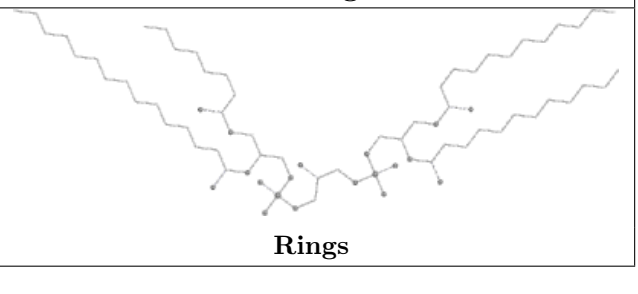


Bond angles

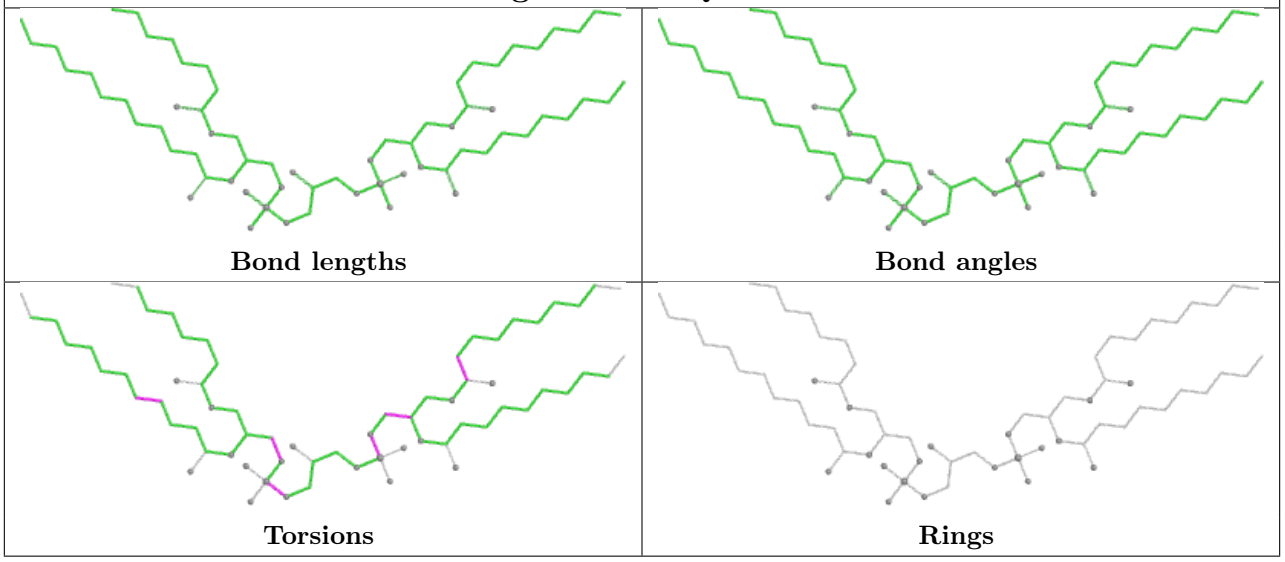


Torsions

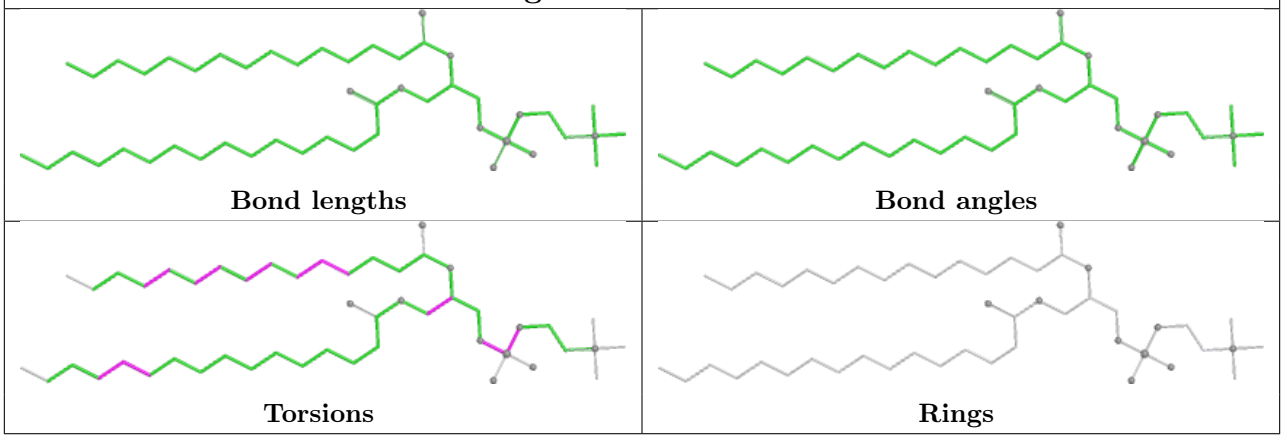


Rings

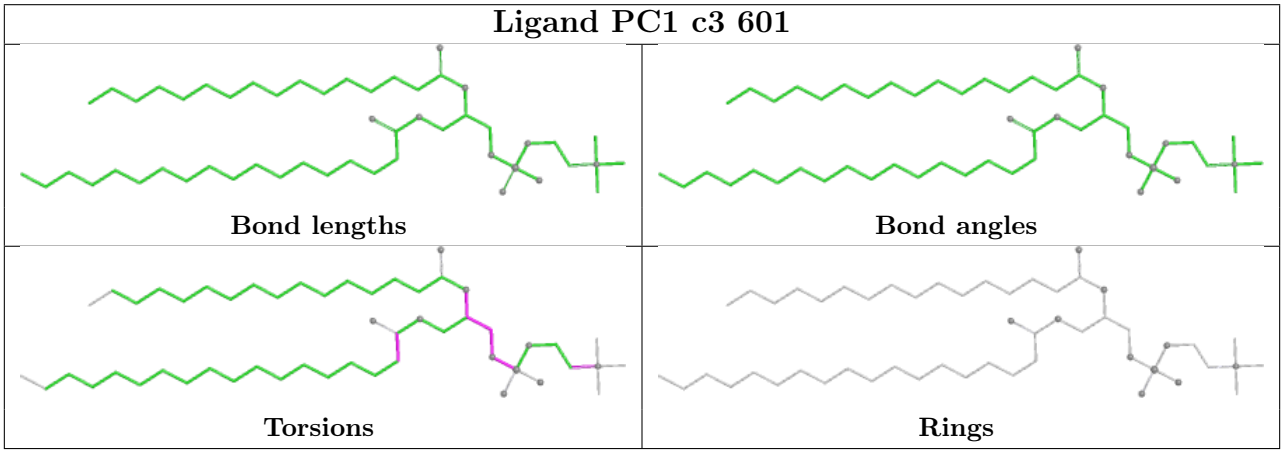
Ligand CDL QB 601



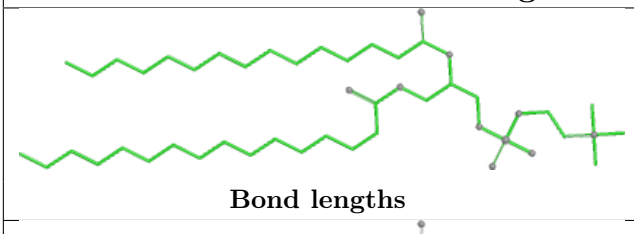
Ligand PC1 c1 704

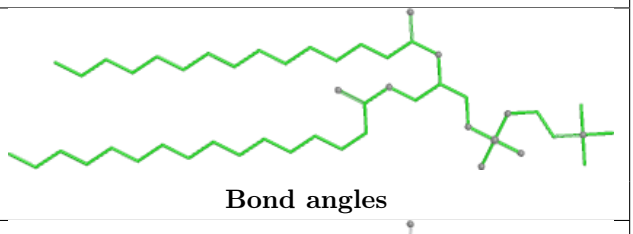


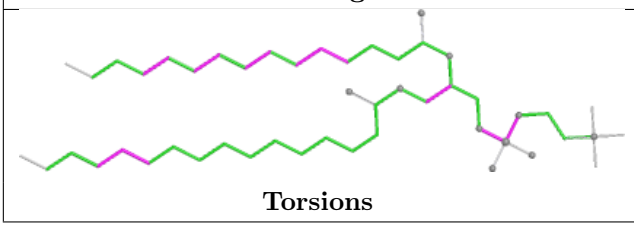
Ligand PC1 c3 601

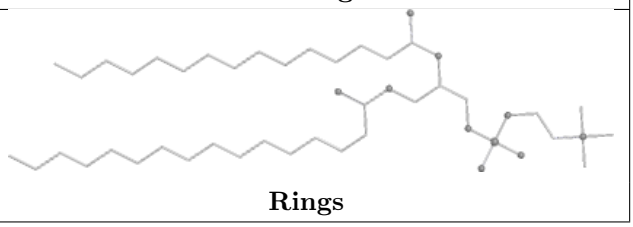


Ligand PC1 C1 706

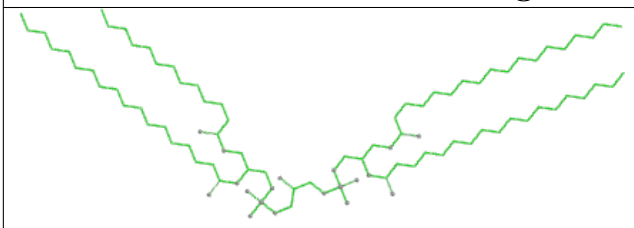

Bond lengths


Bond angles


Torsions


Rings

Ligand CDL C1 712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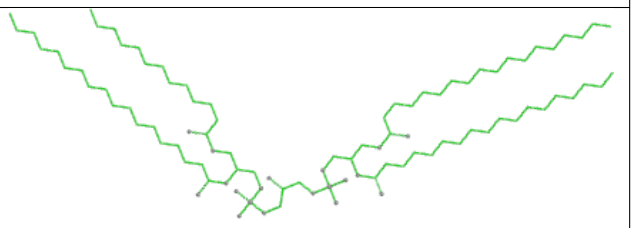
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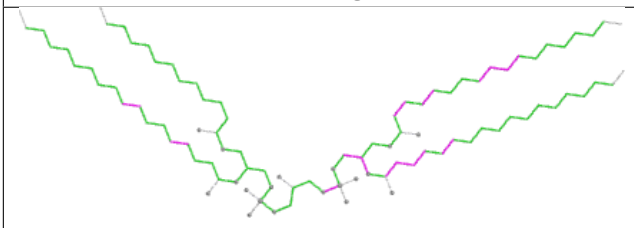
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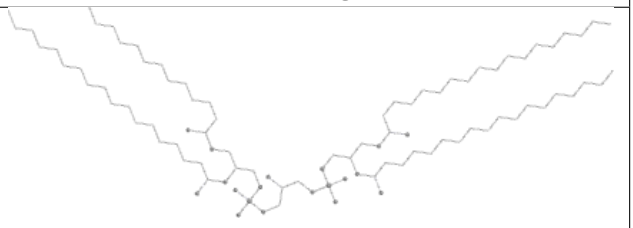
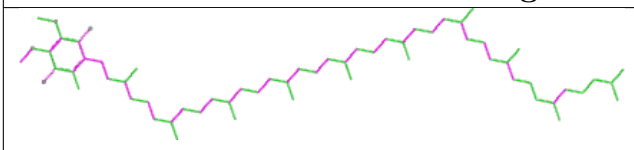

Rings

Ligand U10 SC 102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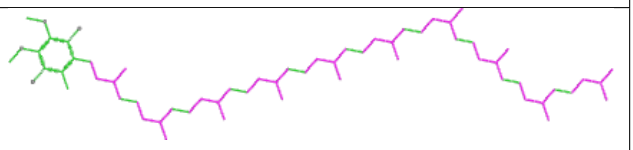
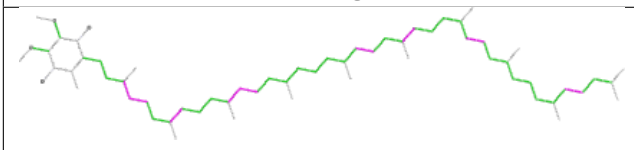
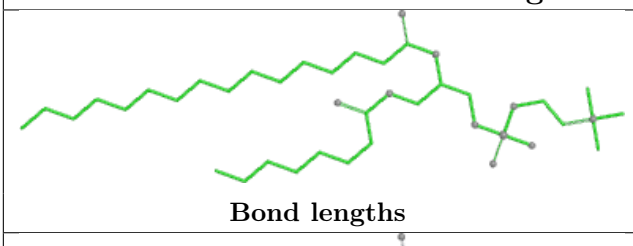

Bond angles


Torsions

Rings

Ligand PC1 2f 302



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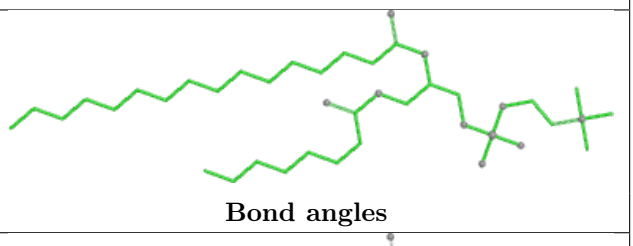
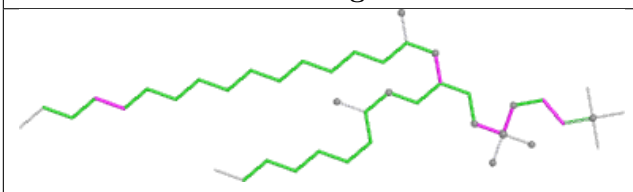


Bond angles



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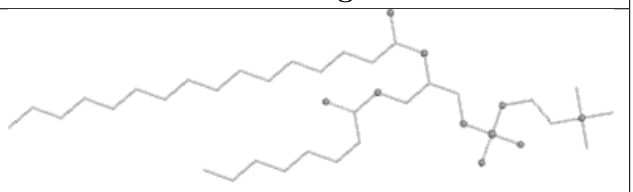
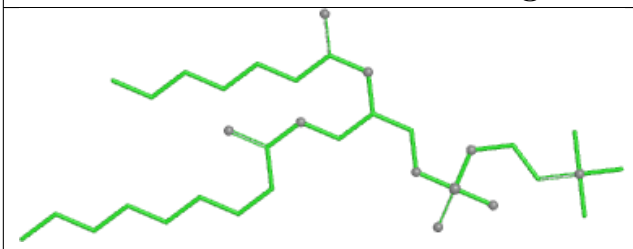


Rings

Ligand PC1 b9 201



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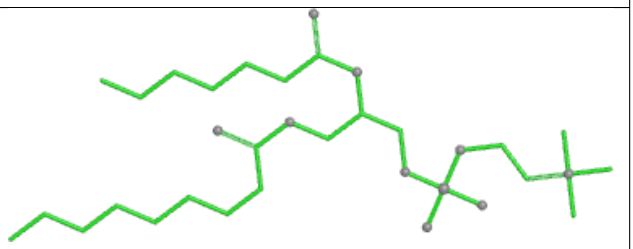
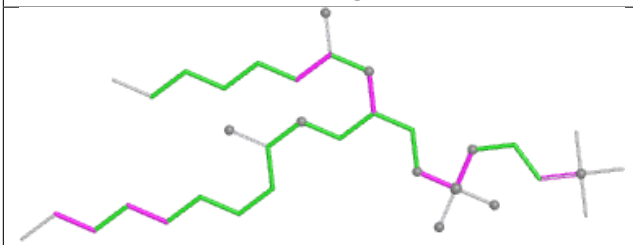


Bond angles



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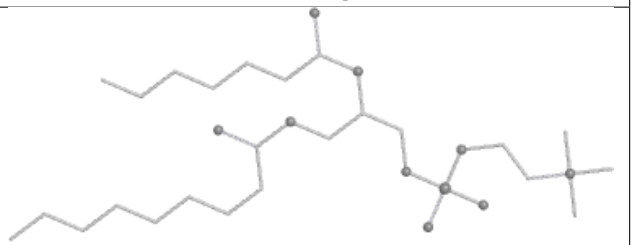
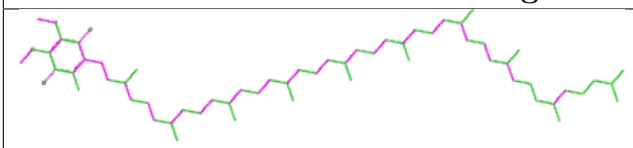


Rings

Ligand U10 B8 301



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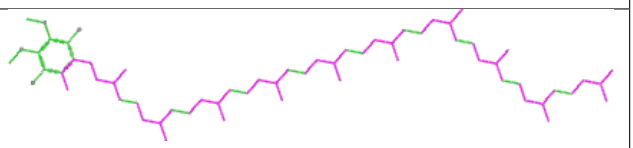
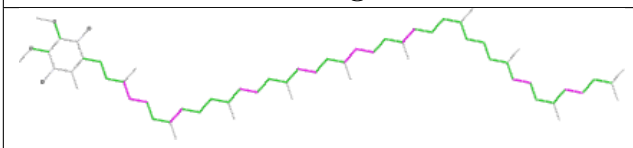


Bond angles



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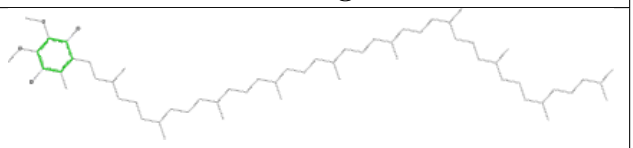
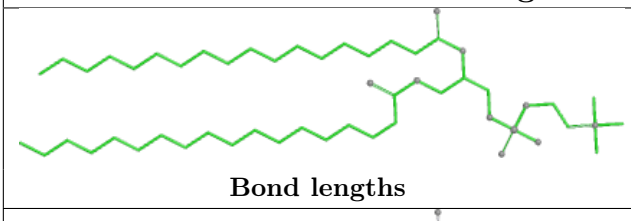


Rings

Ligand PC1 N5 805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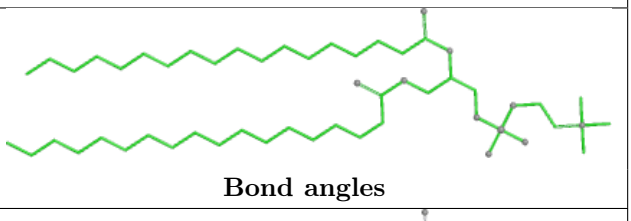
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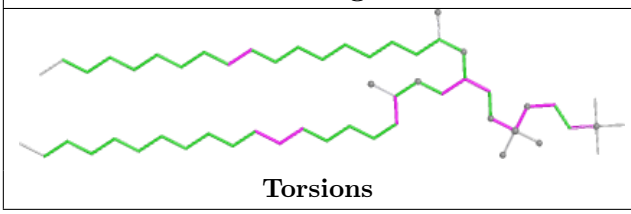
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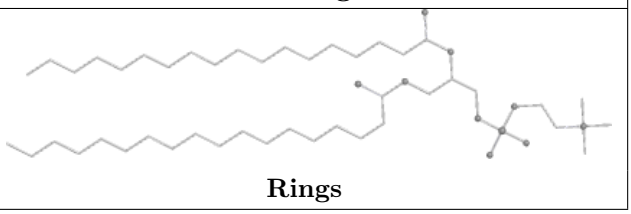
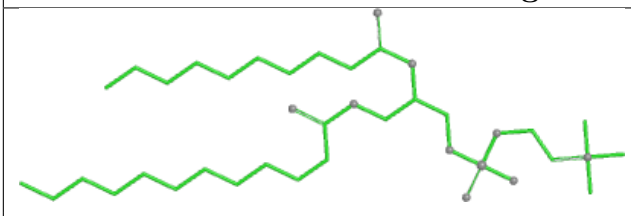

Rings

Ligand PC1 p1 401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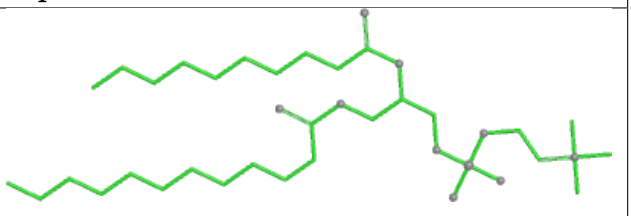
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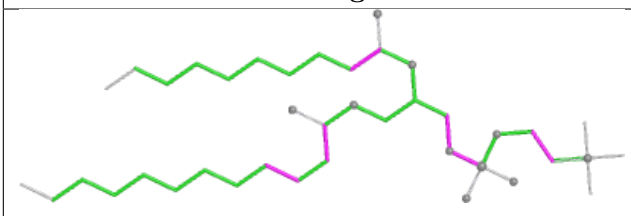
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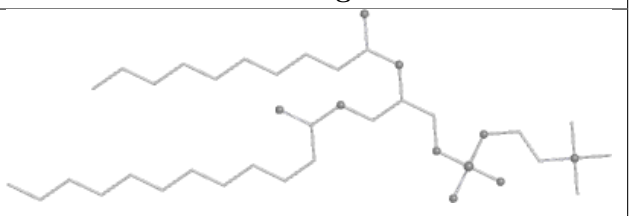
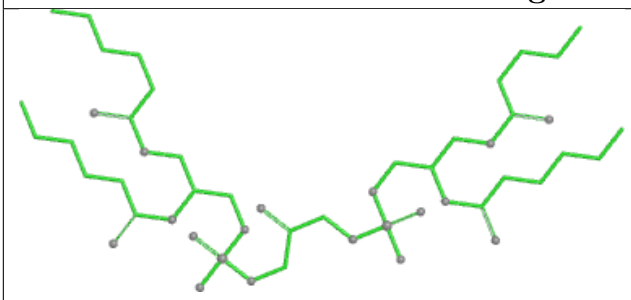

Rings

Ligand CDL a 502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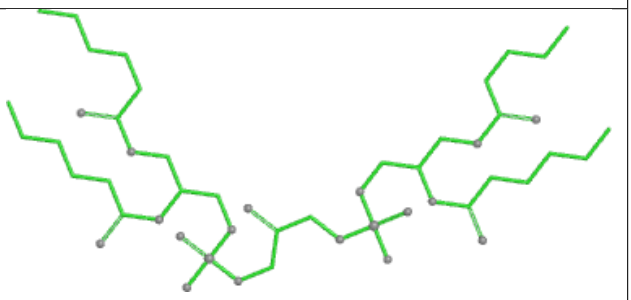
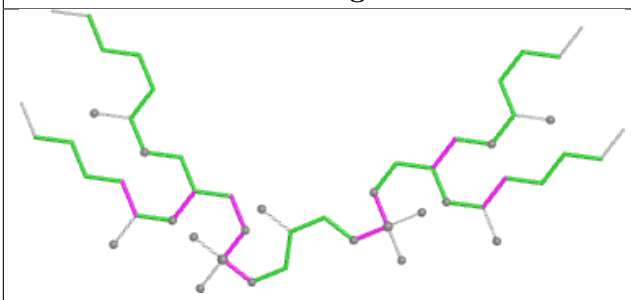
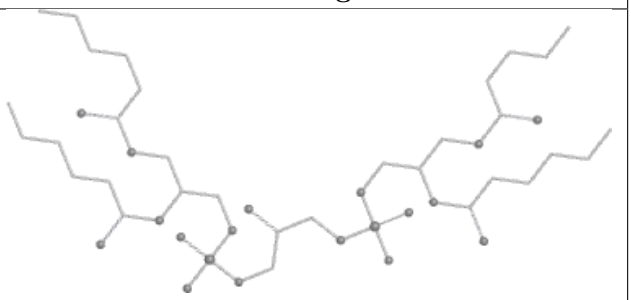
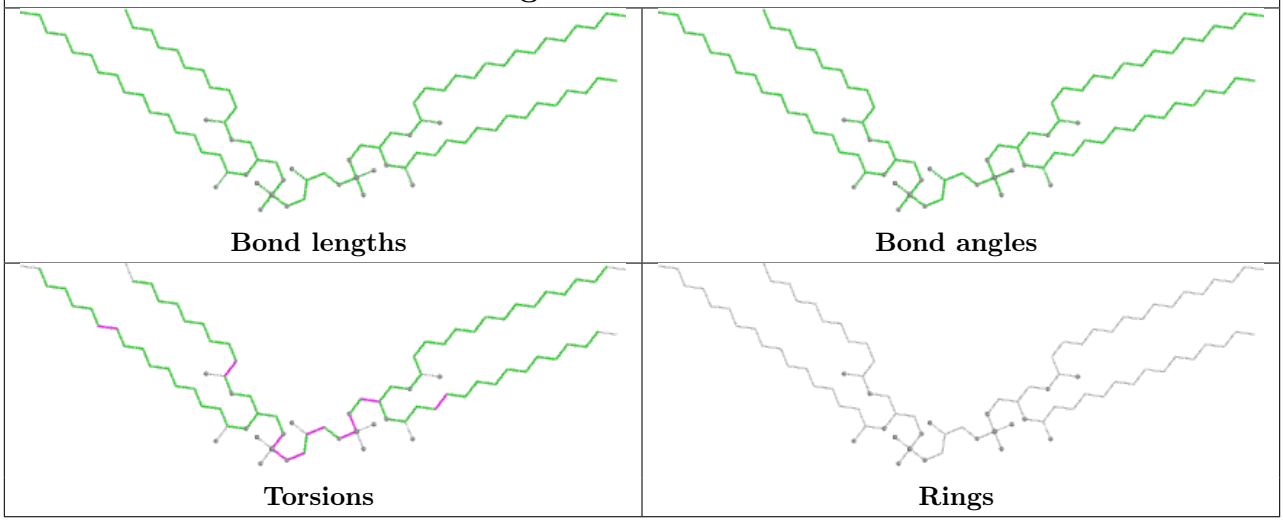

Bond angles

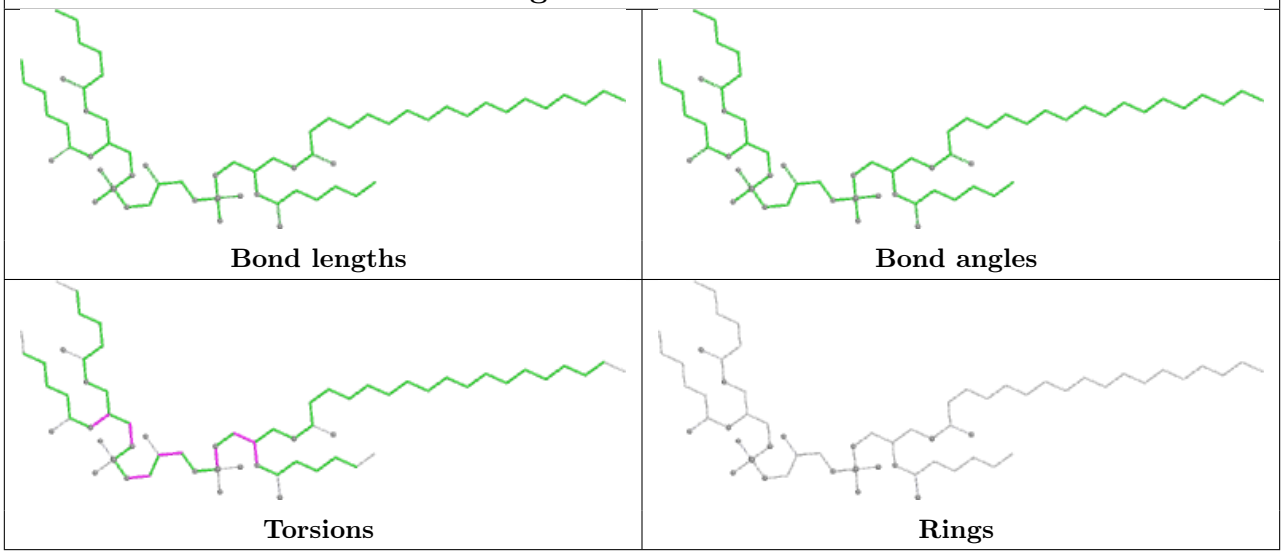

Torsions


Rings

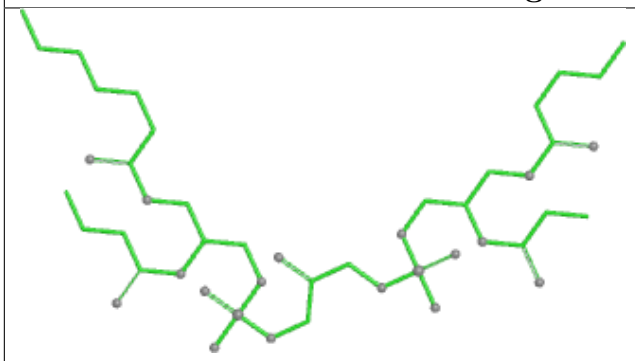
Ligand CDL a9 403



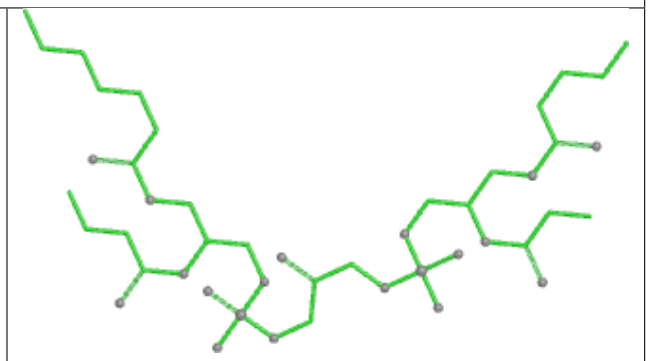
Ligand CDL c 301



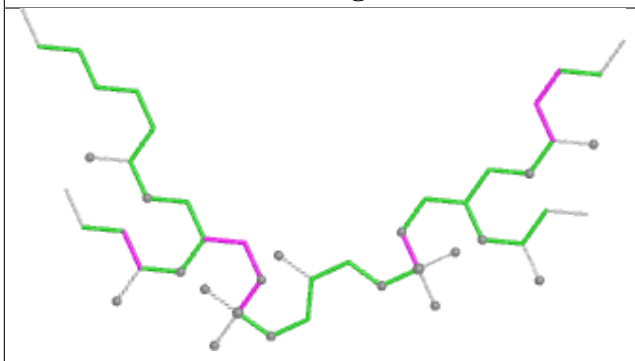
Ligand CDL fs 203



Bond lengths



Bond angles



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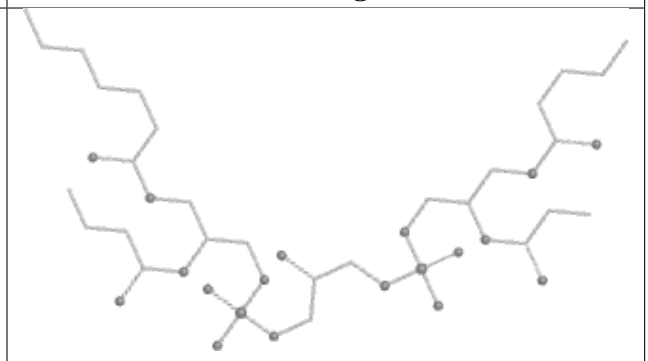
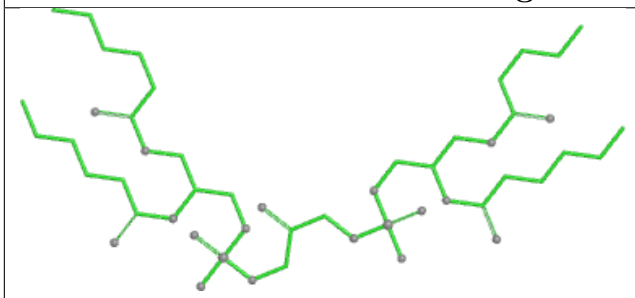


Rings

Ligand CDL 7C 302



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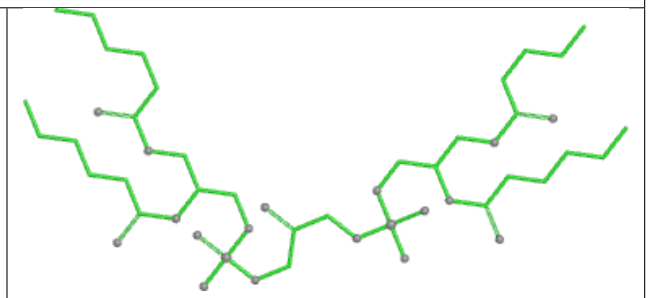
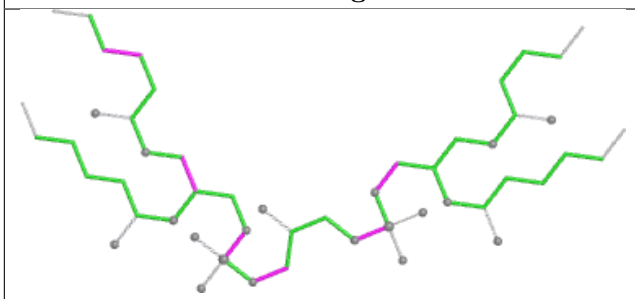
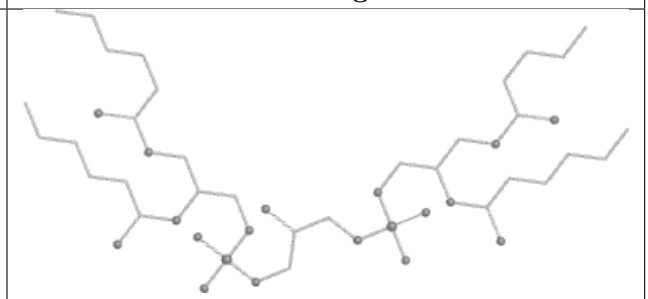


Bond angles

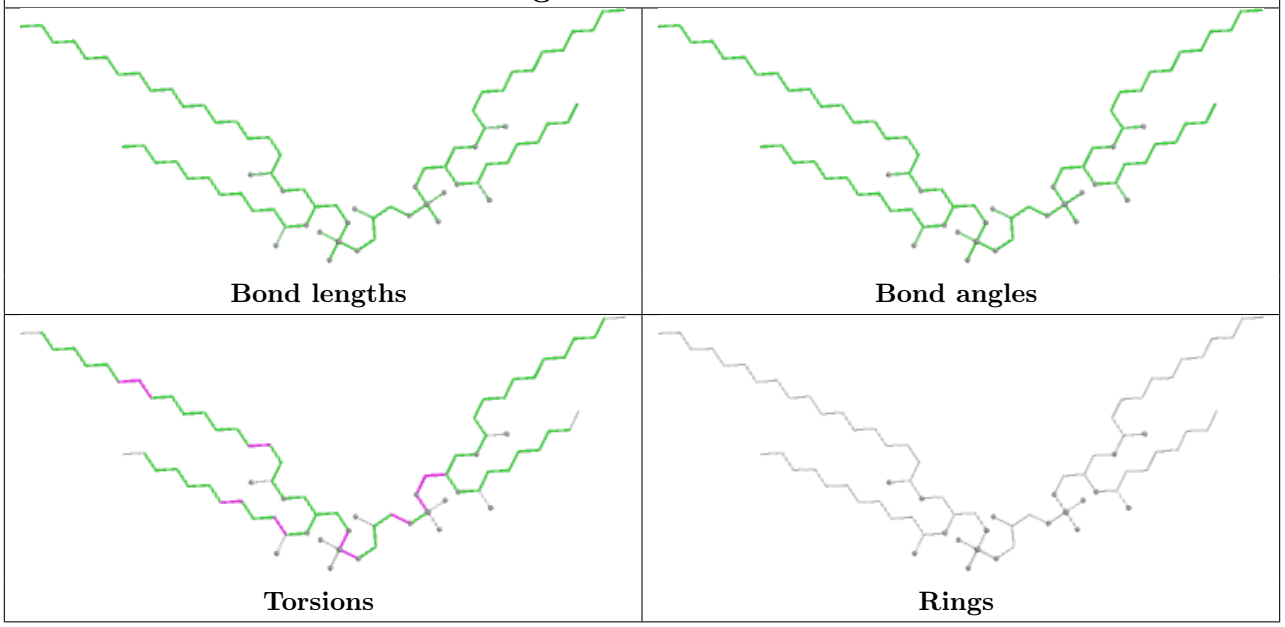


Torsions

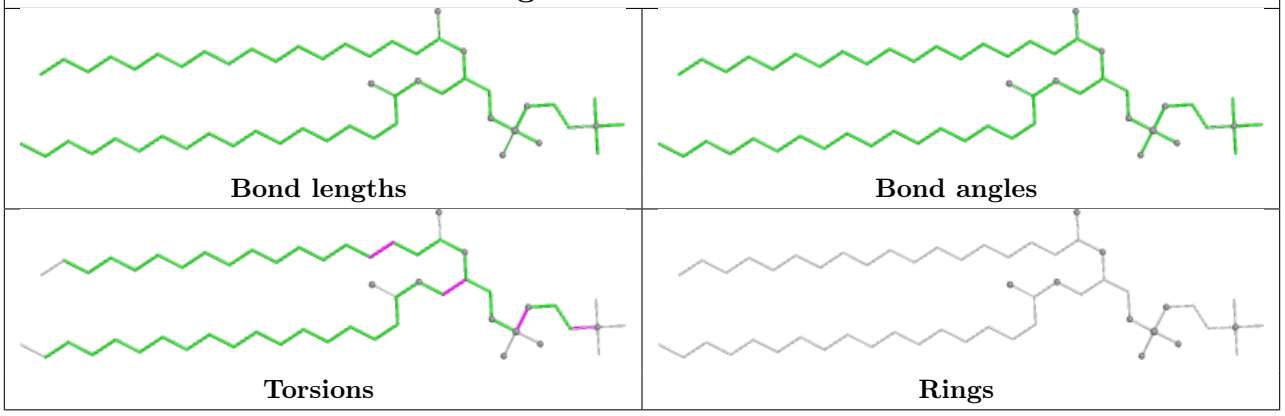


Rings

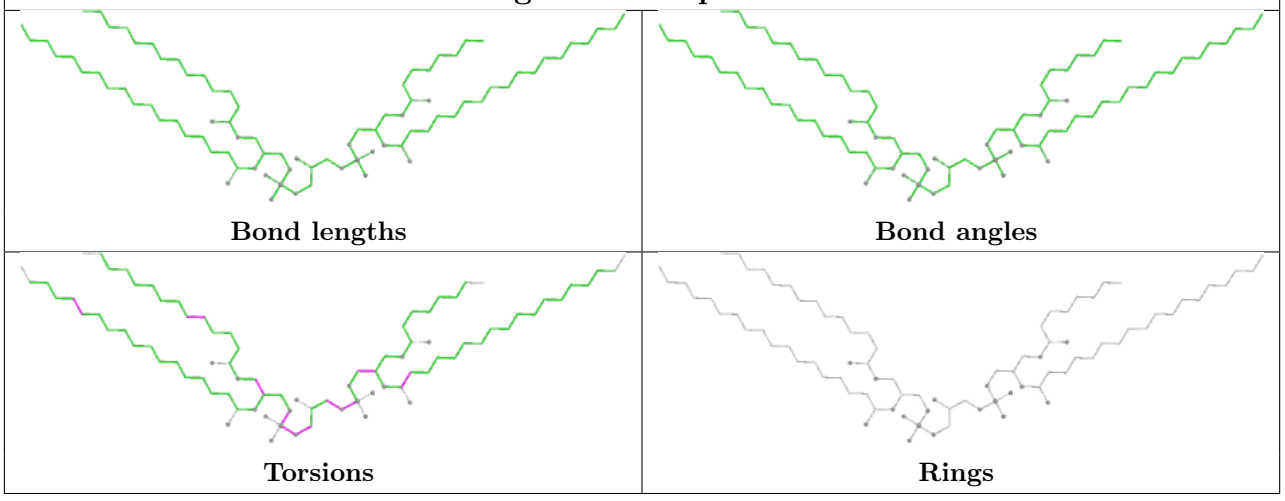
Ligand CDL i 301



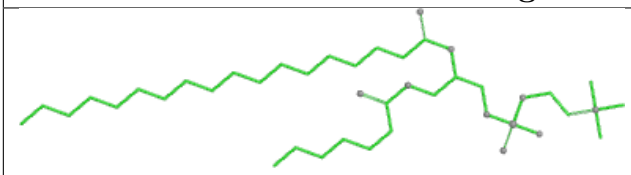
Ligand PC1 m2 405



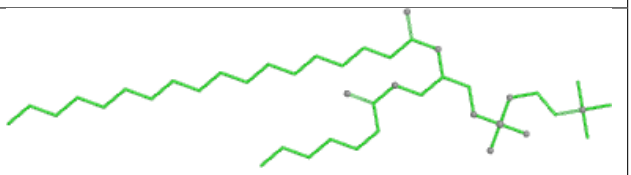
Ligand CDL qG 402



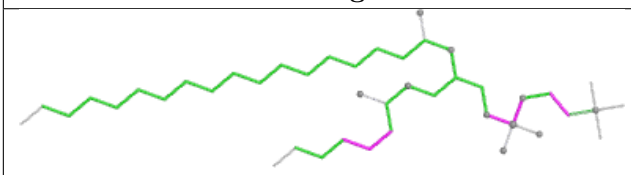
Ligand PC1 7C 303



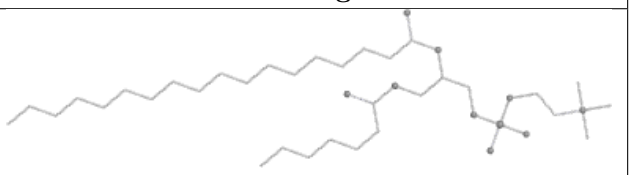
Bond lengths



Bond angles

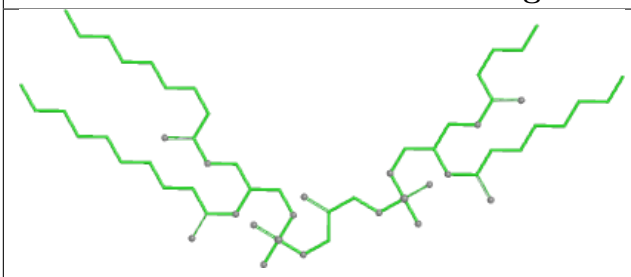


Torsions



Rings

Ligand CDL U 201



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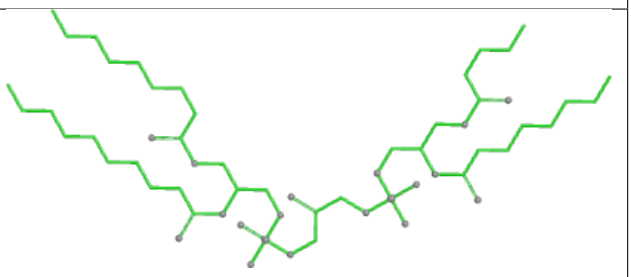
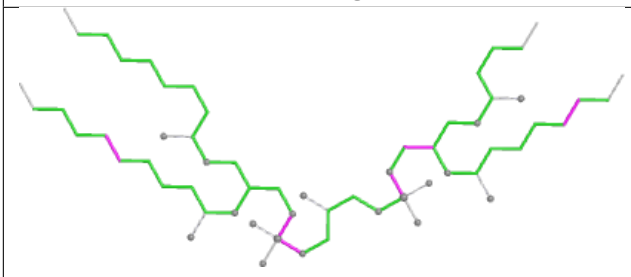


Bond angles



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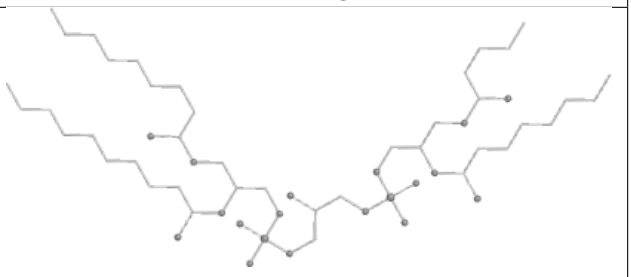
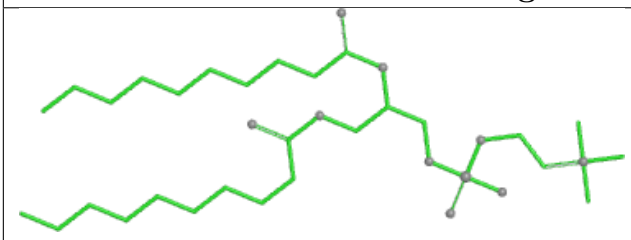


Rings

Ligand PC1 qC 505



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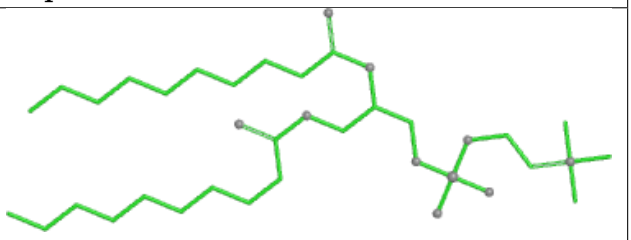
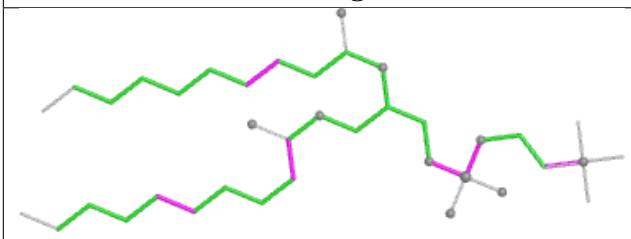


Bond angles



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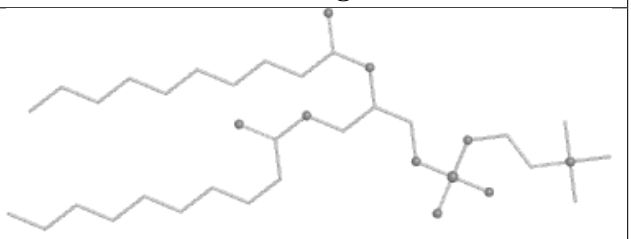
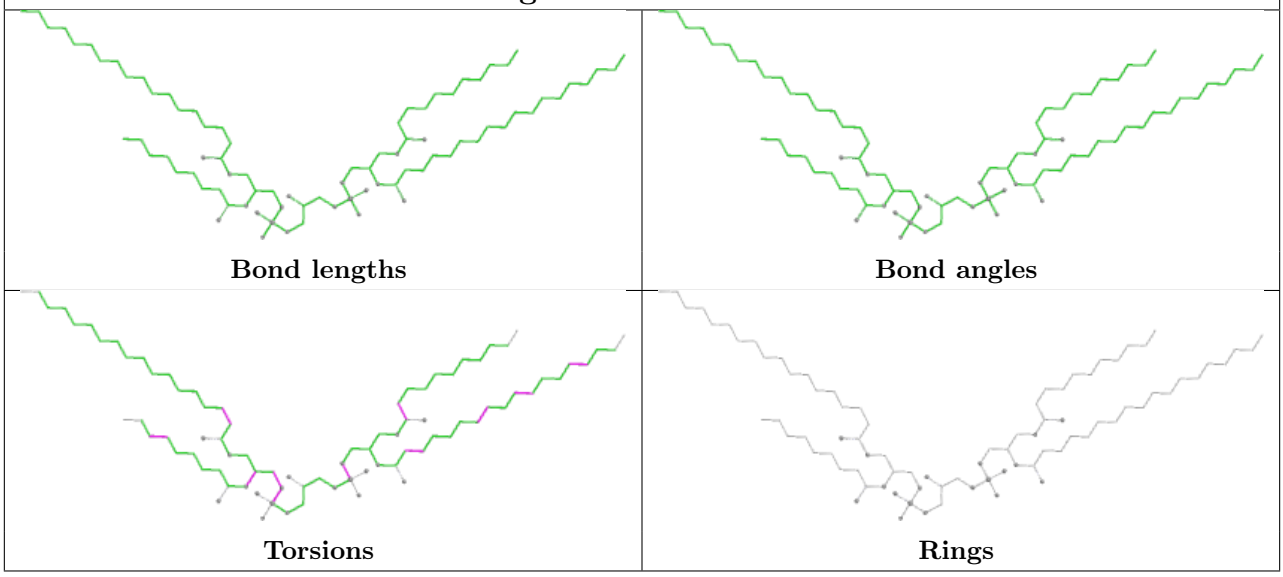
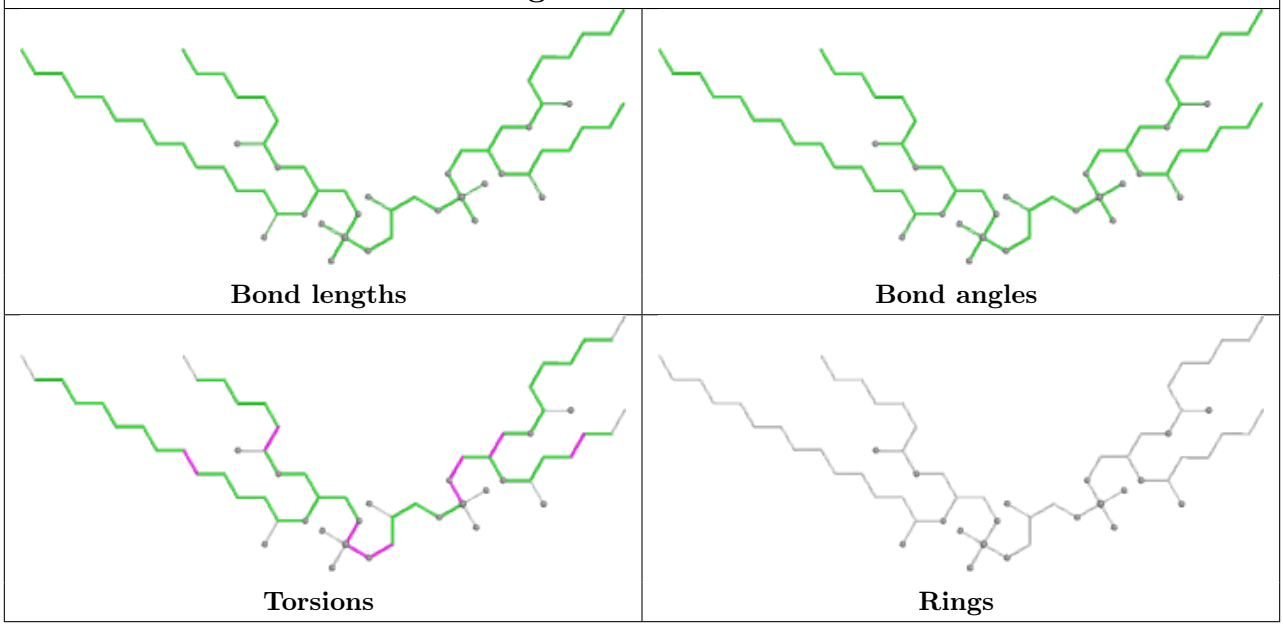


Rings

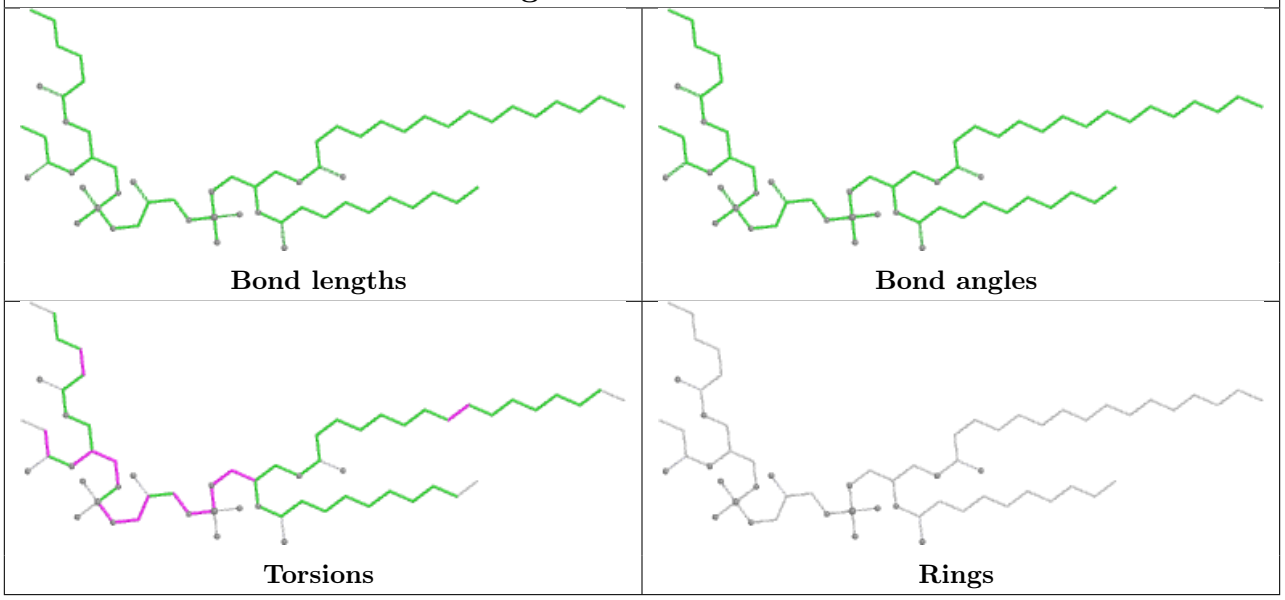
Ligand CDL W 202



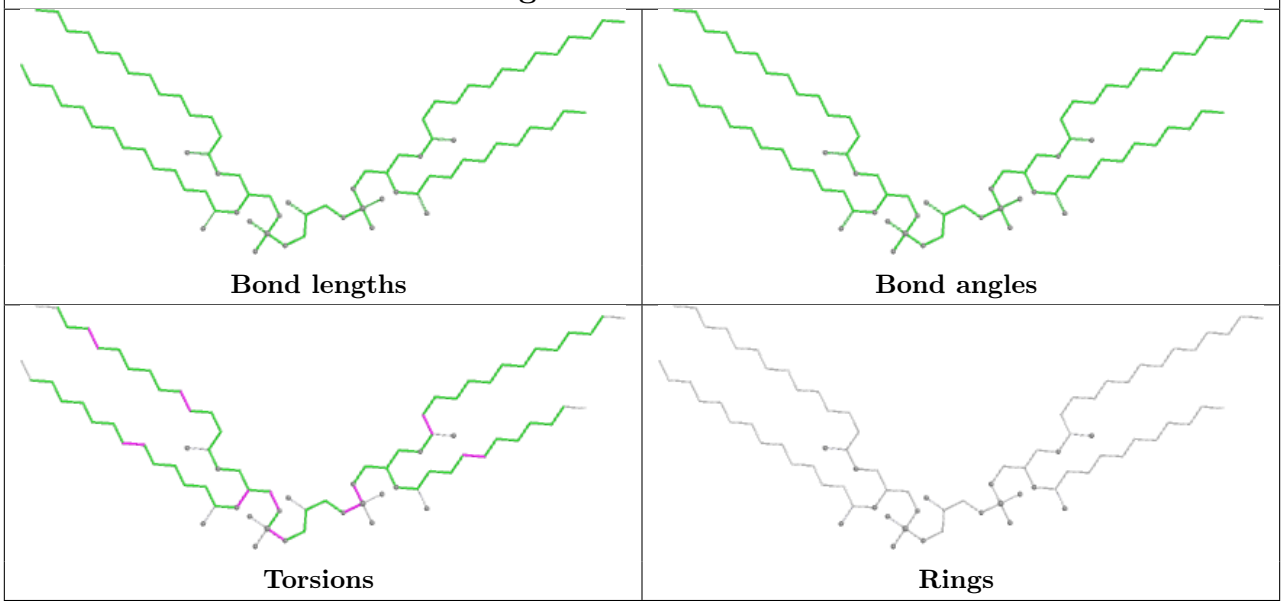
Ligand CDL b 501



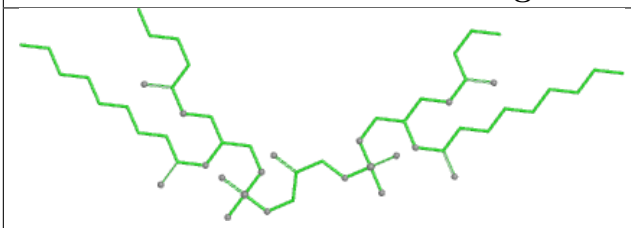
Ligand CDL c1 709



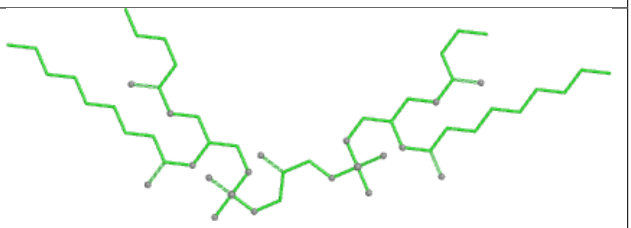
Ligand CDL 5b 201



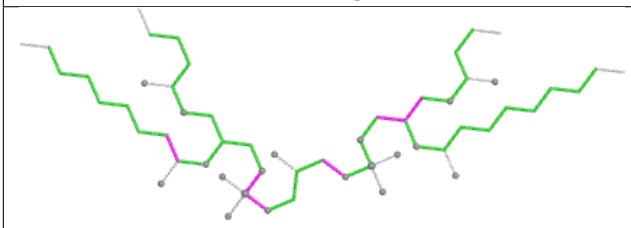
Ligand CDL 2G 203



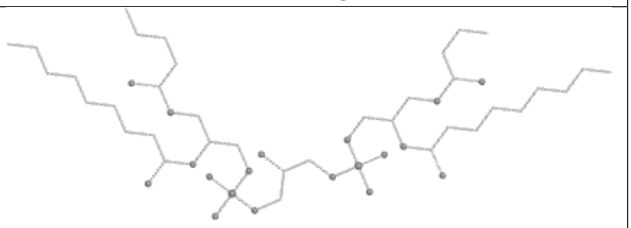
Bond lengths



Bond angles

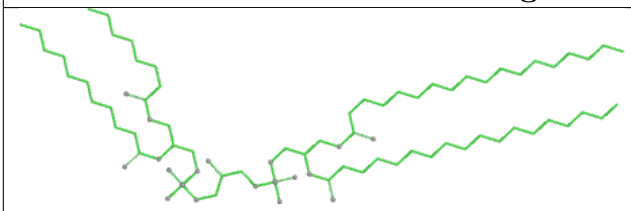


Torsions



Rings

Ligand CDL M 305



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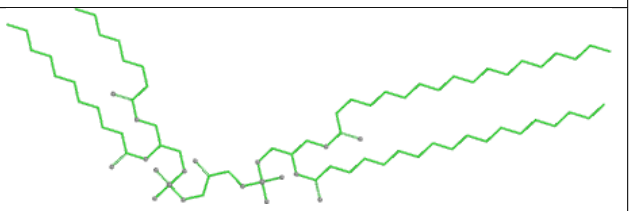
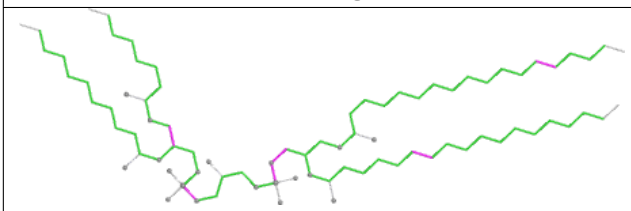


Bond angles



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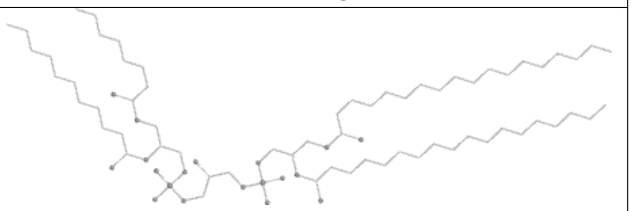
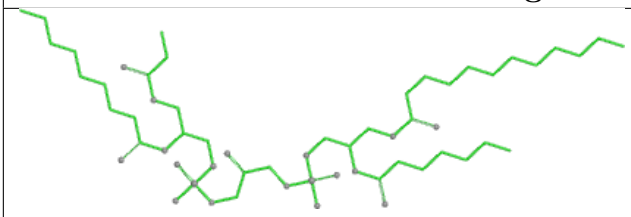


Rings

Ligand CDL T 201



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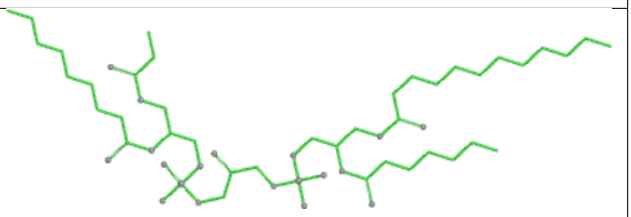

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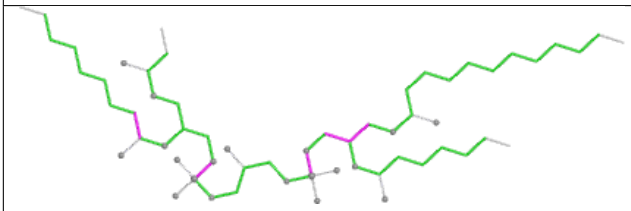

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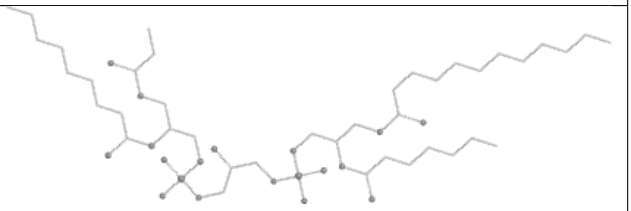
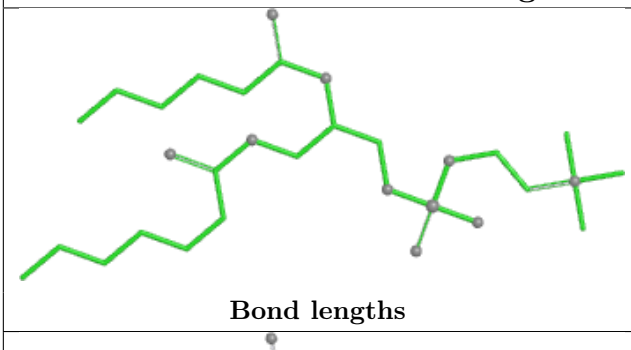


Rings

Ligand PC1 C3 603



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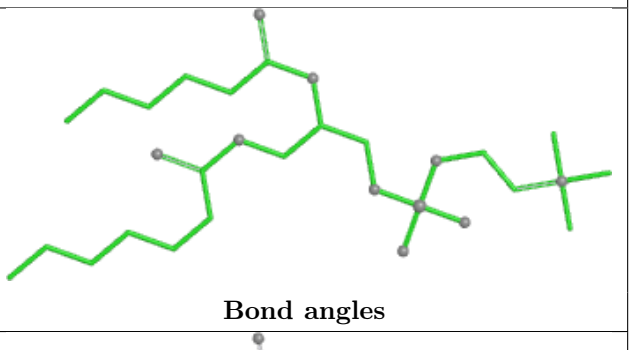
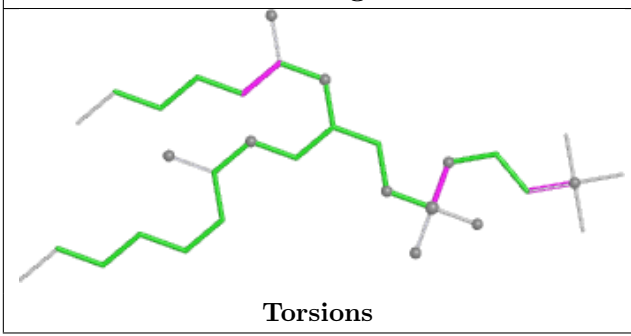


Bond angles



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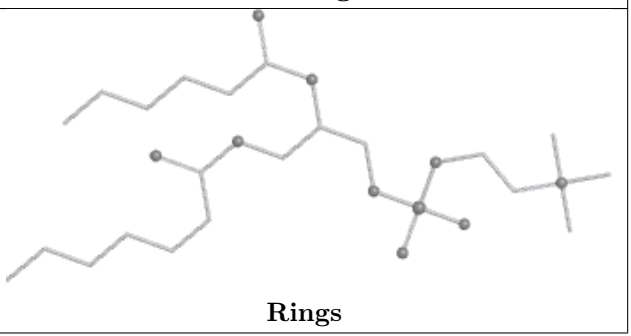
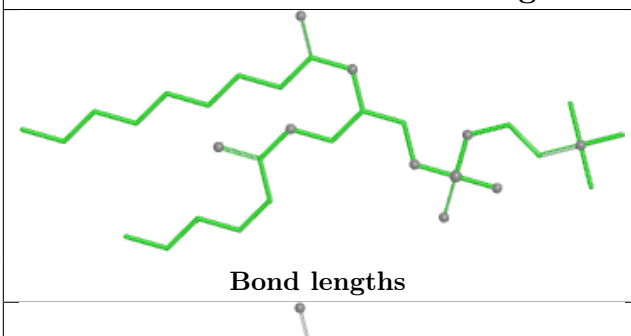


Rings

Ligand PC1 Qe 301



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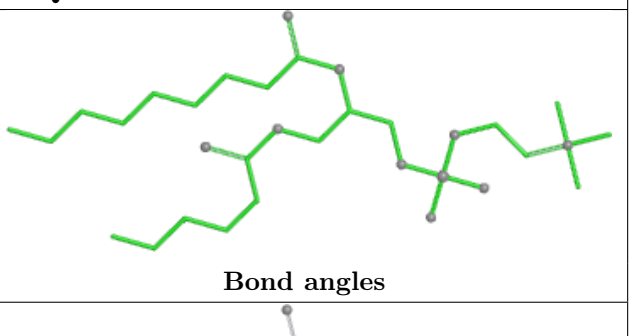

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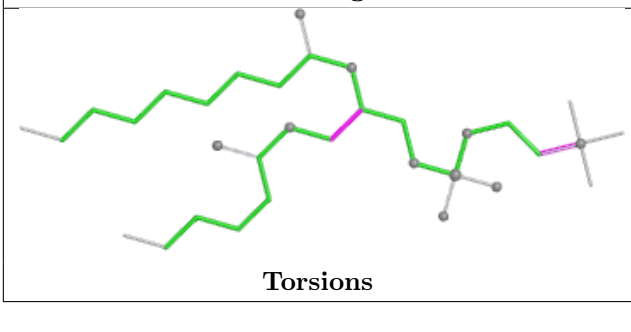

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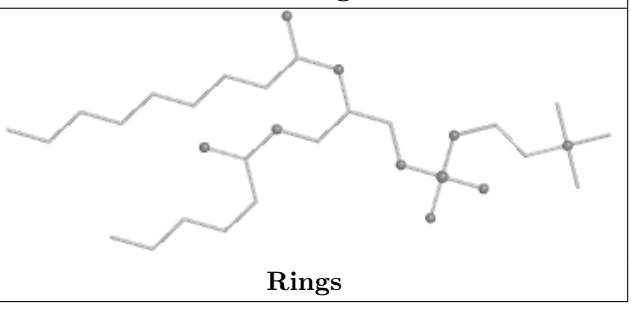
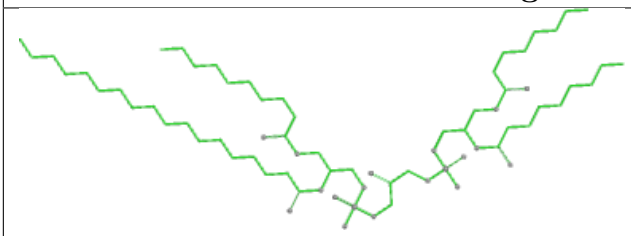


Rings

Ligand CDL t7 201



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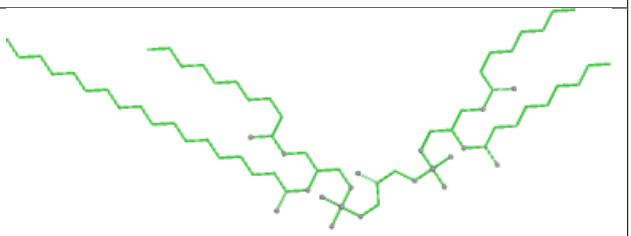
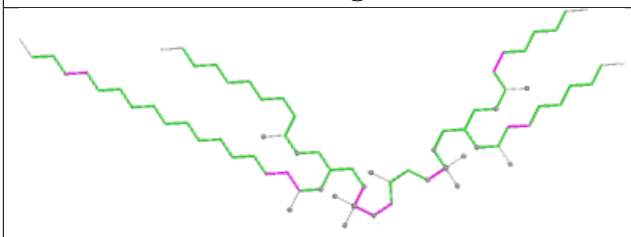


Bond angles



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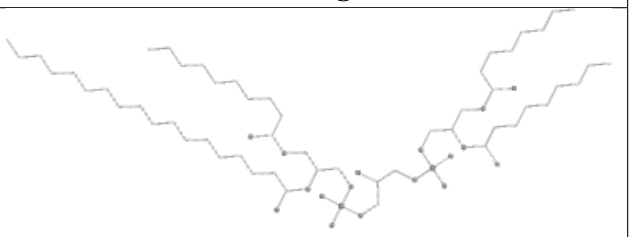
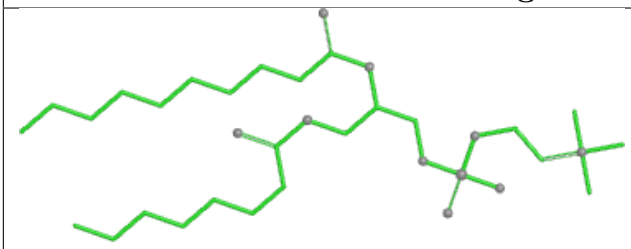


Rings

Ligand PC1 N1 301



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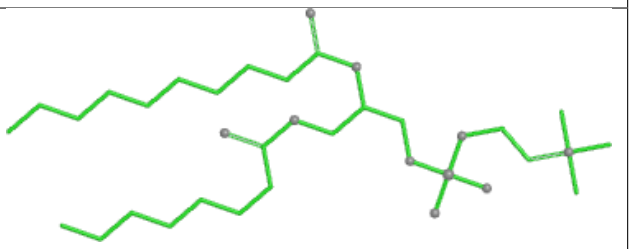
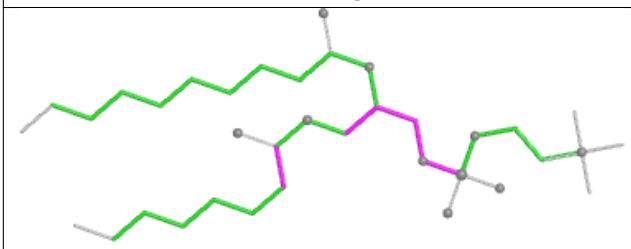


Bond angles



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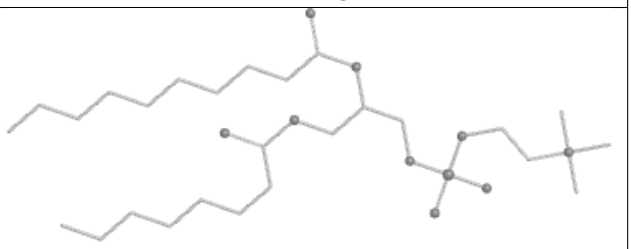
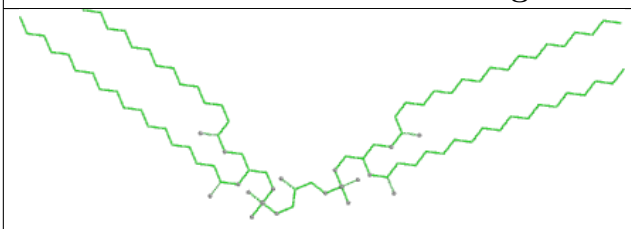


Rings

Ligand CDL 2M 101



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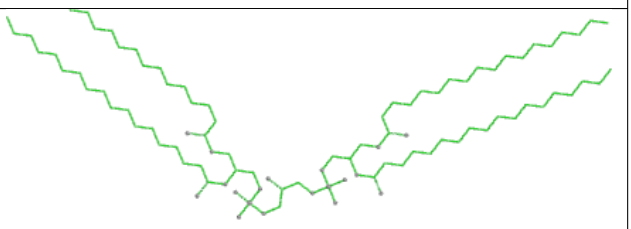
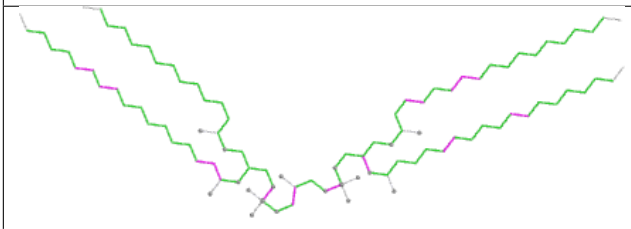


Bond angles



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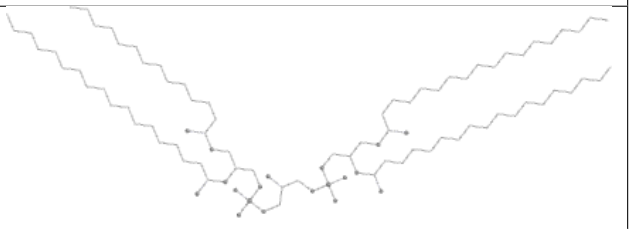
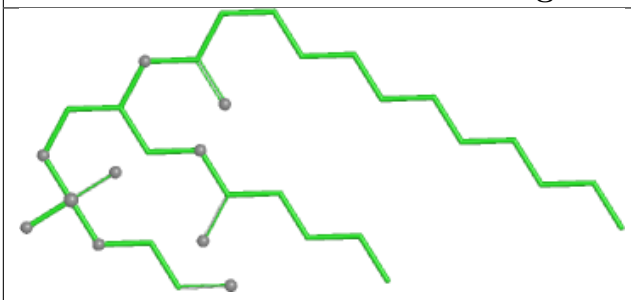


Rings

Ligand 3PE i 303



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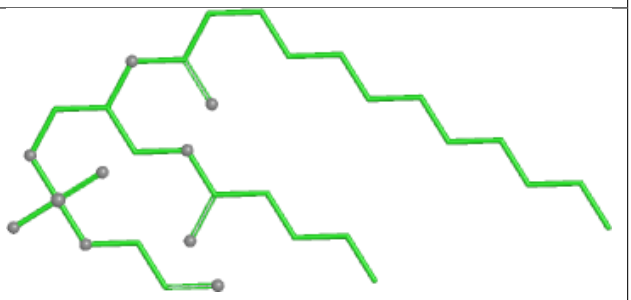
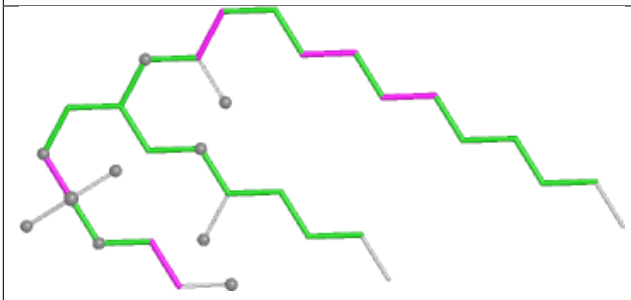
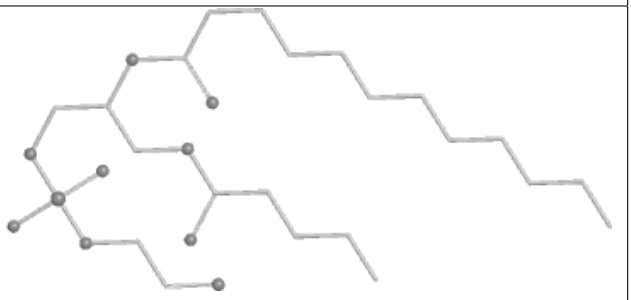


Bond angles

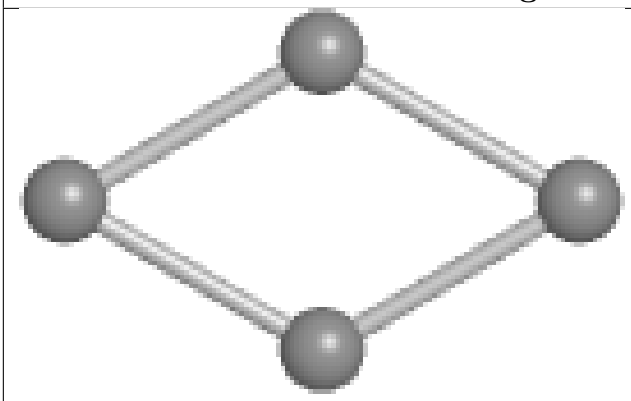


Torsions

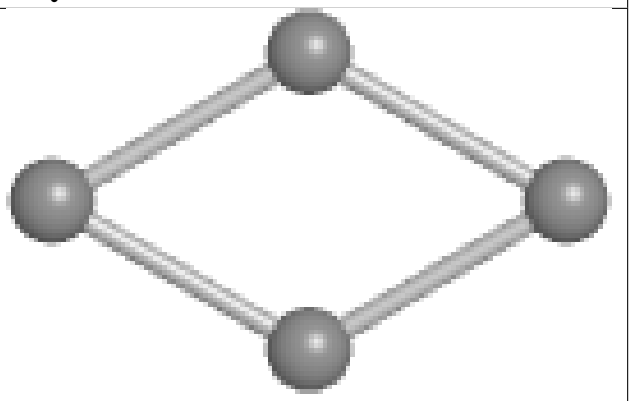


Rings

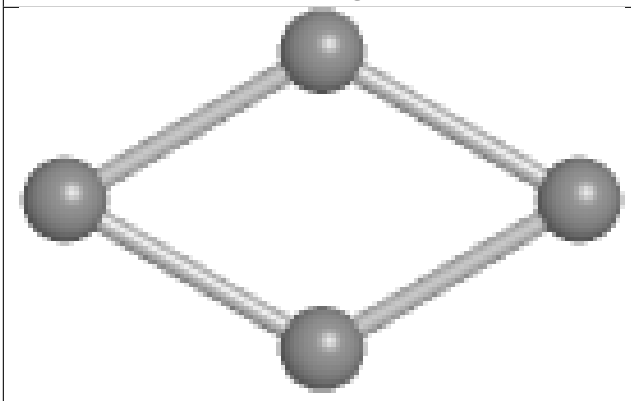
Ligand FES Qe 302



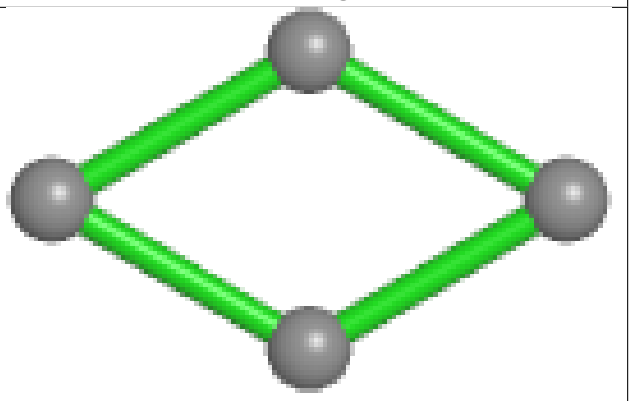
Bond lengths



Bond angles

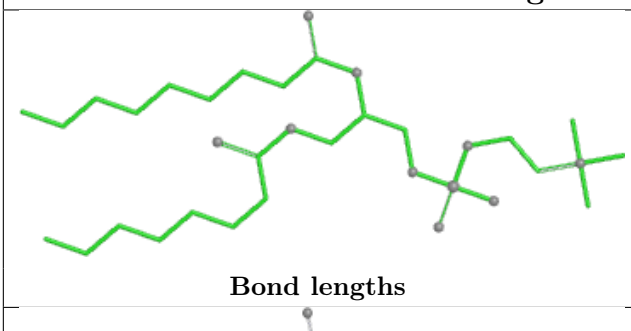


Torsions



Rings

Ligand PC1 D 501



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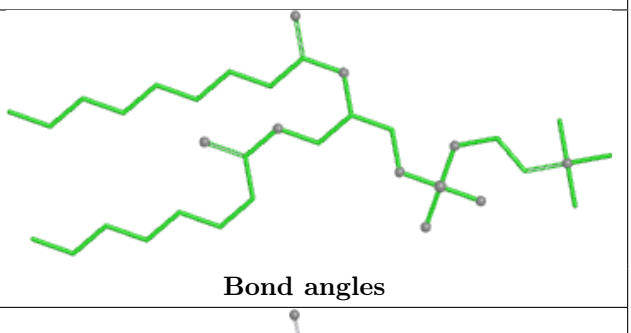
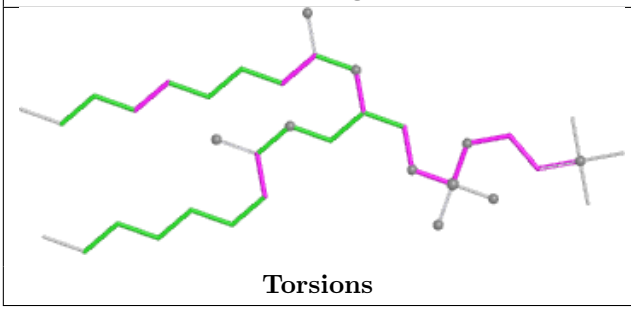
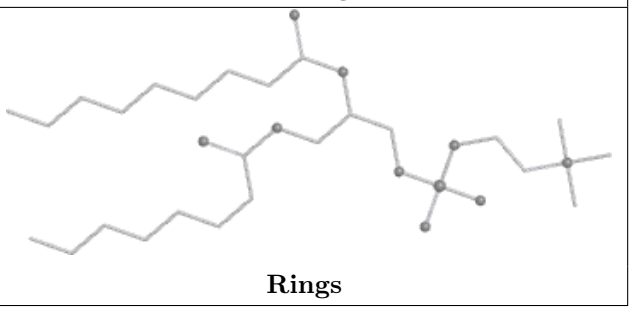


Bond angles

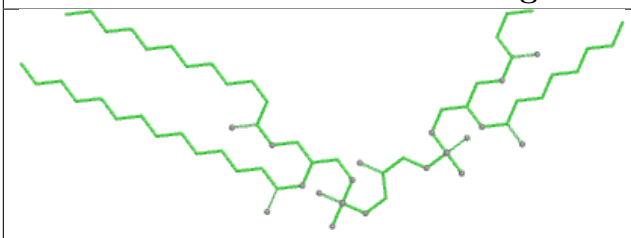


Torsions

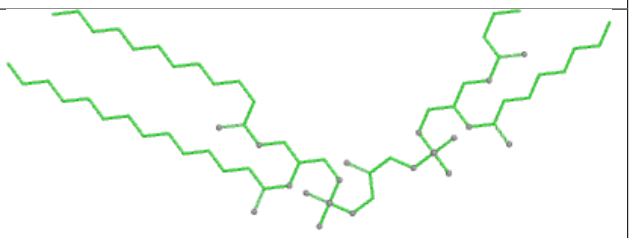


Rings

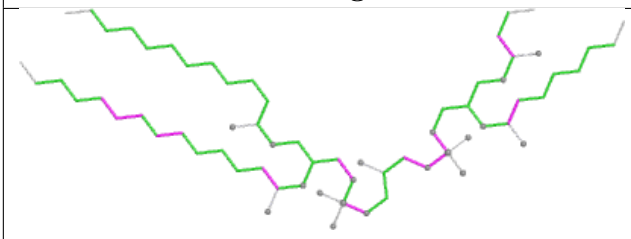
Ligand CDL td 101



Bond lengths



Bond angles



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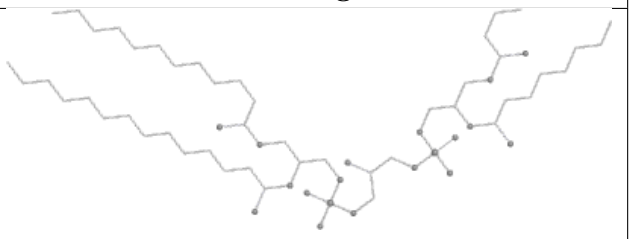
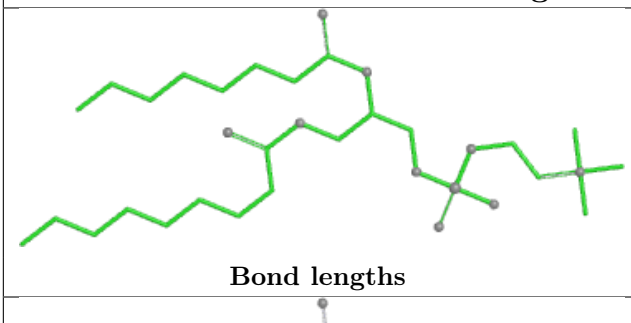
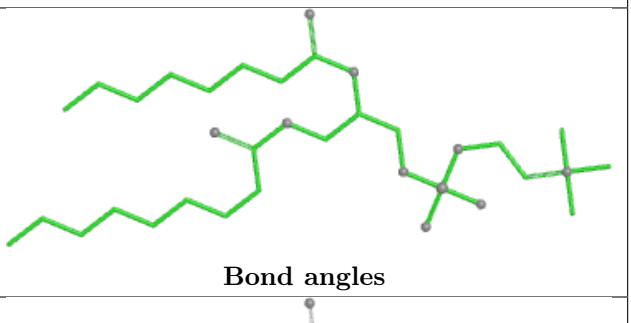


Rings

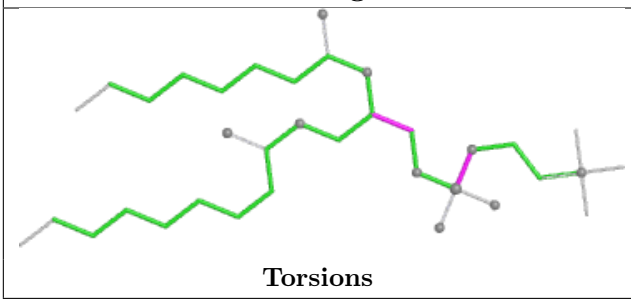
Ligand PC1 v 201



Bond lengths



Bond angles



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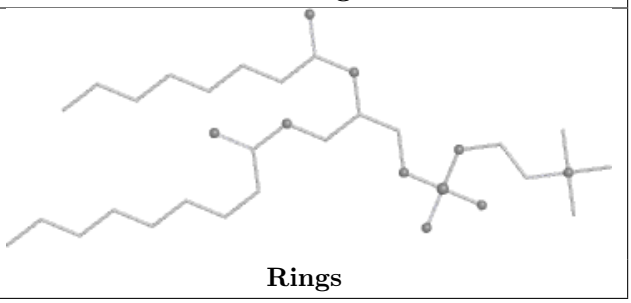
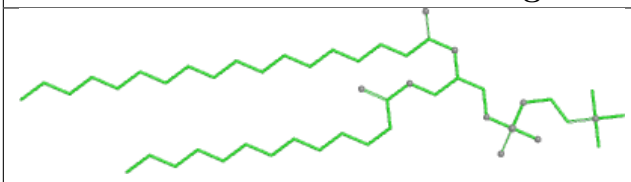


Rings

Ligand PC1 c3 606



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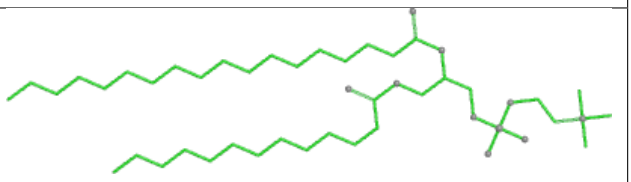
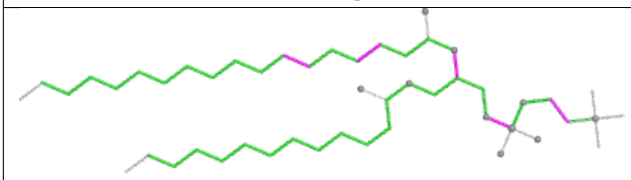


Bond angles



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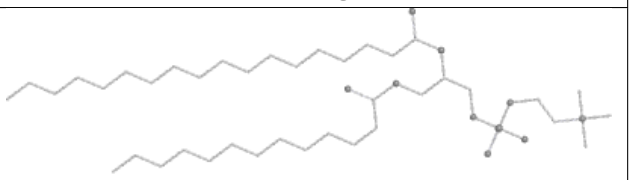
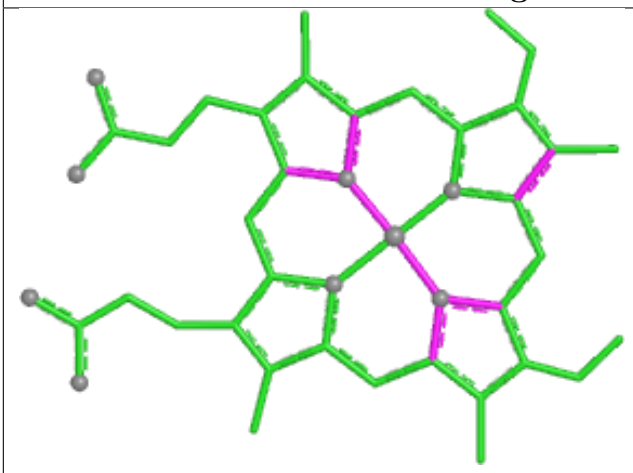


Rings

Ligand HEM Qc 502



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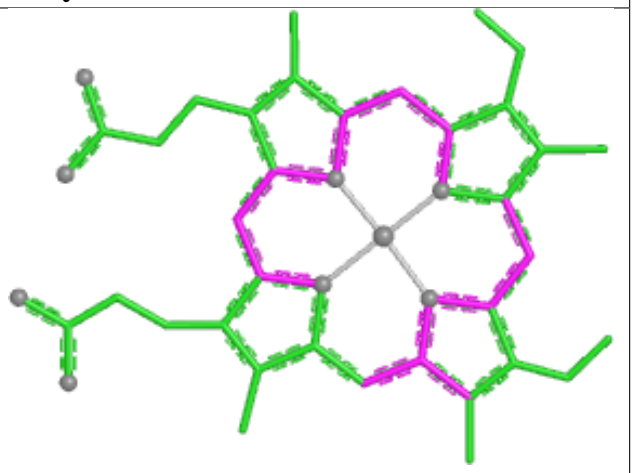
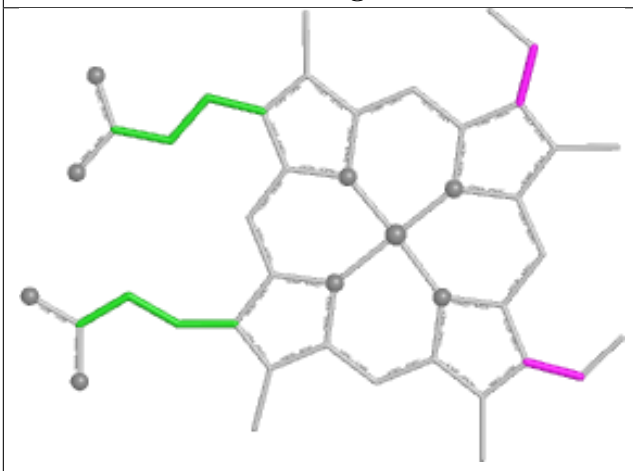
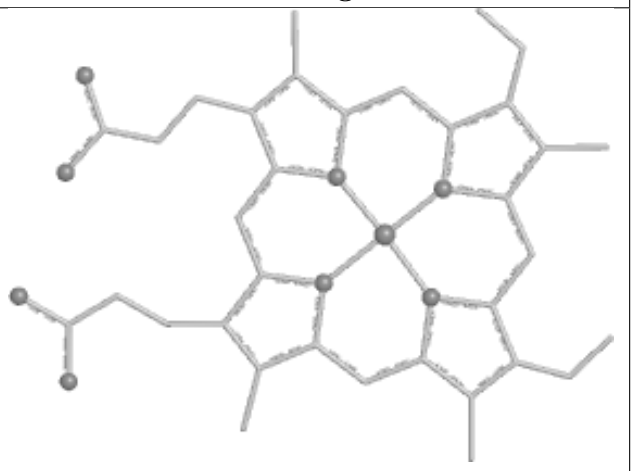


Bond angles

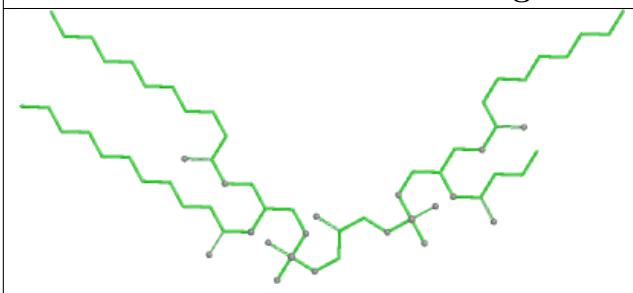


Torsions



Rings

Ligand CDL m3 401



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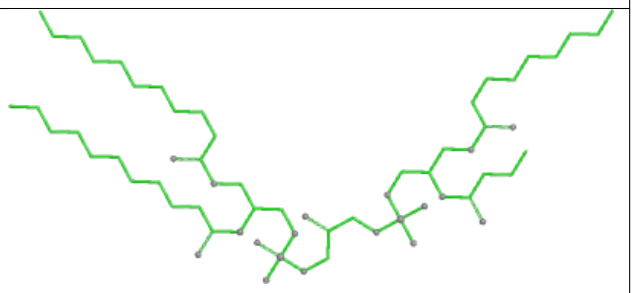
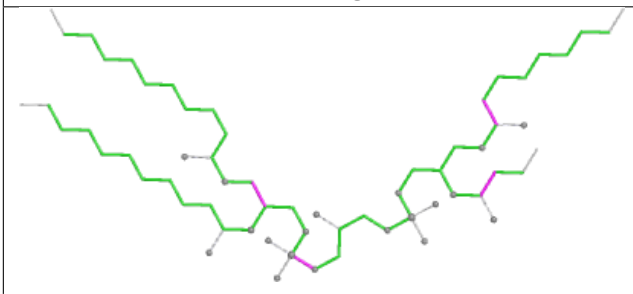


Bond angles



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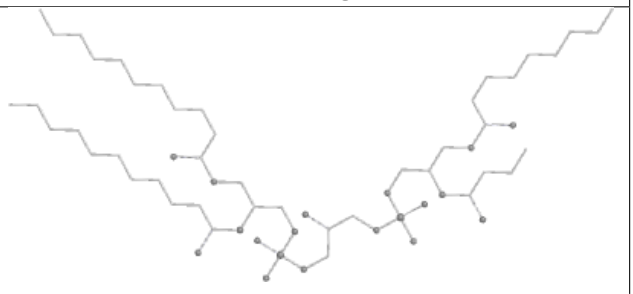
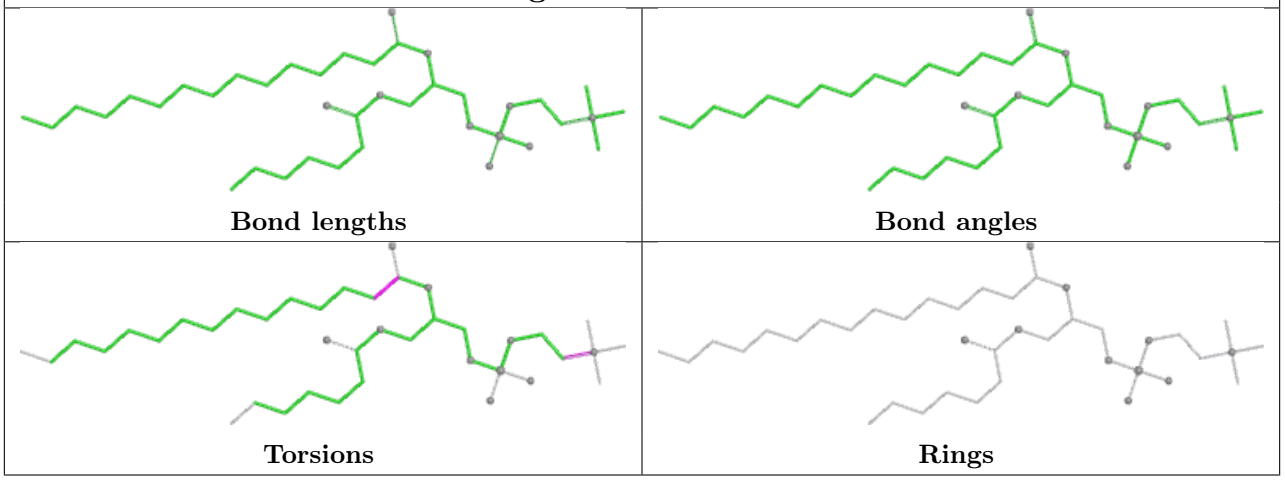
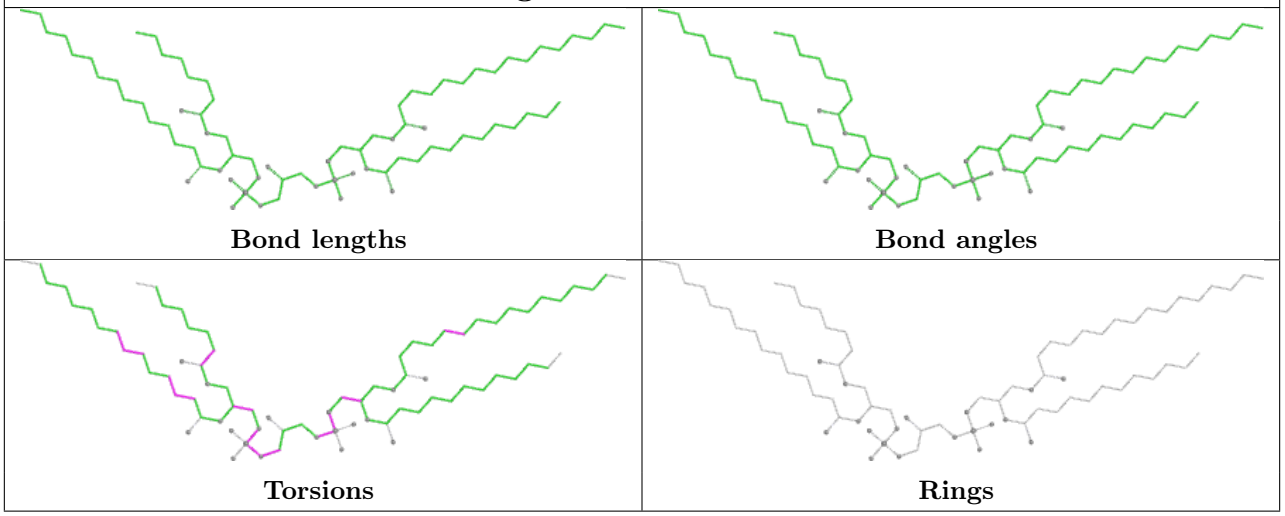


Rings

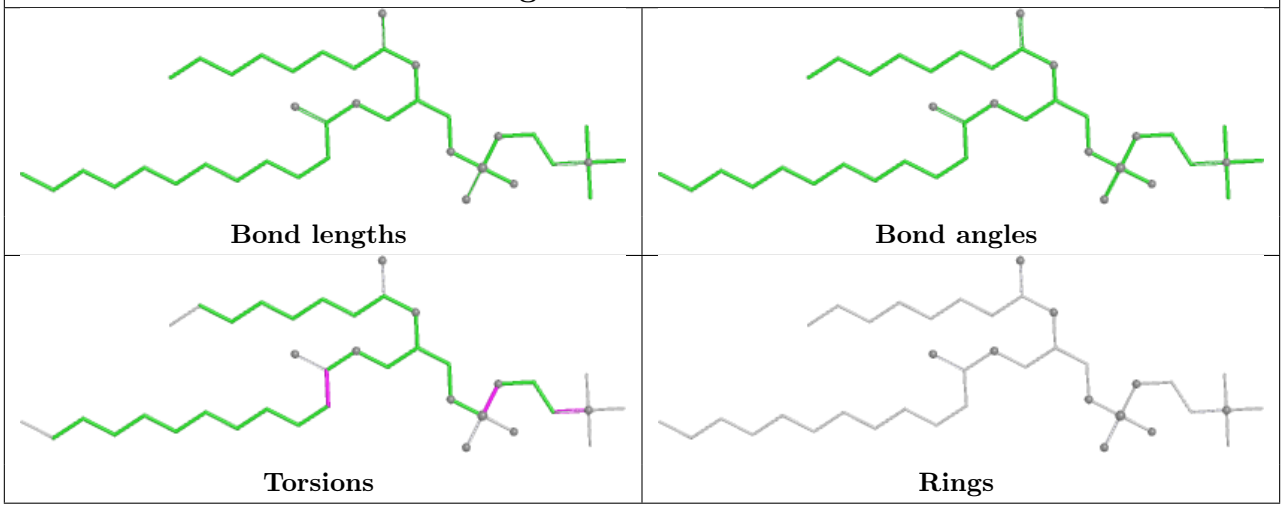
Ligand PC1 fs 204



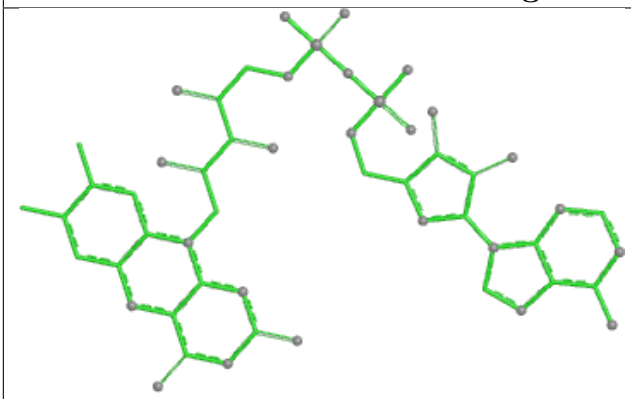
Ligand CDL C1 701



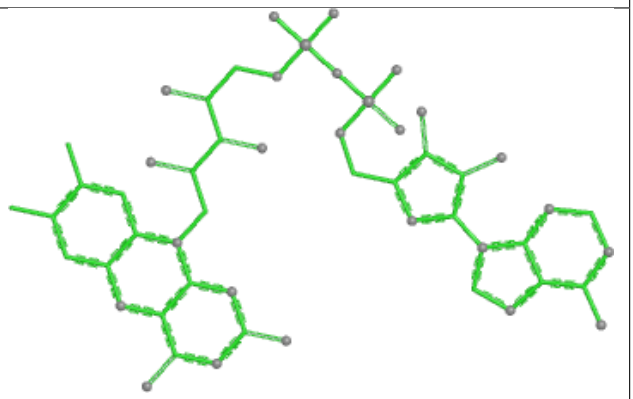
Ligand PC1 C1 710



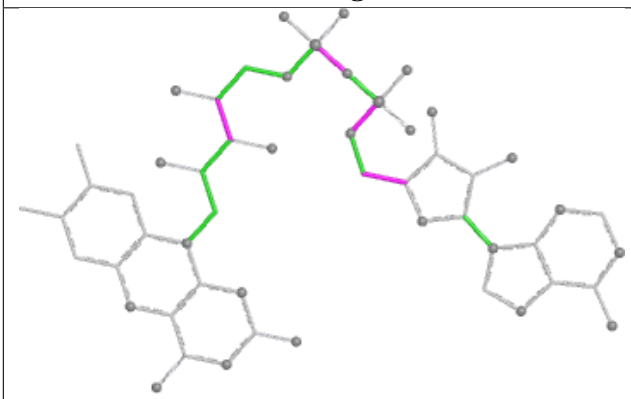
Ligand FAD sa 701



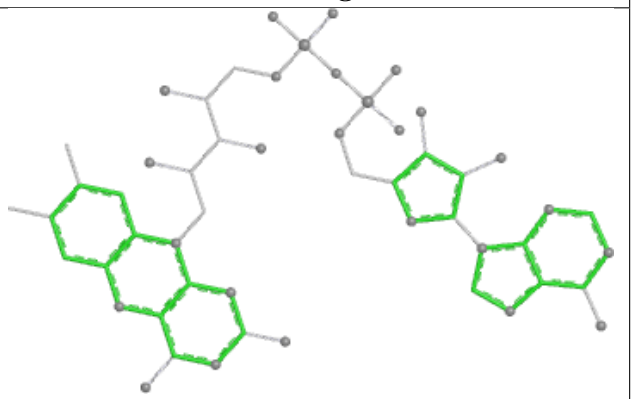
Bond lengths



Bond angles

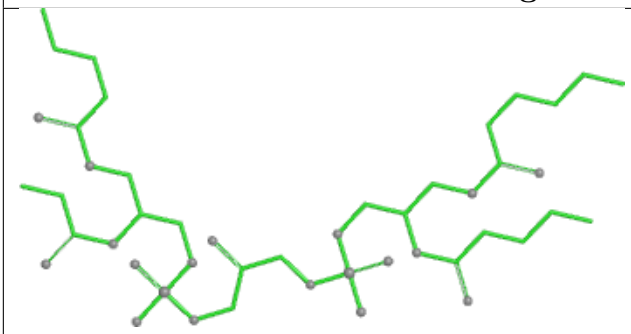


Torsions



Rings

Ligand CDL qc 508



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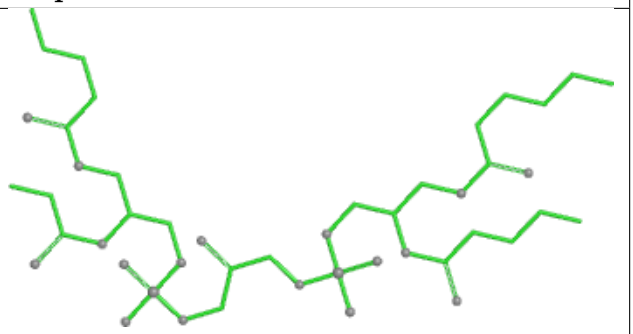
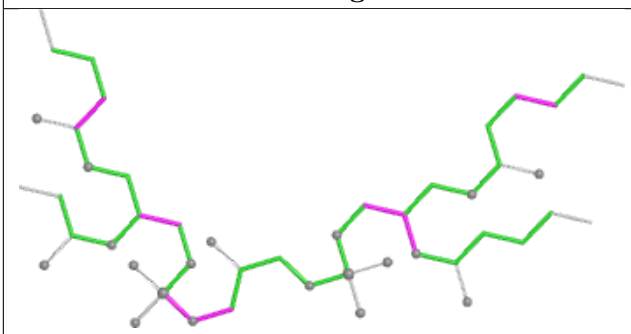
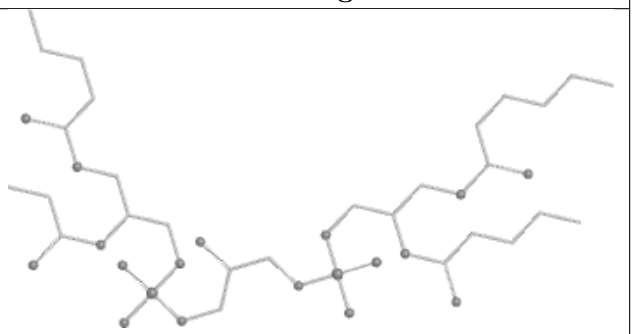


Bond angles

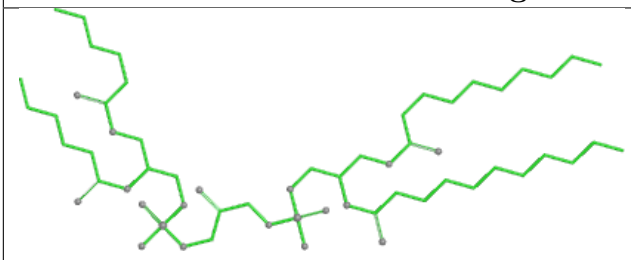


Torsions



Rings

Ligand CDL QD 402



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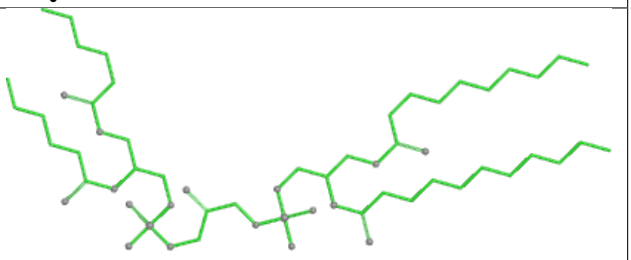
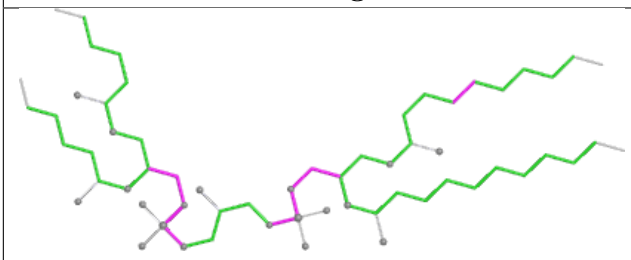
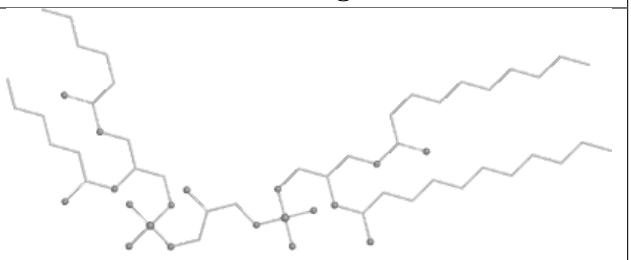


Bond angles

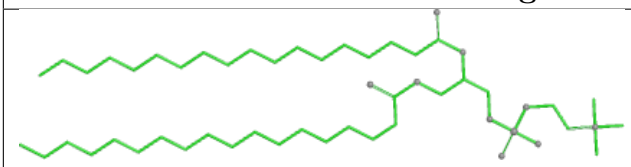


Torsions

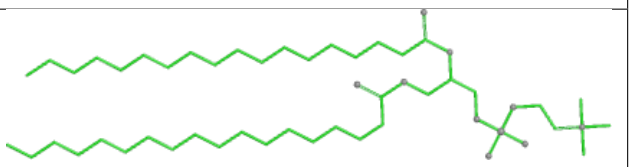


Rings

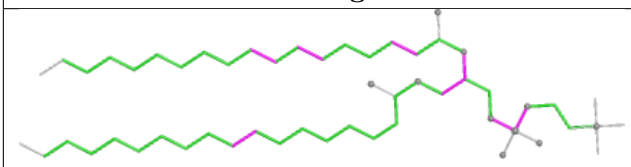
Ligand PC1 T4 303



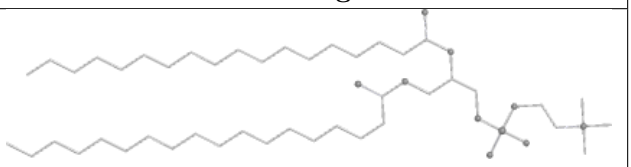
Bond lengths



Bond angles

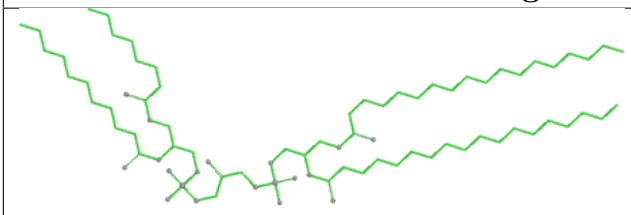


Torsions



Rings

Ligand CDL m 303



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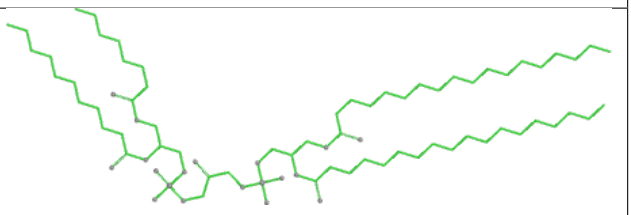
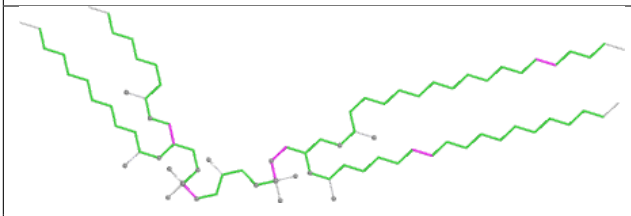
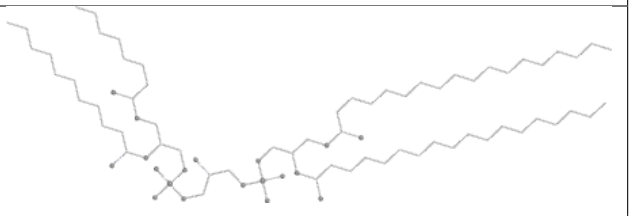


Bond angles

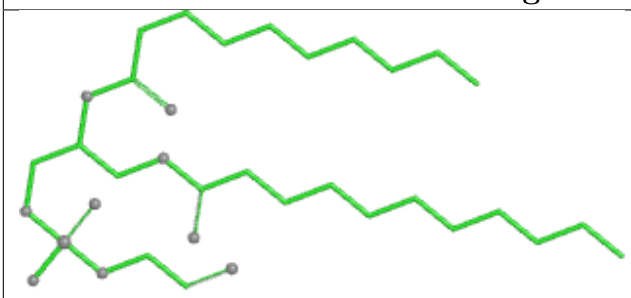


Torsions

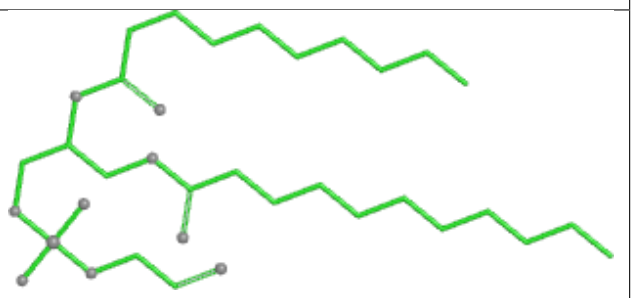


Rings

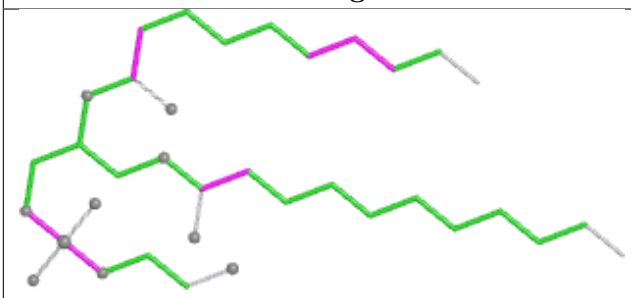
Ligand 3PE n4 601



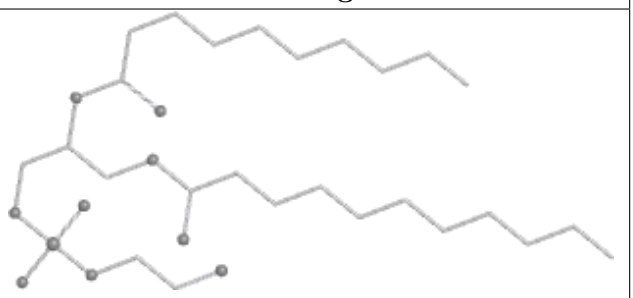
Bond lengths



Bond angles

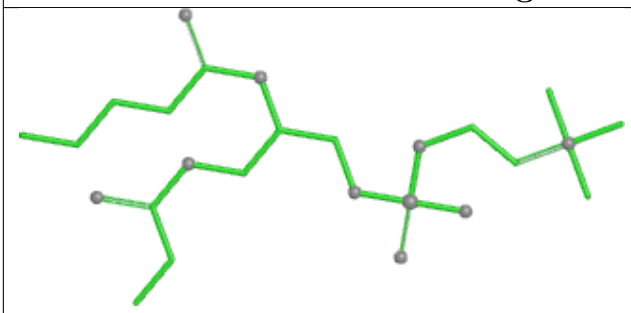


Torsions



Rings

Ligand PC1 AL 302



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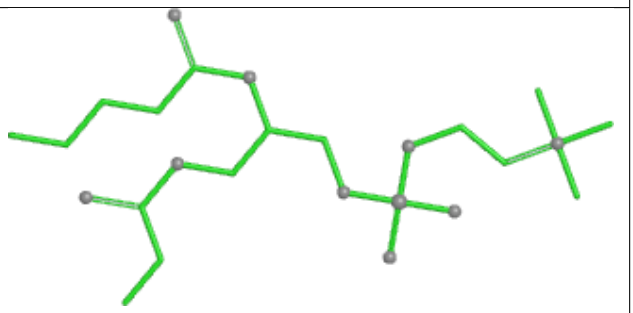
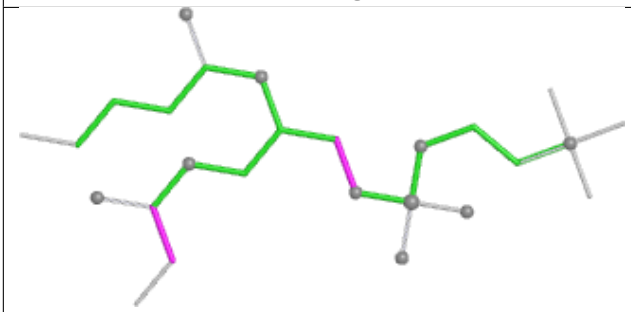
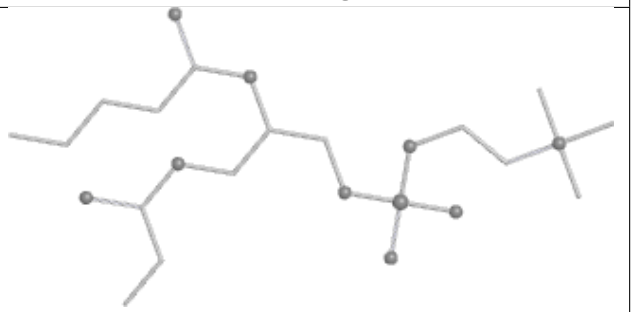


Bond angles

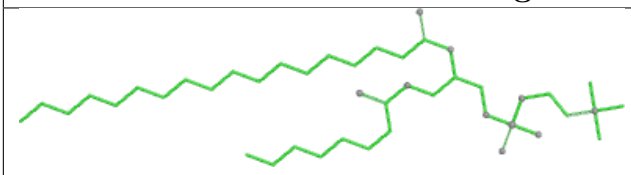


Torsions



Rings

Ligand PC1 QB 602



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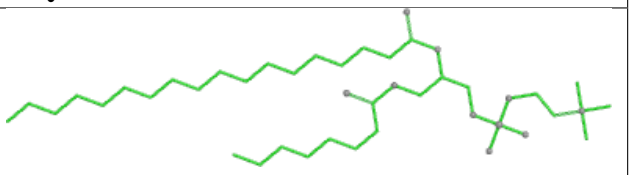
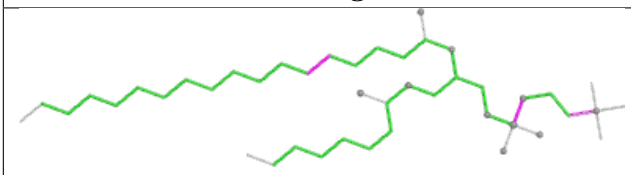
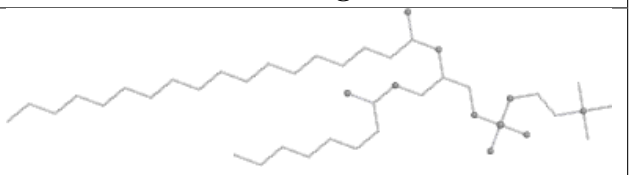


Bond angles

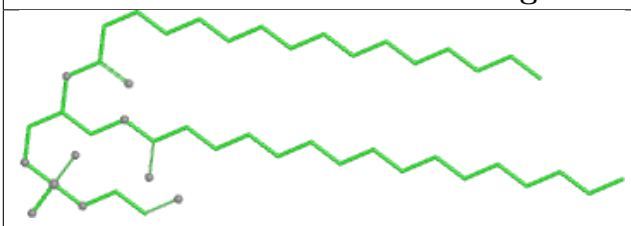


Torsions

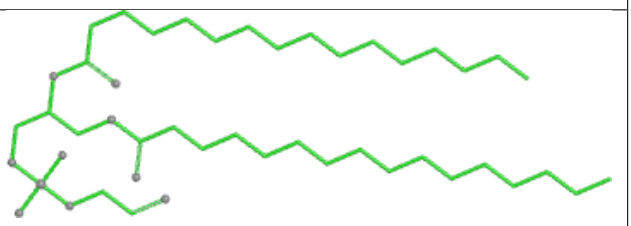


Rings

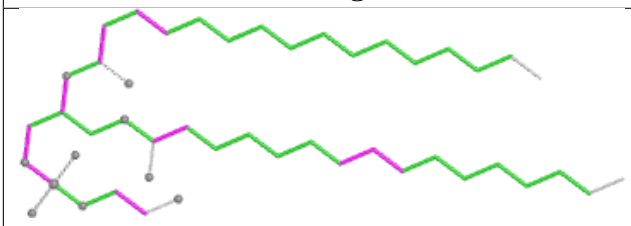
Ligand 3PE T8 601



Bond lengths



Bond angles



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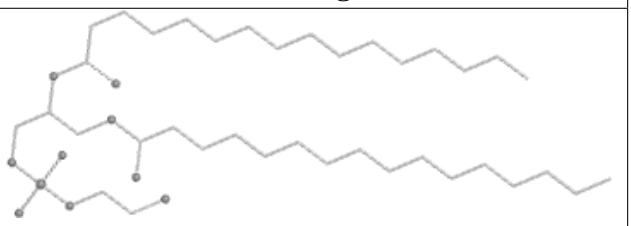
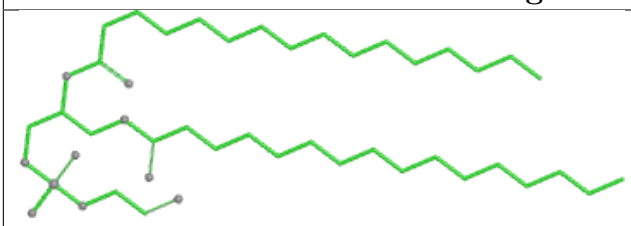


Rings

Ligand 3PE t8 601



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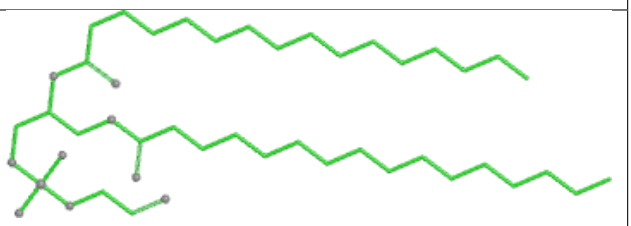
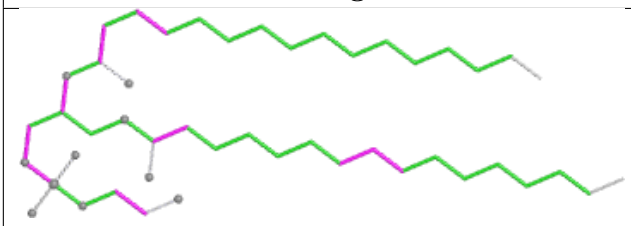


Bond angles



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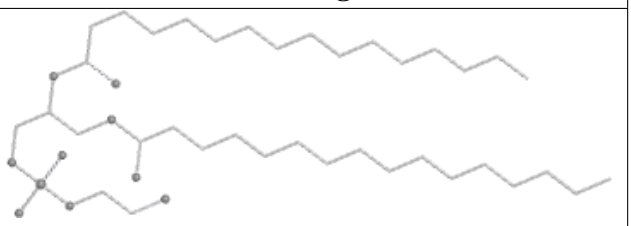
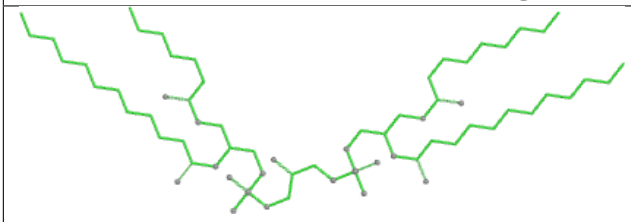


Rings

Ligand CDL C3 604



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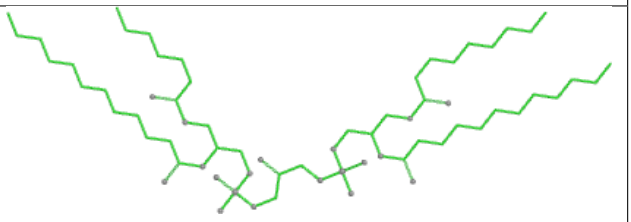
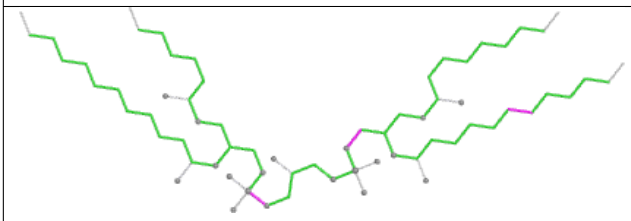


Bond angles



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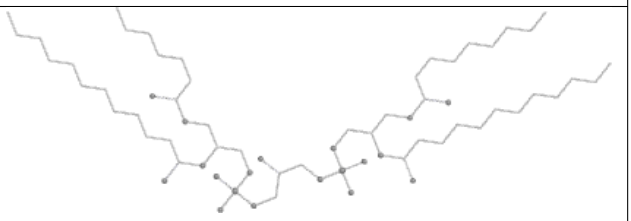
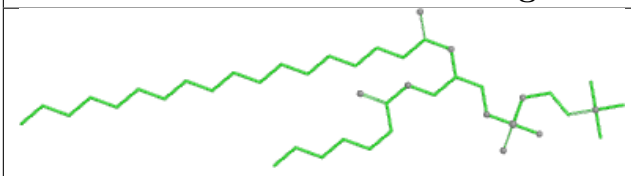


Rings

Ligand PC1 Qe 303



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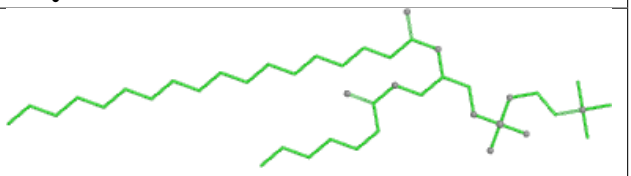
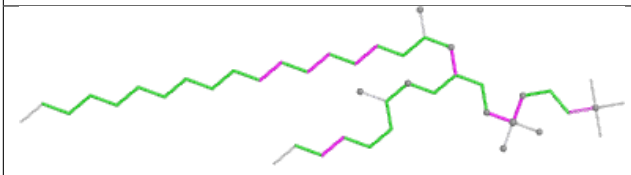


Bond angles



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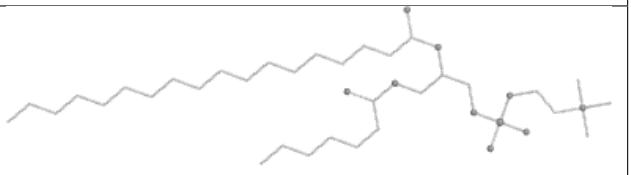
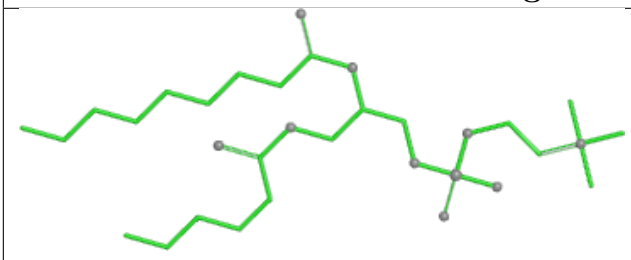


Rings

Ligand PC1 6c 203



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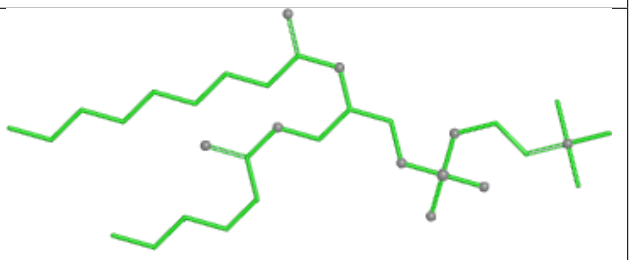

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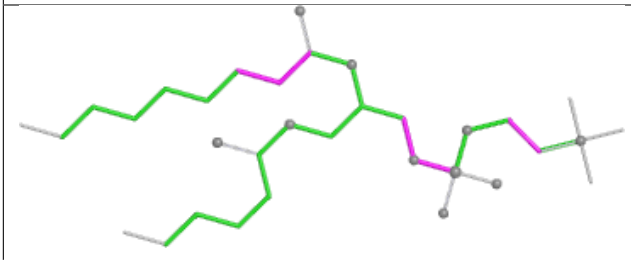

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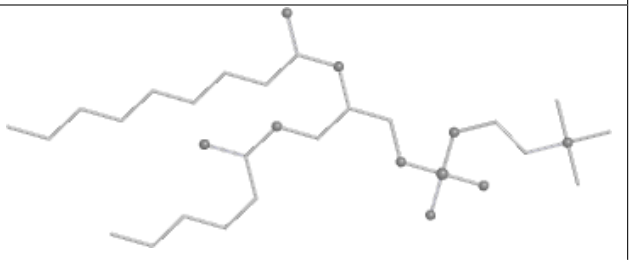
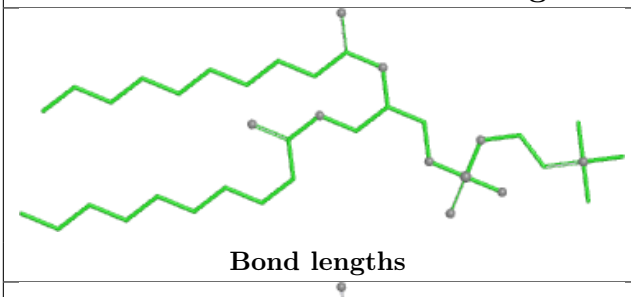


Rings

Ligand PC1 F 401



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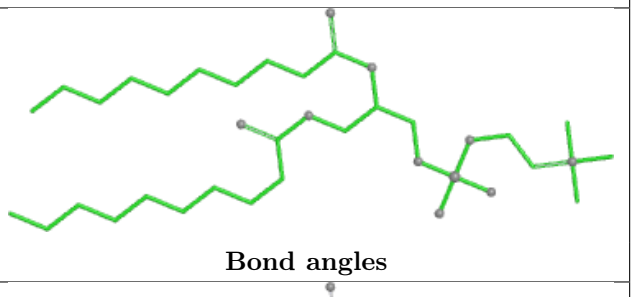
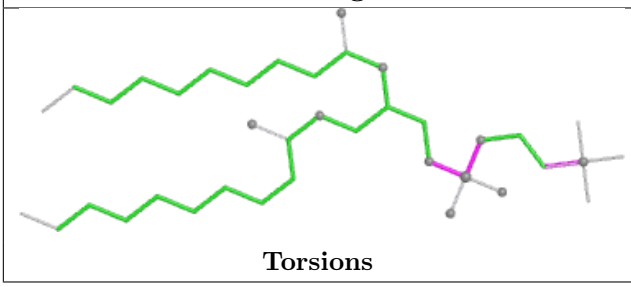
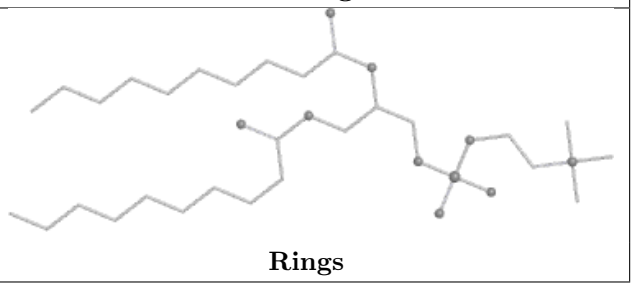


Bond angles

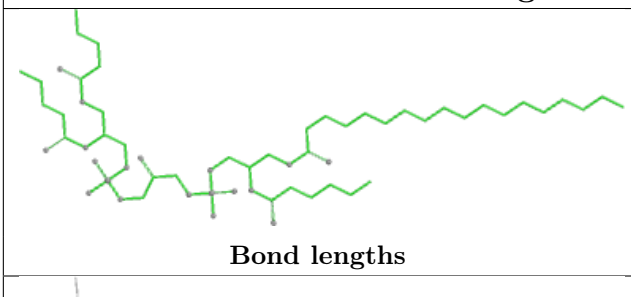


Torsions



Rings

Ligand CDL vb 701



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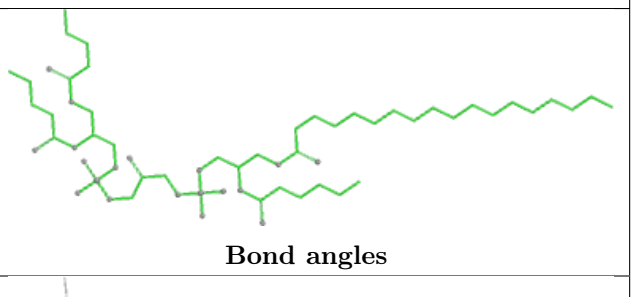
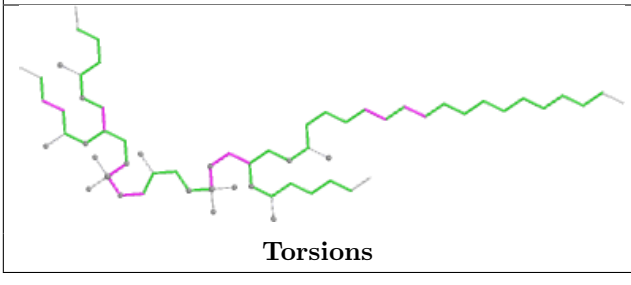


Bond angles



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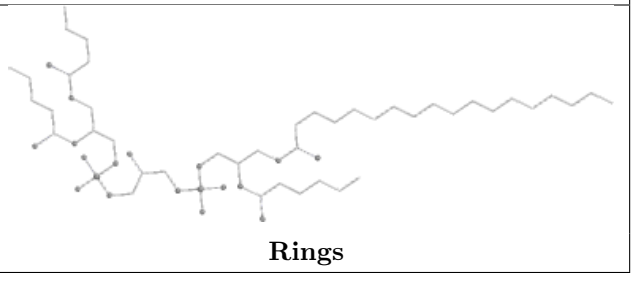
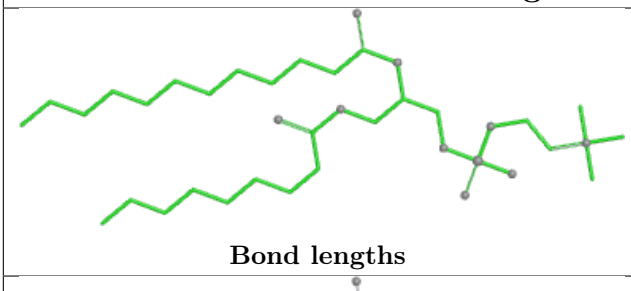


Rings

Ligand PC1 c1 711



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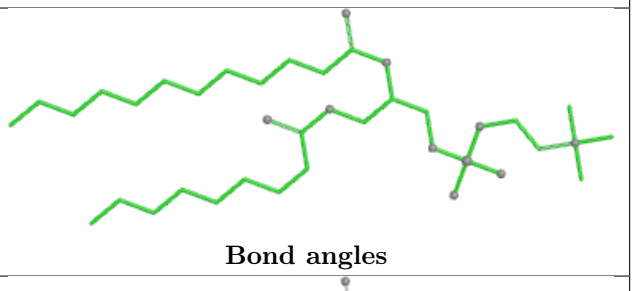
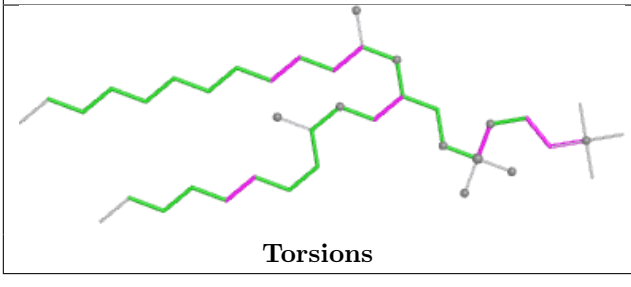
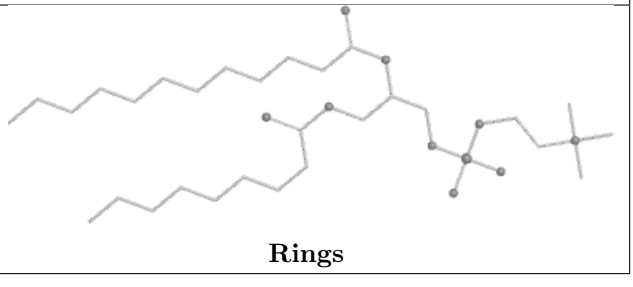


Bond angles

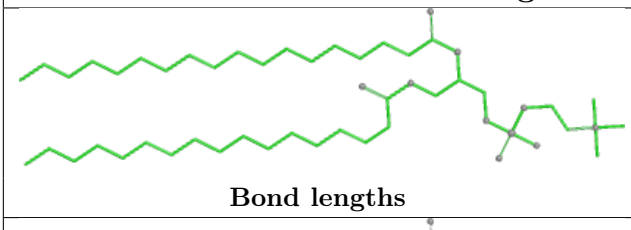


Torsions



Rings

Ligand PC1 N5 803



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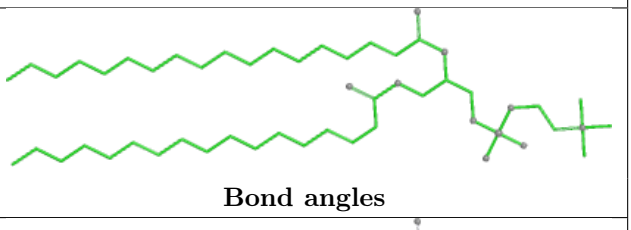
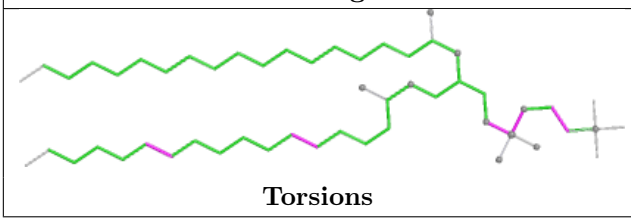


Bond angles



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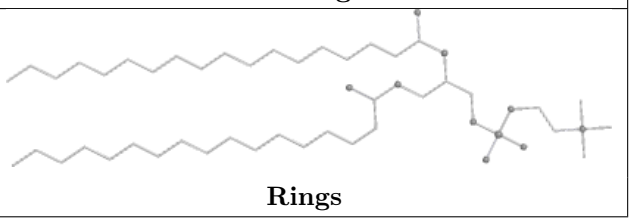
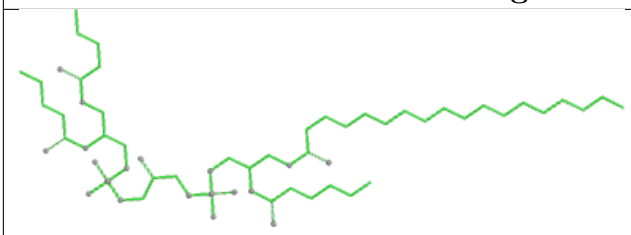


Rings

Ligand CDL VB 701



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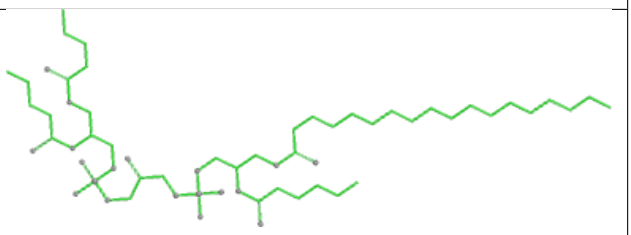
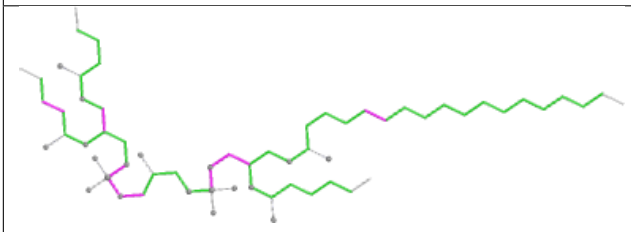
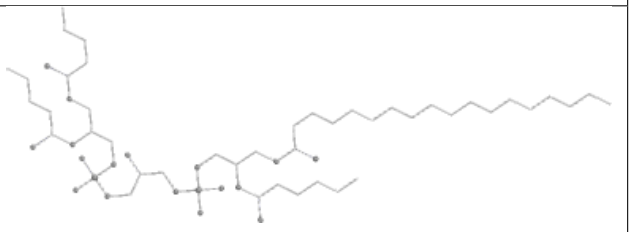


Bond angles

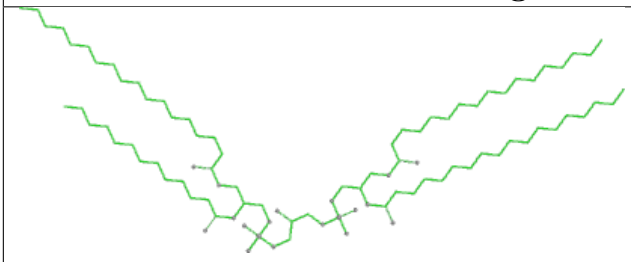


Torsions



Rings

Ligand CDL QH 201



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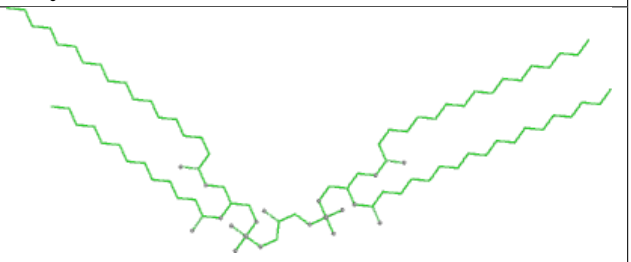
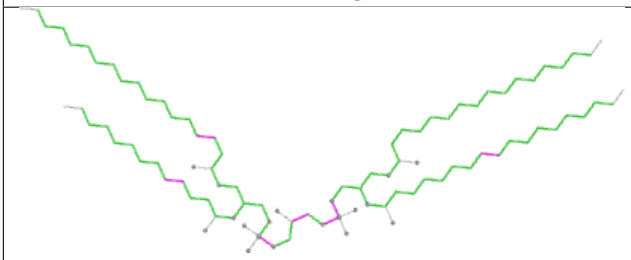
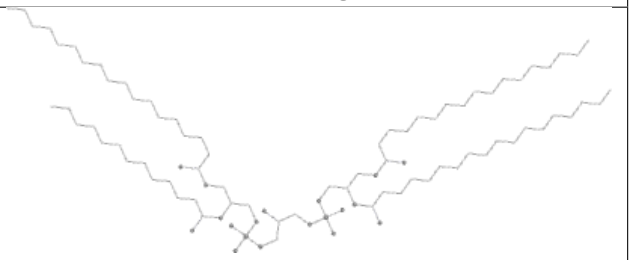


Bond angles

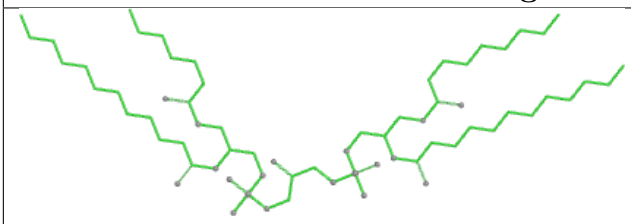


Torsions

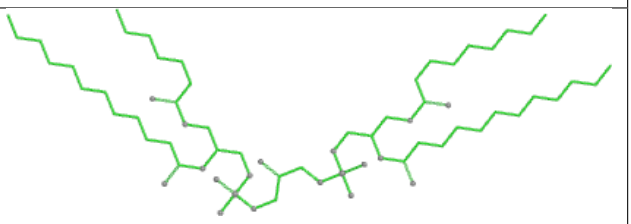


Rings

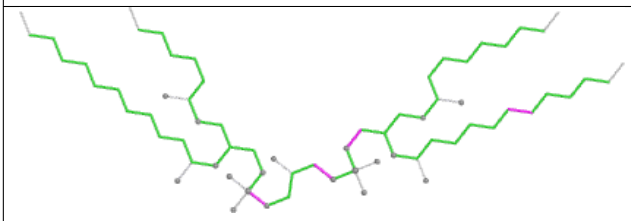
Ligand CDL c3 604



Bond lengths



Bond angles



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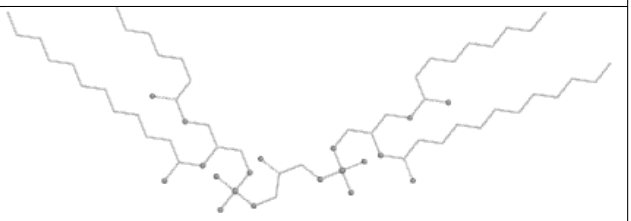
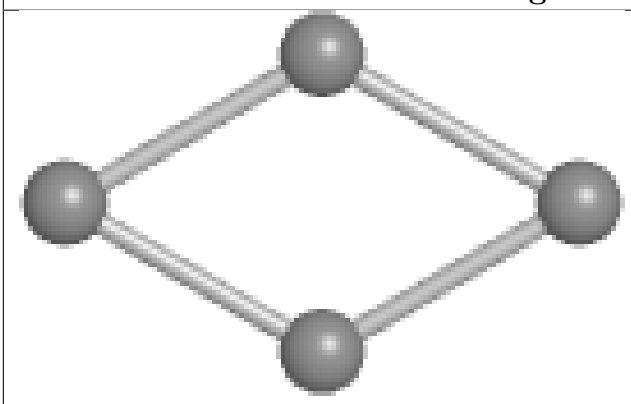


Rings

Ligand FES fs 201



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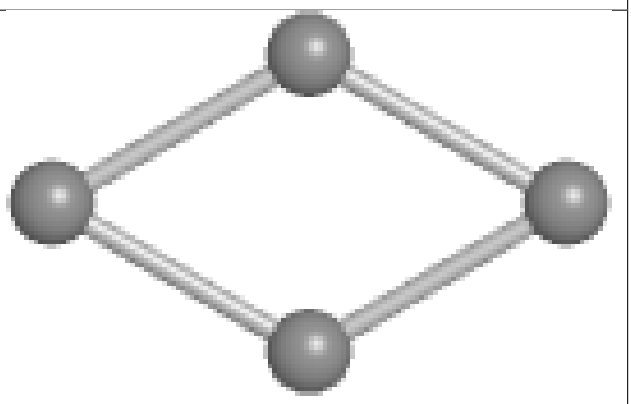

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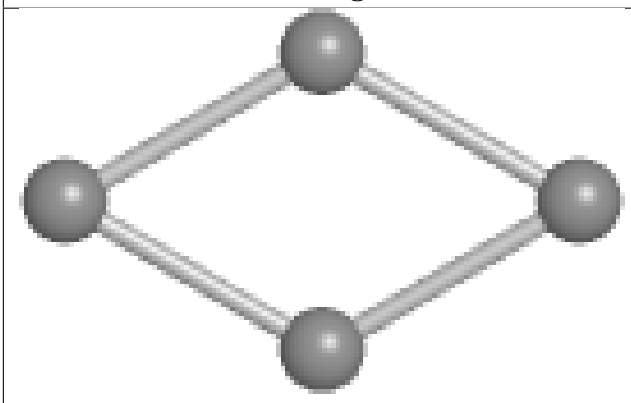

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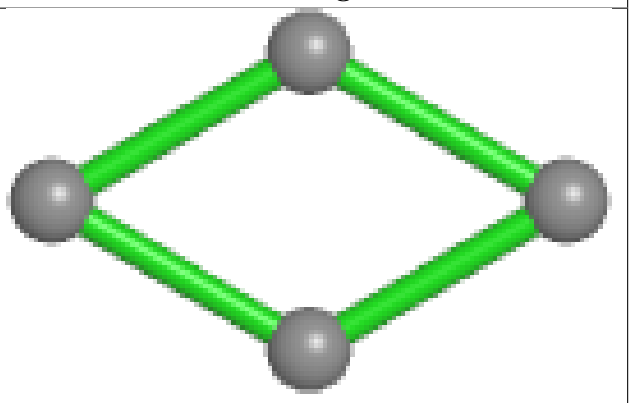
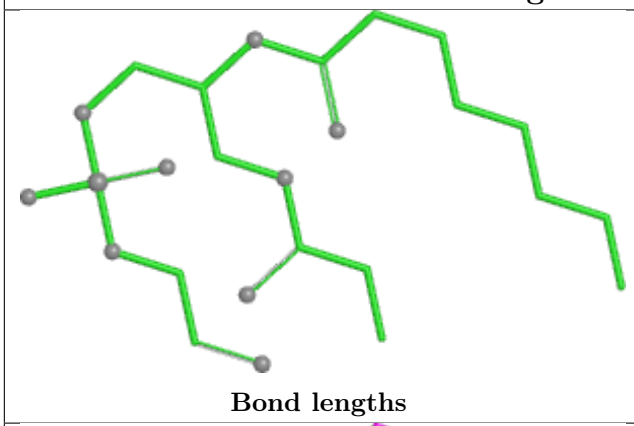


Rings

Ligand 3PE ta 201



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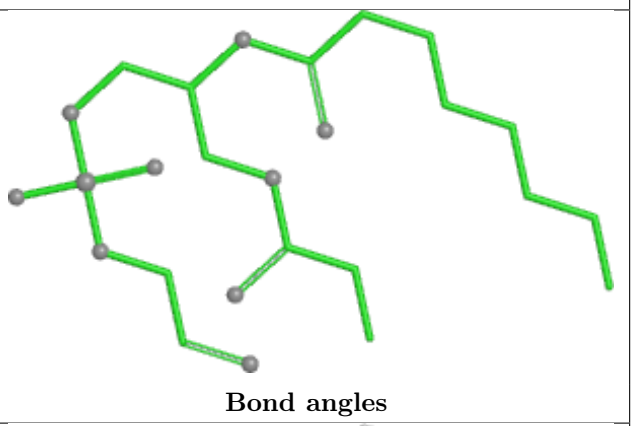
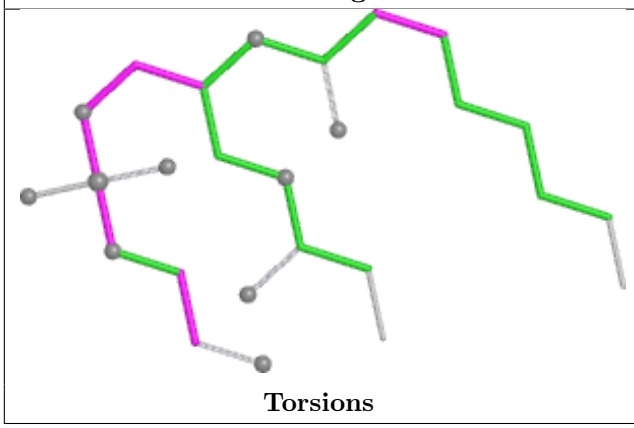


Bond angles



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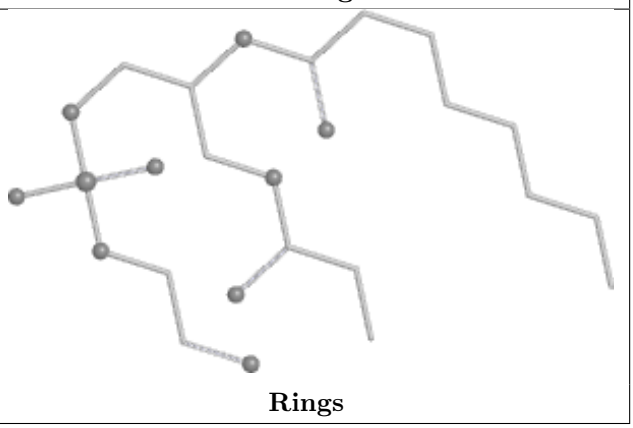
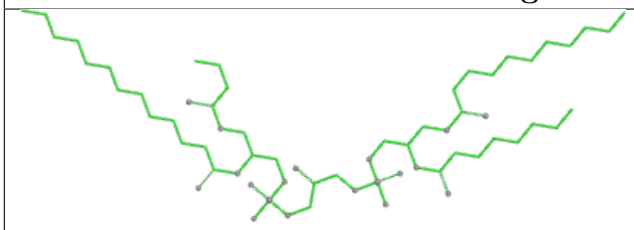


Rings

Ligand CDL M 306



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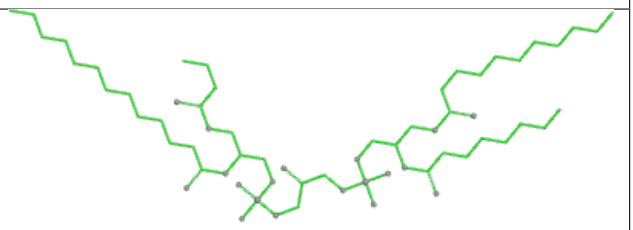
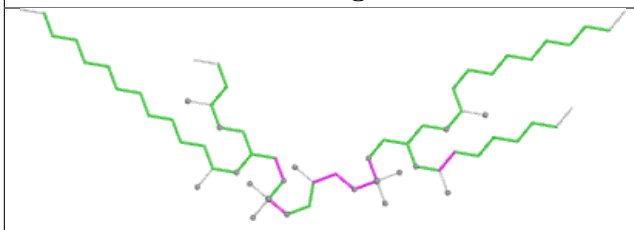


Bond angles



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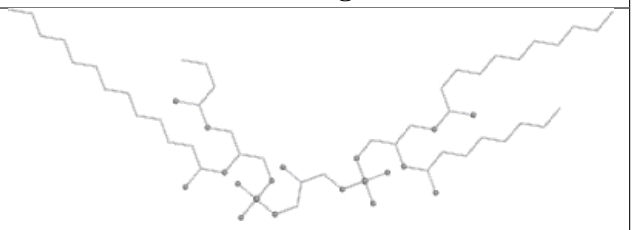
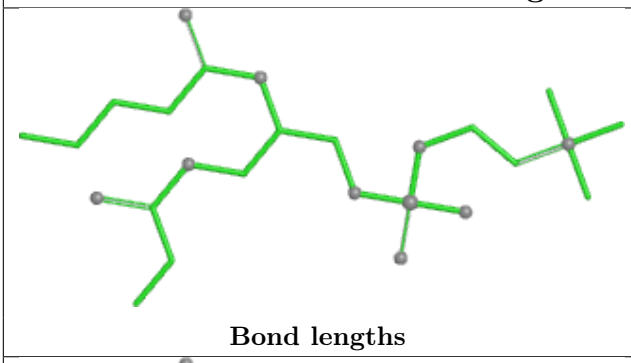


Rings

Ligand PC1 al 302



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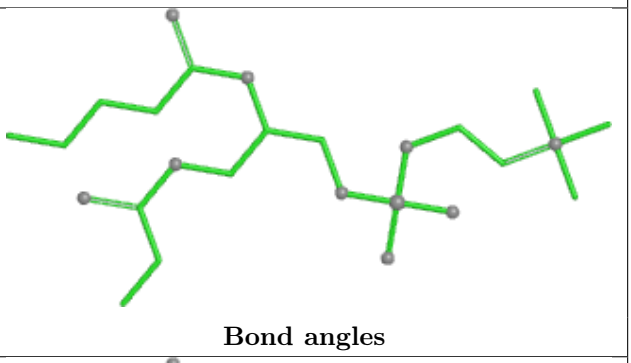
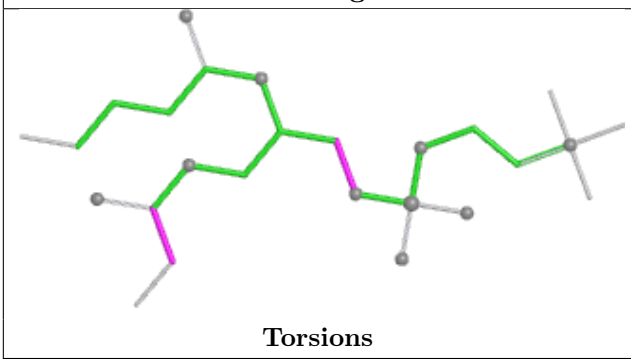


Bond angles



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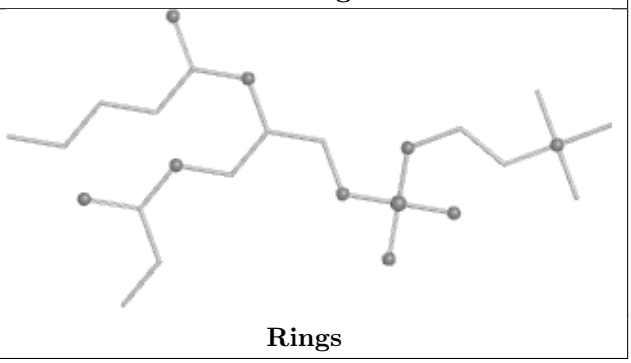
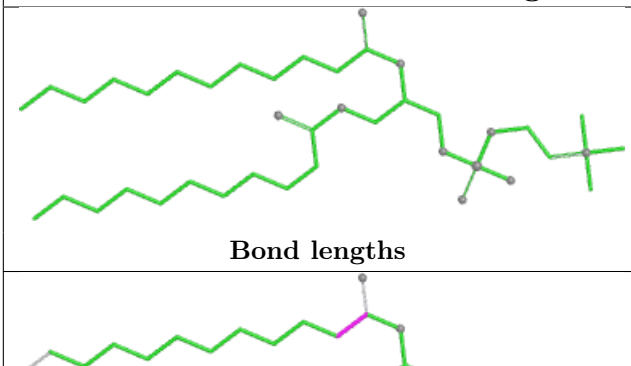


Rings

Ligand PC1 c4 403



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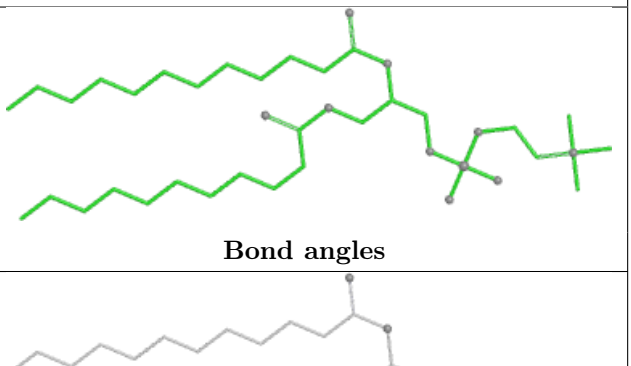

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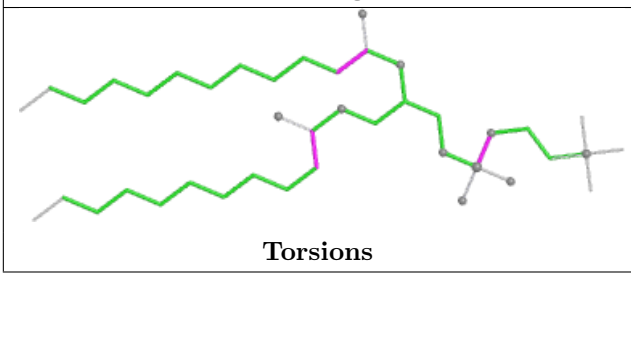

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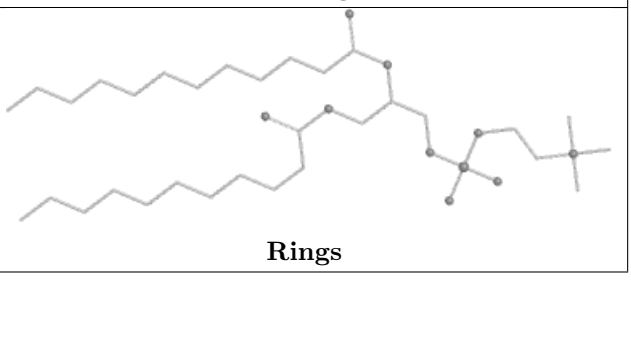
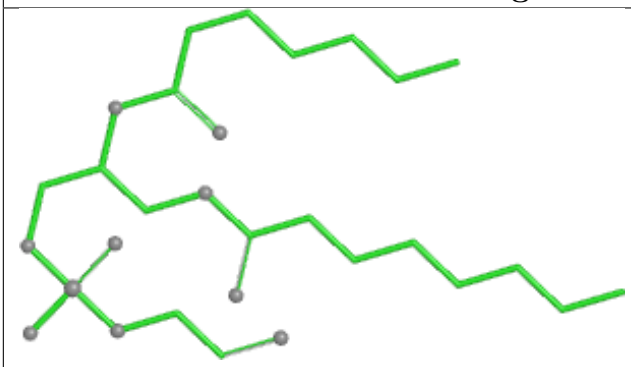


Rings

Ligand 3PE BM 302



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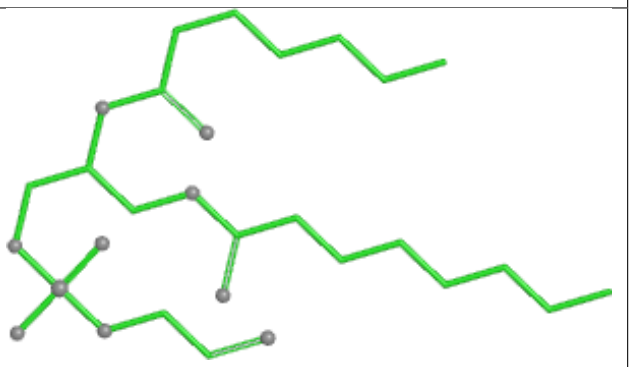
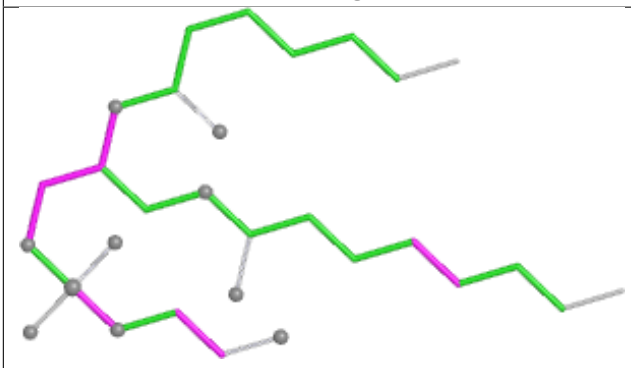


Bond angles



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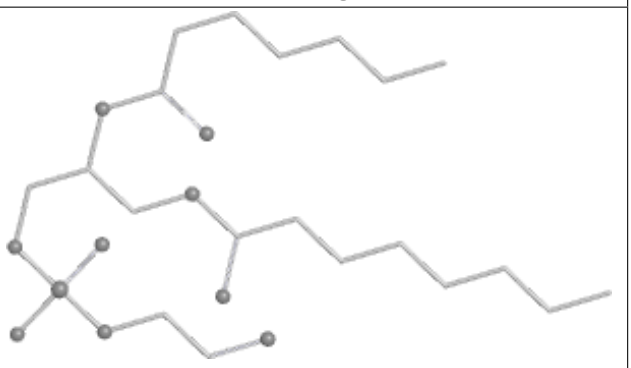
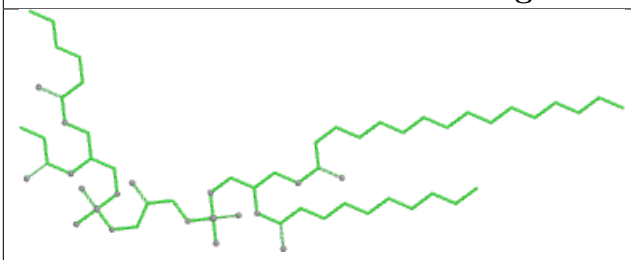


Rings

Ligand CDL C1 708



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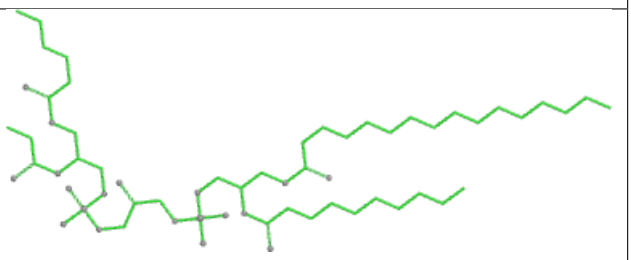
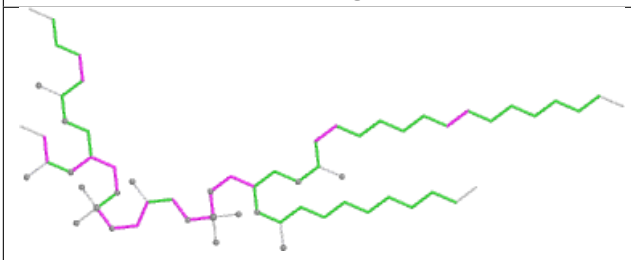


Bond angles



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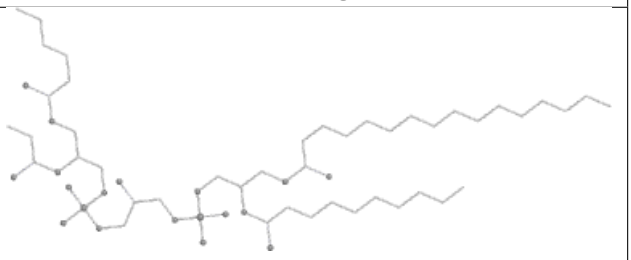
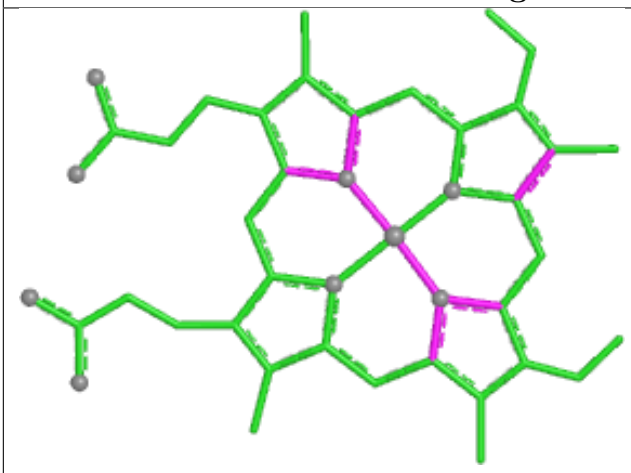


Rings

Ligand HEM qC 501



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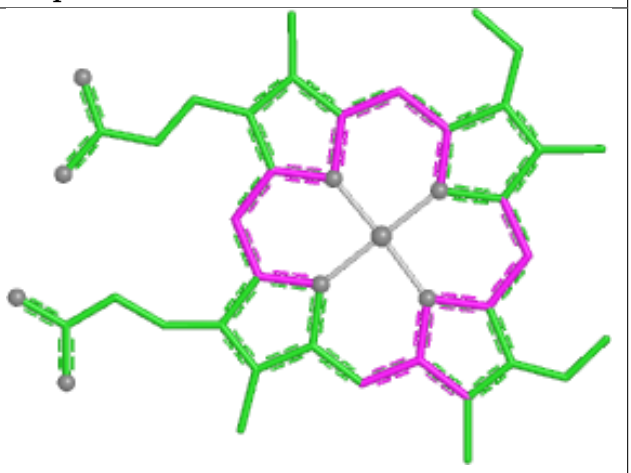

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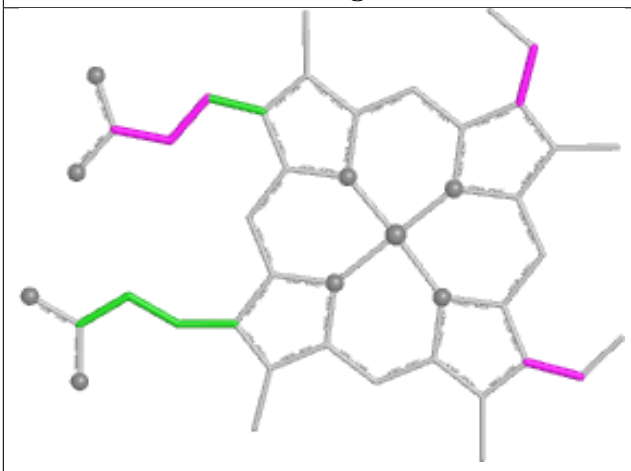

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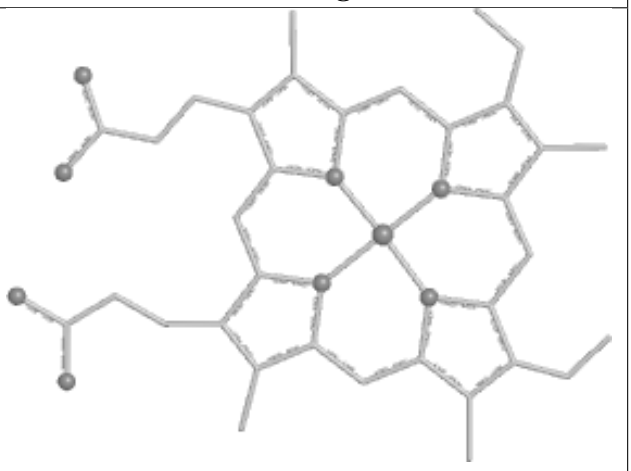
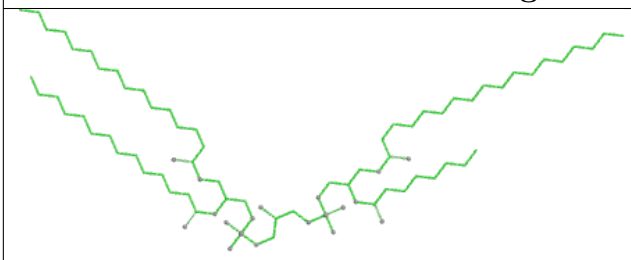


Rings

Ligand CDL th 200



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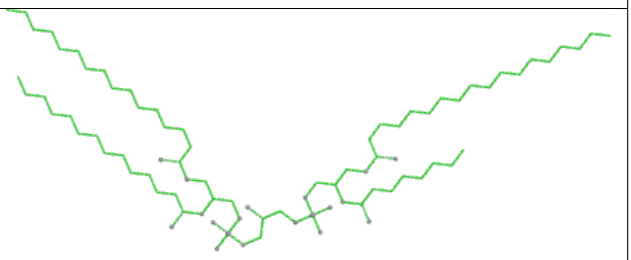
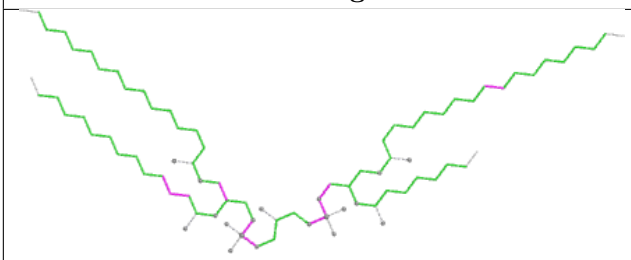


Bond angles



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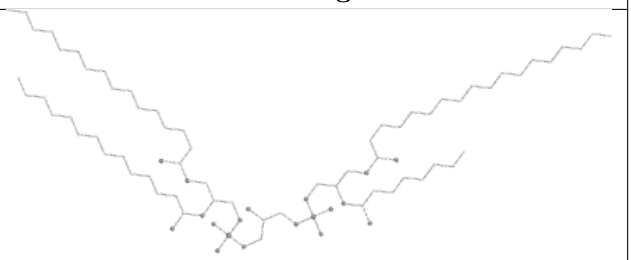
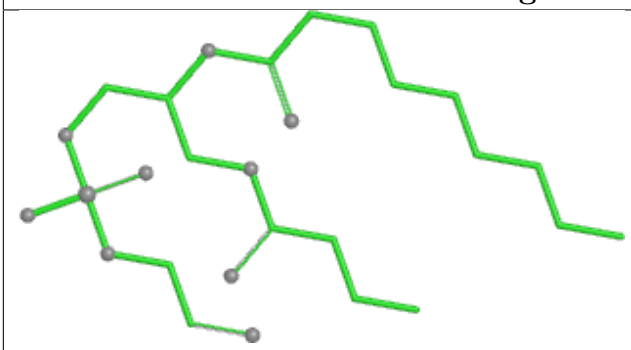


Rings

Ligand 3PE Y5 202



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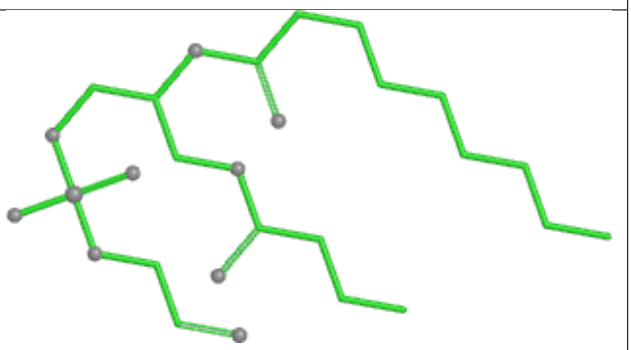

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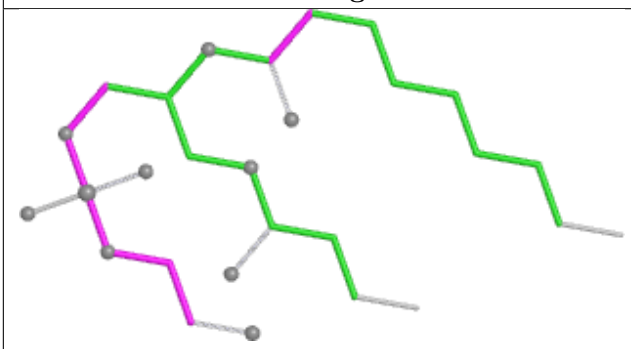

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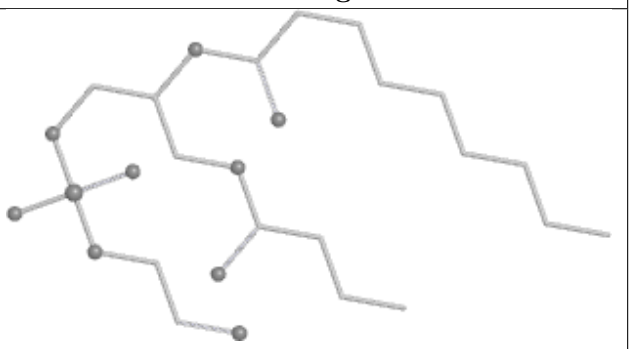
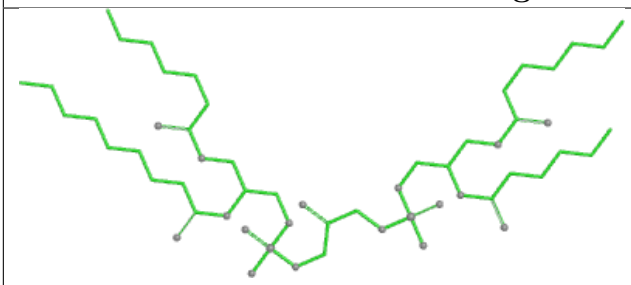


Rings

Ligand CDL m1 405



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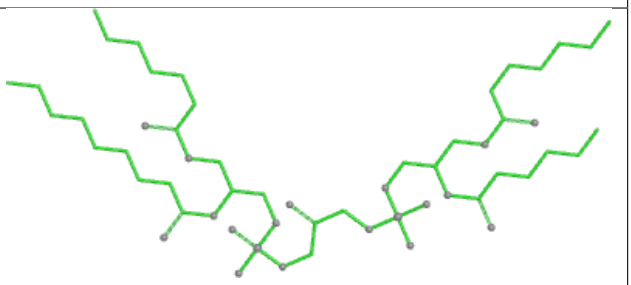
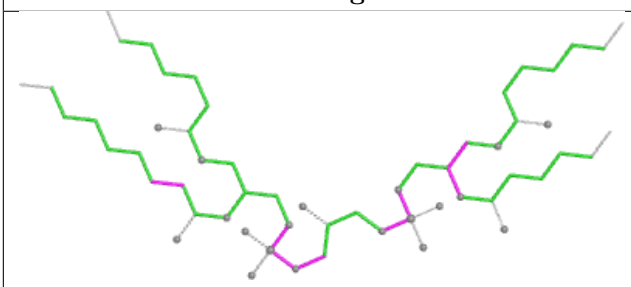


Bond angles



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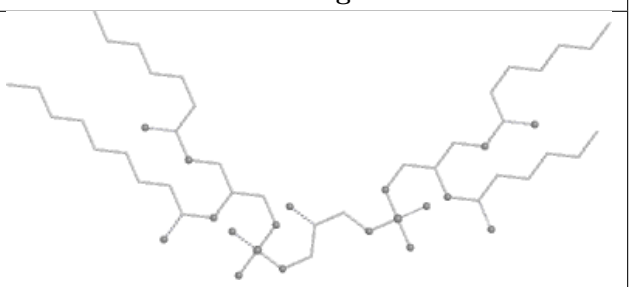
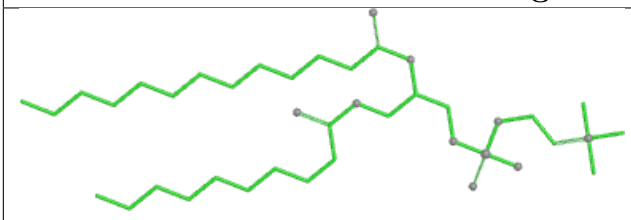


Rings

Ligand PC1 a 503



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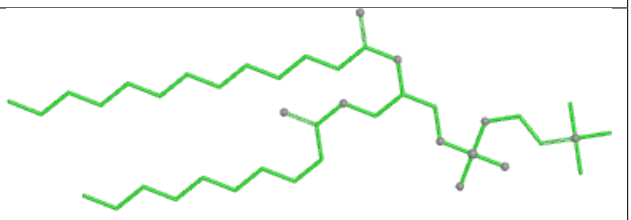
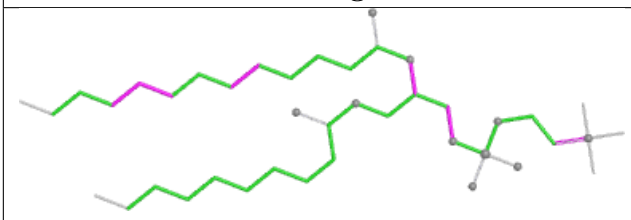


Bond angles



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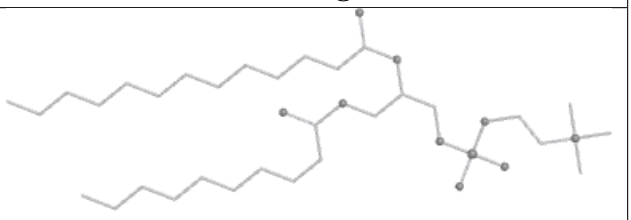
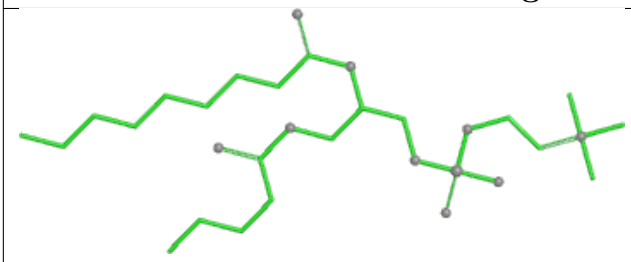
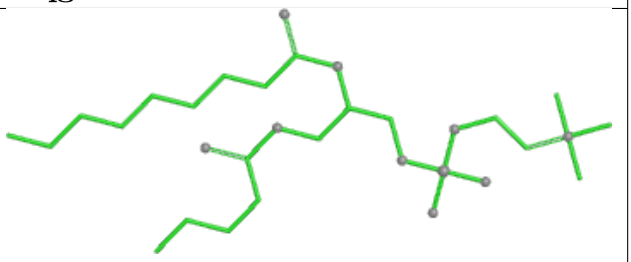


Rings

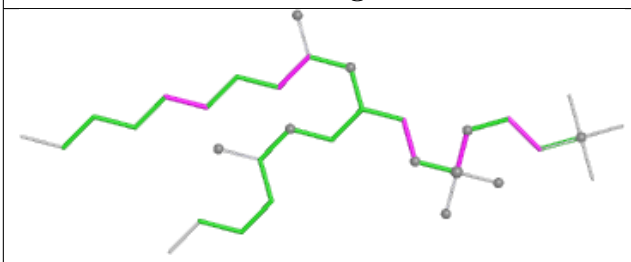
Ligand PC1 qg 401



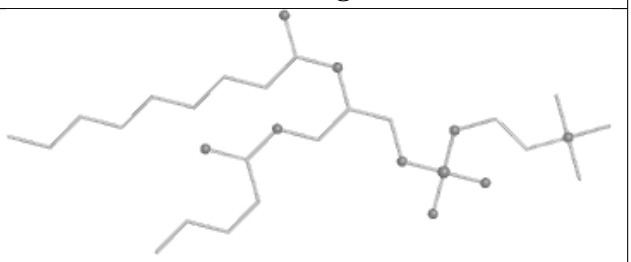
Bond lengths



Bond angles

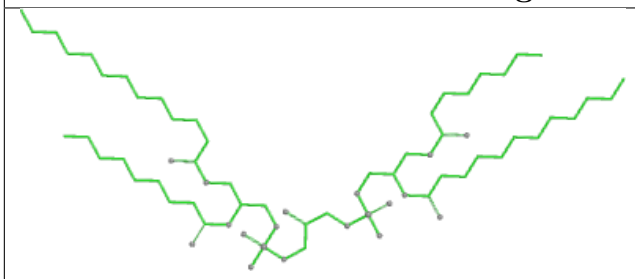


Torsions



Rings

Ligand CDL Y5 201



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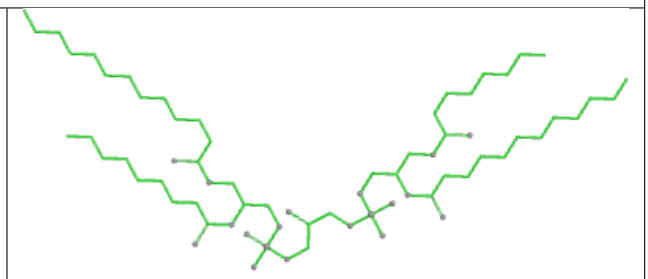
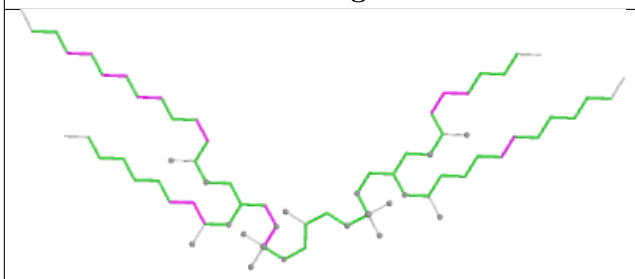
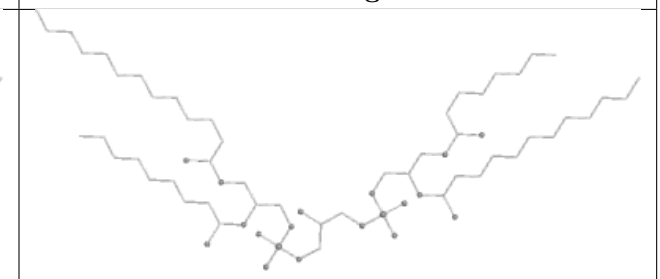


Bond angles

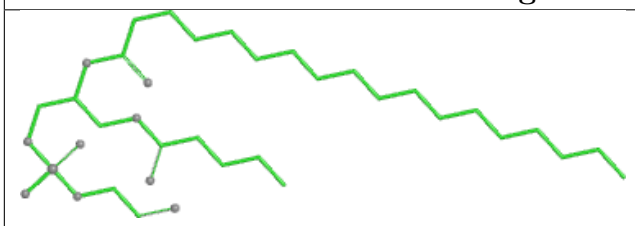


Torsions



Rings

Ligand 3PE m3 402



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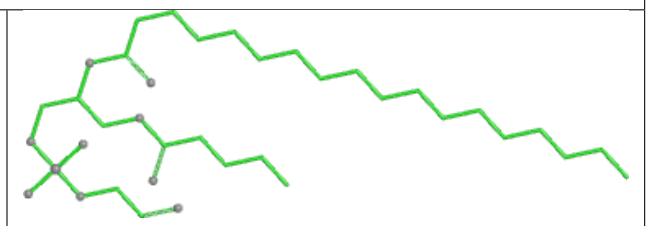

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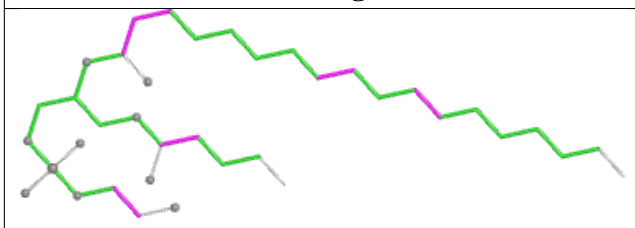

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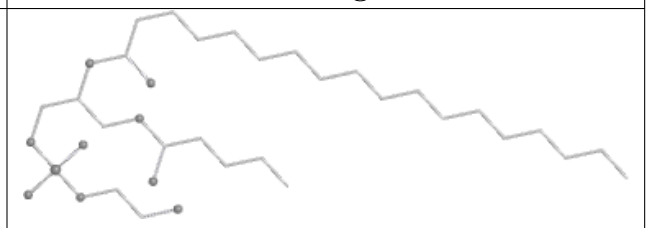
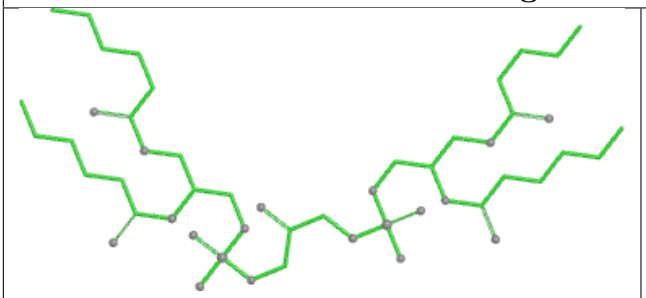
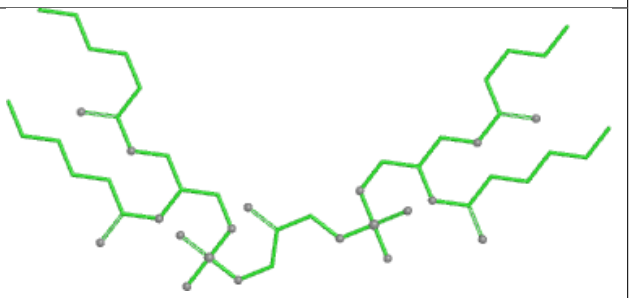


Rings

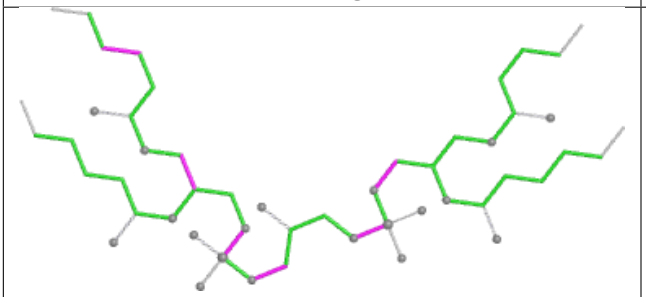
Ligand CDL 7c 302



Bond lengths



Bond angles



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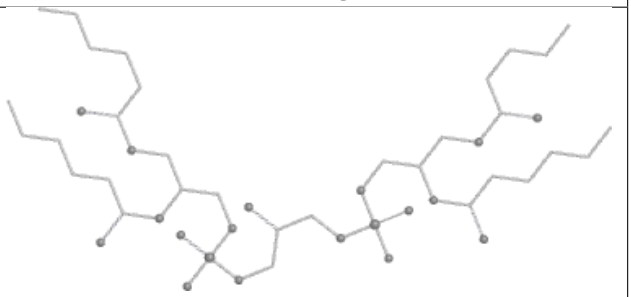
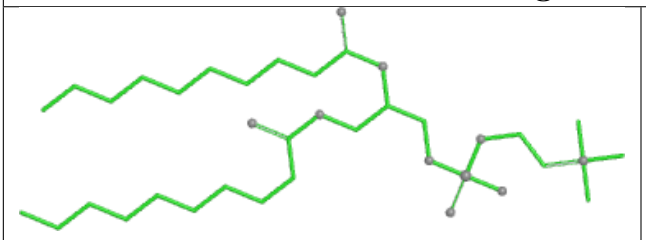


Rings

Ligand PC1 f 402



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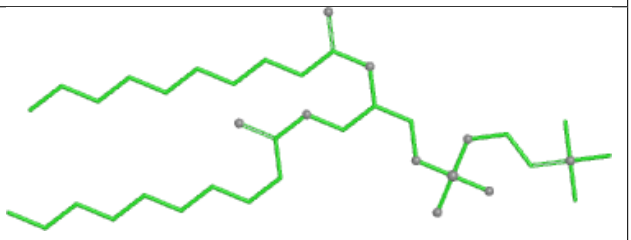
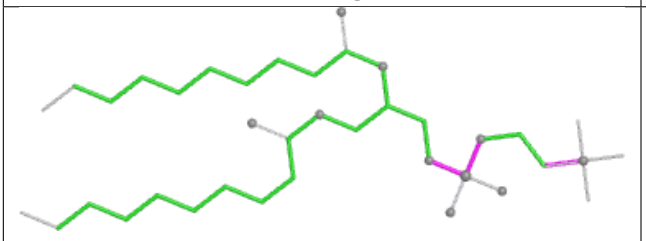


Bond angles



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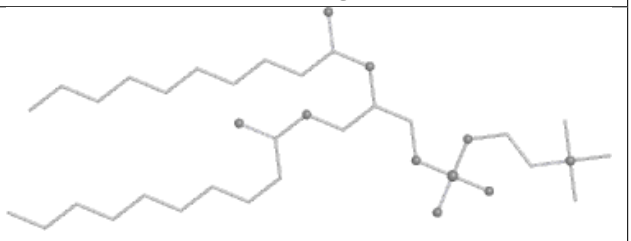
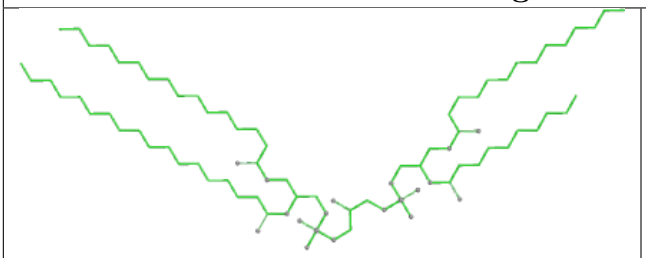


Rings

Ligand CDL bm 301



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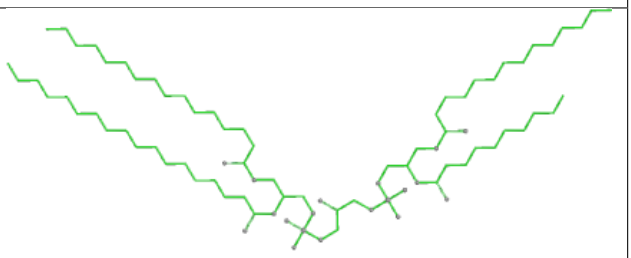
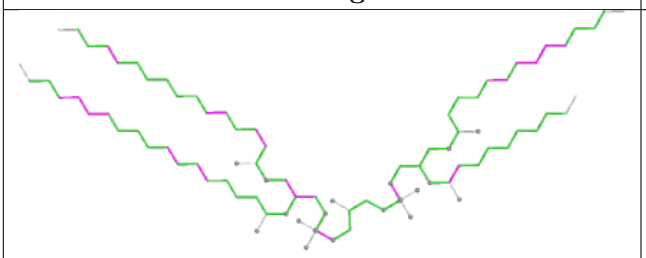


Bond angles



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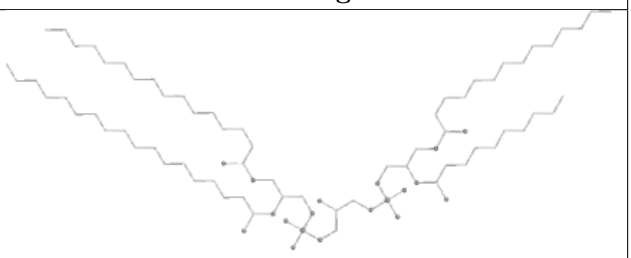
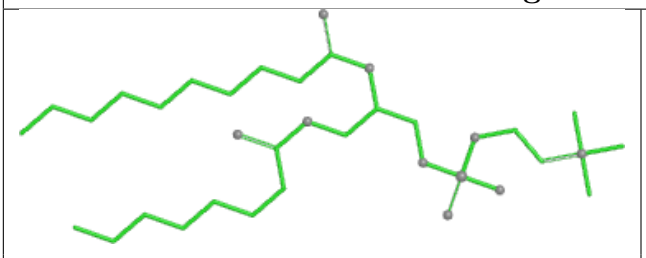


Rings

Ligand PC1 c2 703



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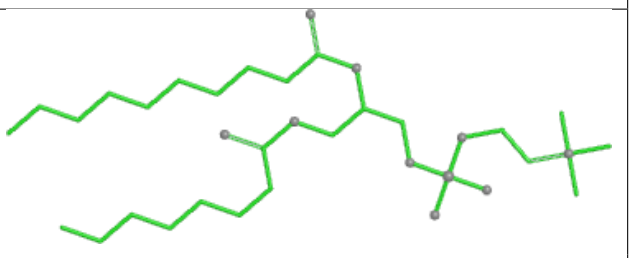
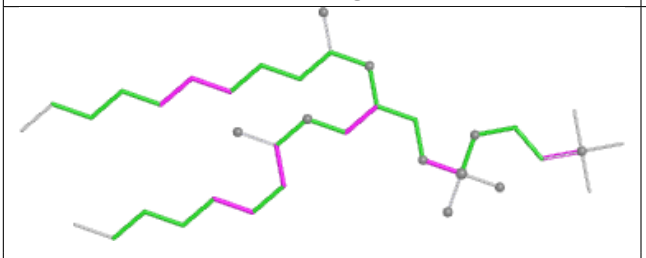
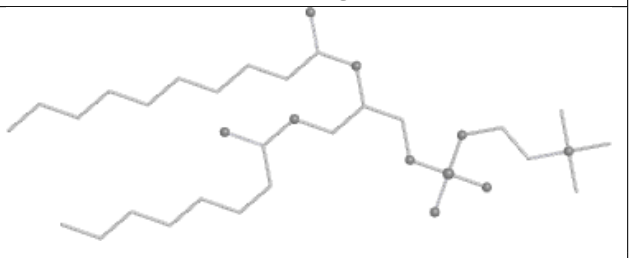


Bond angles

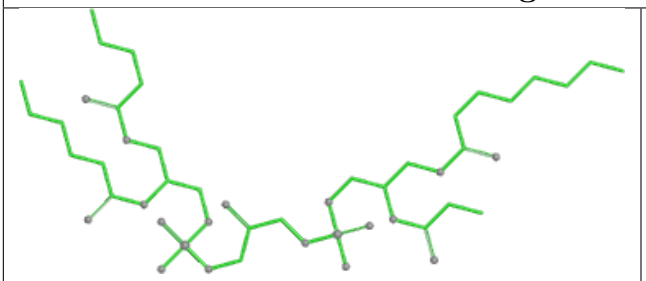


Torsions



Rings

Ligand CDL 2o 101



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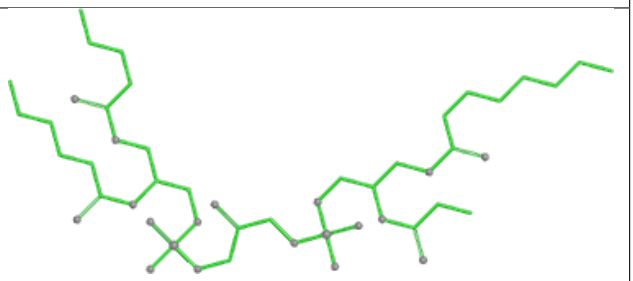

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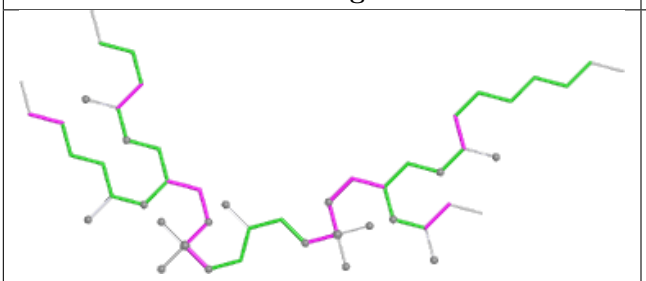

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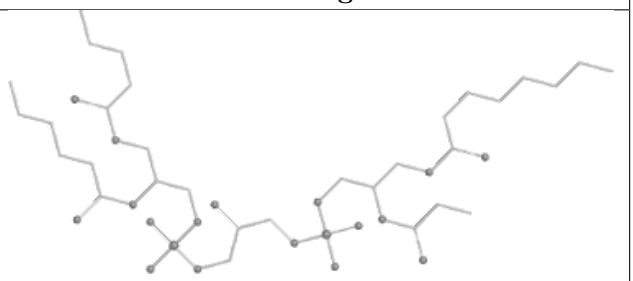
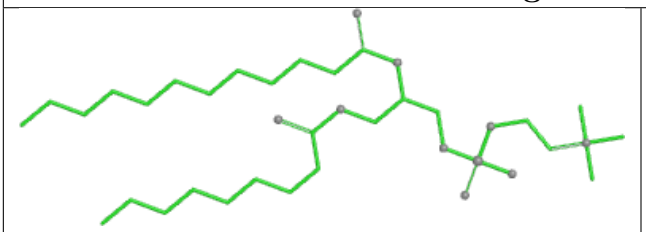
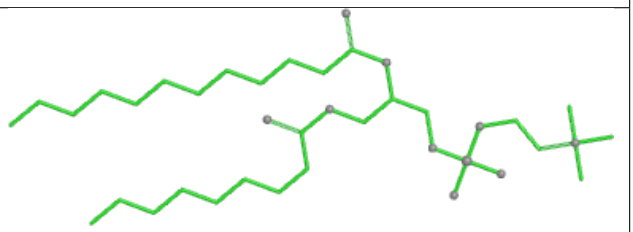


Rings

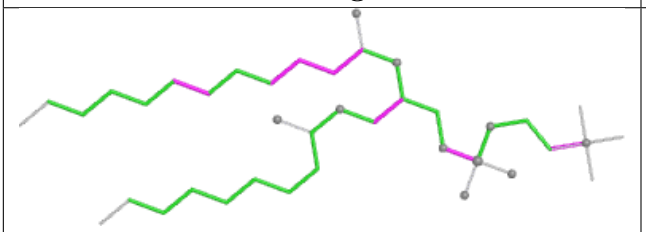
Ligand PC1 c3 602



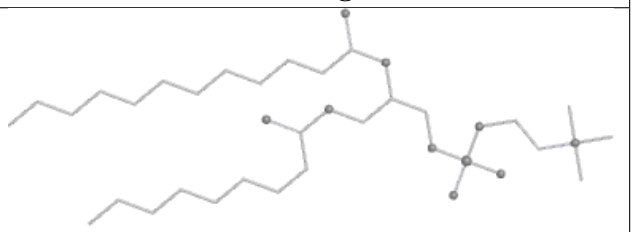
Bond lengths



Bond angles

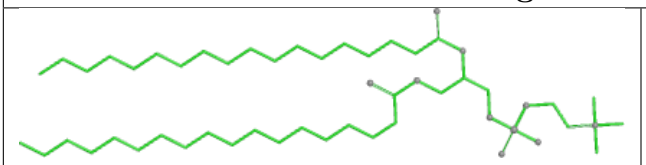


Torsions



Rings

Ligand PC1 m1 401



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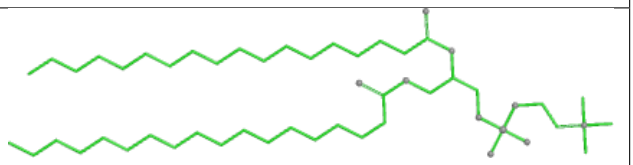
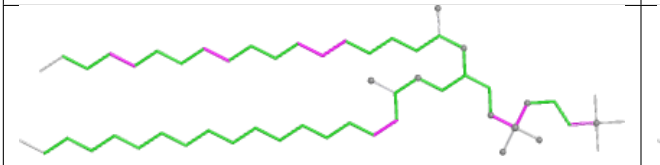


Bond angles



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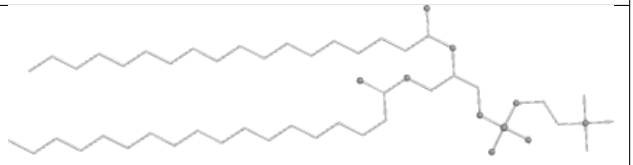
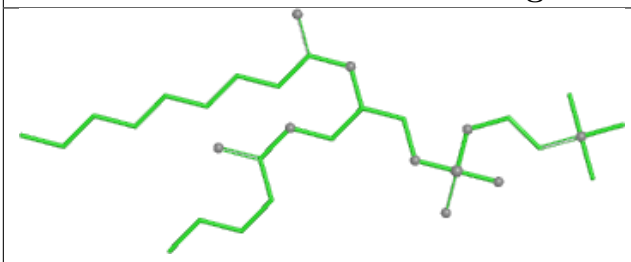


Rings

Ligand PC1 N 302



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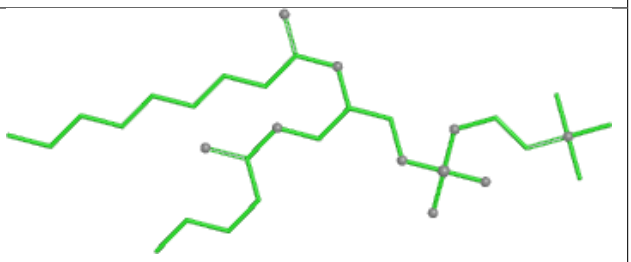
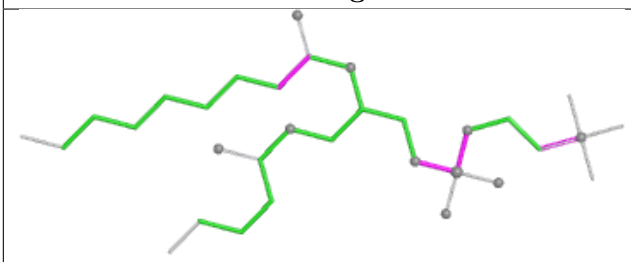


Bond angles



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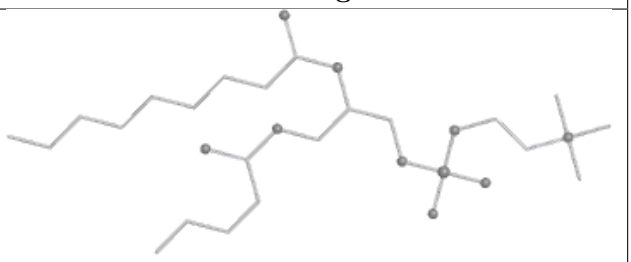
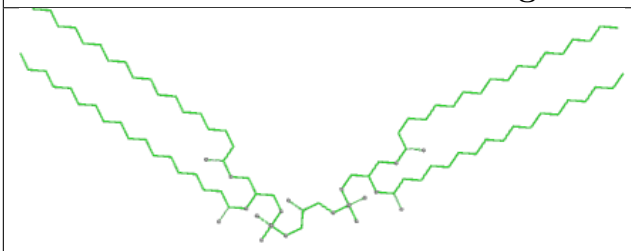


Rings

Ligand CDL qg 402



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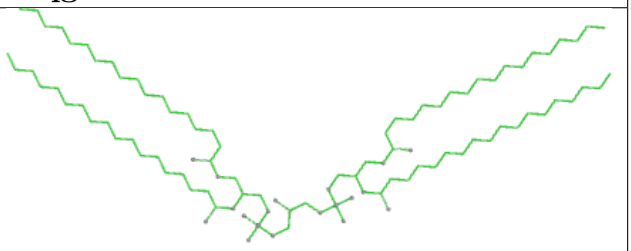
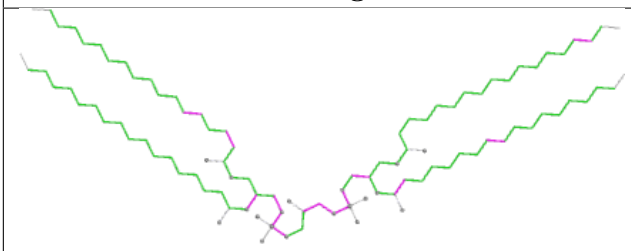
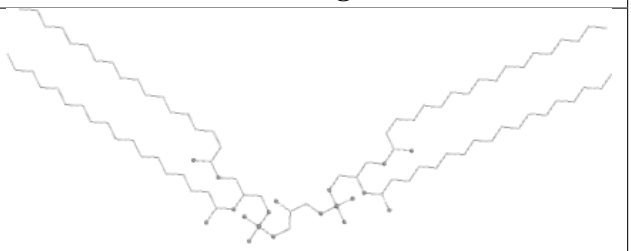


Bond angles

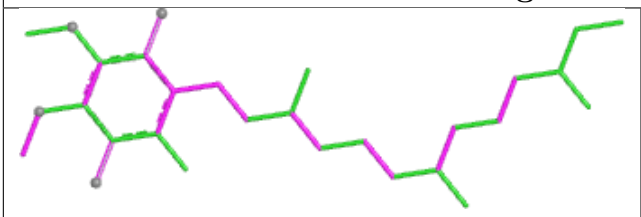


Torsions



Rings

Ligand U10 QC 506



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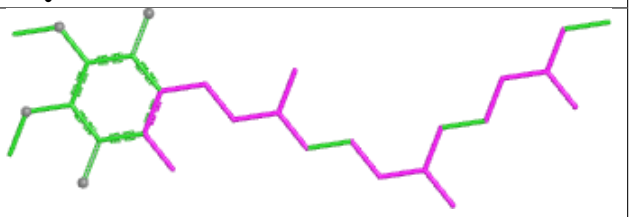
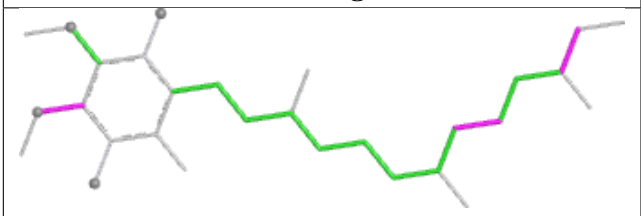


Bond angles



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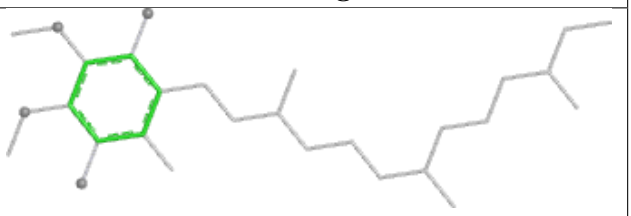
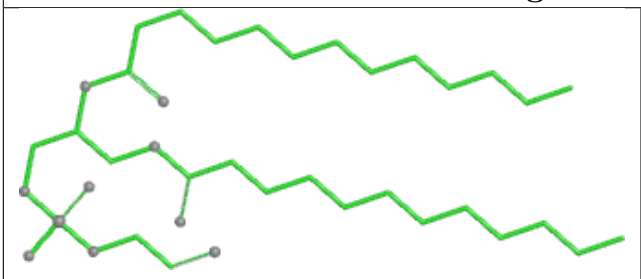
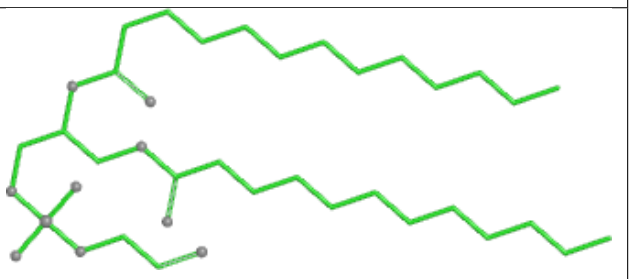


Rings

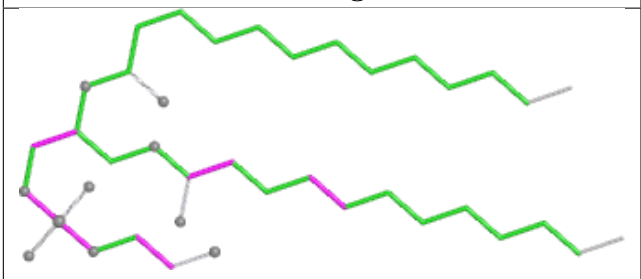
Ligand 3PE sc 101



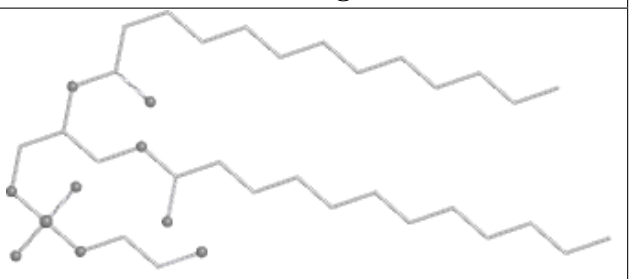
Bond lengths



Bond angles

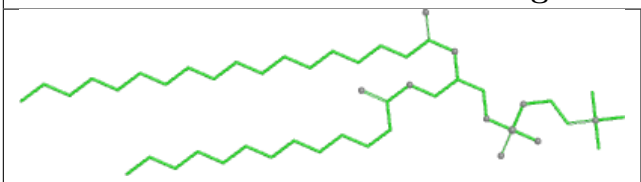


Torsions



Rings

Ligand PC1 v 202



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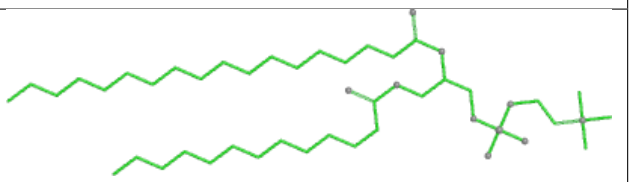

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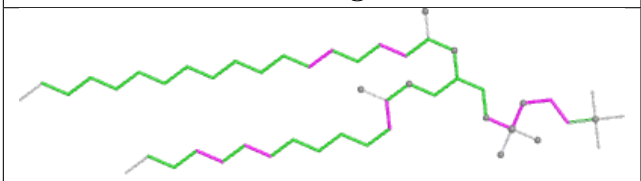

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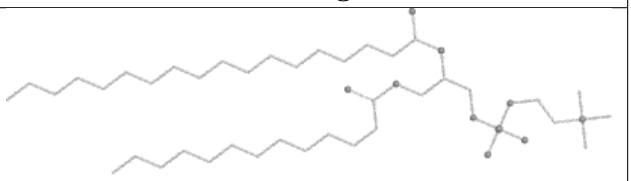
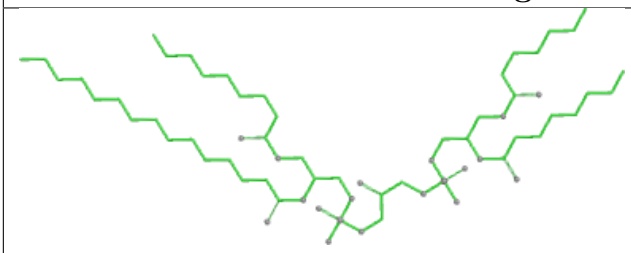


Rings

Ligand CDL A1 102



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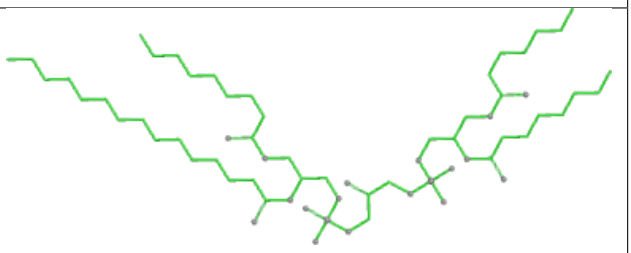

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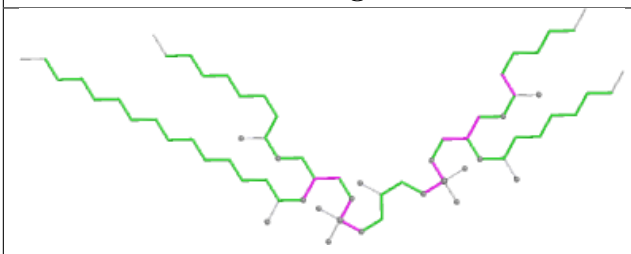

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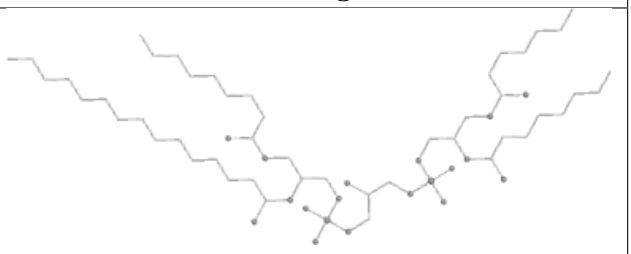
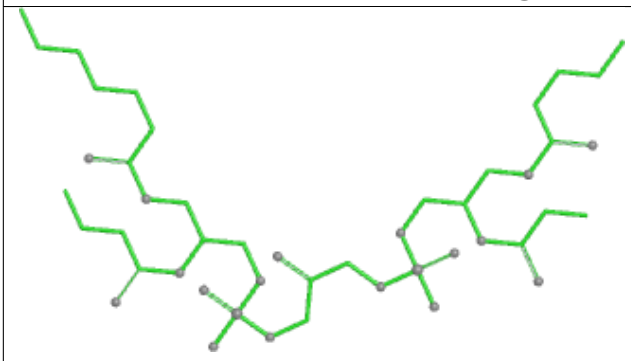


Rings

Ligand CDL FS 204



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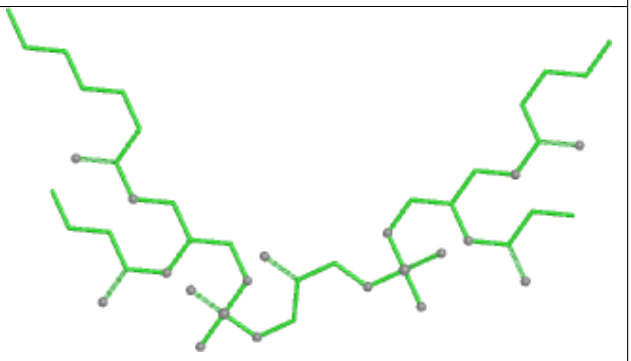

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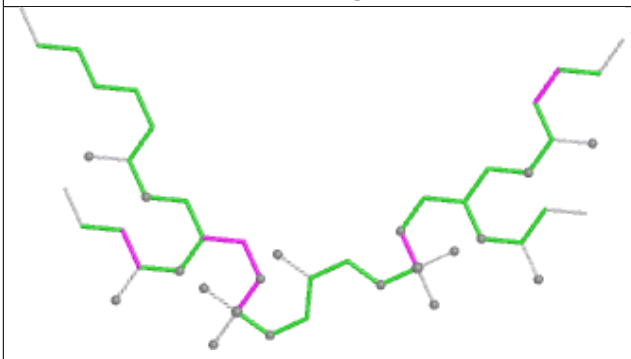

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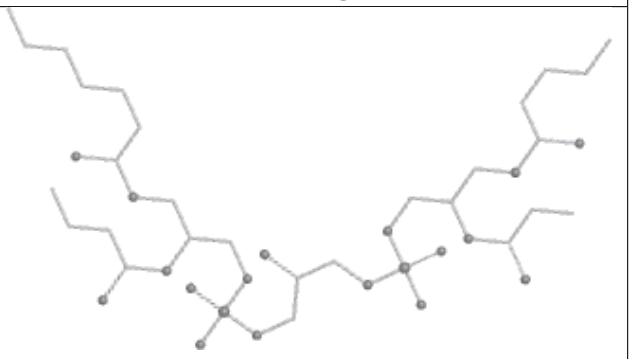
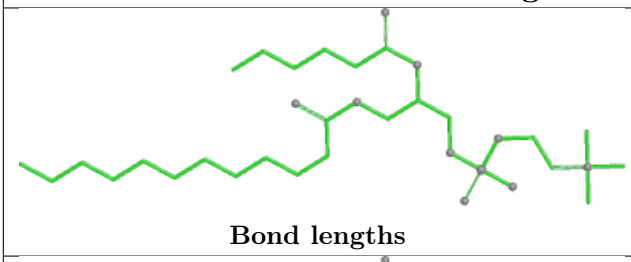


Rings

Ligand PC1 an 304



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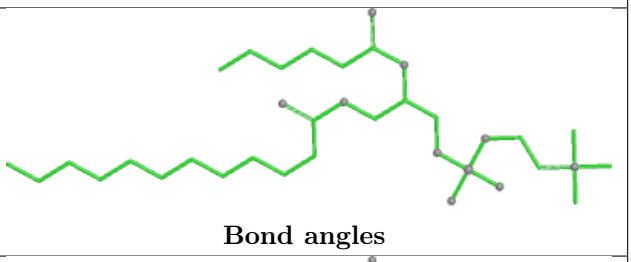

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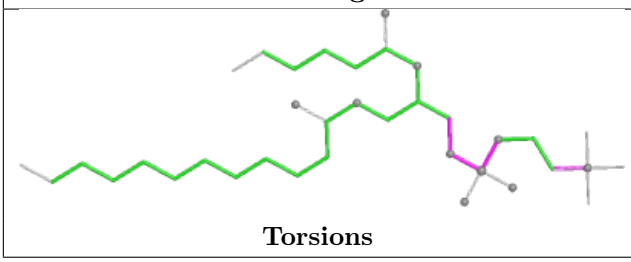

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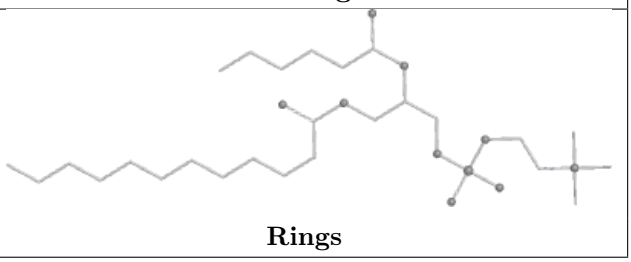
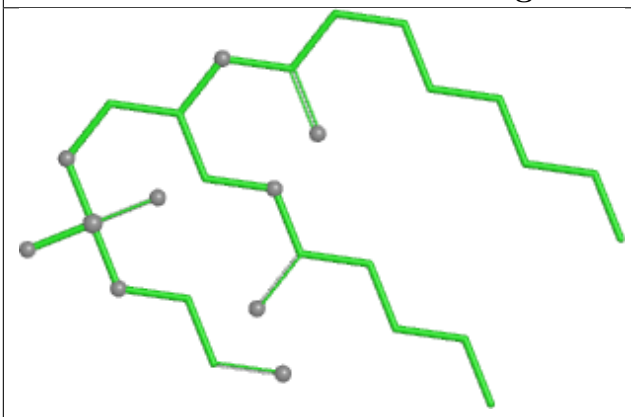


Rings

Ligand 3PE VB 707



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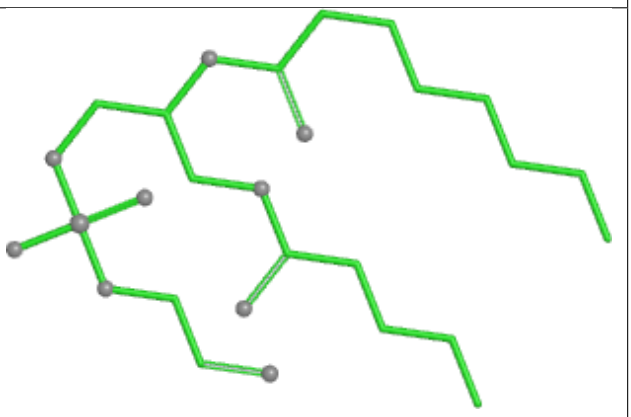
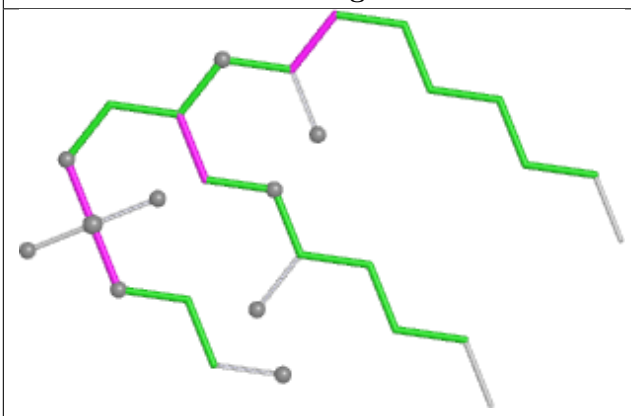


Bond angles



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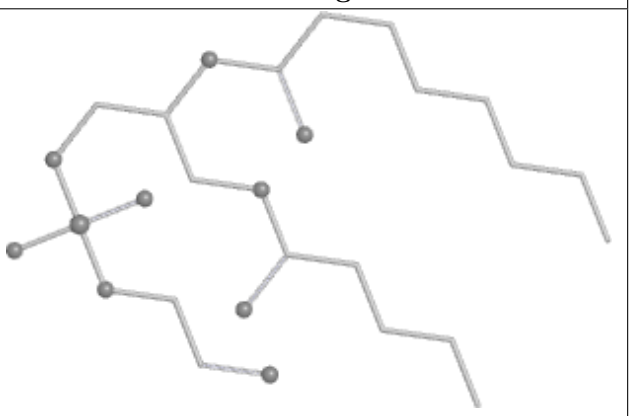
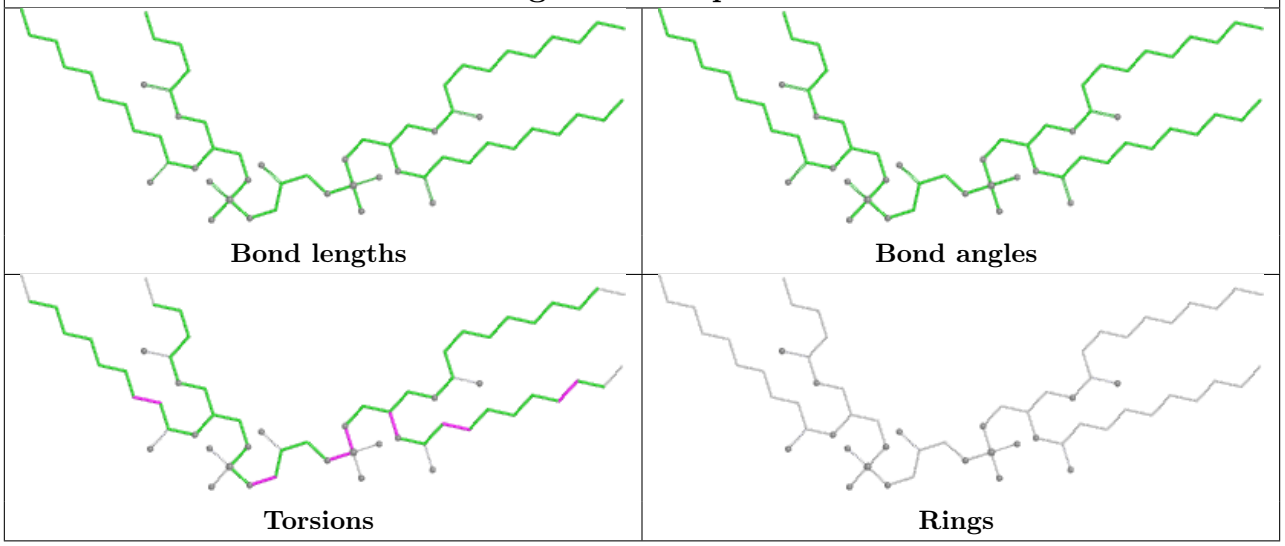
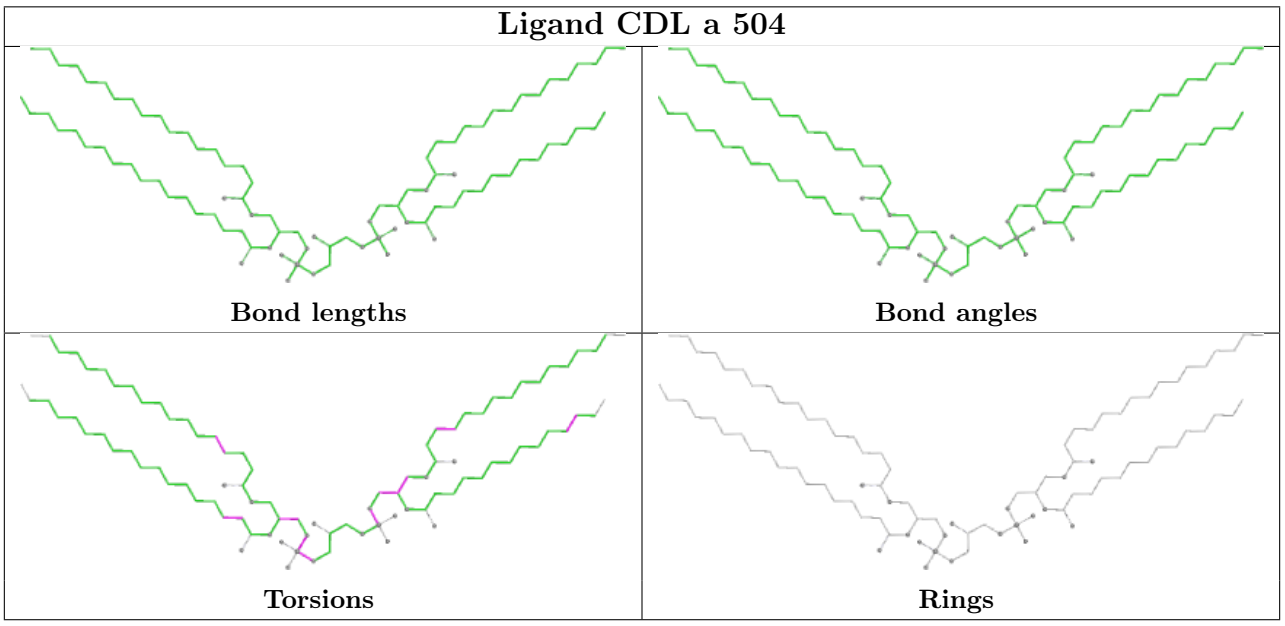


Rings

Ligand CDL q 201



Ligand CDL a 504



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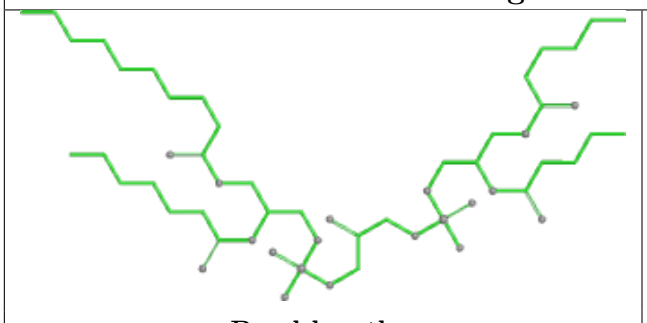

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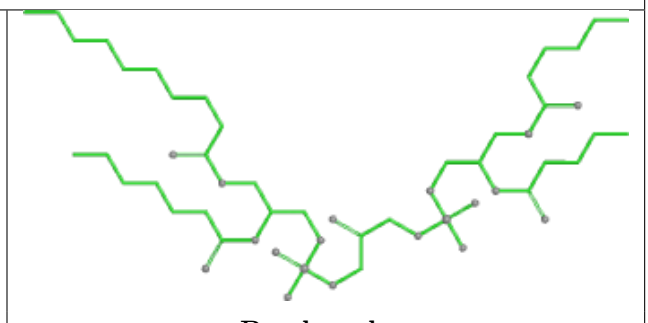

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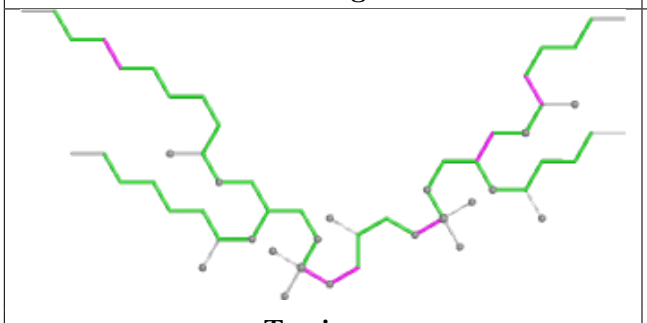

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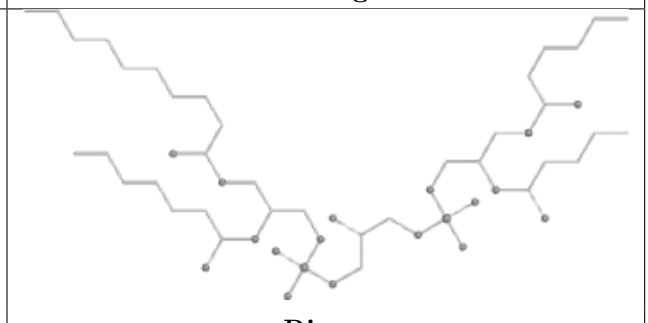
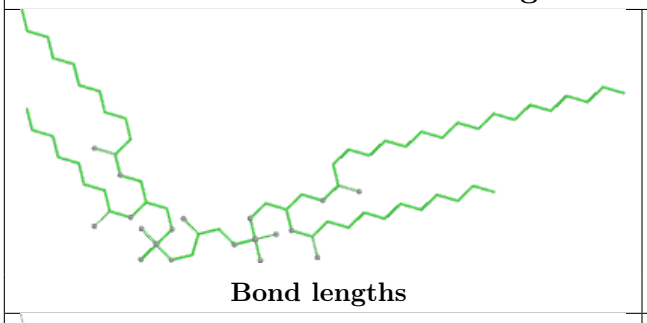


Rings

Ligand CDL a9 402



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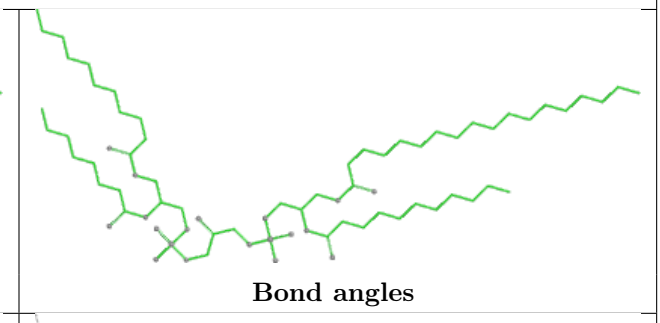
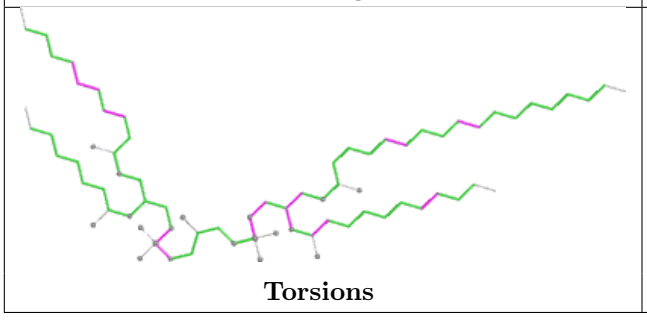


Bond angles



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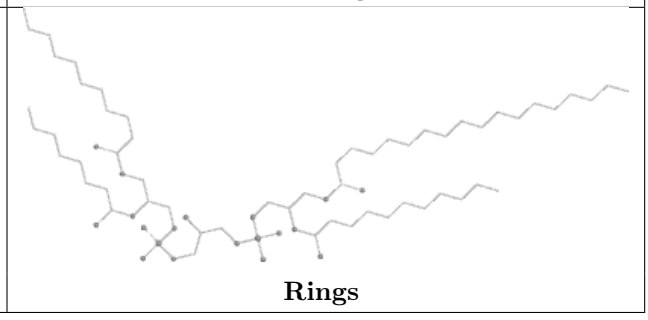
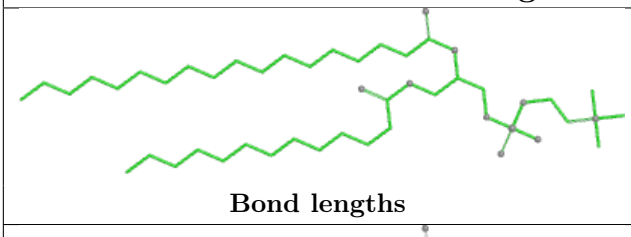


Rings

Ligand PC1 C3 606



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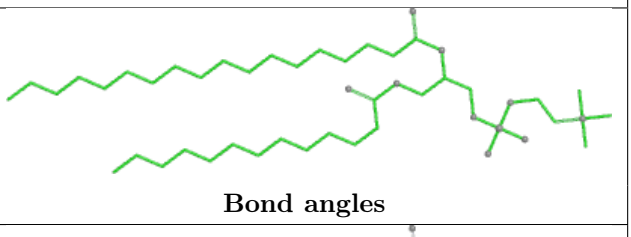
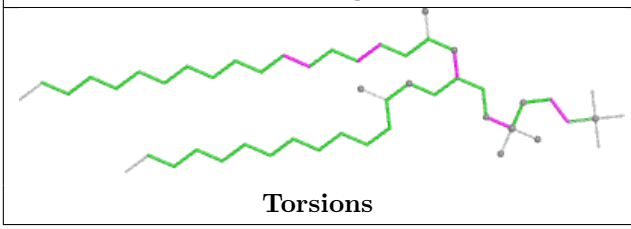


Bond angles



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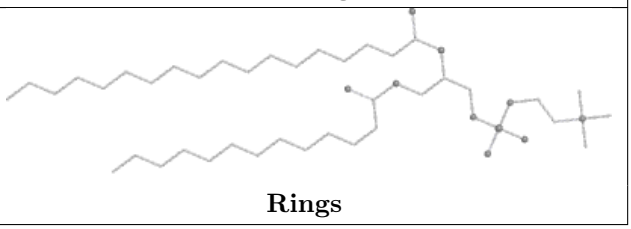
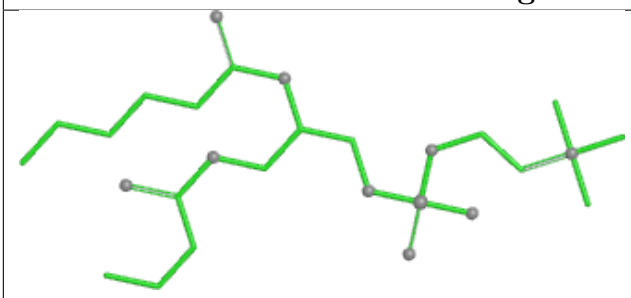


Rings

Ligand PC1 QJ 101



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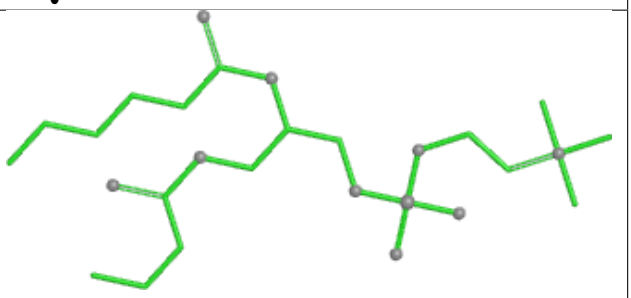

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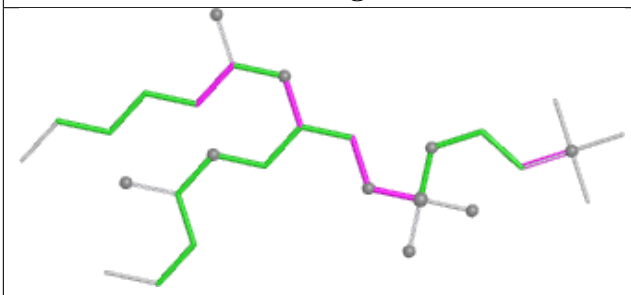

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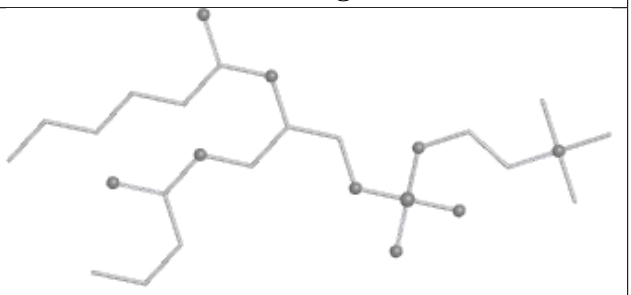
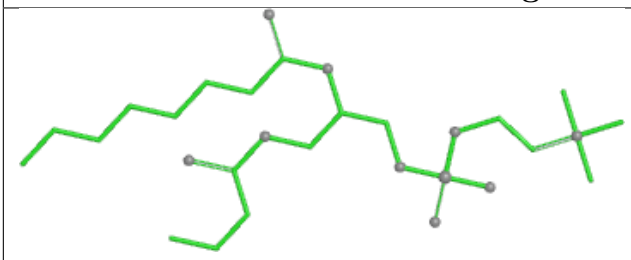


Rings

Ligand PC1 Qi 201



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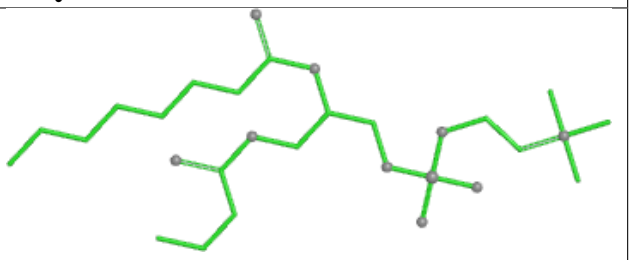

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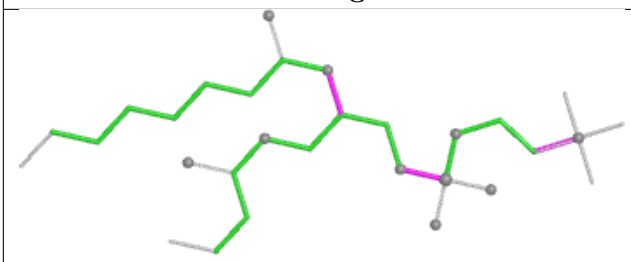

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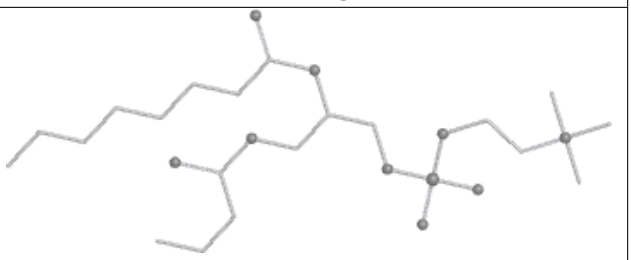
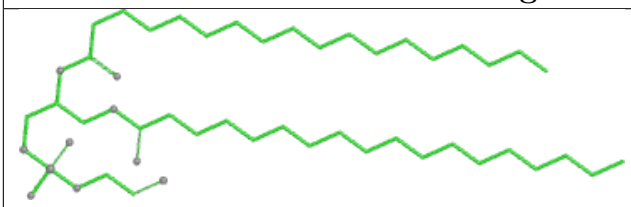


Rings

Ligand 3PE C4 402



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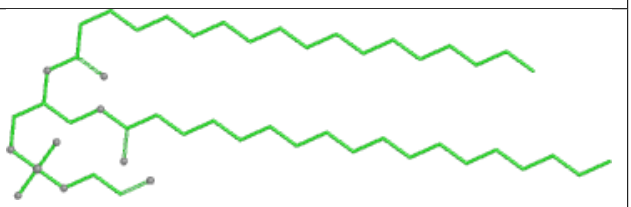

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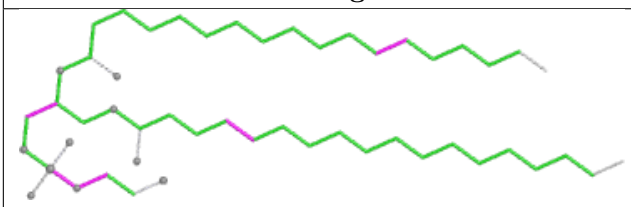

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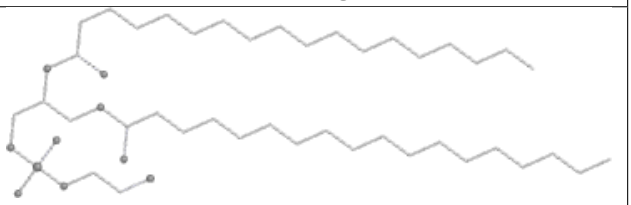
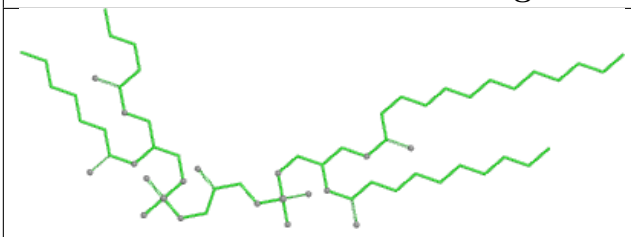


Rings

Ligand CDL 2G 204



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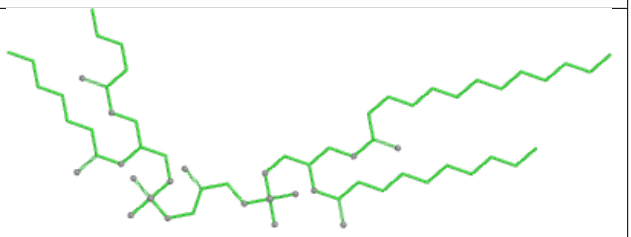

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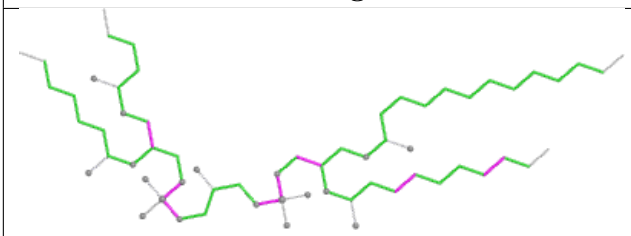

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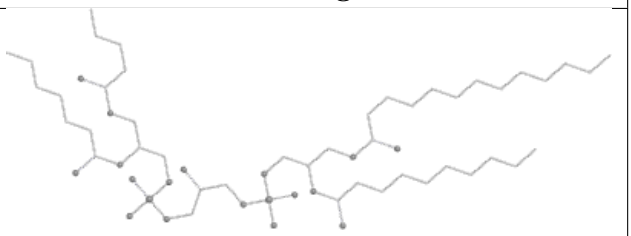
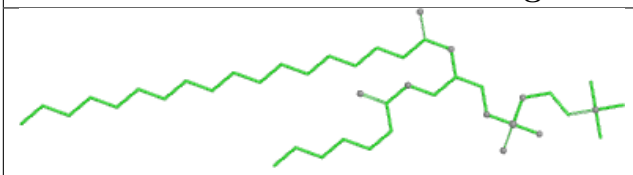


Rings

Ligand PC1 qI 202



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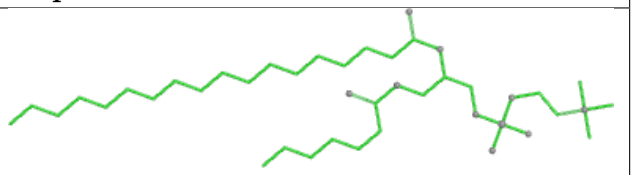
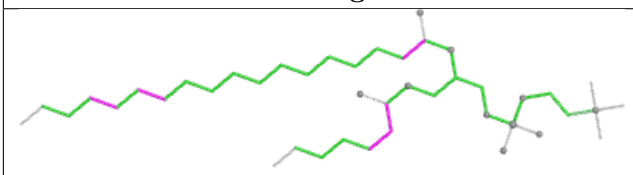
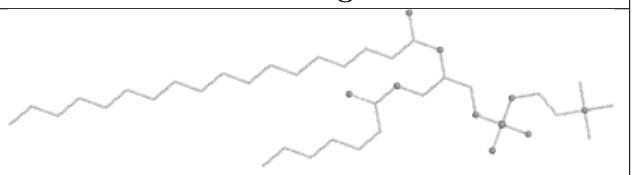


Bond angles

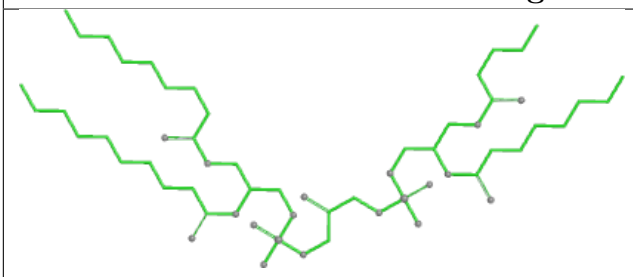


Torsions



Rings

Ligand CDL u 201



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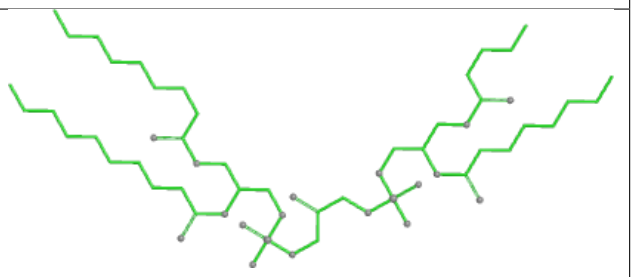
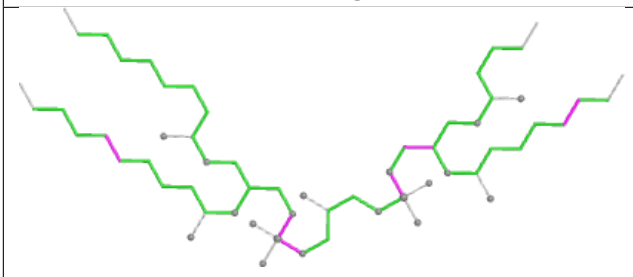


Bond angles



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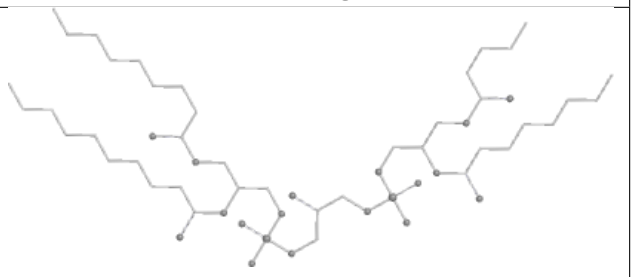
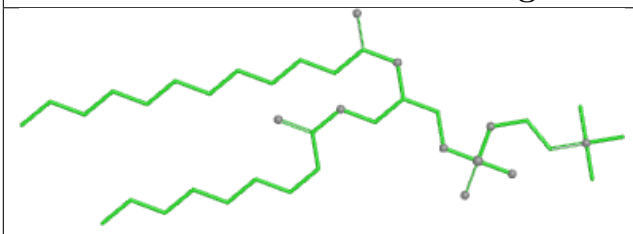


Rings

Ligand PC1 C3 602



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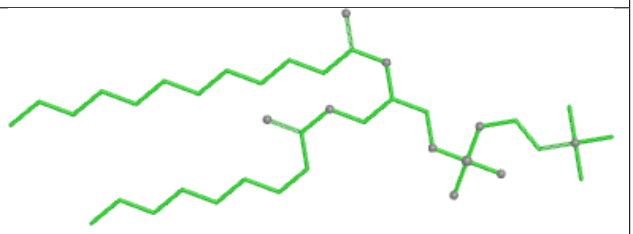

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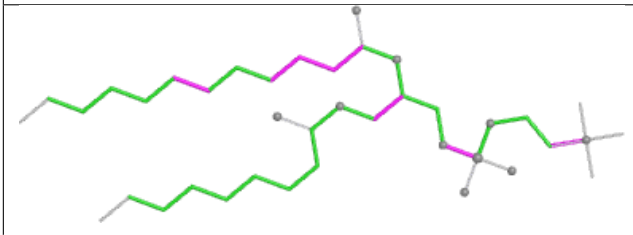

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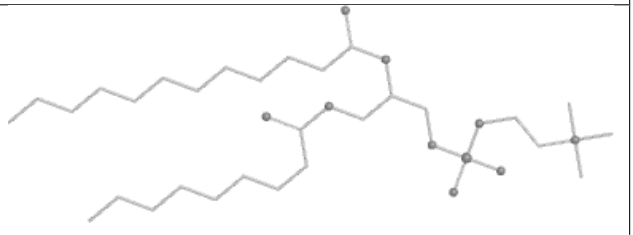
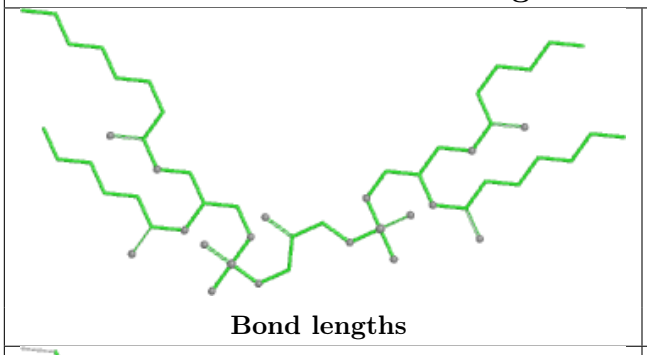


Rings

Ligand CDL M3 403



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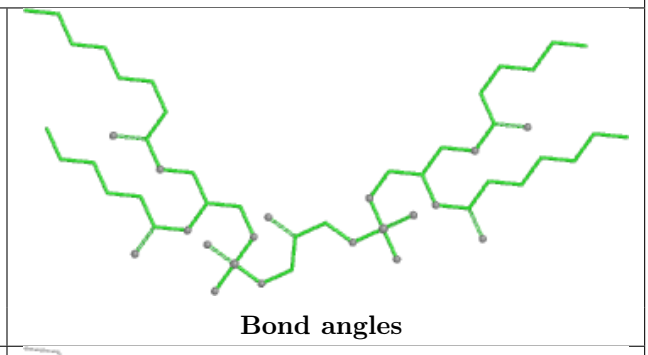

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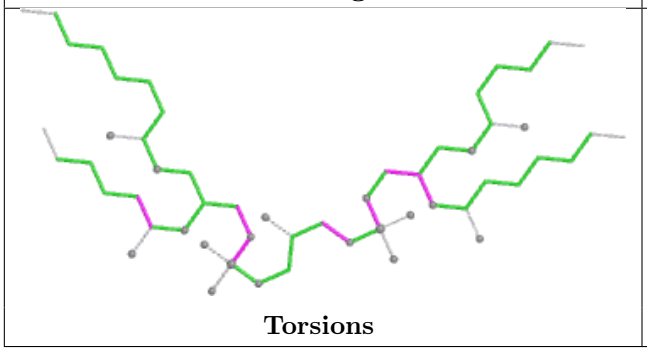

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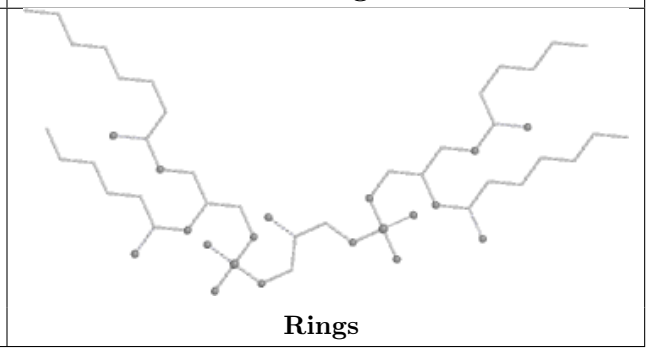
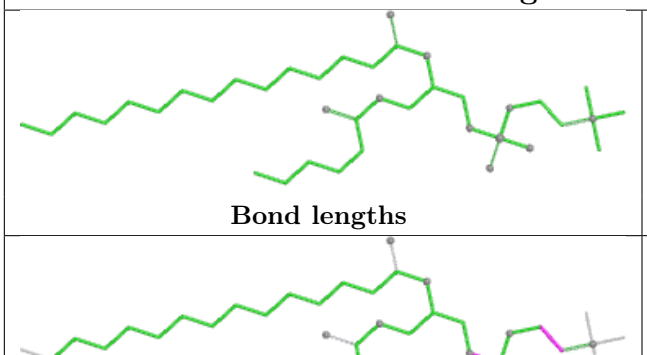


Rings

Ligand PC1 qE 303



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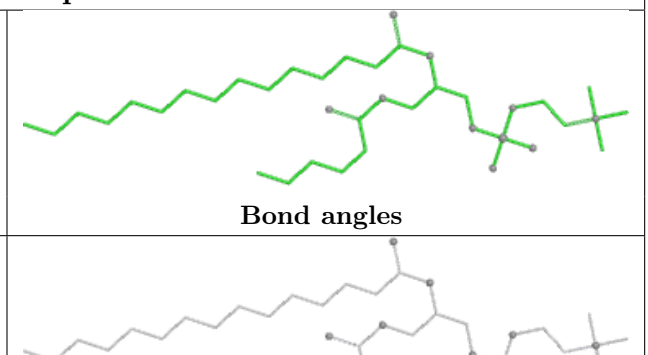

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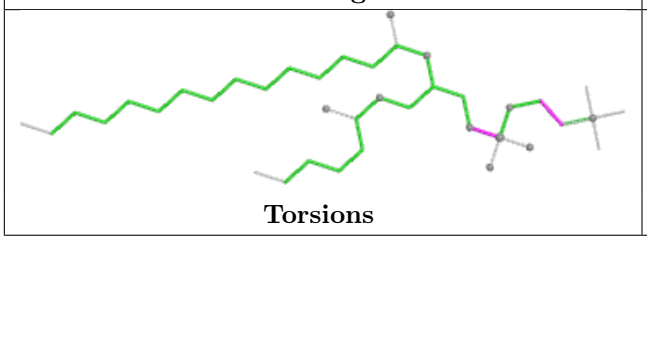

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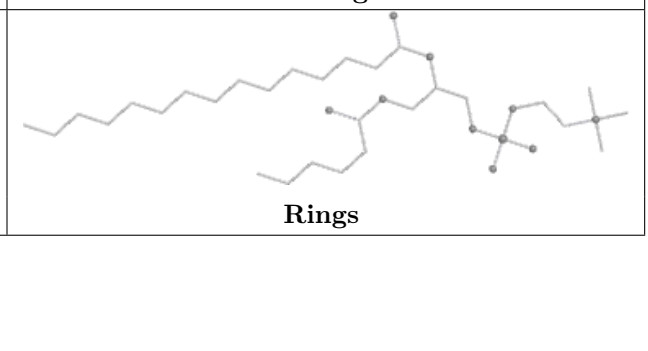
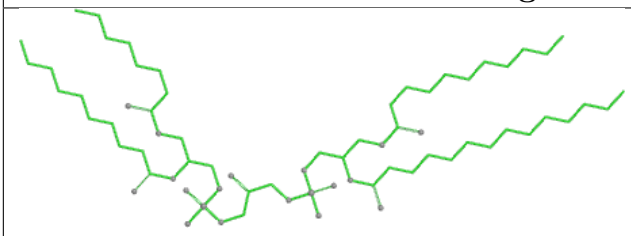


Rings

Ligand CDL Qi 202



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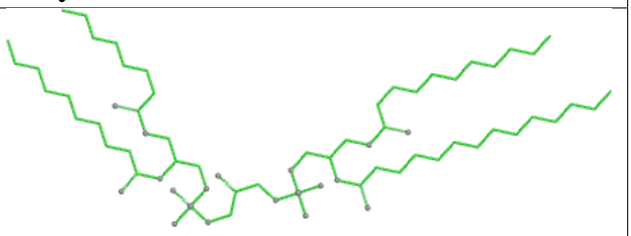
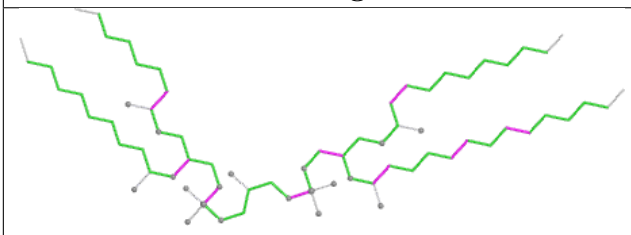


Bond angles



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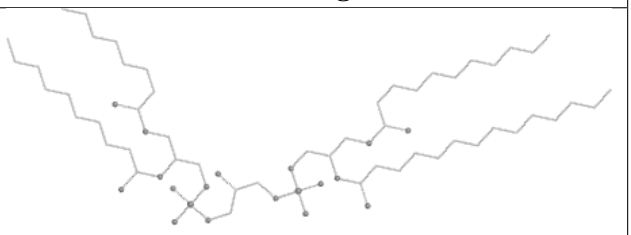
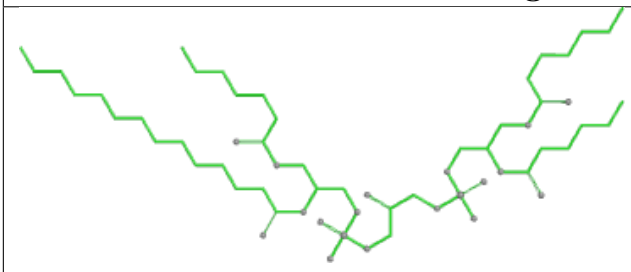


Rings

Ligand CDL B 501



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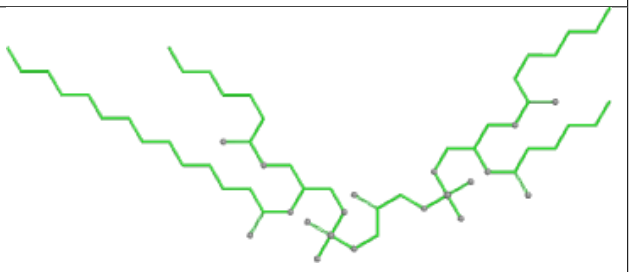
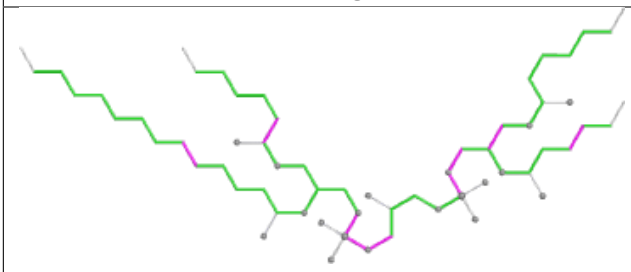


Bond angles



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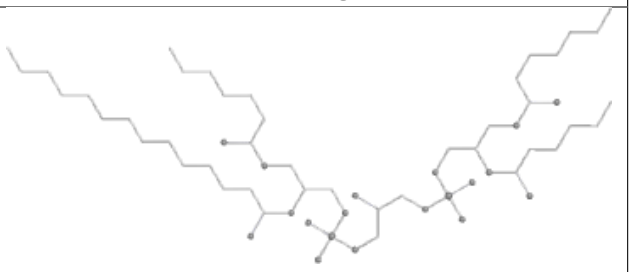
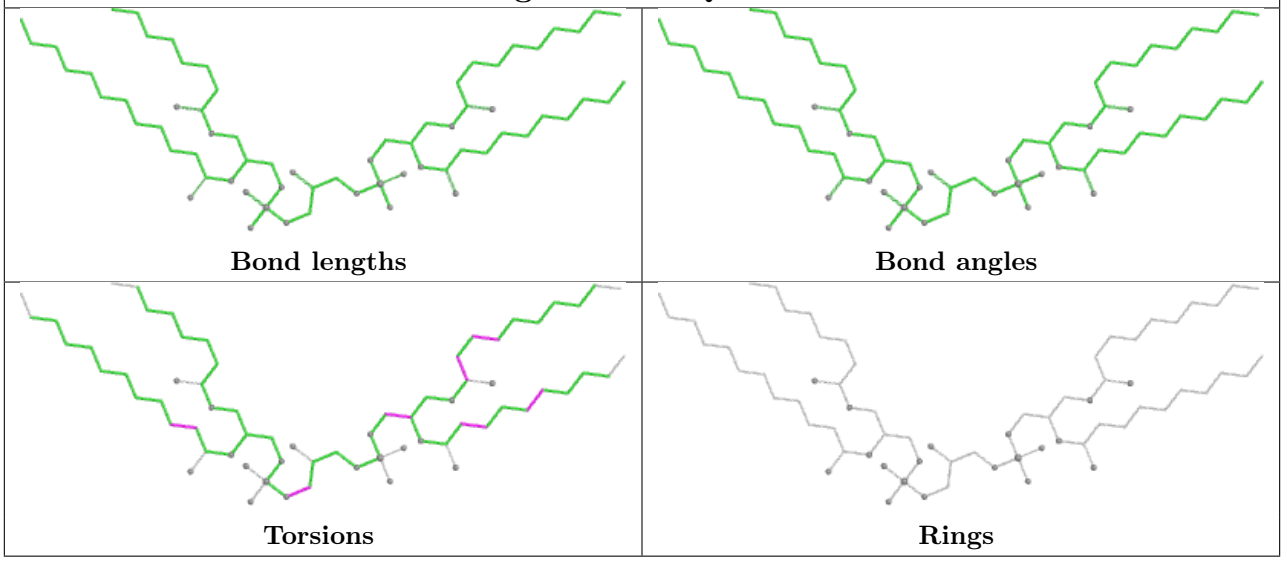
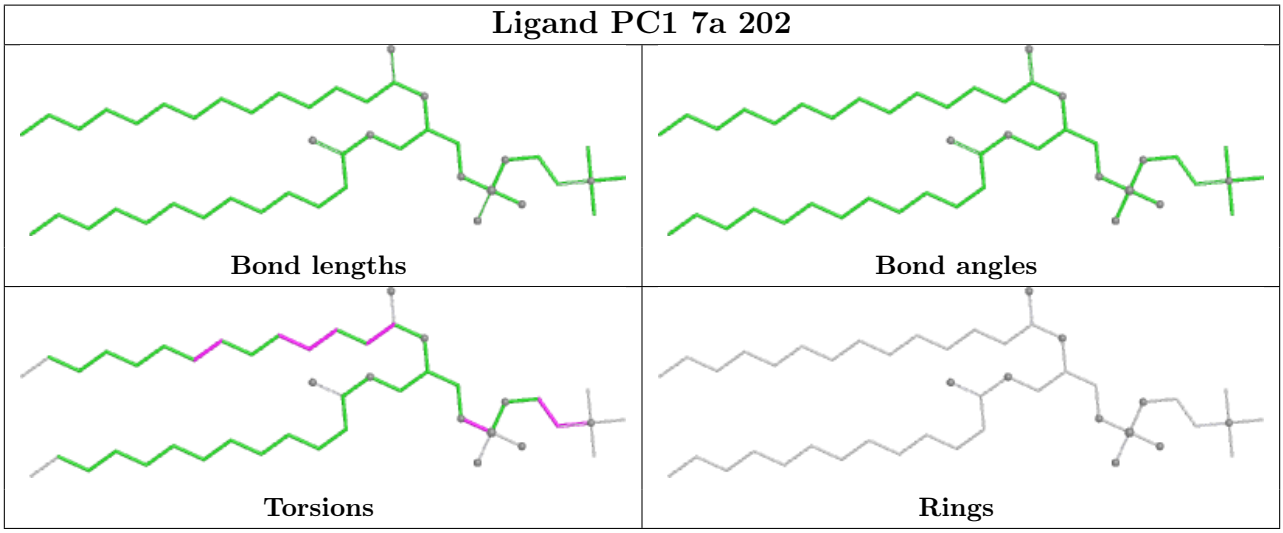


Rings

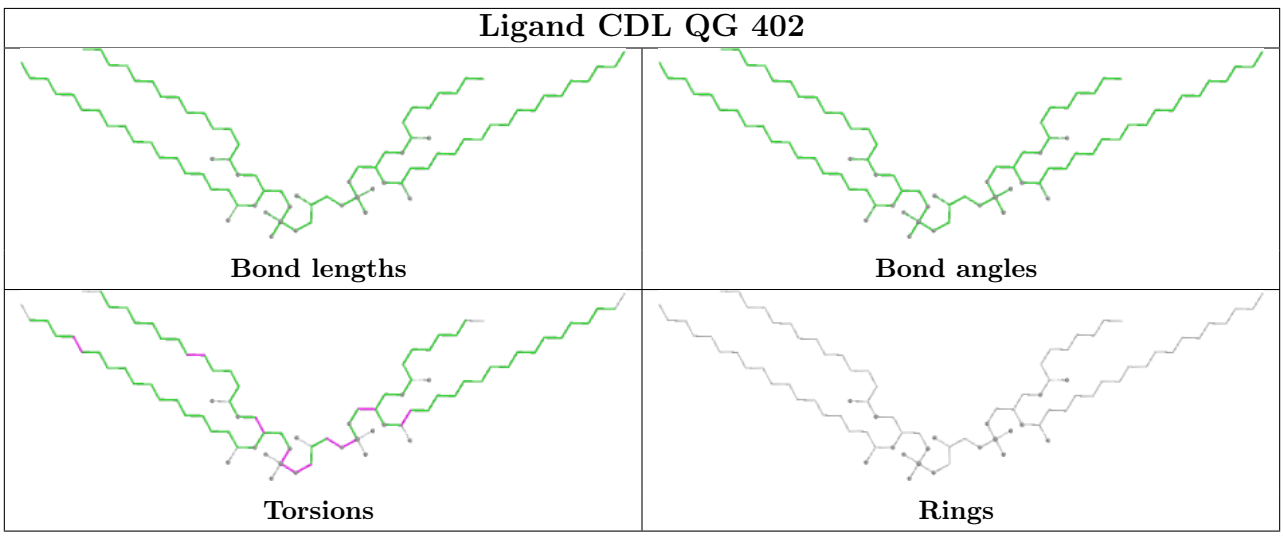
Ligand CDL Qb 601



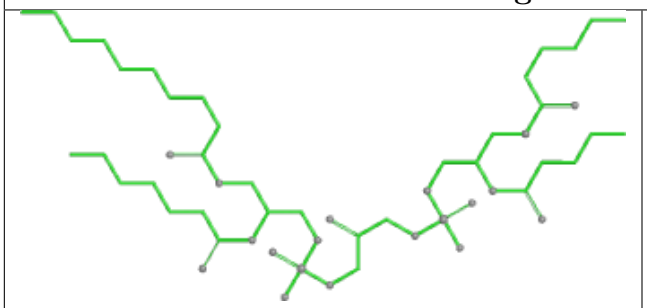
Ligand PC1 7a 202



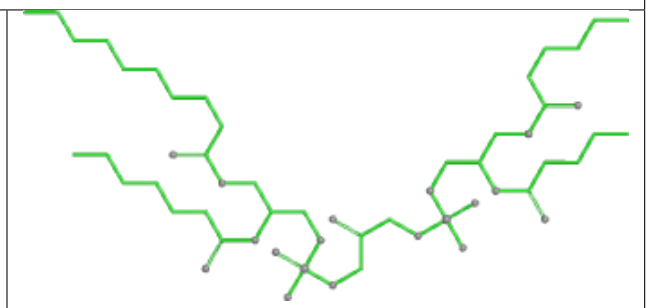
Ligand CDL QG 402



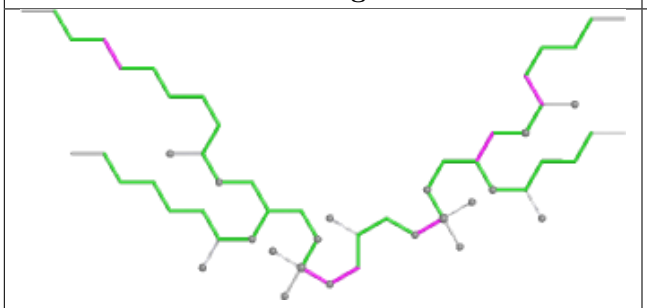
Ligand CDL am 201



Bond lengths



Bond angles



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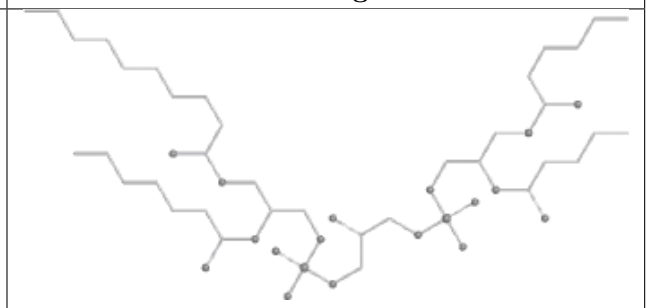
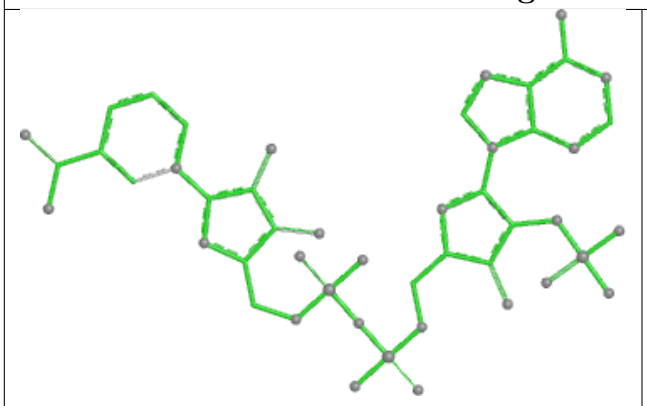
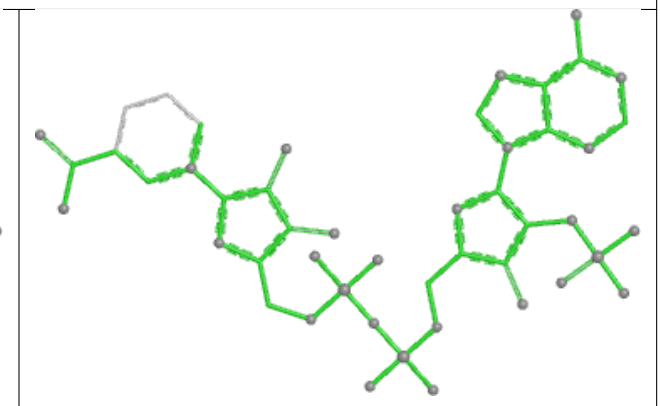


Rings

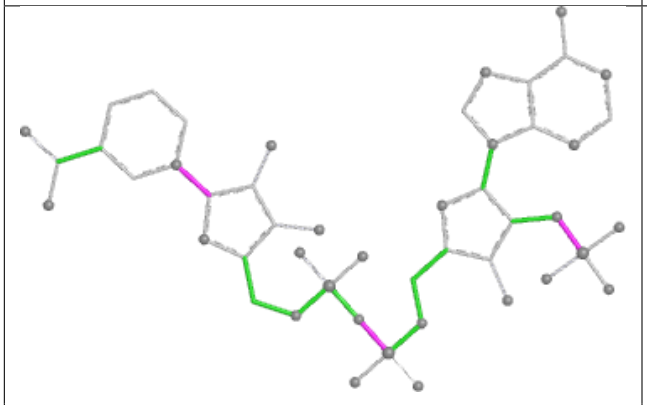
Ligand NDP a9 401



Bond lengths



Bond angles



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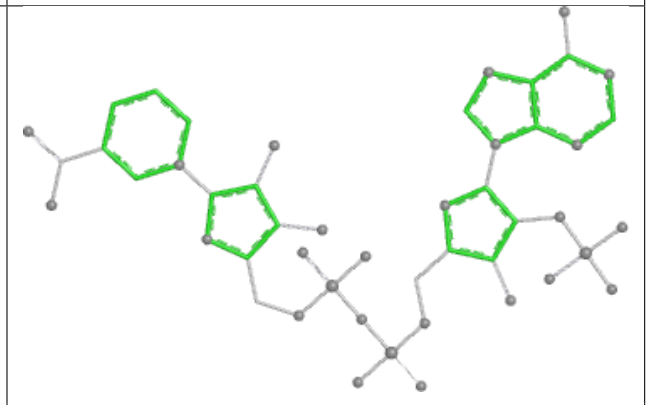
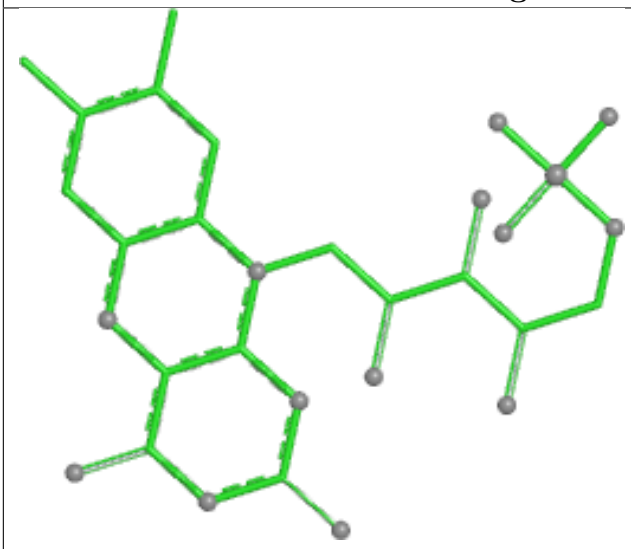


Rings

Ligand FMN V1 501



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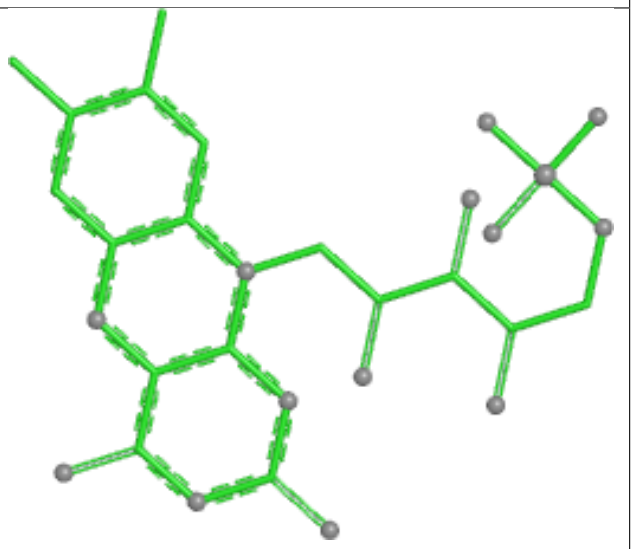

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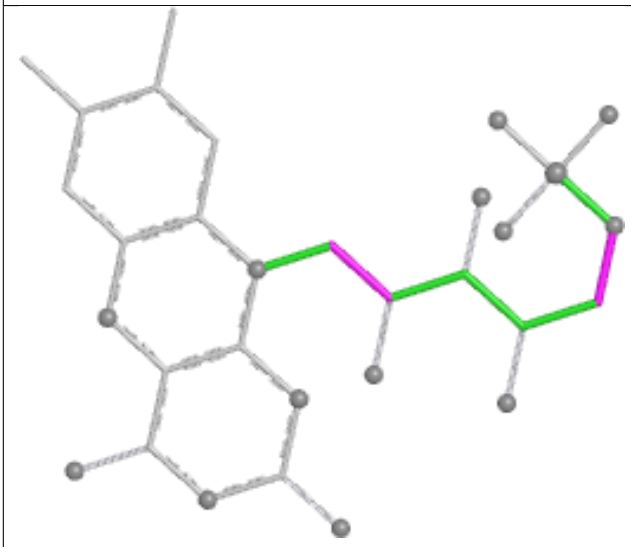
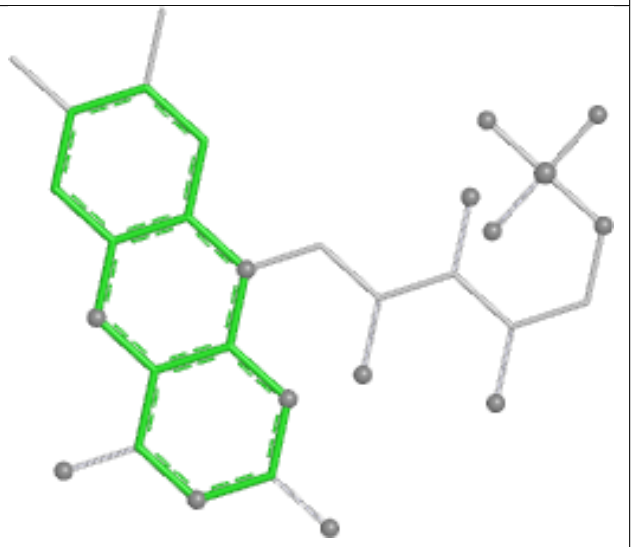
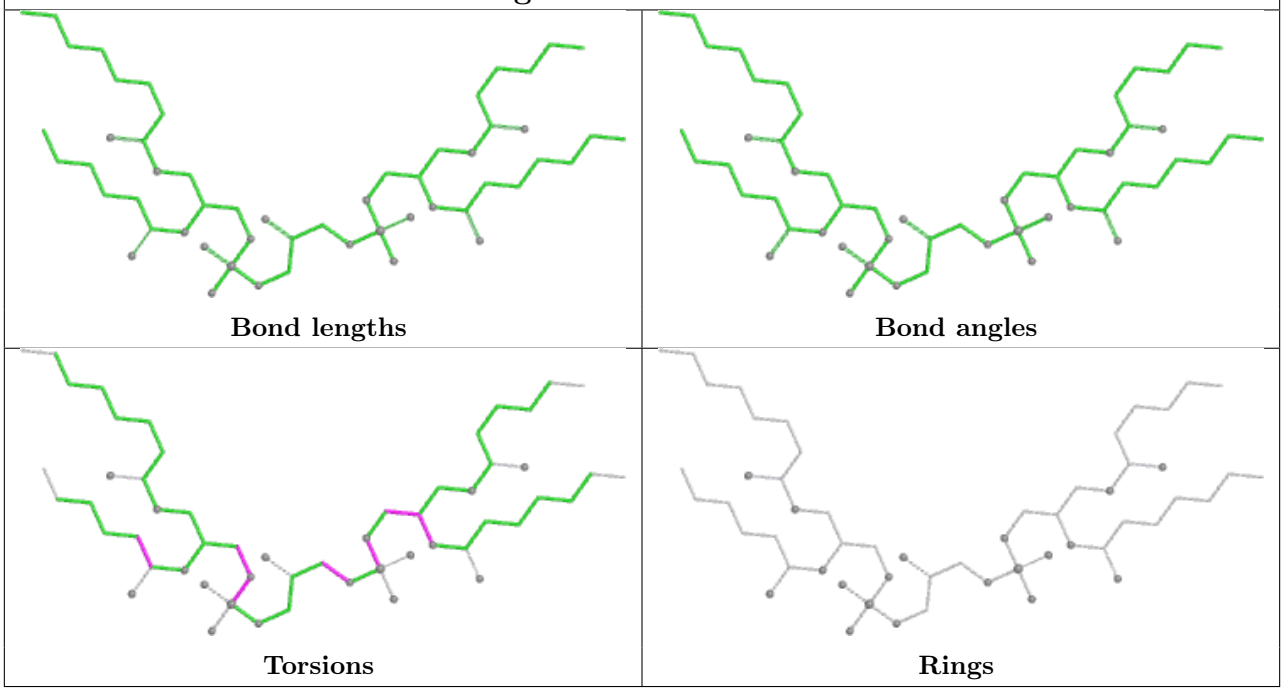


Torsions

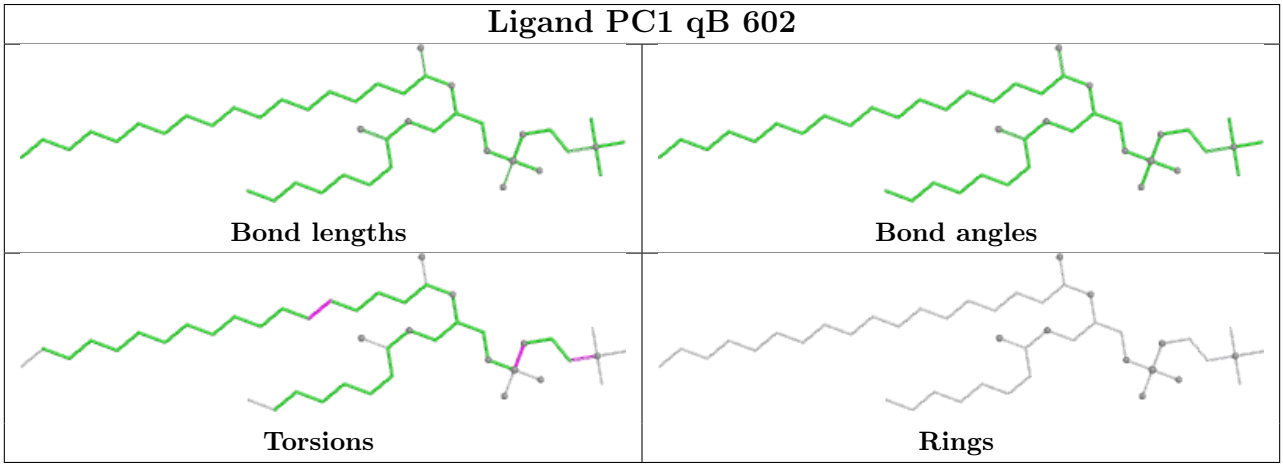


Rings

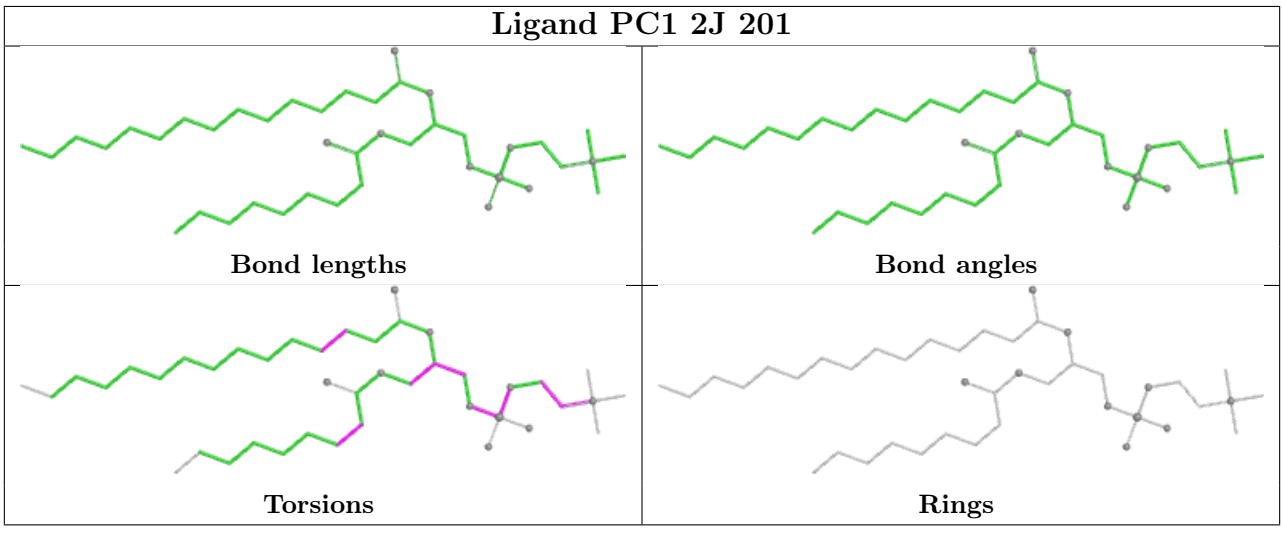
Ligand CDL m3 403



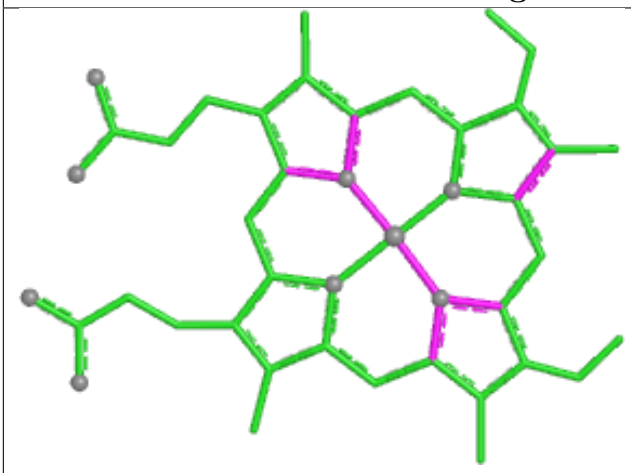
Ligand PC1 qB 602



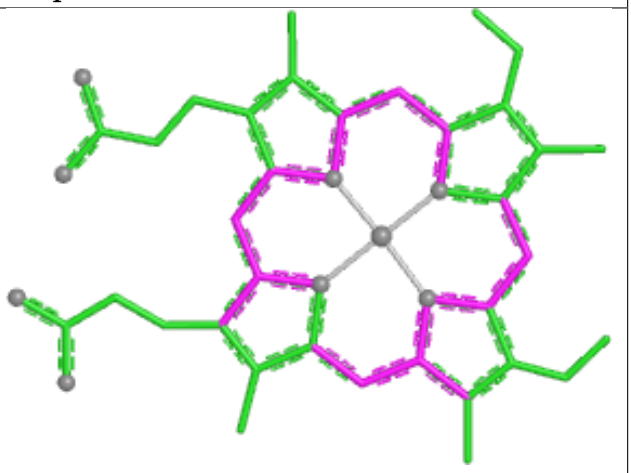
Ligand PC1 2J 201



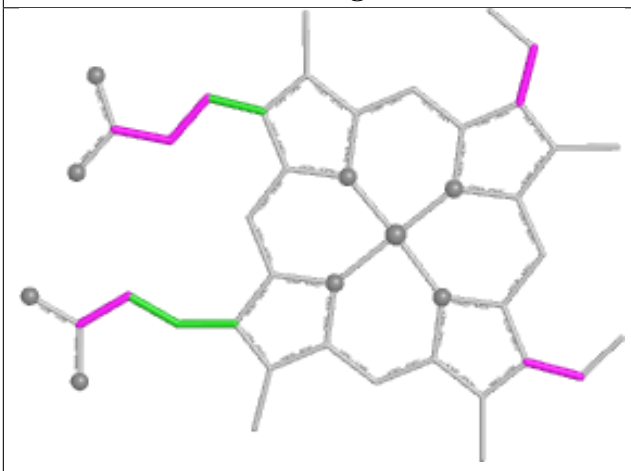
Ligand HEM qC 502



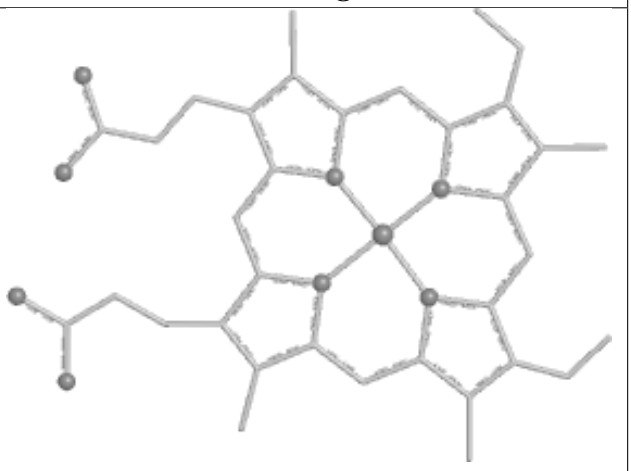
Bond lengths



Bond angles

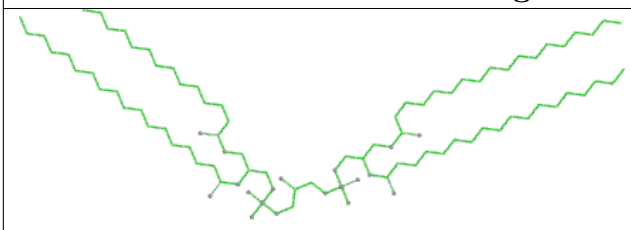


Torsions

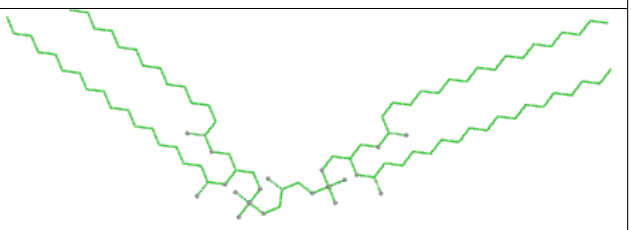


Rings

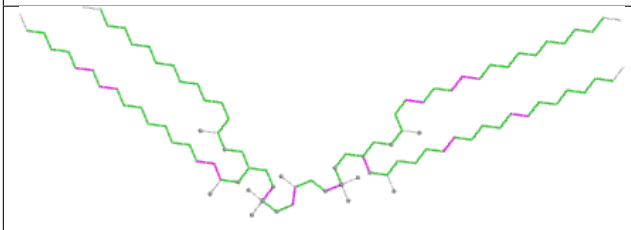
Ligand CDL 2m 101



Bond lengths



Bond angles



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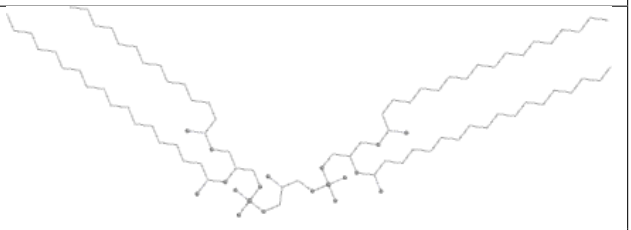
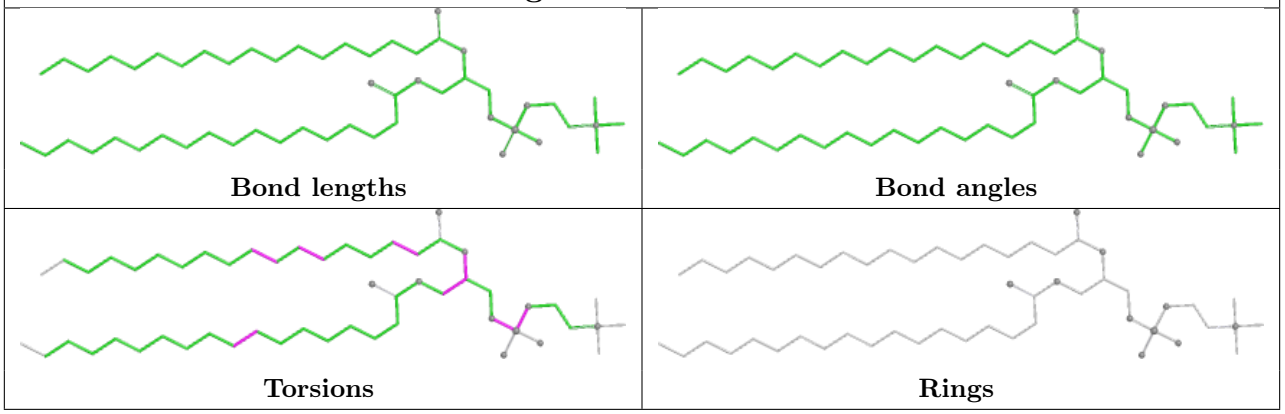
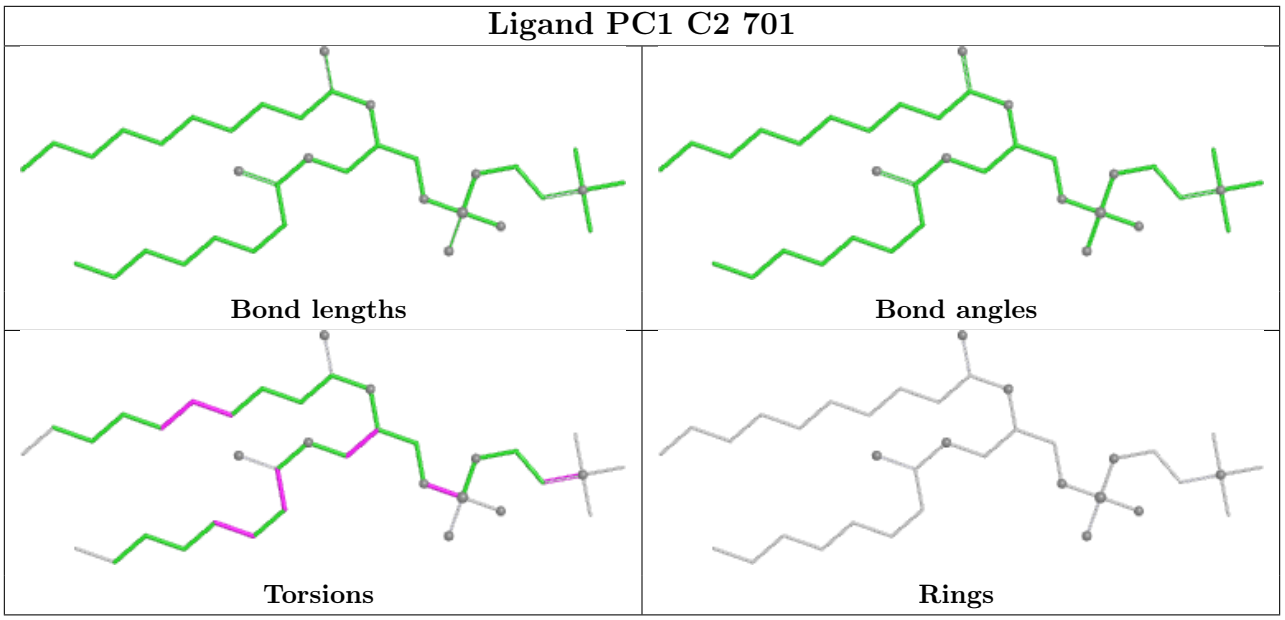


Rings

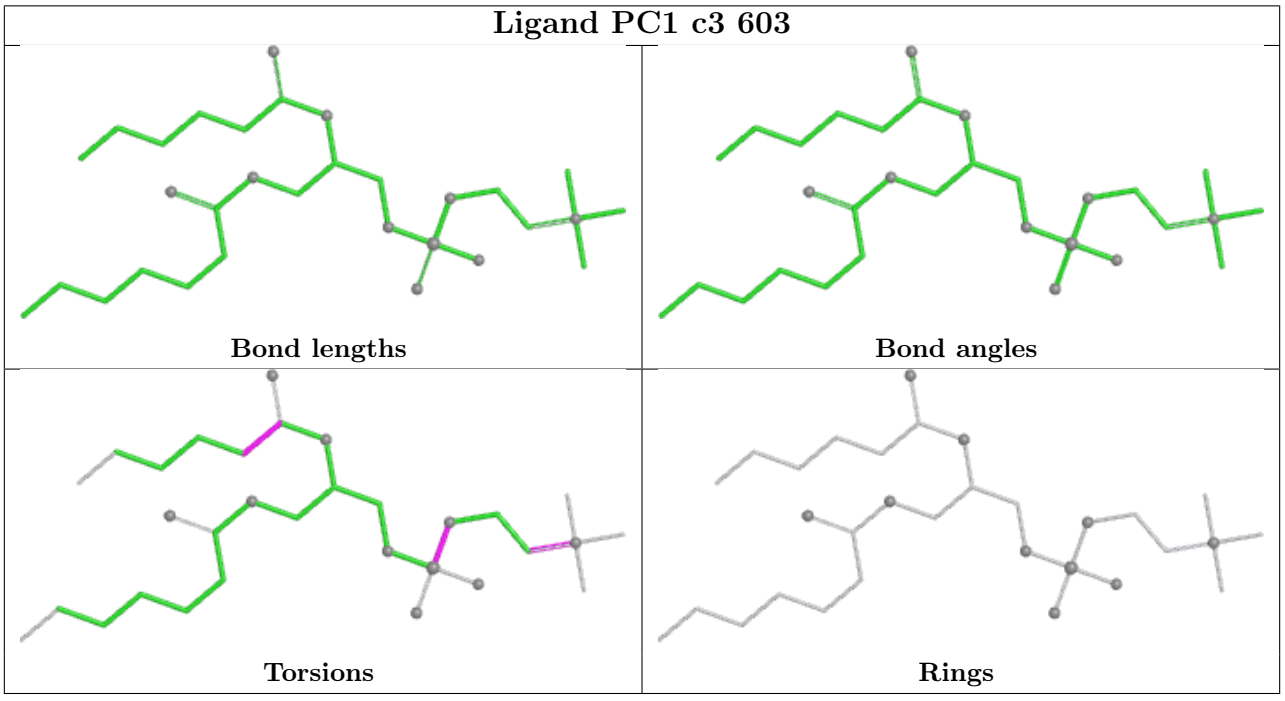
Ligand PC1 t4 303



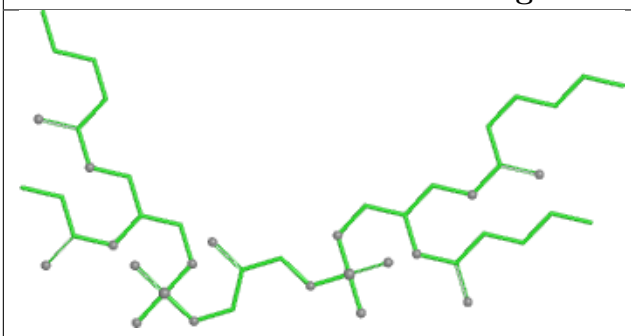
Ligand PC1 C2 701



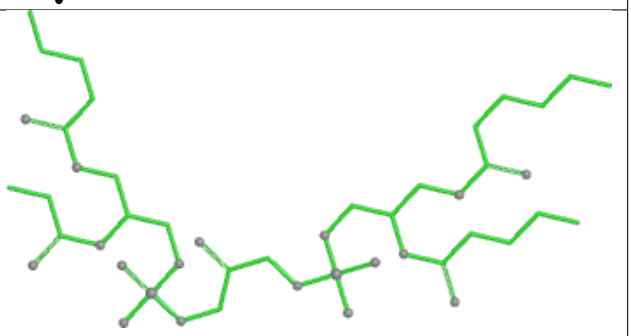
Ligand PC1 c3 603



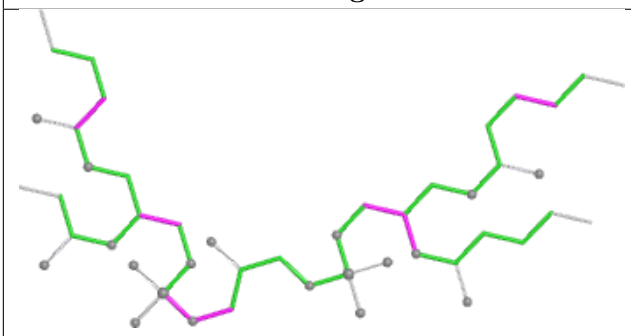
Ligand CDL Qc 508



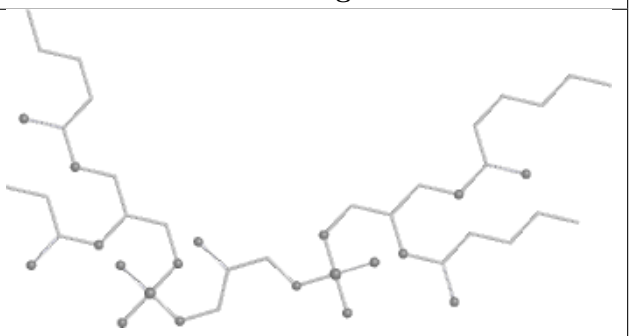
Bond lengths



Bond angles

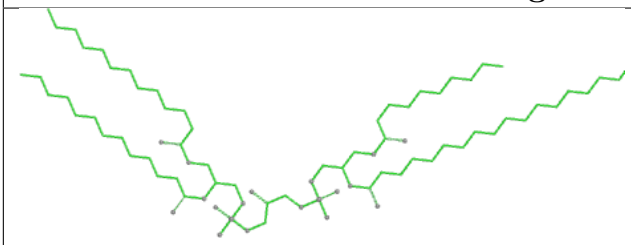


Torsions

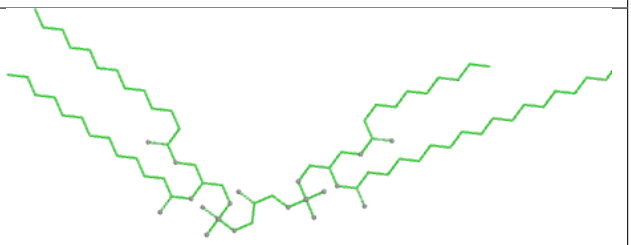


Rings

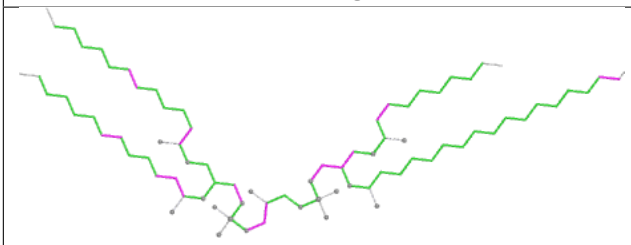
Ligand CDL a 505



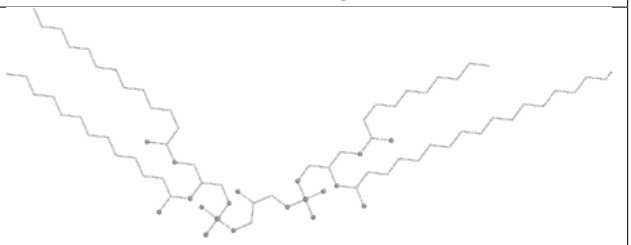
Bond lengths



Bond angles

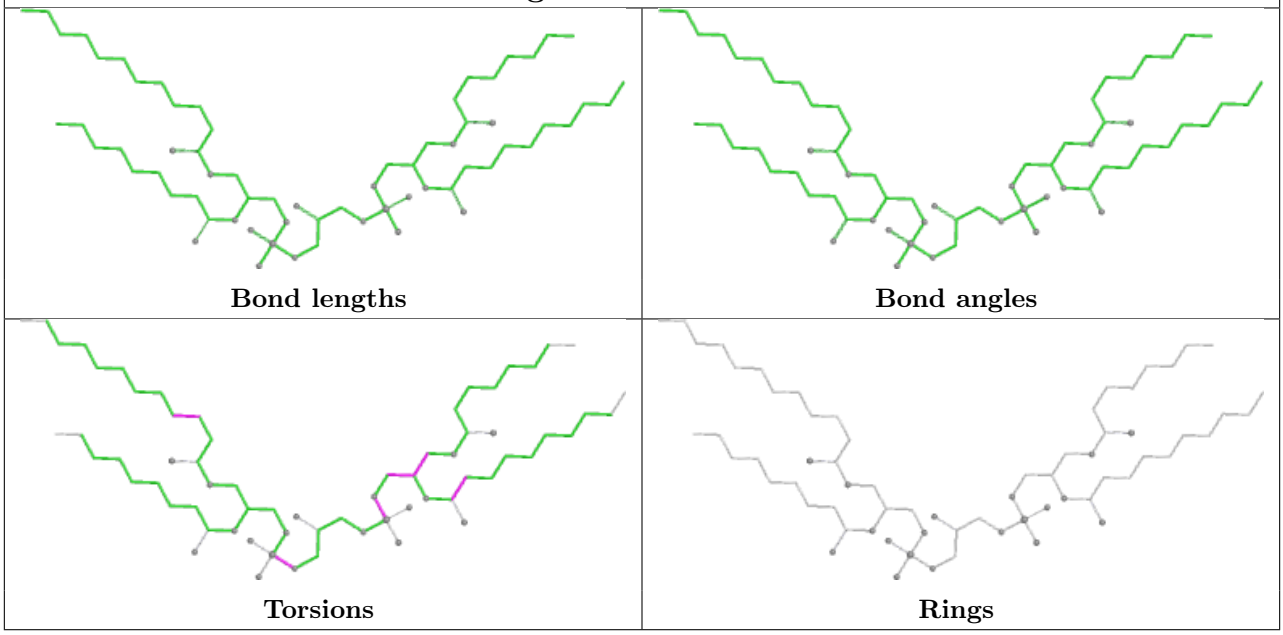


Torsions

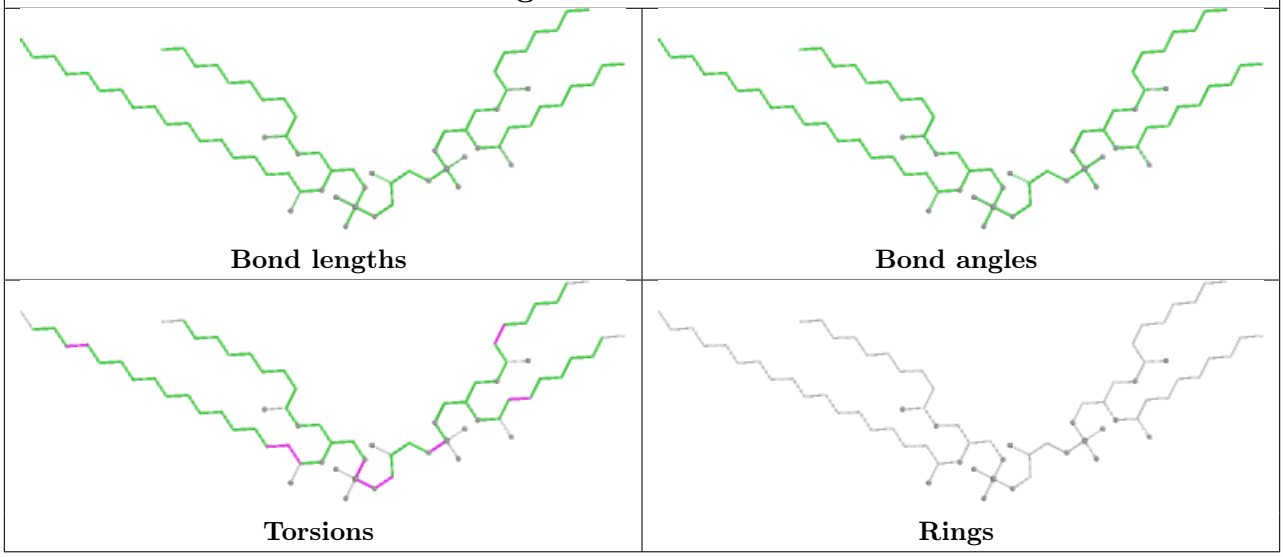


Rings

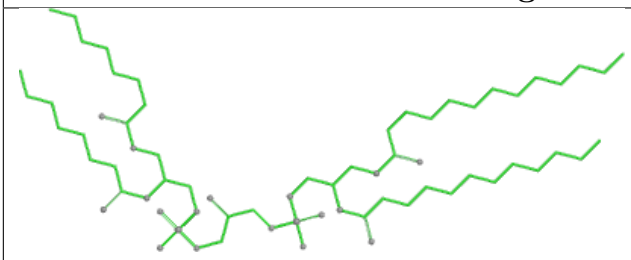
Ligand CDL Z 101



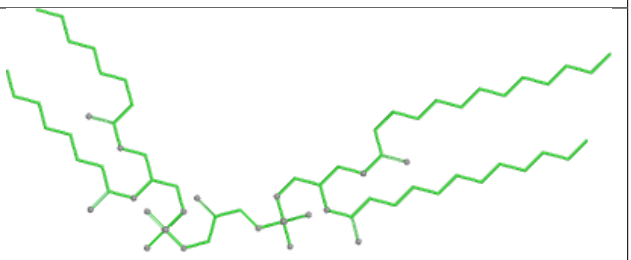
Ligand CDL T7 201



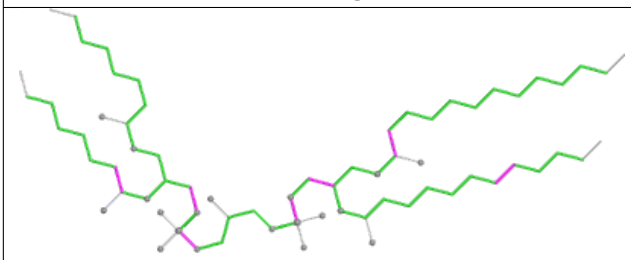
Ligand CDL b8 302



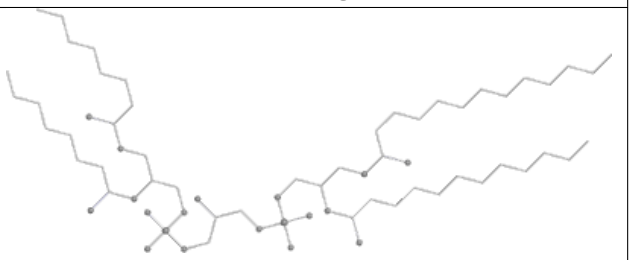
Bond lengths



Bond angles

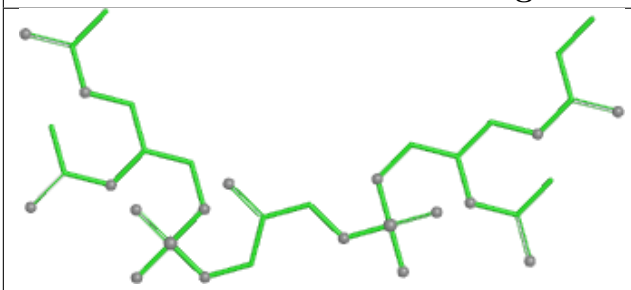


Torsions

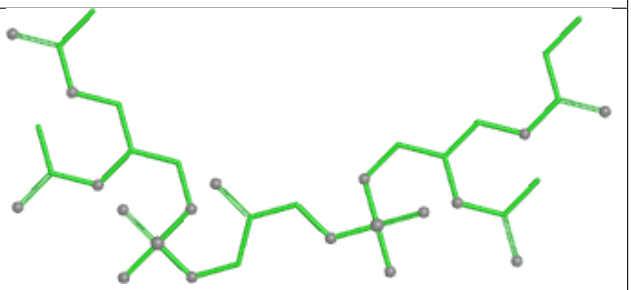


Rings

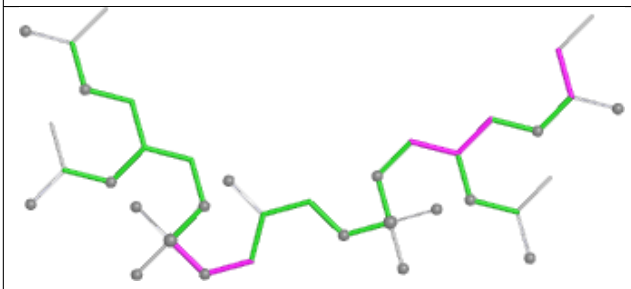
Ligand CDL B4 201



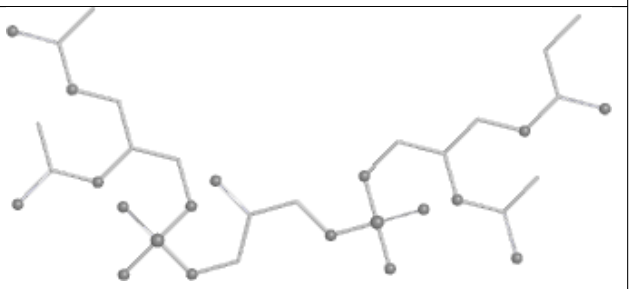
Bond lengths



Bond angles

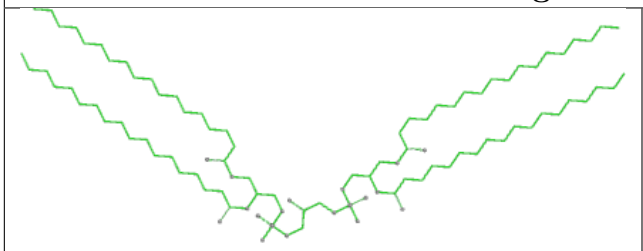


Torsions

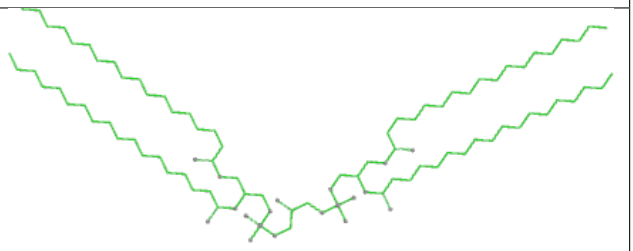


Rings

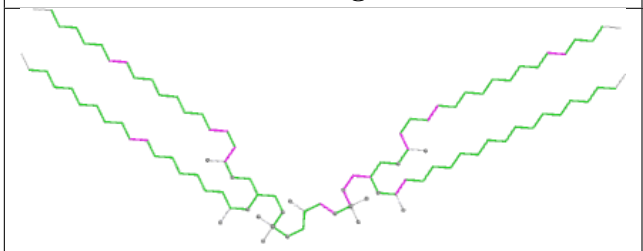
Ligand CDL f 401



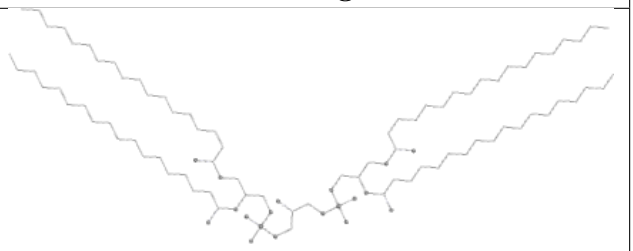
Bond lengths



Bond angles

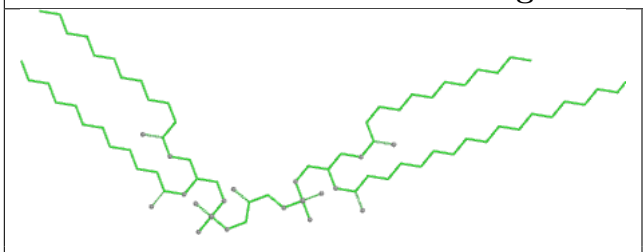


Torsions

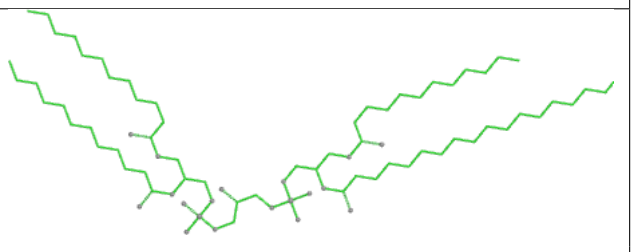


Rings

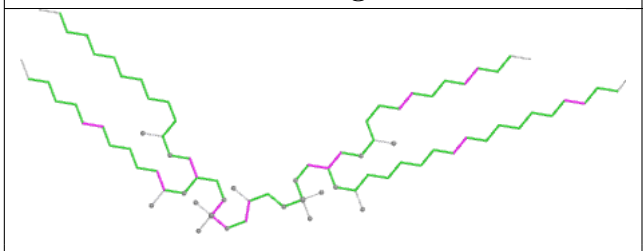
Ligand CDL B3 102



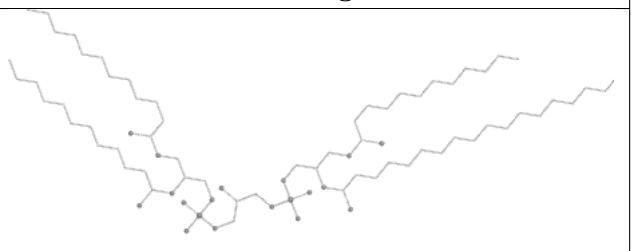
Bond lengths



Bond angles

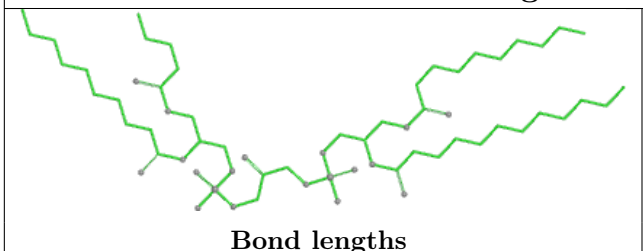


Torsions

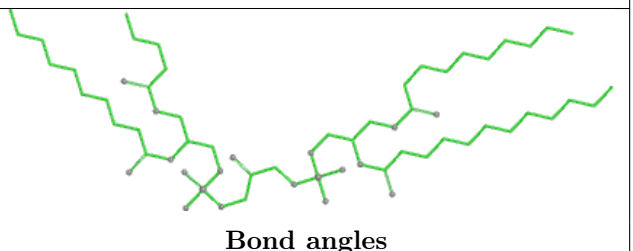


Rings

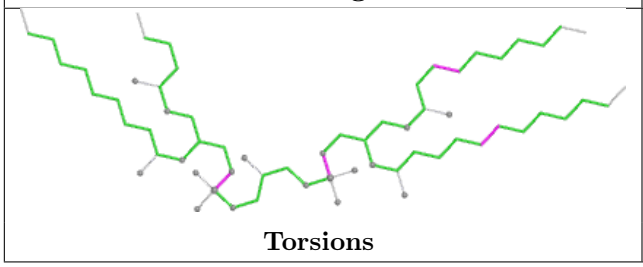
Ligand CDL c1 703



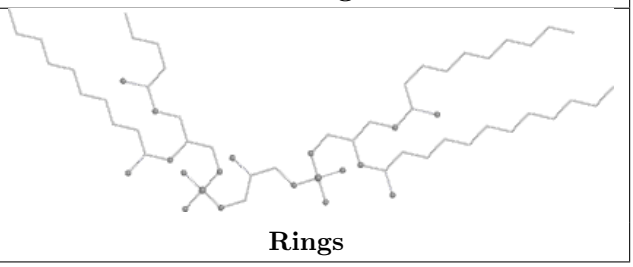
Bond lengths



Bond angles

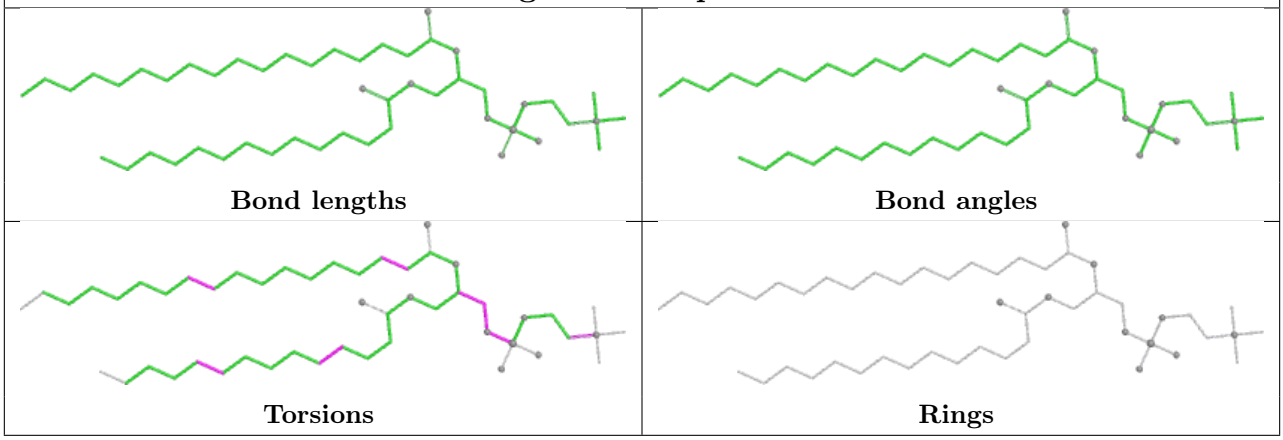


Torsions

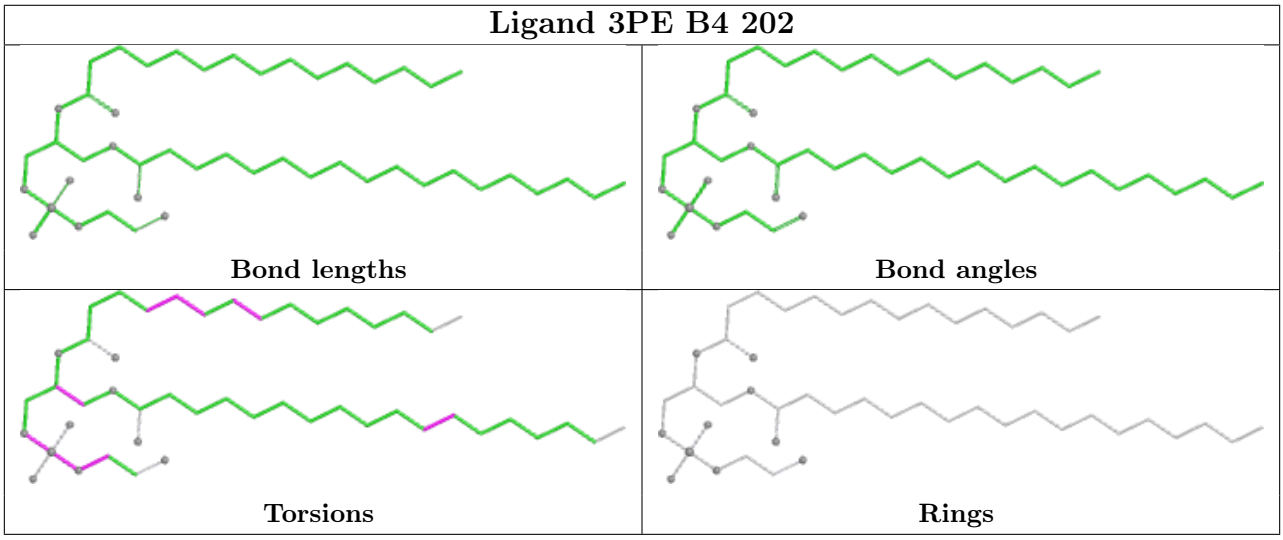


Rings

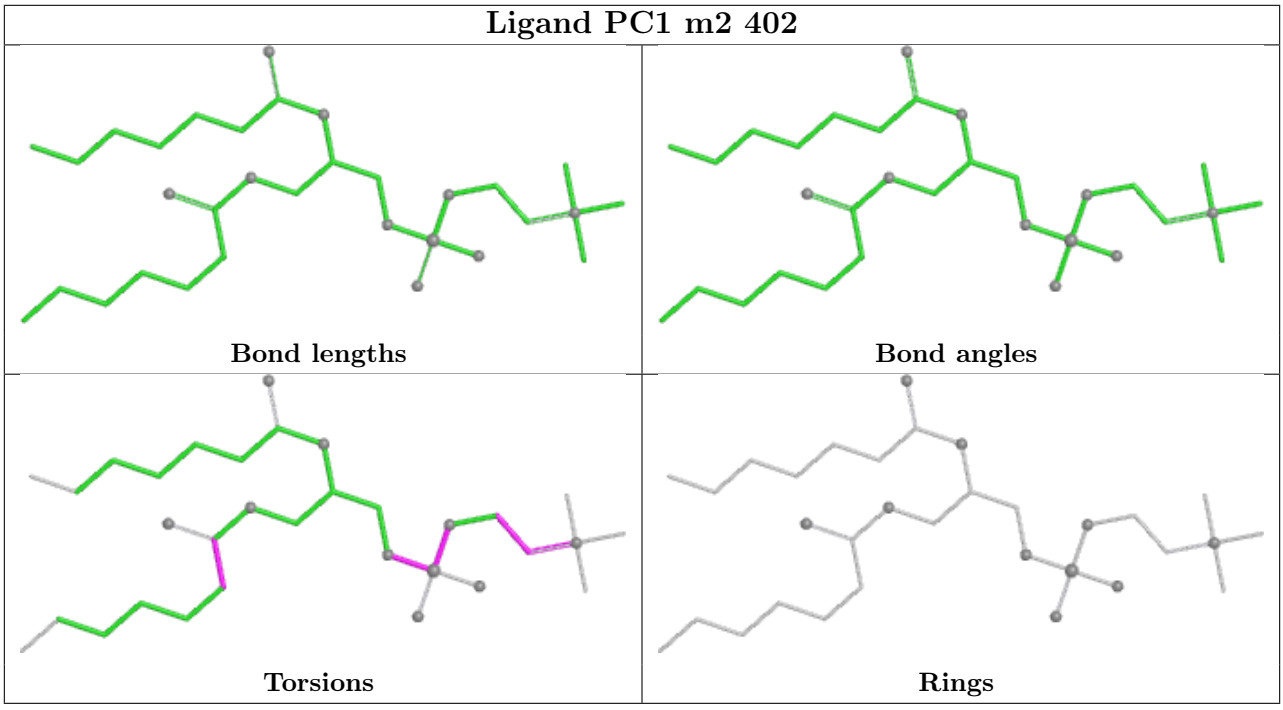
Ligand PC1 qC 507



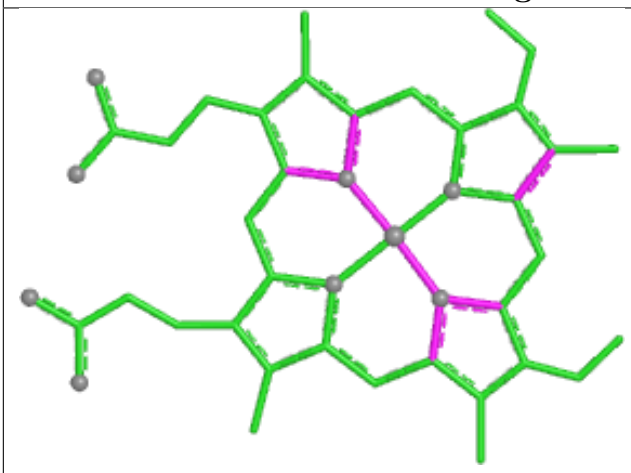
Ligand 3PE B4 202



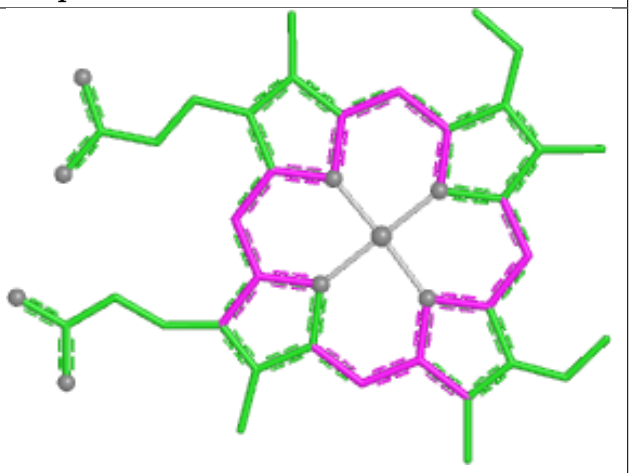
Ligand PC1 m2 402



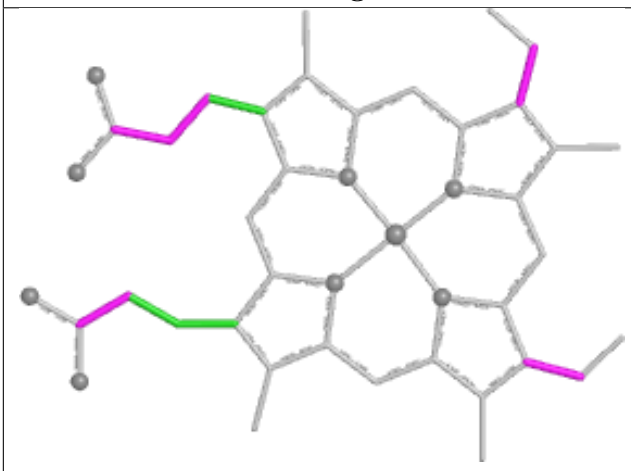
Ligand HEM qc 503



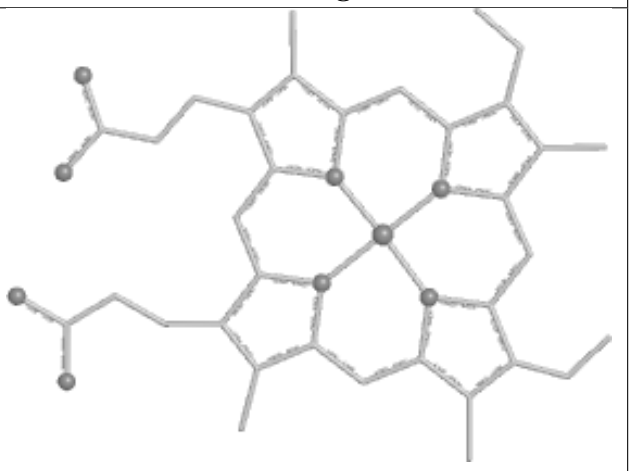
Bond lengths



Bond angles

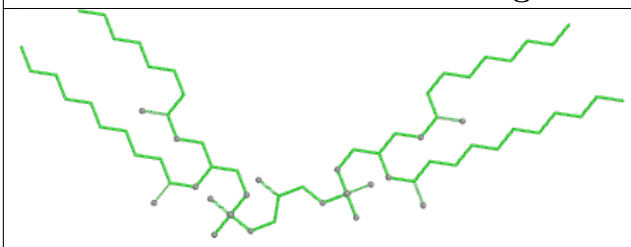


Torsions

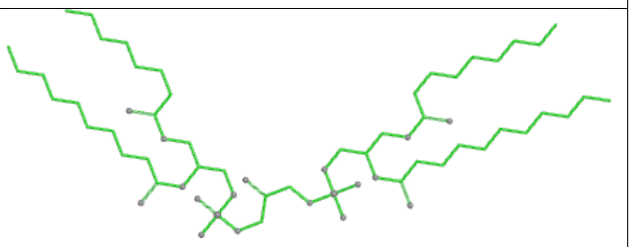


Rings

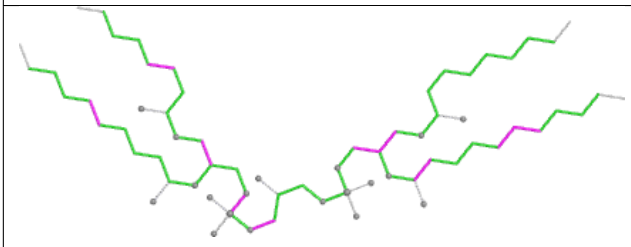
Ligand CDL m1 402



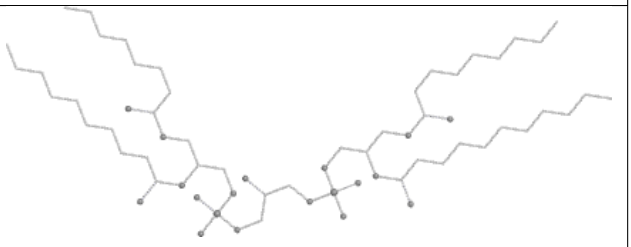
Bond lengths



Bond angles

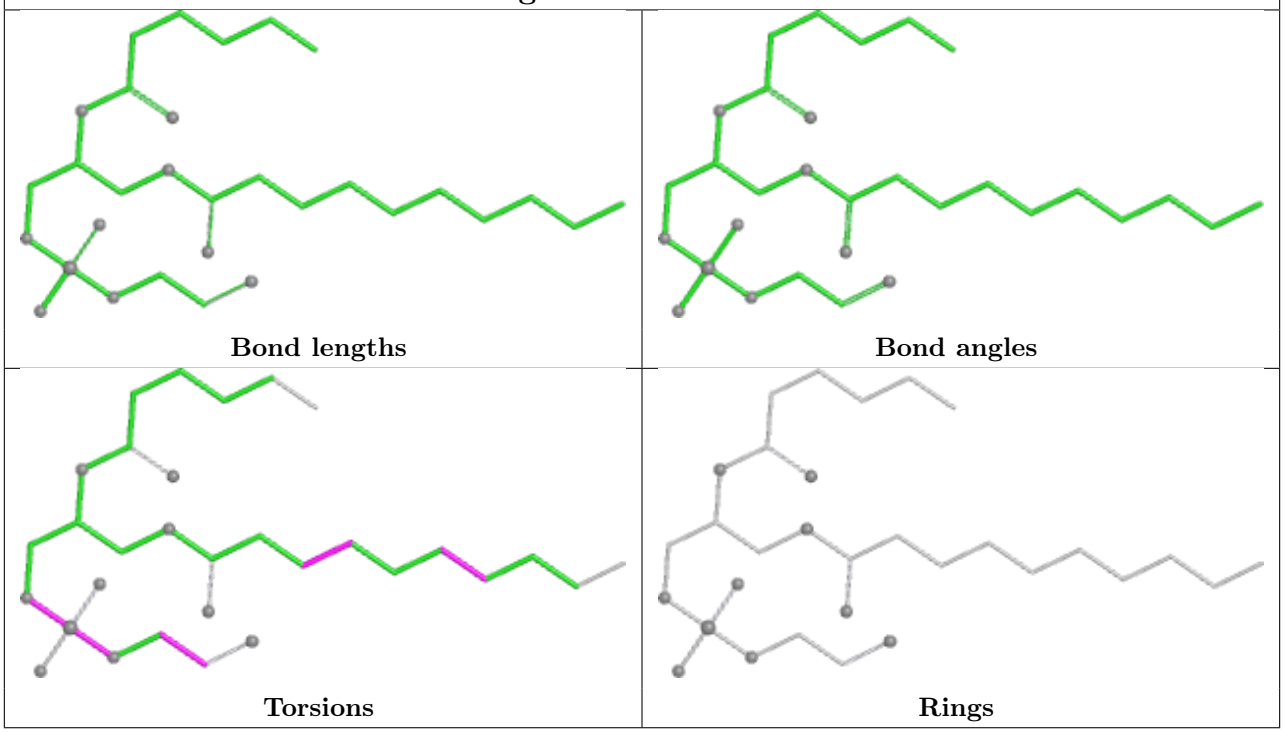


Torsions

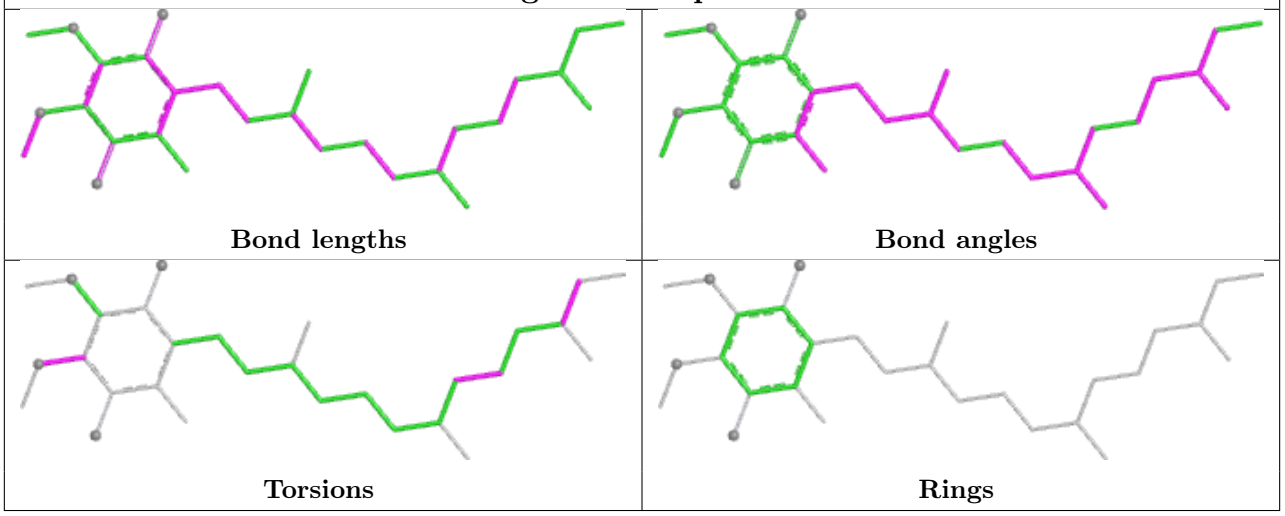


Rings

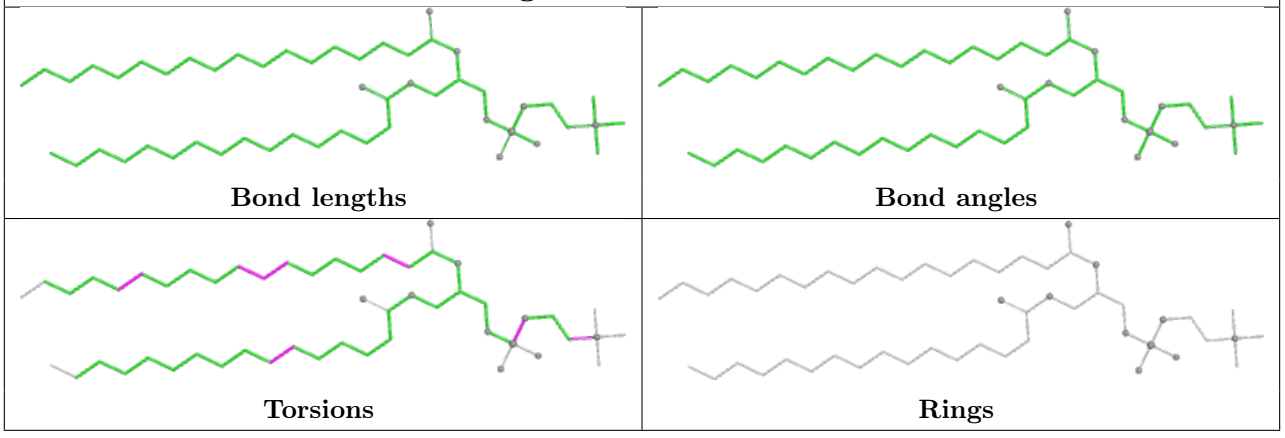
Ligand 3PE m2 408



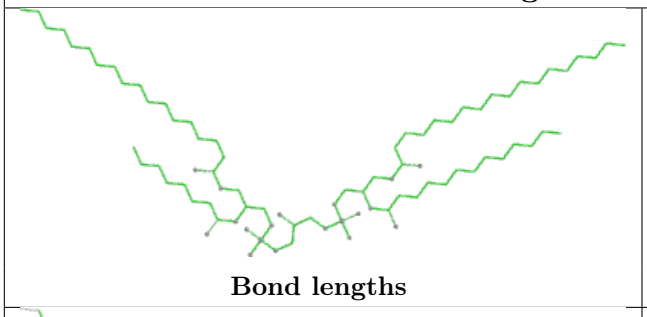
Ligand U10 qC 506



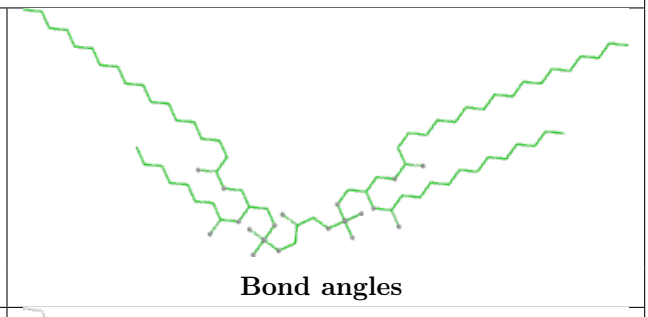
Ligand PC1 N5 801



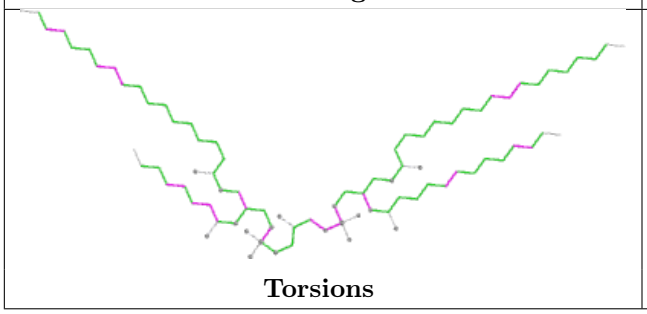
Ligand CDL 7c 301



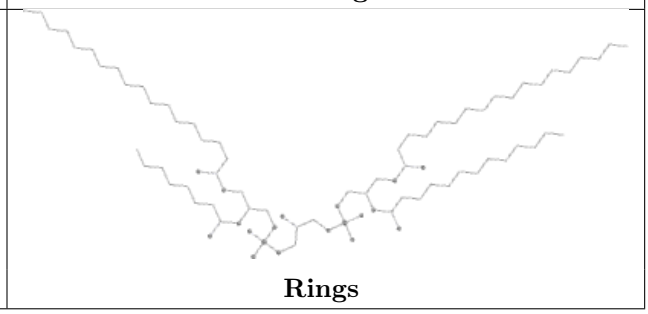
Bond lengths



Bond angles

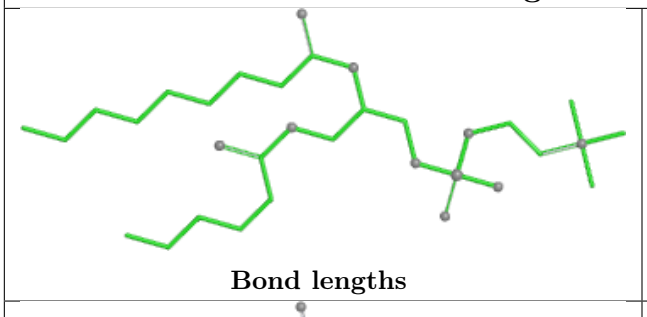


Torsions

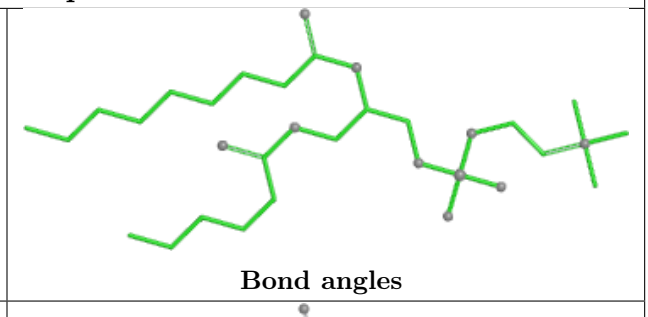


Rings

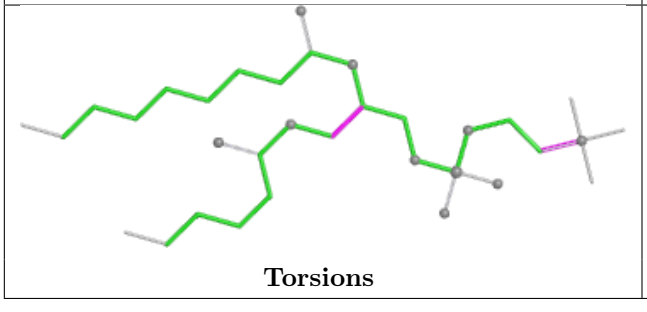
Ligand PC1 qe 301



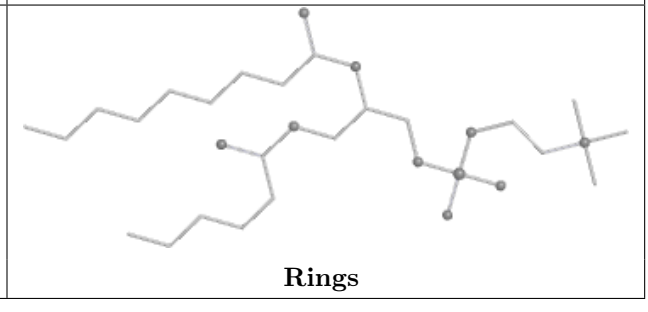
Bond lengths



Bond angles

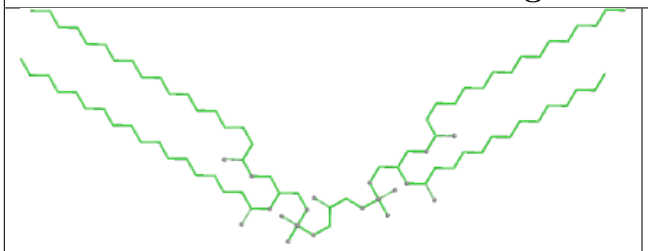


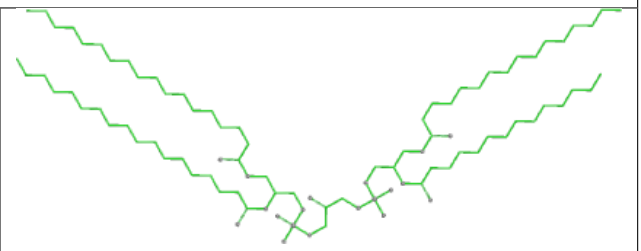
Torsions

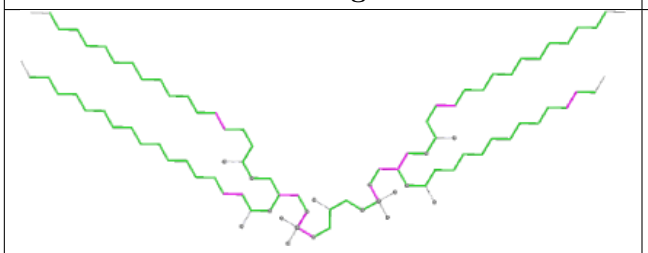


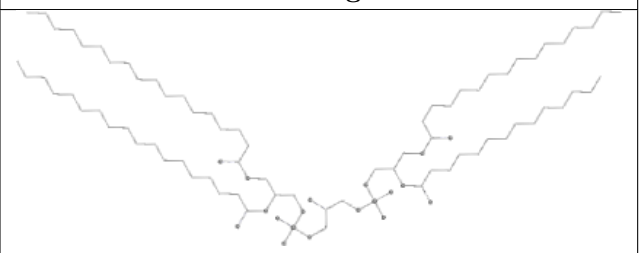
Rings

Ligand CDL A 504

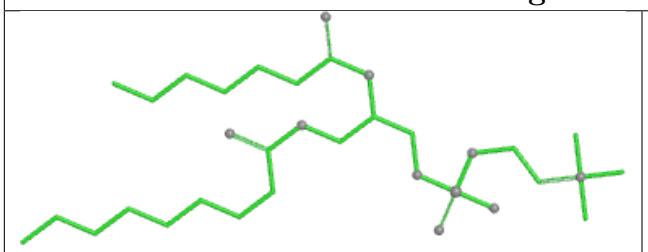

Bond lengths


Bond angles


Torsions


Rings

Ligand PC1 w 204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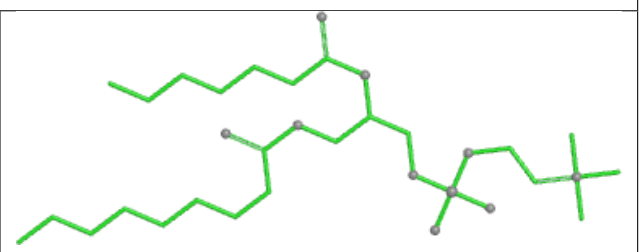
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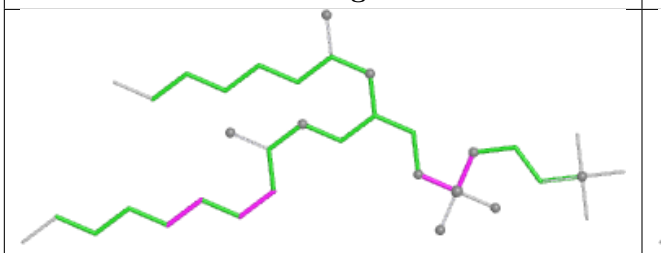
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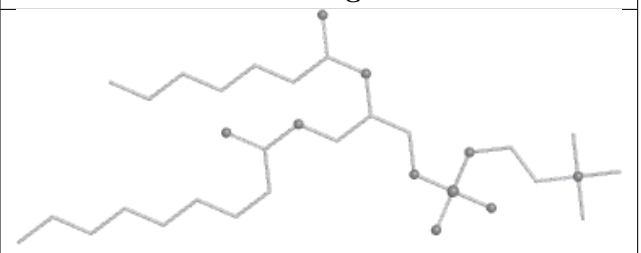
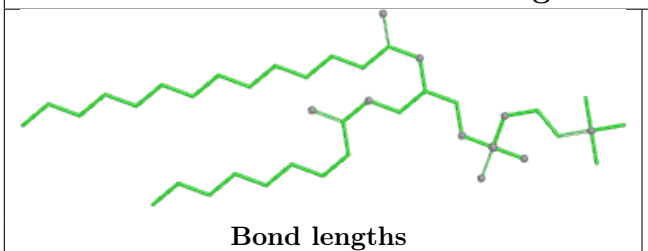

Rings

Ligand PC1 a 501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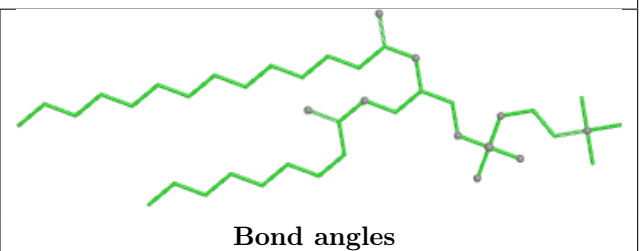
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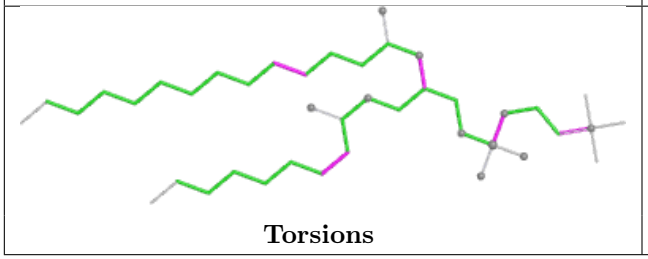
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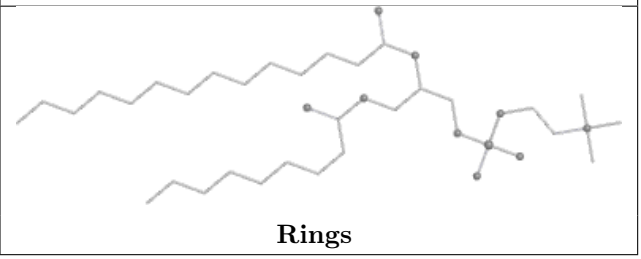
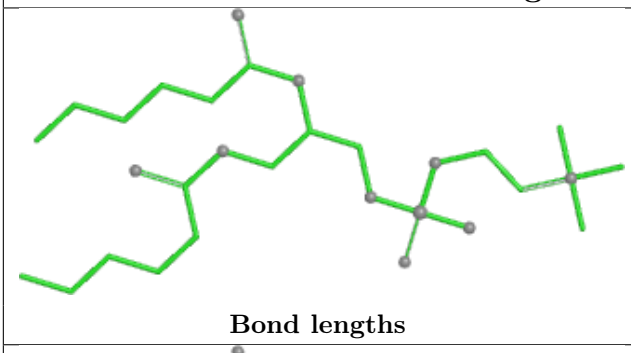

Rings

Ligand PC1 s8 301



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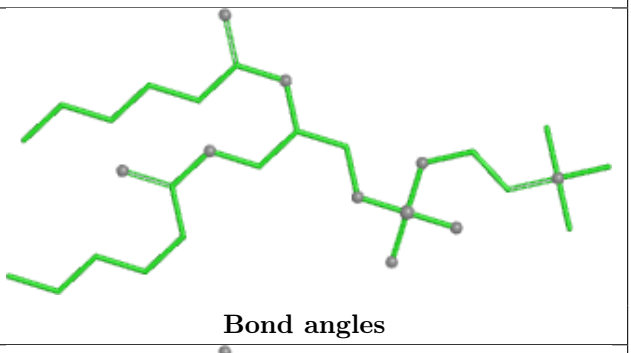
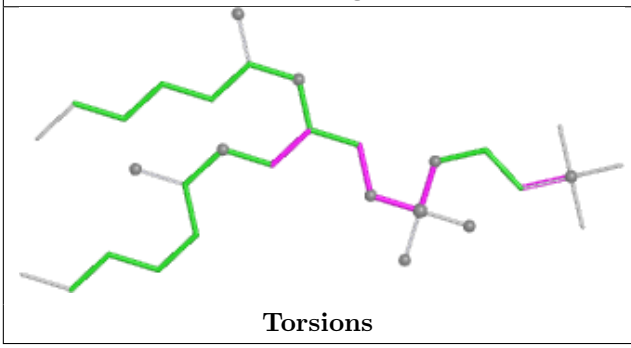


Bond angles



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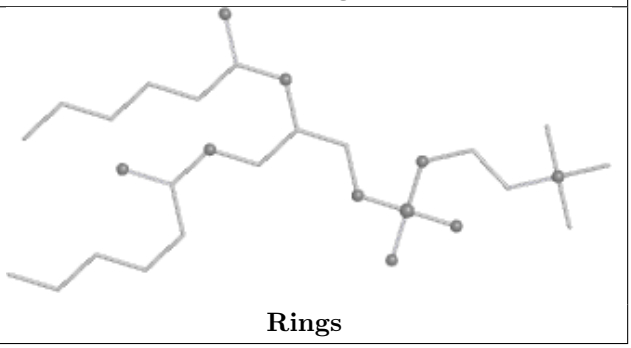
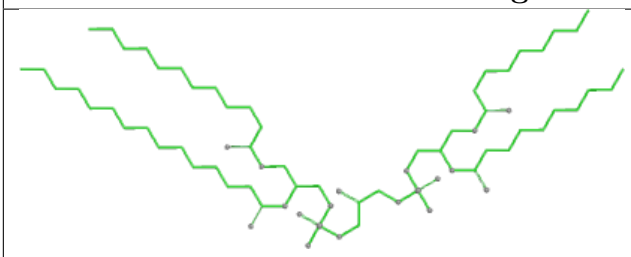


Rings

Ligand CDL M2 404



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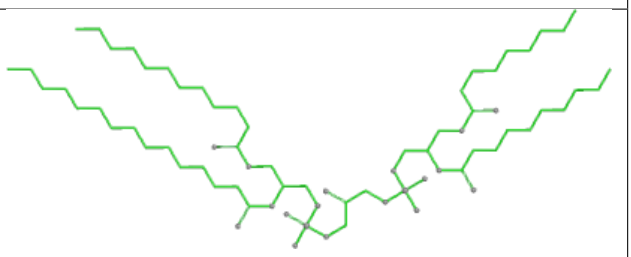
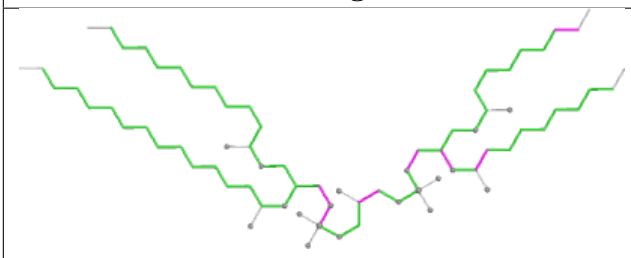


Bond angles



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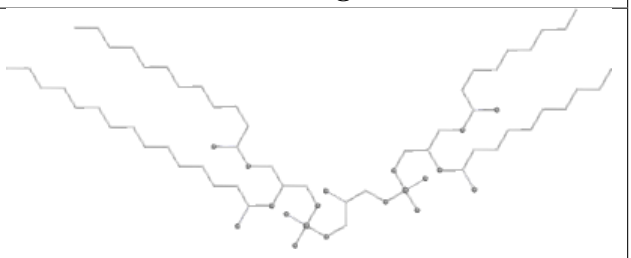
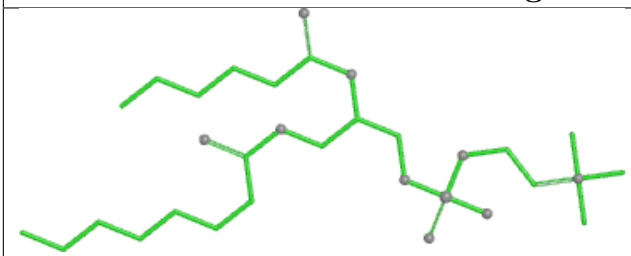


Rings

Ligand PC1 te 102



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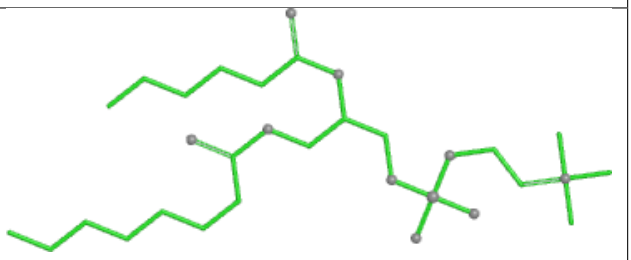
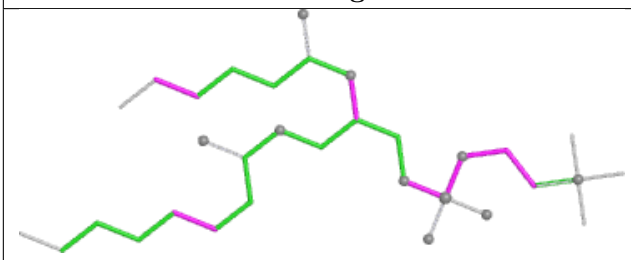


Bond angles



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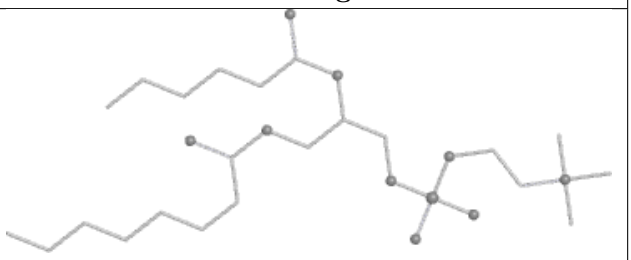
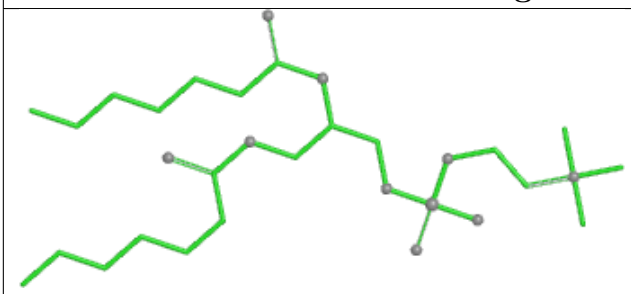


Rings

Ligand PC1 M2 402



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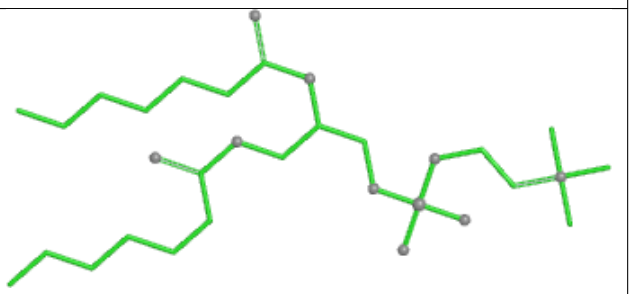

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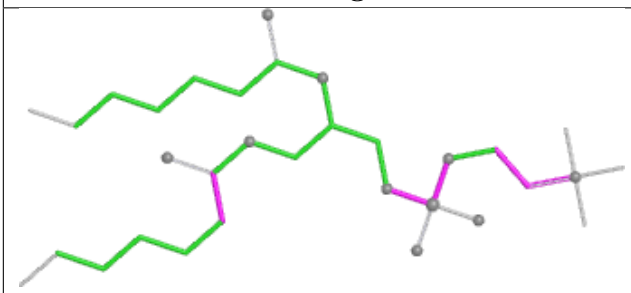

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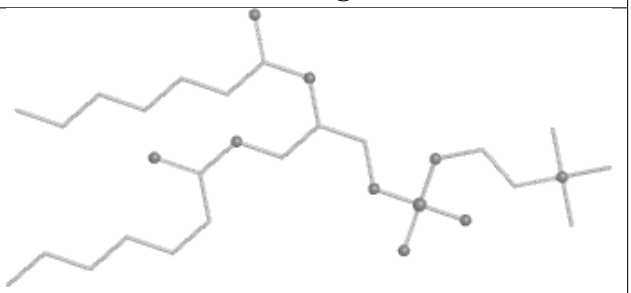
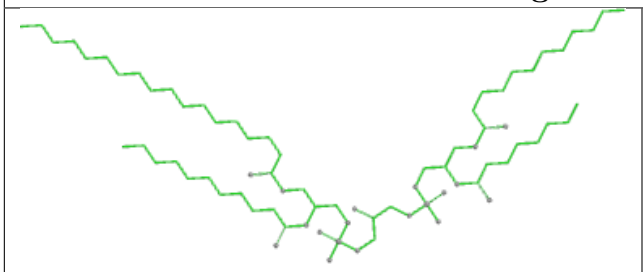


Rings

Ligand CDL I 302



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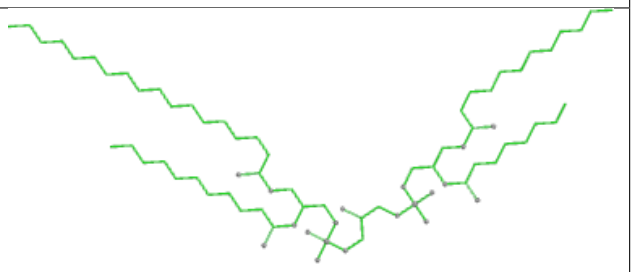

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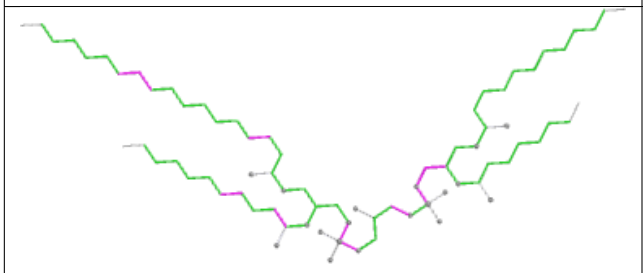

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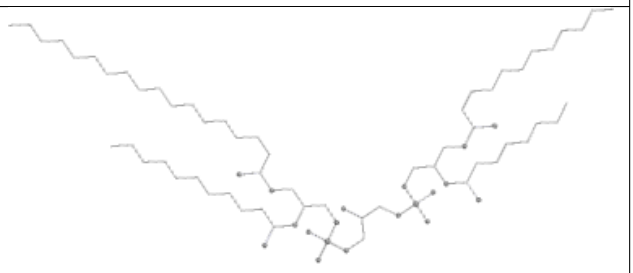
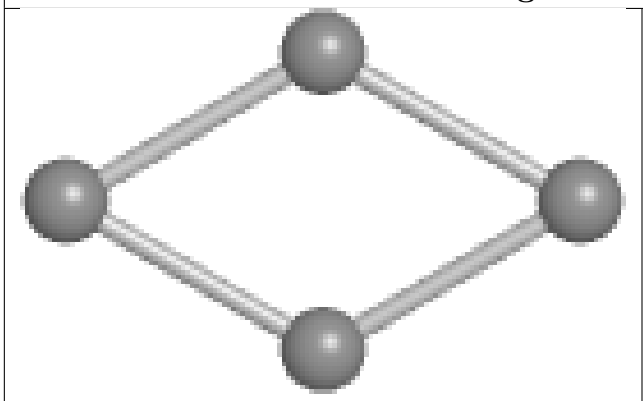


Rings

Ligand FES QE 302



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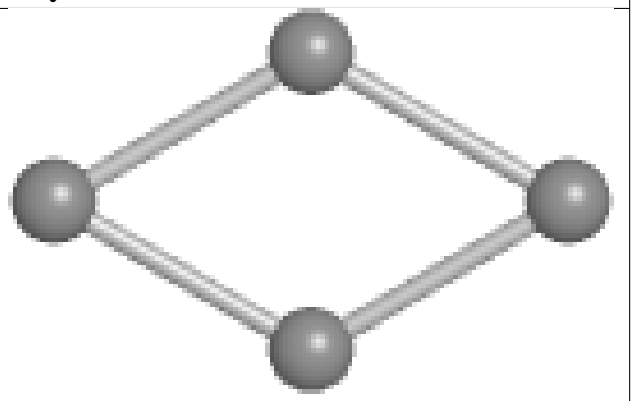

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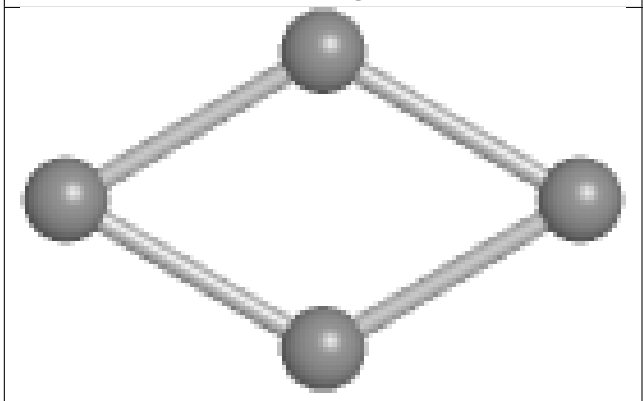

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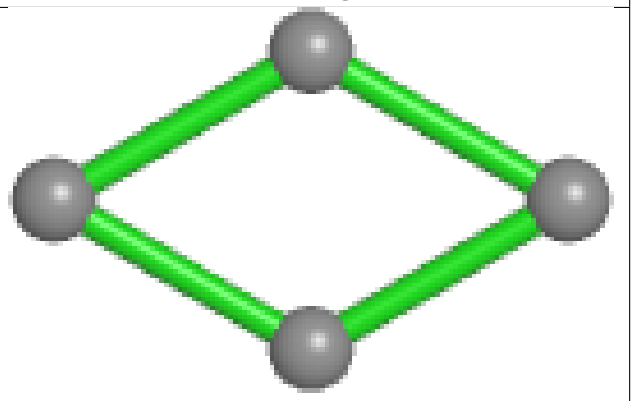
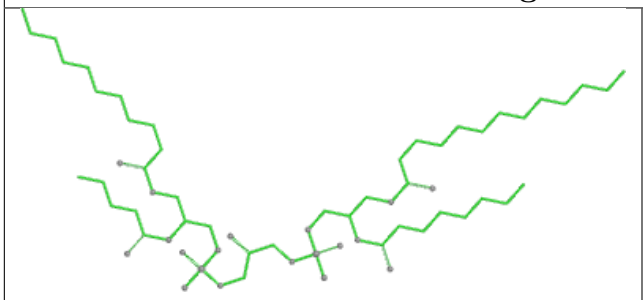


Rings

Ligand CDL y7 501



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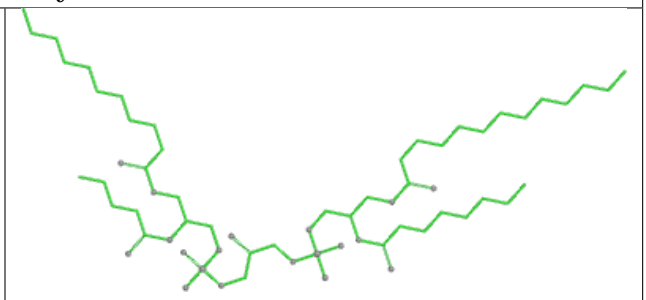
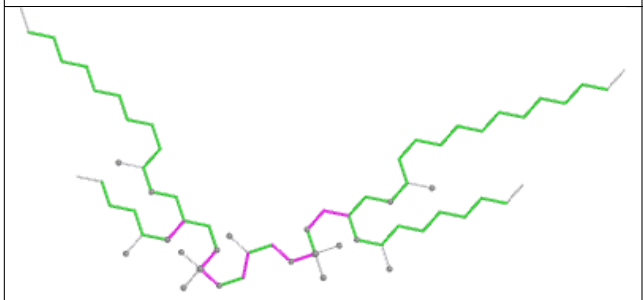


Bond angles



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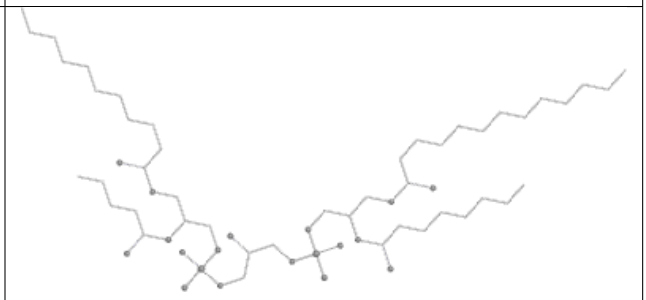
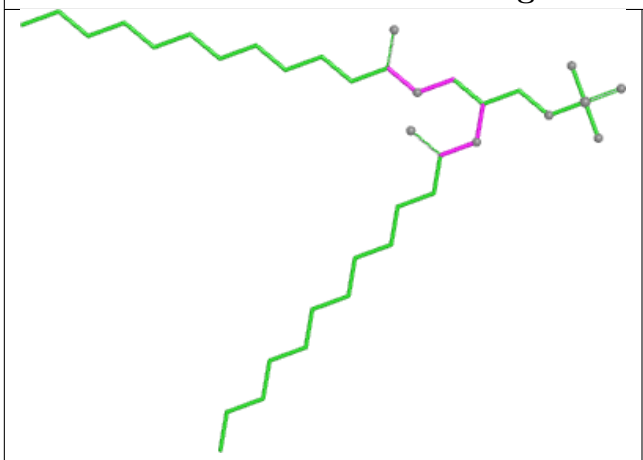


Rings

Ligand PX2 Qh 201



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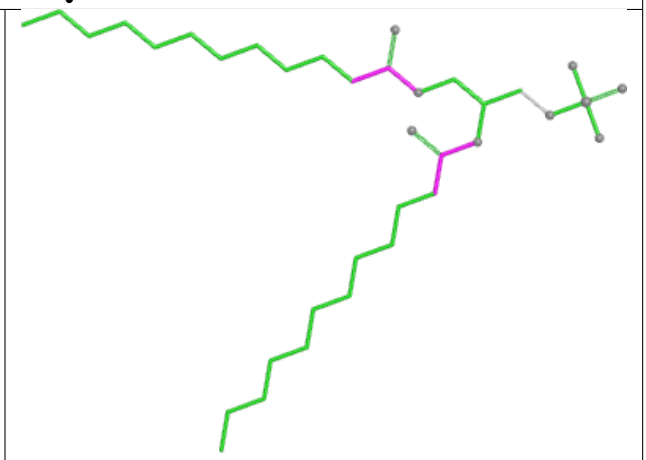
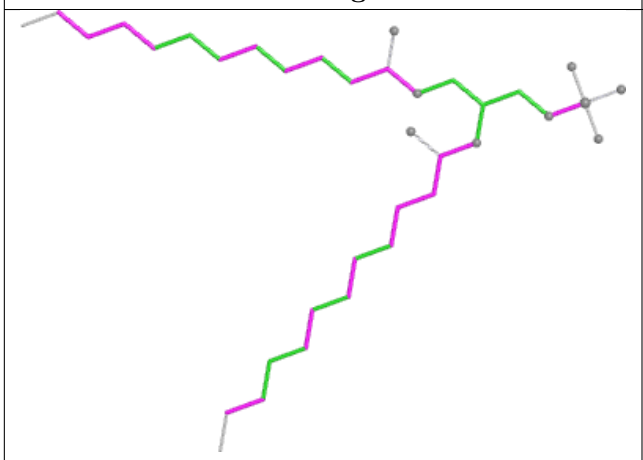


Bond angles



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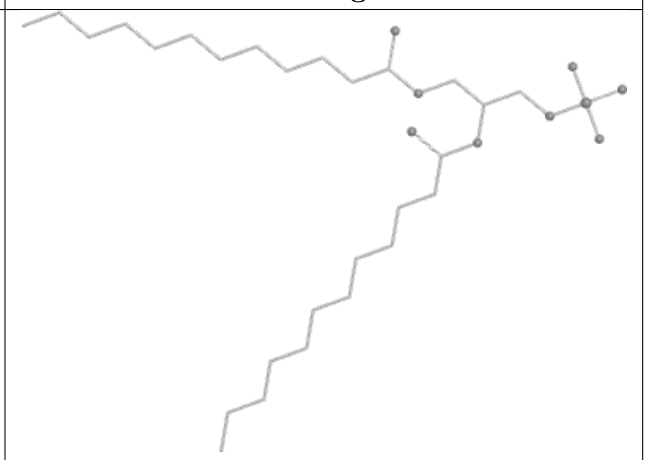
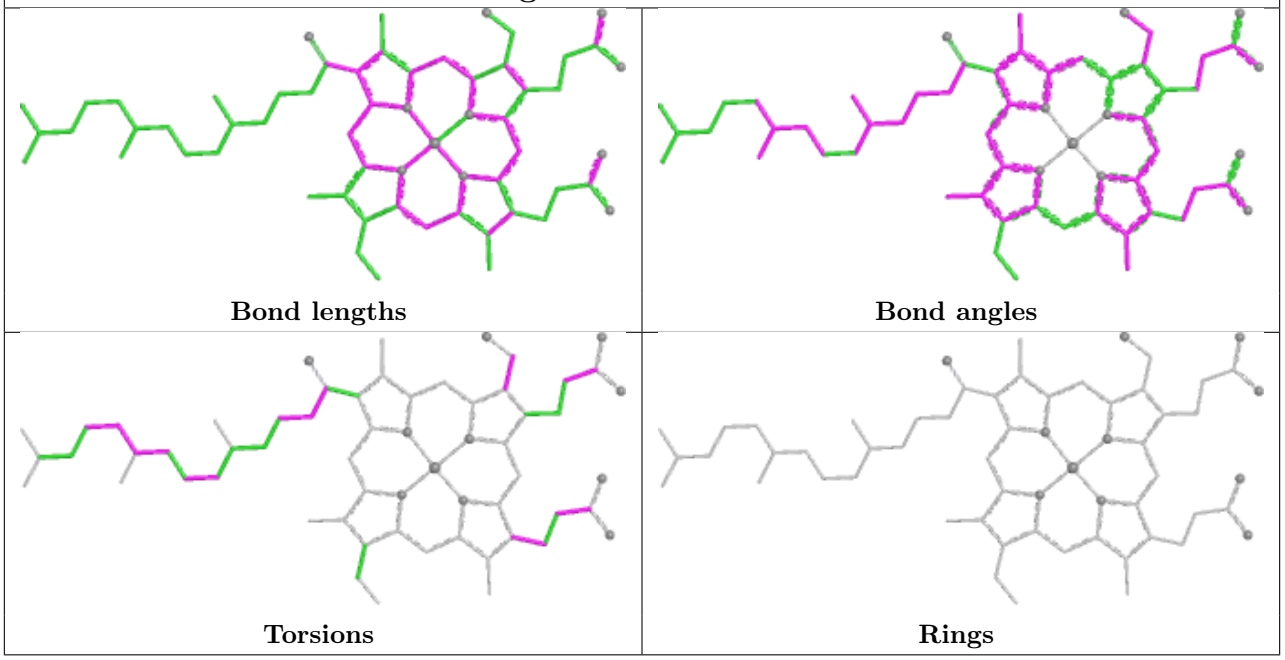
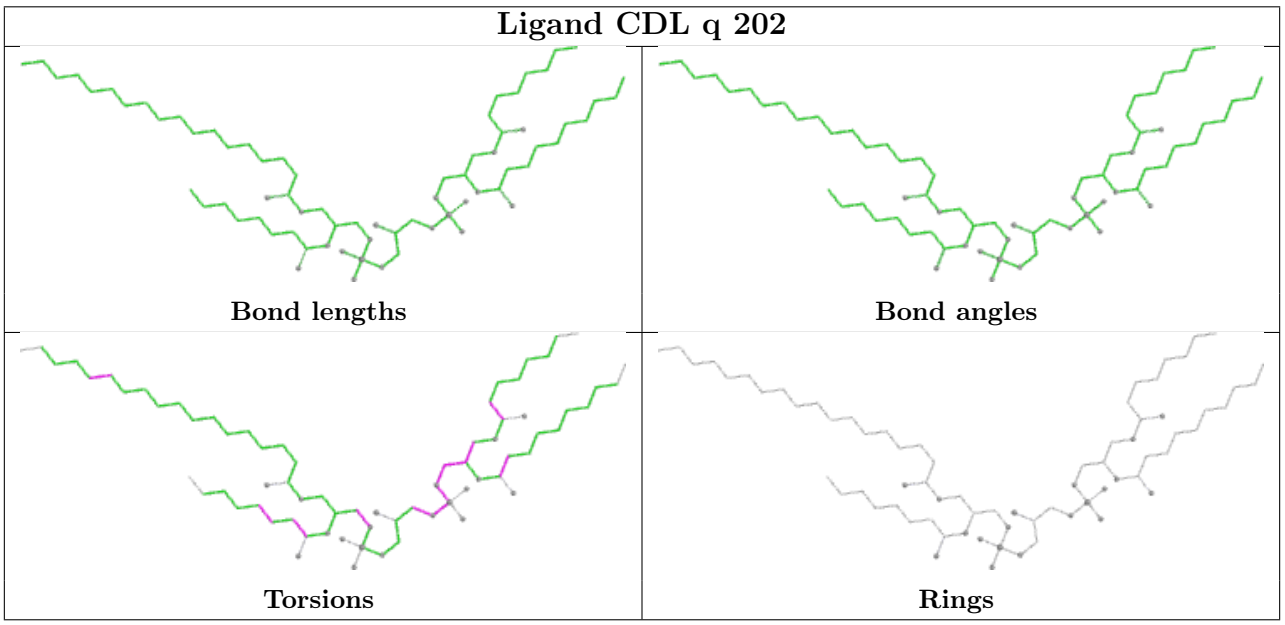


Rings

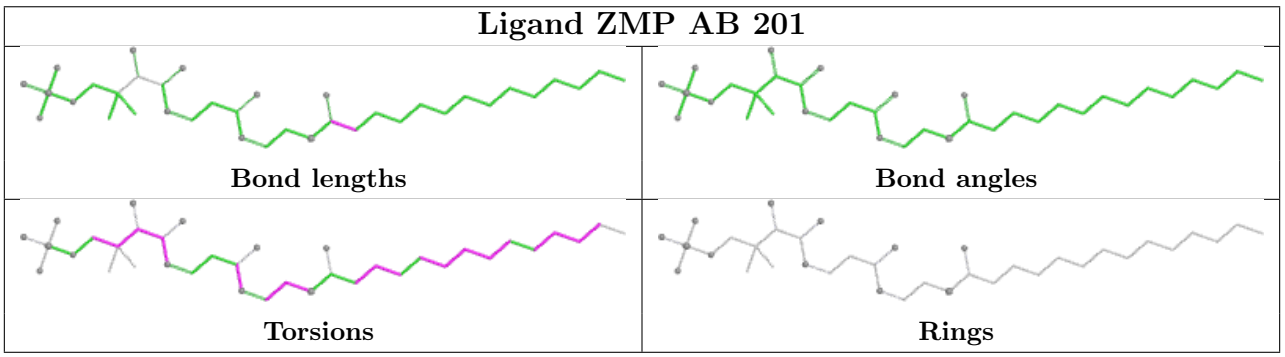
Ligand HEA c1 708



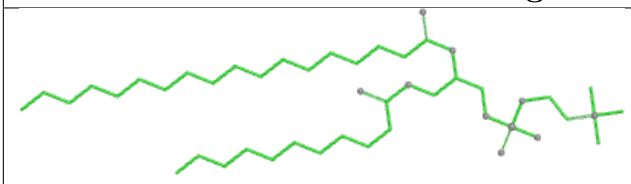
Ligand CDL q 202



Ligand ZMP AB 201



Ligand PC1 2f 301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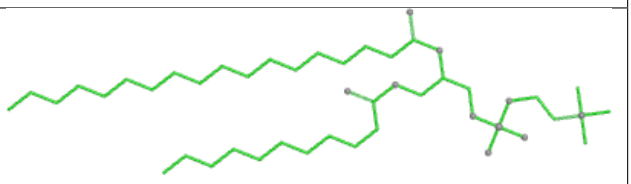
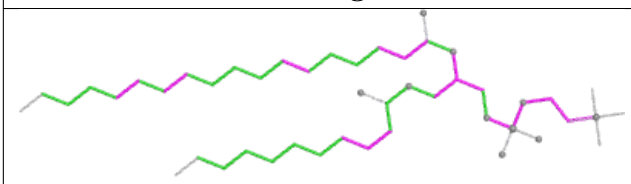
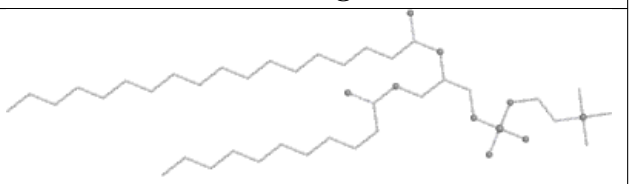
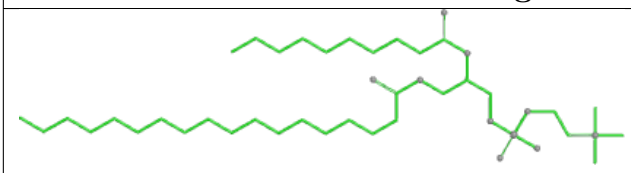

Bond angles


Torsions


Rings

Ligand PC1 M2 407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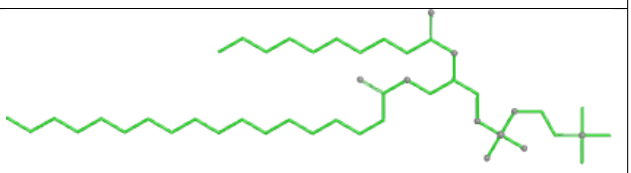
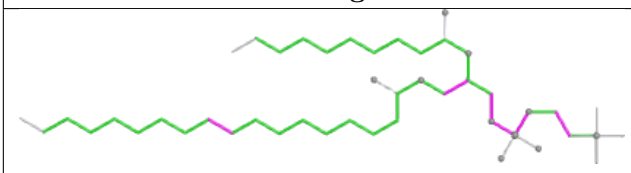

Bond angles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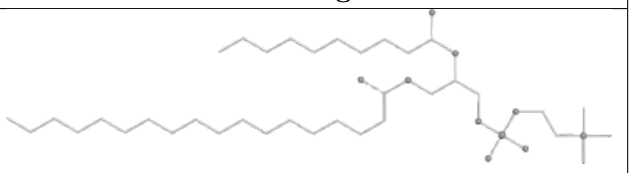
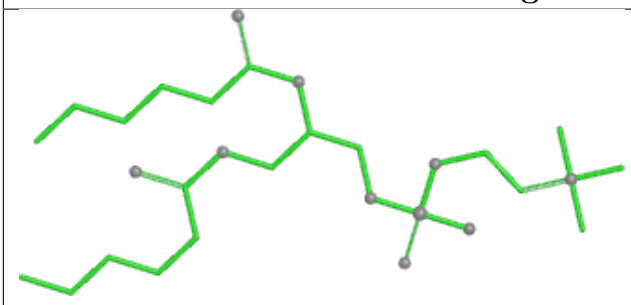

Rings

Ligand PC1 S8 301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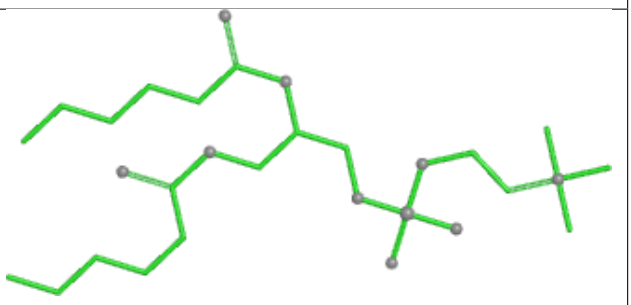
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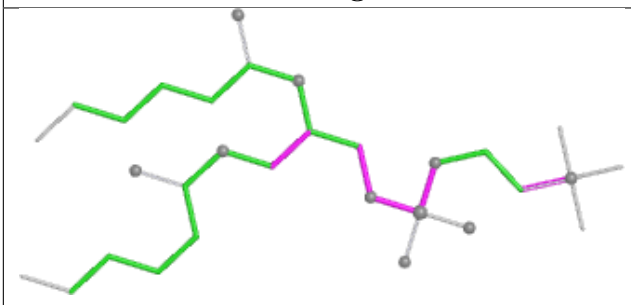
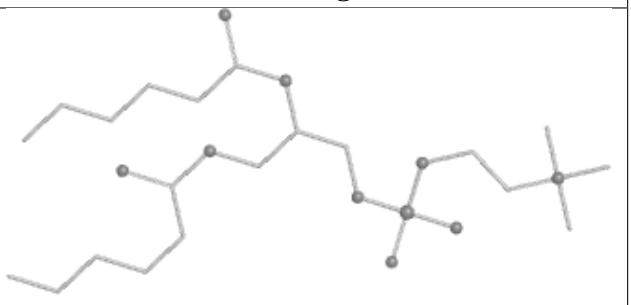
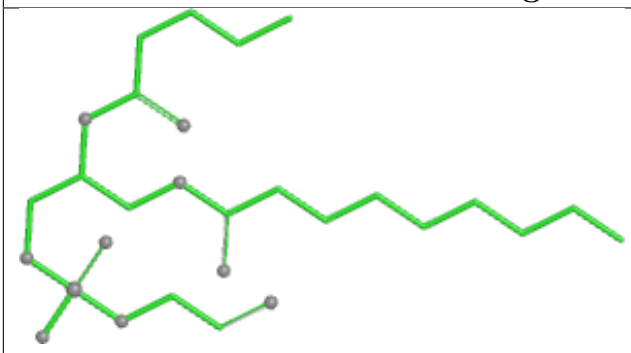
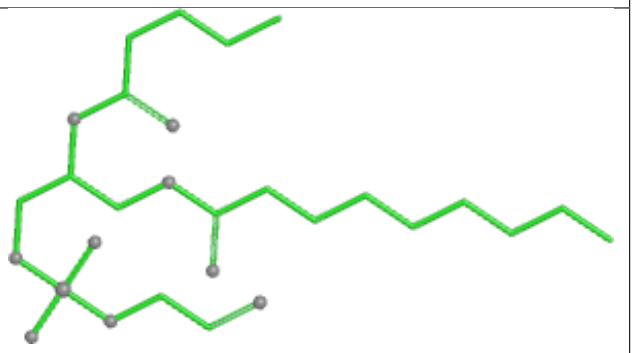

Torsions


Rings

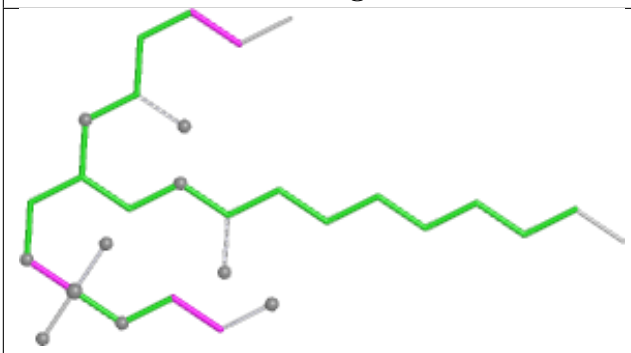
Ligand 3PE an 306



Bond lengths



Bond angles



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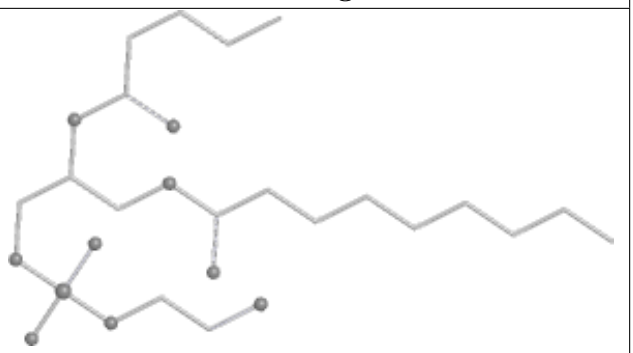
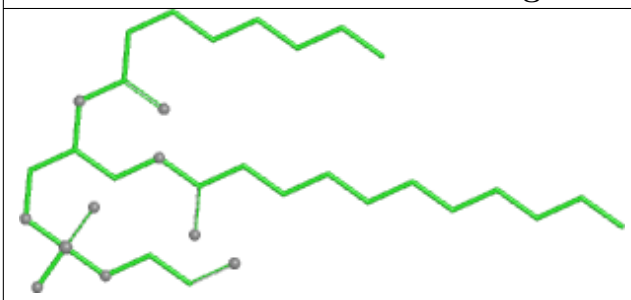


Rings

Ligand 3PE W 203



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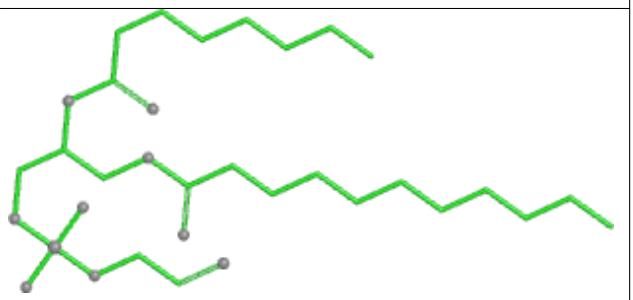

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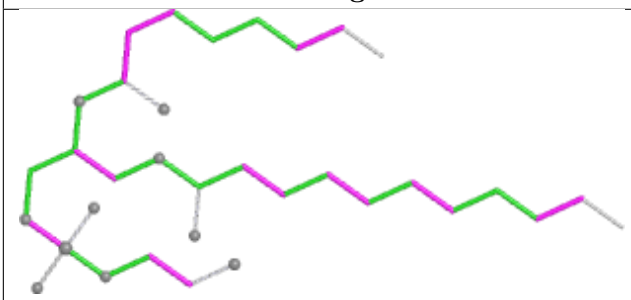

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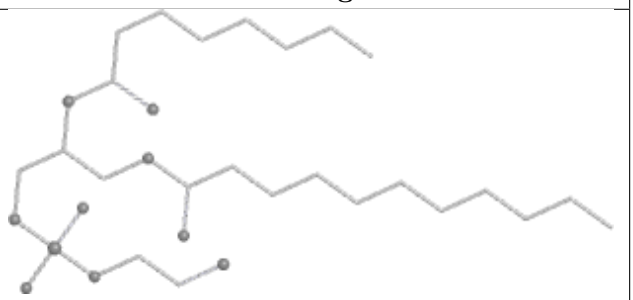
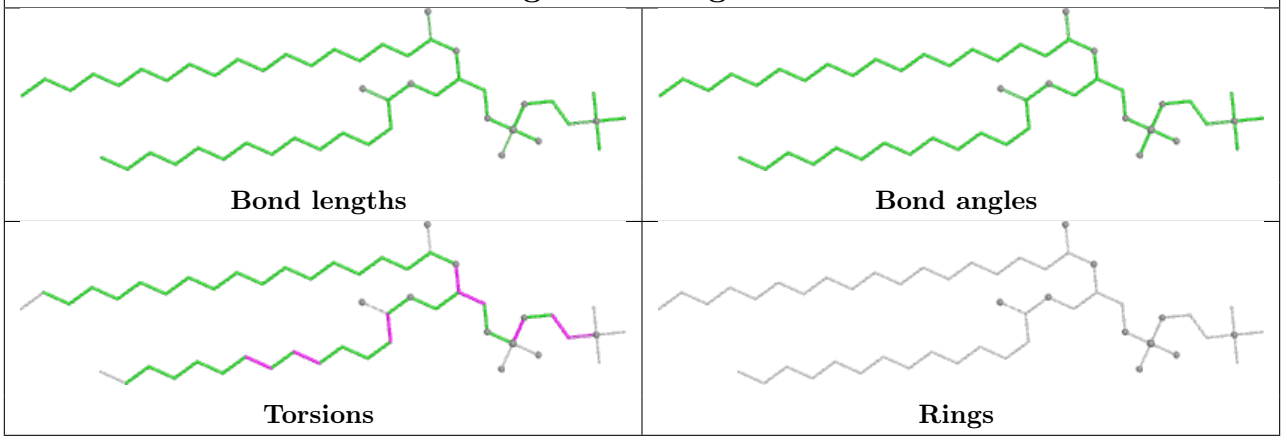
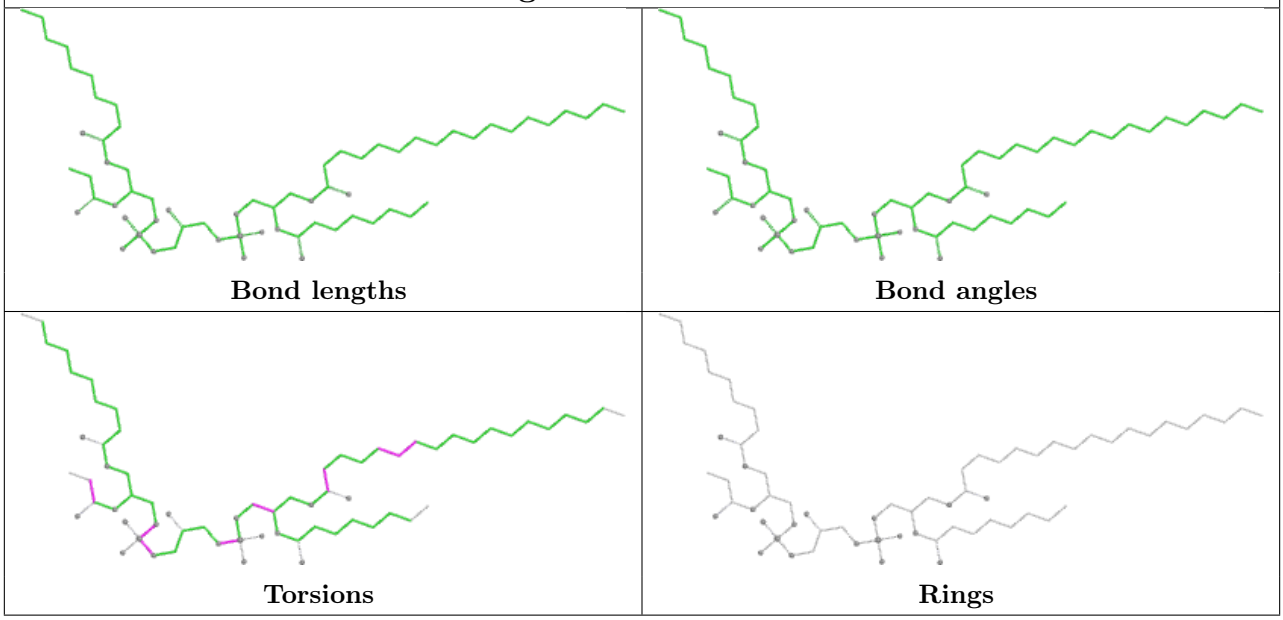


Rings

Ligand PC1 2g 202



Ligand CDL vb 704



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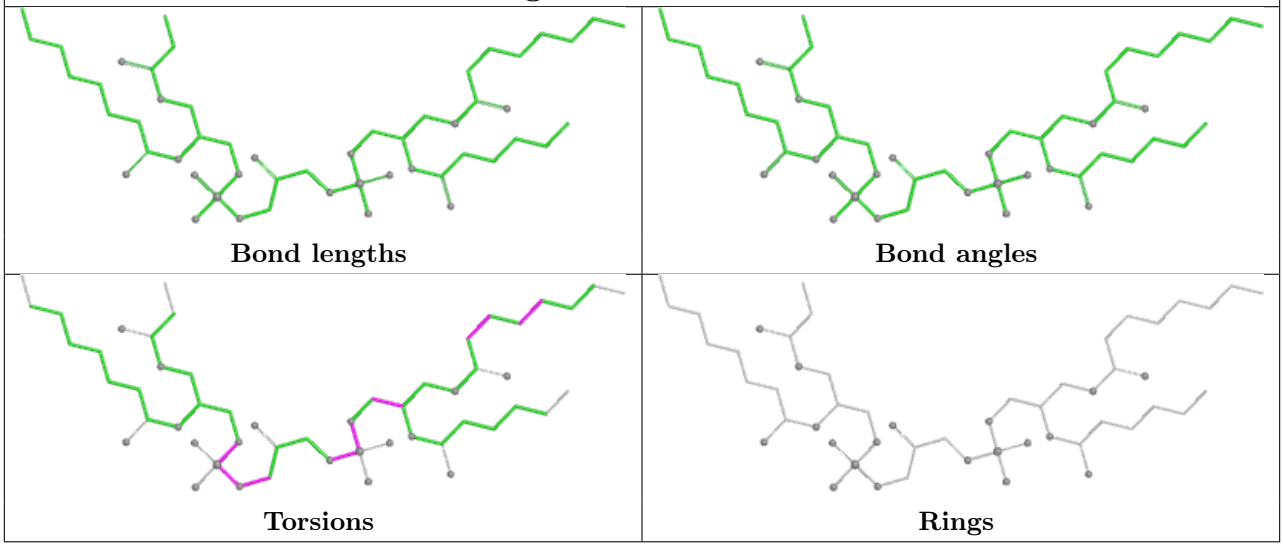
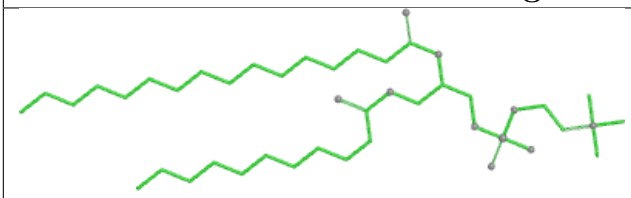
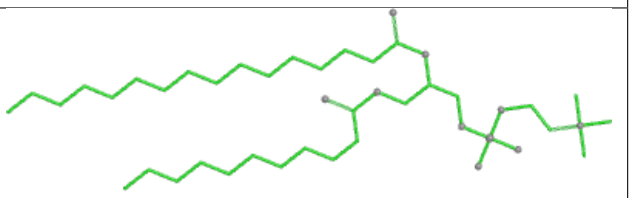
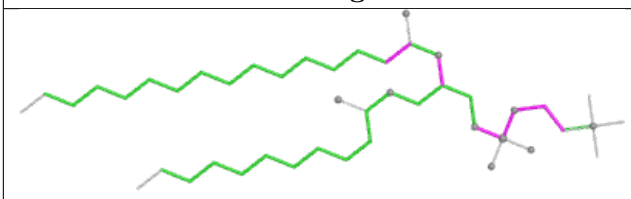
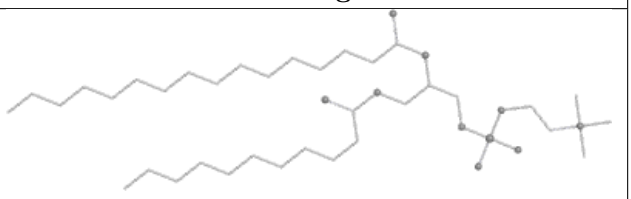
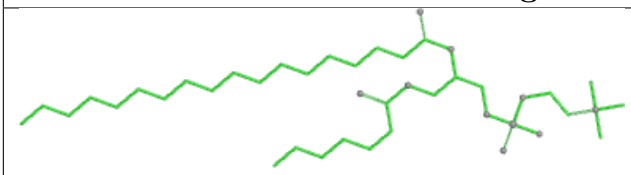
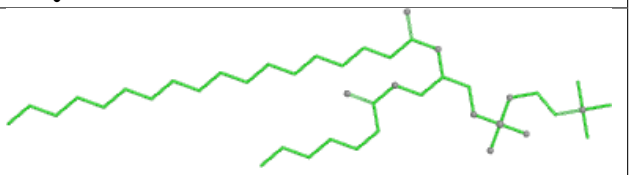
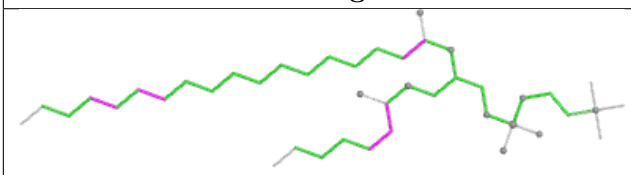
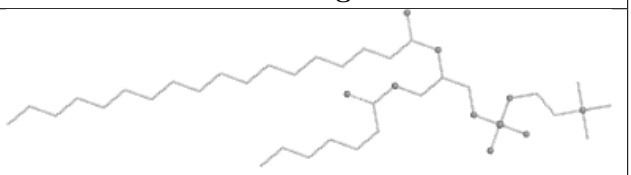
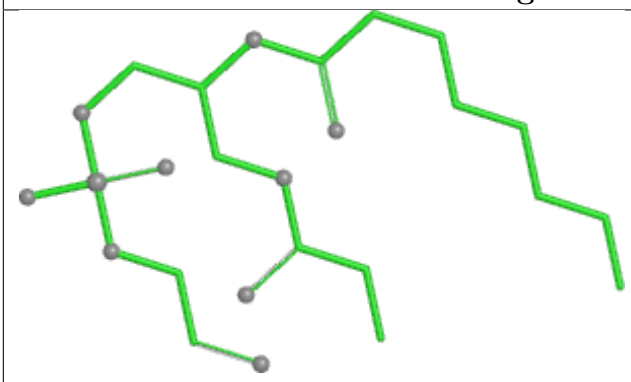


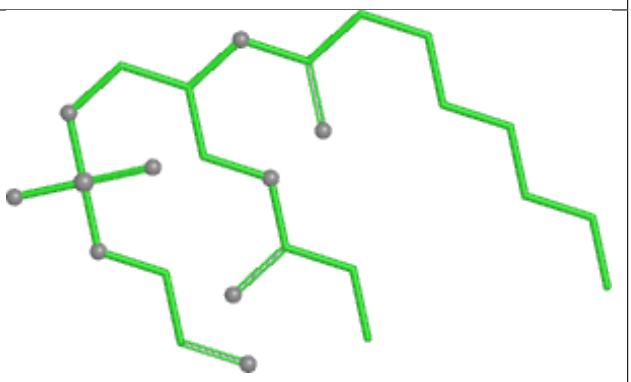
Ligand PC1 c1 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 QI 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE TA 201



Bond lengths



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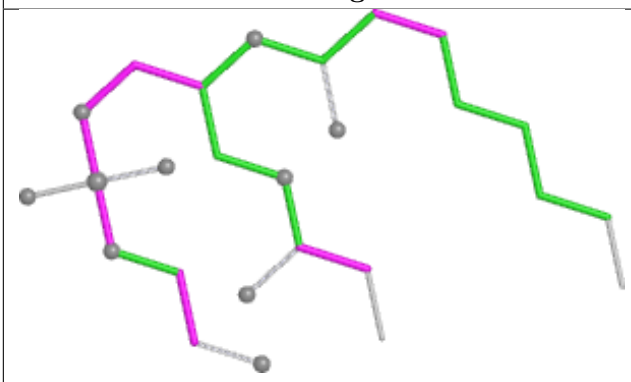
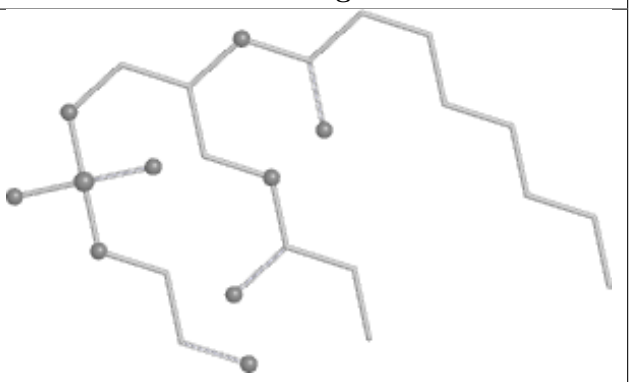
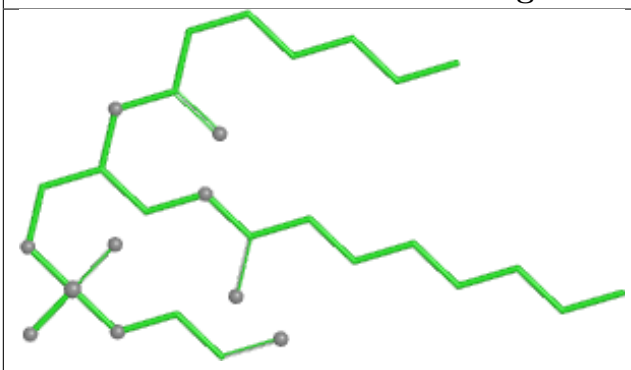


Torsions



Rings

Ligand 3PE bm 302



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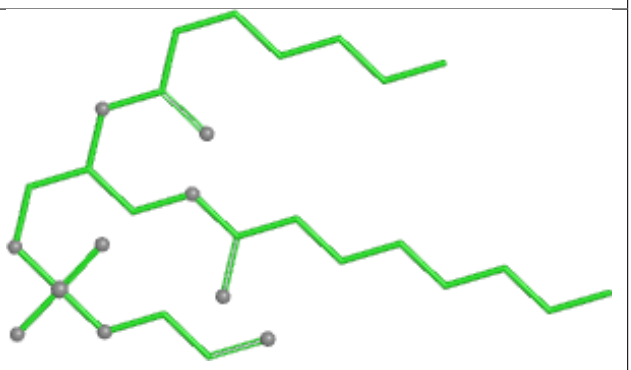

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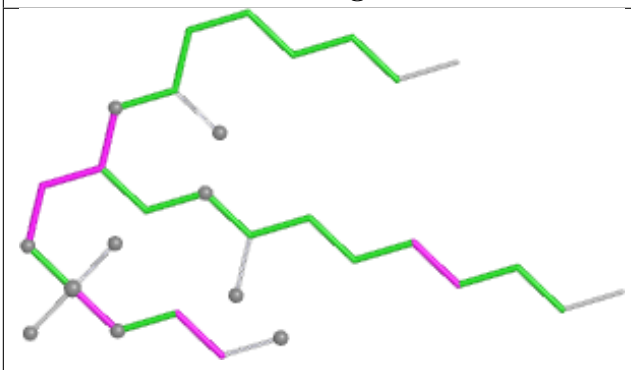

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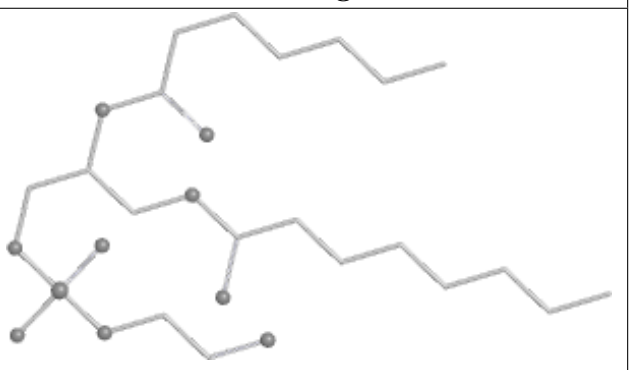
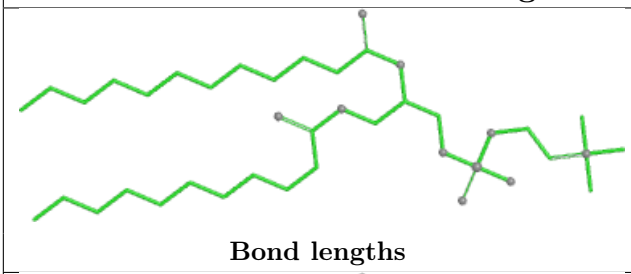


Rings

Ligand PC1 C4 403



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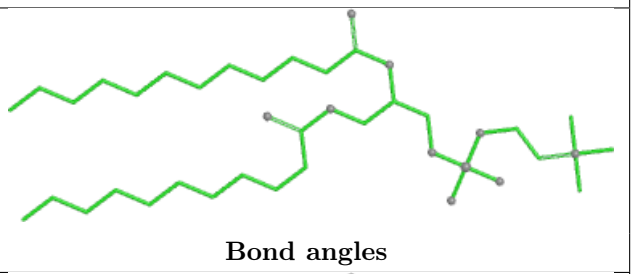
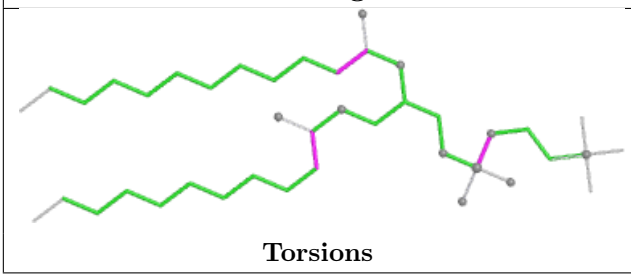


Bond angles



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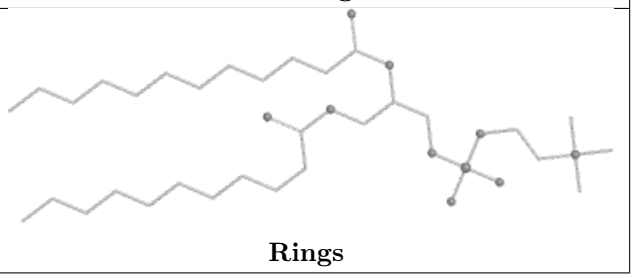
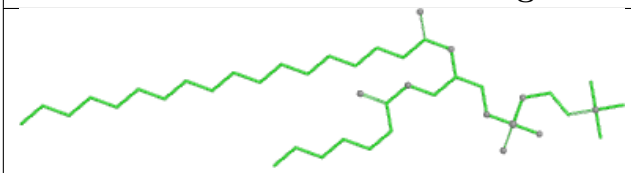


Rings

Ligand PC1 Qb 602



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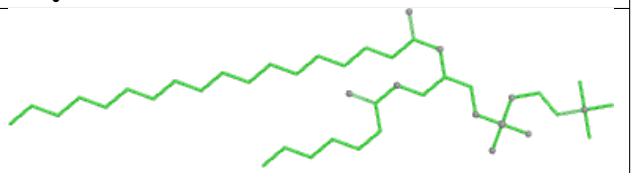

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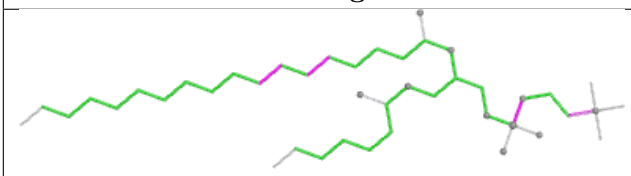

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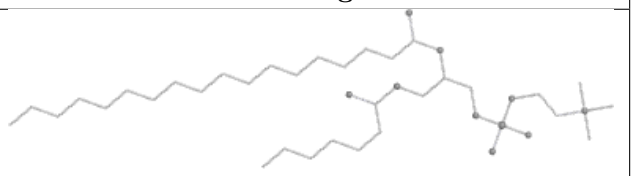
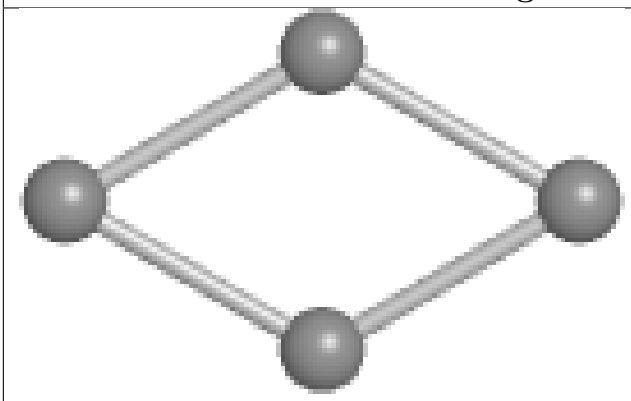


Rings

Ligand FES FX 201



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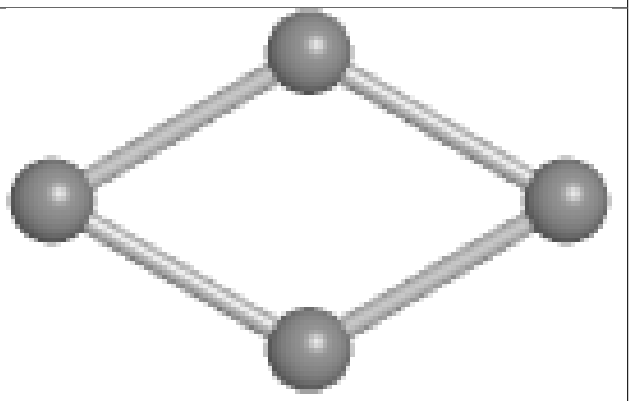

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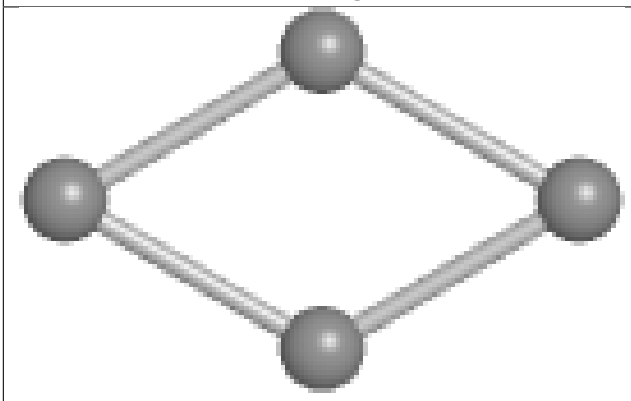

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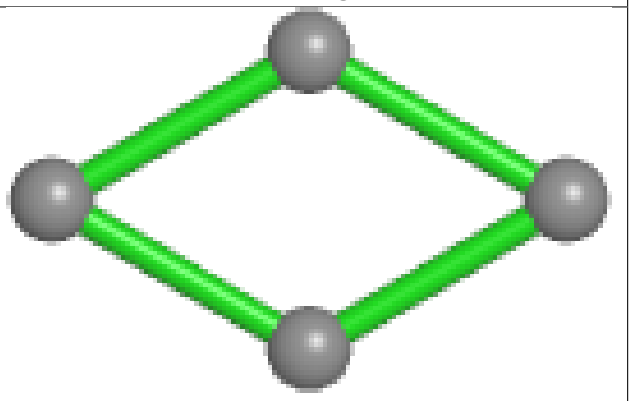
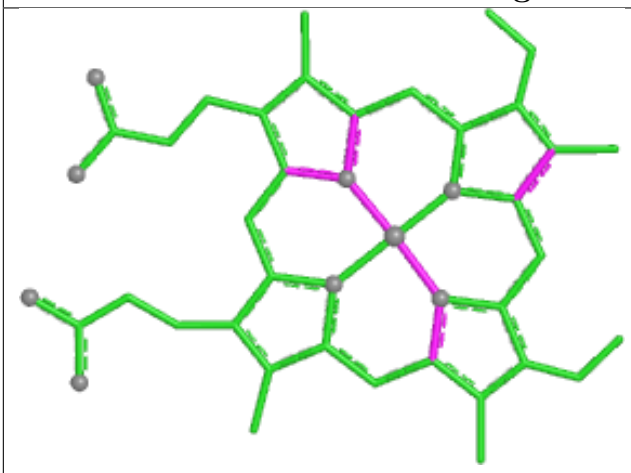


Rings

Ligand HEM y5 203



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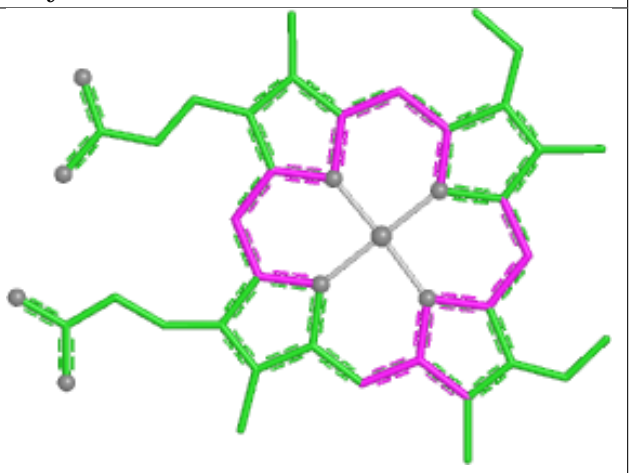

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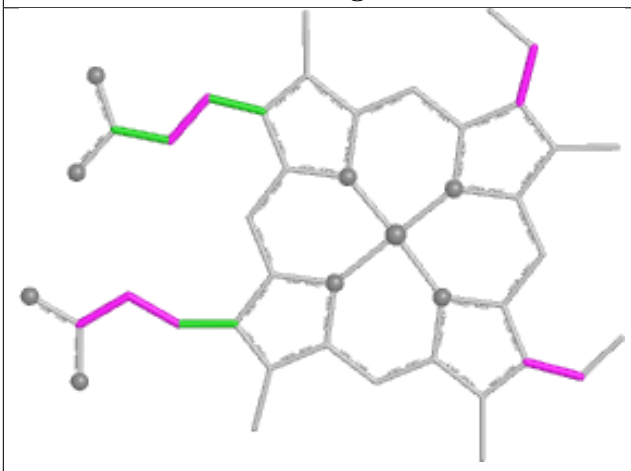

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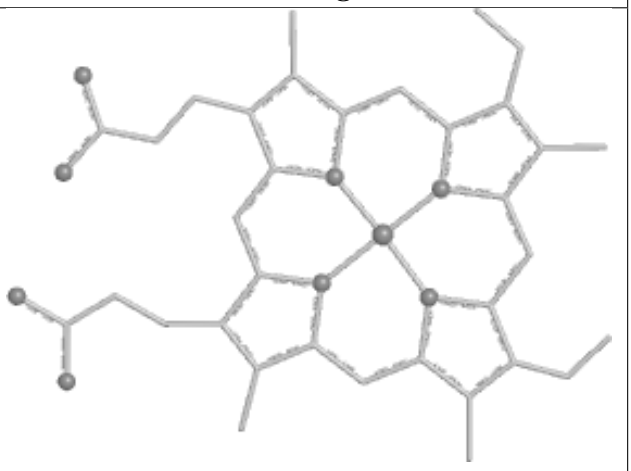
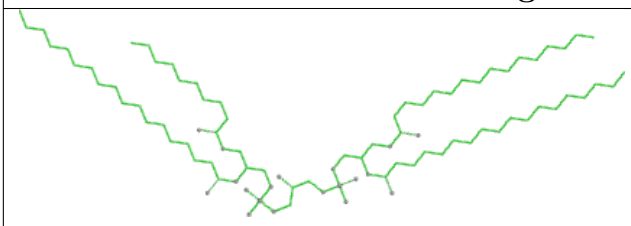


Rings

Ligand CDL n5 806



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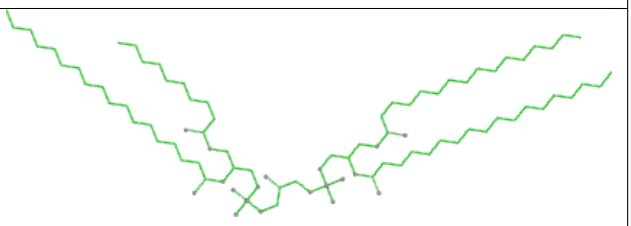
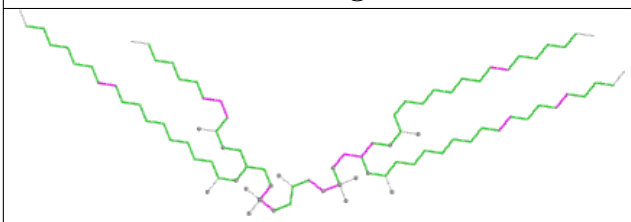


Bond angles



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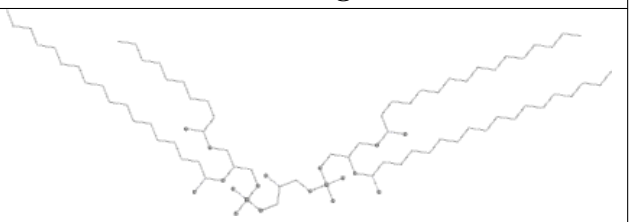
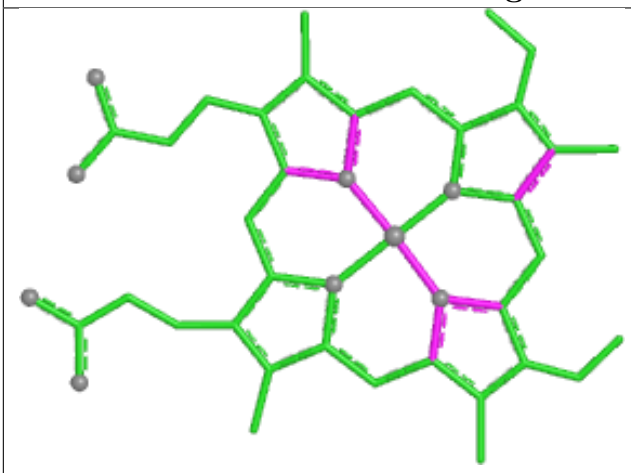


Rings

Ligand HEM QC 501



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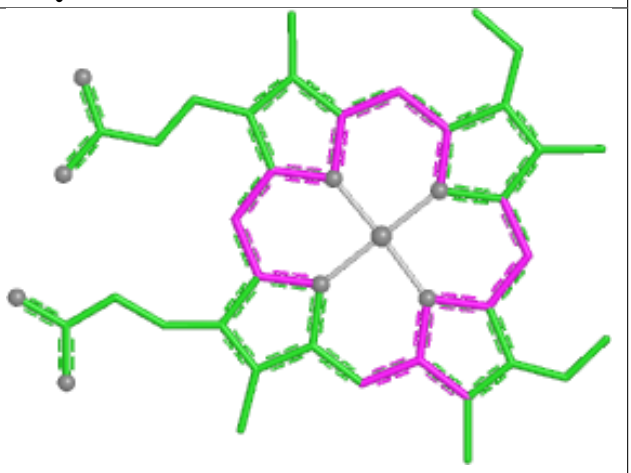
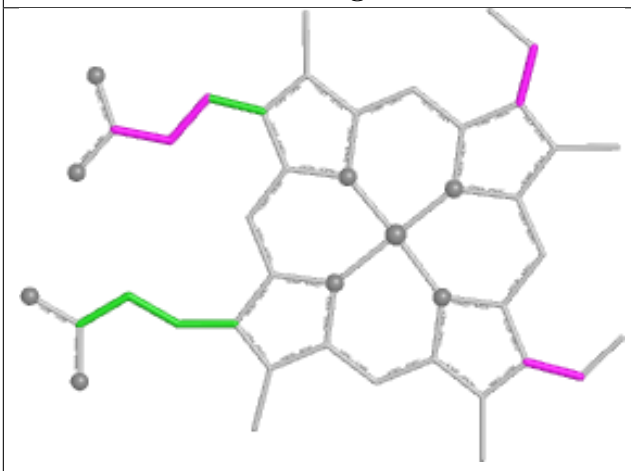
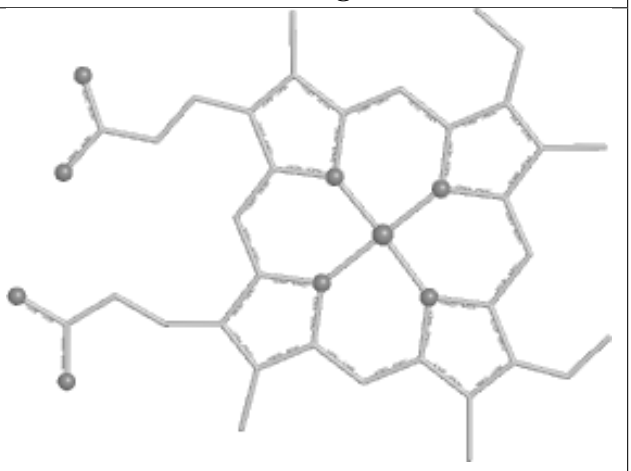


Bond angles

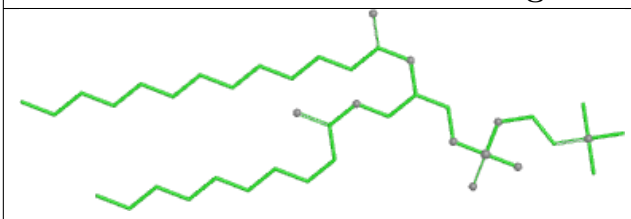


Torsions

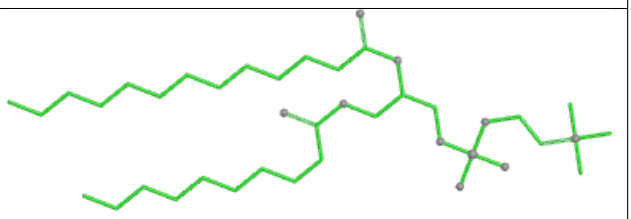


Rings

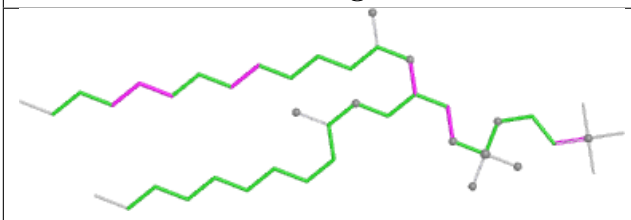
Ligand PC1 A 503



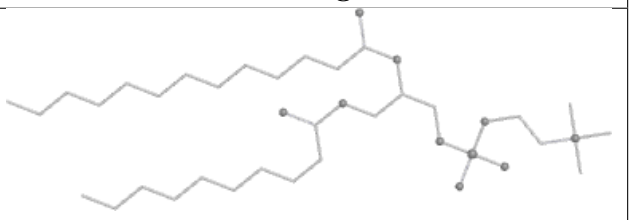
Bond lengths



Bond angles

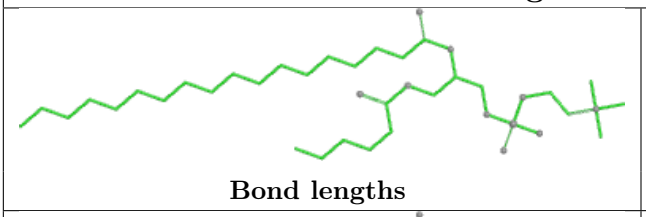


Torsions



Rings

Ligand PC1 qi 203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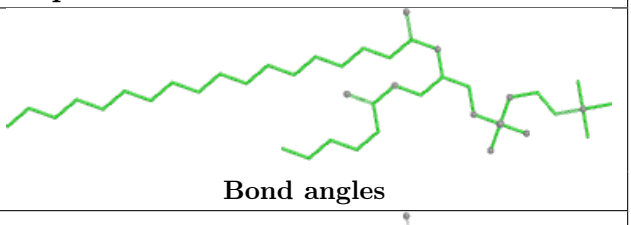
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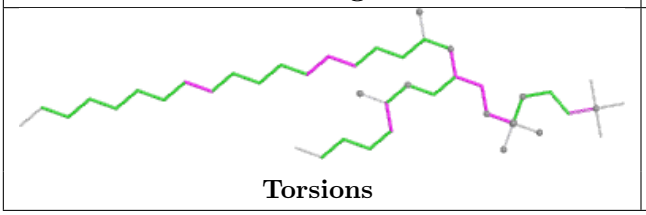
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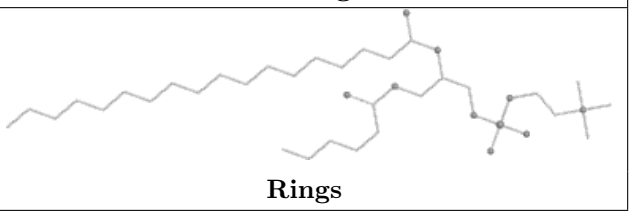
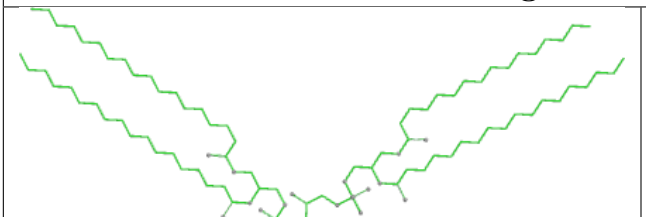

Rings

Ligand CDL c4 401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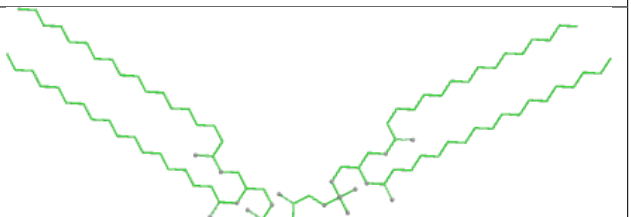
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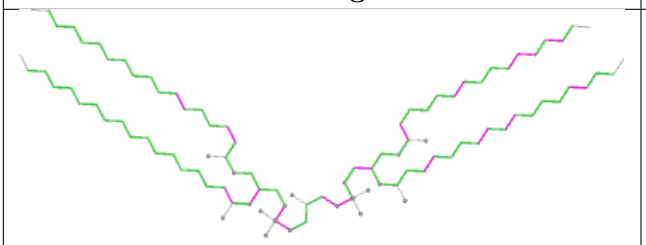
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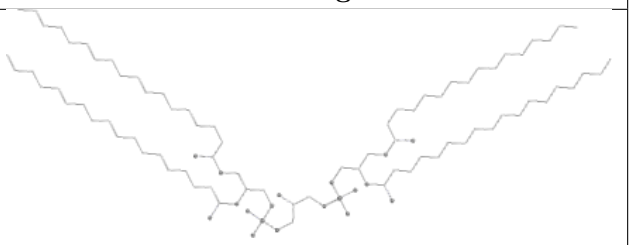
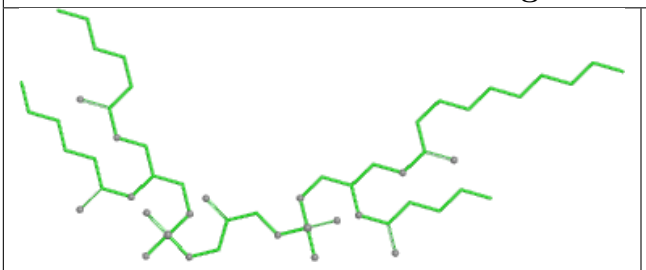

Rings

Ligand CDL t1 601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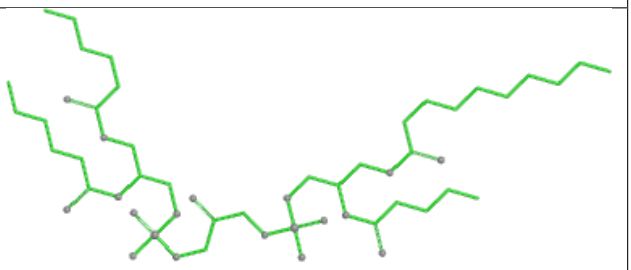
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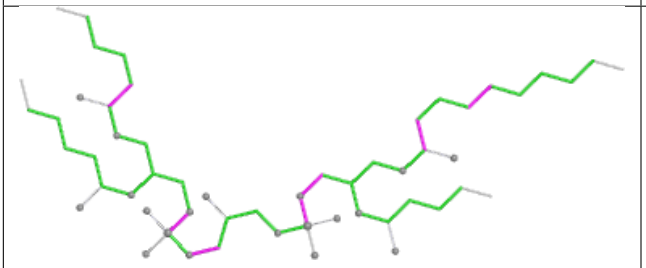
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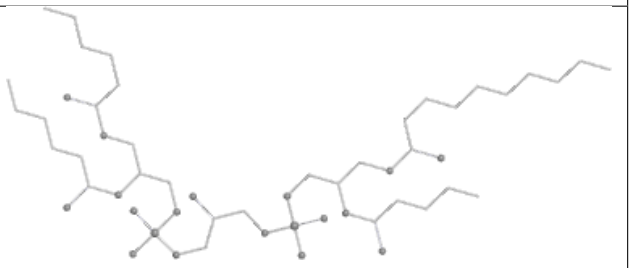
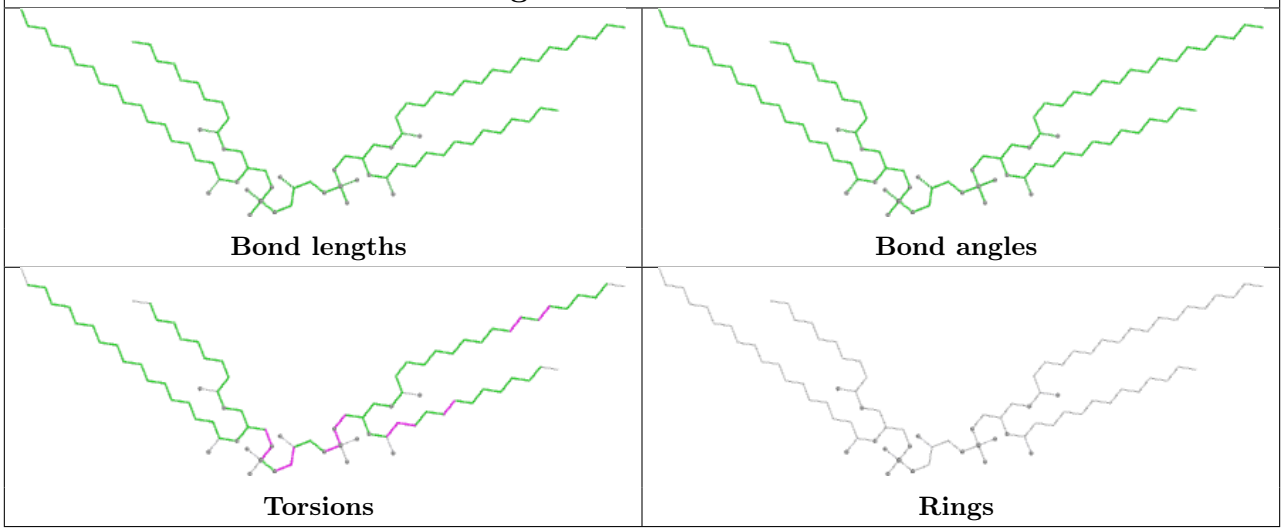
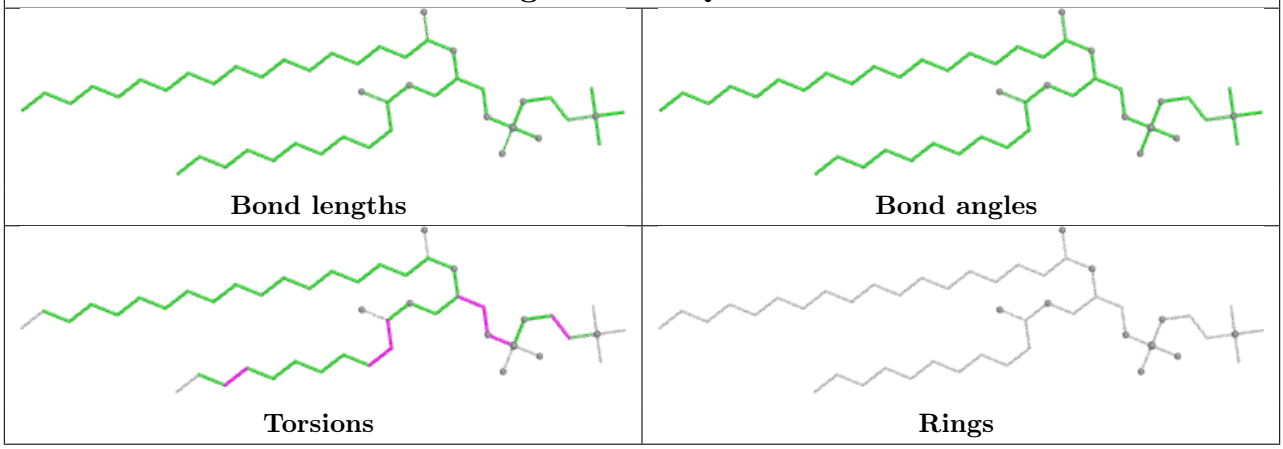

Rings

Ligand CDL AN 302



Ligand PC1 Qc 509



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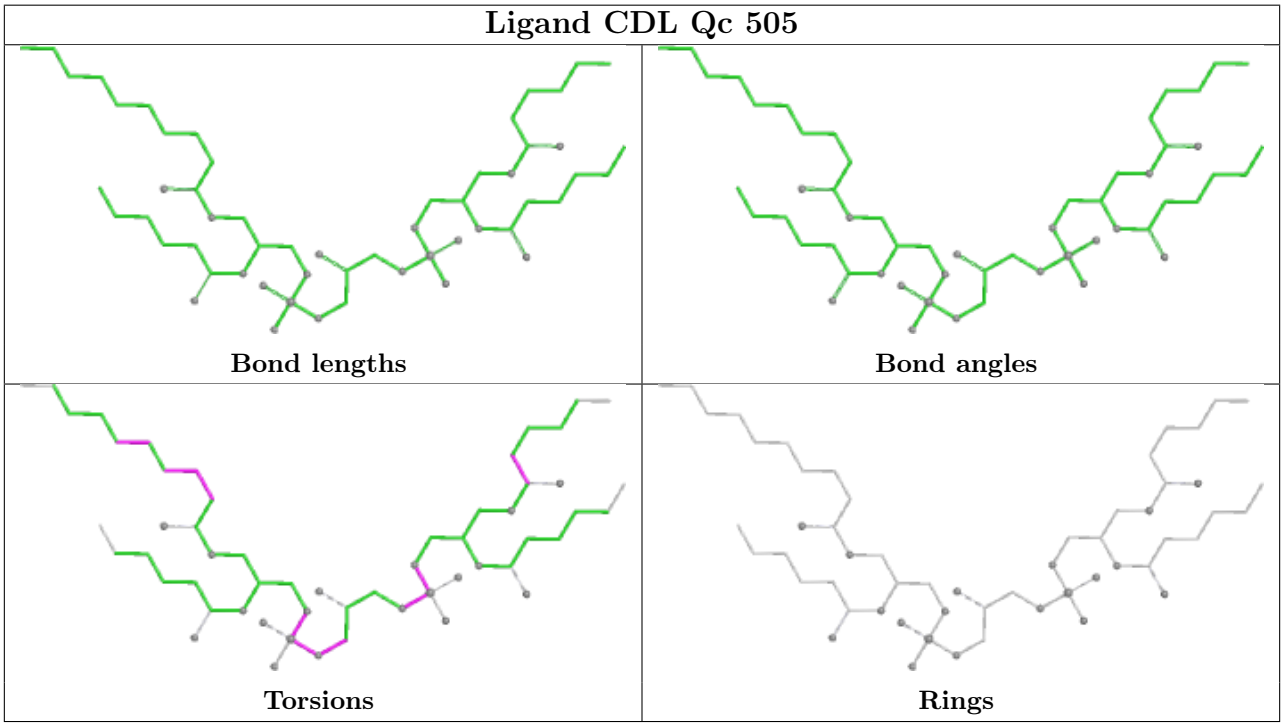
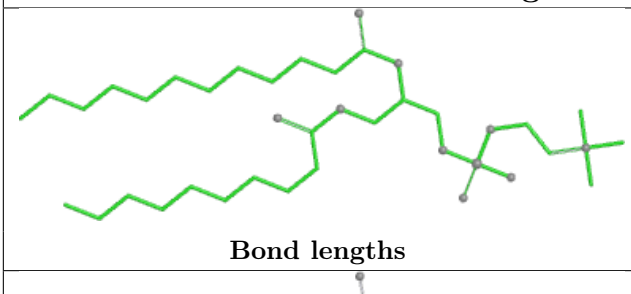


Ligand PC1 J1 400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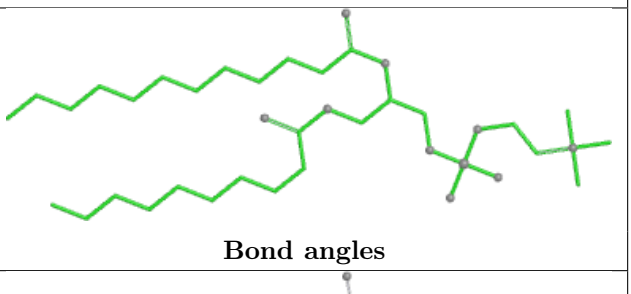
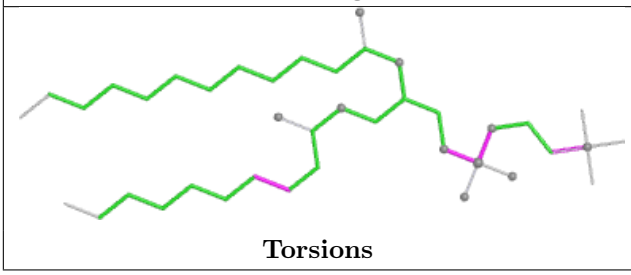
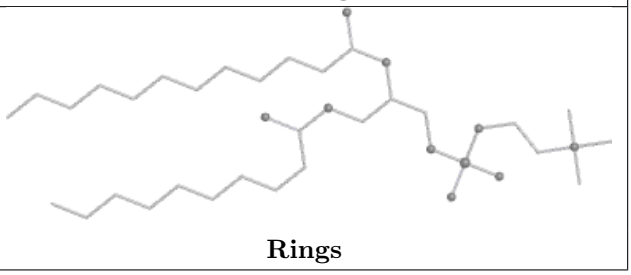
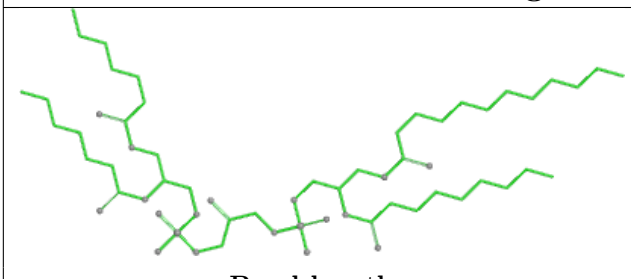

Bond angles


Torsions


Rings

Ligand CDL E 403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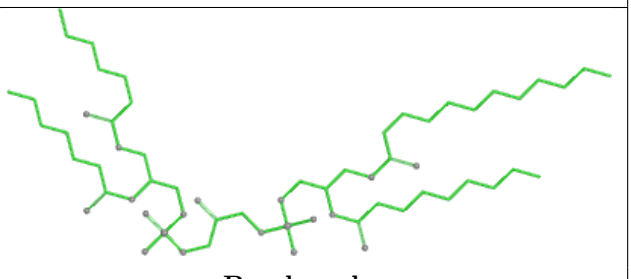
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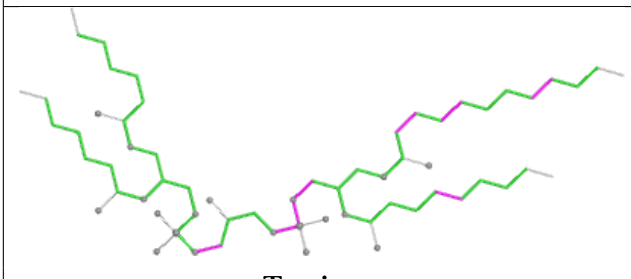
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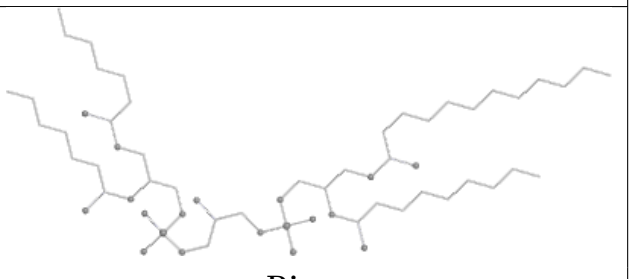
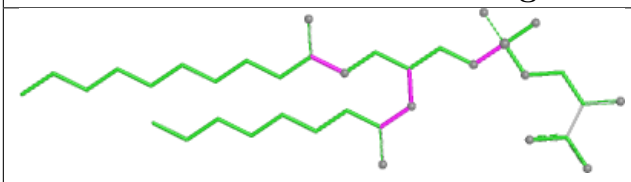

Rings

Ligand P5S m2 406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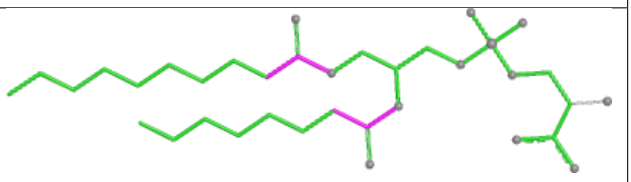
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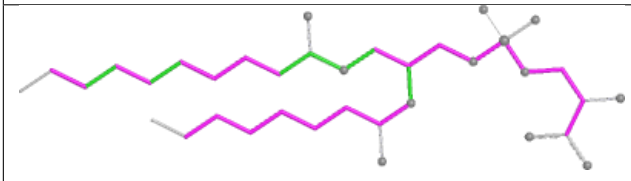
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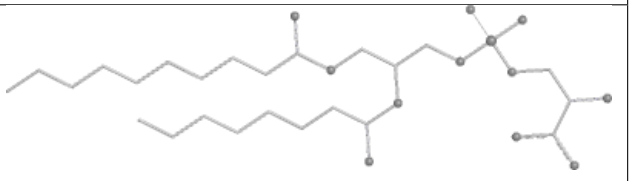
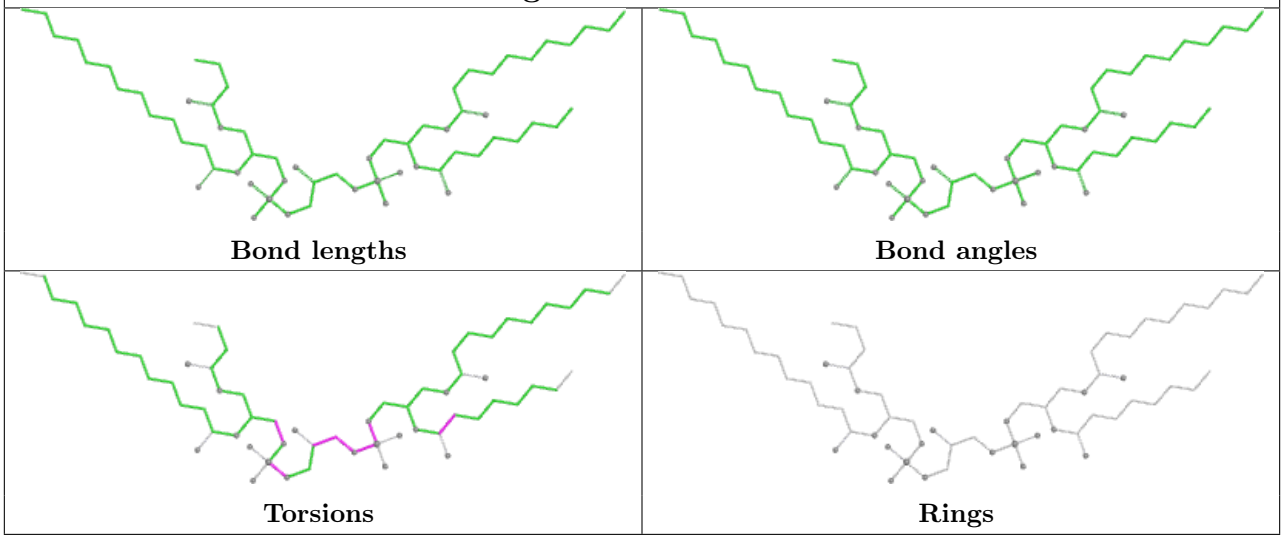
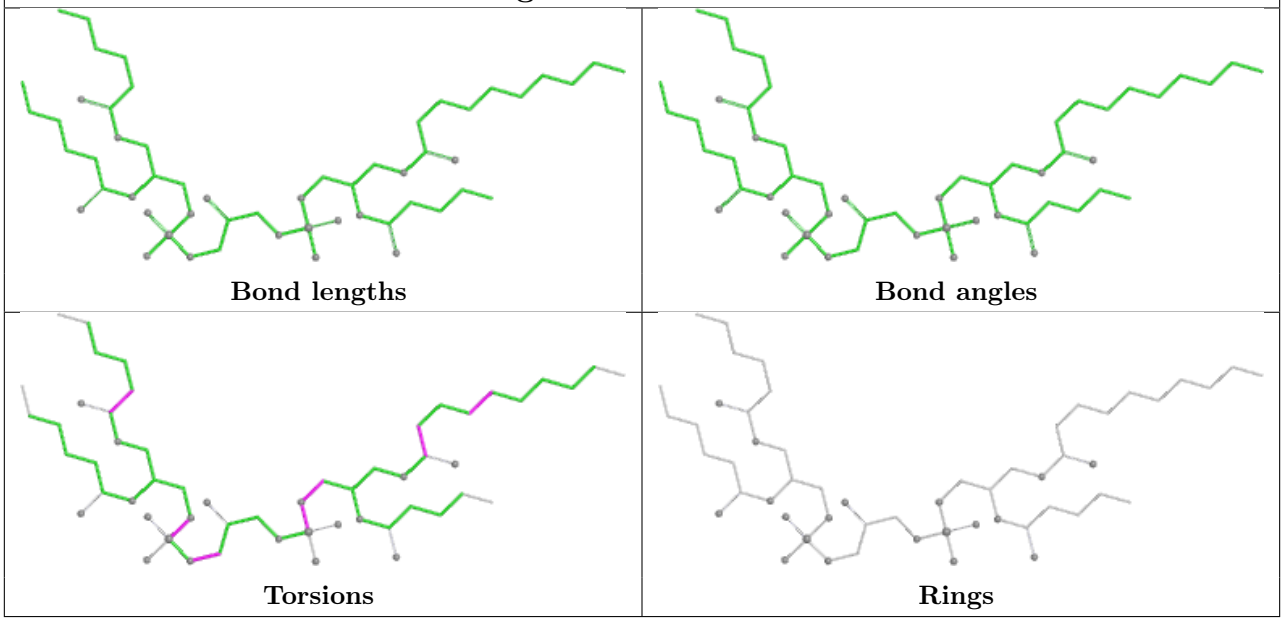

Rings

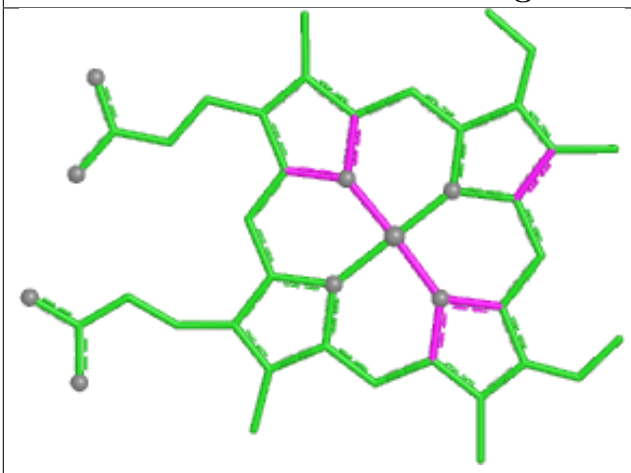
Ligand CDL m 304



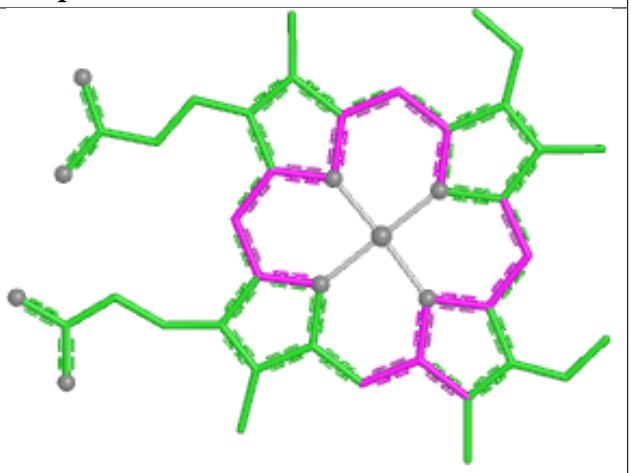
Ligand CDL T1 601



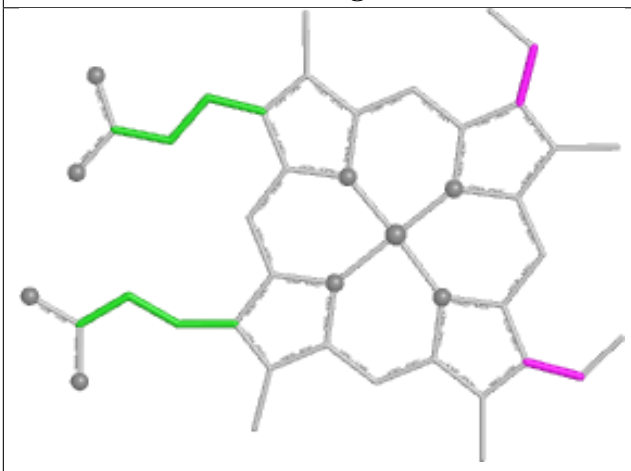
Ligand HEM qc 502



Bond lengths



Bond angles



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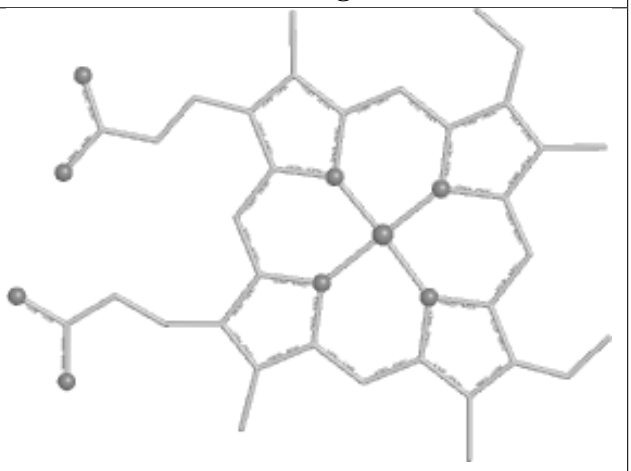
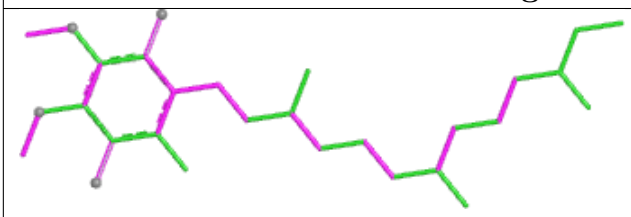


Rings

Ligand U10 Qc 507



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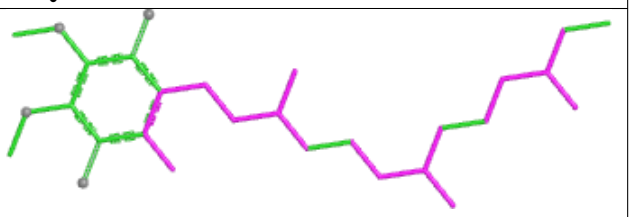

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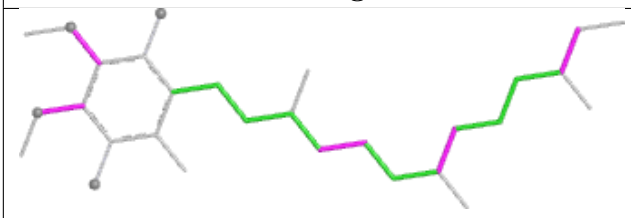

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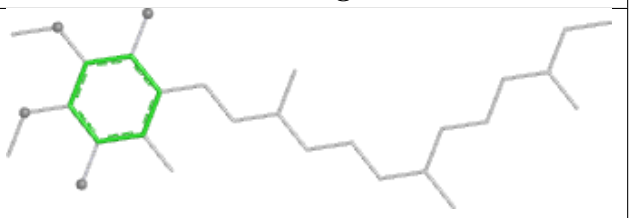
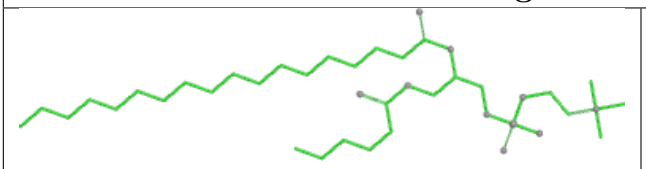


Rings

Ligand PC1 TC 101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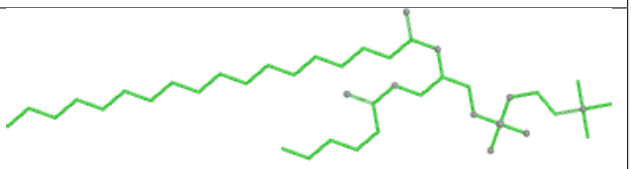
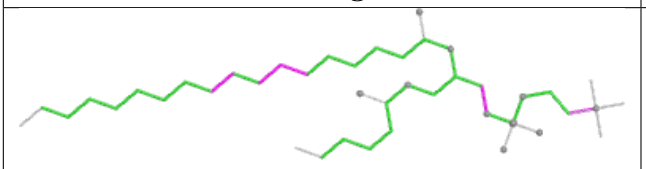

Bond angles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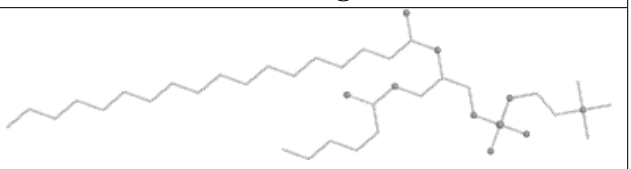
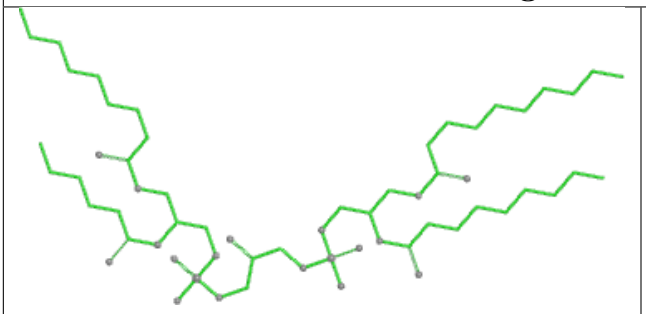

Rings

Ligand CDL 7a 203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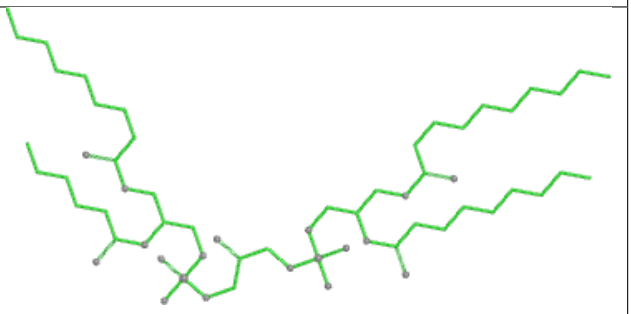
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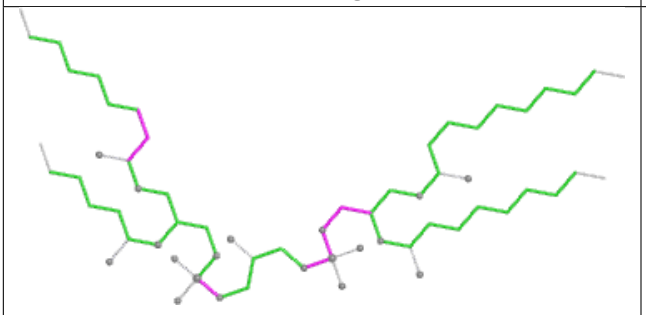
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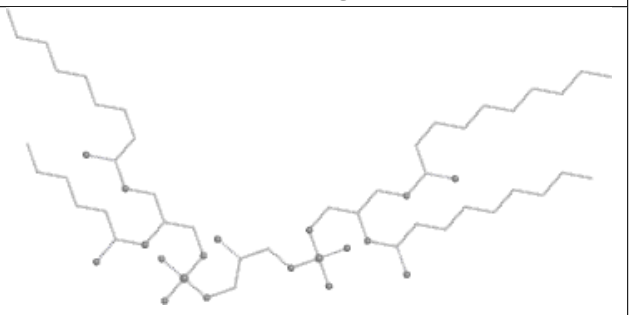
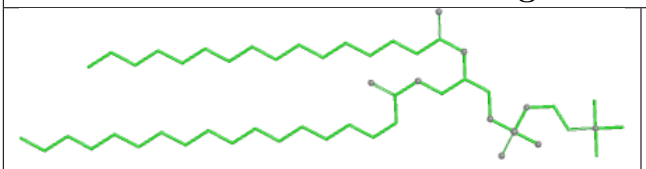

Rings

Ligand PC1 C3 601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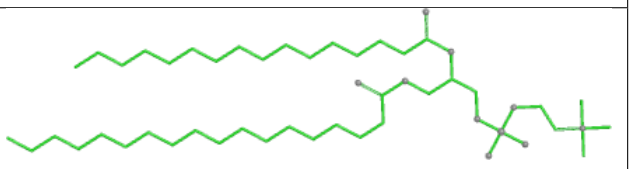
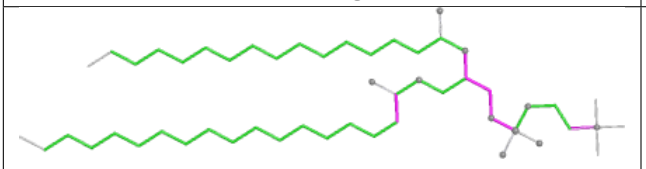

Bond angles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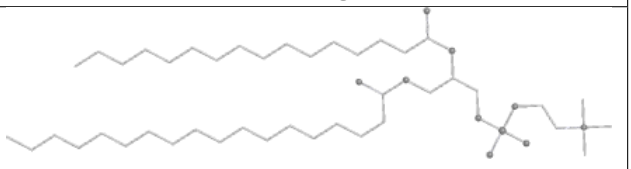
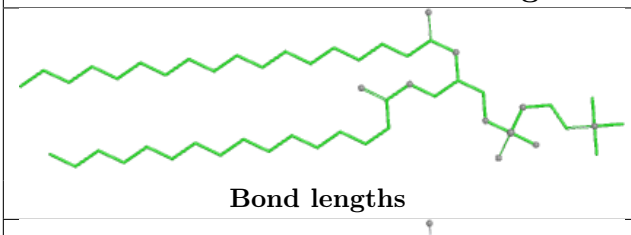

Rings

Ligand PC1 n5 801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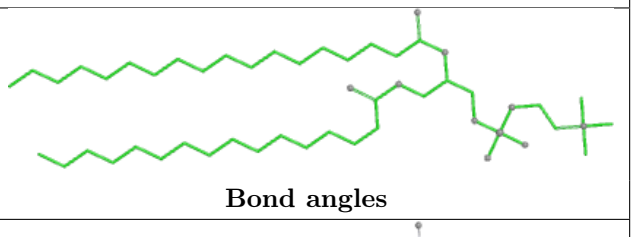
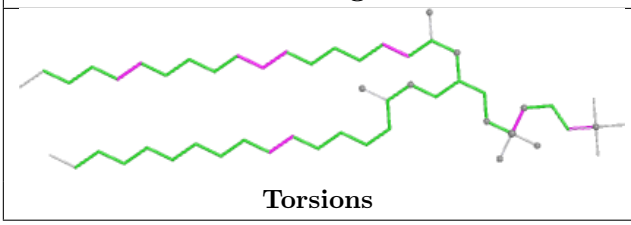
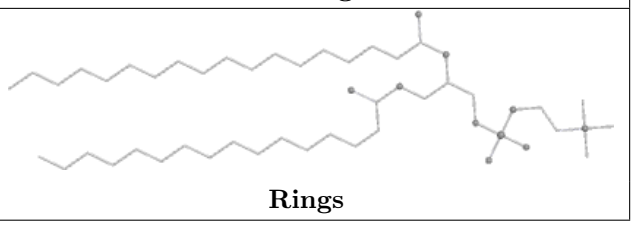
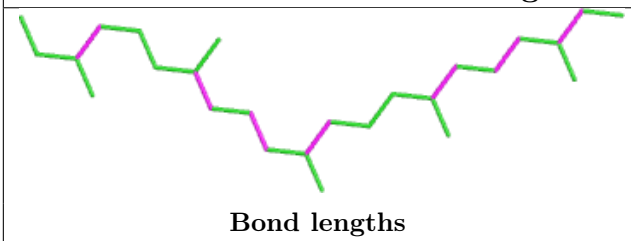

Bond angles


Torsions


Rings

Ligand U10 Qc 501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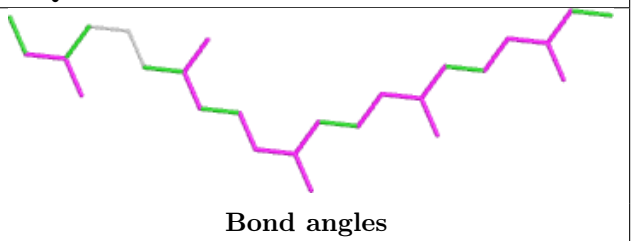
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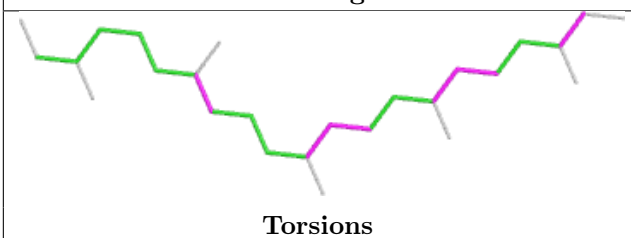
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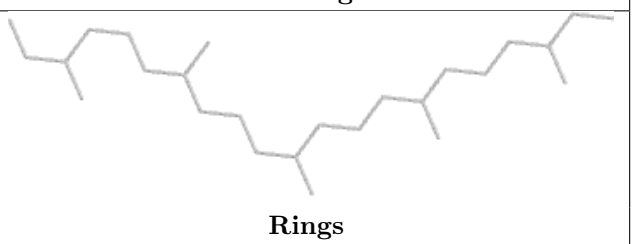
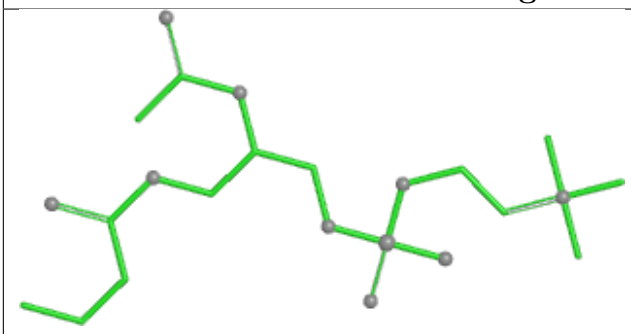

Rings

Ligand PC1 qE 301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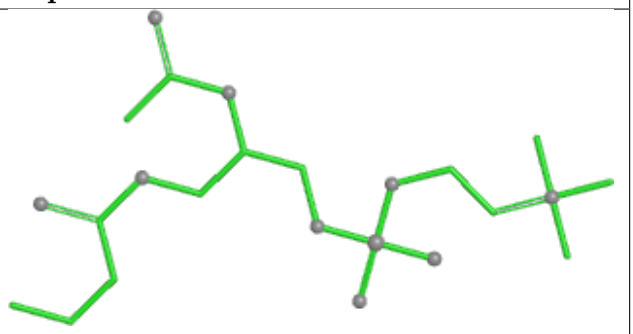
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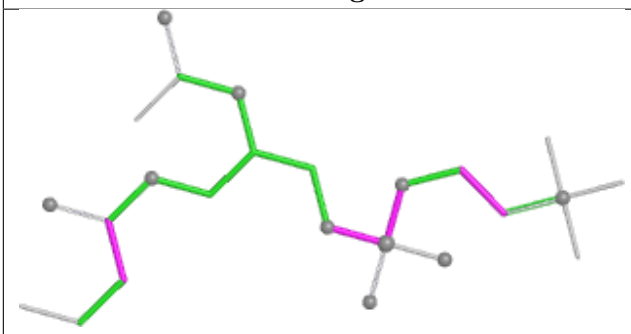
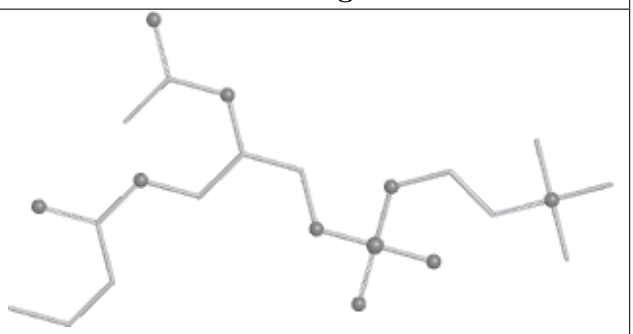
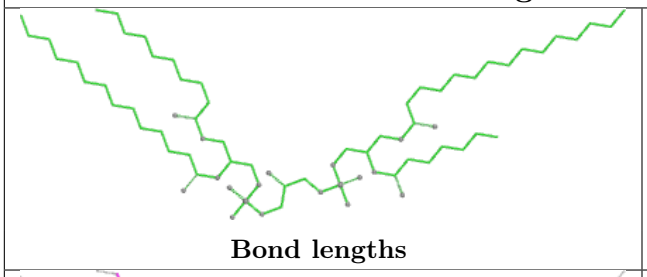

Torsions


Rings

Ligand CDL 6A 201



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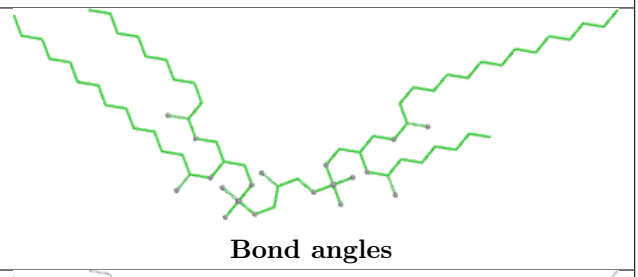

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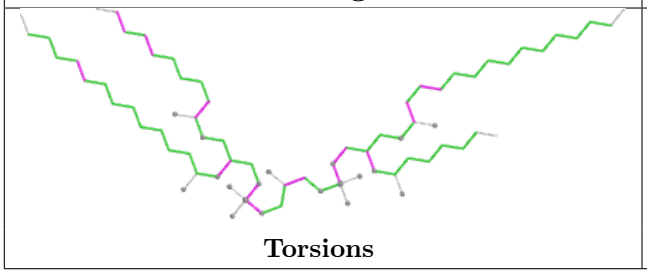

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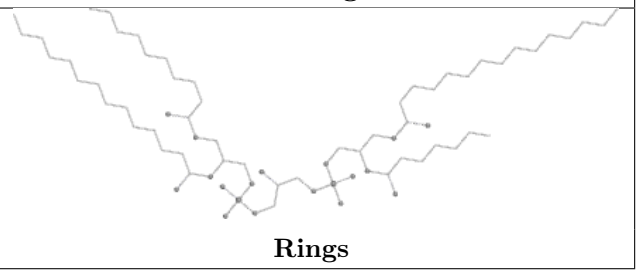
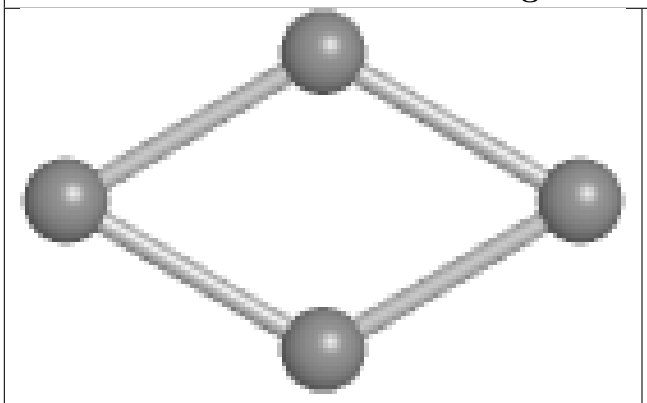


Rings

Ligand FES qE 302



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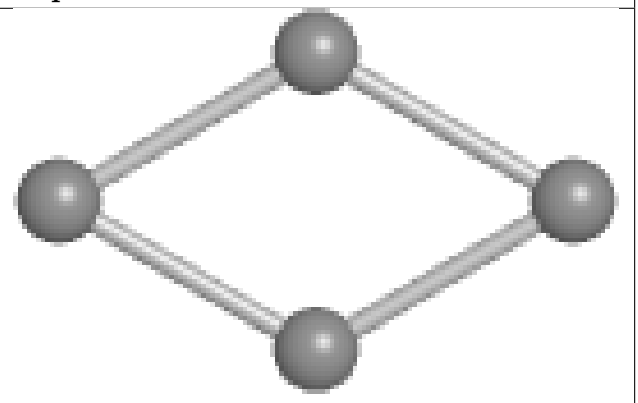

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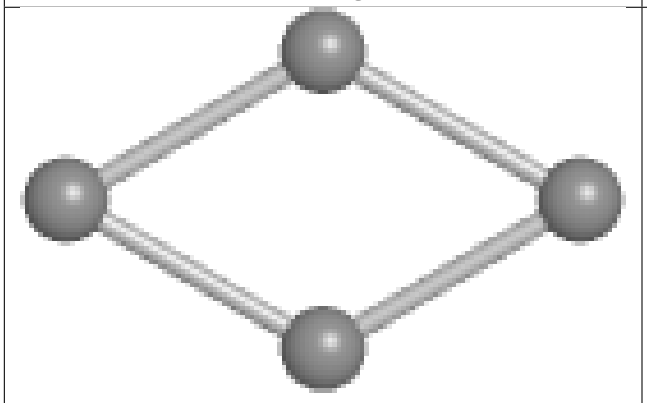

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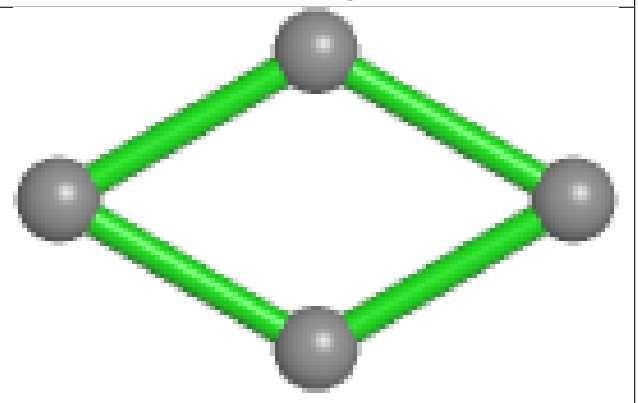
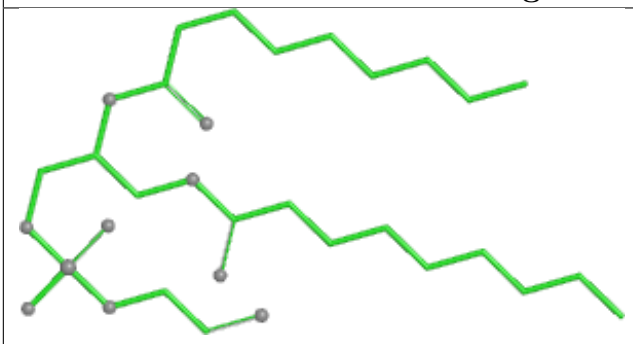


Rings

Ligand 3PE an 305



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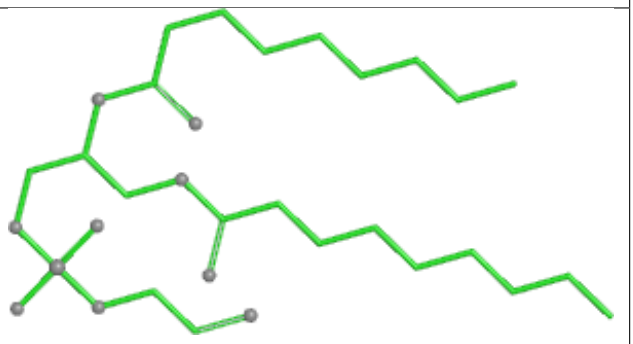
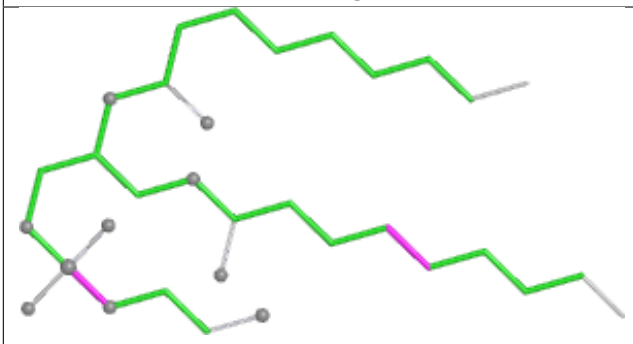


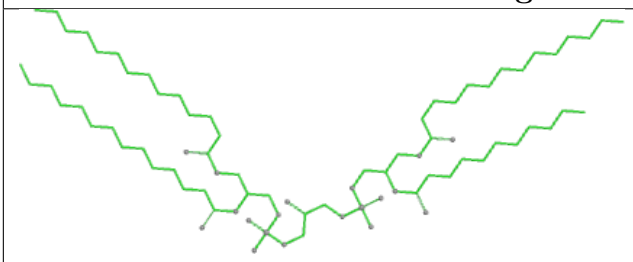
Bond angles



Torsions

Rings

Ligand CDL 5B 201



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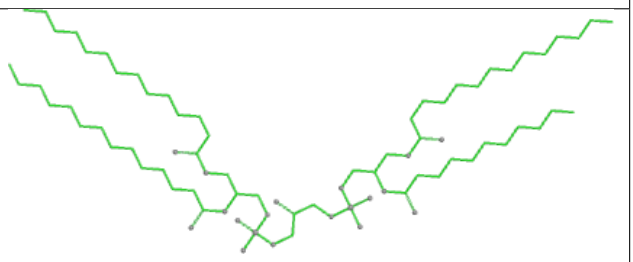
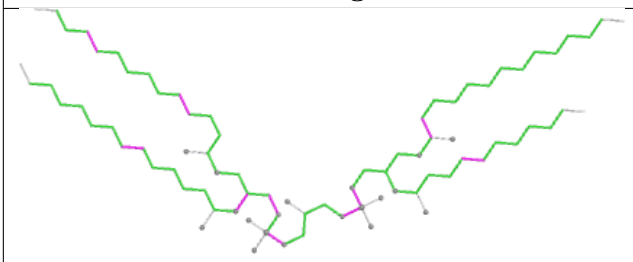


Bond angles



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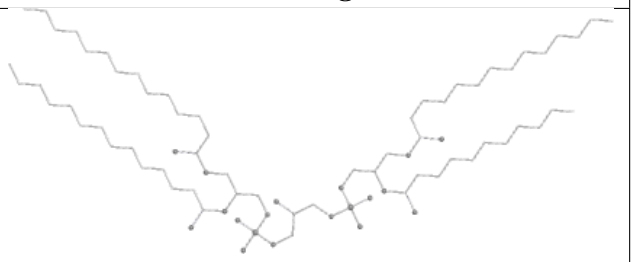
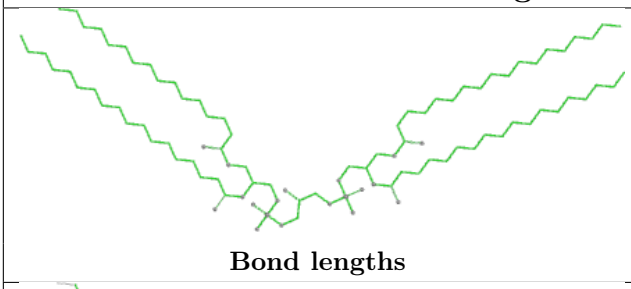


Rings

Ligand CDL 2K 101



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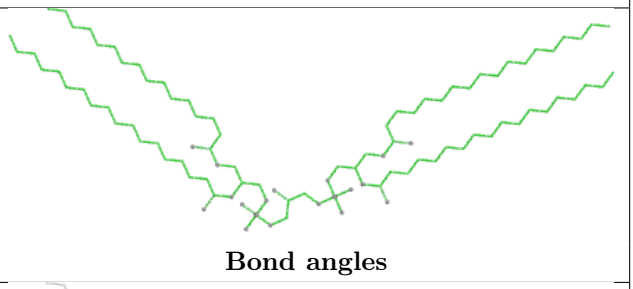

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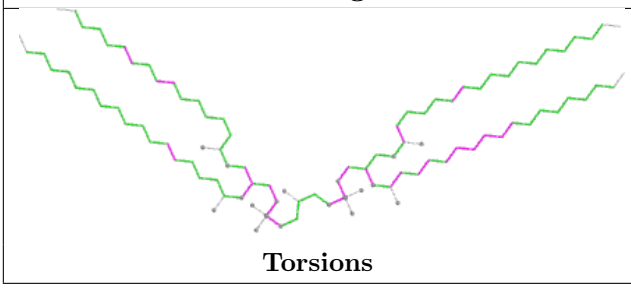

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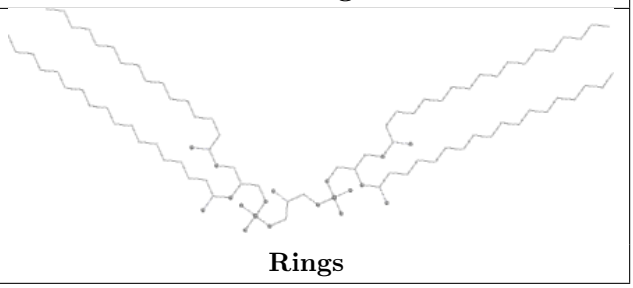
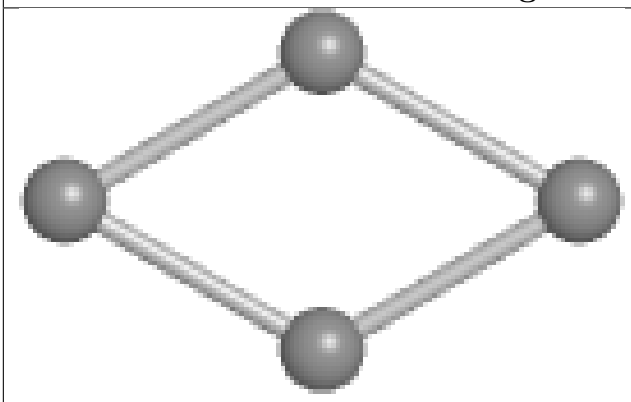


Rings

Ligand FES V2 300



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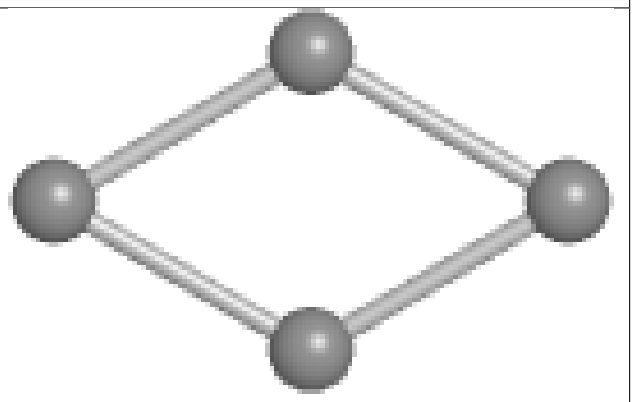

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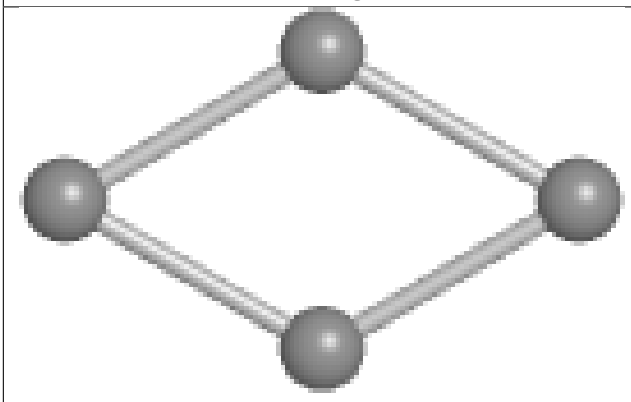

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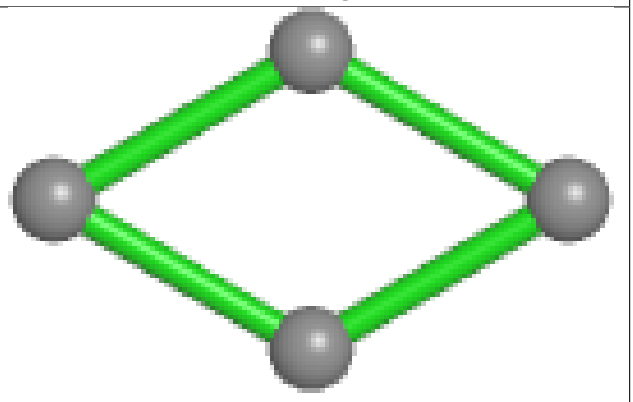
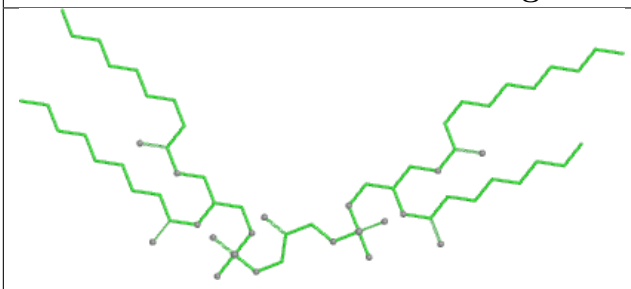


Rings

Ligand CDL m 302



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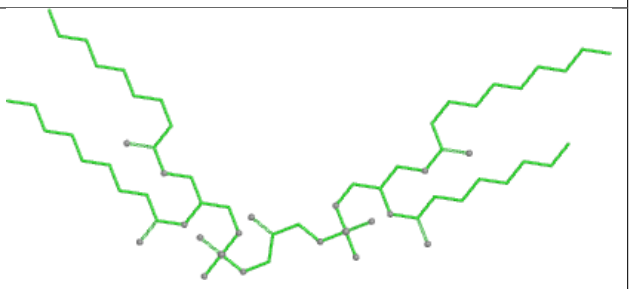

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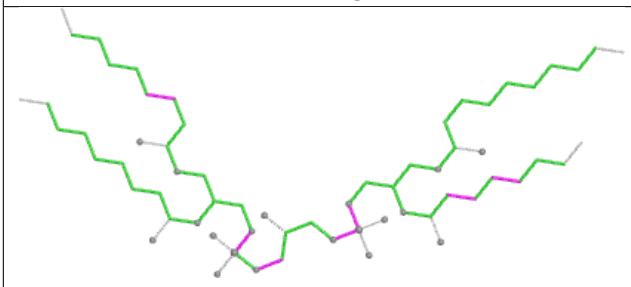

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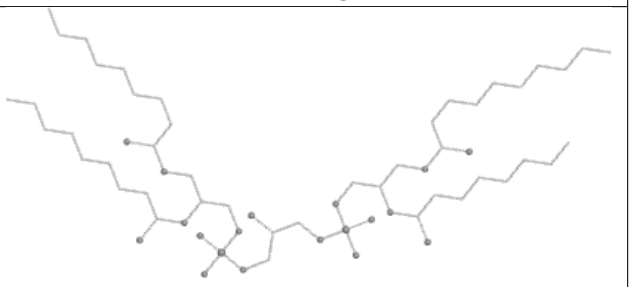
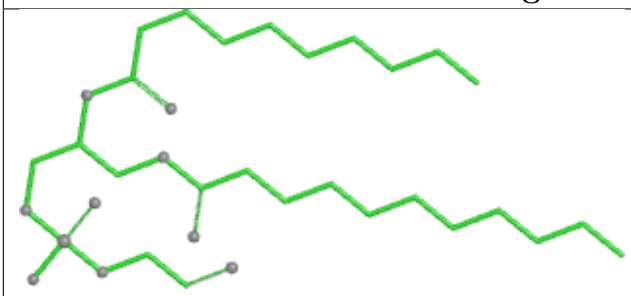


Rings

Ligand 3PE n5 802



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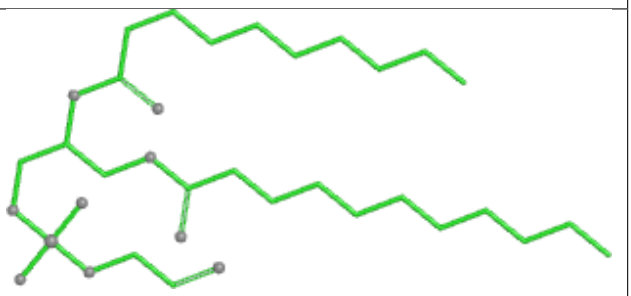

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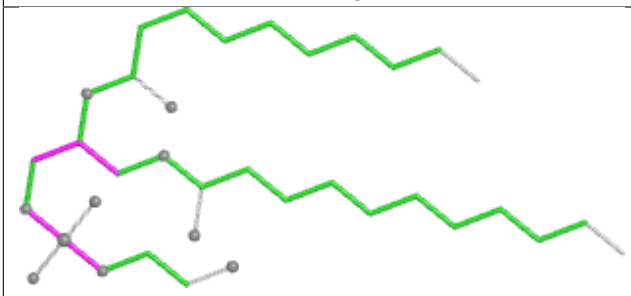

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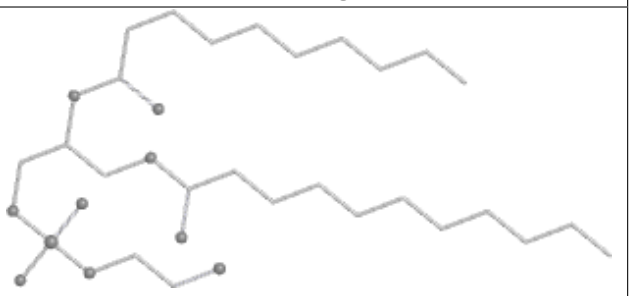
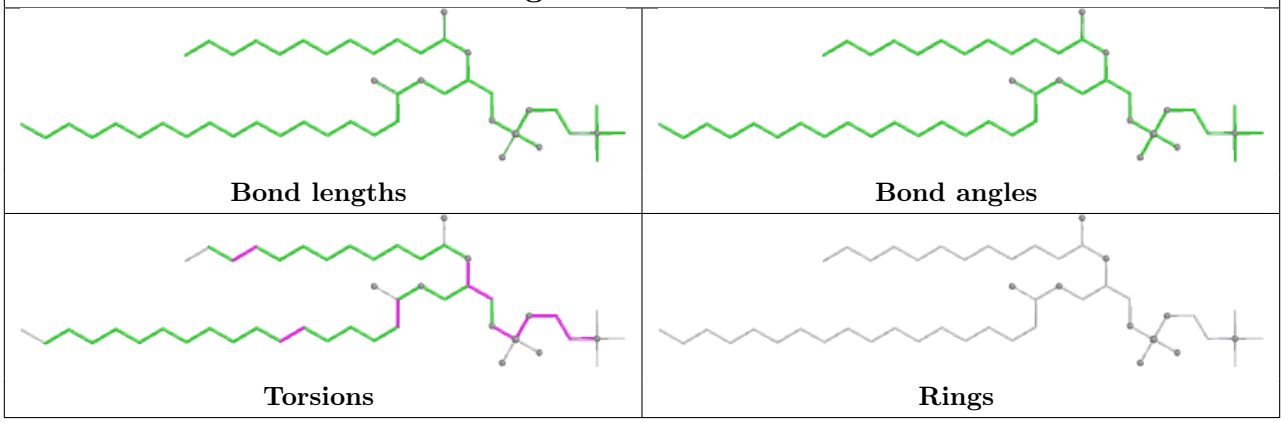
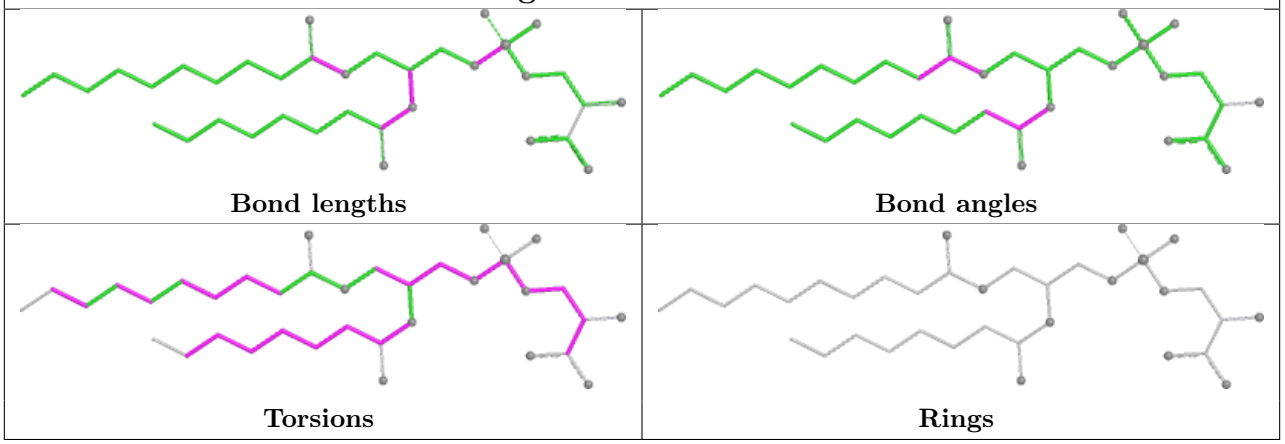


Rings

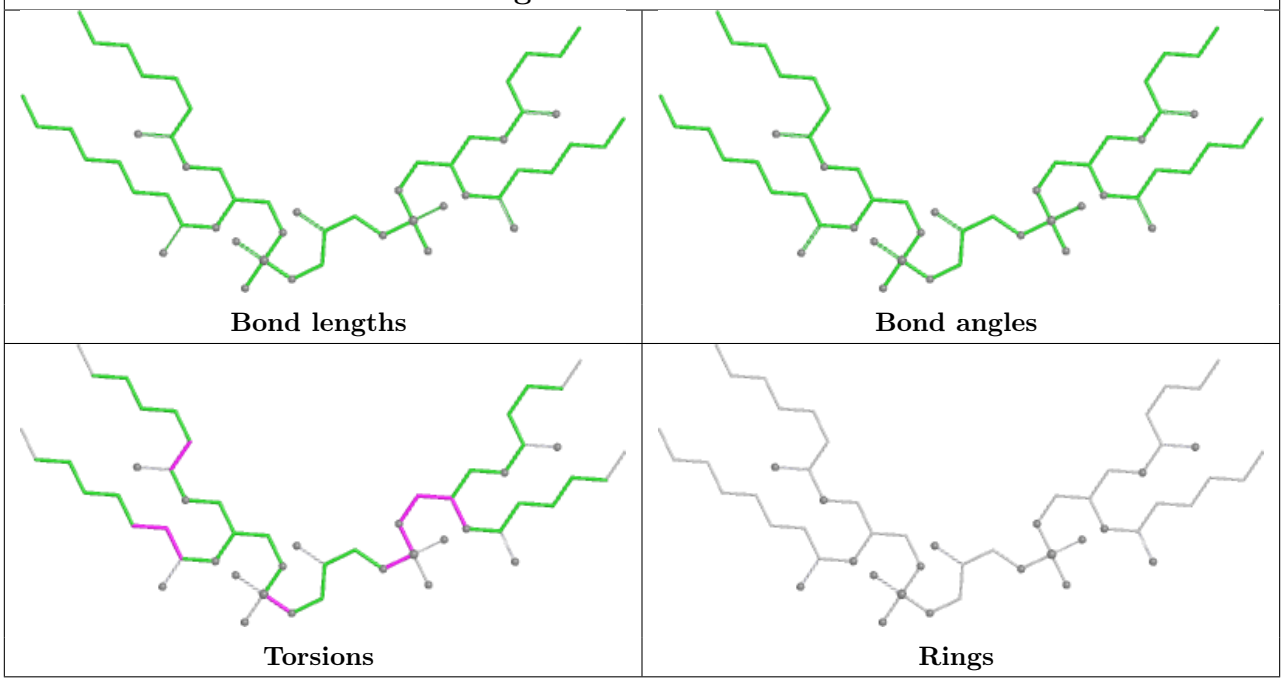
Ligand PC1 t4 301



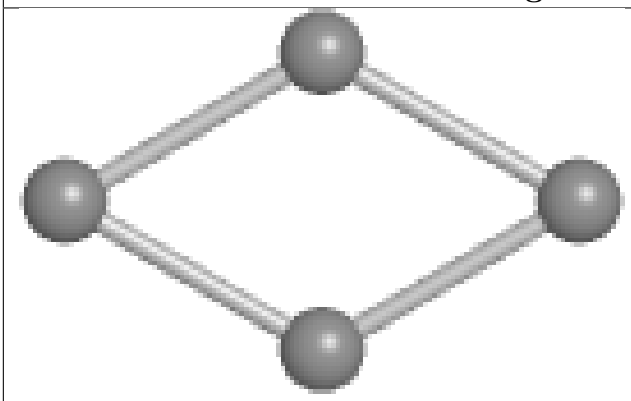
Ligand P5S M2 406



Ligand CDL m2 401



Ligand FES s1 803



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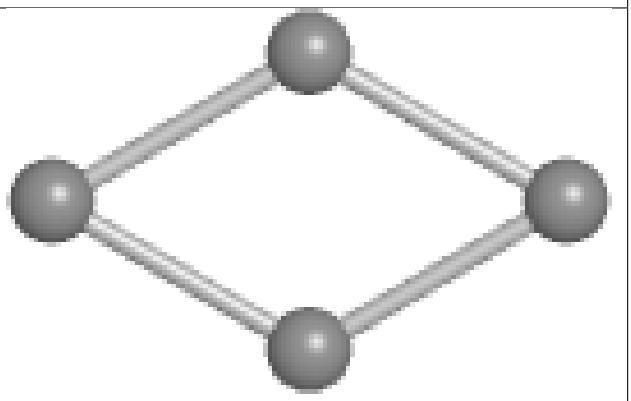
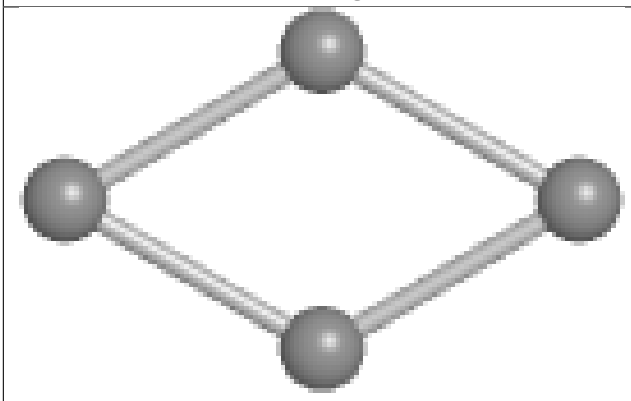
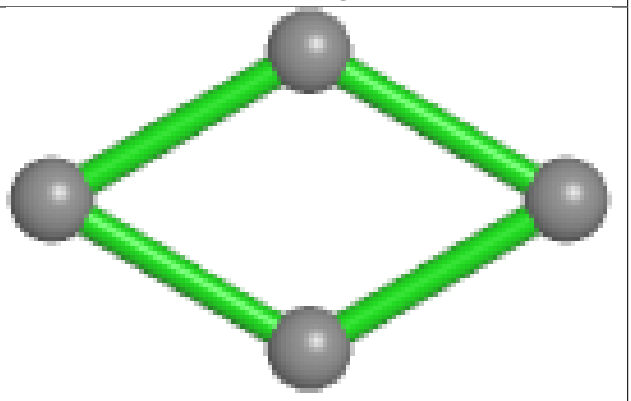


Bond angles

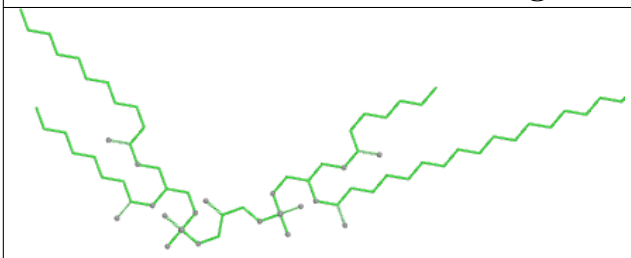


Torsions



Rings

Ligand CDL e 402



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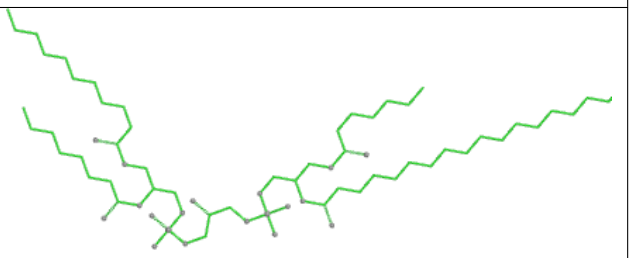
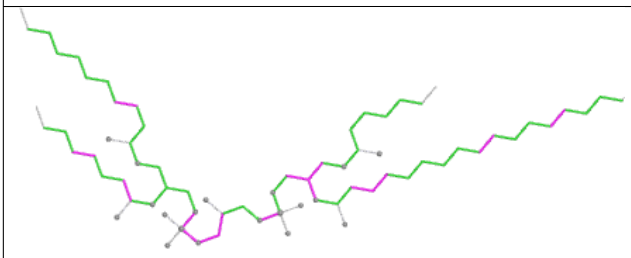


Bond angles



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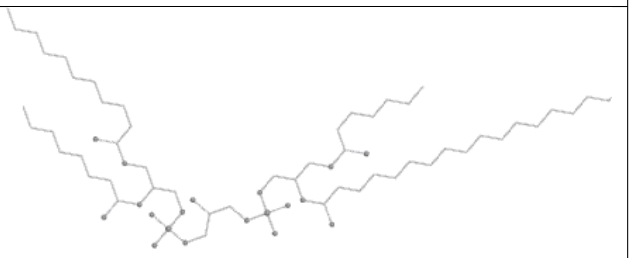
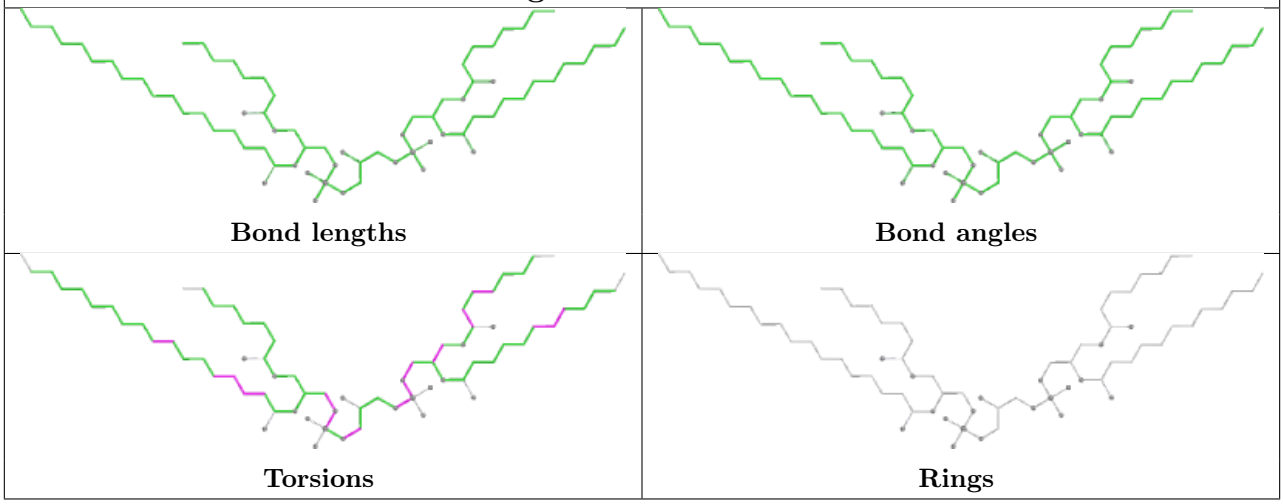
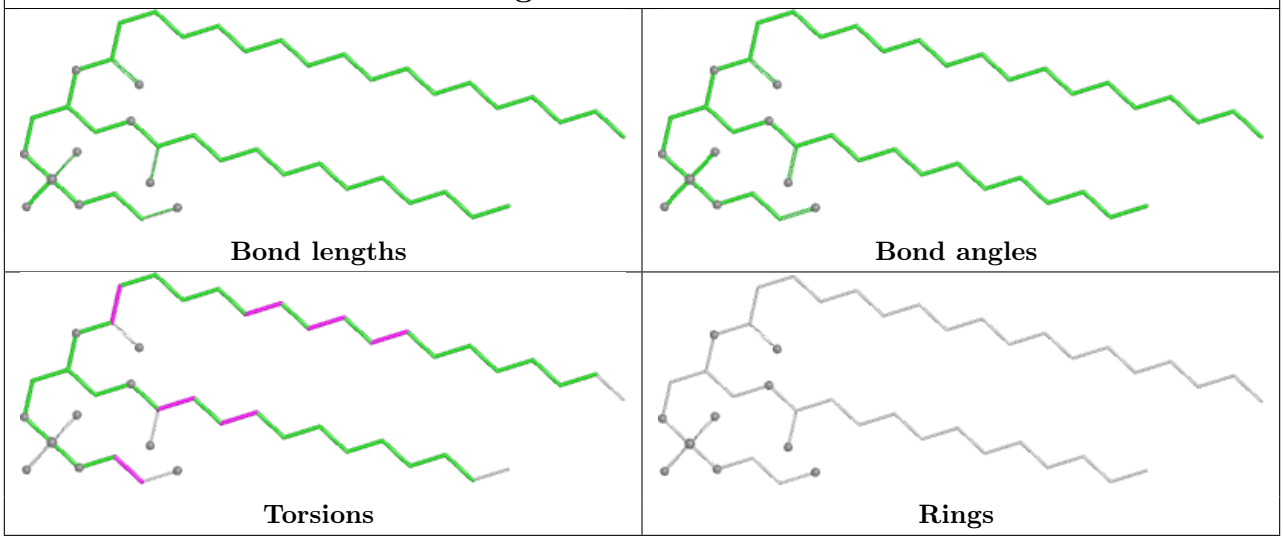


Rings

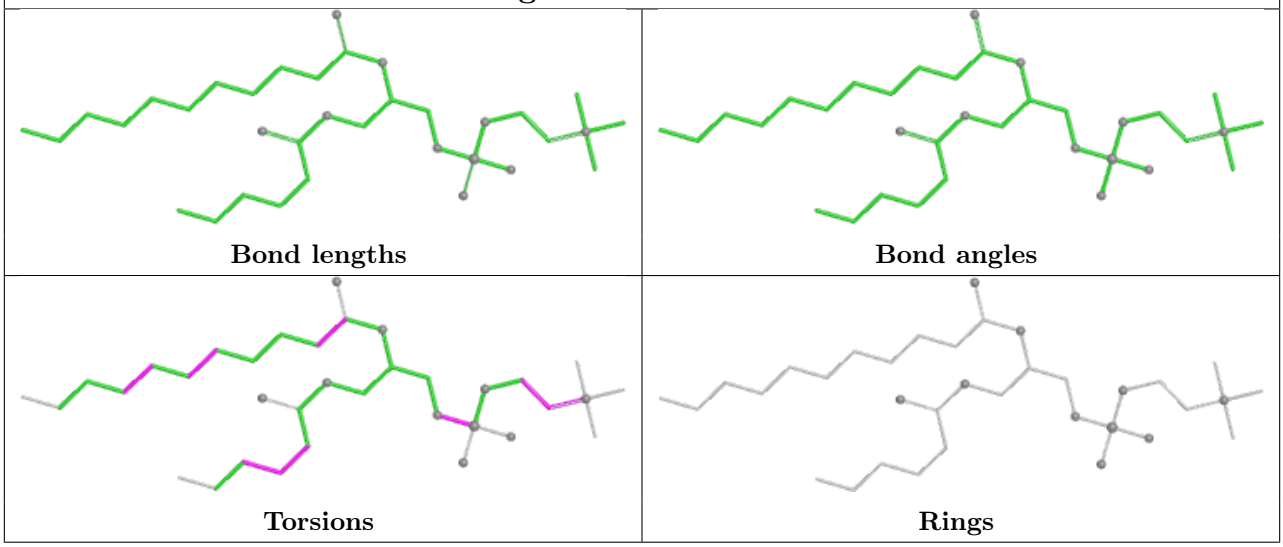
Ligand CDL L 301



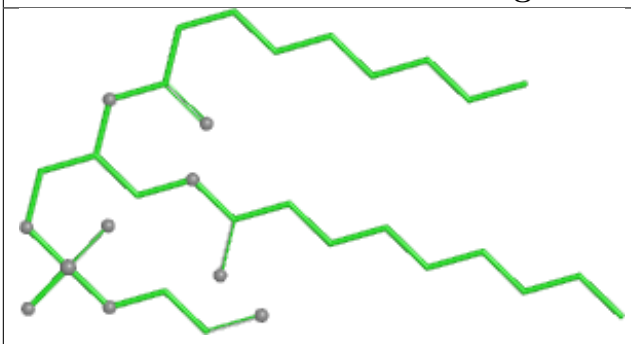
Ligand 3PE AN 303



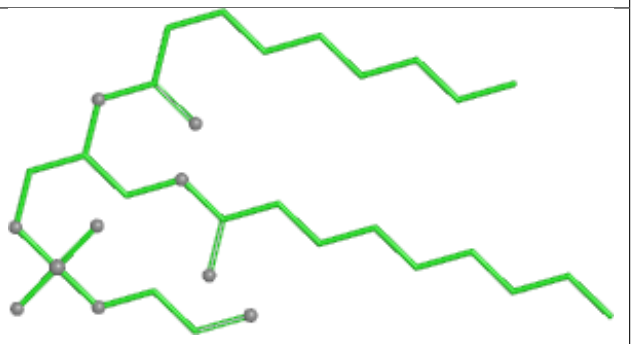
Ligand PC1 6A 202



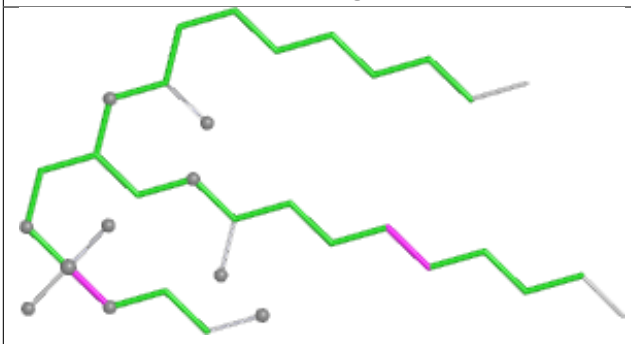
Ligand 3PE AN 305



Bond lengths



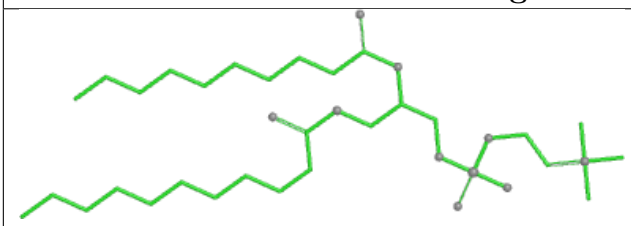
Bond angles



Torsions

Rings

Ligand PC1 AM 202



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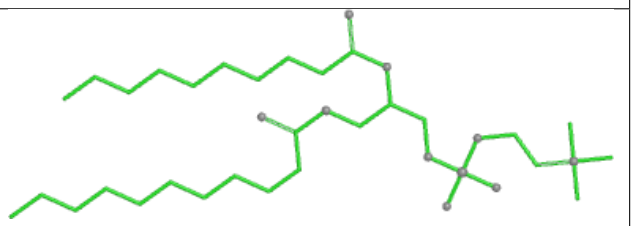
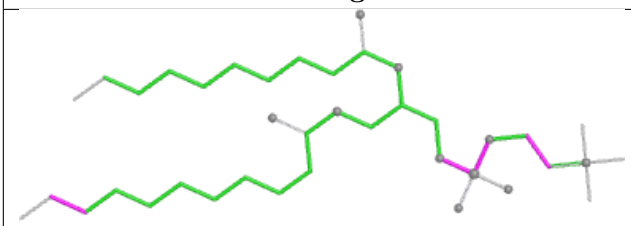
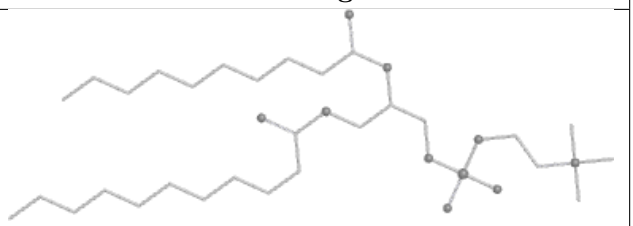


Bond angles

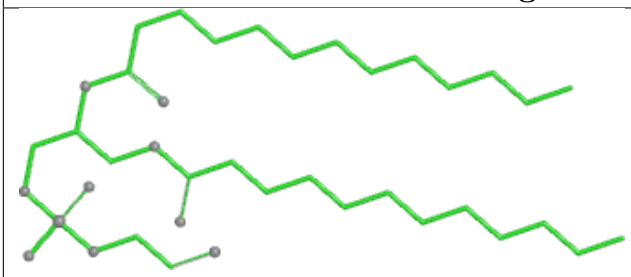


Torsions



Rings

Ligand 3PE SC 101



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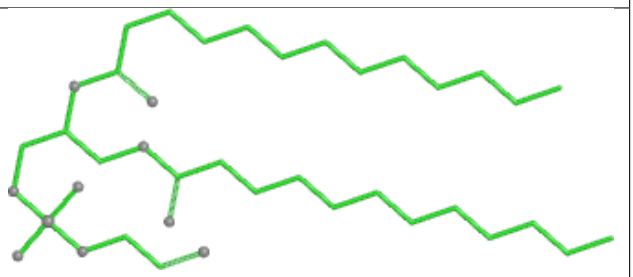
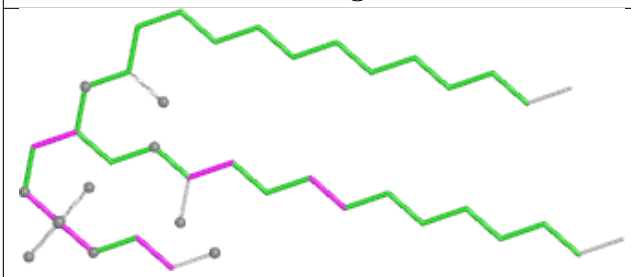


Bond angles



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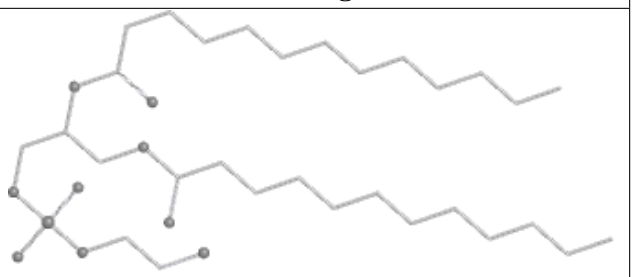
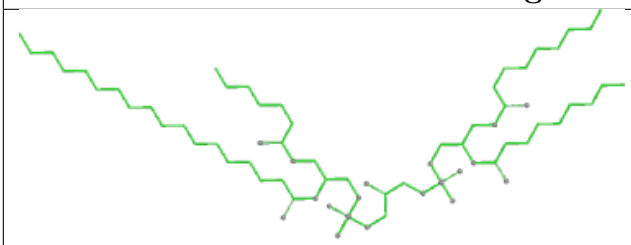


Rings

Ligand CDL T 203



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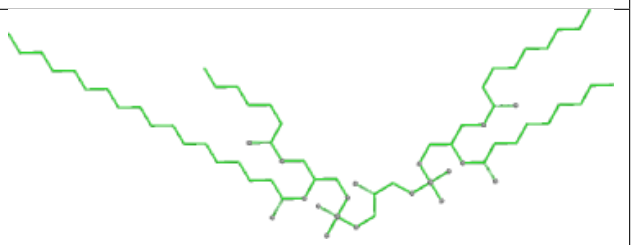
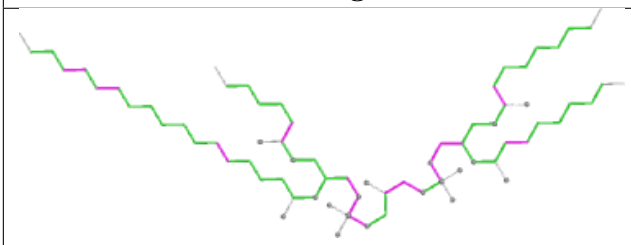
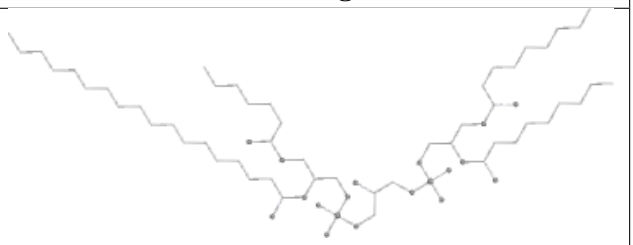


Bond angles

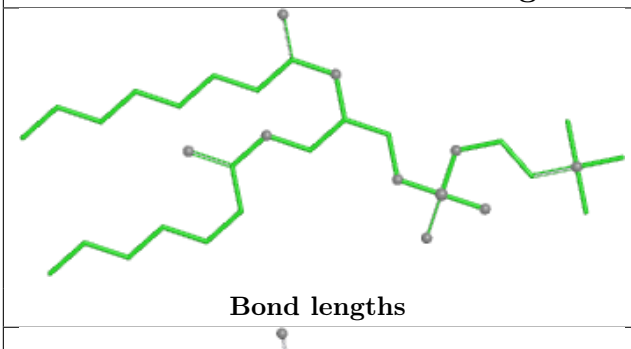


Torsions



Rings

Ligand PC1 T1 602



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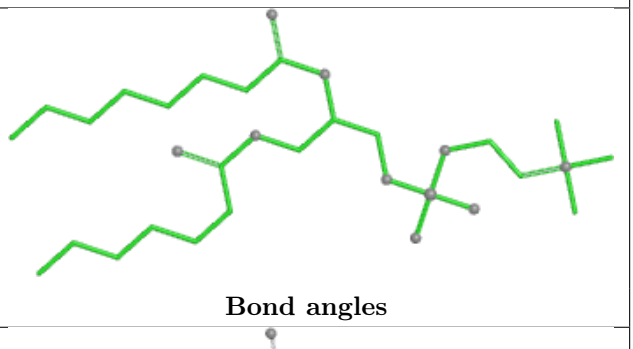
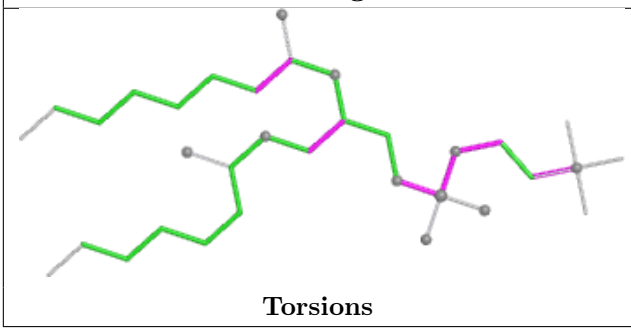


Bond angles



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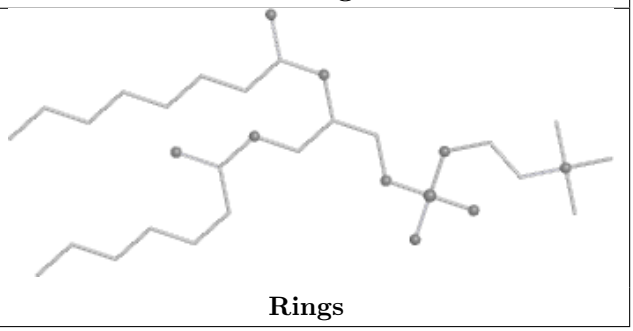
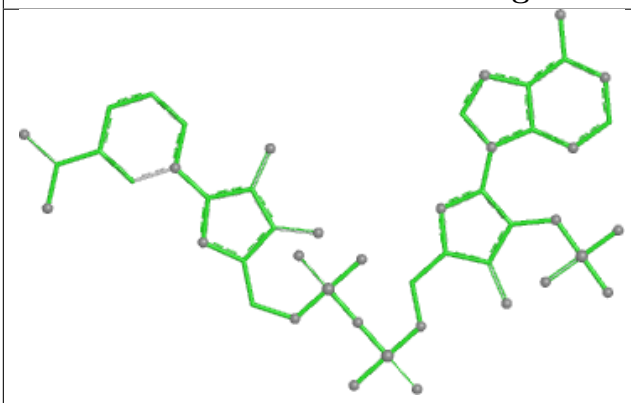


Rings

Ligand NDP A9 401



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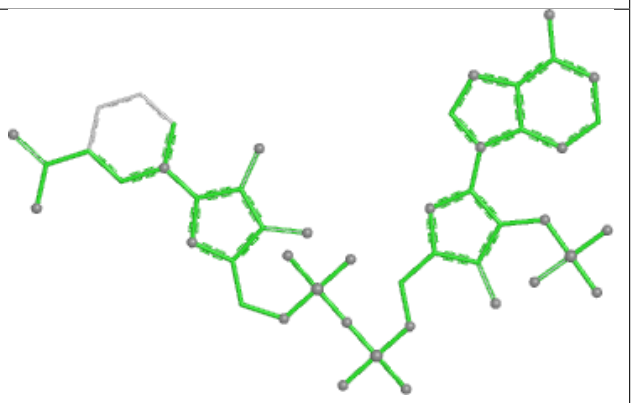
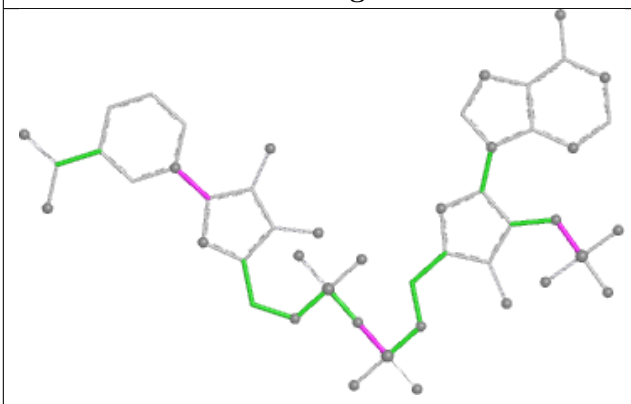


Bond angles



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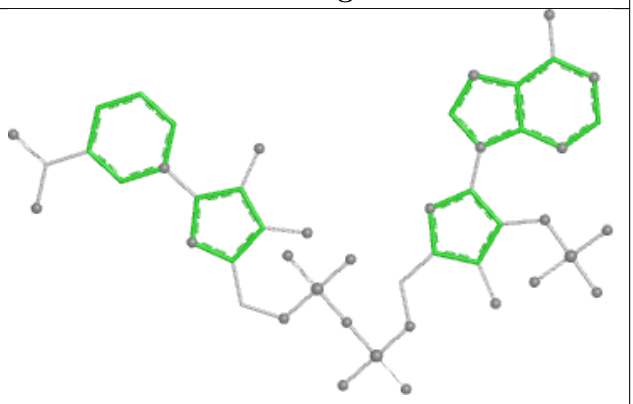
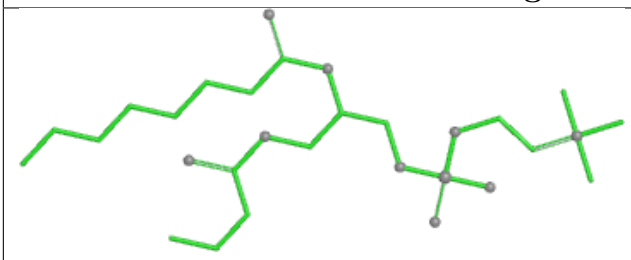


Rings

Ligand PC1 qI 201



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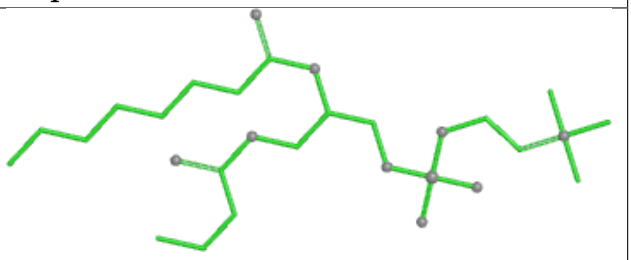

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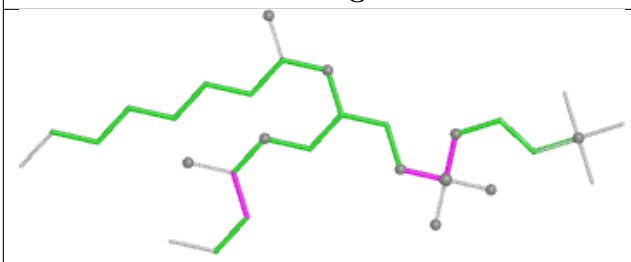

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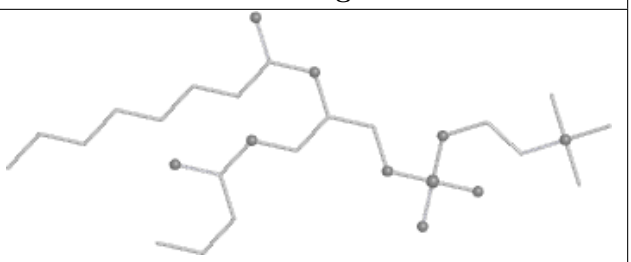
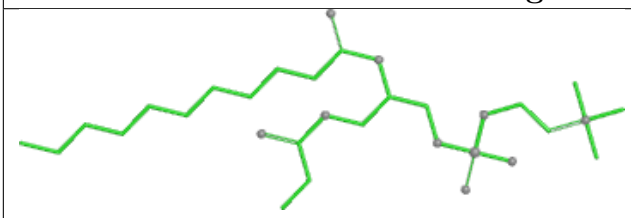


Rings

Ligand PC1 2f 303



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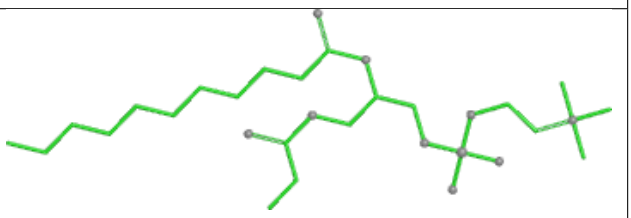
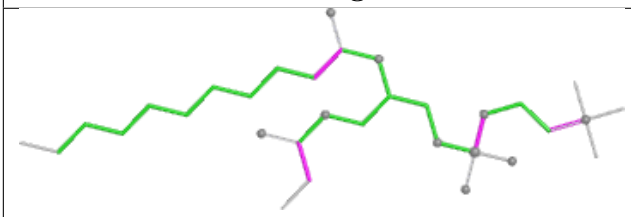
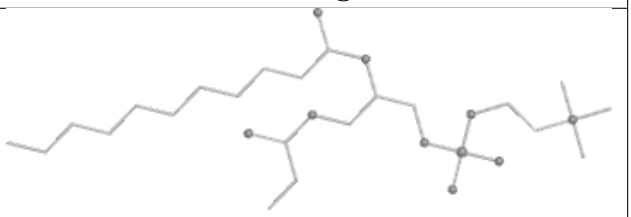


Bond angles

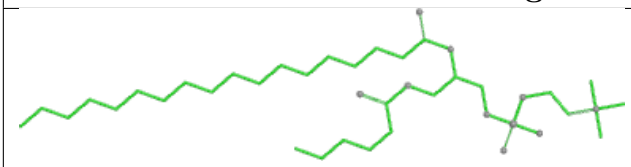


Torsions

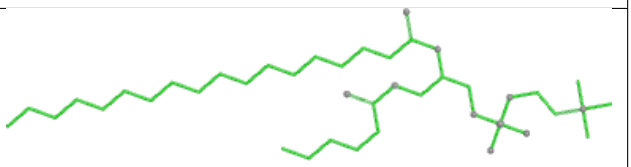


Rings

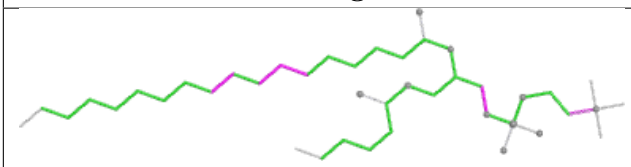
Ligand PC1 tc 101



Bond lengths



Bond angles



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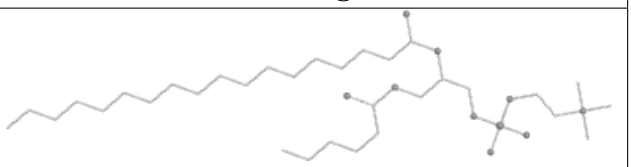
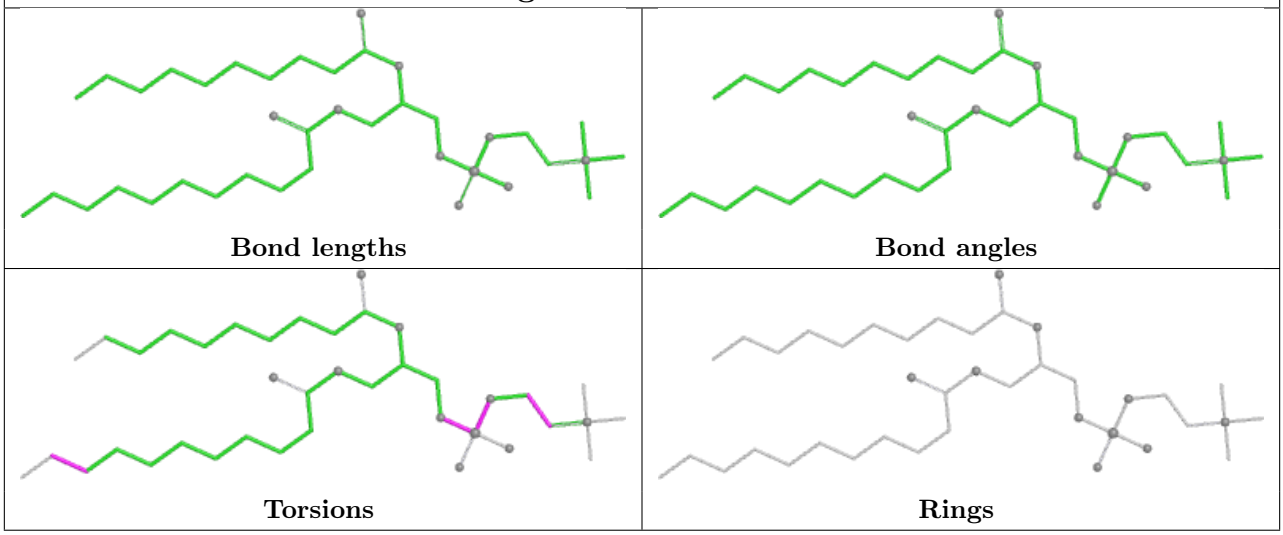
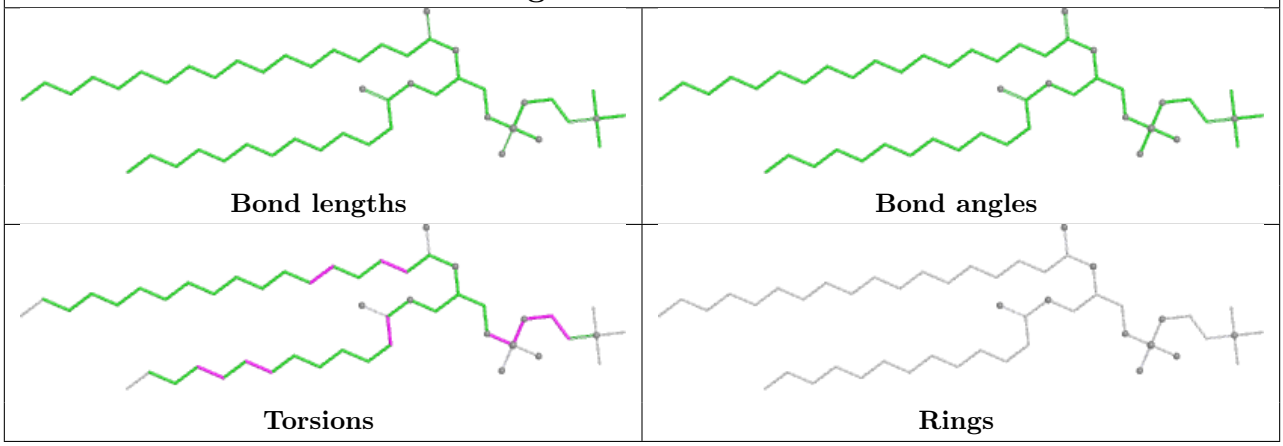


Rings

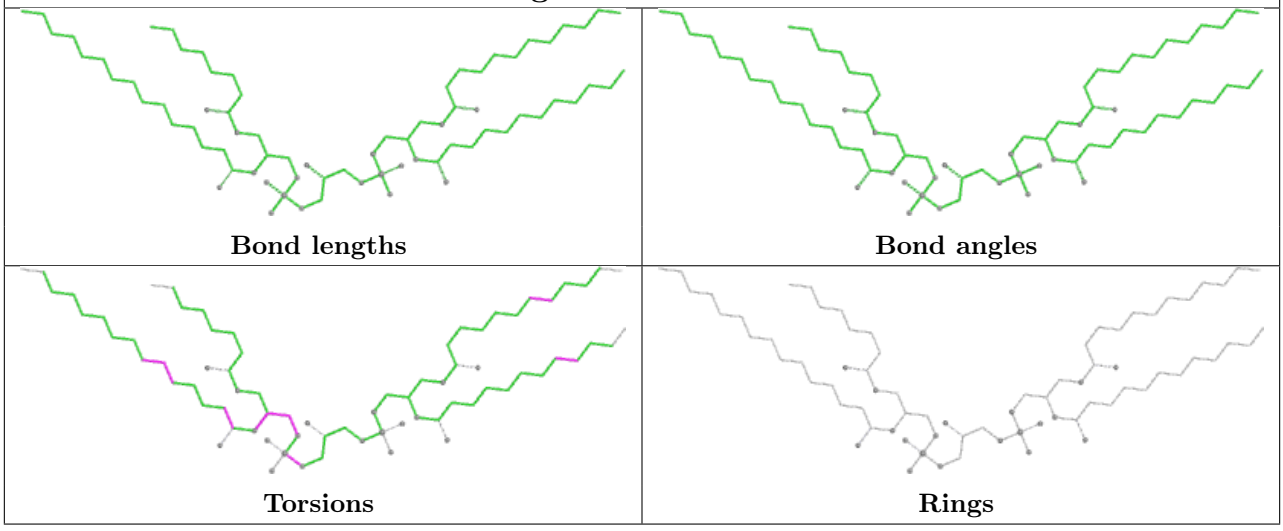
Ligand PC1 am 202



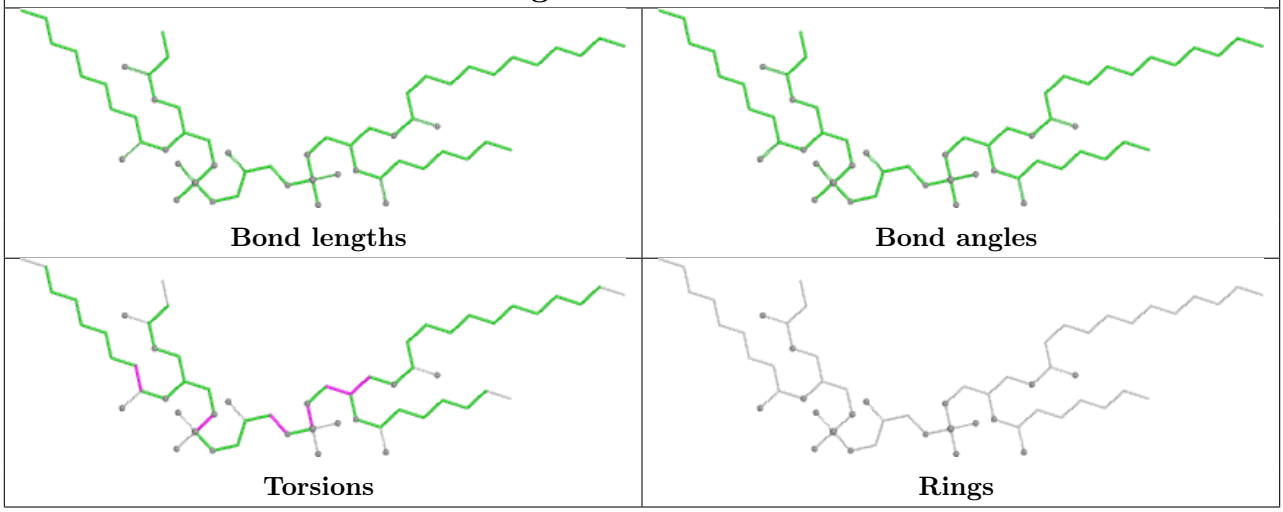
Ligand PC1 V 202



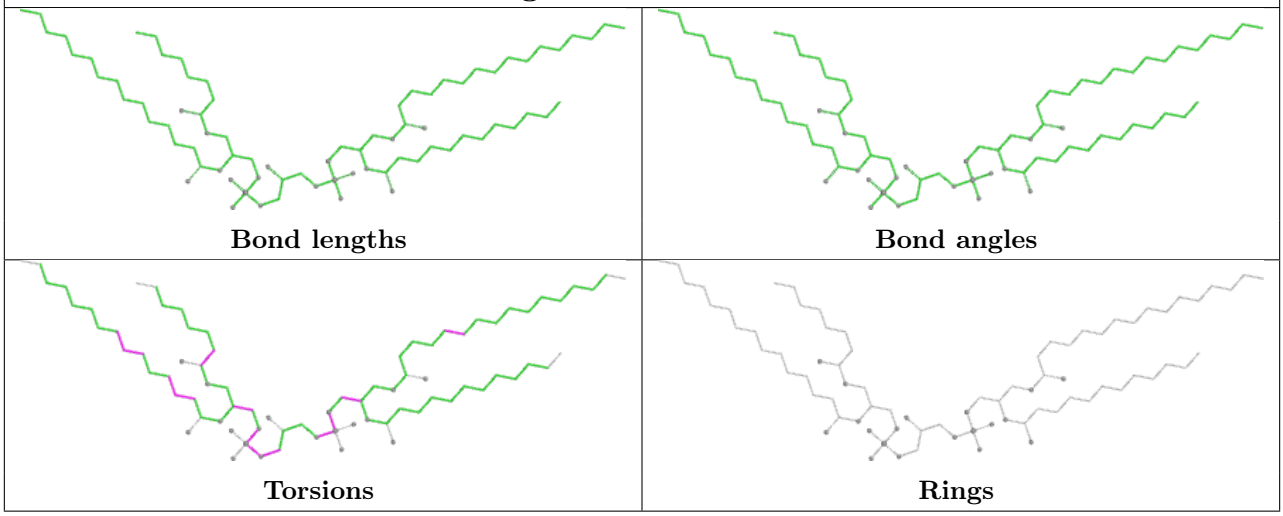
Ligand CDL t 202



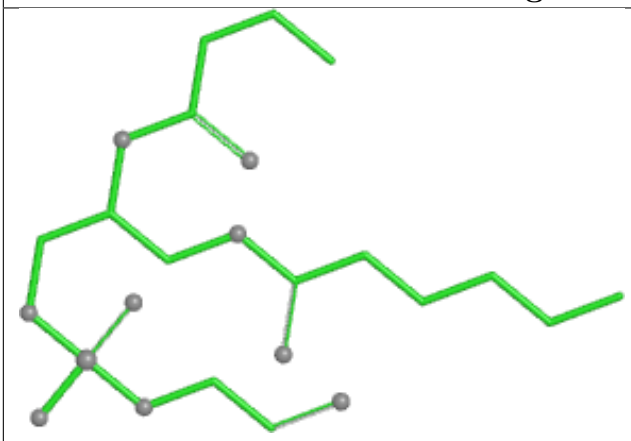
Ligand CDL t 201



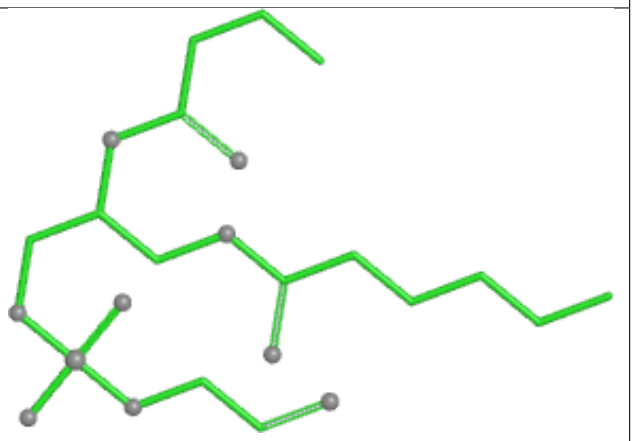
Ligand CDL c1 701



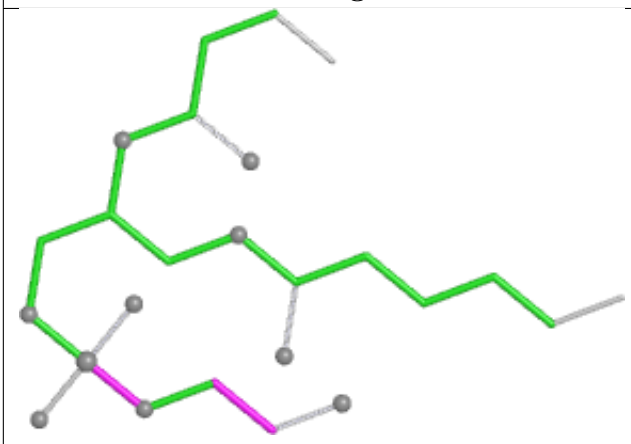
Ligand 3PE t4 302



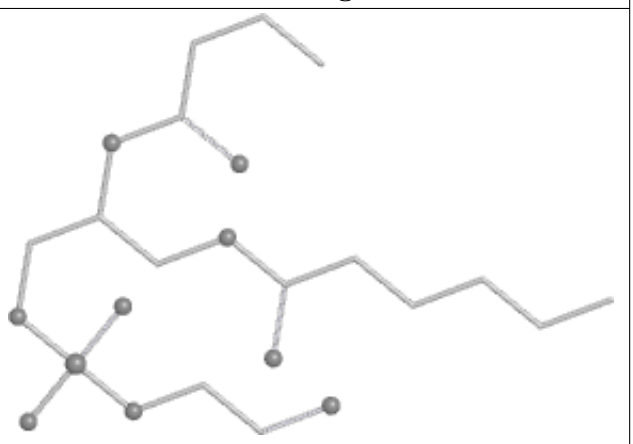
Bond lengths



Bond angles

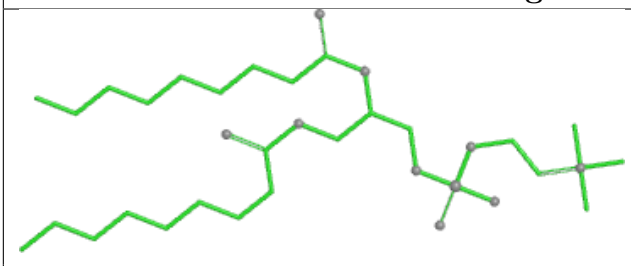


Torsions

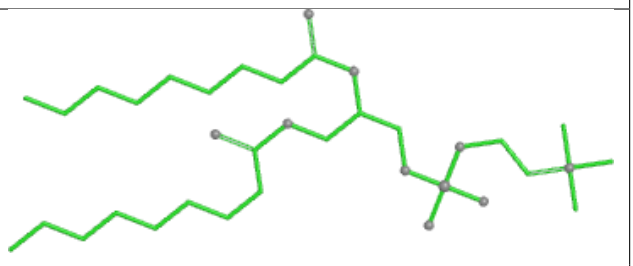


Rings

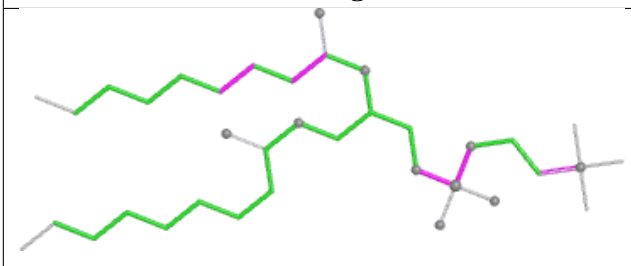
Ligand PC1 m 307



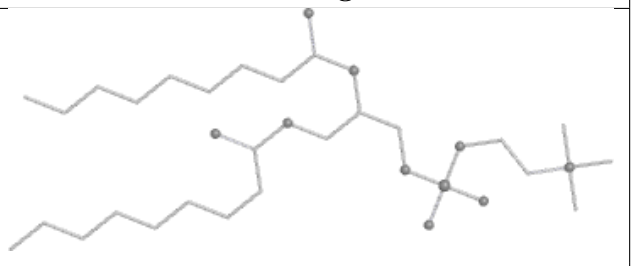
Bond lengths



Bond angles

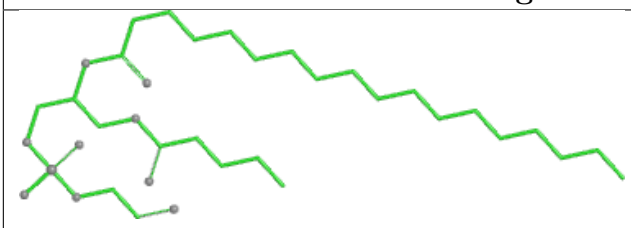


Torsions

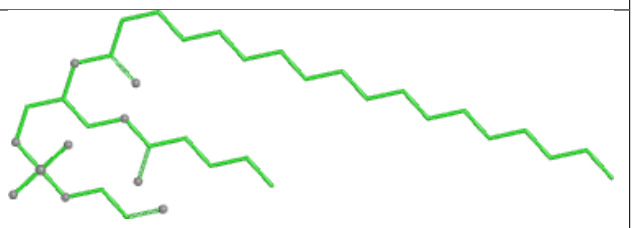


Rings

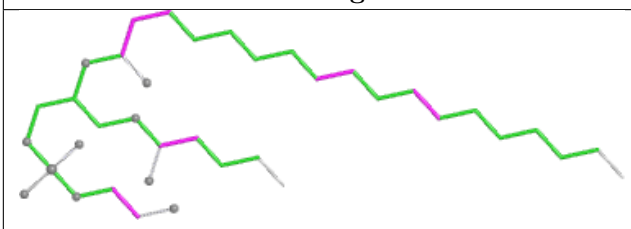
Ligand 3PE M3 402



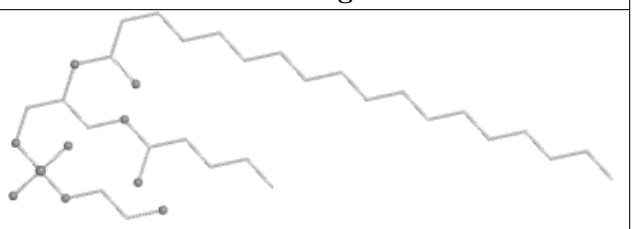
Bond lengths



Bond angles

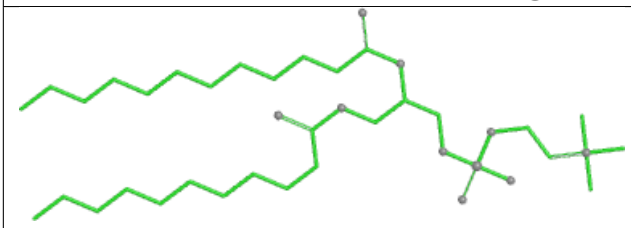


Torsions

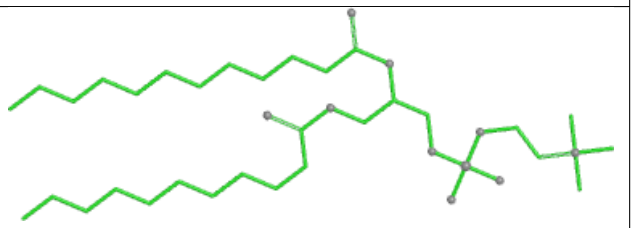


Rings

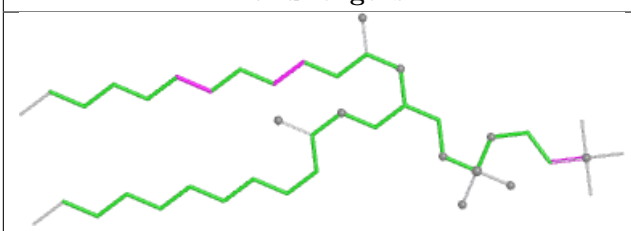
Ligand PC1 N 301



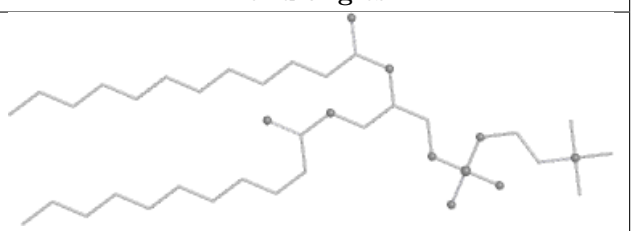
Bond lengths



Bond angles

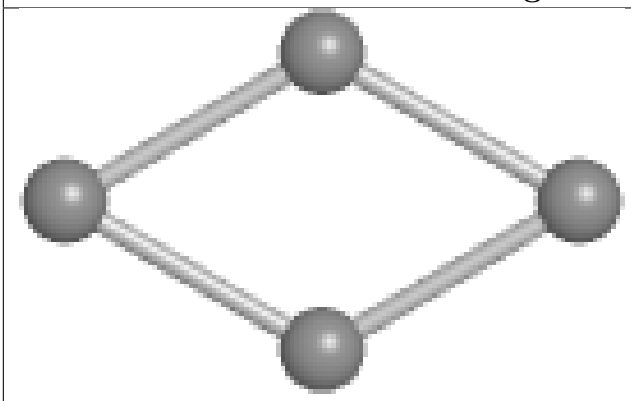


Torsions



Rings

Ligand FES qe 302



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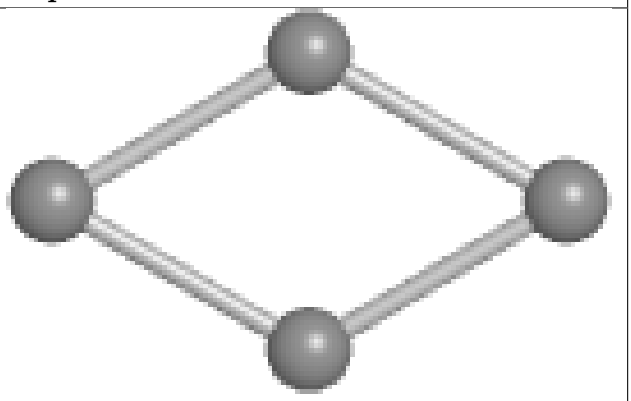
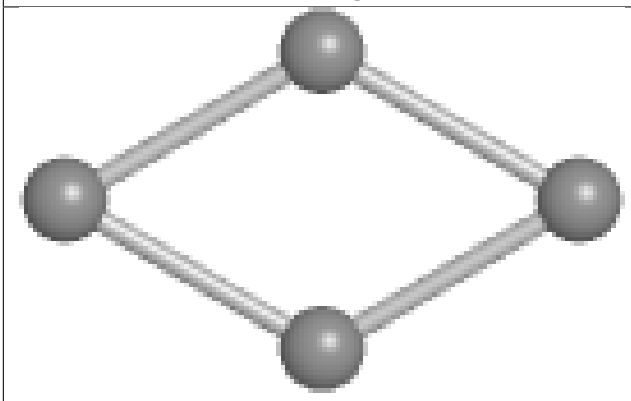
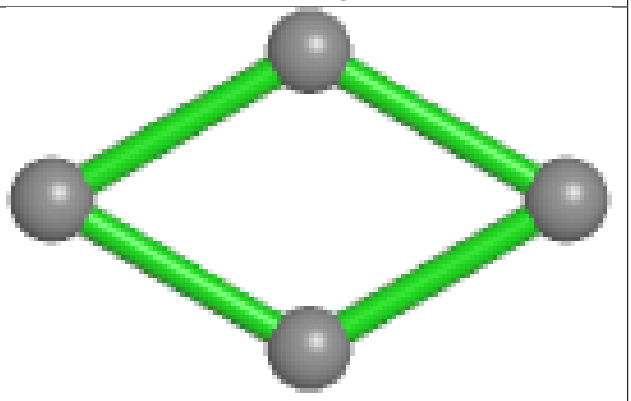


Bond angles

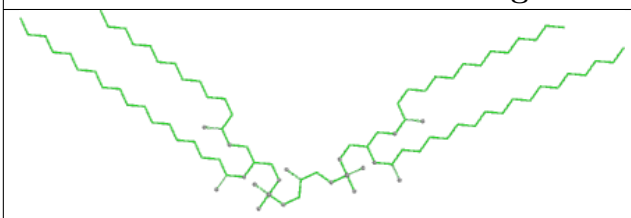


Torsions

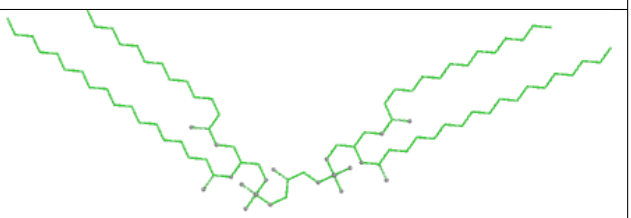


Rings

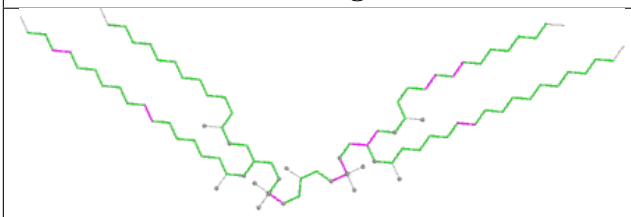
Ligand CDL M1 404



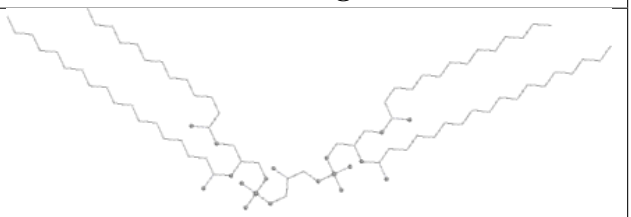
Bond lengths



Bond angles

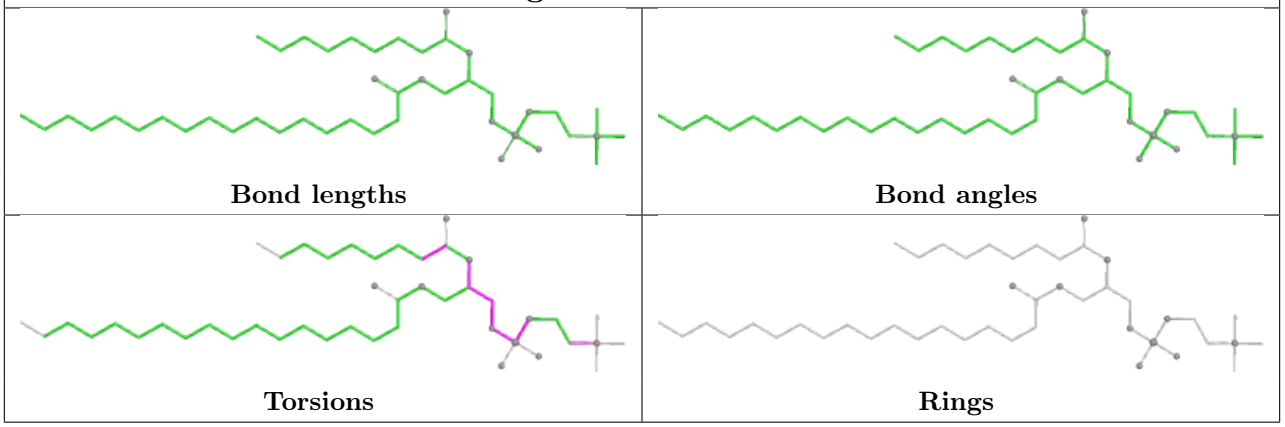


Torsions

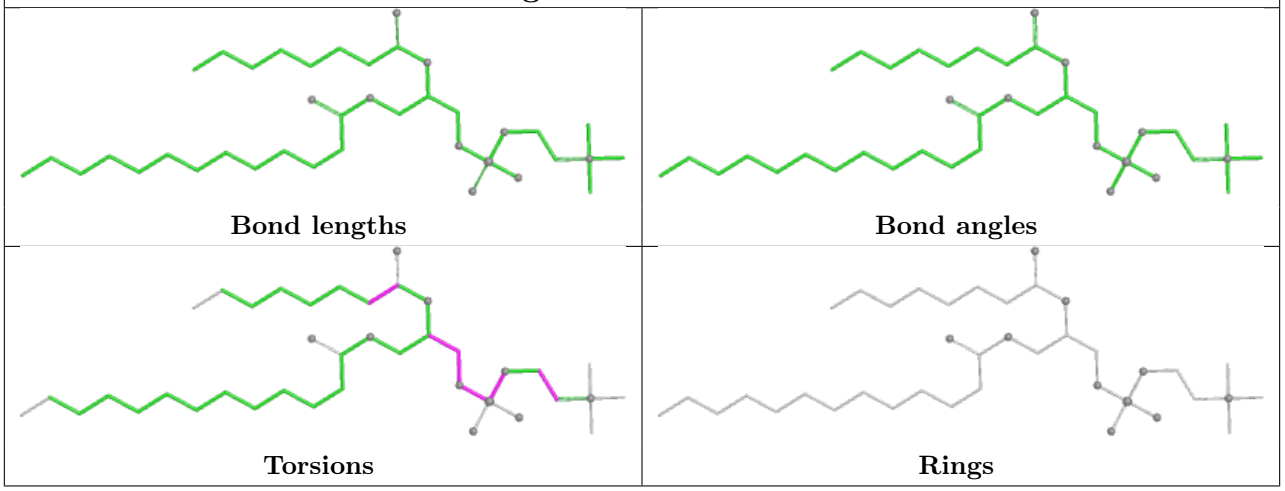


Rings

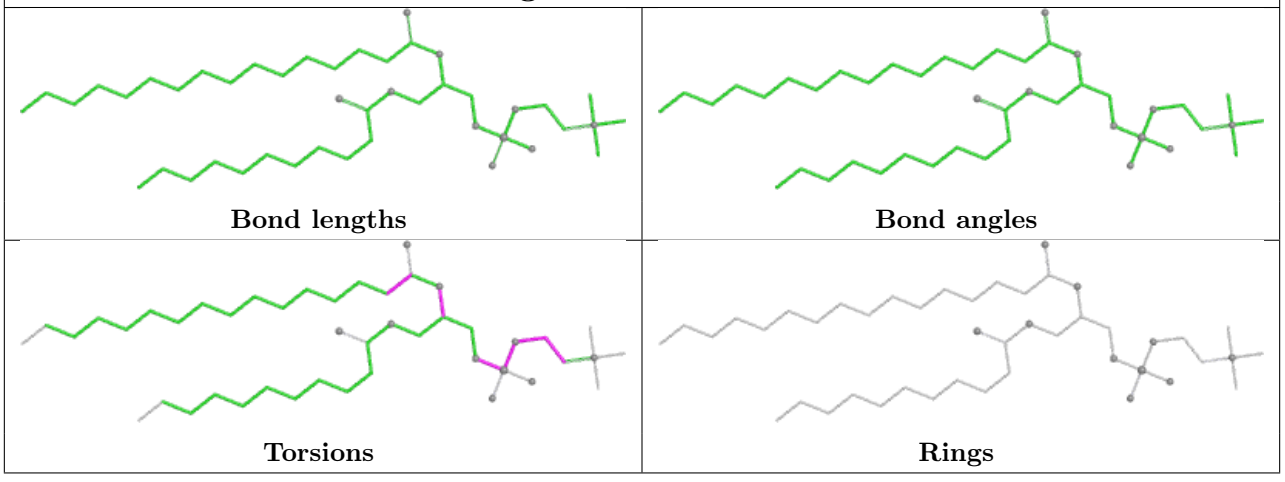
Ligand PC1 m 301



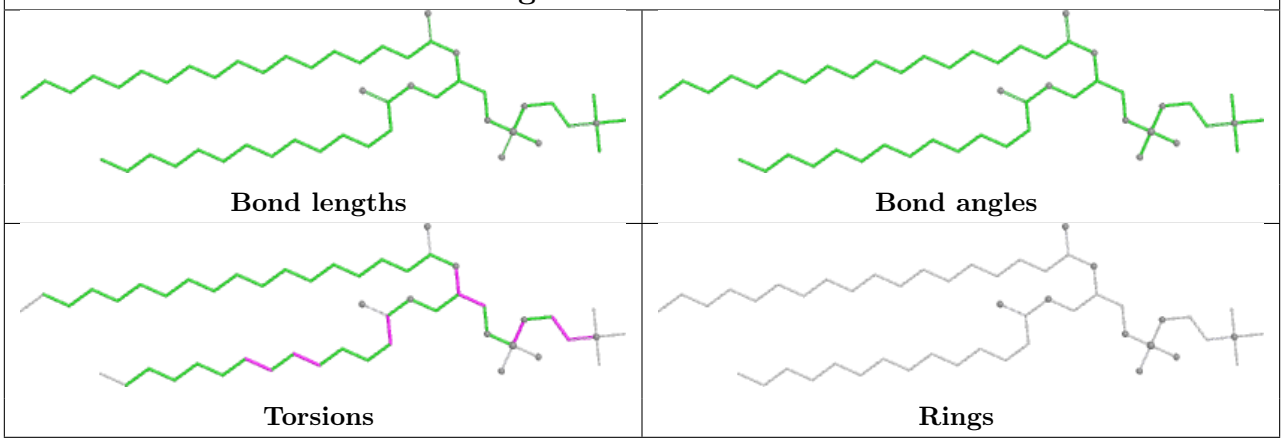
Ligand PC1 n5 804



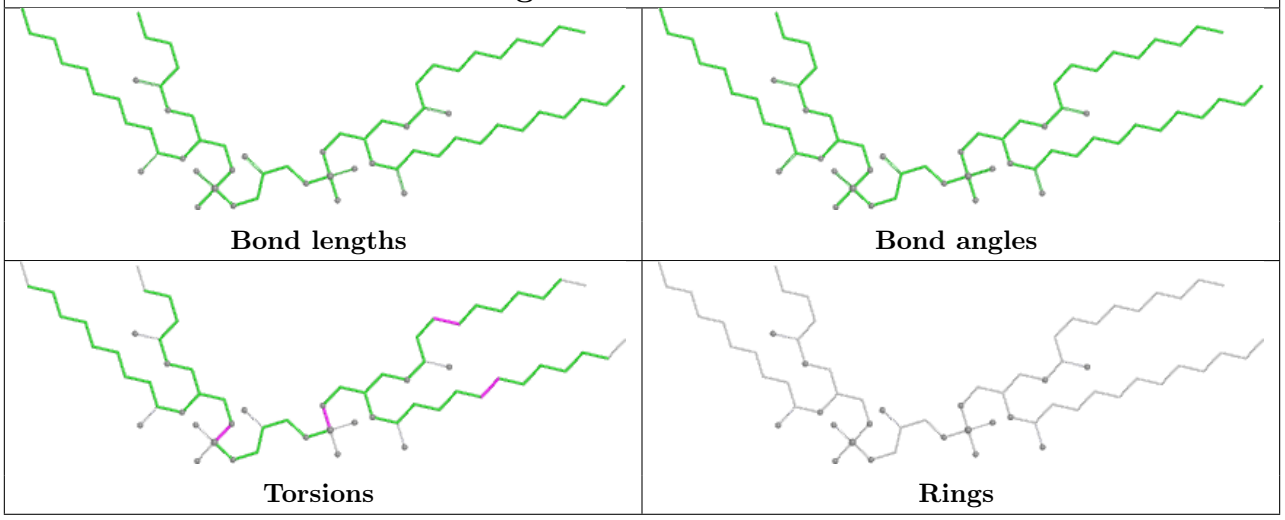
Ligand PC1 C1 709



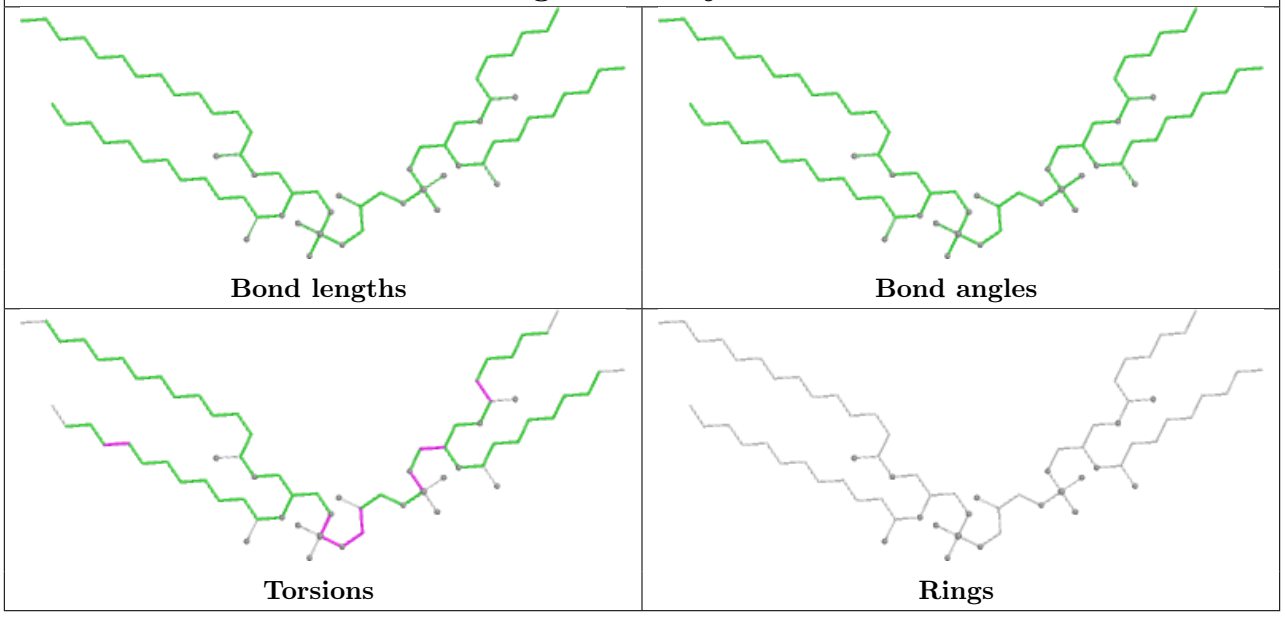
Ligand PC1 2G 202



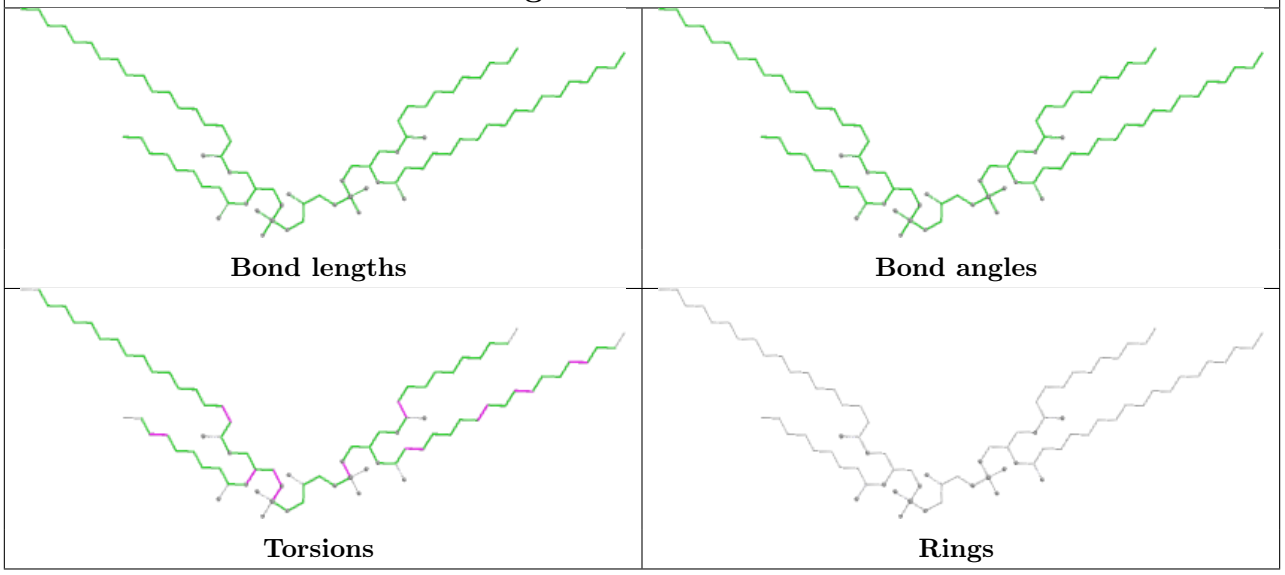
Ligand CDL C1 707



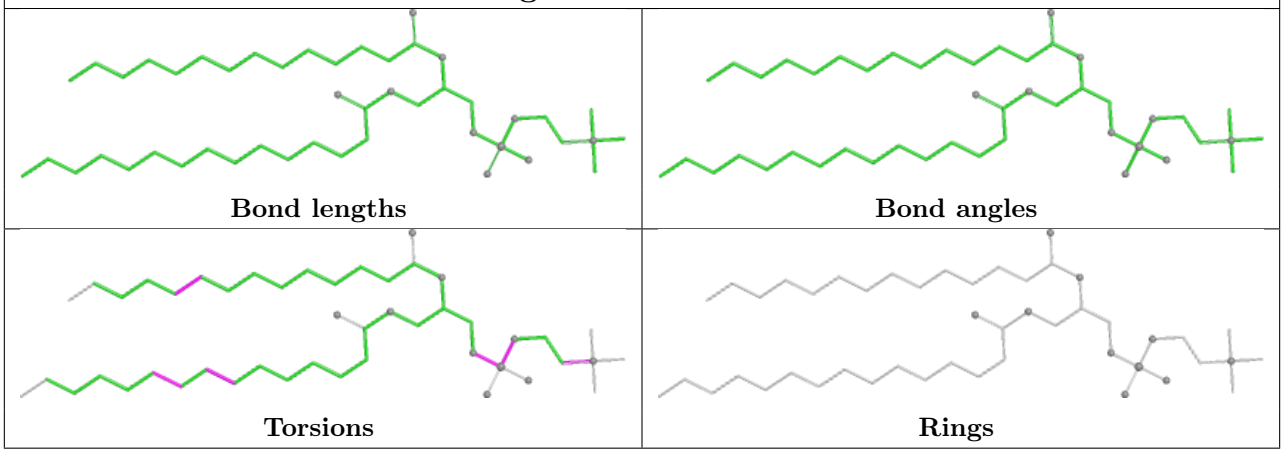
Ligand CDL j 301



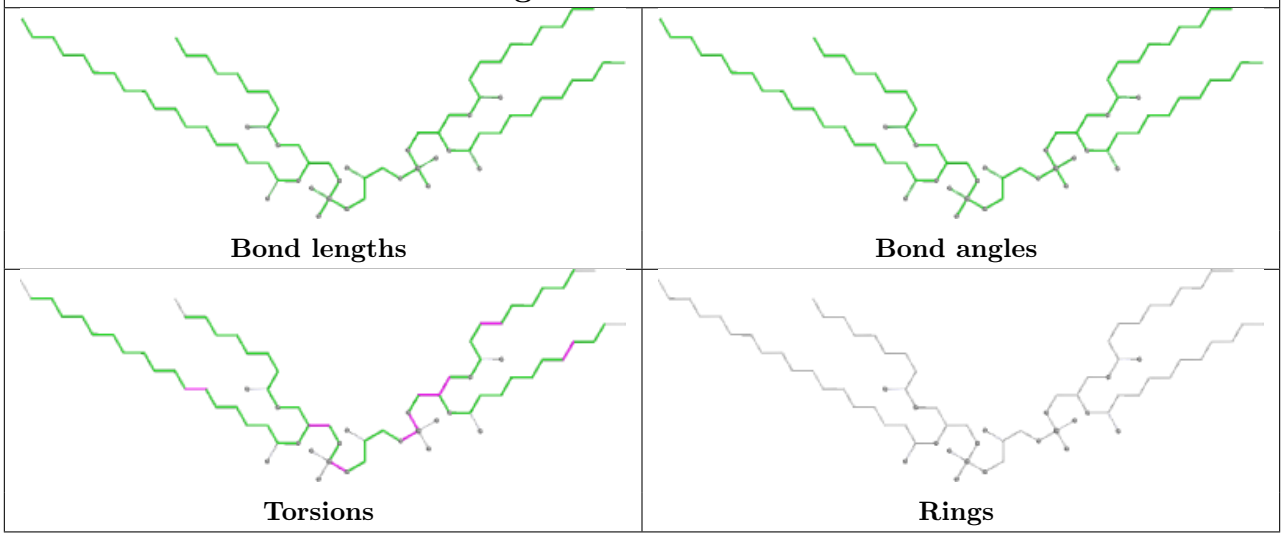
Ligand CDL w 202



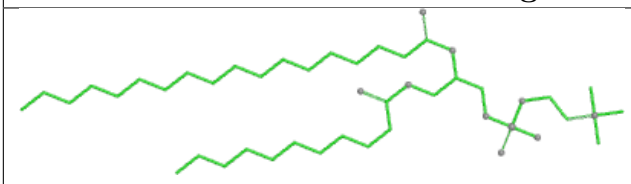
Ligand PC1 5B 202

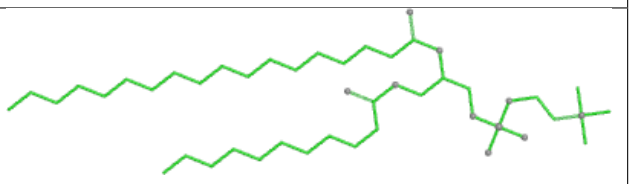


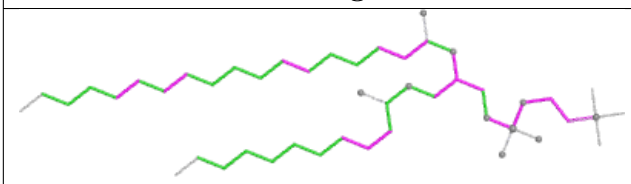
Ligand CDL SD 101

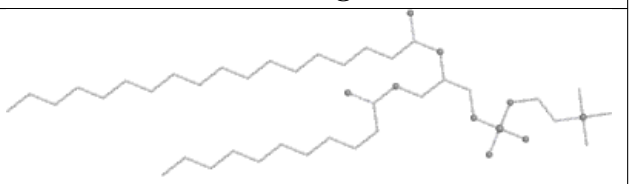


Ligand PC1 2F 301

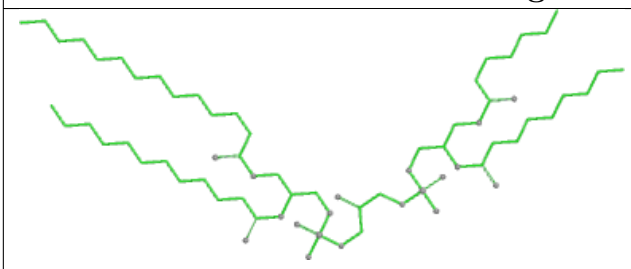

Bond lengths


Bond angles


Torsions


Rings

Ligand CDL J 301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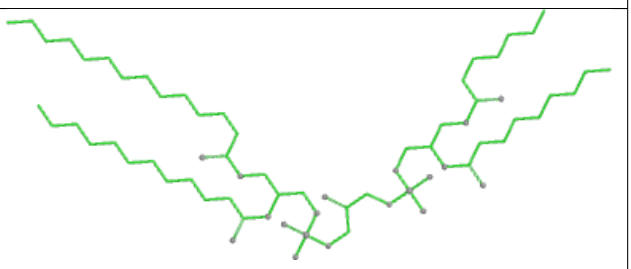
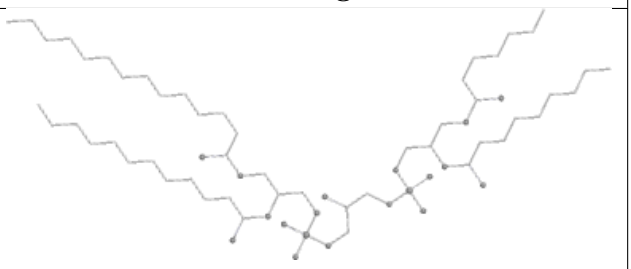
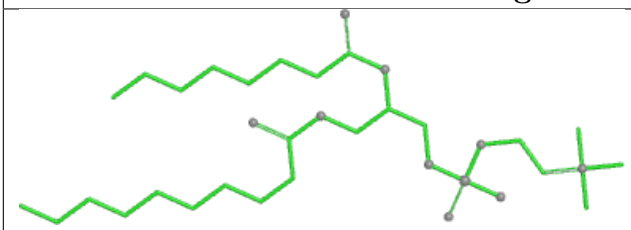

Bond angles

Torsions


Rings

Ligand PC1 QC 508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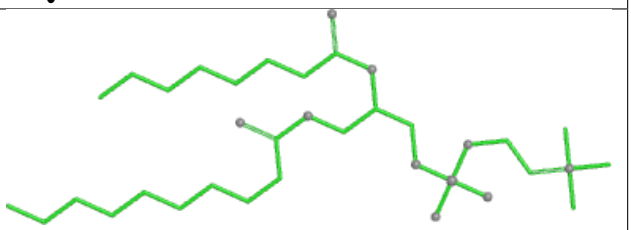
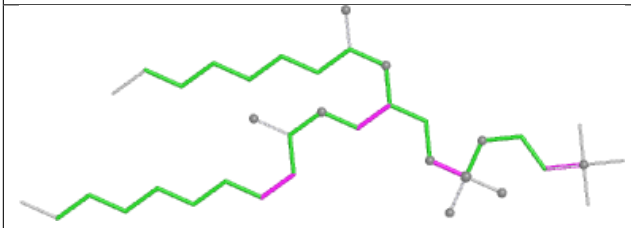
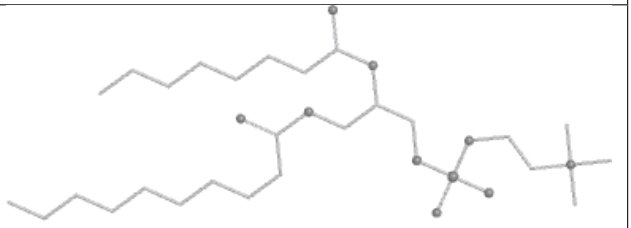
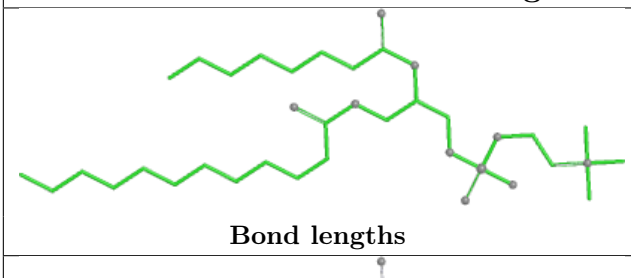

Bond angles


Torsions


Rings

Ligand PC1 c1 707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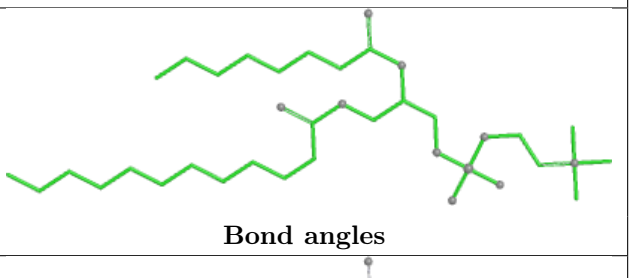
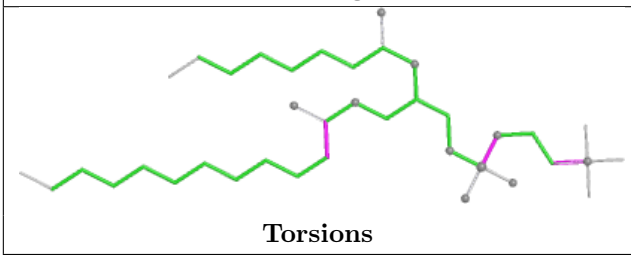
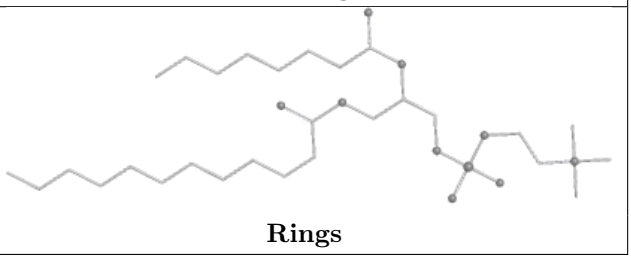
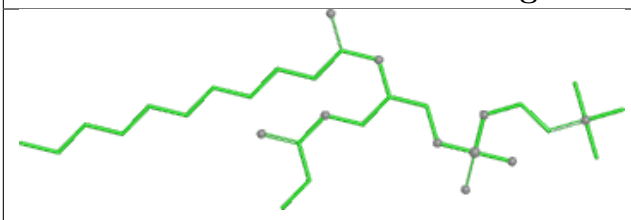

Bond angles


Torsions


Rings

Ligand PC1 2F 303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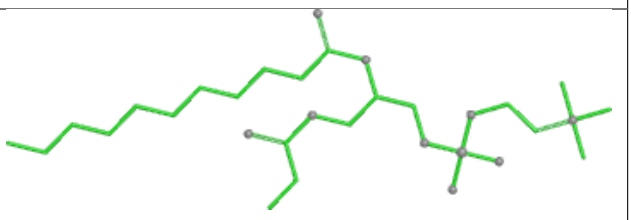
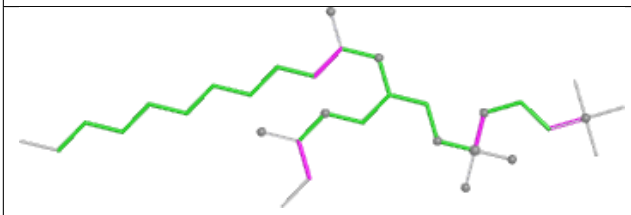

Bond angles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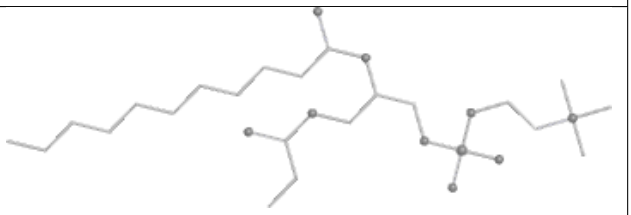
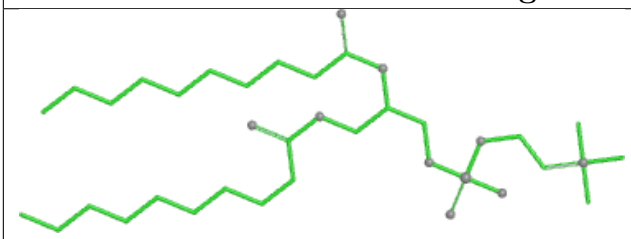

Rings

Ligand PC1 Qc 506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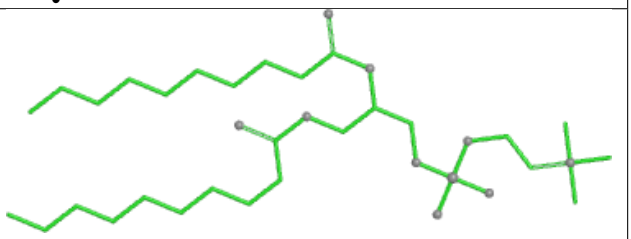
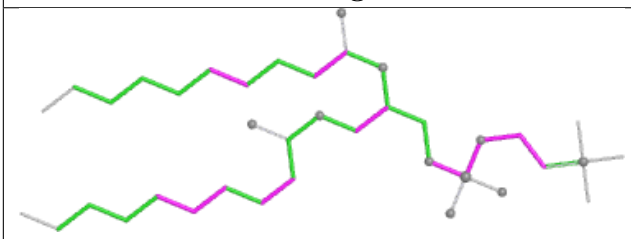
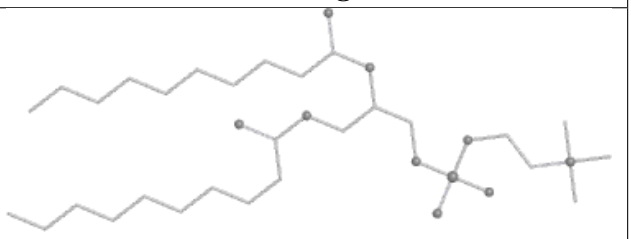
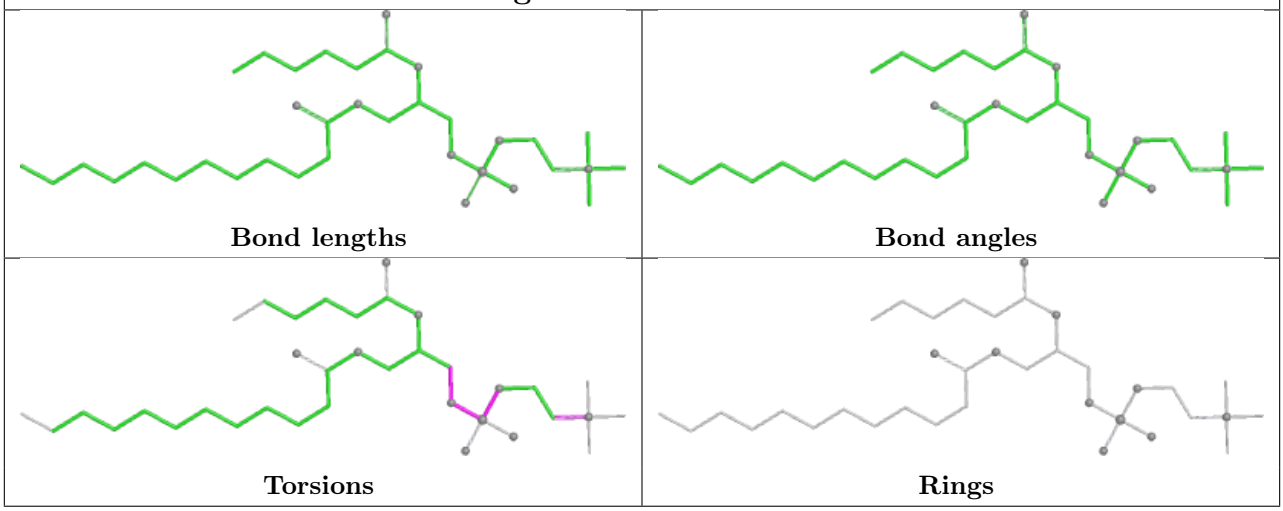

Bond angles

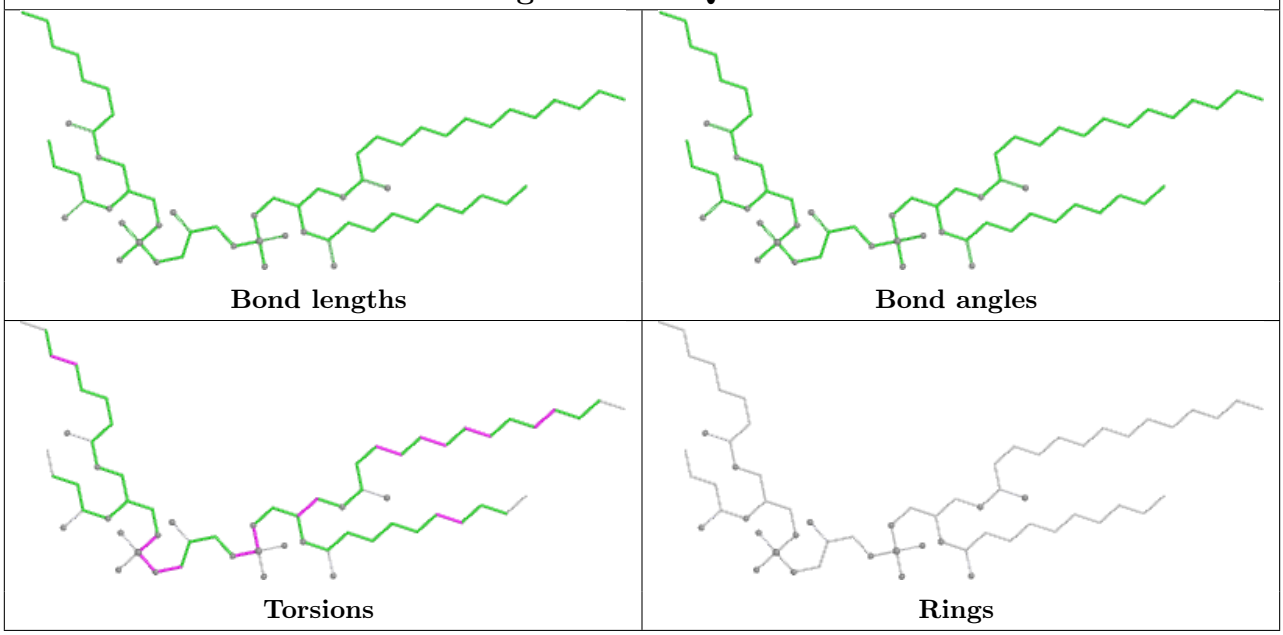

Torsions


Rings

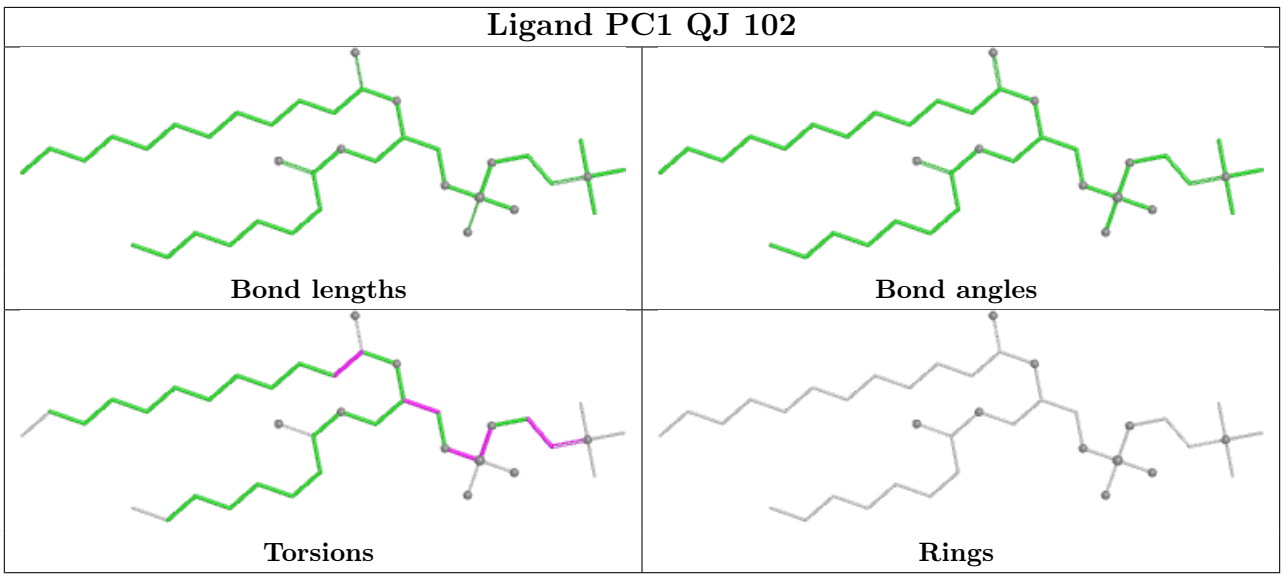
Ligand PC1 AN 304



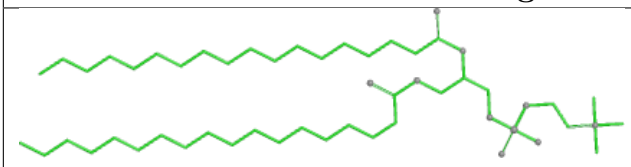
Ligand CDL Qc 504



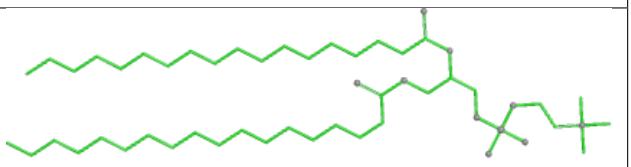
Ligand PC1 QJ 102



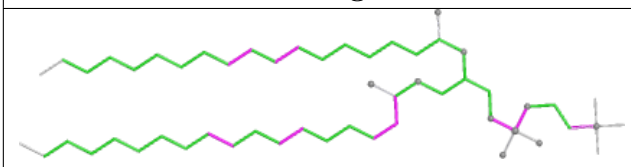
Ligand PC1 N6 301



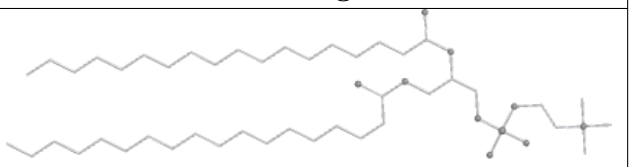
Bond lengths



Bond angles

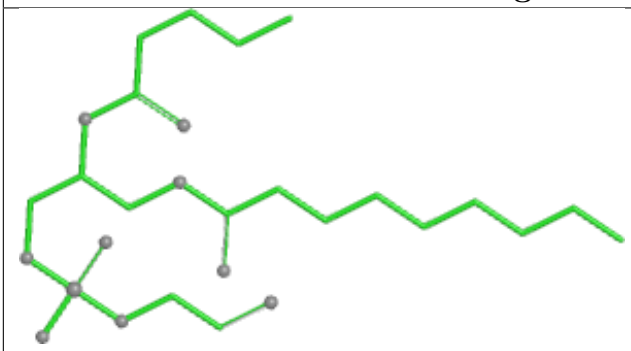


Torsions



Rings

Ligand 3PE AN 306



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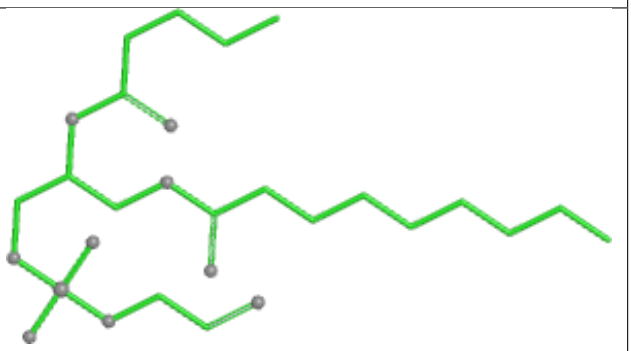
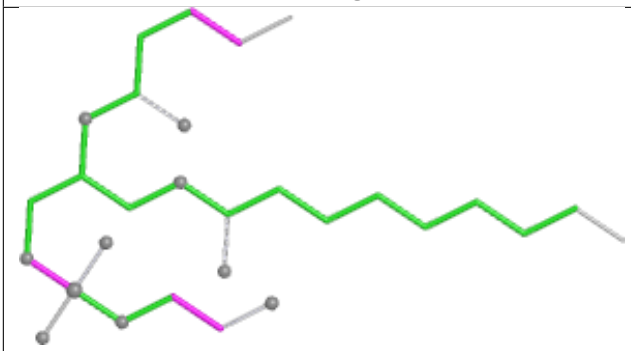
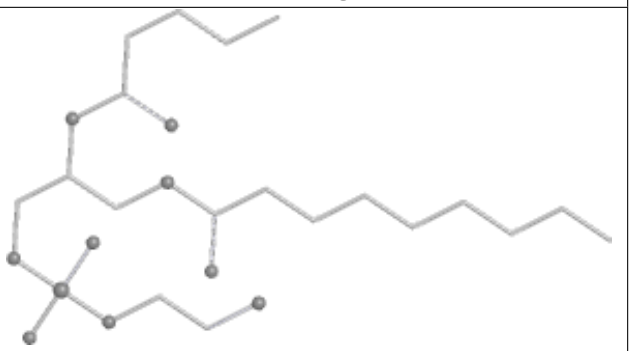


Bond angles

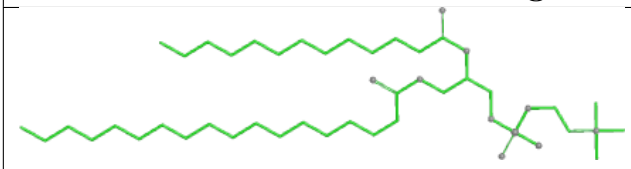


Torsions

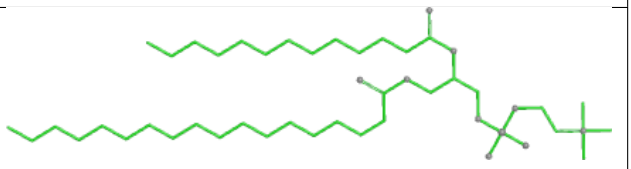


Rings

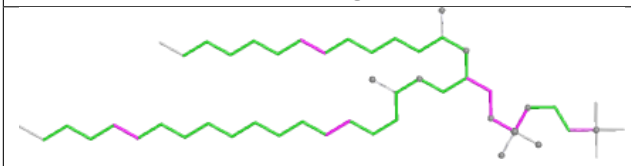
Ligand PC1 w 201



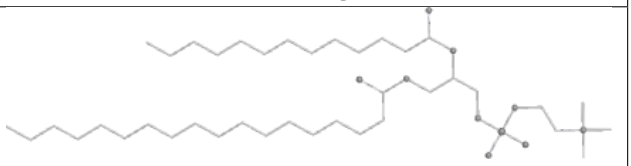
Bond lengths



Bond angles

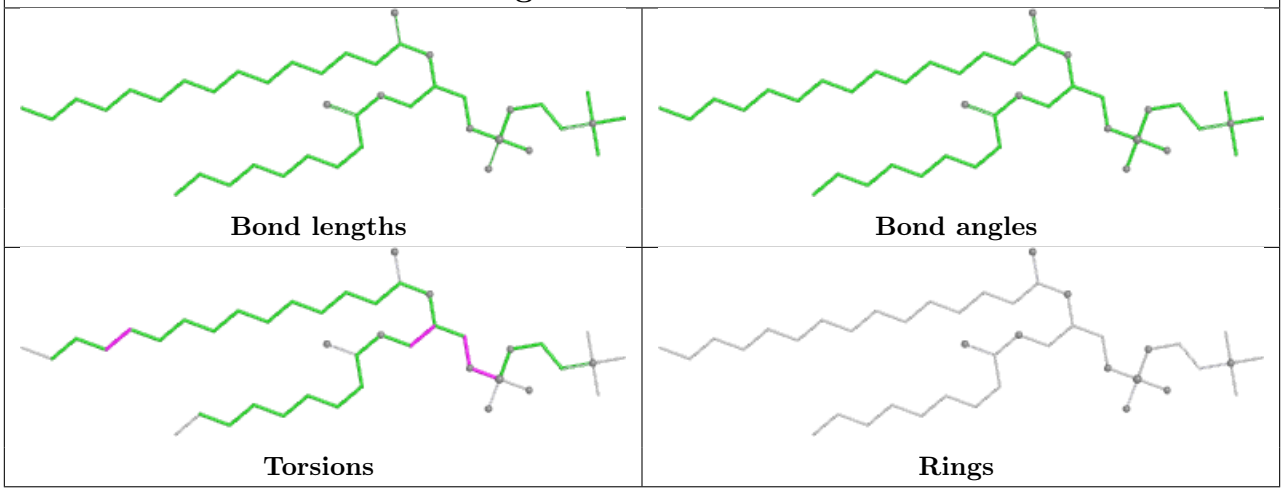


Torsions

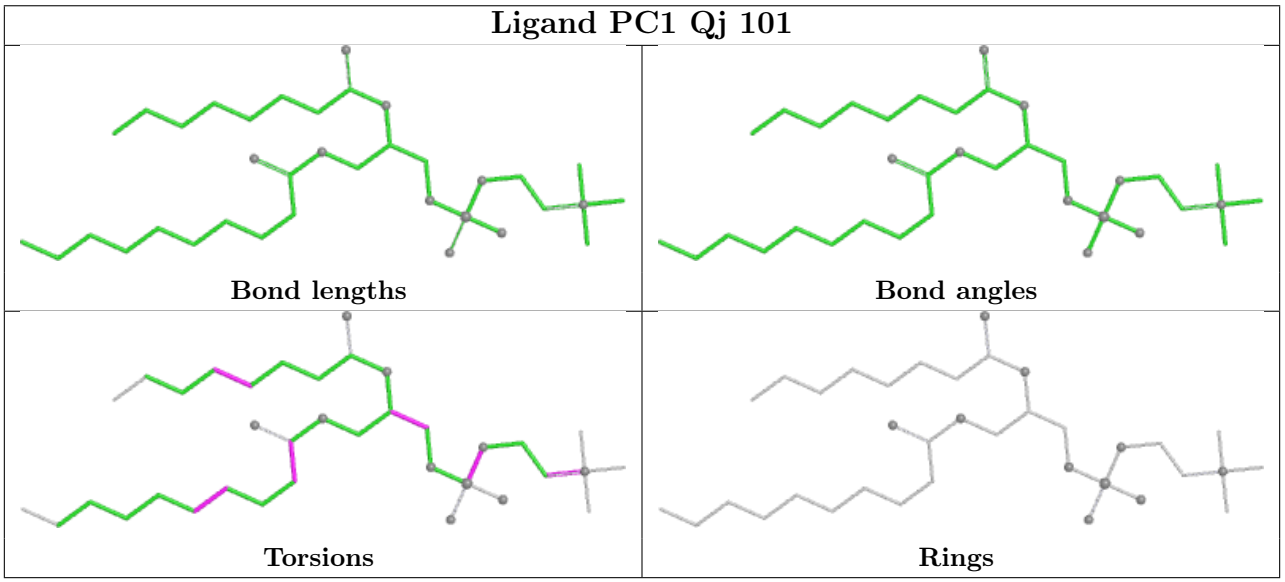


Rings

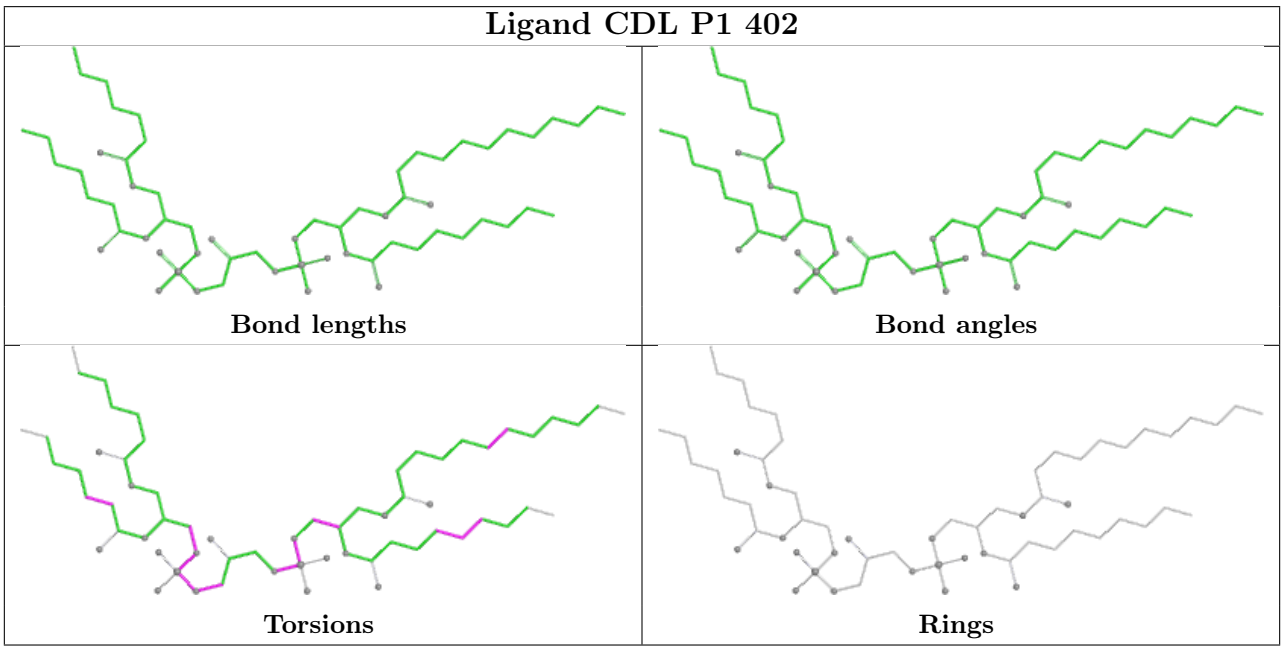
Ligand PC1 M1 403



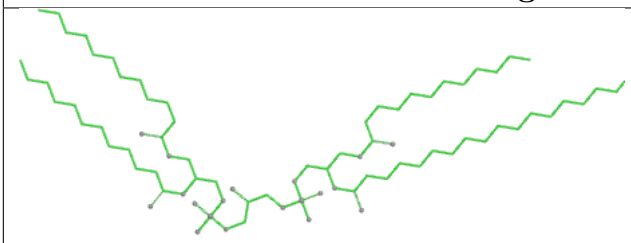
Ligand PC1 Qj 101



Ligand CDL P1 402



Ligand CDL b3 102



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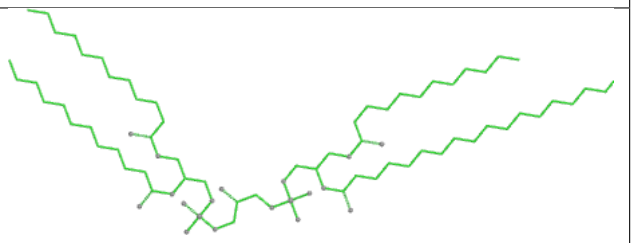
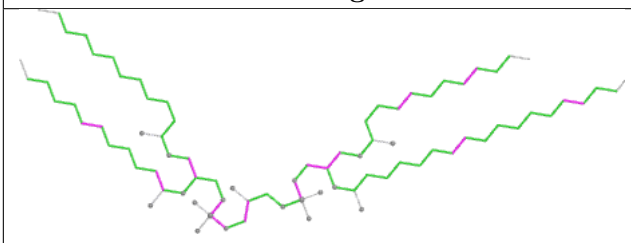
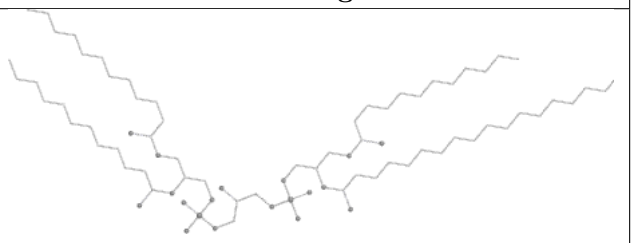


Bond angles

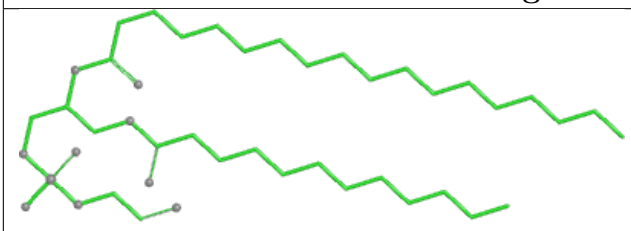


Torsions



Rings

Ligand 3PE an 303



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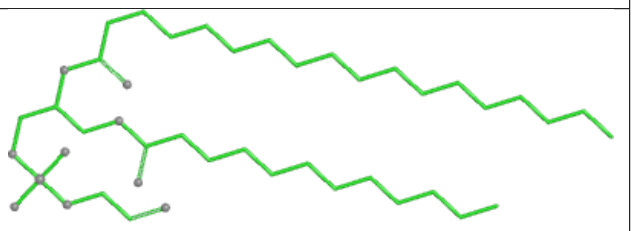
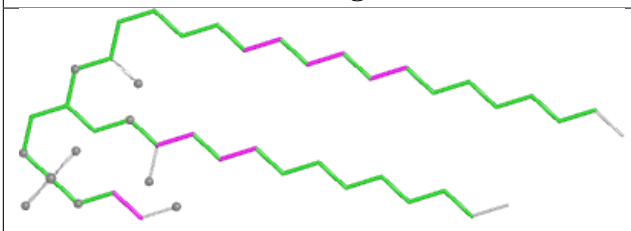


Bond angles



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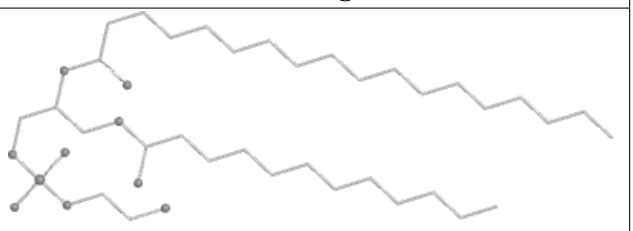
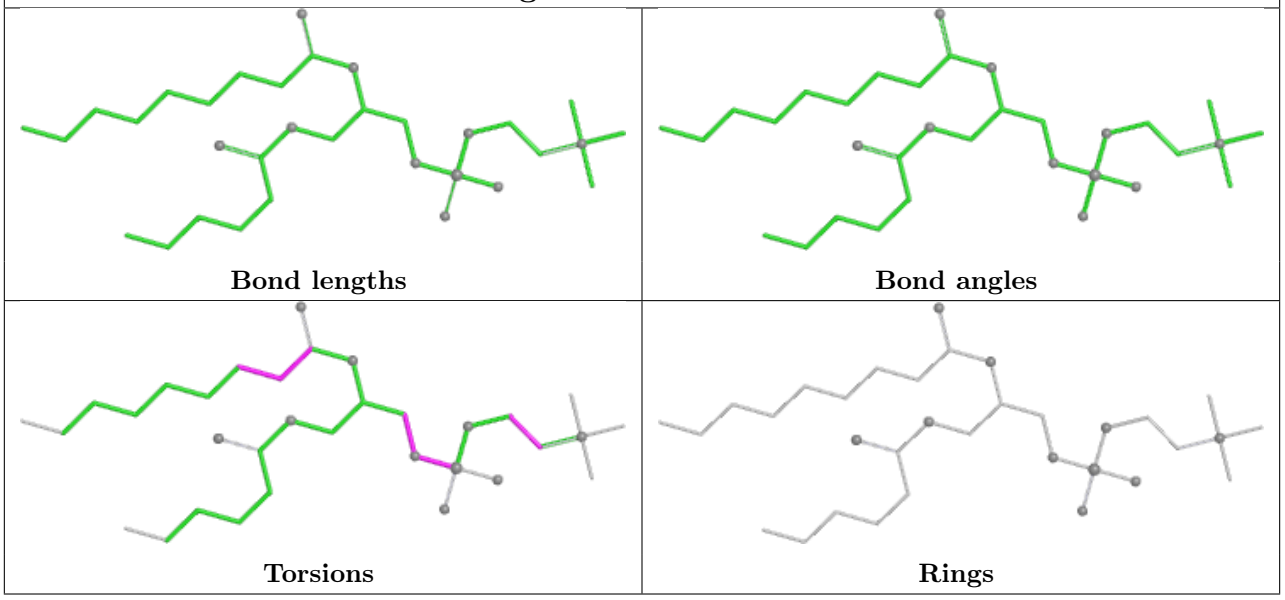
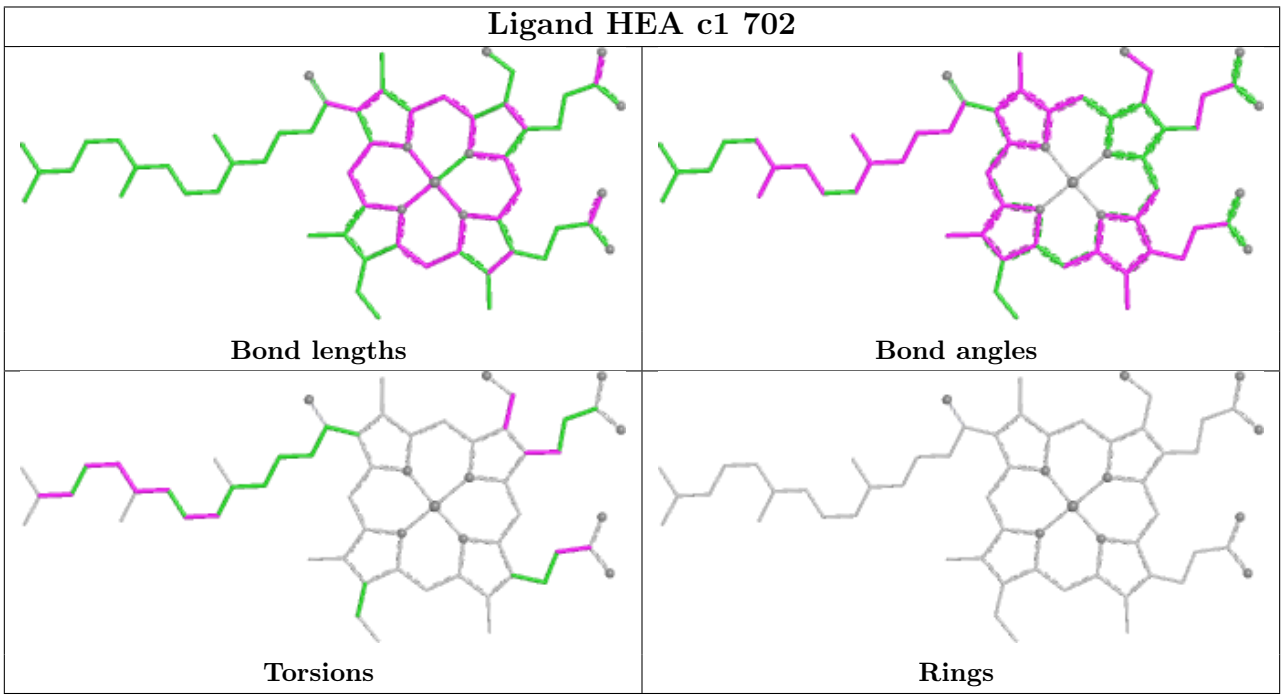


Rings

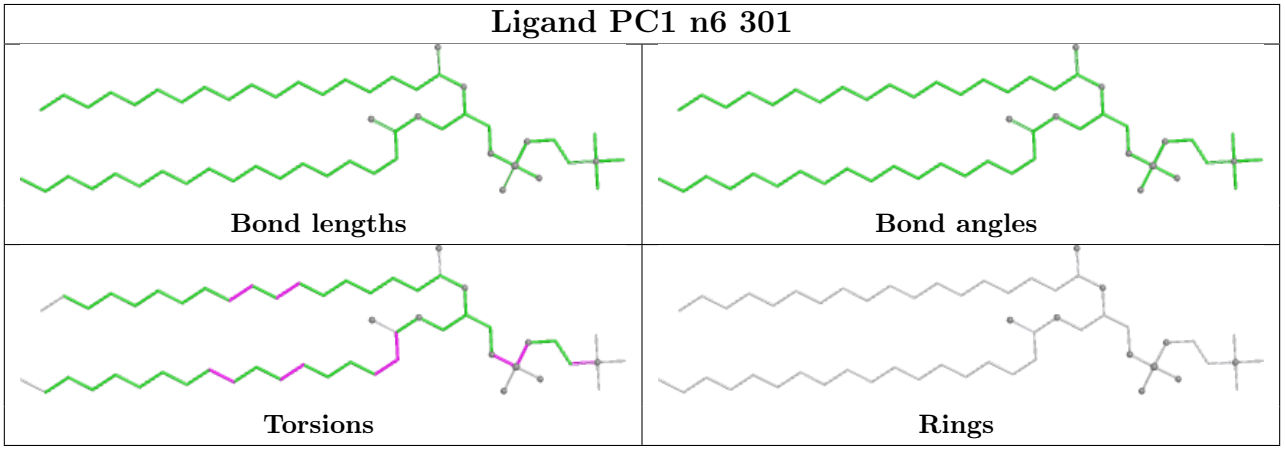
Ligand PC1 6C 201



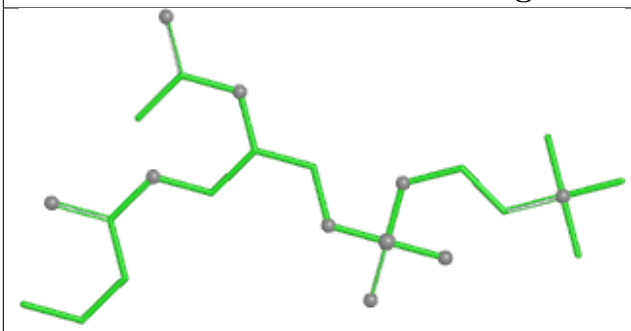
Ligand HEA c1 702



Ligand PC1 n6 301



Ligand PC1 QE 301



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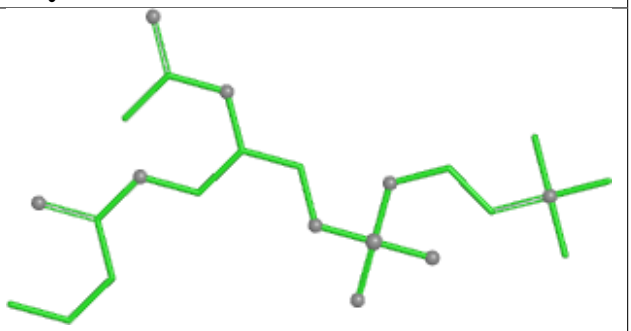
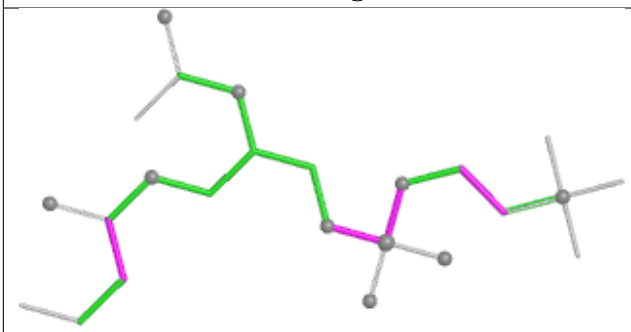
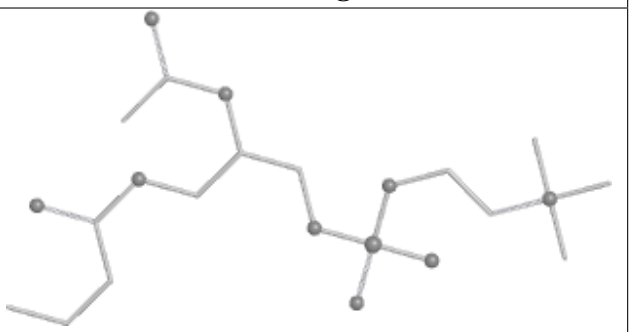


Bond angles

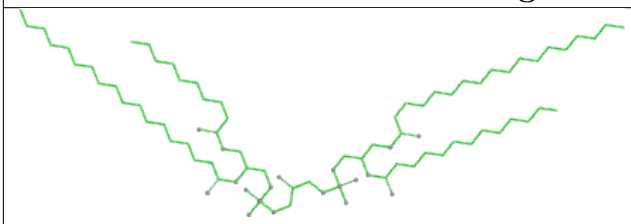


Torsions



Rings

Ligand CDL an 302



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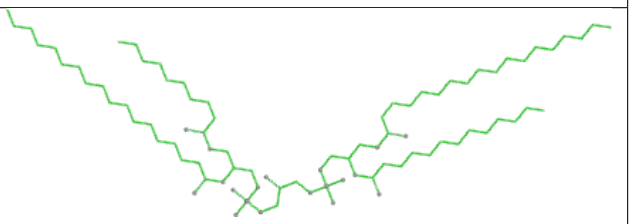
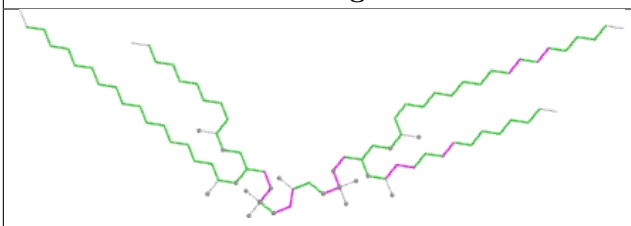


Bond angles



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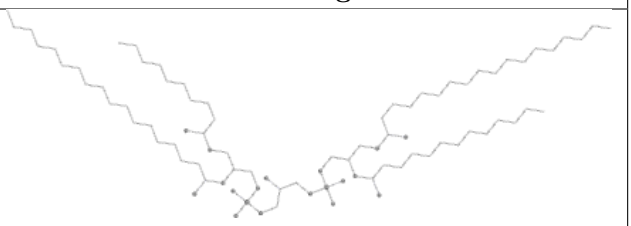
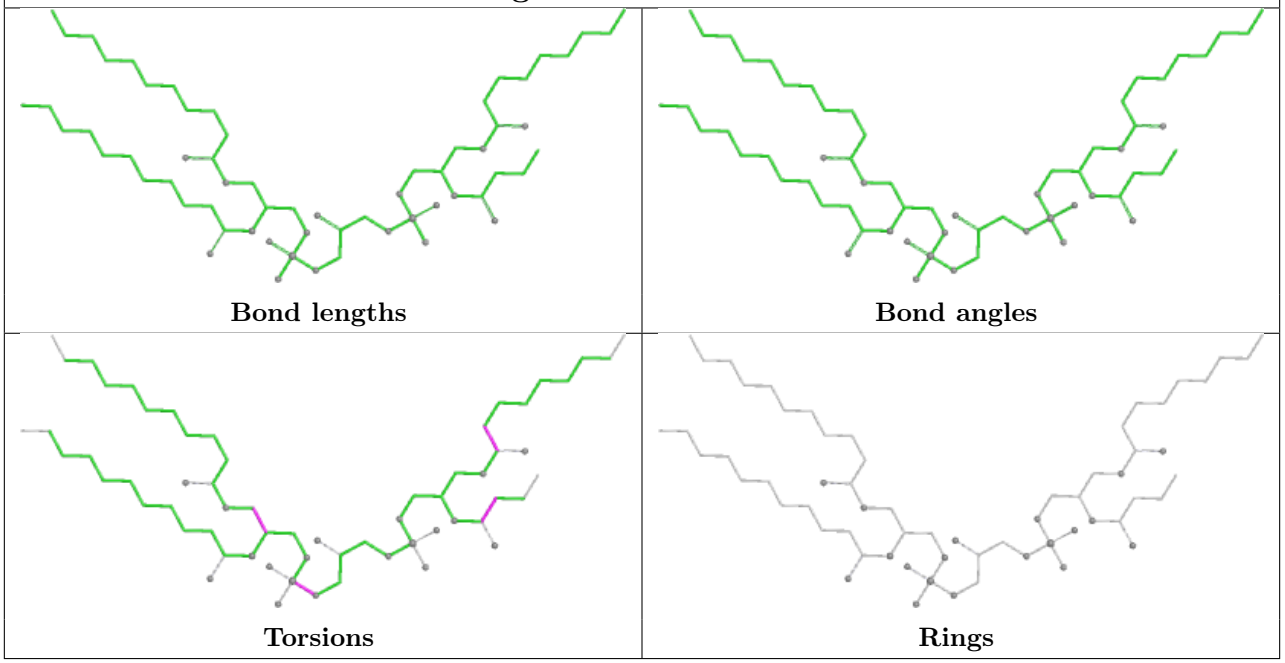


Rings

Ligand CDL M3 401



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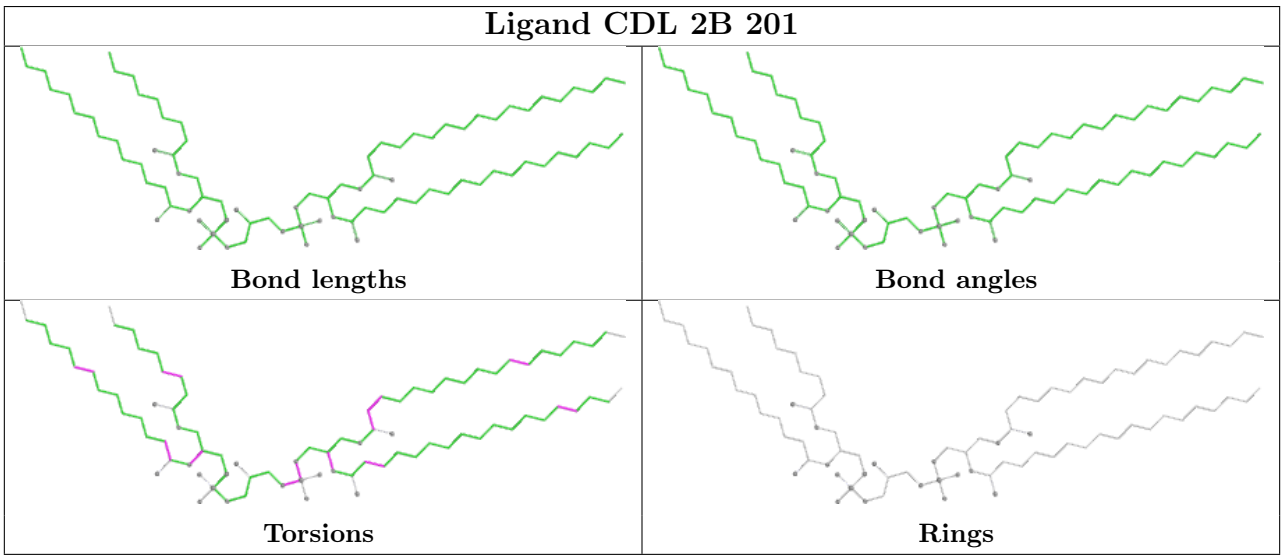

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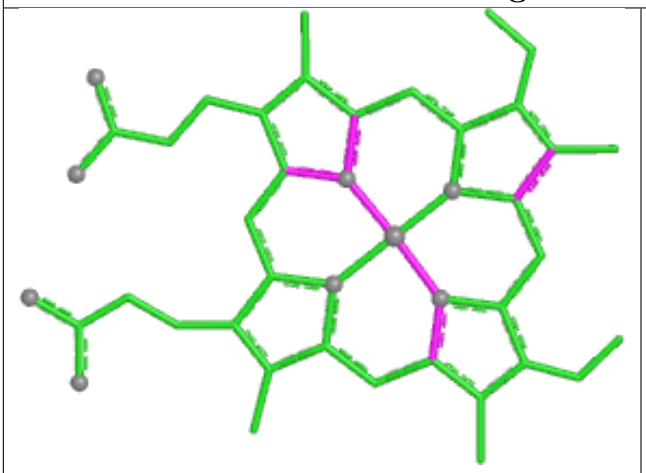

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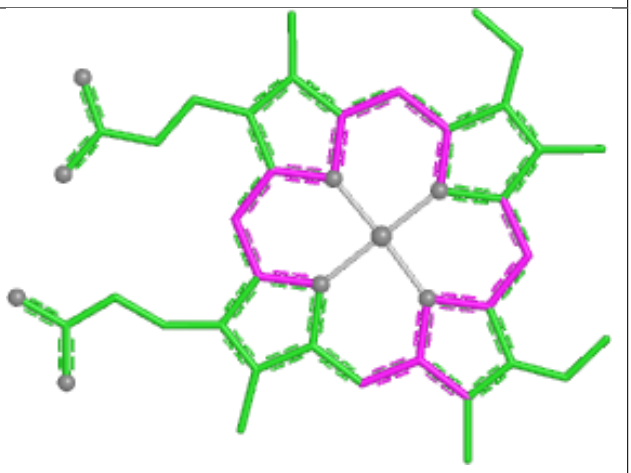
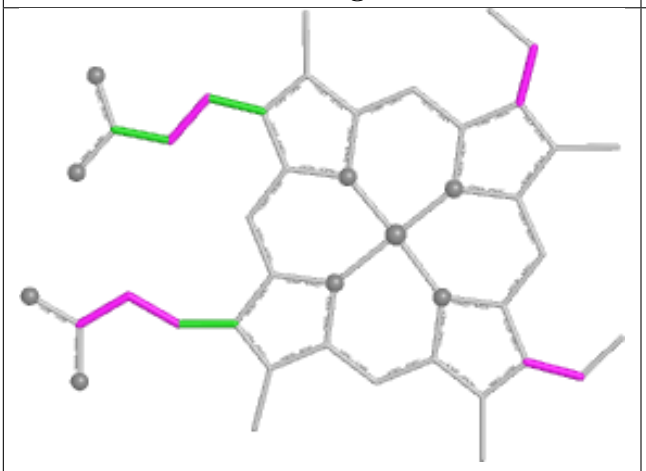


Bond angles



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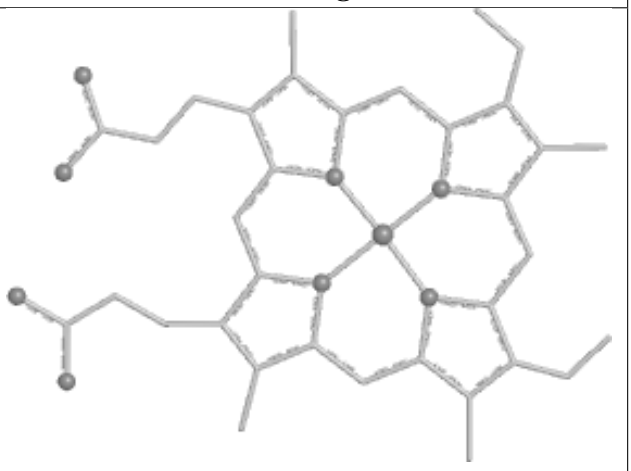
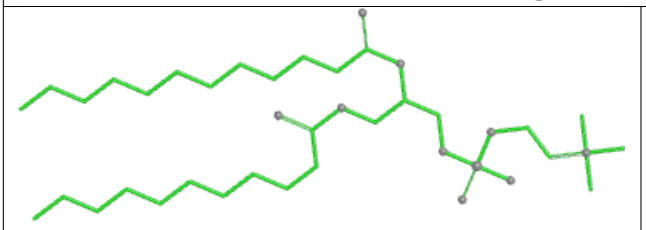


Rings

Ligand PC1 n 301



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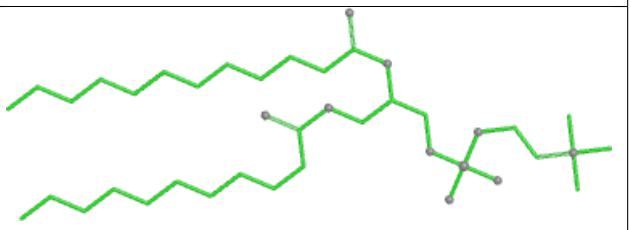
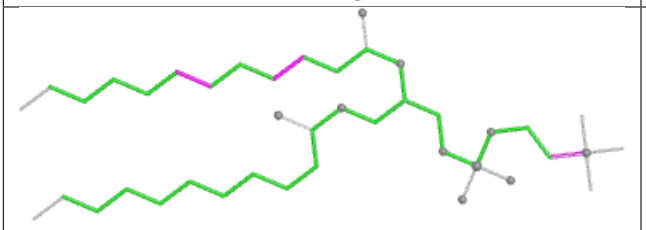


Bond angles



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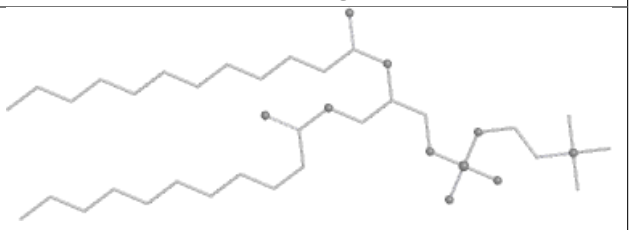
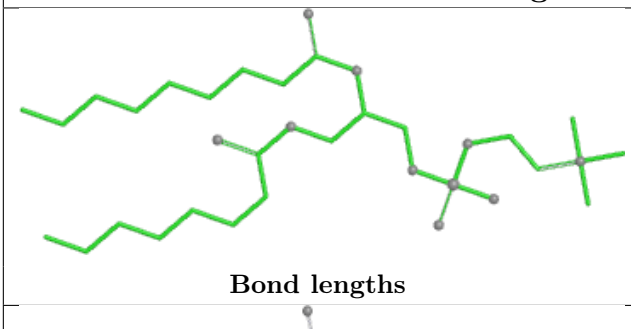


Rings

Ligand PC1 d 501



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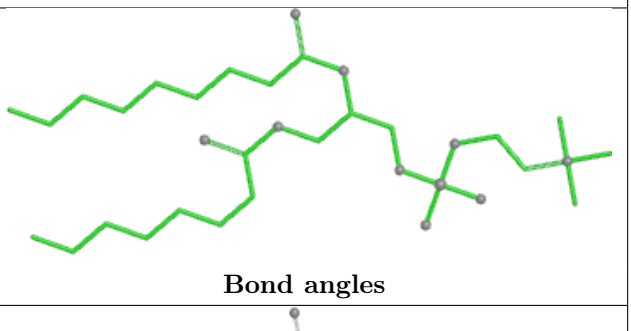

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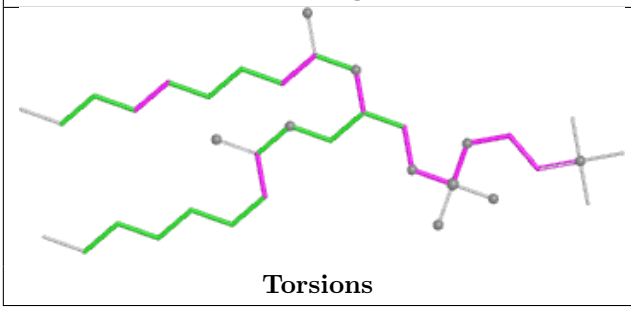

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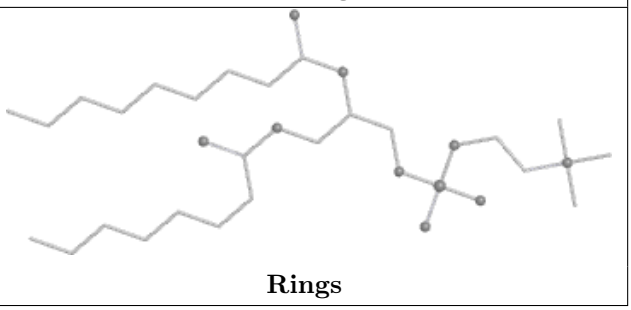
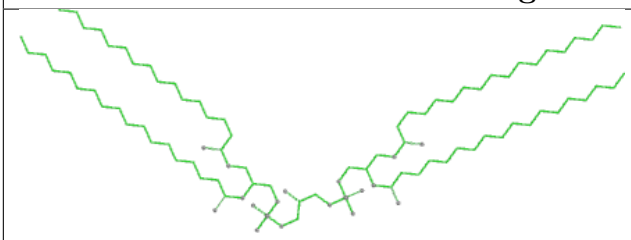


Rings

Ligand CDL 2k 101



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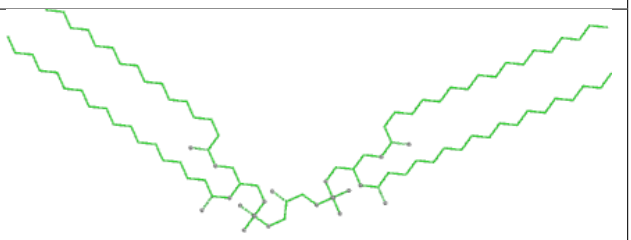

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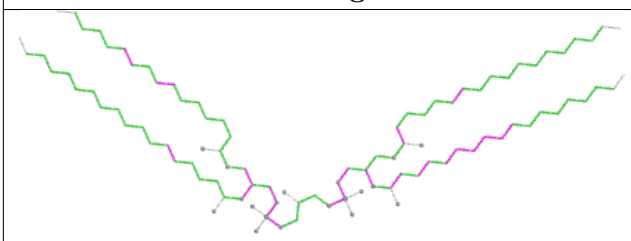

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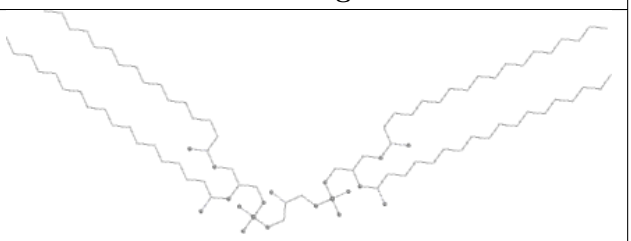
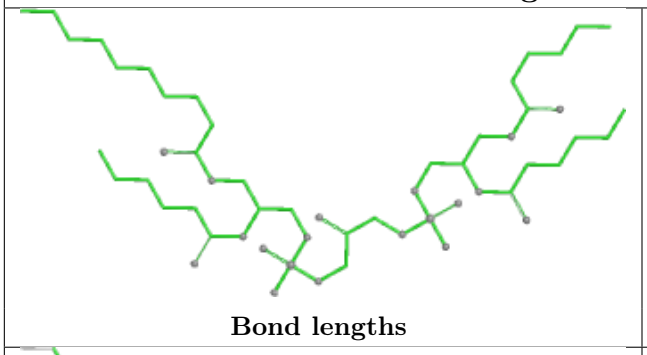


Rings

Ligand CDL qc 505



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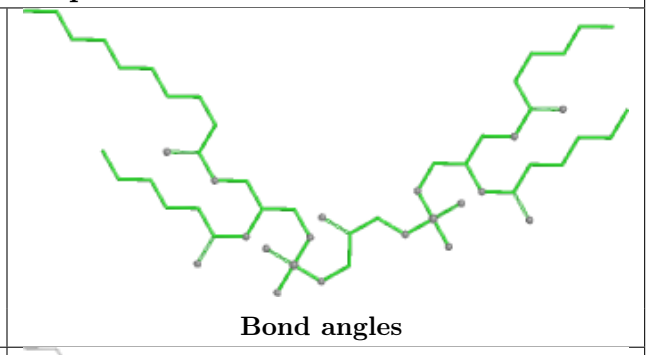
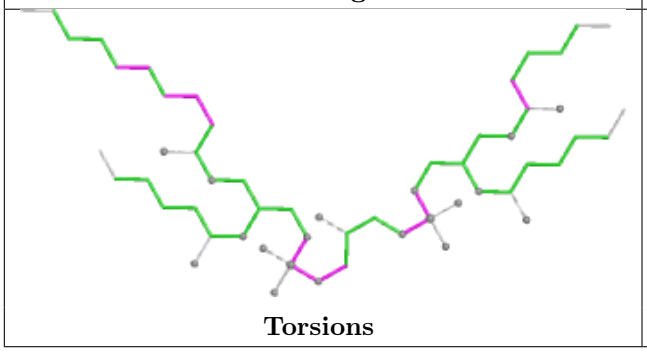


Bond angles



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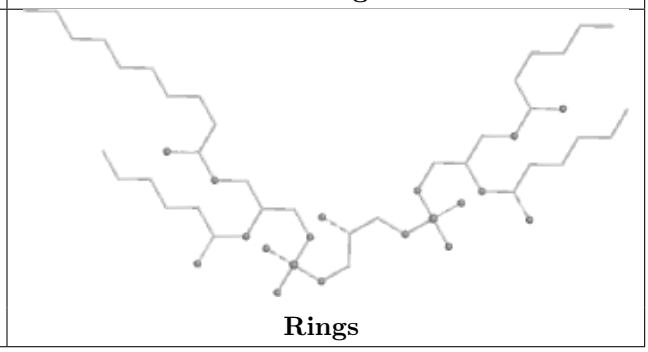
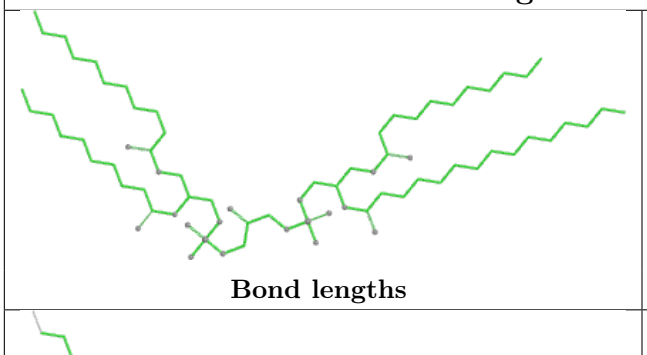


Rings

Ligand CDL 6C 202



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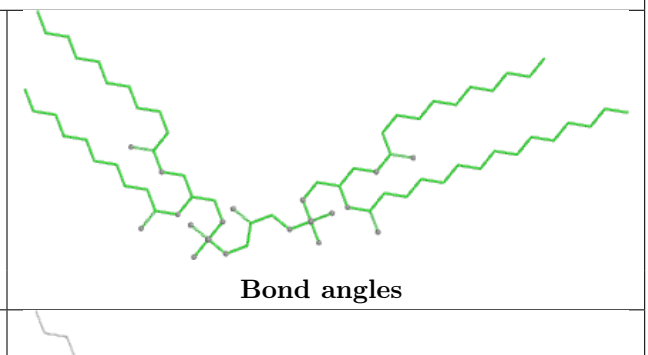
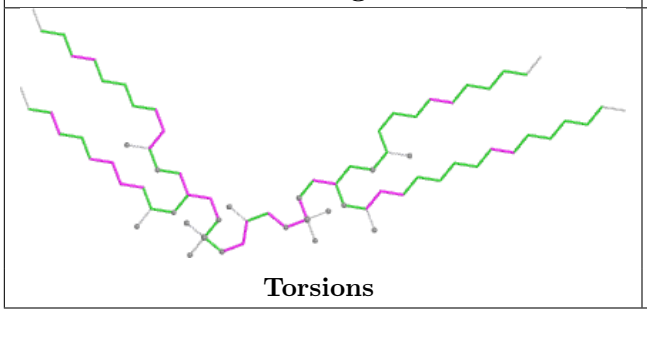


Bond angles



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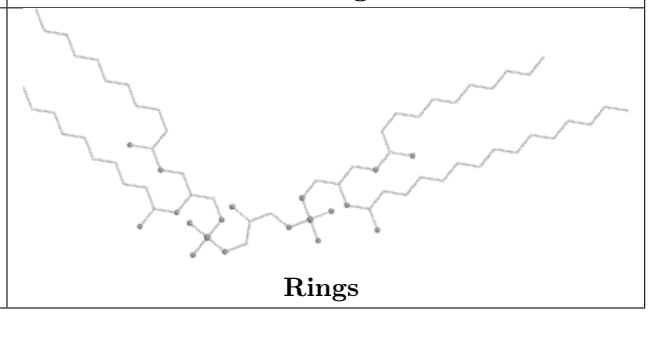
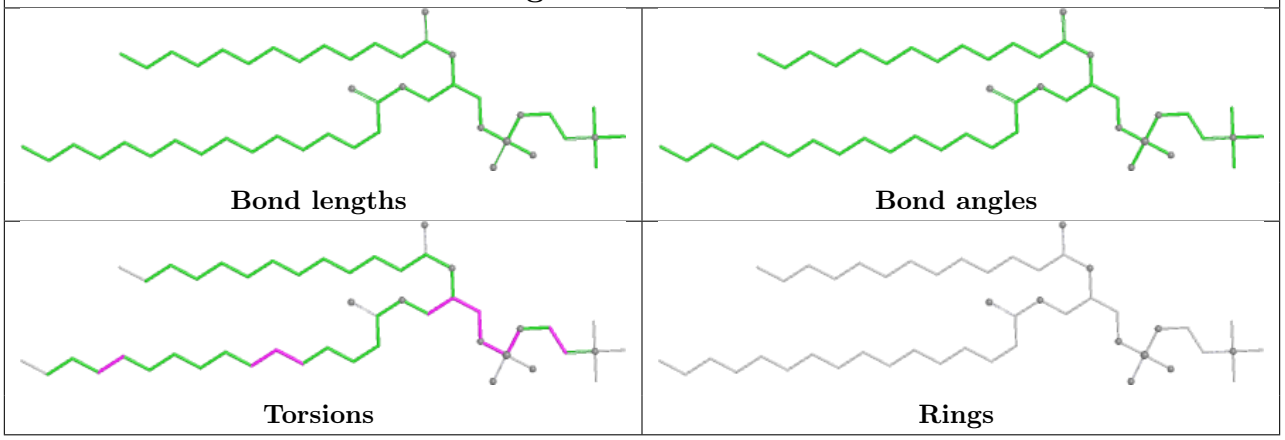
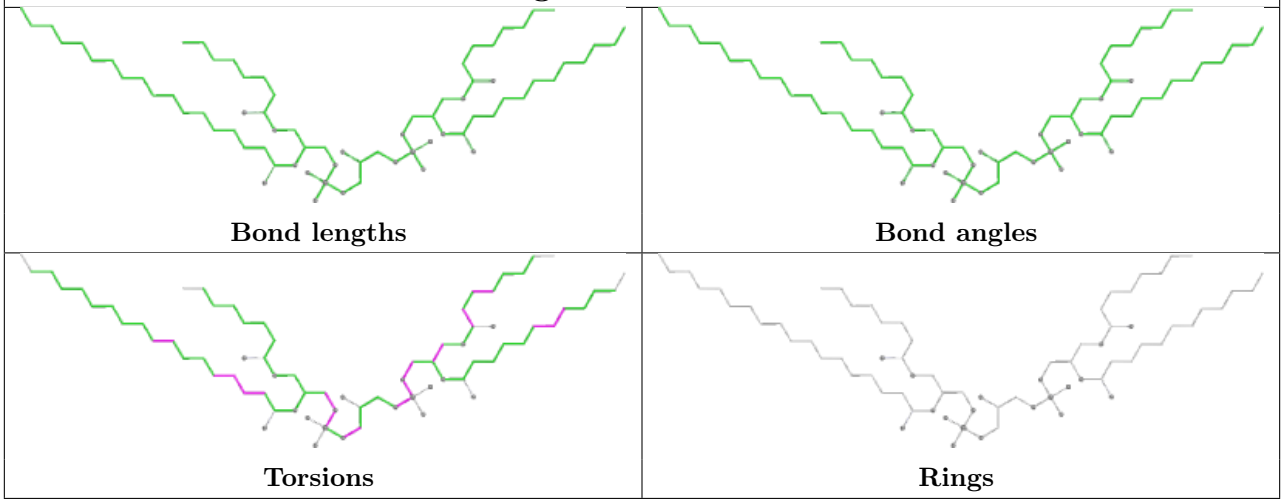


Rings

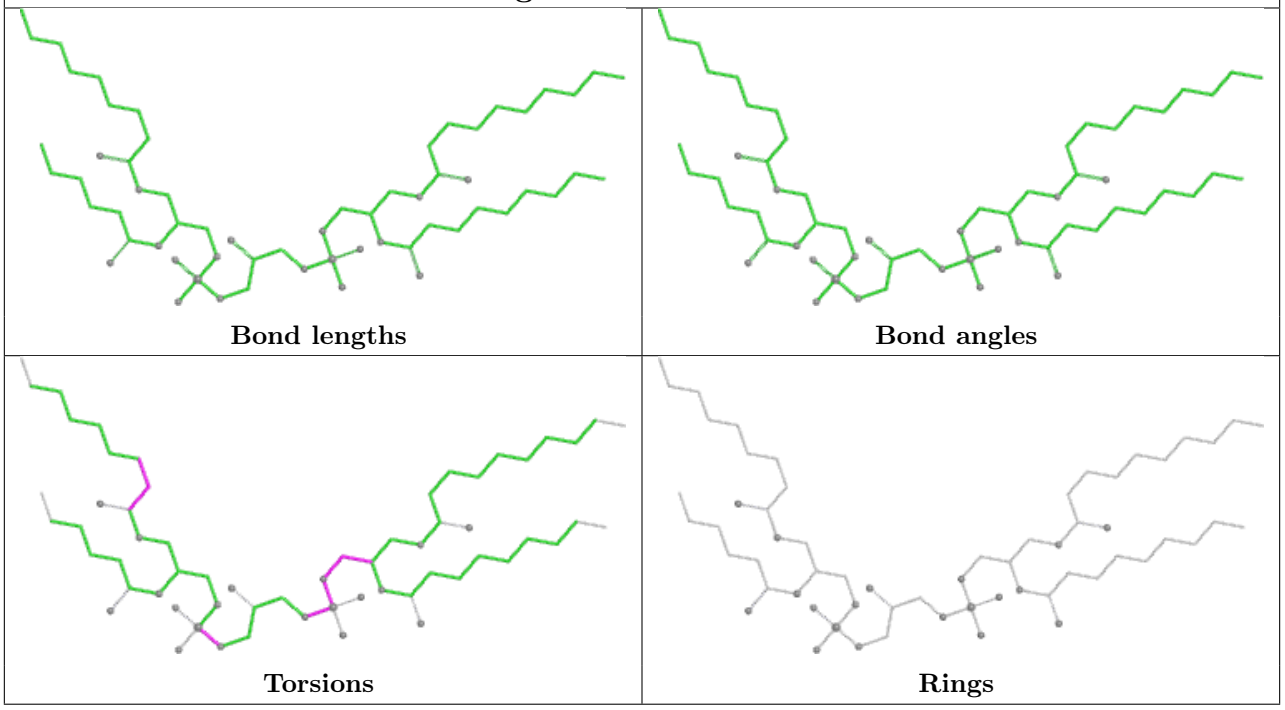
Ligand PC1 tc 102



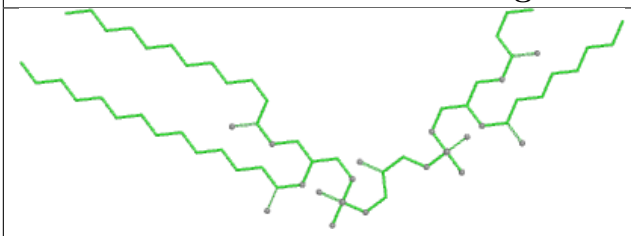
Ligand CDL l 301



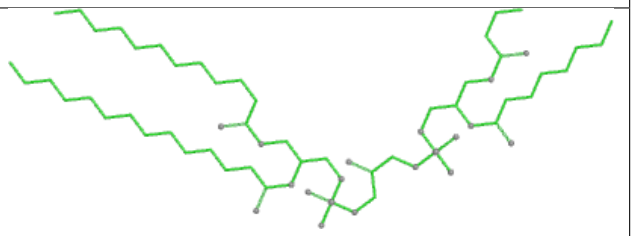
Ligand CDL 7A 203



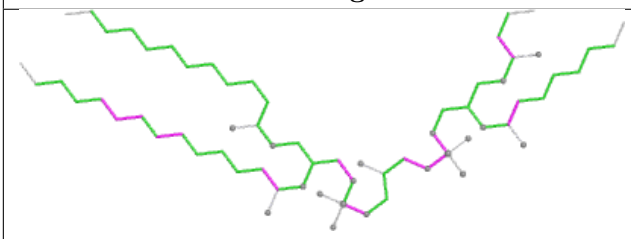
Ligand CDL A1 101



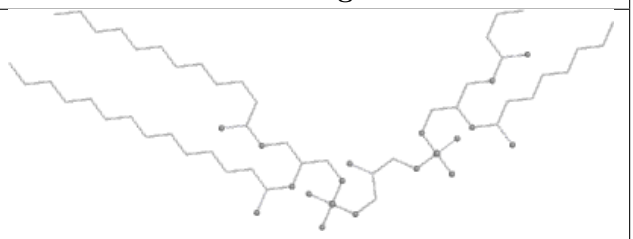
Bond lengths



Bond angles

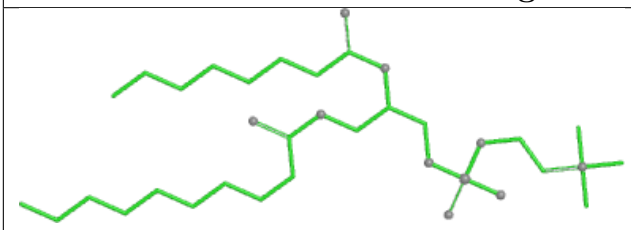


Torsions

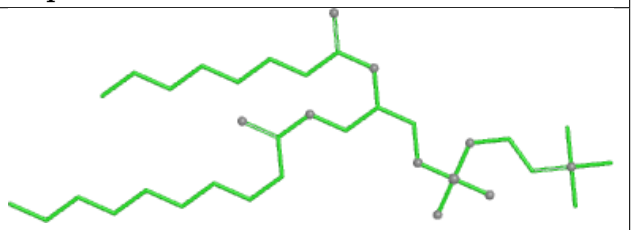


Rings

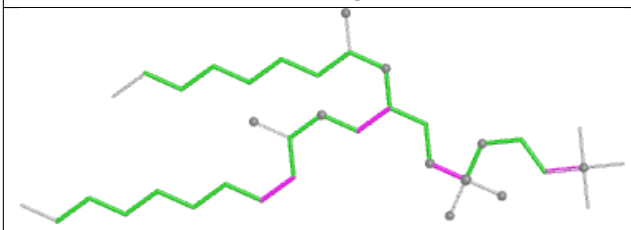
Ligand PC1 qC 508



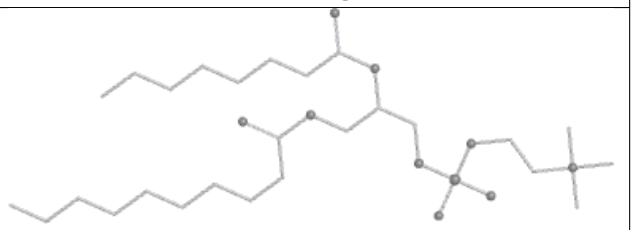
Bond lengths



Bond angles

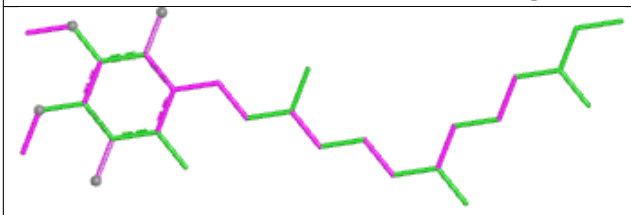


Torsions

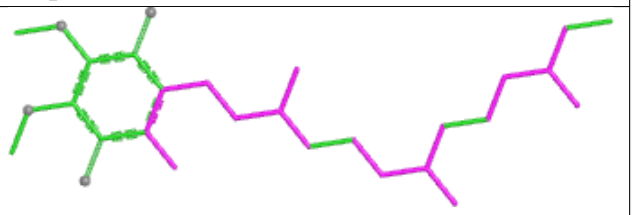


Rings

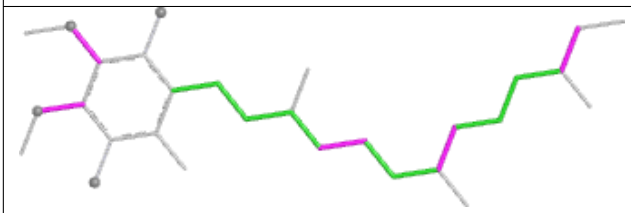
Ligand U10 qc 507



Bond lengths



Bond angles



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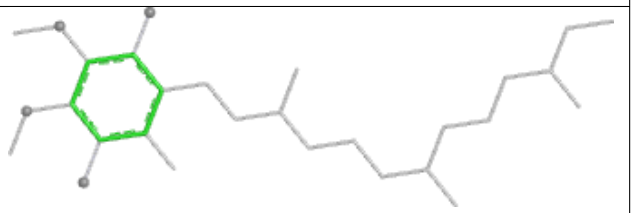
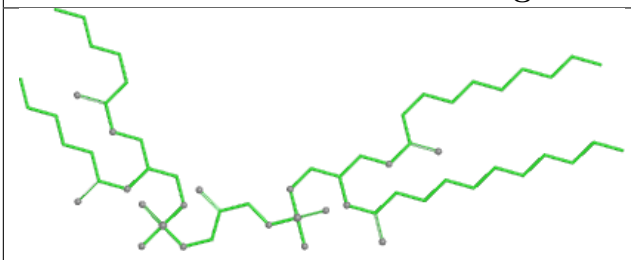


Rings

Ligand CDL qD 402



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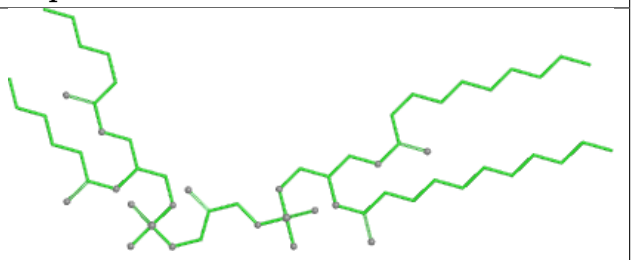
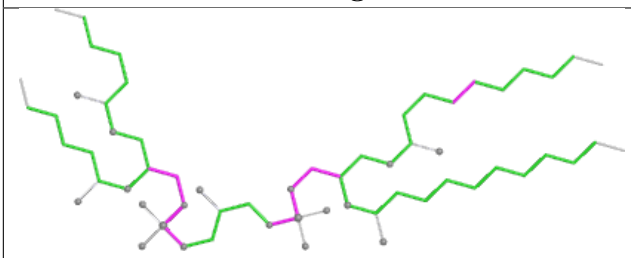


Bond angles



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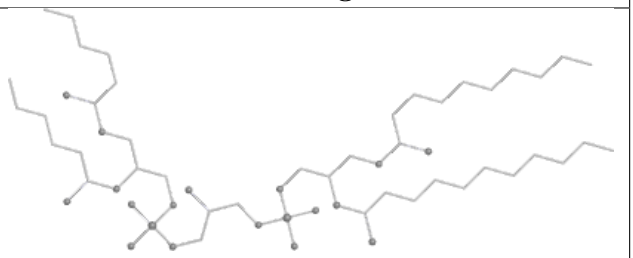
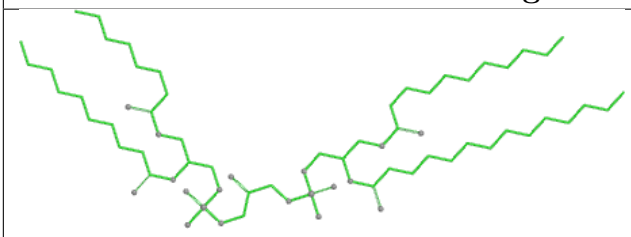
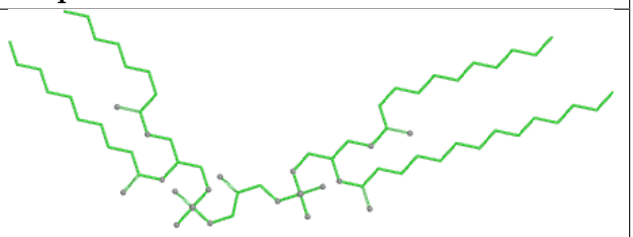


Rings

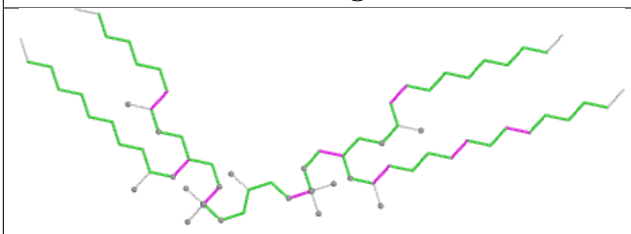
Ligand CDL qi 202



Bond lengths



Bond angles



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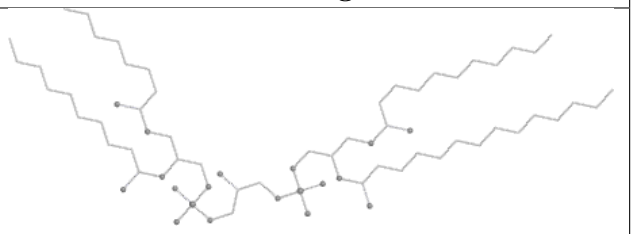
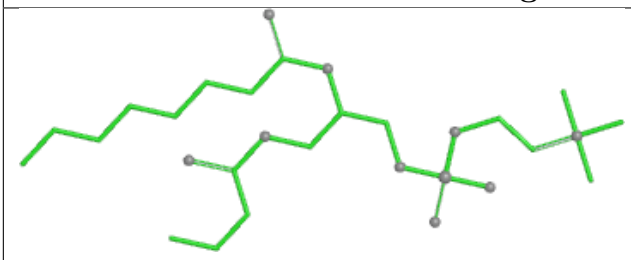


Rings

Ligand PC1 QI 201



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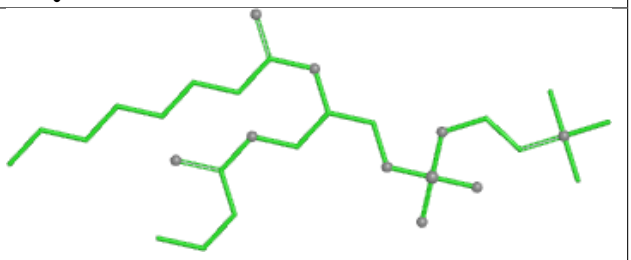
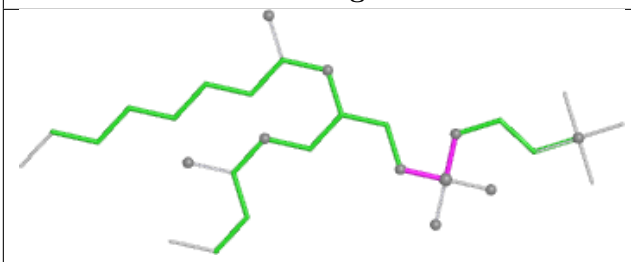


Bond angles



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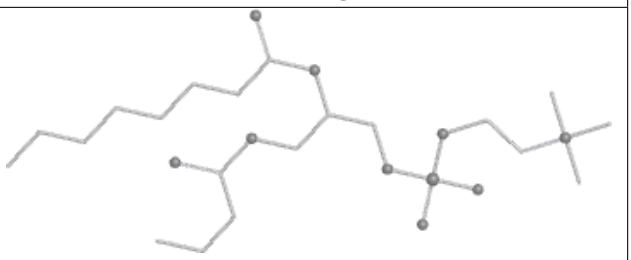
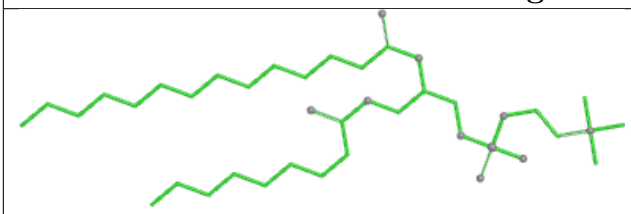
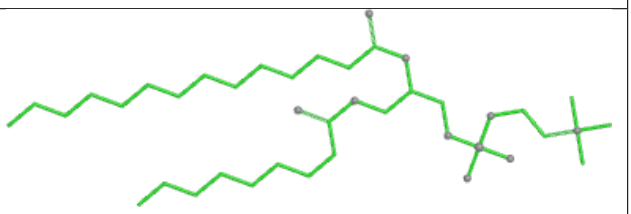


Rings

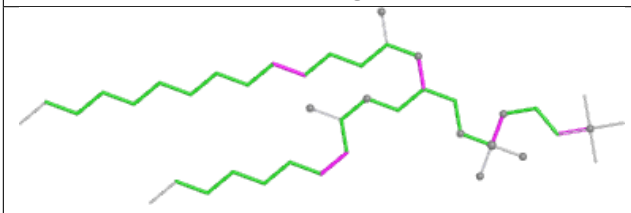
Ligand PC1 A 501



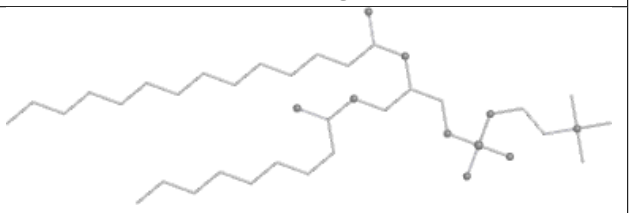
Bond lengths



Bond angles

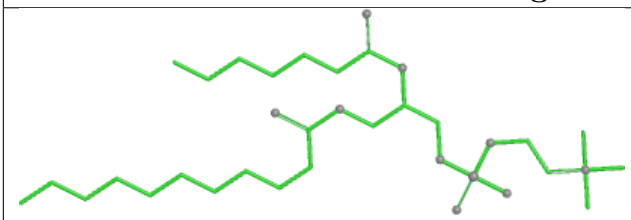


Torsions

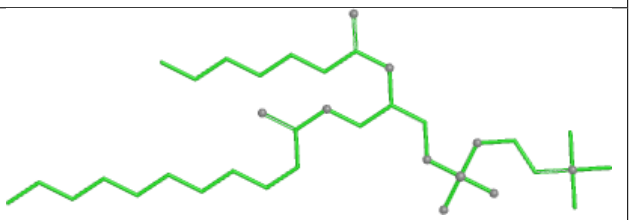


Rings

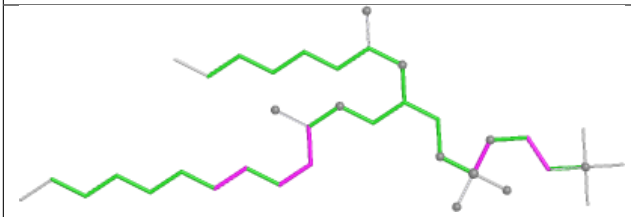
Ligand PC1 n 303



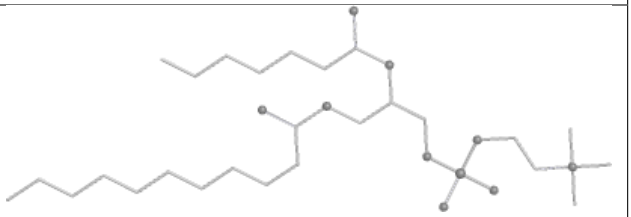
Bond lengths



Bond angles

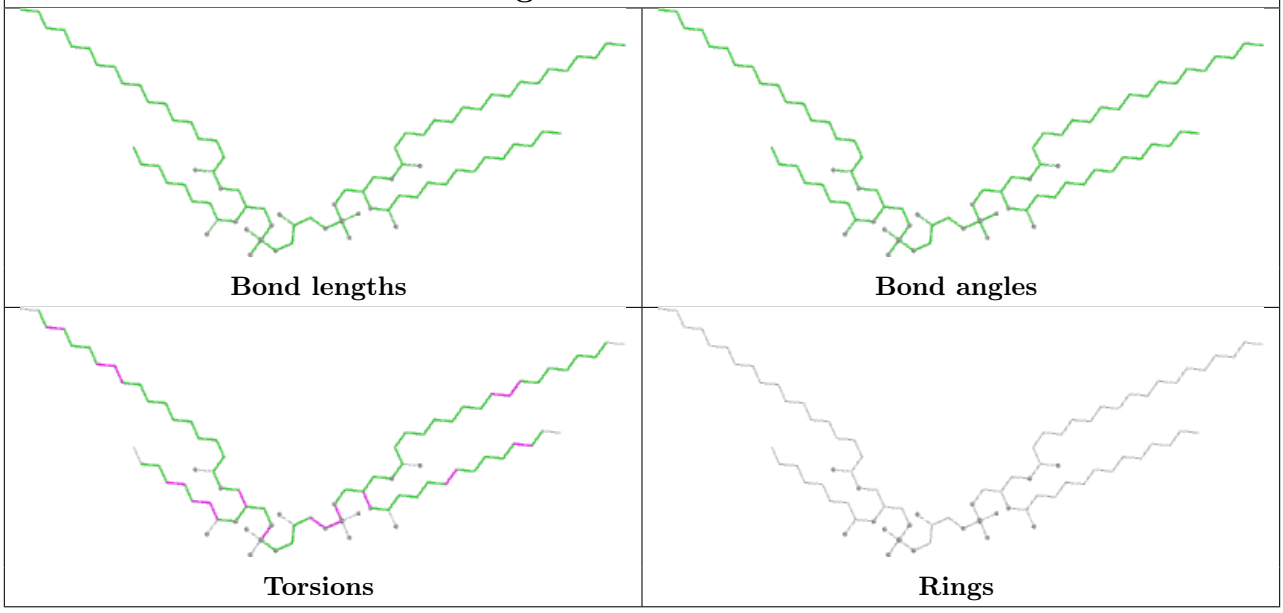


Torsions

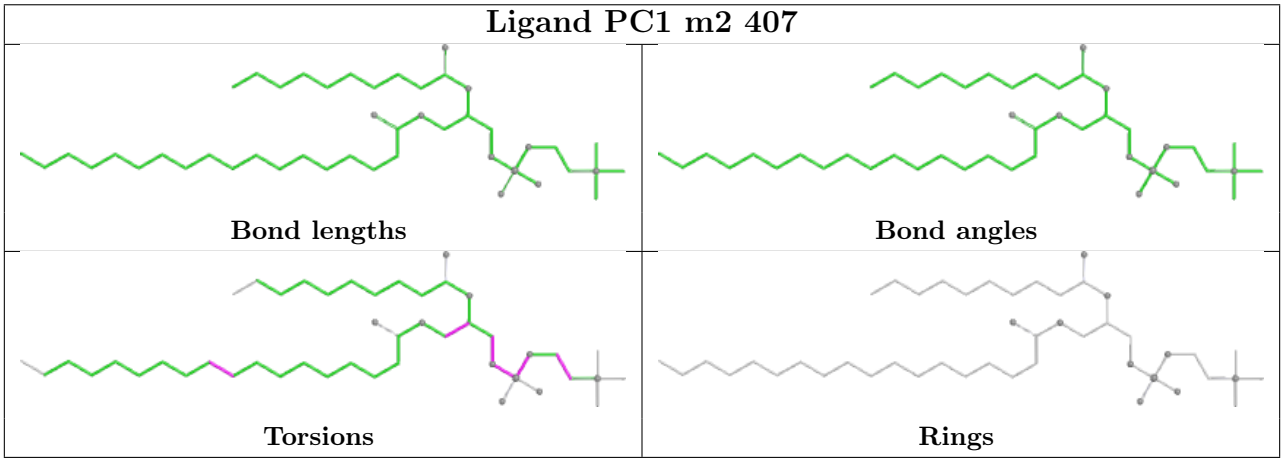


Rings

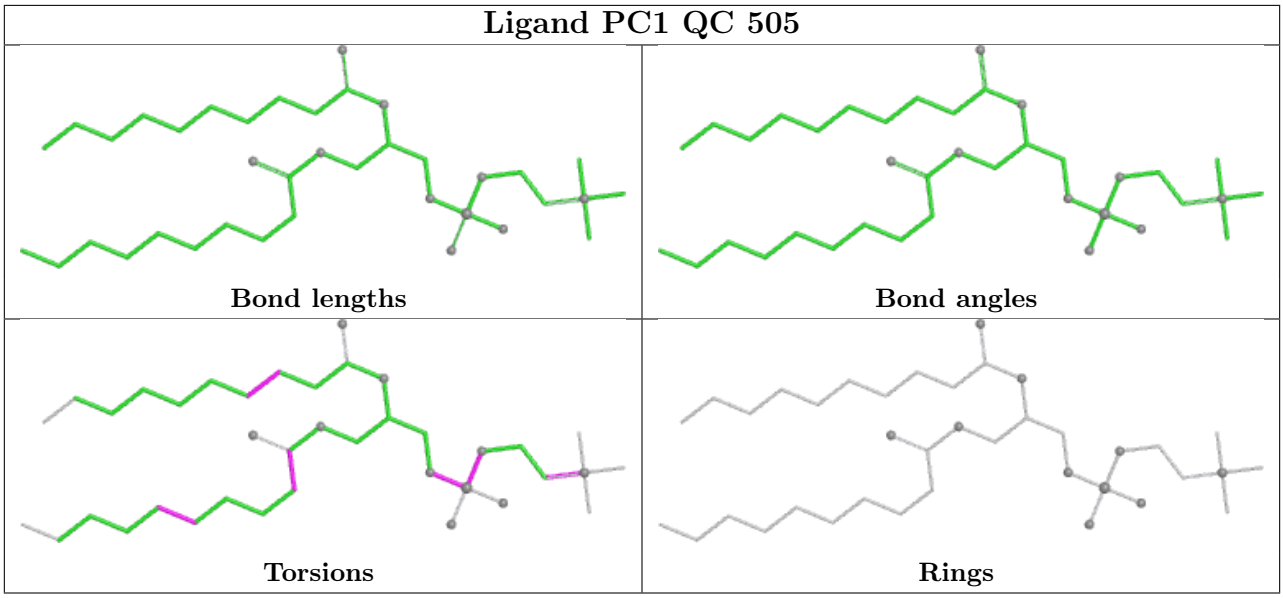
Ligand CDL 7C 301



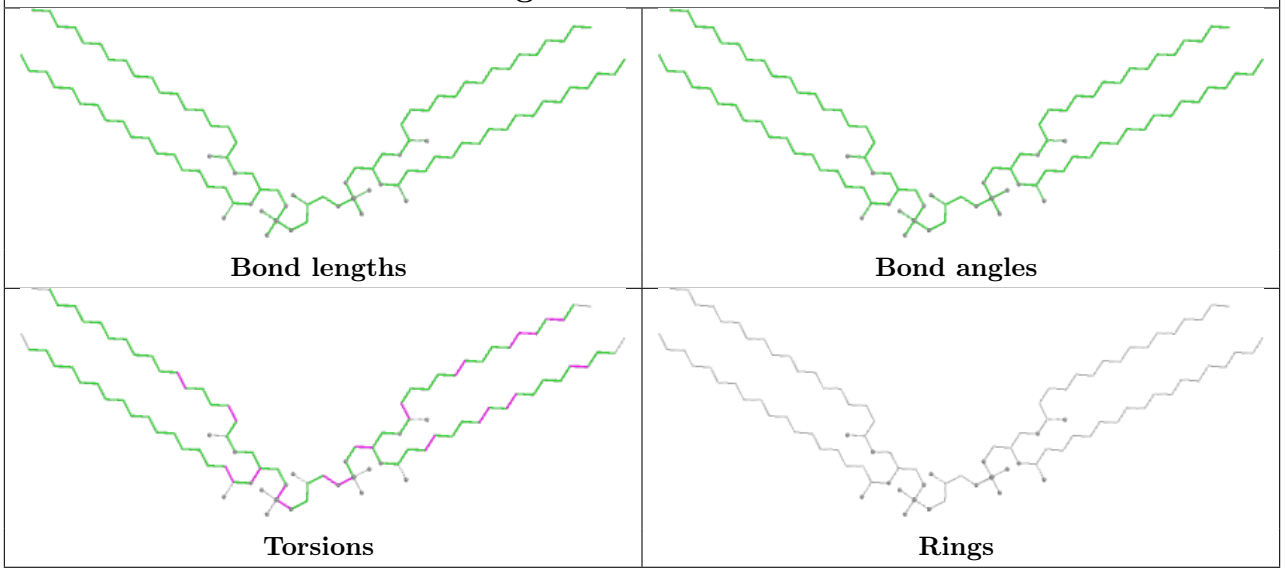
Ligand PC1 m2 407



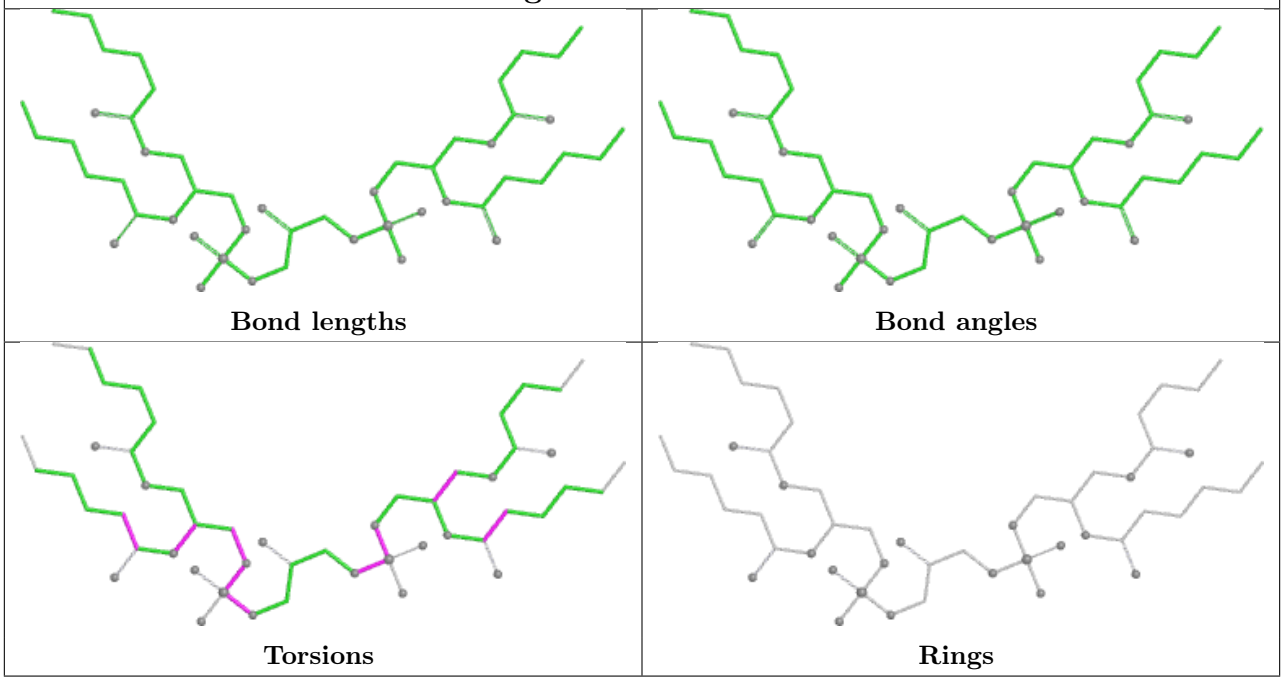
Ligand PC1 QC 505



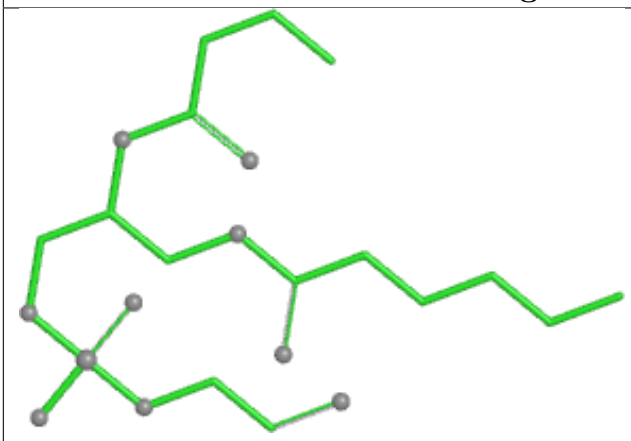
Ligand CDL C4 401



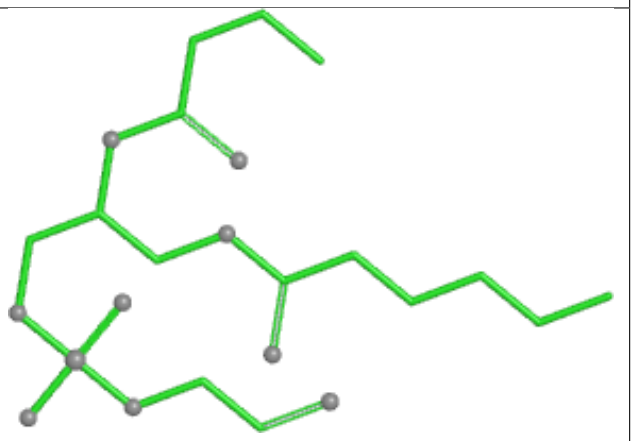
Ligand CDL A 502



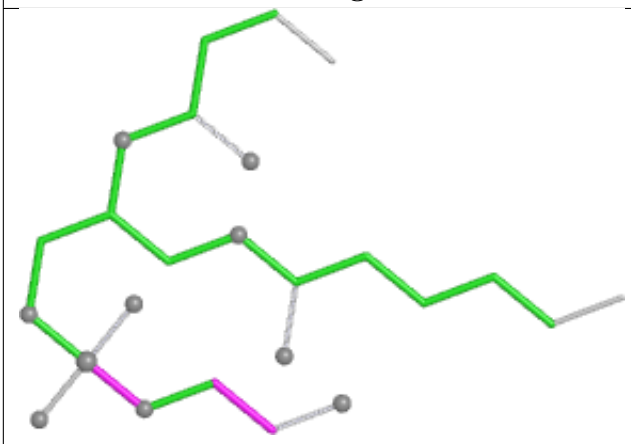
Ligand 3PE T4 302



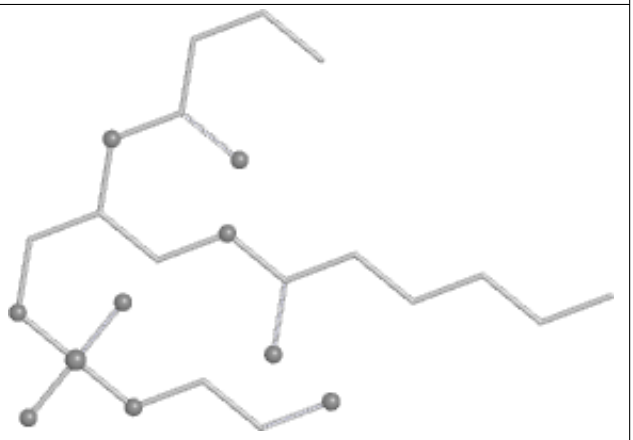
Bond lengths



Bond angles

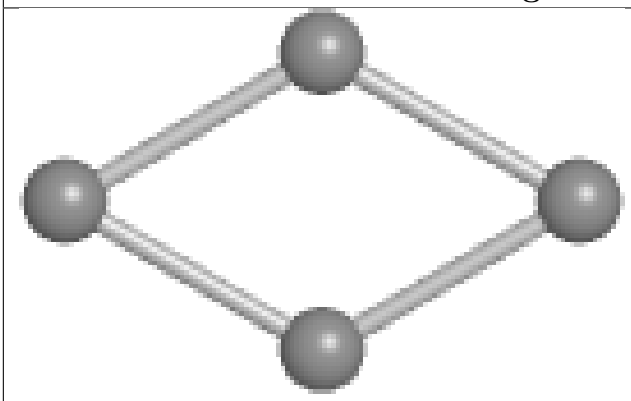


Torsions

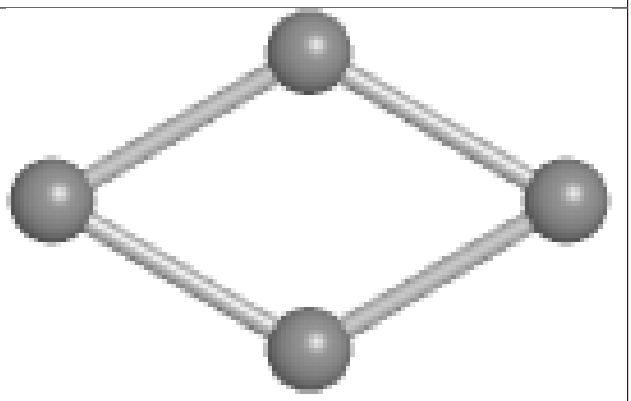


Rings

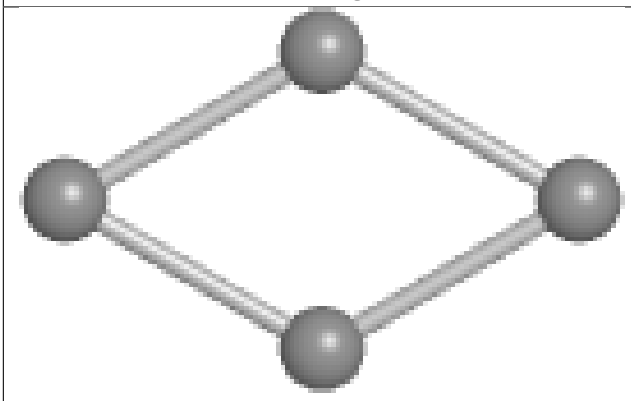
Ligand FES S1 803



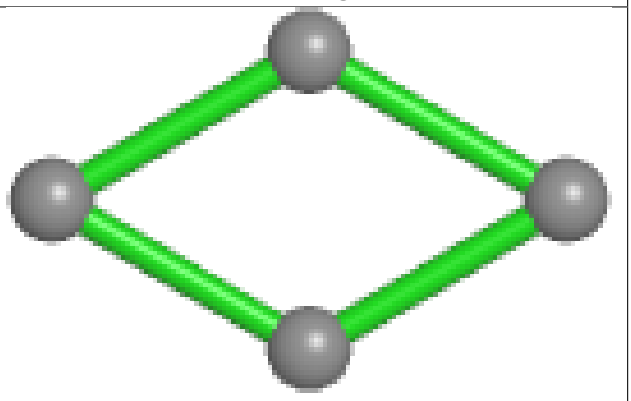
Bond lengths



Bond angles

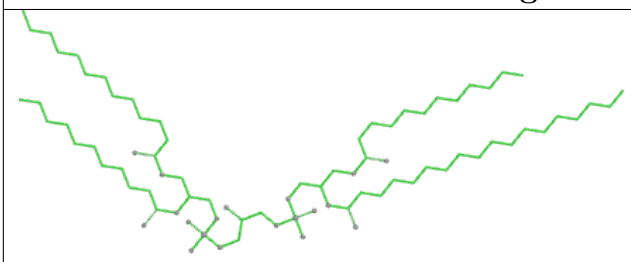


Torsions

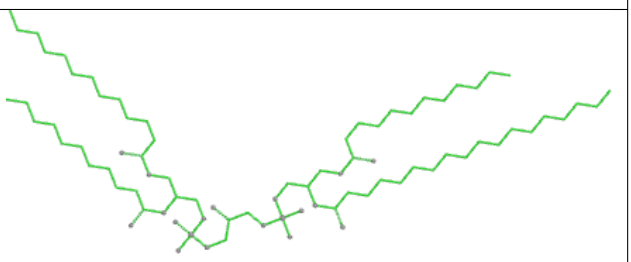


Rings

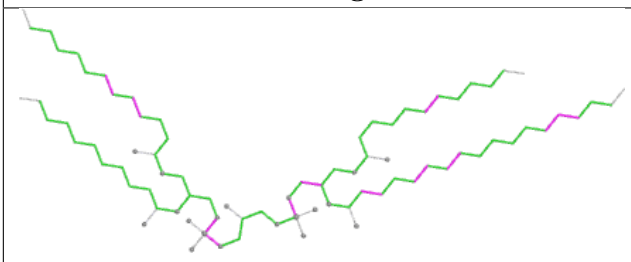
Ligand CDL 6c 202



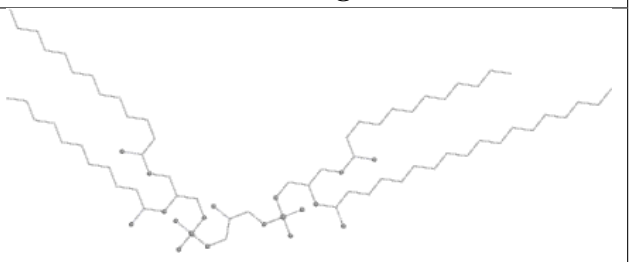
Bond lengths



Bond angles

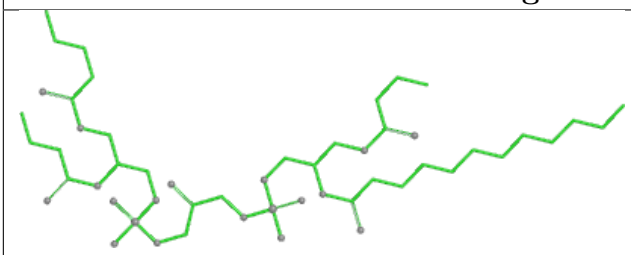


Torsions

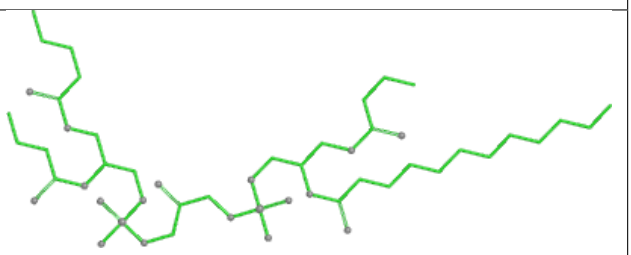


Rings

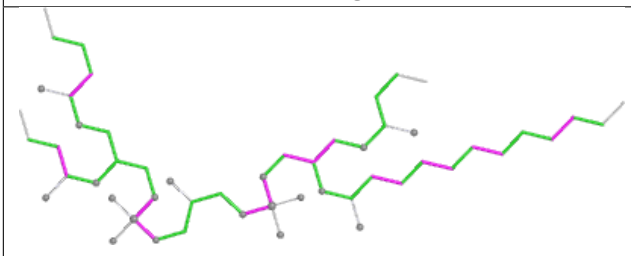
Ligand CDL te 101



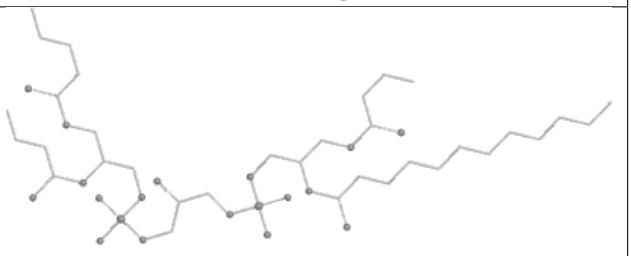
Bond lengths



Bond angles

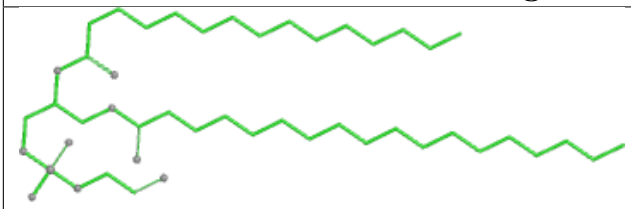


Torsions

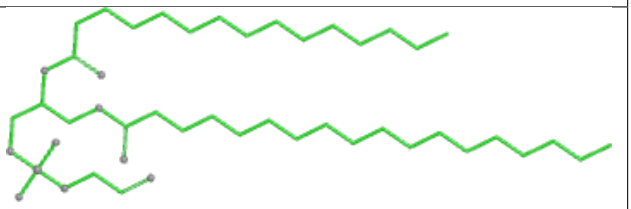


Rings

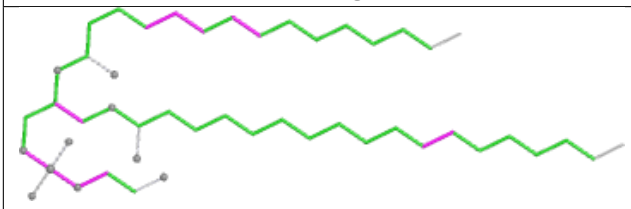
Ligand 3PE b4 202



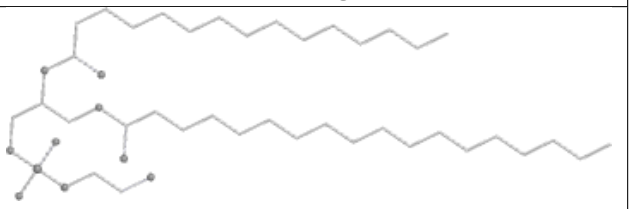
Bond lengths



Bond angles

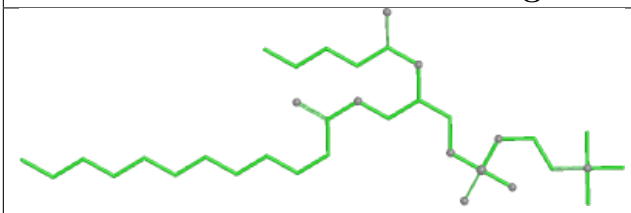


Torsions

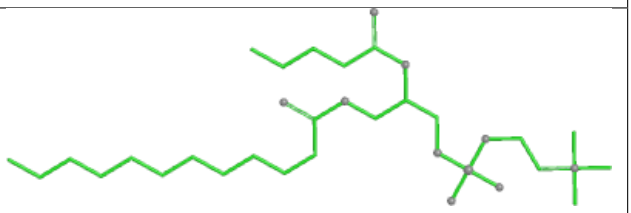


Rings

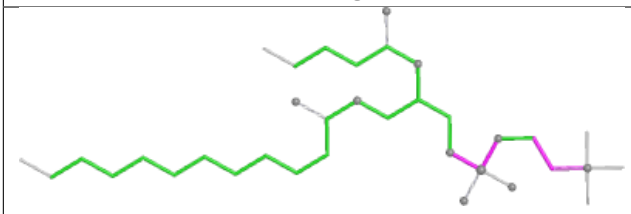
Ligand PC1 M 307



Bond lengths



Bond angles



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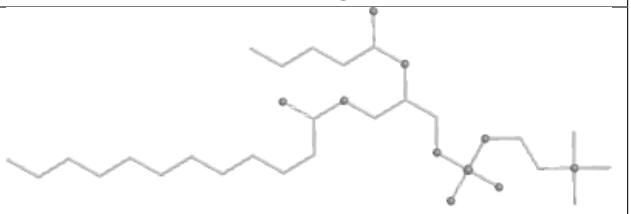
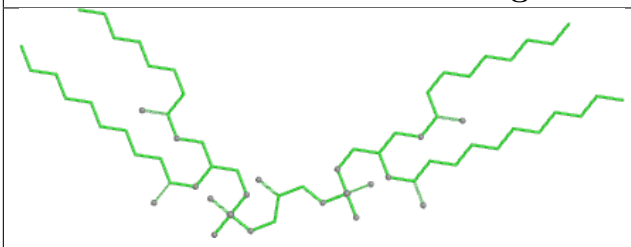
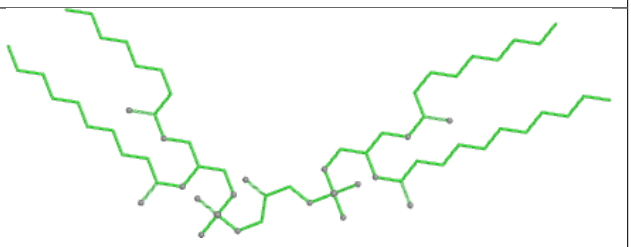


Rings

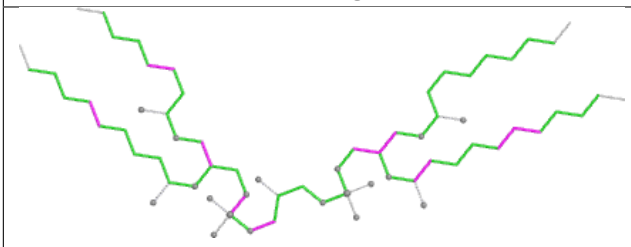
Ligand CDL M1 402



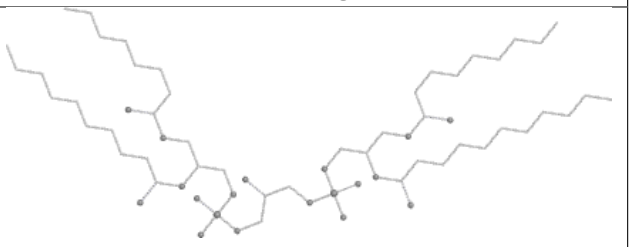
Bond lengths



Bond angles

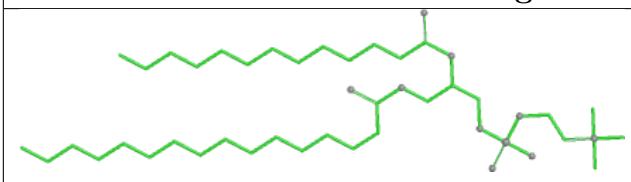


Torsions

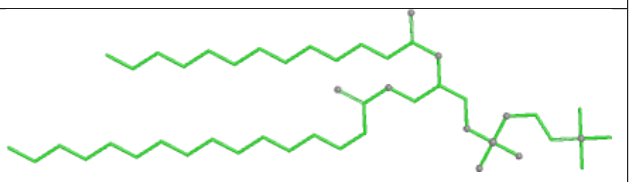


Rings

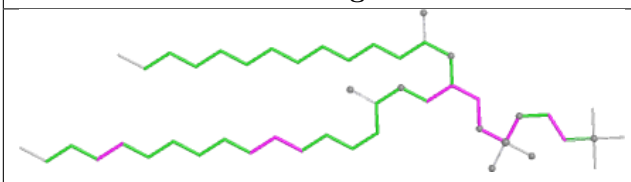
Ligand PC1 TC 102



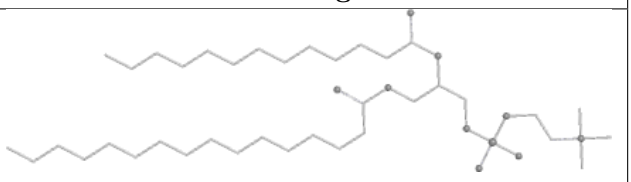
Bond lengths



Bond angles

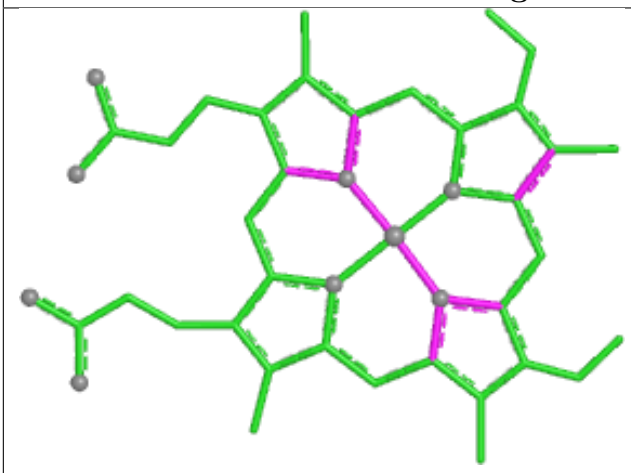


Torsions



Rings

Ligand HEM Qc 503



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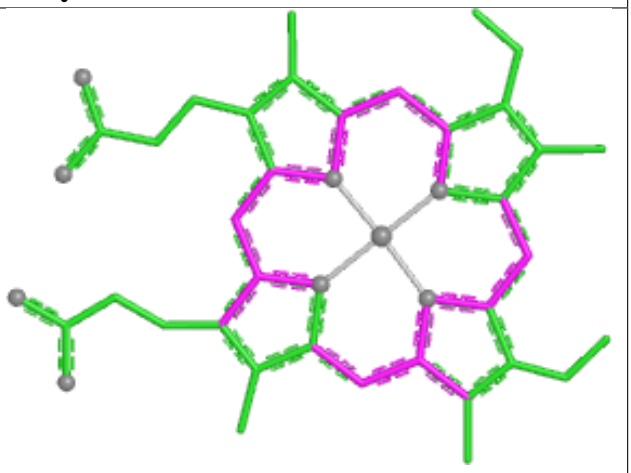
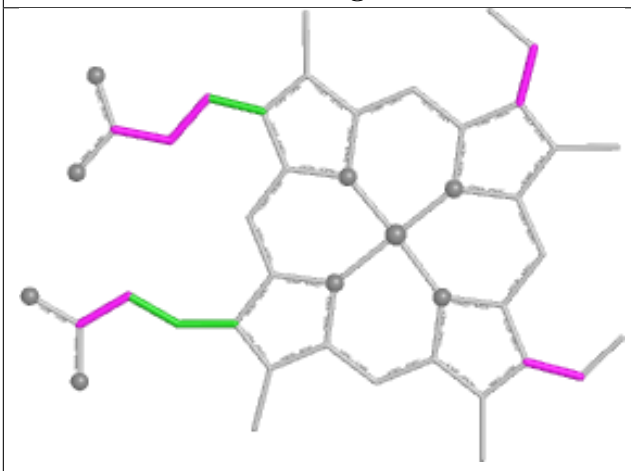


Bond angles



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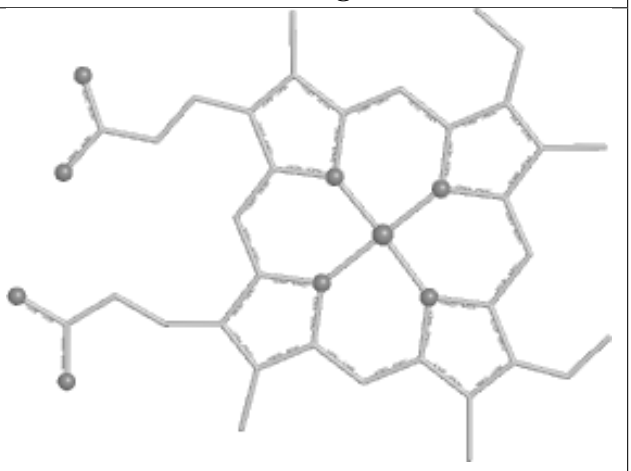
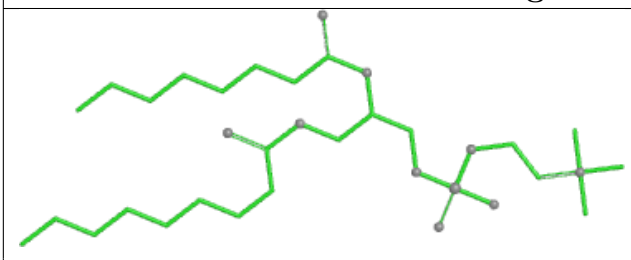
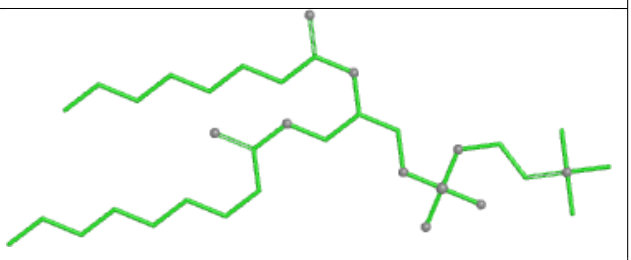


Rings

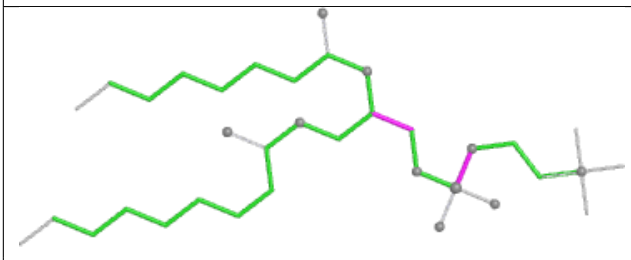
Ligand PC1 V 201



Bond lengths



Bond angles



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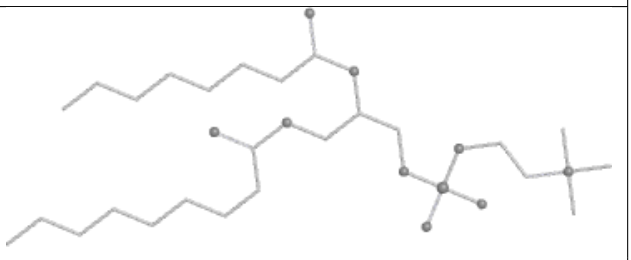
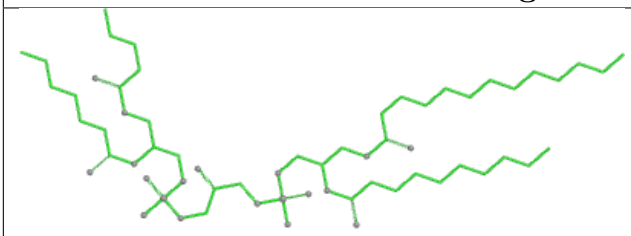
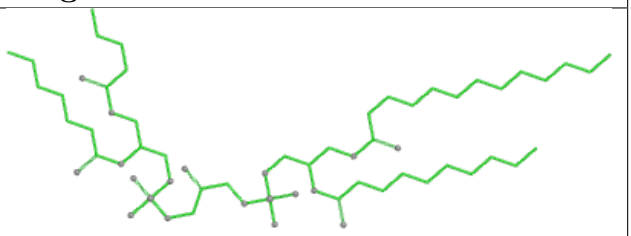


Rings

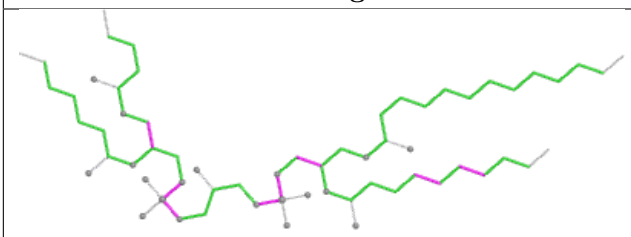
Ligand CDL 2g 204



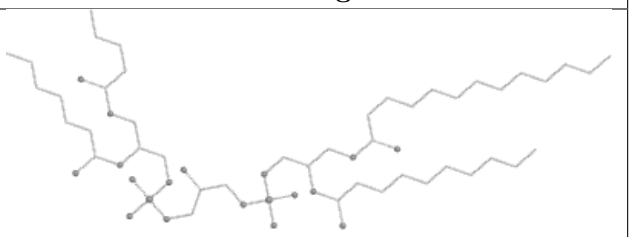
Bond lengths



Bond angles

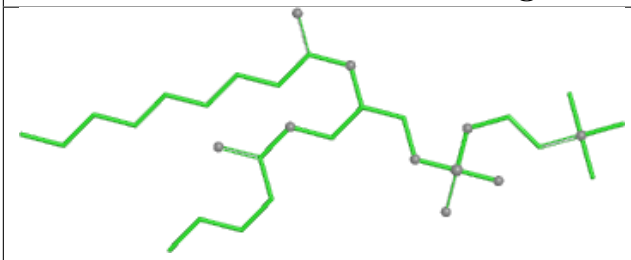


Torsions

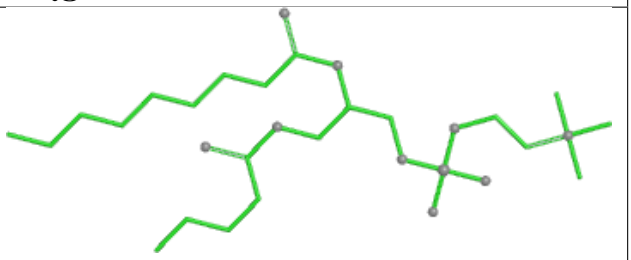


Rings

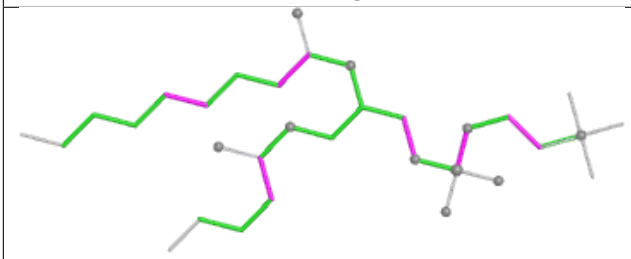
Ligand PC1 Qg 401



Bond lengths



Bond angles



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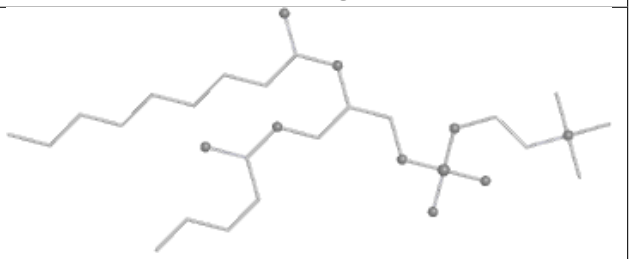
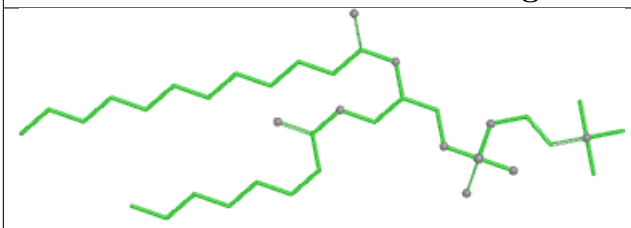
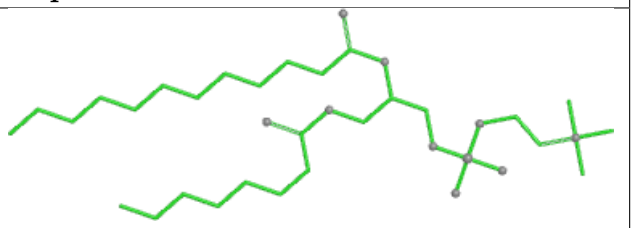


Rings

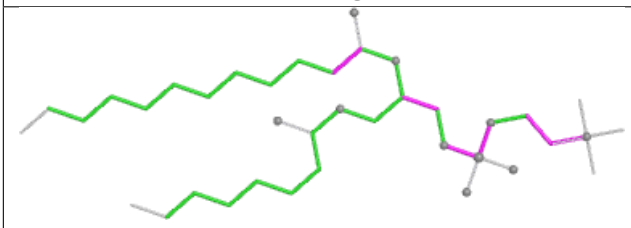
Ligand PC1 qJ 101



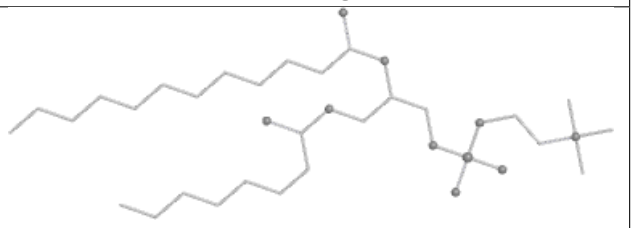
Bond lengths



Bond angles

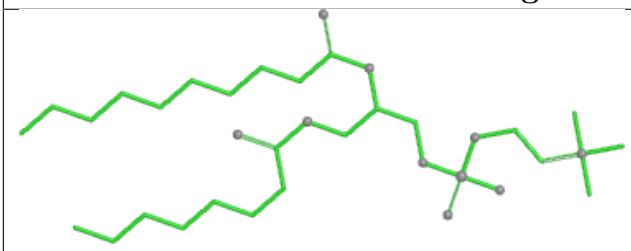


Torsions

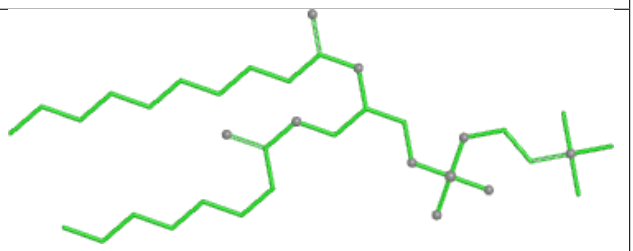


Rings

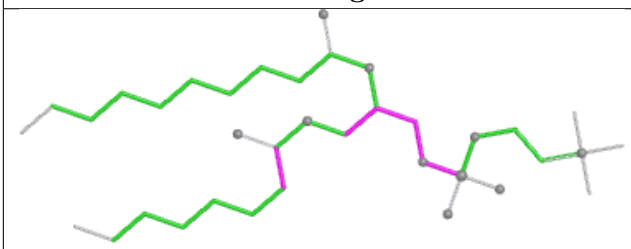
Ligand PC1 n1 301



Bond lengths



Bond angles



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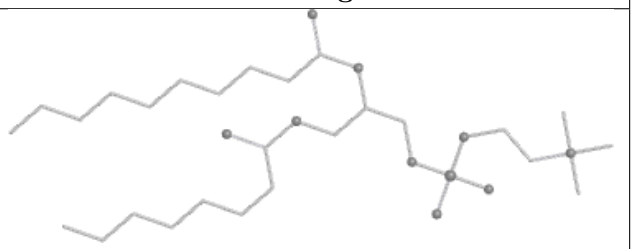
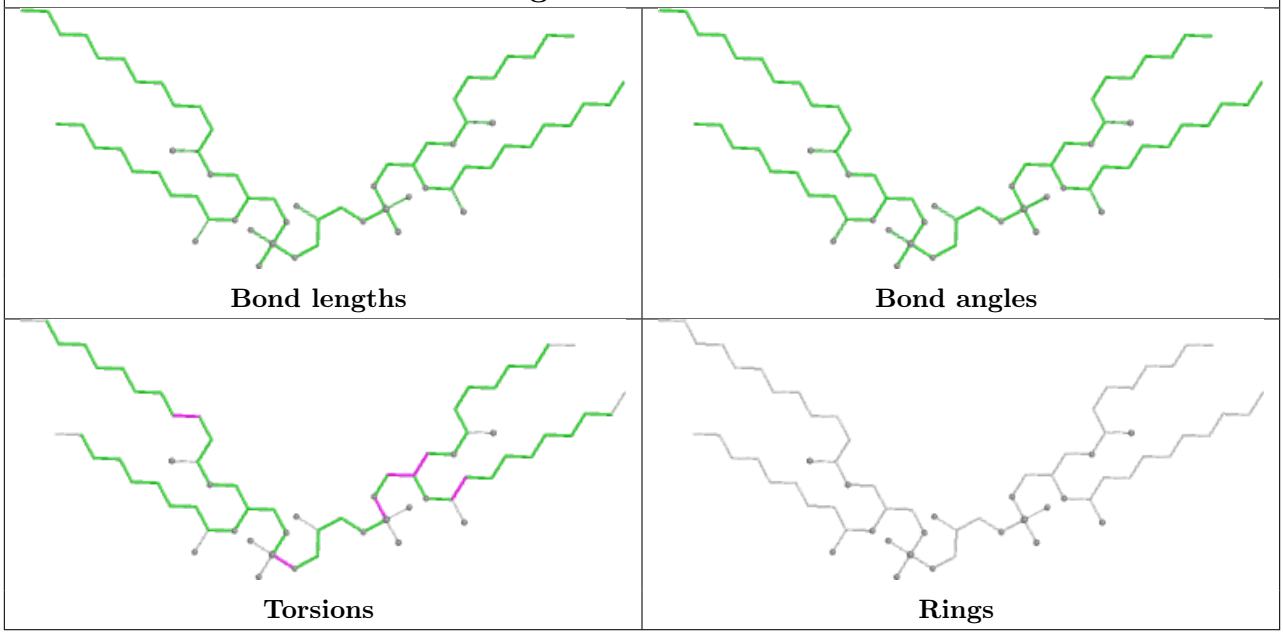
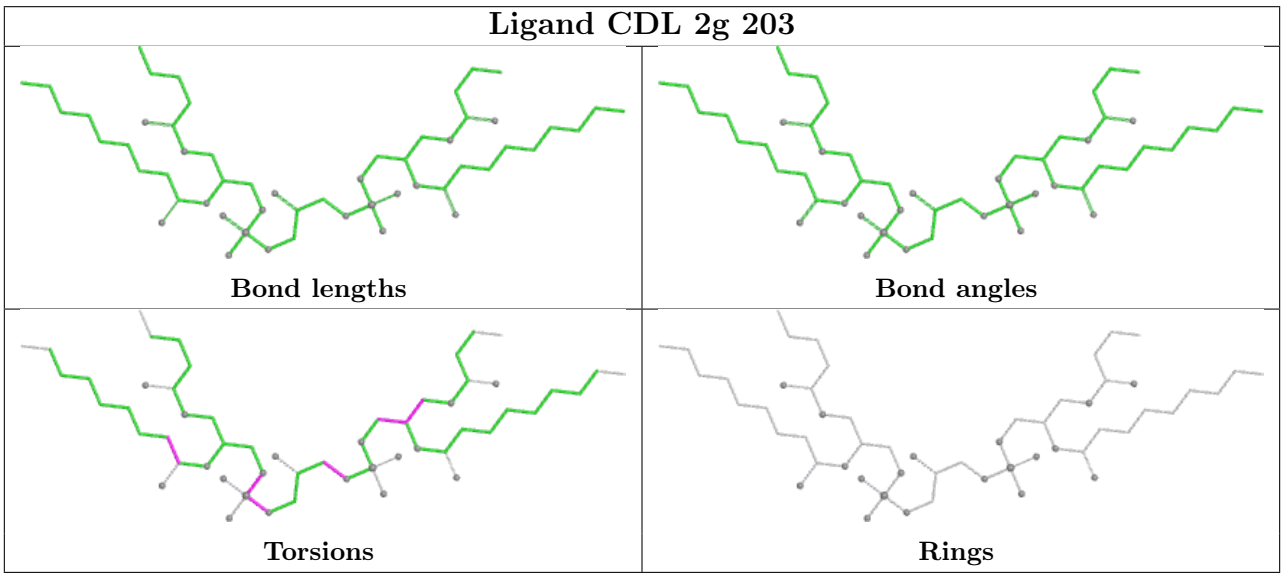


Rings

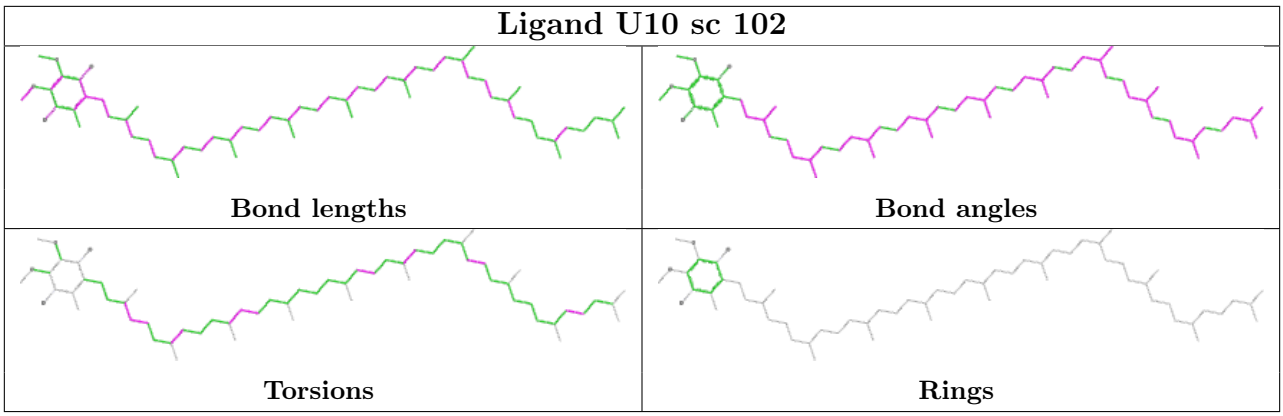
Ligand CDL z 101



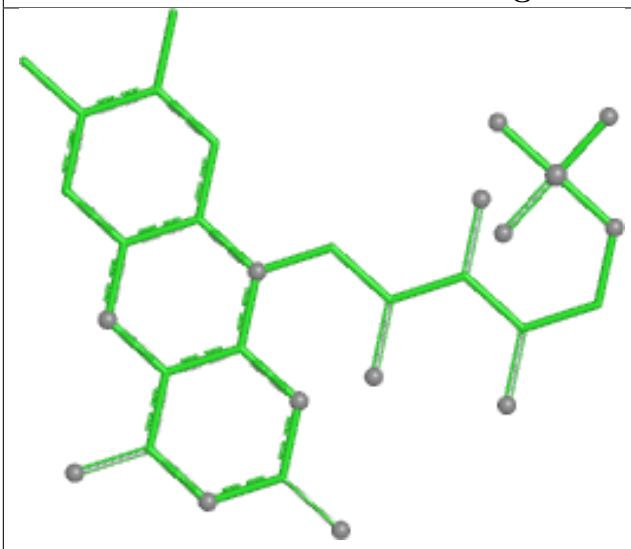
Ligand CDL 2g 203



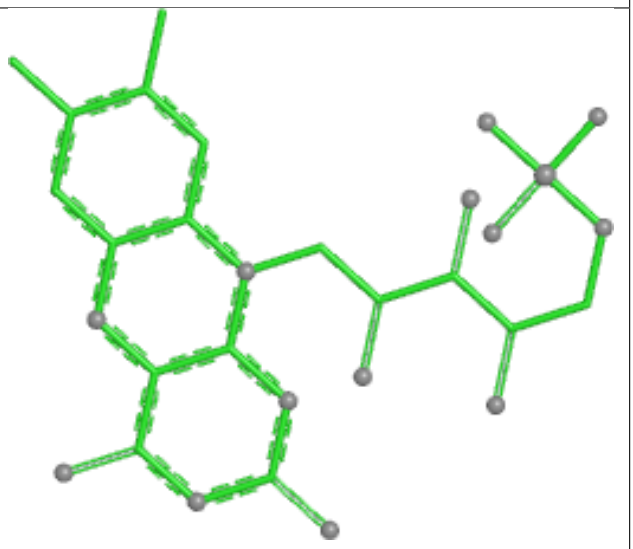
Ligand U10 sc 102



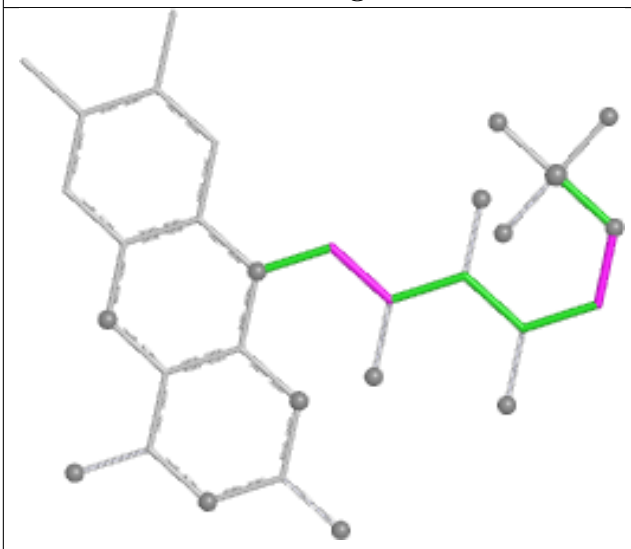
Ligand FMN v1 501



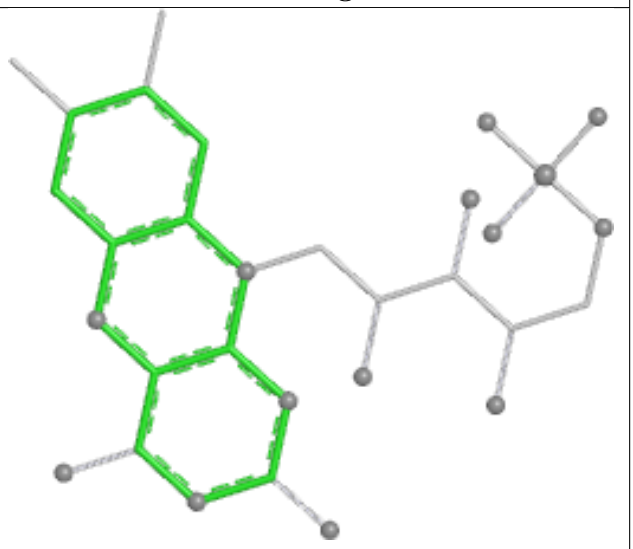
Bond lengths



Bond angles

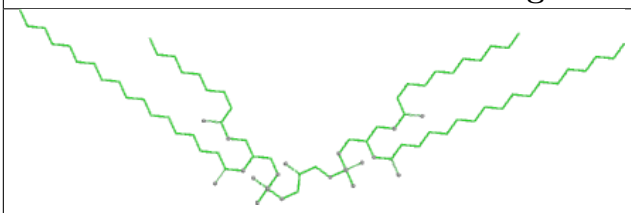


Torsions

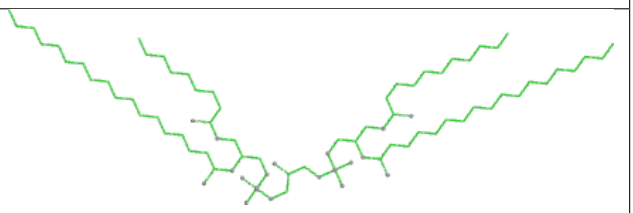


Rings

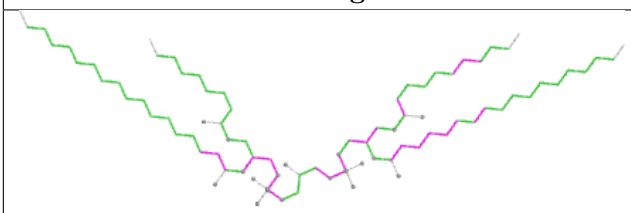
Ligand CDL n 304



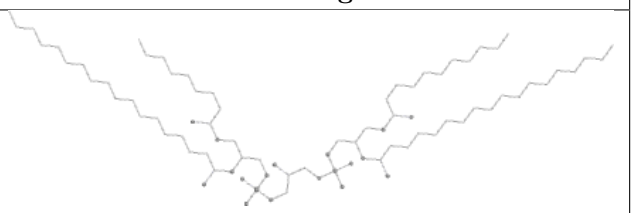
Bond lengths



Bond angles

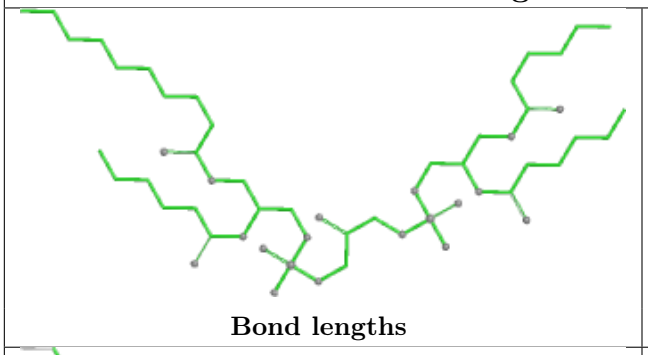


Torsions

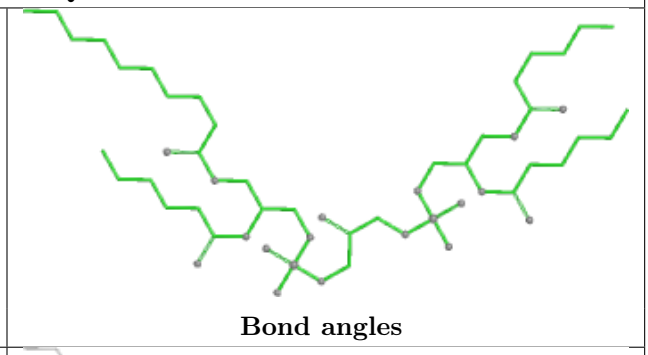


Rings

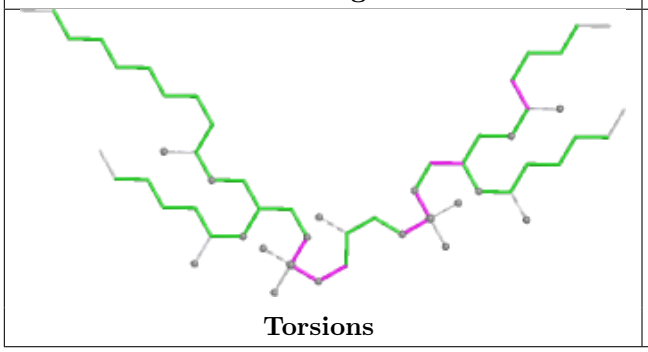
Ligand CDL QC 504



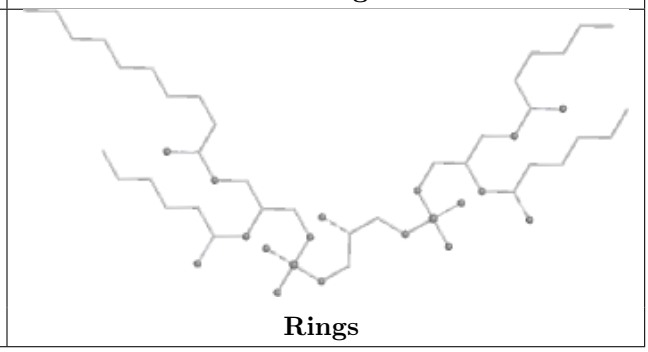
Bond lengths



Bond angles

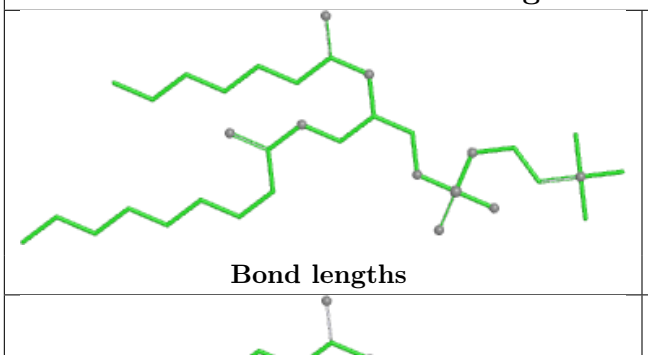


Torsions

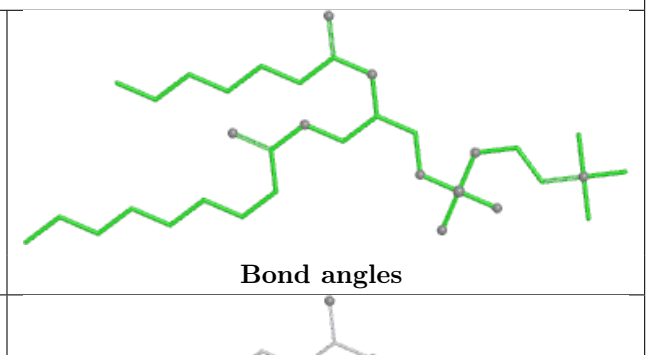


Rings

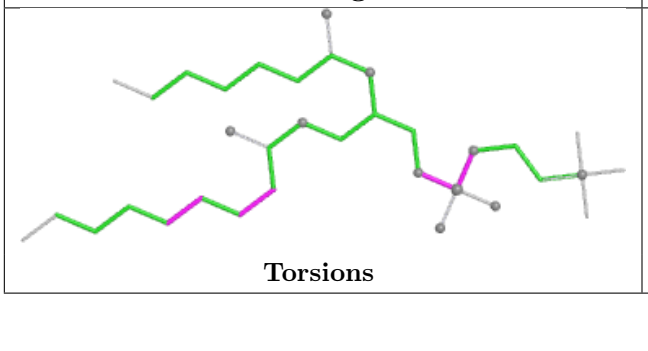
Ligand PC1 W 204



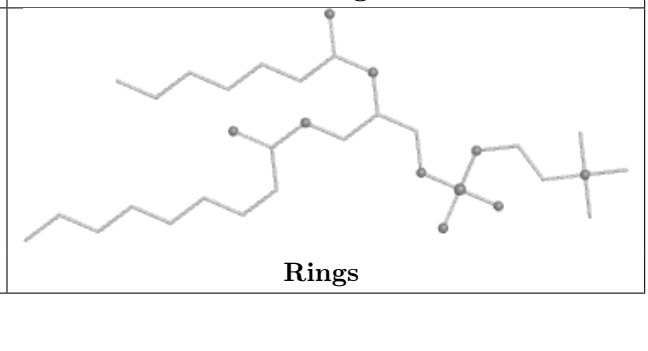
Bond lengths



Bond angles

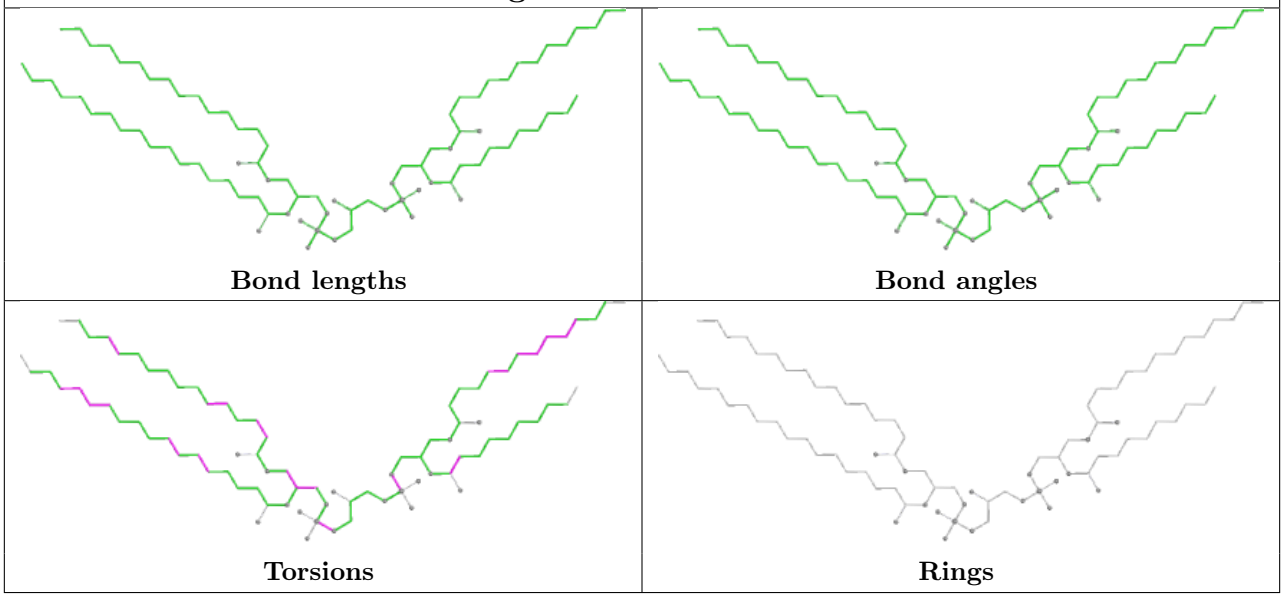


Torsions

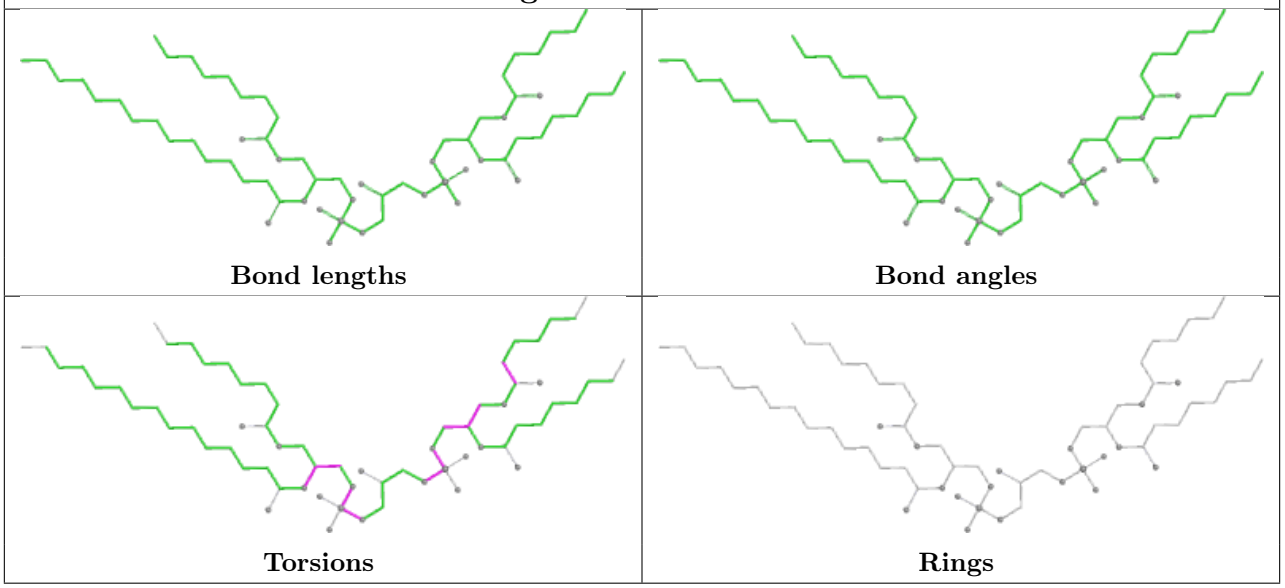


Rings

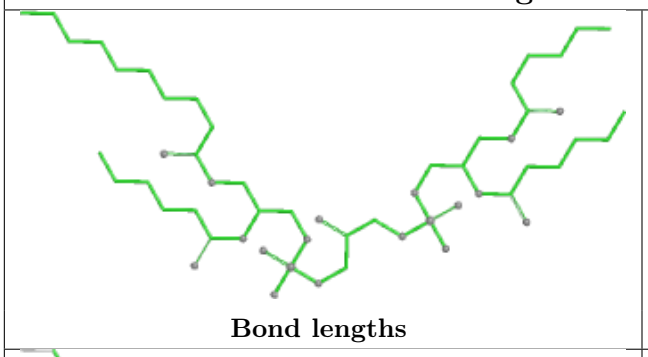
Ligand CDL BM 301



Ligand CDL a1 101



Ligand CDL qC 504



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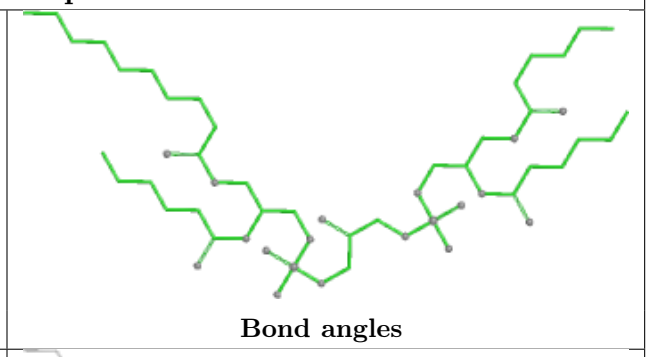
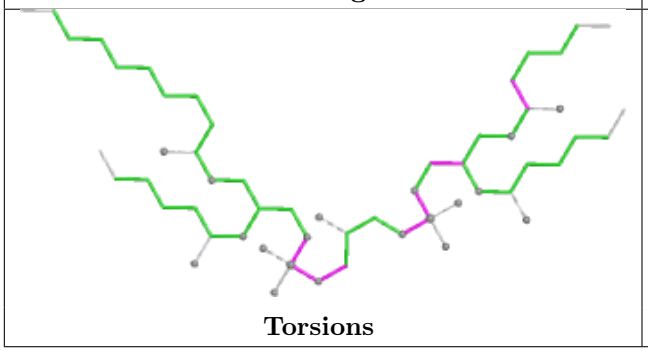
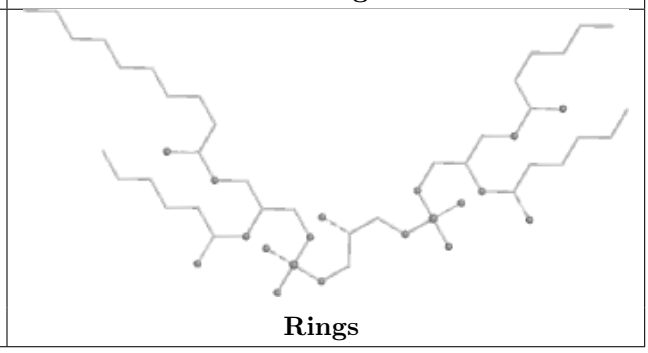


Bond angles

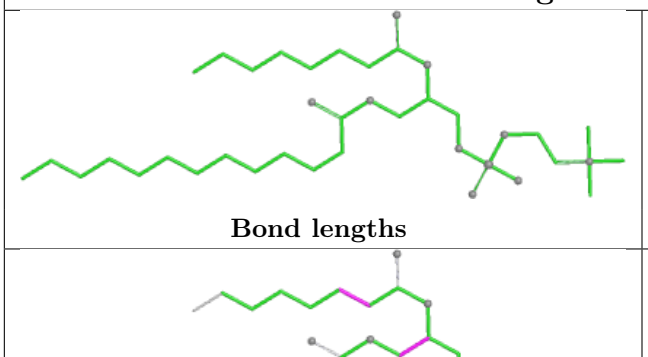


Torsions



Rings

Ligand PC1 i 304



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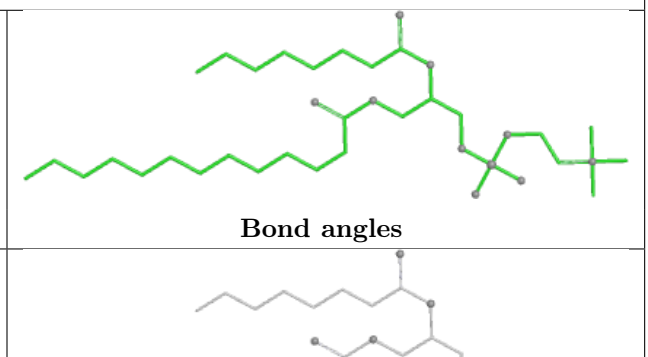
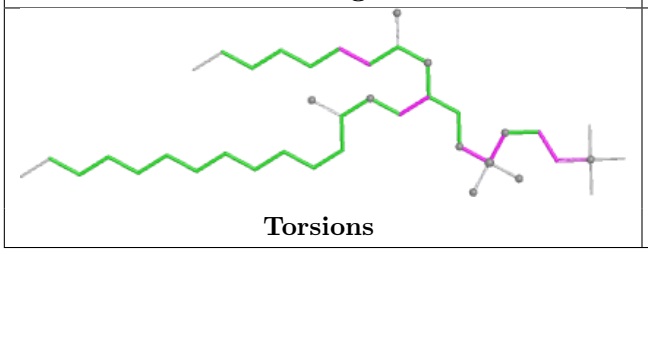


Bond angles



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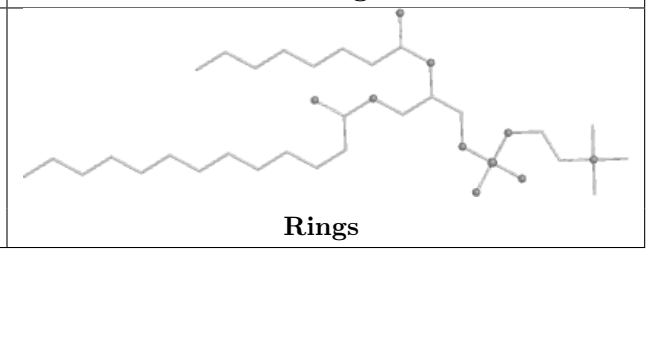
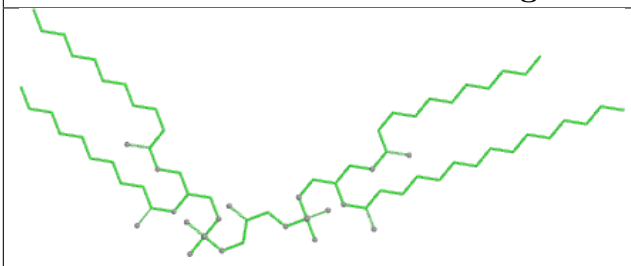


Rings

Ligand CDL 6c 201



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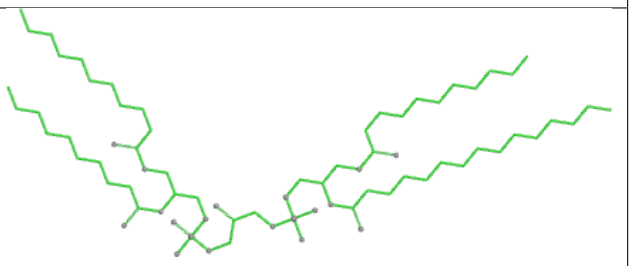
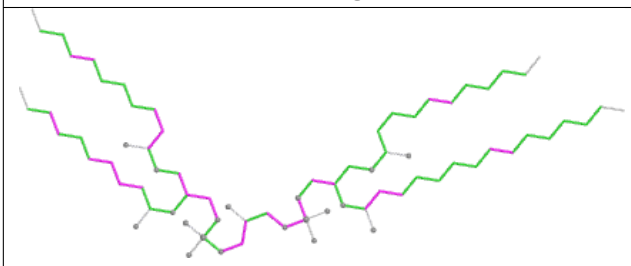


Bond angles



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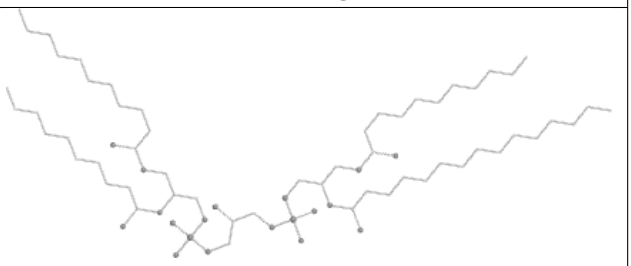
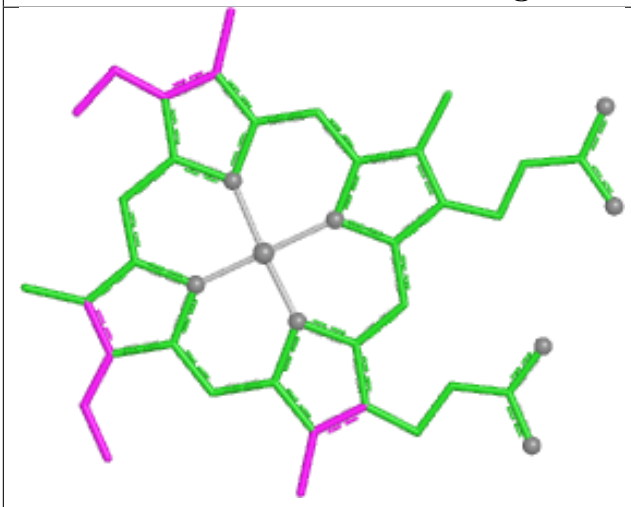


Rings

Ligand HEC qD 401



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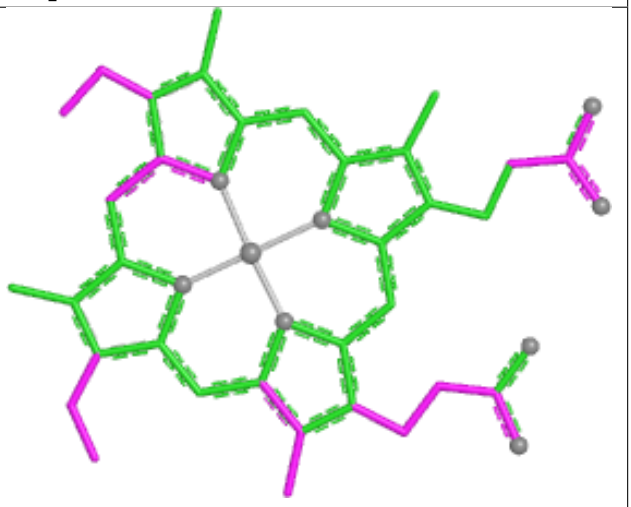

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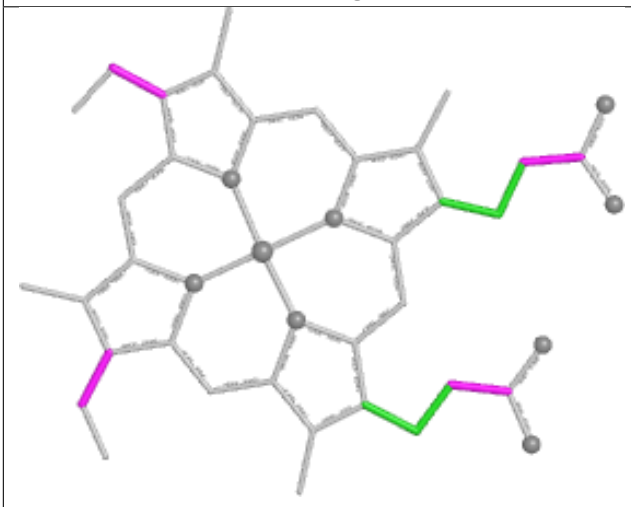

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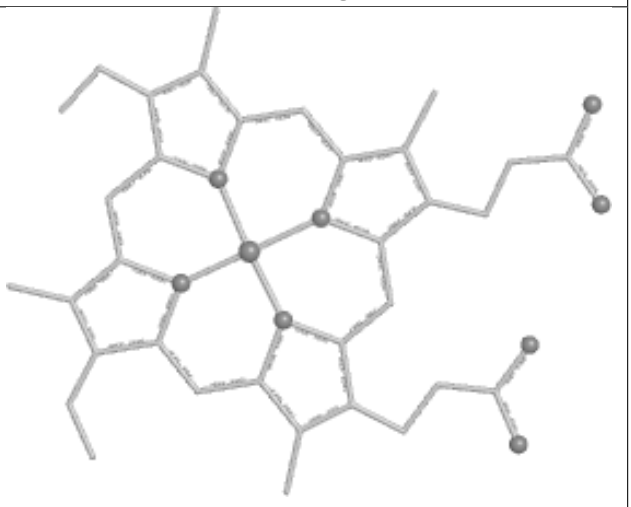
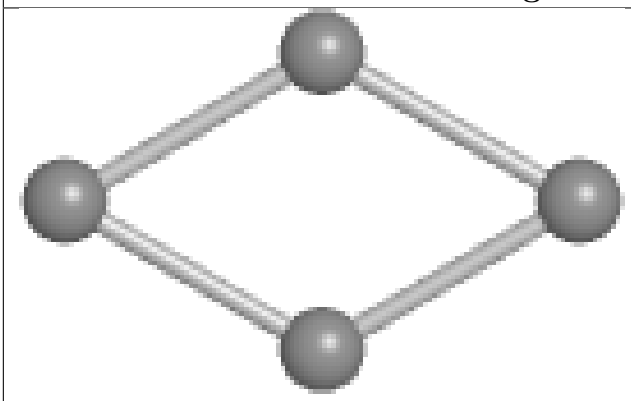


Rings

Ligand FES v2 300



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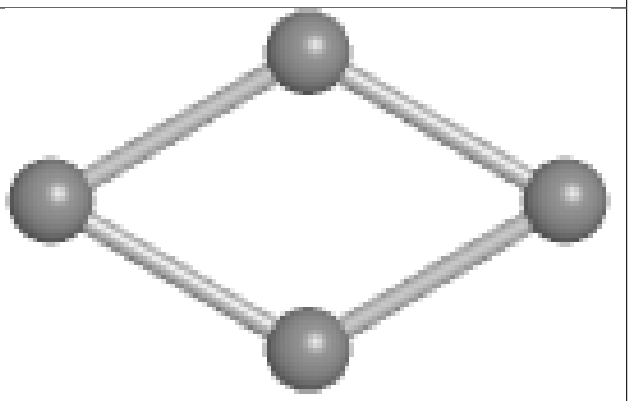

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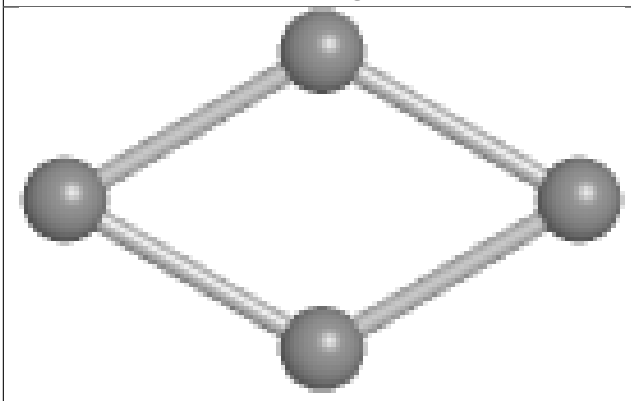

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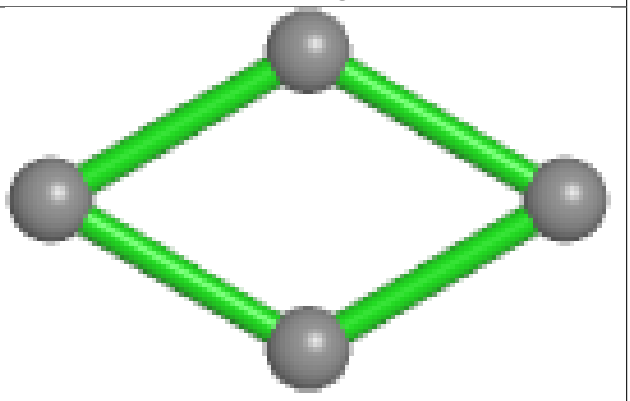
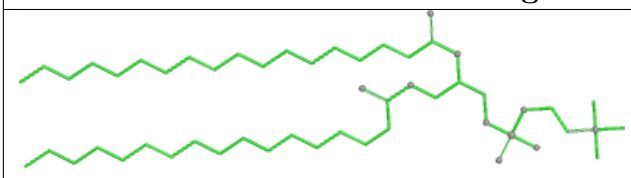


Rings

Ligand PC1 n5 803



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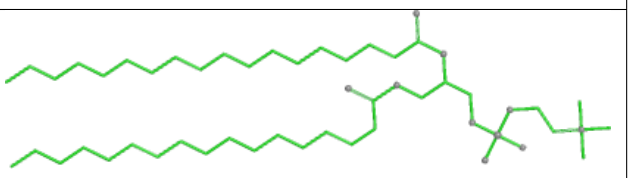

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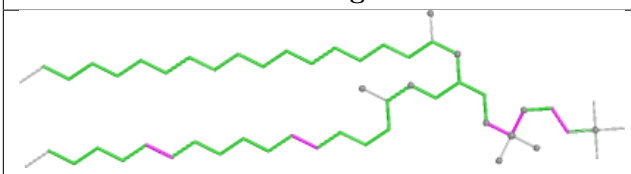

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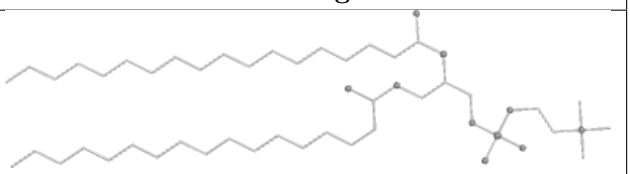
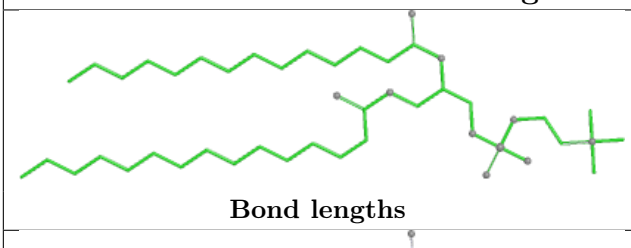


Rings

Ligand PC1 5b 202



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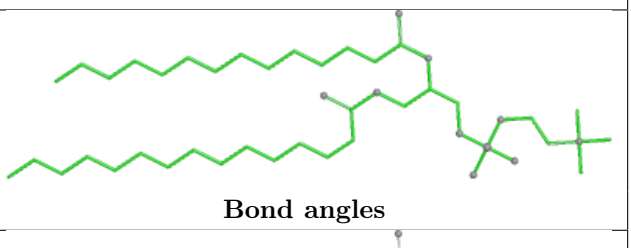
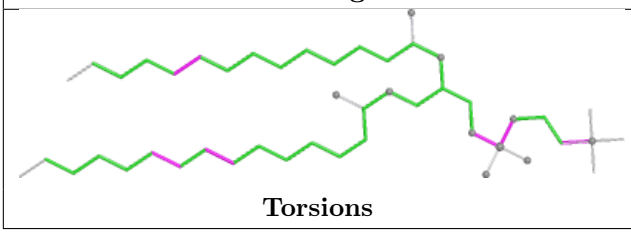


Bond angles



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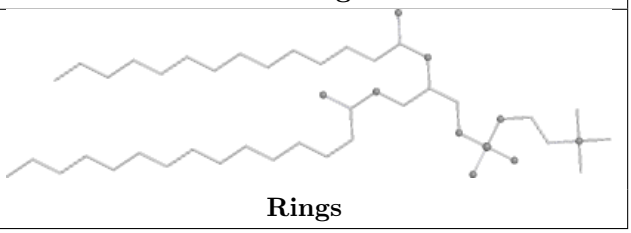
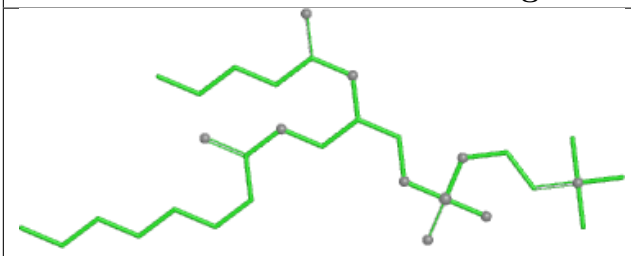


Rings

Ligand PC1 n3 201



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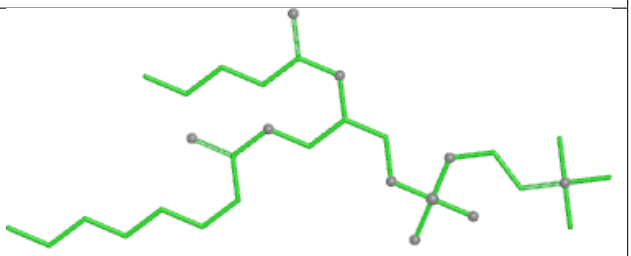

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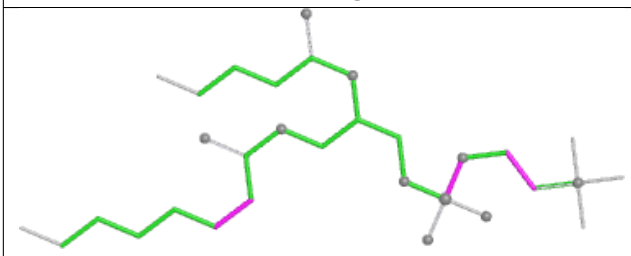

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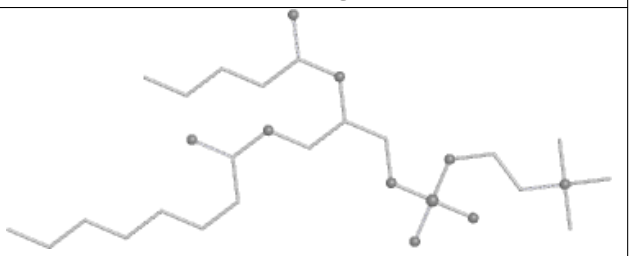
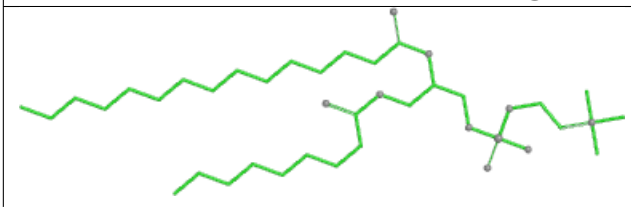


Rings

Ligand PC1 2j 201



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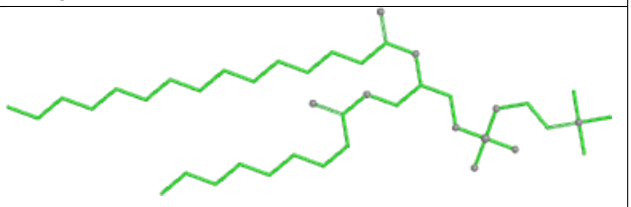

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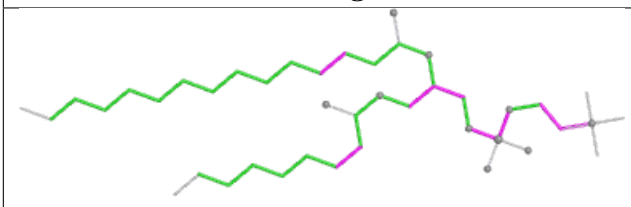

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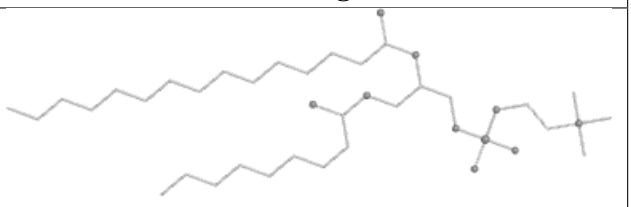
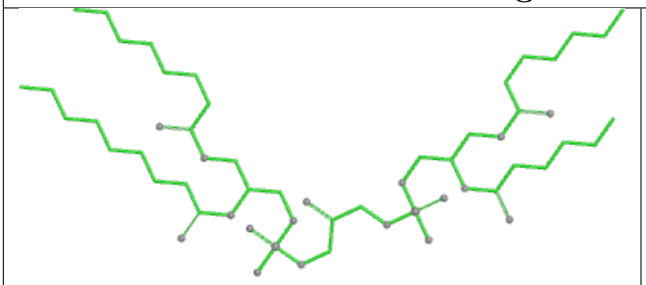


Rings

Ligand CDL P1 403



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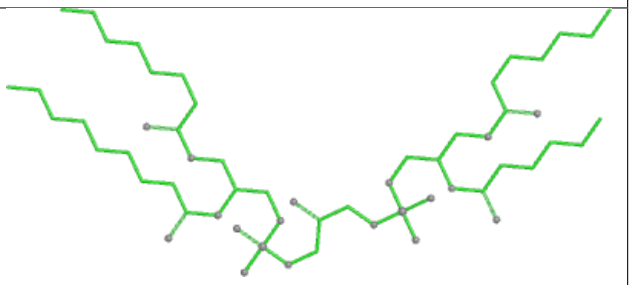
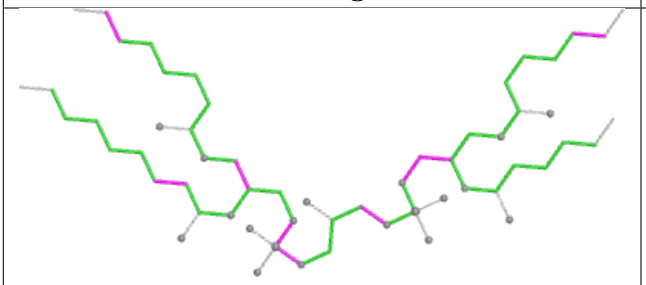


Bond angles



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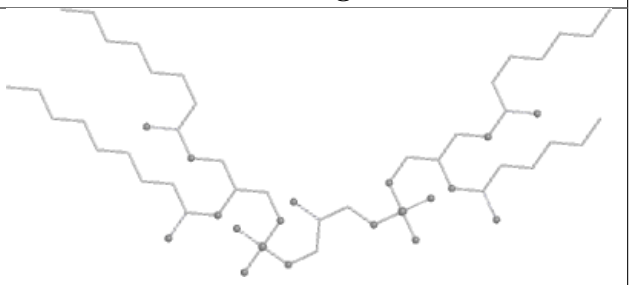
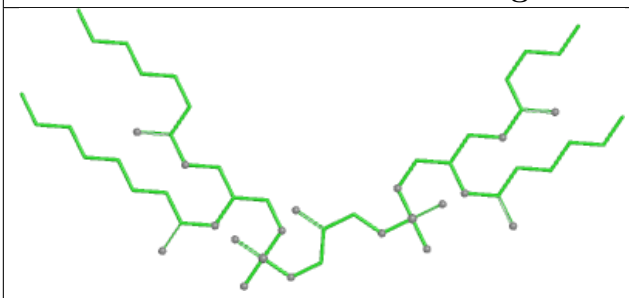
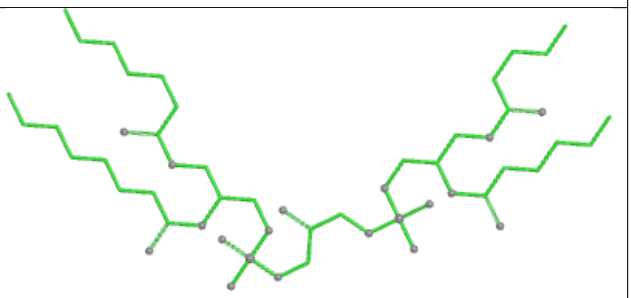


Rings

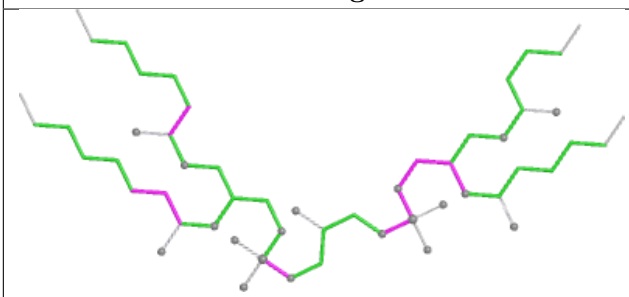
Ligand CDL M2 401



Bond lengths



Bond angles



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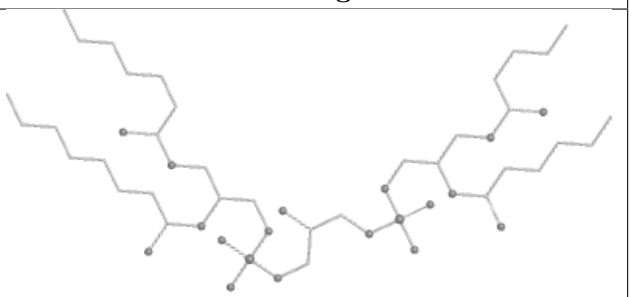
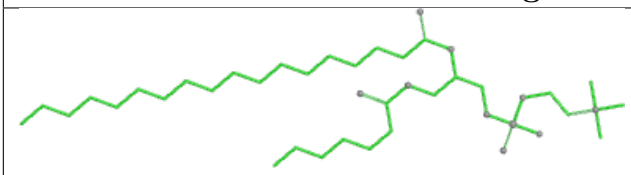


Rings

Ligand PC1 qe 303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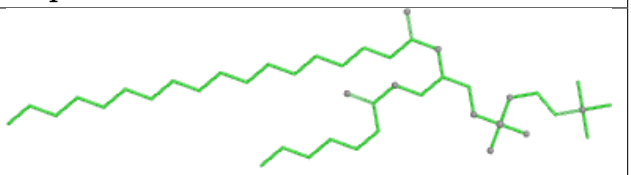
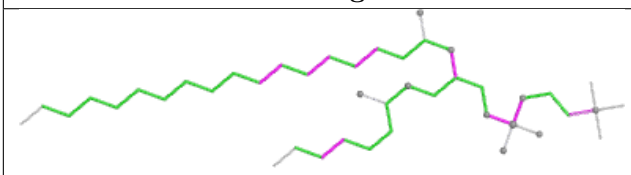

Bond angles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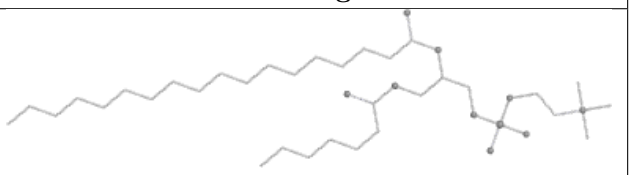
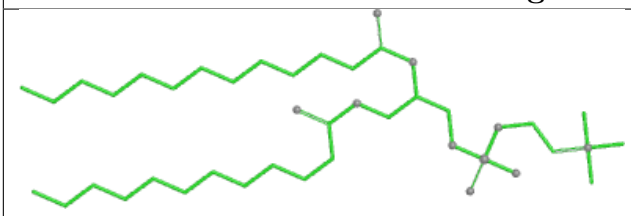
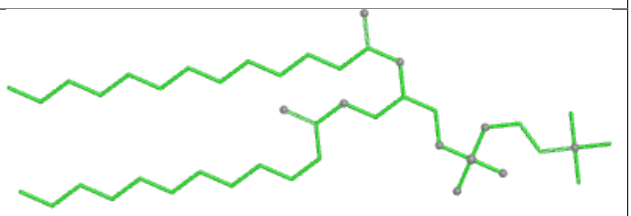
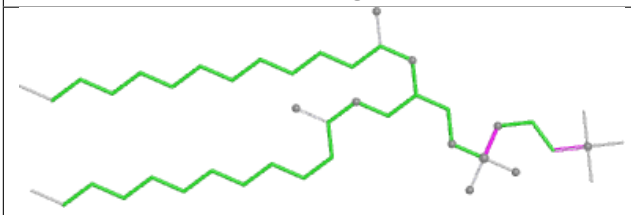
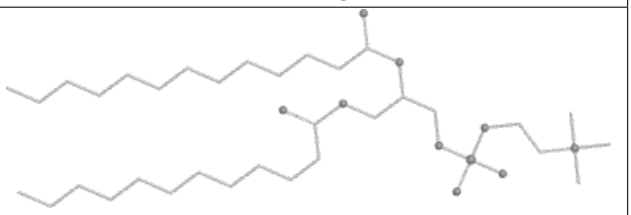

Rings

Ligand PC1 w 205

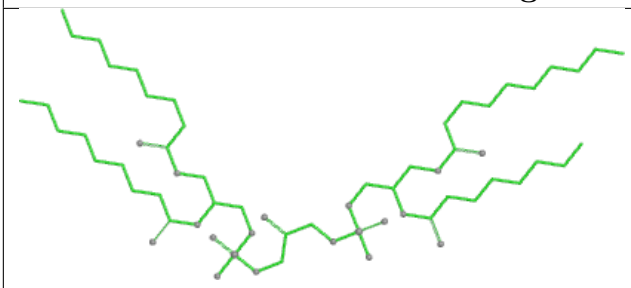

Bond lengths

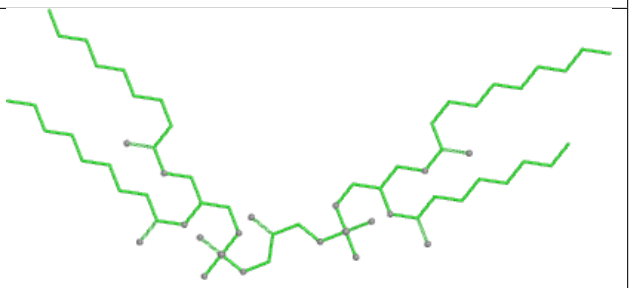

Bond angles


Torsions


Rings

Ligand CDL M 304


Bond lengths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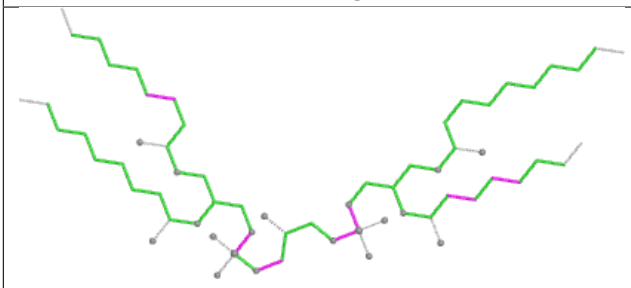
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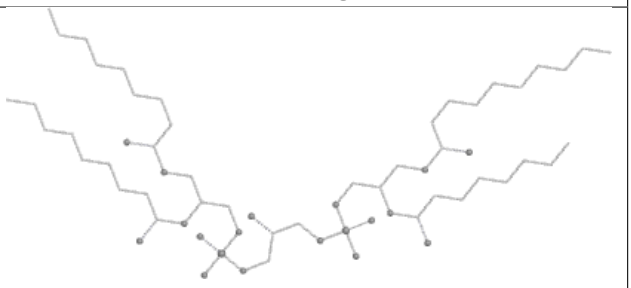
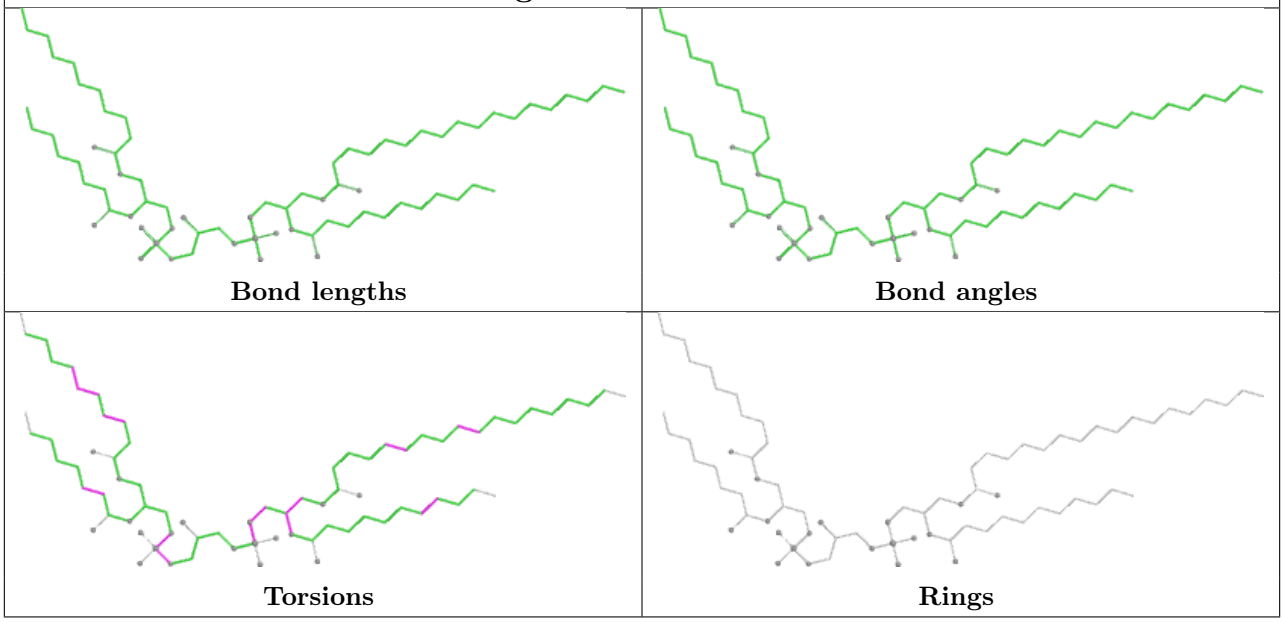
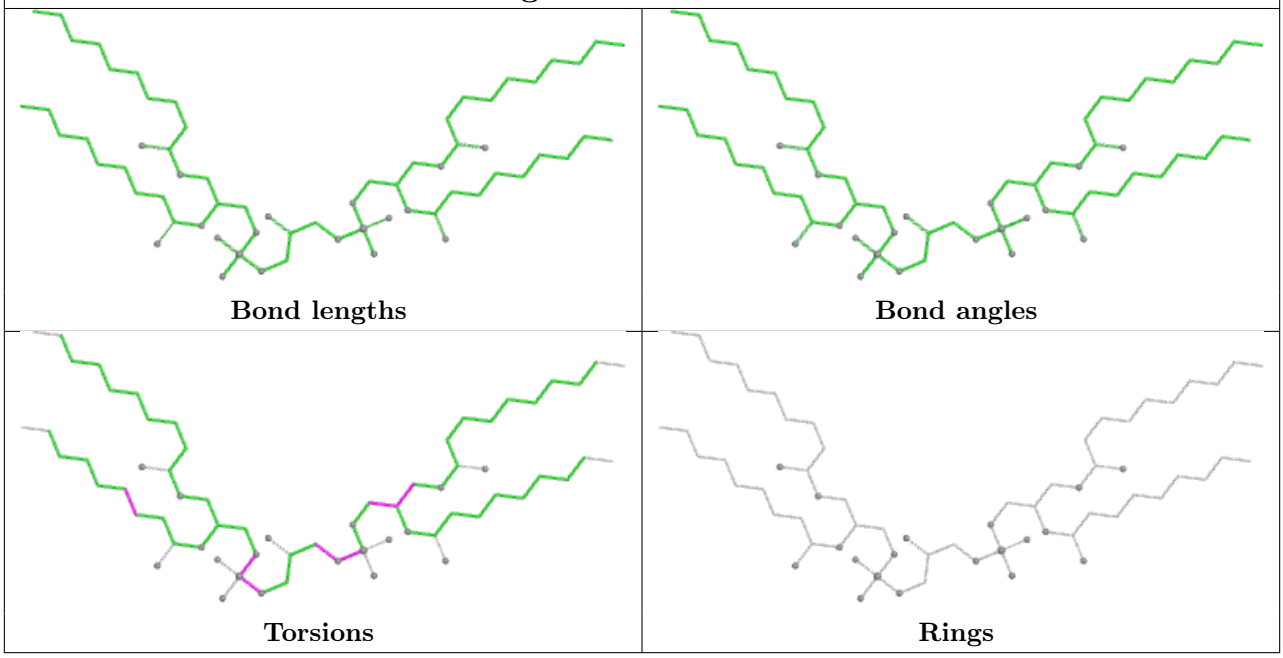

Rings

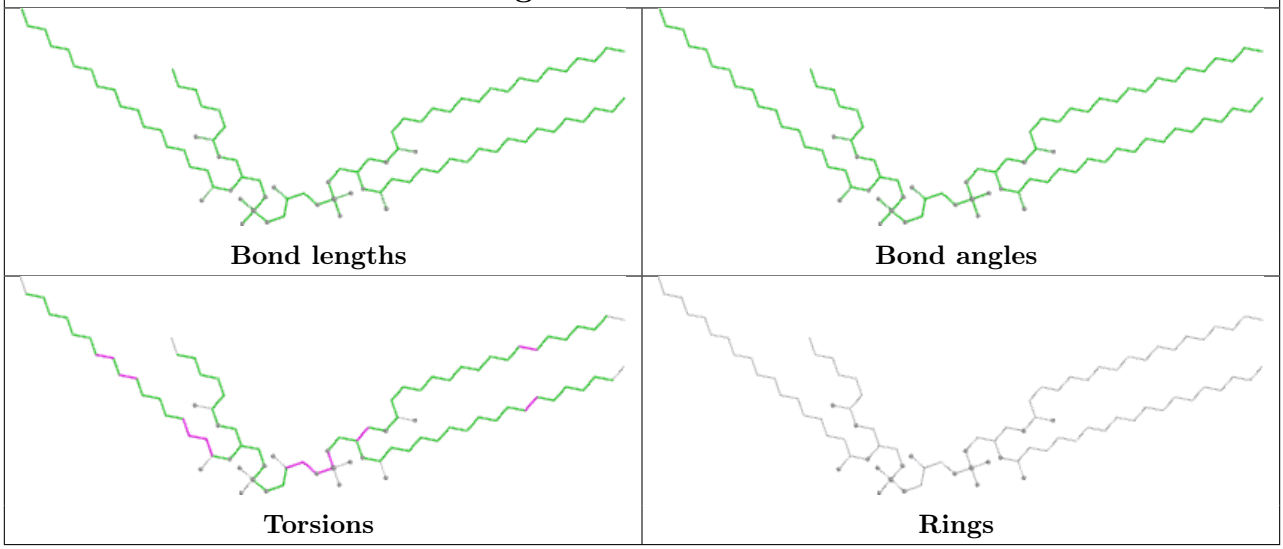
Ligand CDL A9 402



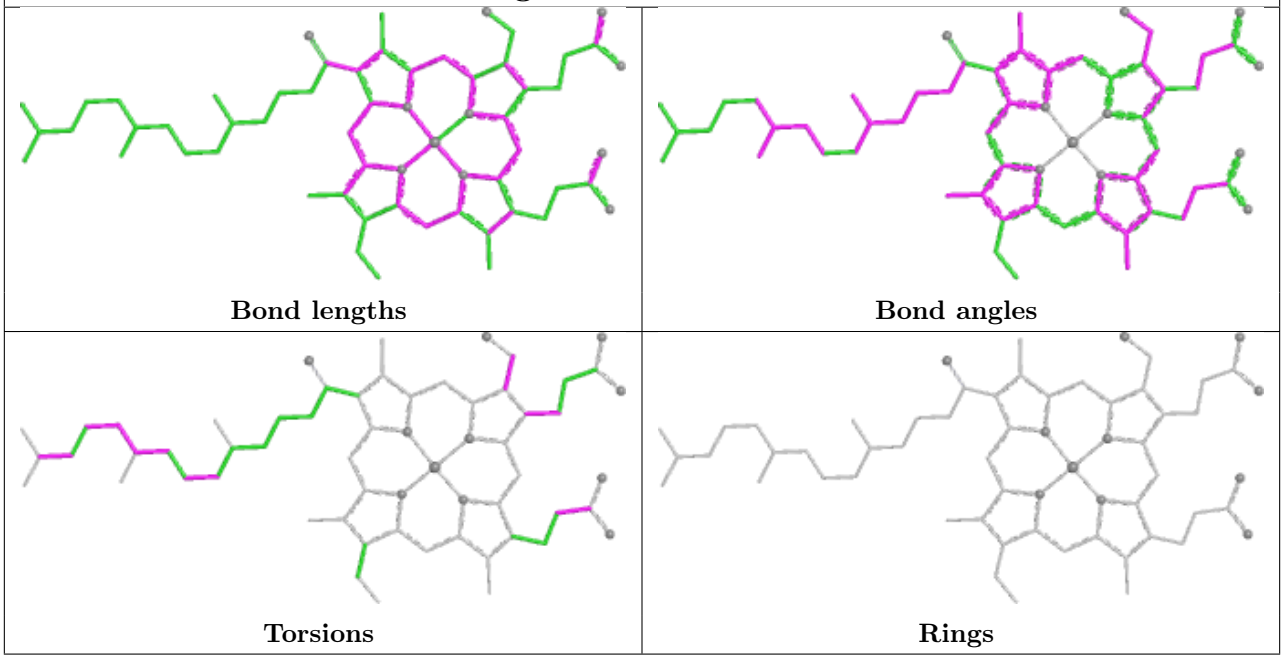
Ligand CDL M 301



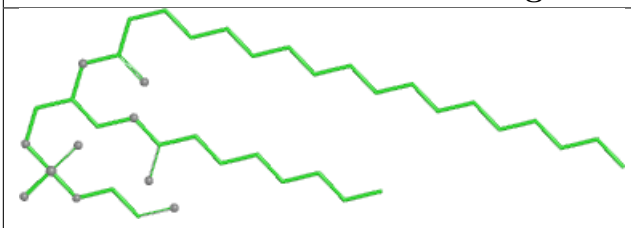
Ligand CDL 2G 201



Ligand HEA C1 702



Ligand 3PE s8 304



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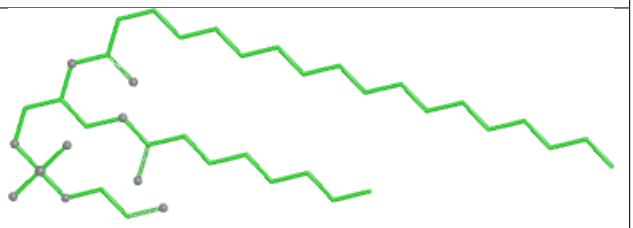
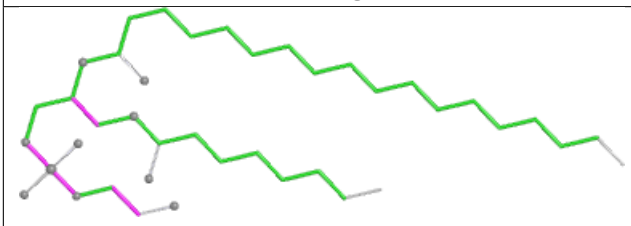


Bond angles



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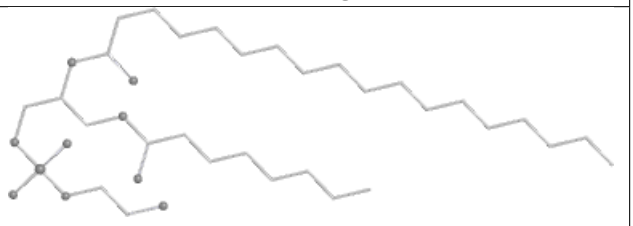
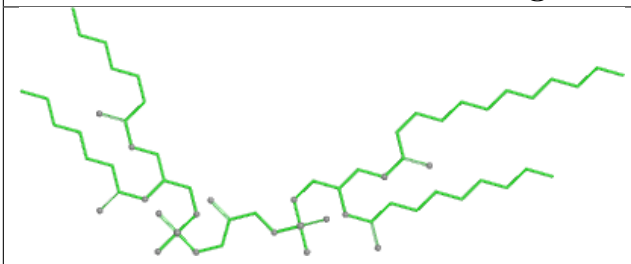


Rings

Ligand CDL e 403



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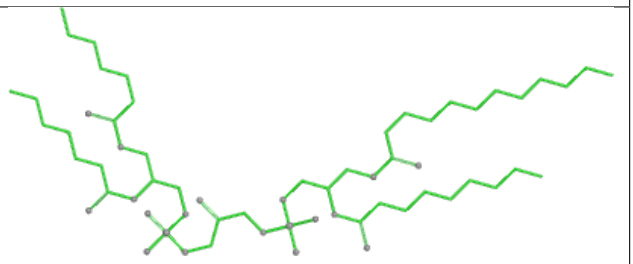
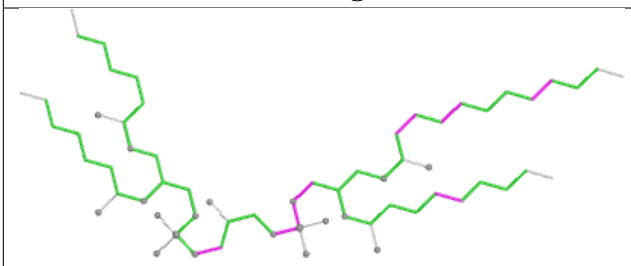


Bond angles



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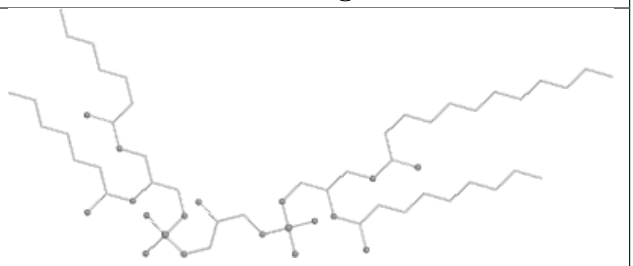
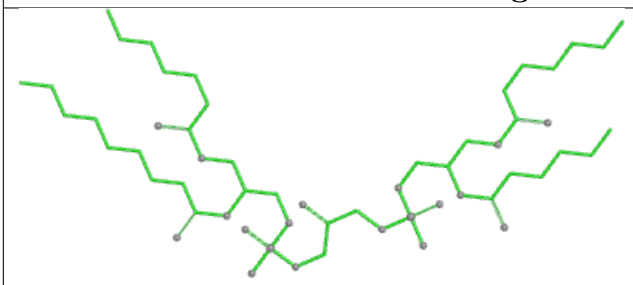


Rings

Ligand CDL M1 405



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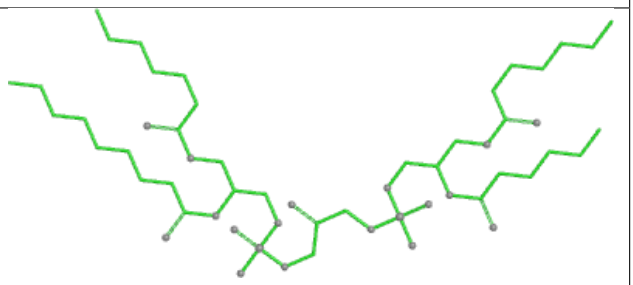
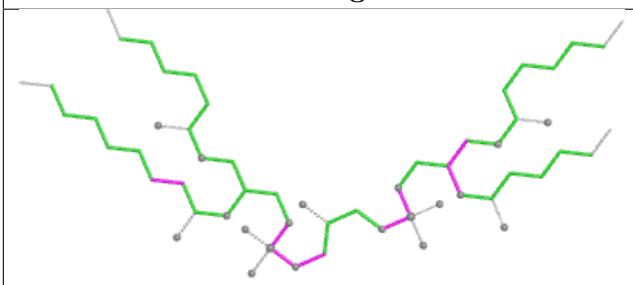


Bond angles



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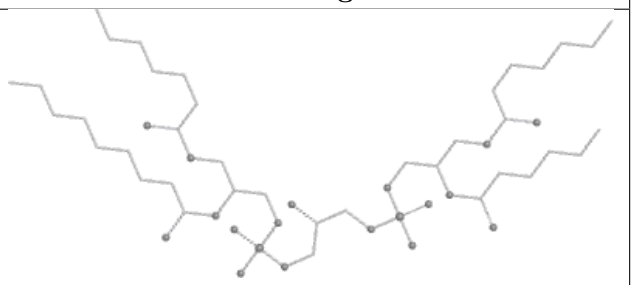
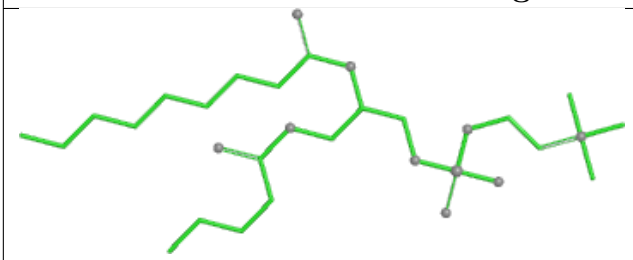


Rings

Ligand PC1 QG 401



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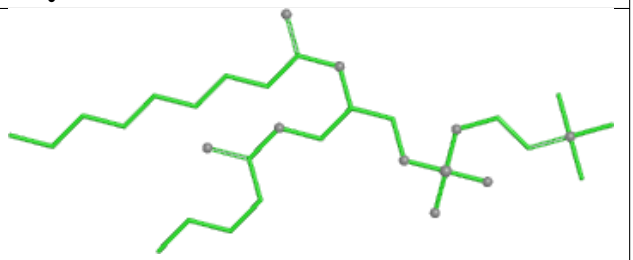
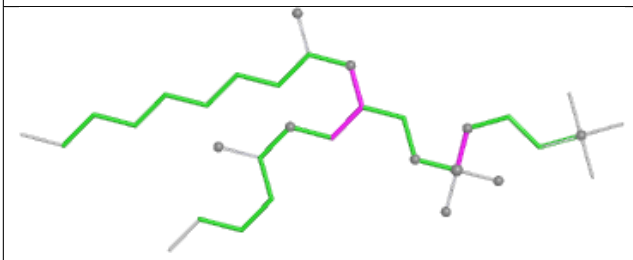
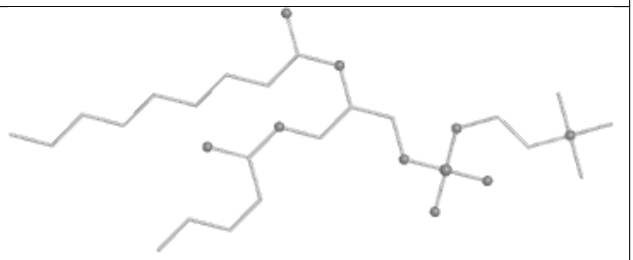


Bond angles

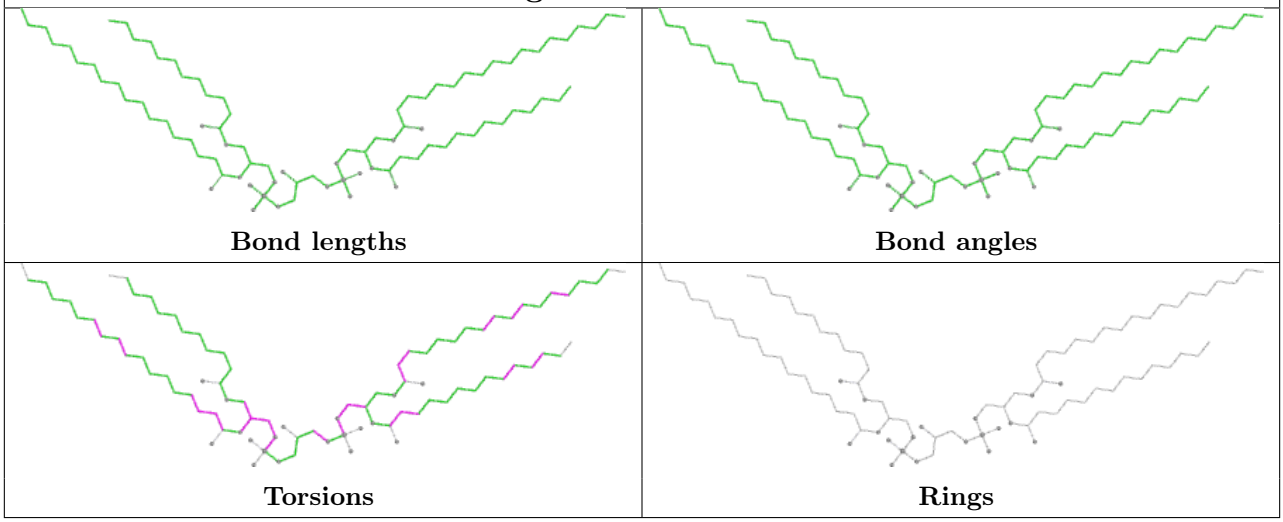


Torsions

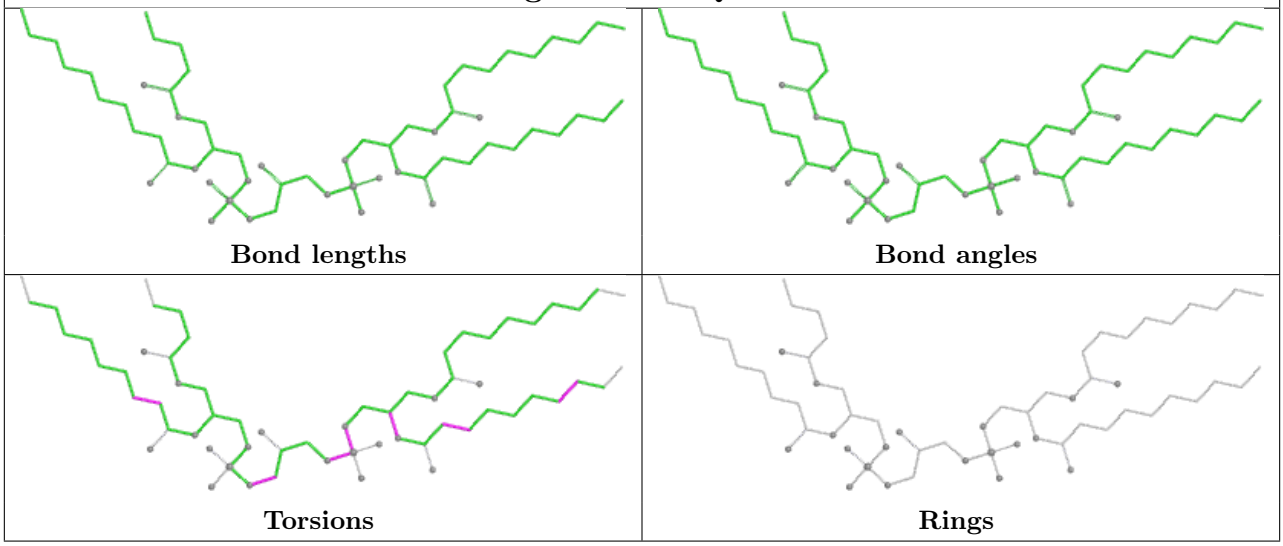


Rings

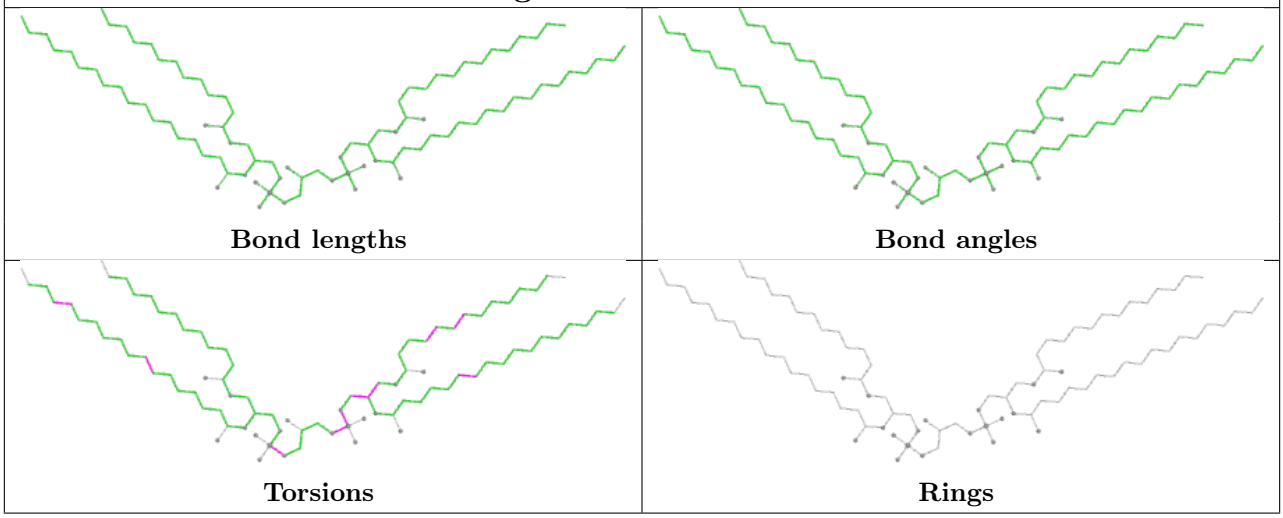
Ligand CDL T 204



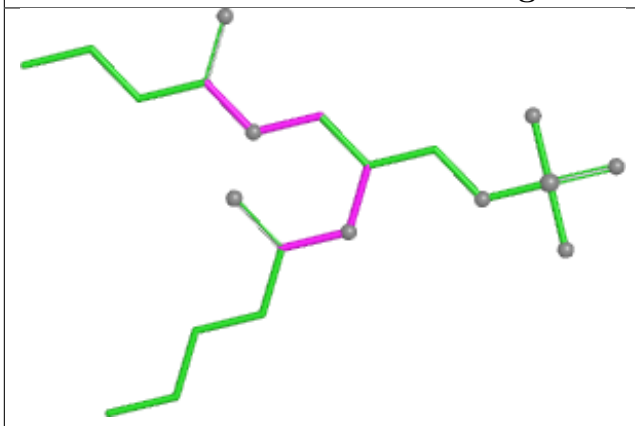
Ligand CDL Q 201



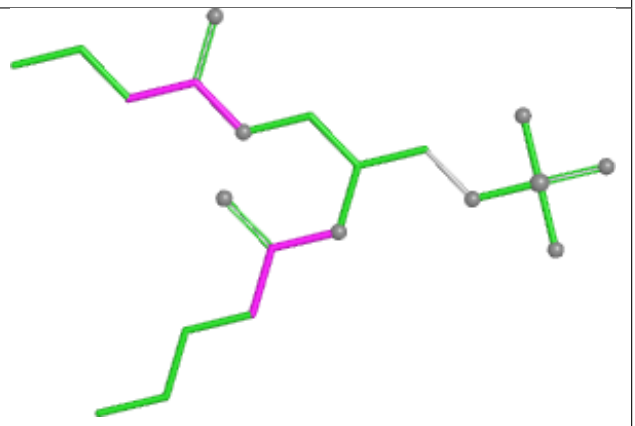
Ligand CDL m1 404



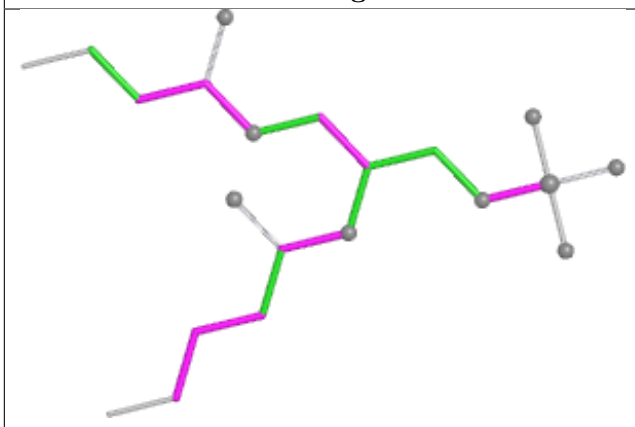
Ligand PX2 Y5 204



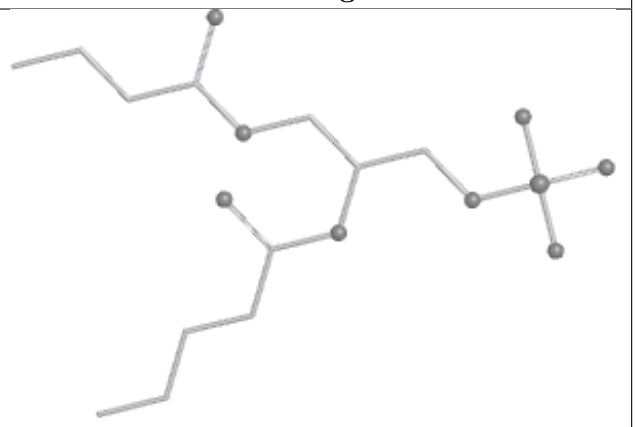
Bond lengths



Bond angles

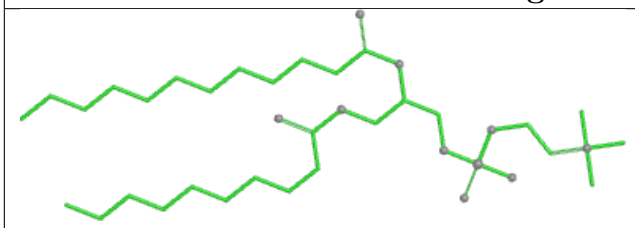


Torsions

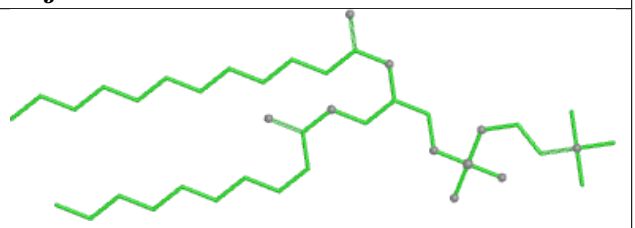


Rings

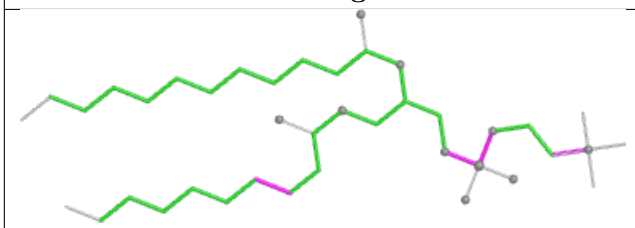
Ligand PC1 j1 400



Bond lengths



Bond angles



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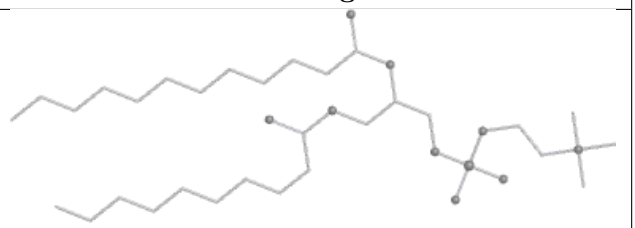
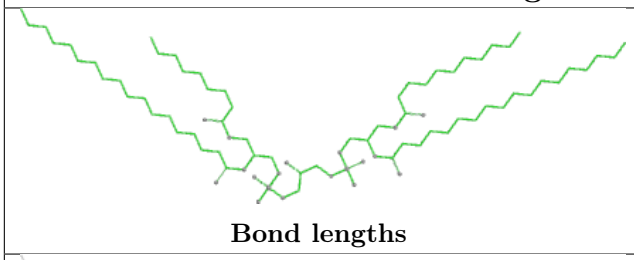


Rings

Ligand CDL N 304



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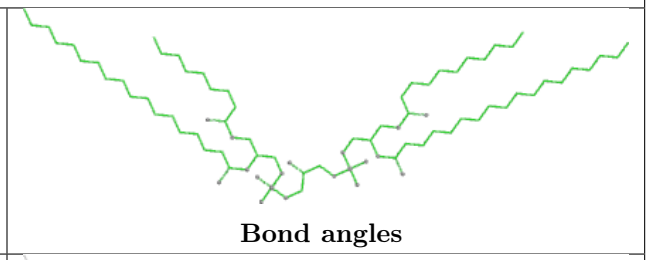
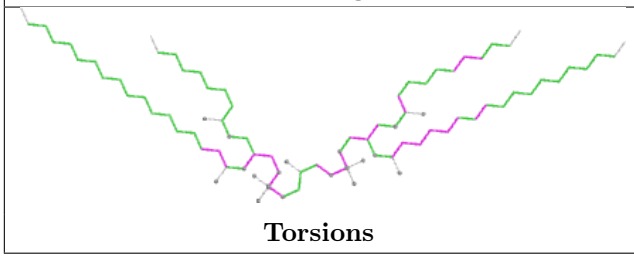
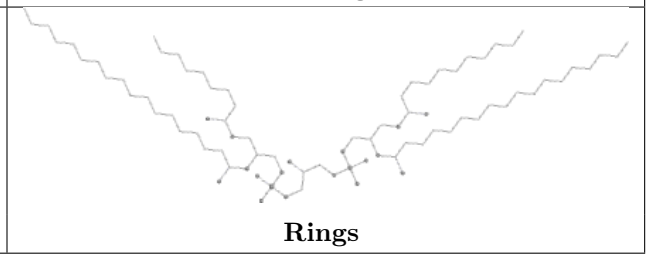


Bond angles

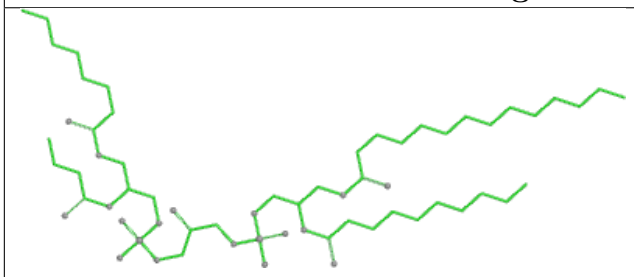


Torsions



Rings

Ligand CDL QC 503



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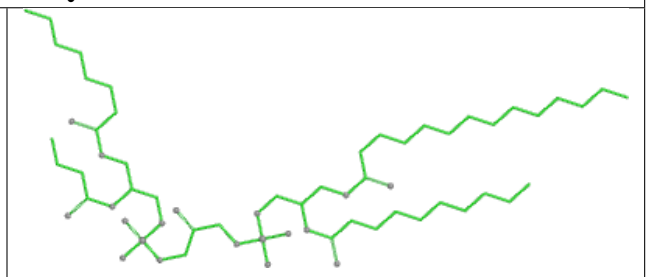
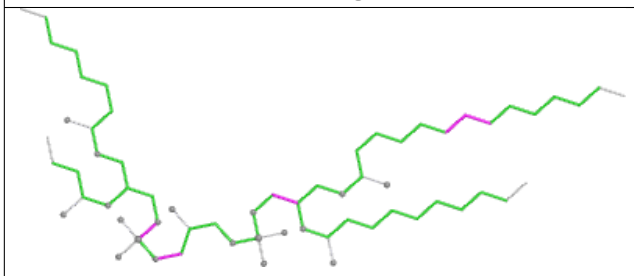


Bond angles



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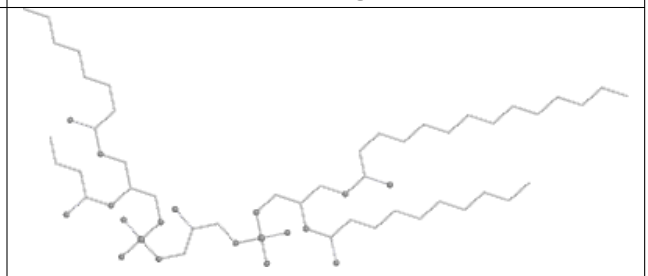
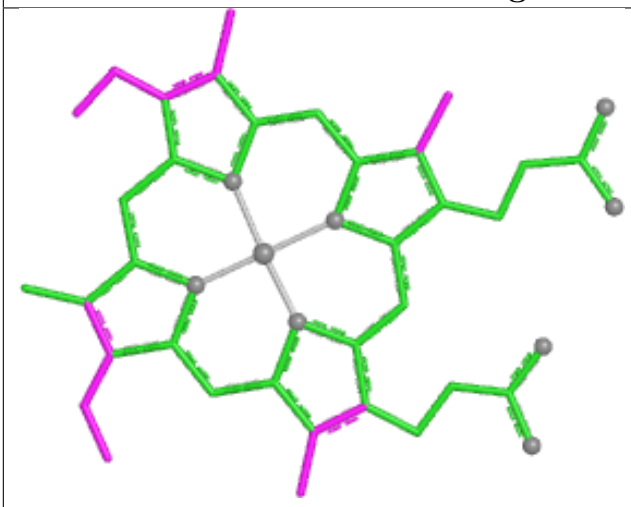


Rings

Ligand HEC QD 401



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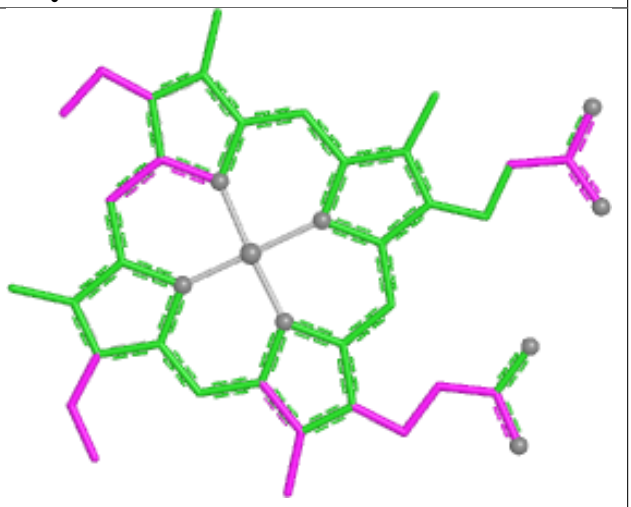
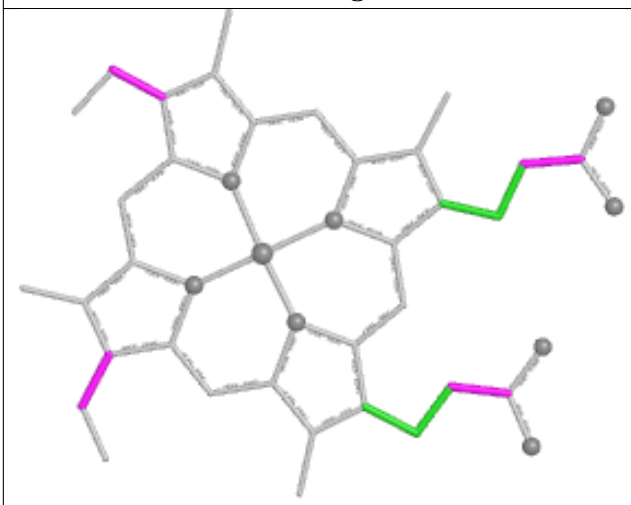


Bond angles



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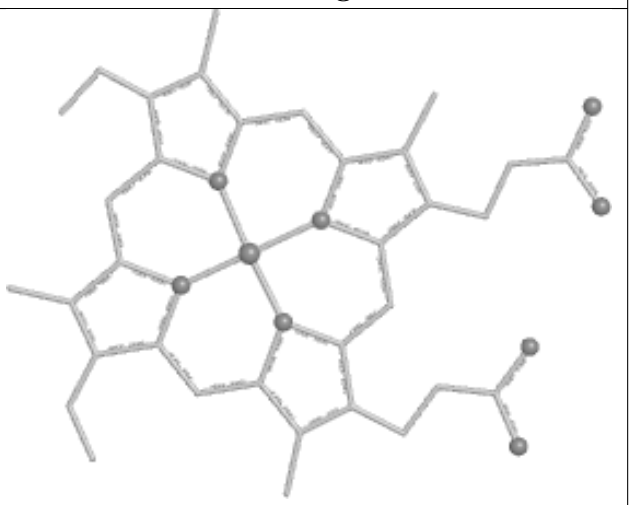
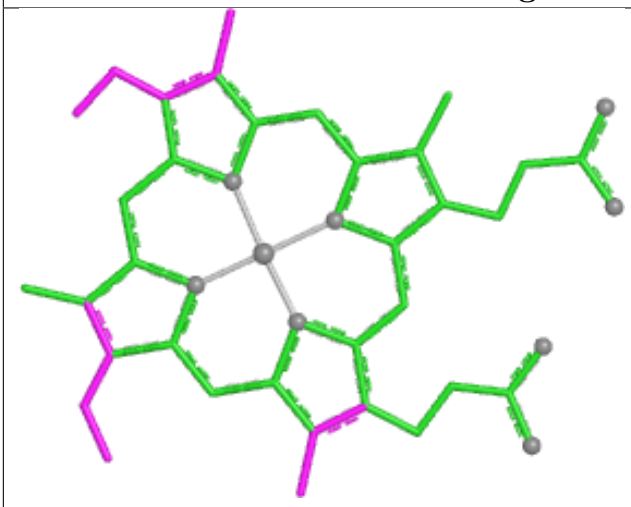


Rings

Ligand HEC 2e 401



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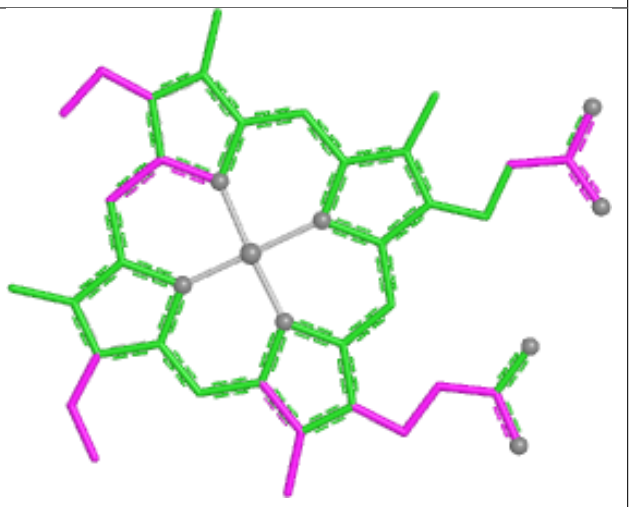
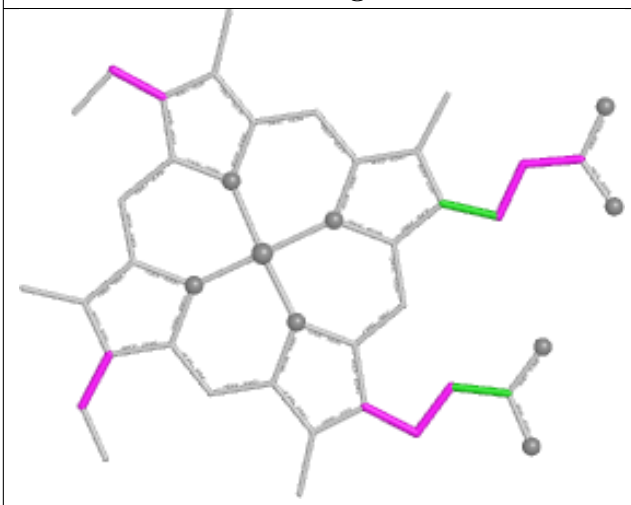


Bond angles



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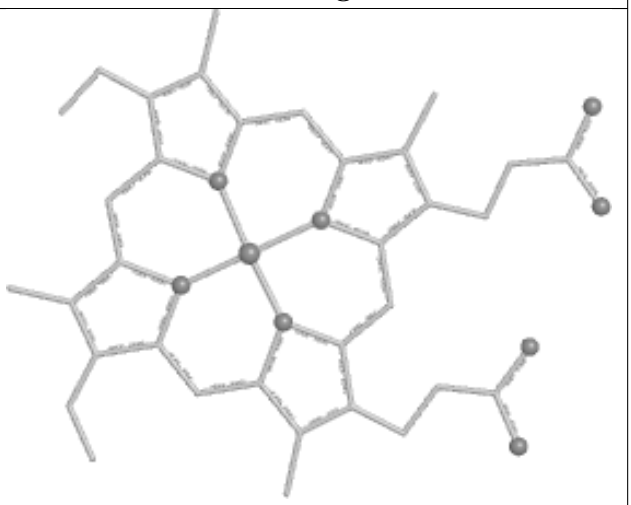
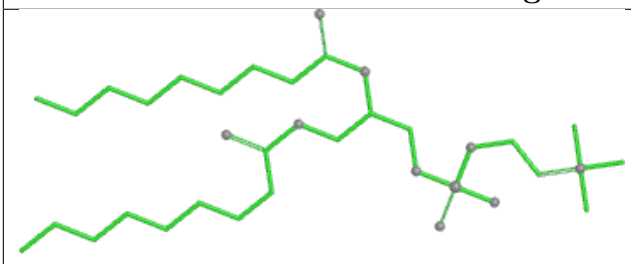
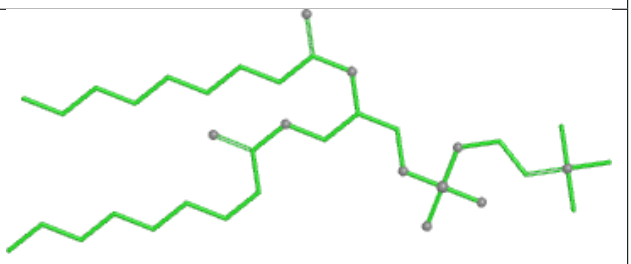


Rings

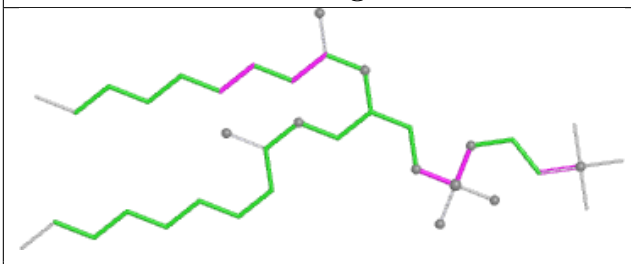
Ligand PC1 M 302



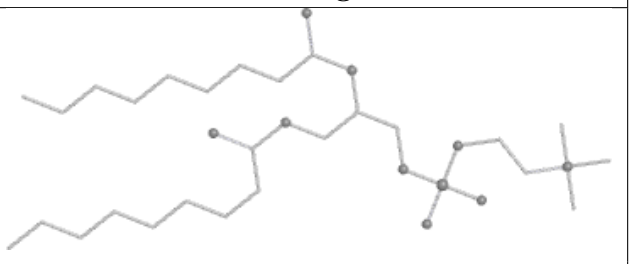
Bond lengths



Bond angles

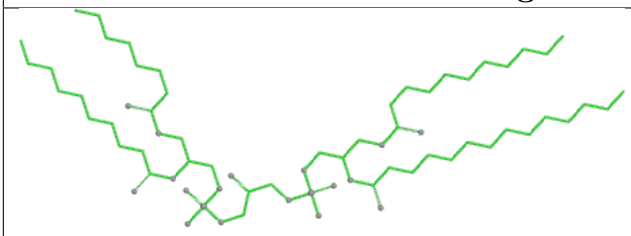


Torsions

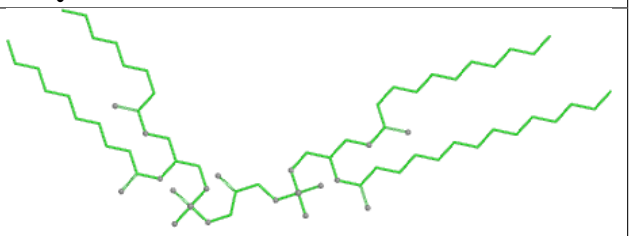


Rings

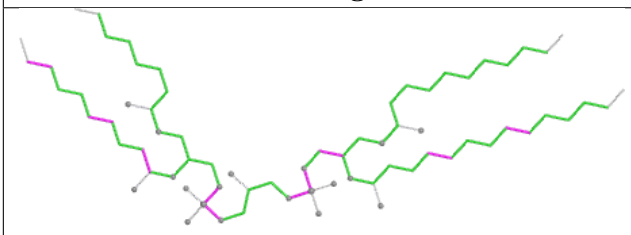
Ligand CDL QI 203



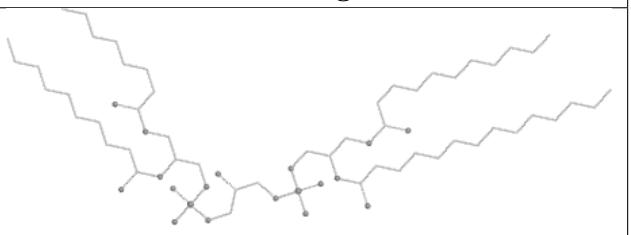
Bond lengths



Bond angles

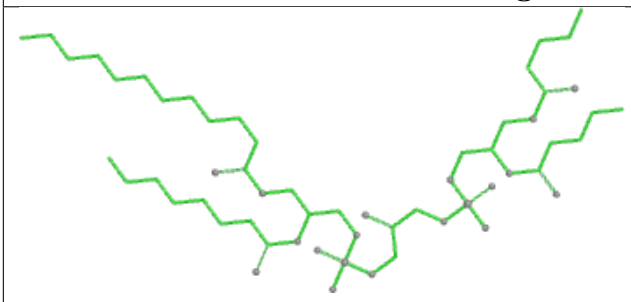


Torsions

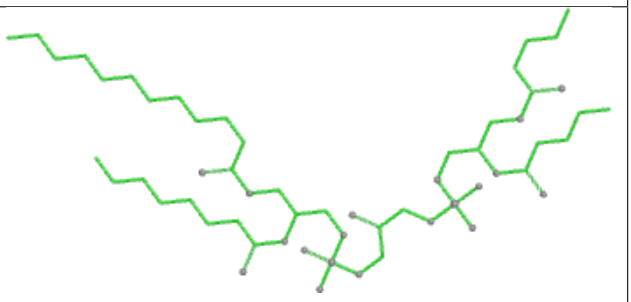


Rings

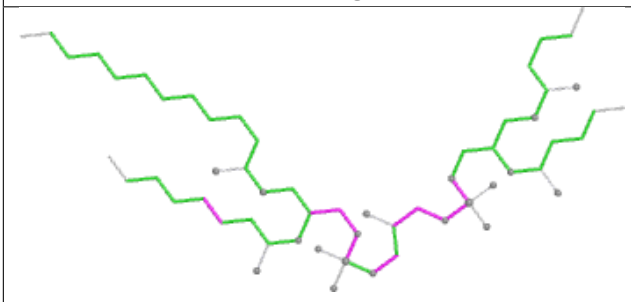
Ligand CDL B3 101



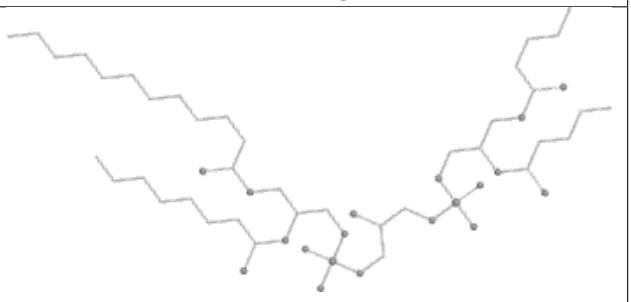
Bond lengths



Bond angles

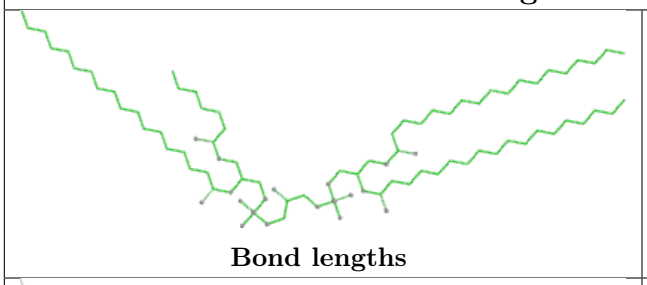


Torsions

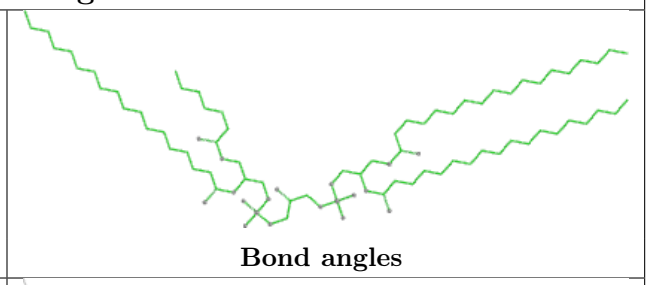


Rings

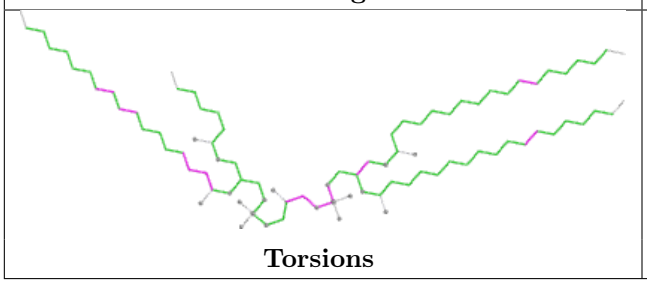
Ligand CDL 2g 201



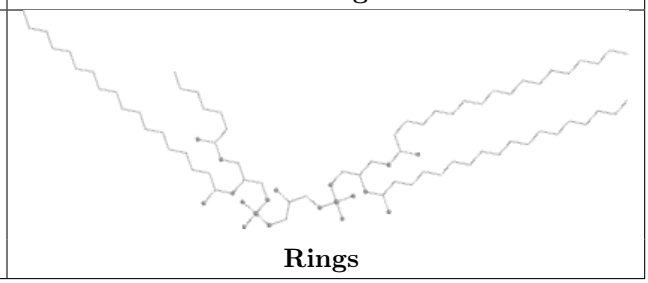
Bond lengths



Bond angles

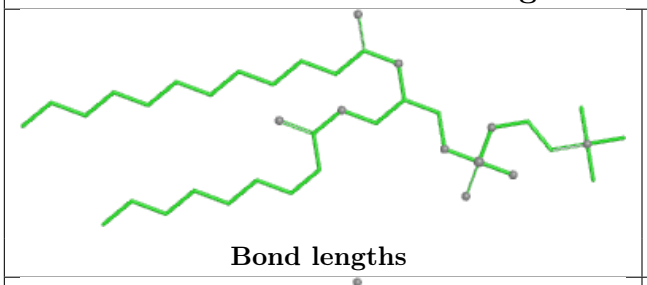


Torsions

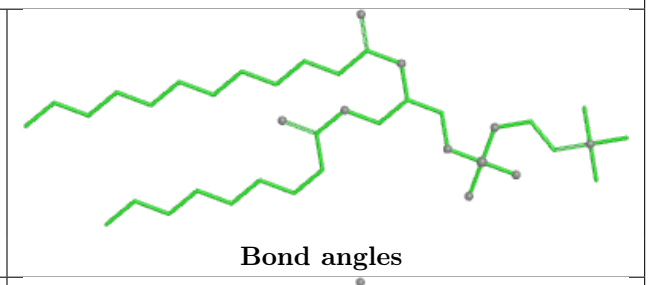


Rings

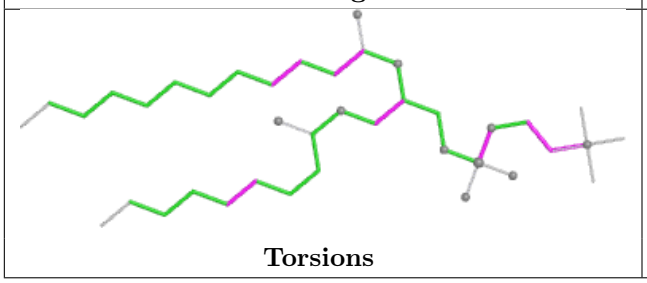
Ligand PC1 C1 711



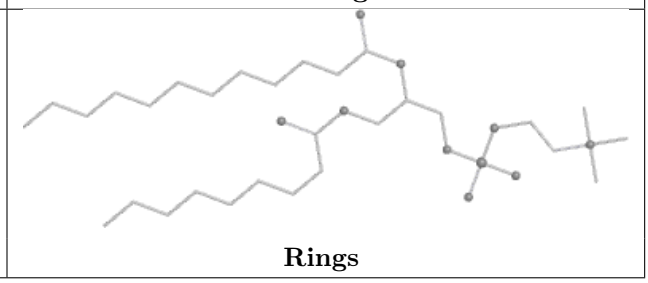
Bond lengths



Bond angles

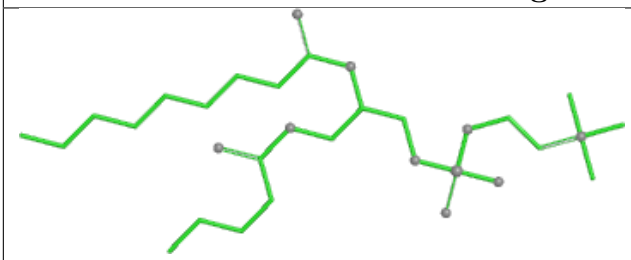


Torsions

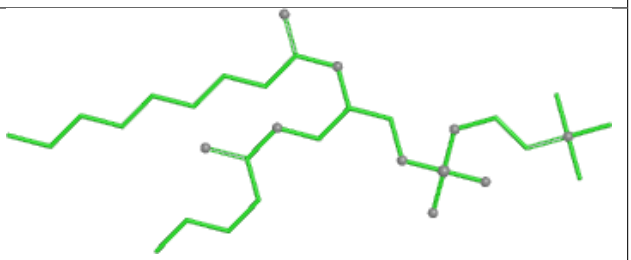


Rings

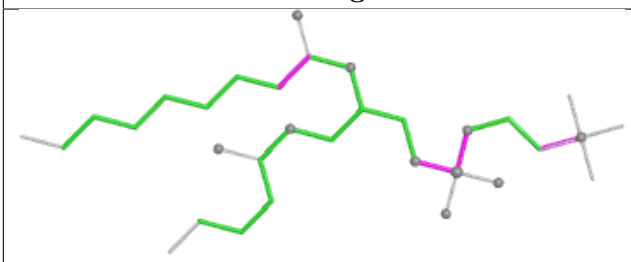
Ligand PC1 n 302



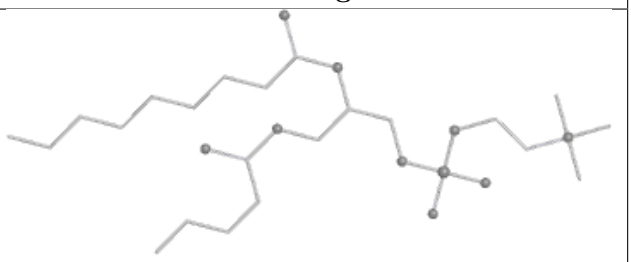
Bond lengths



Bond angles

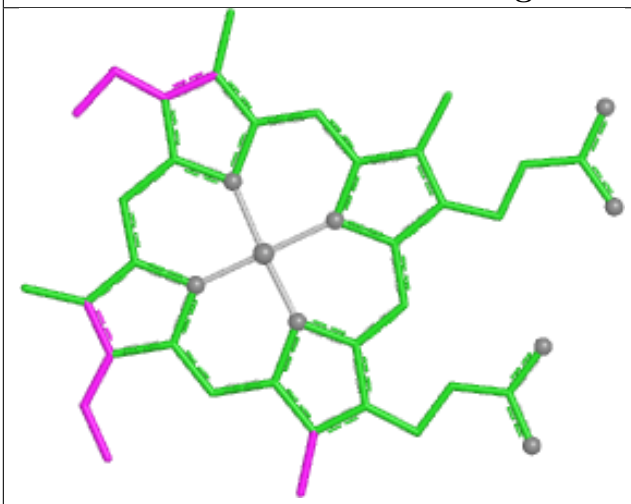


Torsions

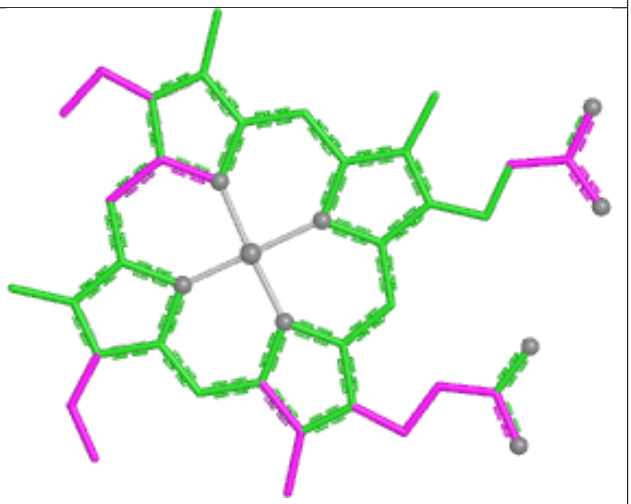


Rings

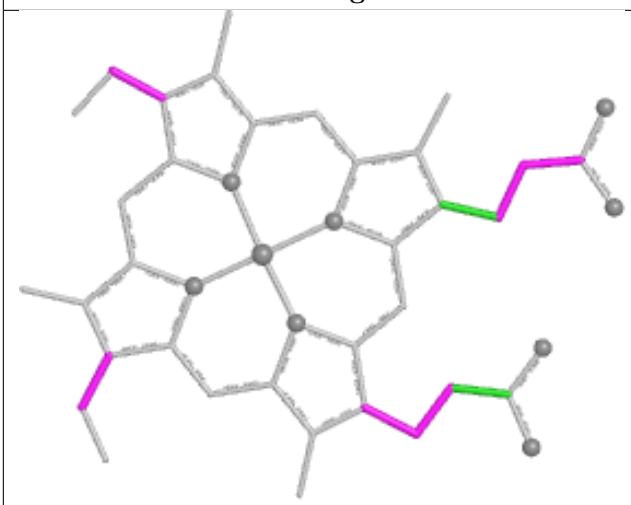
Ligand HEC 2E 401



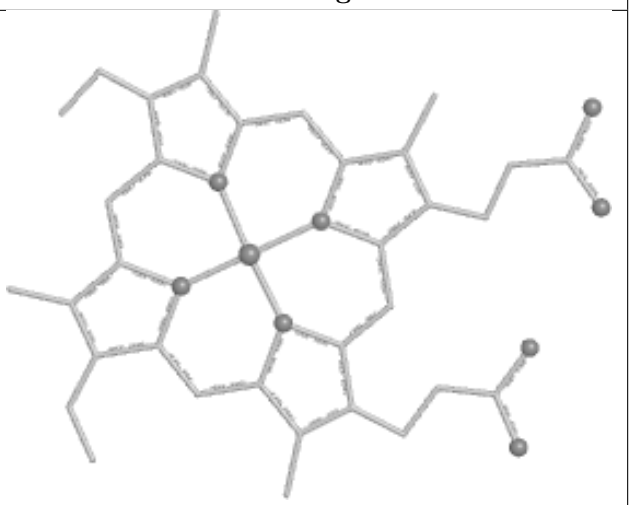
Bond lengths



Bond angles

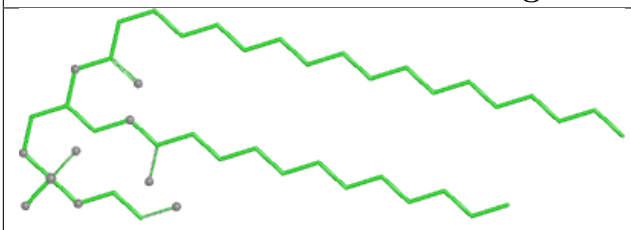


Torsions

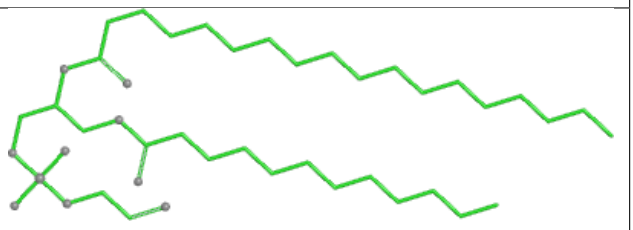


Rings

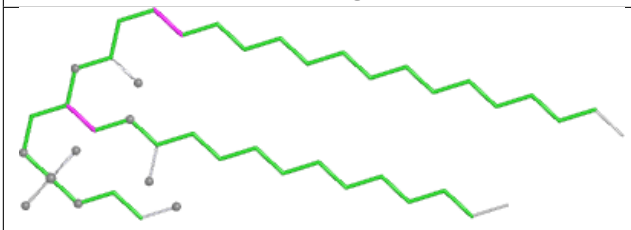
Ligand 3PE an 301



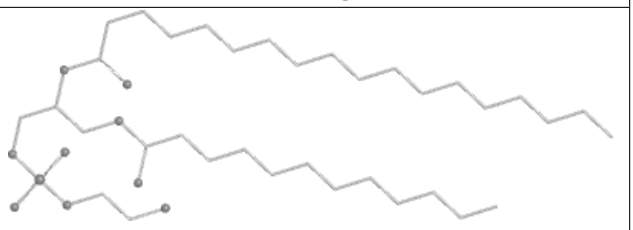
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

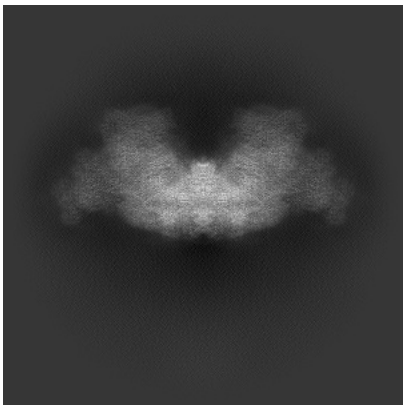
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34373. These allow visual inspection of the internal detail of the map and identification of artifacts.

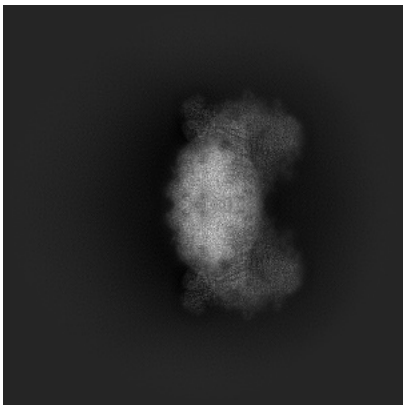
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

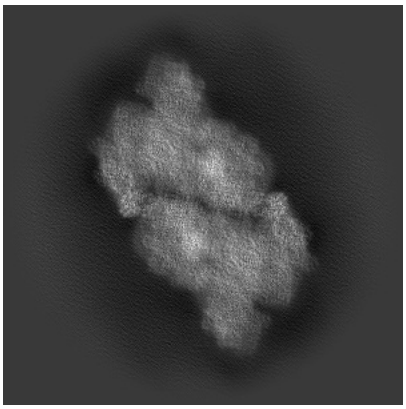
6.1.1 Primary map



X

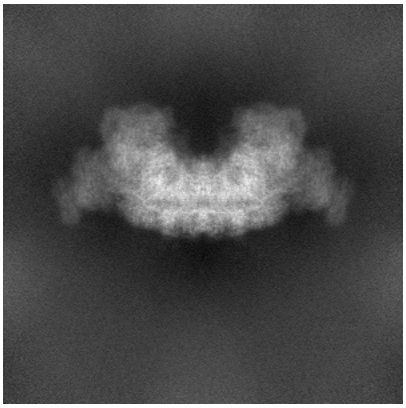


Y

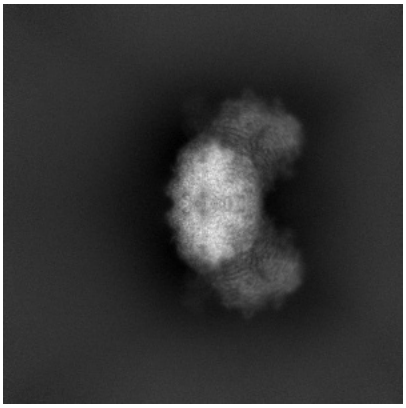


Z

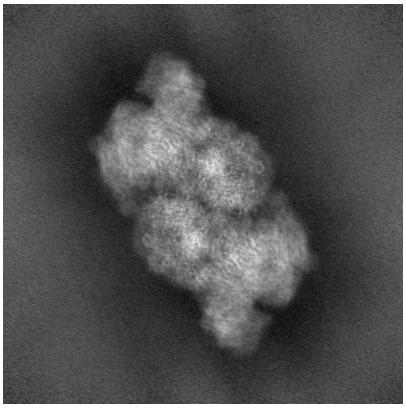
6.1.2 Raw map



X



Y

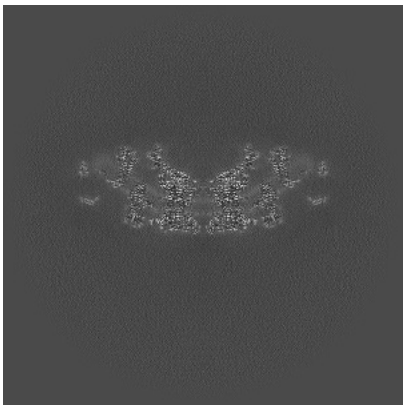


Z

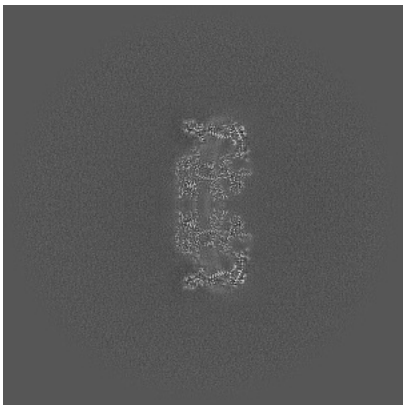
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

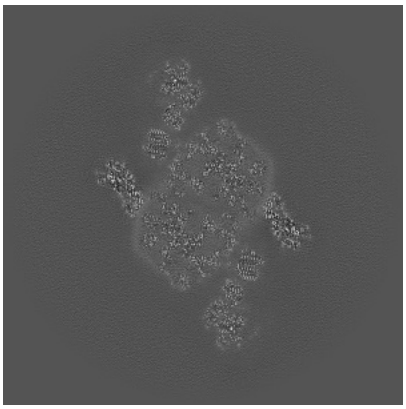
6.2.1 Primary map



X Index: 420

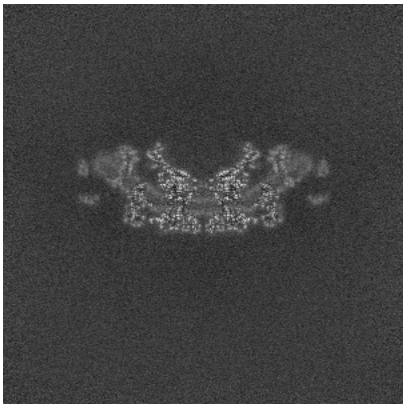


Y Index: 420

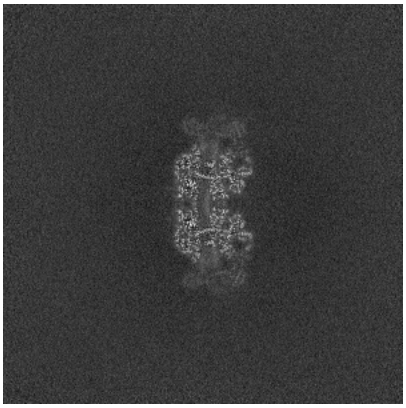


Z Index: 420

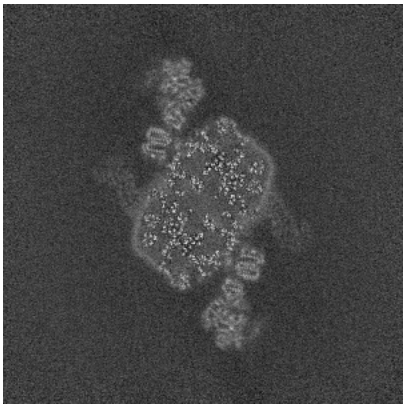
6.2.2 Raw map



X Index: 420



Y Index: 420

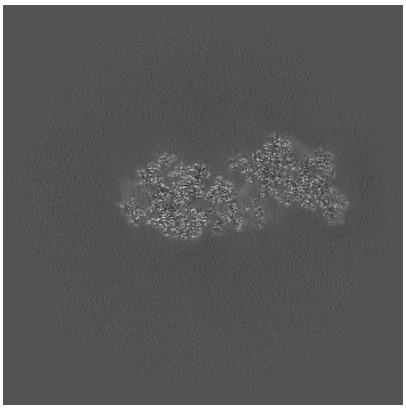


Z Index: 420

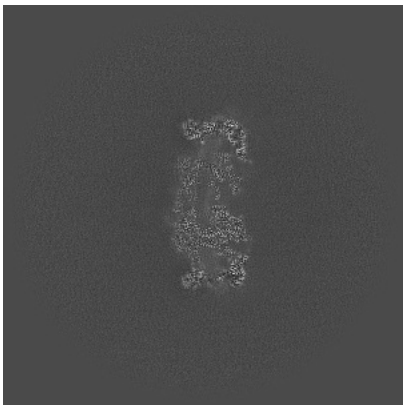
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

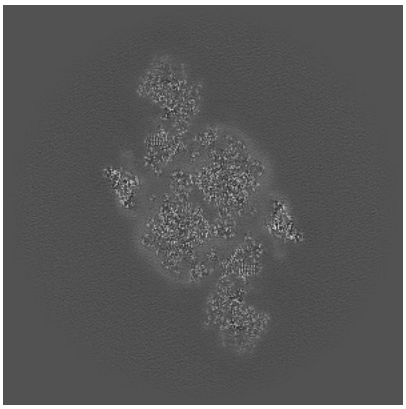
6.3.1 Primary map



X Index: 378

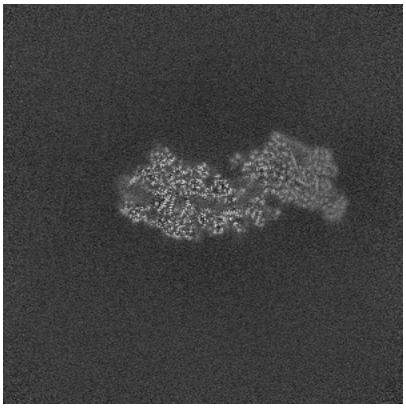


Y Index: 412

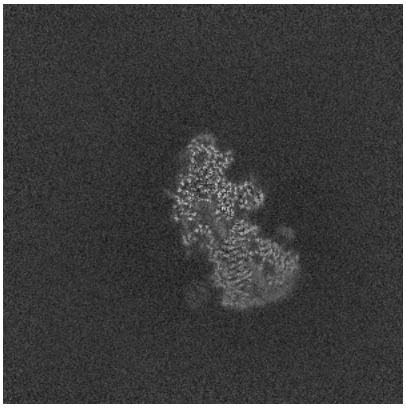


Z Index: 439

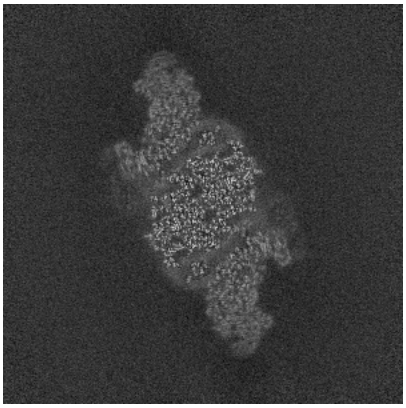
6.3.2 Raw map



X Index: 384



Y Index: 508

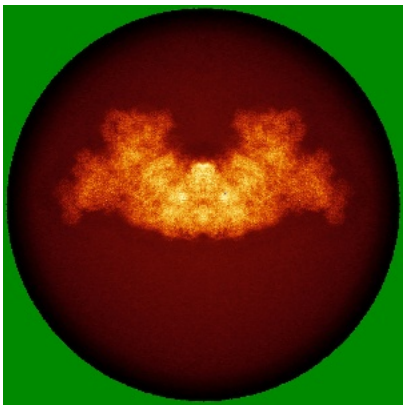


Z Index: 453

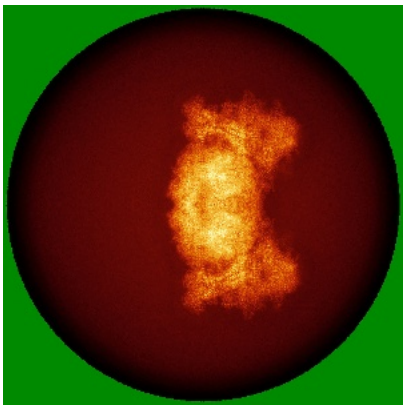
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

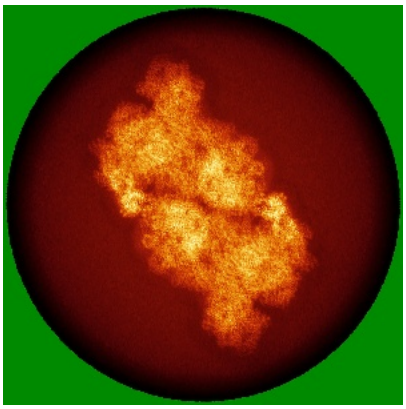
6.4.1 Primary map



X

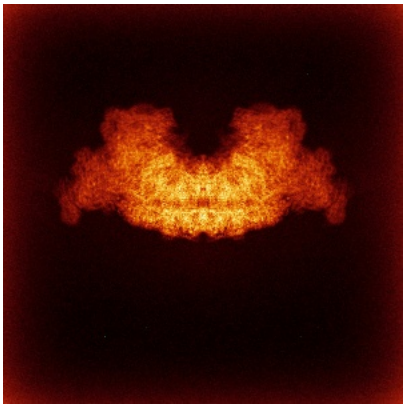


Y

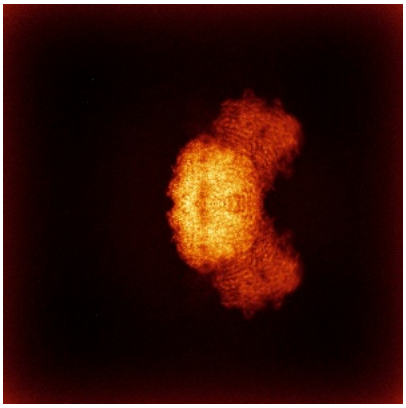


Z

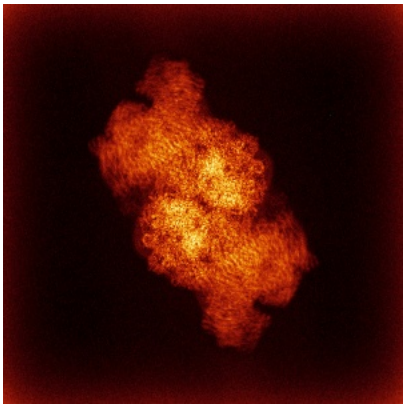
6.4.2 Raw map



X



Y

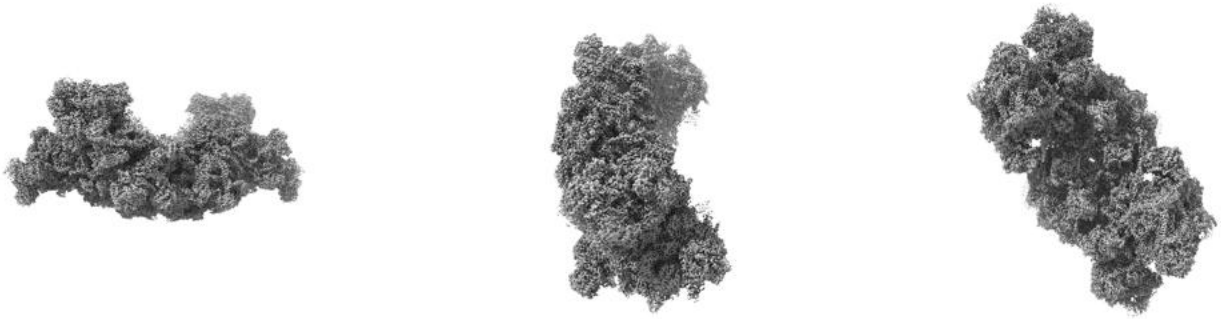


Z

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)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

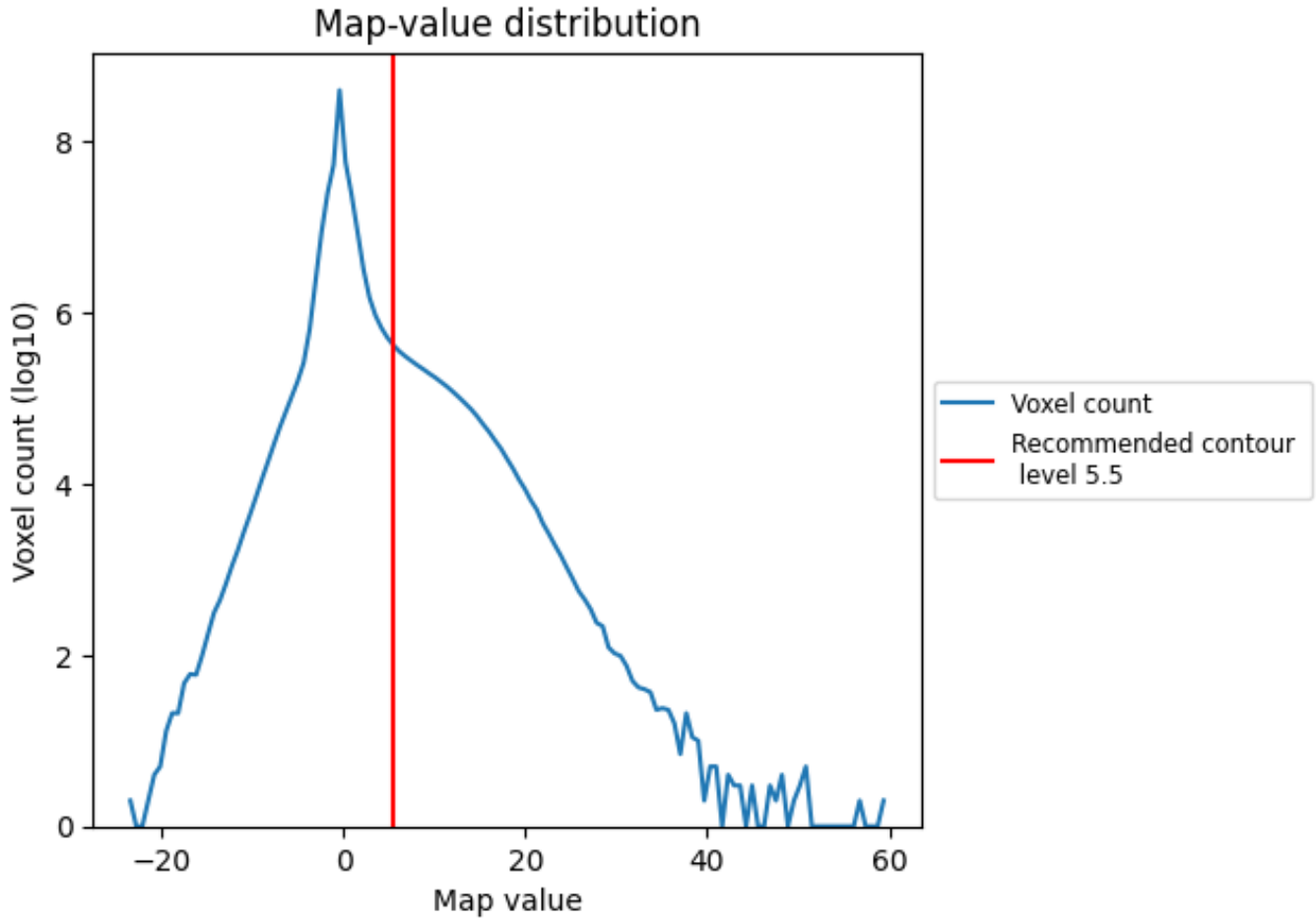
6.6 Mask visualisation (i)

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

7 Map analysis

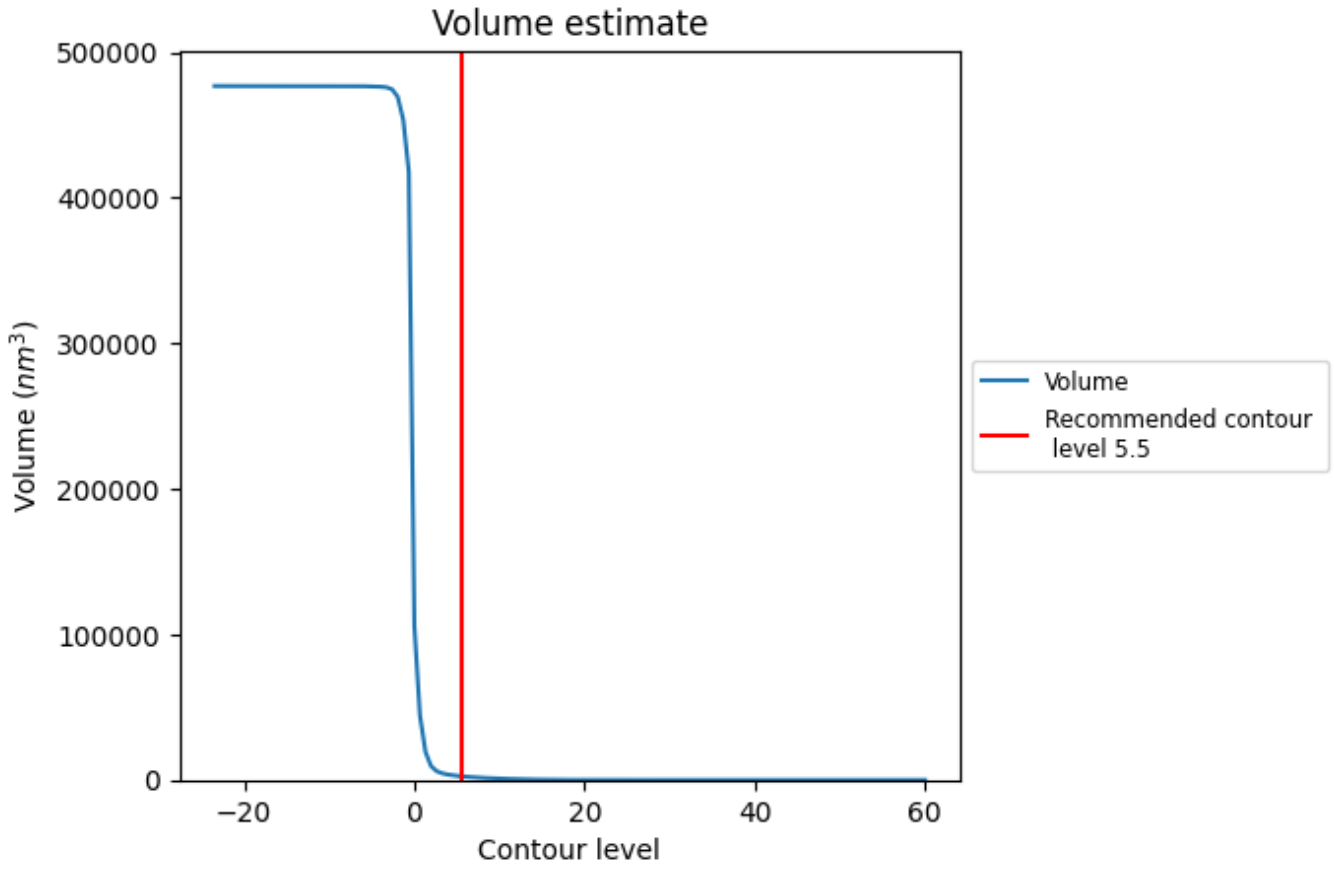
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

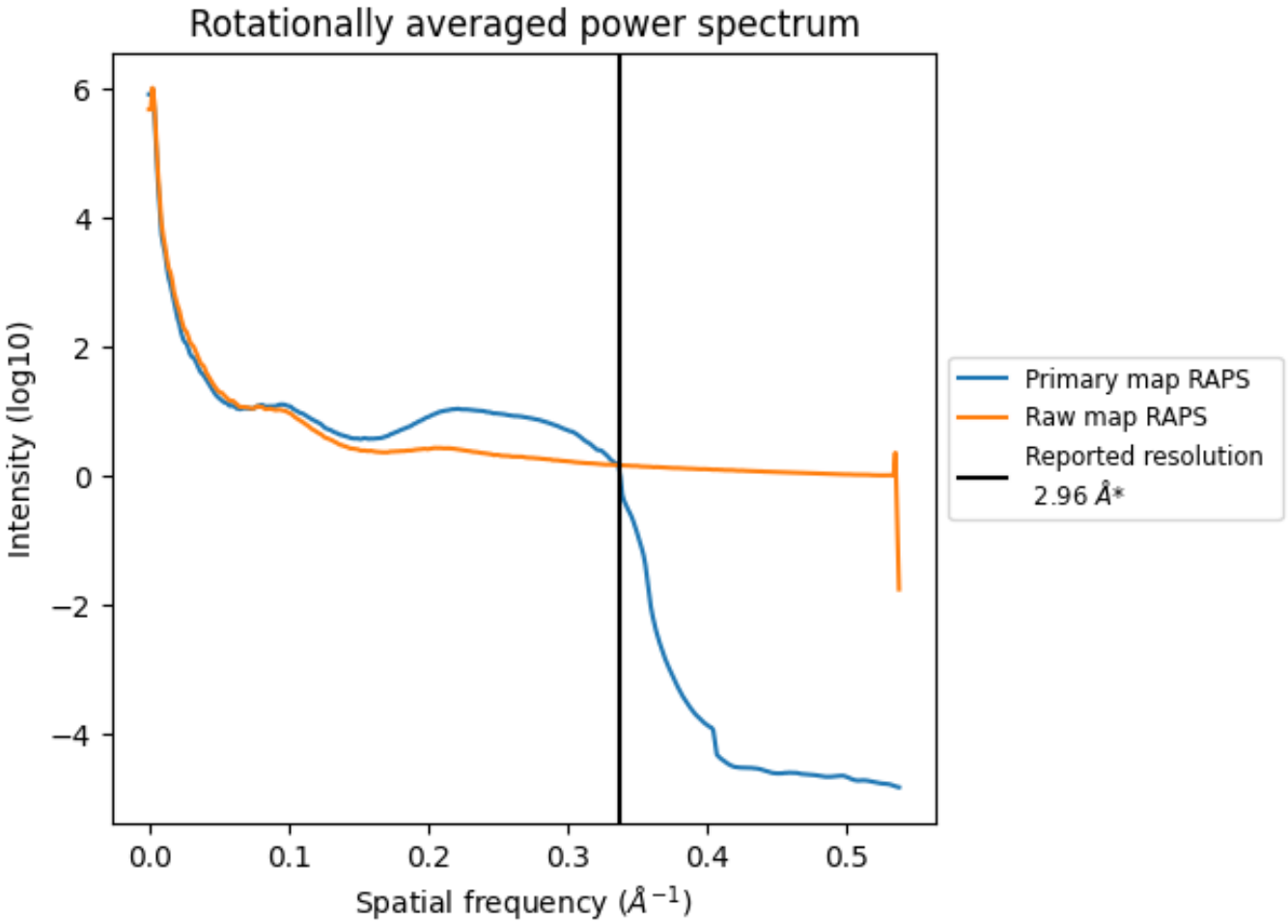
7.2 Volume estimate



The volume at the recommended contour level is 2536 nm^3; this corresponds to an approximate mass of 2290 kDa.

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

7.3 Rotationally averaged power spectrum (i)

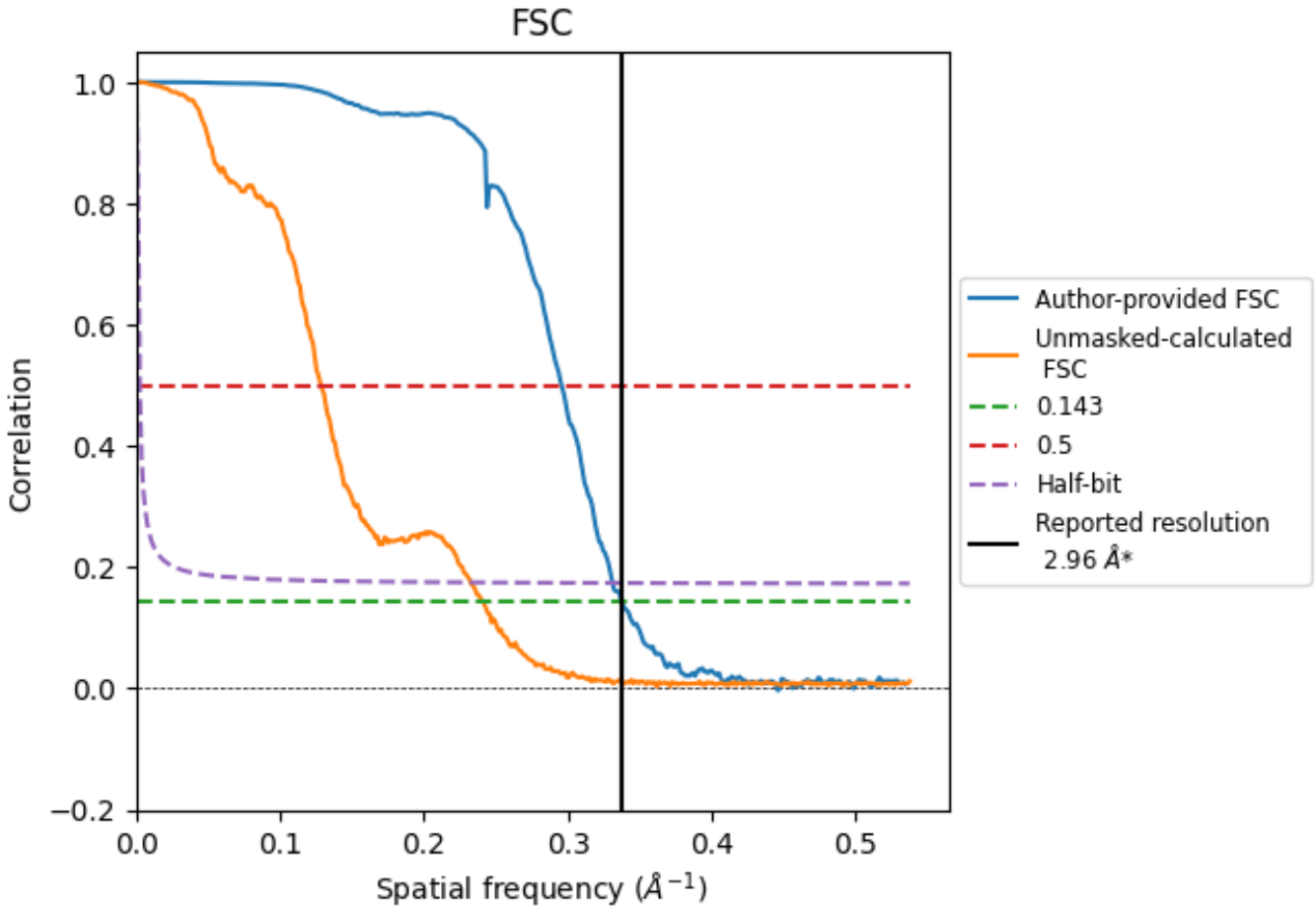


*Reported resolution corresponds to spatial frequency of 0.338 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.338 $Å^{-1}$

8.2 Resolution estimates (i)

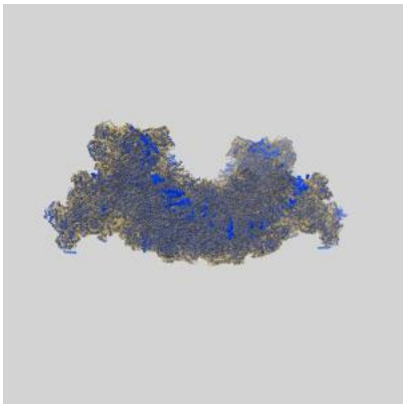
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.38	3.02
Unmasked-calculated*	4.15	7.78	4.30

*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 4.15 differs from the reported value 2.96 by more than 10 %

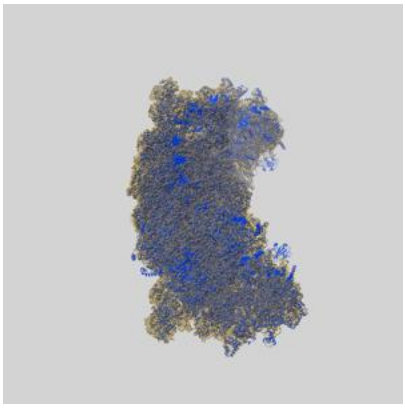
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34373 and PDB model 8GYM. Per-residue inclusion information can be found in section 3 on page 82.

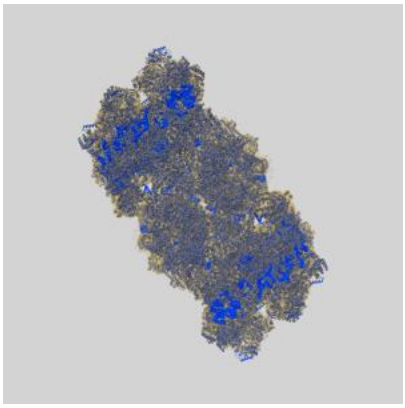
9.1 Map-model overlay



X



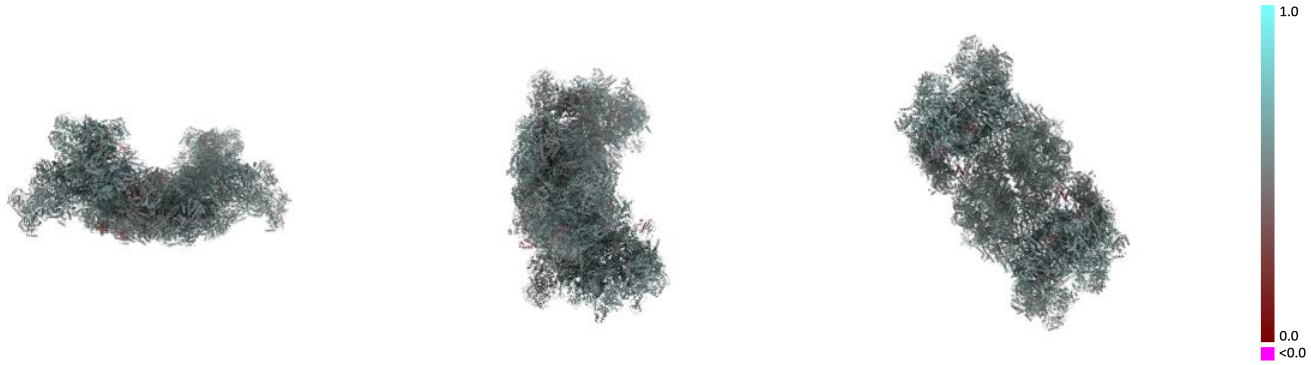
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.5 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.

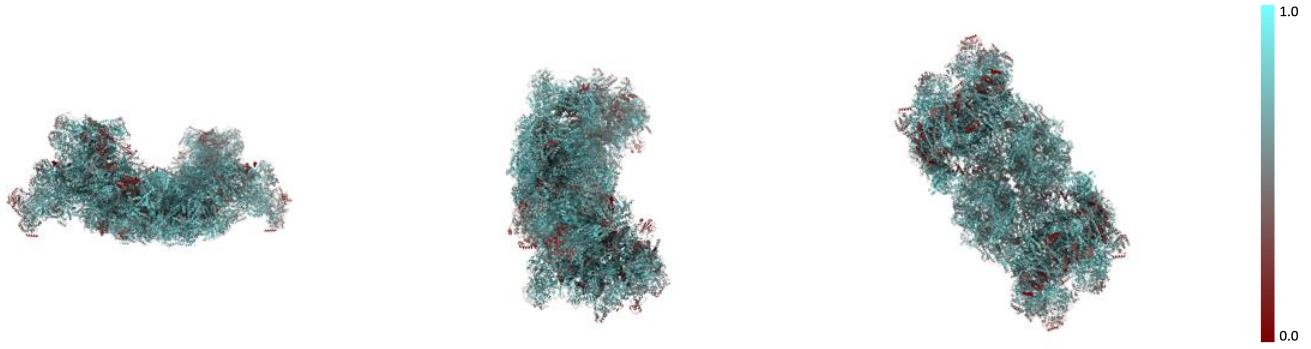
9.2 Q-score mapped to coordinate model



X Y Z

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

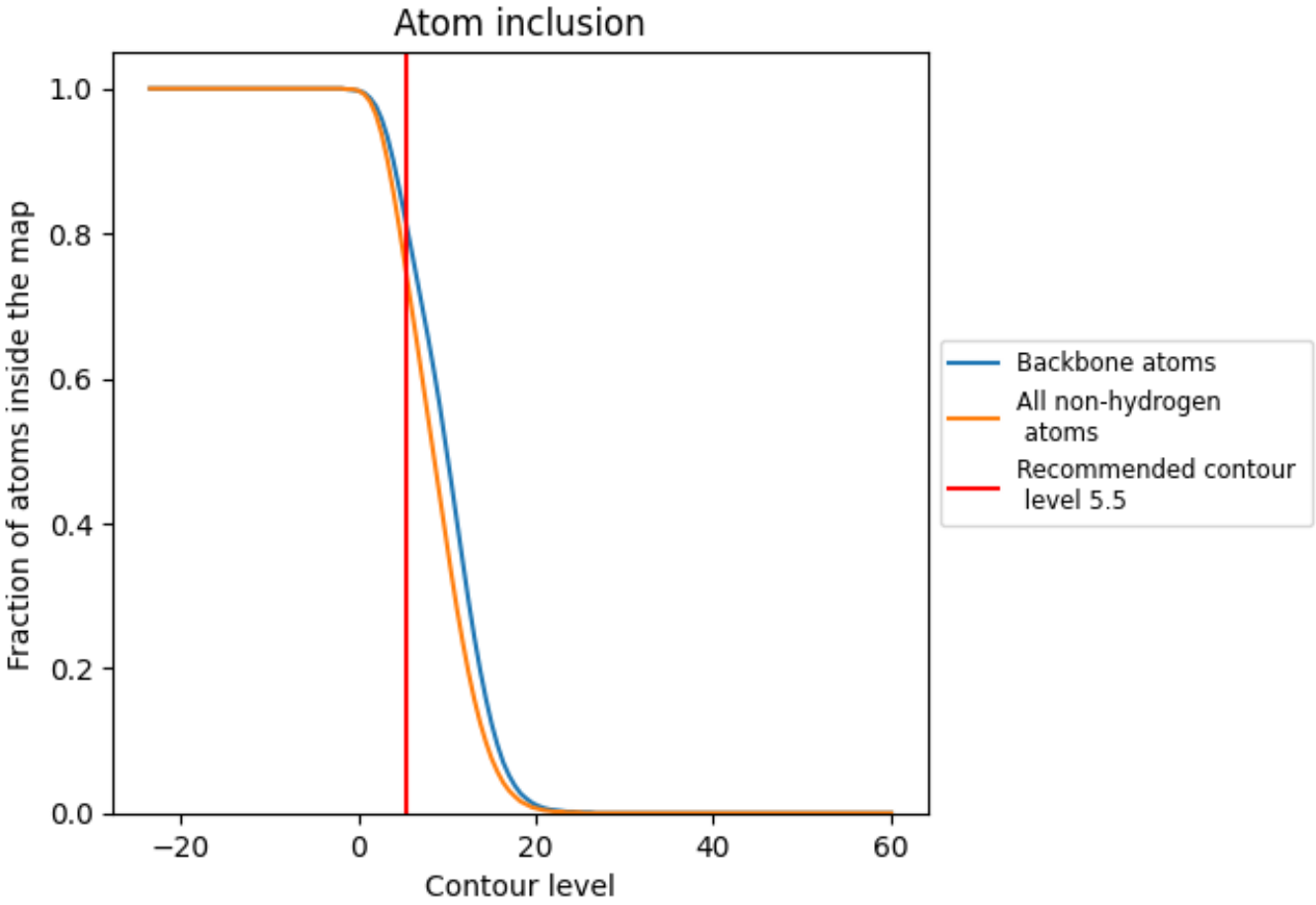
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (5.5).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7380	0.5560
1B	0.8100	0.6000
1T	0.7970	0.5540
1b	0.8100	0.6010
1t	0.7970	0.5530
2B	0.8340	0.6060
2E	0.7130	0.4660
2F	0.8130	0.5170
2G	0.7650	0.5060
2H	0.8350	0.4880
2I	0.7720	0.4860
2J	0.7800	0.4930
2K	0.8000	0.5180
2L	0.8300	0.4930
2M	0.8460	0.5290
2N	0.8180	0.5170
2O	0.8480	0.5140
2T	0.6780	0.5240
2b	0.8340	0.6030
2e	0.7130	0.4670
2f	0.8130	0.5150
2g	0.7650	0.5060
2h	0.8350	0.4860
2i	0.7730	0.4880
2j	0.7870	0.4970
2k	0.8000	0.5180
2l	0.8300	0.5010
2m	0.8470	0.5300
2n	0.8120	0.5150
2o	0.8480	0.5160
2t	0.6780	0.5220
3T	0.6390	0.5110
3t	0.6410	0.5070
4A	0.8030	0.5730
4L	0.8160	0.5960

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Chain	Atom inclusion	Q-score
4T	0.8030	0.5430
4a	0.8020	0.5680
4l	0.8170	0.5960
4t	0.8030	0.5460
5B	0.7820	0.5970
5T	0.6840	0.5250
5b	0.7810	0.5960
5t	0.6800	0.5300
6A	0.8000	0.5630
6B	0.8530	0.5760
6C	0.7880	0.5460
6L	0.7550	0.5430
6T	0.7230	0.5270
6a	0.8000	0.5630
6b	0.8530	0.5740
6c	0.7880	0.5450
6l	0.7550	0.5450
6t	0.7200	0.5280
7A	0.8230	0.5770
7C	0.8020	0.5650
7L	0.8110	0.5670
7a	0.8240	0.5780
7c	0.8040	0.5640
7l	0.8110	0.5640
A	0.8140	0.5690
A1	0.7460	0.5910
A2	0.6140	0.5310
A3	0.8070	0.5960
A5	0.7480	0.5650
A6	0.8350	0.5950
A7	0.6910	0.5550
A8	0.7900	0.5900
A9	0.7510	0.5680
AB	0.7580	0.5870
AC	0.7490	0.5770
AL	0.7400	0.5780
AM	0.7610	0.5800
AN	0.7360	0.5850
B	0.5360	0.4790
B2	0.6960	0.5670
B3	0.6410	0.5610
B4	0.7660	0.5910

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Chain	Atom inclusion	Q-score
B6	0.7870	0.5940
B7	0.7590	0.5710
B8	0.7060	0.5770
B9	0.7830	0.5890
BL	0.8200	0.5960
BM	0.6820	0.5620
BP	0.7100	0.5410
C	0.4500	0.4230
C1	0.8230	0.5670
C2	0.8340	0.5700
C3	0.7730	0.5490
C4	0.7500	0.5810
D	0.7370	0.5490
E	0.7730	0.5550
F	0.7790	0.5610
FS	0.7890	0.5670
FX	0.8450	0.5990
G	0.8250	0.5680
G1	0.8580	0.6060
G2	0.8070	0.5940
G3	0.7790	0.5810
H	0.6900	0.5160
I	0.7220	0.5430
J	0.7560	0.5670
J1	0.7330	0.5750
K	0.7890	0.5600
L	0.7830	0.5580
M	0.7720	0.5630
M1	0.7860	0.5530
M2	0.7850	0.5500
M3	0.7710	0.5560
N	0.7960	0.5660
N1	0.7590	0.5790
N2	0.8230	0.6010
N3	0.7750	0.5840
N4	0.8290	0.5950
N5	0.6770	0.5150
N6	0.7900	0.5960
O	0.8560	0.5710
P	0.7370	0.5430
P1	0.7020	0.5790
P2	0.7180	0.5760

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Chain	Atom inclusion	Q-score
Q	0.8470	0.5690
QA	0.6990	0.5610
QB	0.7790	0.5830
QC	0.7760	0.5860
QD	0.8320	0.5990
QE	0.5560	0.4870
QF	0.7010	0.5690
QG	0.6230	0.5470
QH	0.7790	0.5940
QI	0.7670	0.5880
QJ	0.7840	0.5900
QL	0.5640	0.5540
QM	0.8240	0.5780
Qa	0.6180	0.5490
Qb	0.6790	0.5640
Qc	0.7540	0.5790
Qd	0.7980	0.5920
Qe	0.4930	0.4760
Qf	0.5330	0.5100
Qg	0.6420	0.5560
Qh	0.7650	0.5860
Qi	0.6550	0.5710
Qj	0.7230	0.5720
Ql	0.6760	0.5620
Qm	0.8470	0.5880
R	0.7850	0.5500
S	0.7080	0.5310
S1	0.6940	0.5540
S2	0.7990	0.5820
S3	0.7890	0.5780
S4	0.7180	0.5620
S5	0.7760	0.5920
S6	0.6510	0.5490
S7	0.8210	0.5870
S8	0.8030	0.5750
SA	0.6350	0.4790
SB	0.7420	0.5030
SC	0.7570	0.5080
SD	0.8830	0.5460
T	0.7860	0.5680
T1	0.6060	0.5210
T2	0.2910	0.4730

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Chain	Atom inclusion	Q-score
T3	0.5540	0.5370
T4	0.5530	0.5240
T5	0.7240	0.5610
T6	0.7870	0.5900
T7	0.7060	0.5710
T8	0.7610	0.5850
T9	0.7880	0.5790
TA	0.7180	0.5600
TB	0.7710	0.5940
TC	0.7300	0.5840
TD	0.6320	0.5650
TE	0.6940	0.5760
TF	0.6720	0.5510
TG	0.5440	0.5120
TH	0.7770	0.5800
TX	0.7640	0.5840
U	0.7460	0.5510
U1	0.8220	0.5400
U2	0.8820	0.5480
V	0.7800	0.5590
V1	0.5920	0.5300
V2	0.4610	0.5070
VB	0.8000	0.5600
W	0.7380	0.5490
X	0.8620	0.5820
X1	0.7930	0.5900
Y	0.9100	0.5900
Y0	0.8650	0.5800
Y5	0.7220	0.5380
Y7	0.7200	0.5360
Z	0.7160	0.5390
Z1	0.8050	0.5550
a	0.8120	0.5700
a1	0.7720	0.5880
a2	0.6120	0.5300
a3	0.8090	0.6020
a5	0.7490	0.5670
a6	0.8370	0.5940
a7	0.6910	0.5550
a8	0.7900	0.5880
a9	0.7500	0.5670
ab	0.7580	0.5870

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Chain	Atom inclusion	Q-score
ac	0.7490	0.5750
al	0.7400	0.5760
am	0.7620	0.5790
an	0.7370	0.5850
b	0.5360	0.4790
b2	0.6950	0.5670
b3	0.6420	0.5600
b4	0.7660	0.5880
b6	0.7880	0.5920
b7	0.7600	0.5750
b8	0.7040	0.5770
b9	0.7820	0.5860
bl	0.8200	0.5960
bm	0.6820	0.5610
bp	0.7080	0.5410
c	0.4490	0.4230
c1	0.8230	0.5670
c2	0.8330	0.5690
c3	0.7740	0.5480
c4	0.7540	0.5830
d	0.7360	0.5480
e	0.7750	0.5530
f	0.7810	0.5600
fs	0.7870	0.5670
fx	0.8440	0.5970
g	0.8250	0.5670
g1	0.8570	0.6070
g2	0.8090	0.5930
g3	0.7790	0.5790
h	0.6890	0.5160
i	0.7200	0.5430
j	0.7560	0.5640
j1	0.7320	0.5760
k	0.7900	0.5590
l	0.7840	0.5570
m	0.7700	0.5630
m1	0.7870	0.5530
m2	0.7850	0.5500
m3	0.7710	0.5570
n	0.7940	0.5640
n1	0.7590	0.5790
n2	0.8240	0.6010

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Chain	Atom inclusion	Q-score
n3	0.7750	0.5850
n4	0.8280	0.5930
n5	0.6780	0.5150
n6	0.7890	0.5940
o	0.8550	0.5720
p	0.7360	0.5410
p1	0.7020	0.5790
p2	0.7160	0.5760
q	0.8240	0.5630
qA	0.6980	0.5610
qB	0.7800	0.5820
qC	0.7770	0.5840
qD	0.8340	0.5980
qE	0.5560	0.4890
qF	0.6960	0.5650
qG	0.6220	0.5450
qH	0.7790	0.5920
qI	0.7670	0.5870
qJ	0.7900	0.5910
qL	0.5640	0.5510
qM	0.8240	0.5800
qa	0.6180	0.5470
qb	0.6800	0.5640
qc	0.7530	0.5790
qd	0.7980	0.5920
qe	0.4950	0.4750
qf	0.5280	0.5110
qg	0.6410	0.5570
qh	0.7670	0.5860
qi	0.6550	0.5690
qj	0.7230	0.5720
ql	0.6680	0.5630
qm	0.8470	0.5840
r	0.7840	0.5500
s	0.7080	0.5290
s1	0.6950	0.5540
s2	0.7980	0.5800
s3	0.7890	0.5770
s4	0.7160	0.5620
s5	0.7770	0.5870
s6	0.6500	0.5460
s7	0.8220	0.5870

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Chain	Atom inclusion	Q-score
s8	0.8020	0.5740
sa	0.6340	0.4790
sb	0.7440	0.5050
sc	0.7550	0.5110
sd	0.8830	0.5450
t	0.7870	0.5670
t1	0.6050	0.5210
t2	0.2900	0.4720
t3	0.5550	0.5360
t4	0.5520	0.5230
t5	0.7220	0.5620
t6	0.7830	0.5920
t7	0.7010	0.5710
t8	0.7590	0.5860
t9	0.7880	0.5770
ta	0.7210	0.5600
tb	0.7710	0.5970
tc	0.7330	0.5820
td	0.6110	0.5660
te	0.6960	0.5730
tf	0.6720	0.5500
tg	0.5390	0.5120
th	0.7760	0.5780
tx	0.7640	0.5840
u	0.7460	0.5510
u1	0.8220	0.5380
u2	0.8820	0.5380
v	0.7790	0.5600
v1	0.5920	0.5300
v2	0.4630	0.5090
vb	0.8100	0.5620
w	0.7390	0.5480
x	0.8590	0.5840
x1	0.7950	0.5880
y	0.9100	0.5900
y0	0.8660	0.5810
y5	0.7220	0.5370
y7	0.7210	0.5360
z	0.7180	0.5420
z1	0.8030	0.5530