



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:34 AM UTC

PDB ID : 9IHR / pdb_00009ihr
EMDB ID : EMD-52878
Title : Closed state with NUQM and with flavoprotein (classification state 1) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2025-02-21
Resolution : 2.80 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

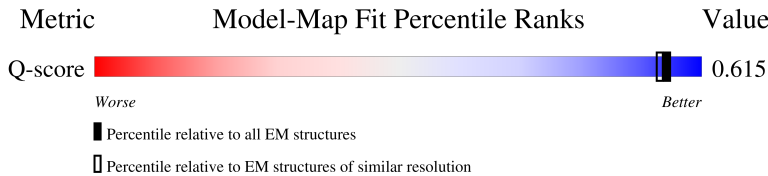
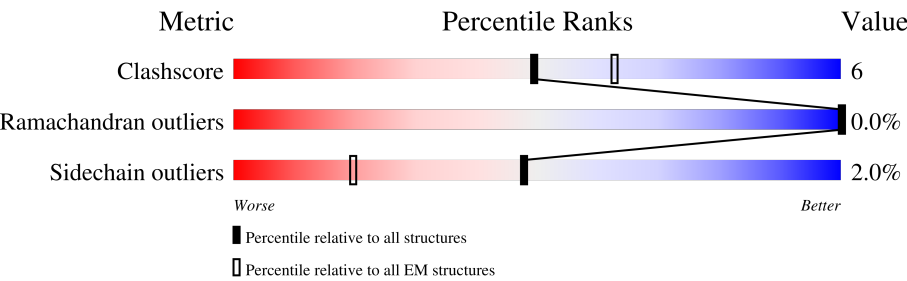
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

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



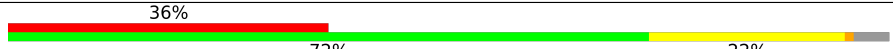
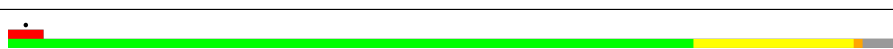
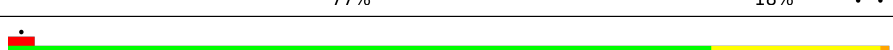
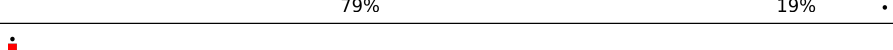
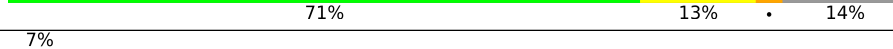
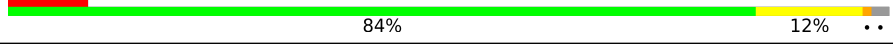
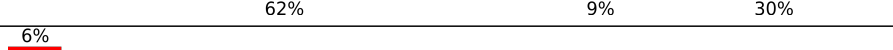
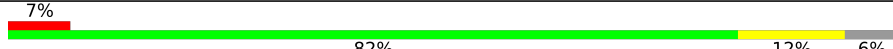
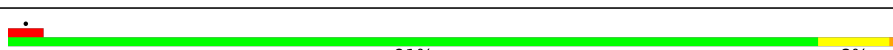
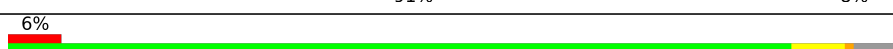
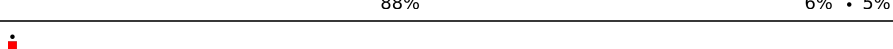
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1	190	21% 75% 13% 11%
2	A	141	82% 16%
3	B	204	71% 15% 14%
4	C	289	70% 13% 17%

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Mol	Chain	Length	Quality of chain
5	D	482	
6	E	241	
7	F	473	
8	G	726	
9	H	353	
10	I	222	
11	J	161	
12	K	82	
13	L	642	
14	M	491	
15	N	523	
16	O	193	
17	P	384	
18	Q	159	
19	R	139	
20	S	90	
21	T	138	
22	U	130	
23	V	134	
24	W	122	
25	X	184	
26	Y	216	
27	Z	147	
28	a	150	
29	b	79	

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Mol	Chain	Length	Quality of chain
30	c	182	
31	d	78	
32	e	106	
33	f	86	
34	g	239	
35	h	182	
36	i	74	
37	j	59	
38	k	61	
39	l	156	
40	m	81	
41	n	111	
42	o	87	
43	p	92	
44	q	140	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	SF4	F	501	-	-	X	-
46	SF4	I	302	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 70216 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 Altered inheritance of mitochondria protein 41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	169	Total	C	N	O	S	0	0
			1383	879	231	272	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	141	Total	C	N	O	S	0	0
			1133	764	166	199	4		

- Molecule 3 is a protein called BA75_00622T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	175	Total	C	N	O	S	0	0
			1407	901	241	249	16		

- Molecule 4 is a protein called NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	240	Total	C	N	O	S	0	0
			1970	1273	331	361	5		

- Molecule 5 is a protein called NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	451	Total	C	N	O	S	0	0
			3621	2310	619	674	18		

- Molecule 6 is a protein called NUHM (24 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	183	Total	C	N	O	S	0	0
			1446	920	239	273	14		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	453	Total	C	N	O	S	0	0
			3500	2213	612	654	21		

- Molecule 8 is a protein called NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	696	Total	C	N	O	S	0	0
			5344	3345	939	1037	23		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	353	Total	C	N	O	S	0	0
			2809	1903	414	478	14		

- Molecule 10 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	192	Total	C	N	O	S	0	0
			1556	988	259	299	10		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	161	Total	C	N	O	S	0	0
			1313	878	180	252	3		

- Molecule 12 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	80	Total	C	N	O	S	0	0
			617	400	93	118	6		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	642	Total	C	N	O	S	0	0
			5115	3454	766	866	29		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	491	Total	C	N	O	S	0	0
			3868	2597	593	663	15		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	506	Total	C	N	O	S	0	0
			4045	2723	594	714	14		

- Molecule 16 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	193	Total	C	N	O	S	0	0
			1575	1019	257	294	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ACE	-	acetylation	UNP E1UWB9

- Molecule 17 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	368	Total	C	N	O	S	0	0
			2922	1862	510	547	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	112	Total	C	N	O	S	0	0
			924	585	161	176	2		

- Molecule 19 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	124	Total	C	N	O	S	0	0
			978	610	179	186	3		

- Molecule 20 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	90	Total	C	N	O		0	0
			697	454	117	126			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	ACE	-	acetylation	UNP E1UWD3

- Molecule 21 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	95	Total	C	N	O	S	0	0
			745	467	119	158	1		

- Molecule 22 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	88	Total	C	N	O		0	0
			681	427	102	152			

- Molecule 23 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	126	Total	C	N	O	S	0	0
			1025	658	165	201	1		

- Molecule 24 is a protein called BA75_04796T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	115	Total	C	N	O	S	0	0
			979	626	177	171	5		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	184	Total	C	N	O	S	0	0
			1450	905	253	282	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	0	ACE	-	acetylation	UNP E1UWB8

- Molecule 26 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	205	Total	C	N	O	S	0	0
			1578	1012	274	289	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	142	Total	C	N	O	S	0	0
			1176	758	212	202	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	ACE	-	acetylation	UNP E1UWD8

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	149	Total	C	N	O	S	0	0
			1215	756	228	225	6		

- Molecule 29 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	78	Total	C	N	O	S	0	0
			641	419	111	109	2		

- Molecule 30 is a protein called BA75_00589T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	182	Total	C	N	O	S	0	0
			1418	902	248	266	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	0	ACE	-	acetylation	UNP E1UWC1

- Molecule 31 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	75	Total	C	N	O	S	0	0
			616	406	106	103	1		

- Molecule 32 is a protein called BA75_05084T0.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	105	Total	C	N	O	S	0	0
			848	531	154	157	6		

- Molecule 33 is a protein called NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	78	Total	C	N	O	S	0	0
			642	428	113	101			

- Molecule 34 is a protein called NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	158	Total	C	N	O	S	0	0
			1280	815	210	252	3		

- Molecule 35 is a protein called NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	131	Total	C	N	O	S	0	0
			1078	699	183	196			

- Molecule 36 is a protein called NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	69	Total	C	N	O	S	0	0
			552	358	95	97	2		

- Molecule 37 is a protein called Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	53	Total	C	N	O	S	0	0
			460	319	76	64	1		

- Molecule 38 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	45	Total	C	N	O	S	0	0
			368	240	71	56	1		

- Molecule 39 is a protein called NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	132	Total	C	N	O	S	0	0
			1082	706	175	200	1		

- Molecule 40 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
40	m	77	Total	C	N	O	0	0
			642	418	116	108		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	105	Total	C	N	O	S	0	0
			861	550	155	155	1		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	80	Total	C	N	O	S	0	0
			682	428	126	122	6		

- Molecule 43 is a protein called NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	90	Total	C	N	O	S	0	0
			740	457	135	144	4		

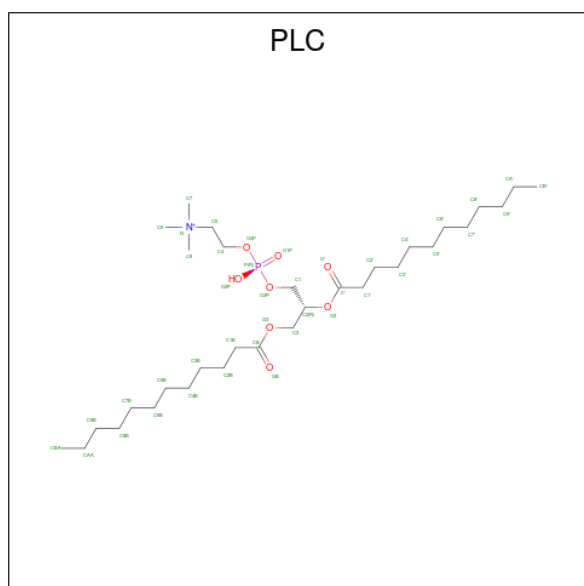
- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	140	Total	C	N	O	S	0	0
			1156	741	201	211	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	0	ACE	-	acetylation	UNP E1UWE0

- Molecule 45 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



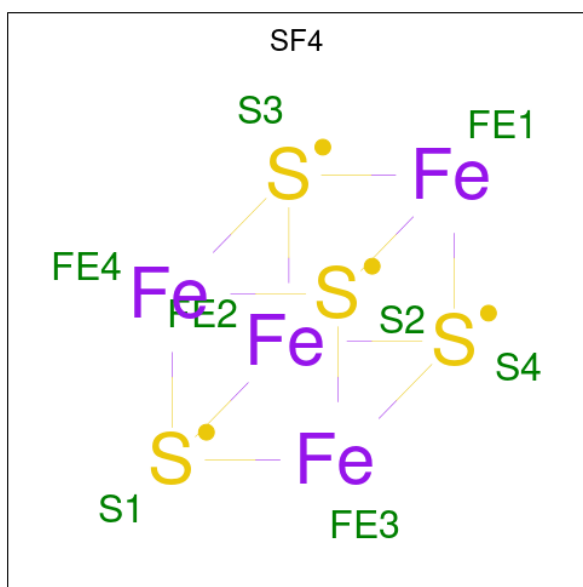
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			31	21	1	8	1	

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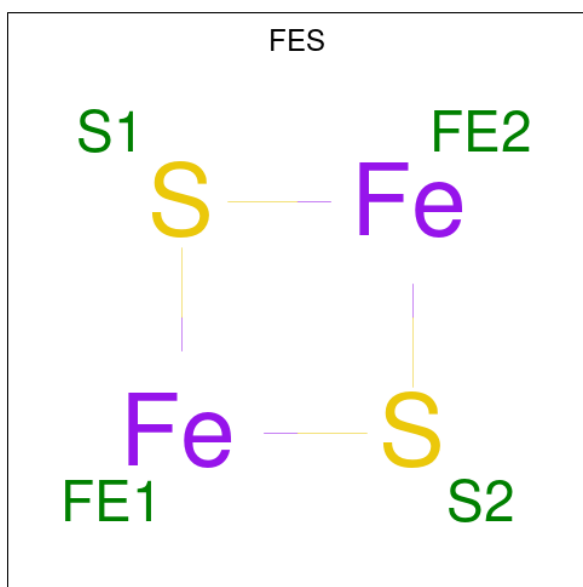
Mol	Chain	Residues	Atoms					AltConf
45	B	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	H	1	Total	C	N	O	P	0
			24	14	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			32	22	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	P	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Z	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	a	1	Total	C	N	O	P	0
			22	12	1	8	1	
45	b	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	d	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	h	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	q	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	q	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



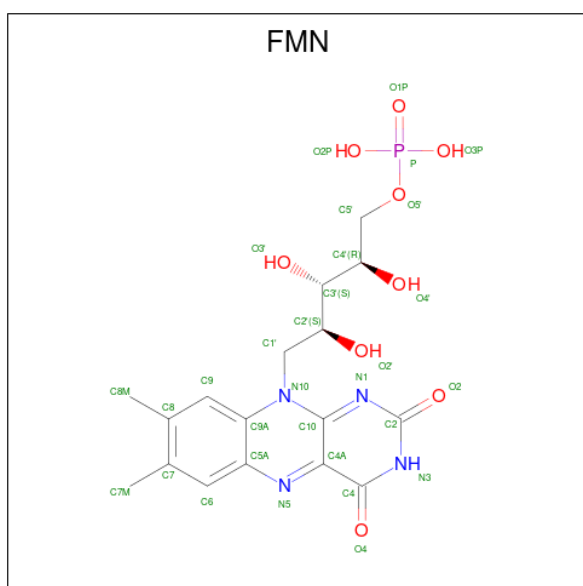
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

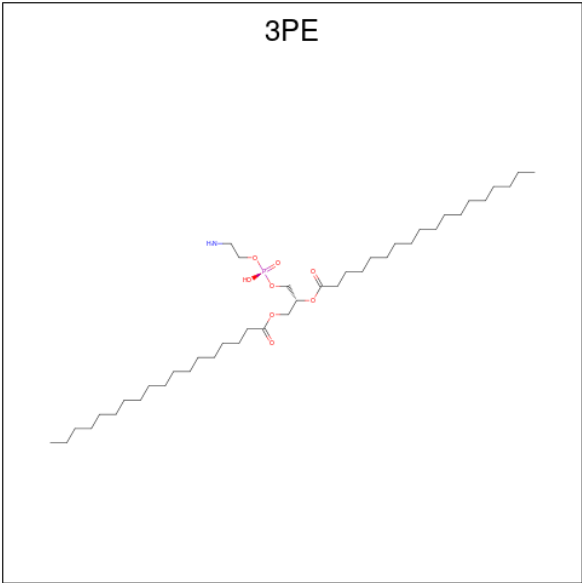


Mol	Chain	Residues	Atoms					AltConf
48	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
49	G	1	Total	K	0
			1	1	

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



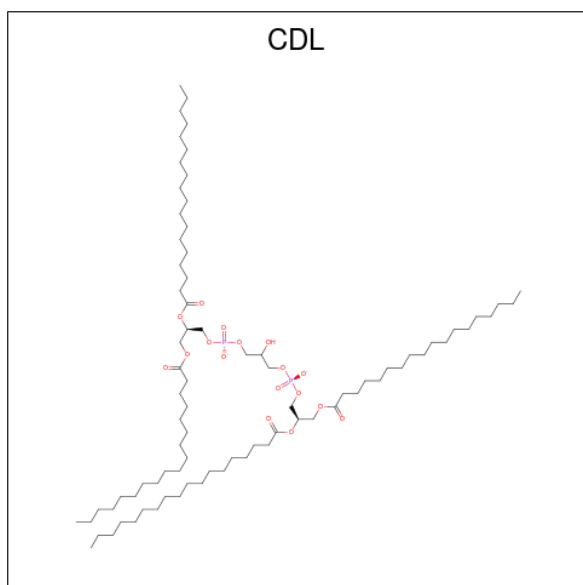
Mol	Chain	Residues	Atoms					AltConf
50	H	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
50	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	L	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			33	23	1	8	1	
50	M	1	Total	C	N	O	P	0
			35	25	1	8	1	

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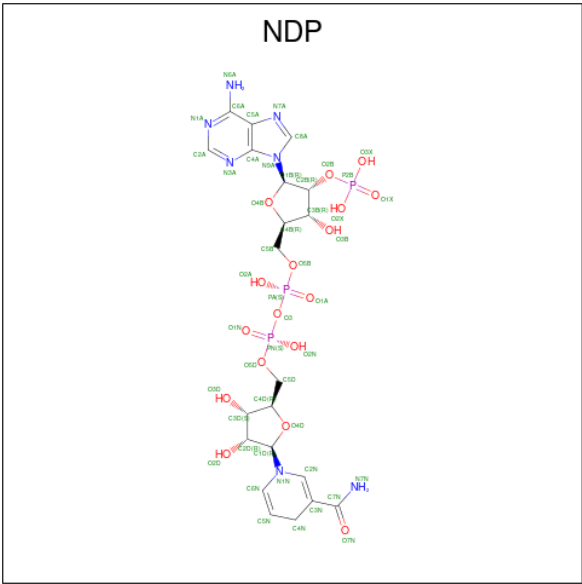
Mol	Chain	Residues	Atoms					AltConf
50	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	Y	1	Total	C	N	O	P	0
			26	16	1	8	1	
50	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	b	1	Total	C	N	O	P	0
			36	26	1	8	1	
50	b	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	b	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	f	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	g	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	j	1	Total	C	N	O	P	0
			27	17	1	8	1	
50	m	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	O	1	Total	C	O	P	0
			75	56	17	2	
51	P	1	Total	C	O	P	0
			42	23	17	2	
51	Z	1	Total	C	O	P	0
			49	30	17	2	
51	a	1	Total	C	O	P	0
			60	41	17	2	
51	b	1	Total	C	O	P	0
			59	40	17	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

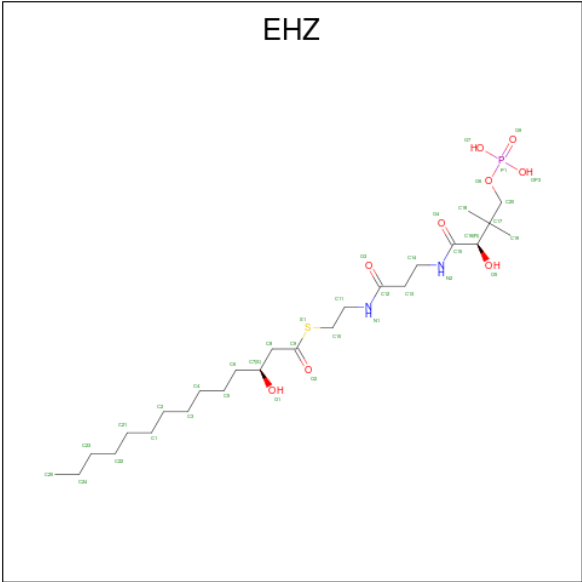


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	R	1	Total	Zn	0
			1	1	

- Molecule 54 is {S}-[2-[3-[[2 {R}))-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S}))-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

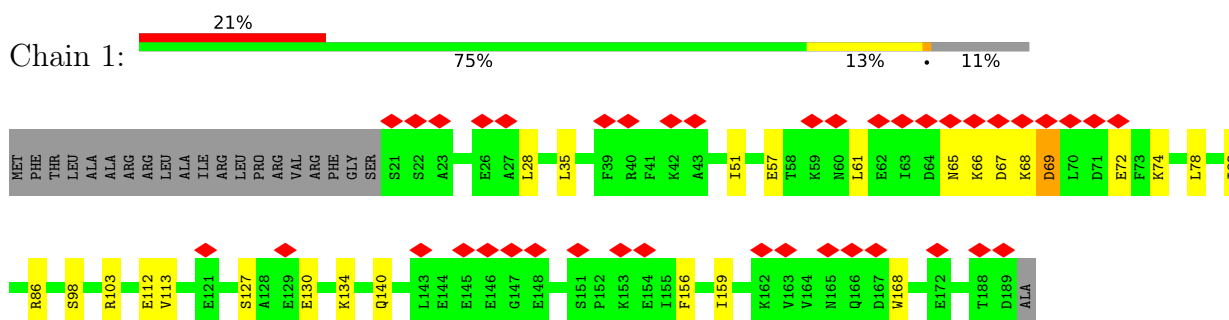


Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

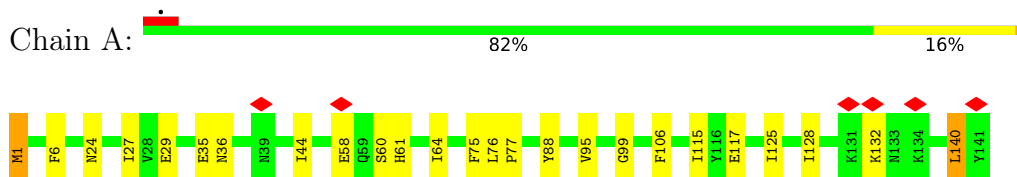
3 Residue-property plots [i](#)

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.

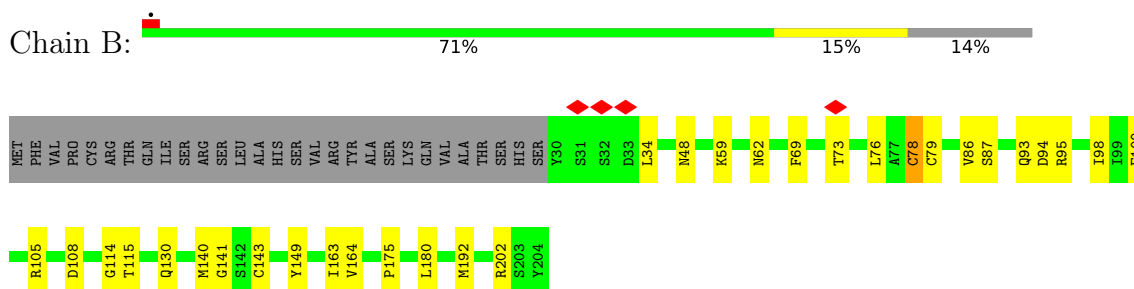
- Molecule 1: Altered inheritance of mitochondria protein 41, mitochondrial



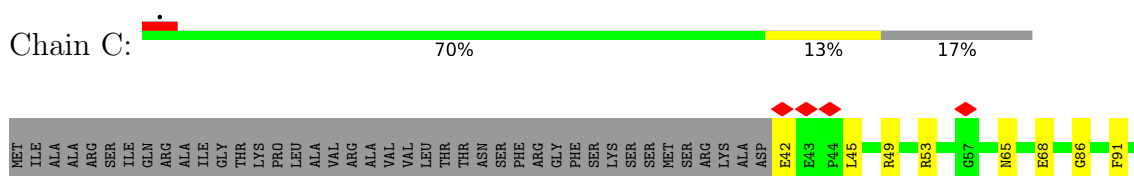
- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

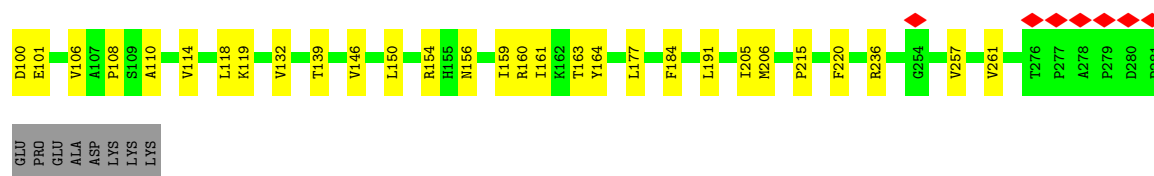


- Molecule 3: BA75_00622T0



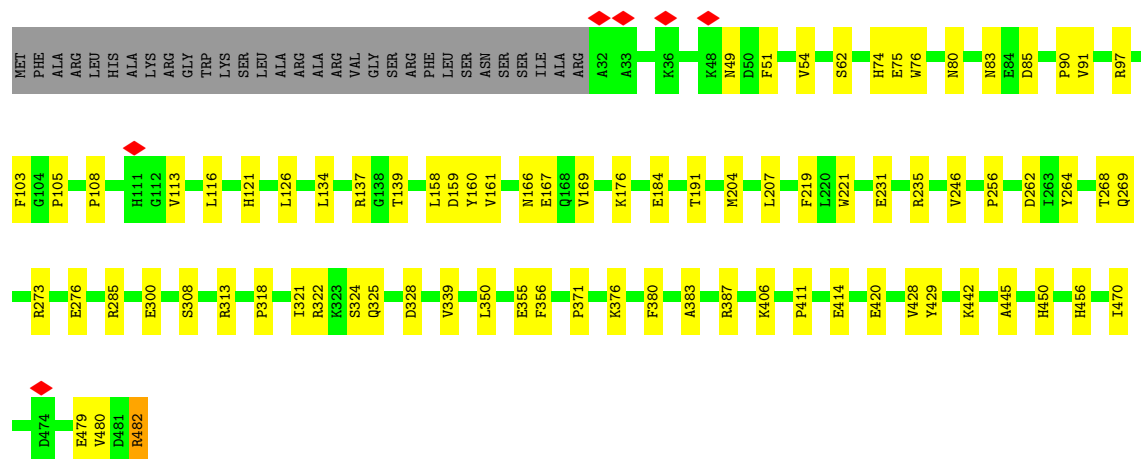
- Molecule 4: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)





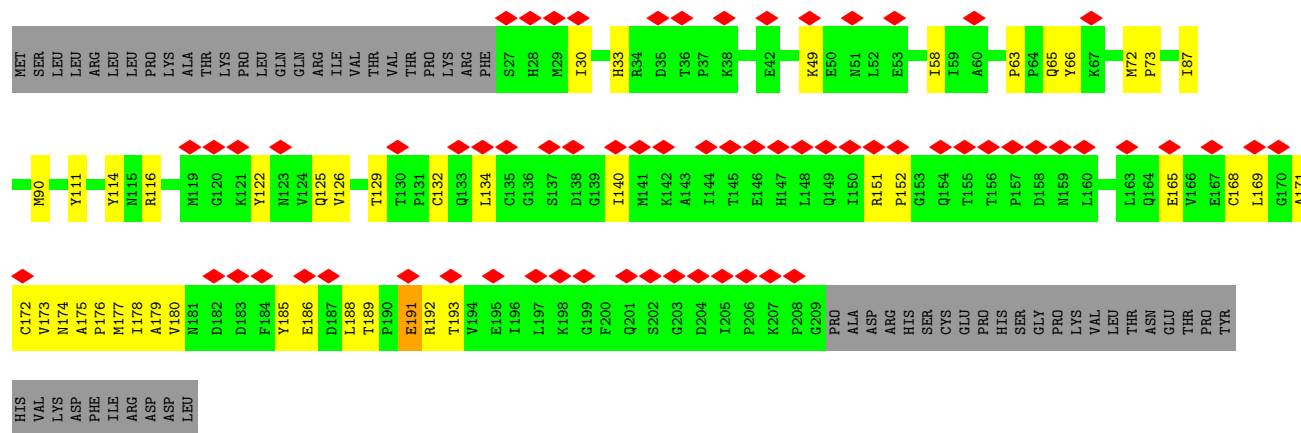
- Molecule 5: NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain D: 77% 16% 6%



- Molecule 6: NUHM (24 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

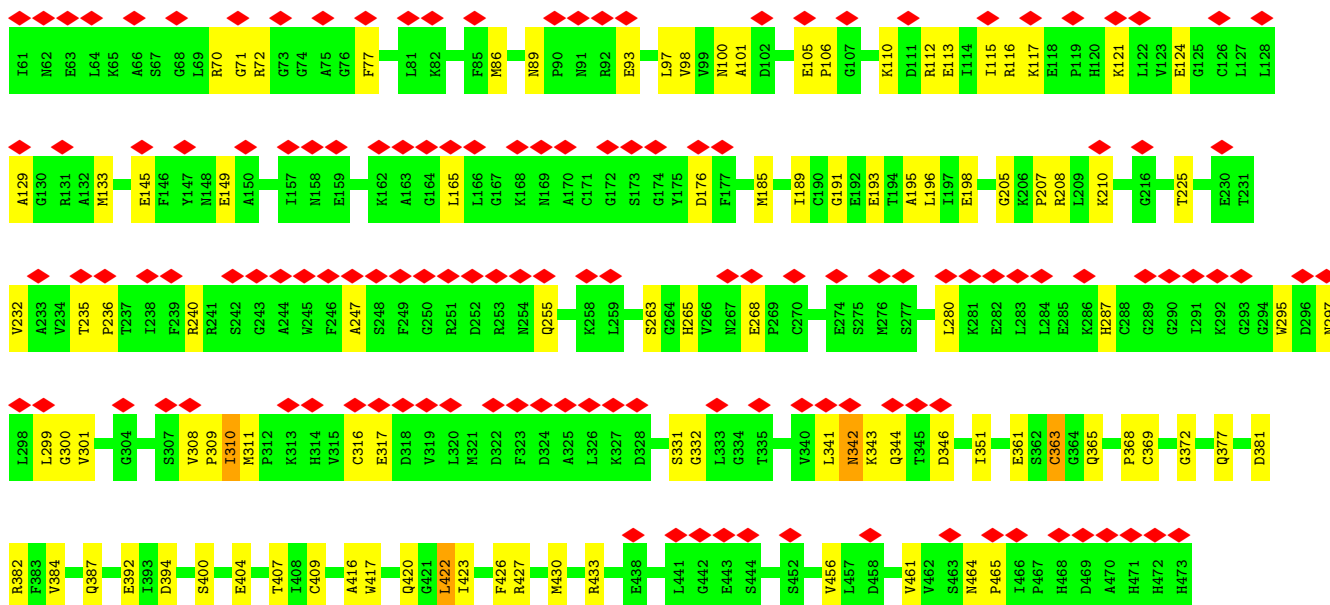
Chain E: 28% 58% 17% 24%



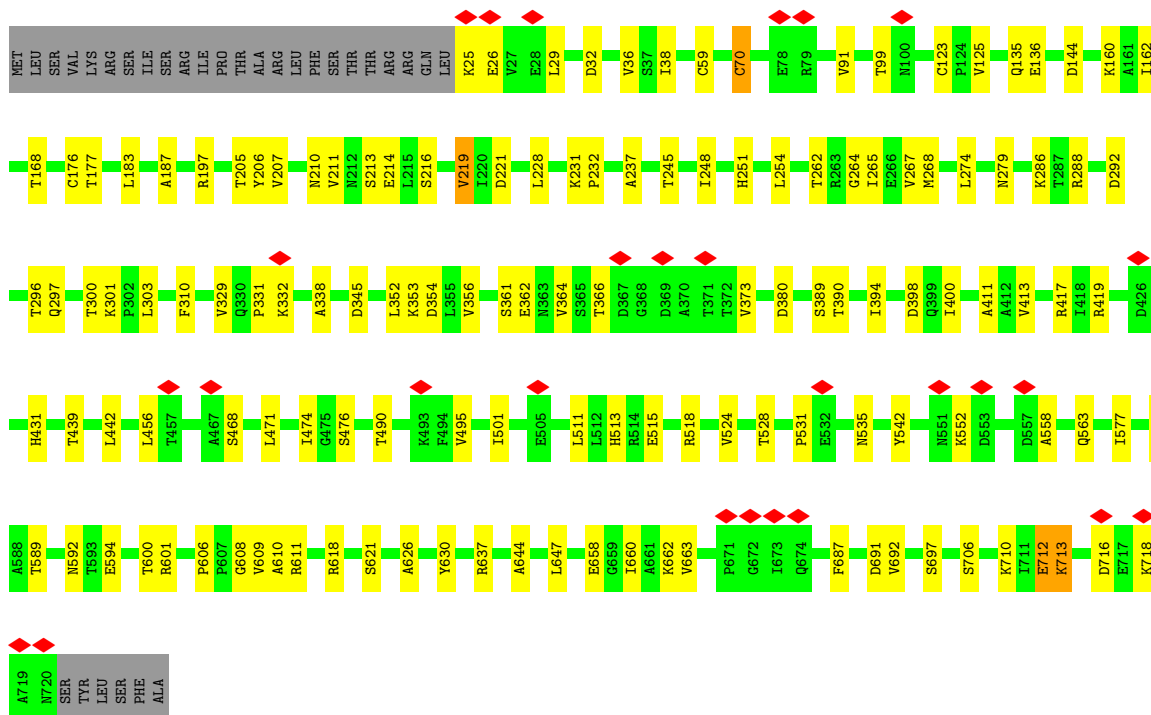
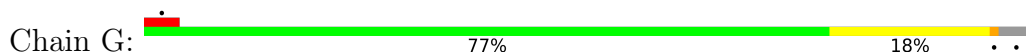
- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 36% 72% 22%

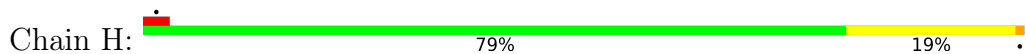


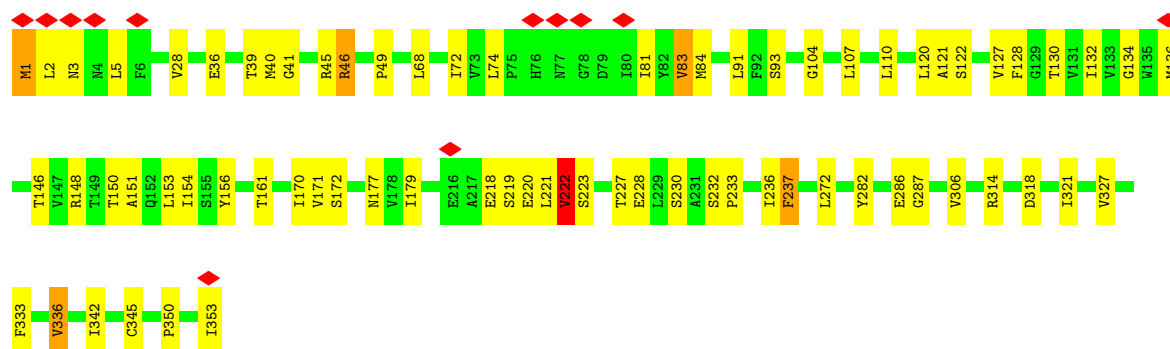


- Molecule 8: NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



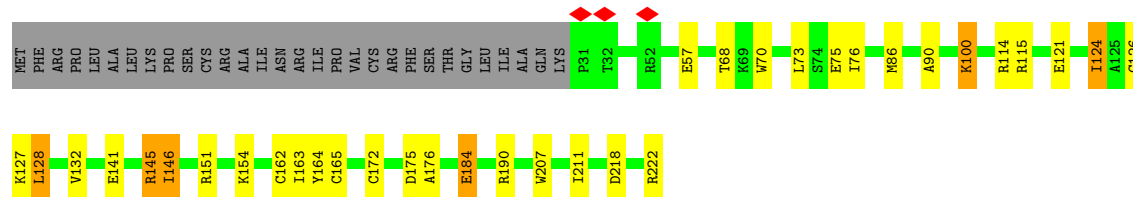
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1





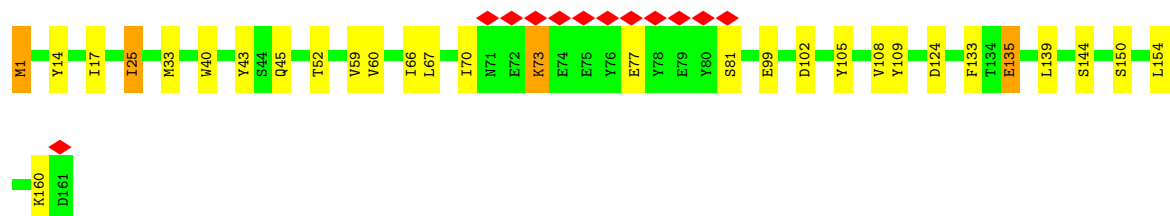
- Molecule 10: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain I: 71% 13% 14%



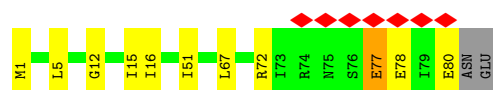
- Molecule 11: NADH-ubiquinone oxidoreductase chain 6

Chain J: 7% 81% 17%



- Molecule 12: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

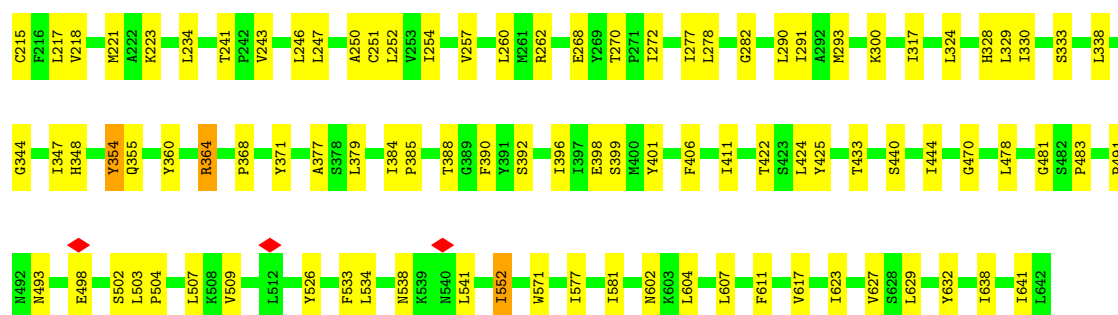
Chain K: 9% 84% 12%



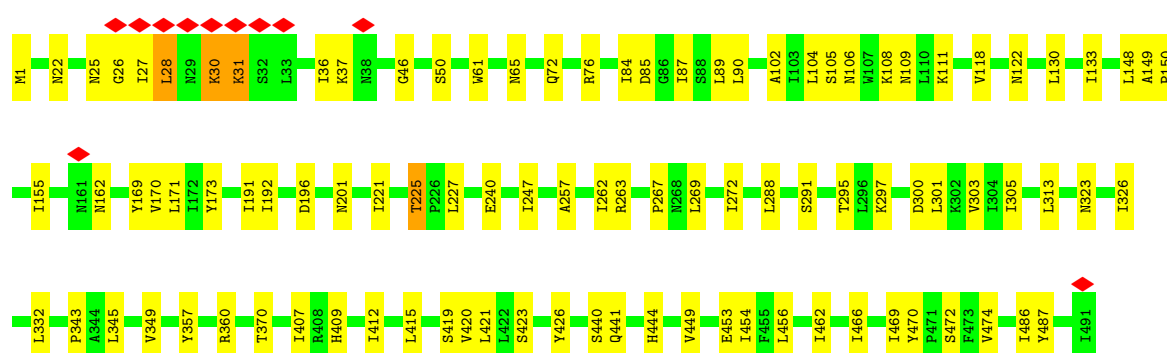
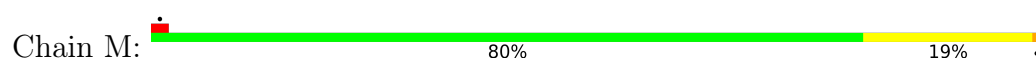
- Molecule 13: NADH-ubiquinone oxidoreductase chain 5

Chain L: 80% 19%

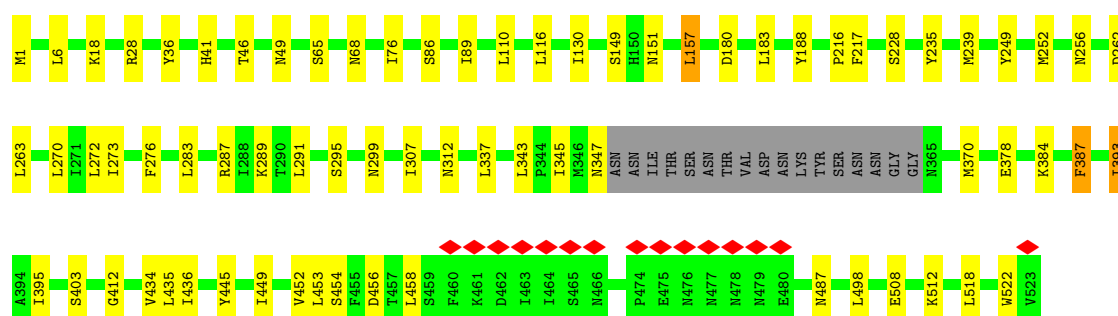
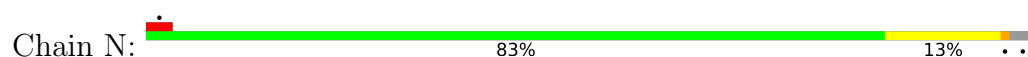




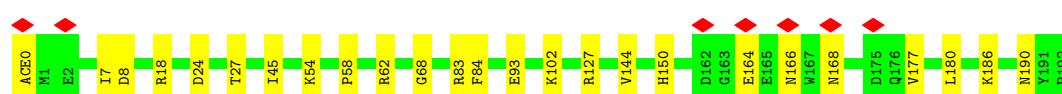
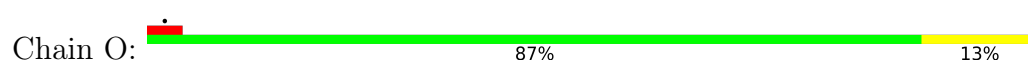
- Molecule 14: NADH-ubiquinone oxidoreductase chain 4



- Molecule 15: NADH-ubiquinone oxidoreductase chain 2

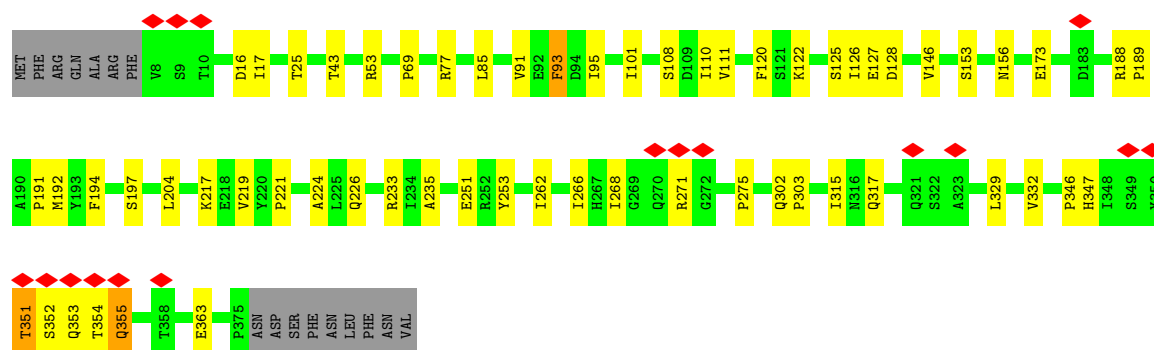


- Molecule 16: NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



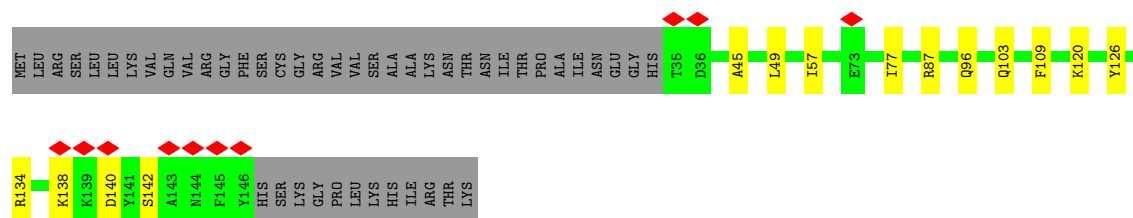
- Molecule 17: NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain P: 



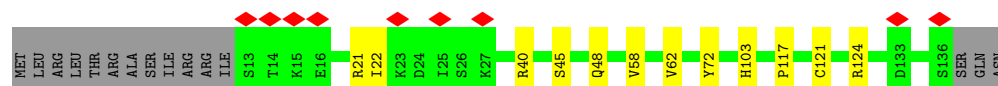
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 



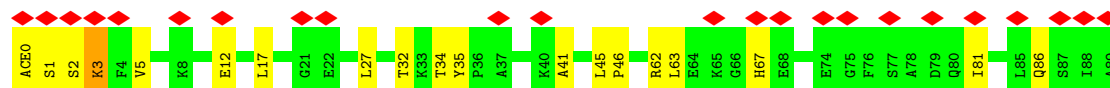
- Molecule 19: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain R: 



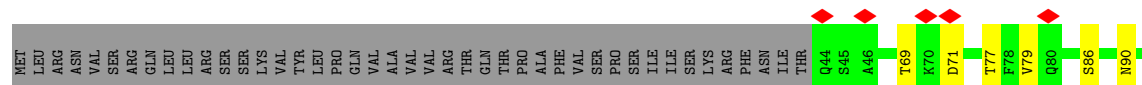
- Molecule 20: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

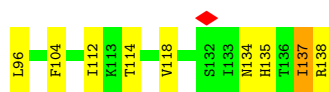
Chain S: 



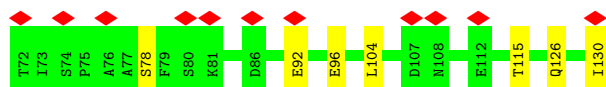
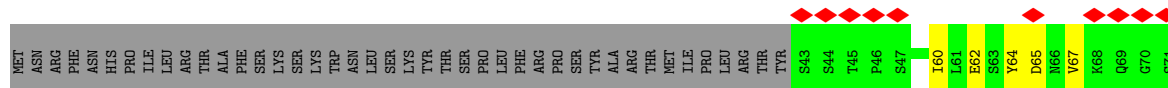
- Molecule 21: Acyl carrier protein

Chain T: 

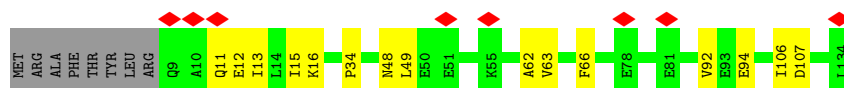
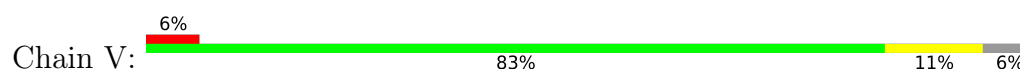




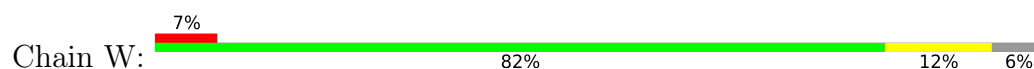
- Molecule 22: Acyl carrier protein



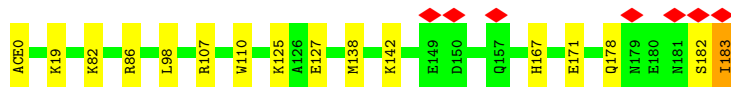
- Molecule 23: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



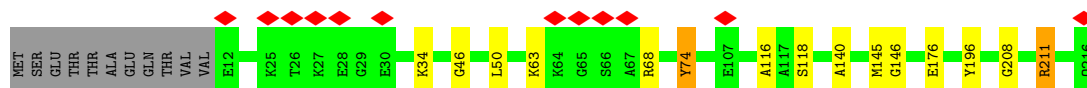
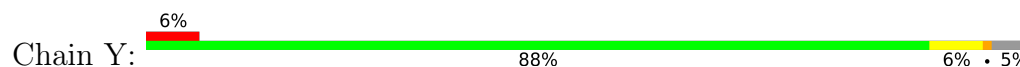
- Molecule 24: BA75_04796T0



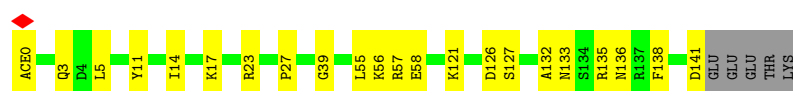
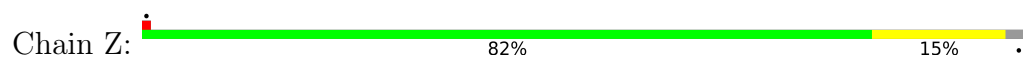
- Molecule 25: NADH-ubiquinone oxidoreductase



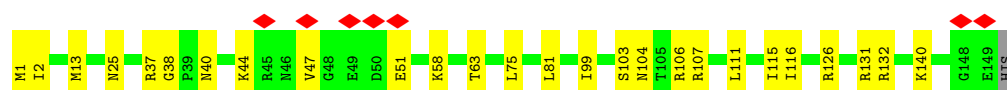
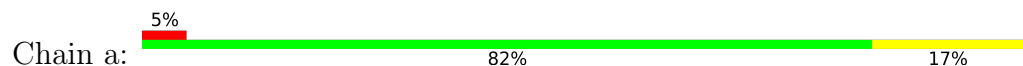
- Molecule 26: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



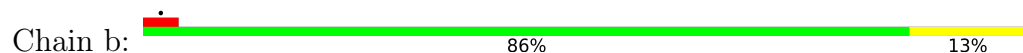
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



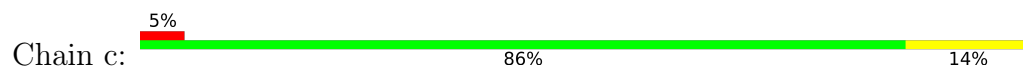
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



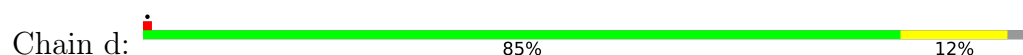
- Molecule 29: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 30: BA75_00589T0



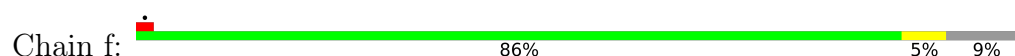
- Molecule 31: Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM

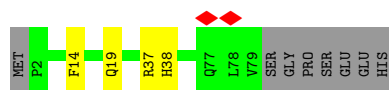


- Molecule 32: BA75_05084T0

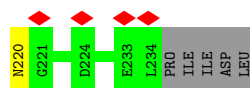
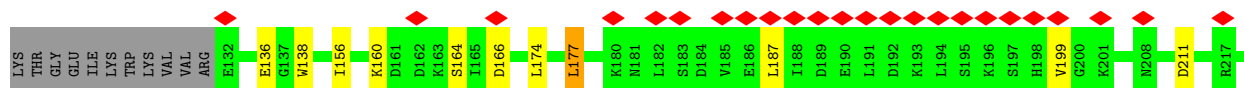
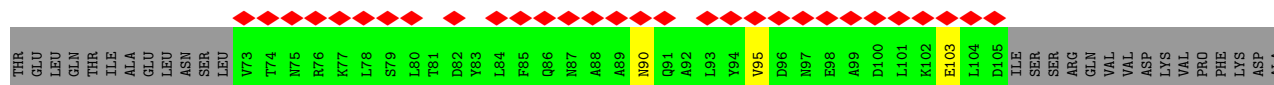


- Molecule 33: NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

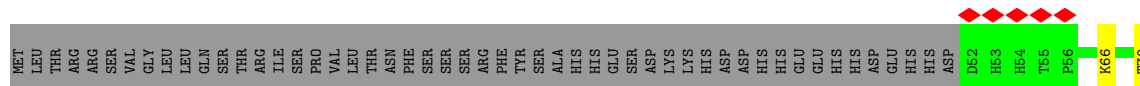




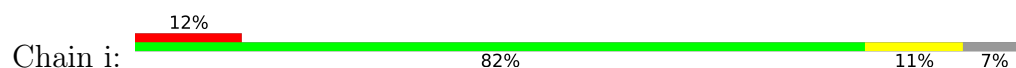
- Molecule 34: NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



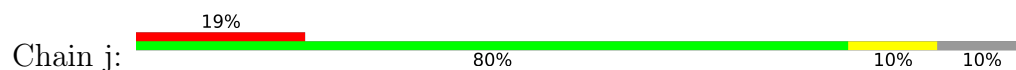
- Molecule 35: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

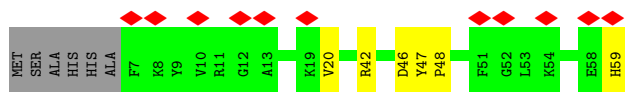


- Molecule 36: NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

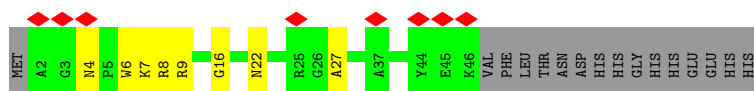


- Molecule 37: Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

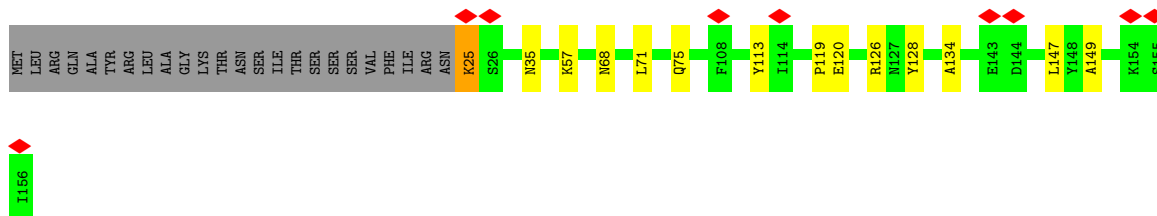
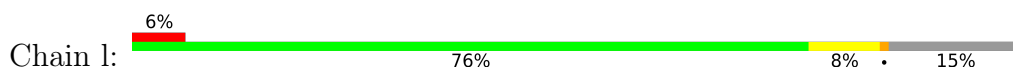




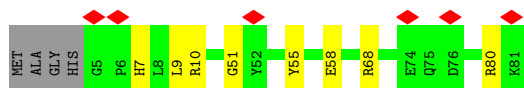
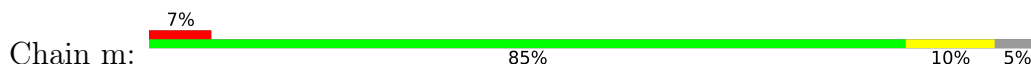
- Molecule 38: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



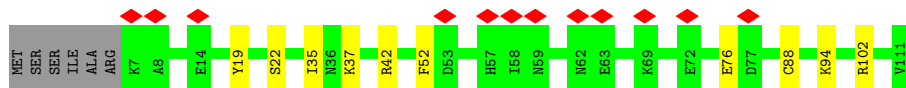
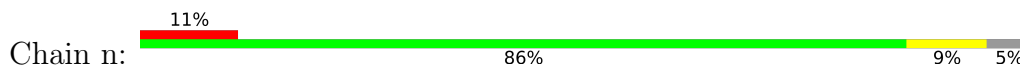
- Molecule 39: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



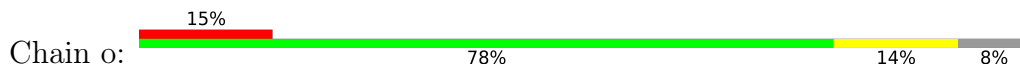
- Molecule 40: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



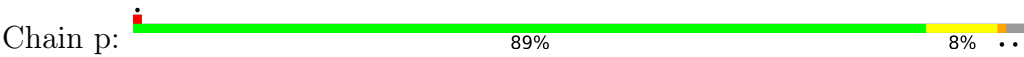
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



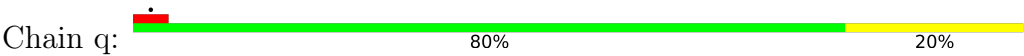
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 43: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53716	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.79	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0127	Depositor
Map size ($\text{\AA}$)	501.66, 501.66, 501.66	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.929, 0.929, 0.929	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PLC, ACE, FME, CDL, 3PE, SF4, ZN, 2MR, FES, FMN, EHZ, NDP

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	1	0.08	0/1405	0.24	0/1896
2	A	0.08	0/1151	0.22	0/1564
3	B	0.09	0/1450	0.24	0/1969
4	C	0.08	0/2033	0.24	0/2770
5	D	0.09	0/3698	0.23	0/5007
6	E	0.08	0/1480	0.24	0/2008
7	F	0.09	0/3579	0.25	0/4832
8	G	0.08	0/5436	0.24	0/7370
9	H	0.08	0/2880	0.24	0/3939
10	I	0.09	0/1596	0.25	0/2164
11	J	0.08	0/1329	0.24	0/1816
12	K	0.07	0/610	0.20	0/828
13	L	0.08	0/5236	0.23	0/7128
14	M	0.09	0/3940	0.24	0/5379
15	N	0.08	0/4110	0.22	0/5609
16	O	0.18	1/1621 (0.1%)	0.24	0/2199
17	P	0.08	0/2985	0.23	0/4035
18	Q	0.07	0/945	0.21	0/1273
19	R	0.08	0/998	0.23	0/1350
20	S	0.26	1/710 (0.1%)	0.30	1/961 (0.1%)
21	T	0.06	0/752	0.19	0/1021
22	U	0.07	0/688	0.21	0/936
23	V	0.08	0/1044	0.20	0/1411
24	W	0.07	0/999	0.19	0/1340
25	X	0.18	1/1475 (0.1%)	0.22	0/1990
26	Y	0.07	0/1615	0.21	0/2175
27	Z	0.20	1/1210 (0.1%)	0.21	0/1639
28	a	0.08	0/1241	0.21	0/1670
29	b	0.08	0/666	0.21	0/911
30	c	0.19	1/1448 (0.1%)	0.25	0/1964
31	d	0.08	0/633	0.18	0/854
32	e	0.07	0/865	0.20	0/1158

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.07	0/663	0.19	0/896
34	g	0.07	0/1293	0.21	0/1735
35	h	0.08	0/1114	0.24	0/1516
36	i	0.11	0/571	0.29	0/777
37	j	0.09	0/484	0.24	0/658
38	k	0.07	0/382	0.22	0/514
39	l	0.08	0/1119	0.25	0/1520
40	m	0.09	0/661	0.21	0/893
41	n	0.07	0/884	0.20	0/1197
42	o	0.08	0/696	0.22	0/933
43	p	0.07	0/756	0.21	0/1020
44	q	0.20	1/1192 (0.1%)	0.25	0/1620
All	All	0.10	6/69643 (0.0%)	0.23	1/94445 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S	0	ACE	C-N	6.19	1.45	1.33
25	X	0	ACE	C-N	6.18	1.45	1.33
16	O	0	ACE	C-N	6.18	1.45	1.33
30	c	0	ACE	C-N	6.18	1.45	1.33
44	q	0	ACE	C-N	6.13	1.45	1.33
27	Z	0	ACE	C-N	6.11	1.45	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S	2	SER	CB-CA-C	-5.58	110.12	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1383	0	1390	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1133	0	1167	24	0
3	B	1407	0	1372	21	0
4	C	1970	0	1905	26	0
5	D	3621	0	3531	56	0
6	E	1446	0	1435	26	0
7	F	3500	0	3459	70	0
8	G	5344	0	5333	82	0
9	H	2809	0	2880	51	0
10	I	1556	0	1499	30	0
11	J	1313	0	1320	30	0
12	K	617	0	657	11	0
13	L	5115	0	5338	80	0
14	M	3868	0	4127	64	0
15	N	4045	0	4327	48	0
16	O	1575	0	1523	15	0
17	P	2922	0	2915	42	0
18	Q	924	0	891	8	0
19	R	978	0	964	8	0
20	S	697	0	736	11	0
21	T	745	0	734	11	0
22	U	681	0	664	7	0
23	V	1025	0	1035	9	0
24	W	979	0	980	9	0
25	X	1450	0	1422	10	0
26	Y	1578	0	1567	13	0
27	Z	1176	0	1165	19	0
28	a	1215	0	1197	21	0
29	b	641	0	620	8	0
30	c	1418	0	1452	19	0
31	d	616	0	624	8	0
32	e	848	0	830	9	0
33	f	642	0	640	4	0
34	g	1280	0	1302	12	0
35	h	1078	0	1036	14	0
36	i	552	0	540	7	0
37	j	460	0	455	2	0
38	k	368	0	348	6	0
39	l	1082	0	1033	11	0
40	m	642	0	635	7	0
41	n	861	0	866	7	0
42	o	682	0	677	7	0
43	p	740	0	700	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	q	1156	0	1115	17	0
45	A	31	0	36	2	0
45	B	31	0	36	1	0
45	D	42	0	64	2	0
45	H	24	0	22	0	0
45	L	109	0	146	7	0
45	M	123	0	183	4	0
45	N	42	0	64	0	0
45	P	31	0	36	3	0
45	Y	72	0	98	1	0
45	Z	42	0	64	0	0
45	a	22	0	18	0	0
45	b	39	0	55	2	0
45	d	42	0	64	4	0
45	h	42	0	64	2	0
45	q	78	0	113	4	0
46	B	8	0	0	0	0
46	F	8	0	0	2	0
46	G	16	0	0	1	0
46	I	16	0	0	3	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	G	1	0	0	0	0
50	H	31	0	36	0	0
50	L	338	0	489	23	0
50	M	35	0	44	0	0
50	N	40	0	57	1	0
50	Y	77	0	108	9	0
50	b	142	0	183	5	0
50	f	51	0	82	7	0
50	g	46	0	69	2	0
50	j	27	0	28	0	0
50	m	25	0	24	0	0
51	O	75	0	97	5	0
51	P	42	0	28	0	0
51	Z	49	0	42	0	0
51	a	60	0	64	2	0
51	b	59	0	62	3	0
52	P	48	0	26	1	0
53	R	1	0	0	0	0
54	T	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	U	37	0	0	1	0
All	All	70216	0	70927	798	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:163:ILE:HG22	3:B:164:VAL:HG13	1.66	0.77
6:E:63:PRO:HG2	6:E:66:TYR:HB2	1.68	0.76
19:R:103:HIS:CD2	19:R:121:CYS:SG	2.80	0.74
8:G:59:CYS:HB3	8:G:70:CYS:HB3	1.71	0.73
13:L:388:THR:HG22	13:L:470:GLY:H	1.52	0.72
10:I:115:ARG:NH2	19:R:72:TYR:O	2.22	0.72
5:D:191:THR:OG1	5:D:328:ASP:O	2.08	0.71
28:a:37:ARG:HH22	28:a:47:VAL:HA	1.56	0.71
9:H:127:VAL:HG11	9:H:153:LEU:HD22	1.73	0.70
21:T:69:THR:HG22	21:T:71:ASP:H	1.56	0.70
5:D:161:VAL:HG11	5:D:204:MET:HG2	1.74	0.70
3:B:86:VAL:HG21	3:B:180:LEU:HD23	1.74	0.68
8:G:286:LYS:NZ	8:G:687:PHE:O	2.26	0.68
3:B:76:LEU:HB2	3:B:114:GLY:HA3	1.74	0.68
8:G:329:VAL:HG23	8:G:331:PRO:HD3	1.77	0.67
8:G:296:THR:HG22	8:G:297:GLN:HG2	1.76	0.66
43:p:44:CYS:SG	43:p:69:LYS:NZ	2.67	0.66
20:S:5:VAL:HG22	20:S:41:ALA:HB1	1.78	0.66
45:L:705:PLC:H61	14:M:370:THR:HA	1.77	0.66
30:c:108:GLU:OE1	30:c:112:LYS:NZ	2.26	0.66
26:Y:208:GLY:O	26:Y:211:ARG:NH2	2.29	0.65
27:Z:23:ARG:HG2	30:c:28:LEU:HD22	1.77	0.65
6:E:169:LEU:HD22	7:F:145:GLU:HG2	1.79	0.65
3:B:86:VAL:HG12	3:B:93:GLN:HB3	1.79	0.65
13:L:324:LEU:HD23	13:L:478:LEU:HD22	1.78	0.65
13:L:440:SER:HB2	13:L:444:ILE:HD12	1.79	0.65
5:D:80:ASN:O	15:N:287:ARG:NH2	2.30	0.64
13:L:604:LEU:HD21	50:L:706:3PE:H2	1.79	0.64
45:L:705:PLC:H42	36:i:18:GLY:HA2	1.77	0.64
28:a:115:ILE:HG23	28:a:116:ILE:HG13	1.79	0.64
3:B:78:CYS:HB3	5:D:160:TYR:HB2	1.78	0.64
10:I:163:ILE:HG13	10:I:165:CYS:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:303:PRO:HA	45:P:502:PLC:H73	1.80	0.64
5:D:429:TYR:HB3	5:D:442:LYS:HB3	1.80	0.63
5:D:480:VAL:O	5:D:482:ARG:NH1	2.31	0.63
13:L:360:TYR:HD2	13:L:433:THR:HG22	1.63	0.63
14:M:22:ASN:HD22	14:M:25:ASN:HD21	1.45	0.63
15:N:384:LYS:NZ	15:N:456:ASP:OD2	2.32	0.63
24:W:84:GLU:OE1	24:W:90:LYS:NZ	2.31	0.63
5:D:231:GLU:OE2	30:c:43:ARG:NH1	2.31	0.63
5:D:285:ARG:NE	10:I:75:GLU:OE2	2.31	0.63
13:L:364:ARG:HH21	13:L:368:PRO:HB3	1.63	0.63
5:D:376:LYS:HD3	5:D:383:ALA:HB1	1.81	0.62
7:F:247:ALA:HA	7:F:255:GLN:HB3	1.79	0.62
45:P:502:PLC:H62	45:P:502:PLC:H12	1.81	0.62
8:G:354:ASP:OD2	8:G:630:TYR:OH	2.18	0.62
4:C:106:VAL:HG11	4:C:114:VAL:HG21	1.82	0.62
5:D:121:HIS:HB2	5:D:126:LEU:HD11	1.82	0.62
9:H:221:LEU:O	9:H:223:SER:N	2.33	0.62
14:M:441:GLN:O	40:m:10:ARG:NH1	2.32	0.62
15:N:180:ASP:OD1	28:a:126:ARG:NH2	2.33	0.62
4:C:101:GLU:OE1	4:C:160:ARG:NH2	2.33	0.61
12:K:12:GLY:O	21:T:138:ARG:NH2	2.32	0.61
18:Q:120:LYS:NZ	18:Q:126:TYR:OH	2.30	0.61
5:D:300:GLU:OE2	23:V:16:LYS:NZ	2.33	0.61
8:G:338:ALA:HB3	8:G:364:VAL:HG12	1.81	0.61
1:l:35:LEU:HB2	1:l:51:ILE:HG21	1.82	0.61
7:F:382:ARG:NH2	7:F:392:GLU:OE1	2.33	0.60
27:Z:57:ARG:NH2	29:b:56:GLU:O	2.34	0.60
9:H:93:SER:OG	9:H:122:SER:O	2.19	0.60
26:Y:176:GLU:OE2	31:d:73:ARG:NH2	2.33	0.60
45:M:1003:PLC:H3A2	15:N:395:ILE:HG21	1.81	0.60
21:T:96:LEU:HD13	21:T:118:VAL:HG11	1.83	0.60
13:L:72:VAL:HG21	13:L:134:LEU:HD12	1.83	0.60
13:L:571:TRP:HB2	14:M:297:LYS:HE2	1.83	0.60
6:E:140:ILE:HG23	6:E:193:THR:HG21	1.84	0.60
15:N:183:LEU:HD13	15:N:188:TYR:HB3	1.83	0.60
19:R:21:ARG:O	19:R:40:ARG:NH2	2.34	0.60
38:k:16:GLY:O	38:k:22:ASN:ND2	2.32	0.60
8:G:419:ARG:NH1	8:G:439:THR:O	2.35	0.60
10:I:100:LYS:HE3	44:q:70:MET:HE2	1.82	0.60
13:L:282:GLY:HA3	13:L:411:ILE:HD12	1.84	0.59
17:P:268:ILE:HG22	17:P:275:PRO:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L:708:3PE:H331	26:Y:140:ALA:HB1	1.84	0.59
17:P:110:ILE:HD13	17:P:235:ALA:HB1	1.84	0.59
7:F:30:TYR:HB2	7:F:32:LYS:HE2	1.85	0.59
14:M:61:TRP:O	34:g:160:LYS:NZ	2.32	0.59
9:H:172:SER:HB2	9:H:350:PRO:HG2	1.85	0.59
13:L:498:GLU:O	13:L:502:SER:OG	2.20	0.59
8:G:531:PRO:O	8:G:535:ASN:ND2	2.32	0.59
42:o:8:GLU:O	42:o:30:ARG:NH1	2.36	0.59
17:P:353:GLN:NE2	24:W:41:ASN:OD1	2.32	0.58
13:L:272:ILE:HG12	50:L:711:3PE:H241	1.84	0.58
14:M:26:GLY:HA2	31:d:24:LYS:HB3	1.84	0.58
4:C:100:ASP:OD1	5:D:176:LYS:NZ	2.36	0.58
10:I:121:GLU:O	10:I:151:ARG:NH1	2.37	0.58
10:I:190:ARG:HD3	17:P:85:LEU:HD21	1.84	0.58
13:L:354:TYR:O	13:L:360:TYR:OH	2.18	0.58
39:l:126:ARG:NH2	42:o:26:ASP:OD2	2.36	0.58
2:A:24:ASN:ND2	9:H:68:LEU:O	2.34	0.58
7:F:456:VAL:HG22	7:F:461:VAL:HG22	1.85	0.58
24:W:31:TYR:HB3	24:W:55:ILE:HD13	1.86	0.58
17:P:217:LYS:NZ	17:P:315:ILE:O	2.31	0.58
15:N:180:ASP:OD2	28:a:132:ARG:NH1	2.37	0.58
3:B:115:THR:HA	3:B:143:CYS:HB3	1.86	0.57
8:G:144:ASP:OD1	30:c:73:ARG:NH2	2.36	0.57
13:L:290:LEU:HA	13:L:293:MET:HE2	1.85	0.57
5:D:108:PRO:HG2	9:H:218:GLU:HG2	1.86	0.57
8:G:123:CYS:SG	8:G:135:GLN:NE2	2.78	0.57
6:E:87:ILE:HA	6:E:90:MET:HE3	1.85	0.57
7:F:70:ARG:O	7:F:72:ARG:NH1	2.38	0.57
8:G:431:HIS:HB2	8:G:442:LEU:HD22	1.86	0.57
28:a:37:ARG:NH2	28:a:51:GLU:OE1	2.38	0.57
34:g:45:ASN:ND2	34:g:103:GLU:OE2	2.33	0.57
8:G:32:ASP:OD2	8:G:99:THR:OG1	2.20	0.57
16:O:18:ARG:HD3	51:O:201:CDL:H331	1.85	0.57
14:M:36:ILE:HG22	14:M:37:LYS:HG3	1.87	0.57
14:M:76:ARG:HH12	35:h:120:LYS:HE2	1.70	0.57
8:G:366:THR:O	8:G:552:LYS:NZ	2.38	0.57
8:G:456:LEU:HD12	8:G:490:THR:HG22	1.85	0.56
11:J:43:TYR:OH	28:a:106:ARG:O	2.22	0.56
4:C:100:ASP:OD2	5:D:325:GLN:NE2	2.38	0.56
14:M:130:LEU:HD23	14:M:133:ILE:HD11	1.85	0.56
4:C:49:ARG:HD2	30:c:45:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:1:FME:O1	33:f:37:ARG:NH1	2.34	0.56
11:J:14:TYR:HA	11:J:17:ILE:HG12	1.87	0.56
16:O:24:ASP:OD2	16:O:83:ARG:NH1	2.34	0.56
33:f:19:GLN:NE2	50:f:101:3PE:O12	2.38	0.56
8:G:254:LEU:HD11	8:G:411:ALA:HB1	1.88	0.56
21:T:77:THR:HG22	21:T:114:THR:HG22	1.88	0.56
13:L:218:VAL:HA	13:L:221:MET:HE2	1.88	0.56
14:M:300:ASP:HB3	14:M:303:VAL:HB	1.88	0.56
8:G:177:THR:N	46:G:802:SF4:S4	2.77	0.56
9:H:45:ARG:NH1	30:c:34:THR:O	2.23	0.56
15:N:228:SER:O	15:N:289:LYS:NZ	2.39	0.56
8:G:660:ILE:HD11	20:S:17:LEU:HD11	1.87	0.56
13:L:187:LEU:HD13	14:M:407:ILE:HA	1.88	0.56
45:M:1002:PLC:H81	35:h:66:LYS:HG2	1.87	0.56
45:h:201:PLC:H11	36:i:15:PRO:HG3	1.87	0.56
8:G:279:ASN:HA	8:G:413:VAL:HG11	1.87	0.56
14:M:300:ASP:OD2	14:M:360:ARG:NH1	2.39	0.56
5:D:321:ILE:HB	5:D:420:GLU:HB2	1.88	0.56
7:F:21:ASP:OD1	7:F:21:ASP:N	2.39	0.56
7:F:198:GLU:OE2	7:F:208:ARG:NE	2.37	0.56
15:N:393:ILE:HG13	31:d:22:ILE:HG23	1.88	0.56
3:B:73:THR:HG22	3:B:100:PHE:HB3	1.89	0.55
14:M:65:ASN:O	14:M:72:GLN:NE2	2.34	0.55
15:N:508:GLU:HG3	15:N:512:LYS:HE3	1.88	0.55
6:E:132:CYS:HA	6:E:175:ALA:HB1	1.88	0.55
8:G:356:VAL:HG13	8:G:361:SER:HB3	1.88	0.55
13:L:211:VAL:HG21	50:L:709:3PE:H331	1.87	0.55
17:P:192:MET:O	17:P:197:SER:OG	2.24	0.55
33:f:37:ARG:HH21	33:f:38:HIS:HB2	1.72	0.55
5:D:49:ASN:ND2	5:D:51:PHE:O	2.39	0.55
9:H:134:GLY:HA3	9:H:146:THR:HG21	1.89	0.55
4:C:53:ARG:NH1	27:Z:5:LEU:O	2.40	0.55
7:F:342:ASN:OD1	7:F:344:GLN:NE2	2.40	0.55
8:G:353:LYS:NZ	8:G:524:VAL:O	2.39	0.55
17:P:43:THR:OG1	17:P:108:SER:OG	2.22	0.55
22:U:60:ILE:HG12	38:k:9:ARG:HH21	1.72	0.55
9:H:171:VAL:HG21	9:H:179:ILE:HG12	1.88	0.55
14:M:462:ILE:HD11	45:M:1002:PLC:H2	1.89	0.55
25:X:19:LYS:HB3	28:a:103:SER:HB2	1.88	0.55
26:Y:118:SER:HB2	26:Y:146:GLY:HA2	1.87	0.55
9:H:72:ILE:HG21	9:H:84:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:127:VAL:HG21	9:H:153:LEU:HD13	1.89	0.55
6:E:186:GLU:OE2	7:F:112:ARG:NH1	2.33	0.55
10:I:90:ALA:HB2	28:a:1:MET:HE1	1.89	0.55
50:Y:302:3PE:H221	50:Y:302:3PE:H321	1.89	0.55
2:A:75:PHE:HB2	9:H:154:ILE:HG23	1.89	0.55
11:J:73:LYS:NZ	21:T:134:ASN:OD1	2.37	0.55
8:G:380:ASP:OD2	20:S:35:TYR:OH	2.24	0.54
13:L:328:HIS:HA	13:L:392:SER:HB2	1.89	0.54
14:M:87:ILE:HD13	14:M:262:ILE:HD13	1.88	0.54
17:P:111:VAL:HG23	17:P:146:VAL:HG11	1.88	0.54
17:P:95:ILE:HA	17:P:101:ILE:HD11	1.89	0.54
2:A:44:ILE:HB	17:P:346:PRO:HB3	1.89	0.54
12:K:15:ILE:HG13	21:T:134:ASN:HD22	1.72	0.54
39:I:71:LEU:HD22	39:I:75:GLN:HG2	1.88	0.54
1:1:57:GLU:HB3	1:1:78:LEU:HD11	1.89	0.54
8:G:542:TYR:OH	8:G:563:GLN:OE1	2.21	0.54
13:L:534:LEU:HD22	41:n:35:ILE:HG12	1.88	0.54
8:G:245:THR:HG23	8:G:601:ARG:HD3	1.89	0.54
24:W:76:MET:HG2	24:W:80:MET:HE3	1.90	0.54
7:F:232:VAL:O	7:F:235:THR:OG1	2.26	0.54
7:F:295:TRP:HZ2	7:F:317:GLU:HG2	1.72	0.54
54:U:201:EHZ:O2	54:U:201:EHZ:O1	2.25	0.54
11:J:135:GLU:OE2	16:O:127:ARG:NH2	2.40	0.54
2:A:35:GLU:OE2	17:P:77:ARG:NH2	2.41	0.53
7:F:124:GLU:OE2	7:F:240:ARG:NH2	2.41	0.53
8:G:237:ALA:HB2	8:G:268:MET:HE2	1.89	0.53
10:I:128:LEU:O	10:I:132:VAL:HG23	2.08	0.53
27:Z:121:LYS:HG2	32:e:73:GLU:HB3	1.90	0.53
3:B:48:ASN:OD1	3:B:202:ARG:NH2	2.42	0.53
11:J:81:SER:OG	17:P:271:ARG:NH1	2.41	0.53
21:T:86:SER:O	21:T:90:ASN:ND2	2.37	0.53
8:G:495:VAL:HA	8:G:501:ILE:HD12	1.89	0.53
9:H:148:ARG:NH1	9:H:220:GLU:OE1	2.39	0.53
1:1:69:ASP:O	1:1:74:LYS:NZ	2.38	0.53
45:A:201:PLC:O2P	17:P:302:GLN:NE2	2.32	0.53
8:G:606:PRO:HB2	8:G:610:ALA:HB3	1.91	0.53
20:S:3:LYS:O	20:S:3:LYS:NZ	2.31	0.53
5:D:387:ARG:NH2	10:I:172:CYS:O	2.39	0.53
6:E:114:TYR:CZ	7:F:185:MET:HG3	2.43	0.53
11:J:139:LEU:HD22	15:N:130:ILE:HD12	1.91	0.53
20:S:12:GLU:HB3	20:S:62:ARG:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:36:TYR:HB3	45:d:101:PLC:H4'2	1.89	0.53
31:d:40:GLY:HA3	45:d:101:PLC:H7'1	1.90	0.53
35:h:89:ARG:NH1	35:h:94:GLY:O	2.40	0.53
3:B:105:ARG:NH1	3:B:130:GLN:O	2.42	0.53
5:D:318:PRO:HB3	5:D:339:VAL:HG21	1.91	0.53
7:F:365:GLN:N	46:F:501:SF4:S3	2.81	0.53
23:V:48:ASN:ND2	23:V:107:ASP:OD1	2.41	0.53
13:L:526:TYR:O	41:n:37:LYS:NZ	2.33	0.52
16:O:144:VAL:O	51:O:201:CDL:O1	2.26	0.52
51:a:201:CDL:H172	30:c:26:LEU:HD13	1.92	0.52
4:C:91:PHE:HB3	4:C:110:ALA:HB1	1.91	0.52
8:G:476:SER:HB3	8:G:513:HIS:HA	1.91	0.52
10:I:57:GLU:OE2	29:b:15:ARG:NH2	2.43	0.52
14:M:148:LEU:HD13	14:M:171:LEU:HD12	1.91	0.52
4:C:118:LEU:HD12	4:C:161:ILE:HD11	1.92	0.52
9:H:81:ILE:HG12	33:f:14:PHE:HB3	1.91	0.52
9:H:151:ALA:HB1	9:H:321:ILE:HD11	1.91	0.52
22:U:96:GLU:OE2	41:n:42:ARG:NH2	2.32	0.52
36:i:64:LEU:HD11	43:p:54:THR:HB	1.91	0.52
7:F:423:ILE:HG12	7:F:430:MET:HE1	1.92	0.52
7:F:404:GLU:OE2	7:F:420:GLN:NE2	2.42	0.52
8:G:251:HIS:HB3	8:G:286:LYS:HD2	1.91	0.52
14:M:61:TRP:CD1	14:M:89:LEU:HD21	2.45	0.52
4:C:42:GLU:N	4:C:42:GLU:OE1	2.43	0.52
13:L:23:ILE:O	13:L:27:SER:OG	2.27	0.52
13:L:268:GLU:OE1	13:L:493:ASN:ND2	2.42	0.52
15:N:252:MET:O	15:N:256:ASN:ND2	2.31	0.52
17:P:233:ARG:NH1	17:P:329:LEU:O	2.43	0.52
5:D:406:LYS:NZ	8:G:136:GLU:OE2	2.43	0.51
9:H:121:ALA:HB1	11:J:52:THR:HB	1.92	0.51
16:O:83:ARG:HB3	16:O:93:GLU:HG3	1.90	0.51
8:G:210:ASN:ND2	8:G:716:ASP:OD1	2.36	0.51
8:G:691:ASP:OD1	8:G:691:ASP:N	2.42	0.51
11:J:105:TYR:HA	32:e:55:ARG:HD3	1.92	0.51
51:O:201:CDL:H531	51:O:201:CDL:H132	1.92	0.51
4:C:119:LYS:NZ	4:C:177:LEU:O	2.42	0.51
5:D:62:SER:OG	15:N:283:LEU:O	2.19	0.51
5:D:308:SER:H	5:D:450:HIS:HE1	1.58	0.51
8:G:609:VAL:HG11	17:P:17:ILE:HB	1.93	0.51
27:Z:135:ARG:NH2	32:e:73:GLU:OE1	2.36	0.51
5:D:105:PRO:HG3	5:D:134:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:5:LEU:HD22	13:L:617:VAL:HG12	1.93	0.51
44:q:111:LEU:O	44:q:114:THR:OG1	2.28	0.51
6:E:174:ASN:ND2	6:E:186:GLU:OE1	2.39	0.51
8:G:345:ASP:OD1	8:G:345:ASP:N	2.40	0.51
37:j:47:TYR:CD2	37:j:48:PRO:HD3	2.46	0.51
5:D:90:PRO:HD3	15:N:370:MET:HE1	1.93	0.51
11:J:99:GLU:HG3	28:a:107:ARG:HD2	1.93	0.51
14:M:449:VAL:HG12	14:M:454:ILE:HG13	1.92	0.51
8:G:587:THR:HG22	8:G:637:ARG:HH21	1.76	0.51
13:L:250:ALA:HB2	13:L:333:SER:HB3	1.93	0.51
7:F:101:ALA:HB1	7:F:115:ILE:HD11	1.93	0.51
50:L:710:3PE:H3A1	14:M:466:ILE:HD13	1.93	0.51
12:K:77:GLU:OE1	12:K:78:GLU:N	2.44	0.51
13:L:88:PRO:HG3	13:L:330:ILE:HG23	1.92	0.51
15:N:287:ARG:NH1	15:N:378:GLU:OE2	2.44	0.51
50:f:101:3PE:H2G1	50:f:101:3PE:H371	1.93	0.51
5:D:380:PHE:HB2	8:G:144:ASP:HB2	1.92	0.50
45:D:501:PLC:H42	10:I:70:TRP:HE1	1.77	0.50
7:F:193:GLU:OE2	7:F:210:LYS:NZ	2.43	0.50
10:I:127:LYS:N	46:I:302:SF4:S1	2.82	0.50
10:I:141:GLU:HB2	10:I:154:LYS:HB3	1.92	0.50
13:L:424:LEU:HD13	45:L:702:PLC:H3A2	1.93	0.50
25:X:178:GLN:O	25:X:182:SER:OG	2.27	0.50
9:H:45:ARG:NH2	10:I:90:ALA:O	2.38	0.50
15:N:46:THR:OG1	15:N:49:ASN:OD1	2.29	0.50
18:Q:140:ASP:OD2	18:Q:142:SER:OG	2.28	0.50
30:c:65:ILE:HG13	30:c:66:VAL:HG13	1.94	0.50
8:G:394:ILE:HB	8:G:417:ARG:HD3	1.93	0.50
8:G:400:ILE:HG12	8:G:471:LEU:HB2	1.92	0.50
13:L:124:MET:HE3	13:L:251:CYS:HA	1.92	0.50
23:V:62:ALA:HB1	30:c:146:PRO:HB3	1.92	0.50
42:o:3:VAL:O	42:o:58:GLN:NE2	2.44	0.50
13:L:169:LEU:HB2	50:L:703:3PE:H231	1.92	0.50
50:L:710:3PE:H3A2	14:M:469:ILE:HD12	1.93	0.50
14:M:196:ASP:OD1	35:h:117:TYR:OH	2.28	0.50
26:Y:116:ALA:HB2	50:Y:303:3PE:H322	1.92	0.50
45:D:501:PLC:H1A2	9:H:327:VAL:HG11	1.94	0.50
11:J:160:LYS:HG3	12:K:72:ARG:HH21	1.77	0.50
13:L:217:LEU:HD13	13:L:277:ILE:HG12	1.94	0.50
25:X:107:ARG:HA	25:X:110:TRP:NE1	2.27	0.50
25:X:183:ILE:HD13	25:X:183:ILE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L:706:3PE:H3C1	50:L:706:3PE:H341	1.93	0.50
18:Q:57:ILE:HG12	18:Q:77:ILE:HG12	1.93	0.50
35:h:107:LYS:NZ	43:p:8:PRO:HG3	2.26	0.50
9:H:219:SER:OG	9:H:314:ARG:NH2	2.45	0.50
9:H:353:ILE:HG12	27:Z:55:LEU:HB3	1.94	0.50
17:P:156:ASN:HD21	17:P:317:GLN:HA	1.77	0.50
26:Y:50:LEU:HG	50:Y:302:3PE:H392	1.94	0.50
44:q:67:ARG:NH2	45:q:402:PLC:O1P	2.34	0.50
14:M:288:LEU:HD21	14:M:419:SER:HB2	1.94	0.50
17:P:226:GLN:NE2	17:P:332:VAL:O	2.43	0.50
2:A:95:VAL:HB	2:A:99:GLY:HA3	1.94	0.50
14:M:486:ILE:HD12	43:p:79:ILE:HG22	1.93	0.50
4:C:160:ARG:NH1	5:D:414:GLU:OE2	2.45	0.49
13:L:385:PRO:HA	13:L:390:PHE:CG	2.46	0.49
13:L:638:ILE:HG22	26:Y:145:MET:HE2	1.93	0.49
18:Q:87:ARG:NH2	18:Q:103:GLN:OE1	2.43	0.49
27:Z:126:ASP:O	27:Z:133:ASN:ND2	2.45	0.49
28:a:40:ASN:OD1	28:a:40:ASN:N	2.44	0.49
7:F:394:ASP:HB2	30:c:66:VAL:HG11	1.93	0.49
11:J:108:VAL:O	32:e:55:ARG:NH1	2.45	0.49
6:E:125:GLN:HB2	6:E:179:ALA:HB3	1.94	0.49
22:U:64:TYR:OH	22:U:92:GLU:OE1	2.28	0.49
7:F:400:SER:HB2	7:F:416:ALA:HB1	1.94	0.49
10:I:114:ARG:HD3	10:I:211:ILE:HG21	1.94	0.49
7:F:297:ASN:OD1	7:F:344:GLN:NE2	2.43	0.49
45:L:705:PLC:H63	36:i:19:TRP:CZ2	2.47	0.49
14:M:85:ASP:CG	14:M:263:ARG:HH22	2.21	0.49
44:q:47:VAL:HG11	44:q:52:GLU:HG3	1.93	0.49
2:A:60:SER:OG	9:H:136:MET:O	2.31	0.49
5:D:159:ASP:HB3	5:D:166:ASN:HD21	1.77	0.49
16:O:62:ARG:NE	51:b:102:CDL:OA4	2.46	0.49
30:c:163:GLU:HA	30:c:166:HIS:CE1	2.48	0.49
1:1:127:SER:N	1:1:130:GLU:OE1	2.42	0.49
7:F:129:ALA:HB1	7:F:133:MET:HE3	1.93	0.49
8:G:310:PHE:HB2	44:q:133:PRO:HB2	1.95	0.49
14:M:191:ILE:HG13	14:M:192:ILE:HG13	1.95	0.49
10:I:184:GLU:OE2	44:q:78:HIS:NE2	2.43	0.49
6:E:126:VAL:HG22	6:E:178:ILE:HD11	1.94	0.49
8:G:618:ARG:NE	8:G:630:TYR:O	2.42	0.49
9:H:36:GLU:HG2	9:H:40:MET:HE2	1.95	0.49
50:Y:302:3PE:H221	50:Y:302:3PE:H352	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:g:220:ASN:HB2	36:i:70:SER:HB2	1.93	0.49
7:F:309:PRO:HD3	7:F:417:TRP:HB3	1.93	0.48
7:F:387:GLN:NE2	7:F:465:PRO:O	2.42	0.48
17:P:127:GLU:OE1	17:P:127:GLU:N	2.42	0.48
30:c:64:ASP:OD1	30:c:65:ILE:N	2.46	0.48
5:D:207:LEU:HB3	5:D:219:PHE:HA	1.94	0.48
13:L:81:LEU:HD23	13:L:262:ARG:HD2	1.94	0.48
15:N:76:ILE:HD12	50:N:602:3PE:H241	1.95	0.48
14:M:90:LEU:HD13	14:M:474:VAL:HG13	1.95	0.48
14:M:111:LYS:HE2	15:N:458:LEU:HB3	1.95	0.48
34:g:156:ILE:HG23	34:g:160:LYS:HD2	1.95	0.48
37:j:42:ARG:NH2	37:j:46:ASP:OD2	2.46	0.48
2:A:61:HIS:CD2	11:J:70:ILE:HD11	2.49	0.48
5:D:387:ARG:NH1	10:I:175:ASP:OD1	2.45	0.48
9:H:91:LEU:HD22	9:H:236:ILE:HG23	1.95	0.48
13:L:250:ALA:HA	13:L:254:ILE:HD13	1.96	0.48
50:L:703:3PE:H382	50:L:703:3PE:H352	1.62	0.48
14:M:423:SER:HA	14:M:426:TYR:CE2	2.49	0.48
7:F:361:GLU:HA	8:G:197:ARG:HH12	1.78	0.48
19:R:45:SER:HB2	19:R:48:GLN:HB2	1.96	0.48
5:D:322:ARG:HG3	5:D:420:GLU:HB3	1.95	0.48
5:D:445:ALA:HB1	5:D:479:GLU:HG2	1.95	0.48
9:H:120:LEU:HD13	9:H:161:THR:HG23	1.96	0.48
43:p:38:VAL:HG21	43:p:79:ILE:HD12	1.96	0.48
5:D:169:VAL:HG22	5:D:428:VAL:HG22	1.96	0.48
7:F:346:ASP:OD1	7:F:433:ARG:NH2	2.47	0.48
8:G:292:ASP:OD1	8:G:697:SER:OG	2.31	0.48
8:G:515:GLU:OE1	8:G:518:ARG:NH1	2.47	0.48
11:J:77:GLU:OE1	26:Y:68:ARG:NH1	2.47	0.48
34:g:174:LEU:HD12	34:g:199:VAL:HG13	1.95	0.48
2:A:61:HIS:HD2	11:J:70:ILE:HD11	1.79	0.48
2:A:64:ILE:HD12	11:J:67:LEU:HB3	1.95	0.48
19:R:117:PRO:HA	19:R:124:ARG:HA	1.96	0.48
7:F:351:ILE:HG13	7:F:422:LEU:HG	1.96	0.47
17:P:191:PRO:HA	52:P:501:NDP:H71N	1.78	0.47
12:K:51:ILE:HD13	15:N:130:ILE:HD11	1.95	0.47
13:L:260:LEU:HD13	13:L:277:ILE:HD13	1.96	0.47
15:N:28:ARG:HG2	15:N:86:SER:OG	2.15	0.47
45:Y:301:PLC:H2A2	40:m:51:GLY:HA3	1.96	0.47
3:B:69:PHE:O	3:B:98:ILE:HA	2.14	0.47
6:E:175:ALA:O	6:E:177:MET:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:100:ASN:ND2	7:F:191:GLY:O	2.40	0.47
7:F:427:ARG:HA	7:F:430:MET:HE2	1.97	0.47
9:H:36:GLU:HG3	9:H:306:VAL:HG13	1.95	0.47
13:L:278:LEU:HG	13:L:411:ILE:HG13	1.96	0.47
14:M:301:LEU:HB3	14:M:349:VAL:HG13	1.96	0.47
19:R:103:HIS:HD2	19:R:121:CYS:SG	2.33	0.47
25:X:142:LYS:NZ	27:Z:58:GLU:OE2	2.46	0.47
35:h:145:ARG:NH2	35:h:147:ASP:OD1	2.47	0.47
1:1:98:SER:HB2	1:1:103:ARG:HA	1.96	0.47
8:G:219:VAL:HG13	8:G:228:LEU:HD13	1.95	0.47
21:T:134:ASN:HB2	26:Y:68:ARG:HH21	1.79	0.47
44:q:28:ASP:OD2	44:q:56:ARG:NH2	2.43	0.47
1:1:86:ARG:NH1	1:1:112:GLU:OE1	2.47	0.47
3:B:115:THR:OG1	3:B:143:CYS:SG	2.67	0.47
4:C:205:ILE:HG23	4:C:206:MET:HG2	1.97	0.47
13:L:611:PHE:HB2	26:Y:74:TYR:HB2	1.97	0.47
15:N:498:LEU:HD12	31:d:15:VAL:HG22	1.97	0.47
10:I:145:ARG:HG3	10:I:151:ARG:HB2	1.96	0.47
15:N:41:HIS:NE2	15:N:68:ASN:OD1	2.44	0.47
15:N:487:ASN:OD1	31:d:19:GLN:NE2	2.38	0.47
20:S:63:LEU:N	20:S:67:HIS:O	2.43	0.47
1:1:83:ILE:HG23	1:1:113:VAL:HG13	1.97	0.47
2:A:36:ASN:HB3	17:P:53:ARG:HH22	1.79	0.47
5:D:85:ASP:OD2	15:N:149:SER:OG	2.31	0.47
6:E:171:ALA:HB3	6:E:177:MET:HE2	1.95	0.47
13:L:18:PHE:HB3	45:h:201:PLC:H1A2	1.96	0.47
5:D:235:ARG:NH1	5:D:262:ASP:OD2	2.41	0.47
7:F:89:ASN:ND2	7:F:93:GLU:O	2.39	0.47
7:F:195:ALA:HB2	7:F:207:PRO:HG3	1.96	0.47
26:Y:46:GLY:HA3	50:Y:302:3PE:H231	1.97	0.47
28:a:75:LEU:HB2	28:a:81:LEU:HD23	1.96	0.47
2:A:58:GLU:HG3	17:P:352:SER:HB3	1.97	0.47
3:B:140:MET:HG2	3:B:175:PRO:HG2	1.97	0.47
5:D:74:HIS:NE2	5:D:75:GLU:OE2	2.47	0.47
8:G:495:VAL:HG22	8:G:501:ILE:HG21	1.97	0.47
27:Z:136:ASN:ND2	27:Z:138:PHE:O	2.46	0.47
14:M:269:LEU:HB3	14:M:272:ILE:HG22	1.97	0.47
8:G:558:ALA:O	44:q:138:ARG:NH2	2.47	0.46
12:K:67:LEU:HD13	15:N:157:LEU:HD11	1.97	0.46
13:L:379:LEU:HD22	13:L:384:ILE:HG13	1.97	0.46
35:h:107:LYS:NZ	43:p:28:GLU:OE1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:PHE:CD1	9:H:110:LEU:HB2	2.50	0.46
5:D:221:TRP:CZ2	10:I:86:MET:HG3	2.51	0.46
8:G:205:THR:O	8:G:207:VAL:N	2.46	0.46
36:i:68:ASN:ND2	43:p:65:GLU:OE1	2.47	0.46
1:l:65:ASN:HB3	1:l:74:LYS:HZ2	1.79	0.46
4:C:45:LEU:HD21	30:c:9:LYS:HA	1.96	0.46
7:F:116:ARG:HB2	7:F:149:GLU:HG3	1.96	0.46
13:L:127:LEU:HD11	13:L:140:TRP:HE3	1.79	0.46
13:L:338:LEU:HD23	13:L:377:ALA:HB2	1.98	0.46
14:M:28:LEU:HB3	14:M:30:LYS:HB3	1.96	0.46
17:P:351:THR:HB	17:P:352:SER:H	1.59	0.46
1:l:61:LEU:HD22	1:l:78:LEU:HD22	1.97	0.46
2:A:125:ILE:HG13	9:H:318:ASP:HB2	1.97	0.46
8:G:160:LYS:O	8:G:168:THR:OG1	2.25	0.46
8:G:262:THR:HG22	8:G:267:VAL:HG22	1.98	0.46
11:J:73:LYS:HB2	21:T:135:HIS:HE1	1.80	0.46
17:P:69:PRO:HB2	17:P:93:PHE:CD1	2.50	0.46
4:C:150:LEU:HB2	4:C:159:ILE:HG22	1.97	0.46
8:G:362:GLU:CD	20:S:62:ARG:HH12	2.23	0.46
13:L:406:PHE:HE2	45:L:704:PLC:H32	1.80	0.46
16:O:127:ARG:NH1	32:e:2:ALA:O	2.48	0.46
21:T:104:PHE:HZ	21:T:118:VAL:HG13	1.81	0.46
7:F:29:VAL:O	7:F:117:LYS:NZ	2.32	0.46
8:G:162:ILE:HB	8:G:211:VAL:HG23	1.98	0.46
8:G:592:ASN:HD21	8:G:594:GLU:HG2	1.81	0.46
9:H:104:GLY:HA3	9:H:107:LEU:HD12	1.96	0.46
13:L:67:VAL:HG11	14:M:326:ILE:HA	1.97	0.46
50:L:707:3PE:H2A2	50:L:708:3PE:H292	1.98	0.46
1:l:140:GLN:NE2	39:l:35:ASN:OD1	2.31	0.46
5:D:97:ARG:HH12	24:W:87:ASN:HA	1.80	0.46
13:L:623:ILE:O	28:a:131:ARG:NH2	2.48	0.46
42:o:39:ARG:HD2	42:o:44:TYR:CD2	2.50	0.46
44:q:37:THR:HG22	44:q:43:LYS:HG2	1.98	0.46
2:A:1:FME:HE2	28:a:63:THR:H	1.80	0.46
5:D:456:HIS:HB2	24:W:2:THR:HG23	1.98	0.46
8:G:264:GLY:HA3	18:Q:96:GLN:NE2	2.31	0.46
50:Y:302:3PE:H3F2	50:Y:302:3PE:H3C1	1.76	0.46
39:l:134:ALA:HB2	39:l:149:ALA:HB2	1.96	0.46
6:E:111:TYR:HB3	7:F:185:MET:HB2	1.98	0.46
7:F:189:ILE:HG12	7:F:363:CYS:HB3	1.99	0.45
27:Z:39:GLY:HA2	50:b:104:3PE:H2B2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:121:LYS:NZ	27:Z:141:ASP:OD1	2.41	0.45
28:a:2:ILE:HD12	51:a:201:CDL:HB4	1.98	0.45
44:q:70:MET:HE1	44:q:81:LEU:HD23	1.97	0.45
2:A:88:TYR:HB2	11:J:133:PHE:CZ	2.51	0.45
3:B:34:LEU:HD21	17:P:128:ASP:HB3	1.96	0.45
50:L:707:3PE:H2B1	50:L:708:3PE:H2B1	1.99	0.45
17:P:219:VAL:HG23	17:P:221:PRO:HD3	1.98	0.45
18:Q:45:ALA:HB1	18:Q:49:LEU:HD12	1.98	0.45
22:U:62:GLU:O	38:k:8:ARG:NH1	2.37	0.45
44:q:69:ASP:HB3	44:q:72:GLU:HG3	1.98	0.45
7:F:422:LEU:HD23	7:F:426:PHE:HB2	1.98	0.45
10:I:172:CYS:HA	46:I:302:SF4:S2	2.57	0.45
14:M:470:TYR:CE2	14:M:472:SER:HB2	2.51	0.45
7:F:377:GLN:NE2	7:F:381:ASP:OD2	2.49	0.45
8:G:706:SER:O	8:G:713:LYS:NZ	2.46	0.45
10:I:172:CYS:SG	10:I:176:ALA:N	2.85	0.45
11:J:40:TRP:O	11:J:45:GLN:HG2	2.15	0.45
4:C:139:THR:HG22	18:Q:109:PHE:HA	1.99	0.45
7:F:176:ASP:OD1	7:F:176:ASP:N	2.44	0.45
13:L:96:VAL:HG11	13:L:246:LEU:HB2	1.99	0.45
14:M:247:ILE:HG23	14:M:343:PRO:HB3	1.97	0.45
15:N:449:ILE:O	15:N:453:LEU:HG	2.17	0.45
30:c:169:TYR:CD1	30:c:175:ILE:HD11	2.52	0.45
13:L:627:VAL:HG21	15:N:262:ASP:HB3	1.99	0.45
20:S:3:LYS:HB3	20:S:86:GLN:HG2	1.99	0.45
13:L:173:PHE:HD1	14:M:421:LEU:HD22	1.82	0.45
13:L:254:ILE:HB	13:L:329:LEU:HD11	1.97	0.45
13:L:629:LEU:HA	13:L:632:TYR:HD2	1.81	0.45
15:N:403:SER:O	15:N:412:GLY:HA3	2.16	0.45
6:E:58:ILE:HG21	6:E:73:PRO:HB2	1.98	0.45
7:F:280:LEU:HD22	7:F:316:CYS:HB3	1.99	0.45
9:H:39:THR:HB	9:H:306:VAL:HG11	1.98	0.45
10:I:162:CYS:SG	10:I:164:TYR:N	2.77	0.45
14:M:225:THR:HG21	14:M:227:LEU:HG	1.98	0.45
29:b:9:TYR:OH	51:b:102:CDL:OA7	2.34	0.45
31:d:59:LEU:HD11	35:h:131:ILE:HD11	1.98	0.45
39:l:120:GLU:OE2	40:m:80:ARG:N	2.50	0.45
5:D:268:THR:HG22	27:Z:14:ILE:HG22	1.97	0.45
5:D:313:ARG:NH2	5:D:355:GLU:OE2	2.40	0.45
5:D:350:LEU:HB3	30:c:175:ILE:HD13	1.99	0.45
7:F:210:LYS:HA	7:F:210:LYS:HD3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:140:TRP:CZ2	13:L:223:LYS:HG3	2.52	0.45
13:L:291:ILE:HD11	13:L:552:ILE:HG12	1.99	0.45
13:L:406:PHE:CZ	39:l:113:TYR:HB2	2.52	0.45
14:M:106:ASN:HA	14:M:109:ASN:HD21	1.82	0.45
50:f:101:3PE:H232	50:f:101:3PE:H261	1.78	0.45
4:C:215:PRO:HA	4:C:220:PHE:CD1	2.52	0.44
5:D:83:ASN:OD1	15:N:151:ASN:ND2	2.50	0.44
6:E:72:MET:HB2	6:E:73:PRO:HD3	1.99	0.44
8:G:274:LEU:HD21	18:Q:134:ARG:HB2	1.98	0.44
9:H:41:GLY:HA2	9:H:46:ARG:HG3	1.99	0.44
14:M:449:VAL:HG13	14:M:453:GLU:HB2	1.99	0.44
17:P:251:GLU:OE1	17:P:253:TYR:OH	2.27	0.44
28:a:99:ILE:HD13	32:e:86:LEU:HD13	1.99	0.44
4:C:261:VAL:HG11	5:D:411:PRO:HG3	1.99	0.44
6:E:173:VAL:HA	7:F:263:SER:HB3	1.98	0.44
9:H:272:LEU:HB3	9:H:282:TYR:HE1	1.81	0.44
9:H:286:GLU:OE2	28:a:58:LYS:NZ	2.40	0.44
50:b:106:3PE:H2A1	50:b:106:3PE:H361	1.98	0.44
44:q:38:ASP:OD1	44:q:42:ASN:N	2.49	0.44
4:C:191:LEU:HA	4:C:215:PRO:HD2	1.98	0.44
8:G:303:LEU:HB2	8:G:577:ILE:HB	1.99	0.44
8:G:338:ALA:HB1	8:G:352:LEU:HD21	1.99	0.44
15:N:116:LEU:HD11	15:N:239:MET:HB3	1.99	0.44
9:H:41:GLY:O	9:H:46:ARG:N	2.50	0.44
14:M:50:SER:OG	14:M:122:ASN:OD1	2.35	0.44
14:M:225:THR:O	14:M:313:LEU:HD13	2.18	0.44
14:M:262:ILE:HD11	14:M:332:LEU:HD21	2.00	0.44
50:f:101:3PE:H221	50:f:101:3PE:H2	1.67	0.44
9:H:353:ILE:HD13	27:Z:56:LYS:HA	2.00	0.44
14:M:162:ASN:HB2	14:M:240:GLU:CD	2.42	0.44
11:J:102:ASP:OD1	28:a:140:LYS:NZ	2.49	0.44
13:L:74:TRP:CD2	50:L:710:3PE:H2D1	2.53	0.44
13:L:533:PHE:CE1	45:L:702:PLC:H31	2.53	0.44
50:L:706:3PE:H392	15:N:273:ILE:HD13	2.00	0.44
50:L:706:3PE:H3H2	50:Y:302:3PE:H2F2	1.99	0.44
25:X:125:LYS:NZ	25:X:171:GLU:OE1	2.33	0.44
50:Y:302:3PE:H342	50:Y:302:3PE:H32	1.99	0.44
34:g:177:LEU:HD22	34:g:187:LEU:HD21	2.00	0.44
45:q:401:PLC:H2'1	45:q:401:PLC:H5'1	1.82	0.44
9:H:227:THR:HG23	9:H:228:GLU:HG2	1.99	0.44
10:I:163:ILE:HG12	46:I:301:SF4:S3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:66:ILE:HD11	12:K:16:ILE:HG12	2.00	0.44
13:L:491:PRO:O	39:l:128:TYR:OH	2.24	0.44
25:X:127:GLU:OE2	25:X:142:LYS:NZ	2.41	0.44
4:C:65:ASN:HB3	4:C:68:GLU:HG2	1.99	0.44
4:C:146:VAL:HB	4:C:163:THR:HG23	2.00	0.44
5:D:54:VAL:HG13	15:N:343:LEU:HB3	1.99	0.44
13:L:4:LEU:O	13:L:8:THR:OG1	2.25	0.44
13:L:243:VAL:O	13:L:247:LEU:HB2	2.18	0.44
13:L:481:GLY:HA3	42:o:32:LEU:HD11	1.98	0.44
15:N:235:TYR:CZ	15:N:239:MET:HG3	2.53	0.44
7:F:28:ASN:ND2	7:F:34:GLY:O	2.50	0.44
8:G:611:ARG:HH22	17:P:16:ASP:CG	2.26	0.44
9:H:81:ILE:HD13	50:f:101:3PE:H3B1	2.00	0.44
13:L:641:ILE:HD11	50:L:706:3PE:H272	1.98	0.44
16:O:102:LYS:NZ	16:O:164:GLU:OE1	2.37	0.44
4:C:86:GLY:HA3	30:c:139:LEU:HD21	1.99	0.43
8:G:398:ASP:OD2	8:G:468:SER:OG	2.35	0.43
50:L:707:3PE:H2I1	15:N:276:PHE:HB2	2.00	0.43
17:P:173:GLU:OE2	17:P:188:ARG:NE	2.40	0.43
29:b:16:TRP:CH2	45:b:101:PLC:H1A1	2.53	0.43
35:h:107:LYS:HE3	35:h:111:ASP:OD2	2.18	0.43
6:E:30:ILE:HG13	6:E:116:ARG:HH12	1.83	0.43
6:E:189:THR:OG1	6:E:191:GLU:OE1	2.35	0.43
25:X:167:HIS:O	25:X:171:GLU:HG2	2.18	0.43
4:C:132:VAL:HB	4:C:184:PHE:HB3	2.00	0.43
9:H:83:VAL:HG23	9:H:84:MET:SD	2.59	0.43
45:L:702:PLC:H4'1	45:L:702:PLC:H7'1	1.62	0.43
15:N:216:PRO:HD3	15:N:270:LEU:HD22	2.00	0.43
3:B:79:CYS:SG	3:B:141:GLY:HA3	2.59	0.43
5:D:97:ARG:NH2	24:W:86:VAL:HG12	2.34	0.43
5:D:126:LEU:HD13	12:K:80:GLU:HG3	1.98	0.43
5:D:167:GLU:HB2	5:D:246:VAL:HB	1.99	0.43
11:J:81:SER:H	26:Y:63:LYS:HB3	1.83	0.43
13:L:396:ILE:O	13:L:399:SER:OG	2.32	0.43
13:L:504:PRO:HD2	13:L:507:LEU:HD12	1.99	0.43
28:a:38:GLY:O	28:a:44:LYS:NZ	2.37	0.43
8:G:658:GLU:HG2	8:G:662:LYS:HE3	2.00	0.43
14:M:440:SER:O	41:n:102:ARG:NH2	2.52	0.43
20:S:45:LEU:HD12	20:S:46:PRO:HD2	1.99	0.43
29:b:48:ARG:NH1	50:b:105:3PE:O22	2.42	0.43
39:l:25:LYS:N	41:n:76:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:213:SER:HB3	8:G:216:SER:HB3	1.99	0.43
8:G:214:GLU:CD	8:G:214:GLU:H	2.26	0.43
14:M:221:ILE:HG23	14:M:257:ALA:HB1	2.01	0.43
16:O:177:VAL:HB	16:O:180:LEU:HD12	2.00	0.43
2:A:115:ILE:HG12	45:b:101:PLC:H4'2	1.99	0.43
5:D:116:LEU:HD22	5:D:470:ILE:HD11	2.00	0.43
7:F:46:TRP:CD2	7:F:165:LEU:HD13	2.54	0.43
9:H:153:LEU:HA	9:H:156:TYR:CE2	2.54	0.43
15:N:291:LEU:HD11	15:N:445:TYR:CD1	2.54	0.43
6:E:168:CYS:SG	7:F:106:PRO:HA	2.58	0.43
13:L:641:ILE:HG12	50:L:706:3PE:H231	2.00	0.43
50:L:706:3PE:H3C1	50:L:706:3PE:H371	2.01	0.43
17:P:204:LEU:HD13	17:P:347:HIS:CD2	2.53	0.43
29:b:31:ILE:HD13	51:b:102:CDL:H552	2.00	0.43
34:g:164:SER:OG	34:g:166:ASP:OD1	2.33	0.43
2:A:117:GLU:HG2	11:J:155:ILE:HD11	2.00	0.43
5:D:273:ARG:HH21	5:D:276:GLU:CD	2.27	0.43
7:F:27:GLN:HB2	7:F:43:ARG:HD3	2.01	0.43
7:F:86:MET:SD	7:F:225:THR:OG1	2.77	0.43
8:G:592:ASN:ND2	8:G:594:GLU:HG2	2.32	0.43
11:J:150:SER:O	11:J:154:LEU:HG	2.18	0.43
13:L:241:THR:HG21	13:L:344:GLY:HA3	2.00	0.43
27:Z:132:ALA:HB2	32:e:85:PHE:CD1	2.53	0.43
35:h:107:LYS:HZ3	43:p:8:PRO:HG3	1.82	0.43
1:1:156:PHE:HA	1:1:159:ILE:HD12	2.01	0.43
7:F:310:ILE:HG12	7:F:311:MET:N	2.33	0.43
8:G:231:LYS:HB3	8:G:232:PRO:HD3	2.01	0.43
8:G:663:VAL:HG21	20:S:32:THR:HA	2.00	0.43
13:L:371:TYR:OH	38:k:27:ALA:O	2.31	0.43
14:M:85:ASP:OD1	14:M:263:ARG:NH2	2.52	0.43
29:b:47:ARG:HG3	29:b:51:LEU:HD12	2.00	0.43
50:g:301:3PE:H272	50:g:301:3PE:H241	1.69	0.43
35:h:70:THR:O	35:h:74:TRP:HD1	2.01	0.43
6:E:122:TYR:HB3	6:E:180:VAL:HG13	2.01	0.42
7:F:113:GLU:OE1	7:F:116:ARG:NH2	2.42	0.42
17:P:194:PHE:HB2	17:P:224:ALA:HB3	2.00	0.42
23:V:34:PRO:HB3	23:V:92:VAL:HG11	2.00	0.42
2:A:29:GLU:HA	45:A:201:PLC:H42	2.00	0.42
7:F:71:GLY:N	7:F:77:PHE:O	2.43	0.42
9:H:230:SER:O	9:H:233:PRO:HD2	2.19	0.42
10:I:73:LEU:HD22	10:I:76:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:54:LYS:O	24:W:58:GLU:HG2	2.19	0.42
44:q:24:GLN:C	45:q:401:PLC:H63	2.44	0.42
4:C:154:ARG:HH22	23:V:94:GLU:CD	2.27	0.42
15:N:249:TYR:HD2	15:N:307:ILE:HG12	1.83	0.42
2:A:76:LEU:HB2	2:A:77:PRO:HD3	2.01	0.42
7:F:98:VAL:HG11	7:F:196:LEU:HD22	2.00	0.42
7:F:198:GLU:HB2	7:F:205:GLY:HA2	2.01	0.42
8:G:248:ILE:HG12	8:G:600:THR:HG22	2.00	0.42
12:K:15:ILE:HD11	21:T:137:ILE:HG23	2.02	0.42
25:X:98:LEU:HD23	25:X:138:MET:HE1	2.00	0.42
34:g:211:ASP:OD1	34:g:211:ASP:N	2.52	0.42
35:h:89:ARG:HB3	35:h:94:GLY:HA2	2.01	0.42
2:A:35:GLU:O	17:P:53:ARG:NH2	2.52	0.42
5:D:139:THR:HG21	5:D:158:LEU:HD21	2.01	0.42
8:G:301:LYS:HD2	17:P:25:THR:HG21	2.01	0.42
8:G:710:LYS:HB2	8:G:712:GLU:HG3	2.01	0.42
13:L:538:ASN:HB3	13:L:541:LEU:HB2	2.01	0.42
14:M:305:ILE:HD12	14:M:345:LEU:HB3	2.01	0.42
15:N:272:LEU:HD12	15:N:434:VAL:HG11	2.01	0.42
5:D:158:LEU:O	5:D:479:GLU:N	2.53	0.42
7:F:33:TYR:HB2	7:F:43:ARG:HH21	1.84	0.42
8:G:221:ASP:CG	8:G:288:ARG:HH22	2.27	0.42
8:G:644:ALA:HB3	8:G:647:LEU:HG	2.02	0.42
9:H:130:THR:HA	9:H:237:PHE:HZ	1.84	0.42
9:H:150:THR:HG23	11:J:60:VAL:HG12	2.02	0.42
13:L:80:LYS:NZ	13:L:483:PRO:O	2.39	0.42
14:M:104:LEU:HB3	14:M:456:LEU:HD21	2.01	0.42
16:O:168:ASN:O	16:O:168:ASN:ND2	2.52	0.42
44:q:47:VAL:HG12	44:q:49:ASP:H	1.85	0.42
3:B:87:SER:HA	3:B:93:GLN:HG2	2.01	0.42
5:D:235:ARG:HG2	5:D:256:PRO:HG3	2.02	0.42
7:F:407:THR:HB	46:F:501:SF4:S1	2.59	0.42
8:G:300:THR:HB	8:G:608:GLY:HA3	2.01	0.42
9:H:333:PHE:O	9:H:336:VAL:HG12	2.19	0.42
14:M:22:ASN:HD22	14:M:25:ASN:ND2	2.14	0.42
14:M:149:ALA:HB3	14:M:150:PRO:HD3	2.02	0.42
15:N:291:LEU:HD23	15:N:449:ILE:HD11	2.02	0.42
15:N:387:PHE:CD1	15:N:454:SER:HB3	2.55	0.42
6:E:152:PRO:HB3	6:E:165:GLU:HG3	2.02	0.42
13:L:398:GLU:HB3	13:L:503:LEU:HD11	2.01	0.42
14:M:46:GLY:HA3	14:M:118:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:357:TYR:HB3	40:m:9:LEU:HB2	2.01	0.42
15:N:312:ASN:ND2	35:h:133:PHE:O	2.52	0.42
2:A:140:LEU:HD12	23:V:13:ILE:HD12	2.02	0.42
6:E:33:HIS:HB2	8:G:206:TYR:CZ	2.55	0.42
7:F:299:LEU:HB2	7:F:343:LYS:HA	2.01	0.42
7:F:361:GLU:HA	8:G:197:ARG:NH1	2.35	0.42
10:I:146:ILE:HG21	19:R:22:ILE:HA	2.01	0.42
7:F:381:ASP:O	7:F:384:VAL:HG12	2.19	0.42
8:G:183:LEU:HA	8:G:187:ALA:HB3	2.01	0.42
8:G:373:VAL:HG11	8:G:531:PRO:HA	2.01	0.42
9:H:128:PHE:O	9:H:132:ILE:HG12	2.20	0.42
50:L:709:3PE:H3D1	14:M:415:LEU:HD23	2.02	0.42
34:g:43:LYS:H	34:g:43:LYS:HD2	1.84	0.42
3:B:78:CYS:HB3	5:D:160:TYR:CB	2.49	0.41
3:B:140:MET:HE2	3:B:180:LEU:HD13	2.01	0.41
7:F:44:GLY:O	7:F:240:ARG:NH1	2.53	0.41
8:G:125:VAL:HG12	10:I:124:ILE:HG13	2.02	0.41
9:H:342:ILE:HD12	50:b:104:3PE:H2A1	2.00	0.41
14:M:102:ALA:O	14:M:105:SER:OG	2.38	0.41
14:M:169:TYR:O	14:M:173:TYR:HB2	2.20	0.41
15:N:65:SER:OG	15:N:518:LEU:O	2.38	0.41
45:d:101:PLC:H72	45:d:101:PLC:H41	1.81	0.41
50:g:301:3PE:H2A2	50:g:301:3PE:H271	1.76	0.41
39:l:147:LEU:O	40:m:68:ARG:NH2	2.53	0.41
41:n:19:TYR:O	41:n:22:SER:OG	2.35	0.41
44:q:14:ASN:HB3	44:q:18:LYS:HB3	2.02	0.41
3:B:62:ASN:HB3	3:B:192:MET:HA	2.02	0.41
7:F:110:LYS:HE3	7:F:110:LYS:HB2	1.78	0.41
15:N:6:LEU:HD13	15:N:110:LEU:HB2	2.02	0.41
22:U:64:TYR:HB3	22:U:67:VAL:HG23	2.01	0.41
50:Y:302:3PE:H242	50:Y:302:3PE:H271	1.91	0.41
13:L:74:TRP:CE3	50:L:710:3PE:H2D1	2.55	0.41
13:L:214:ILE:HD13	13:L:214:ILE:HA	1.94	0.41
13:L:401:TYR:CZ	39:l:119:PRO:HG3	2.55	0.41
14:M:221:ILE:O	14:M:225:THR:HG22	2.20	0.41
17:P:354:THR:OG1	17:P:355:GLN:NE2	2.53	0.41
22:U:96:GLU:HG3	38:k:6:TRP:CH2	2.55	0.41
32:e:28:THR:OG1	35:h:174:ARG:NH1	2.52	0.41
42:o:15:MET:HG2	42:o:20:ILE:HD12	2.03	0.41
2:A:132:LYS:HE2	2:A:132:LYS:HB2	1.85	0.41
7:F:235:THR:OG1	7:F:236:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:332:LYS:HA	8:G:332:LYS:HD3	1.83	0.41
9:H:345:CYS:O	29:b:47:ARG:HD3	2.21	0.41
14:M:31:LYS:HB3	34:g:95:VAL:HG11	2.00	0.41
17:P:120:PHE:HB3	17:P:126:ILE:HG13	2.02	0.41
23:V:63:VAL:HA	23:V:66:PHE:CE1	2.55	0.41
39:l:57:LYS:HD3	39:l:57:LYS:HA	1.86	0.41
7:F:297:ASN:O	7:F:343:LYS:N	2.49	0.41
14:M:409:HIS:ND1	14:M:412:ILE:HG22	2.36	0.41
15:N:384:LYS:HG2	15:N:452:VAL:HG13	2.02	0.41
17:P:153:SER:O	17:P:189:PRO:HD2	2.21	0.41
27:Z:17:LYS:HD3	30:c:167:GLY:HA3	2.01	0.41
2:A:106:PHE:CD1	11:J:144:SER:HB3	2.56	0.41
45:B:302:PLC:H5A2	45:q:401:PLC:H5'2	2.01	0.41
7:F:149:GLU:OE1	7:F:149:GLU:N	2.47	0.41
10:I:207:TRP:CE3	44:q:75:PRO:HB3	2.55	0.41
12:K:16:ILE:HD12	12:K:16:ILE:HA	1.92	0.41
15:N:36:TYR:HE2	16:O:68:GLY:HA2	1.85	0.41
30:c:159:ARG:NH2	30:c:165:GLU:OE2	2.43	0.41
42:o:73:GLU:O	42:o:77:GLN:HG2	2.21	0.41
44:q:88:PRO:HB2	44:q:90:ASN:OD1	2.20	0.41
3:B:59:LYS:NZ	3:B:192:MET:O	2.41	0.41
7:F:265:HIS:HD2	7:F:341:LEU:HA	1.85	0.41
8:G:589:THR:OG1	8:G:637:ARG:NH1	2.49	0.41
10:I:218:ASP:OD2	10:I:222:ARG:NH2	2.53	0.41
11:J:73:LYS:HG3	26:Y:68:ARG:HH22	1.85	0.41
13:L:177:LEU:O	13:L:215:CYS:HB3	2.21	0.41
50:L:707:3PE:H2I2	15:N:434:VAL:HG13	2.02	0.41
14:M:291:SER:O	14:M:295:THR:OG1	2.37	0.41
14:M:444:HIS:CE1	40:m:10:ARG:HH21	2.38	0.41
45:M:1002:PLC:H2	45:M:1002:PLC:H1'1	1.87	0.41
17:P:122:LYS:NZ	45:P:502:PLC:O2P	2.53	0.41
50:f:101:3PE:H2E1	50:f:101:3PE:H2H2	1.88	0.41
3:B:95:ARG:HA	9:H:49:PRO:HA	2.02	0.41
4:C:236:ARG:NH2	24:W:100:GLU:HG3	2.36	0.41
13:L:200:LEU:O	13:L:204:LEU:HG	2.20	0.41
16:O:8:ASP:OD1	16:O:150:HIS:ND1	2.48	0.41
17:P:91:VAL:HG13	19:R:62:VAL:HG11	2.02	0.41
38:k:4:ASN:O	38:k:7:LYS:HG3	2.20	0.41
4:C:108:PRO:HG3	4:C:164:TYR:O	2.21	0.41
5:D:184:GLU:HG2	5:D:371:PRO:HG3	2.02	0.41
5:D:264:TYR:CE1	27:Z:11:TYR:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:176:PRO:HB2	6:E:188:LEU:H	1.86	0.41
7:F:331:SER:OG	7:F:332:GLY:N	2.54	0.41
8:G:389:SER:O	8:G:390:THR:OG1	2.29	0.41
11:J:124:ASP:N	11:J:124:ASP:OD1	2.53	0.41
13:L:93:SER:O	13:L:97:HIS:ND1	2.38	0.41
50:L:711:3PE:H31	50:L:711:3PE:H111	2.02	0.41
16:O:58:PRO:HB3	50:b:106:3PE:H11	2.02	0.41
51:O:201:CDL:H131	51:O:201:CDL:H161	1.77	0.41
51:O:201:CDL:H762	51:O:201:CDL:H792	1.73	0.41
17:P:262:ILE:O	17:P:266:ILE:HG12	2.21	0.41
17:P:363:GLU:OE1	17:P:363:GLU:N	2.54	0.41
25:X:82:LYS:HE3	25:X:86:ARG:NH1	2.35	0.41
27:Z:3:GLN:NE2	30:c:57:PRO:HG3	2.36	0.41
27:Z:127:SER:HA	27:Z:133:ASN:H	1.86	0.41
36:i:72:LYS:HB2	43:p:65:GLU:HG2	2.03	0.41
40:m:55:TYR:HA	40:m:58:GLU:HB2	2.03	0.41
3:B:94:ASP:OD2	9:H:46:ARG:NH2	2.53	0.41
7:F:368:PRO:O	7:F:372:GLY:N	2.34	0.41
8:G:474:ILE:O	8:G:511:LEU:HD12	2.20	0.41
9:H:1:FME:O	9:H:3:ASN:N	2.54	0.41
14:M:155:ILE:HD12	14:M:170:VAL:HG11	2.02	0.41
16:O:7:ILE:HB	16:O:84:PHE:HA	2.03	0.41
6:E:134:LEU:HD22	7:F:265:HIS:HE2	1.86	0.40
7:F:300:GLY:HA3	7:F:310:ILE:HD11	2.02	0.40
8:G:621:SER:HB2	8:G:626:ALA:O	2.21	0.40
10:I:145:ARG:NH1	10:I:151:ARG:HG3	2.36	0.40
13:L:87:VAL:HB	13:L:88:PRO:HD3	2.02	0.40
15:N:89:ILE:HD12	15:N:337:LEU:HB3	2.03	0.40
15:N:295:SER:O	15:N:299:ASN:ND2	2.41	0.40
34:g:26:PHE:CZ	34:g:90:ASN:HB3	2.56	0.40
34:g:136:GLU:HB2	34:g:138:TRP:CD1	2.56	0.40
7:F:25:ILE:O	7:F:121:LYS:NZ	2.55	0.40
8:G:29:LEU:HD22	8:G:91:VAL:HG21	2.03	0.40
10:I:68:THR:HG21	27:Z:27:PRO:O	2.21	0.40
13:L:422:THR:HA	13:L:425:TYR:CZ	2.56	0.40
13:L:577:ILE:HA	13:L:581:ILE:HG22	2.02	0.40
14:M:201:ASN:CG	14:M:267:PRO:HB2	2.46	0.40
15:N:345:ILE:O	15:N:347:ASN:ND2	2.53	0.40
17:P:120:PHE:HB2	17:P:125:SER:HA	2.02	0.40
23:V:15:ILE:HG22	23:V:16:LYS:HG3	2.04	0.40
5:D:76:TRP:CG	13:L:602:ASN:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:65:GLN:HG2	6:E:66:TYR:CD2	2.56	0.40
7:F:97:LEU:HD13	7:F:133:MET:SD	2.62	0.40
9:H:28:VAL:HA	28:a:13:MET:HG2	2.03	0.40
11:J:109:TYR:CE1	28:a:104:ASN:HB3	2.56	0.40
13:L:172:ARG:NH2	14:M:420:VAL:O	2.44	0.40
13:L:234:LEU:HD23	13:L:300:LYS:HD2	2.04	0.40
13:L:257:VAL:HG13	13:L:317:ILE:HD11	2.03	0.40
13:L:347:ILE:HD13	13:L:355:GLN:HG2	2.02	0.40
13:L:422:THR:HA	13:L:425:TYR:CE2	2.56	0.40
16:O:45:ILE:HA	45:d:101:PLC:H31	2.02	0.40
23:V:49:LEU:HG	23:V:106:ILE:HD13	2.03	0.40
41:n:88:CYS:SG	41:n:94:LYS:HE3	2.61	0.40
2:A:36:ASN:HB3	17:P:53:ARG:NH2	2.35	0.40
6:E:178:ILE:HG22	6:E:185:TYR:HB2	2.03	0.40
7:F:280:LEU:HD11	7:F:301:VAL:HG11	2.03	0.40
11:J:25:ILE:HD11	11:J:59:VAL:HG13	2.04	0.40
14:M:272:ILE:HD12	14:M:272:ILE:HA	1.94	0.40
14:M:323:ASN:ND2	14:M:487:TYR:O	2.41	0.40
32:e:62:GLN:O	32:e:66:GLU:HG3	2.22	0.40
1:1:134:LYS:HD3	1:1:168:TRP:CD1	2.57	0.40
4:C:156:ASN:OD1	5:D:324:SER:HB2	2.20	0.40
8:G:216:SER:O	8:G:219:VAL:HB	2.22	0.40
9:H:222:VAL:HG23	9:H:223:SER:H	1.85	0.40
9:H:287:GLY:N	28:a:25:ASN:HD22	2.20	0.40
50:L:707:3PE:H362	50:L:707:3PE:H391	1.86	0.40
20:S:27:LEU:HD13	20:S:81:ILE:HD13	2.04	0.40
22:U:78:SER:HA	22:U:115:THR:HA	2.04	0.40
50:f:101:3PE:H3I3	50:f:101:3PE:H3F2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	167/190 (88%)	158 (95%)	9 (5%)	0	100	100
2	A	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
3	B	173/204 (85%)	168 (97%)	5 (3%)	0	100	100
4	C	238/289 (82%)	234 (98%)	4 (2%)	0	100	100
5	D	448/482 (93%)	438 (98%)	10 (2%)	0	100	100
6	E	181/241 (75%)	175 (97%)	6 (3%)	0	100	100
7	F	451/473 (95%)	428 (95%)	23 (5%)	0	100	100
8	G	694/726 (96%)	679 (98%)	15 (2%)	0	100	100
9	H	351/353 (99%)	343 (98%)	6 (2%)	2 (1%)	21	51
10	I	190/222 (86%)	187 (98%)	3 (2%)	0	100	100
11	J	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
12	K	78/82 (95%)	76 (97%)	2 (3%)	0	100	100
13	L	640/642 (100%)	628 (98%)	11 (2%)	1 (0%)	43	72
14	M	489/491 (100%)	472 (96%)	17 (4%)	0	100	100
15	N	502/523 (96%)	491 (98%)	10 (2%)	1 (0%)	43	72
16	O	191/193 (99%)	190 (100%)	1 (0%)	0	100	100
17	P	366/384 (95%)	356 (97%)	10 (3%)	0	100	100
18	Q	110/159 (69%)	110 (100%)	0	0	100	100
19	R	122/139 (88%)	121 (99%)	1 (1%)	0	100	100
20	S	88/90 (98%)	85 (97%)	3 (3%)	0	100	100
21	T	93/138 (67%)	92 (99%)	1 (1%)	0	100	100
22	U	86/130 (66%)	82 (95%)	4 (5%)	0	100	100
23	V	124/134 (92%)	121 (98%)	3 (2%)	0	100	100
24	W	111/122 (91%)	110 (99%)	1 (1%)	0	100	100
25	X	182/184 (99%)	180 (99%)	2 (1%)	0	100	100
26	Y	203/216 (94%)	195 (96%)	8 (4%)	0	100	100
27	Z	140/147 (95%)	138 (99%)	2 (1%)	0	100	100
28	a	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
29	b	76/79 (96%)	75 (99%)	1 (1%)	0	100	100
30	c	180/182 (99%)	175 (97%)	5 (3%)	0	100	100
31	d	73/78 (94%)	72 (99%)	1 (1%)	0	100	100
32	e	103/106 (97%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	f	76/86 (88%)	76 (100%)	0	0	100	100
34	g	152/239 (64%)	149 (98%)	3 (2%)	0	100	100
35	h	129/182 (71%)	126 (98%)	3 (2%)	0	100	100
36	i	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
37	j	51/59 (86%)	51 (100%)	0	0	100	100
38	k	43/61 (70%)	42 (98%)	1 (2%)	0	100	100
39	l	130/156 (83%)	127 (98%)	3 (2%)	0	100	100
40	m	75/81 (93%)	75 (100%)	0	0	100	100
41	n	103/111 (93%)	103 (100%)	0	0	100	100
42	o	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
43	p	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
44	q	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
All	All	8425/9219 (91%)	8223 (98%)	198 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	H	222	VAL
9	H	2	LEU
15	N	522	TRP
13	L	552	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	152/168 (90%)	146 (96%)	6 (4%)	28	64
2	A	128/128 (100%)	125 (98%)	3 (2%)	44	78
3	B	154/180 (86%)	151 (98%)	3 (2%)	50	81
4	C	214/254 (84%)	213 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	384/408 (94%)	378 (98%)	6 (2%)	55	83
6	E	163/218 (75%)	157 (96%)	6 (4%)	30	65
7	F	369/387 (95%)	357 (97%)	12 (3%)	33	69
8	G	582/610 (95%)	569 (98%)	13 (2%)	45	78
9	H	307/307 (100%)	297 (97%)	10 (3%)	33	69
10	I	166/192 (86%)	159 (96%)	7 (4%)	26	61
11	J	149/149 (100%)	145 (97%)	4 (3%)	39	74
12	K	70/72 (97%)	69 (99%)	1 (1%)	59	85
13	L	576/576 (100%)	565 (98%)	11 (2%)	50	81
14	M	439/439 (100%)	432 (98%)	7 (2%)	55	83
15	N	474/489 (97%)	466 (98%)	8 (2%)	53	83
16	O	169/169 (100%)	164 (97%)	5 (3%)	36	72
17	P	317/332 (96%)	314 (99%)	3 (1%)	70	89
18	Q	95/135 (70%)	94 (99%)	1 (1%)	65	87
19	R	104/118 (88%)	103 (99%)	1 (1%)	68	88
20	S	77/77 (100%)	74 (96%)	3 (4%)	28	64
21	T	87/128 (68%)	84 (97%)	3 (3%)	32	68
22	U	80/120 (67%)	76 (95%)	4 (5%)	22	54
23	V	112/119 (94%)	110 (98%)	2 (2%)	51	82
24	W	107/114 (94%)	105 (98%)	2 (2%)	50	81
25	X	165/165 (100%)	164 (99%)	1 (1%)	78	92
26	Y	163/173 (94%)	159 (98%)	4 (2%)	42	76
27	Z	123/128 (96%)	123 (100%)	0	100	100
28	a	128/129 (99%)	127 (99%)	1 (1%)	73	90
29	b	66/67 (98%)	64 (97%)	2 (3%)	36	72
30	c	159/159 (100%)	157 (99%)	2 (1%)	61	86
31	d	62/65 (95%)	61 (98%)	1 (2%)	55	83
32	e	91/92 (99%)	90 (99%)	1 (1%)	65	87
33	f	64/71 (90%)	64 (100%)	0	100	100
34	g	143/215 (66%)	140 (98%)	3 (2%)	47	79
35	h	118/167 (71%)	115 (98%)	3 (2%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	i	59/63 (94%)	58 (98%)	1 (2%)	53	83
37	j	46/50 (92%)	44 (96%)	2 (4%)	26	60
38	k	32/47 (68%)	32 (100%)	0	100	100
39	l	116/137 (85%)	114 (98%)	2 (2%)	53	83
40	m	64/66 (97%)	63 (98%)	1 (2%)	55	83
41	n	95/100 (95%)	94 (99%)	1 (1%)	65	87
42	o	74/79 (94%)	74 (100%)	0	100	100
43	p	83/85 (98%)	82 (99%)	1 (1%)	63	87
44	q	125/125 (100%)	123 (98%)	2 (2%)	55	83
All	All	7451/8072 (92%)	7301 (98%)	150 (2%)	48	80

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	28	LEU
1	1	66	LYS
1	1	67	ASP
1	1	68	LYS
1	1	69	ASP
1	1	72	GLU
2	A	27	ILE
2	A	128	ILE
2	A	140	LEU
3	B	78	CYS
3	B	108	ASP
3	B	149	TYR
4	C	257	VAL
5	D	91	VAL
5	D	103	PHE
5	D	113	VAL
5	D	269	GLN
5	D	356	PHE
5	D	482	ARG
6	E	49	LYS
6	E	129	THR
6	E	151	ARG
6	E	172	CYS
6	E	191	GLU
6	E	192	ARG

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Mol	Chain	Res	Type
7	F	29	VAL
7	F	105	GLU
7	F	268	GLU
7	F	287	HIS
7	F	308	VAL
7	F	310	ILE
7	F	342	ASN
7	F	363	CYS
7	F	369	CYS
7	F	409	CYS
7	F	422	LEU
7	F	464	ASN
8	G	25	LYS
8	G	26	GLU
8	G	36	VAL
8	G	38	ILE
8	G	70	CYS
8	G	176	CYS
8	G	219	VAL
8	G	265	ILE
8	G	528	THR
8	G	692	VAL
8	G	712	GLU
8	G	713	LYS
8	G	718	LYS
9	H	5	LEU
9	H	46	ARG
9	H	74	LEU
9	H	83	VAL
9	H	170	ILE
9	H	177	ASN
9	H	222	VAL
9	H	232	SER
9	H	237	PHE
9	H	336	VAL
10	I	100	LYS
10	I	124	ILE
10	I	126	CYS
10	I	128	LEU
10	I	145	ARG
10	I	146	ILE
10	I	184	GLU

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Mol	Chain	Res	Type
11	J	25	ILE
11	J	33	MET
11	J	73	LYS
11	J	135	GLU
12	K	77	GLU
13	L	3	LEU
13	L	60	ASN
13	L	83	VAL
13	L	158	PHE
13	L	252	LEU
13	L	270	THR
13	L	348	HIS
13	L	354	TYR
13	L	364	ARG
13	L	509	VAL
13	L	607	LEU
14	M	27	ILE
14	M	28	LEU
14	M	30	LYS
14	M	31	LYS
14	M	84	ILE
14	M	108	LYS
14	M	225	THR
15	N	18	LYS
15	N	157	LEU
15	N	217	PHE
15	N	263	LEU
15	N	387	PHE
15	N	393	ILE
15	N	435	LEU
15	N	436	ILE
16	O	27	THR
16	O	54	LYS
16	O	166	ASN
16	O	186	LYS
16	O	190	ASN
17	P	93	PHE
17	P	351	THR
17	P	355	GLN
18	Q	138	LYS
19	R	58	VAL
20	S	1	SER

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Mol	Chain	Res	Type
20	S	3	LYS
20	S	34	THR
21	T	79	VAL
21	T	112	ILE
21	T	137	ILE
22	U	65	ASP
22	U	104	LEU
22	U	126	GLN
22	U	130	ILE
23	V	11	GLN
23	V	12	GLU
24	W	91	GLN
24	W	109	LYS
25	X	183	ILE
26	Y	34	LYS
26	Y	74	TYR
26	Y	196	TYR
26	Y	211	ARG
28	a	111	LEU
29	b	3	ILE
29	b	53	ASP
30	c	1	SER
30	c	133	LYS
31	d	61	LYS
32	e	98	ASP
34	g	32	LYS
34	g	43	LYS
34	g	177	LEU
35	h	75	LEU
35	h	86	LYS
35	h	104	ILE
36	i	7	HIS
37	j	20	VAL
37	j	59	HIS
39	l	25	LYS
39	l	68	ASN
40	m	7	HIS
41	n	52	PHE
43	p	79	ILE
44	q	27	ASN
44	q	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1	65	ASN
3	B	195	GLN
4	C	179	GLN
4	C	214	HIS
5	D	289	GLN
6	E	201	GLN
7	F	95	GLN
7	F	265	HIS
7	F	297	ASN
7	F	344	GLN
8	G	159	ASN
8	G	443	ASN
8	G	513	HIS
11	J	101	ASN
11	J	121	ASN
12	K	14	ASN
13	L	309	GLN
13	L	447	ASN
14	M	25	ASN
14	M	60	ASN
14	M	131	ASN
14	M	329	ASN
14	M	363	ASN
14	M	366	GLN
14	M	432	ASN
14	M	479	ASN
15	N	390	ASN
15	N	466	ASN
15	N	521	ASN
16	O	168	ASN
17	P	243	GLN
17	P	321	GLN
17	P	353	GLN
17	P	373	ASN
18	Q	70	HIS
18	Q	129	GLN
24	W	9	GLN
24	W	41	ASN
27	Z	77	ASN
28	a	25	ASN
28	a	84	GLN
30	c	75	HIS

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Mol	Chain	Res	Type
32	e	10	HIS
33	f	34	GLN
39	l	63	ASN
39	l	85	HIS
42	o	18	ASN
42	o	58	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	M	1	14	8,9,10	1.52	1 (12%)	8,9,11	1.40	1 (12%)
2	FME	A	1	2	8,9,10	1.52	1 (12%)	8,9,11	1.42	1 (12%)
12	FME	K	1	12	8,9,10	1.51	1 (12%)	8,9,11	1.41	1 (12%)
15	FME	N	1	15	8,9,10	1.52	1 (12%)	8,9,11	1.28	0
13	FME	L	1	13	8,9,10	1.51	1 (12%)	8,9,11	1.47	2 (25%)
9	FME	H	1	9	8,9,10	1.52	1 (12%)	8,9,11	1.47	2 (25%)
5	2MR	D	137	5	10,12,13	2.51	2 (20%)	5,13,15	1.63	1 (20%)
11	FME	J	1	11	8,9,10	1.51	1 (12%)	8,9,11	1.44	2 (25%)

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
14	FME	M	1	14	-	4/7/9/11	-
2	FME	A	1	2	-	4/7/9/11	-
12	FME	K	1	12	-	4/7/9/11	-
15	FME	N	1	15	-	0/7/9/11	-
13	FME	L	1	13	-	3/7/9/11	-
9	FME	H	1	9	-	2/7/9/11	-
5	2MR	D	137	5	-	1/10/13/15	-
11	FME	J	1	11	-	4/7/9/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	137	2MR	CZ-NH2	5.71	1.45	1.33
5	D	137	2MR	CZ-NE	5.10	1.45	1.34
9	H	1	FME	CN-N	3.76	1.45	1.33
2	A	1	FME	CN-N	3.75	1.45	1.33
15	N	1	FME	CN-N	3.75	1.45	1.33
14	M	1	FME	CN-N	3.75	1.45	1.33
11	J	1	FME	CN-N	3.74	1.45	1.33
12	K	1	FME	CN-N	3.74	1.45	1.33
13	L	1	FME	CN-N	3.73	1.45	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	137	2MR	CD-NE-CZ	-2.63	118.43	123.36
13	L	1	FME	O1-CN-N	-2.22	119.58	125.32
13	L	1	FME	CA-N-CN	-2.19	119.45	122.82
12	K	1	FME	O1-CN-N	-2.15	119.76	125.32
9	H	1	FME	CA-N-CN	-2.15	119.52	122.82
9	H	1	FME	O1-CN-N	-2.14	119.80	125.32
11	J	1	FME	O1-CN-N	-2.13	119.83	125.32
14	M	1	FME	O1-CN-N	-2.10	119.90	125.32
2	A	1	FME	O1-CN-N	-2.06	119.99	125.32
11	J	1	FME	CA-N-CN	-2.02	119.71	122.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
2	A	1	FME	C-CA-CB-CG
5	D	137	2MR	O-C-CA-CB
11	J	1	FME	O-C-CA-CB
12	K	1	FME	C-CA-CB-CG
14	M	1	FME	N-CA-CB-CG
14	M	1	FME	CA-CB-CG-SD
2	A	1	FME	N-CA-CB-CG
12	K	1	FME	N-CA-CB-CG
9	H	1	FME	C-CA-CB-CG
11	J	1	FME	N-CA-CB-CG
11	J	1	FME	CB-CG-SD-CE
14	M	1	FME	CB-CG-SD-CE
13	L	1	FME	N-CA-CB-CG
12	K	1	FME	CB-CG-SD-CE
14	M	1	FME	C-CA-CB-CG
9	H	1	FME	CB-CG-SD-CE
13	L	1	FME	CA-CB-CG-SD
2	A	1	FME	CB-CG-SD-CE
11	J	1	FME	CB-CA-N-CN
12	K	1	FME	CB-CA-N-CN
13	L	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	FME	1	0
9	H	1	FME	1	0
11	J	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 2 are monoatomic - leaving 59 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
45	PLC	Z	201	-	41,41,41	0.51	0	47,49,49	0.50	0
54	EHZ	U	201	22	31,36,37	1.58	5 (16%)	36,44,47	1.57	7 (19%)
45	PLC	M	1002	-	38,38,41	0.53	0	44,46,49	0.51	0
45	PLC	A	201	-	30,30,41	0.59	0	36,38,49	0.56	0
46	SF4	F	501	7	0,12,12	-	-	-	-	-
45	PLC	b	101	-	38,38,41	0.53	0	44,46,49	0.55	0
46	SF4	G	801	8	0,12,12	-	-	-	-	-
46	SF4	I	302	10	0,12,12	-	-	-	-	-
50	3PE	Y	303	-	25,25,50	1.21	4 (16%)	28,30,55	1.38	3 (10%)
50	3PE	L	711	-	32,32,50	1.08	4 (12%)	35,37,55	1.16	2 (5%)
47	FES	G	803	8	0,4,4	-	-	-	-	-
48	FMN	F	502	-	33,33,33	2.81	10 (30%)	48,50,50	1.89	14 (29%)
51	CDL	a	201	-	59,59,99	1.12	8 (13%)	65,71,111	1.16	4 (6%)
45	PLC	M	1003	-	41,41,41	0.51	0	47,49,49	0.53	0
45	PLC	Y	304	-	35,35,41	0.54	0	41,43,49	0.58	0
45	PLC	a	202	-	21,21,41	0.69	0	27,29,49	0.67	0
50	3PE	L	706	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
45	PLC	P	502	-	30,30,41	0.58	0	36,38,49	0.59	0
46	SF4	G	802	8	0,12,12	-	-	-	-	-
50	3PE	N	602	-	39,39,50	0.98	4 (10%)	42,44,55	1.13	2 (4%)
50	3PE	f	101	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
50	3PE	m	101	-	24,24,50	1.23	4 (16%)	27,29,55	1.29	2 (7%)
50	3PE	L	709	-	45,45,50	0.91	4 (8%)	48,50,55	1.10	2 (4%)
45	PLC	B	302	-	30,30,41	0.58	0	36,38,49	0.59	0
45	PLC	L	705	-	41,41,41	0.50	0	47,49,49	0.64	1 (2%)
50	3PE	b	106	-	34,34,50	1.04	4 (11%)	37,39,55	1.13	2 (5%)
51	CDL	b	102	-	58,58,99	1.13	8 (13%)	64,70,111	1.20	4 (6%)
47	FES	E	301	6	0,4,4	-	-	-	-	-
45	PLC	d	101	-	41,41,41	0.51	0	47,49,49	0.52	0
50	3PE	L	708	-	34,34,50	1.05	4 (11%)	37,39,55	1.17	2 (5%)
50	3PE	L	703	-	41,41,50	0.96	4 (9%)	44,46,55	1.14	2 (4%)
45	PLC	q	402	-	41,41,41	0.51	0	47,49,49	0.50	0
50	3PE	L	701	-	28,28,50	1.15	4 (14%)	31,33,55	1.14	2 (6%)
45	PLC	h	201	-	41,41,41	0.52	0	47,49,49	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	3PE	M	1004	-	34,34,50	1.04	4 (11%)	37,39,55	1.16	2 (5%)
45	PLC	D	501	-	41,41,41	0.50	0	47,49,49	0.56	0
51	CDL	P	503	-	41,41,99	1.30	7 (17%)	47,53,111	1.35	3 (6%)
52	NDP	P	501	-	51,52,52	4.05	28 (54%)	71,80,80	1.95	14 (19%)
45	PLC	L	702	-	34,34,41	0.56	0	40,42,49	0.55	0
45	PLC	H	401	-	23,23,41	0.68	0	29,31,49	0.69	1 (3%)
50	3PE	H	402	-	30,30,50	1.11	4 (13%)	33,35,55	1.17	2 (6%)
50	3PE	j	101	-	26,26,50	1.18	4 (15%)	29,31,55	1.22	2 (6%)
46	SF4	I	301	10	0,12,12	-	-	-	-	-
51	CDL	O	201	-	74,74,99	1.01	8 (10%)	80,86,111	1.14	4 (5%)
51	CDL	Z	202	-	48,48,99	1.24	8 (16%)	54,60,111	1.30	4 (7%)
45	PLC	N	601	-	41,41,41	0.52	0	47,49,49	0.53	1 (2%)
50	3PE	Y	302	-	50,50,50	0.87	4 (8%)	53,55,55	1.12	2 (3%)
46	SF4	B	301	3	0,12,12	-	-	-	-	-
50	3PE	L	707	-	50,50,50	0.88	4 (8%)	53,55,55	1.10	2 (3%)
54	EHZ	T	201	21	31,36,37	1.58	5 (16%)	36,44,47	1.53	5 (13%)
45	PLC	Y	301	-	35,35,41	0.55	0	41,43,49	0.56	0
50	3PE	g	301	-	45,45,50	0.92	4 (8%)	48,50,55	1.09	2 (4%)
45	PLC	M	1001	-	41,41,41	0.51	0	47,49,49	0.51	0
50	3PE	b	103	-	39,39,50	0.98	4 (10%)	42,44,55	1.14	2 (4%)
50	3PE	b	104	-	35,35,50	1.03	4 (11%)	38,40,55	1.14	2 (5%)
50	3PE	b	105	-	30,30,50	1.11	4 (13%)	33,35,55	1.18	2 (6%)
50	3PE	L	710	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
45	PLC	q	401	-	35,35,41	0.56	0	41,43,49	0.58	0
45	PLC	L	704	-	31,31,41	0.57	0	37,39,49	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PLC	Z	201	-	-	16/45/45/45	-
54	EHZ	U	201	22	-	15/42/44/45	-
45	PLC	M	1002	-	-	14/42/42/45	-
45	PLC	A	201	-	-	13/34/34/45	-
46	SF4	F	501	7	-	-	0/6/5/5
45	PLC	b	101	-	-	5/42/42/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SF4	G	801	8	-	-	0/6/5/5
46	SF4	I	302	10	-	-	0/6/5/5
50	3PE	Y	303	-	-	11/28/28/54	-
50	3PE	L	711	-	-	15/36/36/54	-
51	CDL	a	201	-	-	29/70/70/110	-
48	FMN	F	502	-	-	9/18/18/18	0/3/3/3
47	FES	G	803	8	-	-	0/1/1/1
45	PLC	M	1003	-	-	17/45/45/45	-
45	PLC	Y	304	-	-	13/39/39/45	-
45	PLC	a	202	-	-	5/23/23/45	-
50	3PE	L	706	-	-	22/54/54/54	-
45	PLC	P	502	-	-	7/34/34/45	-
50	3PE	N	602	-	-	15/43/43/54	-
50	3PE	f	101	-	-	21/54/54/54	-
46	SF4	G	802	8	-	-	0/6/5/5
50	3PE	m	101	-	-	12/27/27/54	-
50	3PE	L	709	-	-	27/49/49/54	-
45	PLC	B	302	-	-	14/34/34/45	-
45	PLC	L	705	-	-	18/45/45/45	-
50	3PE	b	106	-	-	15/38/38/54	-
51	CDL	b	102	-	-	19/69/69/110	-
47	FES	E	301	6	-	-	0/1/1/1
45	PLC	d	101	-	-	13/45/45/45	-
50	3PE	L	708	-	-	15/38/38/54	-
50	3PE	L	703	-	-	25/45/45/54	-
45	PLC	q	402	-	-	13/45/45/45	-
50	3PE	L	701	-	-	10/32/32/54	-
45	PLC	h	201	-	-	10/45/45/45	-
50	3PE	M	1004	-	-	21/38/38/54	-
45	PLC	D	501	-	-	9/45/45/45	-
51	CDL	P	503	-	-	16/50/50/110	-
52	NDP	P	501	-	-	10/34/77/77	0/5/5/5
45	PLC	L	702	-	-	14/38/38/45	-
45	PLC	H	401	-	-	19/26/26/45	-
50	3PE	H	402	-	-	16/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	j	101	-	-	15/30/30/54	-
51	CDL	O	201	-	-	34/85/85/110	-
46	SF4	I	301	10	-	-	0/6/5/5
51	CDL	Z	202	-	-	32/58/58/110	-
45	PLC	N	601	-	-	13/45/45/45	-
50	3PE	Y	302	-	-	17/54/54/54	-
54	EHZ	T	201	21	-	22/42/44/45	-
50	3PE	L	707	-	-	15/54/54/54	-
46	SF4	B	301	3	-	-	0/6/5/5
45	PLC	Y	301	-	-	9/39/39/45	-
50	3PE	g	301	-	-	21/49/49/54	-
45	PLC	M	1001	-	-	15/45/45/45	-
50	3PE	b	103	-	-	20/43/43/54	-
50	3PE	b	104	-	-	17/39/39/54	-
50	3PE	b	105	-	-	15/34/34/54	-
50	3PE	L	710	-	-	27/54/54/54	-
45	PLC	q	401	-	-	11/39/39/45	-
45	PLC	L	704	-	-	14/35/35/45	-

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	PA-O3	10.56	1.70	1.59
52	P	501	NDP	C2B-C1B	-8.98	1.31	1.53
52	P	501	NDP	O4B-C1B	8.66	1.62	1.42
52	P	501	NDP	O4D-C1D	8.36	1.61	1.42
52	P	501	NDP	C7N-N7N	7.72	1.55	1.33
52	P	501	NDP	C2D-C1D	-7.35	1.30	1.53
52	P	501	NDP	C6N-C5N	7.19	1.55	1.33
48	F	502	FMN	C10-N1	6.82	1.47	1.33
48	F	502	FMN	C4A-N5	6.65	1.45	1.30
52	P	501	NDP	O4D-C4D	-6.43	1.30	1.45
52	P	501	NDP	P2B-O2B	5.85	1.69	1.59
48	F	502	FMN	C5A-N5	5.59	1.49	1.39
52	P	501	NDP	C6A-N6A	5.48	1.48	1.34
48	F	502	FMN	C2-N1	5.25	1.48	1.36
52	P	501	NDP	O4B-C4B	-5.15	1.33	1.45
54	T	201	EHZ	C12-N1	5.13	1.45	1.33
54	U	201	EHZ	C15-N2	5.13	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	U	201	EHZ	C12-N1	5.13	1.45	1.33
54	T	201	EHZ	C15-N2	5.13	1.45	1.33
52	P	501	NDP	PN-O3	5.01	1.64	1.59
48	F	502	FMN	C9A-N10	4.87	1.49	1.41
52	P	501	NDP	C2N-C3N	4.76	1.48	1.35
48	F	502	FMN	C2-N3	4.58	1.49	1.39
52	P	501	NDP	C5A-C4A	-4.18	1.31	1.39
52	P	501	NDP	O7N-C7N	-4.04	1.15	1.24
48	F	502	FMN	C10-N10	3.93	1.45	1.37
48	F	502	FMN	C4-N3	3.86	1.46	1.38
52	P	501	NDP	O2D-C2D	3.84	1.52	1.43
52	P	501	NDP	C8A-N9A	-3.66	1.31	1.37
52	P	501	NDP	C4N-C3N	3.41	1.56	1.50
48	F	502	FMN	O2-C2	-2.87	1.18	1.24
52	P	501	NDP	C4N-C5N	2.81	1.56	1.49
50	L	703	3PE	O21-C2	-2.75	1.40	1.46
51	b	102	CDL	OB6-CB4	-2.72	1.40	1.46
50	Y	302	3PE	O21-C2	-2.71	1.40	1.46
51	O	201	CDL	OB6-CB4	-2.70	1.40	1.46
51	a	201	CDL	OB6-CB4	-2.70	1.40	1.46
50	g	301	3PE	O21-C2	-2.70	1.40	1.46
48	F	502	FMN	O4-C4	-2.70	1.18	1.23
50	b	104	3PE	O21-C2	-2.69	1.40	1.46
51	Z	202	CDL	OB6-CB4	-2.69	1.40	1.46
51	b	102	CDL	OA6-CA4	-2.69	1.40	1.46
50	b	105	3PE	O21-C2	-2.68	1.40	1.46
50	L	706	3PE	O21-C2	-2.68	1.40	1.46
50	L	711	3PE	O21-C2	-2.67	1.40	1.46
52	P	501	NDP	C6N-N1N	2.67	1.43	1.37
51	P	503	CDL	OA6-CA4	-2.67	1.40	1.46
51	P	503	CDL	OB6-CB4	-2.66	1.40	1.46
50	Y	303	3PE	O21-C2	-2.64	1.40	1.46
50	b	103	3PE	O21-C2	-2.64	1.40	1.46
50	L	708	3PE	O21-C2	-2.63	1.40	1.46
50	L	707	3PE	O21-C2	-2.63	1.40	1.46
50	L	710	3PE	O21-C2	-2.63	1.40	1.46
50	M	1004	3PE	O21-C2	-2.62	1.40	1.46
50	H	402	3PE	O21-C2	-2.62	1.40	1.46
50	L	701	3PE	O21-C2	-2.62	1.40	1.46
50	j	101	3PE	O21-C2	-2.62	1.40	1.46
50	b	106	3PE	O21-C2	-2.61	1.40	1.46
50	f	101	3PE	O21-C2	-2.61	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	N	602	3PE	O21-C2	-2.61	1.40	1.46
52	P	501	NDP	C5A-N7A	-2.52	1.34	1.39
51	Z	202	CDL	OA6-CA5	2.49	1.40	1.35
50	m	101	3PE	O21-C21	2.48	1.40	1.35
51	O	201	CDL	OA8-CA7	2.46	1.40	1.33
54	U	201	EHZ	C9-S1	2.46	1.82	1.76
51	a	201	CDL	OB8-CB7	2.45	1.40	1.33
52	P	501	NDP	C7N-C3N	2.44	1.53	1.48
51	b	102	CDL	OB8-CB7	2.44	1.40	1.33
50	L	707	3PE	O31-C31	2.43	1.40	1.33
52	P	501	NDP	P2B-O1X	2.42	1.58	1.50
51	b	102	CDL	OA8-CA7	2.42	1.40	1.33
54	T	201	EHZ	C9-S1	2.42	1.81	1.76
51	Z	202	CDL	OA8-CA7	2.40	1.40	1.33
50	m	101	3PE	O31-C31	2.40	1.40	1.33
50	Y	303	3PE	O31-C31	2.40	1.40	1.33
51	O	201	CDL	OB8-CB7	2.40	1.40	1.33
51	a	201	CDL	OA6-CA4	-2.40	1.41	1.46
51	P	503	CDL	OA8-CA7	2.40	1.40	1.33
50	j	101	3PE	O31-C31	2.39	1.40	1.33
50	b	104	3PE	O31-C31	2.39	1.40	1.33
50	L	711	3PE	O31-C31	2.39	1.40	1.33
51	Z	202	CDL	OA6-CA4	-2.39	1.41	1.46
50	L	709	3PE	O31-C31	2.39	1.40	1.33
52	P	501	NDP	O3B-C3B	-2.39	1.37	1.43
50	g	301	3PE	O31-C31	2.39	1.40	1.33
50	L	708	3PE	O31-C31	2.39	1.40	1.33
51	Z	202	CDL	OB8-CB7	2.39	1.40	1.33
50	b	106	3PE	O31-C31	2.37	1.40	1.33
50	L	701	3PE	O31-C31	2.37	1.40	1.33
50	L	703	3PE	O31-C31	2.36	1.40	1.33
51	O	201	CDL	OA6-CA5	2.36	1.41	1.34
50	b	103	3PE	O31-C31	2.36	1.40	1.33
50	b	105	3PE	O31-C31	2.36	1.40	1.33
51	P	503	CDL	OB6-CB5	2.36	1.40	1.35
50	f	101	3PE	O31-C31	2.35	1.40	1.33
50	H	402	3PE	O31-C31	2.35	1.40	1.33
50	L	709	3PE	O21-C21	2.35	1.40	1.34
51	a	201	CDL	OA8-CA7	2.35	1.40	1.33
50	m	101	3PE	O21-C2	-2.35	1.41	1.46
50	M	1004	3PE	O31-C31	2.34	1.40	1.33
50	Y	303	3PE	O21-C21	2.34	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	PA-O5B	2.33	1.68	1.59
50	Y	302	3PE	O31-C31	2.33	1.40	1.33
50	N	602	3PE	O31-C31	2.33	1.40	1.33
52	P	501	NDP	O3D-C3D	-2.33	1.37	1.43
50	L	710	3PE	O31-C31	2.33	1.40	1.33
54	U	201	EHZ	O4-C15	-2.32	1.18	1.23
51	a	201	CDL	OA6-CA5	2.31	1.40	1.34
50	L	706	3PE	O31-C3	-2.29	1.40	1.45
51	O	201	CDL	OA6-CA4	-2.27	1.41	1.46
50	L	706	3PE	O31-C31	2.27	1.40	1.33
54	T	201	EHZ	O4-C15	-2.26	1.19	1.23
50	L	709	3PE	O21-C2	-2.24	1.41	1.46
50	L	710	3PE	O31-C3	-2.24	1.40	1.45
50	M	1004	3PE	O31-C3	-2.24	1.40	1.45
50	L	703	3PE	O31-C3	-2.23	1.40	1.45
50	f	101	3PE	O31-C3	-2.22	1.40	1.45
51	Z	202	CDL	OB8-CB6	-2.22	1.40	1.45
50	H	402	3PE	O31-C3	-2.22	1.40	1.45
50	L	701	3PE	O31-C3	-2.22	1.40	1.45
50	N	602	3PE	O31-C3	-2.22	1.40	1.45
50	Y	302	3PE	O31-C3	-2.22	1.40	1.45
51	O	201	CDL	OB8-CB6	-2.22	1.40	1.45
54	T	201	EHZ	O3-C12	-2.22	1.18	1.23
54	U	201	EHZ	O3-C12	-2.21	1.18	1.23
50	b	103	3PE	O31-C3	-2.20	1.40	1.45
50	b	105	3PE	O31-C3	-2.20	1.40	1.45
50	L	708	3PE	O31-C3	-2.19	1.40	1.45
50	L	701	3PE	O21-C21	2.19	1.40	1.34
50	L	711	3PE	O31-C3	-2.19	1.40	1.45
50	Y	303	3PE	O31-C3	-2.19	1.40	1.45
51	a	201	CDL	OA8-CA6	-2.19	1.40	1.45
50	b	104	3PE	O31-C3	-2.18	1.40	1.45
51	b	102	CDL	OB8-CB6	-2.18	1.40	1.45
51	Z	202	CDL	OA8-CA6	-2.18	1.40	1.45
51	P	503	CDL	OA8-CA6	-2.18	1.40	1.45
50	b	106	3PE	O31-C3	-2.18	1.40	1.45
50	N	602	3PE	O21-C21	2.18	1.40	1.34
50	g	301	3PE	O31-C3	-2.18	1.40	1.45
50	b	106	3PE	O21-C21	2.17	1.40	1.34
51	P	503	CDL	OA6-CA5	2.17	1.40	1.34
50	H	402	3PE	O21-C21	2.16	1.40	1.34
50	j	101	3PE	O21-C21	2.16	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	f	101	3PE	O21-C21	2.15	1.40	1.34
50	M	1004	3PE	O21-C21	2.15	1.40	1.34
50	L	706	3PE	O21-C21	2.15	1.40	1.34
51	a	201	CDL	OB8-CB6	-2.15	1.40	1.45
51	b	102	CDL	OA8-CA6	-2.15	1.40	1.45
50	m	101	3PE	O31-C3	-2.15	1.40	1.45
50	L	708	3PE	O21-C21	2.14	1.40	1.34
51	b	102	CDL	OA6-CA5	2.14	1.40	1.34
50	j	101	3PE	O31-C3	-2.14	1.40	1.45
50	L	707	3PE	O31-C3	-2.14	1.40	1.45
52	P	501	NDP	C5B-C4B	2.14	1.58	1.51
51	P	503	CDL	OB8-CB6	-2.14	1.40	1.45
51	Z	202	CDL	OB6-CB5	2.14	1.40	1.34
50	L	710	3PE	O21-C21	2.14	1.40	1.34
51	O	201	CDL	OA8-CA6	-2.13	1.40	1.45
50	L	707	3PE	O21-C21	2.13	1.40	1.34
51	O	201	CDL	OB6-CB5	2.13	1.40	1.34
51	b	102	CDL	OB6-CB5	2.13	1.40	1.34
50	b	103	3PE	O21-C21	2.12	1.40	1.34
50	L	711	3PE	O21-C21	2.12	1.40	1.34
51	a	201	CDL	OB6-CB5	2.12	1.40	1.34
50	L	709	3PE	O31-C3	-2.12	1.40	1.45
50	g	301	3PE	O21-C21	2.11	1.40	1.34
50	b	104	3PE	O21-C21	2.10	1.40	1.34
50	b	105	3PE	O21-C21	2.10	1.40	1.34
50	Y	302	3PE	O21-C21	2.09	1.40	1.34
50	L	703	3PE	O21-C21	2.05	1.40	1.34
52	P	501	NDP	C5D-C4D	2.01	1.57	1.51

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	P	501	NDP	C4A-N9A-C1B	-5.73	113.23	126.63
52	P	501	NDP	N3A-C2A-N1A	-5.64	120.04	128.58
52	P	501	NDP	N6A-C6A-N1A	-5.55	106.02	118.38
51	P	503	CDL	OB6-CB5-C51	5.30	120.55	111.09
48	F	502	FMN	C7M-C7-C6	5.21	128.75	119.57
52	P	501	NDP	C1B-N9A-C8A	5.13	138.47	127.09
54	U	201	EHZ	C8-C9-S1	5.07	119.95	113.56
54	T	201	EHZ	C8-C9-S1	5.06	119.94	113.56
48	F	502	FMN	C9-C8-C7	4.97	126.98	119.69
50	Y	303	3PE	O21-C21-C22	4.95	119.92	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	P	501	NDP	C5A-C4A-N3A	-4.93	119.93	126.72
51	Z	202	CDL	OA6-CA5-C11	4.88	119.78	111.09
50	m	101	3PE	O21-C21-C22	4.84	119.72	111.09
48	F	502	FMN	C8M-C8-C7	-4.37	111.84	120.76
52	P	501	NDP	N9A-C8A-N7A	-4.24	107.92	113.94
50	L	709	3PE	O21-C21-C22	4.20	120.56	111.48
51	Z	202	CDL	OB6-CB5-C51	4.18	120.52	111.48
50	L	711	3PE	O21-C21-C22	4.13	120.42	111.48
50	Y	302	3PE	O21-C21-C22	4.12	120.39	111.48
50	N	602	3PE	O21-C21-C22	4.11	120.36	111.48
52	P	501	NDP	C5A-C6A-N6A	4.09	133.41	123.29
51	O	201	CDL	OA6-CA5-C11	4.06	120.26	111.48
50	H	402	3PE	O21-C21-C22	4.05	120.25	111.48
50	f	101	3PE	O21-C21-C22	4.05	120.24	111.48
50	L	710	3PE	O21-C21-C22	4.05	120.24	111.48
50	j	101	3PE	O21-C21-C22	4.04	120.23	111.48
51	O	201	CDL	OB6-CB5-C51	4.04	120.23	111.48
50	M	1004	3PE	O21-C21-C22	4.03	120.20	111.48
51	a	201	CDL	OB6-CB5-C51	4.02	120.18	111.48
50	b	103	3PE	O21-C21-C22	3.99	120.11	111.48
50	L	708	3PE	O21-C21-C22	3.99	120.10	111.48
50	L	706	3PE	O21-C21-C22	3.99	120.10	111.48
50	b	104	3PE	O21-C21-C22	3.96	120.04	111.48
50	b	105	3PE	O21-C21-C22	3.95	120.02	111.48
50	L	703	3PE	O21-C21-C22	3.93	119.98	111.48
51	P	503	CDL	OA6-CA5-C11	3.91	119.95	111.48
50	L	707	3PE	O21-C21-C22	3.89	119.91	111.48
51	b	102	CDL	OA6-CA5-C11	3.88	119.88	111.48
50	b	106	3PE	O21-C21-C22	3.86	119.83	111.48
50	L	701	3PE	O21-C21-C22	3.83	119.77	111.48
51	b	102	CDL	OB6-CB5-C51	3.80	119.70	111.48
50	g	301	3PE	O21-C21-C22	3.73	119.56	111.48
51	a	201	CDL	OA6-CA5-C11	3.73	119.55	111.48
48	F	502	FMN	C4-N3-C2	-3.51	119.42	125.64
52	P	501	NDP	C2A-N3A-C4A	3.50	120.38	111.83
52	P	501	NDP	N3A-C4A-N9A	2.99	132.26	127.17
51	b	102	CDL	OB8-CB7-C71	2.97	120.17	111.15
50	L	707	3PE	O31-C31-C32	2.92	120.75	111.83
48	F	502	FMN	C7M-C7-C8	-2.85	114.93	120.76
52	P	501	NDP	C5A-N7A-C8A	2.82	107.88	103.45
50	L	703	3PE	O31-C31-C32	2.80	120.38	111.83
51	O	201	CDL	OA8-CA7-C31	2.79	120.35	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	L	709	3PE	O31-C31-C32	2.77	120.28	111.83
50	L	708	3PE	O31-C31-C32	2.77	120.28	111.83
50	b	106	3PE	O31-C31-C32	2.72	120.14	111.83
51	a	201	CDL	OB8-CB7-C71	2.71	120.11	111.83
50	L	710	3PE	O31-C31-C32	2.71	120.11	111.83
51	b	102	CDL	OA8-CA7-C31	2.71	120.10	111.83
50	b	104	3PE	O31-C31-C32	2.71	120.10	111.83
50	b	103	3PE	O31-C31-C32	2.71	120.10	111.83
50	Y	302	3PE	O31-C31-C32	2.71	120.09	111.83
50	g	301	3PE	O31-C31-C32	2.71	120.09	111.83
51	Z	202	CDL	OA8-CA7-C31	2.70	120.05	111.83
50	Y	303	3PE	O31-C31-C32	2.68	120.01	111.83
50	L	711	3PE	O31-C31-C32	2.67	119.98	111.83
50	N	602	3PE	O31-C31-C32	2.66	119.95	111.83
51	Z	202	CDL	OB8-CB7-C71	2.66	119.95	111.83
50	j	101	3PE	O31-C31-C32	2.66	119.94	111.83
51	a	201	CDL	OA8-CA7-C31	2.64	119.90	111.83
54	U	201	EHZ	C10-S1-C9	2.63	109.63	101.84
50	L	706	3PE	O31-C31-C32	2.62	119.83	111.83
48	F	502	FMN	C4A-C4-N3	2.62	119.92	113.25
50	f	101	3PE	O31-C31-C32	2.61	119.79	111.83
51	P	503	CDL	OA8-CA7-C31	2.61	119.78	111.83
50	b	105	3PE	O31-C31-C32	2.60	119.77	111.83
51	O	201	CDL	OB8-CB7-C71	2.60	119.77	111.83
50	M	1004	3PE	O31-C31-C32	2.59	119.74	111.83
50	m	101	3PE	O31-C31-C32	2.58	119.71	111.83
48	F	502	FMN	C9A-C5A-N5	-2.58	119.72	122.45
48	F	502	FMN	O4-C4-C4A	-2.57	119.75	126.53
50	H	402	3PE	O31-C31-C32	2.57	119.67	111.83
52	P	501	NDP	C2B-C1B-N9A	-2.55	109.56	113.75
50	L	701	3PE	O31-C31-C32	2.54	119.57	111.83
45	H	401	PLC	C3-C2-C1	2.44	117.48	111.78
52	P	501	NDP	C4A-N9A-C8A	2.44	108.30	105.74
48	F	502	FMN	C5A-C9A-N10	2.41	120.15	117.97
54	U	201	EHZ	C14-C13-C12	-2.35	108.48	112.39
48	F	502	FMN	C4A-C10-N10	2.35	119.84	116.48
54	T	201	EHZ	C10-S1-C9	2.31	108.68	101.84
54	T	201	EHZ	O2-C9-C8	-2.30	120.11	123.74
48	F	502	FMN	C6-C7-C8	-2.30	116.31	119.69
54	U	201	EHZ	O2-C9-C8	-2.28	120.15	123.74
48	F	502	FMN	C4'-C3'-C2'	-2.27	109.80	113.57
48	F	502	FMN	C10-C4A-N5	-2.21	120.30	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	U	201	EHZ	O2-C9-S1	-2.19	119.89	122.68
50	Y	303	3PE	C2-O21-C21	-2.18	114.00	117.85
52	P	501	NDP	C4A-C5A-N7A	-2.18	108.09	110.58
48	F	502	FMN	C6-C5A-C9A	2.17	122.03	119.05
54	T	201	EHZ	O2-C9-S1	-2.15	119.95	122.68
45	L	705	PLC	C3-C2-C1	2.12	116.73	111.78
54	U	201	EHZ	C16-C15-N2	2.10	120.46	116.48
54	U	201	EHZ	C13-C12-N1	2.09	120.15	116.34
45	N	601	PLC	C3-C2-C1	2.09	116.65	111.78
54	T	201	EHZ	C13-C12-N1	2.03	120.04	116.34
52	P	501	NDP	P2B-O2B-C2B	-2.02	118.04	123.43

There are no chirality outliers.

All (820) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PLC	C1'-C'-O2-C2
45	A	201	PLC	O'-C'-O2-C2
45	A	201	PLC	C1-O3P-P-O1P
45	A	201	PLC	C1-O3P-P-O2P
45	B	302	PLC	O4P-C4-C5-N
45	B	302	PLC	O'-C'-O2-C2
45	B	302	PLC	C1-O3P-P-O1P
45	B	302	PLC	C1-O3P-P-O2P
45	B	302	PLC	C1-O3P-P-O4P
45	D	501	PLC	C1'-C'-O2-C2
45	H	401	PLC	C1-O3P-P-O1P
45	H	401	PLC	C1-O3P-P-O2P
45	H	401	PLC	C1-O3P-P-O4P
45	H	401	PLC	C4-O4P-P-O1P
45	L	702	PLC	O4P-C4-C5-N
45	L	702	PLC	C1'-C'-O2-C2
45	L	702	PLC	C1-O3P-P-O1P
45	L	702	PLC	C1-O3P-P-O2P
45	L	702	PLC	C1-O3P-P-O4P
45	L	704	PLC	C1'-C'-O2-C2
45	L	704	PLC	C1-O3P-P-O2P
45	L	704	PLC	C1-O3P-P-O4P
45	L	705	PLC	O4P-C4-C5-N
45	L	705	PLC	C1-O3P-P-O4P
45	M	1001	PLC	C1-O3P-P-O4P
45	M	1001	PLC	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
45	M	1002	PLC	C1'-C'-O2-C2
45	M	1002	PLC	O'-C'-O2-C2
45	M	1002	PLC	C1-O3P-P-O1P
45	M	1002	PLC	C1-O3P-P-O2P
45	M	1002	PLC	C1-O3P-P-O4P
45	M	1003	PLC	O4P-C4-C5-N
45	M	1003	PLC	C1'-C'-O2-C2
45	M	1003	PLC	C1-O3P-P-O2P
45	M	1003	PLC	C4-O4P-P-O2P
45	M	1003	PLC	C4-O4P-P-O3P
45	N	601	PLC	C1-O3P-P-O2P
45	N	601	PLC	C1-O3P-P-O4P
45	N	601	PLC	C4-O4P-P-O2P
45	P	502	PLC	O2-C2-C3-O3
45	Y	301	PLC	O4P-C4-C5-N
45	Y	301	PLC	C1-O3P-P-O2P
45	Y	301	PLC	C1-O3P-P-O4P
45	Y	304	PLC	C1'-C'-O2-C2
45	Y	304	PLC	O'-C'-O2-C2
45	Y	304	PLC	C1-O3P-P-O2P
45	Y	304	PLC	C1-O3P-P-O4P
45	Z	201	PLC	C1-O3P-P-O2P
45	Z	201	PLC	C1-O3P-P-O4P
45	a	202	PLC	O4P-C4-C5-N
45	a	202	PLC	C1'-C'-O2-C2
45	a	202	PLC	O'-C'-O2-C2
45	b	101	PLC	C1-O3P-P-O2P
45	d	101	PLC	O4P-C4-C5-N
45	d	101	PLC	C4-O4P-P-O1P
45	h	201	PLC	O3P-C1-C2-O2
45	h	201	PLC	O'-C'-O2-C2
45	h	201	PLC	C1-O3P-P-O1P
45	h	201	PLC	C1-O3P-P-O2P
45	h	201	PLC	C1-O3P-P-O4P
45	q	401	PLC	O4P-C4-C5-N
45	q	401	PLC	C1'-C'-O2-C2
45	q	401	PLC	C4-O4P-P-O1P
48	F	502	FMN	C1'-C2'-C3'-O3'
48	F	502	FMN	C1'-C2'-C3'-C4'
50	H	402	3PE	C1-O11-P-O13
50	H	402	3PE	C1-O11-P-O14
50	H	402	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
50	H	402	3PE	O11-C1-C2-O21
50	H	402	3PE	O22-C21-O21-C2
50	L	701	3PE	C11-O13-P-O11
50	L	701	3PE	C11-O13-P-O14
50	L	703	3PE	C1-O11-P-O12
50	L	703	3PE	C1-O11-P-O13
50	L	703	3PE	C1-O11-P-O14
50	L	703	3PE	C11-O13-P-O11
50	L	703	3PE	C11-O13-P-O12
50	L	703	3PE	C11-O13-P-O14
50	L	706	3PE	C22-C21-O21-C2
50	L	707	3PE	C1-O11-P-O12
50	L	707	3PE	C1-O11-P-O13
50	L	707	3PE	O32-C31-O31-C3
50	L	707	3PE	C32-C31-O31-C3
50	L	707	3PE	O22-C21-O21-C2
50	L	707	3PE	C22-C21-O21-C2
50	L	708	3PE	C1-O11-P-O14
50	L	709	3PE	C22-C21-O21-C2
50	L	710	3PE	C11-O13-P-O11
50	L	710	3PE	C11-O13-P-O12
50	L	710	3PE	C11-O13-P-O14
50	L	710	3PE	O21-C2-C3-O31
50	L	711	3PE	C1-O11-P-O12
50	L	711	3PE	C1-O11-P-O13
50	L	711	3PE	C1-O11-P-O14
50	L	711	3PE	C22-C21-O21-C2
50	M	1004	3PE	C1-O11-P-O12
50	M	1004	3PE	C1-O11-P-O13
50	M	1004	3PE	C1-O11-P-O14
50	M	1004	3PE	C11-O13-P-O12
50	M	1004	3PE	O13-C11-C12-N
50	N	602	3PE	C1-O11-P-O13
50	N	602	3PE	C22-C21-O21-C2
50	Y	302	3PE	C1-O11-P-O12
50	Y	302	3PE	C1-O11-P-O13
50	Y	302	3PE	O21-C2-C3-O31
50	Y	302	3PE	O22-C21-O21-C2
50	Y	302	3PE	C22-C21-O21-C2
50	Y	303	3PE	C11-O13-P-O11
50	Y	303	3PE	C11-O13-P-O14
50	b	103	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
50	b	103	3PE	C11-O13-P-O12
50	b	103	3PE	C11-O13-P-O14
50	b	103	3PE	O13-C11-C12-N
50	b	104	3PE	C11-O13-P-O11
50	b	105	3PE	C1-O11-P-O14
50	b	106	3PE	C11-O13-P-O11
50	b	106	3PE	C11-O13-P-O12
50	f	101	3PE	C11-O13-P-O11
50	f	101	3PE	C11-O13-P-O12
50	f	101	3PE	C11-O13-P-O14
50	f	101	3PE	O22-C21-O21-C2
50	f	101	3PE	C22-C21-O21-C2
50	g	301	3PE	C1-O11-P-O12
50	g	301	3PE	C1-O11-P-O14
50	g	301	3PE	C11-O13-P-O11
50	g	301	3PE	C11-O13-P-O12
50	j	101	3PE	C1-O11-P-O12
50	j	101	3PE	C1-O11-P-O13
50	j	101	3PE	C11-O13-P-O12
50	j	101	3PE	O13-C11-C12-N
51	O	201	CDL	CA2-OA2-PA1-OA3
51	O	201	CDL	CA2-OA2-PA1-OA4
51	O	201	CDL	CA2-OA2-PA1-OA5
51	O	201	CDL	CA3-OA5-PA1-OA2
51	O	201	CDL	CA3-OA5-PA1-OA3
51	O	201	CDL	CA3-OA5-PA1-OA4
51	O	201	CDL	C11-CA5-OA6-CA4
51	O	201	CDL	OA9-CA7-OA8-CA6
51	O	201	CDL	C31-CA7-OA8-CA6
51	O	201	CDL	OB7-CB5-OB6-CB4
51	O	201	CDL	C51-CB5-OB6-CB4
51	P	503	CDL	O1-C1-CB2-OB2
51	P	503	CDL	OA6-CA4-CA6-OA8
51	P	503	CDL	OB5-CB3-CB4-OB6
51	P	503	CDL	OB7-CB5-OB6-CB4
51	Z	202	CDL	CA3-OA5-PA1-OA2
51	Z	202	CDL	CA3-OA5-PA1-OA3
51	Z	202	CDL	CA3-OA5-PA1-OA4
51	Z	202	CDL	CB2-OB2-PB2-OB3
51	Z	202	CDL	CB2-OB2-PB2-OB4
51	Z	202	CDL	CB3-OB5-PB2-OB2
51	Z	202	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	Z	202	CDL	OB7-CB5-OB6-CB4
51	a	201	CDL	CA2-OA2-PA1-OA3
51	a	201	CDL	CA2-OA2-PA1-OA4
51	a	201	CDL	CA2-OA2-PA1-OA5
51	a	201	CDL	CB2-OB2-PB2-OB5
51	a	201	CDL	OB6-CB4-CB6-OB8
51	a	201	CDL	C51-CB5-OB6-CB4
51	a	201	CDL	C71-CB7-OB8-CB6
51	b	102	CDL	CA3-OA5-PA1-OA2
51	b	102	CDL	CA3-OA5-PA1-OA3
51	b	102	CDL	CB2-OB2-PB2-OB3
51	b	102	CDL	CB2-OB2-PB2-OB5
52	P	501	NDP	C5B-O5B-PA-O2A
52	P	501	NDP	C5B-O5B-PA-O3
54	T	201	EHZ	C5-C6-C7-C8
54	T	201	EHZ	C11-C10-S1-C9
54	T	201	EHZ	C15-C16-C17-C18
54	T	201	EHZ	C15-C16-C17-C19
54	T	201	EHZ	C15-C16-C17-C20
54	T	201	EHZ	O5-C16-C17-C18
54	T	201	EHZ	O5-C16-C17-C19
54	T	201	EHZ	O5-C16-C17-C20
54	T	201	EHZ	C18-C17-C20-O6
54	T	201	EHZ	C19-C17-C20-O6
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C5-C6-C7-C8
54	U	201	EHZ	S1-C10-C11-N1
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
50	m	101	3PE	C22-C21-O21-C2
51	P	503	CDL	C51-CB5-OB6-CB4
51	Z	202	CDL	C11-CA5-OA6-CA4
50	Y	303	3PE	C22-C21-O21-C2
50	L	703	3PE	O32-C31-O31-C3
50	b	105	3PE	O32-C31-O31-C3
50	f	101	3PE	O32-C31-O31-C3
51	a	201	CDL	OB9-CB7-OB8-CB6
50	L	703	3PE	C32-C31-O31-C3
50	b	105	3PE	C32-C31-O31-C3
50	f	101	3PE	C32-C31-O31-C3
51	Z	202	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	L	702	PLC	OB-CB-O3-C3
50	L	710	3PE	O32-C31-O31-C3
50	N	602	3PE	O32-C31-O31-C3
50	Y	302	3PE	O32-C31-O31-C3
50	Y	303	3PE	O32-C31-O31-C3
50	b	103	3PE	O32-C31-O31-C3
50	j	101	3PE	O32-C31-O31-C3
51	b	102	CDL	OB9-CB7-OB8-CB6
50	m	101	3PE	O22-C21-O21-C2
51	P	503	CDL	C71-CB7-OB8-CB6
45	D	501	PLC	O'-C'-O2-C2
45	M	1003	PLC	O'-C'-O2-C2
45	q	401	PLC	O'-C'-O2-C2
50	L	706	3PE	O22-C21-O21-C2
50	L	709	3PE	O22-C21-O21-C2
50	L	710	3PE	O22-C21-O21-C2
50	N	602	3PE	O22-C21-O21-C2
50	b	104	3PE	O22-C21-O21-C2
51	O	201	CDL	OA7-CA5-OA6-CA4
45	H	401	PLC	C1B-CB-O3-C3
50	N	602	3PE	C32-C31-O31-C3
50	Y	303	3PE	C32-C31-O31-C3
50	b	103	3PE	C32-C31-O31-C3
51	b	102	CDL	C71-CB7-OB8-CB6
45	B	302	PLC	C1'-C'-O2-C2
45	h	201	PLC	C1'-C'-O2-C2
50	H	402	3PE	C22-C21-O21-C2
50	L	710	3PE	C22-C21-O21-C2
50	b	104	3PE	C22-C21-O21-C2
51	Z	202	CDL	C51-CB5-OB6-CB4
45	L	702	PLC	C1B-CB-O3-C3
45	Y	304	PLC	C1B-CB-O3-C3
50	L	710	3PE	C32-C31-O31-C3
50	Y	302	3PE	C32-C31-O31-C3
50	j	101	3PE	C32-C31-O31-C3
51	Z	202	CDL	C31-CA7-OA8-CA6
50	Y	303	3PE	O22-C21-O21-C2
45	H	401	PLC	OB-CB-O3-C3
45	L	705	PLC	OB-CB-O3-C3
51	Z	202	CDL	OA9-CA7-OA8-CA6
51	a	201	CDL	OA9-CA7-OA8-CA6
45	L	702	PLC	O'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
45	L	704	PLC	O'-C'-O2-C2
50	L	711	3PE	O22-C21-O21-C2
51	a	201	CDL	OB7-CB5-OB6-CB4
50	g	301	3PE	C32-C31-O31-C3
51	a	201	CDL	C31-CA7-OA8-CA6
51	P	503	CDL	OB9-CB7-OB8-CB6
45	L	705	PLC	C1B-CB-O3-C3
45	Y	304	PLC	OB-CB-O3-C3
50	g	301	3PE	O32-C31-O31-C3
45	h	201	PLC	C2-C1-O3P-P
50	L	711	3PE	C32-C31-O31-C3
51	O	201	CDL	CB2-C1-CA2-OA2
50	L	709	3PE	C32-C31-O31-C3
52	P	501	NDP	O4D-C1D-N1N-C6N
51	O	201	CDL	O1-C1-CA2-OA2
50	L	709	3PE	O32-C31-O31-C3
45	L	702	PLC	C4'-C5'-C6'-C7'
54	T	201	EHZ	C5-C6-C7-O1
54	U	201	EHZ	C5-C6-C7-O1
50	Y	303	3PE	O21-C2-C3-O31
45	L	705	PLC	C'-C1'-C2'-C3'
51	b	102	CDL	CB5-C51-C52-C53
50	H	402	3PE	C21-C22-C23-C24
50	b	106	3PE	C21-C22-C23-C24
50	j	101	3PE	C31-C32-C33-C34
51	a	201	CDL	CA5-C11-C12-C13
50	b	103	3PE	C22-C21-O21-C2
51	b	102	CDL	C11-CA5-OA6-CA4
45	B	302	PLC	C2-C1-O3P-P
45	M	1002	PLC	CB-C1B-C2B-C3B
50	L	709	3PE	C21-C22-C23-C24
50	b	103	3PE	C21-C22-C23-C24
50	L	711	3PE	O32-C31-O31-C3
50	m	101	3PE	C31-C32-C33-C34
50	M	1004	3PE	C32-C31-O31-C3
50	L	703	3PE	C22-C21-O21-C2
50	L	703	3PE	O22-C21-O21-C2
50	b	103	3PE	O22-C21-O21-C2
51	b	102	CDL	OA7-CA5-OA6-CA4
51	P	503	CDL	CA2-C1-CB2-OB2
51	Z	202	CDL	C71-CB7-OB8-CB6
51	a	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
51	a	201	CDL	OA7-CA5-OA6-CA4
48	F	502	FMN	O2'-C2'-C3'-O3'
50	L	703	3PE	C31-C32-C33-C34
45	D	501	PLC	C3-C2-O2-C'
54	T	201	EHZ	C4-C5-C6-C7
45	Y	301	PLC	C1'-C'-O2-C2
50	b	105	3PE	C22-C21-O21-C2
51	Z	202	CDL	CB5-C51-C52-C53
51	a	201	CDL	CA7-C31-C32-C33
51	O	201	CDL	C14-C15-C16-C17
51	O	201	CDL	C51-C52-C53-C54
54	U	201	EHZ	C1-C2-C3-C4
45	L	702	PLC	C1'-C2'-C3'-C4'
45	q	402	PLC	C1B-C2B-C3B-C4B
50	L	706	3PE	C39-C3A-C3B-C3C
45	M	1002	PLC	C1B-C2B-C3B-C4B
45	d	101	PLC	C7B-C8B-C9B-CAA
45	q	402	PLC	C1'-C2'-C3'-C4'
50	M	1004	3PE	O32-C31-O31-C3
45	L	702	PLC	C3'-C4'-C5'-C6'
45	M	1002	PLC	C3'-C4'-C5'-C6'
45	d	101	PLC	C2B-C3B-C4B-C5B
50	Y	303	3PE	C34-C35-C36-C37
50	L	709	3PE	C38-C39-C3A-C3B
50	b	104	3PE	C31-C32-C33-C34
51	O	201	CDL	CA5-C11-C12-C13
50	L	710	3PE	C3E-C3F-C3G-C3H
50	L	710	3PE	C3D-C3E-C3F-C3G
50	Y	302	3PE	C38-C39-C3A-C3B
45	q	402	PLC	C'-C1'-C2'-C3'
45	a	202	PLC	C1B-CB-O3-C3
45	q	402	PLC	C5'-C6'-C7'-C8'
50	L	711	3PE	C33-C34-C35-C36
50	b	104	3PE	C29-C2A-C2B-C2C
50	g	301	3PE	C23-C24-C25-C26
50	L	710	3PE	C2E-C2F-C2G-C2H
45	d	101	PLC	C6B-C7B-C8B-C9B
51	O	201	CDL	C74-C75-C76-C77
45	q	401	PLC	C1'-C2'-C3'-C4'
50	L	706	3PE	C32-C33-C34-C35
50	b	105	3PE	C24-C25-C26-C27
45	M	1001	PLC	C1B-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
45	Z	201	PLC	C1B-CB-O3-C3
50	L	709	3PE	C25-C26-C27-C28
50	g	301	3PE	C34-C35-C36-C37
50	L	706	3PE	C21-C22-C23-C24
50	L	708	3PE	C21-C22-C23-C24
45	L	705	PLC	C6B-C7B-C8B-C9B
45	d	101	PLC	C1B-C2B-C3B-C4B
50	H	402	3PE	C23-C24-C25-C26
50	L	703	3PE	C29-C2A-C2B-C2C
51	Z	202	CDL	OB9-CB7-OB8-CB6
50	b	103	3PE	C31-C32-C33-C34
45	L	705	PLC	C1'-C'-O2-C2
48	F	502	FMN	O2'-C2'-C3'-C4'
51	Z	202	CDL	C72-C73-C74-C75
54	T	201	EHZ	C1-C2-C3-C4
45	q	402	PLC	C2B-C3B-C4B-C5B
50	Y	303	3PE	C31-C32-C33-C34
45	q	401	PLC	C6'-C7'-C8'-C9'
45	Y	301	PLC	O'-C'-O2-C2
50	b	105	3PE	O22-C21-O21-C2
50	L	709	3PE	C3B-C3C-C3D-C3E
50	Y	302	3PE	C36-C37-C38-C39
45	M	1003	PLC	C3'-C4'-C5'-C6'
50	L	703	3PE	C33-C34-C35-C36
50	b	105	3PE	C31-C32-C33-C34
50	j	101	3PE	C21-C22-C23-C24
45	M	1003	PLC	C1B-CB-O3-C3
45	M	1002	PLC	C5'-C6'-C7'-C8'
45	d	101	PLC	C7'-C8'-C9'-CA'
50	H	402	3PE	C24-C25-C26-C27
50	L	707	3PE	C33-C34-C35-C36
51	Z	202	CDL	C51-C52-C53-C54
50	f	101	3PE	C34-C35-C36-C37
50	f	101	3PE	C3A-C3B-C3C-C3D
50	f	101	3PE	C29-C2A-C2B-C2C
45	Z	201	PLC	C'-C1'-C2'-C3'
45	N	601	PLC	C1B-C2B-C3B-C4B
50	Y	302	3PE	C37-C38-C39-C3A
50	L	706	3PE	C2A-C2B-C2C-C2D
50	L	709	3PE	C26-C27-C28-C29
50	L	703	3PE	C38-C39-C3A-C3B
45	H	401	PLC	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
45	A	201	PLC	C1B-C2B-C3B-C4B
54	U	201	EHZ	C4-C5-C6-C7
45	M	1001	PLC	OB-CB-O3-C3
45	Z	201	PLC	OB-CB-O3-C3
45	A	201	PLC	CB-C1B-C2B-C3B
50	L	708	3PE	O11-C1-C2-O21
45	N	601	PLC	C3'-C4'-C5'-C6'
50	L	706	3PE	C38-C39-C3A-C3B
45	q	402	PLC	CB-C1B-C2B-C3B
50	b	106	3PE	C31-C32-C33-C34
45	H	401	PLC	O2-C2-C3-O3
50	b	104	3PE	O21-C2-C3-O31
50	L	706	3PE	C2B-C2C-C2D-C2E
51	a	201	CDL	C51-C52-C53-C54
54	U	201	EHZ	C2-C1-C21-C22
50	b	106	3PE	C33-C34-C35-C36
50	f	101	3PE	C2B-C2C-C2D-C2E
45	N	601	PLC	C2B-C3B-C4B-C5B
50	M	1004	3PE	C26-C27-C28-C29
50	f	101	3PE	C33-C34-C35-C36
50	b	103	3PE	C3A-C3B-C3C-C3D
45	M	1001	PLC	C1B-C2B-C3B-C4B
54	U	201	EHZ	C21-C1-C2-C3
50	L	709	3PE	C2-C3-O31-C31
50	L	709	3PE	C32-C33-C34-C35
50	L	703	3PE	C24-C25-C26-C27
45	M	1003	PLC	OB-CB-O3-C3
45	q	402	PLC	C3B-C4B-C5B-C6B
45	M	1001	PLC	C5B-C6B-C7B-C8B
45	Y	304	PLC	O3P-C1-C2-C3
45	h	201	PLC	O3P-C1-C2-C3
50	b	103	3PE	O11-C1-C2-C3
50	b	106	3PE	O11-C1-C2-C3
51	P	503	CDL	OB5-CB3-CB4-CB6
45	L	705	PLC	O'-C'-O2-C2
50	L	706	3PE	C23-C24-C25-C26
50	L	706	3PE	C3E-C3F-C3G-C3H
50	M	1004	3PE	C24-C25-C26-C27
50	b	106	3PE	C32-C31-O31-C3
45	N	601	PLC	C'-C1'-C2'-C3'
45	H	401	PLC	C1-C2-C3-O3
45	M	1003	PLC	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
45	P	502	PLC	C1-C2-C3-O3
45	d	101	PLC	C1-C2-C3-O3
50	H	402	3PE	C1-C2-C3-O31
50	L	701	3PE	C1-C2-C3-O31
50	L	706	3PE	C1-C2-C3-O31
50	L	710	3PE	C1-C2-C3-O31
50	L	711	3PE	C1-C2-C3-O31
50	Y	302	3PE	C1-C2-C3-O31
50	Y	303	3PE	C1-C2-C3-O31
50	b	105	3PE	C1-C2-C3-O31
50	L	703	3PE	C32-C33-C34-C35
51	O	201	CDL	C81-C82-C83-C84
50	L	708	3PE	C32-C31-O31-C3
45	Y	304	PLC	C'-C1'-C2'-C3'
50	g	301	3PE	C35-C36-C37-C38
54	U	201	EHZ	C2-C3-C4-C5
50	L	709	3PE	C31-C32-C33-C34
51	Z	202	CDL	CA6-CA4-OA6-CA5
45	M	1003	PLC	C1B-C2B-C3B-C4B
50	g	301	3PE	C38-C39-C3A-C3B
51	O	201	CDL	C34-C35-C36-C37
45	M	1002	PLC	O3P-C1-C2-O2
45	P	502	PLC	O3P-C1-C2-O2
50	b	104	3PE	O11-C1-C2-O21
50	f	101	3PE	O11-C1-C2-O21
51	a	201	CDL	OB5-CB3-CB4-OB6
50	b	104	3PE	C28-C29-C2A-C2B
50	L	707	3PE	C26-C27-C28-C29
50	Y	302	3PE	C39-C3A-C3B-C3C
51	O	201	CDL	C54-C55-C56-C57
50	L	701	3PE	O21-C2-C3-O31
50	L	703	3PE	O21-C2-C3-O31
50	L	711	3PE	O21-C2-C3-O31
51	P	503	CDL	OB6-CB4-CB6-OB8
45	a	202	PLC	OB-CB-O3-C3
50	M	1004	3PE	C29-C2A-C2B-C2C
50	L	703	3PE	C23-C24-C25-C26
50	L	710	3PE	C24-C25-C26-C27
50	b	103	3PE	C36-C37-C38-C39
50	L	701	3PE	C35-C36-C37-C38
50	L	709	3PE	C23-C24-C25-C26
45	d	101	PLC	C8'-C9'-CA'-CB'

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Mol	Chain	Res	Type	Atoms
50	L	710	3PE	C33-C34-C35-C36
50	b	104	3PE	C2B-C2C-C2D-C2E
45	q	402	PLC	C1B-CB-O3-C3
50	g	301	3PE	C2B-C2C-C2D-C2E
45	Y	304	PLC	C1'-C2'-C3'-C4'
45	L	702	PLC	C2-C1-O3P-P
45	L	704	PLC	C2-C1-O3P-P
54	T	201	EHZ	S1-C10-C11-N1
50	L	706	3PE	C32-C31-O31-C3
51	O	201	CDL	C75-C76-C77-C78
45	M	1001	PLC	O3P-C1-C2-C3
45	Y	301	PLC	O3P-C1-C2-C3
50	H	402	3PE	O11-C1-C2-C3
50	M	1004	3PE	O11-C1-C2-C3
50	b	105	3PE	O11-C1-C2-C3
51	b	102	CDL	OA5-CA3-CA4-CA6
50	L	710	3PE	C2A-C2B-C2C-C2D
51	Z	202	CDL	C72-C71-CB7-OB8
51	Z	202	CDL	C31-C32-C33-C34
50	L	710	3PE	C31-C32-C33-C34
52	P	501	NDP	O4D-C4D-C5D-O5D
50	N	602	3PE	C27-C28-C29-C2A
50	b	106	3PE	O32-C31-O31-C3
50	L	708	3PE	O32-C31-O31-C3
54	T	201	EHZ	C1-C21-C22-C23
45	L	705	PLC	C3B-C4B-C5B-C6B
45	M	1002	PLC	C1'-C2'-C3'-C4'
50	N	602	3PE	C1-C2-C3-O31
50	b	103	3PE	C1-C2-C3-O31
50	b	104	3PE	C1-C2-C3-O31
50	M	1004	3PE	C25-C26-C27-C28
50	Y	302	3PE	C22-C23-C24-C25
45	M	1002	PLC	C4B-C5B-C6B-C7B
50	b	104	3PE	C23-C24-C25-C26
45	b	101	PLC	C5B-C6B-C7B-C8B
45	Y	301	PLC	O3P-C1-C2-O2
50	L	703	3PE	O11-C1-C2-O21
50	M	1004	3PE	O11-C1-C2-O21
50	b	103	3PE	O11-C1-C2-O21
50	b	106	3PE	O11-C1-C2-O21
45	H	401	PLC	C2-C1-O3P-P
50	g	301	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
54	T	201	EHZ	O1-C7-C8-C9
54	U	201	EHZ	O1-C7-C8-C9
50	L	701	3PE	C33-C34-C35-C36
50	g	301	3PE	C2A-C2B-C2C-C2D
50	m	101	3PE	C33-C34-C35-C36
50	M	1004	3PE	O21-C2-C3-O31
51	b	102	CDL	OA6-CA4-CA6-OA8
51	b	102	CDL	OB6-CB4-CB6-OB8
52	P	501	NDP	C3D-C4D-C5D-O5D
50	b	104	3PE	C27-C28-C29-C2A
51	O	201	CDL	C11-C12-C13-C14
52	P	501	NDP	PN-O3-PA-O5B
52	P	501	NDP	PA-O3-PN-O5D
50	M	1004	3PE	C27-C28-C29-C2A
54	T	201	EHZ	C6-C7-C8-C9
54	U	201	EHZ	C6-C7-C8-C9
50	b	106	3PE	C26-C27-C28-C29
45	M	1001	PLC	C1'-C'-O2-C2
45	q	402	PLC	OB-CB-O3-C3
45	d	101	PLC	C1'-C2'-C3'-C4'
45	q	401	PLC	C5'-C6'-C7'-C8'
45	H	401	PLC	O3P-C1-C2-C3
45	M	1002	PLC	O3P-C1-C2-C3
45	P	502	PLC	O3P-C1-C2-C3
50	L	703	3PE	O11-C1-C2-C3
50	L	710	3PE	O11-C1-C2-C3
50	f	101	3PE	O11-C1-C2-C3
50	L	706	3PE	O32-C31-O31-C3
45	Z	201	PLC	C4'-C5'-C6'-C7'
51	Z	202	CDL	C73-C74-C75-C76
50	L	707	3PE	C35-C36-C37-C38
50	L	709	3PE	C35-C36-C37-C38
45	N	601	PLC	C3B-C4B-C5B-C6B
45	L	705	PLC	C3-C2-O2-C'
50	L	709	3PE	C3-C2-O21-C21
50	m	101	3PE	C3-C2-O21-C21
51	O	201	CDL	C13-C14-C15-C16
45	A	201	PLC	O3P-C1-C2-O2
45	M	1001	PLC	O3P-C1-C2-O2
50	L	709	3PE	O11-C1-C2-O21
50	L	710	3PE	O11-C1-C2-O21
50	b	105	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
51	b	102	CDL	OA5-CA3-CA4-OA6
50	L	703	3PE	C1-C2-C3-O31
51	P	503	CDL	CA3-CA4-CA6-OA8
51	a	201	CDL	CB3-CB4-CB6-OB8
51	b	102	CDL	CA3-CA4-CA6-OA8
50	g	301	3PE	C22-C21-O21-C2
50	g	301	3PE	C31-C32-C33-C34
45	L	705	PLC	C5B-C6B-C7B-C8B
50	Y	302	3PE	C3B-C3C-C3D-C3E
45	H	401	PLC	C5-C4-O4P-P
50	L	701	3PE	C12-C11-O13-P
50	b	103	3PE	C12-C11-O13-P
50	b	106	3PE	C12-C11-O13-P
50	j	101	3PE	C12-C11-O13-P
50	H	402	3PE	O21-C2-C3-O31
50	N	602	3PE	O21-C2-C3-O31
50	b	103	3PE	O21-C2-C3-O31
50	j	101	3PE	O21-C2-C3-O31
45	L	704	PLC	C2B-C3B-C4B-C5B
50	N	602	3PE	C2D-C2E-C2F-C2G
45	H	401	PLC	C4-C5-N-C6
50	b	104	3PE	C33-C34-C35-C36
52	P	501	NDP	C3B-C4B-C5B-O5B
50	H	402	3PE	C2-C1-O11-P
51	a	201	CDL	C1-CB2-OB2-PB2
45	H	401	PLC	O4P-C4-C5-N
45	L	704	PLC	O4P-C4-C5-N
45	N	601	PLC	O4P-C4-C5-N
45	M	1003	PLC	C7B-C8B-C9B-CAA
45	H	401	PLC	C1'-C'-O2-C2
51	a	201	CDL	C56-C57-C58-C59
45	A	201	PLC	O3P-C1-C2-C3
50	b	104	3PE	O11-C1-C2-C3
51	a	201	CDL	OB5-CB3-CB4-CB6
45	M	1001	PLC	O'-C'-O2-C2
50	g	301	3PE	O22-C21-O21-C2
50	L	706	3PE	C36-C37-C38-C39
48	F	502	FMN	N10-C1'-C2'-O2'
54	U	201	EHZ	C18-C17-C20-O6
50	L	707	3PE	C31-C32-C33-C34
50	L	711	3PE	C2-C1-O11-P
50	M	1004	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
45	N	601	PLC	C1'-C2'-C3'-C4'
45	B	302	PLC	O3P-C1-C2-O2
45	H	401	PLC	O3P-C1-C2-O2
45	M	1003	PLC	O3P-C1-C2-O2
45	Y	304	PLC	O3P-C1-C2-O2
45	A	201	PLC	C4-C5-N-C8
45	Z	201	PLC	C4-C5-N-C8
45	B	302	PLC	C3B-C4B-C5B-C6B
50	L	710	3PE	C35-C36-C37-C38
51	O	201	CDL	C52-C53-C54-C55
45	D	501	PLC	O2-C2-C3-O3
45	M	1003	PLC	O2-C2-C3-O3
45	d	101	PLC	O2-C2-C3-O3
50	L	706	3PE	O21-C2-C3-O31
50	b	105	3PE	O21-C2-C3-O31
45	L	704	PLC	C1-C2-C3-O3
50	j	101	3PE	C1-C2-C3-O31
51	P	503	CDL	CB3-CB4-CB6-OB8
54	T	201	EHZ	C16-C17-C20-O6
45	Y	301	PLC	C1'-C2'-C3'-C4'
45	A	201	PLC	C1-O3P-P-O4P
45	D	501	PLC	C1-O3P-P-O1P
45	H	401	PLC	C4-C5-N-C7
45	H	401	PLC	C4-O4P-P-O3P
45	L	705	PLC	C1-O3P-P-O1P
45	M	1001	PLC	C1-O3P-P-O1P
45	M	1001	PLC	C4-O4P-P-O1P
45	N	601	PLC	C4-O4P-P-O1P
45	N	601	PLC	C4-O4P-P-O3P
45	Z	201	PLC	C4-O4P-P-O1P
45	b	101	PLC	C4-O4P-P-O1P
50	L	706	3PE	C11-O13-P-O12
50	L	706	3PE	O13-C11-C12-N
50	L	707	3PE	C1-O11-P-O14
50	L	707	3PE	C11-O13-P-O12
50	L	708	3PE	C1-O11-P-O12
50	L	708	3PE	C1-O11-P-O13
50	M	1004	3PE	C11-O13-P-O11
50	M	1004	3PE	C11-O13-P-O14
50	N	602	3PE	C1-O11-P-O12
50	Y	302	3PE	C1-O11-P-O14
50	b	104	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
50	b	106	3PE	C1-O11-P-O12
50	g	301	3PE	C1-O11-P-O13
50	g	301	3PE	C11-O13-P-O14
50	j	101	3PE	C11-O13-P-O11
50	j	101	3PE	C11-O13-P-O14
50	m	101	3PE	C11-O13-P-O14
50	m	101	3PE	O13-C11-C12-N
51	O	201	CDL	CB2-OB2-PB2-OB4
51	P	503	CDL	CA2-OA2-PA1-OA3
51	Z	202	CDL	CB2-OB2-PB2-OB5
51	a	201	CDL	CA3-OA5-PA1-OA3
51	b	102	CDL	CA3-OA5-PA1-OA4
50	L	710	3PE	C36-C37-C38-C39
45	L	705	PLC	C2-C1-O3P-P
45	P	502	PLC	C2-C1-O3P-P
50	L	708	3PE	C2-C1-O11-P
50	b	105	3PE	C2-C1-O11-P
51	Z	202	CDL	C1-CA2-OA2-PA1
51	Z	202	CDL	C74-C75-C76-C77
48	F	502	FMN	C5'-O5'-P-O1P
45	L	705	PLC	C2-C3-O3-CB
51	b	102	CDL	C16-C17-C18-C19
50	L	709	3PE	C34-C35-C36-C37
45	d	101	PLC	C'-C1'-C2'-C3'
51	Z	202	CDL	CB7-C71-C72-C73
51	b	102	CDL	C13-C14-C15-C16
45	Y	304	PLC	C3-C2-O2-C'
50	H	402	3PE	C3-C2-O21-C21
51	a	201	CDL	CA6-CA4-OA6-CA5
50	f	101	3PE	C3C-C3D-C3E-C3F
50	L	708	3PE	O11-C1-C2-C3
50	L	709	3PE	O11-C1-C2-C3
45	L	702	PLC	O3P-C1-C2-O2
51	O	201	CDL	OA5-CA3-CA4-OA6
52	P	501	NDP	O4B-C4B-C5B-O5B
45	P	502	PLC	OB-CB-O3-C3
50	j	101	3PE	C33-C34-C35-C36
51	a	201	CDL	C12-C13-C14-C15
51	a	201	CDL	CB7-C71-C72-C73
51	P	503	CDL	C32-C31-CA7-OA8
45	P	502	PLC	C1B-CB-O3-C3
50	L	710	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
45	Y	301	PLC	C2B-C3B-C4B-C5B
51	O	201	CDL	C83-C84-C85-C86
45	N	601	PLC	C4'-C5'-C6'-C7'
51	a	201	CDL	C54-C55-C56-C57
45	Z	201	PLC	C5B-C6B-C7B-C8B
45	L	702	PLC	C3B-C4B-C5B-C6B
50	L	707	3PE	C2A-C2B-C2C-C2D
50	L	709	3PE	C3A-C3B-C3C-C3D
50	g	301	3PE	C24-C25-C26-C27
45	h	201	PLC	C1'-C2'-C3'-C4'
50	L	703	3PE	C28-C29-C2A-C2B
50	b	103	3PE	C34-C35-C36-C37
51	Z	202	CDL	OA6-CA4-CA6-OA8
50	N	602	3PE	C2F-C2G-C2H-C2I
50	L	709	3PE	C36-C37-C38-C39
50	L	708	3PE	C27-C28-C29-C2A
45	A	201	PLC	C2-C1-O3P-P
51	b	102	CDL	CB3-CB4-CB6-OB8
54	U	201	EHZ	C10-C11-N1-C12
51	O	201	CDL	CA3-CA4-OA6-CA5
50	L	709	3PE	C33-C34-C35-C36
45	q	402	PLC	O'-C'-O2-C2
45	M	1001	PLC	C4B-C5B-C6B-C7B
45	q	401	PLC	O3P-C1-C2-O2
50	L	703	3PE	C35-C36-C37-C38
50	b	103	3PE	C2-C1-O11-P
45	M	1003	PLC	C2B-C3B-C4B-C5B
45	H	401	PLC	O'-C'-O2-C2
45	M	1001	PLC	C4'-C5'-C6'-C7'
45	Z	201	PLC	O2-C2-C3-O3
45	Z	201	PLC	C1B-C2B-C3B-C4B
50	b	104	3PE	C32-C33-C34-C35
51	O	201	CDL	C72-C73-C74-C75
45	L	705	PLC	CB-C1B-C2B-C3B
45	D	501	PLC	C6B-C7B-C8B-C9B
45	L	704	PLC	C3B-C4B-C5B-C6B
50	f	101	3PE	C2-C1-O11-P
48	F	502	FMN	O3'-C3'-C4'-C5'
45	B	302	PLC	OB-CB-O3-C3
50	f	101	3PE	C31-C32-C33-C34
50	m	101	3PE	C32-C33-C34-C35
50	N	602	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	L	704	PLC	C2B-C1B-CB-O3
45	d	101	PLC	C3'-C4'-C5'-C6'
50	L	710	3PE	C38-C39-C3A-C3B
51	Z	202	CDL	C72-C71-CB7-OB9
50	H	402	3PE	O31-C31-C32-C33
54	T	201	EHZ	C22-C23-C24-C25
45	M	1003	PLC	O3P-C1-C2-C3
50	b	104	3PE	C2-C1-O11-P
45	M	1001	PLC	C6B-C7B-C8B-C9B
50	L	707	3PE	C34-C35-C36-C37
45	L	704	PLC	C1B-C2B-C3B-C4B
50	L	709	3PE	C37-C38-C39-C3A
50	f	101	3PE	C38-C39-C3A-C3B
45	B	302	PLC	C1B-CB-O3-C3
50	m	101	3PE	O32-C31-O31-C3
45	Z	201	PLC	C6'-C7'-C8'-C9'
50	b	103	3PE	O21-C21-C22-C23
51	O	201	CDL	C36-C37-C38-C39
50	b	105	3PE	C23-C24-C25-C26
45	L	705	PLC	C1'-C2'-C3'-C4'
45	D	501	PLC	C4'-C5'-C6'-C7'
50	L	707	3PE	C37-C38-C39-C3A
50	m	101	3PE	C32-C31-O31-C3
48	F	502	FMN	C4'-C5'-O5'-P
45	L	704	PLC	O3P-C1-C2-O2
45	q	402	PLC	O3P-C1-C2-O2
50	L	706	3PE	O11-C1-C2-O21
50	M	1004	3PE	C1-C2-C3-O31
50	M	1004	3PE	C33-C34-C35-C36
45	L	704	PLC	C1'-C2'-C3'-C4'
50	m	101	3PE	O31-C31-C32-C33
50	L	710	3PE	C3F-C3G-C3H-C3I
45	B	302	PLC	O3P-C1-C2-C3
45	q	401	PLC	O3P-C1-C2-C3
50	L	708	3PE	C33-C34-C35-C36
45	Z	201	PLC	C5'-C6'-C7'-C8'
45	Z	201	PLC	C4-C5-N-C6
45	Z	201	PLC	C4-C5-N-C7
45	D	501	PLC	C3'-C4'-C5'-C6'
50	L	701	3PE	O21-C21-C22-C23
51	Z	202	CDL	C32-C31-CA7-OA8
50	L	710	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
52	P	501	NDP	PN-O3-PA-O2A
50	b	106	3PE	C23-C24-C25-C26
45	q	402	PLC	C1'-C'-O2-C2
45	L	705	PLC	C2B-C1B-CB-O3
50	L	708	3PE	O21-C21-C22-C23
50	L	710	3PE	O31-C31-C32-C33
51	a	201	CDL	C52-C51-CB5-OB6
45	A	201	PLC	C4-C5-N-C6
45	b	101	PLC	C4-C5-N-C7
45	b	101	PLC	C4-C5-N-C8
50	Y	303	3PE	C35-C36-C37-C38
50	L	709	3PE	O31-C31-C32-C33
51	Z	202	CDL	CA7-C31-C32-C33
50	L	703	3PE	C36-C37-C38-C39
45	B	302	PLC	CB-C1B-C2B-C3B
50	L	706	3PE	O31-C31-C32-C33
50	L	709	3PE	O21-C21-C22-C23
45	B	302	PLC	C1B-C2B-C3B-C4B
45	M	1003	PLC	C6B-C7B-C8B-C9B
50	N	602	3PE	C29-C2A-C2B-C2C
50	g	301	3PE	O31-C31-C32-C33
51	a	201	CDL	C12-C11-CA5-OA6
51	O	201	CDL	C82-C83-C84-C85
51	Z	202	CDL	CA3-CA4-CA6-OA8
45	A	201	PLC	C4-C5-N-C7
50	f	101	3PE	C24-C25-C26-C27
50	b	105	3PE	O21-C21-C22-C23
50	b	106	3PE	O21-C21-C22-C23
50	L	701	3PE	C22-C23-C24-C25
51	b	102	CDL	C14-C15-C16-C17
50	L	708	3PE	O21-C2-C3-O31
50	Y	302	3PE	C2B-C2C-C2D-C2E
45	q	401	PLC	C2'-C3'-C4'-C5'
51	P	503	CDL	OA9-CA7-OA8-CA6
45	L	704	PLC	O3P-C1-C2-C3
45	q	402	PLC	O3P-C1-C2-C3
54	U	201	EHZ	C19-C17-C20-O6
51	P	503	CDL	C31-CA7-OA8-CA6
54	T	201	EHZ	C21-C1-C2-C3
50	H	402	3PE	C1-C2-O21-C21
45	Y	304	PLC	C4-C5-N-C7
50	L	709	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
50	L	708	3PE	O22-C21-C22-C23
45	M	1002	PLC	C3B-C4B-C5B-C6B
50	j	101	3PE	C32-C33-C34-C35
51	Z	202	CDL	C32-C31-CA7-OA9
45	h	201	PLC	C7'-C8'-C9'-CA'
50	L	711	3PE	O21-C21-C22-C23
50	Y	302	3PE	C33-C34-C35-C36
48	F	502	FMN	C2'-C3'-C4'-O4'
45	Z	201	PLC	C8'-C9'-CA'-CB'
45	Y	304	PLC	C4-C5-N-C8
50	L	703	3PE	C26-C27-C28-C29
50	L	706	3PE	C33-C34-C35-C36
50	N	602	3PE	C2B-C2C-C2D-C2E
50	f	101	3PE	C39-C3A-C3B-C3C
51	O	201	CDL	C33-C34-C35-C36
45	L	705	PLC	C2B-C1B-CB-OB
50	g	301	3PE	O32-C31-C32-C33
51	O	201	CDL	CA7-C31-C32-C33
50	L	709	3PE	O22-C21-C22-C23
50	b	106	3PE	O22-C21-C22-C23
50	b	105	3PE	O22-C21-C22-C23
50	m	101	3PE	O32-C31-C32-C33
50	L	701	3PE	O22-C21-C22-C23
50	L	709	3PE	O32-C31-C32-C33
45	D	501	PLC	C1-C2-C3-O3
51	a	201	CDL	C52-C51-CB5-OB7
50	M	1004	3PE	O31-C31-C32-C33
50	L	711	3PE	C38-C39-C3A-C3B
50	L	706	3PE	C3D-C3E-C3F-C3G
50	L	710	3PE	O32-C31-C32-C33
45	q	401	PLC	C3'-C4'-C5'-C6'
50	L	708	3PE	O31-C31-C32-C33
50	L	711	3PE	C23-C24-C25-C26
50	N	602	3PE	C32-C33-C34-C35
50	L	706	3PE	O32-C31-C32-C33
50	L	710	3PE	C25-C26-C27-C28
50	f	101	3PE	C2E-C2F-C2G-C2H
50	L	711	3PE	O22-C21-C22-C23

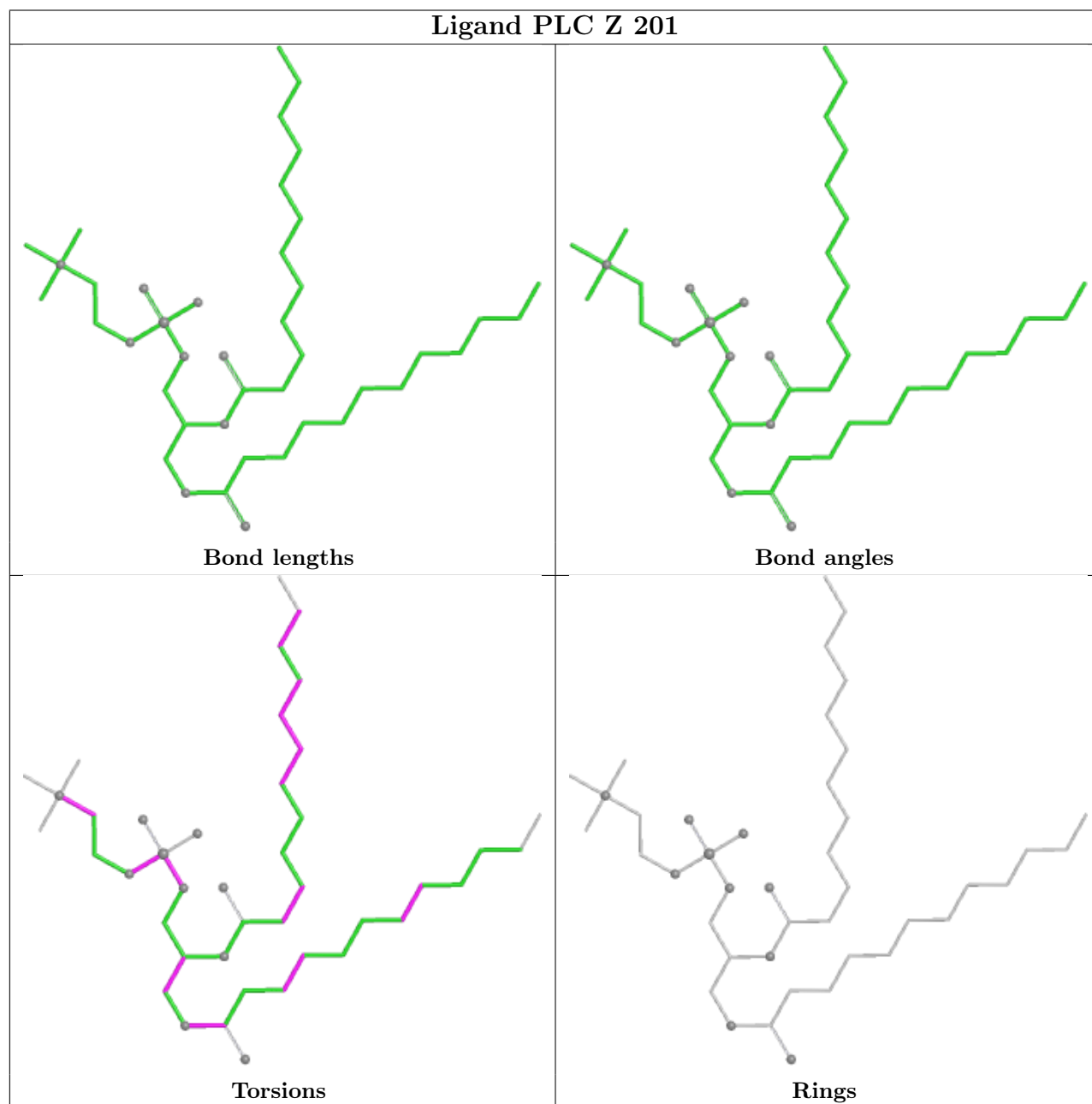
There are no ring outliers.

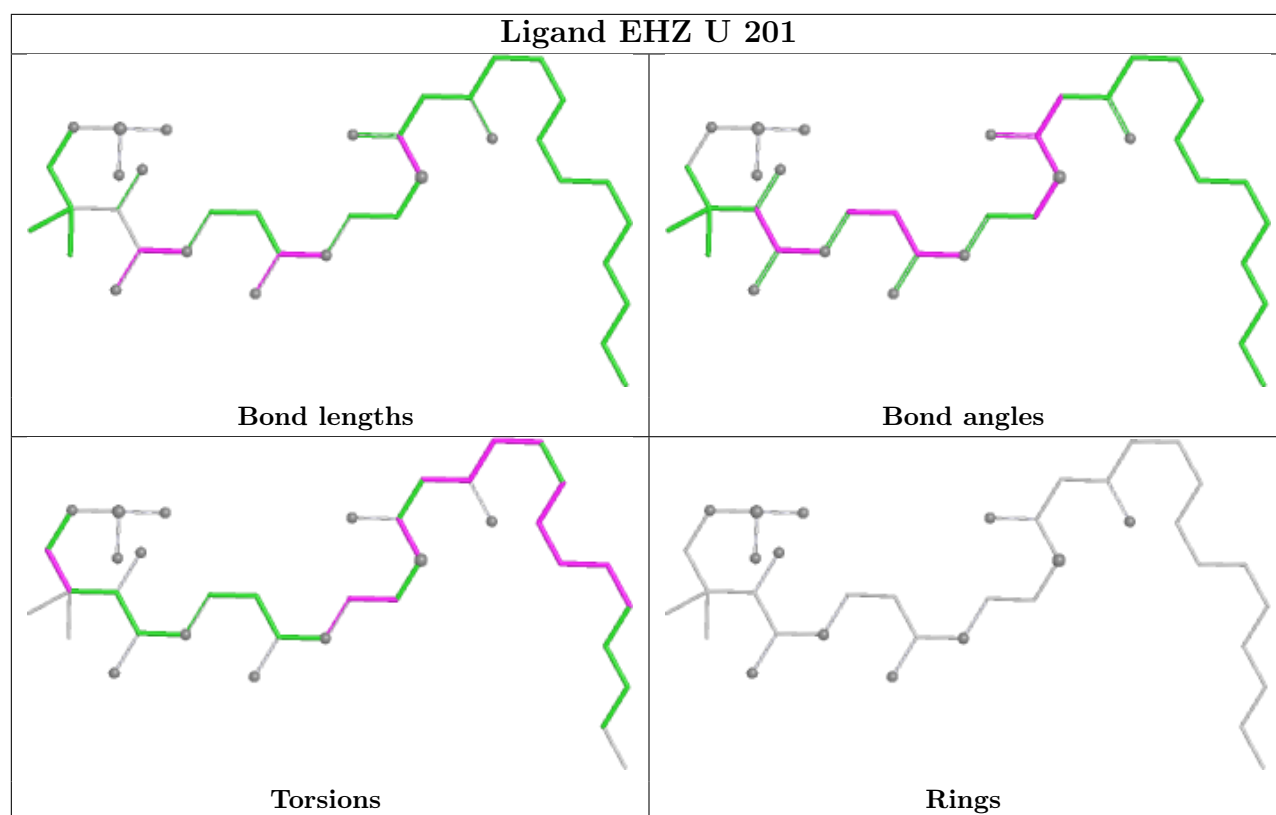
39 monomers are involved in 95 short contacts:

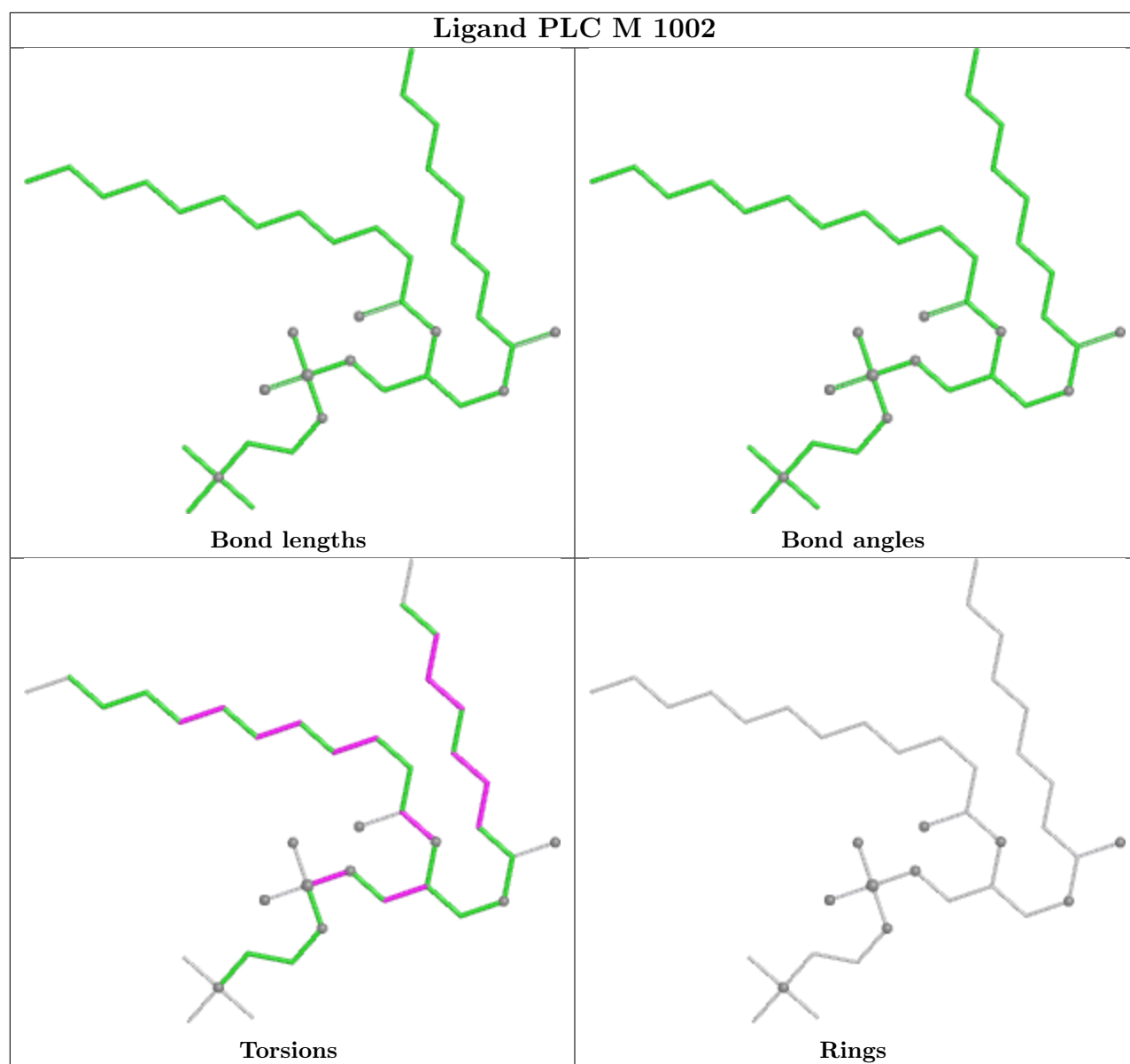
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	U	201	EHZ	1	0
45	M	1002	PLC	3	0
45	A	201	PLC	2	0
46	F	501	SF4	2	0
45	b	101	PLC	2	0
46	I	302	SF4	2	0
50	Y	303	3PE	1	0
50	L	711	3PE	2	0
51	a	201	CDL	2	0
45	M	1003	PLC	1	0
50	L	706	3PE	7	0
45	P	502	PLC	3	0
46	G	802	SF4	1	0
50	N	602	3PE	1	0
50	f	101	3PE	7	0
50	L	709	3PE	2	0
45	B	302	PLC	1	0
45	L	705	PLC	3	0
50	b	106	3PE	2	0
51	b	102	CDL	3	0
45	d	101	PLC	4	0
50	L	708	3PE	3	0
50	L	703	3PE	2	0
45	q	402	PLC	1	0
45	h	201	PLC	2	0
45	D	501	PLC	2	0
52	P	501	NDP	1	0
45	L	702	PLC	3	0
46	I	301	SF4	1	0
51	O	201	CDL	5	0
50	Y	302	3PE	8	0
50	L	707	3PE	5	0
45	Y	301	PLC	1	0
50	g	301	3PE	2	0
50	b	104	3PE	2	0
50	b	105	3PE	1	0
50	L	710	3PE	4	0
45	q	401	PLC	3	0
45	L	704	PLC	1	0

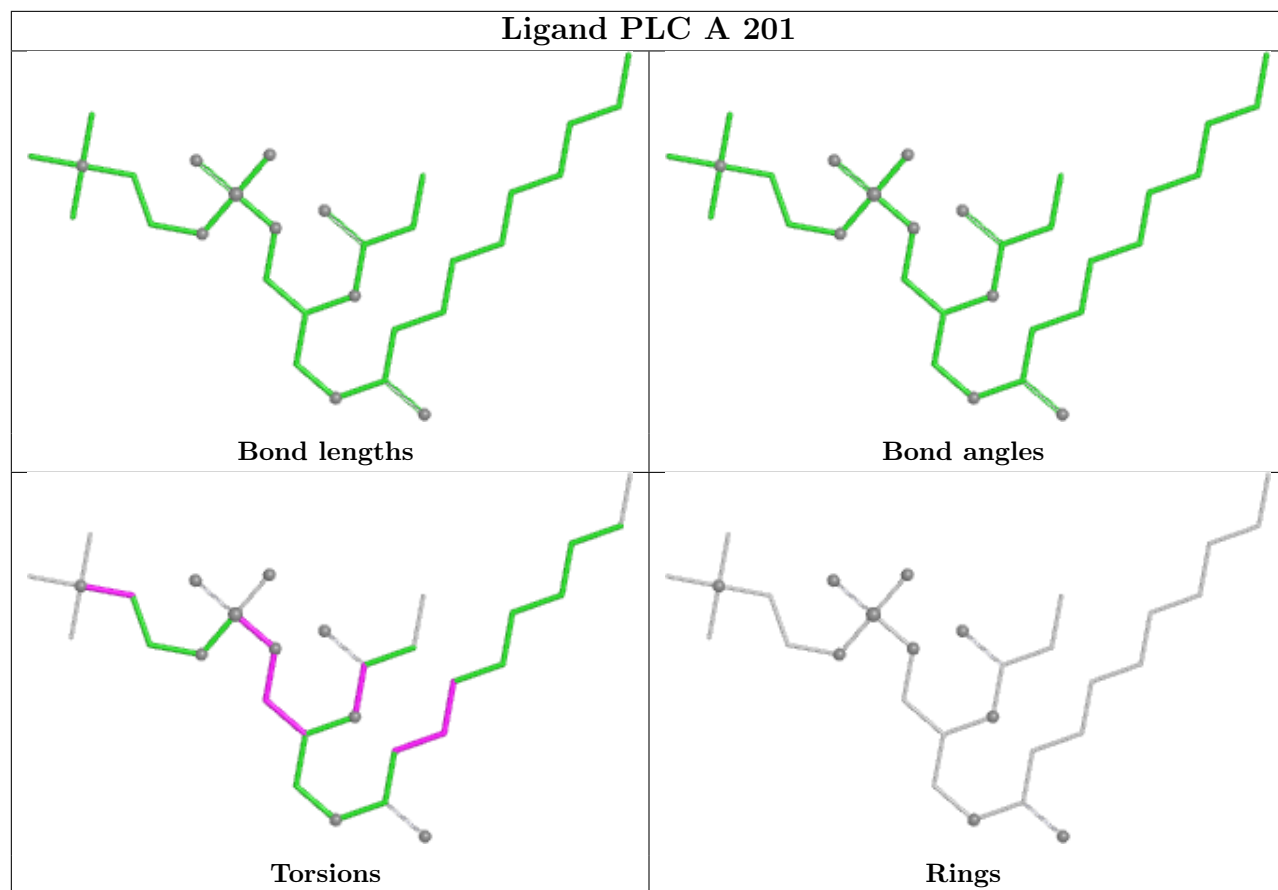
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

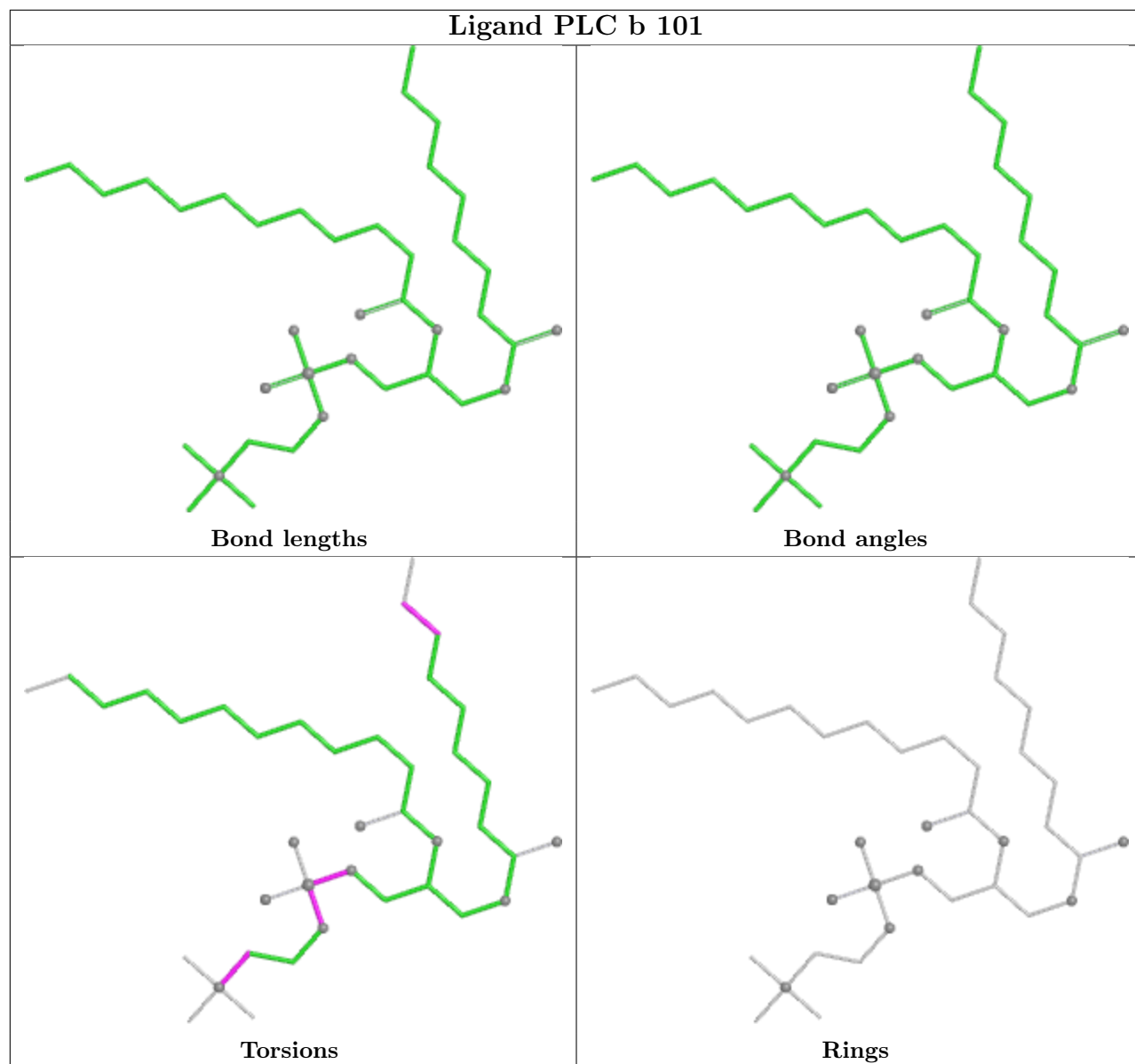
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



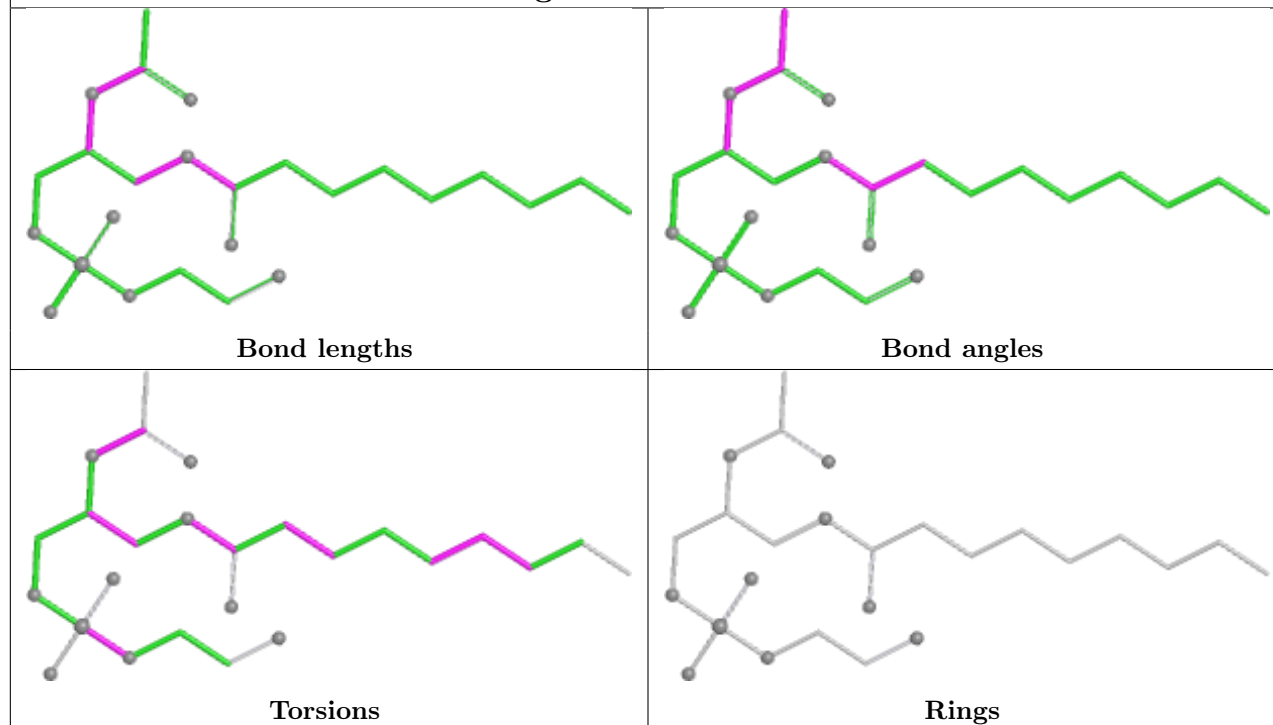




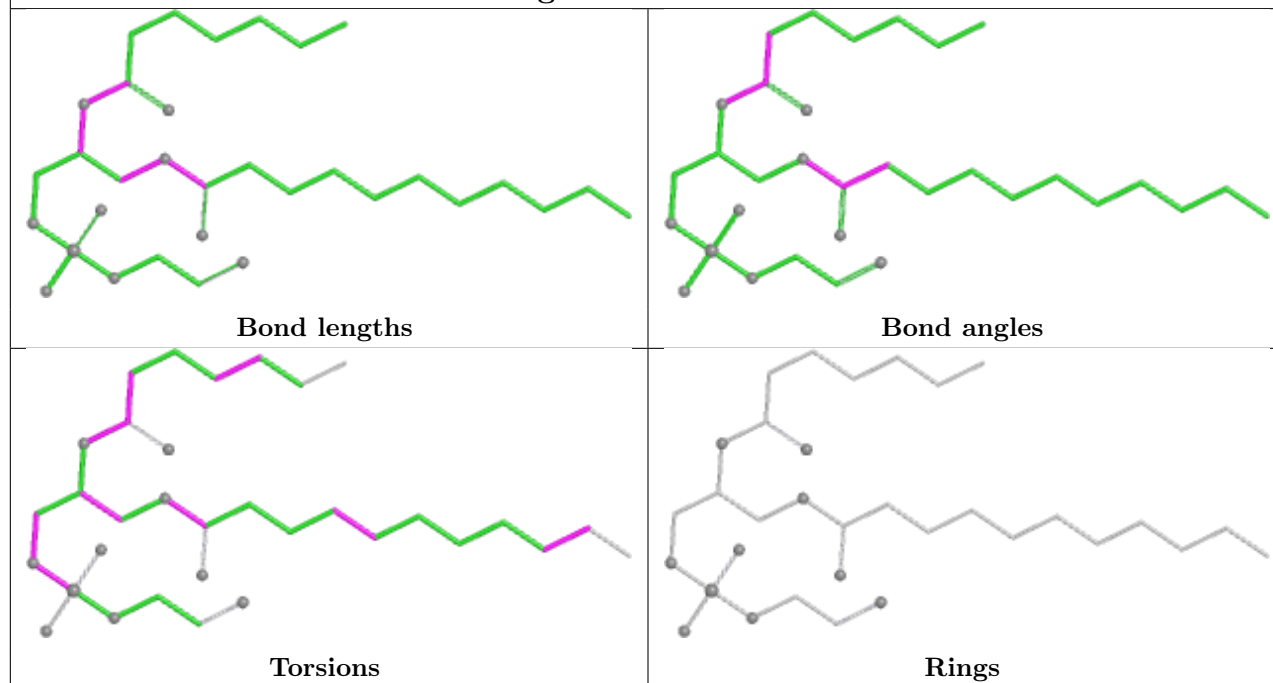


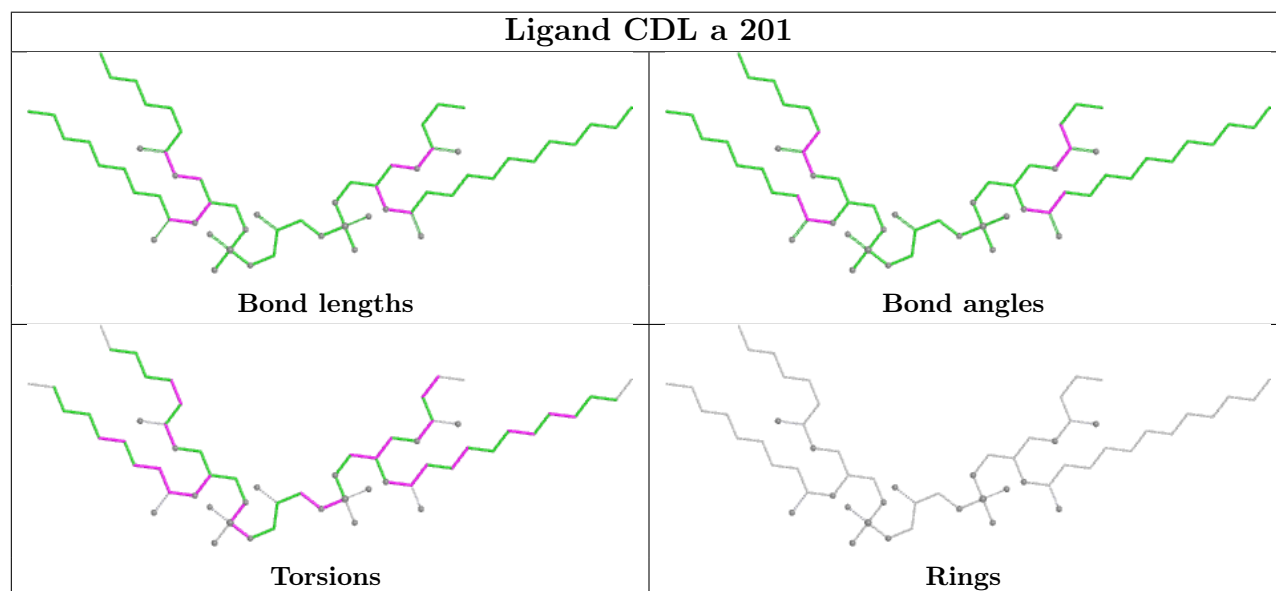
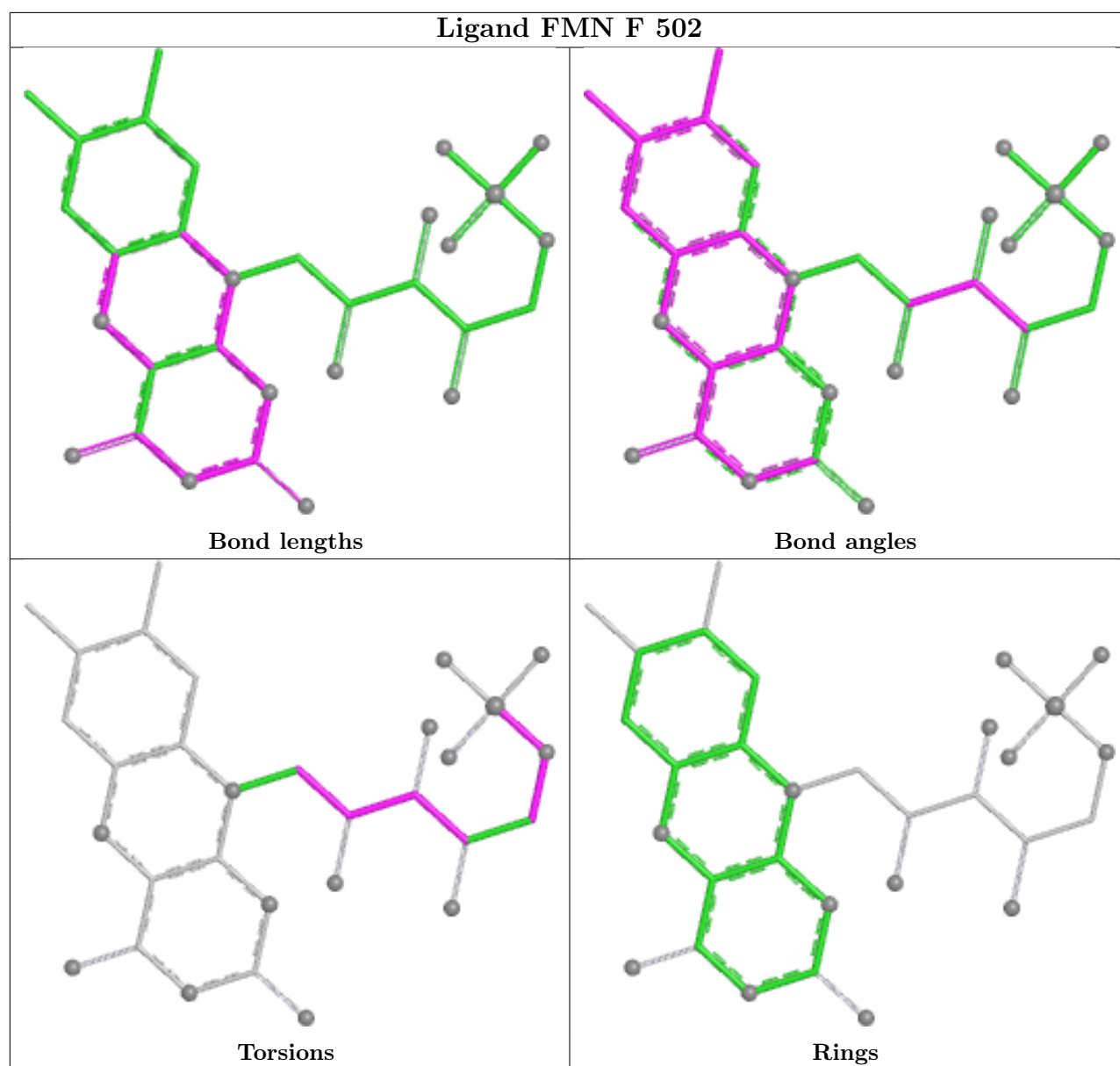


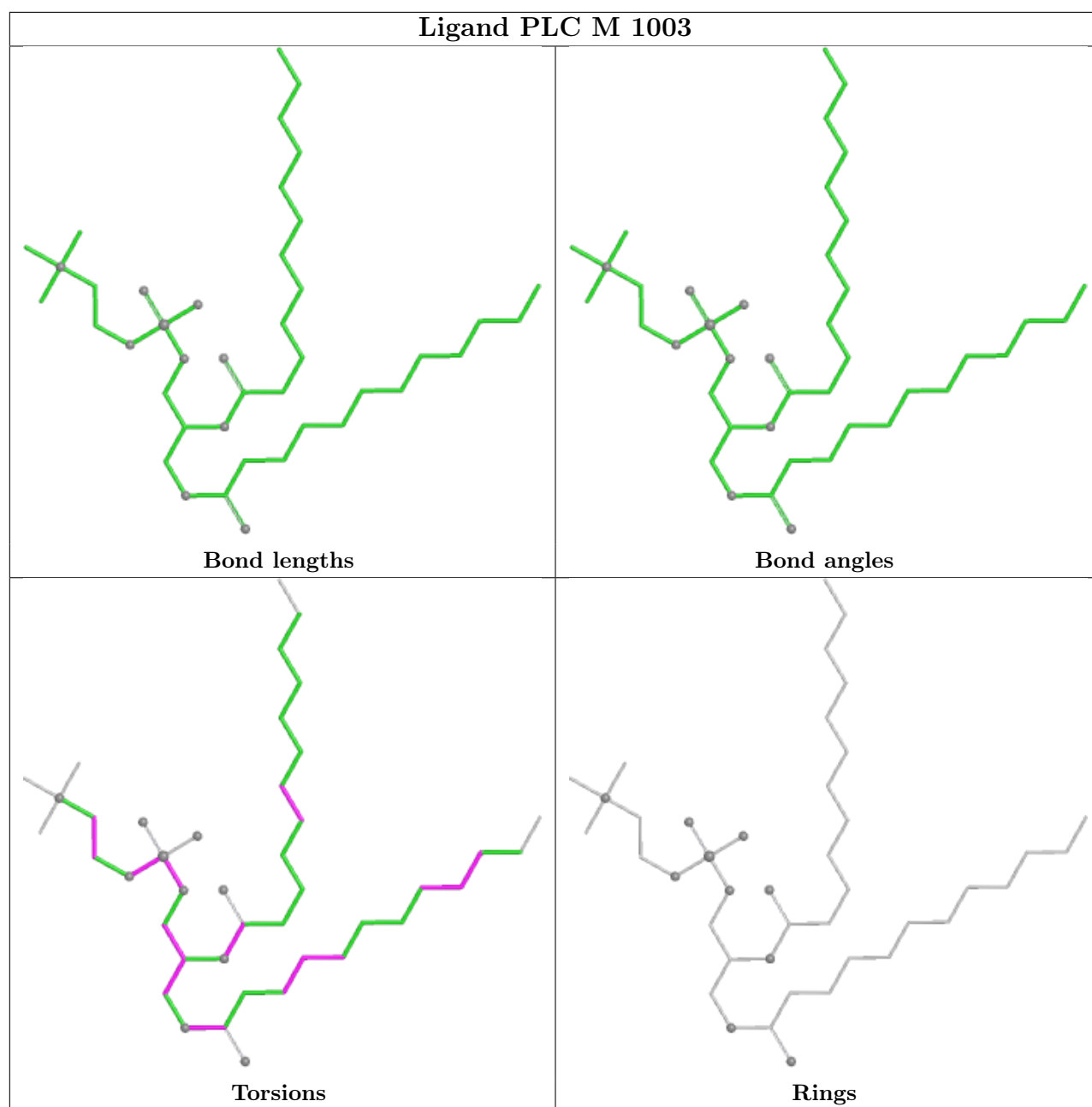
Ligand 3PE Y 303

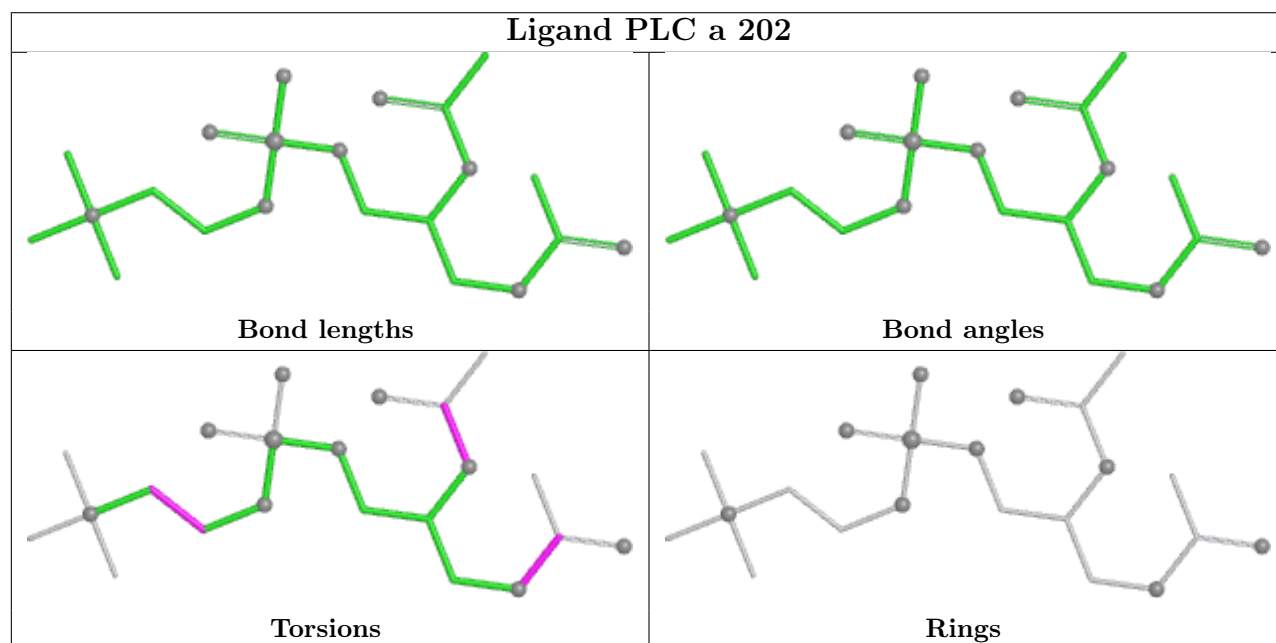
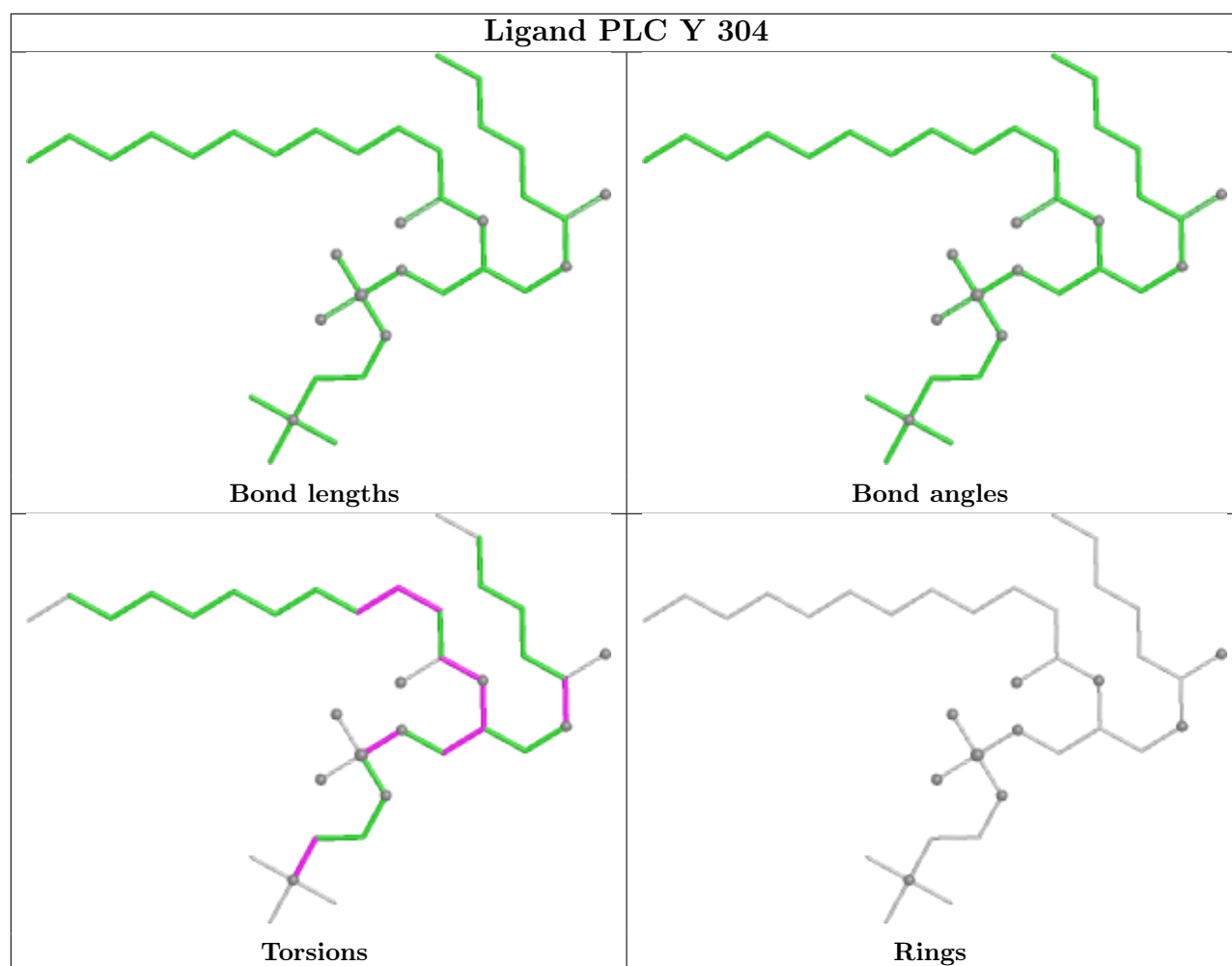


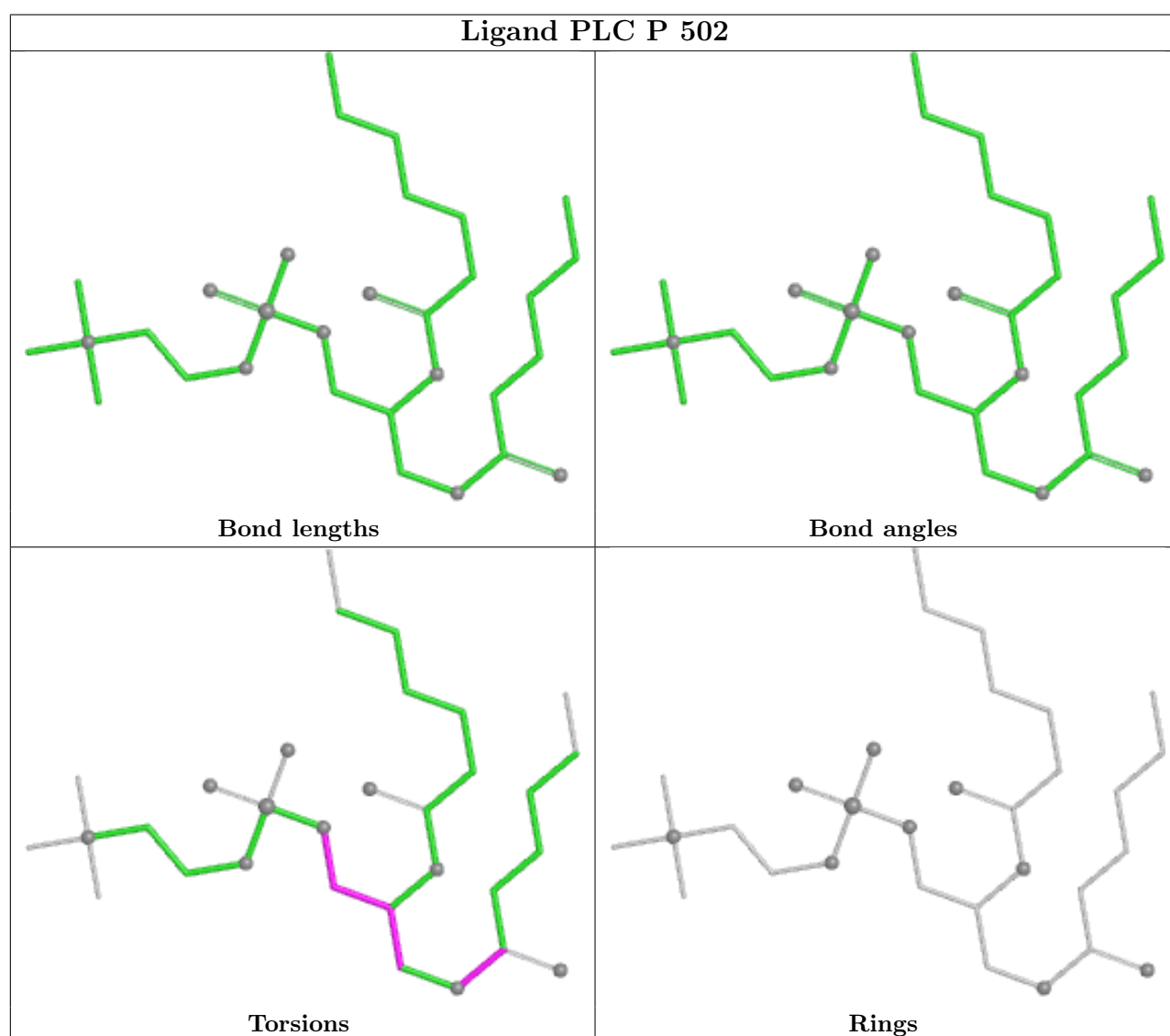
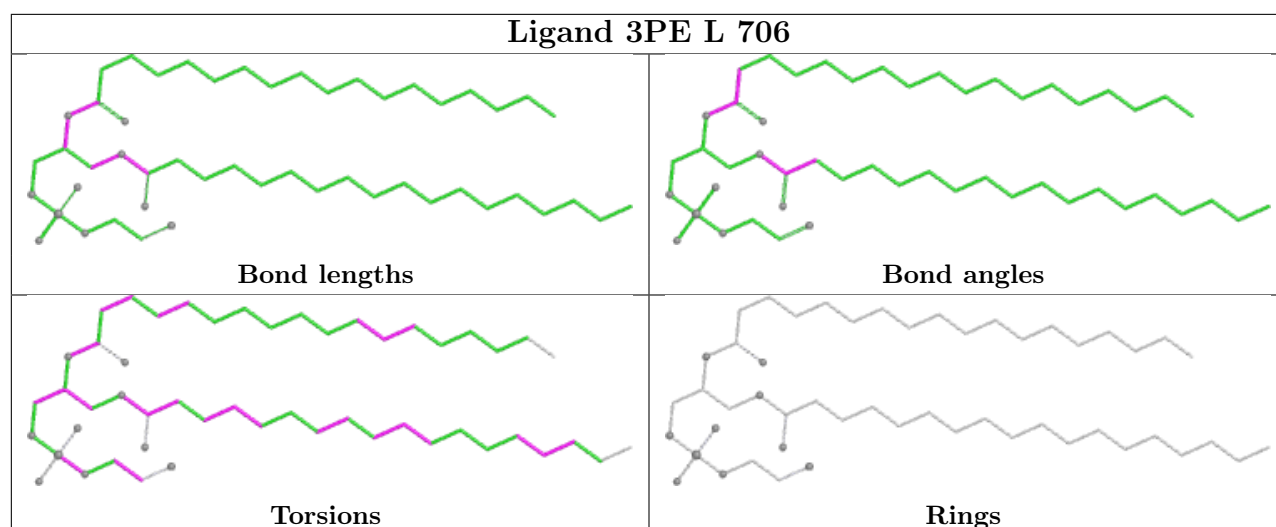
Ligand 3PE L 711

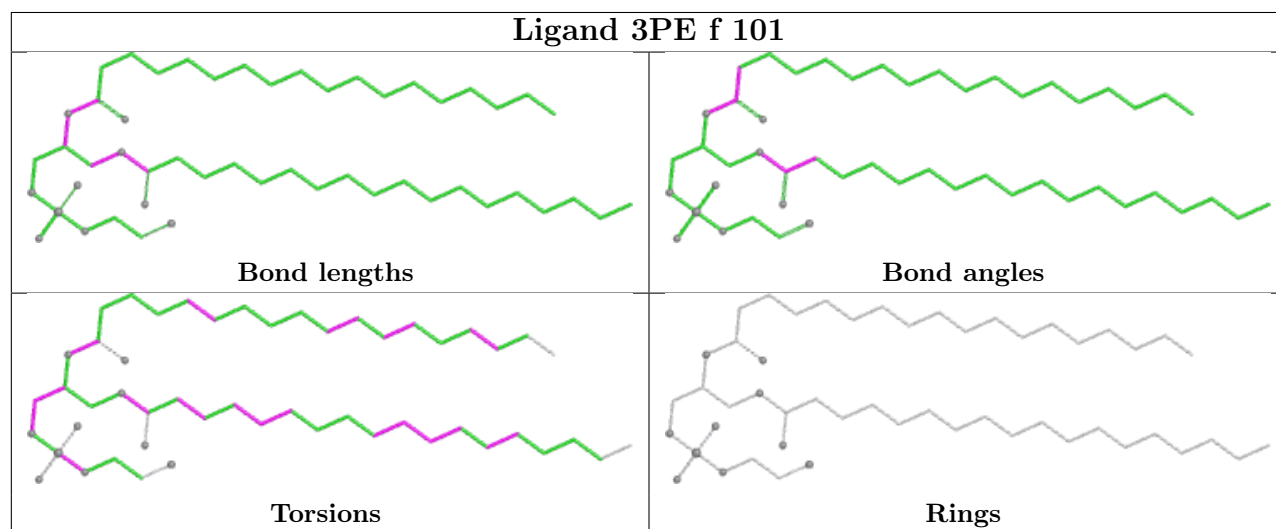
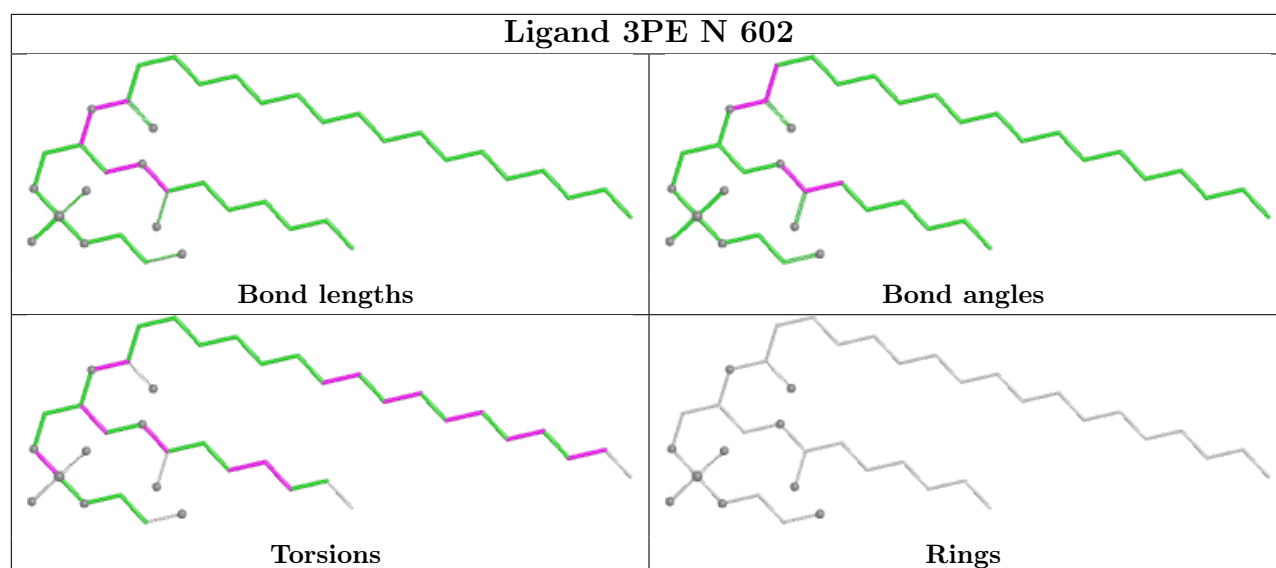


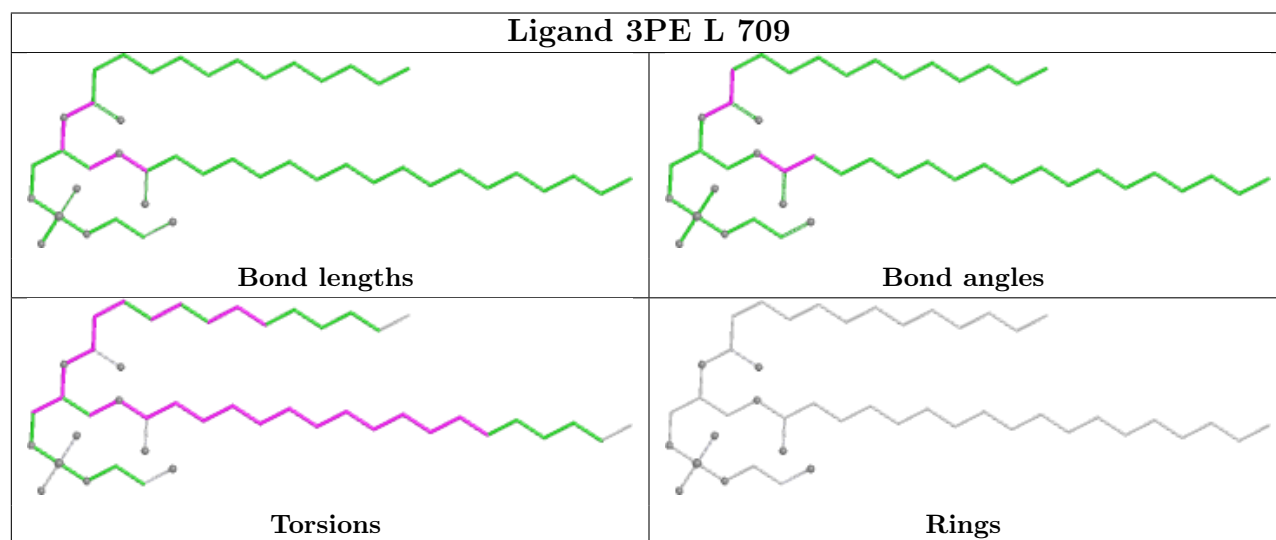
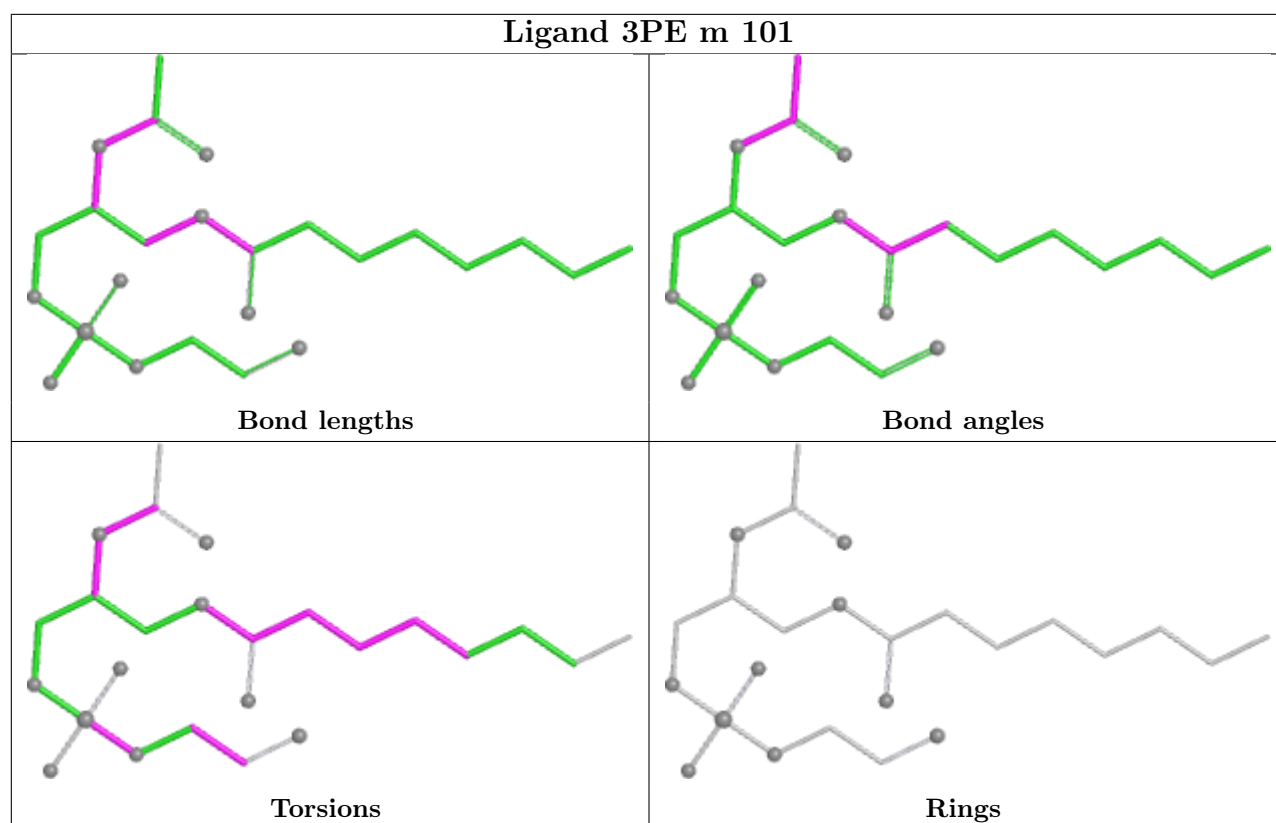


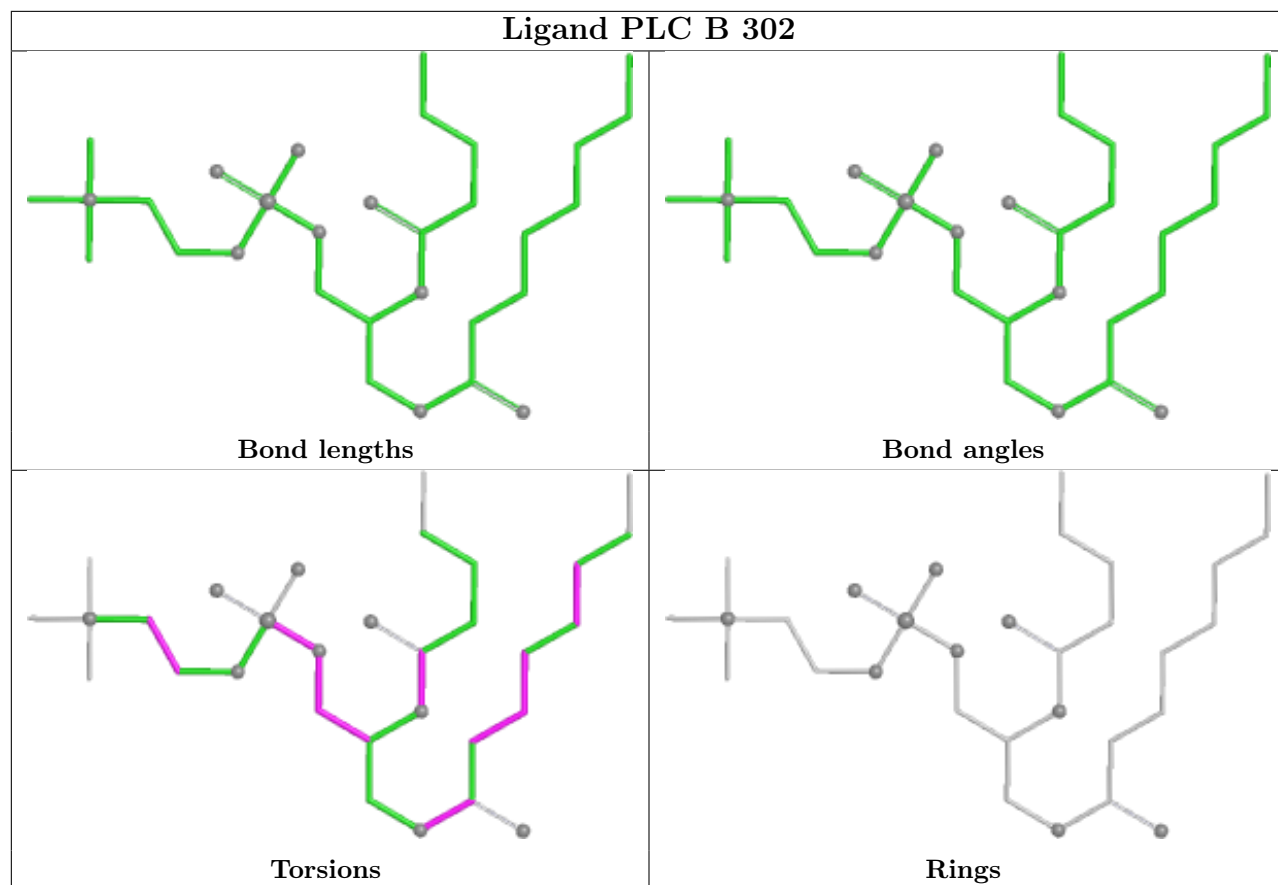


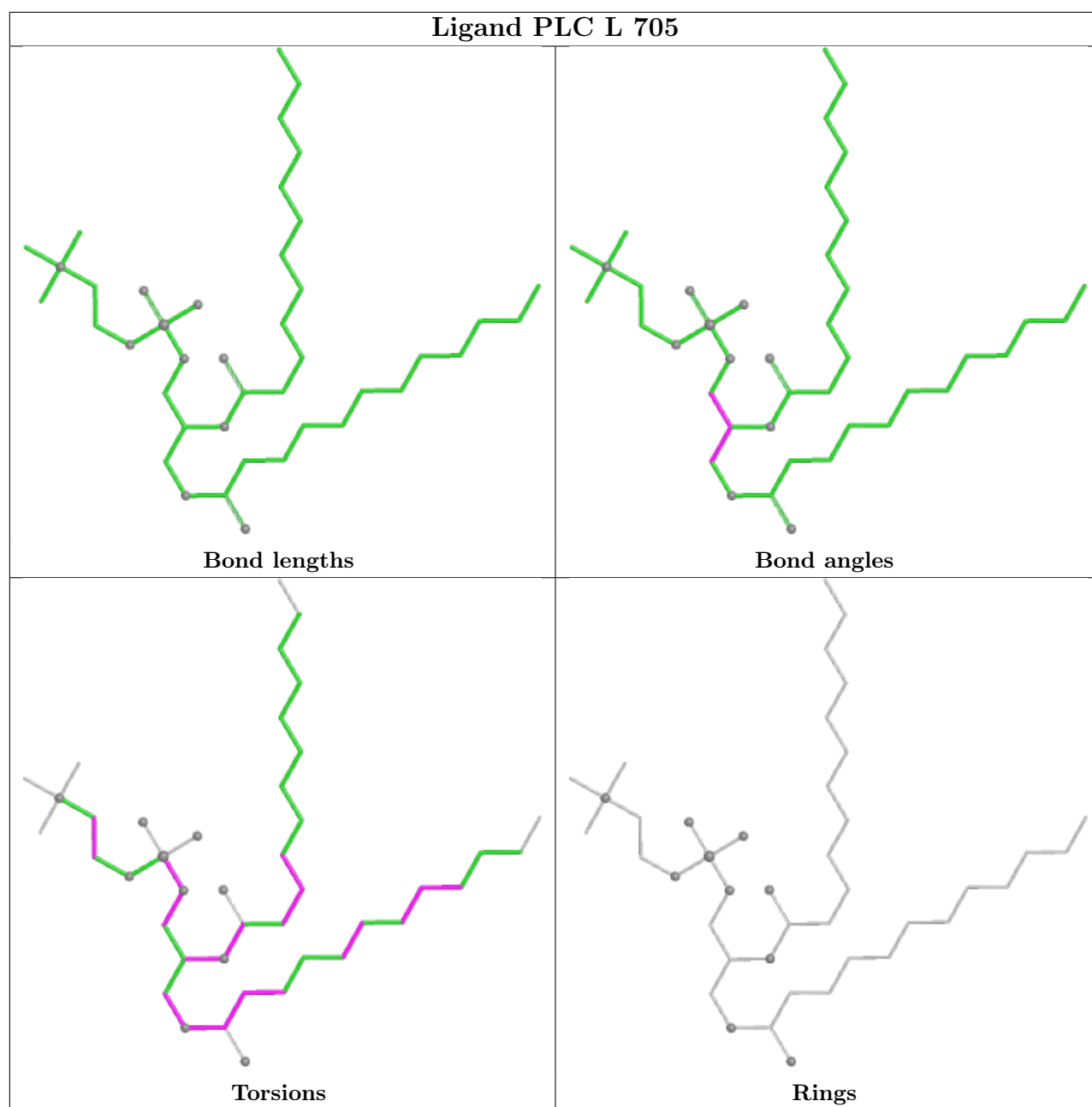


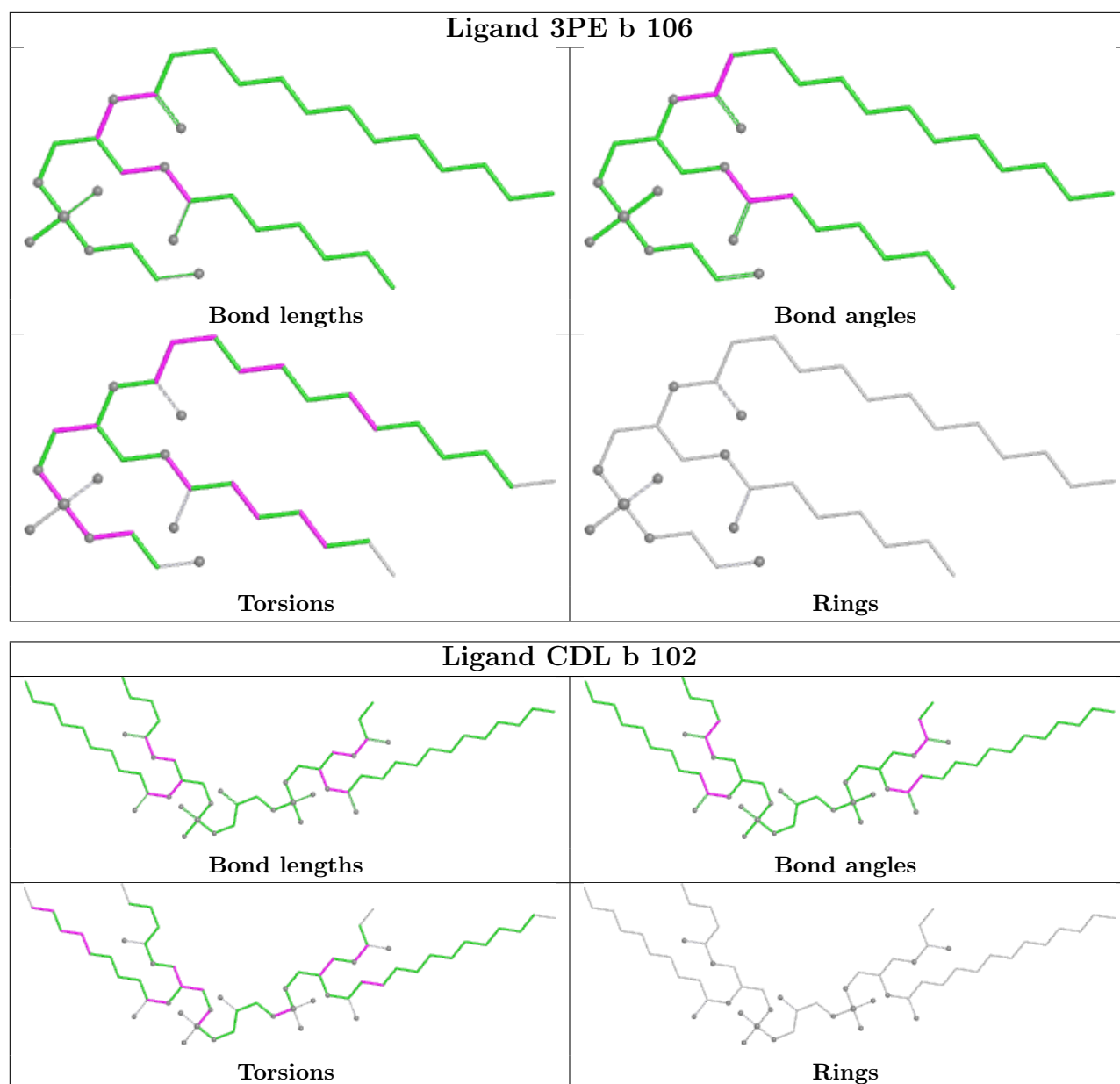


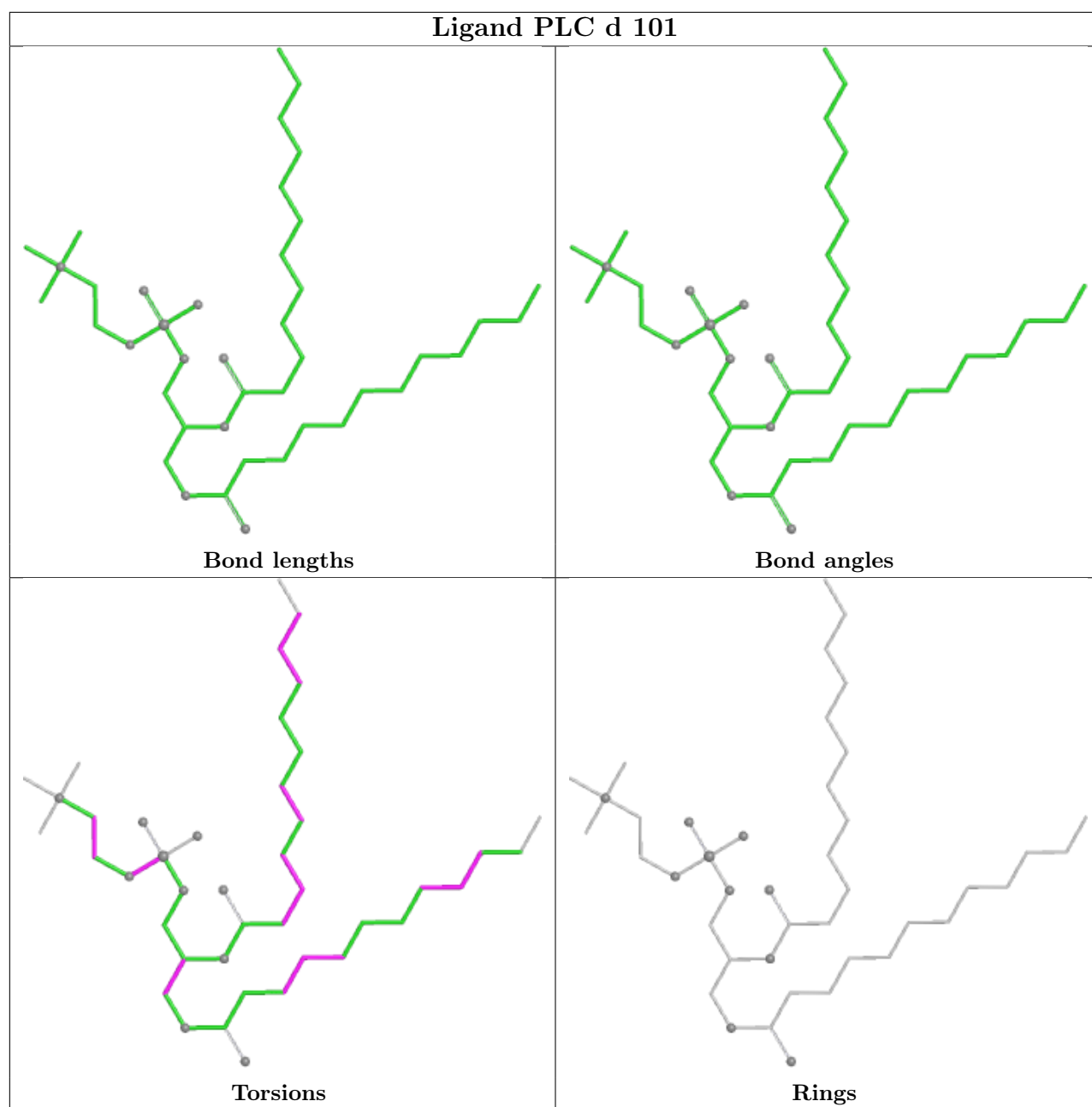


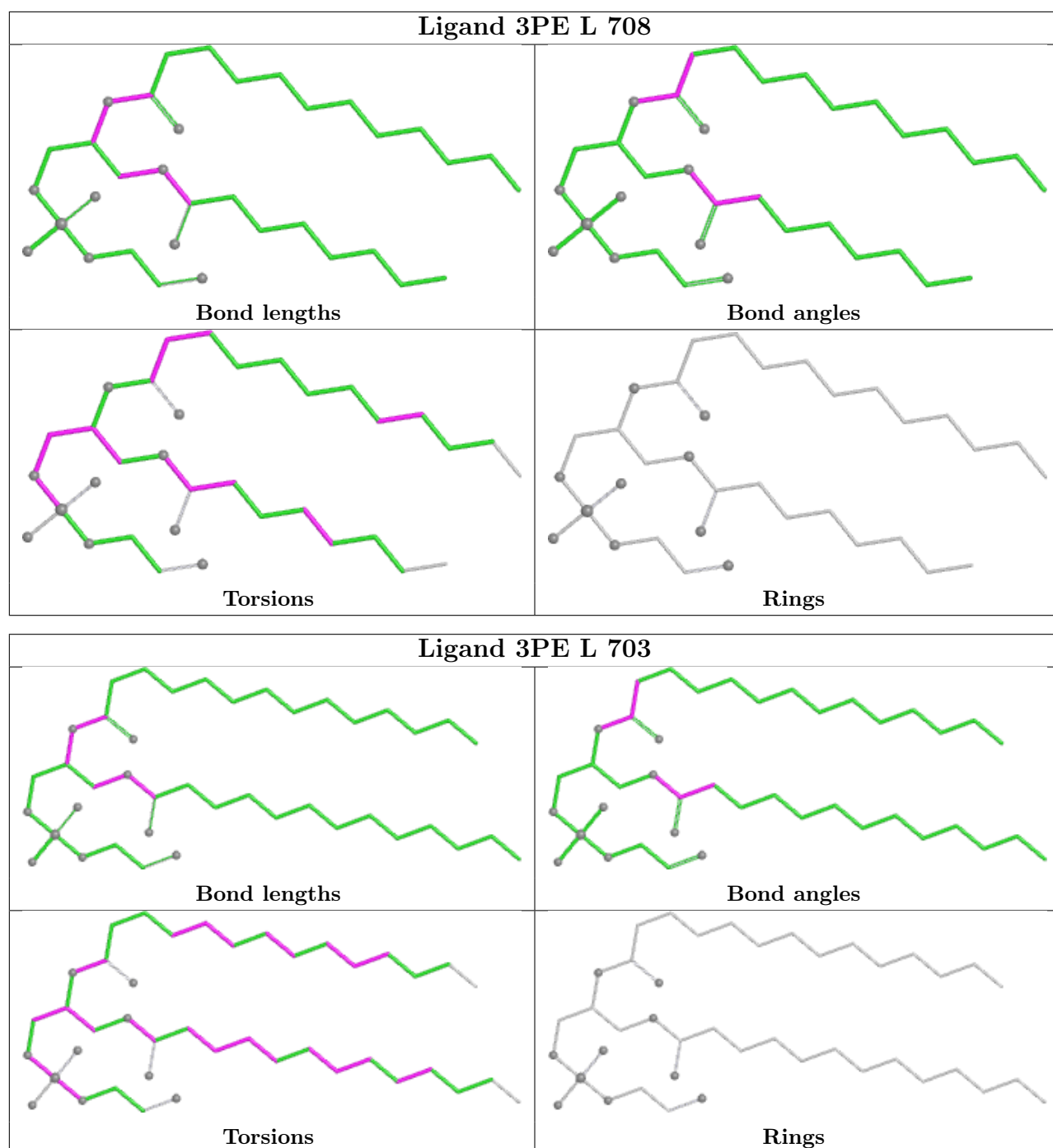


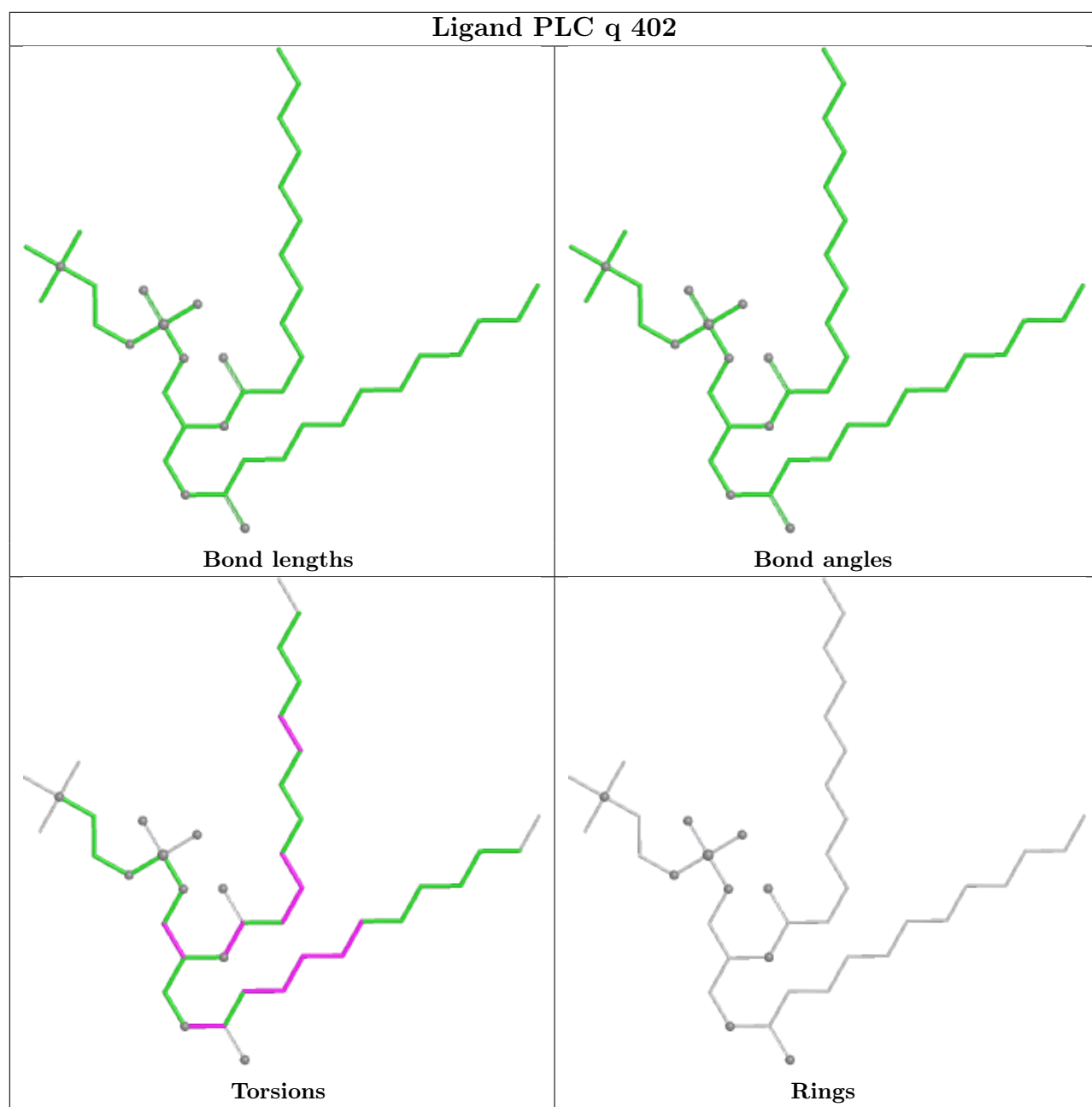


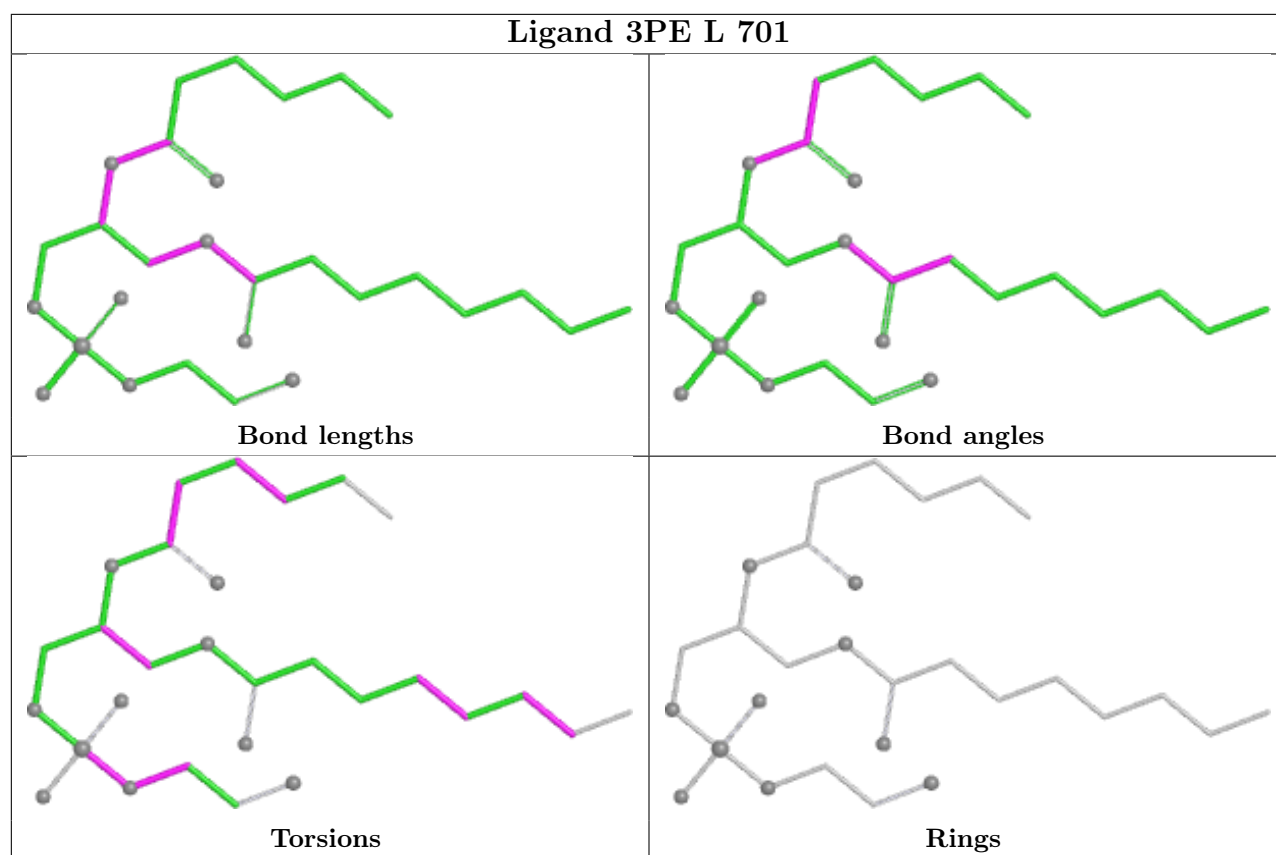


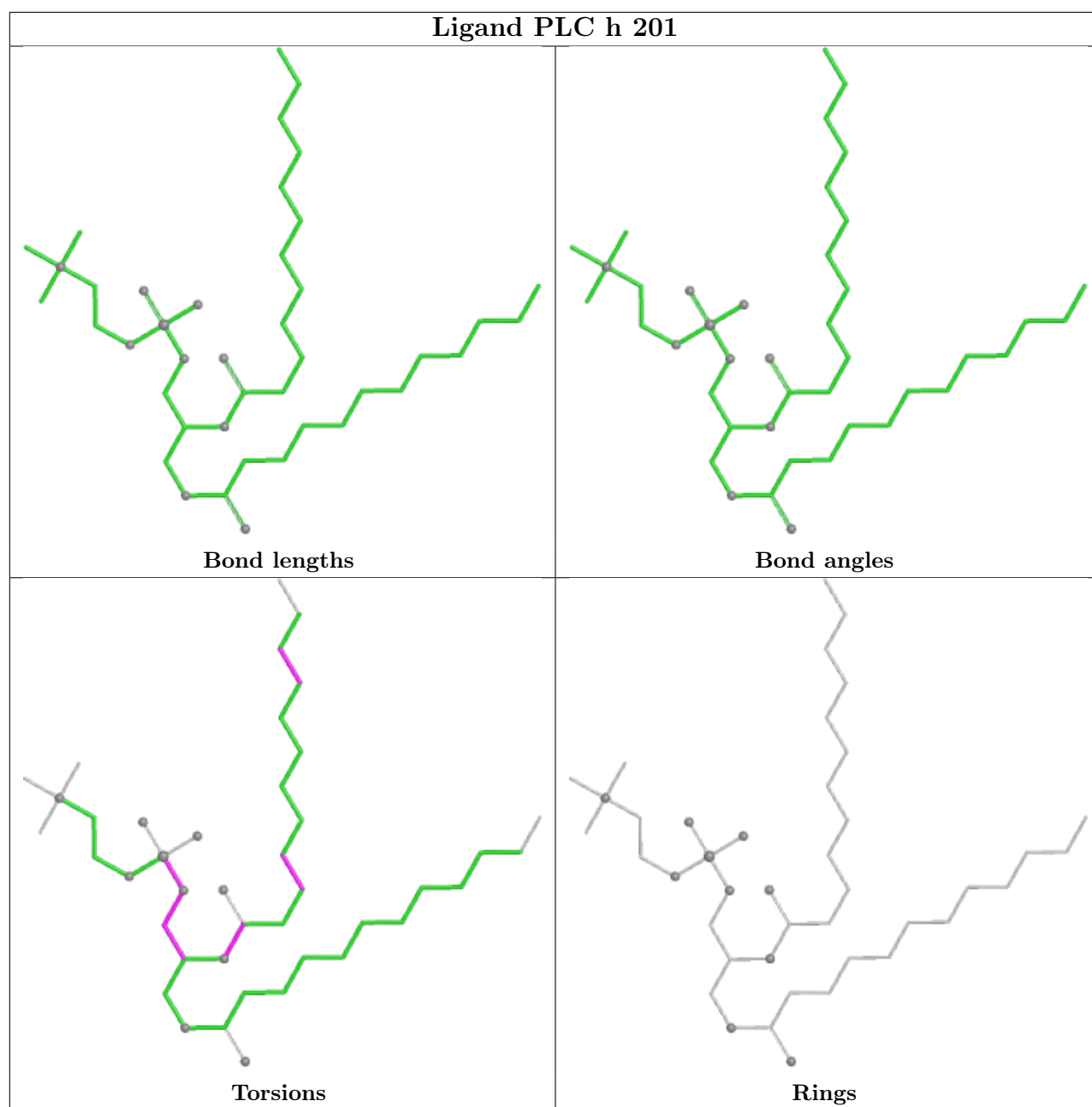


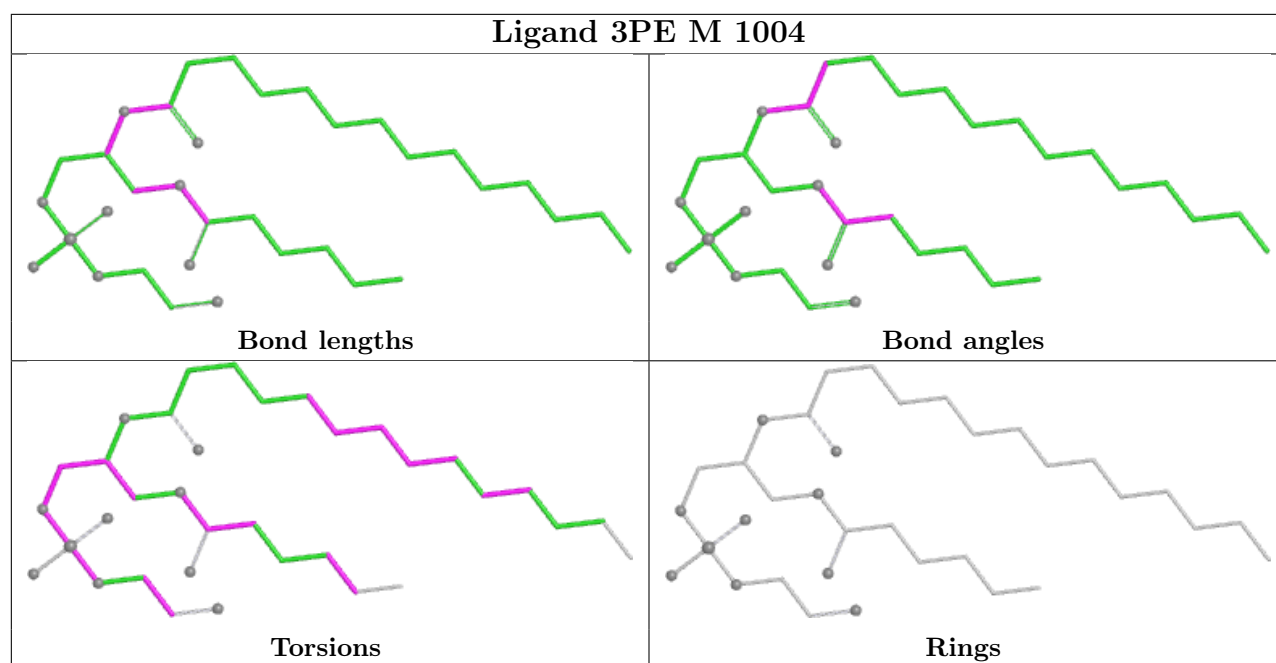


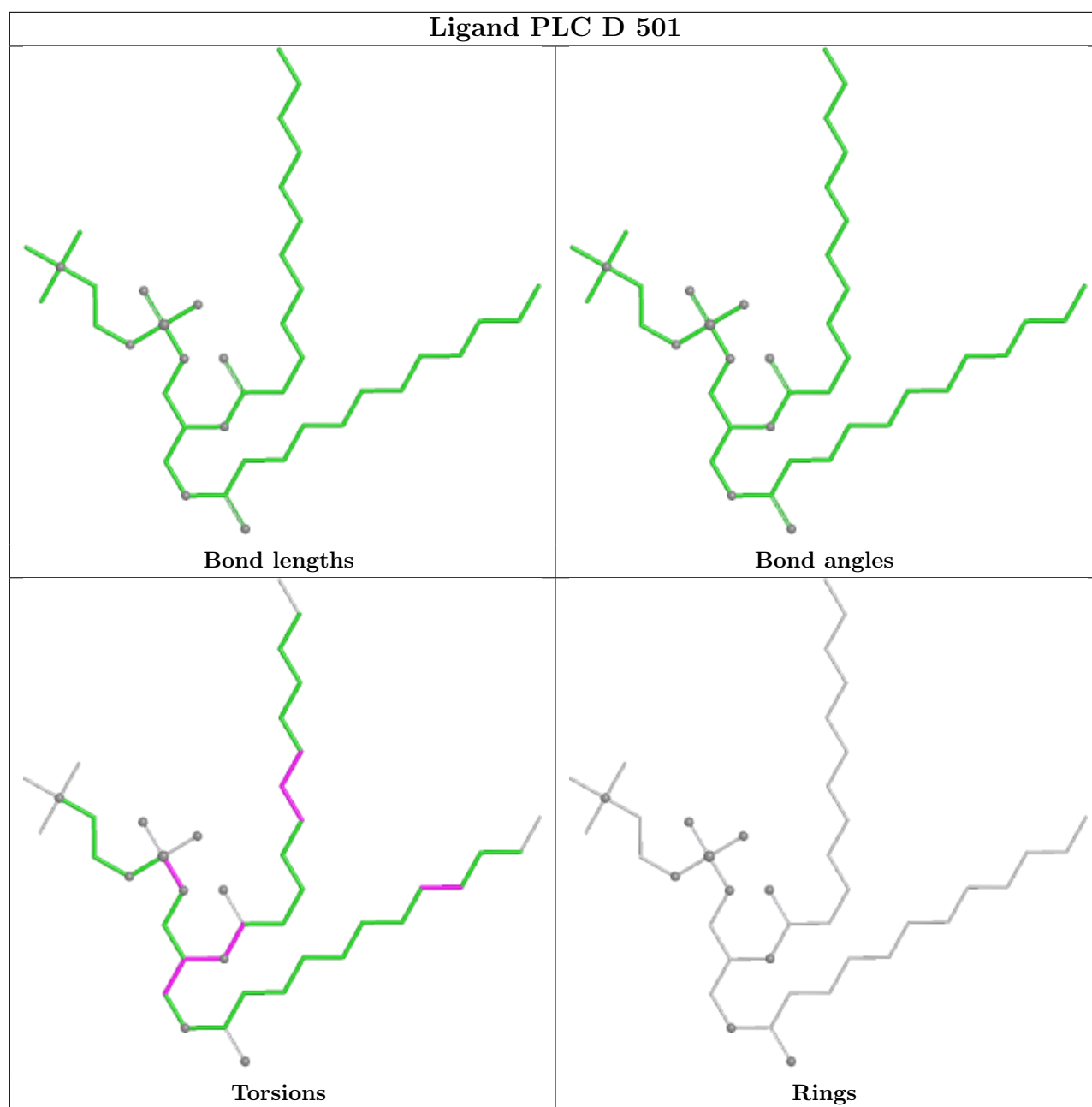


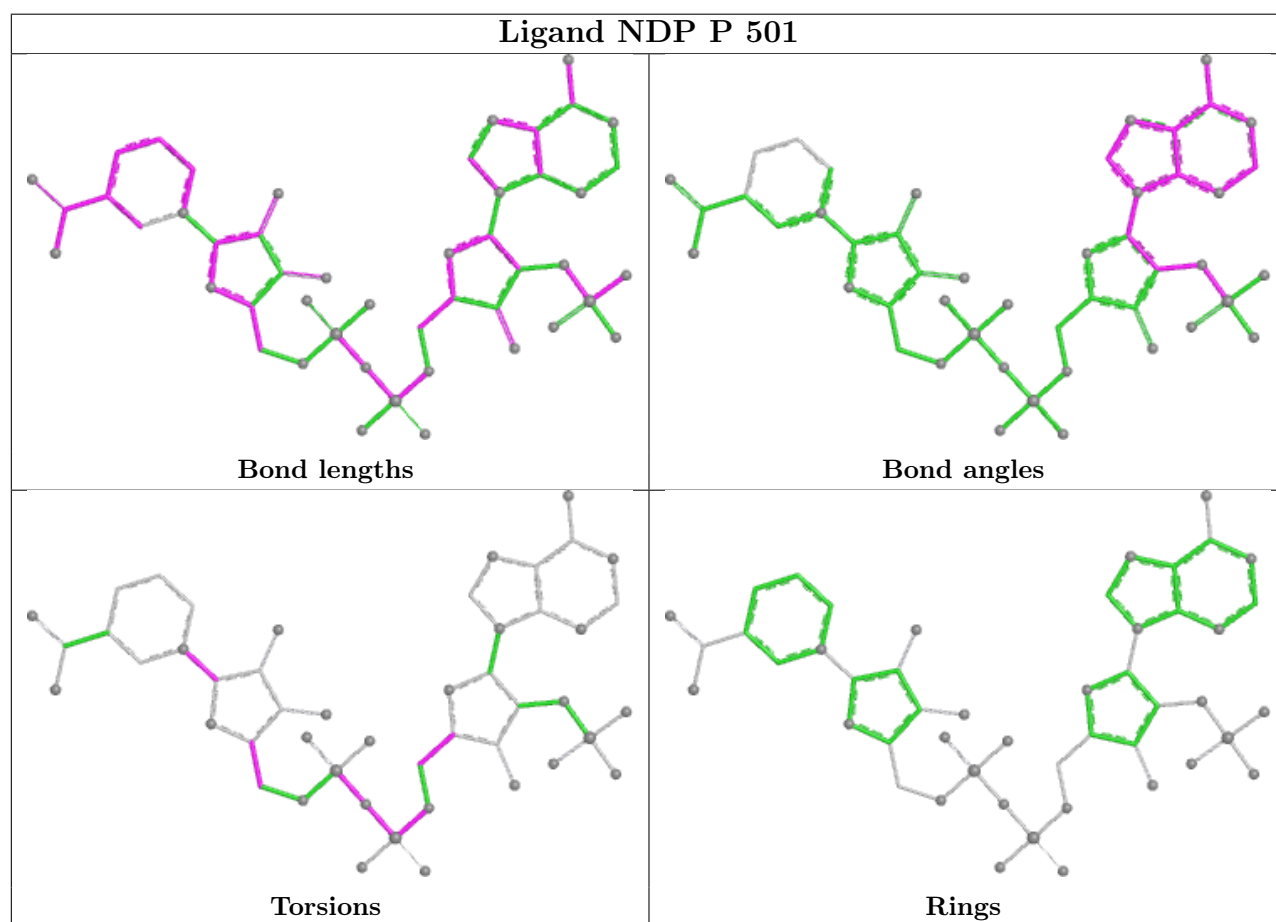
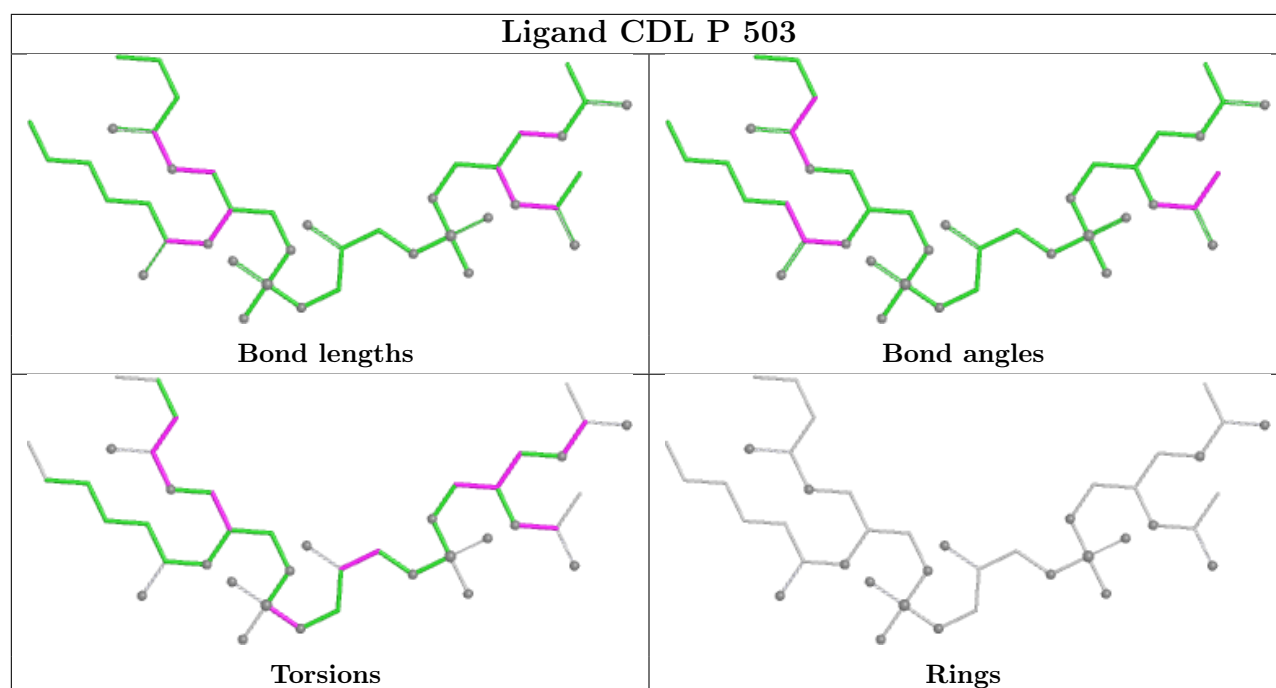


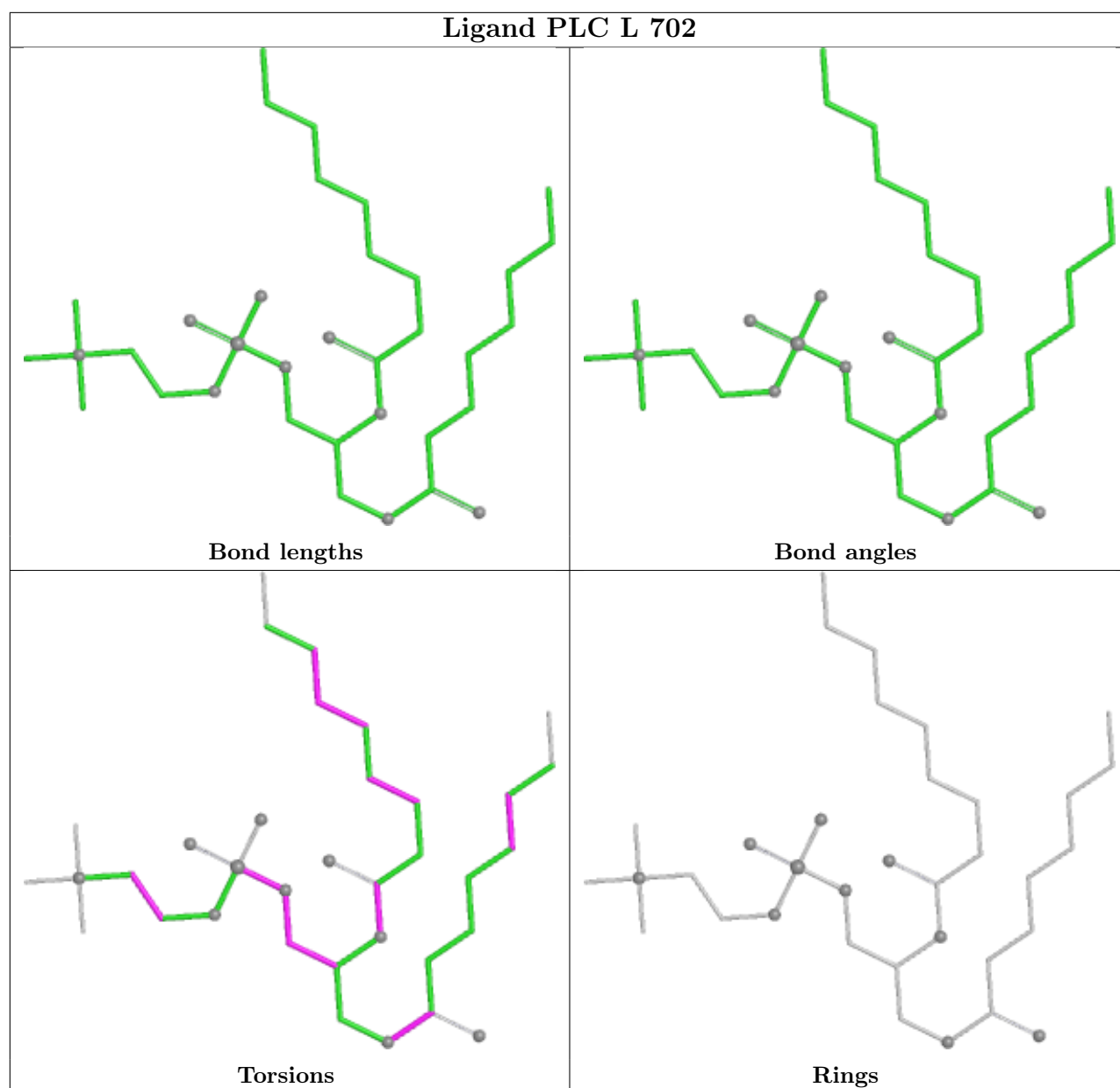


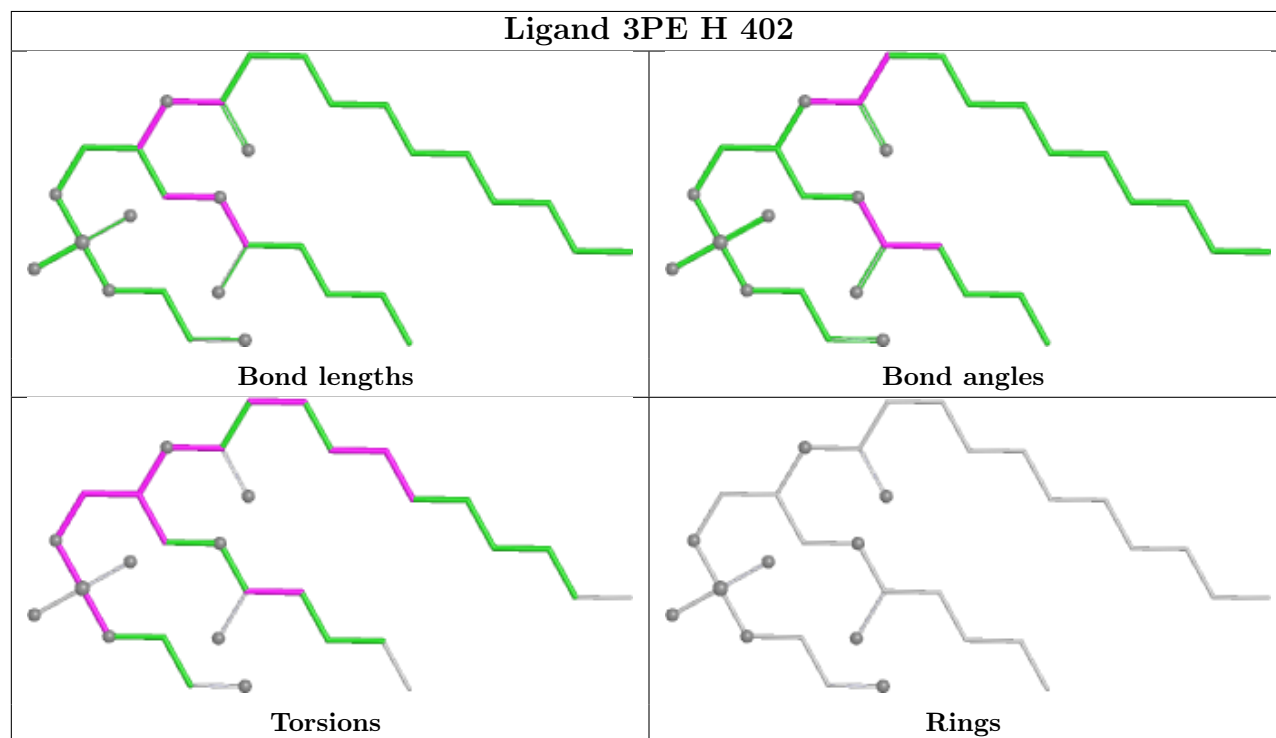
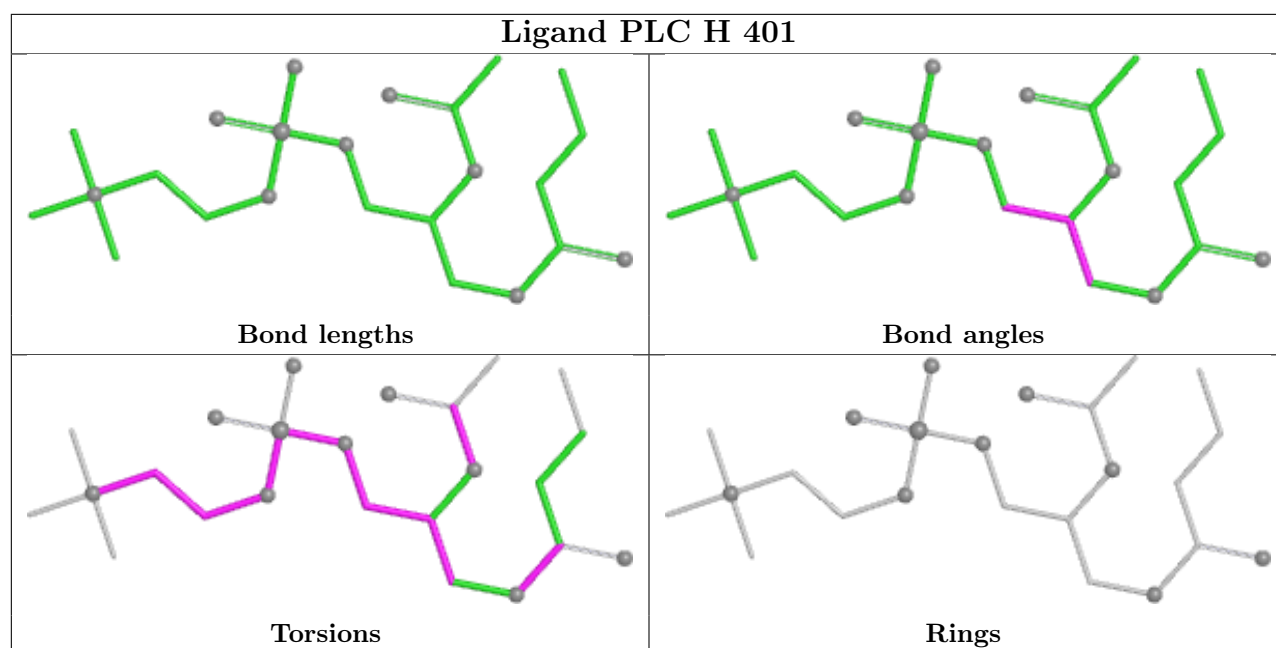




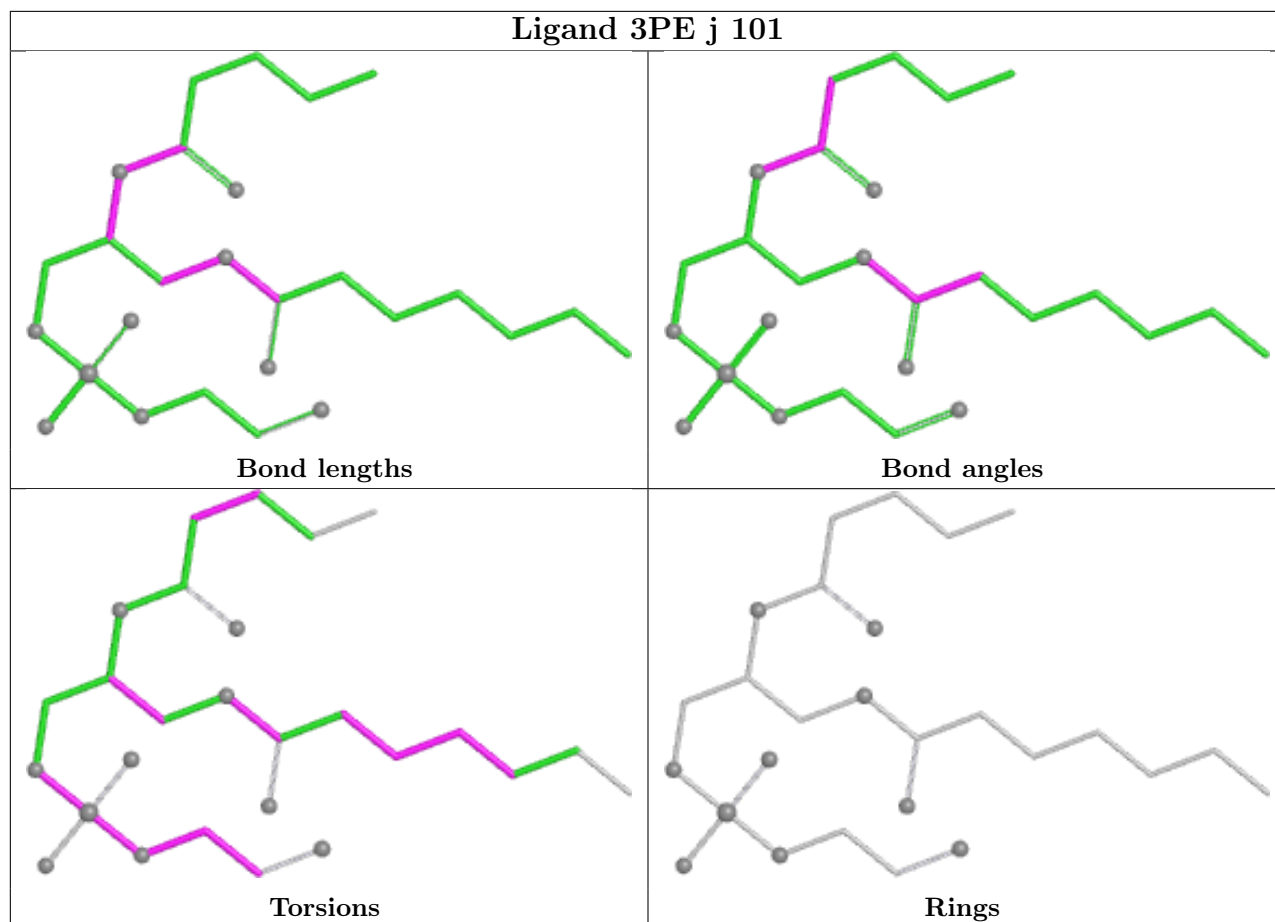




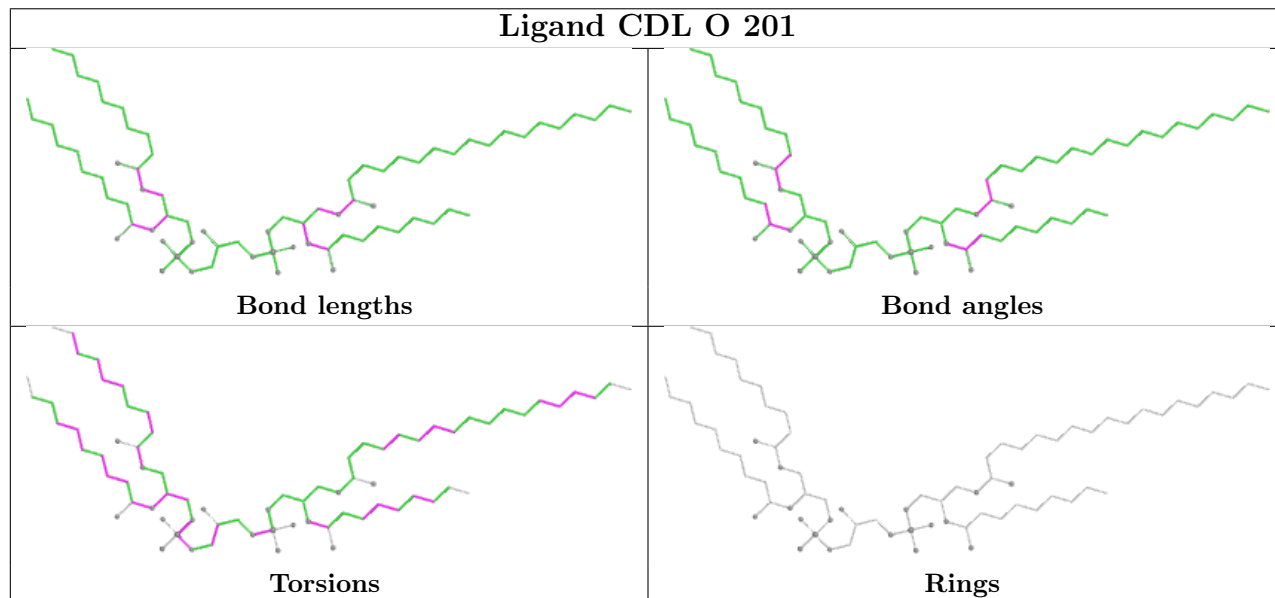


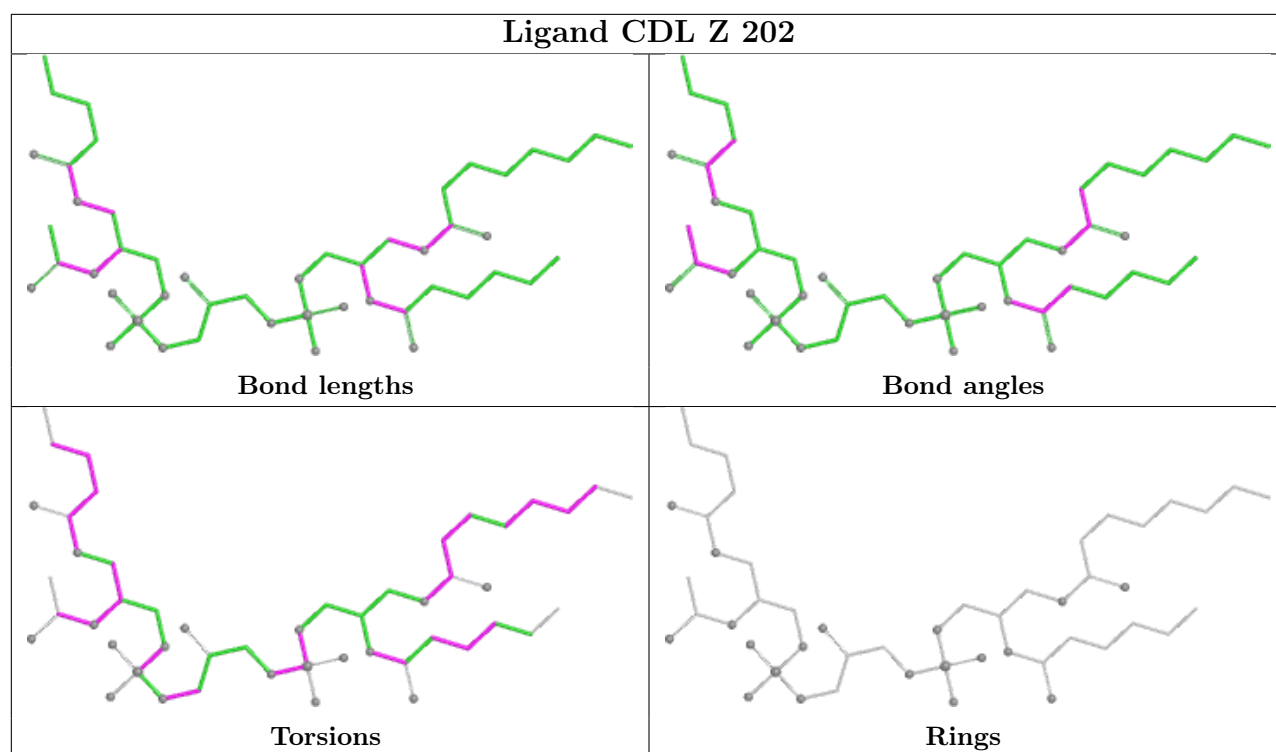


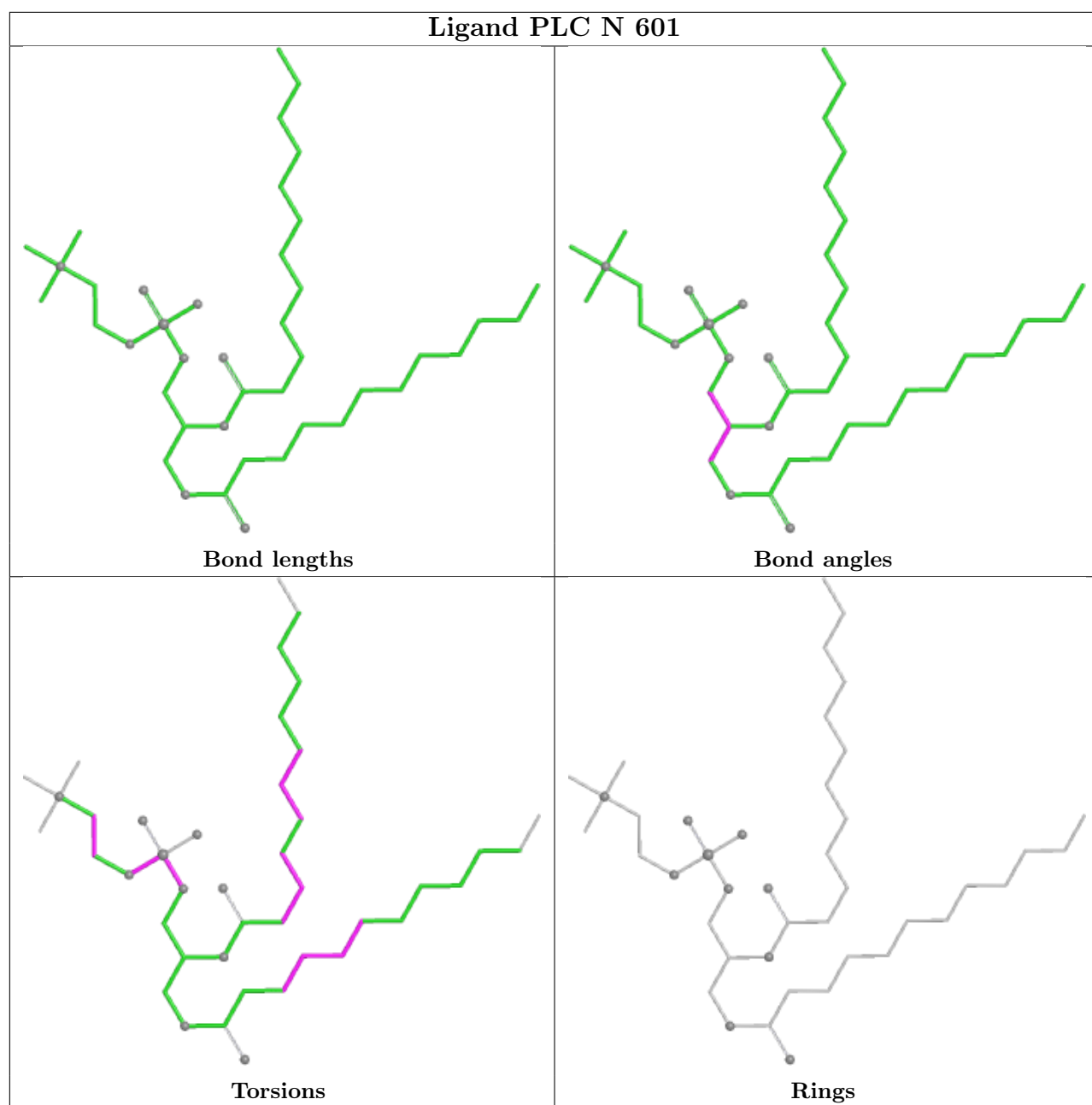
Ligand 3PE j 101

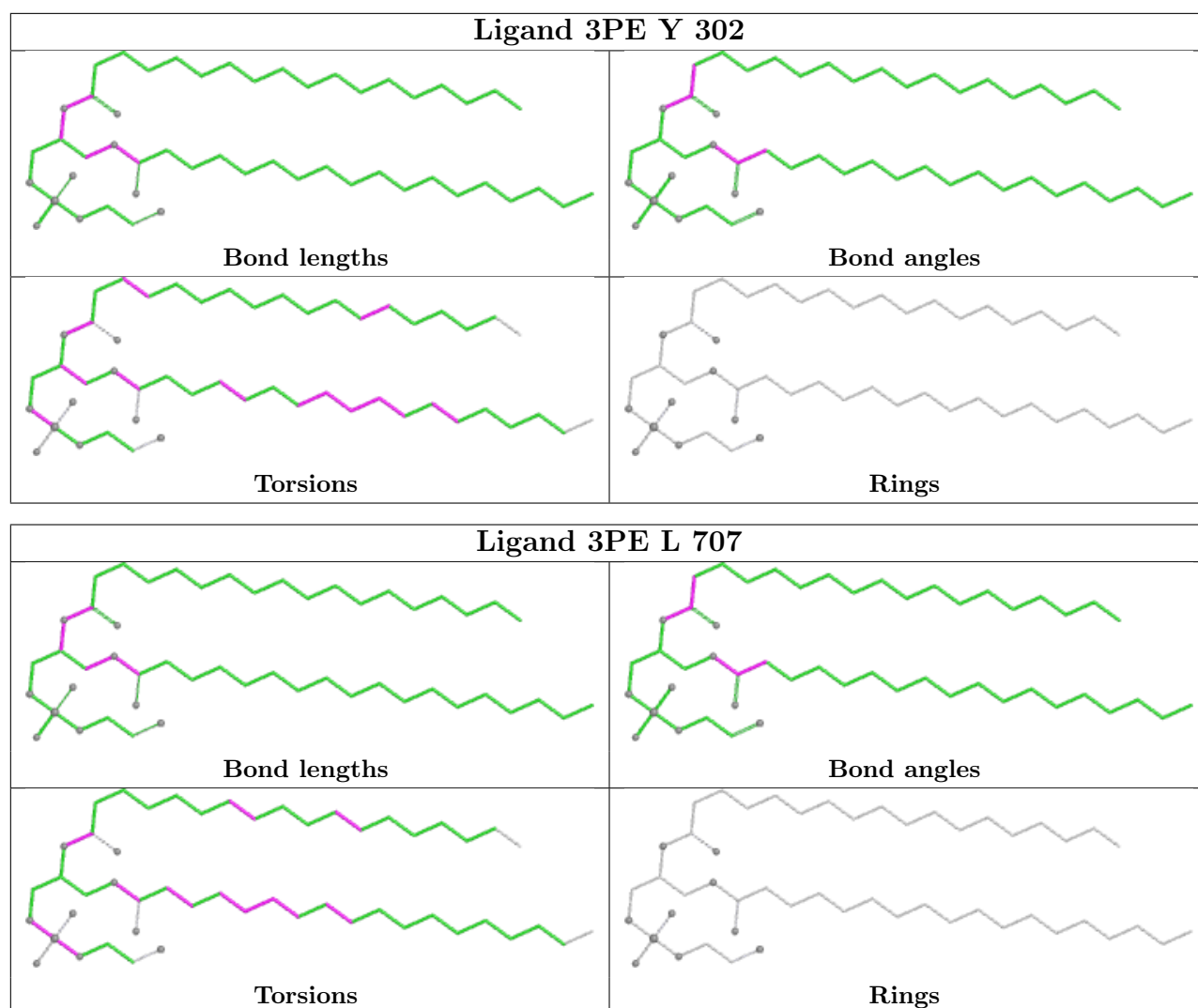


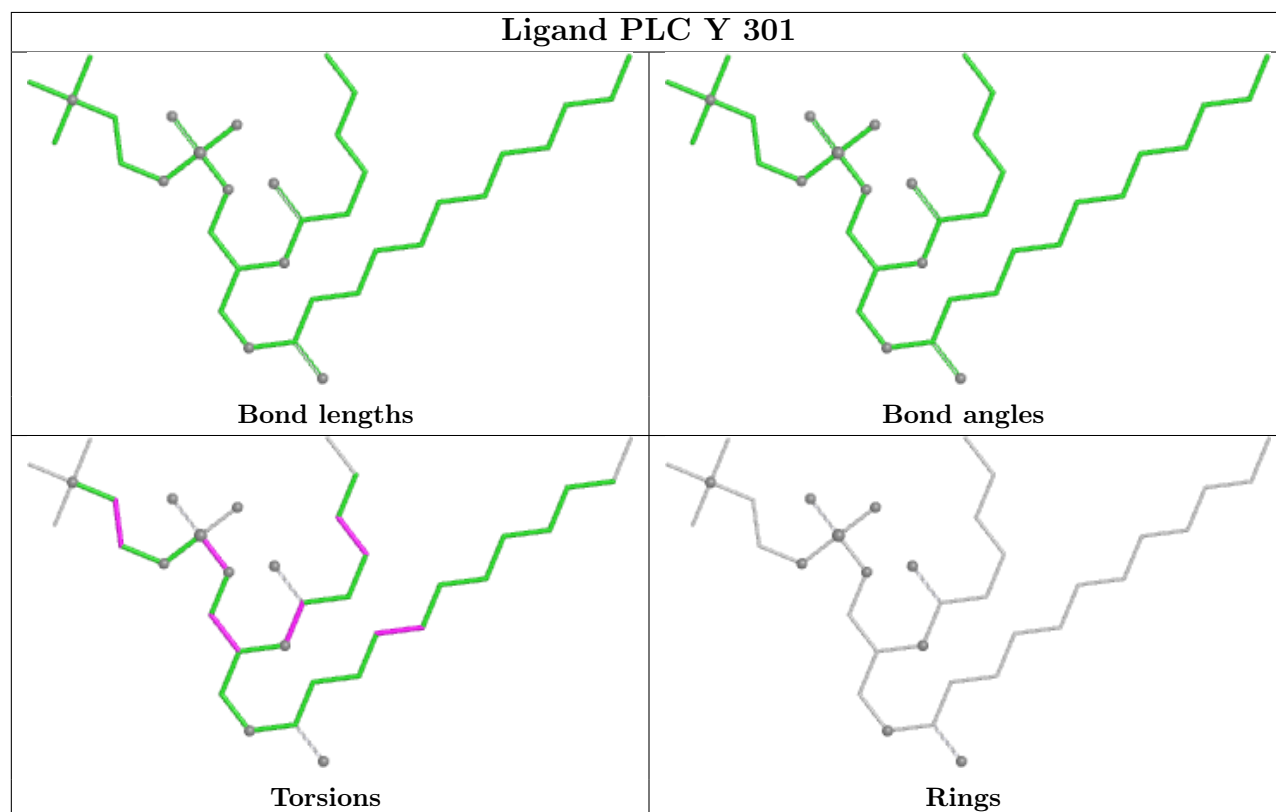
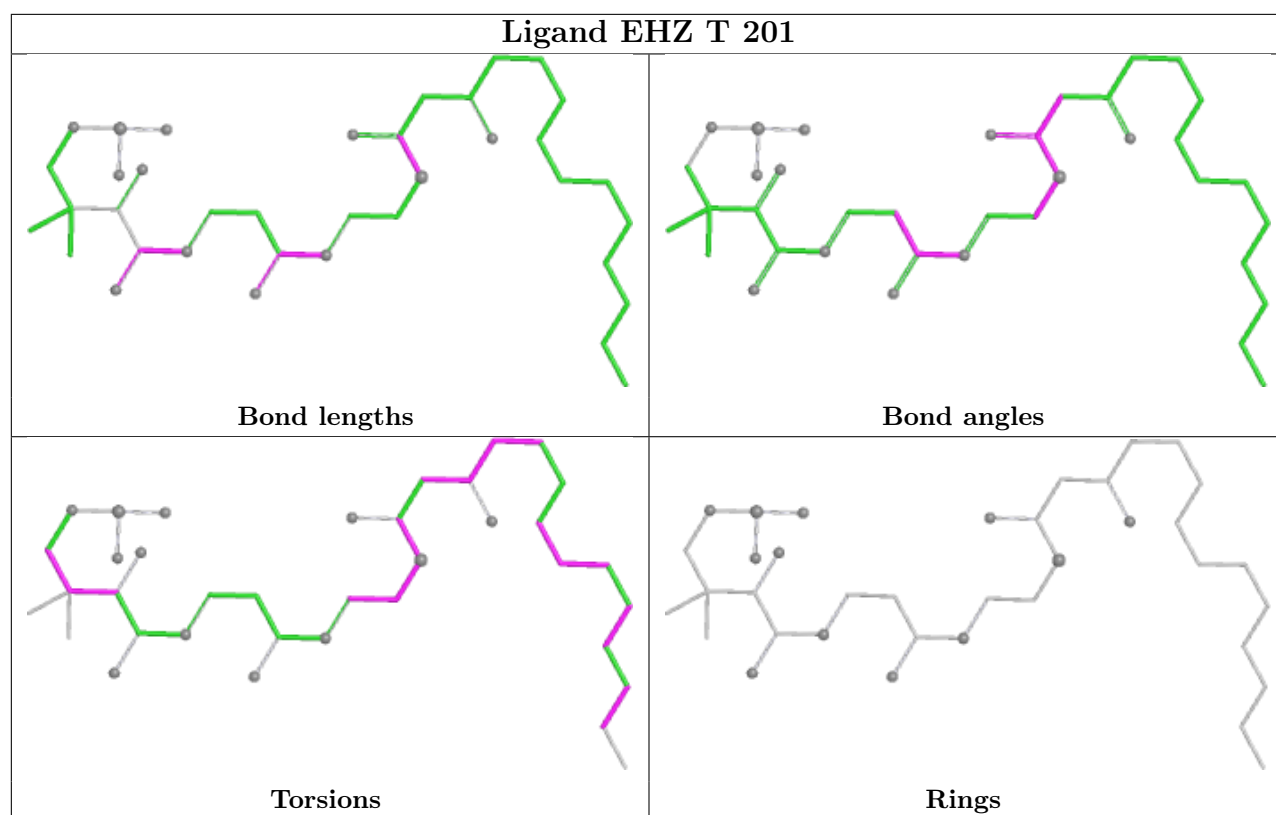
Ligand CDL O 201

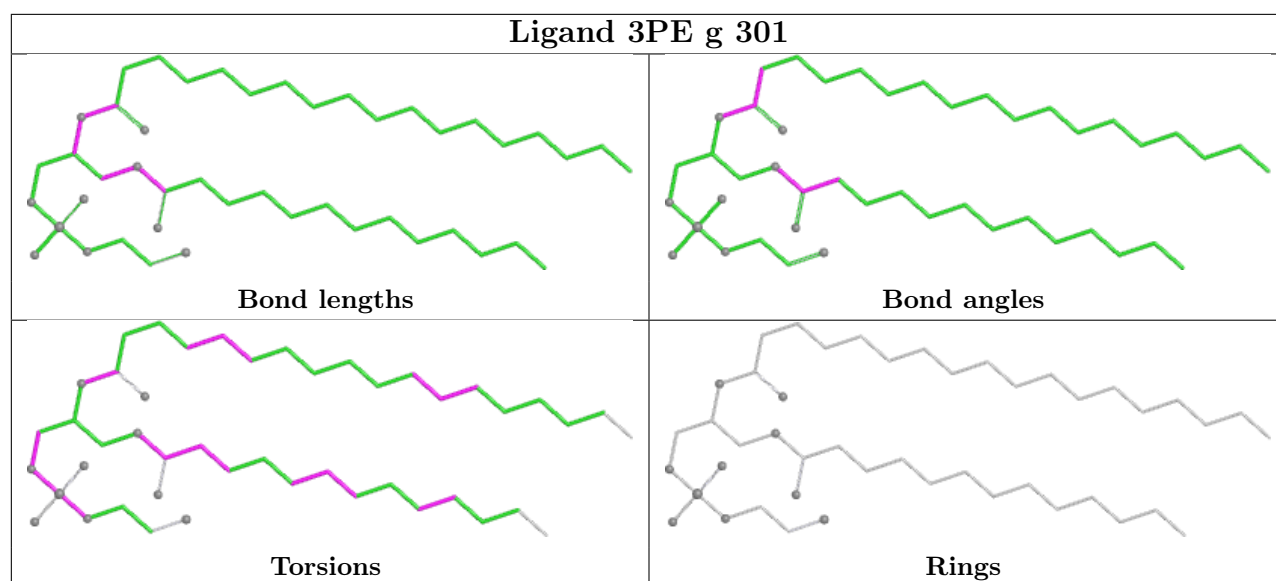


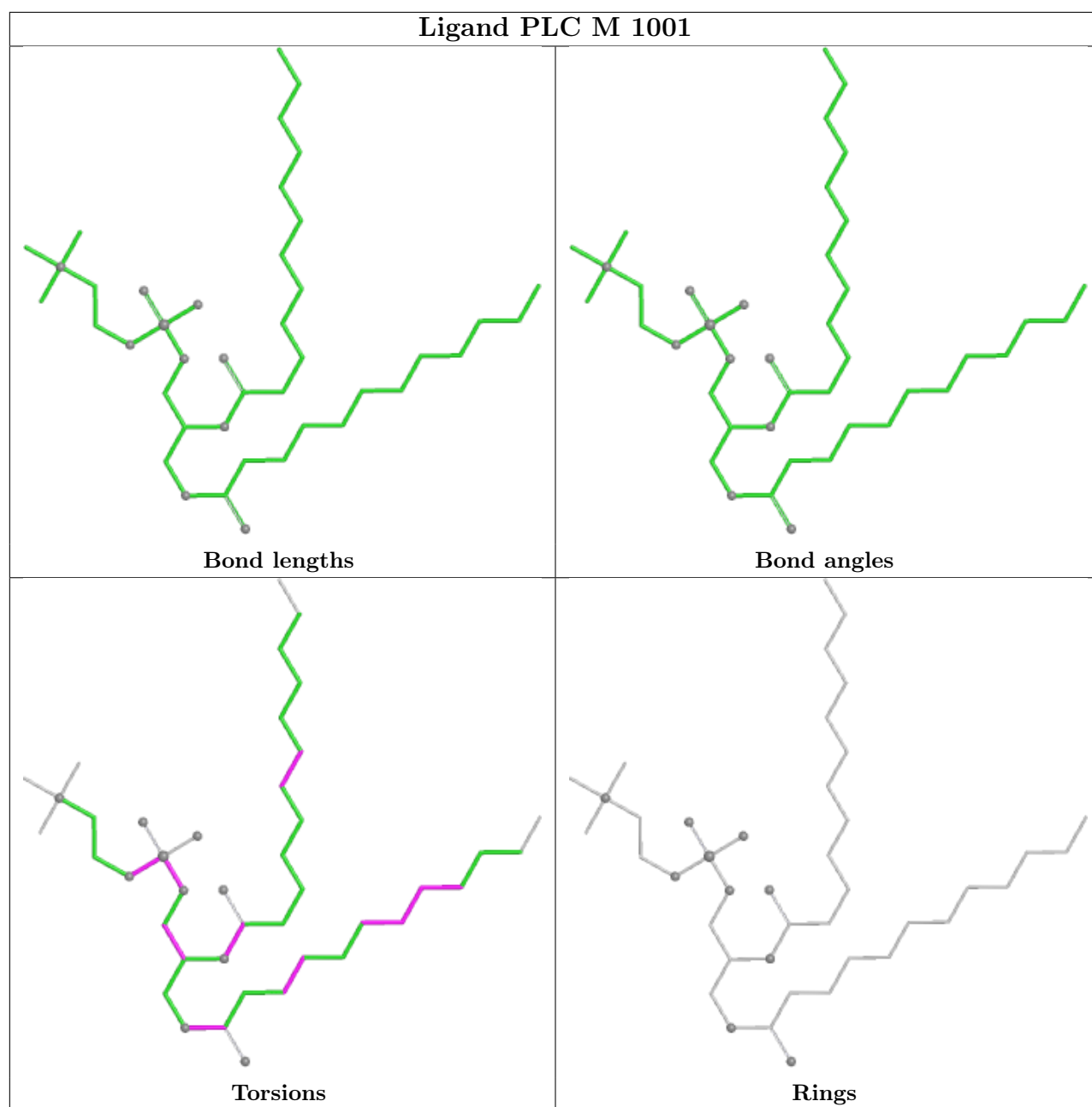


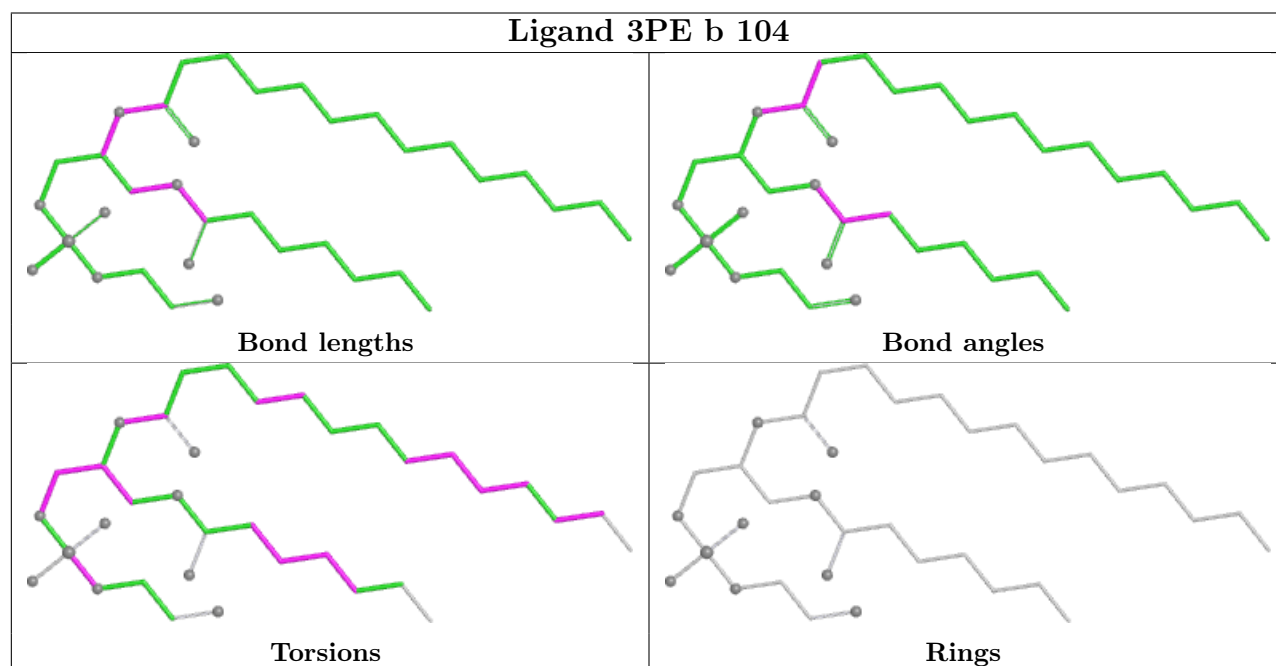
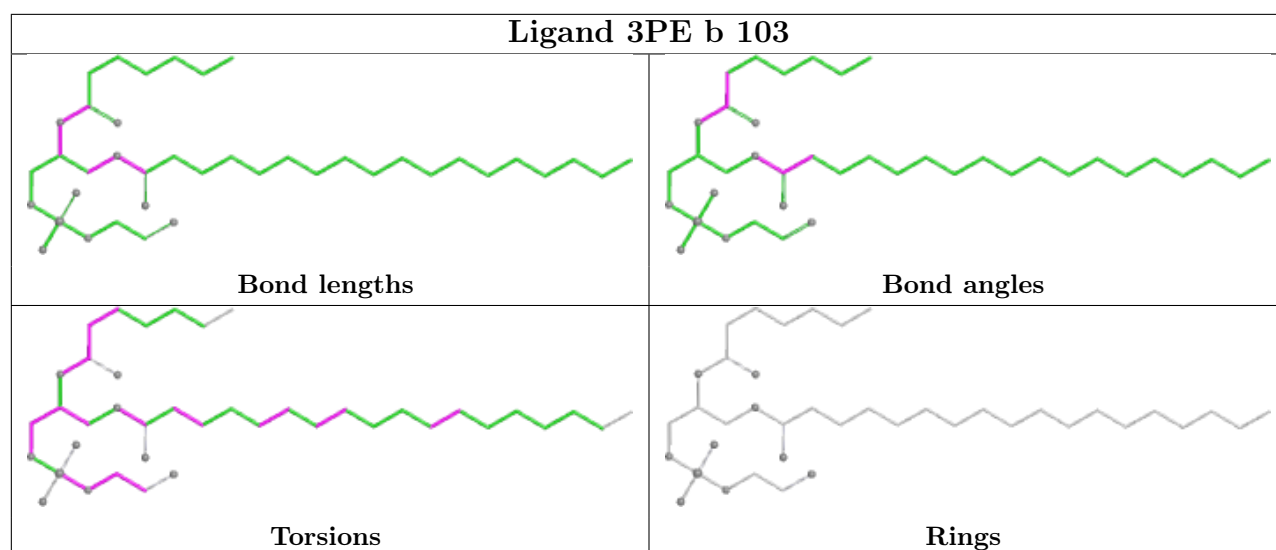


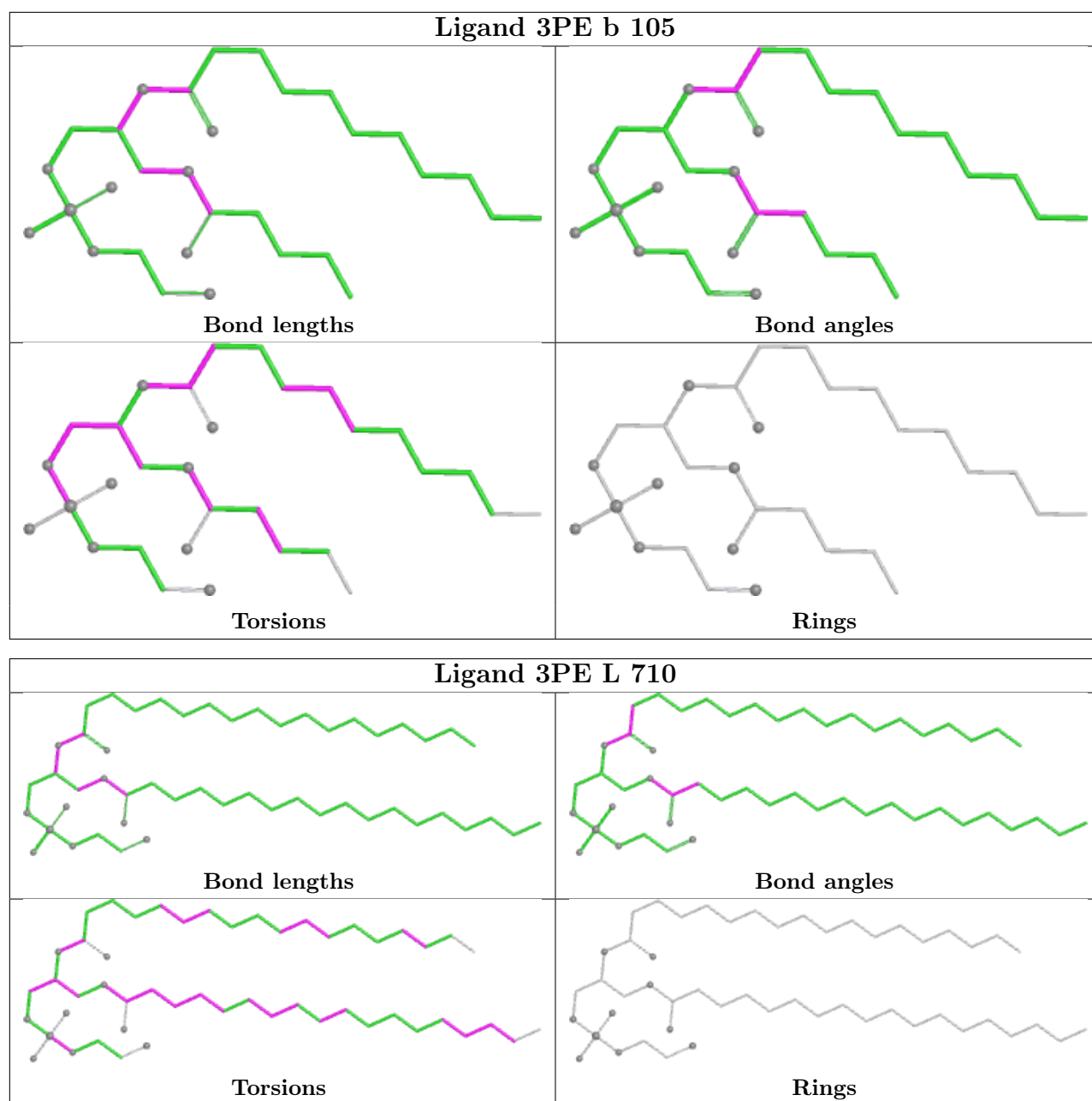


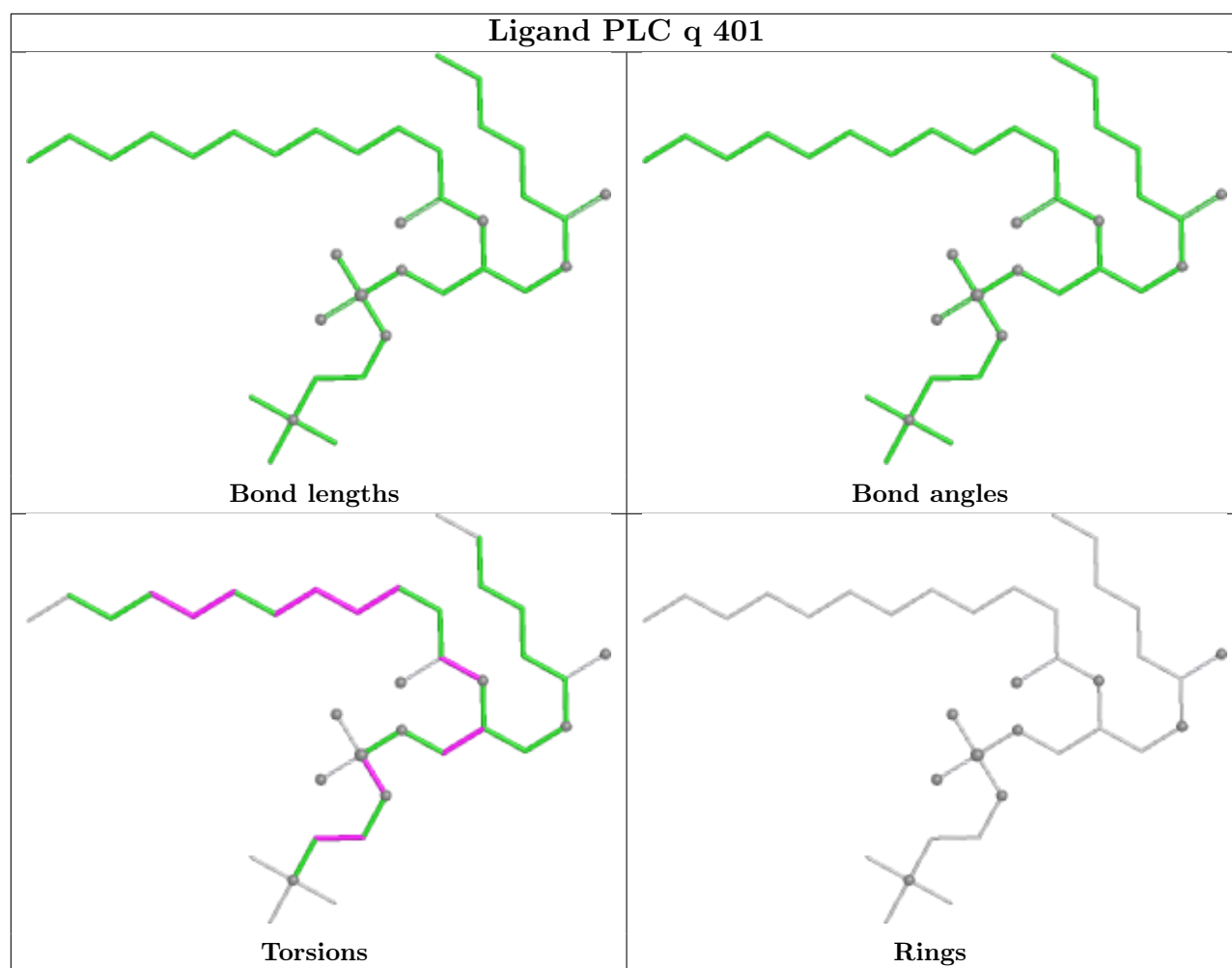


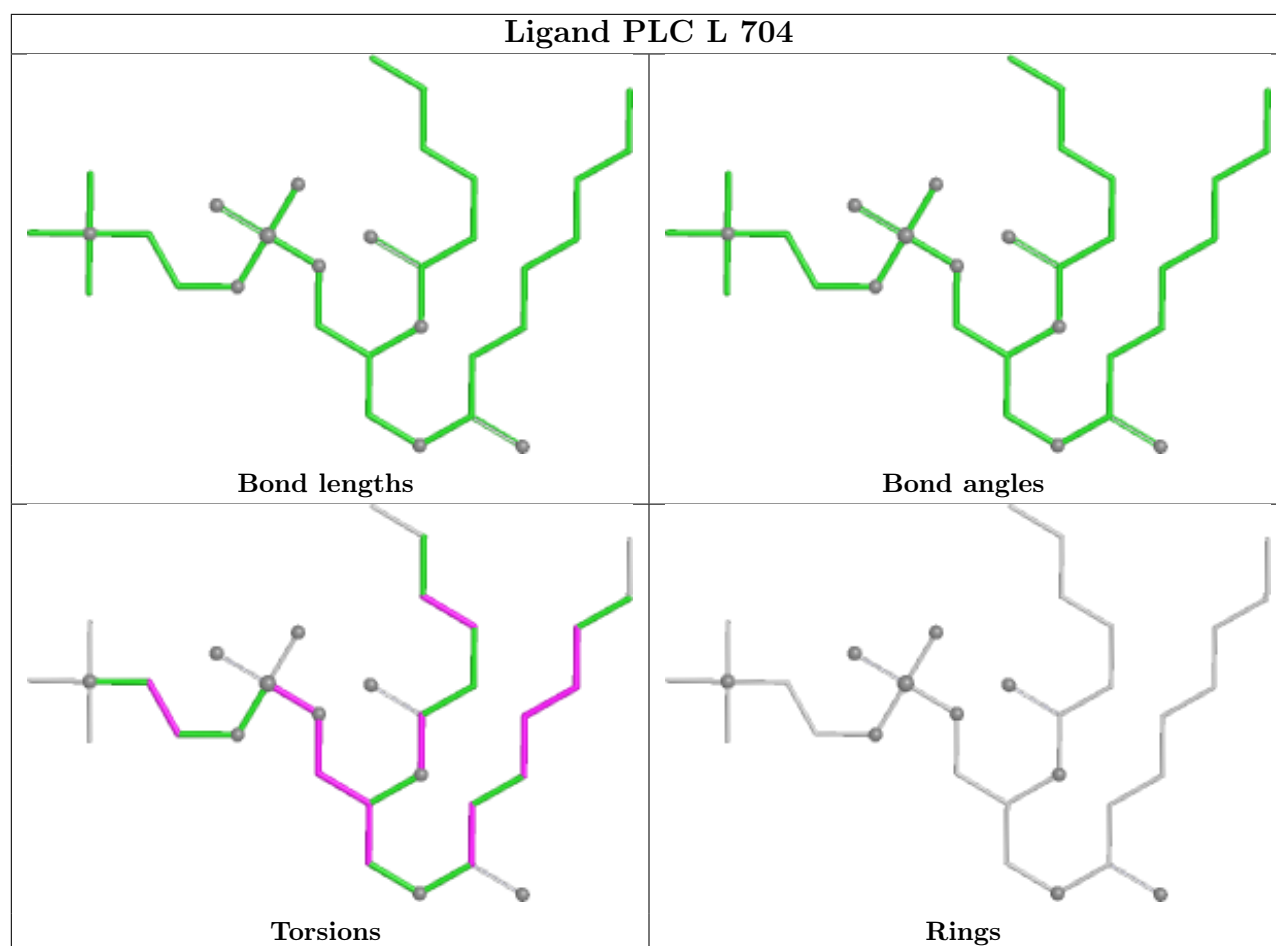












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

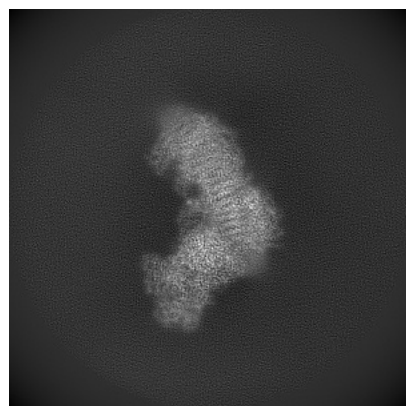
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52878. These allow visual inspection of the internal detail of the map and identification of artifacts.

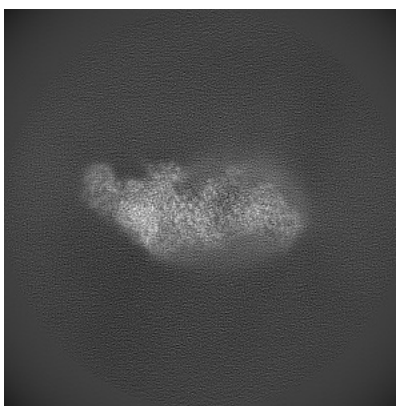
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

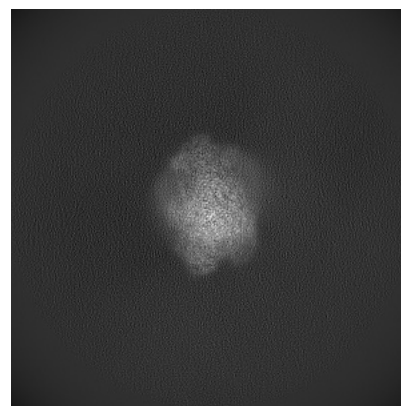
6.1.1 Primary map



X

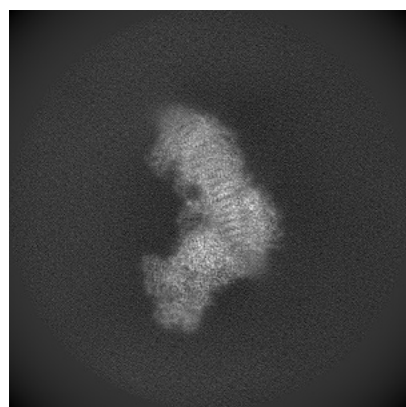


Y

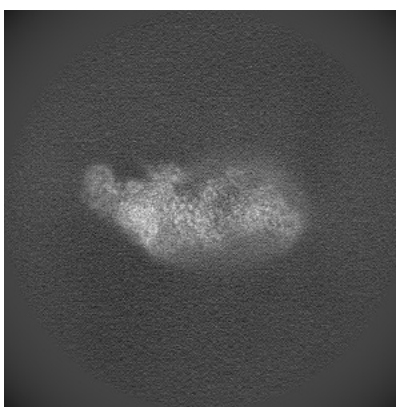


Z

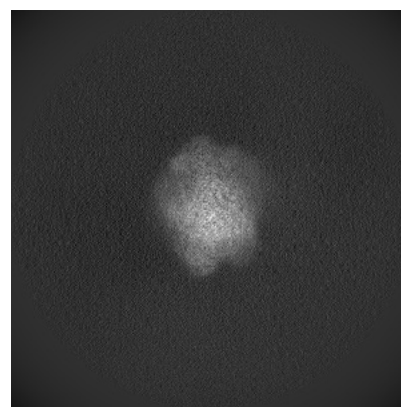
6.1.2 Raw map



X



Y

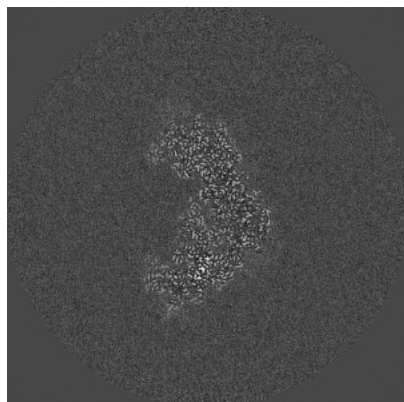


Z

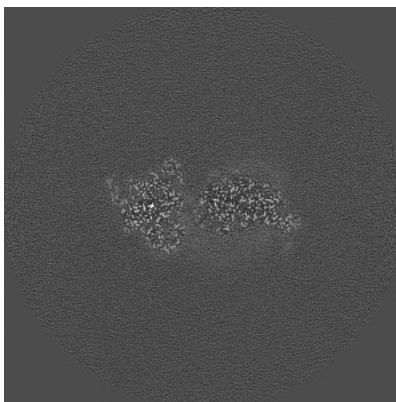
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

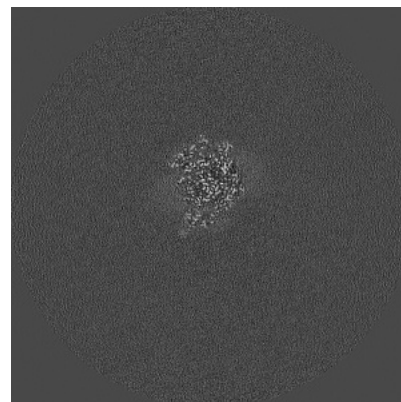
6.2.1 Primary map



X Index: 270

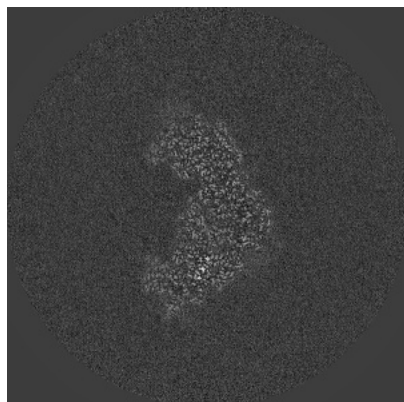


Y Index: 270

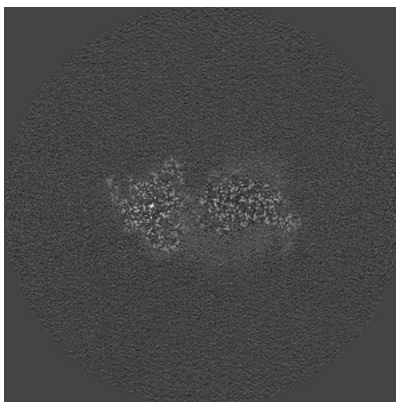


Z Index: 270

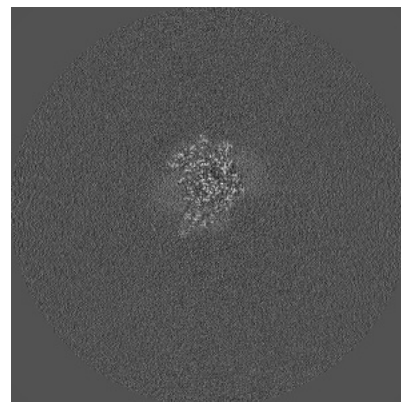
6.2.2 Raw map



X Index: 270



Y Index: 270

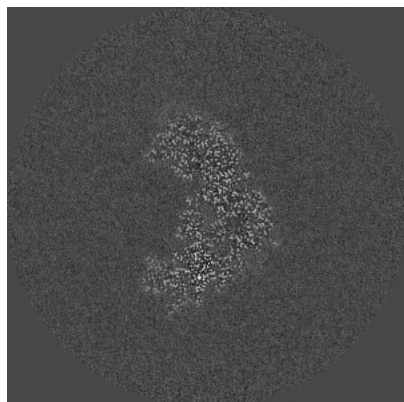


Z Index: 270

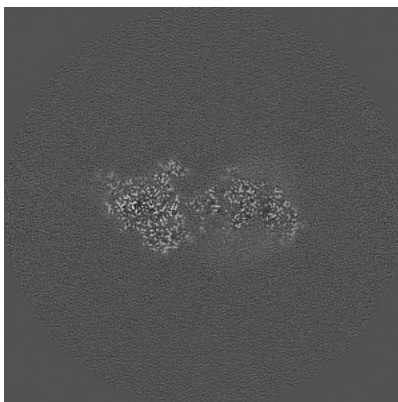
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

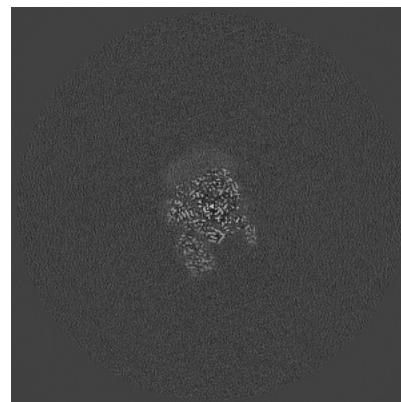
6.3.1 Primary map



X Index: 268

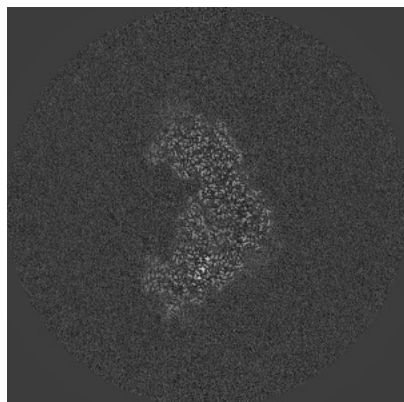


Y Index: 261

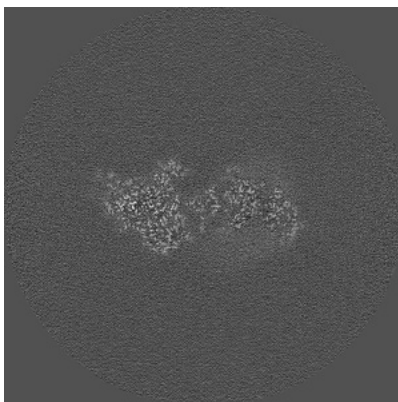


Z Index: 198

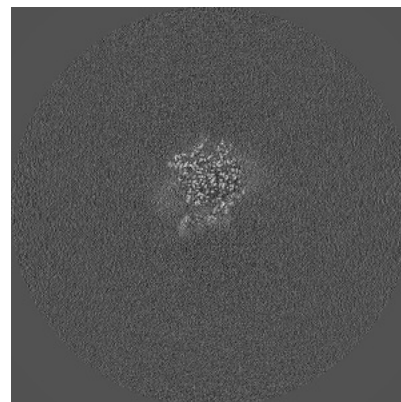
6.3.2 Raw map



X Index: 270



Y Index: 261

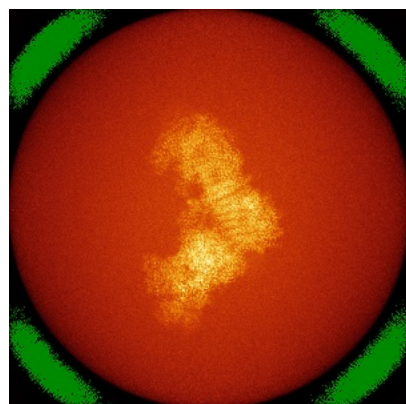


Z Index: 272

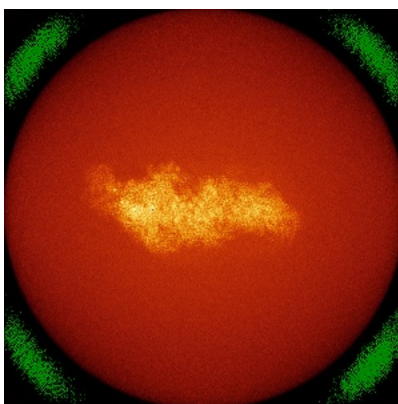
The images above show the largest variance slices of the map in three orthogonal directions.

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

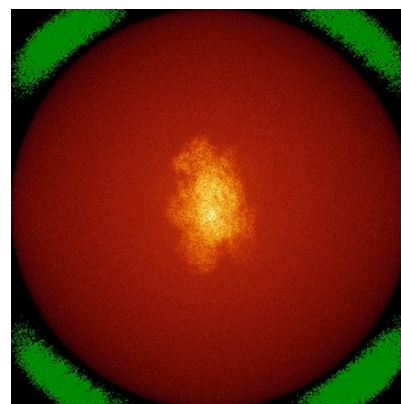
6.4.1 Primary map



X

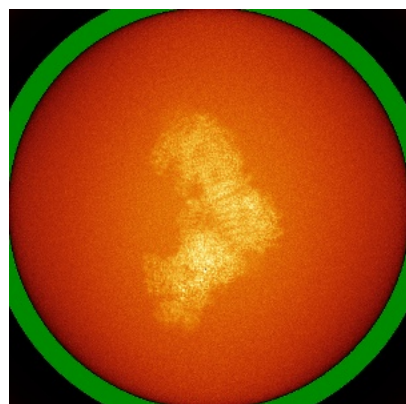


Y

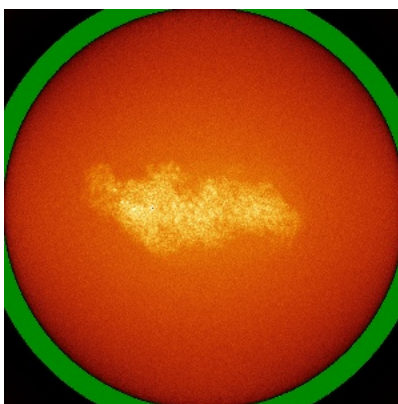


Z

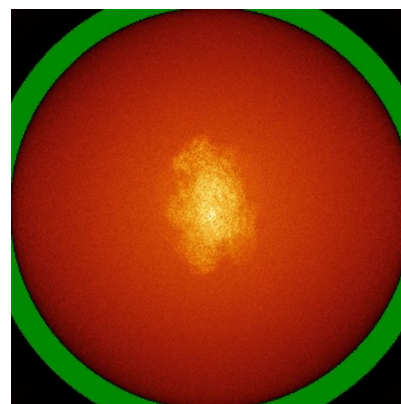
6.4.2 Raw map



X



Y

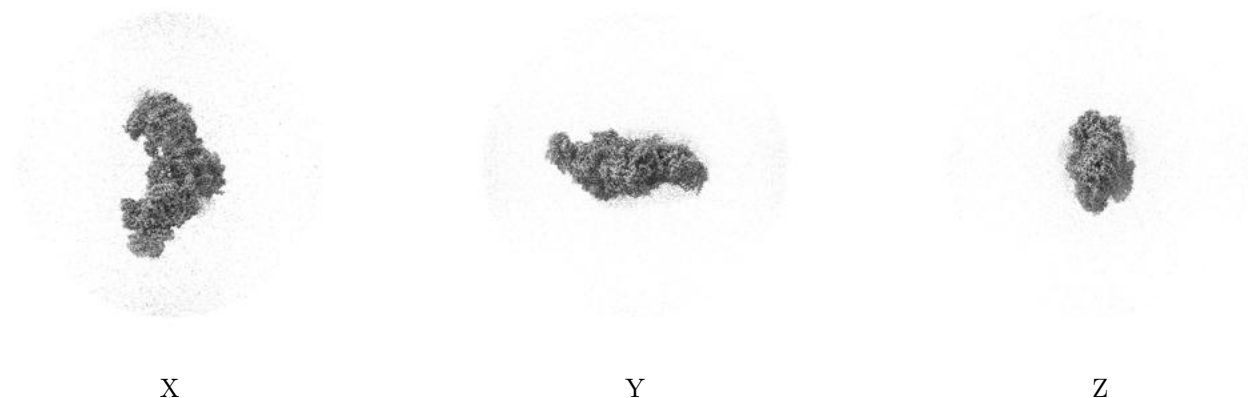


Z

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

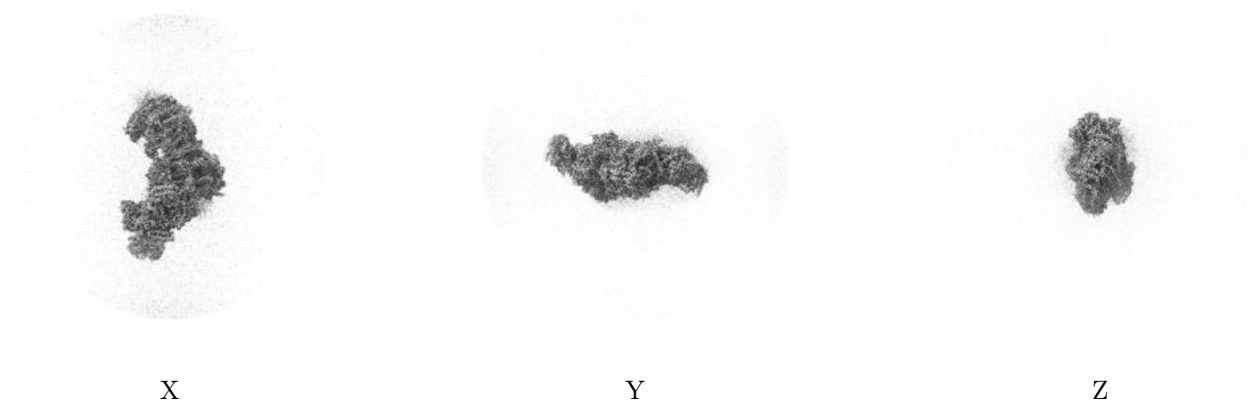
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0127. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

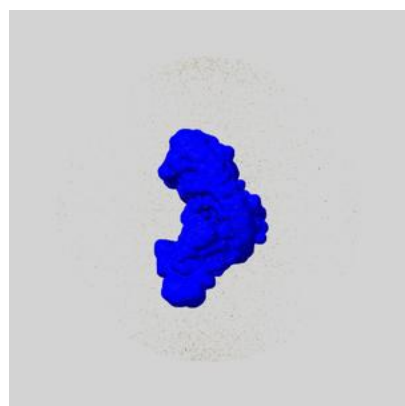
6.6 Mask visualisation [i](#)

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

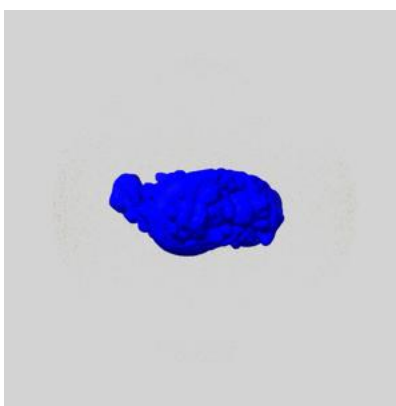
A mask typically either:

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

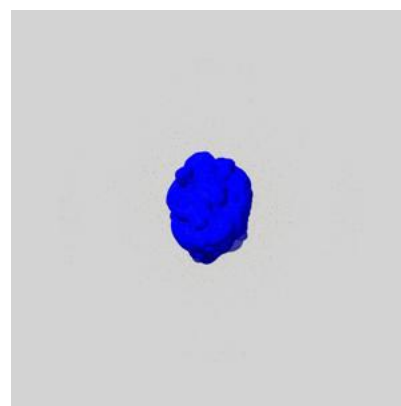
6.6.1 emd_52878_msk_1.map [i](#)



X



Y

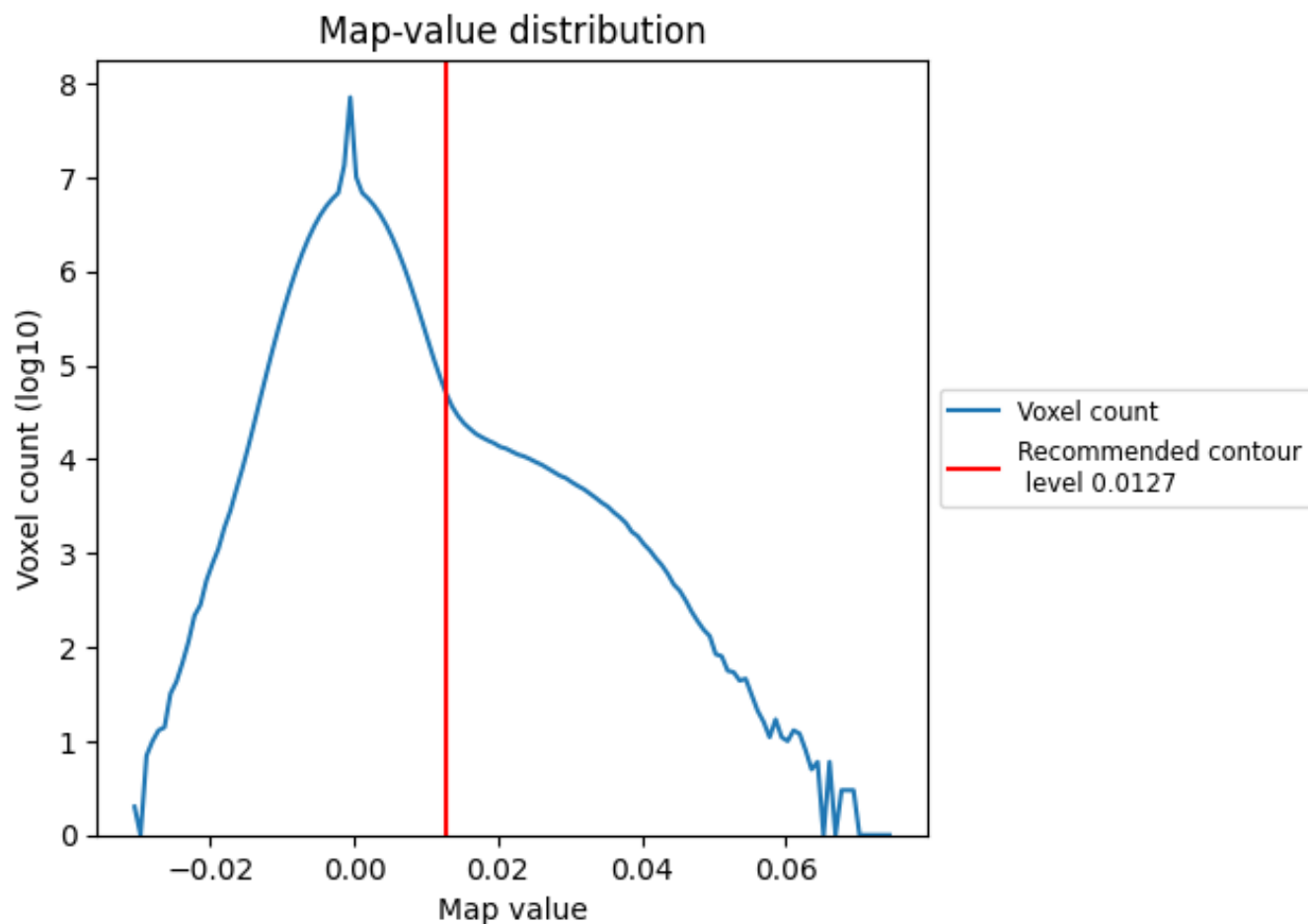


Z

7 Map analysis [i](#)

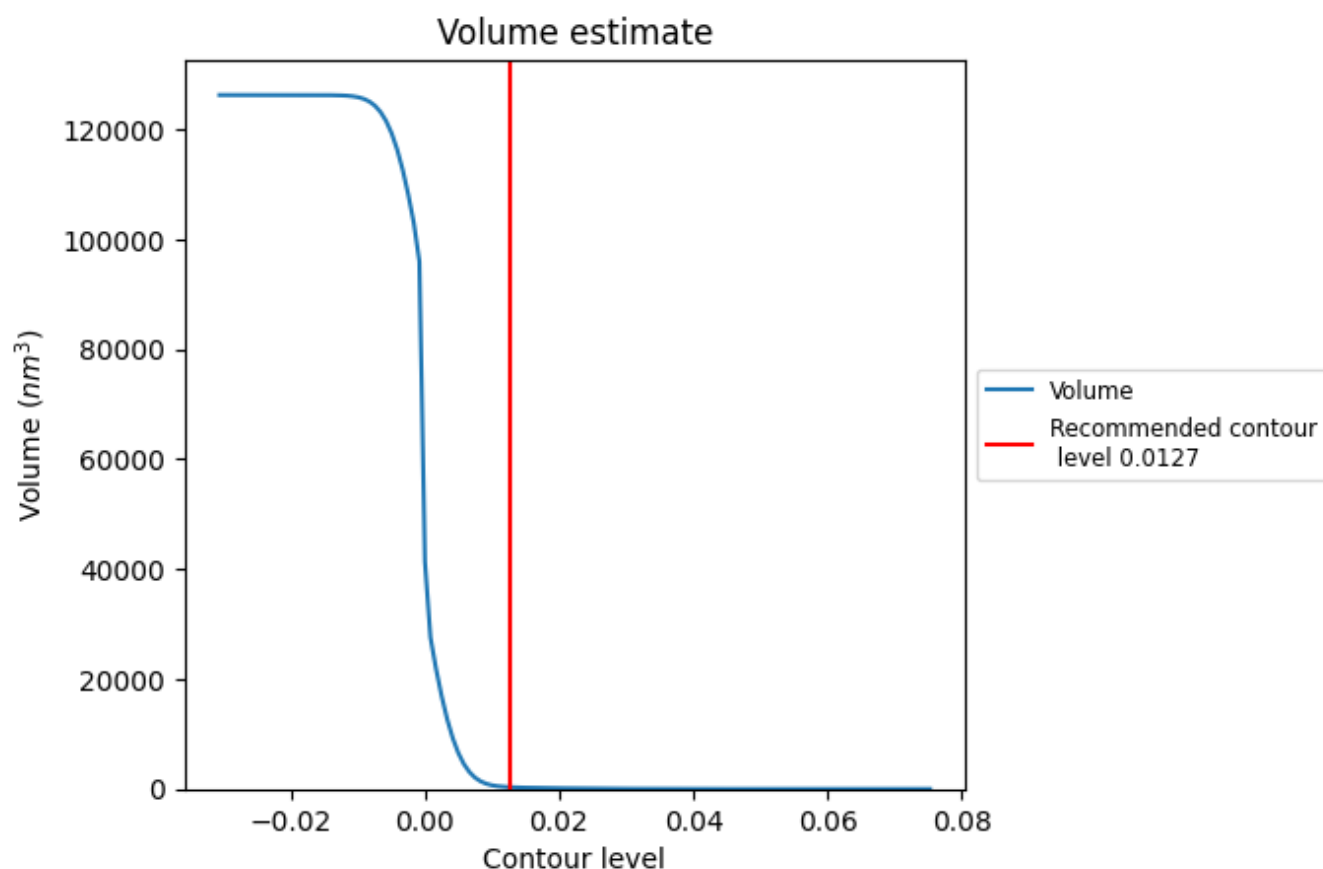
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

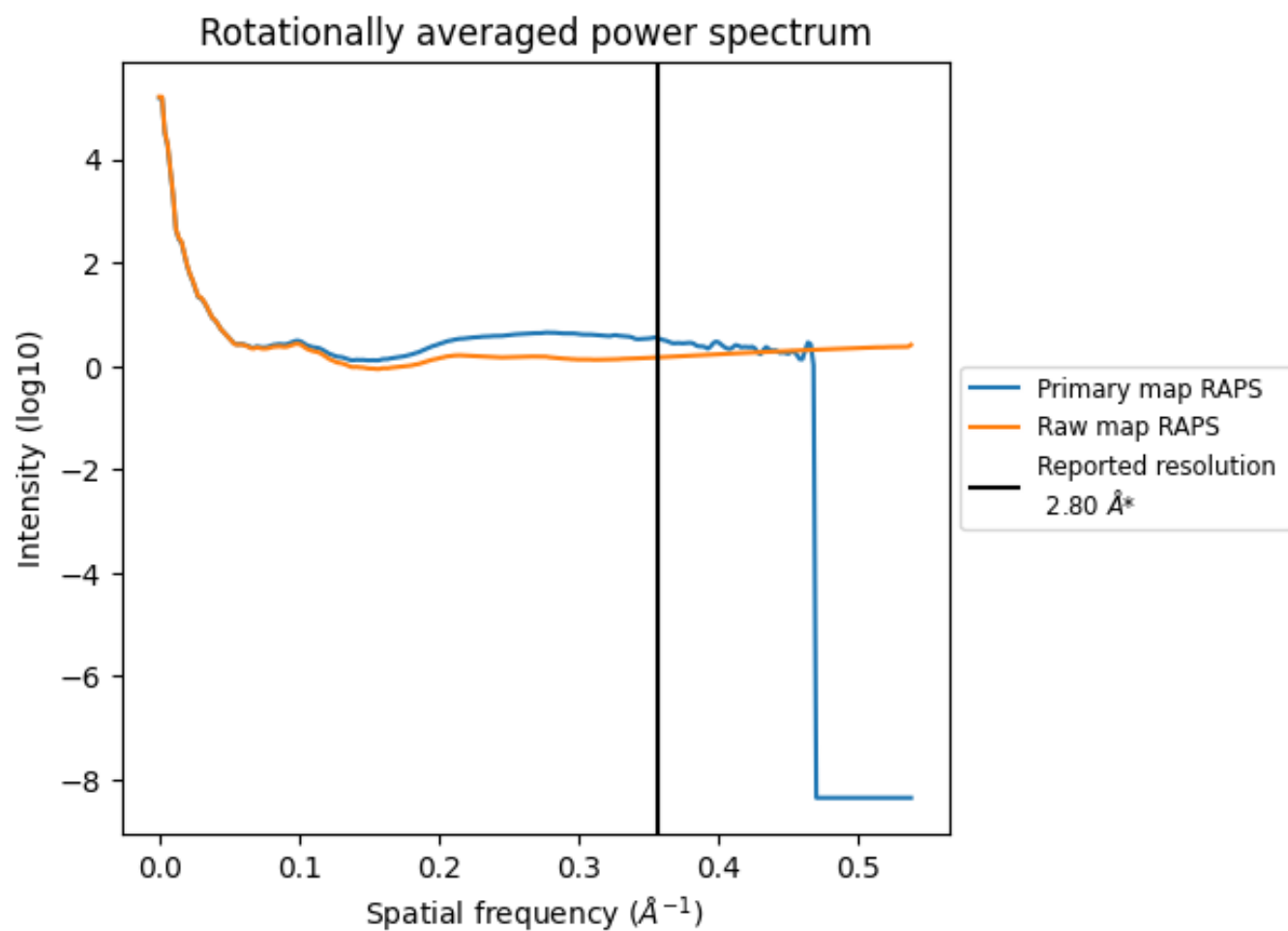
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm^3 ; this corresponds to an approximate mass of 289 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 ⓘ

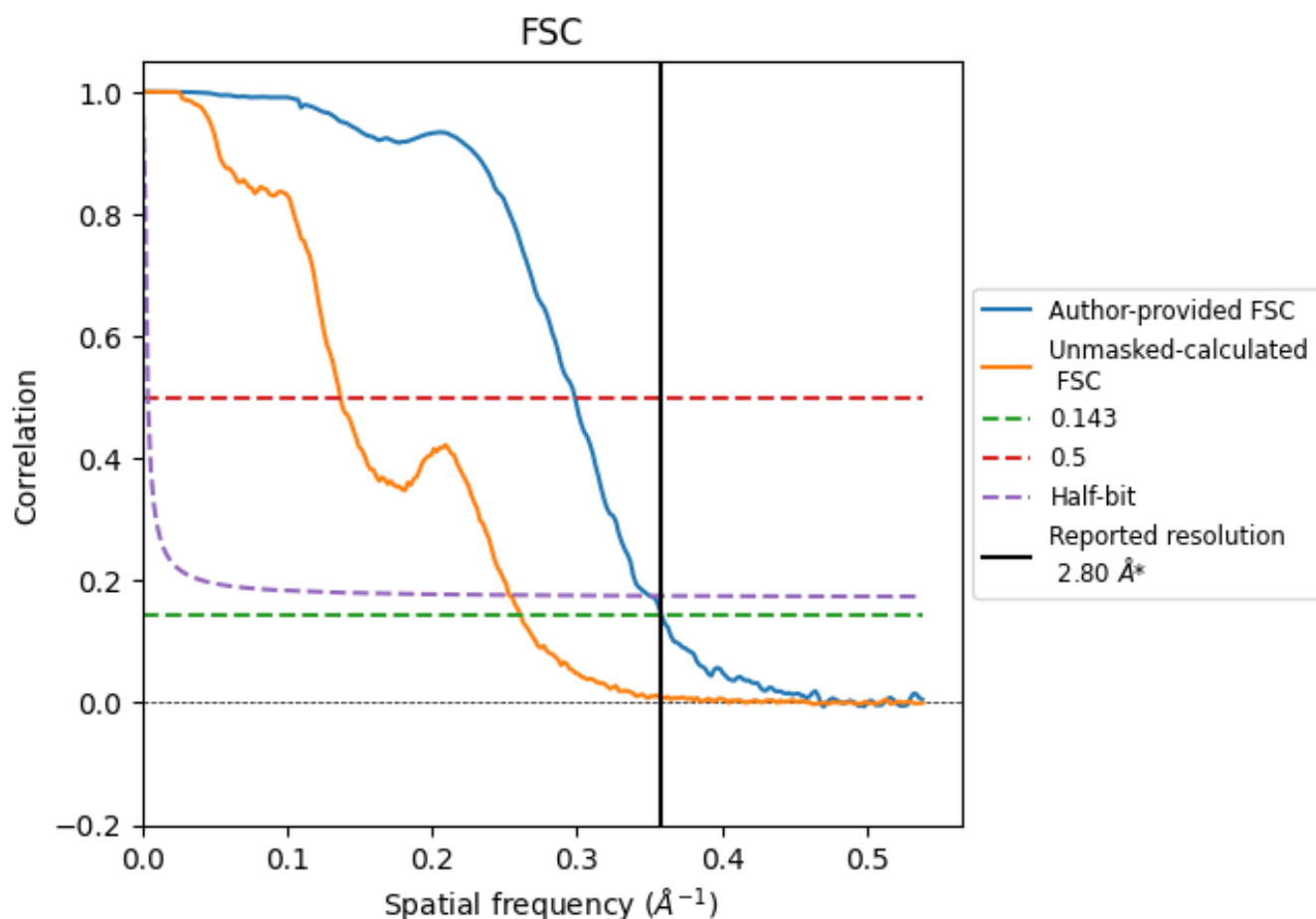


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

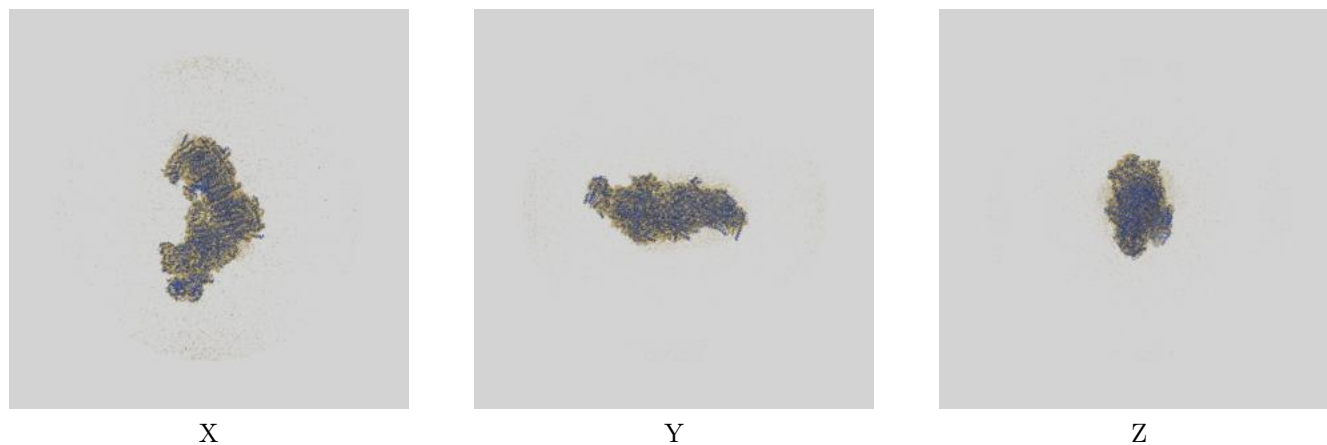
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.79	3.35	2.86
Unmasked-calculated*	3.83	7.31	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

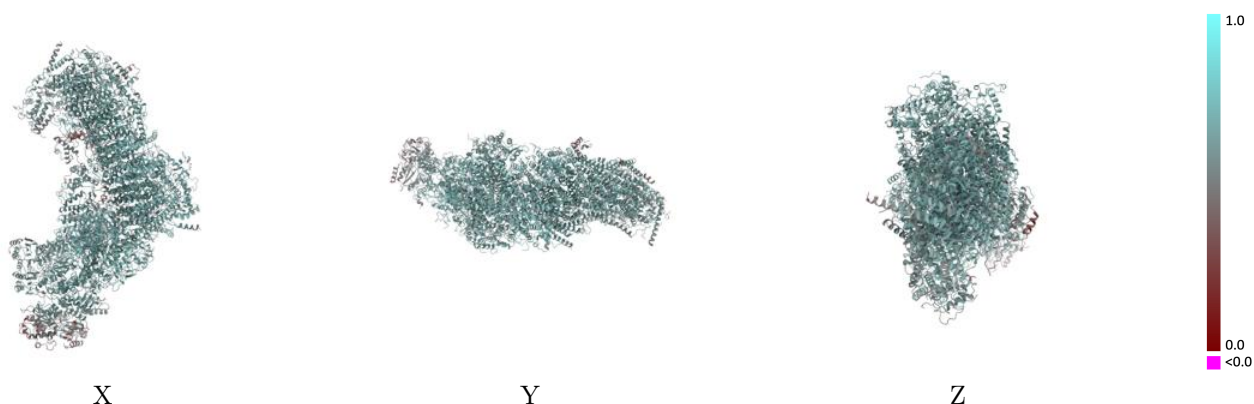
This section contains information regarding the fit between EMDB map EMD-52878 and PDB model 9IHR. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



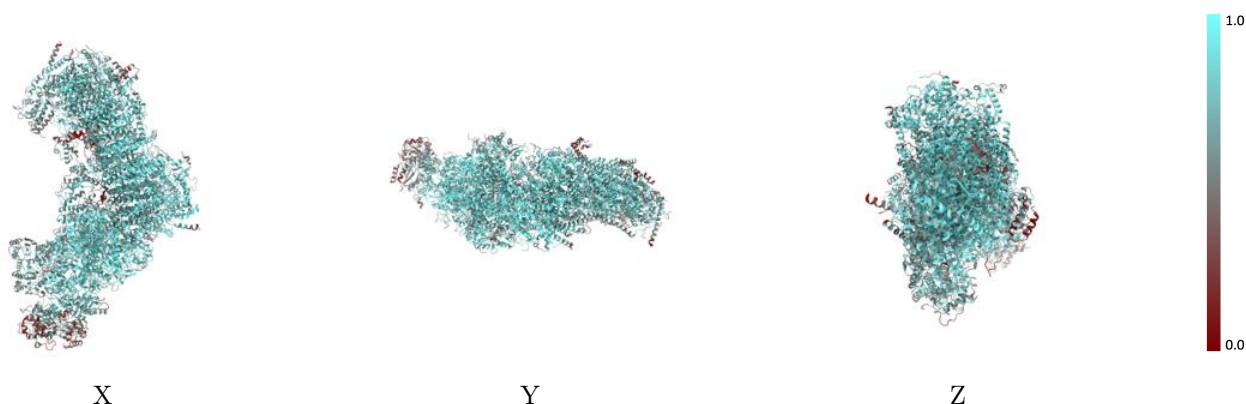
The images above show the 3D surface view of the map at the recommended contour level 0.0127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



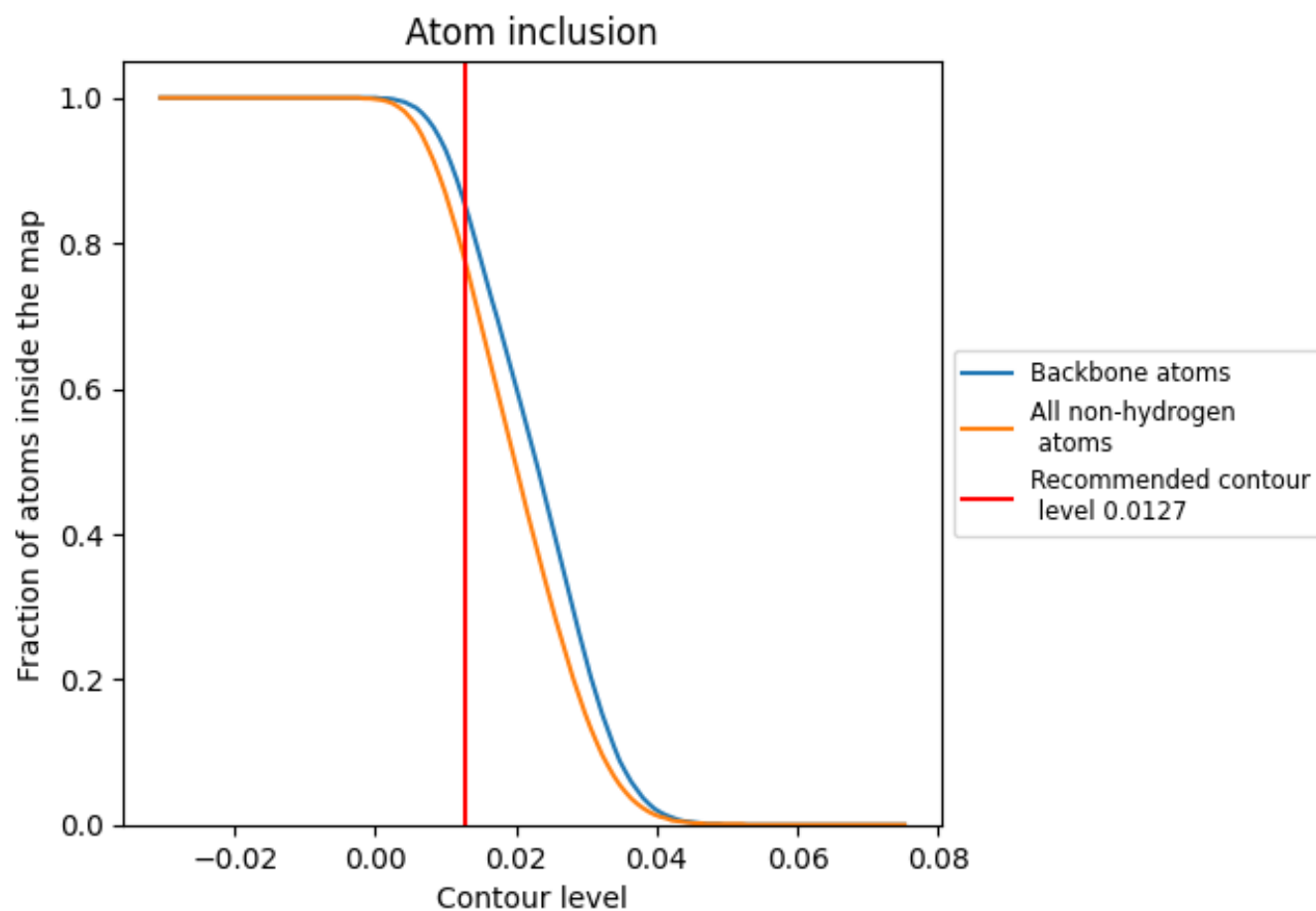
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0127).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.6150
1	 0.5800	 0.5340
A	 0.7960	 0.6320
B	 0.9000	 0.6630
C	 0.8640	 0.6430
D	 0.8890	 0.6600
E	 0.5280	 0.5090
F	 0.5090	 0.5040
G	 0.7890	 0.6120
H	 0.8450	 0.6440
I	 0.9040	 0.6630
J	 0.7650	 0.6120
K	 0.8130	 0.6240
L	 0.8150	 0.6270
M	 0.8800	 0.6540
N	 0.8820	 0.6610
O	 0.8230	 0.6370
P	 0.8000	 0.6190
Q	 0.7730	 0.6260
R	 0.7920	 0.6160
S	 0.5570	 0.5330
T	 0.7250	 0.5980
U	 0.5500	 0.5300
V	 0.7620	 0.6140
W	 0.8210	 0.6360
X	 0.8390	 0.6410
Y	 0.7600	 0.6250
Z	 0.8400	 0.6360
a	 0.8360	 0.6360
b	 0.7370	 0.6320
c	 0.7770	 0.6060
d	 0.8370	 0.6400
e	 0.8450	 0.6370
f	 0.7640	 0.6150
g	 0.4590	 0.5130



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Chain	Atom inclusion	Q-score
h	 0.7250	 0.6030
i	 0.6720	 0.5630
j	 0.6130	 0.5550
k	 0.6100	 0.5360
l	 0.7270	 0.5970
m	 0.7580	 0.6230
n	 0.6710	 0.5570
o	 0.6510	 0.5670
p	 0.8490	 0.6290
q	 0.8270	 0.6340