



Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 09:33 PM JST

PDB ID : 5XTH / pdb_00005xth
EMDB ID : EMD-6775
Title : Cryo-EM structure of human respiratory supercomplex I1III2IV1
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : 2017-06-19
Resolution : 3.90 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

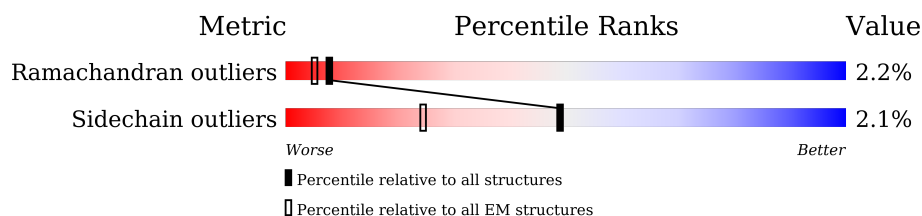
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



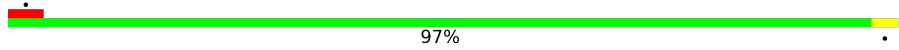

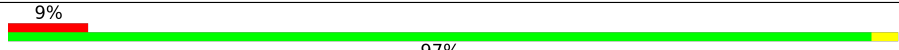
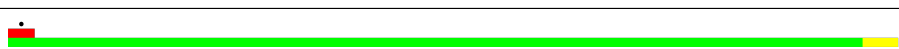
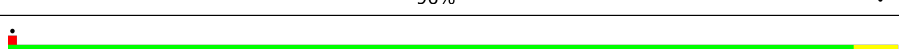
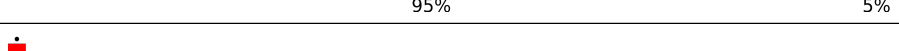
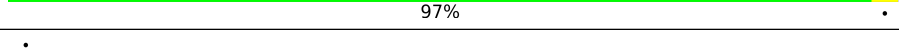
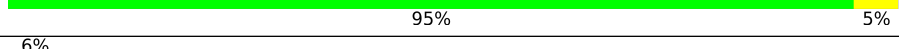
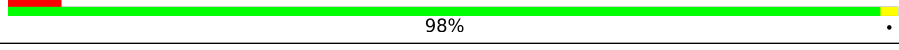
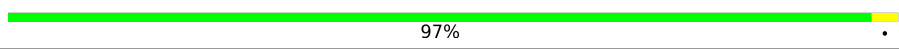
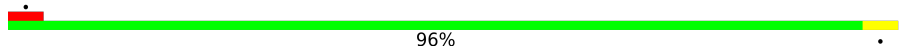
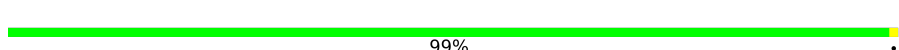
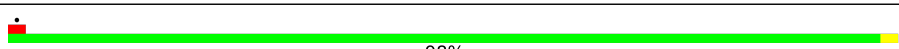

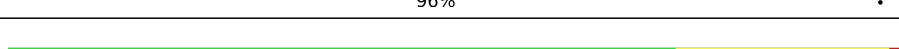
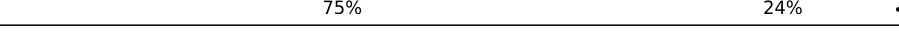
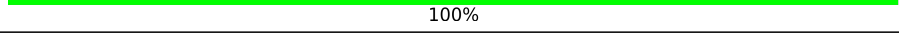
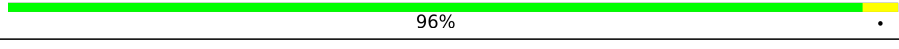
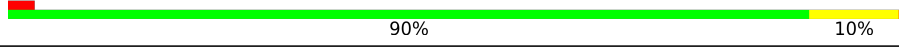
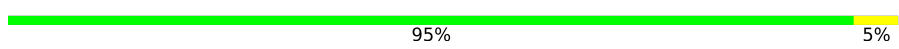
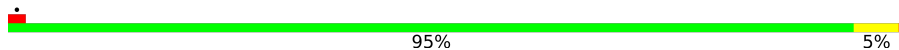
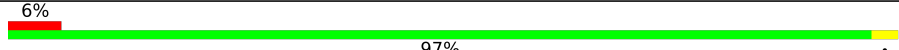

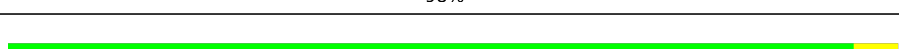
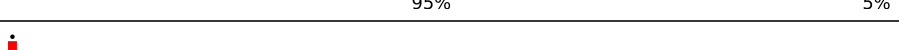
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>6%</div> <div>98%</div> <div>.</div> </div>
2	B	176	<div> <div>99%</div> <div>.</div> </div>
3	C	156	<div> <div>97%</div> <div>.</div> </div>
4	E	113	<div> <div>12%</div> <div>97%</div> <div>.</div> </div>
5	F	83	<div> <div>5%</div> <div>100%</div> </div>
6	G	85	<div> <div>46%</div> <div>98%</div> <div>.</div> </div>
6	X	85	<div> <div>95%</div> <div>5%</div> </div>
7	H	112	<div> <div>10%</div> <div>96%</div> <div>.</div> </div>
8	I	110	<div> <div>5%</div> <div>81%</div> <div>5%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
9	J	337	
10	K	33	
11	L	118	
12	M	687	
13	N	143	
14	O	212	
15	P	208	
16	Q	430	
17	S	70	
18	T	95	
19	U	83	
20	V	140	
21	W	138	
22	Y	59	
23	Z	80	
24	a	138	
25	b	124	
26	c	153	
27	d	171	
28	e	97	
29	f	47	
30	g	119	
31	h	104	
32	i	347	
33	j	115	

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Mol	Chain	Length	Quality of chain
34	k	97	
35	l	603	
36	m	174	
37	n	56	
38	o	128	
39	p	172	
40	r	459	
41	s	318	
42	u	169	
43	v	122	
44	w	320	
45	x	514	
46	y	227	
47	z	261	
48	0	144	
49	1	109	
50	2	98	
51	3	84	
52	4	75	
53	5	73	
54	6	56	
55	7	49	
56	8	47	
57	9	43	
58	AA	81	

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Mol	Chain	Length	Quality of chain
58	AN	81	
59	AB	57	
59	AO	57	
60	AC	196	
60	AP	196	
61	AD	62	
61	AQ	62	
62	AE	74	
62	AR	74	
63	AF	106	
63	AS	106	
64	AG	51	
64	AT	51	
65	AH	241	
65	AU	241	
66	AJ	378	
66	AV	378	
67	AK	419	
67	AW	419	
68	AL	446	
68	AY	446	

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 115642 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 NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3460	2214	599	624	23		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1135	727	202	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	59	Total	C	N	O	S	0	0
			533	354	87	91	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			648	426	110	110	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	124	Total	C	N	O	S	0	0
			1059	697	181	176	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	153	Total	C	N	O	S	0	0
			1236	795	208	222	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	171	Total	C	N	O	S	0	0
			1418	885	262	259	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	97	Total	C	N	O	S	0	0
			810	522	132	152	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			863	546	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2735	1819	421	470	25		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			919	626	132	152	9		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	97	Total	C	N	O	S	0	0
			740	487	113	127	13		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4717	3119	742	823	33		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	174	Total	C	N	O	S	0	0
			1313	879	194	229	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1066	685	192	187	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	172	Total	C	N	O	S	0	0
			1495	961	265	261	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2411	569	619	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2509	1678	380	435	16		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	111	Total	C	N	O	S	0	0
			921	569	187	156	9		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2474	1573	429	464	8		

- Molecule 45 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	514	Total	C	N	O	S	0	0
			4025	2690	623	677	35		

- Molecule 46 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	227	Total	C	N	O	S	0	0
			1822	1184	281	339	18		

- Molecule 47 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	261	Total	C	N	O	S	0	0
			2124	1420	338	353	13		

- Molecule 48 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	144	Total	C	N	O	S	0	0
			1195	777	196	218	4		

- Molecule 49 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	109	Total	C	N	O	S	0	0
			878	558	150	168	2		

- Molecule 50 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	98	Total	C	N	O	S	0	0
			748	464	134	145	5		

- Molecule 51 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	84	Total	C	N	O	S	0	0
			672	431	129	111	1		

- Molecule 52 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	75	Total	C	N	O	S	0	0
			628	395	114	114	5		

- Molecule 53 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			598	388	107	99	4		

- Molecule 54 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	6	56	Total	C	N	O	S	0	0
			441	285	73	80	3		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	7	49	Total	C	N	O	S	0	0
			384	250	65	67	2		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	47	Total	C	N	O	S	0	0
			386	257	65	62	2		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	9	43	Total	C	N	O	0	0
			335	223	53	59		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	81	Total	C	N	O	S	0	0
			694	450	126	117	1		
58	AN	81	Total	C	N	O	S	0	0
			687	444	126	116	1		

- Molecule 59 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	57	Total	C	N	O	S	0	0
			413	261	75	76	1		
59	AO	57	Total	C	N	O	S	0	0
			409	259	74	75	1		

- Molecule 60 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		
60	AP	196	Total	C	N	O	S	0	0
			1521	960	264	290	7		

- Molecule 61 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	62	Total	C	N	O	S	0	0
			509	332	87	89	1		
61	AQ	62	Total	C	N	O	S	0	0
			509	332	87	89	1		

- Molecule 62 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	74	Total	C	N	O	S	0	0
			580	351	108	116	5		
62	AR	74	Total	C	N	O	S	0	0
			580	351	108	116	5		

- Molecule 63 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
63	AS	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

- Molecule 64 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AG	51	Total	C	N	O		0	0
			425	287	72	66			
64	AT	51	Total	C	N	O		0	0
			425	287	72	66			

- Molecule 65 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		
65	AU	241	Total	C	N	O	S	0	0
			1924	1231	329	349	15		

- Molecule 66 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AJ	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		
66	AV	378	Total	C	N	O	S	0	0
			3009	2017	467	509	16		

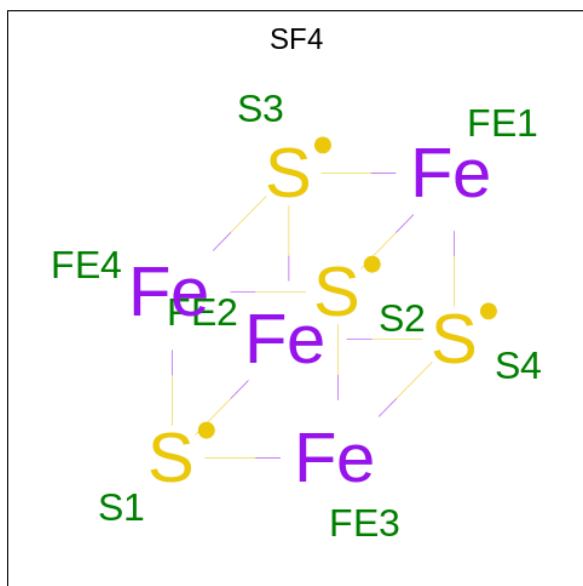
- Molecule 67 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AK	419	Total	C	N	O	S	0	0
			3159	1986	553	610	10		
67	AW	419	Total	C	N	O	S	0	0
			3162	1989	553	610	10		

- Molecule 68 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

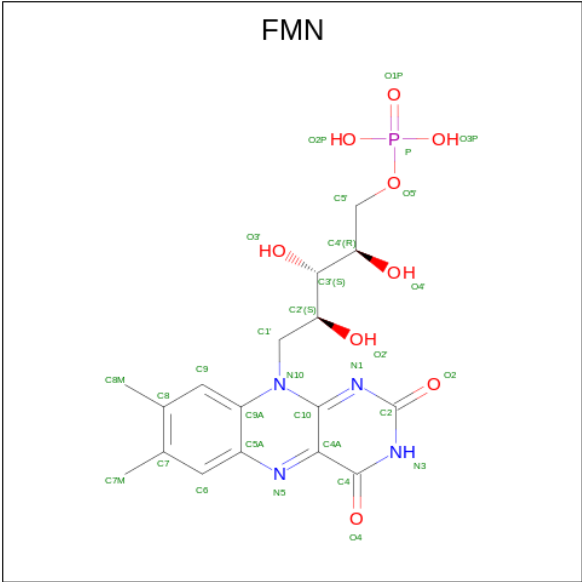
Mol	Chain	Residues	Atoms					AltConf	Trace
68	AL	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		
68	AY	446	Total	C	N	O	S	0	0
			3453	2169	603	661	20		

- Molecule 69 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



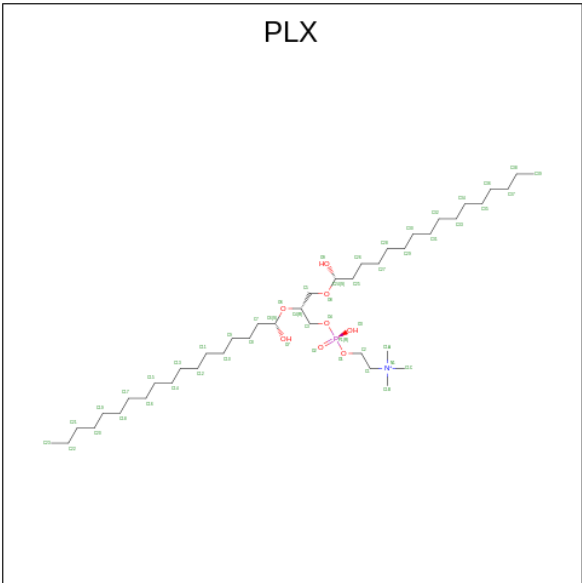
Mol	Chain	Residues	Atoms			AltConf
69	A	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	B	1	Total	Fe	S	0
			8	4	4	
69	C	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	
69	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



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

- Molecule 71 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



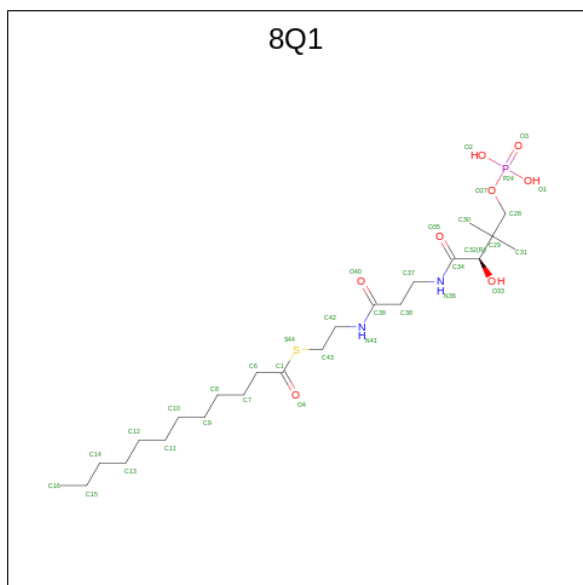
Mol	Chain	Residues	Atoms					AltConf
71	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	U	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	V	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	b	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AL	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AQ	1	Total	C	N	O	P	0
			52	42	1	8	1	
71	AT	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 72 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



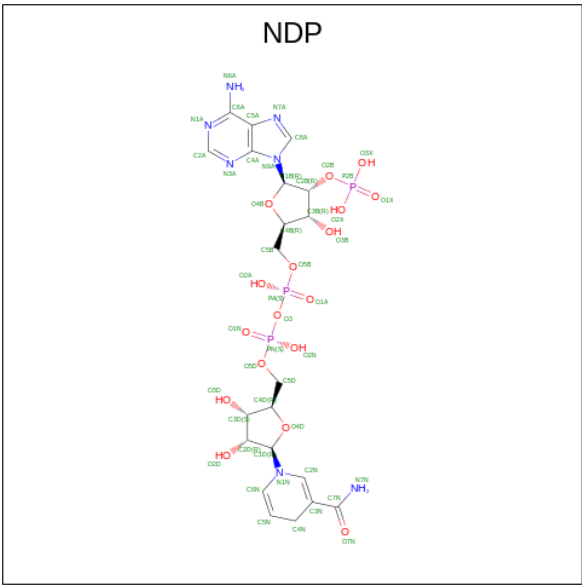
Mol	Chain	Residues	Atoms					AltConf
72	E	1	Total	C	N	O	P	S
			35	23	2	8	1	1

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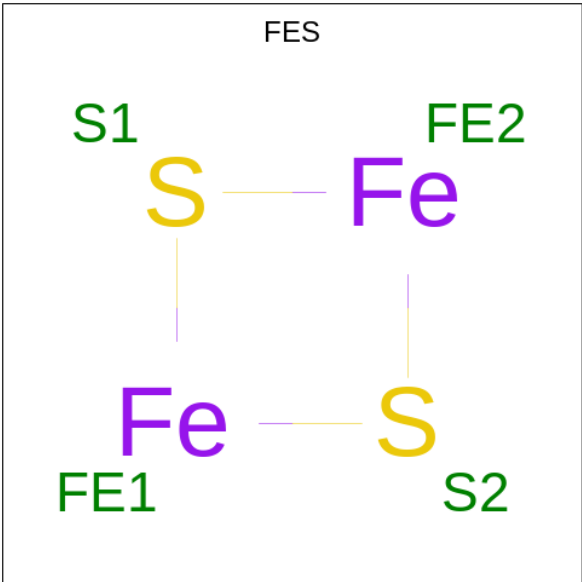
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
72	p	1	35	23	2	8	1	1	0

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



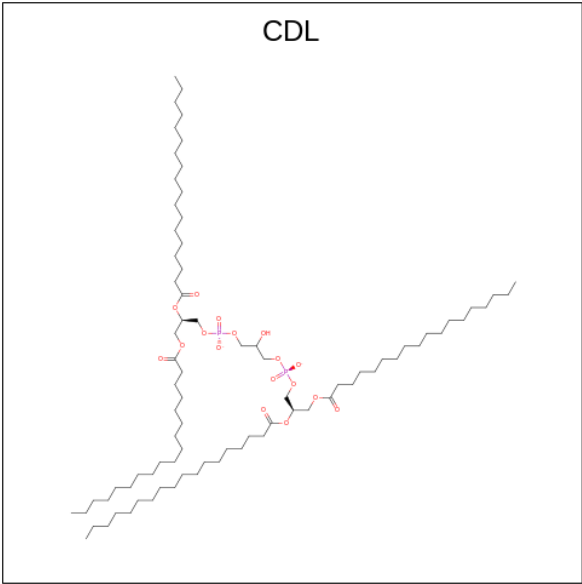
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
73	J	1	48	21	7	17	3	0

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



Mol	Chain	Residues	Atoms			AltConf
74	M	1	Total	Fe	S	0
			4	2	2	
74	O	1	Total	Fe	S	0
			4	2	2	
74	AC	1	Total	Fe	S	0
			4	2	2	
74	AP	1	Total	Fe	S	0
			4	2	2	

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



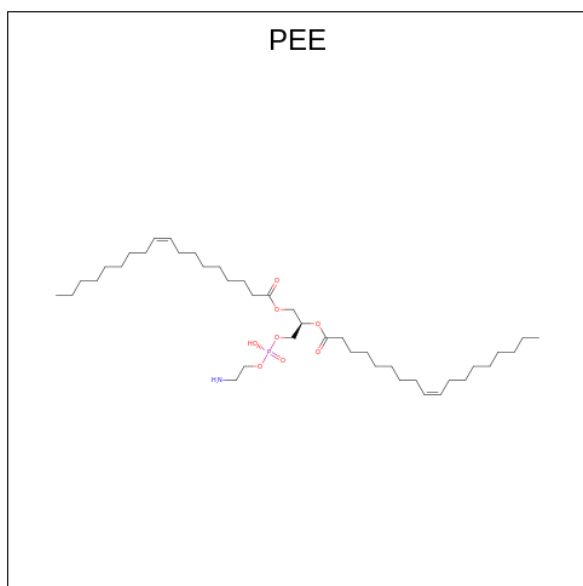
Mol	Chain	Residues	Atoms				AltConf
75	V	1	Total	C	O	P	0
			63	44	17	2	
75	i	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	l	1	Total	C	O	P	0
			64	45	17	2	
75	n	1	Total	C	O	P	0
			64	45	17	2	
75	AA	1	Total	C	O	P	0
			64	45	17	2	
75	AG	1	Total	C	O	P	0
			64	45	17	2	
75	AH	1	Total	C	O	P	0
			64	45	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	AJ	1	Total	C	O	P	0
			64	45	17	2	
75	AJ	1	Total	C	O	P	0
			64	45	17	2	
75	AL	1	Total	C	O	P	0
			64	45	17	2	
75	AN	1	Total	C	O	P	0
			64	45	17	2	
75	AU	1	Total	C	O	P	0
			64	45	17	2	
75	AY	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 76 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
76	V	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	W	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	AH	1	Total	C	N	O	P	0
			49	39	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	AJ	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AL	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AU	1	Total	C	N	O	P	0
			41	31	1	8	1	
76	AV	1	Total	C	N	O	P	0
			49	39	1	8	1	
76	AY	1	Total	C	N	O	P	0
			49	39	1	8	1	

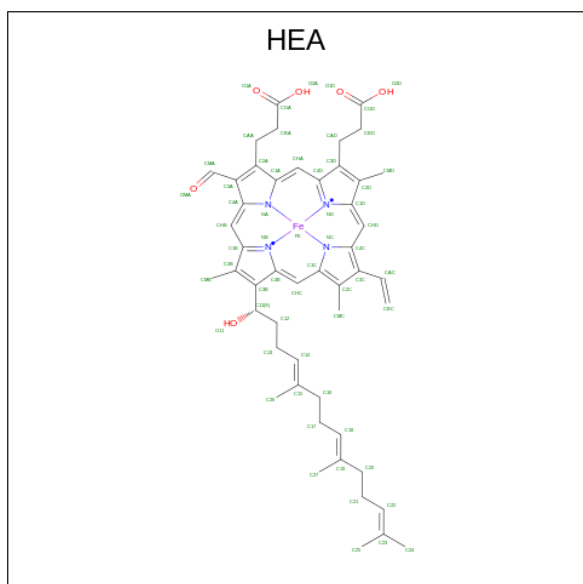
- Molecule 77 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
77	x	1	Total	Cu	0
			1	1	
77	y	2	Total	Cu	0
			2	2	

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

Mol	Chain	Residues	Atoms		AltConf
78	x	1	Total	Mg	0
			1	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

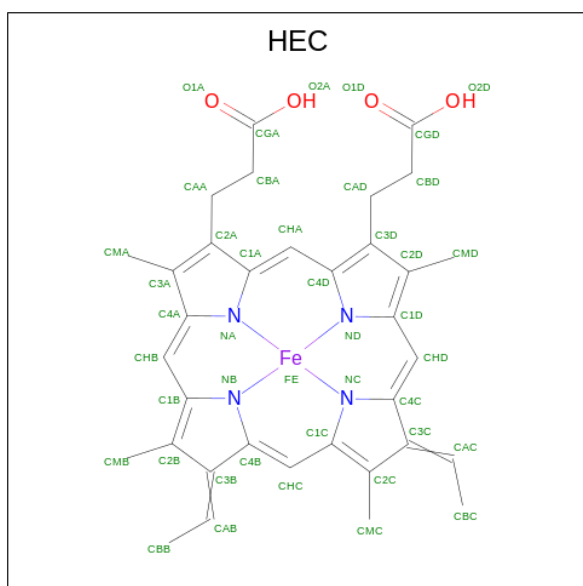


Mol	Chain	Residues	Atoms					AltConf
79	x	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
79	x	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

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

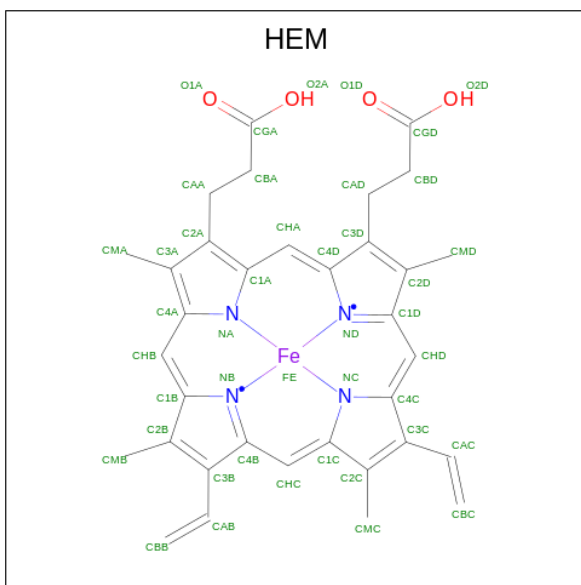
Mol	Chain	Residues	Atoms		AltConf
80	2	1	Total	Zn	0
			1	1	

- Molecule 81 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
81	AH	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
81	AU	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 82 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

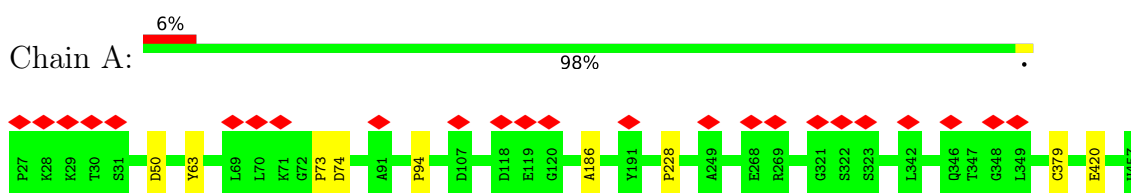


Mol	Chain	Residues	Atoms					AltConf
82	AJ	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AJ	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0
82	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0

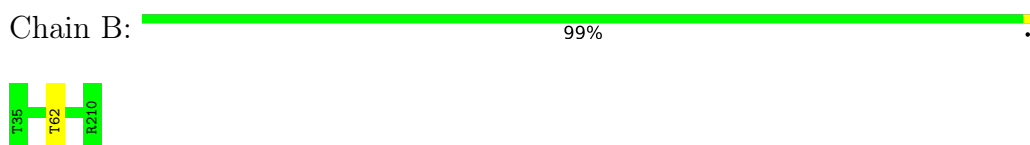
3 Residue-property plots [i](#)

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

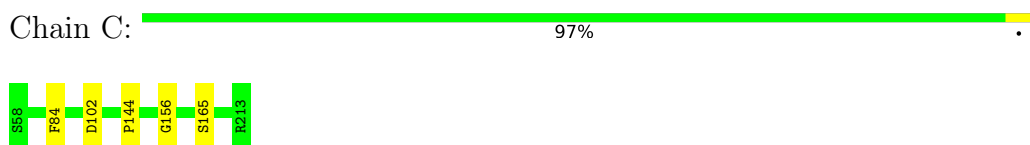
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



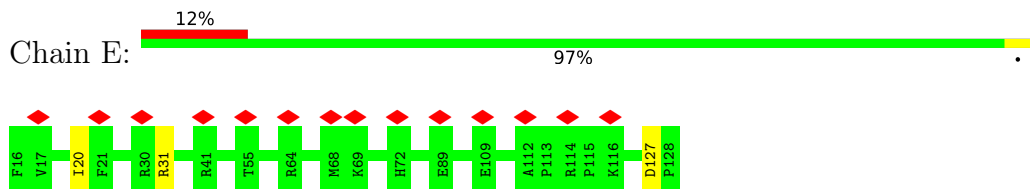
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



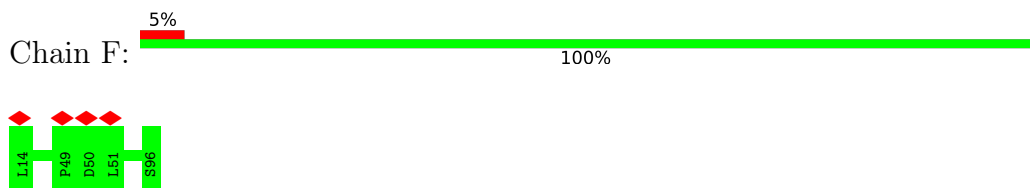
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



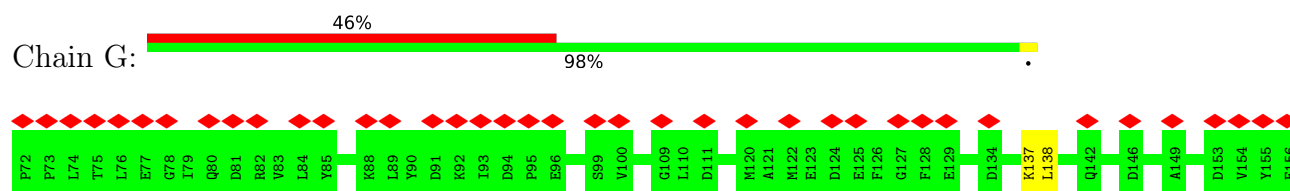
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



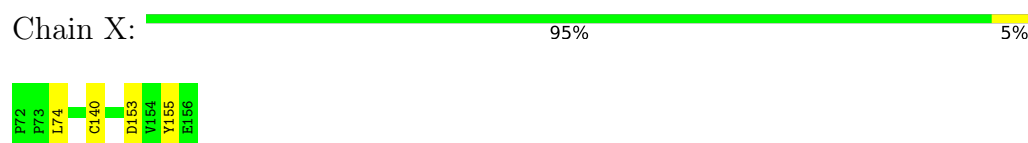
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



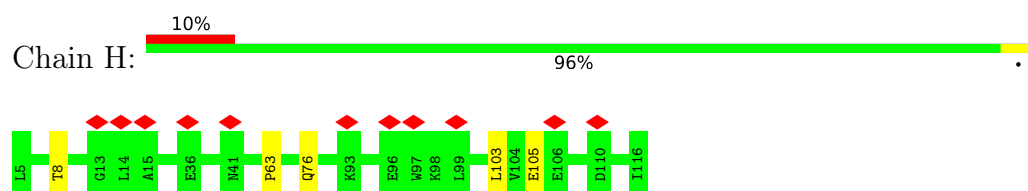
- Molecule 6: Acyl carrier protein, mitochondrial



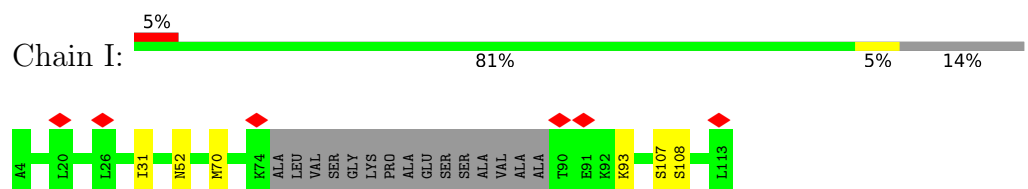
- Molecule 6: Acyl carrier protein, mitochondrial



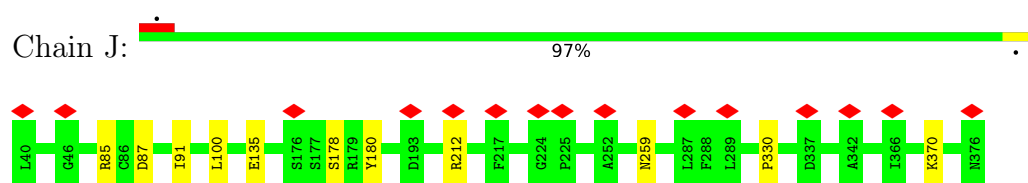
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



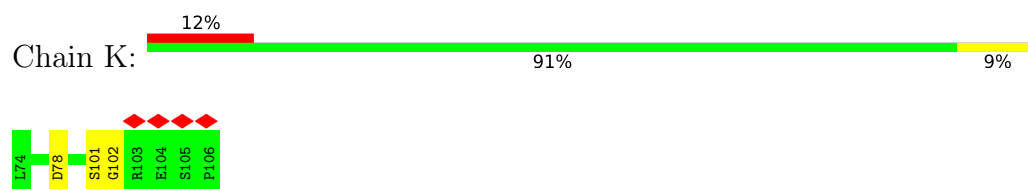
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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

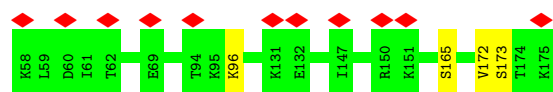


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



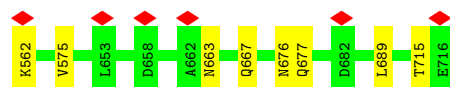
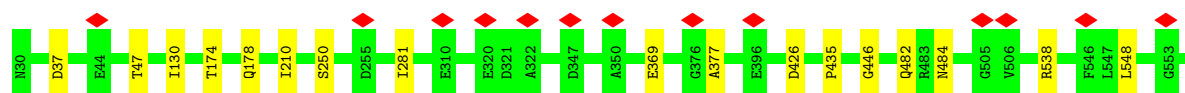
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M: 96%



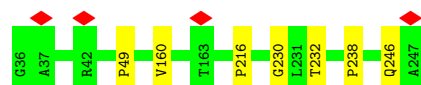
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N: 95% 5%



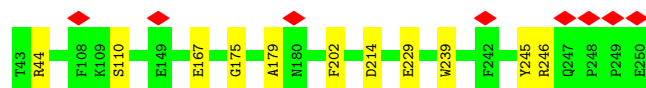
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O: 97%



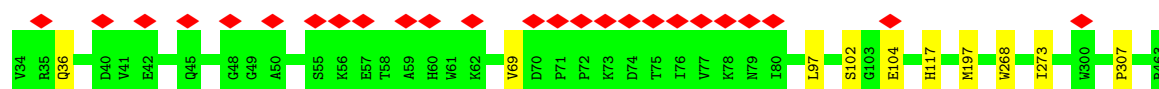
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P: 95% 5%



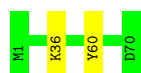
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain Q: 6% 98%



- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 97%



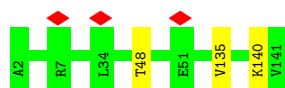
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



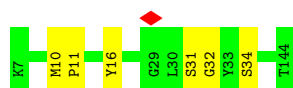
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



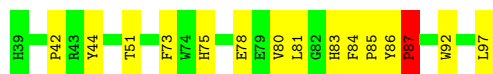
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



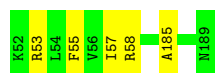
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3




There are no outlier residues recorded for this chain.

- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  96%



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:  90%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  95%



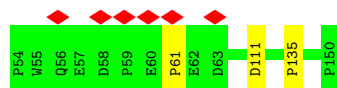
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  95%



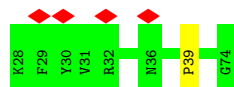
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  97%



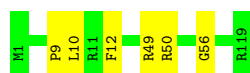
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  98%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  95%



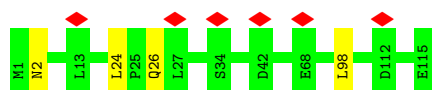
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



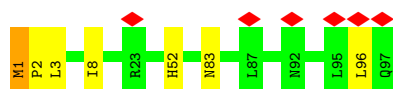
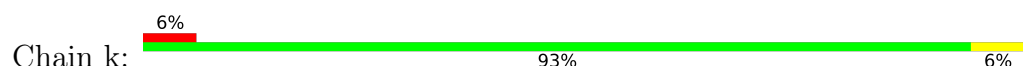
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



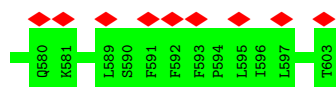
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

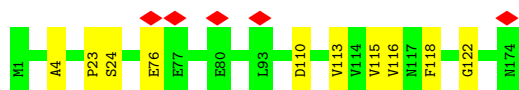


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



- Molecule 36: NADH-ubiquinone oxidoreductase chain 6





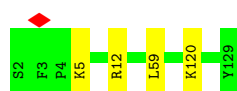
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 96%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 97%



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 98%



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 98%



- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 97%




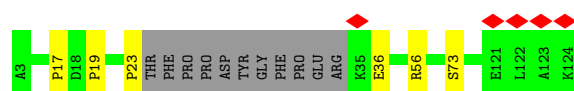
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 97%



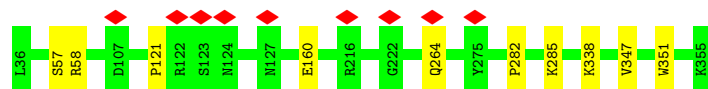
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 

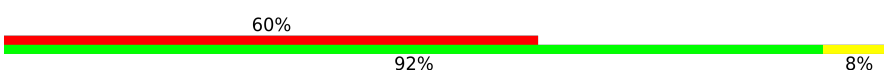


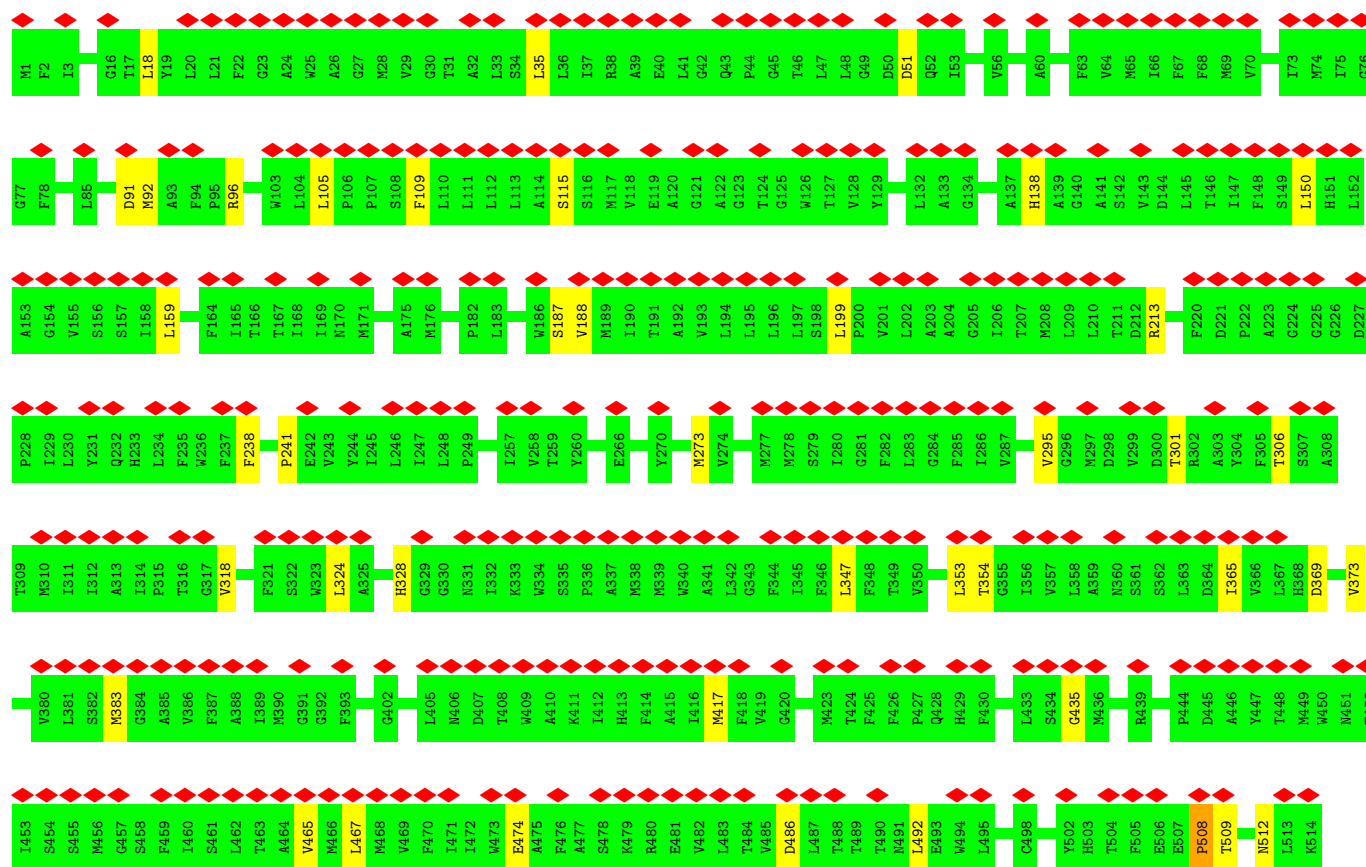
- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain w: 

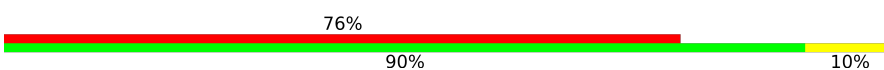


- Molecule 45: Cytochrome c oxidase subunit 1

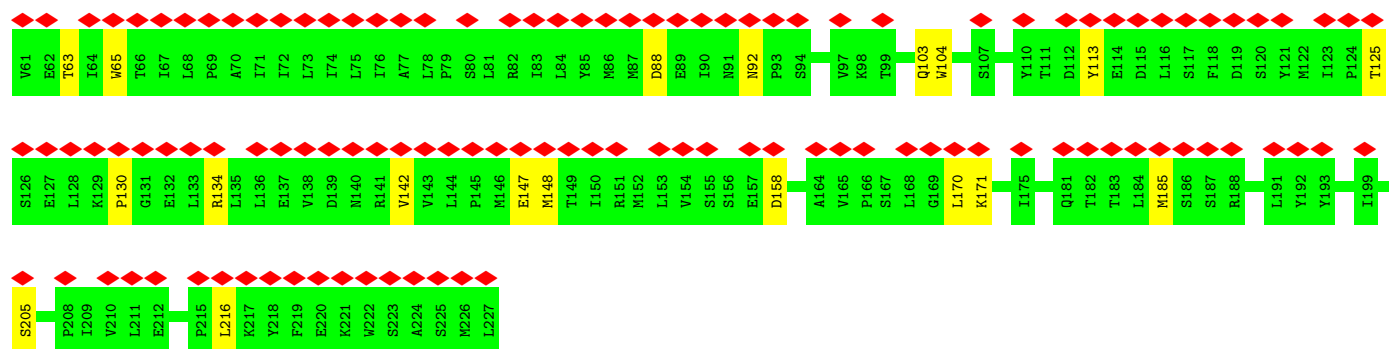
Chain x: 



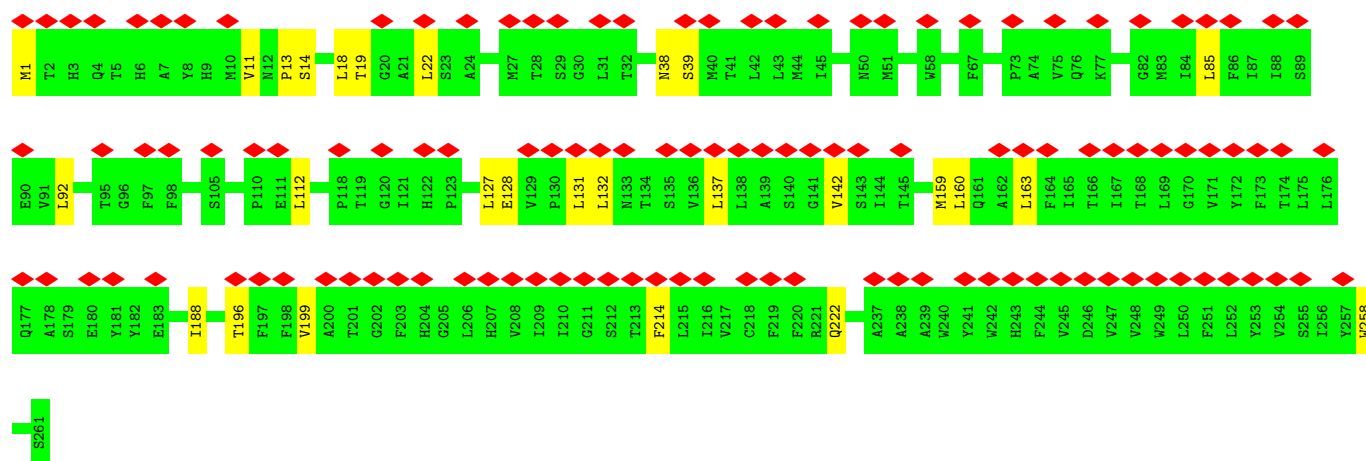
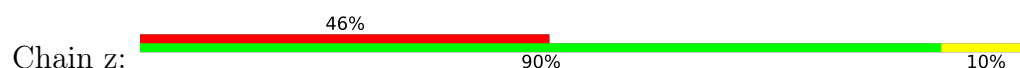
- Molecule 46: Cytochrome c oxidase subunit 2

Chain y: 

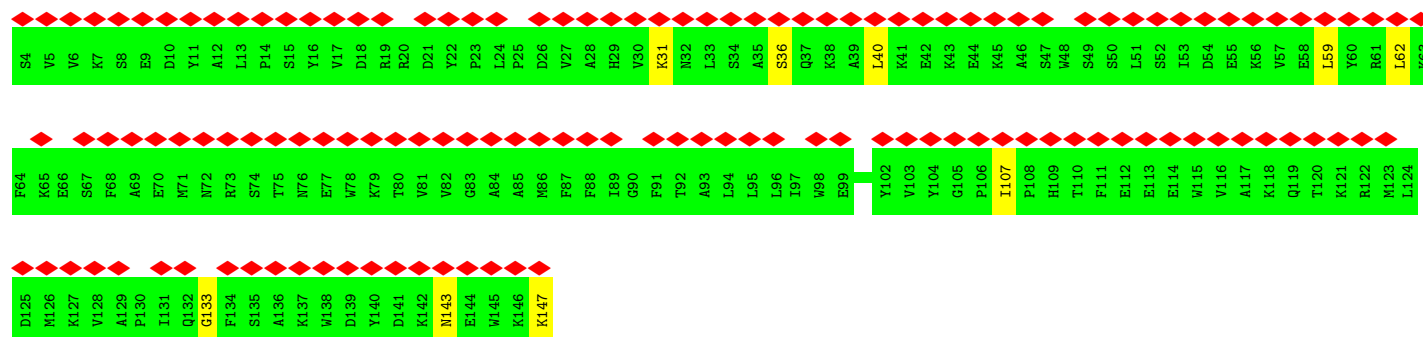
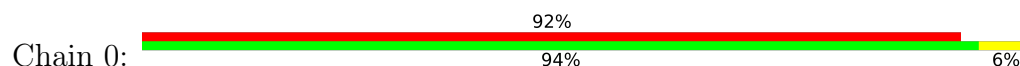




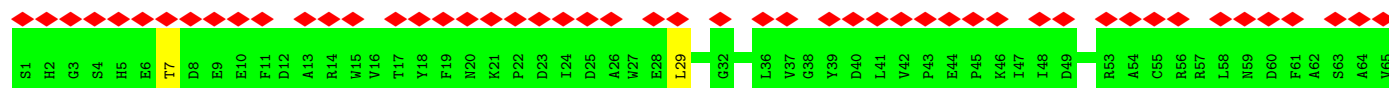
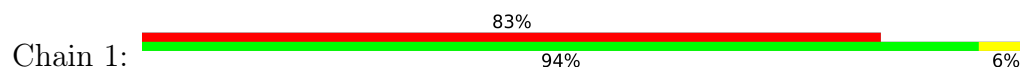
• Molecule 47: Cytochrome c oxidase subunit 3

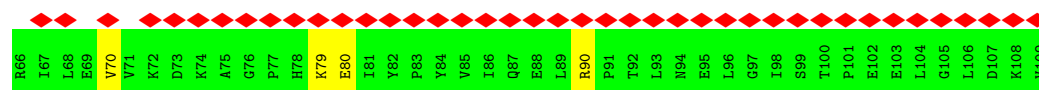


• Molecule 48: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

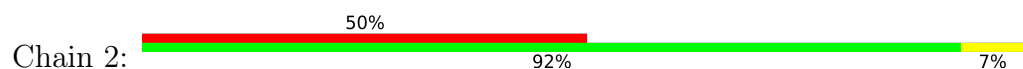


• Molecule 49: Cytochrome c oxidase subunit 5A, mitochondrial

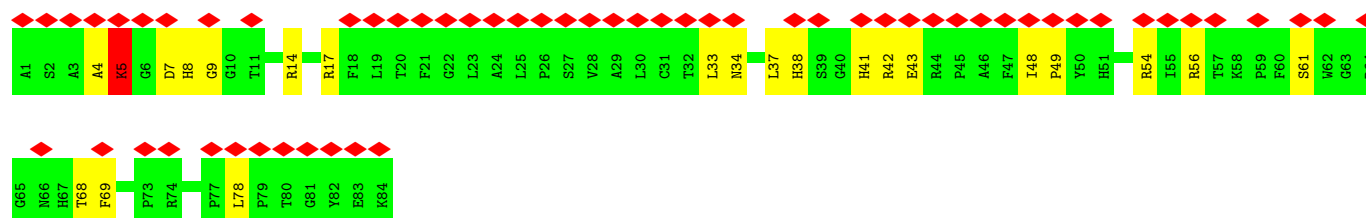
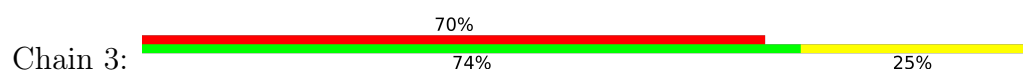




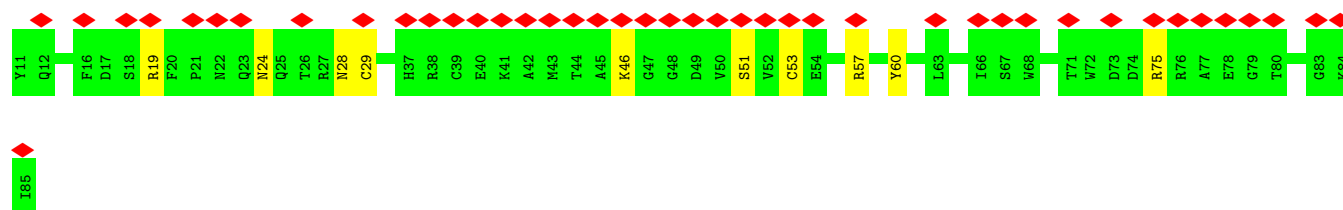
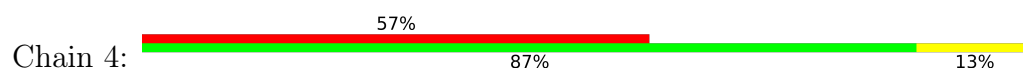
- Molecule 50: Cytochrome c oxidase subunit 5B, mitochondrial



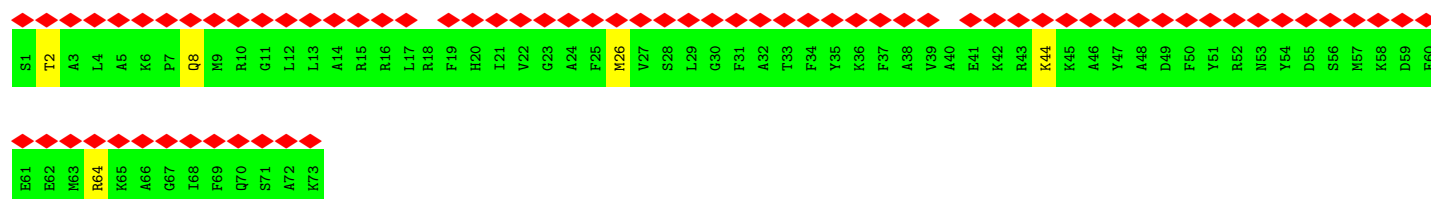
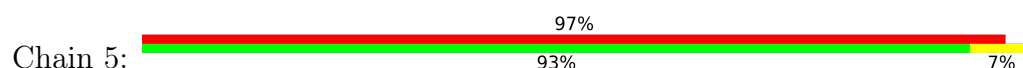
- Molecule 51: Cytochrome c oxidase subunit 6A2, mitochondrial



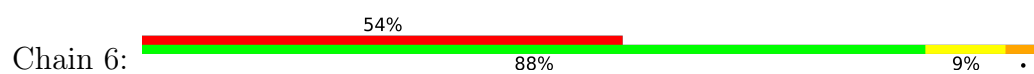
- Molecule 52: Cytochrome c oxidase subunit 6B1



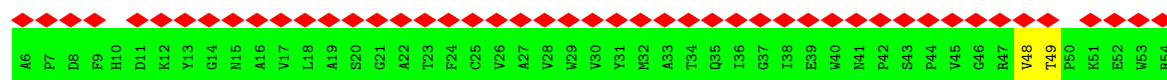
- Molecule 53: Cytochrome c oxidase subunit 6C



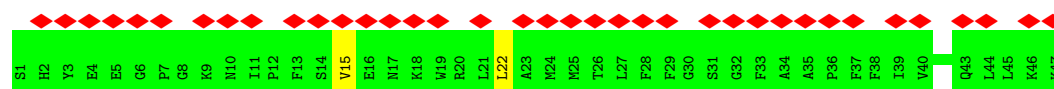
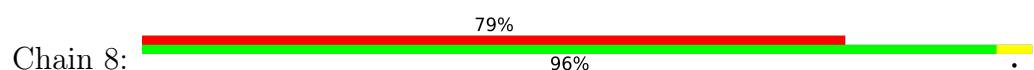
- Molecule 54: Cytochrome c oxidase subunit 7A1, mitochondrial



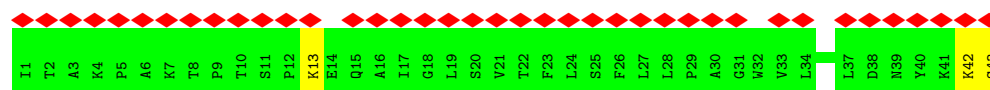
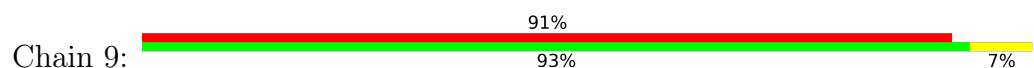
- Molecule 55: Cytochrome c oxidase subunit 7B, mitochondrial



- Molecule 56: Cytochrome c oxidase subunit 7C, mitochondrial



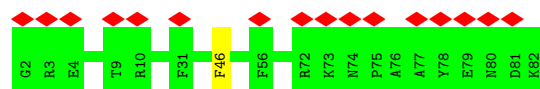
- Molecule 57: Cytochrome c oxidase subunit 8B, mitochondrial



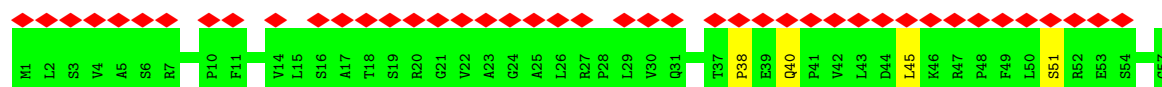
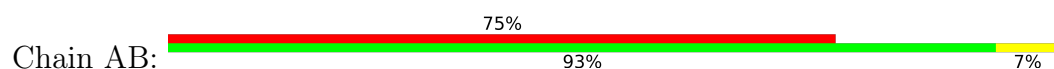
- Molecule 58: Cytochrome b-c1 complex subunit 8




- Molecule 58: Cytochrome b-c1 complex subunit 8

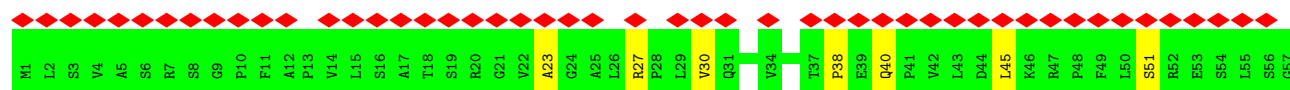


- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial



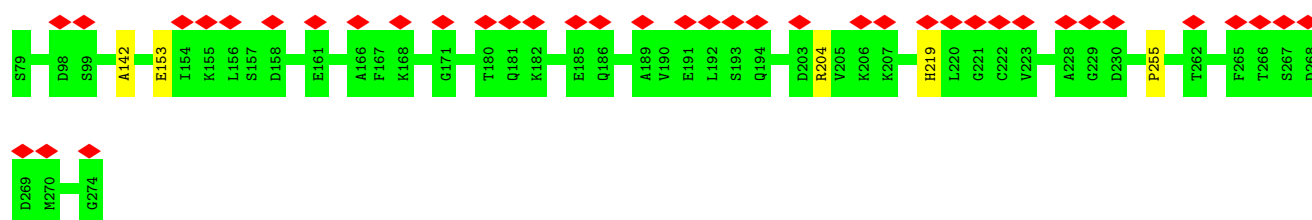
- Molecule 59: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AO: 



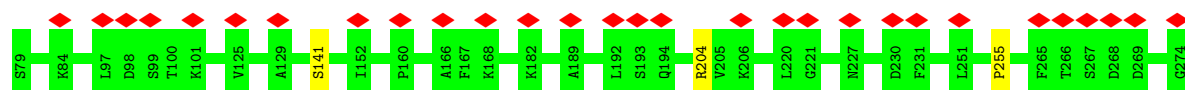
- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AC: 



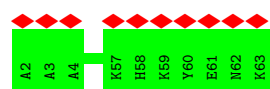
- Molecule 60: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AP: 



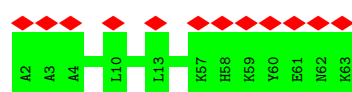
- Molecule 61: Cytochrome b-c1 complex subunit 9

Chain AD: 



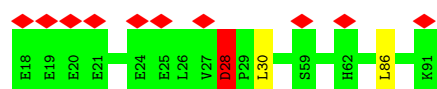
- Molecule 61: Cytochrome b-c1 complex subunit 9

Chain AQ: 

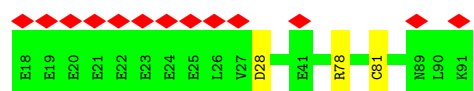


- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial

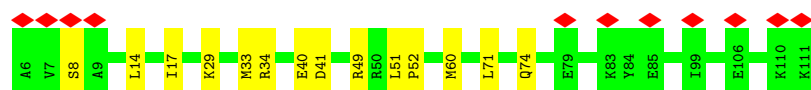
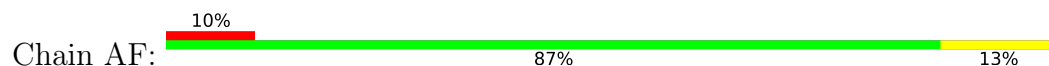
Chain AE: 



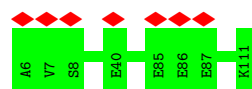
- Molecule 62: Cytochrome b-c1 complex subunit 6, mitochondrial



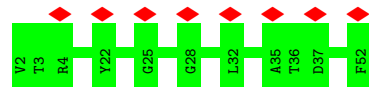
- Molecule 63: Cytochrome b-c1 complex subunit 7



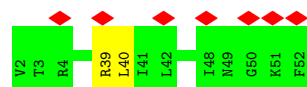
- Molecule 63: Cytochrome b-c1 complex subunit 7



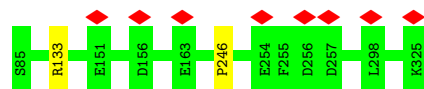
- Molecule 64: Cytochrome b-c1 complex subunit 10



- Molecule 64: Cytochrome b-c1 complex subunit 10



- Molecule 65: Cytochrome c1, heme protein, mitochondrial

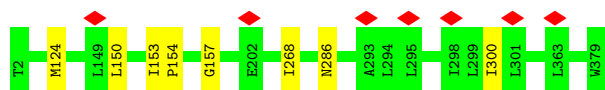


- Molecule 65: Cytochrome c1, heme protein, mitochondrial



- Molecule 66: Cytochrome b

Chain AJ:  98%



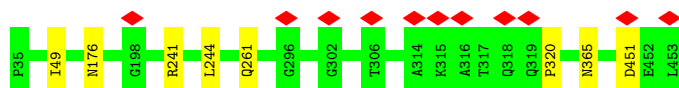
- Molecule 66: Cytochrome b

Chain AV:  96%



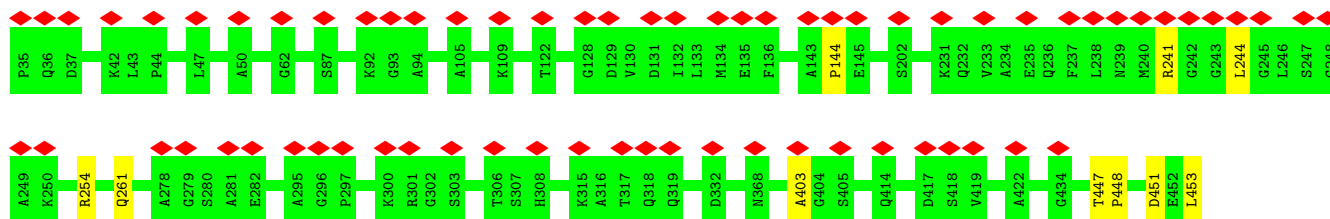
- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AK:  98%



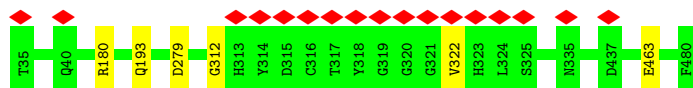
- Molecule 67: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AW:  16%  98%



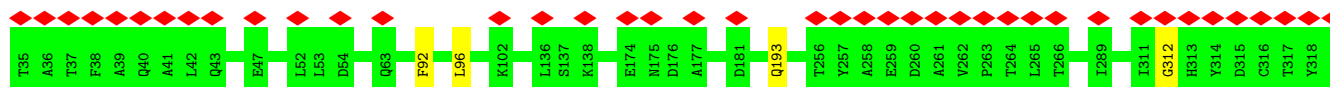
- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AL:  99%



- Molecule 68: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain AY:  12%  97%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0354	Depositor
Map size (\AA)	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 8Q1, ZN, PLX, FES, FMN, PEE, NDP, CDL, HEC, HEM, HEA, SF4, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3398	0.49	0/4590
2	B	0.50	0/1452	0.57	0/1964
3	C	0.58	0/1280	0.57	0/1732
4	E	0.34	0/993	0.53	0/1335
5	F	0.28	0/682	0.53	0/922
6	G	0.33	0/684	0.53	0/926
6	X	0.57	0/698	0.61	0/942
7	H	0.34	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.35	0/2785	0.52	0/3771
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.43	0/3552	0.59	1/4815 (0.0%)
17	S	0.60	0/583	0.64	0/785
18	T	0.32	0/755	0.47	0/1017
19	U	0.52	0/670	0.63	0/920
20	V	0.51	0/1065	0.61	0/1450
21	W	0.57	0/1166	0.68	1/1579 (0.1%)
22	Y	0.52	0/559	0.73	3/763 (0.4%)
23	Z	0.45	0/669	0.53	0/899
24	a	0.68	0/1209	0.65	0/1639
25	b	0.59	1/1095 (0.1%)	0.69	4/1480 (0.3%)
26	c	0.59	0/1287	0.58	0/1761
27	d	0.63	0/1445	0.65	1/1945 (0.1%)
28	e	0.61	0/835	0.62	0/1134
29	f	0.48	0/418	0.58	0/566
30	g	0.64	0/1035	0.63	0/1398
31	h	0.62	0/884	0.65	0/1182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.67	0/2808	0.77	2/3843 (0.1%)
33	j	0.55	0/945	0.69	1/1292 (0.1%)
34	k	0.68	1/751 (0.1%)	0.79	1/1019 (0.1%)
35	l	0.61	2/4840 (0.0%)	0.70	3/6611 (0.0%)
36	m	0.68	0/1346	0.67	0/1832
37	n	0.49	0/484	0.62	0/652
38	o	0.54	0/1093	0.61	0/1479
39	p	0.59	0/1549	0.59	0/2098
40	r	0.70	0/3723	0.76	2/5089 (0.0%)
41	s	0.62	0/2580	0.73	0/3539
42	u	0.57	0/1433	0.61	0/1937
43	v	0.49	0/934	0.67	3/1241 (0.2%)
44	w	0.44	0/2533	0.56	0/3440
45	x	0.60	0/4164	0.76	1/5688 (0.0%)
46	y	0.58	0/1868	0.80	0/2544
47	z	0.56	0/2211	0.69	0/3023
48	0	0.57	0/1229	0.65	1/1658 (0.1%)
49	1	0.50	0/898	0.66	0/1218
50	2	0.56	0/765	0.81	0/1038
51	3	0.55	0/699	0.73	1/950 (0.1%)
52	4	0.55	0/648	0.73	0/877
53	5	0.60	0/611	0.65	0/810
54	6	0.60	0/451	0.71	0/610
55	7	0.58	0/398	0.66	0/546
56	8	0.63	0/399	0.62	0/534
57	9	0.51	0/345	0.65	0/470
58	AA	0.31	0/715	0.48	0/964
58	AN	0.27	0/707	0.49	0/953
59	AB	0.23	0/421	0.60	1/574 (0.2%)
59	AO	0.25	0/417	0.61	1/569 (0.2%)
60	AC	0.24	0/1554	0.43	0/2104
60	AP	0.23	0/1554	0.42	0/2104
61	AD	0.26	0/521	0.42	0/699
61	AQ	0.27	0/521	0.43	0/699
62	AE	0.35	0/587	0.54	1/789 (0.1%)
62	AR	0.27	0/587	0.46	0/789
63	AF	0.42	1/942 (0.1%)	0.52	1/1263 (0.1%)
63	AS	0.27	0/942	0.44	0/1263
64	AG	0.27	0/442	0.48	0/608
64	AT	0.28	0/442	0.49	0/608
65	AH	0.26	0/1983	0.46	0/2691
65	AU	0.27	0/1983	0.45	0/2691
66	AJ	0.31	1/3108 (0.0%)	0.52	1/4254 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
66	AV	0.34	2/3108 (0.1%)	0.54	2/4254 (0.0%)
67	AK	0.27	0/3217	0.49	0/4361
67	AW	0.29	1/3220 (0.0%)	0.48	1/4365 (0.0%)
68	AL	0.27	0/3527	0.47	0/4788
68	AY	0.29	1/3527 (0.0%)	0.50	2/4788 (0.0%)
All	All	0.47	10/115987 (0.0%)	0.60	35/157444 (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
44	w	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	AW	448	PRO	N-CD	5.34	1.55	1.47
66	AJ	154	PRO	N-CD	5.22	1.55	1.47
66	AV	154	PRO	N-CD	5.22	1.55	1.47
34	k	2	PRO	N-CD	5.17	1.55	1.47
25	b	118	PRO	N-CD	5.17	1.55	1.47
68	AY	425	PRO	N-CD	5.08	1.54	1.47
35	l	91	PRO	N-CD	5.03	1.54	1.47
35	l	231	PRO	N-CD	5.02	1.54	1.47
63	AF	52	PRO	N-CD	5.02	1.54	1.47
66	AV	346	PRO	N-CD	5.01	1.54	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	323	THR	C-N-CD	-7.38	104.37	120.60
21	W	31	SER	N-CA-C	-7.00	92.09	111.00
22	Y	92	TRP	N-CA-C	-6.99	92.12	111.00
27	d	2	PRO	N-CA-CB	6.77	111.43	103.30
22	Y	87	PRO	CA-N-CD	-6.56	102.31	111.50
48	0	133	GLY	N-CA-C	6.43	129.17	113.10
25	b	36	PRO	C-N-CD	6.20	141.41	128.40
62	AE	28	ASP	C-N-CD	6.15	141.31	128.40
32	i	323	THR	C-N-CA	6.05	147.42	122.00
43	v	17	PRO	N-CA-CB	5.92	110.40	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	v	23	PRO	N-CA-CB	5.88	110.35	103.30
35	l	197	ASP	C-N-CD	5.87	140.72	128.40
66	AV	345	TYR	C-N-CD	5.82	140.62	128.40
25	b	105	PHE	C-N-CD	5.79	140.57	128.40
66	AV	153	ILE	C-N-CD	5.77	140.52	128.40
34	k	1	MET	C-N-CD	5.75	140.48	128.40
66	AJ	153	ILE	C-N-CD	5.74	140.45	128.40
43	v	19	PRO	N-CA-CB	5.72	110.16	103.30
35	l	90	ILE	C-N-CD	5.71	140.40	128.40
68	AY	424	ILE	C-N-CD	5.67	140.32	128.40
25	b	117	ILE	C-N-CD	5.67	140.31	128.40
35	l	230	HIS	C-N-CD	5.67	140.31	128.40
63	AF	51	LEU	C-N-CD	5.66	140.29	128.40
16	Q	97	LEU	CA-CB-CG	5.64	128.27	115.30
67	AW	447	THR	C-N-CD	5.63	140.22	128.40
59	AB	45	LEU	CA-CB-CG	5.47	127.88	115.30
33	j	98	LEU	CB-CG-CD2	-5.41	101.81	111.00
25	b	37	PRO	CA-N-CD	-5.39	103.95	111.50
68	AY	421	GLY	N-CA-C	-5.38	99.64	113.10
59	AO	45	LEU	CA-CB-CG	5.31	127.50	115.30
51	3	5	LYS	N-CA-C	5.24	125.15	111.00
45	x	435	GLY	N-CA-C	5.22	126.16	113.10
22	Y	86	TYR	C-N-CD	5.14	139.20	128.40
40	r	408	LEU	CA-CB-CG	-5.10	103.57	115.30
40	r	238	LEU	CB-CG-CD2	-5.09	102.34	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	w	338	LYS	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	5	33
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	22	57
3	C	154/156 (99%)	136 (88%)	13 (8%)	5 (3%)	3	26
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	7	35
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	5	30
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	19
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	2	20
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	15
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	33
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	0	8
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	3	25
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	3	25
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	19
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	3	25
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	1	18
16	Q	428/430 (100%)	398 (93%)	23 (5%)	7 (2%)	8	37
17	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	27
18	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	2	21
19	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	11	43
20	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	32
21	W	136/138 (99%)	127 (93%)	4 (3%)	5 (4%)	2	23
22	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	7
23	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	b	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	22
26	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	20
27	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	22	57
28	e	95/97 (98%)	83 (87%)	9 (10%)	3 (3%)	3	26
29	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	32
30	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	18
31	h	102/104 (98%)	86 (84%)	10 (10%)	6 (6%)	1	16
32	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	36
33	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	29
34	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	26
35	l	601/603 (100%)	553 (92%)	38 (6%)	10 (2%)	7	36
36	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	16
37	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	23
38	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	26
39	p	170/172 (99%)	158 (93%)	9 (5%)	3 (2%)	7	35
40	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	33
41	s	316/318 (99%)	285 (90%)	22 (7%)	9 (3%)	4	28
42	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	27
43	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	28
44	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	28
45	x	512/514 (100%)	479 (94%)	29 (6%)	4 (1%)	16	51
46	y	225/227 (99%)	203 (90%)	19 (8%)	3 (1%)	10	41
47	z	259/261 (99%)	249 (96%)	10 (4%)	0	100	100
48	0	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
49	1	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
50	2	96/98 (98%)	86 (90%)	6 (6%)	4 (4%)	2	21
51	3	82/84 (98%)	67 (82%)	10 (12%)	5 (6%)	1	16
52	4	73/75 (97%)	64 (88%)	8 (11%)	1 (1%)	9	39
53	5	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
54	6	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	2	23
55	7	47/49 (96%)	41 (87%)	6 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	8	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
57	9	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
58	AA	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4	30
58	AN	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	10	41
59	AB	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	1	18
59	AO	55/57 (96%)	43 (78%)	6 (11%)	6 (11%)	0	6
60	AC	194/196 (99%)	179 (92%)	10 (5%)	5 (3%)	4	29
60	AP	194/196 (99%)	178 (92%)	13 (7%)	3 (2%)	8	39
61	AD	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
61	AQ	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
62	AE	72/74 (97%)	65 (90%)	5 (7%)	2 (3%)	4	28
62	AR	72/74 (97%)	69 (96%)	2 (3%)	1 (1%)	9	39
63	AF	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	13	46
63	AS	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
64	AG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
64	AT	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
65	AH	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	16	51
65	AU	239/241 (99%)	230 (96%)	7 (3%)	2 (1%)	16	51
66	AJ	376/378 (100%)	363 (96%)	10 (3%)	3 (1%)	16	51
66	AV	376/378 (100%)	359 (96%)	14 (4%)	3 (1%)	16	51
67	AK	417/419 (100%)	390 (94%)	22 (5%)	5 (1%)	11	43
67	AW	417/419 (100%)	397 (95%)	15 (4%)	5 (1%)	11	43
68	AL	444/446 (100%)	405 (91%)	33 (7%)	6 (1%)	9	39
68	AY	444/446 (100%)	413 (93%)	24 (5%)	7 (2%)	8	37
All	All	14029/14219 (99%)	12872 (92%)	849 (6%)	308 (2%)	8	32

All (308) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

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Mol	Chain	Res	Type
12	M	47	THR
12	M	178	GLN
12	M	210	ILE
12	M	369	GLU
13	N	115	PHE
14	O	232	THR
14	O	246	GLN
15	P	167	GLU
17	S	60	TYR
18	T	82	THR
19	U	71	GLN
21	W	34	SER
6	X	155	TYR
22	Y	84	PHE
24	a	58	ARG
26	c	115	ASN
26	c	178	PRO
27	d	2	PRO
31	h	20	ILE
32	i	91	ASN
32	i	323	THR
33	j	24	LEU
33	j	26	GLN
34	k	52	HIS
35	l	450	LEU
36	m	115	VAL
36	m	116	VAL
36	m	118	PHE
37	n	55	VAL
40	r	52	CYS
40	r	346	GLN
44	w	57	SER
44	w	282	PRO
44	w	347	VAL
45	x	328	HIS
45	x	508	PRO
50	2	2	SER
50	2	87	THR
50	2	95	GLN
51	3	4	ALA
51	3	9	GLY
52	4	46	LYS

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Mol	Chain	Res	Type
54	6	2	GLU
66	AJ	268	ILE
67	AK	241	ARG
59	AO	23	ALA
60	AP	141	SER
68	AY	424	ILE
3	C	84	PHE
3	C	165	SER
4	E	20	ILE
4	E	127	ASP
6	G	138	LEU
7	H	105	GLU
8	I	31	ILE
8	I	93	LYS
8	I	107	SER
9	J	87	ASP
11	L	173	SER
12	M	250	SER
12	M	482	GLN
12	M	484	ASN
12	M	562	LYS
12	M	663	ASN
12	M	676	ASN
13	N	19	GLY
13	N	76	ASP
14	O	49	PRO
14	O	160	VAL
16	Q	104	GLU
16	Q	117	HIS
18	T	44	GLN
20	V	135	VAL
20	V	140	LYS
21	W	11	PRO
22	Y	44	TYR
22	Y	51	THR
24	a	57	ILE
24	a	185	ALA
25	b	101	LYS
26	c	170	ARG
30	g	9	PRO
31	h	3	PHE
31	h	24	GLU

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Mol	Chain	Res	Type
31	h	43	CYS
33	j	2	ASN
35	l	73	THR
36	m	122	GLY
37	n	52	SER
40	r	45	ILE
40	r	188	ASN
40	r	250	LEU
40	r	421	HIS
41	s	203	GLY
41	s	213	ILE
41	s	217	ALA
41	s	316	PRO
43	v	56	ARG
44	w	264	GLN
44	w	285	LYS
51	3	5	LYS
60	AC	153	GLU
60	AC	255	PRO
66	AJ	157	GLY
67	AK	176	ASN
59	AO	38	PRO
60	AP	255	PRO
66	AV	157	GLY
66	AV	254	ASP
66	AV	266	PRO
67	AW	244	LEU
68	AY	312	GLY
68	AY	322	VAL
1	A	74	ASP
7	H	8	THR
7	H	63	PRO
8	I	52	ASN
9	J	135	GLU
9	J	178	SER
10	K	101	SER
11	L	165	SER
12	M	538	ARG
12	M	677	GLN
12	M	689	LEU
12	M	715	THR
13	N	113	HIS

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Mol	Chain	Res	Type
14	O	238	PRO
15	P	44	ARG
15	P	179	ALA
15	P	214	ASP
15	P	229	GLU
16	Q	36	GLN
16	Q	197	MET
18	T	83	ARG
6	X	140	CYS
22	Y	85	PRO
25	b	37	PRO
25	b	109	THR
26	c	164	ASN
28	e	61	PRO
28	e	111	ASP
30	g	10	LEU
30	g	12	PHE
30	g	50	ARG
32	i	87	THR
34	k	83	ASN
34	k	96	LEU
35	l	65	ASN
35	l	451	LEU
35	l	549	PRO
35	l	554	ASP
35	l	563	PRO
36	m	4	ALA
36	m	76	GLU
36	m	110	ASP
38	o	5	LYS
38	o	12	ARG
40	r	139	GLN
41	s	38	ASN
42	u	36	CYS
42	u	101	ARG
42	u	143	HIS
43	v	73	SER
44	w	351	TRP
46	y	104	TRP
51	3	61	SER
58	AA	13	HIS
58	AA	29	HIS

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Mol	Chain	Res	Type
59	AB	38	PRO
63	AF	8	SER
65	AH	133	ARG
67	AK	244	LEU
68	AL	180	ARG
68	AL	312	GLY
68	AL	322	VAL
58	AN	46	PHE
59	AO	51	SER
67	AW	241	ARG
67	AW	261	GLN
68	AY	382	SER
1	A	50	ASP
1	A	186	ALA
3	C	156	GLY
7	H	76	GLN
8	I	108	SER
9	J	100	LEU
9	J	330	PRO
9	J	370	LYS
10	K	78	ASP
11	L	172	VAL
12	M	377	ALA
12	M	426	ASP
13	N	42	ASP
13	N	130	THR
14	O	216	PRO
14	O	230	GLY
15	P	175	GLY
15	P	246	ARG
17	S	36	LYS
21	W	16	TYR
6	X	74	LEU
22	Y	42	PRO
22	Y	87	PRO
25	b	115	GLU
26	c	40	PRO
26	c	41	TYR
30	g	49	ARG
30	g	56	GLY
31	h	32	ARG
31	h	45	HIS

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Mol	Chain	Res	Type
32	i	150	ASN
35	l	249	SER
35	l	387	THR
35	l	562	LEU
38	o	59	LEU
38	o	120	LYS
39	p	76	HIS
40	r	251	ASN
41	s	208	VAL
41	s	288	LEU
41	s	289	LEU
42	u	167	PHE
43	v	36	GLU
45	x	51	ASP
59	AB	51	SER
60	AC	142	ALA
60	AC	204	ARG
60	AC	219	HIS
62	AE	86	LEU
67	AK	261	GLN
68	AL	193	GLN
62	AR	28	ASP
65	AU	133	ARG
67	AW	144	PRO
67	AW	403	ALA
68	AY	193	GLN
68	AY	461	PRO
1	A	228	PRO
1	A	420	GLU
7	H	103	LEU
9	J	259	ASN
12	M	281	ILE
12	M	548	LEU
12	M	667	GLN
15	P	110	SER
15	P	202	PHE
15	P	239	TRP
15	P	245	TYR
16	Q	102	SER
20	V	48	THR
6	X	153	ASP
26	c	171	GLY

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Mol	Chain	Res	Type
32	i	92	GLN
36	m	113	VAL
39	p	175	ARG
42	u	144	SER
44	w	58	ARG
44	w	121	PRO
44	w	160	GLU
46	y	103	GLN
54	6	3	ASN
59	AB	40	GLN
62	AE	28	ASP
68	AL	463	GLU
59	AO	27	ARG
59	AO	40	GLN
60	AP	204	ARG
65	AU	246	PRO
68	AY	463	GLU
3	C	102	ASP
6	G	137	LYS
8	I	70	MET
11	L	96	LYS
12	M	446	GLY
13	N	135	GLN
18	T	90	GLY
25	b	41	GLY
29	f	39	PRO
36	m	24	SER
39	p	32	VAL
40	r	205	VAL
45	x	91	ASP
46	y	158	ASP
51	3	49	PRO
65	AH	246	PRO
66	AJ	286	ASN
68	AL	279	ASP
12	M	435	PRO
21	W	10	MET
41	s	241	ILE
1	A	94	PRO
12	M	575	VAL
36	m	23	PRO
50	2	15	GLY

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Mol	Chain	Res	Type
59	AO	30	VAL
3	C	144	PRO
16	Q	307	PRO
21	W	32	GLY
16	Q	69	VAL
67	AK	320	PRO
10	K	102	GLY
32	i	338	PRO
28	e	135	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	75	83
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
6	X	78/79 (99%)	78 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	62	75
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	91	92
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	371/371 (100%)	369 (100%)	2 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	S	59/59 (100%)	59 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	72/72 (100%)	72 (100%)	0	100	100
20	V	102/102 (100%)	102 (100%)	0	100	100
21	W	119/119 (100%)	119 (100%)	0	100	100
22	Y	57/57 (100%)	49 (86%)	8 (14%)	3	17
23	Z	62/63 (98%)	62 (100%)	0	100	100
24	a	124/124 (100%)	122 (98%)	2 (2%)	58	73
25	b	118/118 (100%)	114 (97%)	4 (3%)	32	55
26	c	124/137 (90%)	124 (100%)	0	100	100
27	d	145/154 (94%)	137 (94%)	8 (6%)	18	44
28	e	90/90 (100%)	90 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	105/105 (100%)	105 (100%)	0	100	100
31	h	90/90 (100%)	90 (100%)	0	100	100
32	i	314/314 (100%)	314 (100%)	0	100	100
33	j	102/103 (99%)	102 (100%)	0	100	100
34	k	85/85 (100%)	82 (96%)	3 (4%)	31	54
35	l	531/532 (100%)	510 (96%)	21 (4%)	27	51
36	m	137/137 (100%)	137 (100%)	0	100	100
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	114/114 (100%)	114 (100%)	0	100	100
39	p	157/157 (100%)	156 (99%)	1 (1%)	84	88
40	r	416/416 (100%)	416 (100%)	0	100	100
41	s	278/278 (100%)	278 (100%)	0	100	100
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	89/111 (80%)	89 (100%)	0	100	100
44	w	249/288 (86%)	249 (100%)	0	100	100
45	x	427/427 (100%)	389 (91%)	38 (9%)	8	29
46	y	211/211 (100%)	191 (90%)	20 (10%)	7	25
47	z	226/226 (100%)	199 (88%)	27 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	0	128/128 (100%)	120 (94%)	8 (6%)	15	40
49	1	95/95 (100%)	89 (94%)	6 (6%)	15	40
50	2	81/81 (100%)	76 (94%)	5 (6%)	15	40
51	3	68/68 (100%)	50 (74%)	18 (26%)	0	3
52	4	67/67 (100%)	58 (87%)	9 (13%)	3	17
53	5	58/58 (100%)	53 (91%)	5 (9%)	8	31
54	6	47/47 (100%)	40 (85%)	7 (15%)	2	14
55	7	39/39 (100%)	37 (95%)	2 (5%)	20	45
56	8	40/40 (100%)	38 (95%)	2 (5%)	20	45
57	9	37/37 (100%)	34 (92%)	3 (8%)	9	33
58	AA	74/74 (100%)	68 (92%)	6 (8%)	9	33
58	AN	73/74 (99%)	73 (100%)	0	100	100
59	AB	46/46 (100%)	46 (100%)	0	100	100
59	AO	45/46 (98%)	45 (100%)	0	100	100
60	AC	166/166 (100%)	166 (100%)	0	100	100
60	AP	166/166 (100%)	166 (100%)	0	100	100
61	AD	52/52 (100%)	52 (100%)	0	100	100
61	AQ	52/52 (100%)	52 (100%)	0	100	100
62	AE	61/71 (86%)	59 (97%)	2 (3%)	33	56
62	AR	61/71 (86%)	59 (97%)	2 (3%)	33	56
63	AF	95/95 (100%)	84 (88%)	11 (12%)	4	20
63	AS	95/95 (100%)	95 (100%)	0	100	100
64	AG	42/42 (100%)	42 (100%)	0	100	100
64	AT	42/42 (100%)	40 (95%)	2 (5%)	21	46
65	AH	207/207 (100%)	207 (100%)	0	100	100
65	AU	207/207 (100%)	206 (100%)	1 (0%)	86	90
66	AJ	330/330 (100%)	327 (99%)	3 (1%)	75	83
66	AV	330/330 (100%)	322 (98%)	8 (2%)	44	63
67	AK	334/335 (100%)	331 (99%)	3 (1%)	75	83
67	AW	335/335 (100%)	332 (99%)	3 (1%)	75	83
68	AL	367/367 (100%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	AY	367/367 (100%)	361 (98%)	6 (2%)	58	73
All	All	12164/12289 (99%)	11911 (98%)	253 (2%)	49	67

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	31	ARG
9	J	85	ARG
9	J	91	ILE
9	J	180	TYR
9	J	212	ARG
12	M	130	ILE
12	M	174	THR
16	Q	268	TRP
16	Q	273	ILE
22	Y	73	PHE
22	Y	75	HIS
22	Y	78	GLU
22	Y	80	VAL
22	Y	81	LEU
22	Y	83	HIS
22	Y	87	PRO
22	Y	97	LEU
24	a	53	ARG
24	a	55	PHE
25	b	21	ARG
25	b	38	GLN
25	b	111	LEU
25	b	112	GLU
27	d	54	ARG
27	d	55	TYR
27	d	57	TYR
27	d	60	ARG
27	d	61	GLN
27	d	113	GLN
27	d	115	TYR
27	d	117	GLN
34	k	1	MET
34	k	3	LEU
34	k	8	ILE
35	l	25	ASN
35	l	59	GLN

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Mol	Chain	Res	Type
35	l	87	MET
35	l	88	MET
35	l	94	LEU
35	l	95	PHE
35	l	97	THR
35	l	99	SER
35	l	191	LEU
35	l	193	SER
35	l	195	SER
35	l	196	TRP
35	l	197	ASP
35	l	217	LEU
35	l	218	LEU
35	l	223	LYS
35	l	226	GLN
35	l	447	ASN
35	l	450	LEU
35	l	452	ASN
35	l	513	MET
39	p	124	GLN
45	x	18	LEU
45	x	35	LEU
45	x	92	MET
45	x	96	ARG
45	x	105	LEU
45	x	109	PHE
45	x	115	SER
45	x	138	HIS
45	x	150	LEU
45	x	159	LEU
45	x	187	SER
45	x	188	VAL
45	x	199	LEU
45	x	213	ARG
45	x	238	PHE
45	x	241	PRO
45	x	273	MET
45	x	295	VAL
45	x	301	THR
45	x	306	THR
45	x	318	VAL
45	x	324	LEU

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Mol	Chain	Res	Type
45	x	347	LEU
45	x	353	LEU
45	x	354	THR
45	x	365	ILE
45	x	369	ASP
45	x	373	VAL
45	x	383	MET
45	x	417	MET
45	x	465	VAL
45	x	467	LEU
45	x	474	GLU
45	x	486	ASP
45	x	492	LEU
45	x	508	PRO
45	x	509	THR
45	x	512	ASN
46	y	7	LEU
46	y	31	VAL
46	y	52	HIS
46	y	60	GLU
46	y	63	THR
46	y	65	TRP
46	y	88	ASP
46	y	92	ASN
46	y	113	TYR
46	y	125	THR
46	y	130	PRO
46	y	134	ARG
46	y	142	VAL
46	y	147	GLU
46	y	148	MET
46	y	170	LEU
46	y	171	LYS
46	y	185	MET
46	y	205	SER
46	y	216	LEU
47	z	1	MET
47	z	11	VAL
47	z	13	PRO
47	z	14	SER
47	z	18	LEU
47	z	19	THR

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Mol	Chain	Res	Type
47	z	22	LEU
47	z	38	ASN
47	z	39	SER
47	z	85	LEU
47	z	92	LEU
47	z	112	LEU
47	z	127	LEU
47	z	128	GLU
47	z	131	LEU
47	z	132	LEU
47	z	137	LEU
47	z	142	VAL
47	z	159	MET
47	z	160	LEU
47	z	163	LEU
47	z	188	ILE
47	z	196	THR
47	z	199	VAL
47	z	214	PHE
47	z	222	GLN
47	z	258	TRP
48	0	31	LYS
48	0	36	SER
48	0	40	LEU
48	0	59	LEU
48	0	62	LEU
48	0	107	ILE
48	0	143	ASN
48	0	147	LYS
49	1	7	THR
49	1	29	LEU
49	1	70	VAL
49	1	79	LYS
49	1	80	GLU
49	1	90	ARG
50	2	37	LYS
50	2	53	THR
50	2	74	LEU
50	2	95	GLN
50	2	98	HIS
51	3	5	LYS
51	3	7	ASP

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Mol	Chain	Res	Type
51	3	8	HIS
51	3	14	ARG
51	3	17	ARG
51	3	33	LEU
51	3	34	ASN
51	3	37	LEU
51	3	38	HIS
51	3	41	HIS
51	3	42	ARG
51	3	43	GLU
51	3	48	ILE
51	3	54	ARG
51	3	56	ARG
51	3	68	THR
51	3	69	PHE
51	3	78	LEU
52	4	19	ARG
52	4	24	ASN
52	4	28	ASN
52	4	29	CYS
52	4	51	SER
52	4	53	CYS
52	4	57	ARG
52	4	60	TYR
52	4	75	ARG
53	5	2	THR
53	5	8	GLN
53	5	26	MET
53	5	44	LYS
53	5	64	ARG
54	6	1	PHE
54	6	2	GLU
54	6	3	ASN
54	6	8	LYS
54	6	16	ASN
54	6	23	LYS
54	6	27	THR
55	7	48	VAL
55	7	49	THR
56	8	15	VAL
56	8	22	LEU
57	9	13	LYS

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Mol	Chain	Res	Type
57	9	42	LYS
57	9	43	SER
58	AA	25	ARG
58	AA	40	ARG
58	AA	48	ARG
58	AA	61	THR
58	AA	64	THR
58	AA	66	GLU
62	AE	28	ASP
62	AE	30	LEU
63	AF	14	LEU
63	AF	17	ILE
63	AF	29	LYS
63	AF	33	MET
63	AF	34	ARG
63	AF	40	GLU
63	AF	41	ASP
63	AF	49	ARG
63	AF	60	MET
63	AF	71	LEU
63	AF	74	GLN
66	AJ	124	MET
66	AJ	150	LEU
66	AJ	300	ILE
67	AK	49	ILE
67	AK	365	ASN
67	AK	451	ASP
62	AR	78	ARG
62	AR	81	CYS
64	AT	39	ARG
64	AT	40	LEU
65	AU	292	MET
66	AV	147	THR
66	AV	149	LEU
66	AV	183	PHE
66	AV	185	LEU
66	AV	192	LEU
66	AV	195	LEU
66	AV	299	LEU
66	AV	345	TYR
67	AW	254	ARG
67	AW	451	ASP

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Mol	Chain	Res	Type
67	AW	453	LEU
68	AY	92	PHE
68	AY	96	LEU
68	AY	416	SER
68	AY	418	LEU
68	AY	422	ARG
68	AY	423	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	116	ASN
1	A	164	ASN
1	A	170	GLN
1	A	284	HIS
1	A	313	ASN
1	A	441	HIS
2	B	184	ASN
3	C	95	HIS
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
4	E	70	ASN
5	F	62	GLN
5	F	81	ASN
6	G	80	GLN
6	G	101	ASN
7	H	50	GLN
7	H	73	GLN
7	H	76	GLN
7	H	83	GLN
7	H	111	GLN
8	I	73	GLN
9	J	71	ASN
9	J	102	GLN
9	J	183	ASN
10	K	77	HIS
11	L	71	HIS
11	L	86	ASN
12	M	384	ASN
12	M	425	ASN

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Mol	Chain	Res	Type
12	M	444	HIS
12	M	460	HIS
12	M	464	GLN
12	M	498	GLN
12	M	514	ASN
12	M	688	GLN
13	N	91	HIS
13	N	113	HIS
13	N	135	GLN
14	O	59	ASN
14	O	69	ASN
14	O	189	ASN
14	O	191	ASN
15	P	74	GLN
15	P	82	ASN
15	P	105	ASN
15	P	124	ASN
15	P	247	GLN
16	Q	38	GLN
16	Q	147	ASN
16	Q	182	ASN
16	Q	183	HIS
16	Q	190	HIS
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
16	Q	431	HIS
16	Q	442	HIS
16	Q	454	GLN
17	S	44	HIS
17	S	68	ASN
18	T	64	ASN
21	W	8	GLN
21	W	61	GLN
21	W	112	HIS
21	W	135	HIS
22	Y	75	HIS
24	a	90	ASN
24	a	189	ASN
25	b	14	GLN
25	b	83	HIS
25	b	89	HIS

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Mol	Chain	Res	Type
25	b	126	GLN
26	c	56	ASN
26	c	84	HIS
26	c	154	GLN
27	d	59	HIS
27	d	61	GLN
27	d	85	GLN
27	d	113	GLN
27	d	117	GLN
27	d	138	GLN
30	g	60	GLN
30	g	96	HIS
32	i	83	GLN
32	i	112	HIS
32	i	150	ASN
32	i	186	HIS
32	i	222	ASN
33	j	10	ASN
34	k	7	ASN
34	k	94	ASN
35	l	4	HIS
35	l	59	GLN
35	l	139	GLN
35	l	192	HIS
35	l	199	GLN
35	l	205	ASN
35	l	226	GLN
35	l	248	HIS
35	l	274	GLN
35	l	296	ASN
35	l	320	ASN
35	l	332	HIS
35	l	348	HIS
35	l	394	HIS
35	l	400	ASN
35	l	442	ASN
35	l	446	ASN
35	l	534	HIS
35	l	569	HIS
35	l	580	GLN
36	m	45	ASN
36	m	117	ASN

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Mol	Chain	Res	Type
37	n	40	ASN
38	o	62	ASN
38	o	126	HIS
39	p	75	GLN
40	r	48	ASN
40	r	168	HIS
40	r	390	ASN
40	r	415	GLN
40	r	425	ASN
41	s	93	ASN
41	s	169	GLN
41	s	235	ASN
42	u	30	HIS
42	u	31	HIS
42	u	64	ASN
42	u	77	HIS
42	u	99	HIS
42	u	104	GLN
42	u	143	HIS
43	v	43	GLN
43	v	61	HIS
43	v	85	HIS
43	v	92	HIS
44	w	85	HIS
44	w	111	ASN
44	w	132	GLN
44	w	149	HIS
44	w	257	GLN
45	x	11	ASN
45	x	12	HIS
45	x	43	GLN
45	x	99	ASN
45	x	170	ASN
45	x	256	HIS
45	x	360	ASN
45	x	413	HIS
45	x	512	ASN
46	y	103	GLN
46	y	203	ASN
47	z	6	HIS
47	z	12	ASN
47	z	133	ASN

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Mol	Chain	Res	Type
47	z	148	HIS
47	z	207	HIS
47	z	222	GLN
47	z	232	HIS
48	0	109	HIS
49	1	34	ASN
50	2	66	ASN
51	3	52	HIS
52	4	23	GLN
52	4	24	ASN
52	4	25	GLN
52	4	28	ASN
52	4	37	HIS
54	6	3	ASN
54	6	16	ASN
55	7	10	HIS
55	7	15	ASN
55	7	41	ASN
57	9	39	ASN
58	AA	29	HIS
59	AB	31	GLN
60	AC	80	HIS
60	AC	135	GLN
60	AC	178	HIS
63	AF	23	ASN
63	AF	70	ASN
63	AF	73	HIS
64	AG	16	ASN
65	AH	107	HIS
65	AH	205	HIS
66	AJ	8	ASN
66	AJ	97	HIS
66	AJ	322	GLN
67	AK	167	GLN
67	AK	178	HIS
67	AK	184	ASN
67	AK	206	HIS
67	AK	212	HIS
67	AK	310	HIS
67	AK	311	GLN
67	AK	343	GLN
67	AK	399	GLN

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Mol	Chain	Res	Type
68	AL	87	ASN
68	AL	188	HIS
68	AL	239	HIS
68	AL	240	GLN
68	AL	301	ASN
68	AL	308	ASN
60	AP	135	GLN
60	AP	178	HIS
61	AQ	38	GLN
62	AR	80	HIS
62	AR	84	HIS
63	AS	70	ASN
63	AS	73	HIS
65	AU	284	HIS
66	AV	97	HIS
66	AV	137	GLN
66	AV	255	ASN
66	AV	260	ASN
67	AW	81	HIS
67	AW	139	ASN
67	AW	155	GLN
67	AW	206	HIS
67	AW	212	HIS
67	AW	227	HIS
67	AW	291	HIS
67	AW	298	HIS
67	AW	310	HIS
67	AW	421	ASN
67	AW	446	HIS
68	AY	87	ASN
68	AY	121	ASN
68	AY	152	GLN
68	AY	223	HIS
68	AY	301	ASN
68	AY	342	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 5 are monoatomic - leaving 58 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$
69	SF4	B	301	2	0,12,12	-	-	-		
69	SF4	B	302	2	0,12,12	-	-	-		
71	PLX	b	201	-	51,51,51	0.57	0	55,59,59	0.64	0
75	CDL	AU	403	-	63,63,99	1.24	6 (9%)	69,75,111	1.04	4 (5%)
79	HEA	x	603	45	57,67,67	1.23	6 (10%)	61,103,103	1.47	10 (16%)
76	PEE	V	202	-	50,50,50	1.16	6 (12%)	53,55,55	0.91	2 (3%)
69	SF4	C	301	3	0,12,12	-	-	-		
74	FES	AP	301	60	0,4,4	-	-	-		
74	FES	AC	301	60	0,4,4	-	-	-		
74	FES	M	803	-	0,4,4	-	-	-		
75	CDL	i	401	-	63,63,99	1.21	5 (7%)	69,75,111	1.04	5 (7%)
76	PEE	AY	502	-	48,48,50	1.39	4 (8%)	51,53,55	0.96	2 (3%)
76	PEE	AU	401	-	40,40,50	1.46	4 (10%)	43,45,55	0.95	3 (6%)
81	HEC	AU	402	65	32,50,50	2.28	3 (9%)	24,82,82	1.40	2 (8%)
71	PLX	g	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.58	1 (1%)
73	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.32	4 (7%)
69	SF4	M	802	12	0,12,12	-	-	-		
75	CDL	AA	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
76	PEE	AH	401	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	2 (3%)
82	HEM	AJ	401	66	41,50,50	1.92	6 (14%)	45,82,82	1.60	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	PLX	B	303	-	51,51,51	0.77	1 (1%)	55,59,59	0.68	1 (1%)
75	CDL	V	201	-	61,61,99	1.21	5 (8%)	64,71,111	0.94	3 (4%)
76	PEE	W	201	-	50,50,50	1.14	6 (12%)	53,55,55	0.97	2 (3%)
82	HEM	AJ	402	66	41,50,50	1.89	6 (14%)	45,82,82	1.57	9 (20%)
71	PLX	V	203	-	51,51,51	0.78	1 (1%)	55,59,59	0.60	1 (1%)
75	CDL	l	704	-	63,63,99	1.26	5 (7%)	69,75,111	1.01	4 (5%)
71	PLX	r	502	-	51,51,51	0.64	0	55,59,59	0.67	1 (1%)
75	CDL	AJ	404	-	63,63,99	1.24	5 (7%)	69,75,111	1.03	4 (5%)
71	PLX	AT	101	-	51,51,51	0.75	1 (1%)	55,59,59	0.60	1 (1%)
75	CDL	AJ	405	-	63,63,99	1.13	4 (6%)	69,75,111	1.22	5 (7%)
75	CDL	AN	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.02	4 (5%)
71	PLX	g	201	-	51,51,51	0.82	1 (1%)	55,59,59	0.69	1 (1%)
75	CDL	n	101	-	63,63,99	1.24	5 (7%)	69,75,111	1.07	4 (5%)
69	SF4	A	501	1	0,12,12	-	-	-	-	-
76	PEE	l	701	-	48,48,50	1.34	4 (8%)	51,53,55	0.96	2 (3%)
79	HEA	x	604	45	57,67,67	1.47	6 (10%)	61,103,103	1.47	12 (19%)
69	SF4	M	801	12	0,12,12	-	-	-	-	-
81	HEC	AH	402	65	32,50,50	2.22	3 (9%)	24,82,82	1.35	1 (4%)
75	CDL	l	703	-	63,63,99	1.21	5 (7%)	69,75,111	1.07	4 (5%)
72	8Q1	p	201	-	31,34,34	1.67	5 (16%)	40,43,43	1.57	5 (12%)
72	8Q1	E	201	-	31,34,34	1.64	6 (19%)	40,43,43	1.39	7 (17%)
71	PLX	r	501	-	51,51,51	0.74	1 (1%)	55,59,59	0.65	1 (1%)
71	PLX	AL	501	-	51,51,51	0.77	1 (1%)	55,59,59	0.63	1 (1%)
76	PEE	AL	503	-	48,48,50	1.38	4 (8%)	51,53,55	0.92	2 (3%)
76	PEE	l	702	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
75	CDL	AY	501	-	63,63,99	1.24	5 (7%)	69,75,111	1.01	4 (5%)
76	PEE	AJ	403	-	48,48,50	1.33	4 (8%)	51,53,55	0.99	2 (3%)
82	HEM	AV	401	66	41,50,50	1.97	5 (12%)	45,82,82	1.55	5 (11%)
71	PLX	g	202	-	51,51,51	0.74	1 (1%)	55,59,59	0.61	1 (1%)
71	PLX	AQ	101	-	51,51,51	0.77	1 (1%)	55,59,59	0.61	2 (3%)
74	FES	O	301	14	0,4,4	-	-	-	-	-
75	CDL	AG	101	-	63,63,99	1.15	4 (6%)	69,75,111	1.16	6 (8%)
71	PLX	U	101	-	51,51,51	0.74	1 (1%)	55,59,59	0.72	2 (3%)
75	CDL	AL	502	-	63,63,99	1.24	5 (7%)	69,75,111	1.05	4 (5%)
82	HEM	AV	402	66	41,50,50	1.90	6 (14%)	45,82,82	1.60	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
76	PEE	AV	403	-	48,48,50	1.34	4 (8%)	51,53,55	1.04	2 (3%)
70	FMN	A	502	-	33,33,33	1.39	6 (18%)	48,50,50	1.34	8 (16%)
75	CDL	AH	403	-	63,63,99	1.25	5 (7%)	69,75,111	1.03	4 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	SF4	B	301	2	-	-	0/6/5/5
69	SF4	B	302	2	-	-	0/6/5/5
71	PLX	b	201	-	-	27/55/55/55	-
75	CDL	AU	403	-	-	48/74/74/110	-
79	HEA	x	603	45	-	7/32/76/76	-
76	PEE	V	202	-	-	27/54/54/54	-
69	SF4	C	301	3	-	-	0/6/5/5
74	FES	AP	301	60	-	-	0/1/1/1
74	FES	AC	301	60	-	-	0/1/1/1
74	FES	M	803	-	-	-	0/1/1/1
75	CDL	i	401	-	-	39/74/74/110	-
76	PEE	AY	502	-	-	20/52/52/54	-
76	PEE	AU	401	-	-	17/44/44/54	-
81	HEC	AU	402	65	-	0/10/54/54	-
71	PLX	g	203	-	-	24/55/55/55	-
73	NDP	J	401	-	-	15/30/77/77	0/5/5/5
69	SF4	M	802	12	-	-	0/6/5/5
75	CDL	AA	101	-	-	35/74/74/110	-
76	PEE	AH	401	-	-	27/52/52/54	-
82	HEM	AJ	401	66	-	1/12/54/54	-
71	PLX	B	303	-	-	21/55/55/55	-
75	CDL	V	201	-	-	41/69/69/110	-
76	PEE	W	201	-	-	32/54/54/54	-
82	HEM	AJ	402	66	-	2/12/54/54	-
71	PLX	V	203	-	-	26/55/55/55	-
75	CDL	l	704	-	-	44/74/74/110	-
71	PLX	r	502	-	-	36/55/55/55	-
75	CDL	AJ	404	-	-	33/74/74/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	PLX	AT	101	-	-	23/55/55/55	-
75	CDL	AJ	405	-	-	28/74/74/110	-
75	CDL	AN	101	-	-	40/74/74/110	-
71	PLX	g	201	-	-	25/55/55/55	-
75	CDL	n	101	-	-	33/74/74/110	-
76	PEE	l	701	-	-	32/52/52/54	-
79	HEA	x	604	45	-	5/32/76/76	-
69	SF4	A	501	1	-	-	0/6/5/5
81	HEC	AH	402	65	-	2/10/54/54	-
69	SF4	M	801	12	-	-	0/6/5/5
75	CDL	l	703	-	-	38/74/74/110	-
72	8Q1	p	201	-	-	19/41/41/41	-
72	8Q1	E	201	-	-	18/41/41/41	-
71	PLX	r	501	-	-	28/55/55/55	-
71	PLX	AL	501	-	-	23/55/55/55	-
76	PEE	AL	503	-	-	22/52/52/54	-
76	PEE	l	702	-	-	27/54/54/54	-
75	CDL	AY	501	-	-	36/74/74/110	-
76	PEE	AJ	403	-	-	20/52/52/54	-
82	HEM	AV	401	66	-	3/12/54/54	-
71	PLX	g	202	-	-	25/55/55/55	-
71	PLX	AQ	101	-	-	25/55/55/55	-
75	CDL	AG	101	-	-	38/74/74/110	-
74	FES	O	301	14	-	-	0/1/1/1
71	PLX	U	101	-	-	22/55/55/55	-
75	CDL	AL	502	-	-	43/74/74/110	-
82	HEM	AV	402	66	-	4/12/54/54	-
76	PEE	AV	403	-	-	30/52/52/54	-
70	FMN	A	502	-	-	7/18/18/18	0/3/3/3
75	CDL	AH	403	-	-	42/74/74/110	-

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AJ	401	HEM	C3D-C2D	7.85	1.53	1.36
82	AV	402	HEM	C3D-C2D	7.85	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AJ	402	HEM	C3D-C2D	7.80	1.53	1.36
82	AV	401	HEM	C3D-C2D	7.75	1.53	1.36
81	AU	402	HEC	C3C-C2C	-6.96	1.33	1.40
81	AU	402	HEC	C2B-C3B	-6.69	1.33	1.40
81	AH	402	HEC	C2B-C3B	-6.55	1.33	1.40
81	AH	402	HEC	C3C-C2C	-6.54	1.33	1.40
79	x	604	HEA	C3A-C2A	-6.50	1.31	1.40
82	AV	401	HEM	C3C-C2C	-5.46	1.32	1.40
81	AU	402	HEC	C3D-C2D	5.43	1.53	1.37
81	AH	402	HEC	C3D-C2D	5.38	1.53	1.37
72	p	201	8Q1	C34-N36	5.33	1.45	1.33
72	E	201	8Q1	C34-N36	5.26	1.45	1.33
72	p	201	8Q1	C39-N41	5.24	1.45	1.33
72	E	201	8Q1	C39-N41	4.91	1.44	1.33
70	A	502	FMN	C9A-C5A	4.40	1.48	1.41
75	l	704	CDL	OB8-CB7	4.35	1.46	1.33
75	AH	403	CDL	OA6-CA5	4.34	1.46	1.34
75	AL	502	CDL	OA6-CA5	4.32	1.46	1.34
75	AH	403	CDL	OB8-CB7	4.31	1.45	1.33
75	n	101	CDL	OA6-CA5	4.30	1.46	1.34
76	AY	502	PEE	C39-C38	4.30	1.56	1.31
75	AY	501	CDL	OA6-CA5	4.30	1.46	1.34
75	AG	101	CDL	OB8-CB7	4.30	1.45	1.33
75	AU	403	CDL	OA6-CA5	4.28	1.46	1.34
75	AJ	405	CDL	OA8-CA7	4.28	1.45	1.33
76	AU	401	PEE	C39-C38	4.27	1.56	1.31
75	V	201	CDL	OA6-CA5	4.27	1.46	1.34
75	AJ	404	CDL	OA6-CA5	4.27	1.46	1.34
75	l	703	CDL	OA6-CA5	4.26	1.46	1.34
76	AL	503	PEE	C39-C38	4.26	1.56	1.31
76	AV	403	PEE	C39-C38	4.25	1.56	1.31
76	AL	503	PEE	O3-C30	4.25	1.45	1.33
75	AU	403	CDL	OB8-CB7	4.24	1.45	1.33
76	AJ	403	PEE	C39-C38	4.24	1.56	1.31
75	AG	101	CDL	OA6-CA5	4.23	1.46	1.34
75	l	703	CDL	OB8-CB7	4.23	1.45	1.33
75	AL	502	CDL	OB8-CB7	4.23	1.45	1.33
76	AH	401	PEE	C39-C38	4.23	1.56	1.31
75	AG	101	CDL	OA8-CA7	4.22	1.45	1.33
75	AY	501	CDL	OB8-CB7	4.22	1.45	1.33
76	AY	502	PEE	O3-C30	4.22	1.45	1.33
76	AY	502	PEE	C18-C19	4.21	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	AH	401	PEE	C18-C19	4.20	1.56	1.31
75	V	201	CDL	OB8-CB7	4.20	1.45	1.33
76	AL	503	PEE	C18-C19	4.20	1.56	1.31
76	AH	401	PEE	O3-C30	4.20	1.45	1.33
75	AA	101	CDL	OB8-CB7	4.19	1.45	1.33
75	AJ	404	CDL	OB8-CB7	4.19	1.45	1.33
76	l	701	PEE	C39-C38	4.17	1.56	1.31
75	AA	101	CDL	OA6-CA5	4.17	1.46	1.34
75	AJ	405	CDL	OB8-CB7	4.16	1.45	1.33
75	AN	101	CDL	OA6-CA5	4.16	1.46	1.34
75	l	704	CDL	OA8-CA7	4.15	1.45	1.33
82	AJ	401	HEM	C3C-C2C	-4.15	1.34	1.40
76	AJ	403	PEE	C18-C19	4.15	1.55	1.31
75	l	704	CDL	OA6-CA5	4.15	1.46	1.34
76	l	701	PEE	O3-C30	4.13	1.45	1.33
76	AV	403	PEE	C18-C19	4.13	1.55	1.31
75	AN	101	CDL	OB8-CB7	4.13	1.45	1.33
76	l	701	PEE	C18-C19	4.13	1.55	1.31
76	AV	403	PEE	O3-C30	4.12	1.45	1.33
76	AU	401	PEE	O3-C30	4.12	1.45	1.33
75	n	101	CDL	OB8-CB7	4.11	1.45	1.33
75	AJ	405	CDL	OB6-CB5	4.09	1.45	1.34
76	AU	401	PEE	C19-C18	4.07	1.56	1.28
75	i	401	CDL	OB8-CB7	4.06	1.45	1.33
75	AG	101	CDL	OB6-CB5	4.03	1.45	1.34
82	AV	402	HEM	C3C-C2C	-3.99	1.34	1.40
75	i	401	CDL	OA6-CA5	3.99	1.45	1.34
76	AJ	403	PEE	O3-C30	3.98	1.45	1.33
75	AJ	405	CDL	OA6-CA5	3.98	1.45	1.34
75	AJ	404	CDL	OA8-CA7	3.97	1.44	1.33
82	AJ	402	HEM	C3C-C2C	-3.97	1.34	1.40
75	AY	501	CDL	OA8-CA7	3.96	1.44	1.33
75	AH	403	CDL	OA8-CA7	3.94	1.44	1.33
75	AU	403	CDL	OA8-CA7	3.94	1.44	1.33
79	x	604	HEA	C3A-CMA	-3.92	1.37	1.46
75	n	101	CDL	OA8-CA7	3.91	1.44	1.33
75	AL	502	CDL	OA8-CA7	3.91	1.44	1.33
75	AN	101	CDL	OA8-CA7	3.91	1.44	1.33
75	AA	101	CDL	OA8-CA7	3.90	1.44	1.33
75	l	703	CDL	OA8-CA7	3.82	1.44	1.33
82	AV	402	HEM	C3C-CAC	3.77	1.55	1.47
76	l	702	PEE	C18-C19	3.77	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	V	202	PEE	C18-C19	3.77	1.53	1.31
76	W	201	PEE	C18-C19	3.74	1.53	1.31
75	i	401	CDL	OA8-CA7	3.71	1.44	1.33
76	V	202	PEE	C39-C38	3.71	1.53	1.31
82	AJ	401	HEM	C3C-CAC	3.71	1.55	1.47
76	l	702	PEE	C39-C38	3.69	1.53	1.31
76	W	201	PEE	C39-C38	3.68	1.53	1.31
82	AJ	402	HEM	C3C-CAC	3.60	1.55	1.47
76	AY	502	PEE	O2-C10	3.46	1.44	1.34
76	AL	503	PEE	O2-C10	3.45	1.44	1.34
82	AV	401	HEM	C3C-CAC	3.41	1.54	1.47
75	l	704	CDL	OB6-CB5	3.35	1.43	1.34
76	l	701	PEE	O2-C10	3.33	1.43	1.34
75	AY	501	CDL	OB6-CB5	3.29	1.43	1.34
75	n	101	CDL	OB6-CB5	3.27	1.43	1.34
75	AJ	404	CDL	OB6-CB5	3.24	1.43	1.34
76	AJ	403	PEE	O2-C10	3.23	1.43	1.34
75	AN	101	CDL	OB6-CB5	3.22	1.43	1.34
75	l	703	CDL	OB6-CB5	3.22	1.43	1.34
75	AH	403	CDL	OB6-CB5	3.20	1.43	1.34
79	x	603	HEA	C3C-C2C	-3.18	1.35	1.40
76	AU	401	PEE	O2-C10	3.18	1.43	1.34
75	AA	101	CDL	OB6-CB5	3.15	1.43	1.34
76	AV	403	PEE	O2-C10	3.15	1.43	1.34
75	AU	403	CDL	OB6-CB5	3.14	1.43	1.34
73	J	401	NDP	C6N-C5N	3.13	1.38	1.33
76	AH	401	PEE	O2-C10	3.11	1.43	1.34
75	V	201	CDL	OB6-CB5	3.11	1.43	1.34
75	AL	502	CDL	OB6-CB5	3.10	1.43	1.34
70	A	502	FMN	C8-C7	3.07	1.48	1.40
75	i	401	CDL	OB6-CB5	3.07	1.43	1.34
70	A	502	FMN	C4-N3	-3.03	1.33	1.38
75	V	201	CDL	OA8-CA7	3.01	1.45	1.33
82	AJ	402	HEM	CAB-C3B	2.97	1.55	1.47
71	B	303	PLX	O6-C4	-2.97	1.40	1.44
82	AV	401	HEM	CAB-C3B	2.97	1.55	1.47
82	AJ	401	HEM	CAB-C3B	2.93	1.55	1.47
82	AV	402	HEM	CAB-C3B	2.91	1.55	1.47
71	g	203	PLX	O6-C4	-2.90	1.40	1.44
79	x	603	HEA	C3A-CMA	-2.87	1.39	1.46
71	g	201	PLX	O6-C4	-2.76	1.40	1.44
75	n	101	CDL	OB6-CB4	-2.76	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	V	203	PLX	O6-C4	-2.75	1.40	1.44
79	x	604	HEA	C3C-C2C	-2.75	1.36	1.40
79	x	603	HEA	C4C-NC	2.70	1.41	1.36
71	AL	501	PLX	O6-C4	-2.68	1.41	1.44
75	AL	502	CDL	OB6-CB4	-2.63	1.40	1.46
79	x	604	HEA	C1D-C2D	2.62	1.49	1.44
75	V	201	CDL	OB6-CB4	-2.62	1.40	1.46
75	AH	403	CDL	OB6-CB4	-2.60	1.40	1.46
82	AV	401	HEM	FE-ND	2.60	2.09	1.96
75	AA	101	CDL	OB6-CB4	-2.58	1.40	1.46
71	AQ	101	PLX	O6-C4	-2.58	1.41	1.44
79	x	604	HEA	C1D-ND	-2.57	1.35	1.40
71	U	101	PLX	O6-C4	-2.57	1.41	1.44
75	AJ	404	CDL	OB6-CB4	-2.55	1.40	1.46
75	AN	101	CDL	OB6-CB4	-2.54	1.40	1.46
75	AU	403	CDL	OB6-CB4	-2.52	1.40	1.46
75	i	401	CDL	OB6-CB4	-2.50	1.40	1.46
72	E	201	8Q1	O35-C34	-2.49	1.18	1.23
72	p	201	8Q1	O35-C34	-2.49	1.18	1.23
71	AT	101	PLX	O6-C4	-2.47	1.41	1.44
75	AY	501	CDL	OB6-CB4	-2.46	1.40	1.46
71	g	202	PLX	O6-C4	-2.43	1.41	1.44
76	V	202	PEE	O2-C10	2.39	1.41	1.34
71	r	501	PLX	O6-C4	-2.38	1.41	1.44
76	l	702	PEE	O2-C10	2.38	1.41	1.34
72	E	201	8Q1	C1-S44	2.36	1.81	1.76
75	l	704	CDL	OB6-CB4	-2.36	1.40	1.46
75	l	703	CDL	OB6-CB4	-2.34	1.40	1.46
72	E	201	8Q1	O40-C39	-2.34	1.18	1.23
72	p	201	8Q1	O40-C39	-2.33	1.18	1.23
76	l	702	PEE	O3-C30	2.33	1.40	1.33
70	A	502	FMN	C5A-N5	-2.30	1.35	1.39
76	V	202	PEE	O3-C30	2.25	1.39	1.33
76	l	702	PEE	O2-C2	-2.25	1.41	1.46
76	V	202	PEE	O2-C2	-2.24	1.41	1.46
79	x	603	HEA	C3A-C2A	-2.24	1.37	1.40
76	W	201	PEE	O3-C30	2.24	1.39	1.33
79	x	604	HEA	CMD-C2D	2.24	1.55	1.50
72	p	201	8Q1	C1-S44	2.22	1.81	1.76
76	V	202	PEE	O3-C3	-2.22	1.40	1.45
79	x	603	HEA	C1C-NC	2.22	1.40	1.36
76	W	201	PEE	O2-C10	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	l	702	PEE	O3-C3	-2.20	1.40	1.45
72	E	201	8Q1	C6-C1	2.20	1.53	1.50
76	W	201	PEE	O2-C2	-2.18	1.41	1.46
82	AJ	401	HEM	FE-NB	2.17	2.07	1.96
70	A	502	FMN	C4A-N5	2.16	1.34	1.30
82	AJ	402	HEM	FE-ND	2.16	2.07	1.96
76	W	201	PEE	O3-C3	-2.14	1.40	1.45
82	AV	402	HEM	CAA-C2A	2.13	1.55	1.52
82	AJ	402	HEM	CAA-C2A	2.12	1.55	1.52
70	A	502	FMN	C2-N3	-2.04	1.34	1.39
73	J	401	NDP	C5A-C4A	2.04	1.46	1.40
82	AJ	401	HEM	FE-ND	2.04	2.07	1.96
75	AU	403	CDL	C11-CA5	2.04	1.56	1.50
79	x	603	HEA	CHD-C1D	2.03	1.40	1.35
82	AV	402	HEM	FE-ND	2.01	2.06	1.96

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	AV	402	HEM	C4D-ND-C1D	6.20	111.47	105.07
82	AJ	401	HEM	C4D-ND-C1D	6.12	111.39	105.07
82	AJ	402	HEM	C4D-ND-C1D	6.02	111.30	105.07
72	p	201	8Q1	C6-C1-S44	6.02	120.47	113.46
82	AV	401	HEM	C4D-ND-C1D	5.32	110.57	105.07
73	J	401	NDP	PN-O3-PA	-5.21	114.95	132.83
72	E	201	8Q1	C6-C1-S44	4.57	118.77	113.46
76	l	702	PEE	O2-C10-C11	4.38	120.95	111.50
76	AY	502	PEE	O2-C10-C11	4.31	120.78	111.50
75	AJ	405	CDL	OB6-CB5-C51	4.29	120.74	111.50
75	AL	502	CDL	OA6-CA5-C11	4.26	120.69	111.50
75	AY	501	CDL	OA6-CA5-C11	4.20	120.55	111.50
75	l	703	CDL	OA6-CA5-C11	4.19	120.54	111.50
75	AG	101	CDL	OB6-CB5-C51	4.19	120.53	111.50
75	AH	403	CDL	OA6-CA5-C11	4.16	120.47	111.50
75	AU	403	CDL	OA6-CA5-C11	4.15	120.45	111.50
75	i	401	CDL	OA6-CA5-C11	4.13	120.41	111.50
75	AJ	404	CDL	OA6-CA5-C11	4.12	120.39	111.50
75	V	201	CDL	OB6-CB5-C51	4.09	120.31	111.50
75	l	704	CDL	OA6-CA5-C11	4.09	120.31	111.50
75	AA	101	CDL	OA6-CA5-C11	4.08	120.30	111.50
75	n	101	CDL	OB6-CB5-C51	4.08	120.30	111.50
75	AU	403	CDL	OB6-CB5-C51	4.04	120.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	AJ	404	CDL	OB6-CB5-C51	4.03	120.19	111.50
76	AJ	403	PEE	O2-C10-C11	4.03	120.19	111.50
76	l	701	PEE	O2-C10-C11	4.00	120.13	111.50
75	AA	101	CDL	OB6-CB5-C51	3.99	120.10	111.50
79	x	603	HEA	C17-C18-C19	-3.98	118.09	127.66
75	l	703	CDL	OB6-CB5-C51	3.95	120.02	111.50
75	AN	101	CDL	OA6-CA5-C11	3.95	120.01	111.50
75	n	101	CDL	OA6-CA5-C11	3.93	119.97	111.50
75	AH	403	CDL	OB6-CB5-C51	3.92	119.95	111.50
75	l	704	CDL	OB6-CB5-C51	3.92	119.95	111.50
76	AV	403	PEE	O2-C10-C11	3.91	119.93	111.50
75	AY	501	CDL	OB6-CB5-C51	3.88	119.87	111.50
75	AN	101	CDL	OB6-CB5-C51	3.87	119.83	111.50
75	AL	502	CDL	OB6-CB5-C51	3.85	119.79	111.50
73	J	401	NDP	N3A-C2A-N1A	-3.75	122.81	128.68
76	W	201	PEE	O2-C10-C11	3.69	119.45	111.50
72	p	201	8Q1	O4-C1-C6	-3.65	119.68	123.99
76	V	202	PEE	O2-C10-C11	3.61	119.28	111.50
79	x	604	HEA	C4A-CHB-C1B	3.59	127.29	122.56
75	AG	101	CDL	OA6-CA5-C11	3.58	119.21	111.50
76	AH	401	PEE	O2-C10-C11	3.55	119.16	111.50
75	AJ	405	CDL	OA6-CA5-C11	3.55	119.15	111.50
76	AL	503	PEE	O2-C10-C11	3.51	119.06	111.50
75	i	401	CDL	OB6-CB5-C51	3.49	119.03	111.50
75	V	201	CDL	OA6-CA5-C11	3.45	118.93	111.50
75	AJ	405	CDL	OB8-CB7-C71	3.25	122.11	111.91
76	AU	401	PEE	O2-C10-C11	3.23	118.46	111.50
79	x	603	HEA	C13-C14-C15	-3.13	120.13	127.66
82	AV	401	HEM	C4B-CHC-C1C	3.07	126.61	122.56
76	AV	403	PEE	O3-C30-C31	3.06	121.52	111.91
75	l	703	CDL	OA8-CA7-C31	2.99	121.29	111.91
82	AV	401	HEM	CAD-CBD-CGD	-2.98	107.20	113.60
75	AA	101	CDL	OA8-CA7-C31	2.97	121.22	111.91
79	x	603	HEA	C1B-C2B-C3B	2.93	110.30	106.80
75	AG	101	CDL	CB4-OB6-CB5	-2.90	110.64	117.79
79	x	604	HEA	CBA-CAA-C2A	2.85	117.41	112.60
76	V	202	PEE	O3-C30-C31	2.85	120.85	111.91
82	AJ	401	HEM	C4C-CHD-C1D	2.85	126.32	122.56
76	l	702	PEE	O3-C30-C31	2.84	120.82	111.91
82	AJ	401	HEM	C4B-CHC-C1C	2.83	126.29	122.56
70	A	502	FMN	C4-C4A-N5	2.80	122.22	118.23
72	E	201	8Q1	C43-S44-C1	2.79	110.57	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	AV	401	HEM	C4C-CHD-C1D	2.76	126.21	122.56
75	i	401	CDL	OB8-CB7-C71	2.76	120.57	111.91
70	A	502	FMN	C4A-C10-N1	-2.75	118.34	124.73
75	n	101	CDL	OA8-CA7-C31	2.75	120.54	111.91
75	AG	101	CDL	OB8-CB7-C71	2.74	120.51	111.91
72	E	201	8Q1	C32-C34-N36	2.74	122.03	116.58
75	AL	502	CDL	OA8-CA7-C31	2.72	120.46	111.91
75	l	704	CDL	OA8-CA7-C31	2.72	120.45	111.91
72	p	201	8Q1	C43-S44-C1	2.72	110.34	101.87
75	AJ	405	CDL	OA8-CA7-C31	2.70	120.40	111.91
75	l	703	CDL	OB8-CB7-C71	2.69	120.36	111.91
75	AL	502	CDL	OB8-CB7-C71	2.69	120.36	111.91
75	n	101	CDL	OB8-CB7-C71	2.69	120.34	111.91
75	AN	101	CDL	OA8-CA7-C31	2.68	120.33	111.91
76	W	201	PEE	O3-C30-C31	2.68	120.33	111.91
75	AH	403	CDL	OB8-CB7-C71	2.67	120.30	111.91
82	AV	402	HEM	C4C-CHD-C1D	2.67	126.08	122.56
75	l	704	CDL	OB8-CB7-C71	2.67	120.28	111.91
75	AU	403	CDL	OA8-CA7-C31	2.66	120.25	111.91
75	AJ	404	CDL	OA8-CA7-C31	2.66	120.25	111.91
76	AH	401	PEE	O3-C30-C31	2.65	120.23	111.91
82	AJ	402	HEM	C1B-NB-C4B	2.63	107.79	105.07
79	x	604	HEA	CMD-C2D-C1D	2.62	129.03	125.04
75	AA	101	CDL	OB8-CB7-C71	2.61	120.11	111.91
75	AU	403	CDL	OB8-CB7-C71	2.59	120.05	111.91
79	x	604	HEA	C4D-CHA-C1A	2.59	125.97	122.56
75	AG	101	CDL	OA8-CA7-C31	2.57	119.96	111.91
72	p	201	8Q1	C38-C39-N41	2.55	120.71	116.42
75	AJ	404	CDL	OB8-CB7-C71	2.54	119.87	111.91
75	V	201	CDL	OB8-CB7-C71	2.54	119.86	111.91
75	AY	501	CDL	OA8-CA7-C31	2.52	119.82	111.91
72	E	201	8Q1	O4-C1-C6	-2.52	121.01	123.99
75	AY	501	CDL	OB8-CB7-C71	2.52	119.81	111.91
75	AN	101	CDL	OB8-CB7-C71	2.52	119.81	111.91
81	AH	402	HEC	CMC-C2C-C1C	-2.51	124.61	128.46
75	AH	403	CDL	OA8-CA7-C31	2.50	119.76	111.91
76	AL	503	PEE	O3-C30-C31	2.47	119.66	111.91
82	AV	401	HEM	C1B-NB-C4B	2.46	107.62	105.07
82	AV	402	HEM	C1B-NB-C4B	2.46	107.61	105.07
79	x	604	HEA	CMC-C2C-C3C	2.45	129.27	124.68
73	J	401	NDP	C4A-C5A-N7A	-2.44	106.86	109.40
71	AT	101	PLX	C1C-N1-C1	2.43	119.87	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	i	401	CDL	OA8-CA7-C31	2.42	119.49	111.91
79	x	603	HEA	C17-C16-C15	-2.41	105.04	112.98
70	A	502	FMN	C4A-C10-N10	2.41	120.01	116.48
72	E	201	8Q1	C42-N41-C39	-2.41	118.36	122.84
76	AJ	403	PEE	O3-C30-C31	2.38	119.39	111.91
82	AJ	402	HEM	C4C-CHD-C1D	2.38	125.70	122.56
79	x	604	HEA	C1D-C2D-C3D	-2.37	104.46	106.96
72	E	201	8Q1	C37-N36-C34	-2.37	118.36	122.59
82	AJ	401	HEM	CMC-C2C-C3C	2.37	129.11	124.68
79	x	603	HEA	C16-C17-C18	-2.37	104.10	111.88
79	x	604	HEA	C25-C23-C24	2.36	119.82	114.60
79	x	604	HEA	CMB-C2B-C3B	-2.36	125.84	130.34
71	B	303	PLX	C1C-N1-C1	2.36	119.58	109.92
82	AV	402	HEM	CAD-C3D-C4D	2.35	128.77	124.66
71	AL	501	PLX	C1C-N1-C1	2.35	119.53	109.92
79	x	603	HEA	C20-C19-C18	2.35	125.87	121.12
79	x	603	HEA	CAD-C3D-C4D	2.33	128.72	124.66
71	V	203	PLX	C1C-N1-C1	2.32	119.40	109.92
70	A	502	FMN	O2-C2-N1	-2.31	118.00	121.83
76	AU	401	PEE	O3-C30-C31	2.31	119.16	111.91
76	AY	502	PEE	O3-C30-C31	2.30	119.11	111.91
71	U	101	PLX	C1C-N1-C1	2.29	119.30	109.92
76	l	701	PEE	O3-C30-C31	2.29	119.09	111.91
82	AJ	402	HEM	CAD-C3D-C4D	2.27	128.63	124.66
71	g	203	PLX	C1C-N1-C1	2.27	119.20	109.92
79	x	604	HEA	C13-C14-C15	-2.25	122.25	127.66
70	A	502	FMN	C4-N3-C2	-2.24	121.51	125.64
79	x	604	HEA	C26-C15-C16	2.22	119.00	115.27
75	AJ	405	CDL	OB8-CB7-OB9	-2.21	118.02	123.59
82	AJ	401	HEM	CAD-CBD-CGD	-2.20	108.86	113.60
71	g	201	PLX	C1C-N1-C1	2.20	118.91	109.92
81	AU	402	HEC	CMB-C2B-C1B	-2.20	125.08	128.46
79	x	603	HEA	C4B-C3B-C2B	-2.20	103.66	107.41
73	J	401	NDP	C3D-C2D-C1D	2.19	105.59	101.43
71	g	202	PLX	C1C-N1-C1	2.19	118.89	109.92
79	x	603	HEA	C12-C13-C14	-2.18	106.47	112.23
82	AJ	402	HEM	CMC-C2C-C3C	2.18	128.76	124.68
82	AV	402	HEM	CAD-CBD-CGD	-2.18	108.92	113.60
82	AJ	402	HEM	C4B-CHC-C1C	2.17	125.42	122.56
82	AV	402	HEM	C4A-C3A-C2A	2.16	108.50	107.00
76	AU	401	PEE	C17-C18-C19	-2.15	112.22	126.84
70	A	502	FMN	C4A-C4-N3	2.15	118.65	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AU	402	HEC	C1D-C2D-C3D	-2.14	105.50	107.00
72	E	201	8Q1	O35-C34-N36	-2.14	118.40	122.99
70	A	502	FMN	C10-N1-C2	2.13	121.16	116.90
82	AJ	402	HEM	C4A-C3A-C2A	2.13	108.48	107.00
70	A	502	FMN	N3-C2-N1	2.13	123.56	119.38
72	p	201	8Q1	O4-C1-S44	-2.13	119.85	122.61
71	r	502	PLX	C2-C1-N1	-2.09	108.79	115.78
82	AV	402	HEM	C4B-CHC-C1C	2.09	125.31	122.56
82	AV	402	HEM	CMC-C2C-C3C	2.09	128.59	124.68
71	U	101	PLX	C5-C4-C3	-2.07	106.88	111.79
71	r	501	PLX	C1C-N1-C1	2.06	118.36	109.92
79	x	603	HEA	C27-C19-C18	-2.06	118.41	123.68
82	AJ	402	HEM	C3B-C2B-C1B	2.05	108.01	106.49
75	AG	101	CDL	OB6-CB5-OB7	-2.05	118.76	123.70
71	AQ	101	PLX	C2-C1-N1	-2.04	108.95	115.78
79	x	604	HEA	CBD-CAD-C3D	2.03	118.28	112.63
71	AQ	101	PLX	C1C-N1-C1	2.03	118.22	109.92
79	x	604	HEA	CMC-C2C-C1C	-2.03	125.35	128.46
75	i	401	CDL	OA6-CA5-OA7	-2.01	118.83	123.70
82	AJ	402	HEM	CHD-C1D-ND	2.00	126.61	124.43

There are no chirality outliers.

All (1180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	A	502	FMN	C1'-C2'-C3'-O3'
70	A	502	FMN	C1'-C2'-C3'-C4'
70	A	502	FMN	C3'-C4'-C5'-O5'
70	A	502	FMN	O4'-C4'-C5'-O5'
71	B	303	PLX	C2-O1-P1-O2
71	B	303	PLX	N1-C1-C2-O1
71	U	101	PLX	O7-C6-C7-C8
71	U	101	PLX	O7-C6-O6-C4
71	U	101	PLX	C3-O4-P1-O2
71	U	101	PLX	N1-C1-C2-O1
71	U	101	PLX	O9-C24-C25-C26
71	V	203	PLX	O7-C6-C7-C8
71	V	203	PLX	N1-C1-C2-O1
71	V	203	PLX	O9-C24-C25-C26
71	b	201	PLX	O7-C6-O6-C4
71	b	201	PLX	N1-C1-C2-O1
71	b	201	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
71	g	201	PLX	O7-C6-C7-C8
71	g	201	PLX	O7-C6-O6-C4
71	g	201	PLX	C3-C4-O6-C6
71	g	202	PLX	C2-O1-P1-O4
71	g	202	PLX	C2-O1-P1-O2
71	g	202	PLX	C2-O1-P1-O3
71	g	202	PLX	O9-C24-O8-C5
71	g	203	PLX	O7-C6-O6-C4
71	g	203	PLX	C2-O1-P1-O2
71	g	203	PLX	C25-C24-O8-C5
71	r	501	PLX	C3-O4-P1-O1
71	r	501	PLX	C3-O4-P1-O2
71	r	501	PLX	C3-O4-P1-O3
71	r	501	PLX	O8-C24-C25-C26
71	r	502	PLX	C7-C6-O6-C4
71	r	502	PLX	C3-O4-P1-O1
71	r	502	PLX	C3-O4-P1-O2
71	r	502	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O2
71	r	502	PLX	N1-C1-C2-O1
71	r	502	PLX	O9-C24-C25-C26
71	AL	501	PLX	O7-C6-C7-C8
71	AQ	101	PLX	O7-C6-O6-C4
71	AQ	101	PLX	O6-C4-C5-O8
71	AQ	101	PLX	N1-C1-C2-O1
71	AQ	101	PLX	C25-C24-O8-C5
71	AQ	101	PLX	O9-C24-C25-C26
71	AT	101	PLX	C2-O1-P1-O4
71	AT	101	PLX	O9-C24-O8-C5
72	E	201	8Q1	C1-C6-C7-C8
72	E	201	8Q1	O4-C1-S44-C43
72	E	201	8Q1	C6-C1-S44-C43
72	E	201	8Q1	C29-C32-C34-N36
72	E	201	8Q1	C29-C32-C34-O35
72	E	201	8Q1	C42-C43-S44-C1
72	E	201	8Q1	C28-O27-P24-O3
72	E	201	8Q1	C28-O27-P24-O2
72	E	201	8Q1	C28-O27-P24-O1
72	p	201	8Q1	C1-C6-C7-C8
72	p	201	8Q1	O4-C1-S44-C43
72	p	201	8Q1	C6-C1-S44-C43
72	p	201	8Q1	C28-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
72	p	201	8Q1	C28-C29-C32-O33
72	p	201	8Q1	C30-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-C34
72	p	201	8Q1	C31-C29-C32-O33
72	p	201	8Q1	C28-O27-P24-O2
72	p	201	8Q1	C28-O27-P24-O1
73	J	401	NDP	C5B-O5B-PA-O1A
73	J	401	NDP	C5D-O5D-PN-O1N
75	V	201	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CA2-OA2-PA1-OA3
75	V	201	CDL	CA2-OA2-PA1-OA4
75	V	201	CDL	CA2-OA2-PA1-OA5
75	V	201	CDL	CA3-OA5-PA1-OA3
75	V	201	CDL	CA3-OA5-PA1-OA4
75	V	201	CDL	OA9-CA7-OA8-CA6
75	V	201	CDL	C51-CB5-OB6-CB4
75	i	401	CDL	O1-C1-CA2-OA2
75	i	401	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	CA2-OA2-PA1-OA3
75	i	401	CDL	CA2-OA2-PA1-OA4
75	i	401	CDL	CA2-OA2-PA1-OA5
75	i	401	CDL	CA3-OA5-PA1-OA3
75	i	401	CDL	CA3-OA5-PA1-OA4
75	i	401	CDL	OA6-CA4-CA6-OA8
75	i	401	CDL	CB2-OB2-PB2-OB4
75	i	401	CDL	CB3-OB5-PB2-OB3
75	i	401	CDL	CB3-OB5-PB2-OB4
75	l	703	CDL	CA2-OA2-PA1-OA3
75	l	703	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	CA2-OA2-PA1-OA3
75	l	704	CDL	CA2-OA2-PA1-OA4
75	l	704	CDL	CA3-OA5-PA1-OA2
75	l	704	CDL	CA3-OA5-PA1-OA4
75	l	704	CDL	C11-CA5-OA6-CA4
75	l	704	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CA2-OA2-PA1-OA3
75	n	101	CDL	CA2-OA2-PA1-OA4
75	n	101	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	C11-CA5-OA6-CA4
75	n	101	CDL	CB2-OB2-PB2-OB3
75	n	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
75	n	101	CDL	C51-CB5-OB6-CB4
75	AA	101	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	CB2-OB2-PB2-OB4
75	AA	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	OA9-CA7-OA8-CA6
75	AG	101	CDL	CB2-OB2-PB2-OB4
75	AH	403	CDL	CA2-OA2-PA1-OA3
75	AH	403	CDL	CA2-OA2-PA1-OA4
75	AH	403	CDL	CA3-OA5-PA1-OA2
75	AH	403	CDL	C11-CA5-OA6-CA4
75	AH	403	CDL	CB3-OB5-PB2-OB3
75	AH	403	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	CA3-OA5-PA1-OA2
75	AJ	404	CDL	CA3-OA5-PA1-OA3
75	AJ	404	CDL	CA3-OA5-PA1-OA4
75	AJ	404	CDL	C11-CA5-OA6-CA4
75	AJ	404	CDL	CB3-OB5-PB2-OB2
75	AJ	404	CDL	CB3-OB5-PB2-OB3
75	AJ	404	CDL	CB3-OB5-PB2-OB4
75	AJ	405	CDL	CA3-OA5-PA1-OA4
75	AJ	405	CDL	C51-CB5-OB6-CB4
75	AL	502	CDL	O1-C1-CA2-OA2
75	AL	502	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	C11-CA5-OA6-CA4
75	AL	502	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CB2-OB2-PB2-OB4
75	AL	502	CDL	C71-CB7-OB8-CB6
75	AN	101	CDL	CA3-OA5-PA1-OA3
75	AN	101	CDL	OA7-CA5-OA6-CA4
75	AN	101	CDL	C11-CA5-OA6-CA4
75	AN	101	CDL	CB2-OB2-PB2-OB4
75	AN	101	CDL	CB2-OB2-PB2-OB5
75	AU	403	CDL	CA3-OA5-PA1-OA2
75	AU	403	CDL	CA3-OA5-PA1-OA3
75	AU	403	CDL	C11-CA5-OA6-CA4
75	AU	403	CDL	CB3-OB5-PB2-OB2
75	AU	403	CDL	CB3-OB5-PB2-OB3
75	AU	403	CDL	OB7-CB5-OB6-CB4
75	AY	501	CDL	CB2-C1-CA2-OA2
75	AY	501	CDL	C11-CA5-OA6-CA4
76	V	202	PEE	C2-C1-O3P-P
76	V	202	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
76	W	201	PEE	C4-O4P-P-O3P
76	W	201	PEE	C4-O4P-P-O1P
76	l	701	PEE	C11-C10-O2-C2
76	l	701	PEE	C4-O4P-P-O2P
76	l	701	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C4-O4P-P-O2P
76	AJ	403	PEE	C37-C38-C39-C40
76	AL	503	PEE	C11-C10-O2-C2
76	AL	503	PEE	O4-C10-O2-C2
76	AU	401	PEE	C11-C10-O2-C2
76	AU	401	PEE	C1-O3P-P-O2P
76	AU	401	PEE	C1-O3P-P-O1P
76	AU	401	PEE	C4-O4P-P-O2P
76	AV	403	PEE	O4P-C4-C5-N
76	AV	403	PEE	C39-C40-C41-C42
76	AY	502	PEE	C1-O3P-P-O2P
76	AY	502	PEE	C4-O4P-P-O3P
76	AY	502	PEE	C4-O4P-P-O2P
76	AY	502	PEE	C4-O4P-P-O1P
79	x	603	HEA	C12-C11-C3B-C2B
82	AJ	402	HEM	C1A-C2A-CAA-CBA
82	AV	402	HEM	C1A-C2A-CAA-CBA
82	AV	402	HEM	C3A-C2A-CAA-CBA
75	AL	502	CDL	OB9-CB7-OB8-CB6
75	l	704	CDL	OA9-CA7-OA8-CA6
75	l	704	CDL	OB9-CB7-OB8-CB6
75	n	101	CDL	OA9-CA7-OA8-CA6
75	AA	101	CDL	OB9-CB7-OB8-CB6
75	AN	101	CDL	OB9-CB7-OB8-CB6
75	AU	403	CDL	OB9-CB7-OB8-CB6
75	V	201	CDL	OB7-CB5-OB6-CB4
75	l	704	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB7-CB5-OB6-CB4
75	AJ	404	CDL	OA7-CA5-OA6-CA4
75	AJ	405	CDL	OB7-CB5-OB6-CB4
75	AL	502	CDL	OA7-CA5-OA6-CA4
75	AU	403	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OA7-CA5-OA6-CA4
75	AY	501	CDL	OB7-CB5-OB6-CB4
76	l	701	PEE	O4-C10-O2-C2
76	AU	401	PEE	O4-C10-O2-C2
75	l	704	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
75	l	704	CDL	C71-CB7-OB8-CB6
75	n	101	CDL	C31-CA7-OA8-CA6
75	n	101	CDL	C71-CB7-OB8-CB6
75	AG	101	CDL	C31-CA7-OA8-CA6
75	AN	101	CDL	C71-CB7-OB8-CB6
75	AU	403	CDL	C71-CB7-OB8-CB6
75	l	703	CDL	C51-CB5-OB6-CB4
75	AH	403	CDL	C51-CB5-OB6-CB4
75	AU	403	CDL	C51-CB5-OB6-CB4
75	AY	501	CDL	C51-CB5-OB6-CB4
72	E	201	8Q1	C38-C39-N41-C42
75	AA	101	CDL	C71-CB7-OB8-CB6
75	AH	403	CDL	C71-CB7-OB8-CB6
75	AL	502	CDL	C31-CA7-OA8-CA6
76	W	201	PEE	C17-C18-C19-C20
76	l	701	PEE	C37-C38-C39-C40
76	l	702	PEE	C37-C38-C39-C40
75	AH	403	CDL	OA7-CA5-OA6-CA4
75	n	101	CDL	OB9-CB7-OB8-CB6
76	l	702	PEE	O5-C30-O3-C3
71	AL	501	PLX	C2-C1-N1-C1C
75	l	703	CDL	O1-C1-CA2-OA2
75	l	704	CDL	O1-C1-CA2-OA2
75	AG	101	CDL	O1-C1-CB2-OB2
75	AY	501	CDL	O1-C1-CA2-OA2
75	AY	501	CDL	O1-C1-CB2-OB2
75	AJ	405	CDL	C31-CA7-OA8-CA6
75	AU	403	CDL	C31-CA7-OA8-CA6
75	AH	403	CDL	OB9-CB7-OB8-CB6
75	i	401	CDL	C11-CA5-OA6-CA4
75	AA	101	CDL	C51-CB5-OB6-CB4
76	W	201	PEE	C21-C22-C23-C24
75	AU	403	CDL	OA9-CA7-OA8-CA6
76	V	202	PEE	C20-C21-C22-C23
76	AU	401	PEE	C31-C32-C33-C34
71	r	502	PLX	C16-C17-C18-C19
75	AH	403	CDL	C31-C32-C33-C34
76	l	701	PEE	C32-C33-C34-C35
73	J	401	NDP	O4B-C4B-C5B-O5B
73	J	401	NDP	C3B-C4B-C5B-O5B
76	l	702	PEE	C31-C30-O3-C3
71	r	501	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
71	b	201	PLX	C4-C3-O4-P1
75	AJ	405	CDL	OA9-CA7-OA8-CA6
75	AL	502	CDL	OA9-CA7-OA8-CA6
71	g	203	PLX	C26-C27-C28-C29
79	x	603	HEA	C15-C16-C17-C18
71	b	201	PLX	C14-C15-C16-C17
71	g	203	PLX	C30-C31-C32-C33
71	r	502	PLX	C30-C31-C32-C33
75	AJ	405	CDL	C71-C72-C73-C74
75	AY	501	CDL	C12-C13-C14-C15
76	W	201	PEE	C32-C33-C34-C35
73	J	401	NDP	C1B-C2B-O2B-P2B
75	AY	501	CDL	C31-CA7-OA8-CA6
71	g	202	PLX	C10-C11-C12-C13
72	E	201	8Q1	O40-C39-N41-C42
75	l	703	CDL	CB2-C1-CA2-OA2
75	AA	101	CDL	CA2-C1-CB2-OB2
75	AJ	404	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CB2-C1-CA2-OA2
75	AL	502	CDL	CA2-C1-CB2-OB2
71	r	502	PLX	C12-C13-C14-C15
75	i	401	CDL	C31-C32-C33-C34
75	AH	403	CDL	C31-CA7-OA8-CA6
76	W	201	PEE	C31-C30-O3-C3
75	l	703	CDL	C73-C74-C75-C76
75	l	703	CDL	OB5-CB3-CB4-OB6
76	W	201	PEE	C12-C13-C14-C15
76	l	701	PEE	C34-C35-C36-C37
75	V	201	CDL	O1-C1-CA2-OA2
75	l	703	CDL	O1-C1-CB2-OB2
75	AA	101	CDL	O1-C1-CA2-OA2
75	AJ	404	CDL	O1-C1-CA2-OA2
75	AY	501	CDL	CB5-C51-C52-C53
71	AT	101	PLX	O6-C4-C5-O8
71	r	501	PLX	C12-C13-C14-C15
75	AH	403	CDL	OA9-CA7-OA8-CA6
76	W	201	PEE	O5-C30-O3-C3
75	V	201	CDL	C54-C55-C56-C57
75	i	401	CDL	OA7-CA5-OA6-CA4
71	V	203	PLX	C13-C14-C15-C16
75	l	704	CDL	CB5-C51-C52-C53
75	n	101	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
75	AH	403	CDL	CB5-C51-C52-C53
75	AN	101	CDL	CA5-C11-C12-C13
75	AY	501	CDL	CA7-C31-C32-C33
76	l	702	PEE	C10-C11-C12-C13
76	l	702	PEE	C17-C18-C19-C20
76	AH	401	PEE	C37-C38-C39-C40
75	AN	101	CDL	C71-C72-C73-C74
76	W	201	PEE	C15-C16-C17-C18
75	i	401	CDL	CA5-C11-C12-C13
75	AJ	404	CDL	CA7-C31-C32-C33
75	AL	502	CDL	CA5-C11-C12-C13
75	AU	403	CDL	CA5-C11-C12-C13
76	V	202	PEE	C10-C11-C12-C13
76	l	701	PEE	C30-C31-C32-C33
76	AV	403	PEE	C10-C11-C12-C13
71	r	501	PLX	C27-C28-C29-C30
75	AL	502	CDL	C52-C53-C54-C55
75	AA	101	CDL	OB7-CB5-OB6-CB4
75	AA	101	CDL	CB7-C71-C72-C73
75	AG	101	CDL	CB7-C71-C72-C73
75	AJ	405	CDL	CB7-C71-C72-C73
82	AJ	401	HEM	C3D-CAD-CBD-CGD
82	AV	401	HEM	C3D-CAD-CBD-CGD
75	n	101	CDL	C31-C32-C33-C34
76	AL	503	PEE	C30-C31-C32-C33
75	AL	502	CDL	O1-C1-CB2-OB2
75	i	401	CDL	C31-CA7-OA8-CA6
73	J	401	NDP	C3B-C2B-O2B-P2B
75	AN	101	CDL	C14-C15-C16-C17
75	AY	501	CDL	OA9-CA7-OA8-CA6
76	l	701	PEE	C39-C40-C41-C42
76	V	202	PEE	C17-C18-C19-C20
76	l	701	PEE	C17-C18-C19-C20
75	AH	403	CDL	C33-C34-C35-C36
71	B	303	PLX	C2-O1-P1-O4
71	U	101	PLX	C3-O4-P1-O1
71	b	201	PLX	C3-O4-P1-O1
71	g	201	PLX	C3-O4-P1-O1
71	g	202	PLX	C3-O4-P1-O1
71	g	203	PLX	C2-O1-P1-O4
71	r	502	PLX	C2-O1-P1-O4
75	V	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
75	V	201	CDL	CB3-OB5-PB2-OB2
75	i	401	CDL	CA3-OA5-PA1-OA2
75	i	401	CDL	CB2-OB2-PB2-OB5
75	i	401	CDL	CB3-OB5-PB2-OB2
75	l	703	CDL	CB3-OB5-PB2-OB2
75	l	704	CDL	CA2-OA2-PA1-OA5
75	n	101	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CA2-OA2-PA1-OA5
75	AG	101	CDL	CB2-OB2-PB2-OB5
75	AH	403	CDL	CA2-OA2-PA1-OA5
75	AH	403	CDL	CB3-OB5-PB2-OB2
75	AJ	405	CDL	CA3-OA5-PA1-OA2
75	AL	502	CDL	CB2-OB2-PB2-OB5
75	AL	502	CDL	CB3-OB5-PB2-OB2
75	AN	101	CDL	CA3-OA5-PA1-OA2
75	AY	501	CDL	CA3-OA5-PA1-OA2
76	V	202	PEE	C1-O3P-P-O4P
76	W	201	PEE	C1-O3P-P-O4P
76	l	701	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C4-O4P-P-O3P
76	AU	401	PEE	C1-O3P-P-O4P
76	AU	401	PEE	C4-O4P-P-O3P
76	AY	502	PEE	C1-O3P-P-O4P
75	AY	501	CDL	C71-CB7-OB8-CB6
76	V	202	PEE	C31-C30-O3-C3
71	AL	501	PLX	C12-C13-C14-C15
75	l	703	CDL	CA2-C1-CB2-OB2
75	AG	101	CDL	CA2-C1-CB2-OB2
75	AY	501	CDL	CA2-C1-CB2-OB2
71	AL	501	PLX	C2-C1-N1-C1A
75	l	703	CDL	C71-CB7-OB8-CB6
71	B	303	PLX	O6-C6-C7-C8
71	U	101	PLX	O6-C6-C7-C8
71	g	203	PLX	O8-C24-C25-C26
71	AQ	101	PLX	O8-C24-C25-C26
75	n	101	CDL	C13-C14-C15-C16
75	l	704	CDL	C51-CB5-OB6-CB4
75	AG	101	CDL	C51-CB5-OB6-CB4
71	B	303	PLX	C27-C28-C29-C30
71	g	201	PLX	C13-C14-C15-C16
71	g	201	PLX	C7-C8-C9-C10
71	g	202	PLX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
71	g	203	PLX	C29-C30-C31-C32
71	AQ	101	PLX	C19-C20-C21-C22
71	AT	101	PLX	C7-C8-C9-C10
75	l	704	CDL	C31-C32-C33-C34
75	n	101	CDL	C12-C13-C14-C15
75	AG	101	CDL	C33-C34-C35-C36
75	AJ	405	CDL	C12-C13-C14-C15
75	AY	501	CDL	C32-C33-C34-C35
76	W	201	PEE	C14-C15-C16-C17
76	l	701	PEE	C22-C23-C24-C25
71	g	203	PLX	C34-C35-C36-C37
71	AT	101	PLX	C9-C10-C11-C12
75	AU	403	CDL	C13-C14-C15-C16
76	l	702	PEE	C20-C21-C22-C23
76	AJ	403	PEE	C20-C21-C22-C23
76	AY	502	PEE	C11-C12-C13-C14
75	AL	502	CDL	CA6-CA4-OA6-CA5
75	l	704	CDL	OB7-CB5-OB6-CB4
75	AG	101	CDL	OB7-CB5-OB6-CB4
75	n	101	CDL	CB5-C51-C52-C53
71	AQ	101	PLX	C10-C11-C12-C13
72	p	201	8Q1	C11-C12-C13-C14
76	l	701	PEE	C21-C22-C23-C24
75	AJ	404	CDL	C1-CB2-OB2-PB2
75	AY	501	CDL	OA5-CA3-CA4-OA6
71	AQ	101	PLX	C12-C13-C14-C15
75	V	201	CDL	C71-C72-C73-C74
75	AA	101	CDL	C51-C52-C53-C54
75	AG	101	CDL	C14-C15-C16-C17
75	AL	502	CDL	C51-C52-C53-C54
75	AU	403	CDL	C54-C55-C56-C57
71	r	501	PLX	C13-C14-C15-C16
71	r	502	PLX	C14-C15-C16-C17
75	l	704	CDL	C51-C52-C53-C54
76	V	202	PEE	C12-C13-C14-C15
75	l	703	CDL	CB7-C71-C72-C73
75	l	704	CDL	CB7-C71-C72-C73
75	AA	101	CDL	CA5-C11-C12-C13
71	U	101	PLX	C33-C34-C35-C36
71	b	201	PLX	C16-C17-C18-C19
71	AL	501	PLX	C15-C16-C17-C18
71	AL	501	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
75	AA	101	CDL	C31-C32-C33-C34
76	V	202	PEE	C40-C41-C42-C43
76	l	702	PEE	C33-C34-C35-C36
76	AJ	403	PEE	C13-C14-C15-C16
76	AJ	403	PEE	C11-C12-C13-C14
71	U	101	PLX	C19-C20-C21-C22
71	U	101	PLX	C10-C11-C12-C13
71	U	101	PLX	C35-C36-C37-C38
71	g	203	PLX	C15-C16-C17-C18
71	r	502	PLX	C11-C12-C13-C14
71	r	502	PLX	C10-C11-C12-C13
72	p	201	8Q1	C6-C7-C8-C9
76	AH	401	PEE	C21-C22-C23-C24
75	AN	101	CDL	CB4-CB6-OB8-CB7
71	U	101	PLX	C12-C13-C14-C15
71	U	101	PLX	C9-C10-C11-C12
71	V	203	PLX	C10-C11-C12-C13
71	b	201	PLX	C27-C28-C29-C30
71	b	201	PLX	C29-C30-C31-C32
71	g	202	PLX	C14-C15-C16-C17
71	AQ	101	PLX	C34-C35-C36-C37
72	E	201	8Q1	C12-C13-C14-C15
75	i	401	CDL	C13-C14-C15-C16
75	AL	502	CDL	C32-C33-C34-C35
76	l	702	PEE	C40-C41-C42-C43
76	AL	503	PEE	C32-C33-C34-C35
71	B	303	PLX	C9-C10-C11-C12
71	B	303	PLX	C28-C29-C30-C31
71	r	502	PLX	C9-C10-C11-C12
75	l	704	CDL	C32-C33-C34-C35
75	AJ	405	CDL	C33-C34-C35-C36
75	AU	403	CDL	C31-C32-C33-C34
76	V	202	PEE	C14-C15-C16-C17
76	AH	401	PEE	C11-C12-C13-C14
71	V	203	PLX	C25-C26-C27-C28
71	g	201	PLX	C16-C17-C18-C19
71	AL	501	PLX	C10-C11-C12-C13
75	AY	501	CDL	C14-C15-C16-C17
76	l	702	PEE	C34-C35-C36-C37
76	AH	401	PEE	C22-C23-C24-C25
76	AJ	403	PEE	C22-C23-C24-C25
76	AL	503	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
76	AU	401	PEE	C11-C12-C13-C14
76	AV	403	PEE	C35-C36-C37-C38
76	AY	502	PEE	C19-C20-C21-C22
75	l	704	CDL	CA7-C31-C32-C33
75	AG	101	CDL	CA5-C11-C12-C13
75	AL	502	CDL	CA7-C31-C32-C33
75	AU	403	CDL	CB7-C71-C72-C73
71	U	101	PLX	C7-C8-C9-C10
71	b	201	PLX	C18-C19-C20-C21
71	g	201	PLX	C10-C11-C12-C13
75	l	703	CDL	C51-C52-C53-C54
76	l	702	PEE	C21-C22-C23-C24
71	AL	501	PLX	C2-C1-N1-C1B
71	b	201	PLX	C25-C26-C27-C28
75	l	703	CDL	C11-C12-C13-C14
76	AY	502	PEE	C22-C23-C24-C25
71	V	203	PLX	C32-C33-C34-C35
71	g	202	PLX	C9-C10-C11-C12
75	n	101	CDL	C51-C52-C53-C54
75	AG	101	CDL	C73-C74-C75-C76
75	n	101	CDL	CB7-C71-C72-C73
71	AQ	101	PLX	C15-C16-C17-C18
76	l	701	PEE	C20-C21-C22-C23
71	r	502	PLX	C32-C33-C34-C35
76	AJ	403	PEE	C32-C33-C34-C35
76	AL	503	PEE	C34-C35-C36-C37
72	E	201	8Q1	N41-C42-C43-S44
71	g	203	PLX	C10-C11-C12-C13
71	r	502	PLX	C26-C27-C28-C29
75	AU	403	CDL	C14-C15-C16-C17
76	V	202	PEE	C34-C35-C36-C37
76	AV	403	PEE	C32-C33-C34-C35
76	V	202	PEE	O5-C30-O3-C3
71	B	303	PLX	C12-C13-C14-C15
71	g	203	PLX	C17-C18-C19-C20
75	AG	101	CDL	C72-C73-C74-C75
75	AY	501	CDL	C33-C34-C35-C36
76	W	201	PEE	C37-C38-C39-C40
71	g	203	PLX	C7-C8-C9-C10
71	r	502	PLX	C25-C26-C27-C28
76	AH	401	PEE	C32-C33-C34-C35
71	g	202	PLX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
75	i	401	CDL	C34-C35-C36-C37
75	i	401	CDL	OA9-CA7-OA8-CA6
75	AY	501	CDL	OB9-CB7-OB8-CB6
75	AL	502	CDL	C51-CB5-OB6-CB4
72	p	201	8Q1	C7-C8-C9-C10
75	AH	403	CDL	C32-C33-C34-C35
71	B	303	PLX	O7-C6-C7-C8
71	g	203	PLX	O9-C24-C25-C26
71	r	501	PLX	O9-C24-C25-C26
71	r	502	PLX	O7-C6-C7-C8
71	AT	101	PLX	O9-C24-C25-C26
71	g	203	PLX	C14-C15-C16-C17
71	r	501	PLX	C7-C8-C9-C10
75	i	401	CDL	C11-C12-C13-C14
75	l	703	CDL	C33-C34-C35-C36
75	AU	403	CDL	C53-C54-C55-C56
70	A	502	FMN	O2'-C2'-C3'-O3'
71	AT	101	PLX	C11-C12-C13-C14
75	i	401	CDL	C32-C33-C34-C35
71	r	501	PLX	C35-C36-C37-C38
75	AJ	405	CDL	C52-C53-C54-C55
75	l	703	CDL	OB9-CB7-OB8-CB6
75	AJ	404	CDL	C11-C12-C13-C14
75	AJ	404	CDL	C14-C15-C16-C17
75	AY	501	CDL	C13-C14-C15-C16
76	V	202	PEE	C43-C44-C45-C46
76	l	701	PEE	C13-C14-C15-C16
76	l	701	PEE	C41-C42-C43-C44
75	V	201	CDL	OA7-CA5-OA6-CA4
70	A	502	FMN	O2'-C2'-C3'-C4'
71	V	203	PLX	C11-C12-C13-C14
75	AG	101	CDL	C31-C32-C33-C34
72	p	201	8Q1	C12-C13-C14-C15
76	AV	403	PEE	C41-C42-C43-C44
75	i	401	CDL	CB5-C51-C52-C53
76	AV	403	PEE	C30-C31-C32-C33
76	W	201	PEE	C23-C24-C25-C26
75	l	703	CDL	C31-CA7-OA8-CA6
75	V	201	CDL	C11-CA5-OA6-CA4
76	AH	401	PEE	C11-C10-O2-C2
71	g	201	PLX	C32-C33-C34-C35
71	r	501	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
75	AA	101	CDL	C33-C34-C35-C36
75	AG	101	CDL	C52-C53-C54-C55
75	V	201	CDL	CB5-C51-C52-C53
76	AL	503	PEE	C10-C11-C12-C13
75	n	101	CDL	C55-C56-C57-C58
75	AN	101	CDL	C31-C32-C33-C34
76	AV	403	PEE	C12-C13-C14-C15
76	AU	401	PEE	C33-C34-C35-C36
76	AL	503	PEE	C37-C38-C39-C40
71	r	502	PLX	C36-C37-C38-C39
75	i	401	CDL	C73-C74-C75-C76
76	W	201	PEE	C41-C42-C43-C44
76	l	701	PEE	C15-C16-C17-C18
76	l	702	PEE	C19-C20-C21-C22
75	AL	502	CDL	OB7-CB5-OB6-CB4
76	AV	403	PEE	O4-C10-O2-C2
75	AJ	405	CDL	CB5-C51-C52-C53
75	i	401	CDL	C71-CB7-OB8-CB6
71	r	502	PLX	C20-C21-C22-C23
71	r	502	PLX	C7-C8-C9-C10
76	V	202	PEE	C31-C32-C33-C34
71	AT	101	PLX	C33-C34-C35-C36
75	n	101	CDL	C71-C72-C73-C74
76	l	702	PEE	C31-C32-C33-C34
76	AY	502	PEE	C20-C21-C22-C23
71	b	201	PLX	C30-C31-C32-C33
71	g	202	PLX	C26-C27-C28-C29
76	W	201	PEE	C43-C44-C45-C46
75	i	401	CDL	C51-CB5-OB6-CB4
76	AV	403	PEE	C11-C10-O2-C2
75	AL	502	CDL	OA5-CA3-CA4-OA6
75	AL	502	CDL	OB5-CB3-CB4-OB6
71	AQ	101	PLX	C13-C14-C15-C16
75	AA	101	CDL	C12-C13-C14-C15
71	r	502	PLX	C35-C36-C37-C38
76	AV	403	PEE	C40-C41-C42-C43
76	AH	401	PEE	O4-C10-O2-C2
71	AQ	101	PLX	C18-C19-C20-C21
75	V	201	CDL	C14-C15-C16-C17
71	AL	501	PLX	O6-C4-C5-O8
71	b	201	PLX	C32-C33-C34-C35
75	AH	403	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
76	AL	503	PEE	C12-C13-C14-C15
76	AU	401	PEE	C34-C35-C36-C37
71	B	303	PLX	C29-C30-C31-C32
71	g	203	PLX	C35-C36-C37-C38
76	V	202	PEE	C19-C20-C21-C22
76	W	201	PEE	C19-C20-C21-C22
76	AV	403	PEE	C19-C20-C21-C22
71	r	501	PLX	C9-C10-C11-C12
71	b	201	PLX	C11-C12-C13-C14
75	l	703	CDL	OA9-CA7-OA8-CA6
71	g	202	PLX	C11-C10-C9-C8
71	r	502	PLX	C17-C18-C19-C20
71	AQ	101	PLX	C7-C8-C9-C10
75	l	704	CDL	C13-C14-C15-C16
75	AU	403	CDL	C73-C74-C75-C76
76	l	701	PEE	C23-C24-C25-C26
76	l	701	PEE	C40-C41-C42-C43
76	l	701	PEE	C16-C17-C18-C19
71	g	201	PLX	C2-O1-P1-O4
75	l	703	CDL	CA2-OA2-PA1-OA5
75	AL	502	CDL	CA2-OA2-PA1-OA5
76	AV	403	PEE	C1-O3P-P-O4P
71	B	303	PLX	C15-C16-C17-C18
75	n	101	CDL	C34-C35-C36-C37
76	AV	403	PEE	C33-C34-C35-C36
76	AH	401	PEE	C2-C1-O3P-P
71	AL	501	PLX	C7-C8-C9-C10
75	AG	101	CDL	C34-C35-C36-C37
71	AL	501	PLX	O4-C3-C4-C5
75	l	704	CDL	OB5-CB3-CB4-CB6
76	l	701	PEE	O3P-C1-C2-C3
76	AJ	403	PEE	O3P-C1-C2-C3
71	r	502	PLX	C15-C16-C17-C18
71	AT	101	PLX	C32-C33-C34-C35
75	AG	101	CDL	CA7-C31-C32-C33
75	AY	501	CDL	CB7-C71-C72-C73
71	AQ	101	PLX	C26-C27-C28-C29
71	AT	101	PLX	C18-C19-C20-C21
76	l	702	PEE	C42-C43-C44-C45
71	B	303	PLX	C11-C10-C9-C8
71	AT	101	PLX	C13-C14-C15-C16
71	AT	101	PLX	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
76	AL	503	PEE	C21-C22-C23-C24
75	l	704	CDL	CB2-C1-CA2-OA2
75	i	401	CDL	OB7-CB5-OB6-CB4
75	V	201	CDL	C12-C13-C14-C15
75	AL	502	CDL	C14-C15-C16-C17
75	n	101	CDL	C33-C34-C35-C36
76	W	201	PEE	C33-C34-C35-C36
71	r	501	PLX	C3-C4-C5-O8
75	l	703	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CA3-CA4-CA6-OA8
75	AJ	405	CDL	CB3-CB4-CB6-OB8
75	AL	502	CDL	CA3-CA4-CA6-OA8
75	AL	502	CDL	CB3-CB4-CB6-OB8
75	AN	101	CDL	CB3-CB4-CB6-OB8
75	AU	403	CDL	CA3-CA4-CA6-OA8
76	AV	403	PEE	C1-C2-C3-O3
75	AL	502	CDL	C13-C14-C15-C16
76	AY	502	PEE	C33-C34-C35-C36
71	r	501	PLX	C18-C19-C20-C21
75	AG	101	CDL	C75-C76-C77-C78
76	V	202	PEE	C41-C42-C43-C44
71	g	201	PLX	C26-C27-C28-C29
75	AJ	404	CDL	C15-C16-C17-C18
76	W	201	PEE	C44-C45-C46-C47
76	AJ	403	PEE	C41-C42-C43-C44
75	AJ	404	CDL	CA5-C11-C12-C13
71	U	101	PLX	O8-C24-C25-C26
75	AY	501	CDL	C15-C16-C17-C18
75	AH	403	CDL	C55-C56-C57-C58
75	AL	502	CDL	C31-C32-C33-C34
75	AU	403	CDL	C15-C16-C17-C18
76	l	702	PEE	C12-C13-C14-C15
76	AJ	403	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C39-C40-C41-C42
76	AU	401	PEE	C15-C16-C17-C18
76	AV	403	PEE	C15-C16-C17-C18
75	i	401	CDL	OB9-CB7-OB8-CB6
72	p	201	8Q1	C13-C14-C15-C16
71	AQ	101	PLX	C36-C37-C38-C39
75	AJ	404	CDL	C74-C75-C76-C77
71	b	201	PLX	C20-C21-C22-C23
76	AY	502	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
75	AU	403	CDL	CB5-C51-C52-C53
75	AJ	405	CDL	C55-C56-C57-C58
71	V	203	PLX	C7-C8-C9-C10
75	AN	101	CDL	C55-C56-C57-C58
76	l	701	PEE	C42-C43-C44-C45
75	AJ	404	CDL	CA3-CA4-OA6-CA5
75	AJ	405	CDL	CB6-CB4-OB6-CB5
71	AQ	101	PLX	C31-C32-C33-C34
76	l	702	PEE	C44-C45-C46-C47
76	l	701	PEE	C2-C1-O3P-P
71	AQ	101	PLX	C9-C10-C11-C12
75	V	201	CDL	OA5-CA3-CA4-OA6
71	U	101	PLX	C26-C27-C28-C29
75	AN	101	CDL	C15-C16-C17-C18
75	AJ	405	CDL	CA7-C31-C32-C33
76	AH	401	PEE	C30-C31-C32-C33
71	AL	501	PLX	C34-C35-C36-C37
75	AH	403	CDL	C32-C31-CA7-OA8
76	W	201	PEE	O2-C2-C3-O3
75	l	703	CDL	C75-C76-C77-C78
76	AH	401	PEE	C34-C35-C36-C37
72	p	201	8Q1	C30-C29-C32-O33
75	i	401	CDL	C52-C51-CB5-OB6
71	V	203	PLX	C16-C17-C18-C19
75	AA	101	CDL	C71-C72-C73-C74
76	AV	403	PEE	C13-C14-C15-C16
75	AG	101	CDL	C71-CB7-OB8-CB6
76	AH	401	PEE	C24-C25-C26-C27
75	i	401	CDL	C35-C36-C37-C38
71	U	101	PLX	C11-C10-C9-C8
75	V	201	CDL	C72-C73-C74-C75
75	AH	403	CDL	C15-C16-C17-C18
76	W	201	PEE	C34-C35-C36-C37
75	AJ	405	CDL	C32-C33-C34-C35
71	V	203	PLX	C12-C13-C14-C15
71	g	201	PLX	C17-C18-C19-C20
71	g	201	PLX	C27-C28-C29-C30
75	AJ	404	CDL	C73-C74-C75-C76
75	l	703	CDL	OB5-CB3-CB4-CB6
75	AL	502	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OA5-CA3-CA4-CA6
75	AY	501	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
75	AY	501	CDL	OB5-CB3-CB4-CB6
76	W	201	PEE	O3P-C1-C2-C3
76	AH	401	PEE	C20-C21-C22-C23
71	V	203	PLX	C31-C32-C33-C34
75	AJ	404	CDL	C12-C13-C14-C15
71	B	303	PLX	C30-C31-C32-C33
71	r	501	PLX	C25-C26-C27-C28
75	V	201	CDL	C52-C53-C54-C55
71	U	101	PLX	C28-C29-C30-C31
71	b	201	PLX	C13-C14-C15-C16
71	b	201	PLX	C11-C10-C9-C8
71	b	201	PLX	C36-C37-C38-C39
76	AJ	403	PEE	C40-C41-C42-C43
75	AA	101	CDL	C75-C76-C77-C78
71	U	101	PLX	C27-C28-C29-C30
71	g	201	PLX	C3-C4-C5-O8
71	AL	501	PLX	C3-C4-C5-O8
71	AQ	101	PLX	C3-C4-C5-O8
71	AT	101	PLX	C3-C4-C5-O8
75	V	201	CDL	CB3-CB4-CB6-OB8
75	i	401	CDL	CA3-CA4-CA6-OA8
75	AA	101	CDL	CB3-CB4-CB6-OB8
76	W	201	PEE	C1-C2-C3-O3
71	r	502	PLX	C27-C28-C29-C30
72	p	201	8Q1	C10-C11-C12-C13
72	E	201	8Q1	C7-C8-C9-C10
76	AV	403	PEE	C22-C23-C24-C25
71	r	501	PLX	C28-C29-C30-C31
76	W	201	PEE	C13-C14-C15-C16
76	l	702	PEE	C11-C10-O2-C2
71	AQ	101	PLX	C14-C15-C16-C17
75	V	201	CDL	C53-C54-C55-C56
71	b	201	PLX	C5-C4-O6-C6
71	g	202	PLX	C5-C4-O6-C6
71	AT	101	PLX	C3-O4-P1-O1
76	AV	403	PEE	C4-O4P-P-O3P
75	AJ	404	CDL	C71-C72-C73-C74
71	r	501	PLX	O7-C6-C7-C8
71	b	201	PLX	C35-C36-C37-C38
75	AH	403	CDL	C52-C53-C54-C55
75	l	704	CDL	OA5-CA3-CA4-OA6
75	AN	101	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
76	AJ	403	PEE	O3P-C1-C2-O2
71	AL	501	PLX	C32-C33-C34-C35
71	V	203	PLX	C26-C27-C28-C29
75	AG	101	CDL	OB9-CB7-OB8-CB6
75	l	703	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OB6-CB4-CB6-OB8
75	AH	403	CDL	OB6-CB4-CB6-OB8
75	AL	502	CDL	OA6-CA4-CA6-OA8
75	AL	502	CDL	OB6-CB4-CB6-OB8
75	AU	403	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	C12-C11-CA5-OA6
75	AJ	404	CDL	C31-C32-C33-C34
76	AL	503	PEE	C14-C15-C16-C17
71	g	201	PLX	C20-C21-C22-C23
75	AG	101	CDL	C74-C75-C76-C77
75	AN	101	CDL	C52-C53-C54-C55
71	g	203	PLX	C4-C3-O4-P1
71	r	501	PLX	C4-C3-O4-P1
75	AA	101	CDL	C1-CA2-OA2-PA1
75	AA	101	CDL	C1-CB2-OB2-PB2
75	AA	101	CDL	CB4-CB3-OB5-PB2
75	AH	403	CDL	C1-CA2-OA2-PA1
75	AN	101	CDL	CB4-CB3-OB5-PB2
75	l	704	CDL	C73-C74-C75-C76
76	AV	403	PEE	C34-C35-C36-C37
71	r	501	PLX	C19-C20-C21-C22
75	AU	403	CDL	C74-C75-C76-C77
75	l	703	CDL	C15-C16-C17-C18
75	n	101	CDL	CA5-C11-C12-C13
76	W	201	PEE	O4-C10-O2-C2
76	W	201	PEE	C11-C10-O2-C2
75	AL	502	CDL	C53-C54-C55-C56
71	B	303	PLX	C11-C12-C13-C14
76	AV	403	PEE	C20-C21-C22-C23
75	V	201	CDL	OB5-CB3-CB4-CB6
75	AA	101	CDL	OA5-CA3-CA4-CA6
75	AJ	404	CDL	OB5-CB3-CB4-CB6
75	AN	101	CDL	OA5-CA3-CA4-CA6
75	AU	403	CDL	OB5-CB3-CB4-CB6
76	AY	502	PEE	C14-C15-C16-C17
76	AV	403	PEE	C16-C17-C18-C19
76	AH	401	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
76	l	702	PEE	O4-C10-O2-C2
75	AU	403	CDL	C55-C56-C57-C58
76	AV	403	PEE	C11-C12-C13-C14
75	AA	101	CDL	C35-C36-C37-C38
71	B	303	PLX	C32-C33-C34-C35
76	l	701	PEE	C31-C32-C33-C34
71	r	501	PLX	C30-C31-C32-C33
75	V	201	CDL	C75-C76-C77-C78
75	AU	403	CDL	C71-C72-C73-C74
71	AT	101	PLX	C26-C27-C28-C29
75	AJ	405	CDL	CA6-CA4-OA6-CA5
75	AU	403	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CA6-CA4-OA6-CA5
75	AY	501	CDL	CB3-CB4-OB6-CB5
71	g	202	PLX	C30-C31-C32-C33
75	AG	101	CDL	C11-C12-C13-C14
76	AL	503	PEE	C31-C32-C33-C34
75	AA	101	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	C1-CB2-OB2-PB2
75	AN	101	CDL	CA3-CA4-CA6-OA8
75	AU	403	CDL	C1-CB2-OB2-PB2
75	AY	501	CDL	CA3-CA4-CA6-OA8
71	g	202	PLX	O4-C3-C4-O6
71	AL	501	PLX	O4-C3-C4-O6
71	AQ	101	PLX	O4-C3-C4-O6
75	V	201	CDL	OB5-CB3-CB4-OB6
75	l	703	CDL	OA5-CA3-CA4-OA6
75	AJ	404	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OA5-CA3-CA4-OA6
76	V	202	PEE	C33-C34-C35-C36
71	AL	501	PLX	C6-C7-C8-C9
76	V	202	PEE	C32-C33-C34-C35
71	b	201	PLX	O6-C4-C5-O8
71	r	501	PLX	O6-C4-C5-O8
75	V	201	CDL	OA6-CA4-CA6-OA8
75	V	201	CDL	OB6-CB4-CB6-OB8
75	AA	101	CDL	OA6-CA4-CA6-OA8
75	AG	101	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OA6-CA4-CA6-OA8
75	AJ	405	CDL	OB6-CB4-CB6-OB8
75	AN	101	CDL	OA6-CA4-CA6-OA8
75	AA	101	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
72	E	201	8Q1	C6-C7-C8-C9
75	AH	403	CDL	C12-C13-C14-C15
73	J	401	NDP	C5B-O5B-PA-O3
73	J	401	NDP	C5D-O5D-PN-O3
76	AH	401	PEE	C15-C16-C17-C18
75	l	704	CDL	C12-C13-C14-C15
76	AJ	403	PEE	O4-C10-O2-C2
71	r	502	PLX	C24-C25-C26-C27
75	AJ	404	CDL	C33-C34-C35-C36
71	r	502	PLX	C34-C35-C36-C37
71	g	201	PLX	C35-C36-C37-C38
76	l	701	PEE	C24-C25-C26-C27
76	l	702	PEE	C11-C12-C13-C14
75	AL	502	CDL	C11-C12-C13-C14
75	n	101	CDL	C35-C36-C37-C38
75	n	101	CDL	C11-C12-C13-C14
75	l	704	CDL	CB2-OB2-PB2-OB5
75	AJ	405	CDL	CB2-OB2-PB2-OB5
71	r	501	PLX	C31-C32-C33-C34
76	W	201	PEE	C31-C32-C33-C34
71	r	502	PLX	C4-C3-O4-P1
75	l	704	CDL	CA4-CA3-OA5-PA1
75	AH	403	CDL	CA4-CA3-OA5-PA1
75	AN	101	CDL	C1-CA2-OA2-PA1
75	AN	101	CDL	C1-CB2-OB2-PB2
71	b	201	PLX	C3-O4-P1-O2
71	g	201	PLX	C3-O4-P1-O3
71	g	202	PLX	C3-O4-P1-O2
71	g	202	PLX	C3-O4-P1-O3
71	r	502	PLX	C2-O1-P1-O3
71	AQ	101	PLX	C3-O4-P1-O3
71	AT	101	PLX	C2-O1-P1-O3
73	J	401	NDP	C5B-O5B-PA-O2A
73	J	401	NDP	C5D-O5D-PN-O2N
75	V	201	CDL	CB3-OB5-PB2-OB4
75	i	401	CDL	CB2-OB2-PB2-OB3
75	l	703	CDL	CA2-OA2-PA1-OA4
75	l	703	CDL	CB3-OB5-PB2-OB4
75	l	704	CDL	CA3-OA5-PA1-OA3
75	n	101	CDL	CA3-OA5-PA1-OA3
75	AA	101	CDL	CB2-OB2-PB2-OB3
75	AG	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
75	AG	101	CDL	CB2-OB2-PB2-OB3
75	AL	502	CDL	CA2-OA2-PA1-OA4
75	AL	502	CDL	CB3-OB5-PB2-OB3
75	AL	502	CDL	CB3-OB5-PB2-OB4
75	AN	101	CDL	CA2-OA2-PA1-OA3
75	AN	101	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA3-OA5-PA1-OA4
76	V	202	PEE	C1-O3P-P-O1P
76	AH	401	PEE	C4-O4P-P-O1P
76	AU	401	PEE	C4-O4P-P-O1P
76	AV	403	PEE	C1-O3P-P-O2P
76	AV	403	PEE	C1-O3P-P-O1P
76	AY	502	PEE	C1-O3P-P-O1P
71	g	202	PLX	O4-C3-C4-C5
71	AQ	101	PLX	O4-C3-C4-C5
75	V	201	CDL	OA5-CA3-CA4-CA6
75	l	703	CDL	OA5-CA3-CA4-CA6
75	l	704	CDL	OA5-CA3-CA4-CA6
75	AL	502	CDL	OB5-CB3-CB4-CB6
71	r	501	PLX	C15-C16-C17-C18
75	AL	502	CDL	C33-C34-C35-C36
76	AH	401	PEE	C17-C18-C19-C20
76	AV	403	PEE	C17-C18-C19-C20
71	V	203	PLX	C19-C20-C21-C22
71	U	101	PLX	C25-C24-O8-C5
71	b	201	PLX	C1-C2-O1-P1
71	g	203	PLX	C1-C2-O1-P1
71	r	501	PLX	C25-C24-O8-C5
71	AT	101	PLX	C1-C2-O1-P1
71	AT	101	PLX	C25-C24-O8-C5
76	AH	401	PEE	C5-C4-O4P-P
76	W	201	PEE	C10-C11-C12-C13
71	g	203	PLX	C19-C20-C21-C22
75	V	201	CDL	C74-C75-C76-C77
75	AN	101	CDL	CA2-C1-CB2-OB2
75	AU	403	CDL	CA2-C1-CB2-OB2
75	l	704	CDL	OB5-CB3-CB4-OB6
75	AU	403	CDL	OB5-CB3-CB4-OB6
75	AY	501	CDL	OB5-CB3-CB4-OB6
76	l	701	PEE	O3P-C1-C2-O2
82	AV	401	HEM	C2A-CAA-CBA-CGA
71	AL	501	PLX	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
76	AJ	403	PEE	C11-C10-O2-C2
71	V	203	PLX	C14-C15-C16-C17
76	AH	401	PEE	C14-C15-C16-C17
71	g	203	PLX	C3-C4-C5-O8
71	r	502	PLX	C3-C4-C5-O8
71	AL	501	PLX	N1-C1-C2-O1
75	AG	101	CDL	CA3-CA4-CA6-OA8
81	AH	402	HEC	C1A-C2A-CAA-CBA
81	AH	402	HEC	C3A-C2A-CAA-CBA
82	AJ	402	HEM	C3A-C2A-CAA-CBA
71	g	203	PLX	O6-C4-C5-O8
71	r	502	PLX	O6-C4-C5-O8
75	l	704	CDL	OA6-CA4-CA6-OA8
75	AH	403	CDL	OA6-CA4-CA6-OA8
75	AY	501	CDL	OA6-CA4-CA6-OA8
76	AV	403	PEE	O2-C2-C3-O3
75	AJ	404	CDL	C55-C56-C57-C58
75	AJ	404	CDL	CA4-CA3-OA5-PA1
71	g	201	PLX	C24-C25-C26-C27
75	AJ	404	CDL	C13-C14-C15-C16
71	r	502	PLX	O8-C24-C25-C26
72	E	201	8Q1	O33-C32-C34-O35
71	g	202	PLX	O7-C6-C7-C8
71	B	303	PLX	C20-C21-C22-C23
71	U	101	PLX	C36-C37-C38-C39
75	l	704	CDL	C15-C16-C17-C18
73	J	401	NDP	O4D-C1D-N1N-C6N
76	AL	503	PEE	C33-C34-C35-C36
71	r	502	PLX	C11-C10-C9-C8
75	AH	403	CDL	O1-C1-CB2-OB2
75	AH	403	CDL	C13-C14-C15-C16
75	n	101	CDL	C73-C74-C75-C76
71	g	201	PLX	C14-C15-C16-C17
75	AH	403	CDL	C54-C55-C56-C57
75	V	201	CDL	CA3-CA4-OA6-CA5
75	l	703	CDL	CB6-CB4-OB6-CB5
75	l	704	CDL	CA6-CA4-OA6-CA5
75	AH	403	CDL	CA3-CA4-OA6-CA5
76	l	701	PEE	C3-C2-O2-C10
76	l	702	PEE	C3-C2-O2-C10
75	AA	101	CDL	CB2-C1-CA2-OA2
75	V	201	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
75	i	401	CDL	C32-C31-CA7-OA8
75	AJ	404	CDL	CB4-CB3-OB5-PB2
75	V	201	CDL	C55-C56-C57-C58
75	n	101	CDL	C53-C54-C55-C56
75	AA	101	CDL	OA5-CA3-CA4-OA6
75	l	703	CDL	CA7-C31-C32-C33
76	V	202	PEE	C11-C10-O2-C2
75	n	101	CDL	C15-C16-C17-C18
76	AH	401	PEE	C31-C32-C33-C34
76	AY	502	PEE	C38-C39-C40-C41
75	AN	101	CDL	OB6-CB4-CB6-OB8
71	U	101	PLX	C2-O1-P1-O4
71	V	203	PLX	C3-O4-P1-O1
71	g	203	PLX	C3-O4-P1-O1
75	V	201	CDL	CB2-OB2-PB2-OB5
75	l	703	CDL	CB2-OB2-PB2-OB5
75	AG	101	CDL	CB3-OB5-PB2-OB2
75	AJ	405	CDL	CA2-OA2-PA1-OA5
75	AJ	405	CDL	CB3-OB5-PB2-OB2
75	AU	403	CDL	CA2-OA2-PA1-OA5
76	V	202	PEE	C4-O4P-P-O3P
76	l	701	PEE	C1-O3P-P-O4P
76	l	702	PEE	C4-O4P-P-O3P
76	AH	401	PEE	C1-O3P-P-O4P
76	AL	503	PEE	C4-O4P-P-O3P
71	V	203	PLX	C3-C4-C5-O8
75	AG	101	CDL	CB3-CB4-CB6-OB8
71	V	203	PLX	C29-C30-C31-C32
71	b	201	PLX	C28-C29-C30-C31
71	r	501	PLX	C11-C10-C9-C8
82	AV	402	HEM	C4D-C3D-CAD-CBD
76	AV	403	PEE	C31-C32-C33-C34
76	AY	502	PEE	C40-C41-C42-C43
76	V	202	PEE	C23-C24-C25-C26
75	AN	101	CDL	CB5-C51-C52-C53
75	l	703	CDL	C34-C35-C36-C37
75	l	704	CDL	C1-CB2-OB2-PB2
75	AG	101	CDL	C1-CA2-OA2-PA1
75	AU	403	CDL	CB4-CB3-OB5-PB2
75	AJ	405	CDL	C34-C35-C36-C37
75	AJ	405	CDL	C14-C15-C16-C17
76	V	202	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
76	V	202	PEE	C35-C36-C37-C38
73	J	401	NDP	C2D-C1D-N1N-C6N
75	AG	101	CDL	C51-C52-C53-C54
76	l	702	PEE	C23-C24-C25-C26
76	l	701	PEE	O4P-C4-C5-N
76	AY	502	PEE	O4P-C4-C5-N
71	g	202	PLX	C15-C16-C17-C18
75	AL	502	CDL	C54-C55-C56-C57
75	AY	501	CDL	C52-C53-C54-C55
71	g	201	PLX	C19-C20-C21-C22
75	AJ	405	CDL	C15-C16-C17-C18
71	V	203	PLX	O6-C6-C7-C8
71	g	201	PLX	O6-C6-C7-C8
75	i	401	CDL	C1-CB2-OB2-PB2
75	i	401	CDL	CB4-CB3-OB5-PB2
75	l	703	CDL	CA4-CA3-OA5-PA1
75	AN	101	CDL	C32-C33-C34-C35
71	g	201	PLX	C25-C26-C27-C28
76	W	201	PEE	C11-C12-C13-C14
71	B	303	PLX	C6-C7-C8-C9
71	V	203	PLX	C6-C7-C8-C9
75	l	703	CDL	CB5-C51-C52-C53
75	AG	101	CDL	C71-C72-C73-C74
79	x	603	HEA	CAD-CBD-CGD-O1D
72	E	201	8Q1	O27-C28-C29-C30
72	p	201	8Q1	O27-C28-C29-C31
76	AJ	403	PEE	C15-C16-C17-C18
75	AU	403	CDL	CB3-CB4-OB6-CB5
71	g	203	PLX	C3-C4-O6-C6
71	r	501	PLX	C5-C4-O6-C6
71	AQ	101	PLX	C5-C4-O6-C6
75	AN	101	CDL	CA2-OA2-PA1-OA5
75	V	201	CDL	C11-C12-C13-C14
75	i	401	CDL	C72-C71-CB7-OB8
82	AV	402	HEM	C2D-C3D-CAD-CBD
75	AN	101	CDL	C31-CA7-OA8-CA6
76	V	202	PEE	C21-C22-C23-C24
76	AL	503	PEE	C19-C20-C21-C22
75	AH	403	CDL	C51-C52-C53-C54
79	x	604	HEA	CAD-CBD-CGD-O1D
76	AU	401	PEE	C30-C31-C32-C33
71	V	203	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
72	p	201	8Q1	C42-C43-S44-C1
71	g	201	PLX	O6-C4-C5-O8
75	AA	101	CDL	OB6-CB4-CB6-OB8
76	AL	503	PEE	C16-C17-C18-C19
79	x	604	HEA	CAD-CBD-CGD-O2D
75	AH	403	CDL	C14-C15-C16-C17
76	AV	403	PEE	C14-C15-C16-C17
76	AL	503	PEE	C40-C41-C42-C43
79	x	603	HEA	CAA-CBA-CGA-O1A
75	AH	403	CDL	C32-C31-CA7-OA9
75	AN	101	CDL	OA9-CA7-OA8-CA6
79	x	603	HEA	CAD-CBD-CGD-O2D
75	AU	403	CDL	O1-C1-CA2-OA2
71	B	303	PLX	C7-C8-C9-C10
75	i	401	CDL	C52-C51-CB5-OB7
75	V	201	CDL	C73-C74-C75-C76
75	l	704	CDL	CA3-CA4-CA6-OA8
75	AN	101	CDL	C53-C54-C55-C56
75	AN	101	CDL	C35-C36-C37-C38
71	g	202	PLX	C16-C17-C18-C19
71	r	502	PLX	C28-C29-C30-C31
76	AJ	403	PEE	C36-C37-C38-C39
71	g	201	PLX	O4-C3-C4-O6
75	AH	403	CDL	CB7-C71-C72-C73
71	V	203	PLX	C24-C25-C26-C27
75	AY	501	CDL	C72-C71-CB7-OB8
71	AL	501	PLX	O6-C6-C7-C8
75	AU	403	CDL	C34-C35-C36-C37
76	AL	503	PEE	C23-C24-C25-C26
76	AU	401	PEE	C14-C15-C16-C17
76	AU	401	PEE	C38-C39-C40-C41
76	AY	502	PEE	C36-C37-C38-C39
71	AT	101	PLX	C30-C31-C32-C33
72	E	201	8Q1	O33-C32-C34-N36
76	AU	401	PEE	C42-C43-C44-C45
75	AH	403	CDL	C73-C74-C75-C76
76	W	201	PEE	C35-C36-C37-C38
76	AJ	403	PEE	C19-C20-C21-C22
75	l	703	CDL	C32-C31-CA7-OA8
75	l	704	CDL	C32-C31-CA7-OA8
76	W	201	PEE	C1-C2-O2-C10
76	V	202	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
71	g	202	PLX	C27-C28-C29-C30
75	AA	101	CDL	C15-C16-C17-C18
71	B	303	PLX	C14-C15-C16-C17
71	V	203	PLX	C35-C36-C37-C38
75	AG	101	CDL	C32-C31-CA7-OA8
75	AJ	404	CDL	C52-C51-CB5-OB6
76	AH	401	PEE	C40-C41-C42-C43
76	AV	403	PEE	C36-C37-C38-C39
71	b	201	PLX	C3-C4-C5-O8
75	V	201	CDL	CA3-CA4-CA6-OA8
75	AH	403	CDL	CB3-CB4-CB6-OB8
75	AJ	405	CDL	CA3-CA4-CA6-OA8
76	AH	401	PEE	O3P-C1-C2-O2
75	AN	101	CDL	C12-C11-CA5-OA6
71	AT	101	PLX	C10-C11-C12-C13
73	J	401	NDP	O4D-C4D-C5D-O5D
79	x	604	HEA	CAA-CBA-CGA-O2A
71	r	502	PLX	C33-C34-C35-C36
73	J	401	NDP	O4D-C1D-N1N-C2N
75	l	704	CDL	C35-C36-C37-C38
76	AH	401	PEE	C36-C37-C38-C39
79	x	604	HEA	CAA-CBA-CGA-O1A
71	B	303	PLX	O9-C24-C25-C26
71	AL	501	PLX	C11-C12-C13-C14
76	l	701	PEE	C38-C39-C40-C41
75	AU	403	CDL	O1-C1-CB2-OB2
71	AL	501	PLX	C29-C30-C31-C32
75	l	703	CDL	C32-C31-CA7-OA9
75	AA	101	CDL	C32-C33-C34-C35
76	AL	503	PEE	O2-C10-C11-C12
76	l	702	PEE	C18-C19-C20-C21
75	l	703	CDL	C32-C33-C34-C35
75	AG	101	CDL	C32-C31-CA7-OA9
75	AN	101	CDL	C12-C11-CA5-OA7
75	AU	403	CDL	CB3-CB4-CB6-OB8
76	l	702	PEE	C1-C2-C3-O3
71	b	201	PLX	C24-C25-C26-C27
75	AU	403	CDL	C72-C71-CB7-OB8
76	AL	503	PEE	C41-C42-C43-C44
71	AL	501	PLX	C33-C34-C35-C36
75	AG	101	CDL	C15-C16-C17-C18
76	l	702	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
75	AN	101	CDL	C72-C71-CB7-OB8
71	B	303	PLX	C4-C3-O4-P1
75	AU	403	CDL	C1-CA2-OA2-PA1
75	AJ	404	CDL	C52-C51-CB5-OB7
71	V	203	PLX	C17-C18-C19-C20
79	x	603	HEA	CAA-CBA-CGA-O2A
71	V	203	PLX	C3-O4-P1-O2
71	g	201	PLX	C3-O4-P1-O2
71	AT	101	PLX	C3-O4-P1-O3
75	l	703	CDL	CA3-OA5-PA1-OA3
75	l	704	CDL	CB3-OB5-PB2-OB3
75	n	101	CDL	CB3-OB5-PB2-OB3
75	AJ	405	CDL	CA2-OA2-PA1-OA3
75	AL	502	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CA2-OA2-PA1-OA3
75	AU	403	CDL	CB2-OB2-PB2-OB3
75	AY	501	CDL	CA2-OA2-PA1-OA3
76	l	702	PEE	C4-O4P-P-O1P
76	AH	401	PEE	C1-O3P-P-O1P
76	AJ	403	PEE	C4-O4P-P-O2P
75	AU	403	CDL	OB6-CB4-CB6-OB8
76	l	701	PEE	C33-C34-C35-C36
75	V	201	CDL	C12-C11-CA5-OA7
75	l	704	CDL	C32-C31-CA7-OA9
75	AU	403	CDL	C75-C76-C77-C78
76	AY	502	PEE	C21-C22-C23-C24
82	AV	401	HEM	CAA-CBA-CGA-O2A
76	AJ	403	PEE	O4P-C4-C5-N
71	AT	101	PLX	C25-C26-C27-C28
75	AA	101	CDL	C12-C11-CA5-OA6
71	r	501	PLX	C14-C15-C16-C17
71	b	201	PLX	C25-C24-O8-C5
71	g	202	PLX	C25-C24-O8-C5
71	AL	501	PLX	C1-C2-O1-P1
76	W	201	PEE	C5-C4-O4P-P
76	AJ	403	PEE	C10-C11-C12-C13
75	AY	501	CDL	C51-C52-C53-C54
73	J	401	NDP	C2D-C1D-N1N-C2N
76	l	702	PEE	C41-C42-C43-C44
76	V	202	PEE	C39-C40-C41-C42
75	l	704	CDL	C74-C75-C76-C77
76	l	702	PEE	C32-C33-C34-C35

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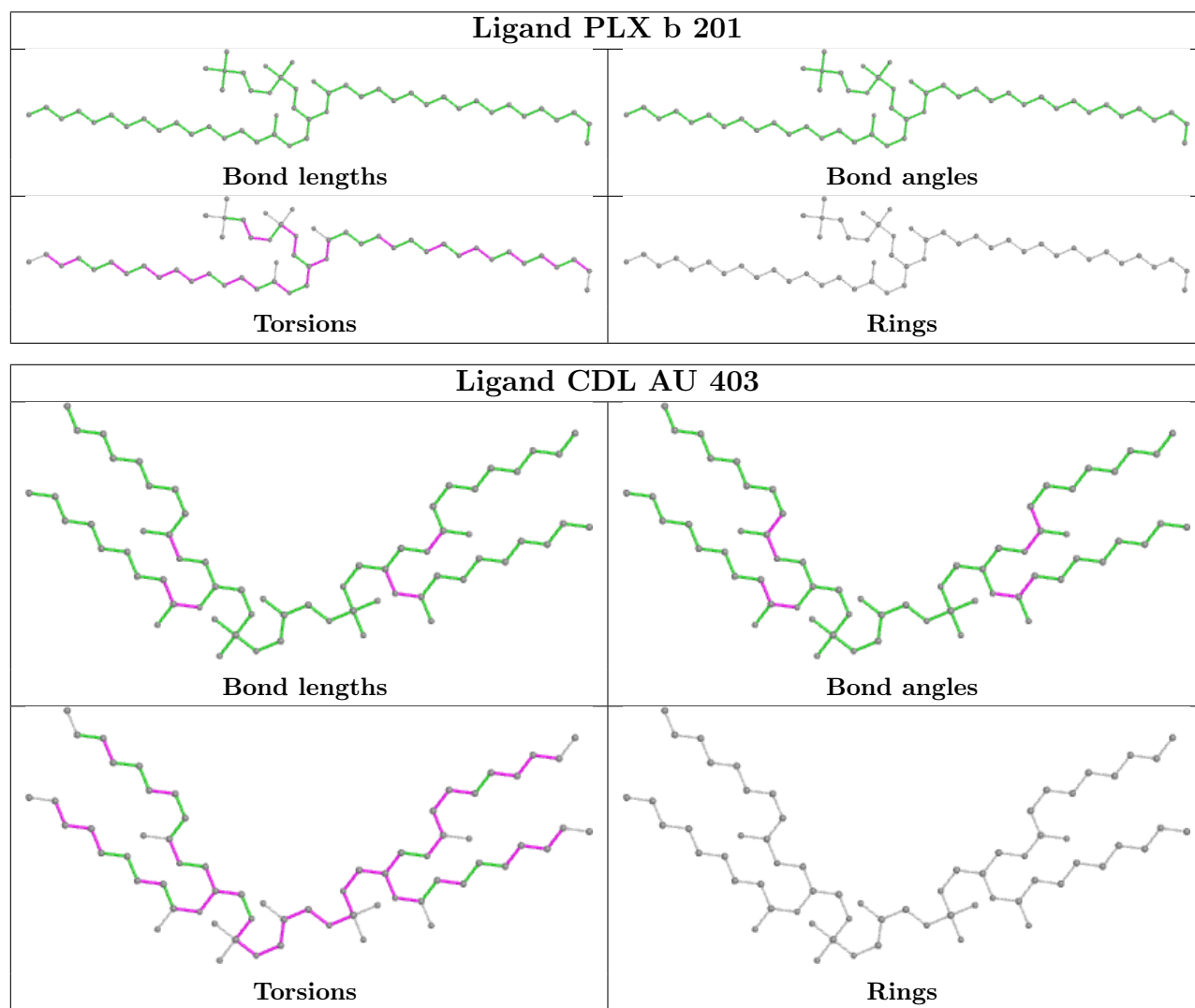
Mol	Chain	Res	Type	Atoms
75	l	704	CDL	C52-C51-CB5-OB6
75	AG	101	CDL	C52-C51-CB5-OB6
75	AJ	404	CDL	C12-C11-CA5-OA6
76	AH	401	PEE	O2-C10-C11-C12
76	AL	503	PEE	O3-C30-C31-C32
76	AY	502	PEE	O3-C30-C31-C32
76	AL	503	PEE	O4-C10-C11-C12
71	g	202	PLX	C6-C7-C8-C9
71	g	202	PLX	C24-C25-C26-C27
71	AQ	101	PLX	C6-C7-C8-C9
79	x	604	HEA	C26-C15-C16-C17
70	A	502	FMN	N10-C1'-C2'-O2'
79	x	603	HEA	O11-C11-C3B-C2B
75	AU	403	CDL	C72-C71-CB7-OB9
76	l	701	PEE	C11-C12-C13-C14
75	AH	403	CDL	C12-C11-CA5-OA6
71	V	203	PLX	C15-C16-C17-C18
75	AH	403	CDL	C12-C11-CA5-OA7
76	AY	502	PEE	O5-C30-C31-C32
75	AA	101	CDL	C12-C11-CA5-OA7
71	g	203	PLX	C36-C37-C38-C39
75	AN	101	CDL	O1-C1-CB2-OB2
75	l	704	CDL	C52-C51-CB5-OB7
75	AJ	404	CDL	C12-C11-CA5-OA7
75	AN	101	CDL	C72-C71-CB7-OB9
71	AT	101	PLX	C17-C18-C19-C20
76	W	201	PEE	C42-C43-C44-C45
75	AY	501	CDL	CA5-C11-C12-C13
75	AA	101	CDL	C52-C51-CB5-OB6

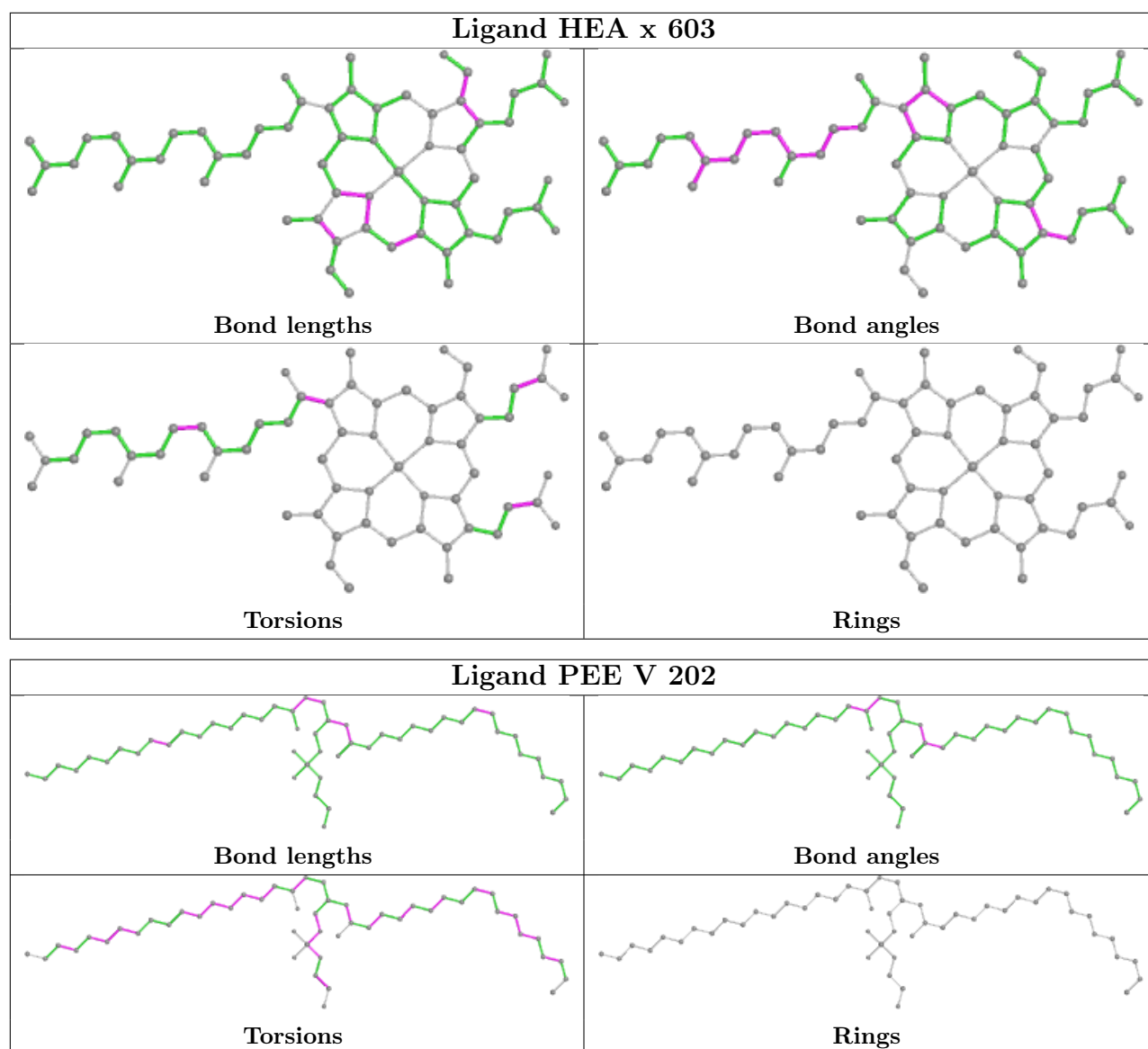
There are no ring outliers.

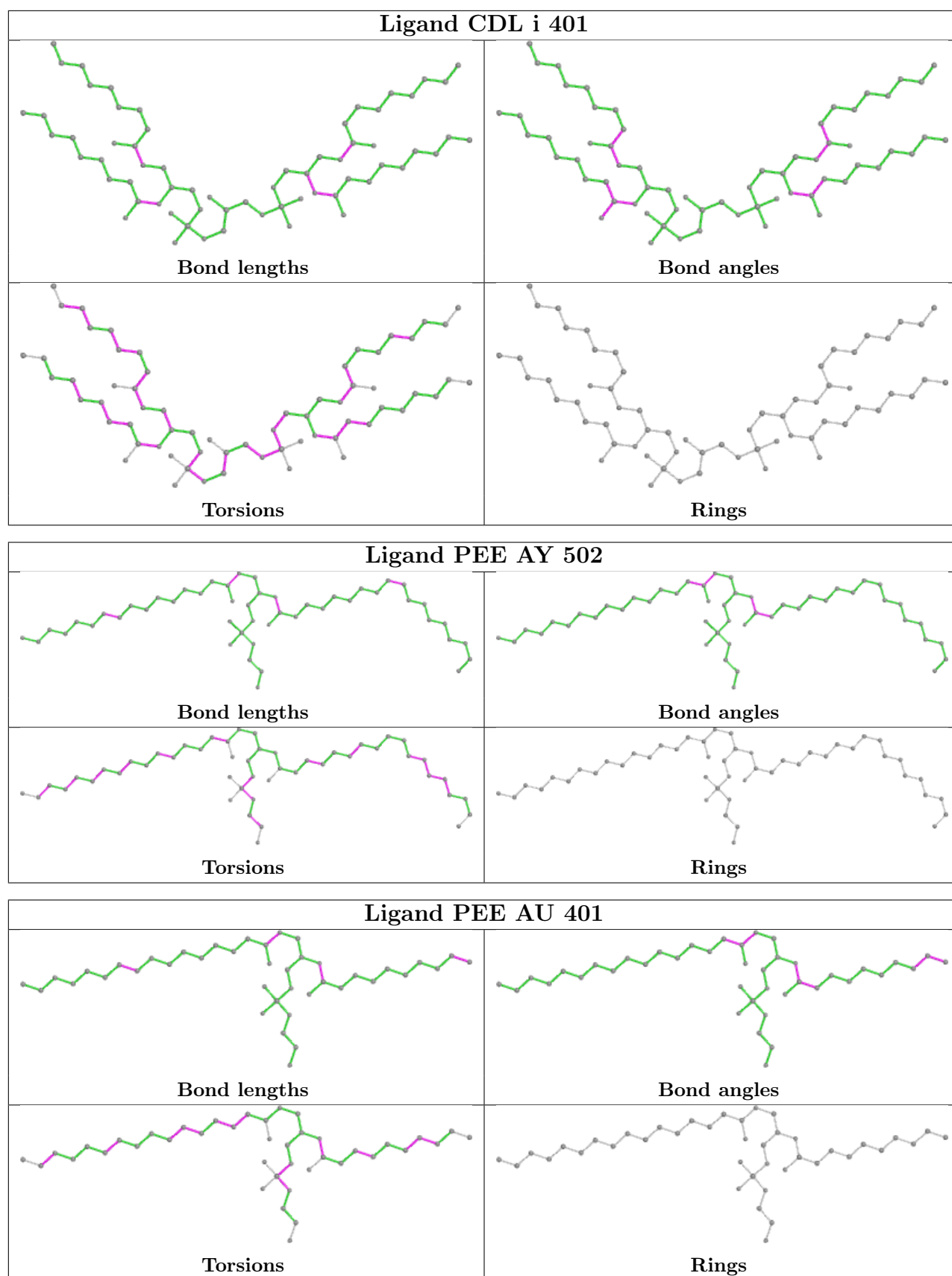
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

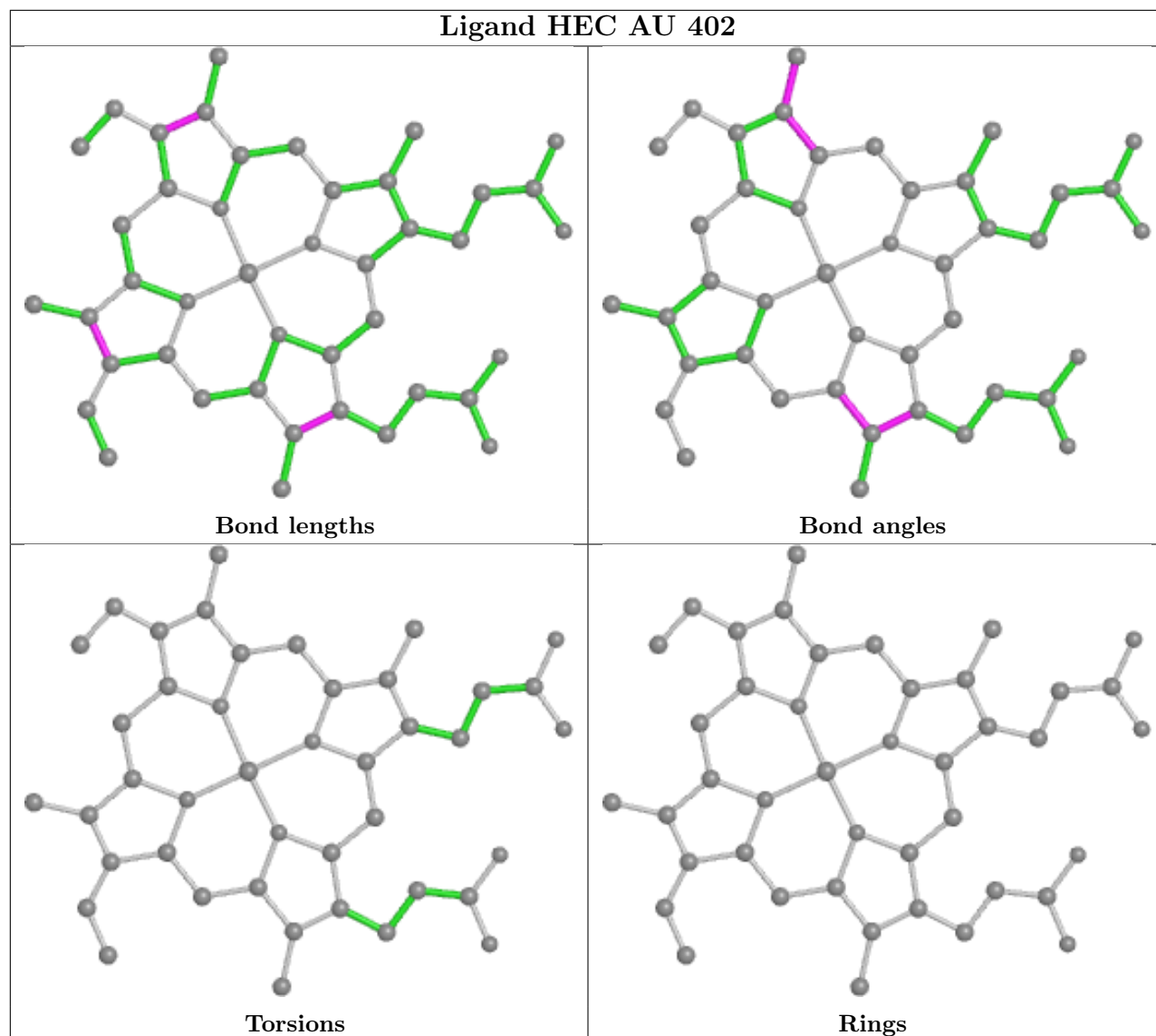
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



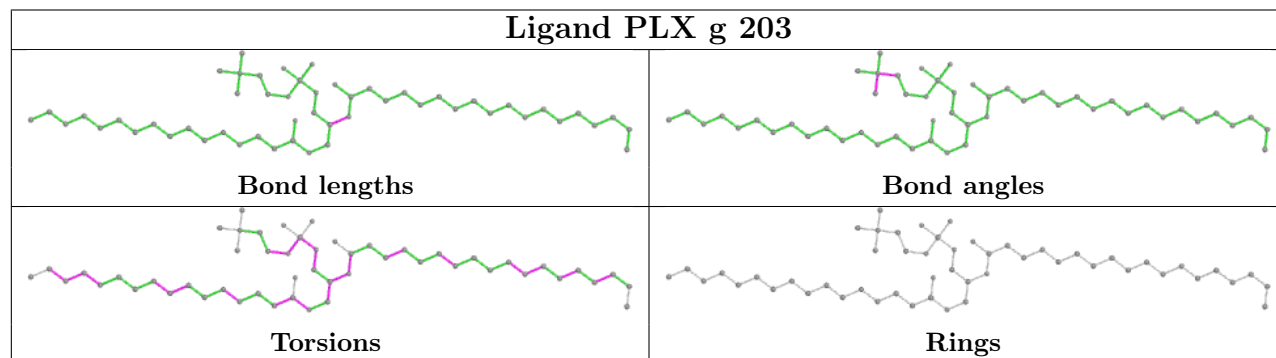


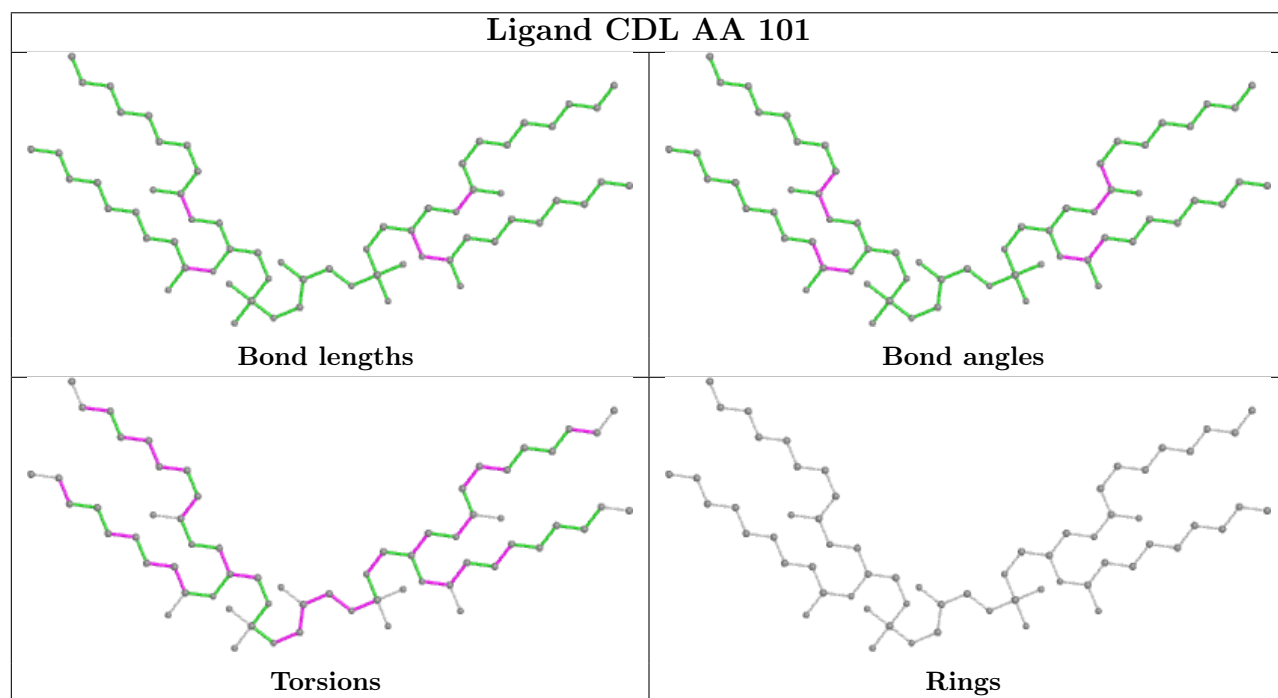
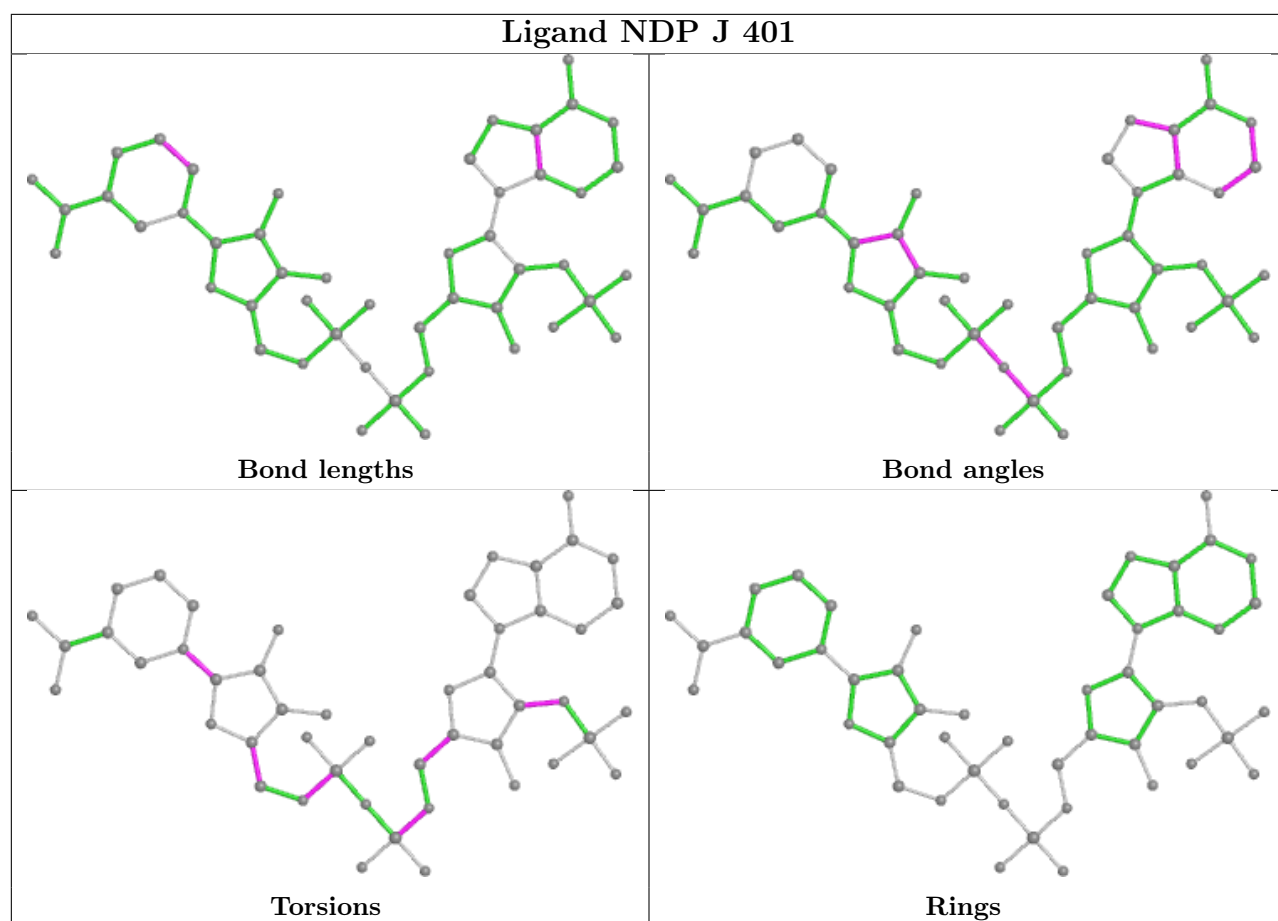


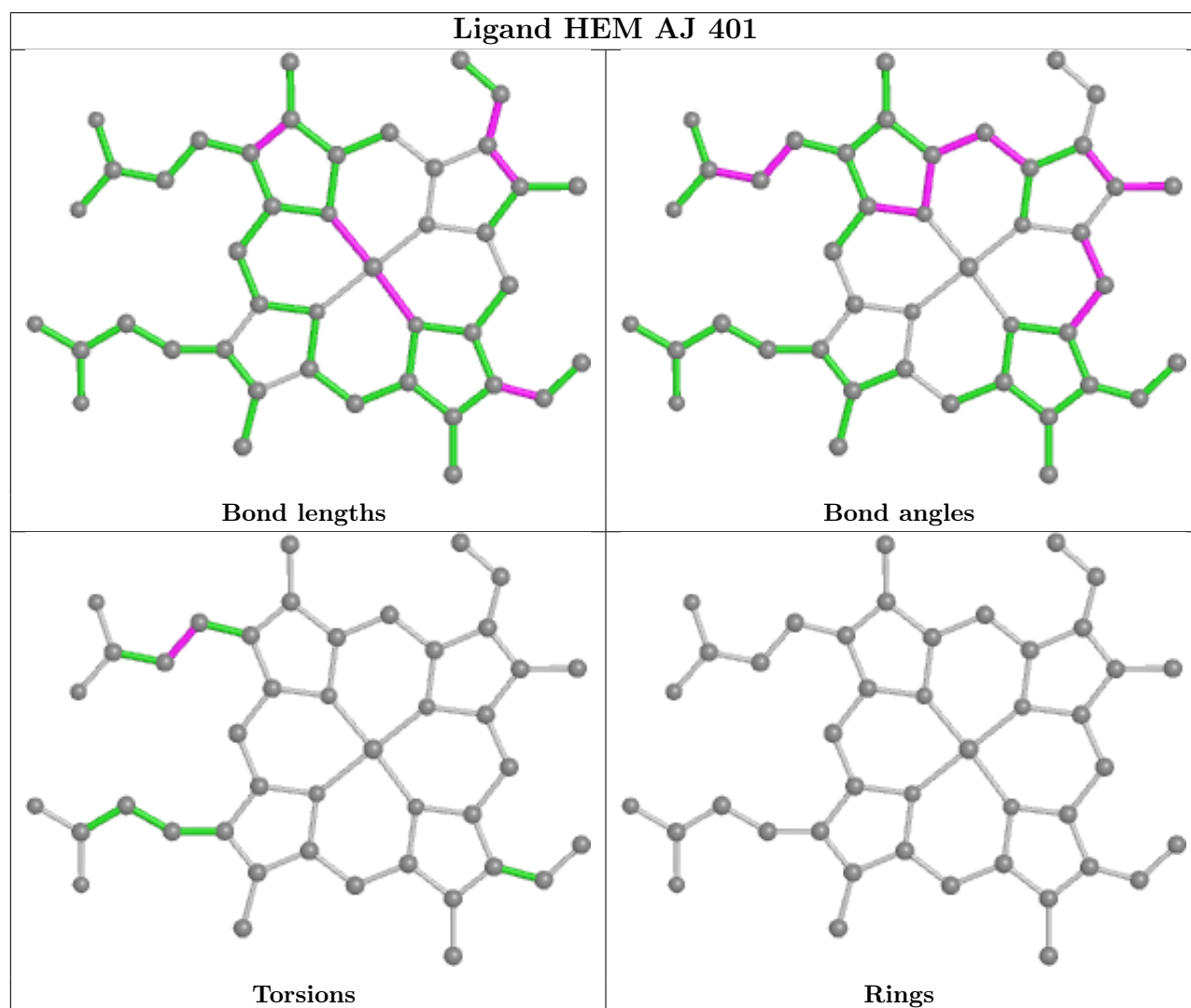
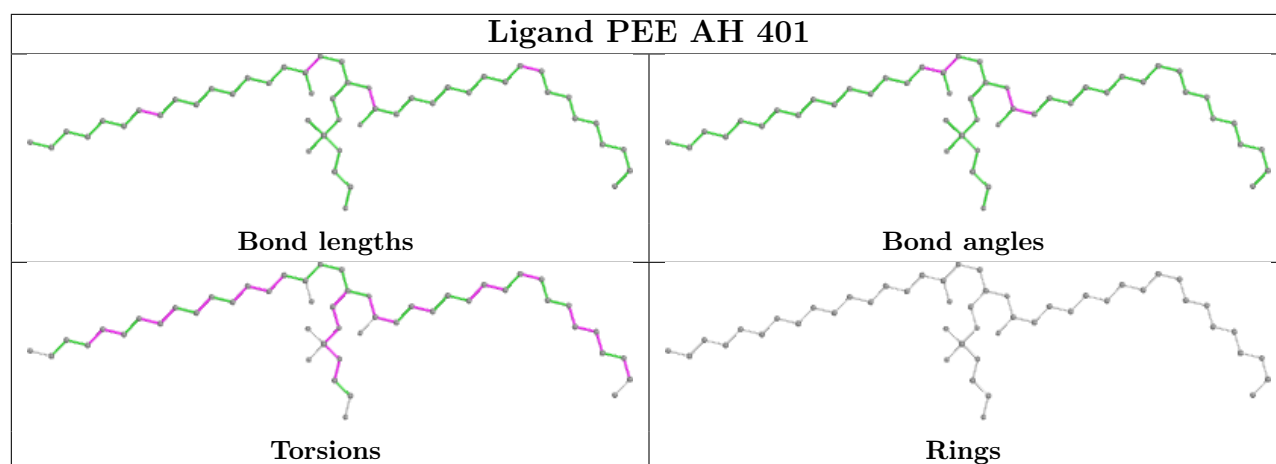
Ligand HEC AU 402

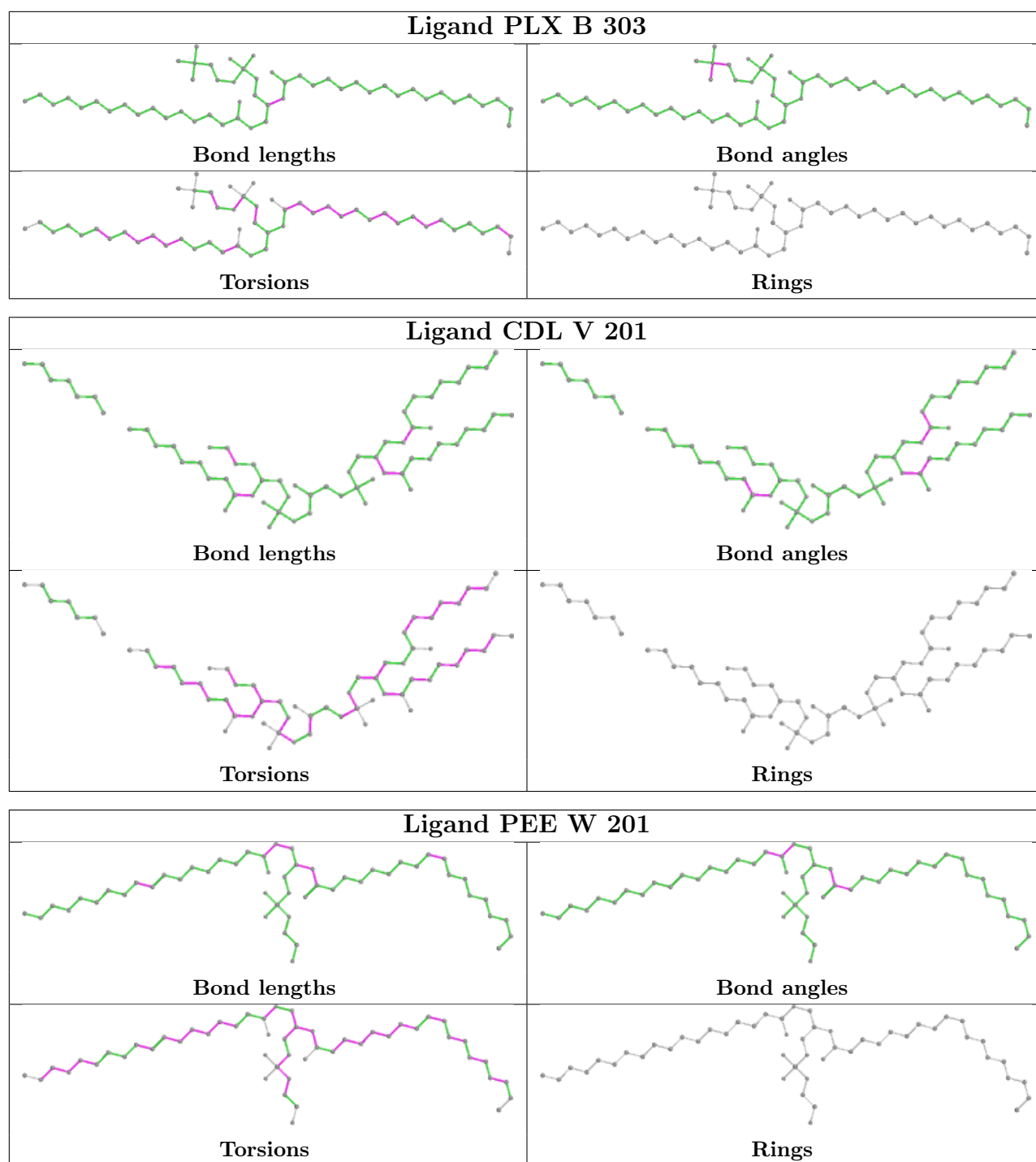


Ligand PLX g 203

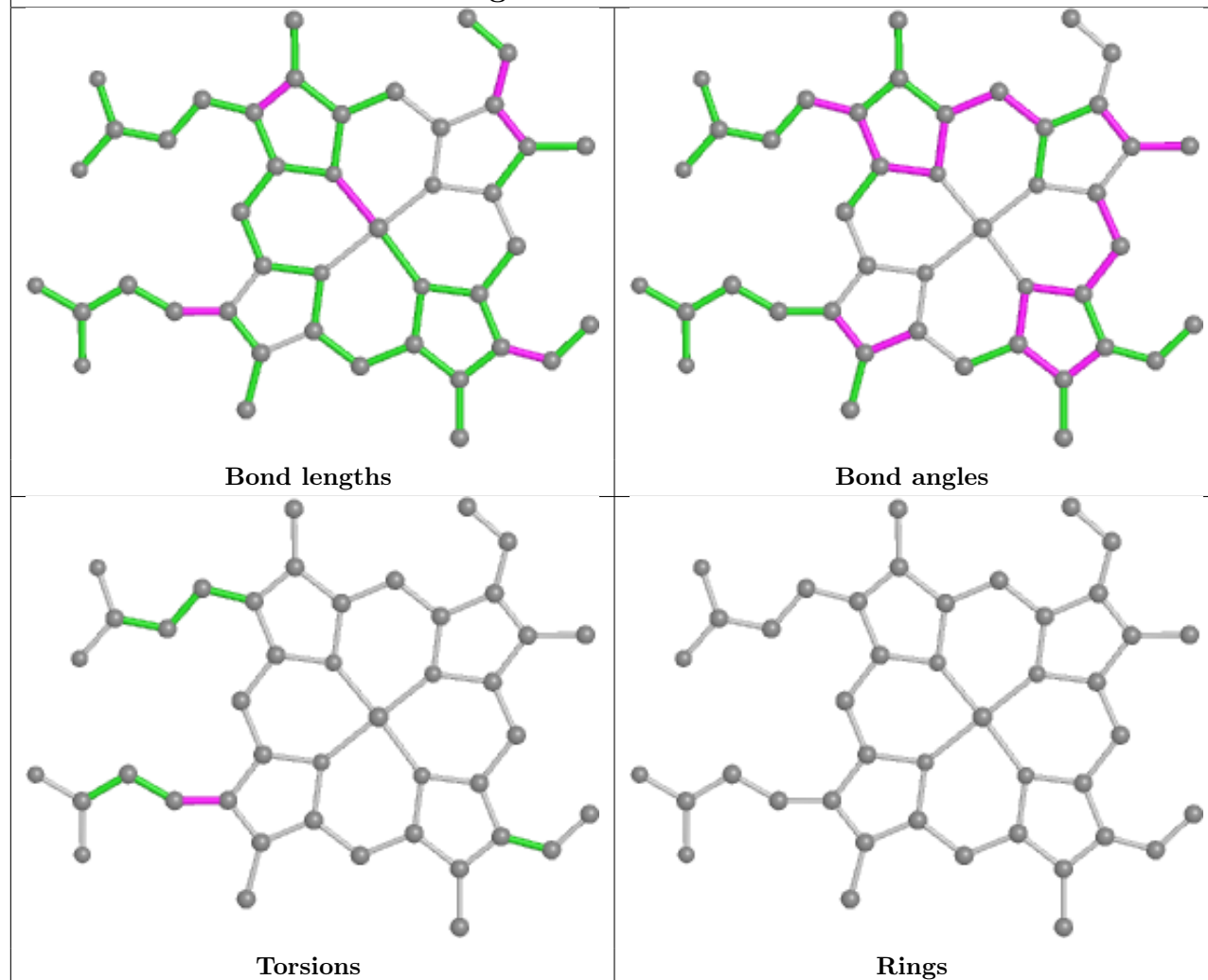




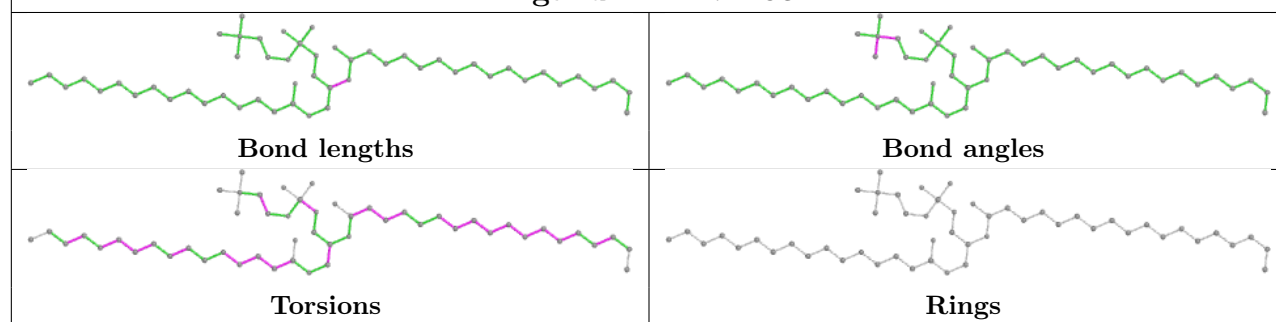


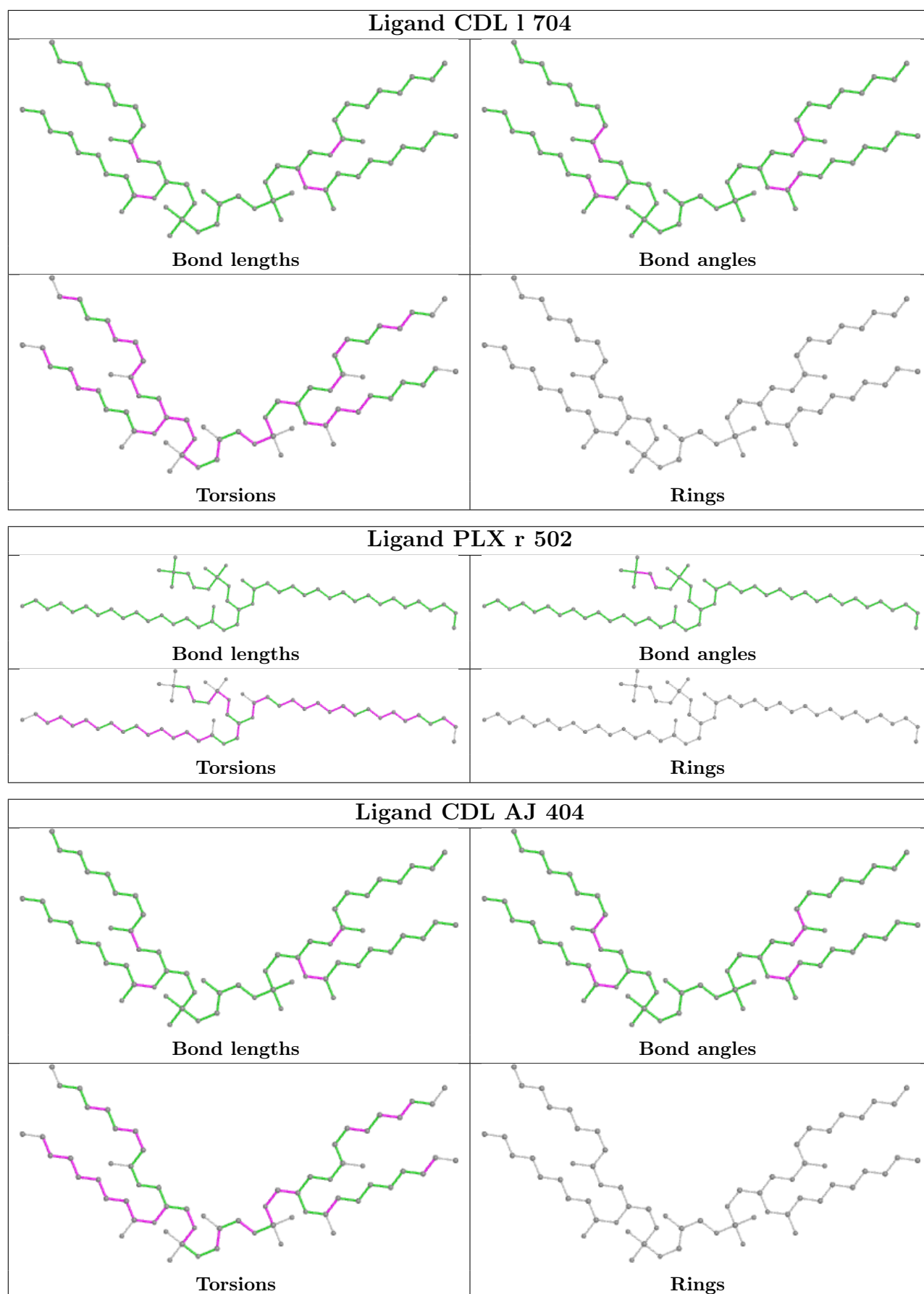


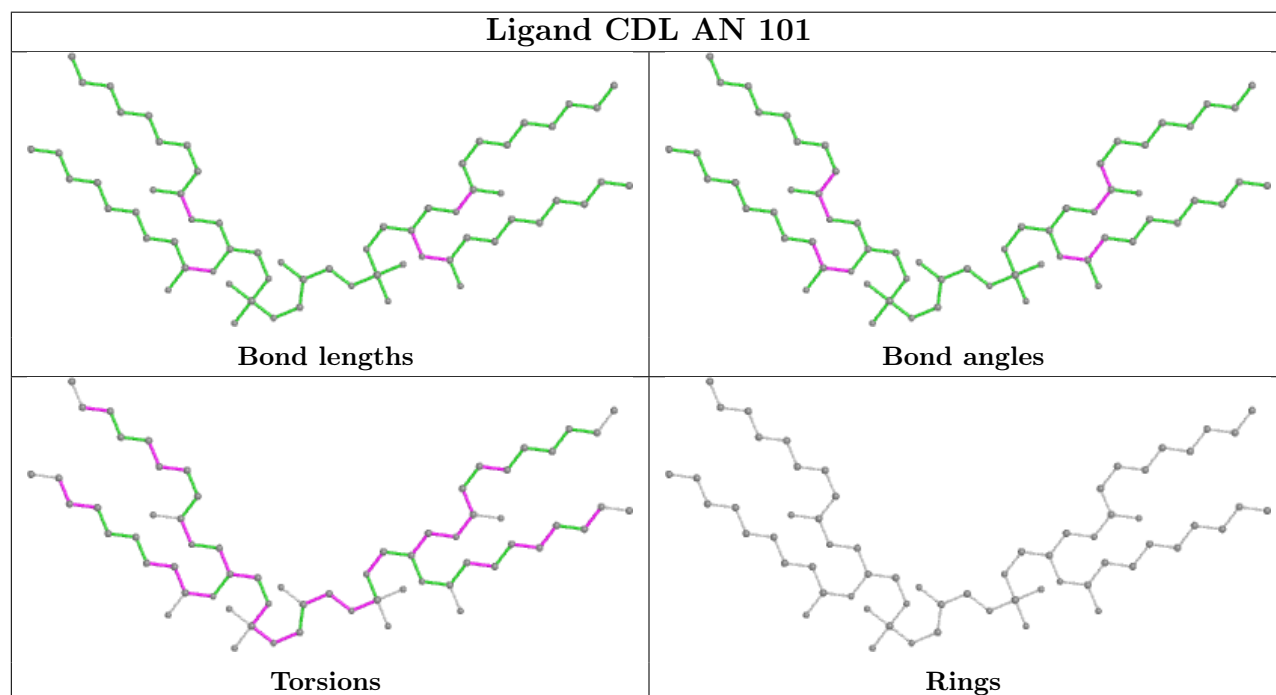
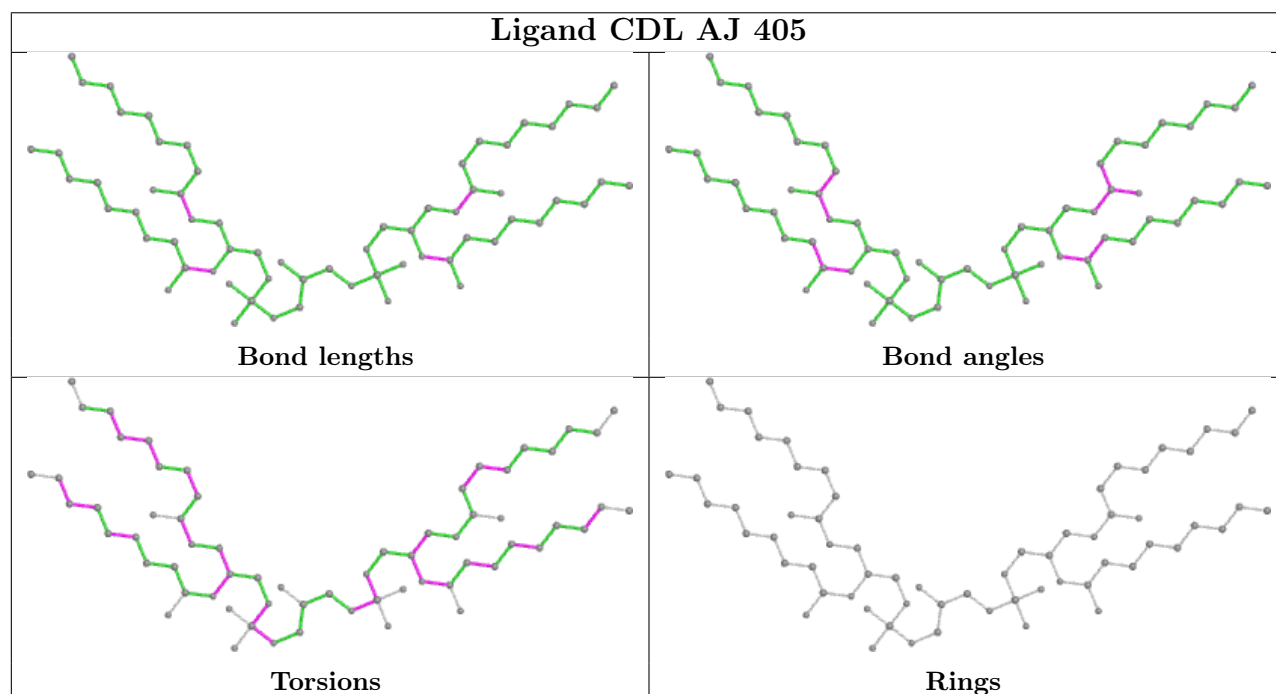
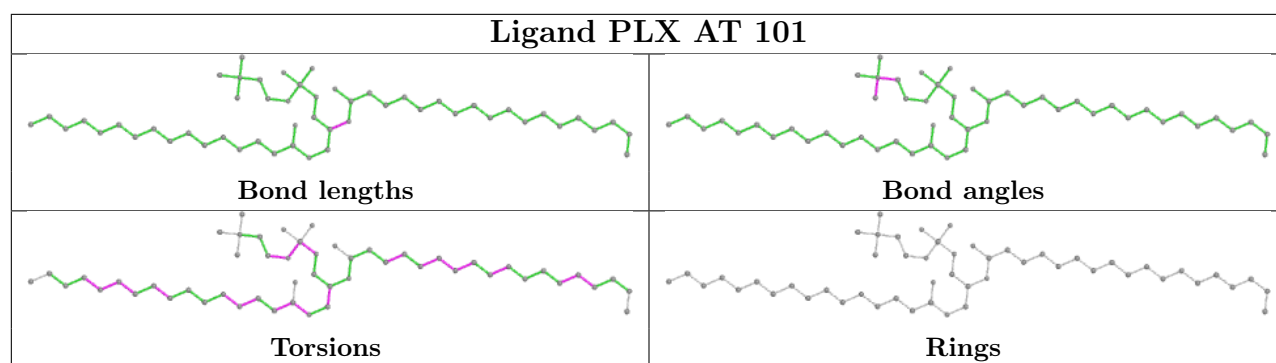
Ligand HEM AJ 402

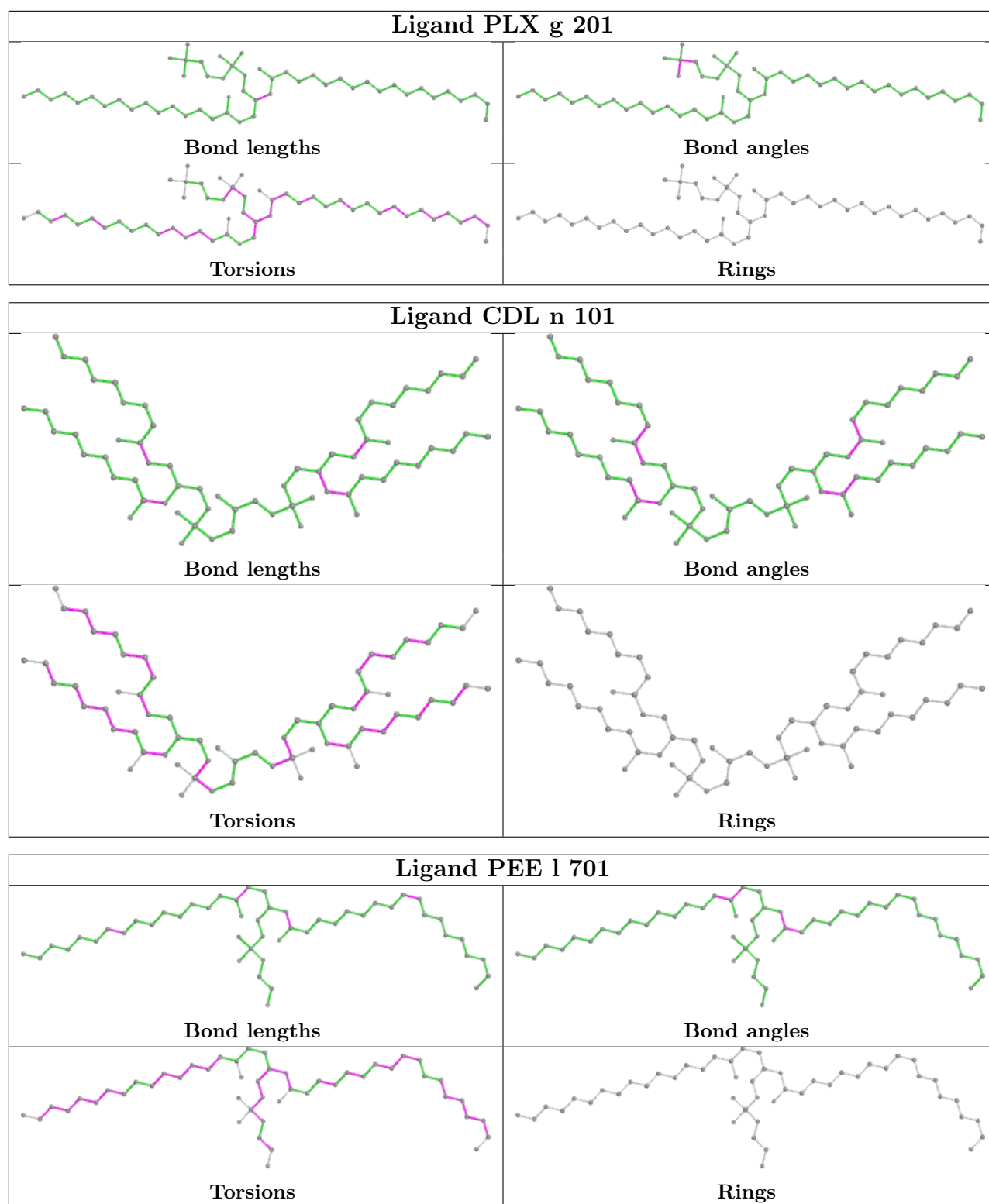


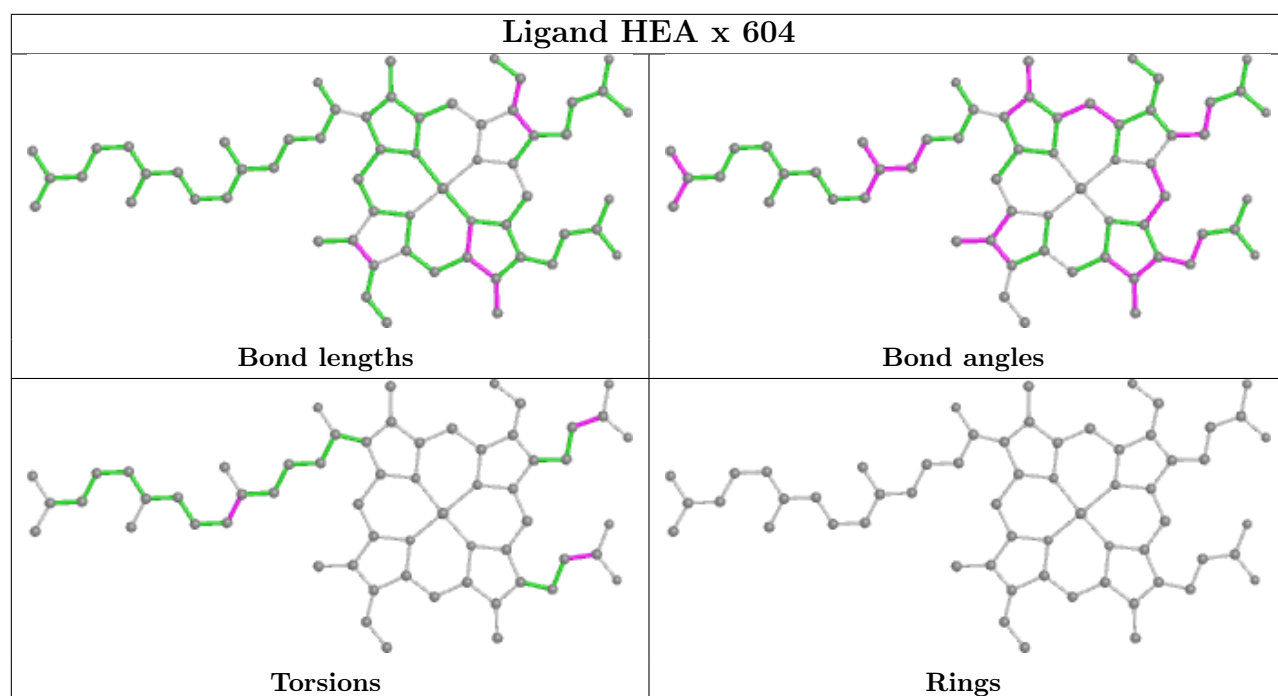
Ligand PLX V 203



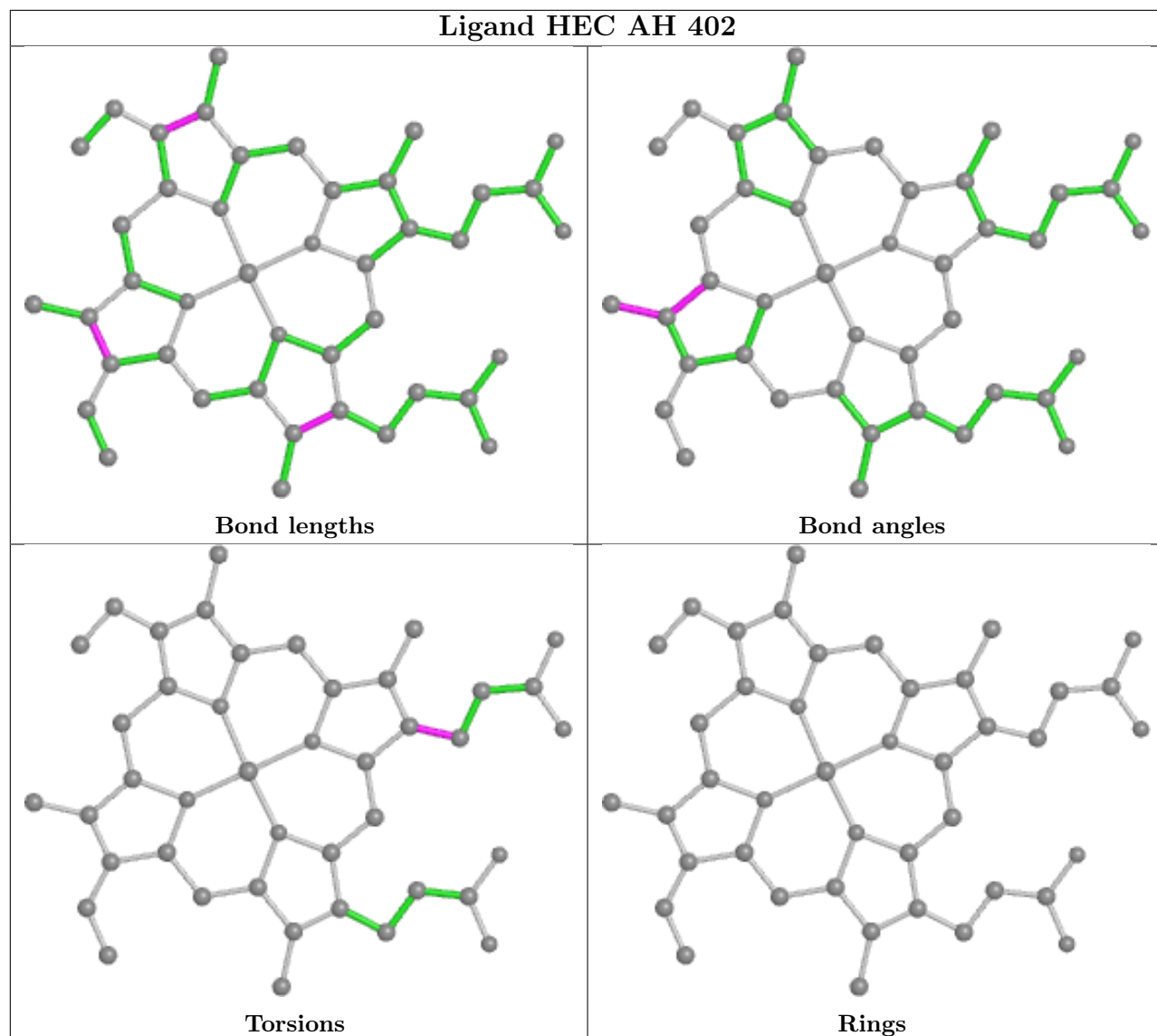


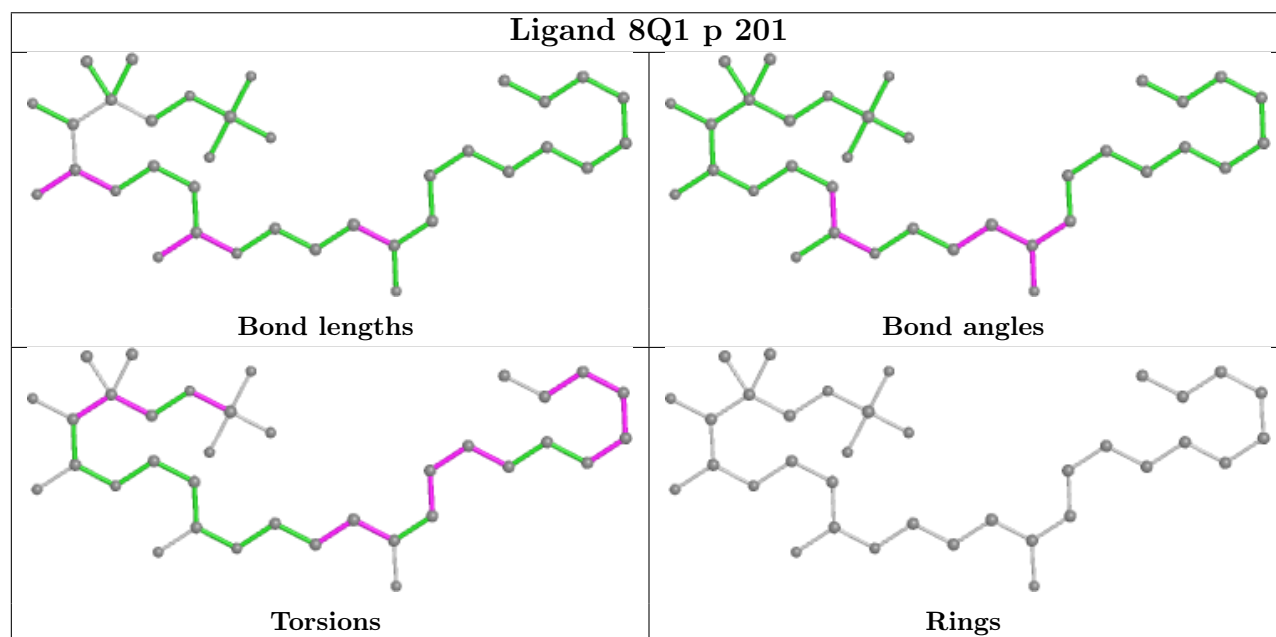
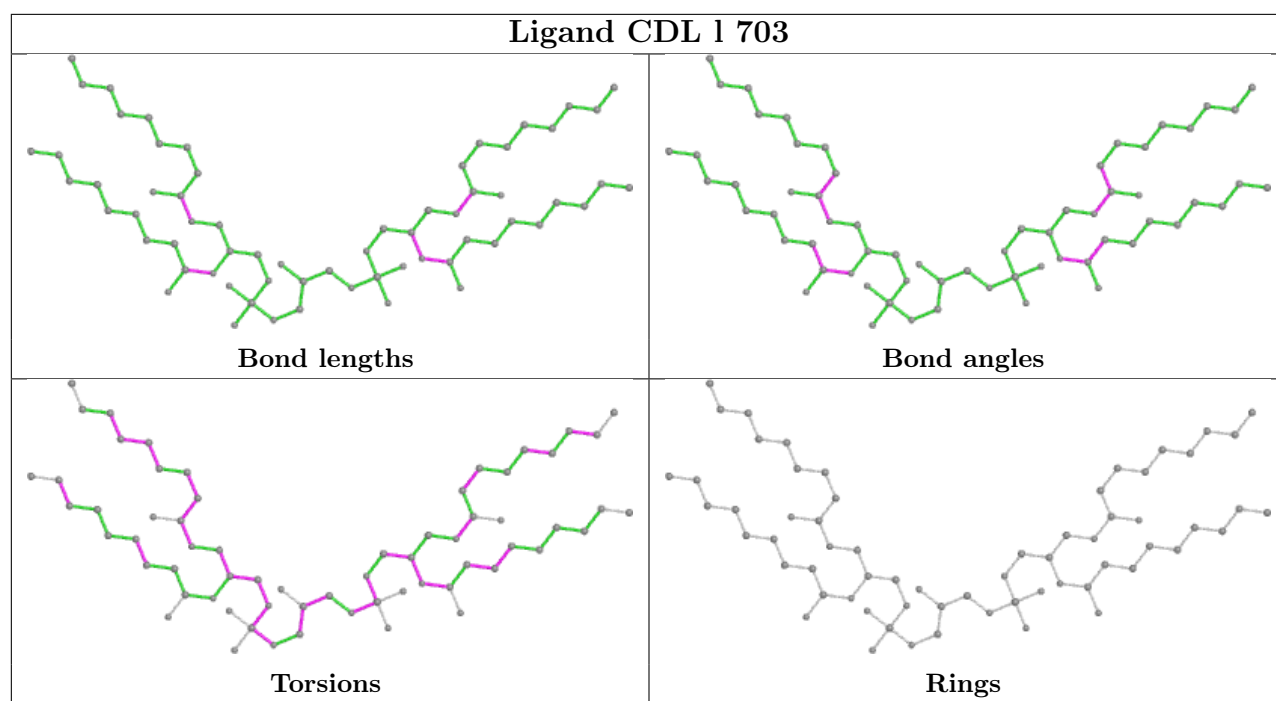


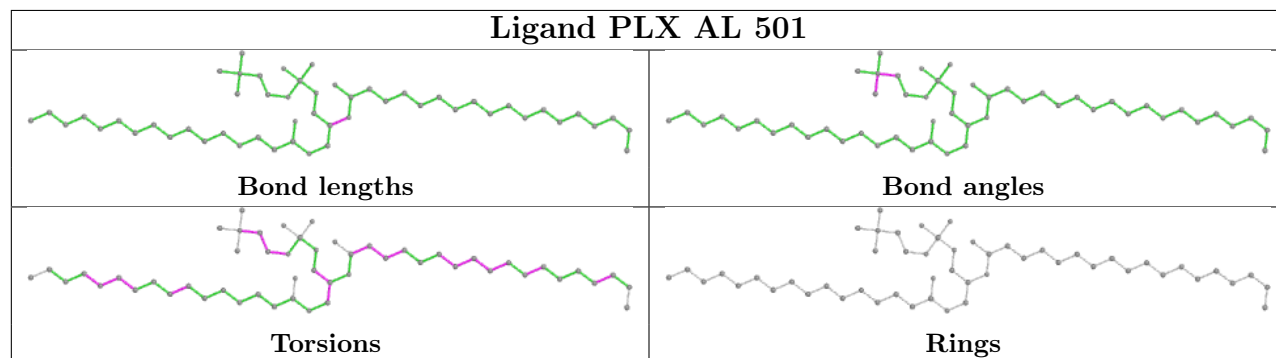
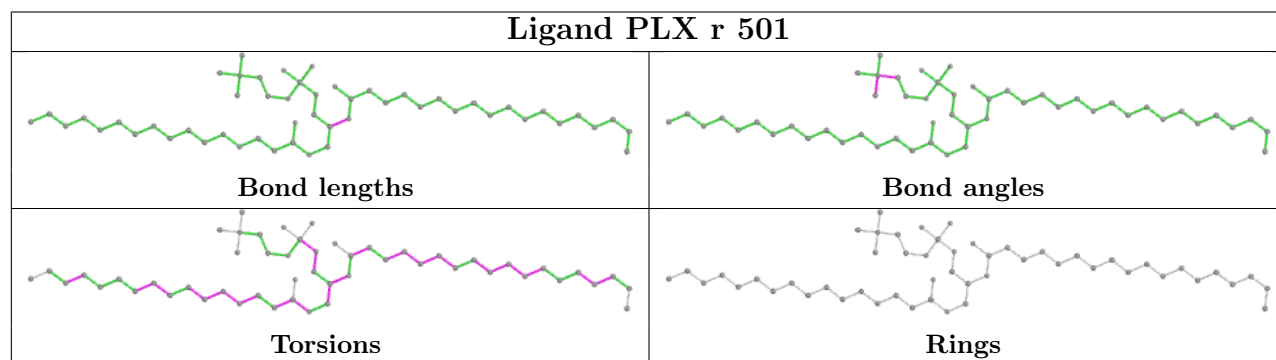
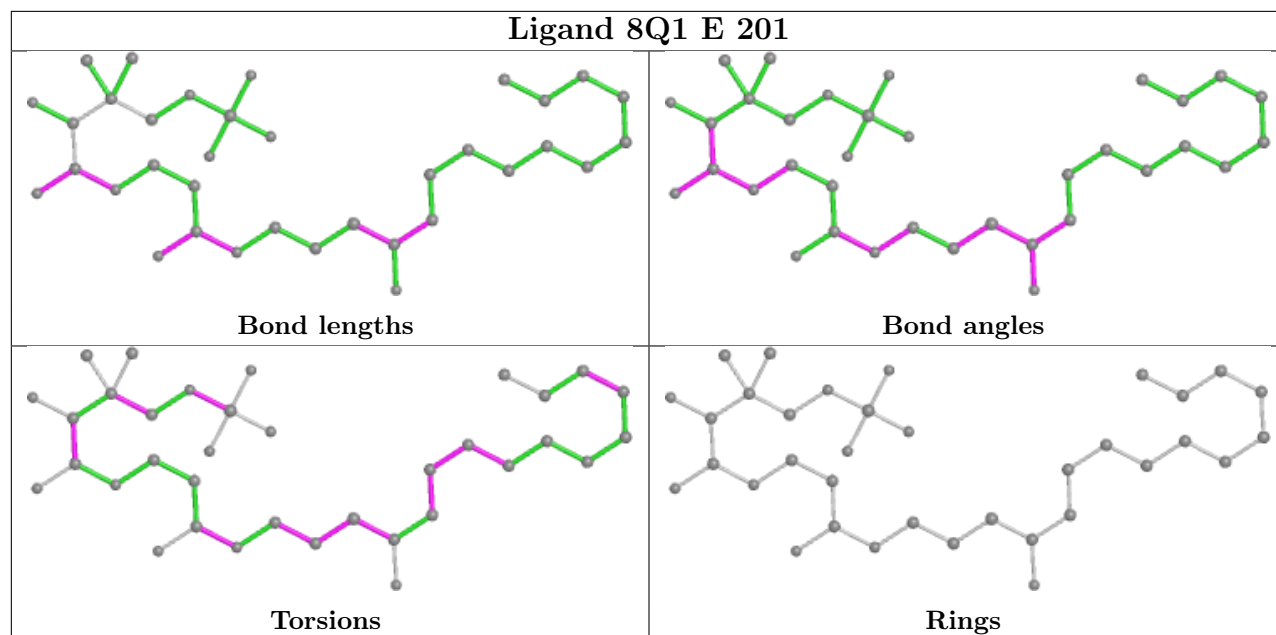


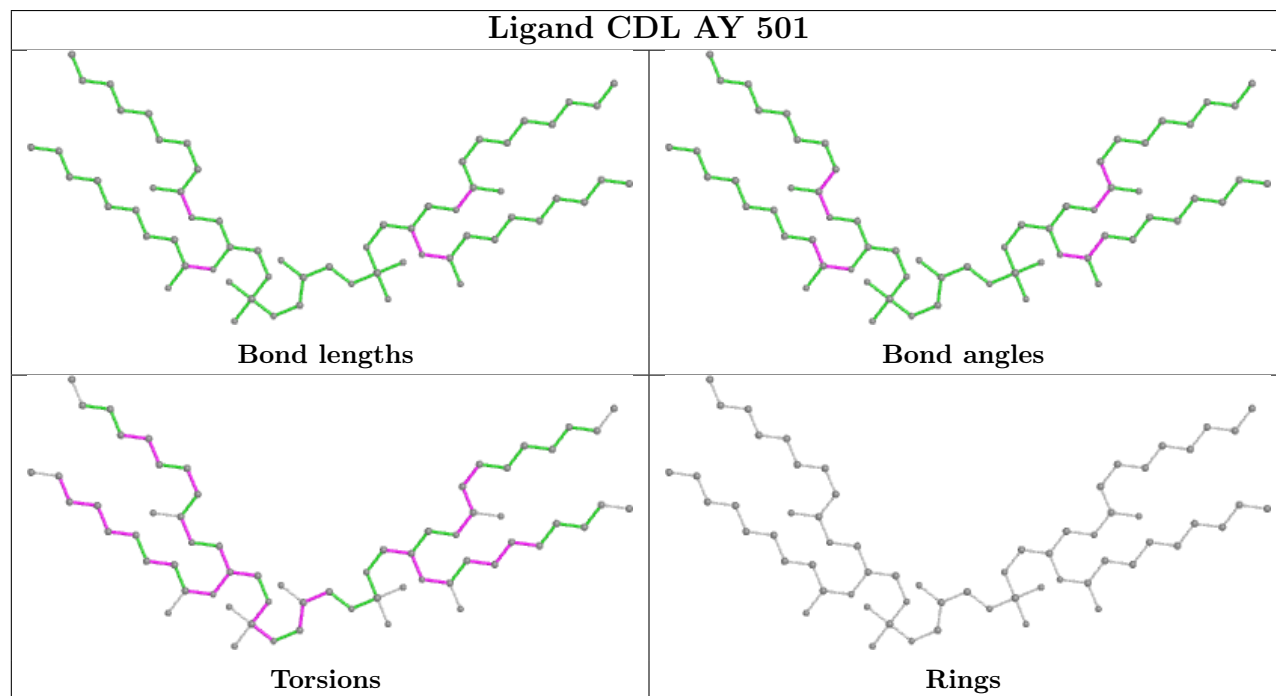
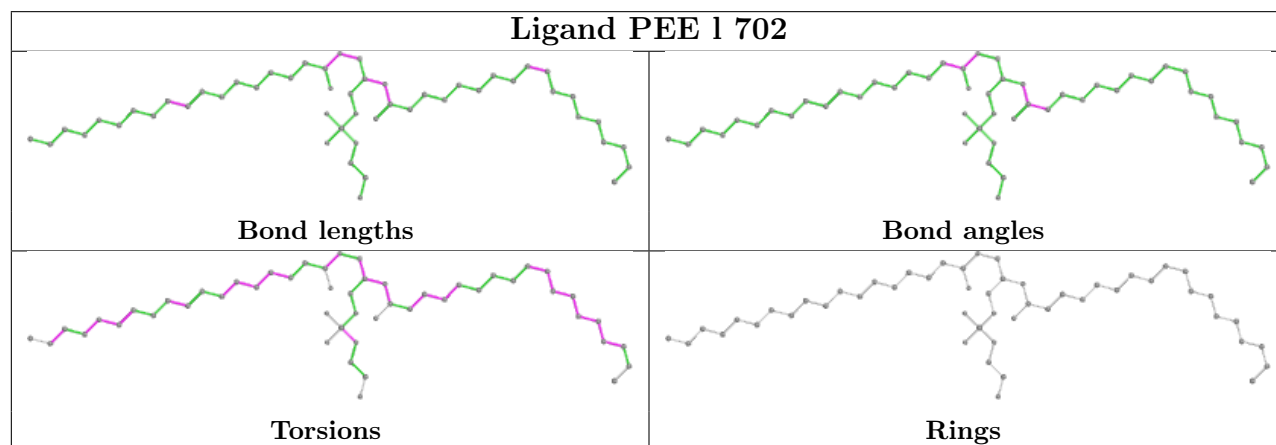
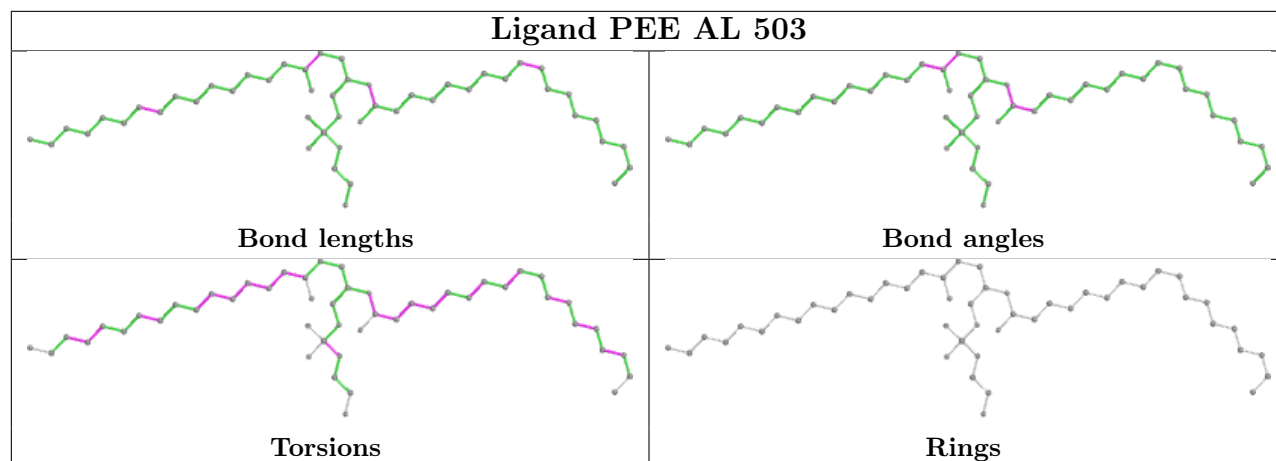


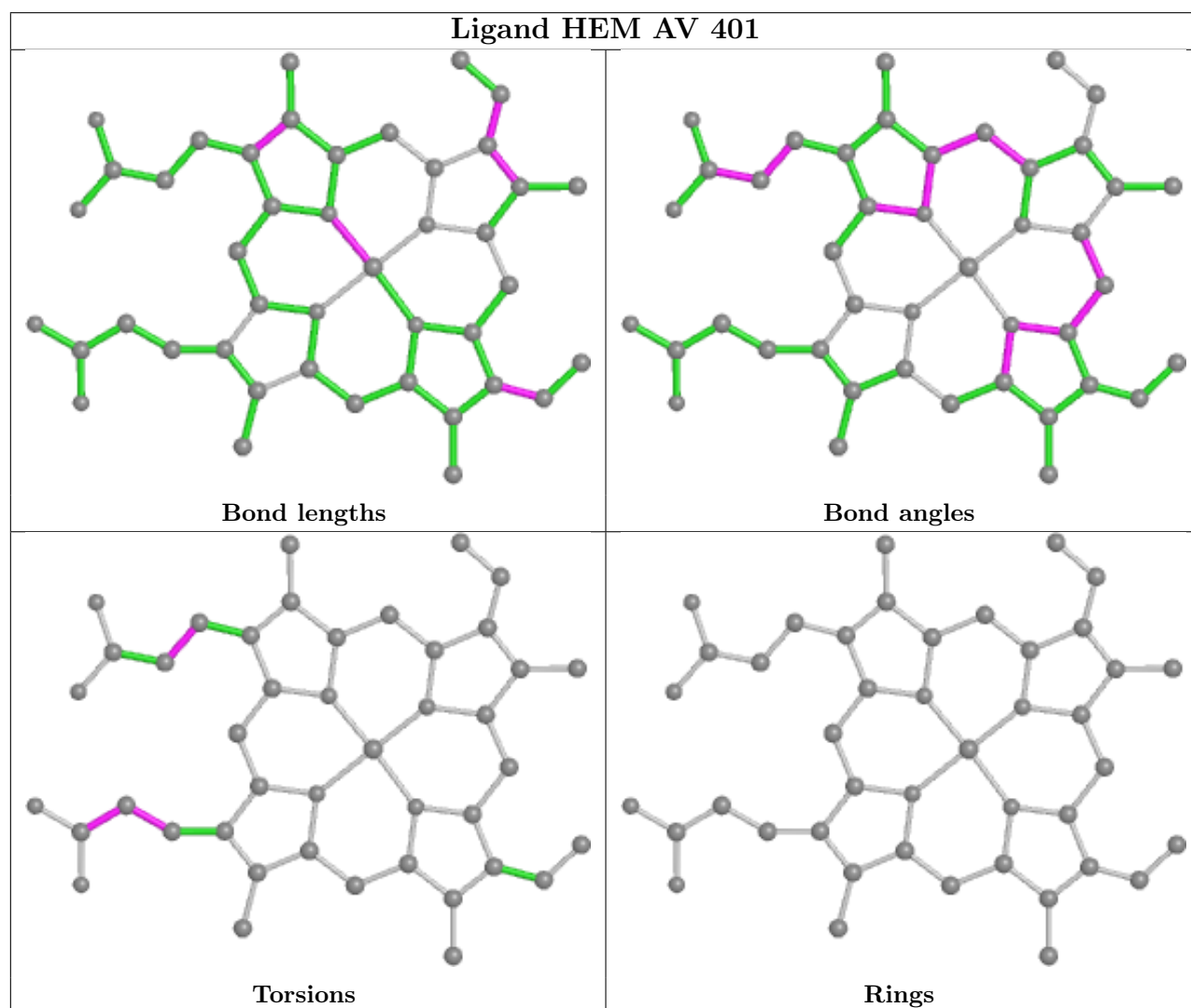
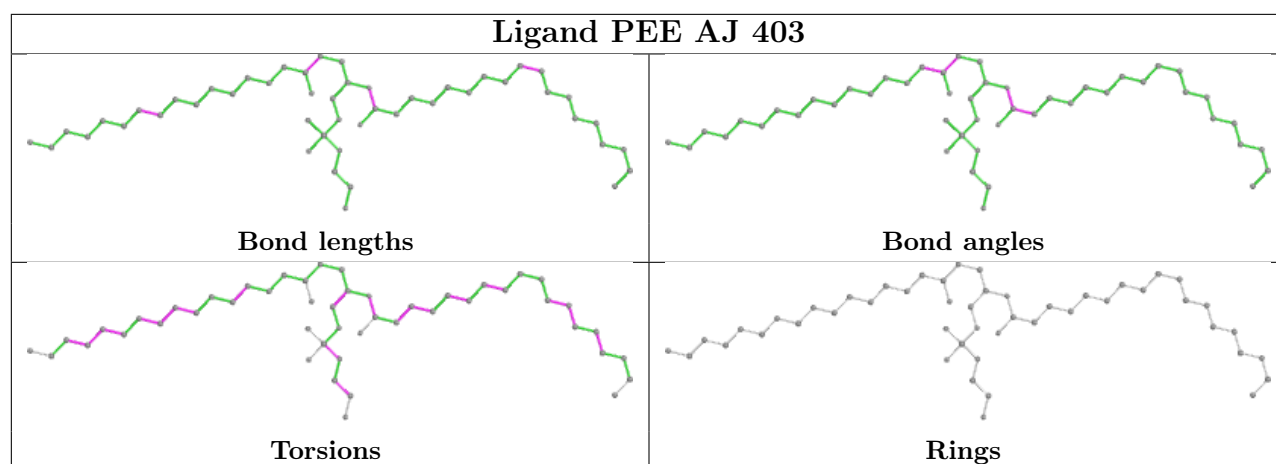
Ligand HEC AH 402

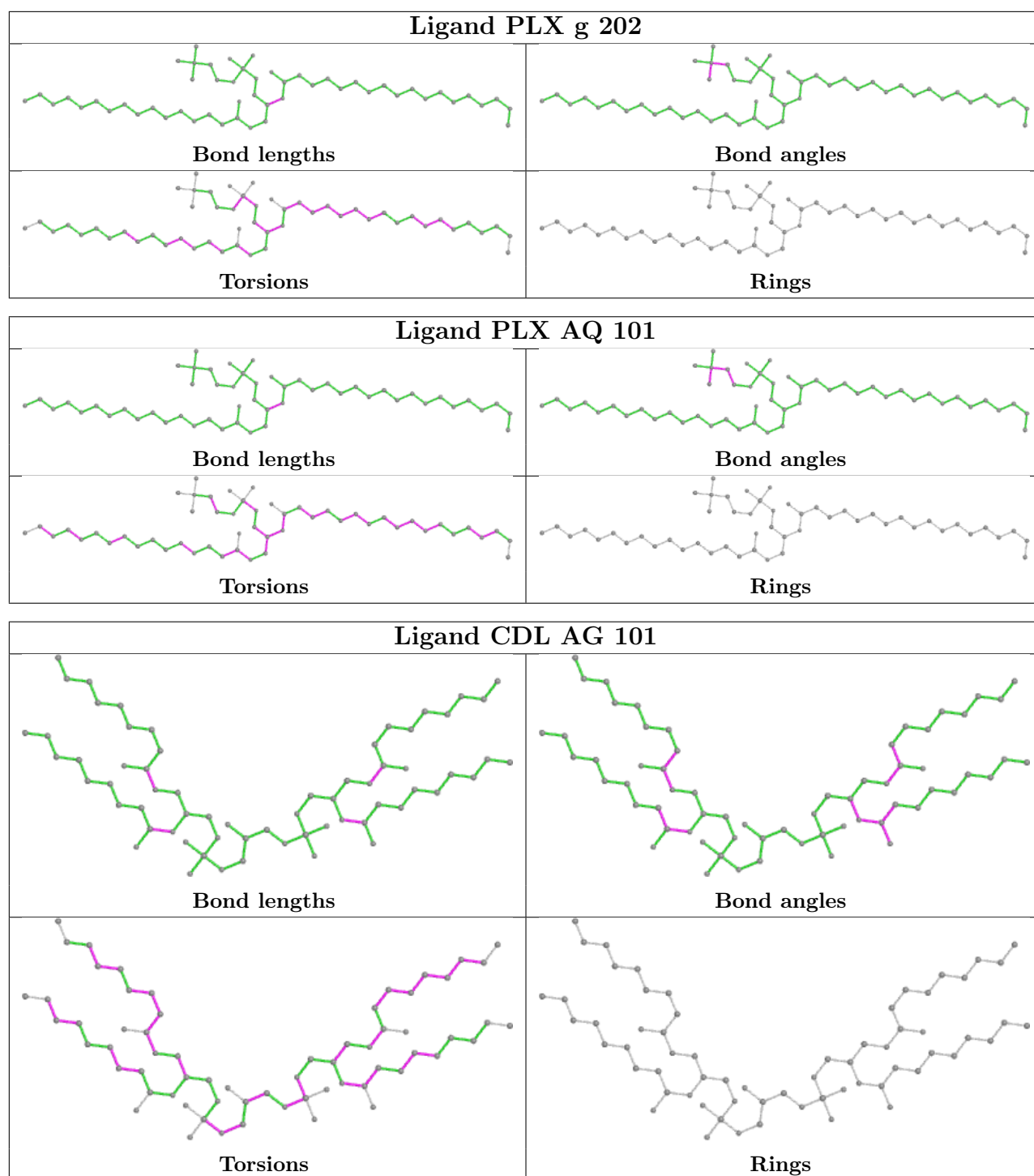


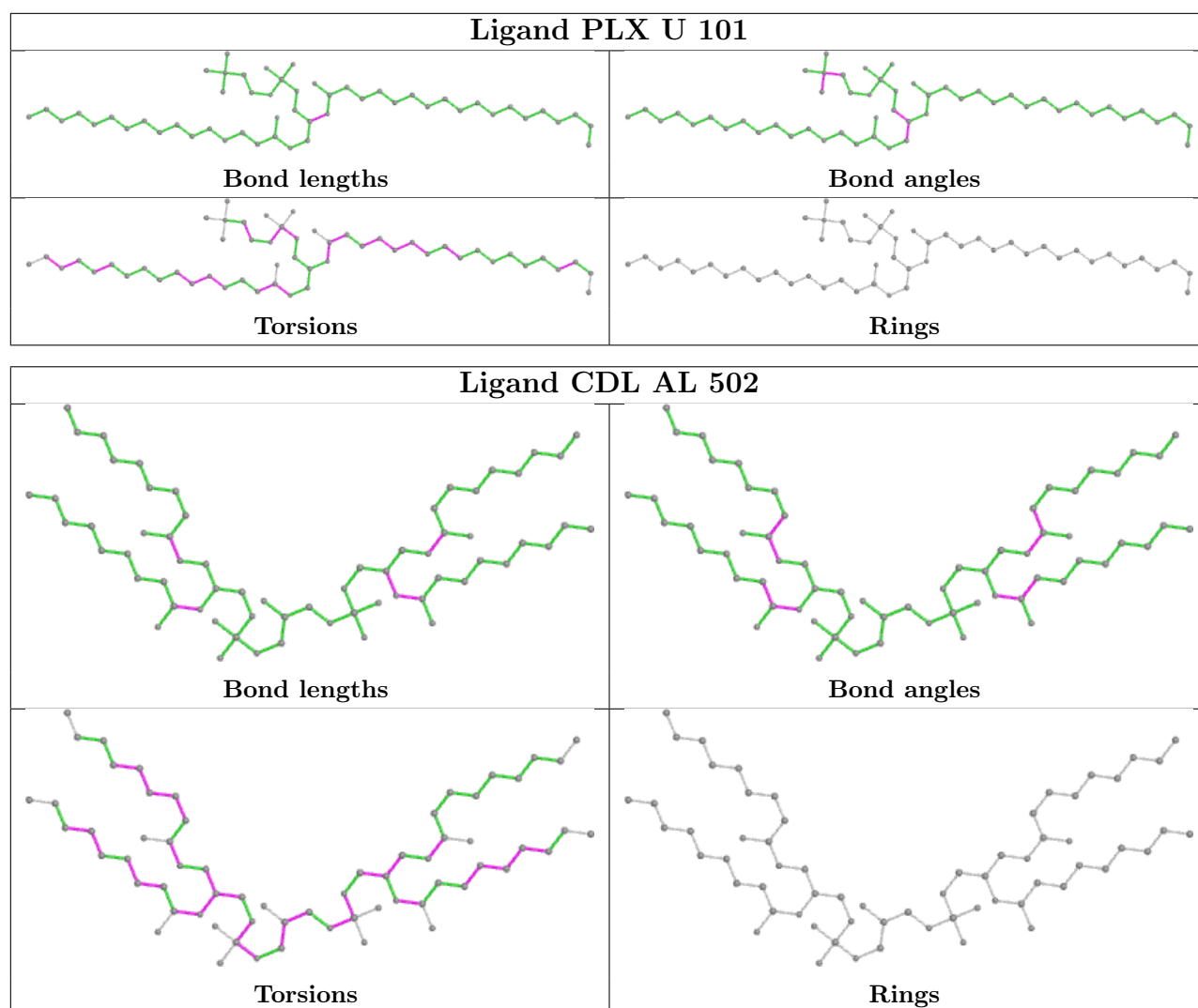




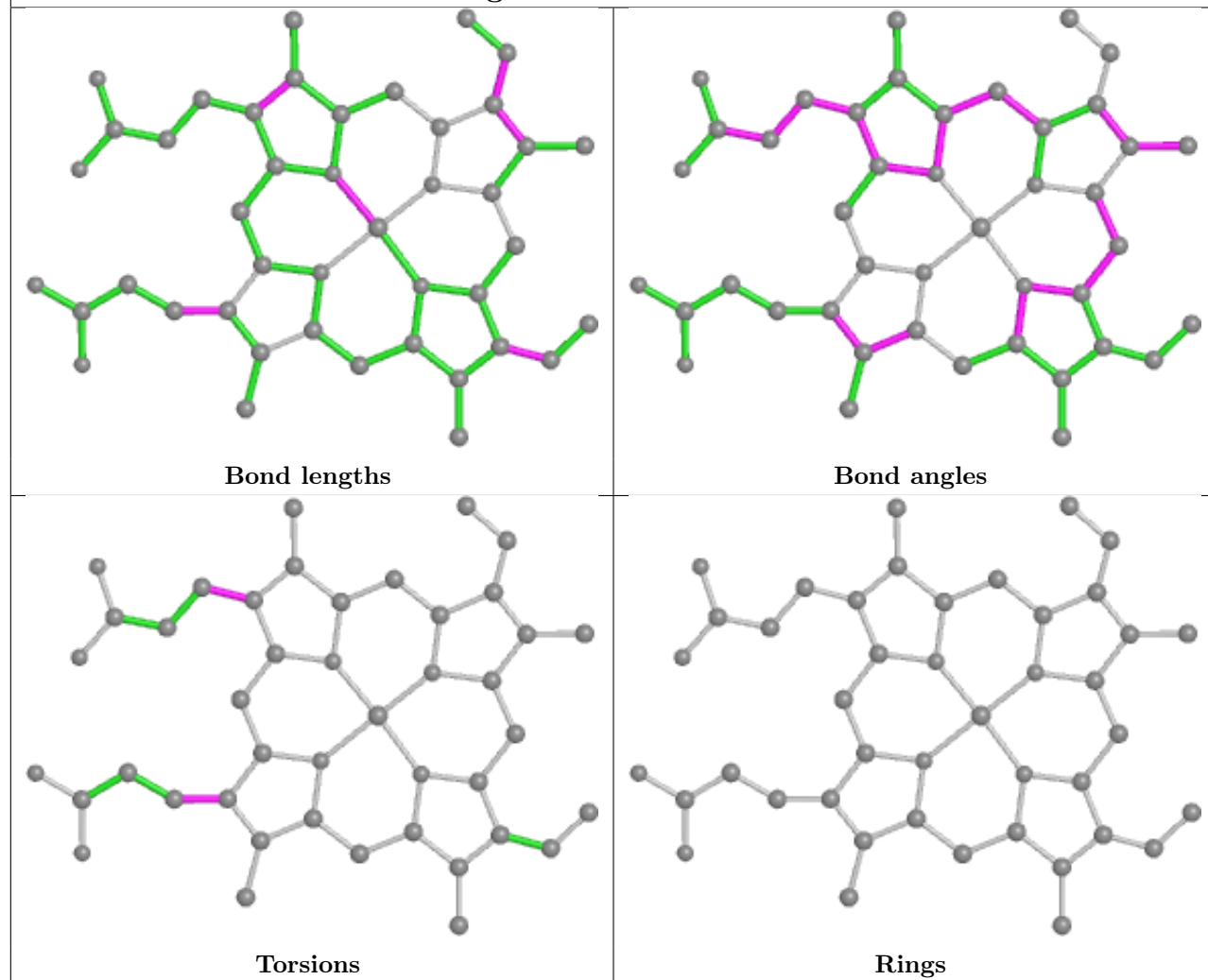




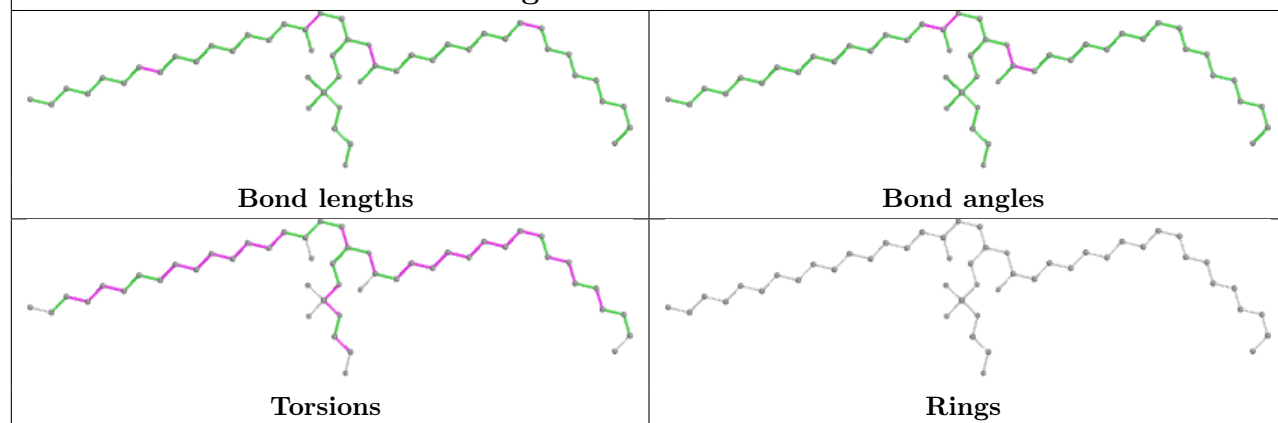


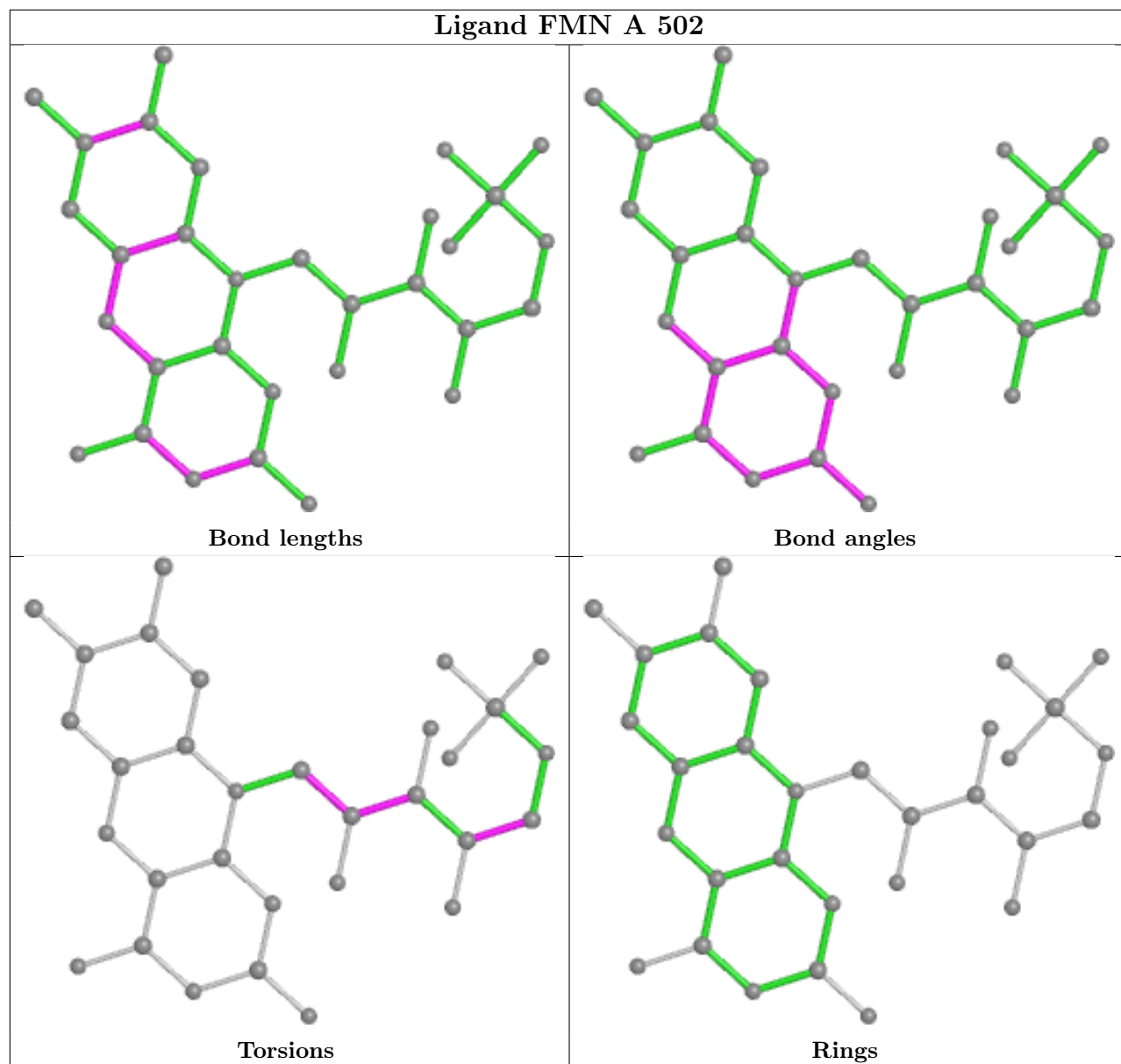


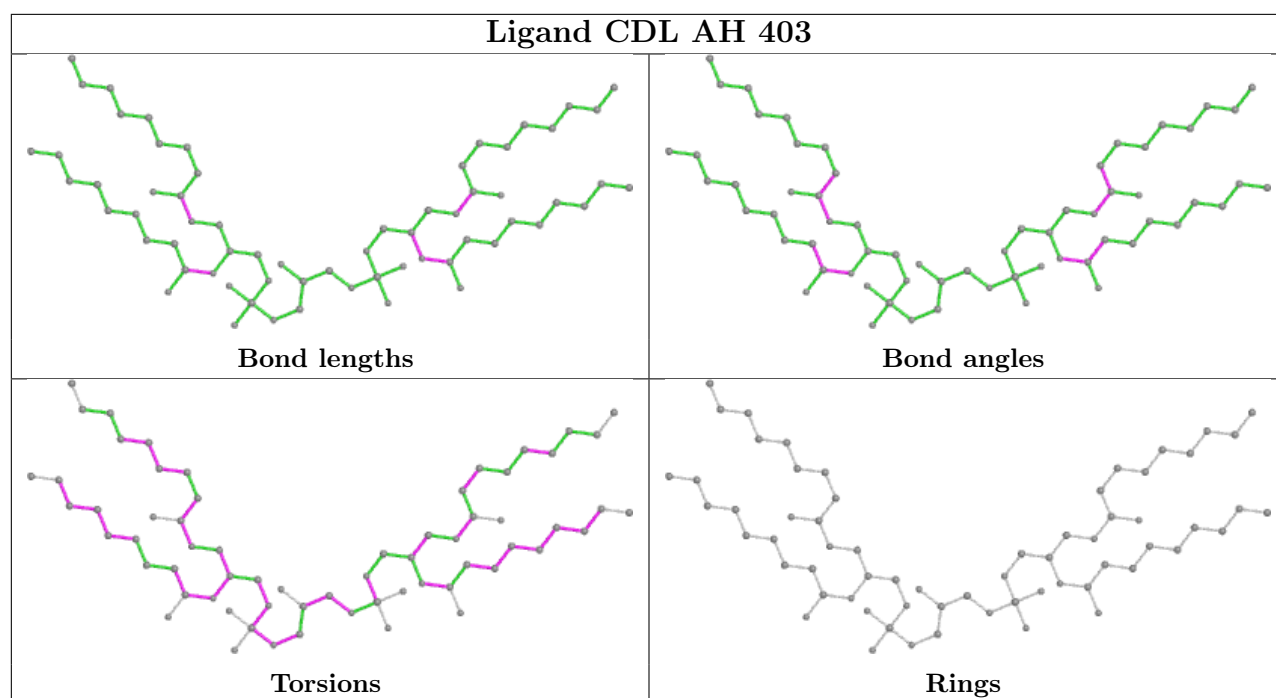
Ligand HEM AV 402



Ligand PEE AV 403







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

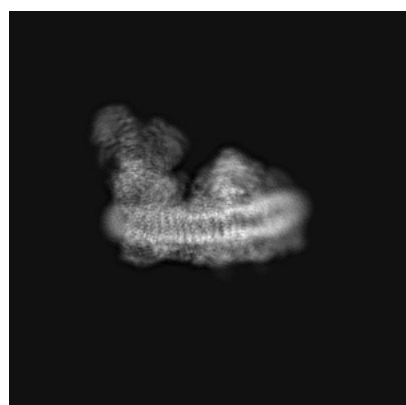
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6775. These allow visual inspection of the internal detail of the map and identification of artifacts.

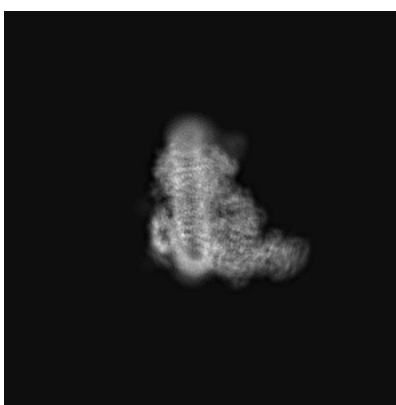
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

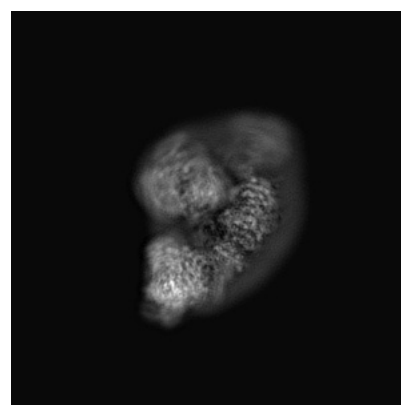
6.1.1 Primary map



X



Y

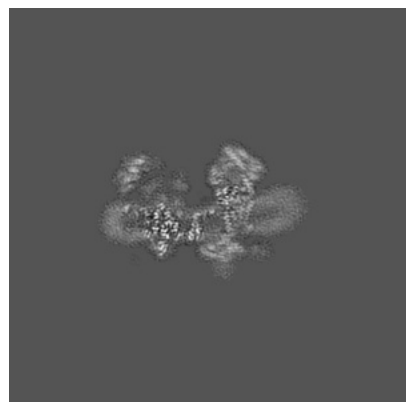


Z

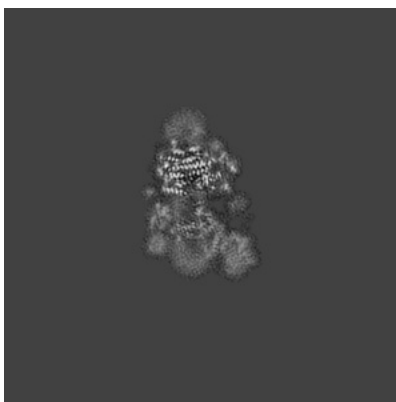
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

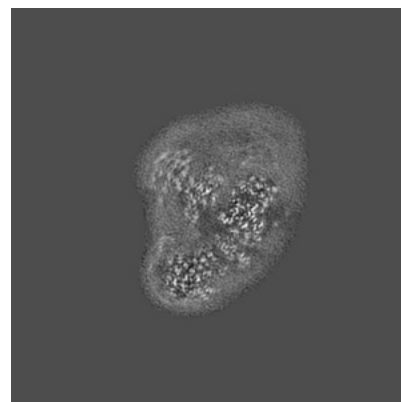
6.2.1 Primary map



X Index: 240



Y Index: 240

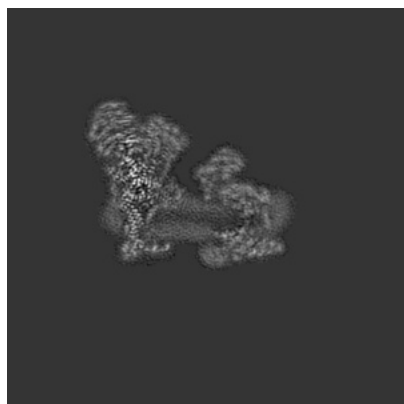


Z Index: 240

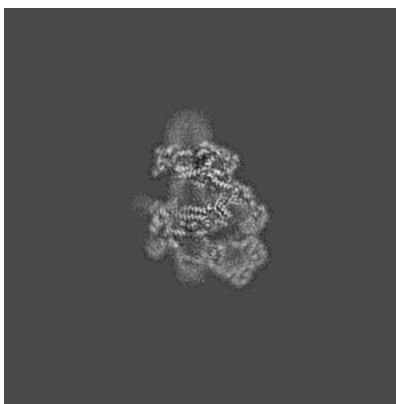
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

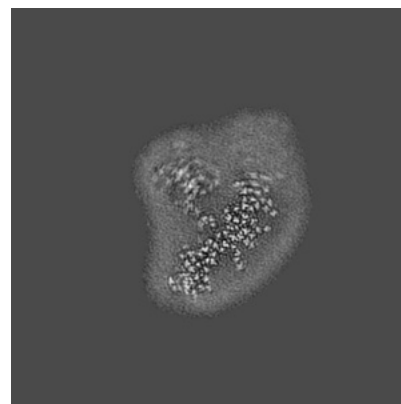
6.3.1 Primary map



X Index: 194



Y Index: 261

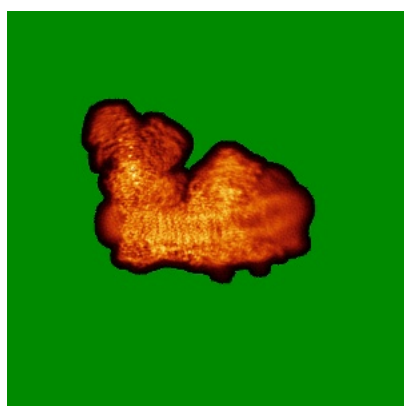


Z Index: 214

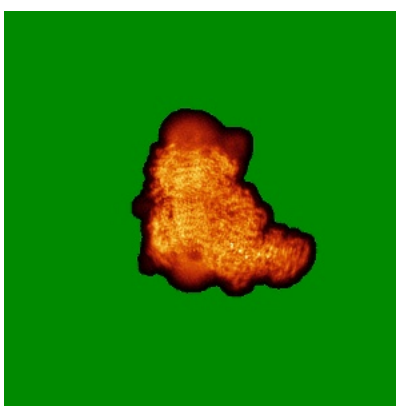
The images above show the largest variance slices of the map in three orthogonal directions.

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

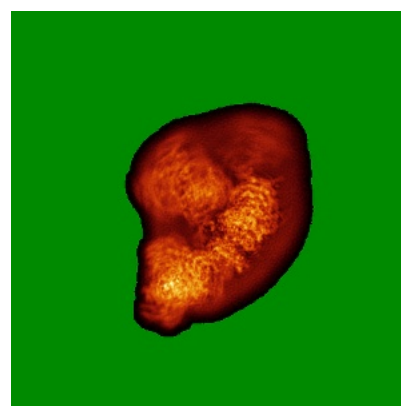
6.4.1 Primary map



X



Y

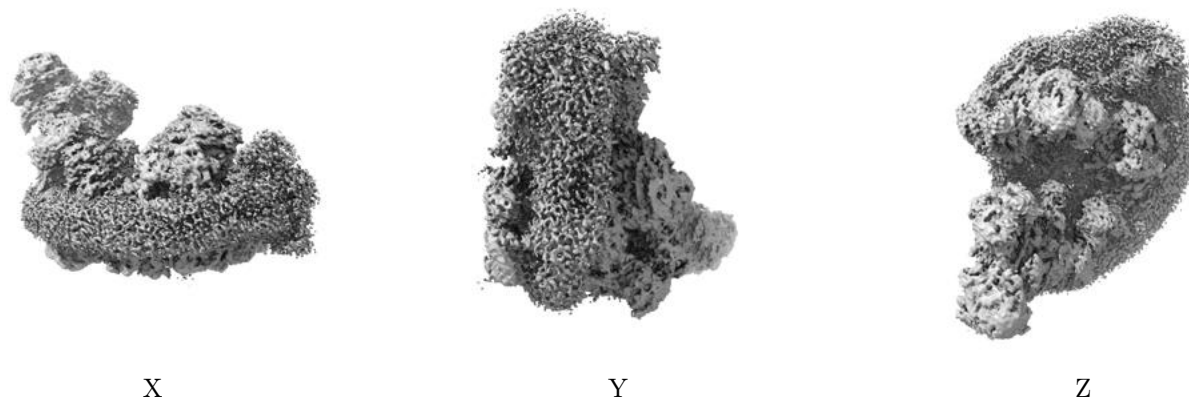


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

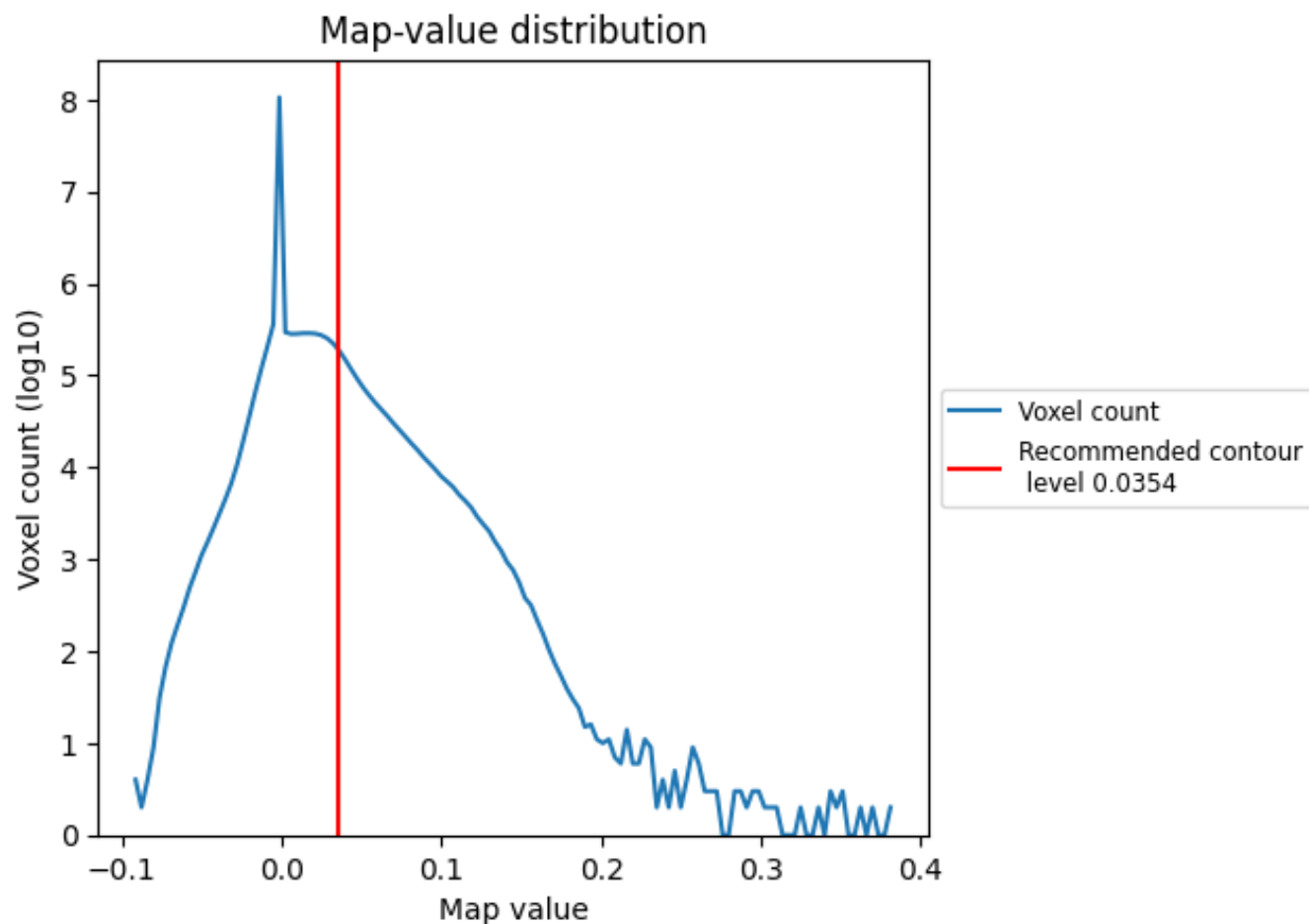
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

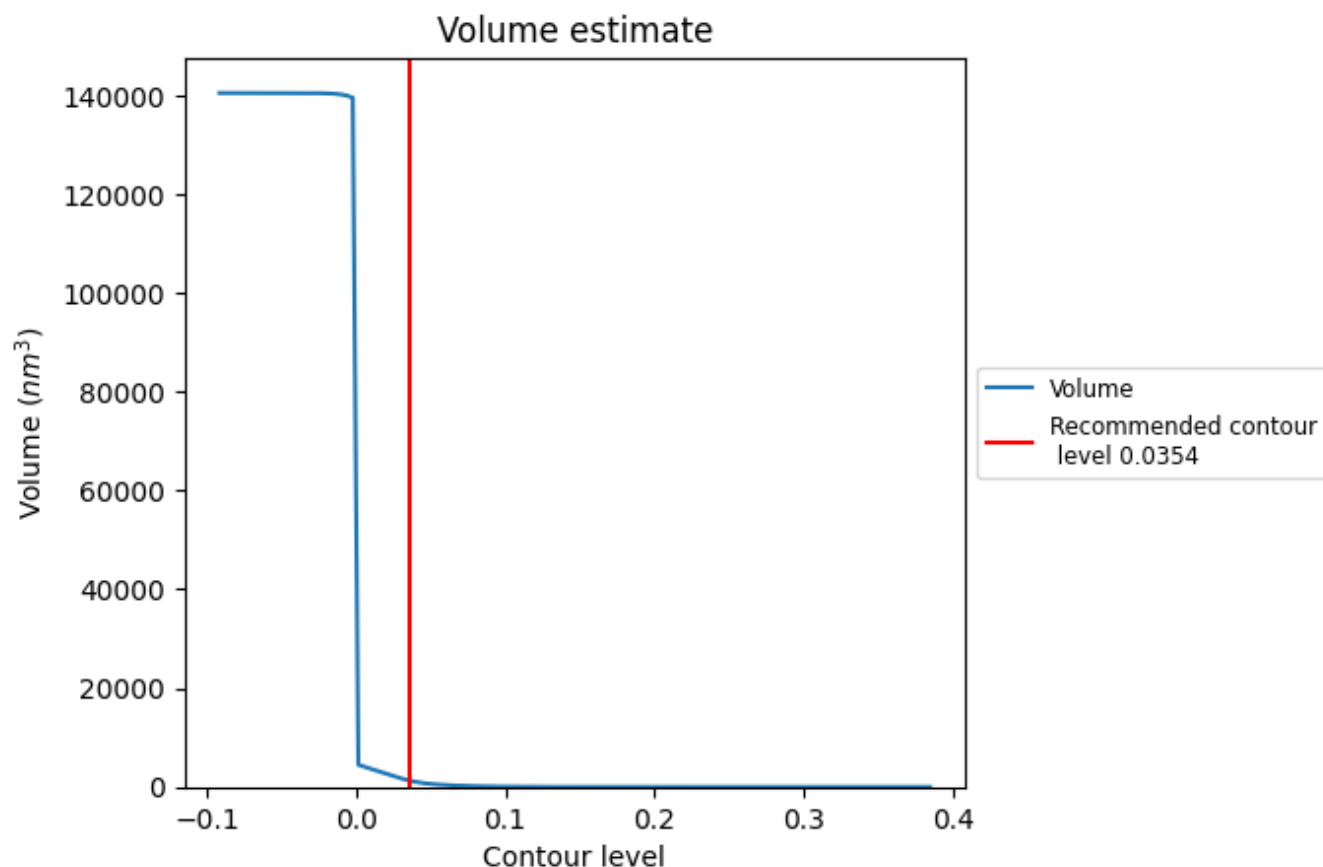
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

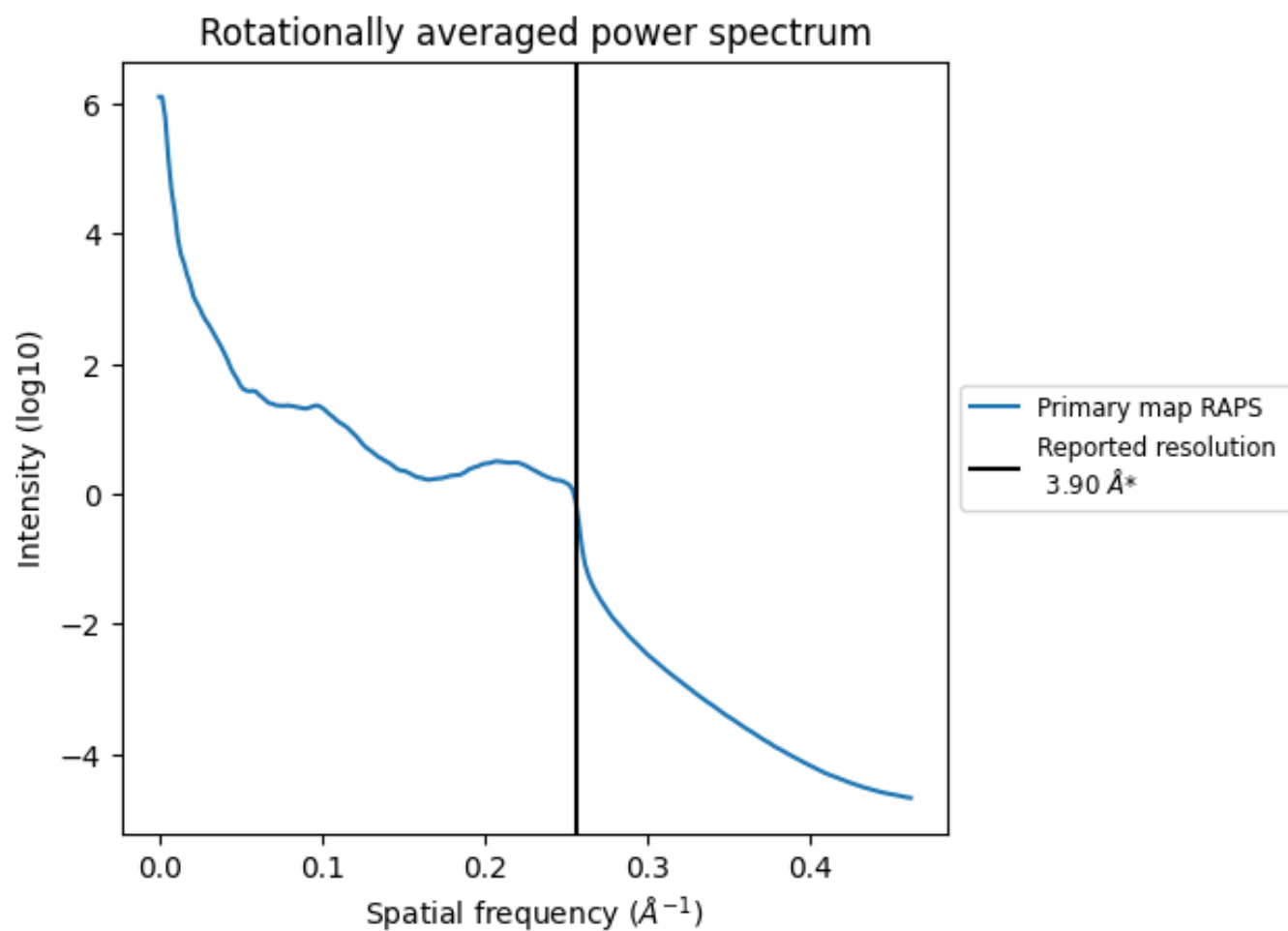
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1319 nm^3 ; this corresponds to an approximate mass of 1191 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

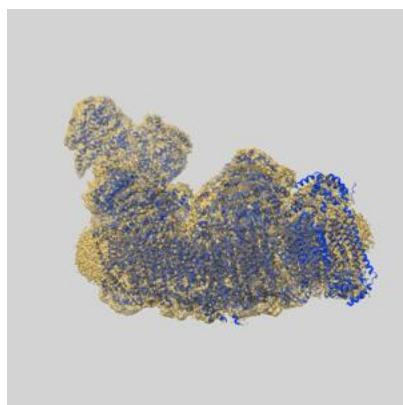
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

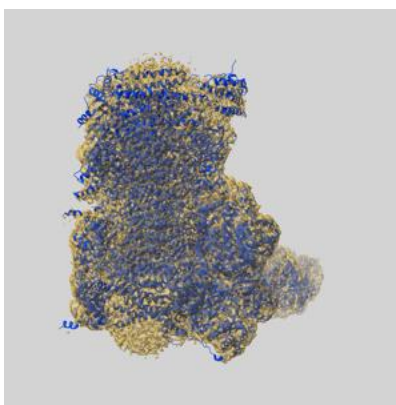
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6775 and PDB model 5XTH. Per-residue inclusion information can be found in section [3](#) on page [26](#).

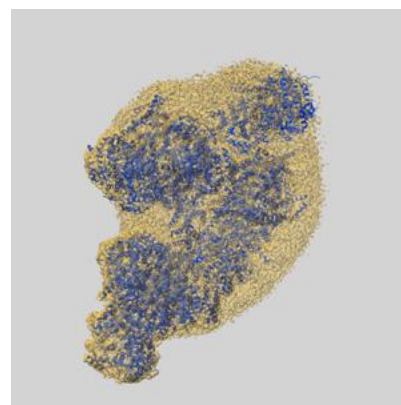
9.1 Map-model overlay [i](#)



X



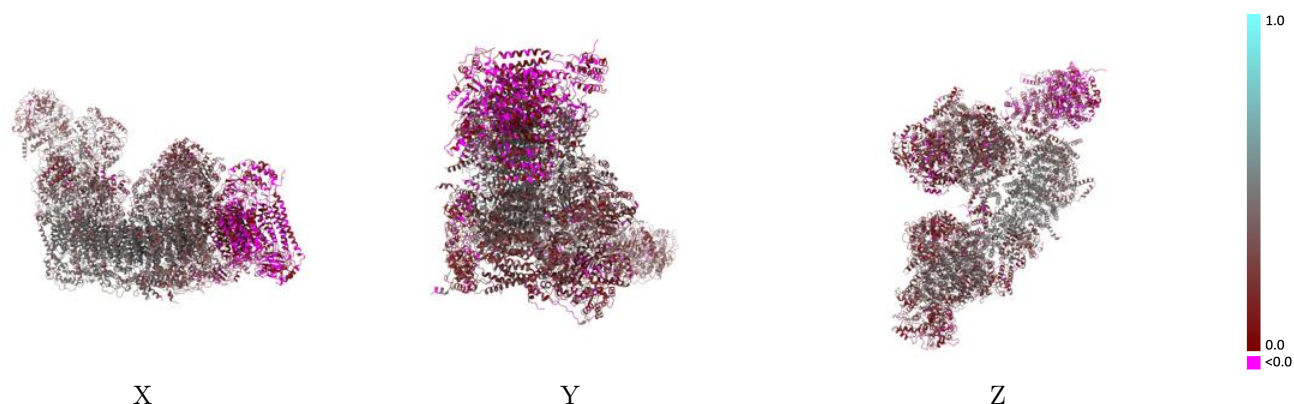
Y



Z

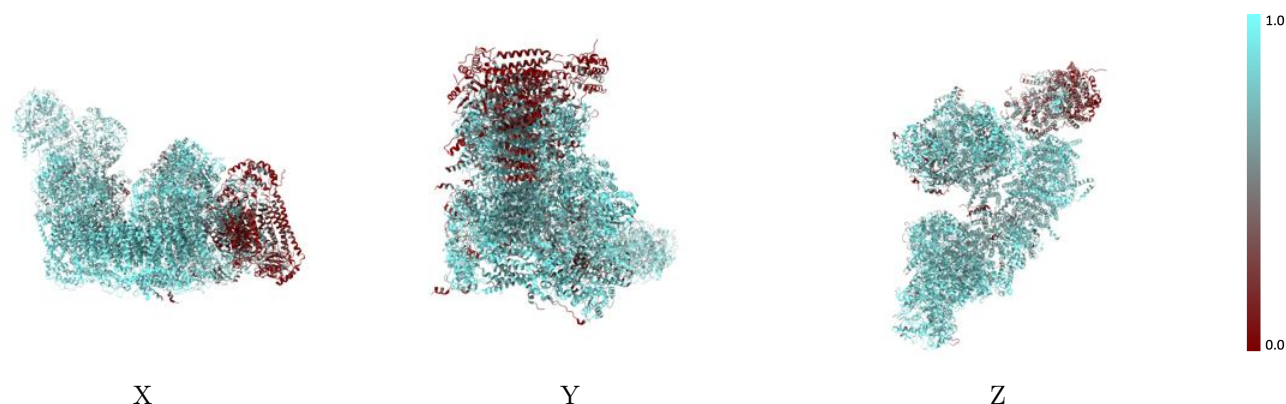
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



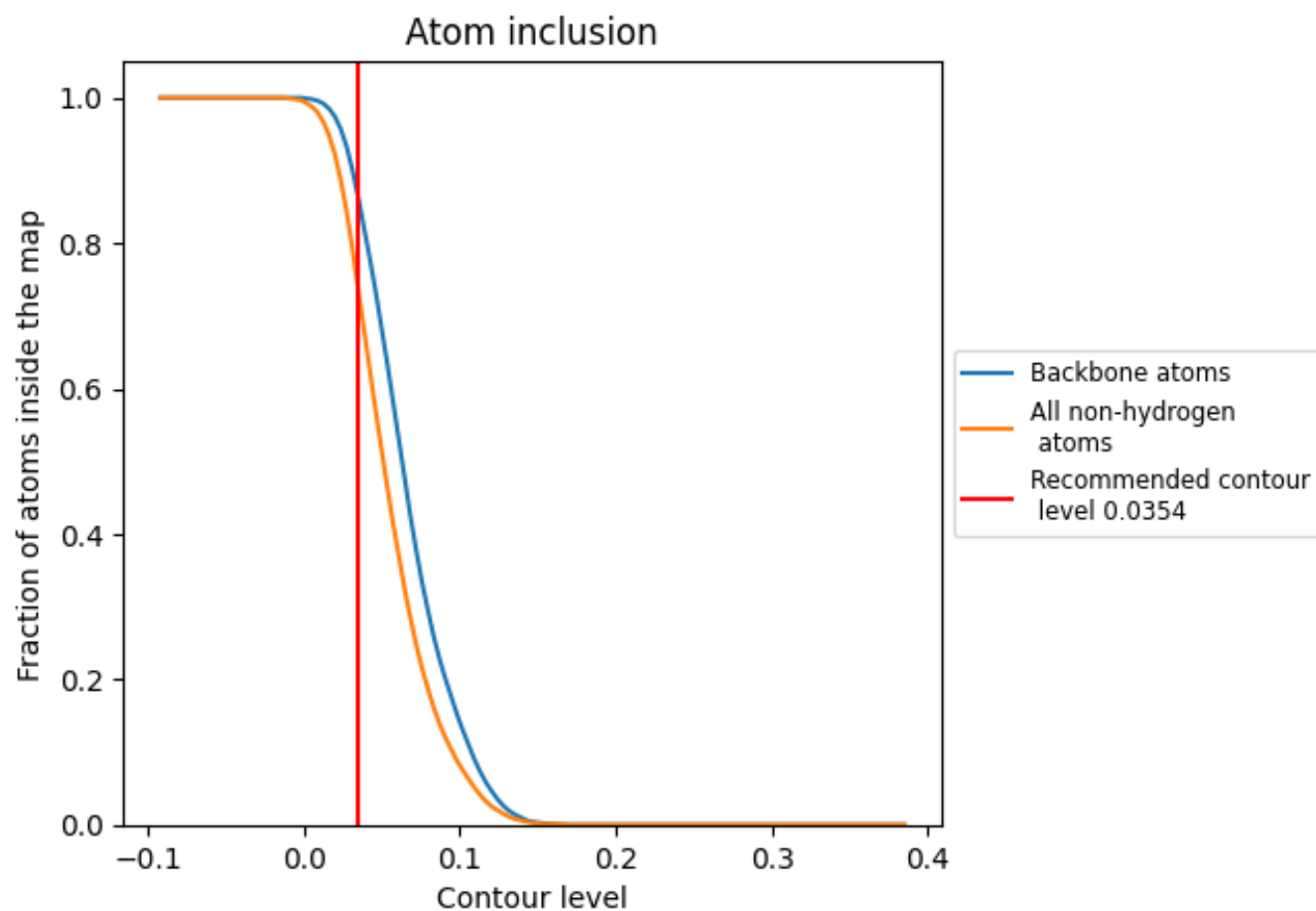
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0354).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.2930
0	 0.1290	 0.0250
1	 0.1760	 0.0530
2	 0.4300	 0.0700
3	 0.2680	 0.0410
4	 0.3500	 0.0370
5	 0.0950	 0.0310
6	 0.3420	 0.0880
7	 0.1040	 0.0240
8	 0.2820	 0.0120
9	 0.1360	 0.0240
A	 0.7830	 0.2470
AA	 0.7190	 0.3250
AB	 0.2280	 0.0740
AC	 0.6510	 0.2070
AD	 0.6410	 0.2820
AE	 0.7310	 0.2250
AF	 0.7020	 0.2830
AG	 0.6360	 0.2600
AH	 0.7730	 0.2990
AJ	 0.7420	 0.3490
AK	 0.8260	 0.2600
AL	 0.7960	 0.3320
AN	 0.6850	 0.1970
AO	 0.1150	 -0.0360
AP	 0.6980	 0.1840
AQ	 0.6500	 0.1980
AR	 0.7170	 0.1870
AS	 0.7790	 0.2640
AT	 0.6440	 0.1700
AU	 0.7820	 0.2360
AV	 0.7580	 0.3070
AW	 0.6950	 0.1790
AY	 0.7270	 0.1890
B	 0.8840	 0.4270











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Chain	Atom inclusion	Q-score
C	 0.9010	 0.4360
E	 0.6870	 0.2550
F	 0.7820	 0.1840
G	 0.4550	 0.1620
H	 0.7200	 0.2130
I	 0.7930	 0.3150
J	 0.8070	 0.2950
K	 0.7540	 0.2440
L	 0.7280	 0.3180
M	 0.7950	 0.2910
N	 0.8210	 0.3440
O	 0.8010	 0.2630
P	 0.7980	 0.3200
Q	 0.8200	 0.3830
S	 0.9090	 0.4250
T	 0.7840	 0.3430
U	 0.8790	 0.4120
V	 0.7820	 0.4030
W	 0.8900	 0.4140
X	 0.8660	 0.3870
Y	 0.8900	 0.3530
Z	 0.8520	 0.3550
a	 0.9170	 0.4530
b	 0.8370	 0.3440
c	 0.8960	 0.4430
d	 0.8900	 0.4060
e	 0.8320	 0.4170
f	 0.7970	 0.3270
g	 0.8480	 0.4350
h	 0.8830	 0.4310
i	 0.8500	 0.4610
j	 0.7550	 0.3810
k	 0.7920	 0.4260
l	 0.8170	 0.4190
m	 0.7980	 0.4080
n	 0.8530	 0.3850
o	 0.8560	 0.4240
p	 0.8950	 0.4010
r	 0.8720	 0.4660
s	 0.8480	 0.4340
u	 0.9120	 0.4080
v	 0.8310	 0.3020

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Chain	Atom inclusion	Q-score
w	 0.8350	 0.3410
x	 0.3690	 0.0410
y	 0.2580	 0.0090
z	 0.4570	 0.0910