



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:45 PM UTC

PDB ID : 8Q48 / pdb_00008q48
EMDB ID : EMD-18141
Title : Outward-facing, closed proteoliposome complex I at 2.5 Å. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-05
Resolution : 2.50 Å(reported)
Based on initial model : 7QSN

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

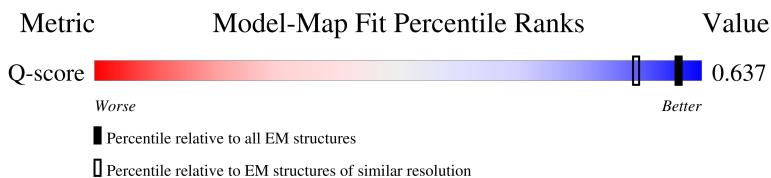
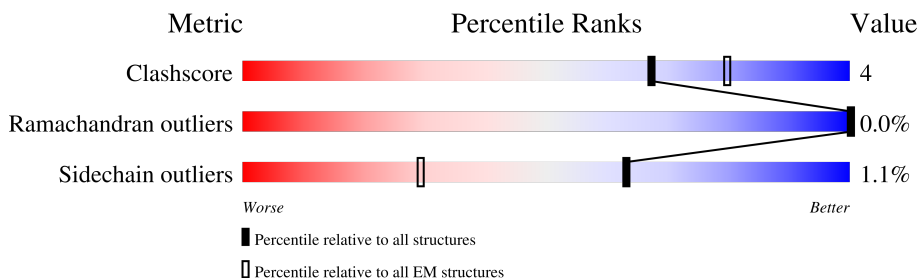
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	216	
3	C	266	
4	D	463	

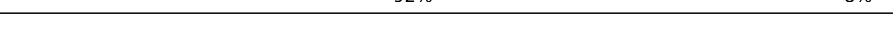
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	 93% 6% .
30	e	106	 88% 6% 7%
31	f	57	 7% 89% 9% .
32	g	154	 57% 8% 34%
33	h	189	 66% 7% 27%
34	i	128	 5% 84% 16% .
35	j	108	 6% 63% . 34%
36	k	98	 77% 6% 17%
37	l	186	 77% 7% 16%
38	m	129	 91% 9% .
39	n	179	 83% 13% .
40	o	137	 74% 15% 11%
41	p	176	 94% 5% .
42	q	145	 92% 8%
43	r	113	 78% 5% . 16%
44	s	109	 34% 7% 59%

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 71395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			921	622	133	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1738	1120	298	317	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	0	0
			3326	2096	594	616	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1345	906	191	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			745	486	112	131	16		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4802	3195	737	827	43		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2754	1781	487	481	5		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	129	Total	C	N	O	S	0	0
			1049	659	188	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			707	454	104	144	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1030	657	176	191	6		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			654	427	109	116	2		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	49	Total	C	N	O	0	0
			414	273	70	71		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			846	544	140	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1154	759	196	197	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	71	Total	C	N	O	S	0	0
			597	390	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1070	686	188	196			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	122	Total	C	N	O	S	0	0
			1048	653	201	185	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	174	Total	C	N	O	S	0	0
			1458	913	269	268	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1212	780	216	211	5		

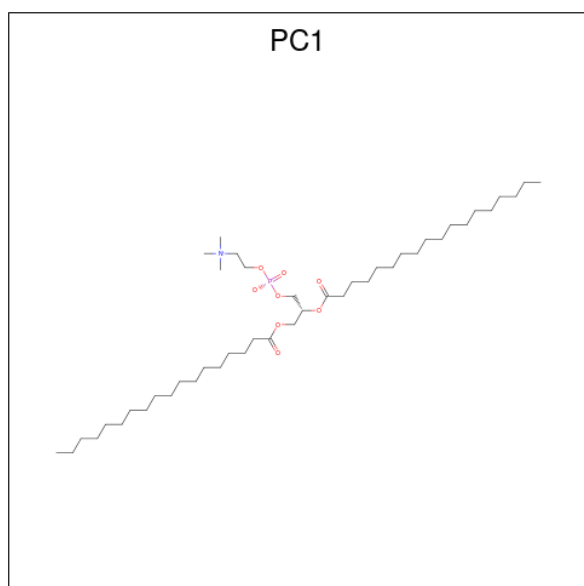
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	95	Total	C	N	O	S	0	0
			776	490	144	139	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	45	Total	C	N	O	S	0	0
			380	238	67	74	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



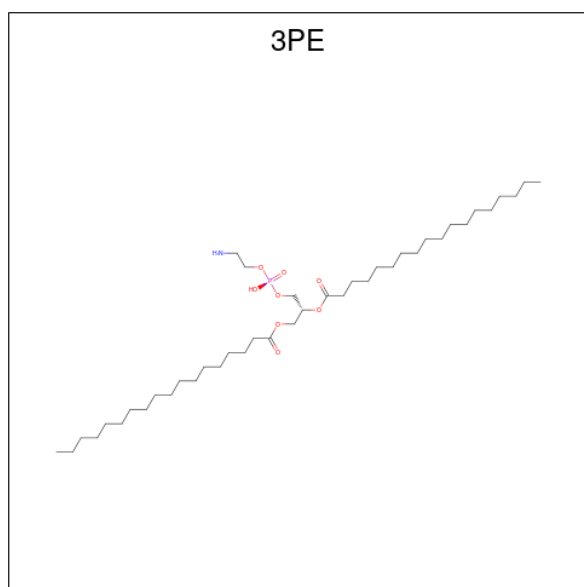
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
45	H	1	Total	C	N	O	P	0
			39	29	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
45	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	g	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			37	27	1	8	1	

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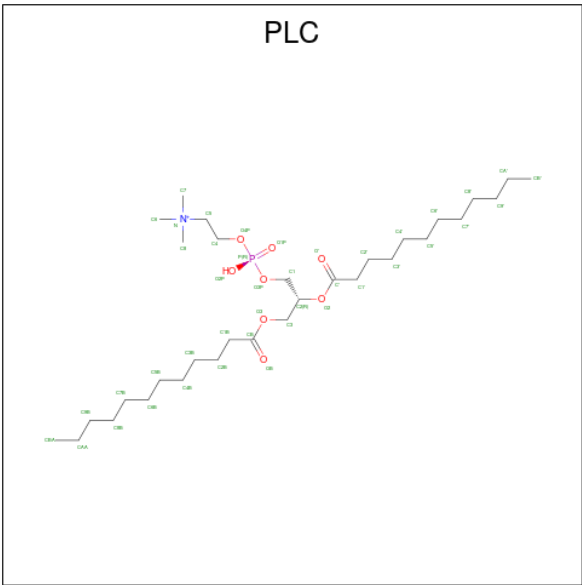
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total 45	C 35	N 1	O 8	P 1	0
46	I	1	Total 51	C 41	N 1	O 8	P 1	0
46	J	1	Total 29	C 19	N 1	O 8	P 1	0
46	J	1	Total 36	C 26	N 1	O 8	P 1	0
46	J	1	Total 44	C 34	N 1	O 8	P 1	0
46	L	1	Total 45	C 35	N 1	O 8	P 1	0
46	M	1	Total 31	C 21	N 1	O 8	P 1	0
46	M	1	Total 50	C 40	N 1	O 8	P 1	0
46	M	1	Total 51	C 41	N 1	O 8	P 1	0
46	M	1	Total 45	C 35	N 1	O 8	P 1	0
46	N	1	Total 49	C 39	N 1	O 8	P 1	0
46	N	1	Total 51	C 41	N 1	O 8	P 1	0
46	P	1	Total 35	C 25	N 1	O 8	P 1	0
46	P	1	Total 45	C 35	N 1	O 8	P 1	0
46	Y	1	Total 41	C 31	N 1	O 8	P 1	0
46	Y	1	Total 27	C 17	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 45	C 35	N 1	O 8	P 1	0
46	Y	1	Total 36	C 26	N 1	O 8	P 1	0

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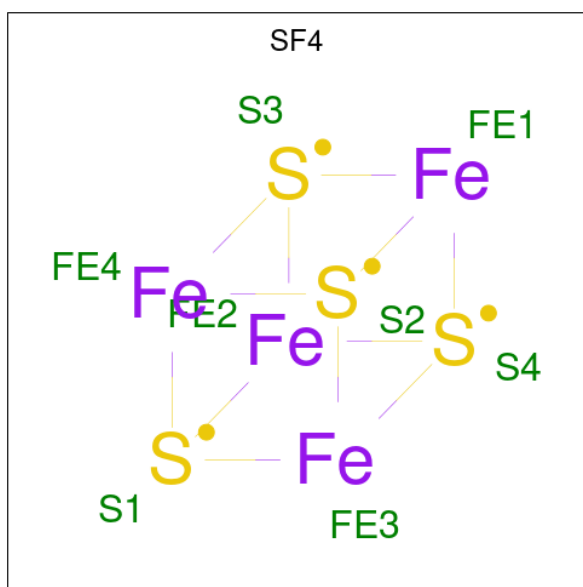
Mol	Chain	Residues	Atoms					AltConf
46	Y	1	Total 43	C 33	N 1	O 8	P 1	0
46	Z	1	Total 51	C 41	N 1	O 8	P 1	0
46	Z	1	Total 41	C 31	N 1	O 8	P 1	0
46	a	1	Total 39	C 29	N 1	O 8	P 1	0
46	b	1	Total 47	C 37	N 1	O 8	P 1	0
46	b	1	Total 51	C 41	N 1	O 8	P 1	0
46	d	1	Total 49	C 39	N 1	O 8	P 1	0
46	f	1	Total 44	C 34	N 1	O 8	P 1	0
46	g	1	Total 34	C 24	N 1	O 8	P 1	0
46	m	1	Total 41	C 31	N 1	O 8	P 1	0
46	m	1	Total 32	C 22	N 1	O 8	P 1	0
46	q	1	Total 51	C 41	N 1	O 8	P 1	0
46	r	1	Total 34	C 24	N 1	O 8	P 1	0

- Molecule 47 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



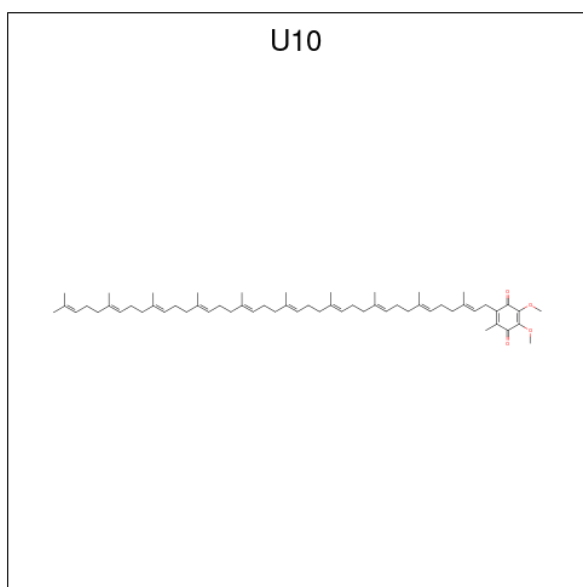
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
47	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	J	1	Total	C	N	O	P	0
			37	27	1	8	1	
47	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	M	1	Total	C	N	O	P	0
			28	18	1	8	1	
47	O	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	P	1	Total	C	N	O	P	0
			32	22	1	8	1	
47	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	Z	1	Total	C	N	O	P	0
			34	24	1	8	1	
47	g	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



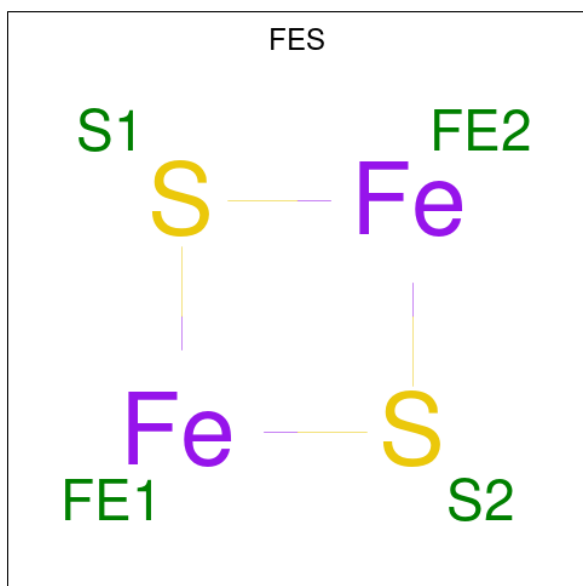
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



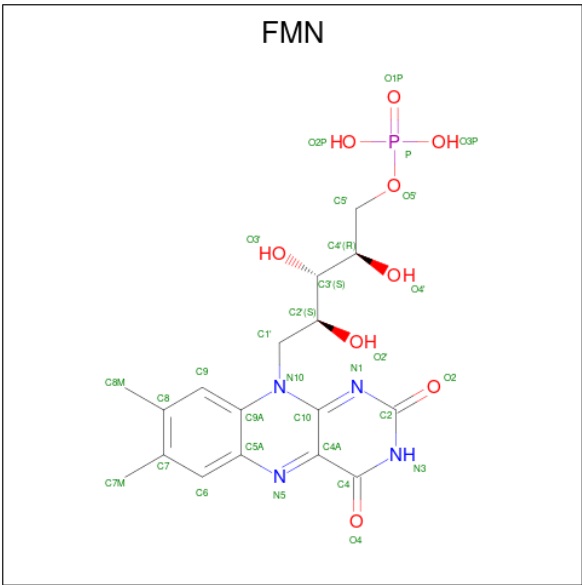
Mol	Chain	Residues	Atoms			AltConf
49	D	1	Total	C	O	0
			63	59	4	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

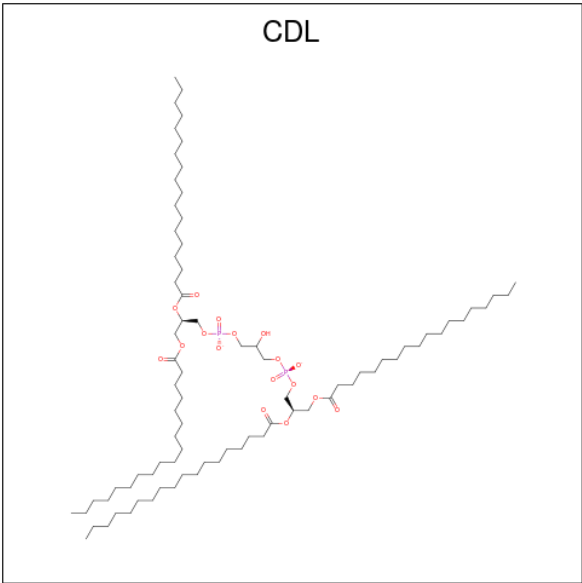


Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
53	H	1	Total	C	O	P	0
			81	62	17	2	
53	L	1	Total	C	O	P	0
			76	57	17	2	
53	M	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			100	81	17	2	
53	P	1	Total	C	O	P	0
			59	40	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	d	1	Total	C	O	P	0
			86	67	17	2	
53	h	1	Total	C	O	P	0
			80	61	17	2	
53	r	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	M	1	Total	Zn	0
			1	1	
54	R	1	Total	Zn	0
			1	1	

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

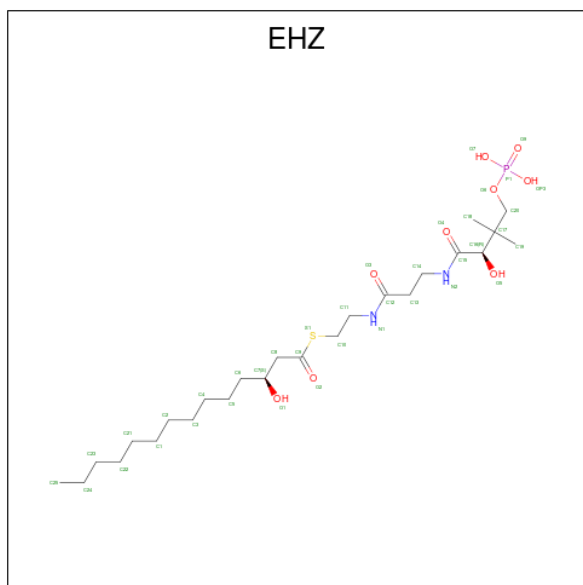
Mol	Chain	Residues	Atoms	AltConf
56	O	1	Total Mg 1 1	0

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



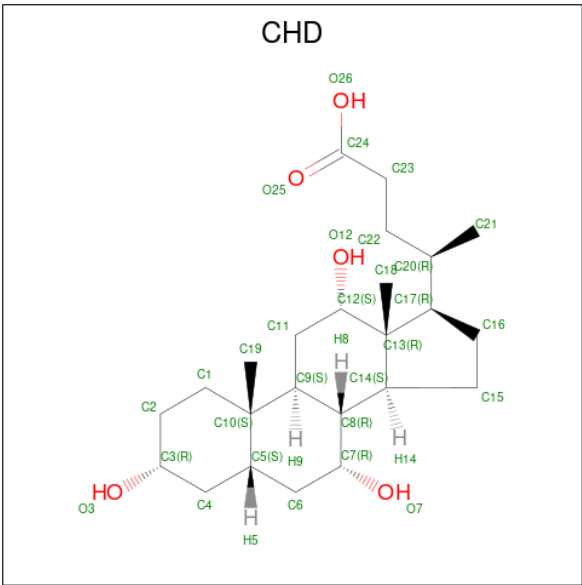
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 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).



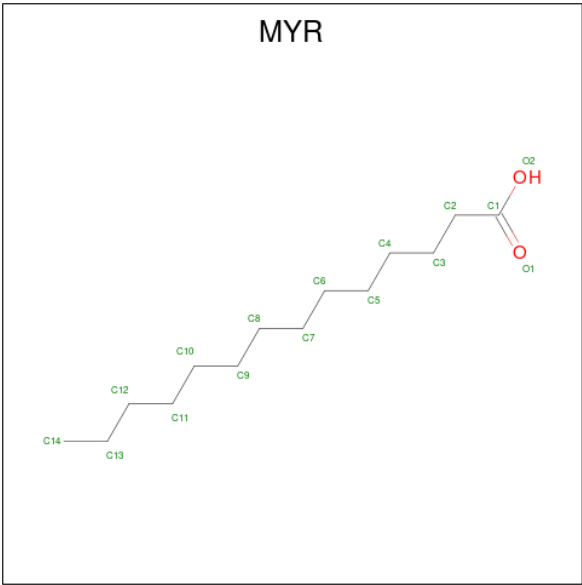
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
59	i	1	Total	C	O	0
			29	24	5	

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	28	Total 28	O 28	0
61	B	68	Total 68	O 68	0
61	C	101	Total 101	O 101	0
61	D	183	Total 183	O 183	0
61	E	2	Total 2	O 2	0
61	F	17	Total 17	O 17	0
61	G	122	Total 122	O 122	0
61	H	78	Total 78	O 78	0
61	I	91	Total 91	O 91	0
61	J	25	Total 25	O 25	0
61	K	19	Total 19	O 19	0
61	L	12	Total 12	O 12	0
61	M	30	Total 30	O 30	0
61	N	35	Total 35	O 35	0
61	O	6	Total 6	O 6	0
61	P	46	Total 46	O 46	0
61	Q	67	Total 67	O 67	0
61	R	20	Total 20	O 20	0
61	V	17	Total 17	O 17	0
61	W	20	Total 20	O 20	0
61	X	8	Total 8	O 8	0
61	Z	17	Total 17	O 17	0

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Mol	Chain	Residues	Atoms		AltConf
61	a	15	Total 15	O 15	0
61	b	4	Total 4	O 4	0
61	d	6	Total 6	O 6	0
61	e	12	Total 12	O 12	0
61	g	1	Total 1	O 1	0
61	h	7	Total 7	O 7	0
61	l	4	Total 4	O 4	0
61	m	3	Total 3	O 3	0
61	p	9	Total 9	O 9	0
61	q	26	Total 26	O 26	0
61	r	22	Total 22	O 22	0
61	s	1	Total 1	O 1	0

3 Residue-property plots

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

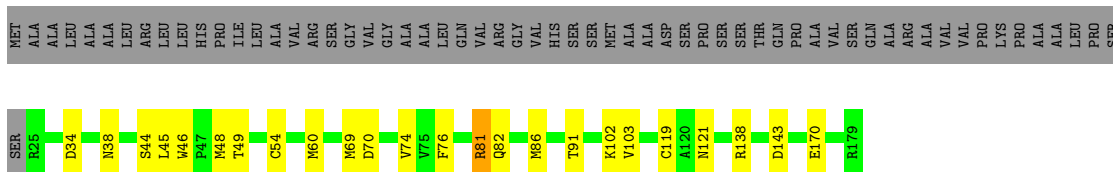
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



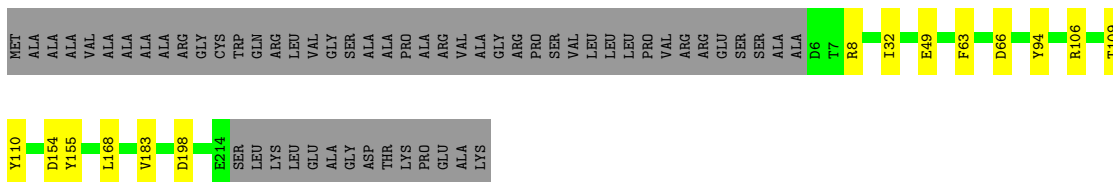
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



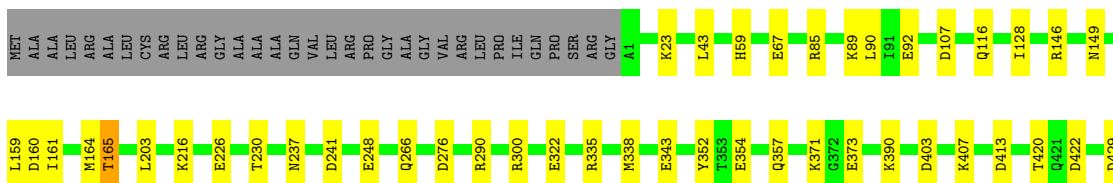
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



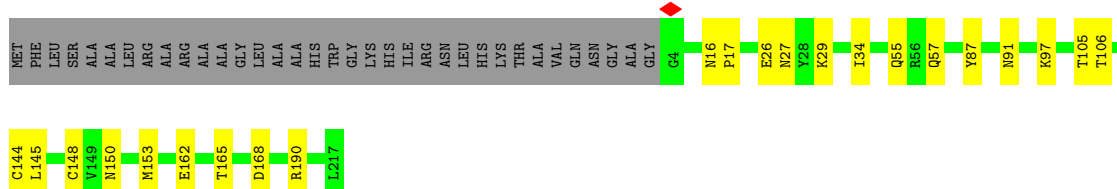
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 

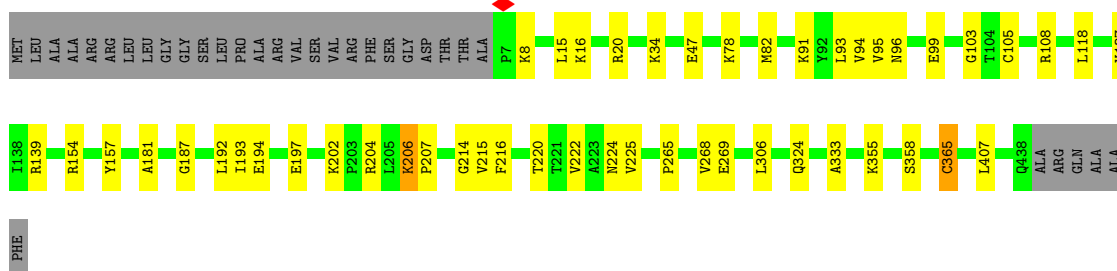


R430

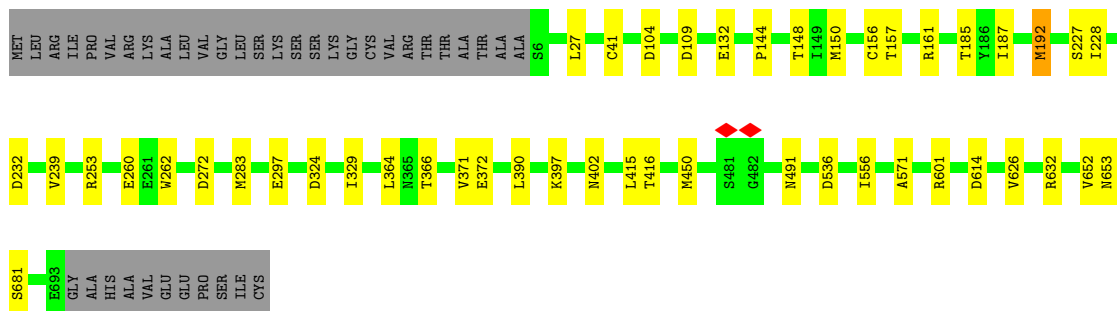
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  77% 9% 14%

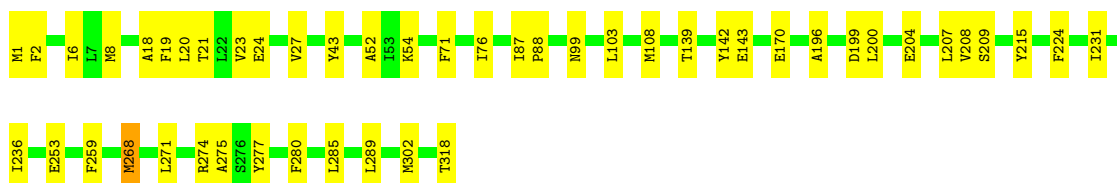
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  83% 10% 7%

- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

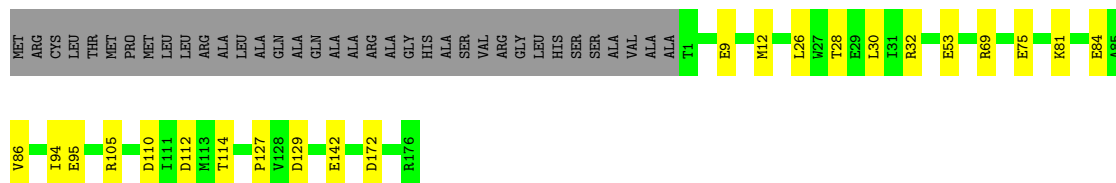
Chain G:  88% 6% 5%

- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  85% 15%

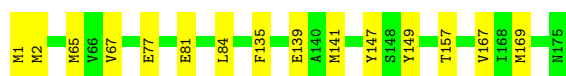
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  73% 10% 17%



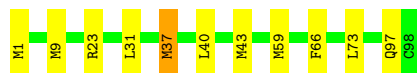
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  91% 9%



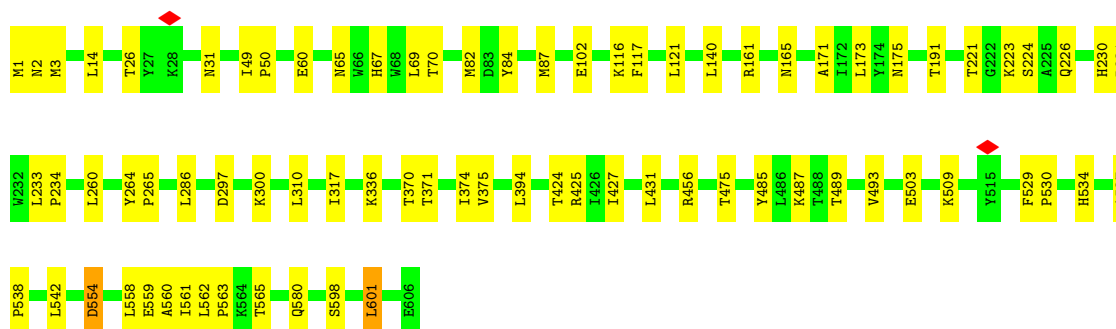
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  89% 10%

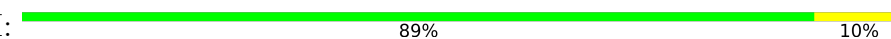


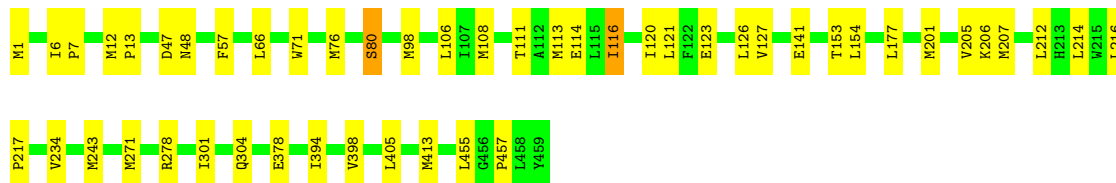
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  87% 13%



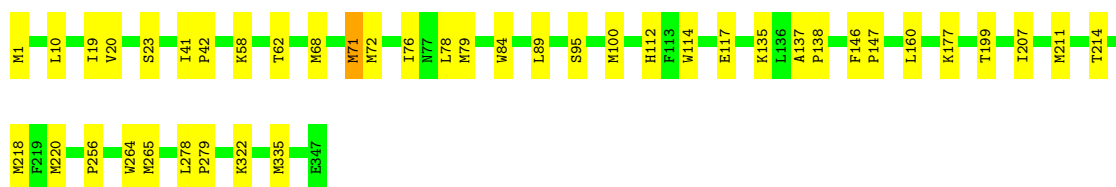
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  89% 10%



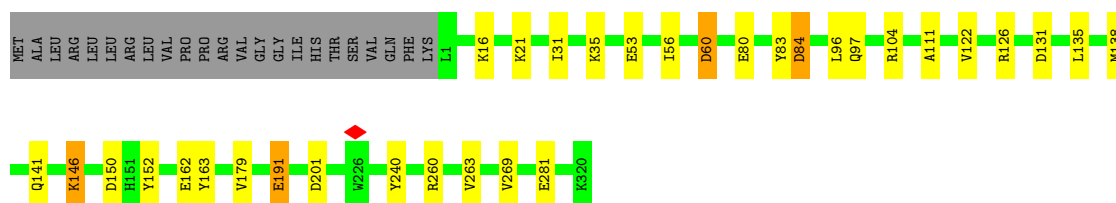
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  88% 12%



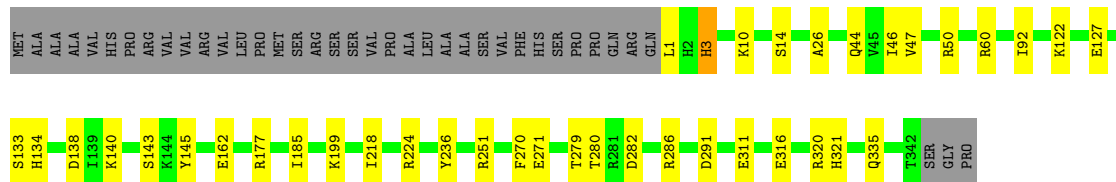
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  84% 8% 7%



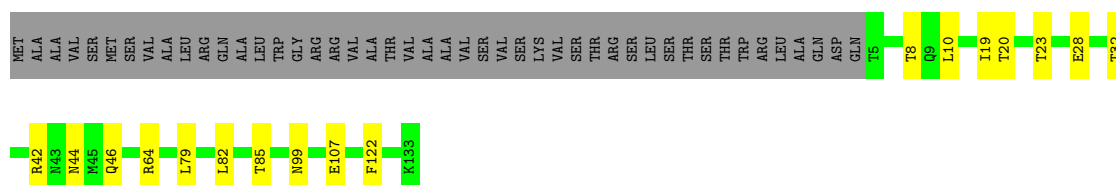
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  80% 10% 10%



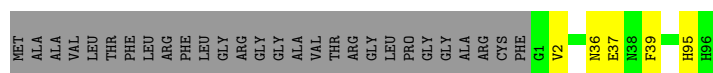
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  64% 10% 26%



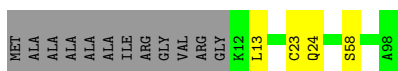
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:  73% 23%



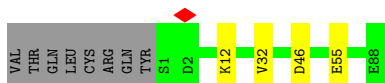
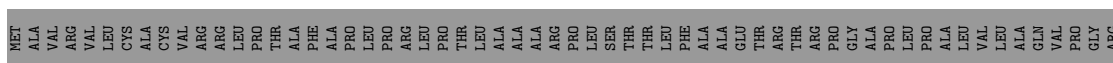
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:  84% 12%



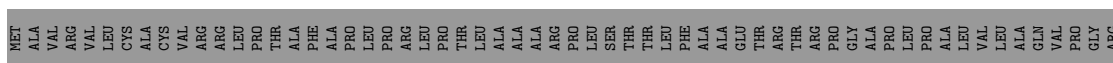
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:  54% 44%

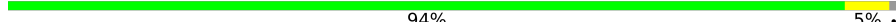


- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:  53% 44%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:  94% 5%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  84% 6% 10%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  90% 9%



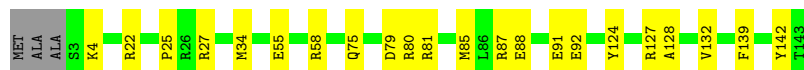
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  94% 5%



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z: 83% 15%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a: 89% 11%



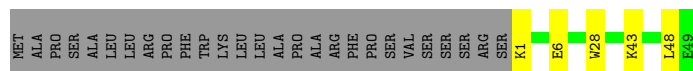
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b: 93% 6%



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c: 58% 7% 36%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d: 93% 6%



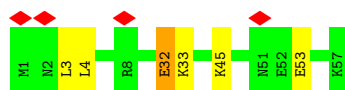
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 88% 6% 7%

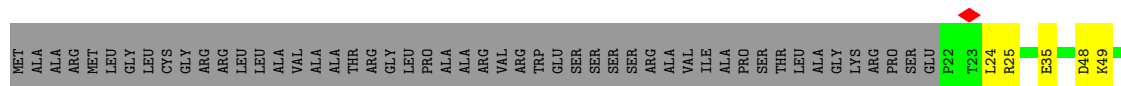


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

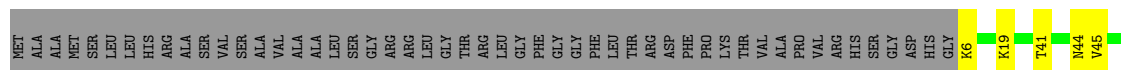
Chain f: 7% 89% 9%



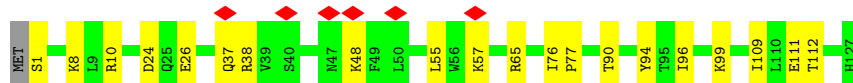
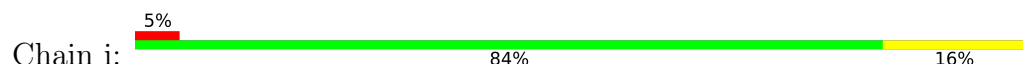
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



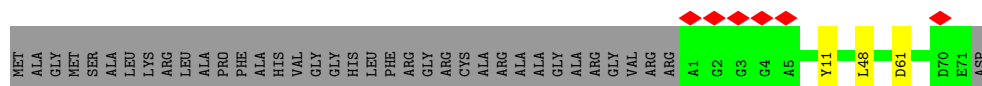
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



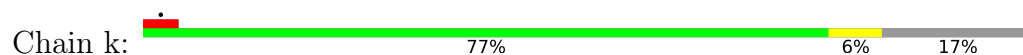
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

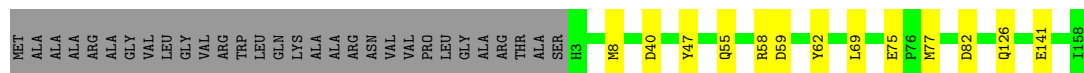


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l: 



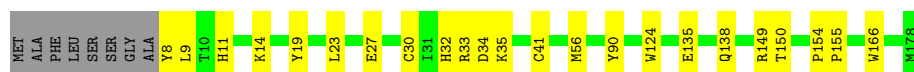
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m: 



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

Chain n: 

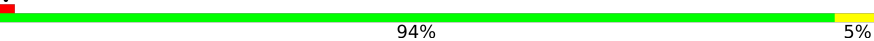


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 

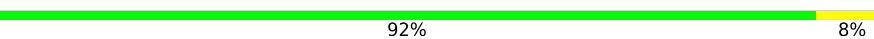


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p: 



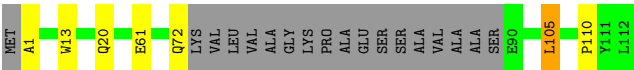
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 

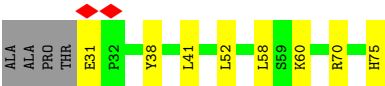
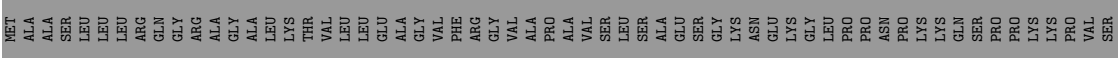


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r: 



● Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	183021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	479.69998, 479.69998, 479.69998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 2MR, CDL, DGT, SF4, CHD, SAC, AYA, EHZ, U10, MG, ZN, FME, PC1, 3PE, NDP, AME, FMN, MYR, K, PLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/936	0.22	0/1281
2	B	0.19	0/1272	0.27	0/1720
3	C	0.18	0/1789	0.25	0/2436
4	D	0.18	0/3537	0.26	0/4794
5	E	0.13	0/1699	0.27	0/2312
6	F	0.13	0/3401	0.26	0/4595
7	G	0.15	0/5367	0.25	0/7274
8	H	0.17	0/2571	0.27	0/3513
9	I	0.20	0/1445	0.28	0/1956
10	J	0.14	0/1370	0.22	0/1859
11	K	0.15	0/745	0.23	0/1008
12	L	0.11	0/4920	0.23	0/6694
13	M	0.14	0/3738	0.23	0/5097
14	N	0.16	0/2792	0.25	0/3800
15	O	0.11	0/2651	0.21	0/3587
16	P	0.15	0/2831	0.24	0/3841
17	Q	0.16	0/1072	0.24	0/1449
18	R	0.16	0/753	0.22	0/1014
19	S	0.11	0/711	0.25	0/956
20	T	0.11	0/719	0.21	0/971
20	U	0.10	0/719	0.21	0/971
21	V	0.14	0/948	0.22	0/1284
22	W	0.13	0/1000	0.23	0/1344
23	X	0.13	0/1439	0.22	0/1942
24	Y	0.11	0/1042	0.19	0/1414
25	Z	0.14	0/1181	0.21	0/1592
26	a	0.15	0/584	0.23	0/786
27	b	0.13	0/667	0.22	0/916
28	c	0.13	0/427	0.19	0/579
29	d	0.13	0/1018	0.21	0/1375
30	e	0.13	0/850	0.22	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.13	0/505	0.23	0/681
32	g	0.11	0/873	0.23	0/1186
33	h	0.12	0/1188	0.21	0/1607
34	i	0.08	0/1127	0.22	0/1534
35	j	0.10	0/624	0.20	0/855
36	k	0.10	0/672	0.19	0/906
37	l	0.10	0/1369	0.23	0/1873
38	m	0.10	0/1088	0.21	0/1472
39	n	0.09	0/1540	0.20	0/2085
40	o	0.11	0/1073	0.21	0/1437
41	p	0.10	0/1491	0.19	0/2011
42	q	0.16	0/1242	0.24	0/1688
43	r	0.15	0/789	0.24	0/1068
44	s	0.10	0/392	0.22	0/531
All	All	0.14	0/68167	0.24	0/92430

There are no bond length outliers.

There are no bond angle outliers.

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	A	921	0	952	10	0
2	B	1241	0	1251	22	0
3	C	1738	0	1685	12	0
4	D	3459	0	3404	39	0
5	E	1659	0	1664	15	0
6	F	3326	0	3282	35	0
7	G	5279	0	5301	30	0
8	H	2509	0	2621	35	0
9	I	1414	0	1370	24	0
10	J	1345	0	1352	14	0
11	K	745	0	785	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	52	0
13	M	3654	0	3852	34	0
14	N	2733	0	2912	34	0
15	O	2589	0	2566	21	0
16	P	2754	0	2773	28	0
17	Q	1049	0	1045	11	0
18	R	740	0	714	4	0
19	S	700	0	719	3	0
20	T	707	0	700	3	0
20	U	707	0	700	5	0
21	V	928	0	972	4	0
22	W	976	0	991	6	0
23	X	1402	0	1381	10	0
24	Y	1030	0	1039	4	0
25	Z	1152	0	1151	22	0
26	a	569	0	568	6	0
27	b	654	0	663	3	0
28	c	414	0	415	4	0
29	d	999	0	988	6	0
30	e	829	0	829	4	0
31	f	492	0	501	5	0
32	g	846	0	798	9	0
33	h	1154	0	1168	9	0
34	i	1097	0	1108	14	0
35	j	597	0	536	2	0
36	k	653	0	642	5	0
37	l	1314	0	1210	7	0
38	m	1070	0	1068	7	0
39	n	1487	0	1433	18	0
40	o	1048	0	1016	13	0
41	p	1458	0	1430	10	0
42	q	1212	0	1183	8	0
43	r	776	0	782	5	0
44	s	380	0	349	8	0
45	A	103	0	128	3	0
45	B	94	0	136	0	0
45	H	126	0	183	4	0
45	I	54	0	88	1	0
45	L	47	0	71	3	0
45	M	35	0	44	0	0
45	Z	44	0	62	0	0
45	d	39	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	g	44	0	65	1	0
45	h	47	0	71	1	0
45	m	54	0	88	0	0
45	q	49	0	75	0	0
46	A	82	0	115	0	0
46	I	51	0	82	0	0
46	J	109	0	143	0	0
46	L	45	0	67	0	0
46	M	177	0	259	0	0
46	N	100	0	157	1	0
46	P	80	0	111	0	0
46	Y	345	0	509	4	0
46	Z	92	0	141	0	0
46	a	39	0	55	0	0
46	b	98	0	153	0	0
46	d	49	0	75	1	0
46	f	44	0	65	0	0
46	g	34	0	42	0	0
46	m	73	0	97	0	0
46	q	51	0	82	1	0
46	r	34	0	42	0	0
47	A	33	0	43	1	0
47	B	42	0	64	0	0
47	J	37	0	51	0	0
47	L	42	0	64	1	0
47	M	28	0	30	0	0
47	O	35	0	47	0	0
47	P	32	0	41	0	0
47	Y	42	0	64	0	0
47	Z	34	0	45	0	0
47	g	42	0	64	1	0
48	B	8	0	0	0	0
48	F	8	0	0	0	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	D	63	0	90	17	0
50	E	4	0	0	0	0
50	G	4	0	0	0	0
51	F	31	0	19	1	0
52	G	1	0	0	0	0
53	H	81	0	109	0	0
53	L	76	0	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	M	100	0	156	2	0
53	N	100	0	156	2	0
53	P	59	0	62	2	0
53	d	151	0	202	1	0
53	h	80	0	104	1	0
53	r	61	0	66	0	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	31	0	12	3	0
56	O	1	0	0	0	0
57	P	48	0	26	2	0
58	T	37	0	0	0	0
58	U	37	0	0	1	0
59	i	29	0	38	6	0
60	o	15	0	27	0	0
61	A	28	0	0	2	0
61	B	68	0	0	7	0
61	C	101	0	0	5	0
61	D	183	0	0	19	0
61	E	2	0	0	0	0
61	F	17	0	0	2	0
61	G	122	0	0	5	0
61	H	78	0	0	7	0
61	I	91	0	0	6	0
61	J	25	0	0	1	0
61	K	19	0	0	0	0
61	L	12	0	0	3	0
61	M	30	0	0	2	0
61	N	35	0	0	4	0
61	O	6	0	0	1	0
61	P	46	0	0	7	0
61	Q	67	0	0	3	0
61	R	20	0	0	0	0
61	V	17	0	0	0	0
61	W	20	0	0	0	0
61	X	8	0	0	2	0
61	Z	17	0	0	1	0
61	a	15	0	0	2	0
61	b	4	0	0	0	0
61	d	6	0	0	0	0
61	e	12	0	0	1	0
61	g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	h	7	0	0	1	0
61	l	4	0	0	1	0
61	m	3	0	0	0	0
61	p	9	0	0	3	0
61	q	26	0	0	2	0
61	r	22	0	0	1	0
61	s	1	0	0	0	0
All	All	71395	0	71766	544	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 4.

All (544) 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)
1:A:33:LYS:O	2:B:81:ARG:NH2	2.10	0.84
4:D:237:ASN:OD1	61:D:601:HOH:O	1.95	0.84
12:L:425:ARG:NH1	47:L:703:PLC:O2P	2.14	0.81
7:G:324:ASP:OD2	61:G:901:HOH:O	1.98	0.81
16:P:14:SER:OG	61:P:601:HOH:O	1.95	0.80
40:o:59:ALA:O	40:o:60:HIS:ND1	2.15	0.80
4:D:429:ASP:OD2	61:D:602:HOH:O	1.98	0.80
13:M:457:PRO:O	32:g:84:ARG:NH2	2.15	0.79
15:O:97:GLN:NE2	15:O:131:ASP:OD1	2.14	0.79
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.00	0.79
16:P:282:ASP:OD2	16:P:286:ARG:NH1	2.15	0.79
3:C:8:ARG:NH1	43:r:61:GLU:OE2	2.16	0.79
40:o:23:THR:OG1	40:o:104:GLU:OE2	2.02	0.78
7:G:109:ASP:OD2	61:G:902:HOH:O	2.02	0.78
13:M:413:MET:SD	61:l:202:HOH:O	2.41	0.78
30:e:40:ILE:HG21	33:h:133:ILE:HD11	1.66	0.78
2:B:48:MET:O	61:B:301:HOH:O	2.01	0.77
26:a:28:ARG:NH1	61:a:202:HOH:O	2.17	0.77
41:p:88:GLU:OE1	61:p:201:HOH:O	2.03	0.77
12:L:165:ASN:ND2	61:L:802:HOH:O	2.17	0.77
16:P:60:ARG:NH2	61:P:603:HOH:O	2.18	0.76
6:F:194:GLU:OE2	6:F:204:ARG:NH1	2.17	0.76
3:C:49:GLU:OE2	61:C:301:HOH:O	2.04	0.76
2:B:82:GLN:OE1	61:B:302:HOH:O	2.03	0.76
10:J:77:GLU:N	10:J:77:GLU:OE1	2.18	0.76
25:Z:88:GLU:OE1	25:Z:127:ARG:NH2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.68	0.75
8:H:204:GLU:OE2	61:H:501:HOH:O	2.04	0.75
16:P:127:GLU:O	16:P:224:ARG:NH2	2.19	0.75
8:H:143:GLU:OE1	61:H:502:HOH:O	2.05	0.75
16:P:44:GLN:NE2	61:P:602:HOH:O	2.18	0.75
9:I:172:ASP:OD1	61:I:301:HOH:O	2.03	0.74
59:i:201:CHD:H212	59:i:201:CHD:H12	1.68	0.74
16:P:10:LYS:NZ	22:W:126:ASP:OD2	2.20	0.74
31:f:53:GLU:N	31:f:53:GLU:OE1	2.21	0.74
4:D:226:GLU:OE1	25:Z:22:ARG:NH1	2.20	0.74
8:H:143:GLU:OE2	61:H:503:HOH:O	2.06	0.74
9:I:81:LYS:NZ	61:I:304:HOH:O	2.12	0.74
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.17	0.74
4:D:266:GLN:OE1	61:D:603:HOH:O	2.05	0.74
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.21	0.73
30:e:20:GLN:OE1	61:e:201:HOH:O	2.06	0.73
1:A:68:GLU:OE2	61:A:301:HOH:O	2.06	0.73
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.20	0.73
14:N:256:PRO:O	61:N:501:HOH:O	2.05	0.73
16:P:335:GLN:N	16:P:335:GLN:OE1	2.22	0.73
6:F:139:ARG:NH1	61:F:601:HOH:O	2.22	0.73
49:D:501:U10:H451	49:D:501:U10:H503	1.70	0.72
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.22	0.72
5:E:144:CYS:O	6:F:139:ARG:NH2	2.22	0.72
11:K:97:GLN:O	14:N:177:LYS:NZ	2.16	0.72
33:h:142:ASP:OD2	61:h:301:HOH:O	2.06	0.72
8:H:318:THR:O	61:H:504:HOH:O	2.07	0.72
16:P:162:GLU:O	16:P:224:ARG:NH1	2.22	0.72
12:L:554:ASP:OD1	61:L:801:HOH:O	2.06	0.72
14:N:20:VAL:O	61:N:502:HOH:O	2.07	0.72
16:P:143:SER:OG	16:P:282:ASP:OD1	2.06	0.72
3:C:198:ASP:OD1	61:C:302:HOH:O	2.08	0.71
4:D:248:GLU:O	61:D:604:HOH:O	2.09	0.71
33:h:140:THR:O	33:h:143:ASN:ND2	2.24	0.71
16:P:60:ARG:NH1	61:P:605:HOH:O	2.23	0.71
12:L:223:LYS:NZ	61:L:803:HOH:O	2.23	0.71
2:B:170:GLU:OE1	61:B:303:HOH:O	2.08	0.71
17:Q:44:ASN:O	61:Q:201:HOH:O	2.09	0.70
20:U:75:GLU:OE2	34:i:8:LYS:NZ	2.23	0.70
2:B:46:TRP:CH2	49:D:501:U10:H401	2.27	0.70
7:G:232:ASP:OD2	61:G:903:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:THR:CG2	25:Z:34:MET:HE1	2.22	0.70
44:s:31:GLU:N	44:s:31:GLU:OE1	2.25	0.70
4:D:203:LEU:O	61:D:605:HOH:O	2.09	0.69
7:G:132:GLU:OE1	61:G:905:HOH:O	2.09	0.69
13:M:378:GLU:OE1	61:M:701:HOH:O	2.10	0.69
4:D:160:ASP:OD1	61:D:606:HOH:O	2.09	0.69
45:I:203:PC1:O12	61:I:302:HOH:O	2.09	0.69
13:M:206:LYS:NZ	61:M:702:HOH:O	2.26	0.69
23:X:94:GLN:OE1	61:X:201:HOH:O	2.09	0.69
25:Z:87:ARG:NH1	25:Z:91:GLU:OE2	2.26	0.69
1:A:42:ASP:OD1	2:B:102:LYS:NZ	2.26	0.69
4:D:422:ASP:OD2	61:D:607:HOH:O	2.10	0.69
7:G:104:ASP:OD2	61:G:904:HOH:O	2.09	0.69
42:q:25:ARG:NE	46:q:202:3PE:O14	2.24	0.69
10:J:139:GLU:OE1	61:J:302:HOH:O	2.11	0.69
26:a:4:GLU:OE1	61:a:201:HOH:O	2.11	0.68
2:B:70:ASP:OD2	61:B:304:HOH:O	2.10	0.68
35:j:61:ASP:OD1	40:o:106:ARG:NH1	2.26	0.68
4:D:413:ASP:OD2	61:D:608:HOH:O	2.11	0.68
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.26	0.68
2:B:76:PHE:CE2	49:D:501:U10:H152	2.29	0.68
8:H:199:ASP:OD2	61:H:505:HOH:O	2.10	0.68
12:L:561:ILE:O	12:L:565:THR:OG1	2.11	0.67
29:d:120:ARG:O	38:m:108:ARG:NH2	2.27	0.67
18:R:2:VAL:HG21	18:R:37:GLU:OE1	1.93	0.67
41:p:88:GLU:OE2	61:p:202:HOH:O	2.10	0.67
42:q:32:ASP:OD2	42:q:58:ARG:NH2	2.27	0.67
9:I:110:ASP:OD1	61:I:303:HOH:O	2.10	0.67
23:X:171:MET:O	61:X:202:HOH:O	2.13	0.67
4:D:107:ASP:OD2	61:D:609:HOH:O	2.13	0.67
1:A:71:LEU:O	10:J:147:TYR:OH	2.10	0.66
11:K:43:MET:SD	14:N:72:MET:HE1	2.35	0.66
3:C:66:ASP:OD2	61:C:303:HOH:O	2.14	0.66
9:I:75:GLU:O	9:I:105:ARG:NH1	2.28	0.66
9:I:142:GLU:O	61:I:305:HOH:O	2.13	0.66
20:U:57:GLU:OE2	35:j:11:TYR:OH	2.12	0.66
1:A:104:TYR:OH	61:A:302:HOH:O	2.10	0.66
53:P:503:CDL:O1	53:P:503:CDL:OB5	2.12	0.65
59:i:201:CHD:O3	59:i:201:CHD:H9	1.96	0.65
15:O:281:GLU:N	15:O:281:GLU:OE1	2.29	0.65
2:B:69:MET:HE3	2:B:74:VAL:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.79	0.65
37:l:59:ASP:OD2	37:l:62:TYR:N	2.28	0.65
44:s:38:TYR:O	44:s:41:LEU:HD11	1.96	0.65
17:Q:85:THR:O	61:Q:202:HOH:O	2.14	0.65
4:D:59:HIS:NE2	61:D:612:HOH:O	2.29	0.65
39:n:34:ASP:OD1	39:n:35:LYS:N	2.28	0.65
2:B:170:GLU:OE2	61:B:305:HOH:O	2.15	0.65
8:H:99:ASN:N	45:H:402:PC1:O12	2.27	0.65
24:Y:80:ARG:NH2	24:Y:85:ASP:OD2	2.30	0.65
8:H:196:ALA:O	61:H:506:HOH:O	2.13	0.64
43:r:72:GLN:N	43:r:72:GLN:OE1	2.30	0.64
2:B:49:THR:HG22	49:D:501:U10:H101	1.79	0.64
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.80	0.64
7:G:415:LEU:O	7:G:416:THR:OG1	2.10	0.64
10:J:141:MET:HA	10:J:141:MET:HE2	1.79	0.63
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.30	0.63
7:G:366:THR:HB	7:G:450:MET:HE3	1.80	0.63
8:H:27:VAL:HG21	8:H:268:MET:HE1	1.81	0.63
43:r:20:GLN:OE1	61:r:301:HOH:O	2.15	0.63
32:g:90:ARG:NH2	41:p:107:GLU:OE2	2.32	0.63
5:E:26:GLU:N	5:E:26:GLU:OE1	2.32	0.62
16:P:145:TYR:HH	57:P:501:NDP:HO2N	1.48	0.62
22:W:110:GLU:OE1	22:W:110:GLU:N	2.31	0.62
12:L:485:TYR:O	12:L:489:THR:OG1	2.18	0.62
15:O:240:TYR:OH	21:V:21:GLU:OE1	2.17	0.62
20:T:12:LYS:HE2	20:T:32:VAL:HG21	1.79	0.62
2:B:60:MET:HE1	49:D:501:U10:H4M3	1.82	0.62
6:F:224:ASN:ND2	51:F:501:FMN:O2	2.33	0.61
12:L:31:ASN:ND2	59:i:201:CHD:H151	2.15	0.61
40:o:32:GLU:N	40:o:32:GLU:OE1	2.34	0.61
8:H:20:LEU:HD21	8:H:231:ILE:HD11	1.82	0.61
7:G:156:CYS:O	7:G:157:THR:OG1	2.18	0.61
10:J:81:GLU:OE1	11:K:23:ARG:NH1	2.34	0.60
9:I:75:GLU:OE2	61:I:306:HOH:O	2.16	0.60
6:F:358:SER:OG	6:F:365:CYS:SG	2.52	0.60
37:l:141:GLU:N	37:l:141:GLU:OE1	2.35	0.59
15:O:162:GLU:OE2	61:O:501:HOH:O	2.16	0.59
4:D:322:GLU:OE1	4:D:322:GLU:N	2.32	0.59
7:G:272:ASP:OD1	7:G:681:SER:OG	2.08	0.59
17:Q:64:ARG:NH1	61:Q:203:HOH:O	2.32	0.59
26:a:34:LYS:NZ	26:a:61:TYR:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ASP:OD1	61:B:306:HOH:O	2.17	0.59
4:D:146:ARG:NH1	61:D:627:HOH:O	2.36	0.59
11:K:9:MET:CE	14:N:79:MET:HE1	2.32	0.59
40:o:82:GLU:N	40:o:82:GLU:OE1	2.32	0.59
41:p:153:LYS:NZ	61:p:203:HOH:O	2.29	0.58
5:E:145:LEU:HD12	5:E:153:MET:SD	2.42	0.58
12:L:2:ASN:OD1	12:L:3:MET:N	2.35	0.58
49:D:501:U10:H151	49:D:501:U10:H211	1.83	0.58
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.86	0.58
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.34	0.58
34:i:111:GLU:OE1	34:i:111:GLU:N	2.36	0.58
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.34	0.58
44:s:70:ARG:NH1	44:s:75:HIS:O	2.37	0.58
4:D:373:GLU:OE1	61:D:610:HOH:O	2.17	0.58
12:L:489:THR:O	12:L:493:VAL:HG22	2.04	0.58
49:D:501:U10:H452	8:H:224:PHE:CG	2.38	0.58
9:I:9:GLU:N	9:I:9:GLU:OE1	2.37	0.57
34:i:37:GLN:NE2	34:i:38:ARG:O	2.37	0.57
2:B:34:ASP:OD1	2:B:38:ASN:ND2	2.37	0.57
25:Z:55:GLU:OE1	25:Z:58:ARG:NH2	2.37	0.57
6:F:118:LEU:HD13	6:F:225:VAL:HG13	1.85	0.57
15:O:146:LYS:NZ	15:O:150:ASP:OD1	2.38	0.57
38:m:74:ASN:OD1	38:m:78:ASN:ND2	2.37	0.57
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.87	0.57
9:I:32:ARG:NH2	25:Z:25:PRO:O	2.35	0.57
9:I:112:ASP:OD1	9:I:114:THR:OG1	2.22	0.56
13:M:141:GLU:N	13:M:141:GLU:OE1	2.37	0.56
37:l:40:ASP:O	38:m:82:ASN:ND2	2.35	0.56
10:J:2:MET:HA	10:J:2:MET:HE2	1.85	0.56
4:D:300:ARG:NH1	61:D:626:HOH:O	2.34	0.56
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.38	0.56
7:G:260:GLU:OE2	7:G:397:LYS:NZ	2.27	0.56
13:M:271:MET:HE2	13:M:271:MET:HA	1.88	0.56
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.37	0.56
8:H:253:GLU:OE2	26:a:25:ARG:NH1	2.39	0.56
15:O:83:TYR:OH	55:O:401:DGT:O3'	2.13	0.56
29:d:45:ASP:OD1	29:d:49:ARG:NH1	2.37	0.56
19:S:23:CYS:SG	19:S:24:GLN:N	2.78	0.56
37:l:58:ARG:NH2	37:l:75:GLU:OE2	2.38	0.56
12:L:542:LEU:O	13:M:278:ARG:NH1	2.38	0.56
16:P:3:HIS:O	16:P:3:HIS:ND1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:4:LEU:HD13	31:f:4:LEU:O	2.05	0.56
9:I:26:LEU:HD12	25:Z:34:MET:HE2	1.86	0.56
37:l:55:GLN:NE2	37:l:69:LEU:O	2.39	0.56
6:F:96:ASN:ND2	6:F:187:GLY:O	2.35	0.55
5:E:105:THR:HG22	5:E:106:THR:H	1.71	0.55
12:L:60:GLU:OE2	12:L:84:TYR:N	2.39	0.55
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.88	0.55
14:N:214:THR:HG22	14:N:218:MET:HE2	1.88	0.55
34:i:10:ARG:NH1	39:n:154:PRO:O	2.39	0.55
31:f:32:GLU:N	31:f:32:GLU:OE1	2.40	0.55
9:I:28:THR:HG22	25:Z:34:MET:HE1	1.87	0.55
18:R:2:VAL:HG22	18:R:39:PHE:CE1	2.42	0.55
11:K:40:LEU:HD13	14:N:71:MET:HB3	1.89	0.55
49:D:501:U10:H151	49:D:501:U10:C21	2.37	0.55
32:g:110:SER:O	41:p:161:ARG:NH2	2.40	0.55
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.89	0.55
2:B:44:SER:O	8:H:54:LYS:NZ	2.40	0.54
12:L:87:MET:HA	12:L:87:MET:HE2	1.89	0.54
23:X:109:CYS:SG	23:X:110:VAL:N	2.80	0.54
49:D:501:U10:C24	49:D:501:U10:H201	2.38	0.54
12:L:191:THR:O	38:m:125:ASN:ND2	2.39	0.54
34:i:99:LYS:NZ	40:o:49:GLN:OE1	2.39	0.54
15:O:80:GLU:N	15:O:80:GLU:OE1	2.38	0.54
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.88	0.54
10:J:157:THR:HG22	11:K:66:PHE:CE2	2.42	0.54
13:M:201:MET:HE1	13:M:212:LEU:HD11	1.90	0.54
36:k:25:LEU:HD21	39:n:41:CYS:HB2	1.88	0.54
2:B:86:MET:HE1	2:B:103:VAL:HG23	1.88	0.54
7:G:556:ILE:HD12	7:G:556:ILE:O	2.08	0.54
13:M:76:MET:O	13:M:80:SER:OG	2.25	0.54
59:i:201:CHD:O7	59:i:201:CHD:H41	2.07	0.54
13:M:98:MET:HE2	13:M:98:MET:HA	1.90	0.54
25:Z:85:MET:HE1	25:Z:124:TYR:CZ	2.44	0.53
11:K:73:LEU:HD21	14:N:41:ILE:HD12	1.90	0.53
15:O:104:ARG:NE	15:O:131:ASP:OD2	2.38	0.53
7:G:148:THR:HG23	7:G:150:MET:SD	2.49	0.53
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.91	0.53
12:L:534:HIS:ND1	45:L:704:PC1:O12	2.39	0.53
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.44	0.53
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.44	0.52
23:X:46:ARG:NE	25:Z:79:ASP:OD2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.43	0.52
33:h:6:LYS:NZ	34:i:26:GLU:OE2	2.41	0.52
45:L:704:PC1:H361	13:M:405:LEU:HD13	1.90	0.52
24:Y:123:LEU:HD12	46:Y:203:3PE:H3I1	1.91	0.52
40:o:26:PRO:O	40:o:33:ARG:NH1	2.42	0.52
4:D:92:GLU:OE2	61:D:611:HOH:O	2.18	0.52
34:i:65:ARG:NH2	59:i:201:CHD:O25	2.43	0.52
1:A:27:LEU:HD12	45:A:201:PC1:H133	1.92	0.52
6:F:206:LYS:HB3	6:F:207:PRO:HA	1.92	0.52
13:M:394:ILE:O	13:M:398:VAL:HG23	2.10	0.52
28:c:1:LYS:NZ	28:c:6:GLU:OE1	2.43	0.52
32:g:70:LEU:O	32:g:74:SER:OG	2.18	0.52
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.92	0.51
14:N:72:MET:HE2	14:N:76:ILE:HG13	1.91	0.51
33:h:44:ASN:ND2	53:h:201:CDL:OB9	2.43	0.51
40:o:72:SER:O	40:o:75:ASN:N	2.43	0.51
7:G:632:ARG:NH2	19:S:58:SER:O	2.40	0.51
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.92	0.51
14:N:135:LYS:NZ	61:N:506:HOH:O	2.35	0.51
12:L:31:ASN:OD1	12:L:31:ASN:N	2.44	0.51
12:L:424:THR:HG23	36:k:52:PHE:CE1	2.45	0.51
13:M:304:GLN:O	29:d:119:VAL:HG11	2.11	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.92	0.51
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.93	0.51
28:c:43:LYS:HG2	28:c:48:LEU:HD11	1.91	0.51
4:D:160:ASP:OD2	61:D:612:HOH:O	2.18	0.51
4:D:164:MET:SD	49:D:501:U10:H251	2.50	0.51
4:D:390:LYS:NZ	61:D:614:HOH:O	2.19	0.50
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.91	0.50
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.91	0.50
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.93	0.50
4:D:43:LEU:H	4:D:43:LEU:HD23	1.76	0.50
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.41	0.50
15:O:138:MET:CE	55:O:401:DGT:HN2	2.25	0.50
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.29	0.50
6:F:103:GLY:O	6:F:333:ALA:HB1	2.11	0.50
8:H:268:MET:CE	8:H:271:LEU:HD12	2.42	0.50
14:N:112:HIS:NE2	61:N:505:HOH:O	2.35	0.50
17:Q:19:ILE:O	17:Q:23:THR:HG23	2.11	0.50
37:l:47:TYR:OH	37:l:77:MET:O	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:g:203:PC1:H132	45:g:203:PC1:O13	2.11	0.50
3:C:94:TYR:OH	61:C:304:HOH:O	2.18	0.50
5:E:55:GLN:OE1	5:E:91:ASN:N	2.40	0.50
49:D:501:U10:H201	49:D:501:U10:C23	2.42	0.50
14:N:76:ILE:HA	14:N:79:MET:HE3	1.93	0.50
2:B:76:PHE:CD2	49:D:501:U10:H152	2.47	0.50
1:A:108:GLN:HB2	10:J:169:MET:HE1	1.93	0.49
16:P:177:ARG:NH2	61:P:611:HOH:O	2.44	0.49
16:P:320:ARG:NH1	61:P:609:HOH:O	2.41	0.49
6:F:47:GLU:OE1	6:F:47:GLU:N	2.45	0.49
7:G:283:MET:HE1	42:q:139:PRO:HG3	1.94	0.49
32:g:48:ASP:OD1	32:g:49:LYS:N	2.46	0.49
11:K:43:MET:CE	14:N:72:MET:HE1	2.43	0.49
39:n:56:MET:HA	39:n:56:MET:HE2	1.95	0.49
2:B:46:TRP:CZ2	49:D:501:U10:H401	2.47	0.49
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.94	0.49
14:N:199:THR:OG1	29:d:1:AME:HT23	2.13	0.49
13:M:205:VAL:HG22	13:M:212:LEU:HD13	1.93	0.49
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.42	0.48
6:F:78:LYS:NZ	6:F:222:VAL:O	2.46	0.48
6:F:99:GLU:OE1	6:F:108:ARG:N	2.46	0.48
25:Z:92:GLU:OE2	30:e:91:TYR:OH	2.25	0.48
45:H:402:PC1:H153	25:Z:139:PHE:O	2.13	0.48
49:D:501:U10:H452	8:H:224:PHE:CD1	2.48	0.48
11:K:37:MET:SD	14:N:68:MET:HE1	2.53	0.48
46:Y:203:3PE:O12	46:Y:205:3PE:N	2.39	0.48
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.41	0.48
25:Z:142:TYR:CE2	26:a:48:MET:HE1	2.49	0.48
8:H:285:LEU:HD12	8:H:289:LEU:HD13	1.94	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.94	0.48
20:U:17:TYR:OH	36:k:11:TRP:NE1	2.40	0.48
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.48
38:m:32:GLN:OE1	39:n:8:TYR:N	2.46	0.48
4:D:403:ASP:O	4:D:407:LYS:NZ	2.43	0.48
45:H:402:PC1:H151	25:Z:139:PHE:CZ	2.48	0.48
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.49	0.48
6:F:306:LEU:C	6:F:306:LEU:HD12	2.39	0.48
13:M:113:MET:HE2	13:M:177:LEU:CD1	2.43	0.47
13:M:127:VAL:HG11	53:M:607:CDL:H842	1.96	0.47
39:n:30:CYS:O	39:n:32:HIS:N	2.47	0.47
27:b:58:ASP:HA	27:b:62:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:200:LEU:HD21	8:H:280:PHE:O	2.13	0.47
14:N:146:PHE:N	14:N:147:PRO:CD	2.78	0.47
7:G:239:VAL:HG23	7:G:253:ARG:HB2	1.97	0.47
16:P:291:ASP:OD1	61:P:604:HOH:O	2.20	0.47
17:Q:8:THR:O	17:Q:8:THR:HG22	2.15	0.47
44:s:41:LEU:HD12	44:s:41:LEU:H	1.78	0.47
4:D:67:GLU:OE1	61:D:613:HOH:O	2.19	0.47
7:G:27:LEU:C	7:G:27:LEU:HD23	2.40	0.47
15:O:260:ARG:HA	15:O:263:VAL:HG22	1.96	0.47
32:g:35:GLU:N	32:g:35:GLU:OE1	2.47	0.47
38:m:21:GLU:O	39:n:14:LYS:NZ	2.48	0.47
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.96	0.47
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.48	0.47
16:P:50:ARG:NH2	57:P:501:NDP:O2X	2.41	0.47
33:h:48:GLY:O	41:p:60:TYR:OH	2.26	0.47
9:I:12:MET:O	27:b:9:LYS:NZ	2.47	0.47
9:I:26:LEU:CD1	25:Z:34:MET:HE2	2.45	0.47
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.48	0.47
7:G:652:VAL:O	7:G:653:ASN:C	2.58	0.47
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.47	0.47
12:L:559:GLU:HG2	13:M:214:LEU:HD13	1.97	0.46
14:N:19:ILE:O	14:N:23:SER:OG	2.20	0.46
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.50	0.46
16:P:270:PHE:CD2	16:P:279:THR:HG22	2.50	0.46
20:U:14:ARG:O	20:U:18:VAL:HG23	2.16	0.46
33:h:109:GLU:O	33:h:113:LEU:HD23	2.16	0.46
12:L:173:LEU:HD13	45:L:704:PC1:H222	1.97	0.46
16:P:138:ASP:N	16:P:138:ASP:OD1	2.48	0.46
12:L:560:ALA:O	12:L:565:THR:HG23	2.16	0.46
22:W:95:VAL:HG12	22:W:95:VAL:O	2.16	0.46
25:Z:27:ARG:NH2	43:r:13:TRP:O	2.48	0.46
31:f:45:LYS:O	41:p:68:ARG:NH1	2.43	0.46
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.79	0.46
49:D:501:U10:C23	49:D:501:U10:C20	2.93	0.46
6:F:197:GLU:OE2	6:F:216:PHE:N	2.45	0.46
46:d:201:3PE:O12	30:e:8:ARG:NH1	2.46	0.46
5:E:34:ILE:HD11	44:s:52:LEU:HD22	1.97	0.46
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.25	0.46
15:O:31:ILE:O	15:O:179:VAL:HG13	2.16	0.46
17:Q:20:THR:HG22	17:Q:99:ASN:O	2.15	0.46
4:D:67:GLU:OE1	4:D:67:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:144:PRO:HD2	7:G:192:MET:HE1	1.98	0.45
40:o:121:MET:SD	40:o:122:ALA:N	2.90	0.45
9:I:95:GLU:OE1	42:q:130:THR:HG21	2.17	0.45
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.97	0.45
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.42	0.45
8:H:277:TYR:OH	9:I:30:LEU:O	2.29	0.45
4:D:159:LEU:HD11	49:D:501:U10:H203	1.98	0.45
42:q:58:ARG:NH1	61:q:302:HOH:O	2.46	0.45
16:P:127:GLU:OE1	16:P:127:GLU:N	2.50	0.45
25:Z:128:ALA:O	25:Z:132:VAL:HG23	2.16	0.45
44:s:41:LEU:HD12	44:s:41:LEU:N	2.31	0.45
8:H:142:TYR:HA	8:H:289:LEU:HD23	1.98	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.45
12:L:601:LEU:HD11	46:Y:209:3PE:H222	1.98	0.45
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.17	0.45
37:l:82:ASP:N	37:l:82:ASP:OD1	2.47	0.45
47:A:206:PLC:H6A1	27:b:29:VAL:HG13	1.98	0.45
13:M:108:MET:CB	13:M:121:LEU:HD13	2.46	0.45
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.23	0.45
26:a:49:GLU:OE1	26:a:52:ARG:NH2	2.49	0.45
2:B:91:THR:HA	2:B:119:CYS:HB3	1.99	0.45
4:D:89:LYS:NZ	61:D:629:HOH:O	2.39	0.45
12:L:224:SER:O	12:L:310:LEU:HD13	2.17	0.45
16:P:133:SER:OG	16:P:134:HIS:N	2.49	0.45
3:C:183:VAL:O	22:W:100:THR:OG1	2.20	0.44
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.51	0.44
16:P:271:GLU:HG2	16:P:280:THR:HG22	1.98	0.44
4:D:165:THR:OG1	8:H:275:ALA:O	2.20	0.44
8:H:207:LEU:O	8:H:209:SER:N	2.49	0.44
15:O:104:ARG:NH1	15:O:126:ARG:O	2.50	0.44
40:o:38:MET:HE3	40:o:40:ALA:O	2.17	0.44
3:C:168:LEU:HD11	4:D:90:LEU:HD23	2.00	0.44
5:E:105:THR:HG22	5:E:106:THR:N	2.32	0.44
7:G:329:ILE:HD11	7:G:626:VAL:HG21	1.98	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.44
10:J:157:THR:HG22	11:K:66:PHE:HE2	1.82	0.44
10:J:67:VAL:HG11	11:K:31:LEU:HD21	1.99	0.44
53:M:607:CDL:H401	53:d:204:CDL:H673	2.00	0.44
14:N:89:LEU:HD12	14:N:95:SER:HA	2.00	0.44
42:q:51:ASP:OD2	61:q:301:HOH:O	2.21	0.44
6:F:15:LEU:O	6:F:20:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:57:PHE:HB3	13:M:113:MET:HE3	1.99	0.44
28:c:48:LEU:HD12	28:c:48:LEU:C	2.43	0.44
34:i:94:TYR:OH	41:p:10:PRO:O	2.34	0.44
3:C:106:ARG:NE	61:C:301:HOH:O	2.34	0.44
7:G:371:VAL:HG22	7:G:450:MET:HE1	1.99	0.44
12:L:260:LEU:HB2	12:L:317:ILE:HD13	1.99	0.44
16:P:26:ALA:HB3	16:P:47:VAL:HG13	2.00	0.44
33:h:41:THR:O	33:h:45:VAL:HG23	2.18	0.44
39:n:138:GLN:NE2	39:n:155:PRO:O	2.48	0.44
8:H:18:ALA:O	8:H:21:THR:OG1	2.31	0.44
12:L:598:SER:CB	14:N:100:MET:HE1	2.47	0.44
20:T:55:GLU:OE2	22:W:36:ARG:NH2	2.50	0.44
24:Y:104:THR:HG22	24:Y:104:THR:O	2.17	0.44
25:Z:81:ARG:NE	61:Z:301:HOH:O	2.44	0.44
5:E:148:CYS:N	6:F:105:CYS:SG	2.91	0.44
12:L:230:HIS:N	12:L:231:PRO:HD3	2.33	0.44
23:X:58:GLU:OE1	23:X:58:GLU:N	2.45	0.44
39:n:135:GLU:OE2	39:n:166:TRP:NE1	2.50	0.44
40:o:56:ASP:OD1	40:o:58:CYS:N	2.51	0.44
6:F:214:GLY:HA3	6:F:220:THR:HG22	1.99	0.44
12:L:14:LEU:HD23	12:L:14:LEU:O	2.18	0.44
14:N:68:MET:HE2	14:N:68:MET:HA	1.99	0.44
6:F:192:LEU:HD23	6:F:192:LEU:O	2.18	0.43
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.52	0.43
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.49	0.43
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.53	0.43
36:k:25:LEU:HD21	39:n:41:CYS:CB	2.48	0.43
3:C:154:ASP:OD1	3:C:155:TYR:N	2.52	0.43
4:D:343:GLU:OE1	4:D:343:GLU:N	2.49	0.43
12:L:558:LEU:C	13:M:214:LEU:HD11	2.44	0.43
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.51	0.43
18:R:95:HIS:O	18:R:95:HIS:ND1	2.51	0.43
34:i:76:ILE:HB	34:i:77:PRO:HD3	2.01	0.43
12:L:286:LEU:C	12:L:286:LEU:HD13	2.43	0.43
17:Q:79:LEU:HD22	17:Q:82:LEU:HD22	1.99	0.43
2:B:45:LEU:O	2:B:74:VAL:HA	2.18	0.43
5:E:16:ASN:HB2	5:E:17:PRO:HD2	2.00	0.43
6:F:93:LEU:C	6:F:93:LEU:HD23	2.43	0.43
8:H:43:TYR:OH	61:H:507:HOH:O	2.16	0.43
12:L:562:LEU:HB2	12:L:563:PRO:HD3	1.99	0.43
16:P:251:ARG:NH1	16:P:321:HIS:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:55:LEU:HD13	34:i:55:LEU:C	2.43	0.43
12:L:161:ARG:NH1	39:n:90:TYR:O	2.48	0.43
3:C:32:ILE:HG21	3:C:63:PHE:CE2	2.54	0.43
7:G:297:GLU:OE1	7:G:297:GLU:N	2.42	0.43
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.54	0.43
12:L:297:ASP:OD2	12:L:300:LYS:N	2.42	0.43
14:N:72:MET:HA	14:N:72:MET:HE3	2.00	0.43
34:i:90:THR:HG22	34:i:96:ILE:HD12	2.01	0.43
4:D:413:ASP:OD1	61:D:615:HOH:O	2.21	0.43
5:E:150:ASN:HB3	5:E:162:GLU:HB3	2.01	0.43
12:L:26:THR:HG23	12:L:26:THR:O	2.19	0.43
1:A:18:VAL:HG21	8:H:76:ILE:CG1	2.49	0.43
10:J:84:LEU:HD22	53:P:503:CDL:H521	2.00	0.43
32:g:122:GLU:OE2	41:p:166:ARG:NH2	2.52	0.43
39:n:8:TYR:C	39:n:9:LEU:HD12	2.43	0.43
3:C:109:THR:OG1	3:C:110:TYR:N	2.51	0.42
13:M:47:ASP:OD1	13:M:48:ASN:N	2.51	0.42
34:i:109:ILE:HG22	34:i:111:GLU:H	1.84	0.42
17:Q:10:LEU:N	17:Q:10:LEU:HD12	2.33	0.42
6:F:137:TYR:HB2	6:F:192:LEU:HD21	2.01	0.42
8:H:19:PHE:O	8:H:23:VAL:HG23	2.20	0.42
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.02	0.42
14:N:265:MET:HA	14:N:265:MET:HE2	2.01	0.42
21:V:77:GLU:OE1	21:V:77:GLU:N	2.49	0.42
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.01	0.42
9:I:28:THR:HG21	25:Z:34:MET:HE1	2.01	0.42
25:Z:75:GLN:NE2	25:Z:79:ASP:OD1	2.52	0.42
7:G:227:SER:OG	7:G:228:ILE:N	2.53	0.42
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.02	0.42
16:P:46:ILE:N	16:P:46:ILE:HD12	2.35	0.42
16:P:270:PHE:HD2	16:P:279:THR:HG22	1.85	0.42
6:F:268:VAL:HG22	6:F:269:GLU:N	2.34	0.42
8:H:236:ILE:HG23	8:H:259:PHE:CE1	2.55	0.42
31:f:3:LEU:HD12	31:f:3:LEU:C	2.44	0.42
40:o:59:ALA:O	40:o:60:HIS:CG	2.72	0.42
45:A:202:PC1:O13	45:A:202:PC1:H142	2.20	0.42
14:N:220:MET:HE1	53:N:402:CDL:H712	2.02	0.42
19:S:13:LEU:H	19:S:13:LEU:HD23	1.85	0.42
4:D:230:THR:HG21	25:Z:22:ARG:HH12	1.84	0.42
8:H:139:THR:CG2	10:J:65:MET:HE2	2.50	0.42
12:L:171:ALA:O	12:L:175:ASN:ND2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:475:THR:O	40:o:51:VAL:HG21	2.20	0.42
15:O:84:ASP:N	15:O:84:ASP:OD1	2.51	0.42
4:D:161:ILE:O	4:D:161:ILE:HG22	2.20	0.42
7:G:185:THR:O	7:G:187:ILE:N	2.52	0.42
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.50	0.42
14:N:207:ILE:HG22	14:N:211:MET:HE2	2.00	0.42
6:F:407:LEU:C	6:F:407:LEU:HD23	2.44	0.41
7:G:364:LEU:HD12	7:G:491:ASN:HB3	2.02	0.41
12:L:31:ASN:HD22	59:i:201:CHD:H151	1.83	0.41
13:M:114:GLU:OE1	13:M:116:ILE:N	2.53	0.41
15:O:60:ASP:OD1	15:O:60:ASP:N	2.53	0.41
5:E:190:ARG:NH1	6:F:265:PRO:O	2.52	0.41
7:G:41:CYS:O	7:G:161:ARG:NH2	2.42	0.41
13:M:123:GLU:OE2	13:M:154:LEU:HD23	2.20	0.41
34:i:112:THR:O	34:i:112:THR:HG22	2.19	0.41
12:L:370:THR:HG22	12:L:374:ILE:HD12	2.01	0.41
13:M:6:ILE:HB	13:M:7:PRO:HD3	2.02	0.41
42:q:49:TYR:HB2	42:q:61:TRP:CE2	2.55	0.41
45:A:202:PC1:H133	10:J:149:TYR:CE2	2.56	0.41
11:K:9:MET:HE2	14:N:79:MET:HE1	2.03	0.41
12:L:69:LEU:HD21	13:M:455:LEU:HD11	2.03	0.41
15:O:53:GLU:OE2	15:O:126:ARG:NH1	2.54	0.41
29:d:5:ARG:NE	29:d:85:VAL:HG13	2.35	0.41
58:U:101:EHZ:O3	39:n:11:HIS:NE2	2.48	0.41
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.51	0.41
2:B:138:ARG:NH1	61:B:310:HOH:O	2.39	0.41
8:H:108:MET:HE1	45:H:402:PC1:H362	2.02	0.41
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.56	0.41
14:N:10:LEU:CD1	53:N:402:CDL:H272	2.50	0.41
5:E:87:TYR:CD1	6:F:181:ALA:HB3	2.56	0.41
6:F:202:LYS:NZ	61:F:602:HOH:O	2.33	0.41
12:L:140:LEU:O	12:L:140:LEU:HD23	2.20	0.41
38:m:115:ILE:HG12	38:m:120:LEU:HD23	2.02	0.41
2:B:121:ASN:HB3	9:I:114:THR:HG22	2.02	0.41
49:D:501:U10:H512	8:H:52:ALA:HB2	2.02	0.41
6:F:82:MET:O	6:F:91:LYS:NZ	2.44	0.41
6:F:157:TYR:CD2	44:s:58:LEU:HD22	2.56	0.41
6:F:306:LEU:HD12	6:F:306:LEU:O	2.21	0.41
8:H:71:PHE:O	8:H:215:TYR:OH	2.36	0.41
9:I:84:GLU:HB2	9:I:94:ILE:HD12	2.02	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:160:LEU:HD21	46:N:403:3PE:H2B2	2.03	0.41
15:O:191:GLU:OE2	55:O:401:DGT:O3'	2.30	0.41
39:n:23:LEU:O	39:n:27:GLU:N	2.44	0.41
4:D:338:MET:HE1	9:I:127:PRO:HA	2.02	0.41
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.41
12:L:65:ASN:OD1	12:L:65:ASN:N	2.54	0.41
39:n:149:ARG:O	39:n:150:THR:HG23	2.20	0.41
5:E:148:CYS:H	6:F:105:CYS:HG	1.67	0.40
6:F:204:ARG:HD2	17:Q:122:PHE:CZ	2.56	0.40
7:G:372:GLU:O	7:G:402:ASN:ND2	2.54	0.40
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.03	0.40
47:g:202:PLC:H6A1	45:h:202:PC1:H2I1	2.02	0.40
4:D:161:ILE:O	4:D:161:ILE:CG2	2.69	0.40
12:L:82:MET:HE2	12:L:82:MET:HA	2.02	0.40
13:M:126:LEU:HD21	13:M:153:THR:HG21	2.04	0.40
36:k:2:LYS:NZ	36:k:3:MET:O	2.54	0.40
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.52	0.40
43:r:105:LEU:HD22	43:r:110:PRO:HB3	2.04	0.40
6:F:192:LEU:HD23	6:F:192:LEU:C	2.46	0.40
12:L:371:THR:O	12:L:375:VAL:HG23	2.21	0.40
14:N:278:LEU:HB3	14:N:279:PRO:HD3	2.02	0.40
15:O:56:ILE:HD11	15:O:96:LEU:CD1	2.51	0.40
3:C:66:ASP:O	21:V:82:GLN:NE2	2.51	0.40
16:P:185:ILE:O	16:P:185:ILE:HG22	2.20	0.40
23:X:79:GLU:HB3	23:X:80:PRO:HD3	2.03	0.40
24:Y:109:ILE:HD11	46:Y:203:3PE:H2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
2	B	153/216 (71%)	148 (97%)	5 (3%)	0	100	100
3	C	207/266 (78%)	202 (98%)	5 (2%)	0	100	100
4	D	427/463 (92%)	419 (98%)	8 (2%)	0	100	100
5	E	212/249 (85%)	199 (94%)	13 (6%)	0	100	100
6	F	430/464 (93%)	421 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	663 (97%)	23 (3%)	0	100	100
8	H	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	55
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	578 (96%)	26 (4%)	0	100	100
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	341 (99%)	4 (1%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	340/380 (90%)	334 (98%)	6 (2%)	0	100	100
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
18	R	94/124 (76%)	93 (99%)	1 (1%)	0	100	100
19	S	85/99 (86%)	82 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
20	U	86/156 (55%)	86 (100%)	0	0	100	100
21	V	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
22	W	113/128 (88%)	110 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
25	Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
30	e	97/106 (92%)	96 (99%)	1 (1%)	0	100	100
31	f	55/57 (96%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	69 (100%)	0	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	n	169/179 (94%)	162 (96%)	7 (4%)	0	100	100
40	o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	p	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	s	43/109 (39%)	43 (100%)	0	0	100	100
All	All	8193/9213 (89%)	7993 (98%)	199 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	208	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	129 (98%)	2 (2%)	57	80
3	C	190/228 (83%)	190 (100%)	0	100	100
4	D	370/392 (94%)	365 (99%)	5 (1%)	59	81
5	E	183/205 (89%)	181 (99%)	2 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	346/368 (94%)	339 (98%)	7 (2%)	48	75
7	G	578/608 (95%)	576 (100%)	2 (0%)	86	94
8	H	274/274 (100%)	270 (98%)	4 (2%)	57	80
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	141/141 (100%)	140 (99%)	1 (1%)	76	89
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	70
12	L	533/533 (100%)	524 (98%)	9 (2%)	53	78
13	M	412/412 (100%)	409 (99%)	3 (1%)	76	89
14	N	315/315 (100%)	312 (99%)	3 (1%)	68	86
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	69
16	P	296/327 (90%)	290 (98%)	6 (2%)	48	75
17	Q	116/153 (76%)	115 (99%)	1 (1%)	70	87
18	R	79/97 (81%)	79 (100%)	0	100	100
19	S	77/82 (94%)	77 (100%)	0	100	100
20	T	81/135 (60%)	81 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	86
22	W	107/114 (94%)	105 (98%)	2 (2%)	50	76
23	X	154/155 (99%)	151 (98%)	3 (2%)	50	76
24	Y	101/102 (99%)	100 (99%)	1 (1%)	68	86
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	88
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	45 (100%)	0	100	100
29	d	105/105 (100%)	105 (100%)	0	100	100
30	e	89/96 (93%)	87 (98%)	2 (2%)	45	73
31	f	54/54 (100%)	52 (96%)	2 (4%)	30	57
32	g	92/131 (70%)	90 (98%)	2 (2%)	45	73
33	h	121/158 (77%)	120 (99%)	1 (1%)	73	88
34	i	120/121 (99%)	118 (98%)	2 (2%)	53	78
35	j	61/84 (73%)	60 (98%)	1 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	79
37	l	140/159 (88%)	138 (99%)	2 (1%)	59	81
38	m	113/114 (99%)	112 (99%)	1 (1%)	70	87
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	109 (99%)	1 (1%)	70	87
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	130/130 (100%)	128 (98%)	2 (2%)	57	80
43	r	85/97 (88%)	84 (99%)	1 (1%)	63	83
44	s	44/92 (48%)	43 (98%)	1 (2%)	44	72
All	All	7218/7891 (92%)	7137 (99%)	81 (1%)	63	84

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
2	B	81	ARG
4	D	23	LYS
4	D	128	ILE
4	D	165	THR
4	D	216	LYS
4	D	420	THR
5	E	29	LYS
5	E	97	LYS
6	F	8	LYS
6	F	16	LYS
6	F	34	LYS
6	F	206	LYS
6	F	324	GLN
6	F	355	LYS
6	F	365	CYS
7	G	192	MET
7	G	536	ASP
8	H	8	MET
8	H	103	LEU
8	H	268	MET
8	H	274	ARG
10	J	135	PHE
11	K	37	MET
11	K	59	MET

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Mol	Chain	Res	Type
12	L	116	LYS
12	L	336	LYS
12	L	394	LEU
12	L	487	LYS
12	L	503	GLU
12	L	509	LYS
12	L	554	ASP
12	L	580	GLN
12	L	601	LEU
13	M	80	SER
13	M	116	ILE
13	M	207	MET
14	N	71	MET
14	N	322	LYS
14	N	335	MET
15	O	16	LYS
15	O	21	LYS
15	O	35	LYS
15	O	60	ASP
15	O	84	ASP
15	O	146	LYS
15	O	191	GLU
16	P	1	LEU
16	P	3	HIS
16	P	122	LYS
16	P	140	LYS
16	P	199	LYS
16	P	316	GLU
17	Q	107	GLU
21	V	6	LYS
22	W	56	LYS
22	W	98	GLN
23	X	15	GLN
23	X	41	GLU
23	X	43	MET
24	Y	119	LEU
25	Z	4	LYS
30	e	53	LYS
30	e	90	LYS
31	f	32	GLU
31	f	33	LYS
32	g	24	LEU

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Mol	Chain	Res	Type
32	g	25	ARG
33	h	19	LYS
34	i	48	LYS
34	i	57	LYS
35	j	48	LEU
36	k	81	LYS
37	l	8	MET
37	l	126	GLN
38	m	111	LYS
40	o	112	LYS
42	q	43	LYS
42	q	107	LYS
43	r	105	LEU
44	s	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
2	B	94	ASN
3	C	19	HIS
3	C	46	ASN
3	C	88	ASN
4	D	27	HIS
4	D	79	HIS
4	D	98	GLN
4	D	135	GLN
4	D	190	HIS
4	D	201	GLN
4	D	217	ASN
5	E	42	HIS
6	F	257	ASN
7	G	7	ASN
7	G	51	ASN
7	G	155	GLN
7	G	401	HIS
7	G	402	ASN
7	G	655	GLN
8	H	235	ASN
8	H	317	GLN
12	L	165	ASN
12	L	170	GLN

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Mol	Chain	Res	Type
12	L	269	ASN
12	L	471	ASN
12	L	541	ASN
13	M	83	HIS
13	M	138	ASN
13	M	139	GLN
13	M	144	ASN
13	M	175	ASN
13	M	338	HIS
13	M	415	GLN
14	N	63	GLN
14	N	289	ASN
15	O	76	ASN
15	O	107	GLN
15	O	114	HIS
15	O	288	GLN
16	P	243	GLN
18	R	90	GLN
20	T	74	GLN
23	X	29	HIS
24	Y	88	ASN
25	Z	60	GLN
27	b	51	ASN
28	c	9	HIS
30	e	6	GLN
30	e	44	HIS
32	g	27	GLN
32	g	57	ASN
33	h	124	HIS
33	h	135	HIS
34	i	127	HIS
41	p	143	HIS
42	q	112	ASN
43	r	24	GLN
44	s	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 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$
34	SAC	i	1	34	7,8,9	1.73	1 (14%)	7,9,11	1.49	1 (14%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	8,9,11	1.36	1 (12%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	8,9,11	1.38	1 (12%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	8,9,11	1.38	2 (25%)
4	2MR	D	85	4	10,12,13	2.47	2 (20%)	5,13,15	1.29	1 (20%)
38	SAC	m	1	38	7,8,9	1.73	1 (14%)	7,9,11	1.22	1 (14%)
14	FME	N	1	14	8,9,10	1.53	1 (12%)	8,9,11	1.24	0
27	AYA	b	1	27	6,7,8	1.87	1 (16%)	6,8,10	1.33	1 (16%)
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.33	1 (16%)
42	AME	q	1	42	9,10,11	1.53	1 (11%)	9,11,13	1.25	0
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.35	1 (11%)
43	AYA	r	1	43	6,7,8	1.88	2 (33%)	6,8,10	1.40	1 (16%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.42	1 (12%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	8,9,11	1.48	2 (25%)
13	FME	M	1	13	8,9,10	1.49	1 (12%)	8,9,11	1.40	1 (12%)

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
34	SAC	i	1	34	-	4/7/8/10	-
10	FME	J	1	10	-	3/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SAC	m	1	38	-	0/7/8/10	-
14	FME	N	1	14	-	1/7/9/11	-
27	AYA	b	1	27	-	0/5/6/8	-
24	AYA	Y	1	24	-	0/5/6/8	-
42	AME	q	1	42	-	4/9/10/12	-
29	AME	d	1	29	-	0/9/10/12	-
43	AYA	r	1	43	-	1/5/6/8	-
12	FME	L	1	12	-	1/7/9/11	-
8	FME	H	1	8	-	1/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.53	1.45	1.33
4	D	85	2MR	CZ-NE	5.13	1.45	1.34
14	N	1	FME	CN-N	3.80	1.45	1.33
10	J	1	FME	CN-N	3.76	1.45	1.33
11	K	1	FME	CN-N	3.73	1.45	1.33
12	L	1	FME	CN-N	3.72	1.45	1.33
1	A	1	FME	CN-N	3.69	1.45	1.33
13	M	1	FME	CN-N	3.67	1.45	1.33
8	H	1	FME	CN-N	3.66	1.45	1.33
38	m	1	SAC	C1A-N	3.55	1.45	1.34
34	i	1	SAC	C1A-N	3.53	1.45	1.34
42	q	1	AME	CT1-N	3.53	1.45	1.34
29	d	1	AME	CT1-N	3.49	1.45	1.34
27	b	1	AYA	CT-N	3.48	1.45	1.34
43	r	1	AYA	CT-N	3.45	1.45	1.34
24	Y	1	AYA	CT-N	3.43	1.45	1.34
43	r	1	AYA	OT-CT	-2.08	1.18	1.23
24	Y	1	AYA	OT-CT	-2.01	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.83	120.81	116.12
29	d	1	AME	CT2-CT1-N	2.52	120.30	116.12
43	r	1	AYA	CM-CT-N	2.51	120.28	116.12
27	b	1	AYA	CM-CT-N	2.30	119.94	116.12
24	Y	1	AYA	CM-CT-N	2.28	119.90	116.12
38	m	1	SAC	C2A-C1A-N	2.18	119.73	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	FME	CA-N-CN	-2.17	119.48	122.82
4	D	85	2MR	CD-NE-CZ	-2.17	119.30	123.36
12	L	1	FME	O1-CN-N	-2.11	119.88	125.32
8	H	1	FME	O1-CN-N	-2.09	119.91	125.32
1	A	1	FME	O1-CN-N	-2.08	119.95	125.32
10	J	1	FME	O1-CN-N	-2.08	119.96	125.32
11	K	1	FME	O1-CN-N	-2.07	119.96	125.32
1	A	1	FME	CA-N-CN	-2.03	119.70	122.82
13	M	1	FME	O1-CN-N	-2.01	120.13	125.32

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
10	J	1	FME	O1-CN-N-CA
34	i	1	SAC	C-CA-CB-OG
42	q	1	AME	C-CA-CB-CG
43	r	1	AYA	O-C-CA-CB
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CA-CB-CG-SD
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
42	q	1	AME	N-CA-CB-CG
34	i	1	SAC	N-CA-CB-OG
13	M	1	FME	C-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
42	q	1	AME	C-CA-N-CT1
10	J	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
11	K	1	FME	CB-CA-N-CN
14	N	1	FME	CB-CA-N-CN
42	q	1	AME	CB-CA-N-CT1
8	H	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	1	AME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 4 are monoatomic - leaving 87 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	$\# Z > 2$
46	3PE	A	205	-	44,44,50	0.92	4 (9%)	47,49,55	1.11	2 (4%)
45	PC1	m	202	-	53,53,53	0.94	4 (7%)	59,61,61	1.01	2 (3%)
45	PC1	g	203	-	43,43,53	1.04	4 (9%)	49,51,61	1.01	2 (4%)
45	PC1	M	606	-	34,34,53	1.17	4 (11%)	40,42,61	1.02	2 (5%)
46	3PE	Z	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	Y	209	-	42,42,50	0.95	4 (9%)	45,47,55	1.06	2 (4%)
45	PC1	L	704	-	46,46,53	1.01	4 (8%)	52,54,61	1.03	2 (3%)
46	3PE	Y	202	-	26,26,50	1.18	4 (15%)	29,31,55	1.20	2 (6%)
60	MYR	o	201	40	13,14,15	0.42	0	12,13,15	0.87	0
47	PLC	P	504	-	31,31,41	0.58	0	37,39,49	0.53	0
45	PC1	H	403	-	38,38,53	1.10	4 (10%)	44,46,61	1.10	2 (4%)
46	3PE	A	204	-	36,36,50	1.02	4 (11%)	39,41,55	1.08	2 (5%)
46	3PE	Y	205	-	50,50,50	0.87	4 (8%)	53,55,55	1.03	2 (3%)
51	FMN	F	501	-	33,33,33	2.72	10 (30%)	48,50,50	1.74	13 (27%)
46	3PE	g	201	-	33,33,50	1.06	4 (12%)	36,38,55	1.17	2 (5%)
46	3PE	M	602	-	30,30,50	1.10	4 (13%)	33,35,55	1.21	2 (6%)
45	PC1	B	204	-	47,47,53	1.00	4 (8%)	53,55,61	1.13	2 (3%)
46	3PE	M	603	-	49,49,50	0.88	4 (8%)	52,54,55	1.03	2 (3%)
47	PLC	Y	208	-	41,41,41	0.50	0	47,49,49	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	r	201	-	60,60,99	1.12	8 (13%)	66,72,111	1.13	4 (6%)
45	PC1	q	201	-	48,48,53	0.99	4 (8%)	54,56,61	0.96	2 (3%)
53	CDL	L	701	-	75,75,99	1.00	8 (10%)	81,87,111	1.09	4 (4%)
46	3PE	P	502	-	34,34,50	1.04	4 (11%)	37,39,55	1.10	2 (5%)
46	3PE	a	101	-	38,38,50	0.99	4 (10%)	41,43,55	1.09	2 (4%)
45	PC1	H	402	-	47,47,53	1.02	4 (8%)	53,55,61	1.04	2 (3%)
45	PC1	I	203	-	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
46	3PE	d	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.04	2 (3%)
46	3PE	I	204	-	50,50,50	0.88	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	f	101	-	43,43,50	0.94	4 (9%)	46,48,55	1.09	2 (4%)
45	PC1	B	202	-	45,45,53	1.03	4 (8%)	51,53,61	0.98	2 (3%)
46	3PE	J	202	-	35,35,50	1.02	4 (11%)	38,40,55	1.16	2 (5%)
47	PLC	B	203	-	41,41,41	0.52	0	47,49,49	0.54	0
46	3PE	J	201	-	28,28,50	1.14	4 (14%)	31,33,55	1.20	2 (6%)
57	NDP	P	501	-	51,52,52	3.99	27 (52%)	71,80,80	1.91	13 (18%)
45	PC1	d	202	-	38,38,53	1.13	4 (10%)	44,46,61	1.03	2 (4%)
46	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.14	2 (4%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
48	SF4	B	201	2	0,12,12	-	-	-	-	-
45	PC1	h	202	-	46,46,53	1.01	4 (8%)	52,54,61	1.02	2 (3%)
46	3PE	M	604	-	50,50,50	0.87	4 (8%)	53,55,55	1.07	2 (3%)
47	PLC	J	203	-	36,36,41	0.53	0	42,44,49	0.53	0
46	3PE	Z	204	-	40,40,50	0.97	4 (10%)	43,45,55	1.05	2 (4%)
58	EHZ	T	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.68	8 (22%)
48	SF4	I	202	9	0,12,12	-	-	-	-	-
49	U10	D	501	-	63,63,63	1.87	25 (39%)	78,79,79	1.43	18 (23%)
45	PC1	H	404	-	38,38,53	1.12	4 (10%)	44,46,61	0.96	2 (4%)
53	CDL	h	201	-	79,79,99	0.98	8 (10%)	85,91,111	1.17	5 (5%)
46	3PE	m	203	-	31,31,50	1.09	4 (12%)	34,36,55	1.19	2 (5%)
46	3PE	L	702	-	44,44,50	0.92	4 (9%)	47,49,55	1.07	2 (4%)
47	PLC	O	403	-	34,34,41	0.56	0	40,42,49	0.57	0
45	PC1	Z	201	-	43,43,53	1.05	4 (9%)	49,51,61	1.03	2 (4%)
45	PC1	A	202	-	34,34,53	1.18	4 (11%)	40,42,61	0.97	2 (5%)
53	CDL	d	203	-	64,64,99	1.08	8 (12%)	70,76,111	1.08	4 (5%)
46	3PE	Y	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.07	2 (3%)
55	DGT	O	401	56	32,33,33	3.31	14 (43%)	48,52,52	1.94	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PC1	A	201	-	34,34,53	1.17	4 (11%)	40,42,61	1.05	2 (5%)
48	SF4	I	201	9	0,12,12	-	-	-		
46	3PE	Y	204	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
47	PLC	L	703	-	41,41,41	0.52	0	47,49,49	0.51	0
53	CDL	P	503	-	58,58,99	1.13	8 (13%)	64,70,111	1.16	4 (6%)
47	PLC	M	608	-	27,27,41	0.62	0	33,35,49	0.55	0
46	3PE	b	101	-	46,46,50	0.90	4 (8%)	49,51,55	1.01	2 (4%)
50	FES	E	301	5	0,4,4	-	-	-		
53	CDL	d	204	-	85,85,99	0.94	8 (9%)	91,97,111	1.11	4 (4%)
50	FES	G	803	7	0,4,4	-	-	-		
48	SF4	F	502	6	0,12,12	-	-	-		
45	PC1	A	203	-	32,32,53	1.21	4 (12%)	38,40,61	1.12	2 (5%)
46	3PE	M	605	-	44,44,50	0.92	3 (6%)	47,49,55	1.01	2 (4%)
46	3PE	Y	207	-	35,35,50	1.03	4 (11%)	38,40,55	1.14	2 (5%)
46	3PE	P	505	-	44,44,50	0.91	4 (9%)	47,49,55	1.10	2 (4%)
59	CHD	i	201	-	32,32,32	3.27	10 (31%)	51,51,51	2.42	19 (37%)
58	EHZ	U	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.63	6 (16%)
48	SF4	G	801	7	0,12,12	-	-	-		
53	CDL	N	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
47	PLC	A	206	-	32,32,41	0.57	0	38,40,49	0.57	0
46	3PE	N	403	-	50,50,50	0.88	4 (8%)	53,55,55	1.07	2 (3%)
53	CDL	H	401	-	80,80,99	0.98	8 (10%)	86,92,111	1.06	4 (4%)
46	3PE	b	102	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	r	202	-	33,33,50	1.05	4 (12%)	36,38,55	1.10	2 (5%)
53	CDL	M	607	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	4 (3%)
46	3PE	N	401	-	48,48,50	0.88	4 (8%)	51,53,55	1.06	2 (3%)
46	3PE	Y	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.13	2 (4%)
47	PLC	g	202	-	41,41,41	0.51	0	47,49,49	0.54	0
46	3PE	Y	206	-	44,44,50	0.93	4 (9%)	47,49,55	1.09	2 (4%)
47	PLC	Z	203	-	33,33,41	0.56	0	39,41,49	0.61	0
46	3PE	q	202	-	50,50,50	0.88	4 (8%)	53,55,55	1.06	2 (3%)
46	3PE	J	204	-	43,43,50	0.94	4 (9%)	46,48,55	1.08	2 (4%)

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
46	3PE	A	205	-	-	17/48/48/54	-
45	PC1	m	202	-	-	16/57/57/57	-
45	PC1	g	203	-	-	19/47/47/57	-
45	PC1	M	606	-	-	18/38/38/57	-
46	3PE	Z	202	-	-	23/54/54/54	-
46	3PE	Y	209	-	-	23/46/46/54	-
45	PC1	L	704	-	-	22/50/50/57	-
46	3PE	Y	202	-	-	10/30/30/54	-
60	MYR	o	201	40	-	8/12/12/13	-
47	PLC	P	504	-	-	16/34/34/45	-
45	PC1	H	403	-	-	14/42/42/57	-
46	3PE	A	204	-	-	12/40/40/54	-
46	3PE	Y	205	-	-	20/54/54/54	-
51	FMN	F	501	-	-	6/18/18/18	0/3/3/3
46	3PE	g	201	-	-	24/37/37/54	-
46	3PE	M	602	-	-	11/34/34/54	-
45	PC1	B	204	-	-	16/51/51/57	-
46	3PE	M	603	-	-	22/53/53/54	-
47	PLC	Y	208	-	-	17/45/45/45	-
53	CDL	r	201	-	-	31/71/71/110	-
45	PC1	q	201	-	-	18/52/52/57	-
53	CDL	L	701	-	-	28/86/86/110	-
46	3PE	P	502	-	-	12/38/38/54	-
46	3PE	a	101	-	-	12/42/42/54	-
45	PC1	H	402	-	-	22/51/51/57	-
45	PC1	I	203	-	-	25/57/57/57	-
46	3PE	d	201	-	-	14/52/52/54	-
46	3PE	I	204	-	-	22/54/54/54	-
46	3PE	f	101	-	-	24/47/47/54	-
45	PC1	B	202	-	-	17/49/49/57	-
46	3PE	J	202	-	-	18/39/39/54	-
47	PLC	B	203	-	-	17/45/45/45	-
46	3PE	J	201	-	-	14/32/32/54	-
57	NDP	P	501	-	-	12/34/77/77	0/5/5/5
45	PC1	d	202	-	-	21/42/42/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	m	201	-	-	18/44/44/54	-
48	SF4	G	802	7	-	-	0/6/5/5
48	SF4	B	201	2	-	-	0/6/5/5
45	PC1	h	202	-	-	21/50/50/57	-
46	3PE	M	604	-	-	17/54/54/54	-
47	PLC	J	203	-	-	12/40/40/45	-
46	3PE	Z	204	-	-	15/44/44/54	-
58	EHZ	T	101	20	-	14/42/44/45	-
49	U10	D	501	-	-	21/63/87/87	0/1/1/1
48	SF4	I	202	9	-	-	0/6/5/5
45	PC1	H	404	-	-	16/42/42/57	-
53	CDL	h	201	-	-	40/90/90/110	-
46	3PE	m	203	-	-	16/35/35/54	-
46	3PE	L	702	-	-	28/48/48/54	-
47	PLC	O	403	-	-	10/38/38/45	-
45	PC1	Z	201	-	-	18/47/47/57	-
45	PC1	A	202	-	-	12/38/38/57	-
53	CDL	d	203	-	-	32/75/75/110	-
46	3PE	Y	203	-	-	26/54/54/54	-
55	DGT	O	401	56	-	3/22/34/34	0/3/3/3
45	PC1	A	201	-	-	19/38/38/57	-
48	SF4	I	201	9	-	-	0/6/5/5
46	3PE	Y	204	-	-	26/54/54/54	-
47	PLC	L	703	-	-	12/45/45/45	-
53	CDL	P	503	-	-	26/69/69/110	-
47	PLC	M	608	-	-	12/31/31/45	-
46	3PE	b	101	-	-	15/50/50/54	-
50	FES	E	301	5	-	-	0/1/1/1
53	CDL	d	204	-	-	48/96/96/110	-
50	FES	G	803	7	-	-	0/1/1/1
48	SF4	F	502	6	-	-	0/6/5/5
45	PC1	A	203	-	-	18/36/36/57	-
46	3PE	M	605	-	-	16/48/48/54	-
46	3PE	Y	207	-	-	17/39/39/54	-
46	3PE	P	505	-	-	24/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CHD	i	201	-	-	2/9/74/74	0/4/4/4
58	EHZ	U	101	20	-	17/42/44/45	-
48	SF4	G	801	7	-	-	0/6/5/5
53	CDL	N	402	-	-	43/110/110/110	-
47	PLC	A	206	-	-	9/36/36/45	-
46	3PE	N	403	-	-	23/54/54/54	-
53	CDL	H	401	-	-	37/91/91/110	-
46	3PE	b	102	-	-	22/54/54/54	-
46	3PE	r	202	-	-	16/37/37/54	-
53	CDL	M	607	-	-	47/110/110/110	-
46	3PE	N	401	-	-	21/52/52/54	-
46	3PE	Y	201	-	-	16/44/44/54	-
47	PLC	g	202	-	-	14/45/45/45	-
46	3PE	Y	206	-	-	17/48/48/54	-
47	PLC	Z	203	-	-	15/37/37/45	-
46	3PE	q	202	-	-	19/54/54/54	-
46	3PE	J	204	-	-	26/47/47/54	-

All (375) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.20	1.70	1.59
59	i	201	CHD	C11-C12	9.10	1.68	1.53
57	P	501	NDP	C2B-C1B	-9.04	1.30	1.53
55	O	401	DGT	O6-C6	8.81	1.40	1.23
57	P	501	NDP	O4B-C1B	8.56	1.61	1.42
57	P	501	NDP	O4D-C1D	8.18	1.60	1.42
57	P	501	NDP	C7N-N7N	7.64	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.35	1.30	1.53
59	i	201	CHD	C16-C15	7.13	1.73	1.54
57	P	501	NDP	C6N-C5N	7.09	1.54	1.33
55	O	401	DGT	C5-N7	6.74	1.52	1.39
57	P	501	NDP	O4D-C4D	-6.57	1.30	1.45
51	F	501	FMN	C10-N1	6.48	1.46	1.33
51	F	501	FMN	C4A-N5	6.48	1.44	1.30
59	i	201	CHD	C20-C17	-6.17	1.43	1.54
57	P	501	NDP	P2B-O2B	5.66	1.69	1.59
59	i	201	CHD	C13-C17	5.52	1.64	1.55
51	F	501	FMN	C5A-N5	5.46	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	i	201	CHD	C8-C9	5.34	1.64	1.53
57	P	501	NDP	C6A-N6A	5.32	1.47	1.34
59	i	201	CHD	O12-C12	-5.27	1.34	1.43
57	P	501	NDP	O4B-C4B	-5.24	1.33	1.45
55	O	401	DGT	PB-O3B	5.11	1.65	1.59
58	U	101	EHZ	C12-N1	5.08	1.45	1.33
55	O	401	DGT	PA-O3A	5.07	1.65	1.59
58	T	101	EHZ	C12-N1	5.04	1.45	1.33
55	O	401	DGT	PB-O3A	5.01	1.64	1.59
58	U	101	EHZ	C15-N2	4.98	1.45	1.33
58	T	101	EHZ	C15-N2	4.97	1.45	1.33
51	F	501	FMN	C2-N1	4.92	1.47	1.36
51	F	501	FMN	C9A-N10	4.86	1.49	1.41
55	O	401	DGT	C2-N2	4.83	1.45	1.34
55	O	401	DGT	C2-N1	4.78	1.49	1.37
59	i	201	CHD	C6-C5	4.61	1.61	1.53
57	P	501	NDP	C2N-C3N	4.56	1.47	1.35
51	F	501	FMN	C2-N3	4.49	1.48	1.39
57	P	501	NDP	C5A-C4A	-4.40	1.31	1.39
55	O	401	DGT	C8-N9	-4.30	1.27	1.37
55	O	401	DGT	C2-N3	4.30	1.43	1.33
57	P	501	NDP	PN-O3	4.26	1.64	1.59
57	P	501	NDP	O7N-C7N	-4.19	1.14	1.24
59	i	201	CHD	C15-C14	4.09	1.62	1.54
55	O	401	DGT	C4-N9	-3.96	1.28	1.38
57	P	501	NDP	C8A-N9A	-3.94	1.30	1.37
57	P	501	NDP	O2D-C2D	3.74	1.52	1.43
51	F	501	FMN	C4-N3	3.67	1.45	1.38
59	i	201	CHD	C6-C7	3.58	1.59	1.52
51	F	501	FMN	C10-N10	3.58	1.45	1.37
49	D	501	U10	C4-C5	-3.32	1.39	1.48
57	P	501	NDP	C4N-C3N	3.26	1.56	1.50
49	D	501	U10	C51-C49	3.12	1.57	1.51
49	D	501	U10	C31-C29	3.10	1.57	1.51
49	D	501	U10	C3-C2	-2.98	1.40	1.48
51	F	501	FMN	O2-C2	-2.95	1.18	1.24
49	D	501	U10	C20-C19	2.94	1.57	1.50
46	M	605	3PE	O21-C2	-2.85	1.39	1.46
45	d	202	PC1	O21-C2	-2.85	1.39	1.46
53	M	607	CDL	OB6-CB4	-2.85	1.39	1.46
53	d	204	CDL	OB6-CB4	-2.80	1.40	1.46
53	H	401	CDL	OA6-CA4	-2.79	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Z	201	PC1	O21-C2	-2.77	1.40	1.46
46	J	204	3PE	O21-C2	-2.76	1.40	1.46
57	P	501	NDP	C4N-C5N	2.76	1.56	1.49
49	D	501	U10	C30-C29	2.75	1.57	1.50
46	I	204	3PE	O21-C2	-2.75	1.40	1.46
53	r	201	CDL	OA6-CA4	-2.73	1.40	1.46
53	d	203	CDL	OA6-CA4	-2.73	1.40	1.46
46	Y	204	3PE	O21-C2	-2.73	1.40	1.46
53	P	503	CDL	OB6-CB4	-2.73	1.40	1.46
45	A	203	PC1	O21-C2	-2.72	1.40	1.46
46	Y	209	3PE	O21-C2	-2.72	1.40	1.46
57	P	501	NDP	C5A-N7A	-2.72	1.34	1.39
53	r	201	CDL	OB6-CB4	-2.72	1.40	1.46
46	d	201	3PE	O21-C2	-2.72	1.40	1.46
55	O	401	DGT	C1'-N9	-2.71	1.41	1.48
46	A	205	3PE	O21-C2	-2.71	1.40	1.46
46	Y	202	3PE	O21-C2	-2.71	1.40	1.46
53	L	701	CDL	OA6-CA4	-2.71	1.40	1.46
53	P	503	CDL	OA6-CA4	-2.71	1.40	1.46
45	g	203	PC1	O21-C2	-2.71	1.40	1.46
45	B	202	PC1	O21-C2	-2.70	1.40	1.46
46	b	101	3PE	O21-C2	-2.70	1.40	1.46
53	H	401	CDL	OB6-CB4	-2.70	1.40	1.46
53	M	607	CDL	OA6-CA4	-2.70	1.40	1.46
45	A	201	PC1	O21-C2	-2.70	1.40	1.46
46	g	201	3PE	O21-C2	-2.70	1.40	1.46
51	F	501	FMN	O4-C4	-2.69	1.18	1.23
45	h	202	PC1	O21-C2	-2.69	1.40	1.46
46	Y	207	3PE	O21-C2	-2.69	1.40	1.46
45	H	404	PC1	O21-C2	-2.68	1.40	1.46
45	M	606	PC1	O21-C2	-2.68	1.40	1.46
53	d	203	CDL	OB6-CB4	-2.67	1.40	1.46
46	J	202	3PE	O21-C2	-2.66	1.40	1.46
53	L	701	CDL	OB6-CB4	-2.66	1.40	1.46
46	M	604	3PE	O21-C2	-2.66	1.40	1.46
45	H	403	PC1	O21-C2	-2.65	1.40	1.46
46	N	401	3PE	O21-C2	-2.65	1.40	1.46
45	A	202	PC1	O21-C2	-2.65	1.40	1.46
46	N	403	3PE	O21-C2	-2.65	1.40	1.46
45	L	704	PC1	O21-C2	-2.64	1.40	1.46
46	Z	204	3PE	O21-C2	-2.64	1.40	1.46
53	N	402	CDL	OA6-CA4	-2.64	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	q	202	3PE	O21-C2	-2.64	1.40	1.46
46	M	602	3PE	O21-C2	-2.64	1.40	1.46
45	m	202	PC1	O21-C2	-2.63	1.40	1.46
46	Z	202	3PE	O21-C2	-2.63	1.40	1.46
46	Y	206	3PE	O21-C2	-2.62	1.40	1.46
49	D	501	U10	C15-C14	2.62	1.57	1.50
46	A	204	3PE	O21-C2	-2.62	1.40	1.46
46	P	502	3PE	O21-C2	-2.62	1.40	1.46
45	H	402	PC1	O21-C2	-2.61	1.40	1.46
46	Y	201	3PE	O21-C2	-2.60	1.40	1.46
53	N	402	CDL	OB6-CB4	-2.60	1.40	1.46
45	I	203	PC1	O21-C2	-2.60	1.40	1.46
46	m	201	3PE	O21-C2	-2.60	1.40	1.46
53	h	201	CDL	OA6-CA4	-2.60	1.40	1.46
46	b	102	3PE	O21-C2	-2.60	1.40	1.46
46	f	101	3PE	O21-C2	-2.60	1.40	1.46
53	h	201	CDL	OB6-CB4	-2.58	1.40	1.46
46	M	603	3PE	O21-C2	-2.58	1.40	1.46
46	a	101	3PE	O21-C2	-2.58	1.40	1.46
46	J	201	3PE	O21-C2	-2.57	1.40	1.46
49	D	501	U10	C41-C39	2.56	1.56	1.51
46	r	202	3PE	O21-C2	-2.53	1.40	1.46
46	m	203	3PE	O21-C2	-2.52	1.40	1.46
45	B	204	PC1	O21-C2	-2.50	1.40	1.46
46	Y	205	3PE	O21-C2	-2.48	1.40	1.46
53	d	204	CDL	OA6-CA4	-2.47	1.40	1.46
49	D	501	U10	C35-C34	2.47	1.56	1.50
57	P	501	NDP	O3D-C3D	-2.46	1.36	1.43
46	P	505	3PE	O21-C2	-2.46	1.40	1.46
45	q	201	PC1	O21-C2	-2.45	1.40	1.46
49	D	501	U10	C26-C24	2.45	1.56	1.51
45	H	404	PC1	O31-C31	2.44	1.40	1.33
46	L	702	3PE	O21-C2	-2.44	1.40	1.46
57	P	501	NDP	O3B-C3B	-2.44	1.36	1.43
45	M	606	PC1	O31-C31	2.44	1.40	1.33
49	D	501	U10	C6-C1	2.43	1.39	1.35
53	L	701	CDL	OB8-CB7	2.43	1.40	1.33
53	L	701	CDL	OA8-CA7	2.43	1.40	1.33
45	d	202	PC1	O31-C31	2.43	1.40	1.33
58	T	101	EHZ	O3-C12	-2.42	1.18	1.23
57	P	501	NDP	C6N-N1N	2.42	1.43	1.37
53	P	503	CDL	OA8-CA7	2.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	h	202	PC1	O31-C31	2.41	1.40	1.33
46	Y	209	3PE	O31-C31	2.41	1.40	1.33
45	q	201	PC1	O31-C31	2.41	1.40	1.33
45	L	704	PC1	O31-C3	-2.41	1.39	1.45
53	r	201	CDL	OB8-CB7	2.41	1.40	1.33
53	M	607	CDL	OB8-CB7	2.41	1.40	1.33
53	M	607	CDL	OA8-CA7	2.40	1.40	1.33
46	J	202	3PE	O31-C31	2.40	1.40	1.33
46	N	403	3PE	O31-C31	2.40	1.40	1.33
53	H	401	CDL	OA8-CA7	2.40	1.40	1.33
45	A	203	PC1	O31-C31	2.39	1.40	1.33
53	d	204	CDL	OA8-CA7	2.39	1.40	1.33
46	J	204	3PE	O31-C3	-2.39	1.39	1.45
58	U	101	EHZ	C9-S1	2.39	1.81	1.76
46	a	101	3PE	O31-C31	2.38	1.40	1.33
46	A	204	3PE	O31-C31	2.38	1.40	1.33
53	N	402	CDL	OA8-CA7	2.38	1.40	1.33
46	A	205	3PE	O31-C31	2.37	1.40	1.33
45	A	201	PC1	O31-C31	2.37	1.40	1.33
45	A	202	PC1	O31-C31	2.37	1.40	1.33
53	P	503	CDL	OB8-CB7	2.37	1.40	1.33
46	Z	204	3PE	O31-C31	2.37	1.40	1.33
46	L	702	3PE	O31-C31	2.37	1.40	1.33
49	D	501	U10	C16-C14	2.37	1.56	1.51
53	N	402	CDL	OB8-CB7	2.36	1.40	1.33
45	Z	201	PC1	O31-C31	2.36	1.40	1.33
46	I	204	3PE	O31-C31	2.36	1.40	1.33
46	Y	206	3PE	O31-C31	2.36	1.40	1.33
53	h	201	CDL	OA8-CA6	-2.35	1.39	1.45
46	M	604	3PE	O31-C31	2.35	1.40	1.33
46	Y	203	3PE	O21-C2	-2.35	1.41	1.46
46	f	101	3PE	O31-C31	2.35	1.40	1.33
58	T	101	EHZ	C9-S1	2.35	1.81	1.76
49	D	501	U10	C1M-C1	2.35	1.55	1.50
46	Y	207	3PE	O31-C31	2.35	1.40	1.33
58	T	101	EHZ	O4-C15	-2.34	1.18	1.23
45	m	202	PC1	O31-C31	2.34	1.40	1.33
53	r	201	CDL	OA8-CA7	2.34	1.40	1.33
46	q	202	3PE	O31-C31	2.34	1.40	1.33
49	D	501	U10	C40-C39	2.34	1.56	1.50
53	h	201	CDL	OB8-CB7	2.34	1.40	1.33
45	H	403	PC1	O31-C31	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	b	101	3PE	O31-C31	2.34	1.40	1.33
46	m	201	3PE	O31-C31	2.34	1.40	1.33
45	I	203	PC1	O31-C31	2.33	1.40	1.33
53	d	203	CDL	OB8-CB7	2.33	1.40	1.33
46	d	201	3PE	O31-C31	2.33	1.40	1.33
53	H	401	CDL	OB8-CB7	2.33	1.40	1.33
46	Y	201	3PE	O31-C31	2.33	1.40	1.33
49	D	501	U10	C7-C8	2.32	1.54	1.50
58	U	101	EHZ	O4-C15	-2.32	1.18	1.23
53	d	203	CDL	OA8-CA7	2.32	1.40	1.33
46	M	603	3PE	O31-C3	-2.32	1.40	1.45
46	M	602	3PE	O31-C31	2.32	1.40	1.33
46	m	203	3PE	O31-C31	2.32	1.40	1.33
57	P	501	NDP	C7N-C3N	2.32	1.53	1.48
46	P	502	3PE	O31-C31	2.32	1.40	1.33
46	Y	205	3PE	O31-C31	2.32	1.40	1.33
46	N	401	3PE	O31-C3	-2.31	1.40	1.45
53	d	204	CDL	OB8-CB6	-2.31	1.40	1.45
46	Y	205	3PE	O31-C3	-2.31	1.40	1.45
49	D	501	U10	C46-C44	2.31	1.56	1.51
46	g	201	3PE	O31-C3	-2.31	1.40	1.45
58	U	101	EHZ	O3-C12	-2.31	1.18	1.23
45	B	202	PC1	O31-C31	2.31	1.40	1.33
46	J	201	3PE	O31-C31	2.30	1.40	1.33
53	r	201	CDL	OA8-CA6	-2.30	1.40	1.45
46	M	603	3PE	O31-C31	2.30	1.40	1.33
46	P	505	3PE	O31-C31	2.30	1.40	1.33
46	r	202	3PE	O31-C31	2.30	1.40	1.33
45	B	204	PC1	O31-C3	-2.29	1.40	1.45
46	g	201	3PE	O31-C31	2.29	1.40	1.33
46	Y	204	3PE	O31-C3	-2.29	1.40	1.45
53	h	201	CDL	OB8-CB6	-2.29	1.40	1.45
46	Y	202	3PE	O31-C31	2.29	1.40	1.33
46	P	502	3PE	O31-C3	-2.29	1.40	1.45
53	H	401	CDL	OB8-CB6	-2.29	1.40	1.45
53	h	201	CDL	OA8-CA7	2.28	1.40	1.33
45	H	402	PC1	O31-C31	2.28	1.40	1.33
46	m	203	3PE	O31-C3	-2.28	1.40	1.45
46	M	605	3PE	O31-C3	-2.27	1.40	1.45
46	m	201	3PE	O31-C3	-2.27	1.40	1.45
45	g	203	PC1	O31-C3	-2.27	1.40	1.45
45	q	201	PC1	O21-C21	2.27	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	N	401	3PE	O31-C31	2.27	1.40	1.33
49	D	501	U10	C6-C5	-2.27	1.40	1.46
49	D	501	U10	C50-C49	2.27	1.56	1.50
53	d	203	CDL	OA8-CA6	-2.27	1.40	1.45
46	Y	207	3PE	O31-C3	-2.26	1.40	1.45
57	P	501	NDP	P2B-O1X	2.26	1.57	1.50
46	J	201	3PE	O31-C3	-2.26	1.40	1.45
46	b	102	3PE	O31-C31	2.26	1.39	1.33
46	Z	202	3PE	O31-C31	2.26	1.39	1.33
45	B	204	PC1	O31-C31	2.26	1.39	1.33
55	O	401	DGT	PG-O1G	-2.25	1.46	1.54
45	B	202	PC1	O31-C3	-2.25	1.40	1.45
46	d	201	3PE	O31-C3	-2.25	1.40	1.45
46	Y	206	3PE	O31-C3	-2.25	1.40	1.45
45	B	204	PC1	O21-C21	2.25	1.40	1.34
45	H	402	PC1	O31-C3	-2.25	1.40	1.45
46	I	204	3PE	O31-C3	-2.25	1.40	1.45
46	r	202	3PE	O31-C3	-2.25	1.40	1.45
46	b	102	3PE	O31-C3	-2.25	1.40	1.45
45	L	704	PC1	O31-C31	2.24	1.39	1.33
46	Y	201	3PE	O31-C3	-2.24	1.40	1.45
49	D	501	U10	C1-C2	-2.24	1.39	1.47
45	d	202	PC1	O31-C3	-2.24	1.40	1.45
53	h	201	CDL	OB6-CB5	2.24	1.40	1.34
46	Y	203	3PE	O31-C31	2.24	1.39	1.33
46	M	605	3PE	O31-C31	2.24	1.39	1.33
55	O	401	DGT	PG-O2G	-2.24	1.46	1.54
45	g	203	PC1	O31-C31	2.24	1.39	1.33
49	D	501	U10	O4-C4	2.24	1.42	1.36
46	Y	203	3PE	O31-C3	-2.23	1.40	1.45
46	Y	204	3PE	O31-C31	2.23	1.39	1.33
46	Y	203	3PE	O21-C21	2.23	1.40	1.34
46	J	204	3PE	O31-C31	2.23	1.39	1.33
46	Z	202	3PE	O31-C3	-2.23	1.40	1.45
45	I	203	PC1	O31-C3	-2.23	1.40	1.45
46	f	101	3PE	O31-C3	-2.22	1.40	1.45
46	Y	202	3PE	O31-C3	-2.22	1.40	1.45
45	H	403	PC1	O31-C3	-2.22	1.40	1.45
46	b	101	3PE	O31-C3	-2.22	1.40	1.45
53	N	402	CDL	OB8-CB6	-2.21	1.40	1.45
46	M	602	3PE	O31-C3	-2.21	1.40	1.45
45	I	203	PC1	O21-C21	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	M	603	3PE	O21-C21	2.21	1.40	1.34
53	h	201	CDL	OA6-CA5	2.21	1.40	1.34
46	Z	204	3PE	O31-C3	-2.21	1.40	1.45
53	N	402	CDL	OA6-CA5	2.21	1.40	1.34
46	q	202	3PE	O31-C3	-2.20	1.40	1.45
53	P	503	CDL	OB8-CB6	-2.20	1.40	1.45
53	N	402	CDL	OB6-CB5	2.20	1.40	1.34
53	d	203	CDL	OB6-CB5	2.20	1.40	1.34
53	d	203	CDL	OB8-CB6	-2.20	1.40	1.45
46	Y	205	3PE	O21-C21	2.20	1.40	1.34
46	L	702	3PE	O31-C3	-2.20	1.40	1.45
57	P	501	NDP	PA-O5B	2.20	1.68	1.59
53	M	607	CDL	OA8-CA6	-2.19	1.40	1.45
46	M	604	3PE	O31-C3	-2.19	1.40	1.45
59	i	201	CHD	C13-C12	-2.19	1.51	1.54
46	L	702	3PE	O21-C21	2.19	1.40	1.34
55	O	401	DGT	C4-N3	2.19	1.39	1.34
53	r	201	CDL	OB8-CB6	-2.19	1.40	1.45
46	P	502	3PE	O21-C21	2.18	1.40	1.34
45	L	704	PC1	O21-C21	2.18	1.40	1.34
46	m	201	3PE	O21-C21	2.18	1.40	1.34
53	L	701	CDL	OB6-CB5	2.18	1.40	1.34
46	Y	201	3PE	O21-C21	2.18	1.40	1.34
46	A	204	3PE	O21-C21	2.18	1.40	1.34
53	d	203	CDL	OA6-CA5	2.18	1.40	1.34
46	Y	209	3PE	O31-C3	-2.18	1.40	1.45
46	f	101	3PE	O21-C21	2.18	1.40	1.34
46	q	202	3PE	O21-C21	2.17	1.40	1.34
53	d	204	CDL	OB8-CB7	2.17	1.39	1.33
46	P	505	3PE	O21-C21	2.17	1.40	1.34
46	m	203	3PE	O21-C21	2.17	1.40	1.34
53	H	401	CDL	OA8-CA6	-2.17	1.40	1.45
49	D	501	U10	C25-C24	2.17	1.56	1.50
49	D	501	U10	C21-C19	2.17	1.55	1.51
45	A	202	PC1	O21-C21	2.17	1.40	1.34
45	h	202	PC1	O21-C21	2.17	1.40	1.34
45	g	203	PC1	O21-C21	2.16	1.40	1.34
45	A	203	PC1	O31-C3	-2.16	1.40	1.45
46	N	403	3PE	O21-C21	2.16	1.40	1.34
46	P	505	3PE	O31-C3	-2.16	1.40	1.45
45	H	403	PC1	O21-C21	2.16	1.40	1.34
53	M	607	CDL	OB8-CB6	-2.16	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	a	101	3PE	O21-C21	2.16	1.40	1.34
45	H	402	PC1	O21-C21	2.16	1.40	1.34
53	r	201	CDL	OB6-CB5	2.16	1.40	1.34
46	A	204	3PE	O31-C3	-2.15	1.40	1.45
53	d	204	CDL	OA8-CA6	-2.15	1.40	1.45
46	Z	204	3PE	O21-C21	2.15	1.40	1.34
45	A	202	PC1	O31-C3	-2.15	1.40	1.45
46	J	202	3PE	O31-C3	-2.15	1.40	1.45
53	r	201	CDL	OA6-CA5	2.15	1.40	1.34
46	A	205	3PE	O31-C3	-2.14	1.40	1.45
53	H	401	CDL	OB6-CB5	2.14	1.40	1.34
46	b	102	3PE	O21-C21	2.14	1.40	1.34
45	H	404	PC1	O31-C3	-2.14	1.40	1.45
53	P	503	CDL	OA6-CA5	2.14	1.40	1.34
46	g	201	3PE	O21-C21	2.14	1.40	1.34
53	d	204	CDL	OA6-CA5	2.14	1.40	1.34
45	B	202	PC1	O21-C21	2.13	1.40	1.34
45	q	201	PC1	O31-C3	-2.13	1.40	1.45
45	A	201	PC1	O21-C21	2.13	1.40	1.34
46	a	101	3PE	O31-C3	-2.13	1.40	1.45
53	N	402	CDL	OA8-CA6	-2.12	1.40	1.45
46	Z	202	3PE	O21-C21	2.12	1.40	1.34
45	h	202	PC1	O31-C3	-2.12	1.40	1.45
46	r	202	3PE	O21-C21	2.12	1.40	1.34
46	J	201	3PE	O21-C21	2.12	1.40	1.34
45	m	202	PC1	O31-C3	-2.12	1.40	1.45
46	N	403	3PE	O31-C3	-2.11	1.40	1.45
45	Z	201	PC1	O31-C3	-2.11	1.40	1.45
53	L	701	CDL	OB8-CB6	-2.11	1.40	1.45
45	M	606	PC1	O21-C21	2.10	1.40	1.34
46	b	101	3PE	O21-C21	2.10	1.40	1.34
46	d	201	3PE	O21-C21	2.10	1.40	1.34
45	Z	201	PC1	O21-C21	2.10	1.40	1.34
46	Y	206	3PE	O21-C21	2.10	1.40	1.34
45	A	201	PC1	O31-C3	-2.10	1.40	1.45
46	M	602	3PE	O21-C21	2.09	1.40	1.34
46	I	204	3PE	O21-C21	2.09	1.40	1.34
46	Y	202	3PE	O21-C21	2.09	1.40	1.34
46	Y	207	3PE	O21-C21	2.09	1.40	1.34
53	P	503	CDL	OA8-CA6	-2.09	1.40	1.45
46	N	401	3PE	O21-C21	2.08	1.40	1.34
45	m	202	PC1	O21-C21	2.08	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Y	209	3PE	O21-C21	2.08	1.40	1.34
45	H	404	PC1	O21-C21	2.08	1.40	1.34
46	Y	204	3PE	O21-C21	2.08	1.40	1.34
57	P	501	NDP	C5B-C4B	2.08	1.57	1.51
45	A	203	PC1	O21-C21	2.07	1.40	1.34
53	M	607	CDL	OA6-CA5	2.07	1.40	1.34
46	M	604	3PE	O21-C21	2.07	1.40	1.34
49	D	501	U10	O3-C3	2.07	1.41	1.36
49	D	501	U10	C36-C34	2.07	1.55	1.51
53	L	701	CDL	OA8-CA6	-2.07	1.40	1.45
45	M	606	PC1	O31-C3	-2.06	1.40	1.45
46	A	205	3PE	O21-C21	2.06	1.40	1.34
53	H	401	CDL	OA6-CA5	2.05	1.40	1.34
53	L	701	CDL	OA6-CA5	2.05	1.40	1.34
46	J	202	3PE	O21-C21	2.05	1.40	1.34
53	P	503	CDL	OB6-CB5	2.05	1.40	1.34
46	J	204	3PE	O21-C21	2.05	1.40	1.34
49	D	501	U10	C22-C23	2.04	1.56	1.50
45	d	202	PC1	O21-C21	2.04	1.40	1.34
53	d	204	CDL	OB6-CB5	2.03	1.40	1.34
53	M	607	CDL	OB6-CB5	2.00	1.39	1.34

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	C8-N9-C4	7.54	120.16	106.03
59	i	201	CHD	C13-C17-C20	-6.35	111.79	119.48
59	i	201	CHD	C14-C13-C12	5.94	112.84	107.42
57	P	501	NDP	N6A-C6A-N1A	-5.67	105.76	118.38
57	P	501	NDP	N3A-C2A-N1A	-5.66	120.01	128.58
59	i	201	CHD	C17-C13-C14	5.56	105.69	100.11
57	P	501	NDP	C4A-N9A-C1B	-5.25	114.35	126.63
58	U	101	EHZ	C8-C9-S1	5.22	120.14	113.56
57	P	501	NDP	C5A-C4A-N3A	-5.19	119.57	126.72
58	T	101	EHZ	C8-C9-S1	5.18	120.09	113.56
53	h	201	CDL	OB6-CB5-C51	4.94	122.16	111.48
45	B	204	PC1	O21-C21-C22	4.87	122.01	111.48
57	P	501	NDP	C1B-N9A-C8A	4.77	137.68	127.09
51	F	501	FMN	C7M-C7-C6	4.58	127.65	119.57
51	F	501	FMN	C9-C8-C7	4.55	126.37	119.69
59	i	201	CHD	C17-C13-C12	4.46	121.68	117.67
46	Y	203	3PE	O21-C21-C22	4.28	120.74	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	m	201	3PE	O21-C21-C22	4.28	120.73	111.48
46	m	203	3PE	O21-C21-C22	4.26	120.69	111.48
46	M	602	3PE	O21-C21-C22	4.23	120.62	111.48
53	d	204	CDL	OB6-CB5-C51	4.22	120.61	111.48
59	i	201	CHD	C18-C13-C12	-4.20	104.85	109.06
46	A	205	3PE	O21-C21-C22	4.18	120.53	111.48
46	Y	206	3PE	O21-C21-C22	4.15	120.46	111.48
46	Y	201	3PE	O21-C21-C22	4.14	120.44	111.48
45	H	402	PC1	O21-C21-C22	4.13	120.41	111.48
57	P	501	NDP	C5A-C6A-N6A	4.12	133.48	123.29
53	h	201	CDL	OA6-CA5-C11	4.07	120.29	111.48
46	J	202	3PE	O21-C21-C22	4.07	120.29	111.48
46	P	505	3PE	O21-C21-C22	4.06	120.27	111.48
46	f	101	3PE	O21-C21-C22	4.06	120.27	111.48
45	I	203	PC1	O21-C21-C22	4.06	120.26	111.48
53	L	701	CDL	OA6-CA5-C11	4.05	120.24	111.48
46	N	403	3PE	O21-C21-C22	4.05	120.23	111.48
53	N	402	CDL	OB6-CB5-C51	4.04	120.22	111.48
57	P	501	NDP	N9A-C8A-N7A	-4.04	108.21	113.94
45	A	203	PC1	O21-C21-C22	4.04	120.22	111.48
46	q	202	3PE	O21-C21-C22	4.03	120.20	111.48
53	M	607	CDL	OA6-CA5-C11	4.03	120.19	111.48
46	a	101	3PE	O21-C21-C22	4.02	120.17	111.48
46	Y	207	3PE	O21-C21-C22	4.01	120.17	111.48
46	J	201	3PE	O21-C21-C22	4.01	120.16	111.48
45	H	403	PC1	O21-C21-C22	4.00	120.14	111.48
46	g	201	3PE	O21-C21-C22	4.00	120.12	111.48
46	Y	202	3PE	O21-C21-C22	3.98	120.08	111.48
46	b	102	3PE	O21-C21-C22	3.97	120.06	111.48
53	H	401	CDL	OA6-CA5-C11	3.97	120.06	111.48
46	M	604	3PE	O21-C21-C22	3.96	120.05	111.48
46	Z	202	3PE	O21-C21-C22	3.96	120.05	111.48
46	J	204	3PE	O21-C21-C22	3.96	120.05	111.48
45	A	201	PC1	O21-C21-C22	3.93	119.98	111.48
46	I	204	3PE	O21-C21-C22	3.92	119.97	111.48
53	P	503	CDL	OA6-CA5-C11	3.91	119.95	111.48
46	Y	205	3PE	O21-C21-C22	3.91	119.94	111.48
53	M	607	CDL	OB6-CB5-C51	3.90	119.92	111.48
45	L	704	PC1	O21-C21-C22	3.90	119.92	111.48
46	A	204	3PE	O21-C21-C22	3.89	119.89	111.48
53	P	503	CDL	OB6-CB5-C51	3.89	119.89	111.48
46	L	702	3PE	O21-C21-C22	3.88	119.87	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	Z	201	PC1	O21-C21-C22	3.88	119.86	111.48
59	i	201	CHD	C18-C13-C17	-3.85	105.17	111.20
46	P	502	3PE	O21-C21-C22	3.84	119.79	111.48
46	Y	204	3PE	O21-C21-C22	3.84	119.78	111.48
53	r	201	CDL	OB6-CB5-C51	3.82	119.75	111.48
59	i	201	CHD	C18-C13-C14	-3.82	105.22	111.20
53	d	204	CDL	OA6-CA5-C11	3.79	119.68	111.48
46	N	401	3PE	O21-C21-C22	3.76	119.61	111.48
45	g	203	PC1	O21-C21-C22	3.74	119.57	111.48
45	M	606	PC1	O21-C21-C22	3.74	119.57	111.48
53	H	401	CDL	OB6-CB5-C51	3.73	119.54	111.48
46	M	603	3PE	O21-C21-C22	3.72	119.52	111.48
46	Y	209	3PE	O21-C21-C22	3.71	119.50	111.48
53	d	203	CDL	OA6-CA5-C11	3.70	119.49	111.48
45	d	202	PC1	O21-C21-C22	3.69	119.45	111.48
46	r	202	3PE	O21-C21-C22	3.68	119.45	111.48
45	B	202	PC1	O21-C21-C22	3.68	119.45	111.48
45	m	202	PC1	O21-C21-C22	3.67	119.41	111.48
53	L	701	CDL	OB6-CB5-C51	3.66	119.39	111.48
53	r	201	CDL	OA6-CA5-C11	3.65	119.38	111.48
45	h	202	PC1	O21-C21-C22	3.65	119.38	111.48
46	Z	204	3PE	O21-C21-C22	3.61	119.29	111.48
45	q	201	PC1	O21-C21-C22	3.58	119.22	111.48
57	P	501	NDP	C2A-N3A-C4A	3.58	120.56	111.83
53	N	402	CDL	OA6-CA5-C11	3.56	119.19	111.48
58	T	101	EHZ	C13-C12-N1	3.56	122.83	116.34
49	D	501	U10	C20-C19-C21	3.56	121.40	115.23
46	d	201	3PE	O21-C21-C22	3.50	119.05	111.48
45	A	202	PC1	O21-C21-C22	3.50	119.05	111.48
59	i	201	CHD	C1-C10-C5	3.48	112.73	107.75
55	O	401	DGT	C1'-N9-C8	-3.47	120.14	127.91
51	F	501	FMN	C4-N3-C2	-3.44	119.54	125.64
46	M	605	3PE	O21-C21-C22	3.39	118.82	111.48
46	b	101	3PE	O21-C21-C22	3.30	118.63	111.48
51	F	501	FMN	C8M-C8-C7	-3.22	114.18	120.76
49	D	501	U10	C40-C39-C41	3.20	120.78	115.23
57	P	501	NDP	N3A-C4A-N9A	3.15	132.52	127.17
55	O	401	DGT	C2-N1-C6	-3.11	119.47	125.11
59	i	201	CHD	C6-C5-C4	-3.06	107.73	111.23
45	H	403	PC1	O31-C31-C32	2.99	120.22	111.15
45	h	202	PC1	O31-C31-C32	2.96	120.87	111.83
45	H	404	PC1	O31-C31-C32	2.95	120.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	i	201	CHD	C23-C22-C20	-2.94	108.97	114.46
51	F	501	FMN	C4A-C10-N10	2.93	120.68	116.48
53	M	607	CDL	OB8-CB7-C71	2.92	120.75	111.83
53	M	607	CDL	OA8-CA7-C31	2.91	120.72	111.83
49	D	501	U10	C10-C9-C11	2.90	120.25	115.23
45	A	203	PC1	O31-C31-C32	2.88	120.62	111.83
53	d	204	CDL	OA8-CA7-C31	2.88	120.62	111.83
49	D	501	U10	C25-C24-C26	2.88	120.22	115.23
46	M	605	3PE	O31-C31-C32	2.87	120.60	111.83
59	i	201	CHD	C16-C17-C13	2.86	106.32	103.54
46	P	505	3PE	O31-C31-C32	2.86	120.55	111.83
45	m	202	PC1	O31-C31-C32	2.85	120.54	111.83
49	D	501	U10	C20-C19-C18	-2.85	116.31	123.63
46	Y	204	3PE	O31-C31-C32	2.85	120.52	111.83
46	r	202	3PE	O31-C31-C32	2.85	120.52	111.83
55	O	401	DGT	O2G-PG-O3B	2.84	114.17	104.64
46	Y	207	3PE	O31-C31-C32	2.84	120.50	111.83
46	J	202	3PE	O31-C31-C32	2.84	119.77	111.15
53	L	701	CDL	OA8-CA7-C31	2.84	120.50	111.83
45	d	202	PC1	O31-C31-C32	2.83	120.46	111.83
46	m	201	3PE	O31-C31-C32	2.83	120.45	111.83
46	Y	206	3PE	O31-C31-C32	2.82	120.44	111.83
45	L	704	PC1	O31-C31-C32	2.82	120.42	111.83
53	r	201	CDL	OA8-CA7-C31	2.82	120.42	111.83
46	N	401	3PE	O31-C31-C32	2.82	120.42	111.83
46	g	201	3PE	O31-C31-C32	2.81	120.41	111.83
57	P	501	NDP	C5A-N7A-C8A	2.80	107.84	103.45
59	i	201	CHD	C15-C14-C8	2.79	122.19	118.36
46	Z	204	3PE	O31-C31-C32	2.79	120.33	111.83
46	Y	205	3PE	O31-C31-C32	2.79	120.33	111.83
59	i	201	CHD	C1-C2-C3	2.79	114.17	110.48
55	O	401	DGT	O1G-PG-O3B	2.78	113.97	104.64
53	d	203	CDL	OA8-CA7-C31	2.77	120.30	111.83
46	f	101	3PE	O31-C31-C32	2.77	120.29	111.83
46	J	201	3PE	O31-C31-C32	2.77	120.27	111.83
45	B	204	PC1	O31-C31-C32	2.76	120.26	111.83
46	N	403	3PE	O31-C31-C32	2.76	120.25	111.83
45	H	402	PC1	O31-C31-C32	2.75	120.23	111.83
53	d	204	CDL	OB8-CB7-C71	2.75	120.22	111.83
46	M	602	3PE	O31-C31-C32	2.74	120.20	111.83
53	d	203	CDL	OB6-CB5-C51	2.73	120.95	110.93
53	P	503	CDL	OA8-CA7-C31	2.72	120.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	r	201	CDL	OB8-CB7-C71	2.72	120.14	111.83
53	h	201	CDL	OB8-CB7-C71	2.71	120.11	111.83
45	Z	201	PC1	O31-C31-C32	2.71	120.10	111.83
46	I	204	3PE	O31-C31-C32	2.71	120.10	111.83
46	P	502	3PE	O31-C31-C32	2.71	120.10	111.83
45	g	203	PC1	O31-C31-C32	2.69	120.05	111.83
49	D	501	U10	C40-C39-C38	-2.69	116.71	123.63
46	J	204	3PE	O31-C31-C32	2.69	120.03	111.83
46	L	702	3PE	O31-C31-C32	2.69	120.03	111.83
53	H	401	CDL	OA8-CA7-C31	2.68	120.02	111.83
46	q	202	3PE	O31-C31-C32	2.68	120.01	111.83
46	Y	209	3PE	O31-C31-C32	2.68	120.00	111.83
53	N	402	CDL	OA8-CA7-C31	2.67	119.98	111.83
45	A	201	PC1	O31-C31-C32	2.67	119.97	111.83
45	B	202	PC1	O31-C31-C32	2.67	119.97	111.83
46	m	203	3PE	O31-C31-C32	2.66	119.95	111.83
53	h	201	CDL	OA8-CA7-C31	2.66	119.94	111.83
46	Y	201	3PE	O31-C31-C32	2.66	119.93	111.83
46	Y	202	3PE	O31-C31-C32	2.65	119.92	111.83
49	D	501	U10	C15-C14-C16	2.65	119.83	115.23
46	A	204	3PE	O31-C31-C32	2.63	119.86	111.83
46	d	201	3PE	O31-C31-C32	2.63	119.84	111.83
53	P	503	CDL	OB8-CB7-C71	2.62	119.83	111.83
46	M	603	3PE	O31-C31-C32	2.62	119.82	111.83
51	F	501	FMN	C6-C7-C8	-2.61	115.85	119.69
46	Y	203	3PE	O31-C31-C32	2.61	119.79	111.83
46	b	101	3PE	O31-C31-C32	2.60	119.78	111.83
46	M	604	3PE	O31-C31-C32	2.60	119.78	111.83
53	d	203	CDL	OB8-CB7-C71	2.60	119.76	111.83
58	T	101	EHZ	C10-S1-C9	2.59	109.50	101.84
45	A	202	PC1	O31-C31-C32	2.59	119.72	111.83
46	Z	202	3PE	O31-C31-C32	2.58	119.70	111.83
45	M	606	PC1	O31-C31-C32	2.57	119.66	111.83
46	a	101	3PE	O31-C31-C32	2.56	119.63	111.83
49	D	501	U10	C45-C44-C46	2.55	119.65	115.23
45	q	201	PC1	O31-C31-C32	2.54	119.59	111.83
46	A	205	3PE	O31-C31-C32	2.54	119.59	111.83
49	D	501	U10	C7-C8-C9	2.54	131.20	126.83
59	i	201	CHD	C4-C3-C2	2.53	113.71	110.62
45	I	203	PC1	O31-C31-C32	2.53	119.55	111.83
46	b	102	3PE	O31-C31-C32	2.52	119.53	111.83
53	H	401	CDL	OB8-CB7-C71	2.51	119.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	F	501	FMN	C4A-C4-N3	2.50	119.62	113.25
58	U	101	EHZ	C10-S1-C9	2.50	109.22	101.84
51	F	501	FMN	O4-C4-C4A	-2.49	119.97	126.53
51	F	501	FMN	C5A-C9A-N10	2.49	120.22	117.97
55	O	401	DGT	C5-C6-N1	2.47	119.55	113.25
58	T	101	EHZ	C11-N1-C12	-2.47	118.22	122.82
55	O	401	DGT	C2'-C3'-C4'	2.46	107.79	102.80
55	O	401	DGT	O1A-PA-O2A	-2.45	101.04	112.44
53	L	701	CDL	OB8-CB7-C71	2.45	119.31	111.83
53	N	402	CDL	OB8-CB7-C71	2.44	119.27	111.83
49	D	501	U10	C25-C24-C23	-2.43	117.38	123.63
49	D	501	U10	C30-C29-C31	2.43	119.45	115.23
58	U	101	EHZ	C13-C12-N1	2.40	120.71	116.34
55	O	401	DGT	O1B-PB-O2B	-2.39	101.31	112.44
45	H	404	PC1	O21-C21-C22	2.39	119.69	110.93
58	U	101	EHZ	O2-C9-C8	-2.38	120.00	123.74
57	P	501	NDP	C2B-C1B-N9A	-2.37	109.85	113.75
55	O	401	DGT	O6-C6-C5	-2.36	120.31	126.53
58	T	101	EHZ	O3-C12-N1	-2.35	118.42	123.03
58	U	101	EHZ	C19-C17-C16	2.35	112.77	108.77
58	T	101	EHZ	O2-C9-S1	-2.32	119.73	122.68
51	F	501	FMN	C9A-C5A-N5	-2.32	119.99	122.45
49	D	501	U10	C50-C49-C51	2.32	119.25	115.23
59	i	201	CHD	C9-C11-C12	-2.32	111.26	114.29
58	T	101	EHZ	C14-N2-C15	-2.28	118.44	122.55
49	D	501	U10	C56-C54-C55	2.28	119.84	114.59
51	F	501	FMN	C10-C4A-N5	-2.28	120.16	124.81
58	T	101	EHZ	O2-C9-C8	-2.27	120.17	123.74
58	U	101	EHZ	O2-C9-S1	-2.22	119.85	122.68
59	i	201	CHD	C19-C10-C9	-2.20	108.22	111.18
57	P	501	NDP	C4A-C5A-N7A	-2.20	108.06	110.58
55	O	401	DGT	C5-C4-N9	-2.18	101.75	105.66
49	D	501	U10	C35-C34-C36	2.18	119.00	115.23
59	i	201	CHD	C16-C17-C20	-2.16	108.90	112.18
49	D	501	U10	C35-C34-C33	-2.16	118.09	123.63
55	O	401	DGT	C1'-N9-C4	-2.15	119.70	125.50
55	O	401	DGT	N9-C8-N7	-2.14	109.43	113.40
57	P	501	NDP	C4A-N9A-C8A	2.13	107.97	105.74
55	O	401	DGT	C6-C5-N7	2.12	134.16	130.29
51	F	501	FMN	C6-C5A-C9A	2.11	121.95	119.05
49	D	501	U10	C45-C44-C43	-2.09	118.26	123.63
51	F	501	FMN	C7M-C7-C8	-2.09	116.50	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	D	501	U10	C1M-C1-C6	-2.08	121.04	124.45
55	O	401	DGT	N9-C4-N3	2.06	130.07	125.95
59	i	201	CHD	C15-C14-C13	2.03	105.51	103.54
53	h	201	CDL	OB6-CB5-OB7	-2.03	118.95	123.70
59	i	201	CHD	C9-C10-C5	2.02	111.33	108.51
49	D	501	U10	C7-C6-C1	-2.02	121.43	124.89

There are no chirality outliers.

All (1517) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PC1	C1-O11-P-O14
45	A	201	PC1	C1-O11-P-O13
45	A	201	PC1	O11-C1-C2-O21
45	A	201	PC1	C22-C21-O21-C2
45	A	202	PC1	C11-O13-P-O12
45	A	203	PC1	C11-O13-P-O12
45	A	203	PC1	C11-O13-P-O11
45	A	203	PC1	O22-C21-O21-C2
45	A	203	PC1	C22-C21-O21-C2
45	B	202	PC1	C11-O13-P-O14
45	B	202	PC1	C11-O13-P-O11
45	B	204	PC1	C11-O13-P-O11
45	B	204	PC1	O22-C21-O21-C2
45	H	402	PC1	C11-O13-P-O12
45	H	402	PC1	C11-O13-P-O14
45	H	402	PC1	C11-O13-P-O11
45	H	402	PC1	C1-O11-P-O14
45	H	402	PC1	C1-O11-P-O13
45	H	403	PC1	C1-O11-P-O12
45	H	403	PC1	C1-O11-P-O13
45	H	403	PC1	O13-C11-C12-N
45	H	403	PC1	O22-C21-O21-C2
45	H	403	PC1	C22-C21-O21-C2
45	I	203	PC1	C11-O13-P-O11
45	I	203	PC1	O13-C11-C12-N
45	M	606	PC1	C11-O13-P-O12
45	M	606	PC1	C11-O13-P-O14
45	M	606	PC1	C11-O13-P-O11
45	M	606	PC1	O22-C21-O21-C2
45	M	606	PC1	C22-C21-O21-C2
45	Z	201	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
45	Z	201	PC1	C1-O11-P-O13
45	d	202	PC1	C1-O11-P-O14
45	d	202	PC1	C1-O11-P-O13
45	g	203	PC1	C11-O13-P-O12
45	g	203	PC1	C11-O13-P-O14
45	g	203	PC1	C11-O13-P-O11
45	g	203	PC1	C1-O11-P-O12
45	g	203	PC1	C1-O11-P-O13
45	g	203	PC1	O13-C11-C12-N
45	h	202	PC1	C11-O13-P-O14
45	h	202	PC1	C11-O13-P-O11
45	m	202	PC1	C11-O13-P-O12
45	q	201	PC1	C11-O13-P-O12
45	q	201	PC1	C11-O13-P-O11
45	q	201	PC1	C1-O11-P-O14
46	A	205	3PE	C11-O13-P-O14
46	A	205	3PE	O22-C21-O21-C2
46	I	204	3PE	C1-O11-P-O13
46	I	204	3PE	C11-O13-P-O14
46	I	204	3PE	O11-C1-C2-O21
46	I	204	3PE	C22-C21-O21-C2
46	J	201	3PE	C1-O11-P-O12
46	J	201	3PE	C1-O11-P-O13
46	J	201	3PE	C1-O11-P-O14
46	J	201	3PE	C11-O13-P-O11
46	J	201	3PE	C11-O13-P-O14
46	J	201	3PE	C12-C11-O13-P
46	J	201	3PE	C22-C21-O21-C2
46	J	202	3PE	C1-O11-P-O14
46	J	202	3PE	C11-O13-P-O11
46	J	202	3PE	C11-O13-P-O12
46	J	202	3PE	C11-O13-P-O14
46	J	204	3PE	C1-O11-P-O12
46	J	204	3PE	C1-O11-P-O13
46	J	204	3PE	C1-O11-P-O14
46	J	204	3PE	O13-C11-C12-N
46	J	204	3PE	O11-C1-C2-O21
46	L	702	3PE	C1-O11-P-O12
46	L	702	3PE	C1-O11-P-O13
46	L	702	3PE	C11-O13-P-O12
46	L	702	3PE	C22-C21-O21-C2
46	M	602	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	M	602	3PE	C1-O11-P-O14
46	M	602	3PE	C22-C21-O21-C2
46	M	603	3PE	O13-C11-C12-N
46	M	604	3PE	C1-O11-P-O12
46	M	604	3PE	C1-O11-P-O13
46	M	604	3PE	C1-O11-P-O14
46	M	605	3PE	C11-O13-P-O11
46	N	401	3PE	C1-O11-P-O13
46	N	403	3PE	C11-O13-P-O11
46	N	403	3PE	C22-C21-O21-C2
46	P	505	3PE	C11-O13-P-O11
46	P	505	3PE	C11-O13-P-O14
46	P	505	3PE	C12-C11-O13-P
46	P	505	3PE	C22-C21-O21-C2
46	Y	201	3PE	C1-O11-P-O12
46	Y	202	3PE	C1-O11-P-O12
46	Y	202	3PE	C1-O11-P-O13
46	Y	202	3PE	C1-O11-P-O14
46	Y	202	3PE	C11-O13-P-O11
46	Y	202	3PE	C11-O13-P-O14
46	Y	202	3PE	C22-C21-O21-C2
46	Y	203	3PE	C11-O13-P-O14
46	Y	203	3PE	C22-C21-O21-C2
46	Y	204	3PE	C1-O11-P-O14
46	Y	204	3PE	C11-O13-P-O11
46	Y	204	3PE	C11-O13-P-O12
46	Y	204	3PE	C22-C21-O21-C2
46	Y	205	3PE	C1-O11-P-O13
46	Y	207	3PE	C1-O11-P-O14
46	Y	207	3PE	C11-O13-P-O11
46	Y	207	3PE	C11-O13-P-O12
46	Y	207	3PE	O13-C11-C12-N
46	Y	207	3PE	O22-C21-O21-C2
46	Y	209	3PE	C1-O11-P-O12
46	Y	209	3PE	C11-O13-P-O11
46	Y	209	3PE	C22-C21-O21-C2
46	Z	202	3PE	C11-O13-P-O11
46	Z	202	3PE	C11-O13-P-O14
46	Z	202	3PE	C12-C11-O13-P
46	Z	202	3PE	O13-C11-C12-N
46	Z	204	3PE	C11-O13-P-O14
46	Z	204	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	a	101	3PE	C1-O11-P-O12
46	a	101	3PE	C1-O11-P-O13
46	a	101	3PE	O22-C21-O21-C2
46	b	101	3PE	C1-O11-P-O12
46	b	101	3PE	C1-O11-P-O13
46	b	102	3PE	C1-O11-P-O13
46	b	102	3PE	C1-O11-P-O14
46	b	102	3PE	O22-C21-O21-C2
46	d	201	3PE	C11-O13-P-O11
46	d	201	3PE	C11-O13-P-O12
46	d	201	3PE	C11-O13-P-O14
46	f	101	3PE	C1-O11-P-O12
46	f	101	3PE	C1-O11-P-O13
46	f	101	3PE	C11-O13-P-O11
46	f	101	3PE	C11-O13-P-O12
46	f	101	3PE	C11-O13-P-O14
46	g	201	3PE	C1-O11-P-O13
46	g	201	3PE	C1-O11-P-O14
46	g	201	3PE	O21-C2-C3-O31
46	g	201	3PE	O22-C21-O21-C2
46	m	201	3PE	C1-O11-P-O12
46	m	201	3PE	C1-O11-P-O13
46	m	201	3PE	C1-O11-P-O14
46	m	201	3PE	C11-O13-P-O11
46	m	201	3PE	C11-O13-P-O12
46	m	201	3PE	O22-C21-O21-C2
46	m	203	3PE	C11-O13-P-O11
46	m	203	3PE	C11-O13-P-O12
46	m	203	3PE	C11-O13-P-O14
46	m	203	3PE	O22-C21-O21-C2
46	q	202	3PE	C11-O13-P-O11
46	q	202	3PE	C11-O13-P-O12
46	q	202	3PE	C11-O13-P-O14
46	q	202	3PE	O21-C2-C3-O31
46	q	202	3PE	O22-C21-O21-C2
47	A	206	PLC	C1-O3P-P-O1P
47	B	203	PLC	C1-O3P-P-O1P
47	B	203	PLC	C1-O3P-P-O2P
47	B	203	PLC	C1-O3P-P-O4P
47	B	203	PLC	C4-O4P-P-O2P
47	B	203	PLC	C4-O4P-P-O3P
47	J	203	PLC	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
47	J	203	PLC	C4-O4P-P-O2P
47	J	203	PLC	C4-O4P-P-O3P
47	L	703	PLC	C4-O4P-P-O1P
47	L	703	PLC	C4-O4P-P-O2P
47	L	703	PLC	C4-O4P-P-O3P
47	M	608	PLC	C5-C4-O4P-P
47	M	608	PLC	C1-O3P-P-O1P
47	M	608	PLC	C1-O3P-P-O2P
47	M	608	PLC	C1-O3P-P-O4P
47	M	608	PLC	C4-O4P-P-O3P
47	P	504	PLC	C1-O3P-P-O1P
47	P	504	PLC	C4-O4P-P-O1P
47	P	504	PLC	C4-O4P-P-O2P
47	P	504	PLC	C4-O4P-P-O3P
47	Y	208	PLC	C1-O3P-P-O2P
47	Y	208	PLC	C4-O4P-P-O1P
47	Z	203	PLC	O3P-C1-C2-O2
47	Z	203	PLC	O4P-C4-C5-N
47	Z	203	PLC	O'-C'-O2-C2
47	Z	203	PLC	C4-O4P-P-O1P
47	Z	203	PLC	C4-O4P-P-O2P
47	Z	203	PLC	C4-O4P-P-O3P
47	g	202	PLC	C1-C2-O2-C'
47	g	202	PLC	C1-O3P-P-O2P
47	g	202	PLC	C1-O3P-P-O4P
49	D	501	U10	C20-C19-C21-C22
53	H	401	CDL	O1-C1-CA2-OA2
53	H	401	CDL	CA2-OA2-PA1-OA4
53	H	401	CDL	CA2-OA2-PA1-OA5
53	H	401	CDL	C11-CA5-OA6-CA4
53	H	401	CDL	CB2-OB2-PB2-OB3
53	H	401	CDL	OB5-CB3-CB4-OB6
53	H	401	CDL	OB6-CB4-CB6-OB8
53	L	701	CDL	CA2-OA2-PA1-OA3
53	L	701	CDL	CA2-OA2-PA1-OA4
53	L	701	CDL	CA2-OA2-PA1-OA5
53	L	701	CDL	CB2-OB2-PB2-OB5
53	M	607	CDL	C1-CA2-OA2-PA1
53	M	607	CDL	OA7-CA5-OA6-CA4
53	M	607	CDL	C11-CA5-OA6-CA4
53	M	607	CDL	CB3-OB5-PB2-OB4
53	M	607	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
53	N	402	CDL	OB6-CB4-CB6-OB8
53	P	503	CDL	CA3-OA5-PA1-OA2
53	P	503	CDL	CA3-OA5-PA1-OA3
53	P	503	CDL	C11-CA5-OA6-CA4
53	P	503	CDL	C1-CB2-OB2-PB2
53	P	503	CDL	CB3-OB5-PB2-OB2
53	P	503	CDL	CB3-OB5-PB2-OB3
53	P	503	CDL	C51-CB5-OB6-CB4
53	d	203	CDL	O1-C1-CA2-OA2
53	d	203	CDL	CB3-OB5-PB2-OB3
53	d	203	CDL	CB3-OB5-PB2-OB4
53	d	203	CDL	OB7-CB5-OB6-CB4
53	d	204	CDL	CA3-OA5-PA1-OA2
53	d	204	CDL	CA3-OA5-PA1-OA3
53	d	204	CDL	C11-CA5-OA6-CA4
53	d	204	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CA3-OA5-PA1-OA2
53	h	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB2-OB2-PB2-OB5
53	h	201	CDL	CB3-OB5-PB2-OB2
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	CB3-OB5-PB2-OB4
53	h	201	CDL	OB7-CB5-OB6-CB4
53	h	201	CDL	C51-CB5-OB6-CB4
53	r	201	CDL	CA3-OA5-PA1-OA2
53	r	201	CDL	CA3-OA5-PA1-OA4
57	P	501	NDP	C5B-O5B-PA-O1A
57	P	501	NDP	C5B-O5B-PA-O2A
57	P	501	NDP	C5B-O5B-PA-O3
57	P	501	NDP	C5D-O5D-PN-O3
57	P	501	NDP	C5D-O5D-PN-O2N
58	T	101	EHZ	C5-C6-C7-C8
58	T	101	EHZ	S1-C10-C11-N1
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	S1-C10-C11-N1
58	U	101	EHZ	C15-C16-C17-C19
58	U	101	EHZ	C15-C16-C17-C20

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Mol	Chain	Res	Type	Atoms
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
45	H	403	PC1	O32-C31-O31-C3
45	H	403	PC1	C32-C31-O31-C3
46	J	201	3PE	C32-C31-O31-C3
45	H	404	PC1	O32-C31-O31-C3
45	d	202	PC1	O32-C31-O31-C3
45	g	203	PC1	O32-C31-O31-C3
45	h	202	PC1	O32-C31-O31-C3
45	m	202	PC1	O32-C31-O31-C3
46	A	205	3PE	O32-C31-O31-C3
46	J	201	3PE	O32-C31-O31-C3
46	M	602	3PE	O32-C31-O31-C3
46	P	502	3PE	O32-C31-O31-C3
46	Y	205	3PE	O32-C31-O31-C3
46	Y	206	3PE	O32-C31-O31-C3
46	g	201	3PE	O32-C31-O31-C3
46	m	201	3PE	O32-C31-O31-C3
53	M	607	CDL	OA9-CA7-OA8-CA6
53	N	402	CDL	OB9-CB7-OB8-CB6
53	P	503	CDL	OA9-CA7-OA8-CA6
53	r	201	CDL	OA9-CA7-OA8-CA6
46	Y	201	3PE	O32-C31-O31-C3
45	A	201	PC1	O22-C21-O21-C2
46	I	204	3PE	O22-C21-O21-C2
46	J	201	3PE	O22-C21-O21-C2
46	J	202	3PE	O22-C21-O21-C2
46	L	702	3PE	O22-C21-O21-C2
46	M	602	3PE	O22-C21-O21-C2
46	N	403	3PE	O22-C21-O21-C2
46	P	505	3PE	O22-C21-O21-C2
46	Y	202	3PE	O22-C21-O21-C2
46	Y	203	3PE	O22-C21-O21-C2
46	Y	204	3PE	O22-C21-O21-C2
47	B	203	PLC	O'-C'-O2-C2
53	H	401	CDL	OA7-CA5-OA6-CA4
53	M	607	CDL	OB7-CB5-OB6-CB4
53	N	402	CDL	OB7-CB5-OB6-CB4
53	P	503	CDL	OA7-CA5-OA6-CA4
53	P	503	CDL	OB7-CB5-OB6-CB4
53	d	204	CDL	OA7-CA5-OA6-CA4
53	d	204	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
45	H	404	PC1	C32-C31-O31-C3
45	d	202	PC1	C32-C31-O31-C3
45	h	202	PC1	C32-C31-O31-C3
45	m	202	PC1	C32-C31-O31-C3
46	A	205	3PE	C32-C31-O31-C3
46	M	602	3PE	C32-C31-O31-C3
46	P	502	3PE	C32-C31-O31-C3
46	Y	205	3PE	C32-C31-O31-C3
46	Y	207	3PE	C32-C31-O31-C3
46	r	202	3PE	C32-C31-O31-C3
47	J	203	PLC	C1B-CB-O3-C3
53	M	607	CDL	C31-CA7-OA8-CA6
53	P	503	CDL	C31-CA7-OA8-CA6
53	h	201	CDL	C71-CB7-OB8-CB6
45	B	204	PC1	C22-C21-O21-C2
46	A	205	3PE	C22-C21-O21-C2
46	J	202	3PE	C22-C21-O21-C2
46	Y	207	3PE	C22-C21-O21-C2
46	a	101	3PE	C22-C21-O21-C2
46	b	102	3PE	C22-C21-O21-C2
46	g	201	3PE	C22-C21-O21-C2
46	m	201	3PE	C22-C21-O21-C2
46	m	203	3PE	C22-C21-O21-C2
46	q	202	3PE	C22-C21-O21-C2
47	B	203	PLC	C1'-C'-O2-C2
47	Z	203	PLC	C1'-C'-O2-C2
53	N	402	CDL	C51-CB5-OB6-CB4
53	d	203	CDL	C51-CB5-OB6-CB4
46	d	201	3PE	O32-C31-O31-C3
49	D	501	U10	C18-C19-C21-C22
45	H	402	PC1	C32-C31-O31-C3
45	g	203	PC1	C32-C31-O31-C3
46	Y	201	3PE	C32-C31-O31-C3
46	Y	204	3PE	C32-C31-O31-C3
46	Y	206	3PE	C32-C31-O31-C3
46	Z	202	3PE	C32-C31-O31-C3
46	d	201	3PE	C32-C31-O31-C3
46	g	201	3PE	C32-C31-O31-C3
46	m	201	3PE	C32-C31-O31-C3
46	m	203	3PE	C32-C31-O31-C3
53	N	402	CDL	C71-CB7-OB8-CB6
53	d	203	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	r	201	CDL	C31-CA7-OA8-CA6
46	I	204	3PE	O32-C31-O31-C3
46	Y	204	3PE	O32-C31-O31-C3
46	Y	207	3PE	O32-C31-O31-C3
46	Y	209	3PE	O32-C31-O31-C3
46	m	203	3PE	O32-C31-O31-C3
46	r	202	3PE	O32-C31-O31-C3
53	h	201	CDL	OB9-CB7-OB8-CB6
46	Y	209	3PE	O22-C21-O21-C2
49	D	501	U10	C16-C17-C18-C19
53	d	204	CDL	O1-C1-CA2-OA2
45	B	204	PC1	C32-C31-O31-C3
45	L	704	PC1	C32-C31-O31-C3
46	N	401	3PE	C32-C31-O31-C3
46	Y	209	3PE	C32-C31-O31-C3
46	f	101	3PE	C32-C31-O31-C3
46	f	101	3PE	O32-C31-O31-C3
47	J	203	PLC	OB-CB-O3-C3
53	d	203	CDL	OA9-CA7-OA8-CA6
45	m	202	PC1	C22-C21-O21-C2
46	f	101	3PE	C22-C21-O21-C2
45	L	704	PC1	O32-C31-O31-C3
46	I	204	3PE	C32-C31-O31-C3
45	H	402	PC1	O32-C31-O31-C3
46	N	401	3PE	O32-C31-O31-C3
46	Z	202	3PE	O32-C31-O31-C3
45	m	202	PC1	O22-C21-O21-C2
49	D	501	U10	C14-C16-C17-C18
49	D	501	U10	C24-C26-C27-C28
49	D	501	U10	C44-C46-C47-C48
49	D	501	U10	C49-C51-C52-C53
45	B	204	PC1	O32-C31-O31-C3
53	d	203	CDL	C71-CB7-OB8-CB6
53	r	201	CDL	C11-CA5-OA6-CA4
53	d	203	CDL	OB9-CB7-OB8-CB6
46	f	101	3PE	O22-C21-O21-C2
53	d	203	CDL	CB2-C1-CA2-OA2
53	d	204	CDL	CB2-C1-CA2-OA2
45	A	203	PC1	C32-C31-O31-C3
46	P	505	3PE	C32-C31-O31-C3
53	N	402	CDL	C31-CA7-OA8-CA6
53	d	204	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C31-CA7-OA8-CA6
53	L	701	CDL	O1-C1-CB2-OB2
46	P	505	3PE	O32-C31-O31-C3
53	d	204	CDL	OA9-CA7-OA8-CA6
45	A	203	PC1	C21-C22-C23-C24
47	J	203	PLC	CB-C1B-C2B-C3B
58	T	101	EHZ	C5-C6-C7-O1
45	A	203	PC1	O32-C31-O31-C3
45	M	606	PC1	O11-C1-C2-O21
53	L	701	CDL	C11-CA5-OA6-CA4
46	b	101	3PE	O21-C2-C3-O31
46	J	202	3PE	C21-C22-C23-C24
47	Z	203	PLC	C1B-CB-O3-C3
49	D	501	U10	C25-C24-C26-C27
46	Y	209	3PE	C31-C32-C33-C34
49	D	501	U10	C34-C36-C37-C38
45	m	202	PC1	C21-C22-C23-C24
45	q	201	PC1	C21-C22-C23-C24
45	q	201	PC1	C31-C32-C33-C34
53	N	402	CDL	OA9-CA7-OA8-CA6
53	h	201	CDL	OA9-CA7-OA8-CA6
45	H	402	PC1	C21-C22-C23-C24
45	I	203	PC1	C21-C22-C23-C24
45	d	202	PC1	C21-C22-C23-C24
46	M	605	3PE	C21-C22-C23-C24
46	N	401	3PE	C21-C22-C23-C24
46	P	505	3PE	C21-C22-C23-C24
46	Y	205	3PE	C31-C32-C33-C34
53	H	401	CDL	CB5-C51-C52-C53
46	M	603	3PE	C31-C32-C33-C34
46	Y	204	3PE	C21-C22-C23-C24
53	d	203	CDL	CB7-C71-C72-C73
53	L	701	CDL	OA7-CA5-OA6-CA4
53	r	201	CDL	OA7-CA5-OA6-CA4
45	h	202	PC1	C21-C22-C23-C24
46	Z	204	3PE	C32-C31-O31-C3
53	H	401	CDL	CB2-C1-CA2-OA2
47	Z	203	PLC	OB-CB-O3-C3
46	M	604	3PE	C22-C21-O21-C2
46	M	604	3PE	O22-C21-O21-C2
46	a	101	3PE	C31-C32-C33-C34
46	f	101	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	CB5-C51-C52-C53
45	Z	201	PC1	C32-C31-O31-C3
46	g	201	3PE	C2-C1-O11-P
46	Z	204	3PE	O32-C31-O31-C3
47	A	206	PLC	C5B-C6B-C7B-C8B
47	Y	208	PLC	C'-C1'-C2'-C3'
53	d	204	CDL	CA3-CA4-OA6-CA5
45	I	203	PC1	C22-C21-O21-C2
45	L	704	PC1	C22-C21-O21-C2
46	Z	204	3PE	C22-C21-O21-C2
47	g	202	PLC	C1'-C'-O2-C2
53	N	402	CDL	C11-CA5-OA6-CA4
46	L	702	3PE	C31-C32-C33-C34
49	D	501	U10	C23-C24-C26-C27
45	L	704	PC1	C32-C33-C34-C35
46	A	204	3PE	C24-C25-C26-C27
46	Y	204	3PE	C2E-C2F-C2G-C2H
45	A	203	PC1	C24-C25-C26-C27
46	Y	202	3PE	C24-C25-C26-C27
46	g	201	3PE	C33-C34-C35-C36
46	m	201	3PE	C35-C36-C37-C38
53	H	401	CDL	C56-C57-C58-C59
53	M	607	CDL	C54-C55-C56-C57
53	M	607	CDL	C72-C73-C74-C75
53	N	402	CDL	C35-C36-C37-C38
46	d	201	3PE	C31-C32-C33-C34
53	H	401	CDL	CA7-C31-C32-C33
46	J	204	3PE	C36-C37-C38-C39
46	M	604	3PE	C26-C27-C28-C29
46	M	604	3PE	C2B-C2C-C2D-C2E
46	f	101	3PE	C26-C27-C28-C29
47	B	203	PLC	C4'-C5'-C6'-C7'
53	h	201	CDL	C58-C59-C60-C61
46	A	205	3PE	C34-C35-C36-C37
46	I	204	3PE	C34-C35-C36-C37
46	J	204	3PE	C26-C27-C28-C29
46	Y	207	3PE	C38-C39-C3A-C3B
46	a	101	3PE	C39-C3A-C3B-C3C
46	b	102	3PE	C2C-C2D-C2E-C2F
46	g	201	3PE	C35-C36-C37-C38
47	Y	208	PLC	C2'-C3'-C4'-C5'
47	Y	208	PLC	C7'-C8'-C9'-CA'

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Mol	Chain	Res	Type	Atoms
53	N	402	CDL	C16-C17-C18-C19
53	N	402	CDL	C79-C80-C81-C82
46	A	205	3PE	C2E-C2F-C2G-C2H
46	Z	202	3PE	C26-C27-C28-C29
46	m	201	3PE	C22-C23-C24-C25
46	q	202	3PE	C36-C37-C38-C39
53	M	607	CDL	C57-C58-C59-C60
53	N	402	CDL	C81-C82-C83-C84
53	d	204	CDL	C32-C33-C34-C35
45	M	606	PC1	C21-C22-C23-C24
46	q	202	3PE	C21-C22-C23-C24
53	N	402	CDL	CB7-C71-C72-C73
46	r	202	3PE	C35-C36-C37-C38
53	d	204	CDL	C51-C52-C53-C54
45	Z	201	PC1	C22-C21-O21-C2
45	B	204	PC1	C28-C29-C2A-C2B
53	M	607	CDL	C14-C15-C16-C17
58	U	101	EHZ	C5-C6-C7-C8
45	H	402	PC1	C2B-C2C-C2D-C2E
46	Y	203	3PE	C3E-C3F-C3G-C3H
46	Y	206	3PE	C2C-C2D-C2E-C2F
45	L	704	PC1	C21-C22-C23-C24
46	Y	201	3PE	C21-C22-C23-C24
45	A	202	PC1	C23-C24-C25-C26
45	B	204	PC1	C34-C35-C36-C37
45	g	203	PC1	C26-C27-C28-C29
46	N	403	3PE	C3A-C3B-C3C-C3D
46	Y	205	3PE	C28-C29-C2A-C2B
46	Z	202	3PE	C24-C25-C26-C27
46	b	101	3PE	C27-C28-C29-C2A
47	O	403	PLC	C2'-C3'-C4'-C5'
53	L	701	CDL	C13-C14-C15-C16
53	M	607	CDL	C33-C34-C35-C36
53	N	402	CDL	C76-C77-C78-C79
45	m	202	PC1	C3A-C3B-C3C-C3D
46	A	205	3PE	C38-C39-C3A-C3B
46	d	201	3PE	C28-C29-C2A-C2B
53	d	204	CDL	C37-C38-C39-C40
53	d	204	CDL	C62-C63-C64-C65
45	M	606	PC1	C33-C34-C35-C36
53	L	701	CDL	C36-C37-C38-C39
46	M	605	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
53	M	607	CDL	CB5-C51-C52-C53
46	A	205	3PE	C25-C26-C27-C28
46	J	202	3PE	C27-C28-C29-C2A
46	N	401	3PE	C35-C36-C37-C38
46	N	403	3PE	C32-C33-C34-C35
46	Y	209	3PE	C2E-C2F-C2G-C2H
46	Z	202	3PE	C39-C3A-C3B-C3C
46	Z	202	3PE	C2A-C2B-C2C-C2D
47	g	202	PLC	O'-C'-O2-C2
46	b	101	3PE	C2A-C2B-C2C-C2D
46	f	101	3PE	C23-C24-C25-C26
46	r	202	3PE	C33-C34-C35-C36
53	N	402	CDL	C38-C39-C40-C41
53	L	701	CDL	CA2-C1-CB2-OB2
45	I	203	PC1	C22-C23-C24-C25
45	m	202	PC1	C2A-C2B-C2C-C2D
45	q	201	PC1	C2C-C2D-C2E-C2F
46	Y	206	3PE	C32-C33-C34-C35
53	N	402	CDL	C19-C20-C21-C22
53	d	203	CDL	C31-C32-C33-C34
53	N	402	CDL	CA5-C11-C12-C13
53	h	201	CDL	CB7-C71-C72-C73
45	B	204	PC1	C3B-C3C-C3D-C3E
46	A	205	3PE	C2B-C2C-C2D-C2E
46	Y	206	3PE	C36-C37-C38-C39
46	Y	206	3PE	C28-C29-C2A-C2B
46	Z	202	3PE	C3C-C3D-C3E-C3F
53	M	607	CDL	C13-C14-C15-C16
53	N	402	CDL	C58-C59-C60-C61
53	P	503	CDL	C71-C72-C73-C74
53	d	204	CDL	C58-C59-C60-C61
53	d	204	CDL	C79-C80-C81-C82
53	d	204	CDL	C82-C83-C84-C85
45	Z	201	PC1	O32-C31-O31-C3
45	B	202	PC1	C33-C34-C35-C36
45	Z	201	PC1	C32-C33-C34-C35
46	J	202	3PE	C2E-C2F-C2G-C2H
46	q	202	3PE	C32-C33-C34-C35
53	H	401	CDL	C12-C13-C14-C15
53	P	503	CDL	C75-C76-C77-C78
53	h	201	CDL	C33-C34-C35-C36
46	N	401	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
45	I	203	PC1	C26-C27-C28-C29
47	J	203	PLC	C2'-C3'-C4'-C5'
45	Z	201	PC1	C31-C32-C33-C34
46	Y	201	3PE	C31-C32-C33-C34
46	Y	206	3PE	C31-C32-C33-C34
47	Y	208	PLC	C4'-C5'-C6'-C7'
53	M	607	CDL	C83-C84-C85-C86
45	H	404	PC1	C22-C21-O21-C2
46	J	204	3PE	C22-C21-O21-C2
46	Y	205	3PE	C22-C21-O21-C2
46	P	505	3PE	C2-C1-O11-P
46	M	603	3PE	C25-C26-C27-C28
46	M	605	3PE	C23-C24-C25-C26
46	N	401	3PE	C27-C28-C29-C2A
53	d	203	CDL	C36-C37-C38-C39
53	d	203	CDL	C72-C73-C74-C75
45	g	203	PC1	C32-C33-C34-C35
46	A	204	3PE	C27-C28-C29-C2A
46	Y	206	3PE	C21-C22-C23-C24
46	I	204	3PE	C37-C38-C39-C3A
46	J	204	3PE	C24-C25-C26-C27
46	b	102	3PE	C32-C33-C34-C35
53	h	201	CDL	C31-C32-C33-C34
45	B	202	PC1	C38-C39-C3A-C3B
53	M	607	CDL	C41-C42-C43-C44
45	I	203	PC1	O22-C21-O21-C2
45	L	704	PC1	O22-C21-O21-C2
46	Z	204	3PE	O22-C21-O21-C2
53	N	402	CDL	OA7-CA5-OA6-CA4
46	M	605	3PE	C22-C23-C24-C25
45	B	204	PC1	C37-C38-C39-C3A
45	L	704	PC1	C3B-C3C-C3D-C3E
46	J	202	3PE	C2C-C2D-C2E-C2F
46	M	604	3PE	C35-C36-C37-C38
53	N	402	CDL	C22-C23-C24-C25
45	h	202	PC1	C29-C2A-C2B-C2C
46	A	205	3PE	C27-C28-C29-C2A
46	f	101	3PE	C34-C35-C36-C37
53	d	203	CDL	C38-C39-C40-C41
45	d	202	PC1	C32-C33-C34-C35
46	b	101	3PE	C2C-C2D-C2E-C2F
45	H	402	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	Y	204	3PE	C2C-C2D-C2E-C2F
46	b	102	3PE	C36-C37-C38-C39
47	Y	208	PLC	C3B-C4B-C5B-C6B
45	Z	201	PC1	C22-C23-C24-C25
46	N	401	3PE	C25-C26-C27-C28
46	m	203	3PE	C26-C27-C28-C29
53	L	701	CDL	C31-CA7-OA8-CA6
53	P	503	CDL	C78-C79-C80-C81
45	d	202	PC1	C22-C21-O21-C2
46	P	502	3PE	C22-C21-O21-C2
46	Y	201	3PE	C22-C21-O21-C2
46	r	202	3PE	C22-C21-O21-C2
53	r	201	CDL	C51-CB5-OB6-CB4
58	T	101	EHZ	C12-C13-C14-N2
45	H	404	PC1	C31-C32-C33-C34
46	J	204	3PE	C21-C22-C23-C24
46	J	201	3PE	C33-C34-C35-C36
45	Z	201	PC1	O22-C21-O21-C2
45	d	202	PC1	C38-C39-C3A-C3B
45	g	203	PC1	C25-C26-C27-C28
47	Z	203	PLC	C2B-C3B-C4B-C5B
46	I	204	3PE	C36-C37-C38-C39
47	L	703	PLC	C7'-C8'-C9'-CA'
57	P	501	NDP	O4B-C4B-C5B-O5B
57	P	501	NDP	C3B-C4B-C5B-O5B
46	Z	204	3PE	C32-C33-C34-C35
46	f	101	3PE	C32-C33-C34-C35
53	M	607	CDL	C18-C19-C20-C21
53	d	204	CDL	C35-C36-C37-C38
46	Z	204	3PE	C2D-C2E-C2F-C2G
53	N	402	CDL	C23-C24-C25-C26
45	L	704	PC1	C22-C23-C24-C25
45	M	606	PC1	C32-C33-C34-C35
46	a	101	3PE	C3B-C3C-C3D-C3E
58	U	101	EHZ	C5-C6-C7-O1
45	H	404	PC1	C32-C33-C34-C35
46	L	702	3PE	C34-C35-C36-C37
47	L	703	PLC	C7B-C8B-C9B-CAA
47	P	504	PLC	C7'-C8'-C9'-CA'
53	d	204	CDL	C61-C62-C63-C64
46	r	202	3PE	O22-C21-O21-C2
45	A	203	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
53	r	201	CDL	OB5-CB3-CB4-OB6
45	I	203	PC1	C32-C33-C34-C35
46	Z	202	3PE	C2D-C2E-C2F-C2G
46	m	201	3PE	C33-C34-C35-C36
46	r	202	3PE	C23-C24-C25-C26
47	P	504	PLC	C1'-C'-O2-C2
46	Y	204	3PE	C25-C26-C27-C28
46	q	202	3PE	C34-C35-C36-C37
53	N	402	CDL	C71-C72-C73-C74
46	Z	204	3PE	C21-C22-C23-C24
53	d	204	CDL	CB7-C71-C72-C73
45	B	204	PC1	C32-C33-C34-C35
53	M	607	CDL	C62-C63-C64-C65
45	L	704	PC1	O21-C2-C3-O31
47	O	403	PLC	O2-C2-C3-O3
47	P	504	PLC	O2-C2-C3-O3
53	h	201	CDL	OB6-CB4-CB6-OB8
46	M	603	3PE	C3C-C3D-C3E-C3F
46	J	202	3PE	C32-C31-O31-C3
46	Y	209	3PE	C2C-C2D-C2E-C2F
45	M	606	PC1	C31-C32-C33-C34
53	H	401	CDL	C61-C62-C63-C64
46	J	202	3PE	C29-C2A-C2B-C2C
46	Y	203	3PE	C2E-C2F-C2G-C2H
45	I	203	PC1	C25-C26-C27-C28
46	N	401	3PE	C24-C25-C26-C27
46	Y	201	3PE	C26-C27-C28-C29
46	b	102	3PE	C3C-C3D-C3E-C3F
53	M	607	CDL	C40-C41-C42-C43
49	D	501	U10	C46-C47-C48-C49
47	g	202	PLC	C4B-C5B-C6B-C7B
46	Y	205	3PE	O22-C21-O21-C2
45	Z	201	PC1	C25-C26-C27-C28
45	h	202	PC1	C24-C25-C26-C27
46	Z	202	3PE	C34-C35-C36-C37
53	M	607	CDL	C59-C60-C61-C62
53	d	204	CDL	C80-C81-C82-C83
46	N	401	3PE	C38-C39-C3A-C3B
53	H	401	CDL	C51-CB5-OB6-CB4
46	J	204	3PE	C32-C33-C34-C35
46	m	201	3PE	C24-C25-C26-C27
53	L	701	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
53	N	402	CDL	C34-C35-C36-C37
45	h	202	PC1	C25-C26-C27-C28
60	o	201	MYR	C7-C8-C9-C10
58	T	101	EHZ	C1-C2-C3-C4
46	b	101	3PE	C33-C34-C35-C36
45	m	202	PC1	C23-C24-C25-C26
45	A	201	PC1	O11-C1-C2-C3
45	H	402	PC1	O11-C1-C2-C3
45	M	606	PC1	O11-C1-C2-C3
46	I	204	3PE	O11-C1-C2-C3
46	J	204	3PE	O11-C1-C2-C3
47	M	608	PLC	O3P-C1-C2-C3
47	Z	203	PLC	O3P-C1-C2-C3
53	H	401	CDL	OB5-CB3-CB4-CB6
53	r	201	CDL	OB5-CB3-CB4-CB6
45	H	404	PC1	O22-C21-O21-C2
46	J	204	3PE	O22-C21-O21-C2
46	P	502	3PE	O22-C21-O21-C2
46	Y	201	3PE	O22-C21-O21-C2
46	M	603	3PE	C38-C39-C3A-C3B
46	N	403	3PE	C2E-C2F-C2G-C2H
45	H	403	PC1	C21-C22-C23-C24
46	I	204	3PE	C28-C29-C2A-C2B
45	L	704	PC1	C39-C3A-C3B-C3C
45	d	202	PC1	C33-C34-C35-C36
46	M	605	3PE	C35-C36-C37-C38
46	r	202	3PE	C36-C37-C38-C39
53	H	401	CDL	C34-C35-C36-C37
51	F	501	FMN	O3'-C3'-C4'-C5'
45	A	201	PC1	C1-C2-C3-O31
46	P	505	3PE	C1-C2-C3-O31
46	Y	207	3PE	C1-C2-C3-O31
46	b	102	3PE	C1-C2-C3-O31
46	f	101	3PE	C1-C2-C3-O31
47	B	203	PLC	C1-C2-C3-O3
47	J	203	PLC	C1-C2-C3-O3
47	L	703	PLC	C1-C2-C3-O3
49	D	501	U10	C19-C21-C22-C23
53	L	701	CDL	CA3-CA4-CA6-OA8
45	Z	201	PC1	C38-C39-C3A-C3B
46	r	202	3PE	C22-C23-C24-C25
53	M	607	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
53	M	607	CDL	C77-C78-C79-C80
45	H	402	PC1	C38-C39-C3A-C3B
45	I	203	PC1	C2D-C2E-C2F-C2G
46	Y	205	3PE	C32-C33-C34-C35
46	L	702	3PE	C36-C37-C38-C39
46	Y	205	3PE	C36-C37-C38-C39
47	A	206	PLC	C1B-C2B-C3B-C4B
45	A	203	PC1	C11-C12-N-C14
53	M	607	CDL	CA5-C11-C12-C13
53	L	701	CDL	OA9-CA7-OA8-CA6
46	N	403	3PE	C22-C23-C24-C25
45	H	403	PC1	C2-C1-O11-P
45	d	202	PC1	O22-C21-O21-C2
53	r	201	CDL	OB7-CB5-OB6-CB4
53	M	607	CDL	C74-C75-C76-C77
53	d	204	CDL	C76-C77-C78-C79
46	J	202	3PE	O32-C31-O31-C3
51	F	501	FMN	C5'-O5'-P-O1P
46	P	505	3PE	C1-C2-O21-C21
45	M	606	PC1	C24-C25-C26-C27
46	N	401	3PE	C3B-C3C-C3D-C3E
46	P	505	3PE	C27-C28-C29-C2A
46	f	101	3PE	C35-C36-C37-C38
45	B	202	PC1	C34-C35-C36-C37
45	q	201	PC1	O11-C1-C2-O21
46	A	205	3PE	O11-C1-C2-O21
46	d	201	3PE	O11-C1-C2-O21
47	Y	208	PLC	C1'-C'-O2-C2
46	M	605	3PE	C28-C29-C2A-C2B
45	H	404	PC1	C35-C36-C37-C38
47	O	403	PLC	C4'-C5'-C6'-C7'
46	g	201	3PE	C38-C39-C3A-C3B
45	A	202	PC1	C33-C34-C35-C36
46	A	204	3PE	C33-C34-C35-C36
46	L	702	3PE	C39-C3A-C3B-C3C
46	M	602	3PE	C22-C23-C24-C25
47	O	403	PLC	C1B-C2B-C3B-C4B
46	N	401	3PE	C33-C34-C35-C36
46	d	201	3PE	C39-C3A-C3B-C3C
45	B	202	PC1	O21-C2-C3-O31
46	A	205	3PE	O21-C2-C3-O31
46	Y	204	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	Z	204	3PE	O21-C2-C3-O31
53	d	204	CDL	C64-C65-C66-C67
46	Z	204	3PE	C35-C36-C37-C38
46	Y	203	3PE	C33-C34-C35-C36
53	d	204	CDL	C44-C45-C46-C47
58	U	101	EHZ	O5-C16-C17-C18
58	U	101	EHZ	O5-C16-C17-C19
45	H	402	PC1	C33-C34-C35-C36
46	Y	203	3PE	C34-C35-C36-C37
53	M	607	CDL	C35-C36-C37-C38
55	O	401	DGT	PB-O3A-PA-O2A
46	A	204	3PE	C2-C3-O31-C31
45	I	203	PC1	C3F-C3G-C3H-C3I
46	Y	201	3PE	C24-C25-C26-C27
53	H	401	CDL	C31-CA7-OA8-CA6
46	M	605	3PE	C25-C26-C27-C28
53	N	402	CDL	C31-C32-C33-C34
45	m	202	PC1	C39-C3A-C3B-C3C
46	m	201	3PE	C2-C1-O11-P
47	J	203	PLC	C2-C1-O3P-P
47	g	202	PLC	C2-C1-O3P-P
53	d	203	CDL	C1-CB2-OB2-PB2
46	I	204	3PE	C3D-C3E-C3F-C3G
47	B	203	PLC	C2'-C3'-C4'-C5'
46	Y	204	3PE	C22-C23-C24-C25
57	P	501	NDP	O4D-C1D-N1N-C6N
46	P	505	3PE	C33-C34-C35-C36
53	L	701	CDL	C58-C59-C60-C61
45	Z	201	PC1	C3B-C3C-C3D-C3E
45	A	203	PC1	O11-C1-C2-C3
45	L	704	PC1	O11-C1-C2-C3
46	M	603	3PE	O11-C1-C2-C3
46	M	605	3PE	O11-C1-C2-C3
46	N	403	3PE	O11-C1-C2-C3
46	m	201	3PE	O11-C1-C2-C3
46	r	202	3PE	O11-C1-C2-C3
45	I	203	PC1	C37-C38-C39-C3A
46	A	204	3PE	C37-C38-C39-C3A
46	q	202	3PE	C3F-C3G-C3H-C3I
53	N	402	CDL	C57-C58-C59-C60
47	M	608	PLC	C'-C1'-C2'-C3'
46	M	603	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
45	I	203	PC1	C32-C31-O31-C3
45	L	704	PC1	C37-C38-C39-C3A
47	Z	203	PLC	C6B-C7B-C8B-C9B
46	N	403	3PE	C3B-C3C-C3D-C3E
46	Y	201	3PE	C2D-C2E-C2F-C2G
46	Y	209	3PE	C25-C26-C27-C28
45	B	202	PC1	C1-C2-C3-O31
45	B	204	PC1	C1-C2-C3-O31
45	L	704	PC1	C1-C2-C3-O31
45	h	202	PC1	C1-C2-C3-O31
46	J	202	3PE	C1-C2-C3-O31
46	Z	204	3PE	C1-C2-C3-O31
46	b	101	3PE	C1-C2-C3-O31
47	O	403	PLC	C1-C2-C3-O3
47	Z	203	PLC	C1-C2-C3-O3
53	H	401	CDL	CB3-CB4-CB6-OB8
53	d	204	CDL	CB3-CB4-CB6-OB8
53	h	201	CDL	CB3-CB4-CB6-OB8
46	b	101	3PE	C2D-C2E-C2F-C2G
53	N	402	CDL	C44-C45-C46-C47
46	M	603	3PE	C22-C23-C24-C25
46	Z	202	3PE	C22-C23-C24-C25
46	M	602	3PE	O11-C1-C2-O21
46	Y	204	3PE	O11-C1-C2-O21
46	r	202	3PE	O11-C1-C2-O21
47	M	608	PLC	O3P-C1-C2-O2
53	M	607	CDL	OA5-CA3-CA4-OA6
53	d	203	CDL	OA5-CA3-CA4-OA6
53	H	401	CDL	C63-C64-C65-C66
58	U	101	EHZ	O3-C12-C13-C14
46	Y	204	3PE	C26-C27-C28-C29
46	J	204	3PE	C28-C29-C2A-C2B
47	A	206	PLC	C2-C1-O3P-P
51	F	501	FMN	C4'-C5'-O5'-P
53	M	607	CDL	C31-C32-C33-C34
45	A	201	PC1	O21-C2-C3-O31
45	d	202	PC1	O21-C2-C3-O31
45	h	202	PC1	O21-C2-C3-O31
46	J	204	3PE	O21-C2-C3-O31
46	L	702	3PE	O21-C2-C3-O31
47	Z	203	PLC	O2-C2-C3-O3
47	g	202	PLC	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
53	L	701	CDL	OA6-CA4-CA6-OA8
53	r	201	CDL	OA6-CA4-CA6-OA8
46	b	101	3PE	C24-C25-C26-C27
46	q	202	3PE	C3D-C3E-C3F-C3G
47	P	504	PLC	O'-C'-O2-C2
53	M	607	CDL	C16-C17-C18-C19
45	A	201	PC1	C32-C31-O31-C3
45	H	404	PC1	C3B-C3C-C3D-C3E
46	Y	204	3PE	C39-C3A-C3B-C3C
57	P	501	NDP	PN-O3-PA-O5B
45	A	203	PC1	C32-C33-C34-C35
53	N	402	CDL	C32-C33-C34-C35
53	d	203	CDL	C44-C45-C46-C47
53	N	402	CDL	C21-C22-C23-C24
53	N	402	CDL	C78-C79-C80-C81
60	o	201	MYR	C11-C10-C9-C8
46	P	505	3PE	C29-C2A-C2B-C2C
46	g	201	3PE	C34-C35-C36-C37
46	Z	202	3PE	C22-C21-O21-C2
51	F	501	FMN	C2'-C3'-C4'-O4'
46	I	204	3PE	C24-C25-C26-C27
53	d	204	CDL	C71-C72-C73-C74
46	M	605	3PE	C26-C27-C28-C29
46	Y	203	3PE	C38-C39-C3A-C3B
47	B	203	PLC	O2-C'-C1'-C2'
45	B	202	PC1	C21-C22-C23-C24
46	Y	204	3PE	C3F-C3G-C3H-C3I
46	Y	204	3PE	O11-C1-C2-C3
46	Y	209	3PE	O11-C1-C2-C3
53	M	607	CDL	OA5-CA3-CA4-CA6
53	d	203	CDL	OA5-CA3-CA4-CA6
46	Y	209	3PE	C29-C2A-C2B-C2C
45	A	201	PC1	O32-C31-O31-C3
46	Y	203	3PE	C24-C25-C26-C27
47	Y	208	PLC	C5B-C6B-C7B-C8B
46	M	604	3PE	C31-C32-C33-C34
53	N	402	CDL	CB5-C51-C52-C53
45	I	203	PC1	C3D-C3E-C3F-C3G
46	M	603	3PE	C32-C31-O31-C3
53	d	204	CDL	C41-C42-C43-C44
47	P	504	PLC	C'-C1'-C2'-C3'
46	q	202	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
47	Y	208	PLC	O'-C'-O2-C2
53	H	401	CDL	OB7-CB5-OB6-CB4
53	d	204	CDL	C32-C31-CA7-OA8
53	H	401	CDL	OA9-CA7-OA8-CA6
53	r	201	CDL	C16-C17-C18-C19
45	A	203	PC1	C11-C12-N-C13
45	A	203	PC1	C11-C12-N-C15
46	N	401	3PE	C2A-C2B-C2C-C2D
46	r	202	3PE	C3-C2-O21-C21
47	Y	208	PLC	C1-C2-O2-C'
47	A	206	PLC	CB-C1B-C2B-C3B
45	H	402	PC1	O11-C1-C2-O21
46	M	603	3PE	O11-C1-C2-O21
46	N	403	3PE	O11-C1-C2-O21
46	Y	209	3PE	O11-C1-C2-O21
46	a	101	3PE	O11-C1-C2-O21
46	m	201	3PE	O11-C1-C2-O21
46	L	702	3PE	C3D-C3E-C3F-C3G
46	N	403	3PE	C26-C27-C28-C29
45	d	202	PC1	C1-C2-C3-O31
45	g	203	PC1	C1-C2-C3-O31
46	J	204	3PE	C1-C2-C3-O31
46	L	702	3PE	C1-C2-C3-O31
46	Z	202	3PE	C1-C2-C3-O31
46	g	201	3PE	C1-C2-C3-O31
46	q	202	3PE	C1-C2-C3-O31
53	N	402	CDL	CB3-CB4-CB6-OB8
53	d	203	CDL	CB3-CB4-CB6-OB8
53	d	204	CDL	CA3-CA4-CA6-OA8
46	b	101	3PE	C26-C27-C28-C29
58	U	101	EHZ	C3-C4-C5-C6
46	Y	206	3PE	C29-C2A-C2B-C2C
49	D	501	U10	C12-C11-C9-C10
53	r	201	CDL	C72-C73-C74-C75
45	M	606	PC1	C12-C11-O13-P
46	A	205	3PE	C12-C11-O13-P
46	J	202	3PE	C12-C11-O13-P
46	M	603	3PE	C12-C11-O13-P
46	M	605	3PE	C12-C11-O13-P
46	N	403	3PE	C12-C11-O13-P
46	Y	204	3PE	C12-C11-O13-P
46	Y	207	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
46	Z	204	3PE	C12-C11-O13-P
46	b	102	3PE	C12-C11-O13-P
46	g	201	3PE	C12-C11-O13-P
46	m	201	3PE	C12-C11-O13-P
46	m	203	3PE	C12-C11-O13-P
46	q	202	3PE	C12-C11-O13-P
47	O	403	PLC	C5-C4-O4P-P
45	B	204	PC1	O21-C2-C3-O31
46	A	204	3PE	O21-C2-C3-O31
46	b	102	3PE	O21-C2-C3-O31
46	f	101	3PE	O21-C2-C3-O31
47	J	203	PLC	O2-C2-C3-O3
47	L	703	PLC	O2-C2-C3-O3
53	d	204	CDL	OB6-CB4-CB6-OB8
46	Y	209	3PE	C36-C37-C38-C39
46	Y	205	3PE	C22-C23-C24-C25
46	Y	209	3PE	C27-C28-C29-C2A
45	I	203	PC1	O32-C31-O31-C3
53	r	201	CDL	C51-C52-C53-C54
46	Z	204	3PE	C25-C26-C27-C28
53	L	701	CDL	C62-C63-C64-C65
53	h	201	CDL	C11-CA5-OA6-CA4
46	Y	203	3PE	C3A-C3B-C3C-C3D
46	b	102	3PE	C3F-C3G-C3H-C3I
45	H	402	PC1	C24-C25-C26-C27
45	h	202	PC1	C34-C35-C36-C37
53	L	701	CDL	C53-C54-C55-C56
45	q	201	PC1	O13-C11-C12-N
47	L	703	PLC	O4P-C4-C5-N
47	M	608	PLC	O4P-C4-C5-N
47	Y	208	PLC	O4P-C4-C5-N
47	g	202	PLC	O4P-C4-C5-N
55	O	401	DGT	PA-O3A-PB-O1B
58	U	101	EHZ	C1-C2-C3-C4
46	N	403	3PE	C2A-C2B-C2C-C2D
46	Z	202	3PE	C32-C33-C34-C35
53	h	201	CDL	C52-C53-C54-C55
46	A	205	3PE	C28-C29-C2A-C2B
60	o	201	MYR	C1-C2-C3-C4
46	M	603	3PE	C39-C3A-C3B-C3C
45	A	202	PC1	C36-C37-C38-C39
53	H	401	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
53	N	402	CDL	C62-C63-C64-C65
45	A	202	PC1	C11-C12-N-C14
47	B	203	PLC	C1B-CB-O3-C3
53	H	401	CDL	C71-CB7-OB8-CB6
53	L	701	CDL	C32-C33-C34-C35
46	g	201	3PE	C31-C32-C33-C34
46	N	403	3PE	C2C-C2D-C2E-C2F
53	M	607	CDL	C52-C53-C54-C55
53	N	402	CDL	C82-C83-C84-C85
46	A	205	3PE	O11-C1-C2-C3
46	M	602	3PE	O11-C1-C2-C3
46	Y	206	3PE	O11-C1-C2-C3
46	a	101	3PE	O11-C1-C2-C3
46	d	201	3PE	O11-C1-C2-C3
53	h	201	CDL	OA5-CA3-CA4-CA6
46	Z	202	3PE	O22-C21-O21-C2
53	H	401	CDL	C74-C75-C76-C77
58	T	101	EHZ	C18-C17-C20-O6
46	Y	209	3PE	C22-C23-C24-C25
46	Y	206	3PE	C25-C26-C27-C28
45	L	704	PC1	C24-C25-C26-C27
46	L	702	3PE	C3B-C3C-C3D-C3E
45	L	704	PC1	C23-C24-C25-C26
46	A	204	3PE	C35-C36-C37-C38
46	M	603	3PE	O32-C31-O31-C3
46	Z	202	3PE	C21-C22-C23-C24
53	M	607	CDL	C39-C40-C41-C42
58	U	101	EHZ	C11-C10-S1-C9
45	L	704	PC1	C25-C26-C27-C28
45	H	403	PC1	C23-C24-C25-C26
53	h	201	CDL	OA7-CA5-OA6-CA4
45	L	704	PC1	O11-C1-C2-O21
46	M	605	3PE	O11-C1-C2-O21
46	Y	206	3PE	O11-C1-C2-O21
53	N	402	CDL	OA5-CA3-CA4-OA6
53	h	201	CDL	OA5-CA3-CA4-OA6
46	Y	205	3PE	C35-C36-C37-C38
46	Y	204	3PE	C38-C39-C3A-C3B
45	A	202	PC1	C11-C12-N-C13
45	H	404	PC1	C11-C12-N-C13
45	A	203	PC1	O21-C2-C3-O31
45	H	404	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	g	203	PC1	O21-C2-C3-O31
46	P	505	3PE	O21-C2-C3-O31
46	Z	202	3PE	O21-C2-C3-O31
53	P	503	CDL	OA6-CA4-CA6-OA8
53	d	203	CDL	OB6-CB4-CB6-OB8
53	d	204	CDL	OA6-CA4-CA6-OA8
45	H	403	PC1	C29-C2A-C2B-C2C
46	A	205	3PE	C1-C2-C3-O31
46	Y	204	3PE	C1-C2-C3-O31
47	P	504	PLC	C1-C2-C3-O3
53	r	201	CDL	CA3-CA4-CA6-OA8
53	H	401	CDL	C58-C59-C60-C61
47	B	203	PLC	OB-CB-O3-C3
47	B	203	PLC	C1B-C2B-C3B-C4B
46	d	201	3PE	C21-C22-C23-C24
47	J	203	PLC	C'-C1'-C2'-C3'
53	r	201	CDL	CB7-C71-C72-C73
46	P	502	3PE	C33-C34-C35-C36
46	J	204	3PE	C2A-C2B-C2C-C2D
53	d	203	CDL	C40-C41-C42-C43
53	H	401	CDL	OB9-CB7-OB8-CB6
46	L	702	3PE	C33-C34-C35-C36
46	M	603	3PE	C34-C35-C36-C37
46	b	102	3PE	C29-C2A-C2B-C2C
45	A	201	PC1	C11-O13-P-O12
45	A	201	PC1	C11-O13-P-O14
45	A	201	PC1	C11-O13-P-O11
45	A	201	PC1	C1-O11-P-O12
45	A	202	PC1	C11-O13-P-O14
45	A	202	PC1	C11-O13-P-O11
45	A	202	PC1	C1-O11-P-O14
45	A	202	PC1	C11-C12-N-C15
45	B	204	PC1	C11-O13-P-O14
45	H	402	PC1	C1-O11-P-O12
45	I	203	PC1	C11-O13-P-O12
45	L	704	PC1	C11-O13-P-O12
45	L	704	PC1	C11-O13-P-O14
45	L	704	PC1	C11-O13-P-O11
45	M	606	PC1	C1-O11-P-O14
45	Z	201	PC1	C11-O13-P-O14
45	Z	201	PC1	C11-C12-N-C15
45	d	202	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	d	202	PC1	C1-O11-P-O12
45	g	203	PC1	C1-O11-P-O14
45	m	202	PC1	C11-O13-P-O14
45	m	202	PC1	C11-O13-P-O11
45	q	201	PC1	C11-O13-P-O14
46	A	204	3PE	C11-O13-P-O14
46	J	201	3PE	O13-C11-C12-N
46	J	202	3PE	O13-C11-C12-N
46	L	702	3PE	C11-O13-P-O11
46	L	702	3PE	C11-O13-P-O14
46	M	603	3PE	C11-O13-P-O12
46	M	605	3PE	C11-O13-P-O14
46	N	401	3PE	C11-O13-P-O14
46	P	502	3PE	C11-O13-P-O11
46	P	502	3PE	C11-O13-P-O12
46	P	502	3PE	C11-O13-P-O14
46	P	505	3PE	C11-O13-P-O12
46	P	505	3PE	O13-C11-C12-N
46	Y	201	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O14
46	Y	203	3PE	C1-O11-P-O13
46	Y	203	3PE	C1-O11-P-O14
46	Y	203	3PE	C11-O13-P-O11
46	Y	203	3PE	C11-O13-P-O12
46	Y	205	3PE	C1-O11-P-O14
46	Y	207	3PE	C11-O13-P-O14
46	Y	209	3PE	C1-O11-P-O13
46	Y	209	3PE	C11-O13-P-O14
46	g	201	3PE	C1-O11-P-O12
46	g	201	3PE	C11-O13-P-O11
46	g	201	3PE	C11-O13-P-O12
46	g	201	3PE	C11-O13-P-O14
46	g	201	3PE	O13-C11-C12-N
46	r	202	3PE	C1-O11-P-O14
47	M	608	PLC	C4-O4P-P-O1P
47	O	403	PLC	C1-O3P-P-O1P
47	Y	208	PLC	C1-O3P-P-O4P
53	H	401	CDL	CA2-OA2-PA1-OA3
53	L	701	CDL	CB2-OB2-PB2-OB3
53	M	607	CDL	CB3-OB5-PB2-OB2
53	M	607	CDL	CB3-OB5-PB2-OB3
53	N	402	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
53	d	203	CDL	CA3-OA5-PA1-OA3
53	d	203	CDL	CB3-OB5-PB2-OB2
53	d	204	CDL	CB3-OB5-PB2-OB2
53	d	204	CDL	CB3-OB5-PB2-OB3
53	d	204	CDL	CB3-OB5-PB2-OB4
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA3-OA5-PA1-OA3
53	r	201	CDL	CA2-OA2-PA1-OA3
53	r	201	CDL	CA3-OA5-PA1-OA3
53	r	201	CDL	CB3-OB5-PB2-OB2
53	r	201	CDL	CB3-OB5-PB2-OB3
53	r	201	CDL	CB3-OB5-PB2-OB4
58	U	101	EHZ	O5-C16-C17-C20
45	q	201	PC1	C25-C26-C27-C28
53	d	203	CDL	C34-C35-C36-C37
53	P	503	CDL	C51-C52-C53-C54
53	r	201	CDL	C71-C72-C73-C74
46	N	403	3PE	O31-C31-C32-C33
49	D	501	U10	C12-C11-C9-C8
45	H	402	PC1	C2-C1-O11-P
45	H	404	PC1	C2-C1-O11-P
45	M	606	PC1	C2-C1-O11-P
46	Z	202	3PE	C2-C1-O11-P
47	Y	208	PLC	C2-C1-O3P-P
53	r	201	CDL	CA4-CA3-OA5-PA1
45	M	606	PC1	C23-C24-C25-C26
53	N	402	CDL	C55-C56-C57-C58
60	o	201	MYR	C9-C10-C11-C12
45	B	202	PC1	C31-C32-C33-C34
53	h	201	CDL	C75-C76-C77-C78
46	I	204	3PE	C2F-C2G-C2H-C2I
46	b	102	3PE	C3E-C3F-C3G-C3H
46	Y	203	3PE	C31-C32-C33-C34
46	A	204	3PE	C26-C27-C28-C29
46	Y	203	3PE	C1-C2-O21-C21
46	Y	205	3PE	C3-C2-O21-C21
53	N	402	CDL	CA6-CA4-OA6-CA5
46	M	602	3PE	C32-C33-C34-C35
47	g	202	PLC	C4'-C5'-C6'-C7'
53	r	201	CDL	C54-C55-C56-C57
45	H	404	PC1	C34-C35-C36-C37
53	d	203	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
45	H	404	PC1	C11-C12-N-C15
45	q	201	PC1	O11-C1-C2-C3
47	Y	208	PLC	O3P-C1-C2-C3
46	Y	209	3PE	C34-C35-C36-C37
53	r	201	CDL	C31-C32-C33-C34
53	H	401	CDL	C53-C54-C55-C56
51	F	501	FMN	C2'-C3'-C4'-C5'
46	L	702	3PE	C32-C33-C34-C35
46	L	702	3PE	C26-C27-C28-C29
53	r	201	CDL	C18-C19-C20-C21
46	Y	202	3PE	O11-C1-C2-O21
47	L	703	PLC	O3P-C1-C2-O2
45	H	402	PC1	C28-C29-C2A-C2B
53	M	607	CDL	C21-C22-C23-C24
45	I	203	PC1	C23-C24-C25-C26
46	M	603	3PE	C33-C34-C35-C36
60	o	201	MYR	C6-C7-C8-C9
45	A	203	PC1	C2-C1-O11-P
45	h	202	PC1	C2-C1-O11-P
46	M	603	3PE	C28-C29-C2A-C2B
45	M	606	PC1	O21-C2-C3-O31
46	J	202	3PE	O21-C2-C3-O31
46	Y	207	3PE	O21-C2-C3-O31
47	B	203	PLC	O2-C2-C3-O3
47	M	608	PLC	C2B-C1B-CB-O3
46	L	702	3PE	C25-C26-C27-C28
45	h	202	PC1	C22-C21-O21-C2
53	L	701	CDL	C64-C65-C66-C67
45	B	202	PC1	C27-C28-C29-C2A
53	L	701	CDL	C35-C36-C37-C38
45	H	404	PC1	C1-C2-C3-O31
46	q	202	3PE	C33-C34-C35-C36
46	q	202	3PE	C25-C26-C27-C28
46	Y	205	3PE	C3C-C3D-C3E-C3F
46	d	201	3PE	C2A-C2B-C2C-C2D
57	P	501	NDP	C3D-C4D-C5D-O5D
53	d	204	CDL	C71-CB7-OB8-CB6
45	q	201	PC1	C23-C24-C25-C26
46	I	204	3PE	C39-C3A-C3B-C3C
46	J	204	3PE	C39-C3A-C3B-C3C
45	H	404	PC1	C11-C12-N-C14
45	Z	201	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
45	d	202	PC1	C36-C37-C38-C39
45	H	403	PC1	C24-C25-C26-C27
47	g	202	PLC	C3B-C4B-C5B-C6B
58	U	101	EHZ	C1-C21-C22-C23
45	h	202	PC1	O22-C21-O21-C2
45	g	203	PC1	C29-C2A-C2B-C2C
53	d	204	CDL	OB9-CB7-OB8-CB6
49	D	501	U10	C35-C34-C36-C37
45	h	202	PC1	C23-C24-C25-C26
46	I	204	3PE	C3B-C3C-C3D-C3E
45	q	201	PC1	C32-C33-C34-C35
46	q	202	3PE	C29-C2A-C2B-C2C
46	N	401	3PE	C34-C35-C36-C37
45	H	402	PC1	C2F-C2G-C2H-C2I
60	o	201	MYR	C2-C3-C4-C5
46	J	204	3PE	C32-C31-O31-C3
53	M	607	CDL	C73-C74-C75-C76
51	F	501	FMN	O3'-C3'-C4'-O4'
45	A	201	PC1	C33-C34-C35-C36
45	I	203	PC1	C29-C2A-C2B-C2C
46	P	502	3PE	O21-C2-C3-O31
46	M	603	3PE	C3E-C3F-C3G-C3H
46	b	101	3PE	O21-C21-C22-C23
46	b	102	3PE	C34-C35-C36-C37
47	O	403	PLC	C1'-C2'-C3'-C4'
45	h	202	PC1	C26-C27-C28-C29
45	h	202	PC1	C36-C37-C38-C39
45	h	202	PC1	C37-C38-C39-C3A
46	a	101	3PE	C35-C36-C37-C38
45	B	202	PC1	C39-C3A-C3B-C3C
53	L	701	CDL	CA4-CA3-OA5-PA1
59	i	201	CHD	C22-C23-C24-O26
46	N	401	3PE	C37-C38-C39-C3A
58	U	101	EHZ	N1-C12-C13-C14
47	P	504	PLC	C4'-C5'-C6'-C7'
45	Z	201	PC1	C11-C12-N-C14
45	A	201	PC1	C22-C23-C24-C25
46	A	204	3PE	C22-C23-C24-C25
46	I	204	3PE	C35-C36-C37-C38
53	M	607	CDL	C34-C35-C36-C37
45	I	203	PC1	C38-C39-C3A-C3B
46	N	401	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
47	P	504	PLC	C2'-C3'-C4'-C5'
45	q	201	PC1	C1-C2-O21-C21
46	L	702	3PE	C1-C2-O21-C21
46	m	203	3PE	C1-C2-O21-C21
46	m	203	3PE	C3-C2-O21-C21
53	h	201	CDL	CB6-CB4-OB6-CB5
45	g	203	PC1	O22-C21-O21-C2
45	H	403	PC1	C27-C28-C29-C2A
46	J	204	3PE	C33-C34-C35-C36
46	N	403	3PE	O21-C21-C22-C23
58	T	101	EHZ	C3-C4-C5-C6
46	J	201	3PE	C35-C36-C37-C38
46	N	401	3PE	C29-C2A-C2B-C2C
46	N	403	3PE	C25-C26-C27-C28
46	L	702	3PE	C2-C3-O31-C31
46	f	101	3PE	C22-C23-C24-C25
46	g	201	3PE	C39-C3A-C3B-C3C
53	H	401	CDL	C17-C18-C19-C20
45	B	204	PC1	C2B-C2C-C2D-C2E
53	P	503	CDL	OA5-CA3-CA4-OA6
53	P	503	CDL	OB5-CB3-CB4-OB6
46	Z	202	3PE	C35-C36-C37-C38
47	A	206	PLC	O2-C'-C1'-C2'
53	d	204	CDL	CA7-C31-C32-C33
53	M	607	CDL	C11-C12-C13-C14
46	P	502	3PE	C2-C1-O11-P
46	Z	204	3PE	C2-C1-O11-P
49	D	501	U10	C50-C49-C51-C52
45	B	204	PC1	C36-C37-C38-C39
46	Y	202	3PE	O11-C1-C2-C3
46	b	101	3PE	C39-C3A-C3B-C3C
45	I	203	PC1	C31-C32-C33-C34
46	Y	203	3PE	O21-C2-C3-O31
46	Y	206	3PE	O21-C2-C3-O31
46	m	201	3PE	C38-C39-C3A-C3B
46	N	401	3PE	C23-C24-C25-C26
53	H	401	CDL	C13-C14-C15-C16
53	h	201	CDL	C76-C77-C78-C79
45	m	202	PC1	C2C-C2D-C2E-C2F
46	I	204	3PE	C25-C26-C27-C28
46	a	101	3PE	C37-C38-C39-C3A
49	D	501	U10	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
49	D	501	U10	C48-C49-C51-C52
46	Y	204	3PE	C3D-C3E-C3F-C3G
47	O	403	PLC	C6'-C7'-C8'-C9'
53	r	201	CDL	C53-C54-C55-C56
47	J	203	PLC	C1B-C2B-C3B-C4B
46	P	505	3PE	C24-C25-C26-C27
46	N	403	3PE	C2-C1-O11-P
46	Y	209	3PE	C2-C1-O11-P
46	b	102	3PE	C2-C1-O11-P
53	L	701	CDL	CB4-CB3-OB5-PB2
46	M	604	3PE	C2D-C2E-C2F-C2G
46	J	204	3PE	O32-C31-O31-C3
45	g	203	PC1	C22-C21-O21-C2
45	h	202	PC1	C22-C23-C24-C25
46	a	101	3PE	C21-C22-C23-C24
46	J	204	3PE	O21-C21-C22-C23
46	P	502	3PE	C36-C37-C38-C39
45	A	203	PC1	C1-C2-C3-O31
45	M	606	PC1	C1-C2-C3-O31
46	A	204	3PE	C1-C2-C3-O31
53	L	701	CDL	CA5-C11-C12-C13
45	h	202	PC1	C2D-C2E-C2F-C2G
53	L	701	CDL	C63-C64-C65-C66
46	J	202	3PE	O11-C1-C2-O21
45	H	404	PC1	C33-C34-C35-C36
46	r	202	3PE	C24-C25-C26-C27
59	i	201	CHD	C22-C23-C24-O25
45	B	202	PC1	C22-C23-C24-C25
46	Y	205	3PE	C3D-C3E-C3F-C3G
53	M	607	CDL	C51-C52-C53-C54
47	P	504	PLC	C4-C5-N-C6
47	P	504	PLC	C4-C5-N-C7
46	M	604	3PE	C38-C39-C3A-C3B
46	M	603	3PE	C36-C37-C38-C39
46	M	604	3PE	C32-C33-C34-C35
46	f	101	3PE	C38-C39-C3A-C3B
46	b	102	3PE	O11-C1-C2-C3
46	Y	209	3PE	C28-C29-C2A-C2B
46	m	203	3PE	C24-C25-C26-C27
46	Y	203	3PE	C25-C26-C27-C28
45	B	204	PC1	C2-C1-O11-P
46	f	101	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
46	m	203	3PE	C28-C29-C2A-C2B
46	m	203	3PE	C29-C2A-C2B-C2C
53	H	401	CDL	C11-C12-C13-C14
47	g	202	PLC	C8'-C9'-CA'-CB'
45	I	203	PC1	C3B-C3C-C3D-C3E
46	L	702	3PE	C23-C24-C25-C26
45	B	202	PC1	C28-C29-C2A-C2B
49	D	501	U10	C29-C31-C32-C33
53	M	607	CDL	C76-C77-C78-C79
53	N	402	CDL	C37-C38-C39-C40
46	J	204	3PE	C34-C35-C36-C37
53	h	201	CDL	C16-C17-C18-C19
47	B	203	PLC	C3'-C4'-C5'-C6'
46	Y	207	3PE	C35-C36-C37-C38
45	A	201	PC1	C11-C12-N-C14
45	d	202	PC1	C11-C12-N-C15
47	P	504	PLC	C4-C5-N-C8
45	d	202	PC1	C3B-C3C-C3D-C3E
46	M	603	3PE	C3A-C3B-C3C-C3D
53	d	203	CDL	C37-C38-C39-C40
53	r	201	CDL	C17-C18-C19-C20
46	N	401	3PE	O21-C21-C22-C23
53	L	701	CDL	C56-C57-C58-C59
53	d	204	CDL	CA5-C11-C12-C13
53	h	201	CDL	CB3-CB4-OB6-CB5
45	Z	201	PC1	C34-C35-C36-C37
46	Y	203	3PE	C32-C33-C34-C35
53	H	401	CDL	C71-C72-C73-C74
53	H	401	CDL	C37-C38-C39-C40
53	h	201	CDL	C11-C12-C13-C14
46	Y	207	3PE	C36-C37-C38-C39
46	d	201	3PE	C22-C23-C24-C25
45	m	202	PC1	C38-C39-C3A-C3B
46	L	702	3PE	C27-C28-C29-C2A
53	d	203	CDL	OA7-CA5-OA6-CA4
45	d	202	PC1	C11-C12-N-C14
46	Y	206	3PE	C1-C2-C3-O31
47	g	202	PLC	C1-C2-C3-O3
53	P	503	CDL	CA3-CA4-CA6-OA8
46	M	605	3PE	C2B-C2C-C2D-C2E
46	q	202	3PE	C39-C3A-C3B-C3C
45	I	203	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
46	N	403	3PE	C34-C35-C36-C37
45	B	202	PC1	C36-C37-C38-C39
47	A	206	PLC	O'-C'-C1'-C2'
46	Y	203	3PE	C12-C11-O13-P
58	U	101	EHZ	C15-C16-C17-C18
53	M	607	CDL	C36-C37-C38-C39
46	N	403	3PE	C27-C28-C29-C2A
53	M	607	CDL	C12-C11-CA5-OA6
45	g	203	PC1	C27-C28-C29-C2A
46	Y	201	3PE	C33-C34-C35-C36
53	r	201	CDL	C11-C12-C13-C14
46	M	605	3PE	O21-C2-C3-O31
47	Z	203	PLC	C7B-C8B-C9B-CAA
45	B	202	PC1	O31-C31-C32-C33
47	Y	208	PLC	C2B-C1B-CB-O3
53	d	204	CDL	OB5-CB3-CB4-CB6
46	P	505	3PE	C35-C36-C37-C38
45	A	201	PC1	C11-C12-N-C13
53	M	607	CDL	C80-C81-C82-C83
53	P	503	CDL	C12-C11-CA5-OA6
46	J	204	3PE	C35-C36-C37-C38
53	d	203	CDL	C75-C76-C77-C78
45	Z	201	PC1	C36-C37-C38-C39
46	Y	204	3PE	C35-C36-C37-C38
46	J	204	3PE	C37-C38-C39-C3A
53	H	401	CDL	C62-C63-C64-C65
46	f	101	3PE	C3F-C3G-C3H-C3I
45	H	402	PC1	O21-C21-C22-C23
46	b	102	3PE	O31-C31-C32-C33
45	A	202	PC1	O13-C11-C12-N
47	P	504	PLC	O4P-C4-C5-N
57	P	501	NDP	PN-O3-PA-O1A
45	h	202	PC1	C2B-C2C-C2D-C2E
53	d	204	CDL	C81-C82-C83-C84
46	Y	203	3PE	C39-C3A-C3B-C3C
45	q	201	PC1	O31-C31-C32-C33
46	g	201	3PE	O21-C21-C22-C23
45	H	403	PC1	C22-C23-C24-C25
46	M	604	3PE	C2E-C2F-C2G-C2H
53	h	201	CDL	C38-C39-C40-C41
46	Y	209	3PE	C37-C38-C39-C3A
53	N	402	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
58	T	101	EHZ	C2-C1-C21-C22
45	A	201	PC1	C11-C12-N-C15
46	b	101	3PE	C36-C37-C38-C39
53	d	204	CDL	C52-C51-CB5-OB6
46	M	604	3PE	O11-C1-C2-O21
49	D	501	U10	C45-C44-C46-C47
45	H	402	PC1	C31-C32-C33-C34
53	P	503	CDL	C72-C71-CB7-OB8
46	M	603	3PE	C29-C2A-C2B-C2C
47	B	203	PLC	O'-C'-C1'-C2'
53	M	607	CDL	OB9-CB7-OB8-CB6
45	g	203	PC1	C2A-C2B-C2C-C2D
46	b	102	3PE	C35-C36-C37-C38
47	L	703	PLC	O2-C'-C1'-C2'
46	m	203	3PE	C27-C28-C29-C2A
46	Y	203	3PE	C22-C23-C24-C25
45	m	202	PC1	C2B-C2C-C2D-C2E
46	Z	202	3PE	C3B-C3C-C3D-C3E
53	N	402	CDL	C72-C71-CB7-OB8
53	r	201	CDL	C32-C31-CA7-OA8
45	d	202	PC1	C11-C12-N-C13
46	P	505	3PE	C25-C26-C27-C28
53	M	607	CDL	C24-C25-C26-C27
46	N	403	3PE	C2D-C2E-C2F-C2G
46	P	505	3PE	O21-C21-C22-C23
46	f	101	3PE	O21-C21-C22-C23
47	M	608	PLC	O2-C2-C3-O3
49	D	501	U10	C51-C52-C53-C54
53	d	204	CDL	C60-C61-C62-C63
45	d	202	PC1	C3A-C3B-C3C-C3D
53	d	204	CDL	C32-C31-CA7-OA9
46	N	401	3PE	C2F-C2G-C2H-C2I
53	M	607	CDL	C71-CB7-OB8-CB6
46	L	702	3PE	O21-C21-C22-C23
46	Y	204	3PE	O31-C31-C32-C33
47	A	206	PLC	C2B-C1B-CB-O3
45	L	704	PC1	C27-C28-C29-C2A
45	q	201	PC1	C29-C2A-C2B-C2C
46	P	505	3PE	C36-C37-C38-C39
45	B	202	PC1	C24-C25-C26-C27
46	M	604	3PE	C3D-C3E-C3F-C3G
58	T	101	EHZ	C19-C17-C20-O6

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Mol	Chain	Res	Type	Atoms
46	M	604	3PE	O21-C21-C22-C23
46	Y	203	3PE	C32-C31-O31-C3
45	A	203	PC1	C3-C2-O21-C21
46	L	702	3PE	C3-C2-O21-C21
46	Y	203	3PE	C3-C2-O21-C21
46	N	403	3PE	O32-C31-O31-C3
57	P	501	NDP	O4D-C4D-C5D-O5D
46	I	204	3PE	C2C-C2D-C2E-C2F
46	Y	206	3PE	C33-C34-C35-C36
53	d	203	CDL	C52-C51-CB5-OB6
58	T	101	EHZ	C21-C1-C2-C3
46	Y	203	3PE	O32-C31-O31-C3
46	Y	203	3PE	C2-C1-O11-P
53	d	203	CDL	C1-CA2-OA2-PA1
53	d	204	CDL	C1-CA2-OA2-PA1
46	M	602	3PE	C24-C25-C26-C27
46	g	201	3PE	O22-C21-C22-C23
53	N	402	CDL	C52-C51-CB5-OB7
46	Y	201	3PE	O21-C21-C22-C23
46	Y	205	3PE	O31-C31-C32-C33
46	Y	207	3PE	C23-C24-C25-C26
53	N	402	CDL	C43-C44-C45-C46
46	f	101	3PE	C3D-C3E-C3F-C3G
53	h	201	CDL	C15-C16-C17-C18
46	m	203	3PE	O31-C31-C32-C33
45	q	201	PC1	O32-C31-C32-C33
46	J	204	3PE	C3B-C3C-C3D-C3E
46	L	702	3PE	C21-C22-C23-C24
46	Y	209	3PE	C2A-C2B-C2C-C2D
46	N	403	3PE	C32-C31-O31-C3
46	P	505	3PE	C3F-C3G-C3H-C3I
46	r	202	3PE	C37-C38-C39-C3A
45	I	203	PC1	C11-C12-N-C15
46	Y	206	3PE	C38-C39-C3A-C3B
47	g	202	PLC	C2'-C3'-C4'-C5'
53	P	503	CDL	CB5-C51-C52-C53
46	r	202	3PE	C32-C33-C34-C35
53	P	503	CDL	O1-C1-CA2-OA2
46	L	702	3PE	C35-C36-C37-C38
46	Y	206	3PE	C35-C36-C37-C38
46	b	102	3PE	C38-C39-C3A-C3B
53	M	607	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C56-C57-C58-C59
53	P	503	CDL	C72-C71-CB7-OB9
53	d	204	CDL	C72-C71-CB7-OB8
45	B	202	PC1	O32-C31-C32-C33
53	N	402	CDL	C72-C71-CB7-OB9
53	d	204	CDL	C52-C51-CB5-OB7
46	Y	205	3PE	C26-C27-C28-C29
60	o	201	MYR	C11-C12-C13-C14
53	h	201	CDL	C52-C51-CB5-OB6
46	M	605	3PE	C39-C3A-C3B-C3C
46	P	505	3PE	O22-C21-C22-C23
46	b	102	3PE	O32-C31-C32-C33
46	f	101	3PE	O22-C21-C22-C23
47	A	206	PLC	C2B-C1B-CB-OB
47	L	703	PLC	O'-C'-C1'-C2'
47	Y	208	PLC	C2B-C1B-CB-OB
45	q	201	PC1	C22-C23-C24-C25
46	J	201	3PE	C1-C2-C3-O31
45	m	202	PC1	C28-C29-C2A-C2B
46	Y	204	3PE	O32-C31-C32-C33
53	P	503	CDL	C12-C11-CA5-OA7
53	r	201	CDL	C32-C31-CA7-OA9
46	b	101	3PE	O31-C31-C32-C33
46	d	201	3PE	C26-C27-C28-C29
45	I	203	PC1	C11-C12-N-C13
45	I	203	PC1	C11-C12-N-C14
46	M	604	3PE	O22-C21-C22-C23
46	I	204	3PE	C29-C2A-C2B-C2C
46	Y	207	3PE	O31-C31-C32-C33
46	Y	205	3PE	C2A-C2B-C2C-C2D
53	P	503	CDL	C31-C32-C33-C34
47	L	703	PLC	C5'-C6'-C7'-C8'
46	L	702	3PE	O22-C21-C22-C23
45	A	202	PC1	O31-C31-C32-C33
46	I	204	3PE	O21-C21-C22-C23
53	L	701	CDL	C52-C51-CB5-OB6
45	L	704	PC1	C3D-C3E-C3F-C3G
53	h	201	CDL	C73-C74-C75-C76
46	Y	205	3PE	C2B-C2C-C2D-C2E
53	H	401	CDL	CB7-C71-C72-C73
45	d	202	PC1	O21-C21-C22-C23
46	A	204	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	M	603	3PE	O21-C21-C22-C23
46	Y	204	3PE	O21-C21-C22-C23
46	g	201	3PE	O31-C31-C32-C33
47	O	403	PLC	C2B-C1B-CB-O3
53	d	203	CDL	C11-CA5-OA6-CA4
55	O	401	DGT	PA-O3A-PB-O2B
46	Y	205	3PE	O32-C31-C32-C33
45	H	402	PC1	C27-C28-C29-C2A
53	H	401	CDL	C59-C60-C61-C62
53	d	204	CDL	C36-C37-C38-C39
46	Y	201	3PE	C32-C33-C34-C35
60	o	201	MYR	C3-C4-C5-C6
46	Y	201	3PE	C2F-C2G-C2H-C2I
46	P	502	3PE	C21-C22-C23-C24
46	b	102	3PE	C21-C22-C23-C24
53	h	201	CDL	C52-C51-CB5-OB7

There are no ring outliers.

27 monomers are involved in 59 short contacts:

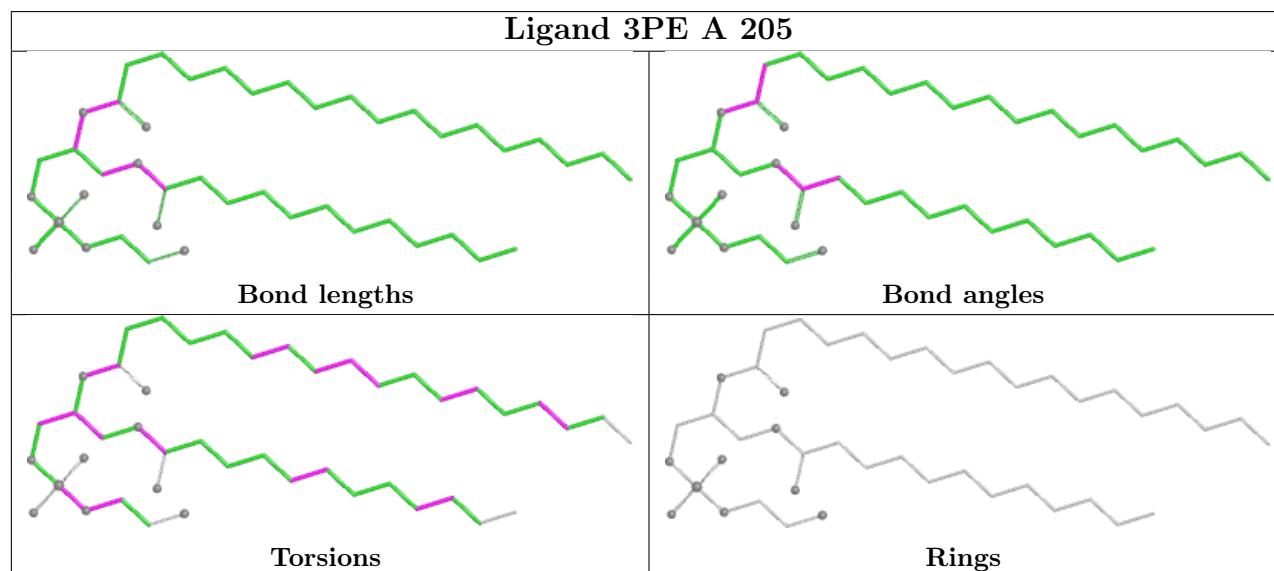
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	g	203	PC1	1	0
46	Y	209	3PE	1	0
45	L	704	PC1	3	0
46	Y	205	3PE	1	0
51	F	501	FMN	1	0
45	H	402	PC1	4	0
45	I	203	PC1	1	0
46	d	201	3PE	1	0
57	P	501	NDP	2	0
45	h	202	PC1	1	0
49	D	501	U10	17	0
53	h	201	CDL	1	0
45	A	202	PC1	2	0
46	Y	203	3PE	3	0
55	O	401	DGT	3	0
45	A	201	PC1	1	0
47	L	703	PLC	1	0
53	P	503	CDL	2	0
53	d	204	CDL	1	0
59	i	201	CHD	6	0
58	U	101	EHZ	1	0

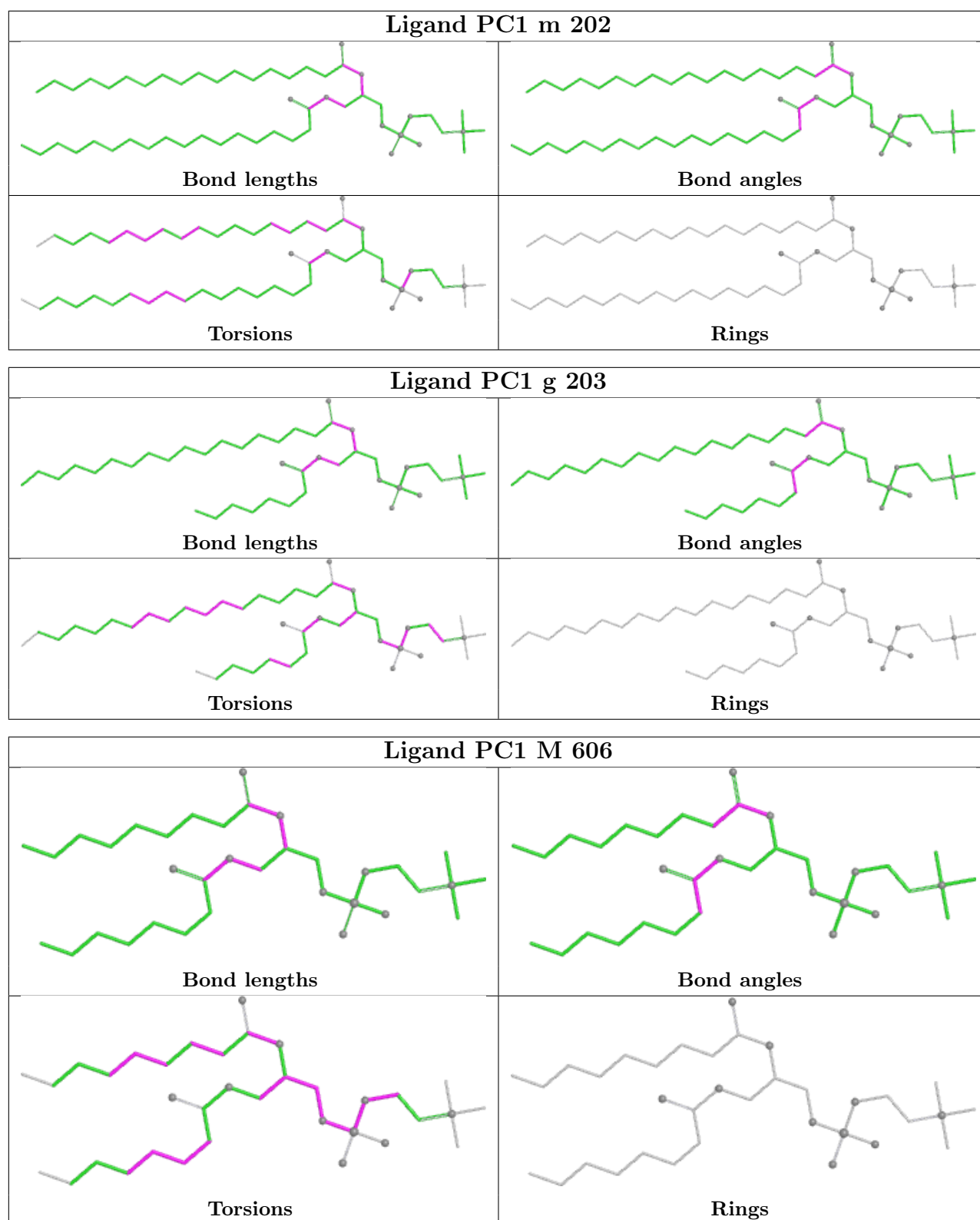
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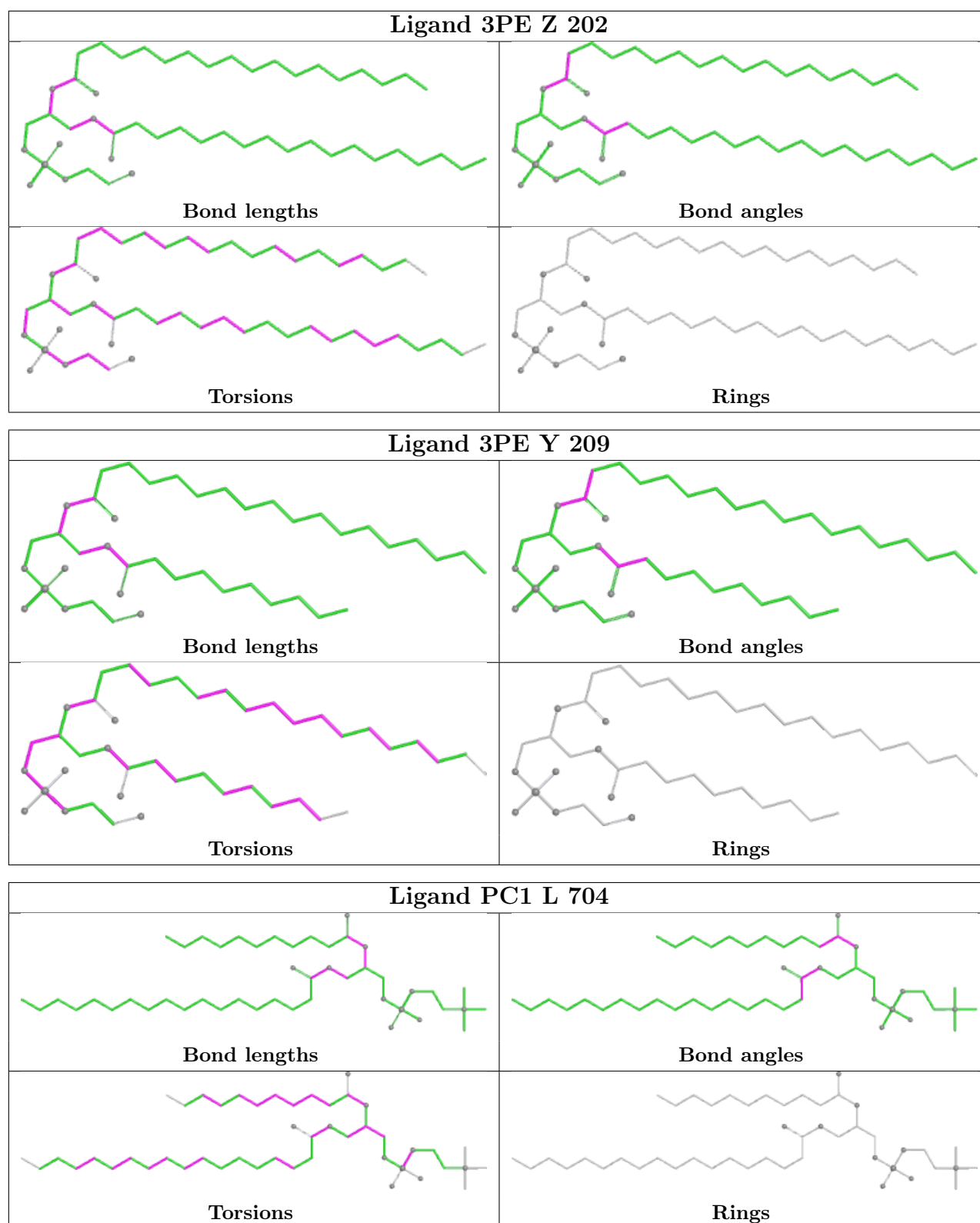
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	N	402	CDL	2	0
47	A	206	PLC	1	0
46	N	403	3PE	1	0
53	M	607	CDL	2	0
47	g	202	PLC	1	0
46	q	202	3PE	1	0

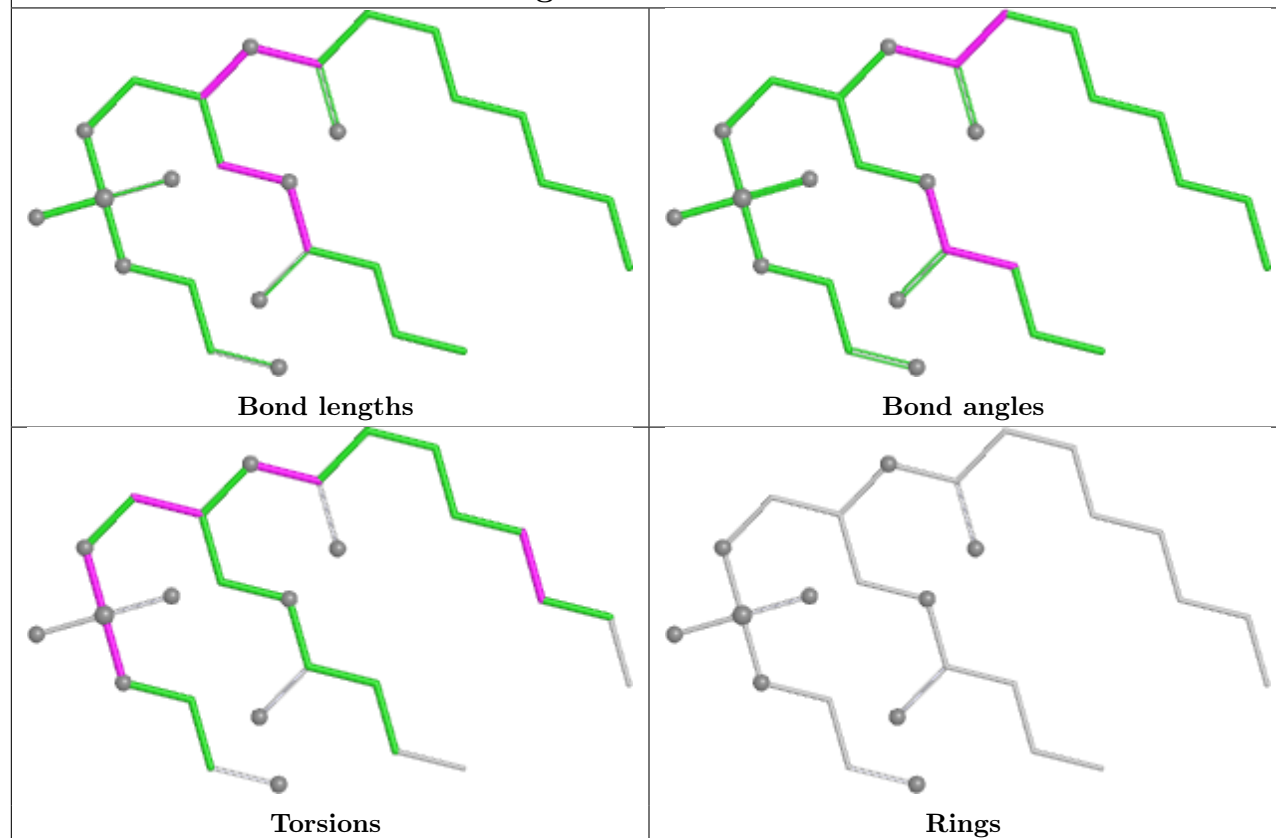
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



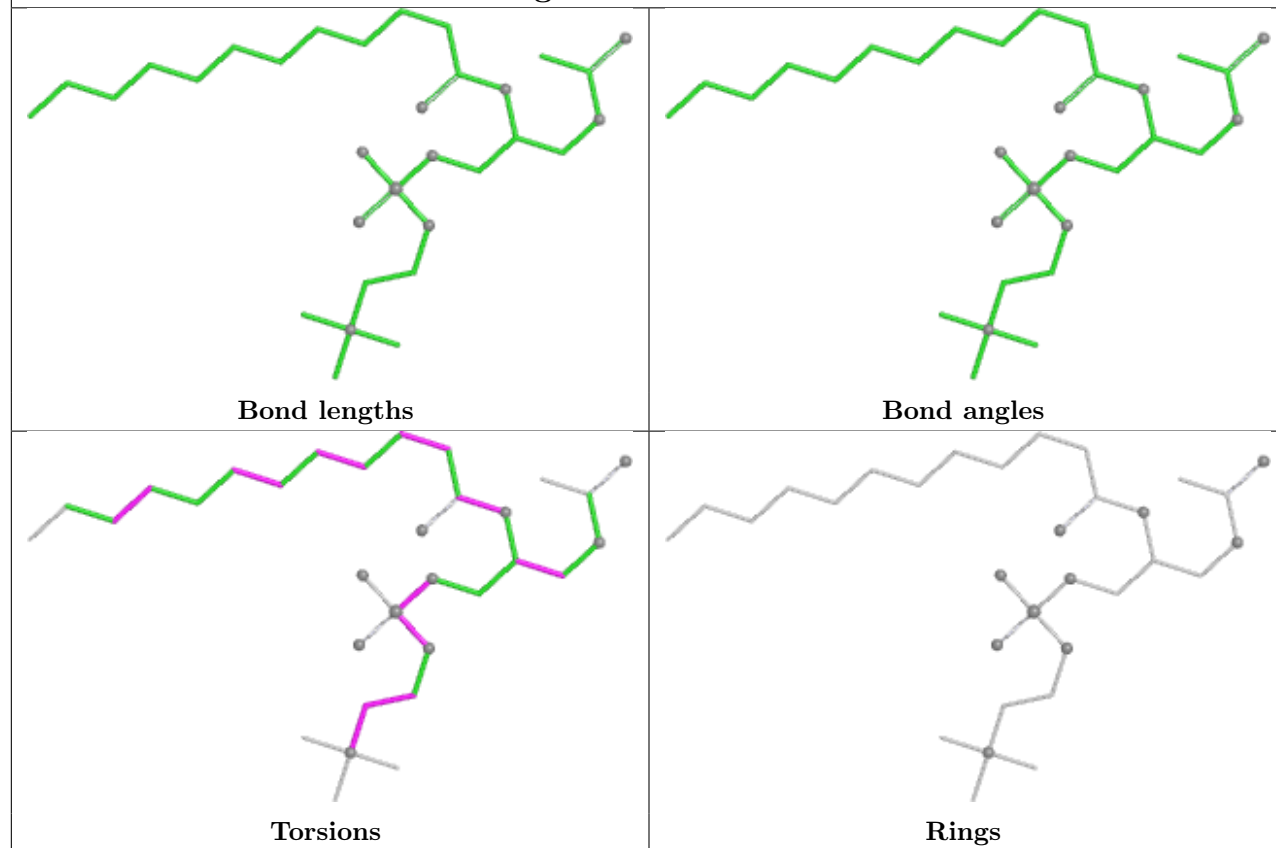


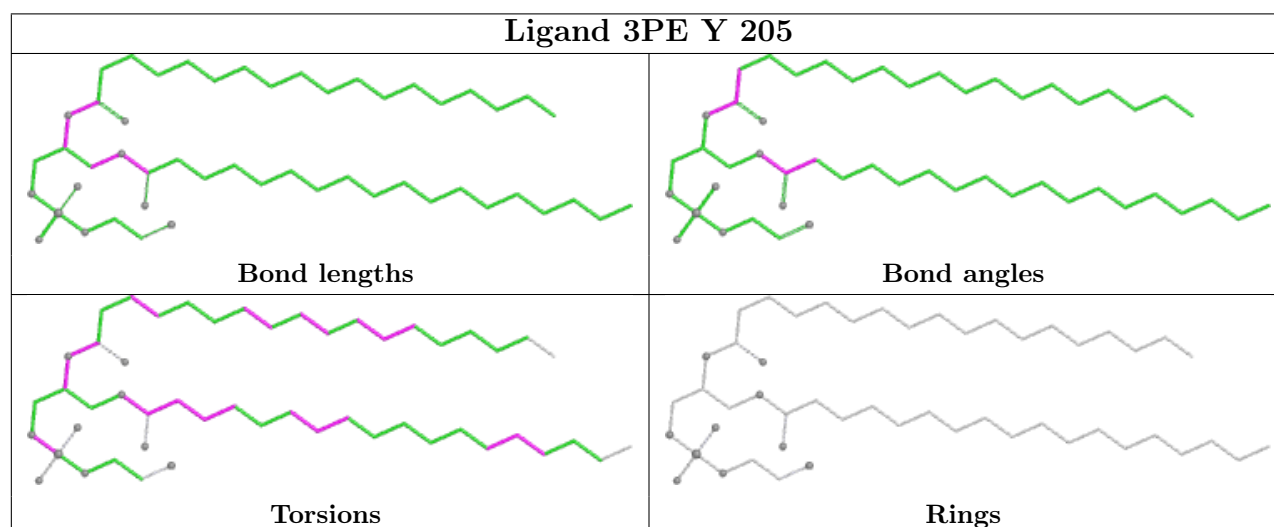
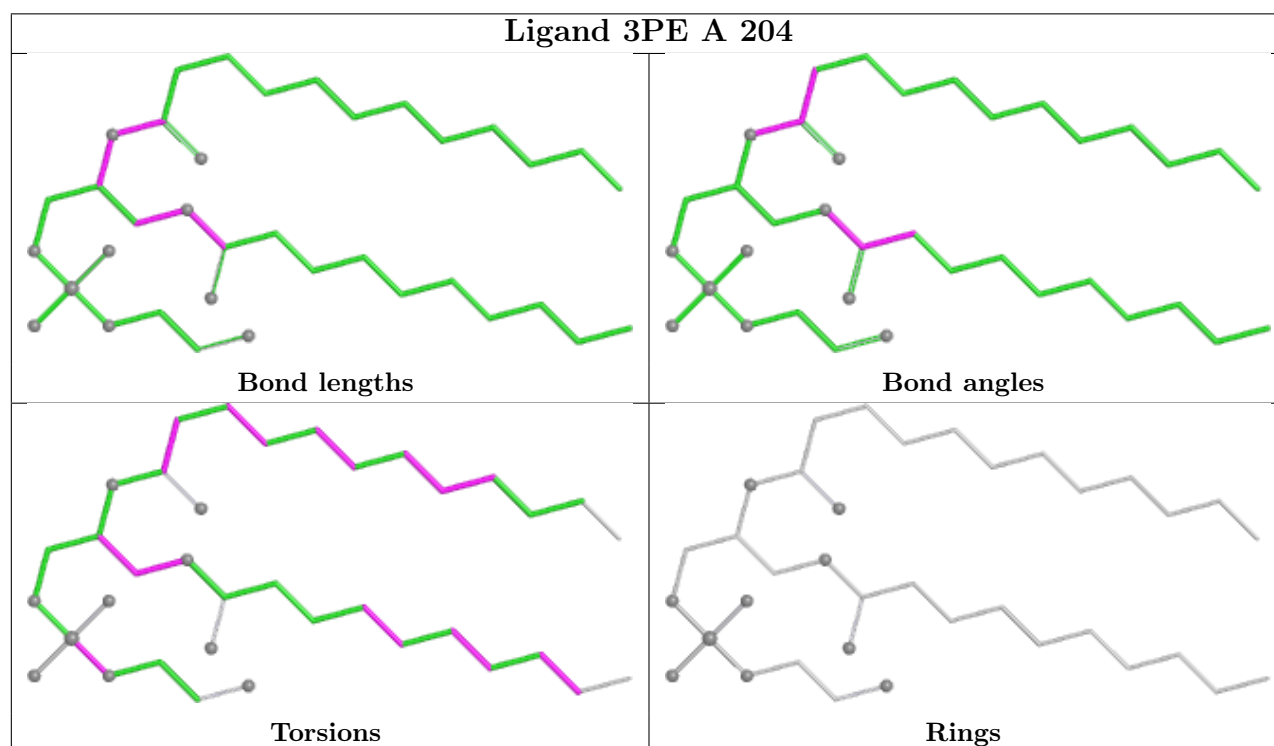
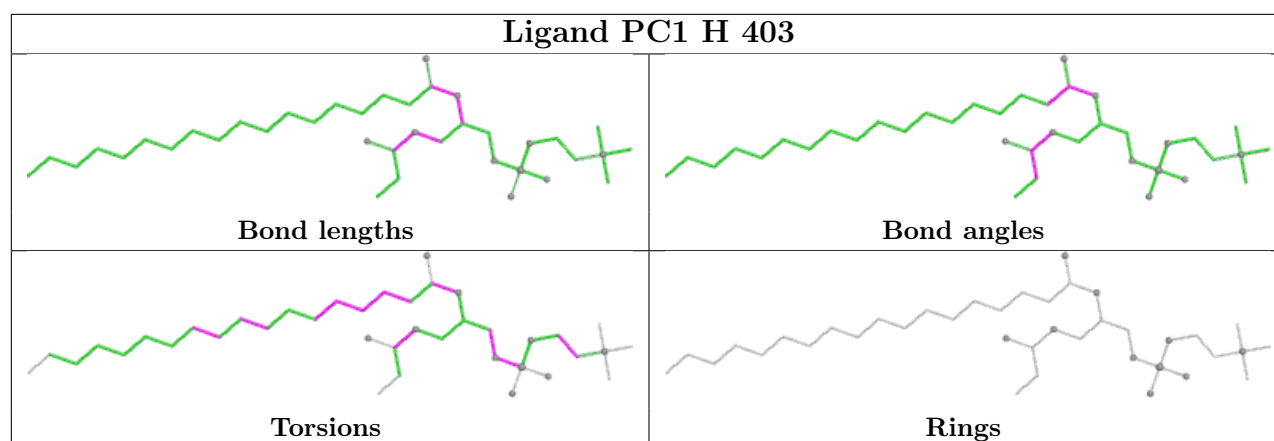


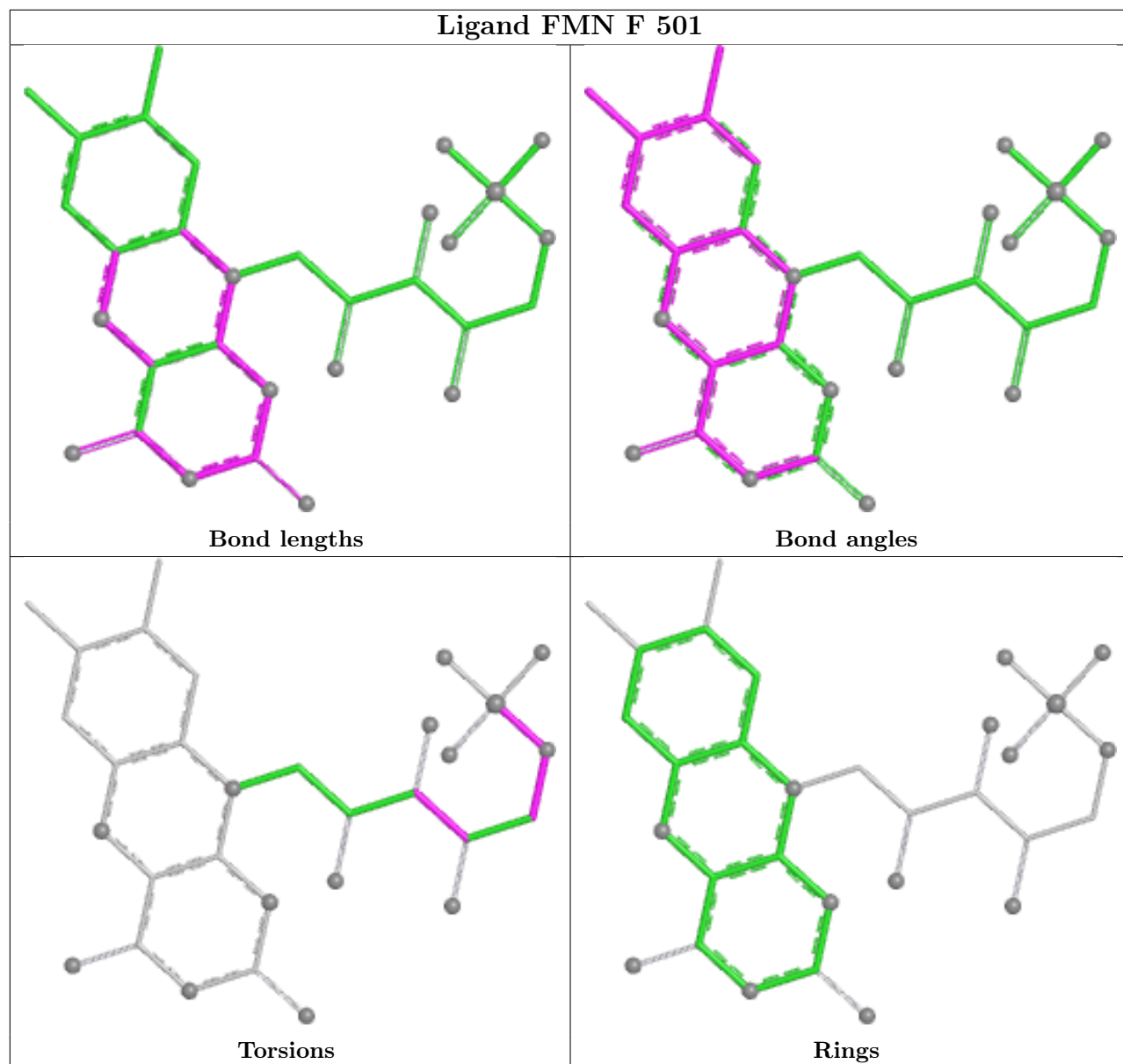
Ligand 3PE Y 202



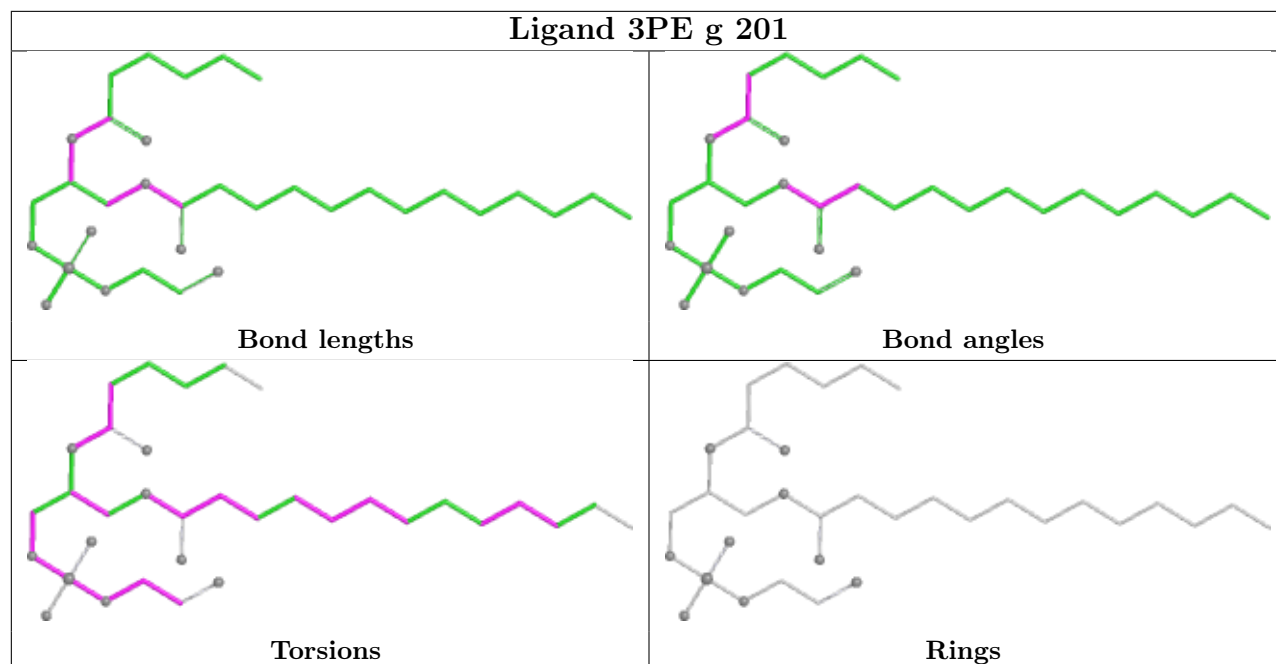
Ligand PLC P 504



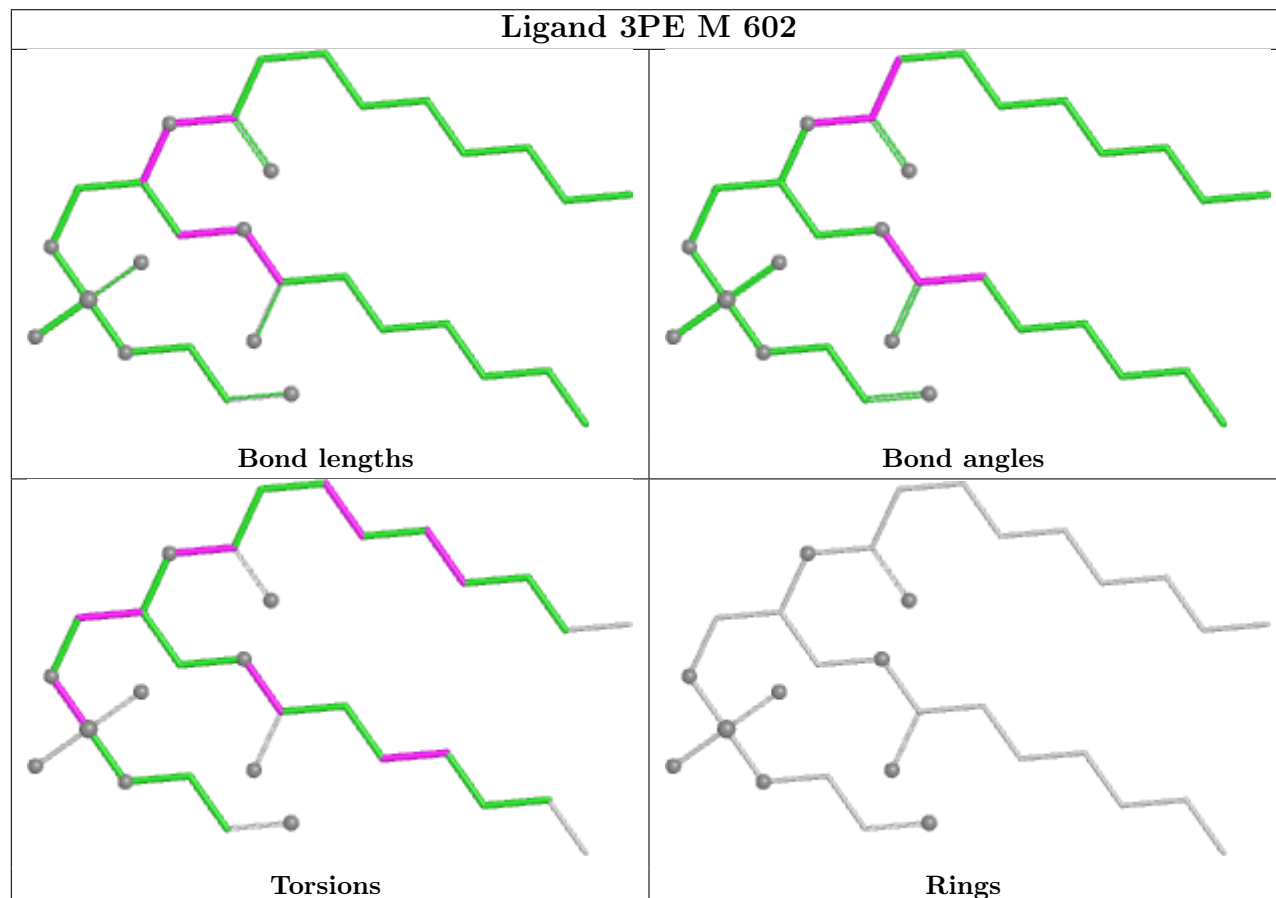


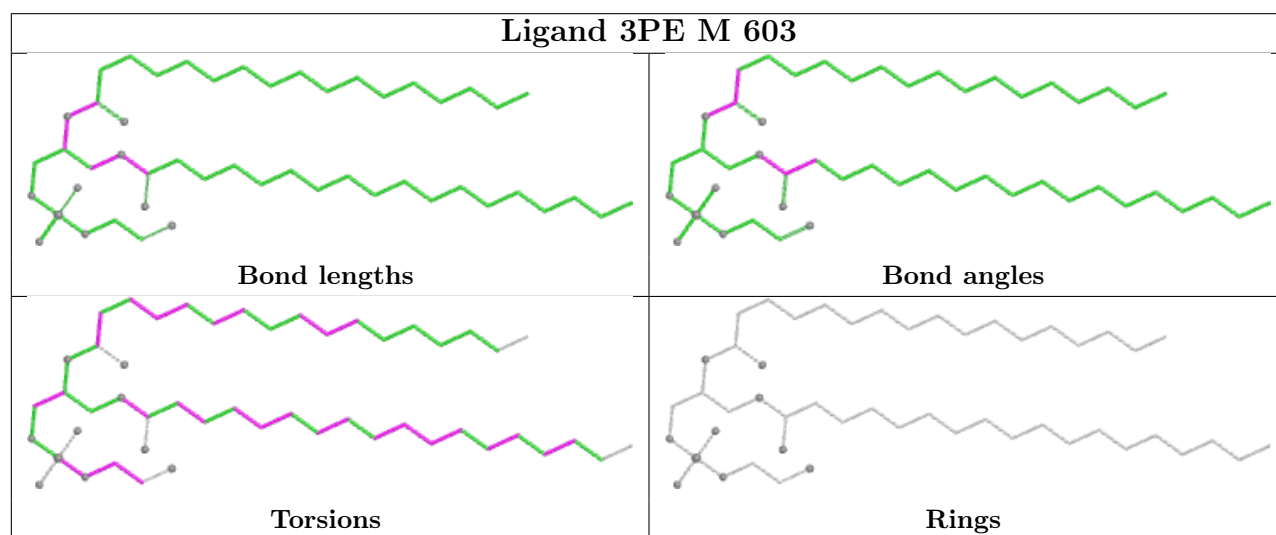
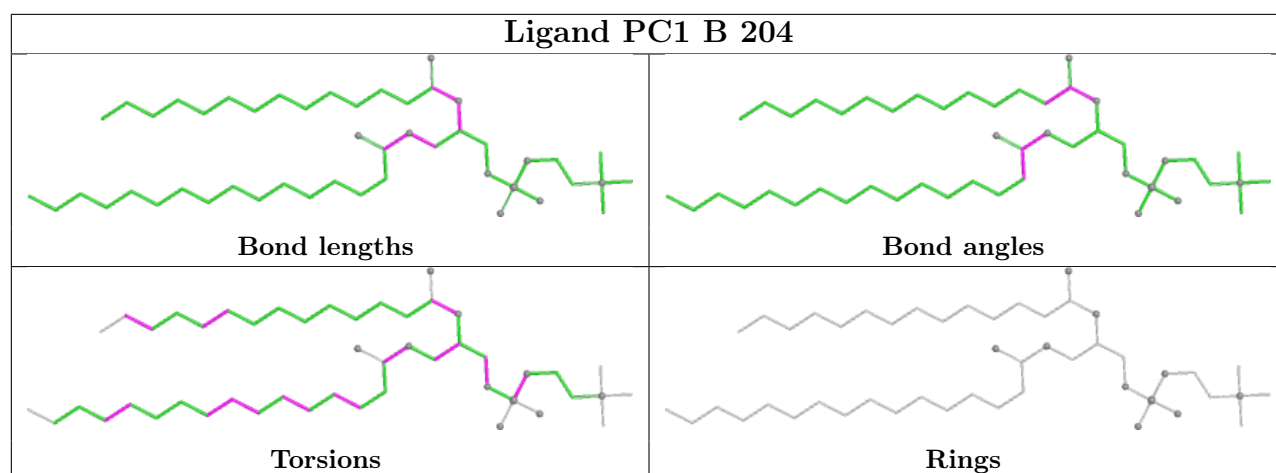


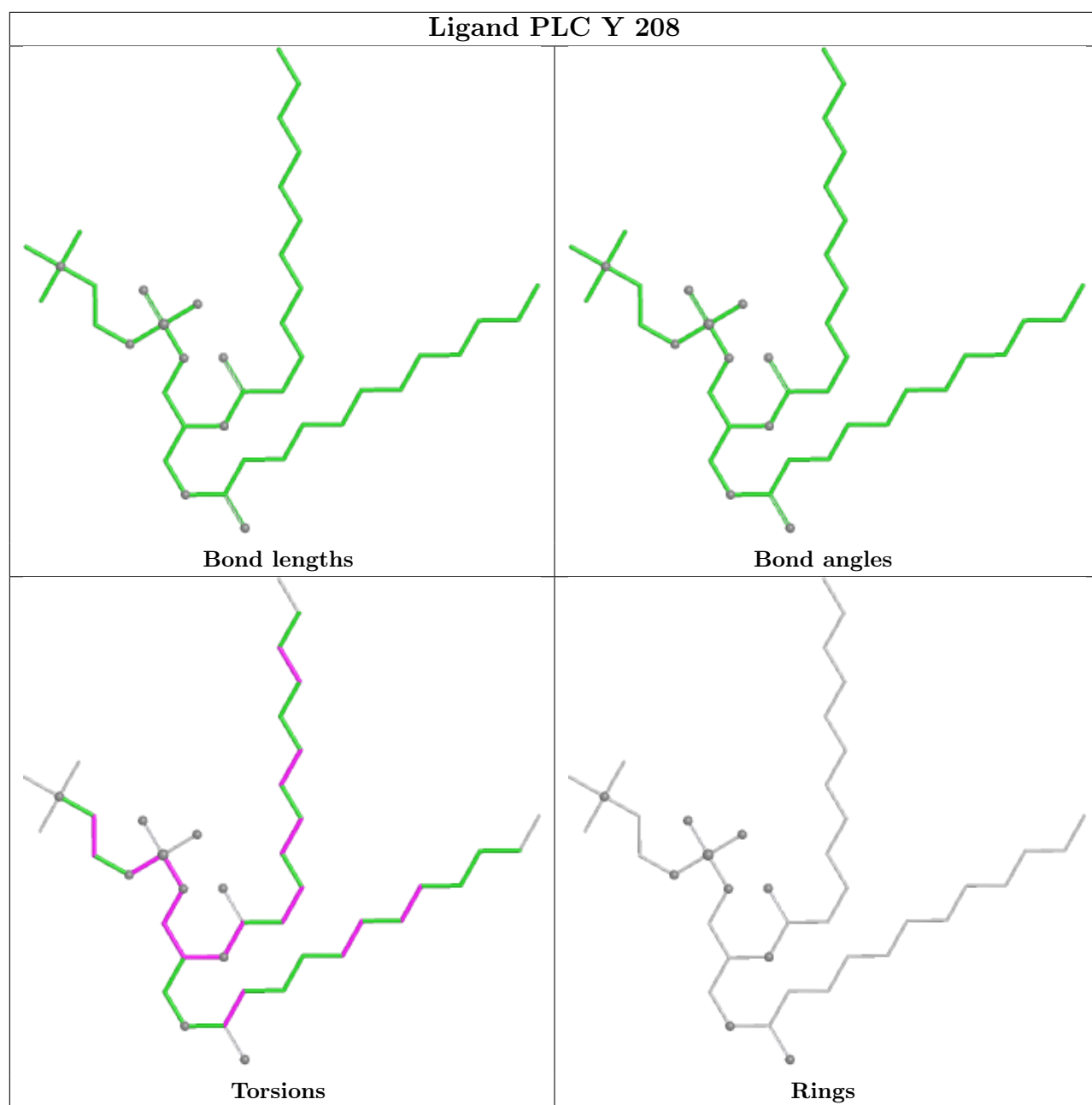
Ligand 3PE g 201

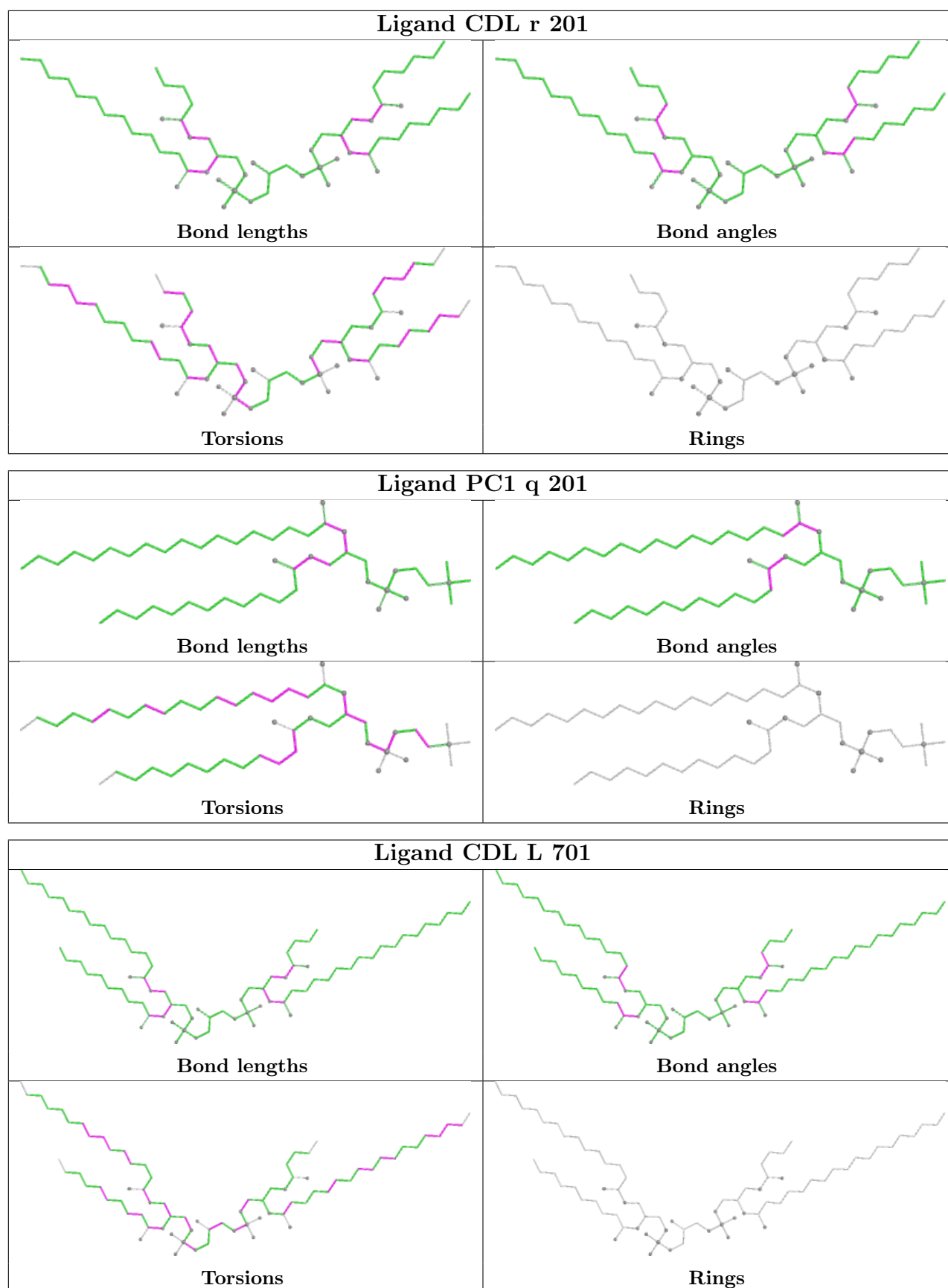


Ligand 3PE M 602

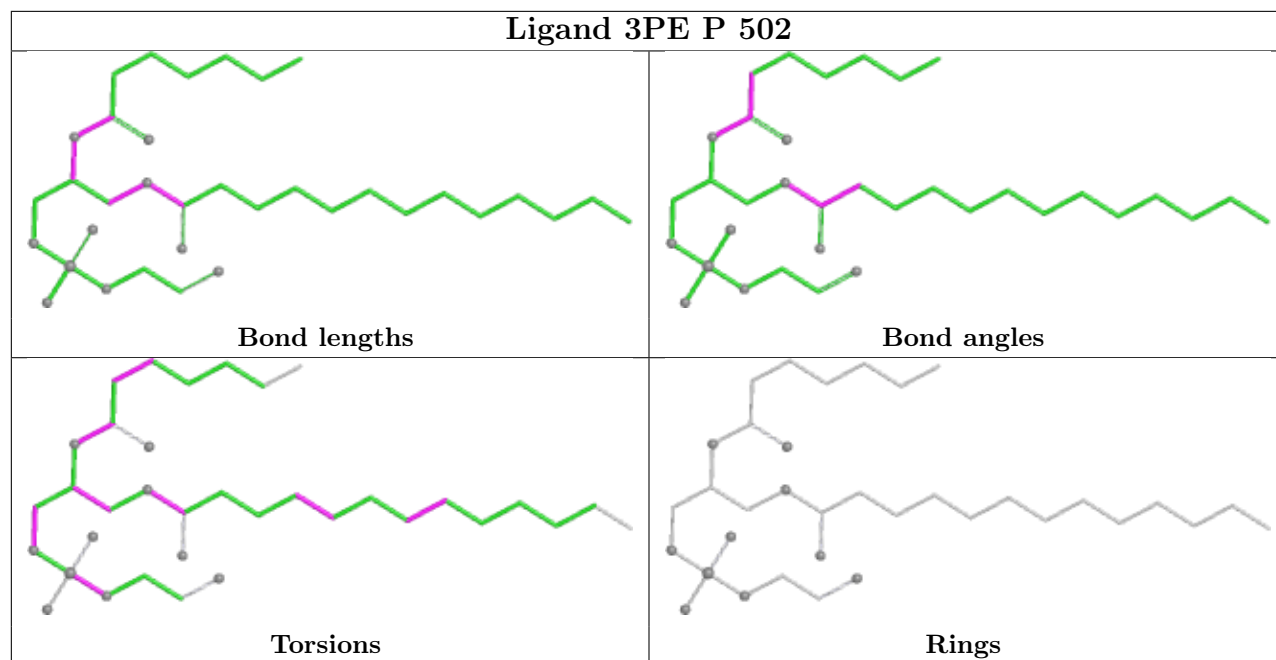




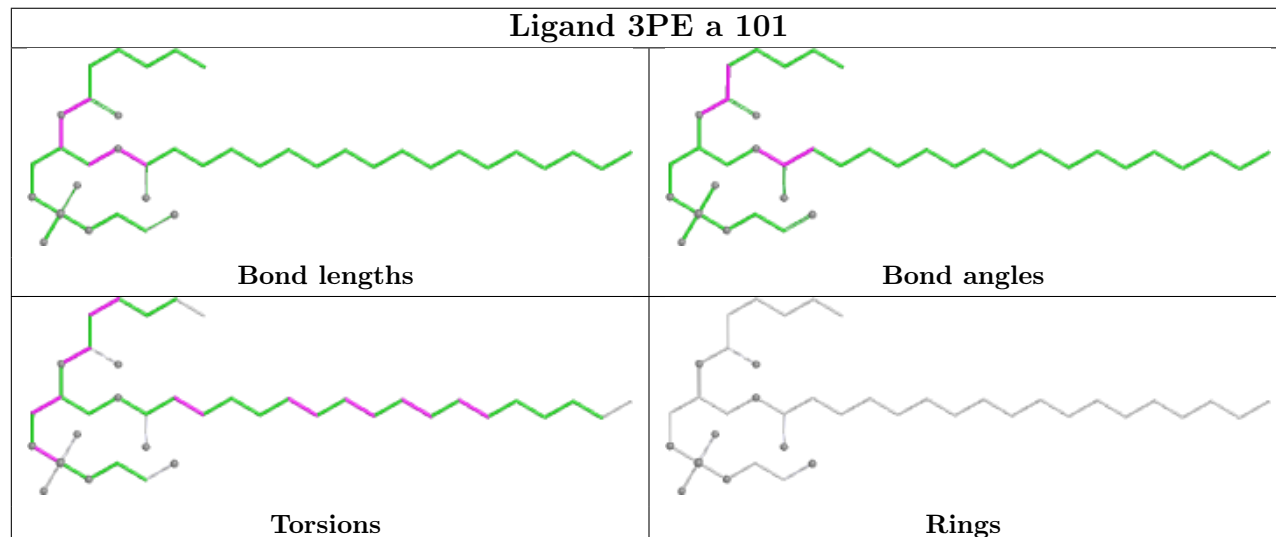




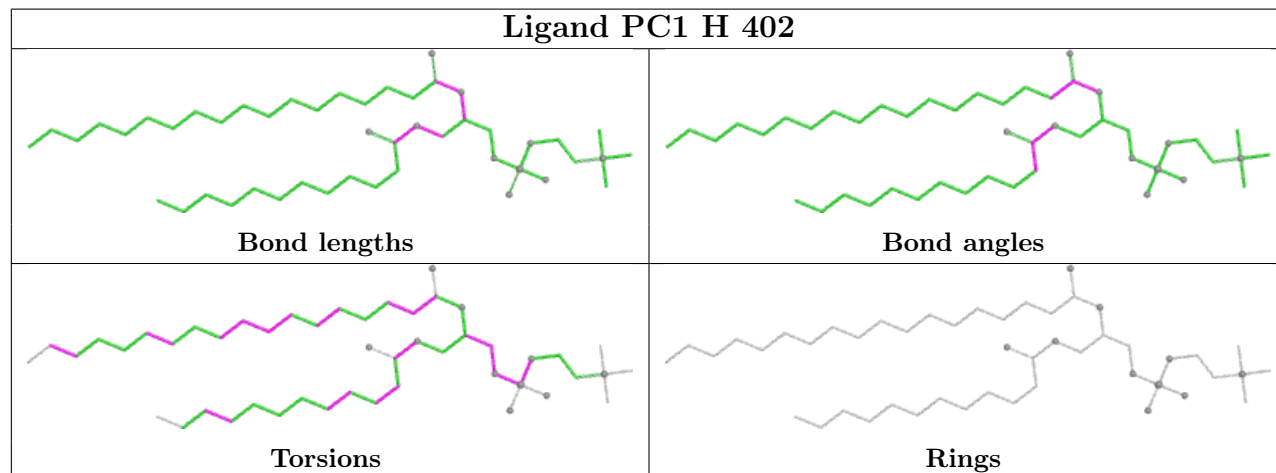
Ligand 3PE P 502

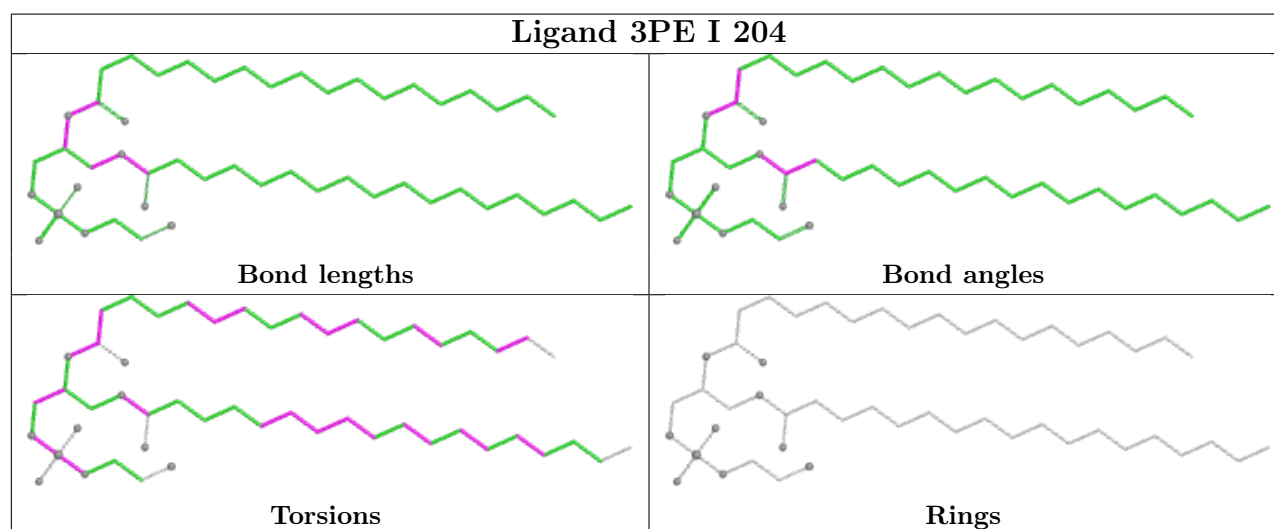
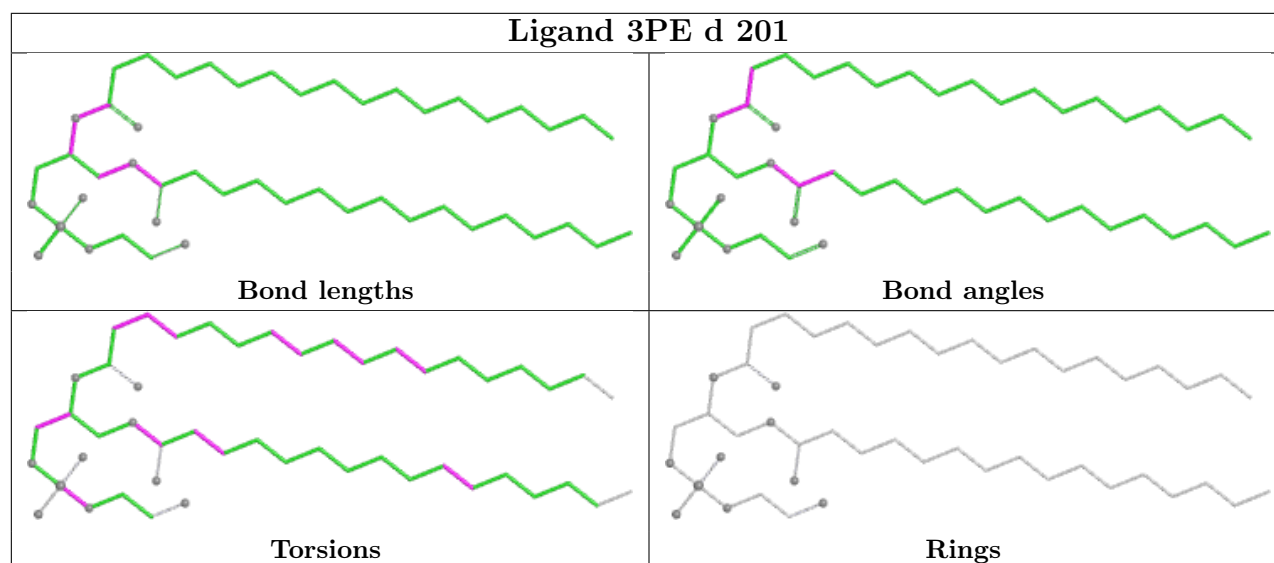
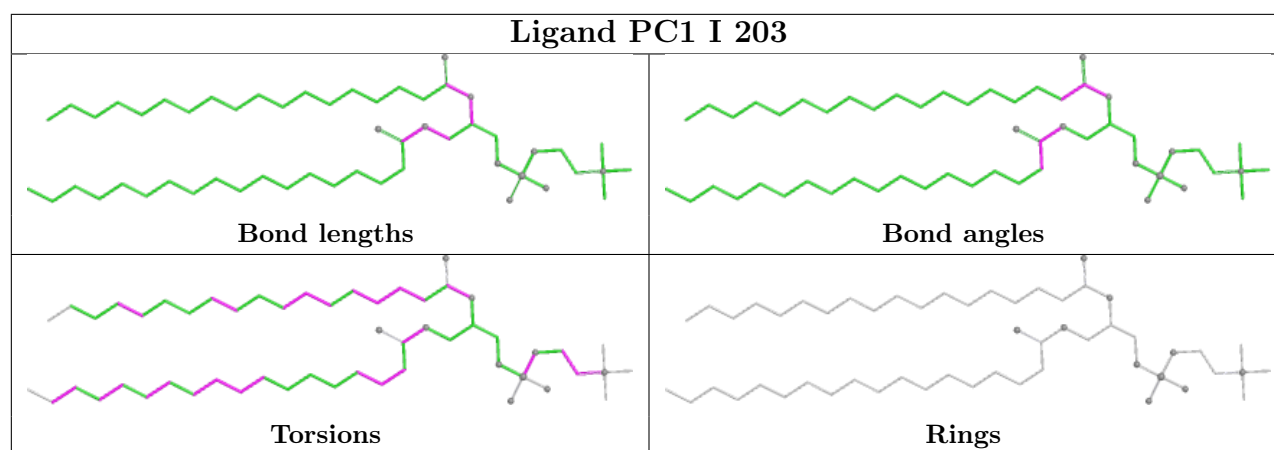


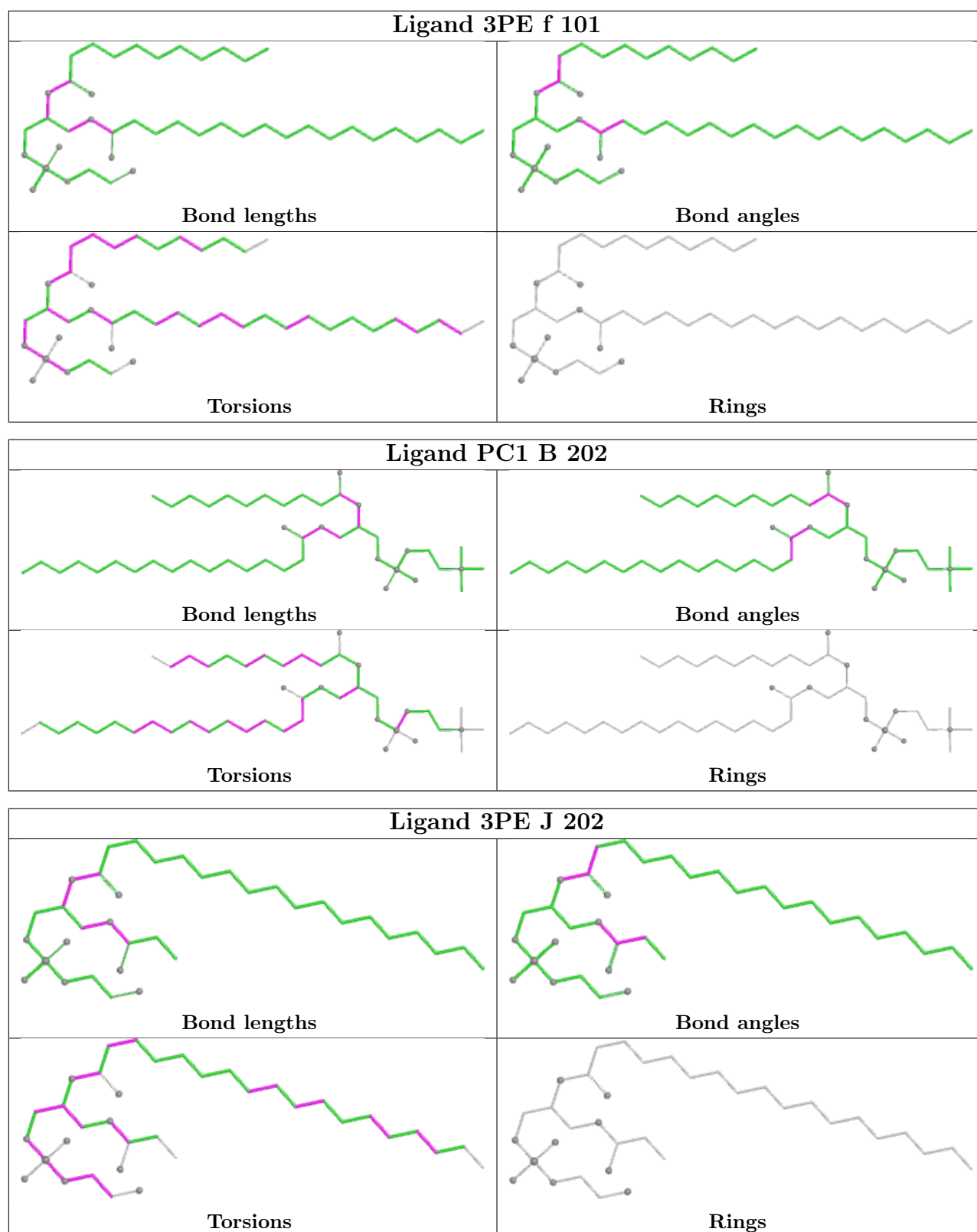
Ligand 3PE a 101

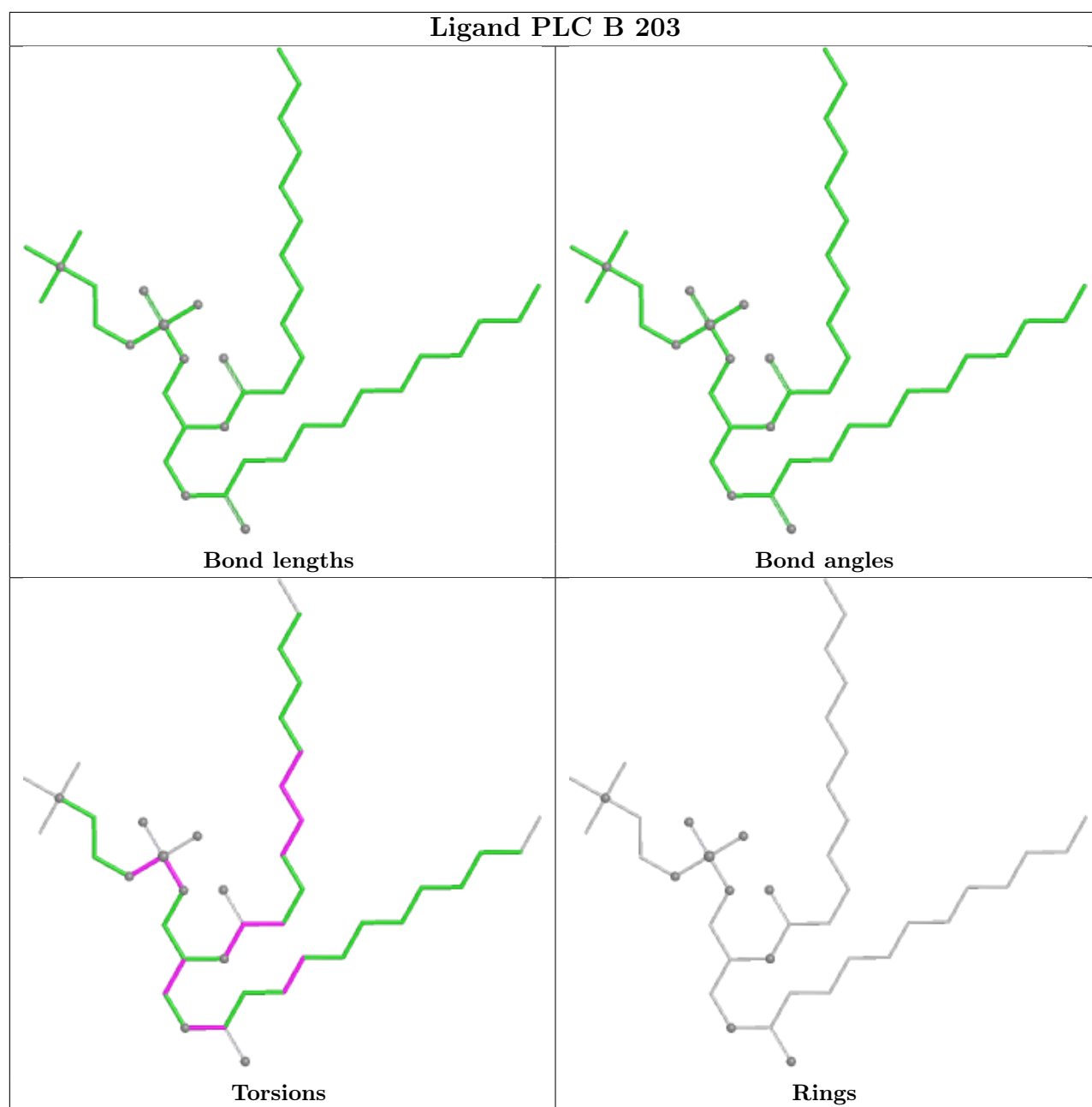


Ligand PC1 H 402

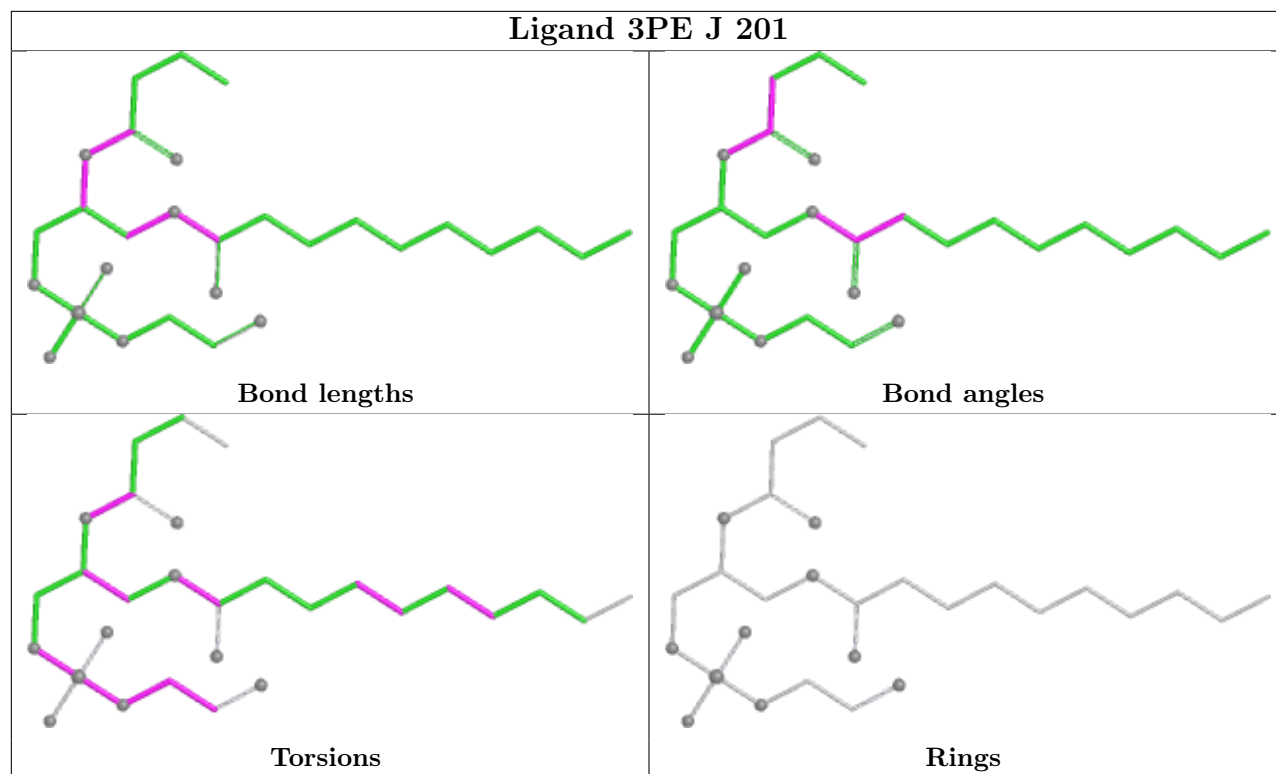




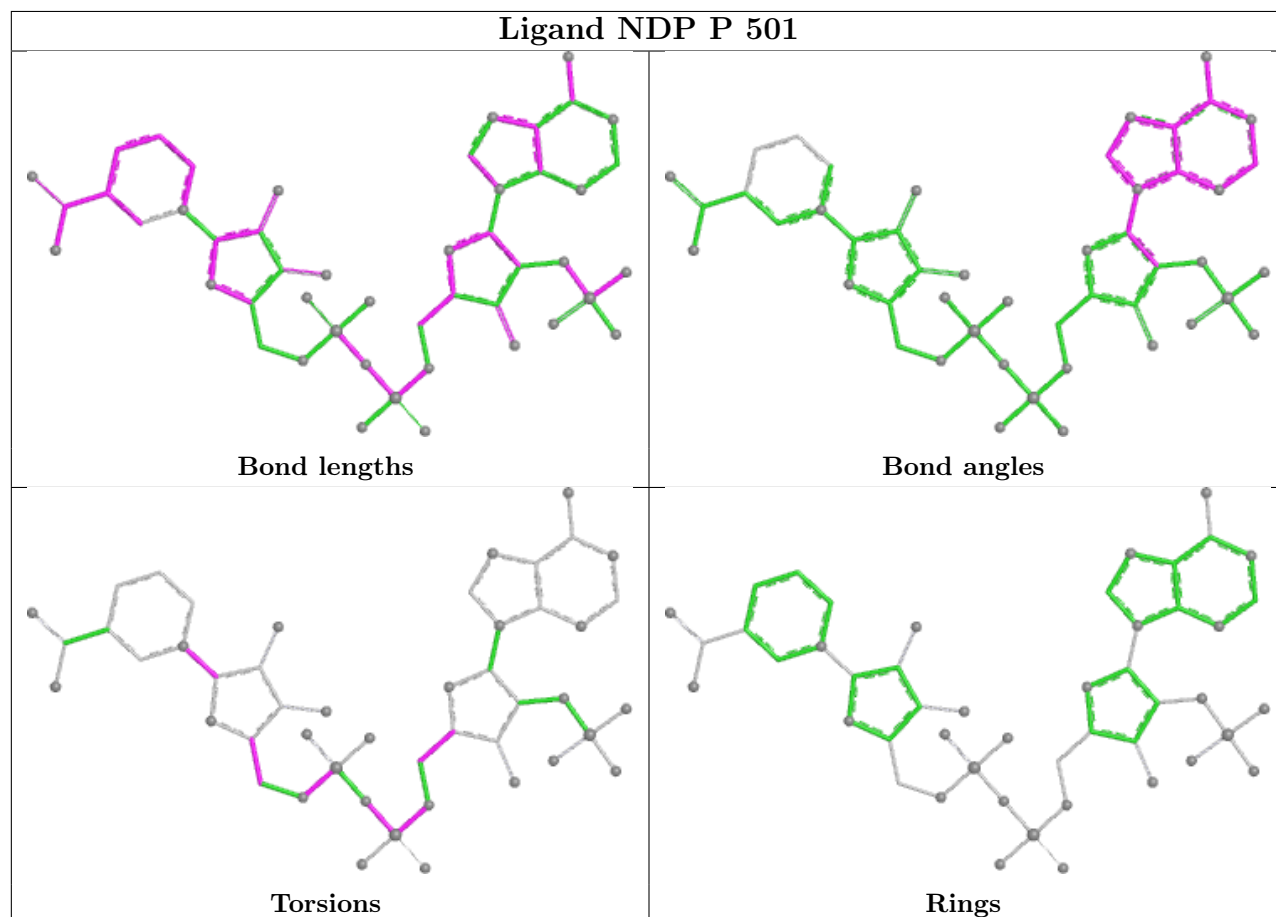


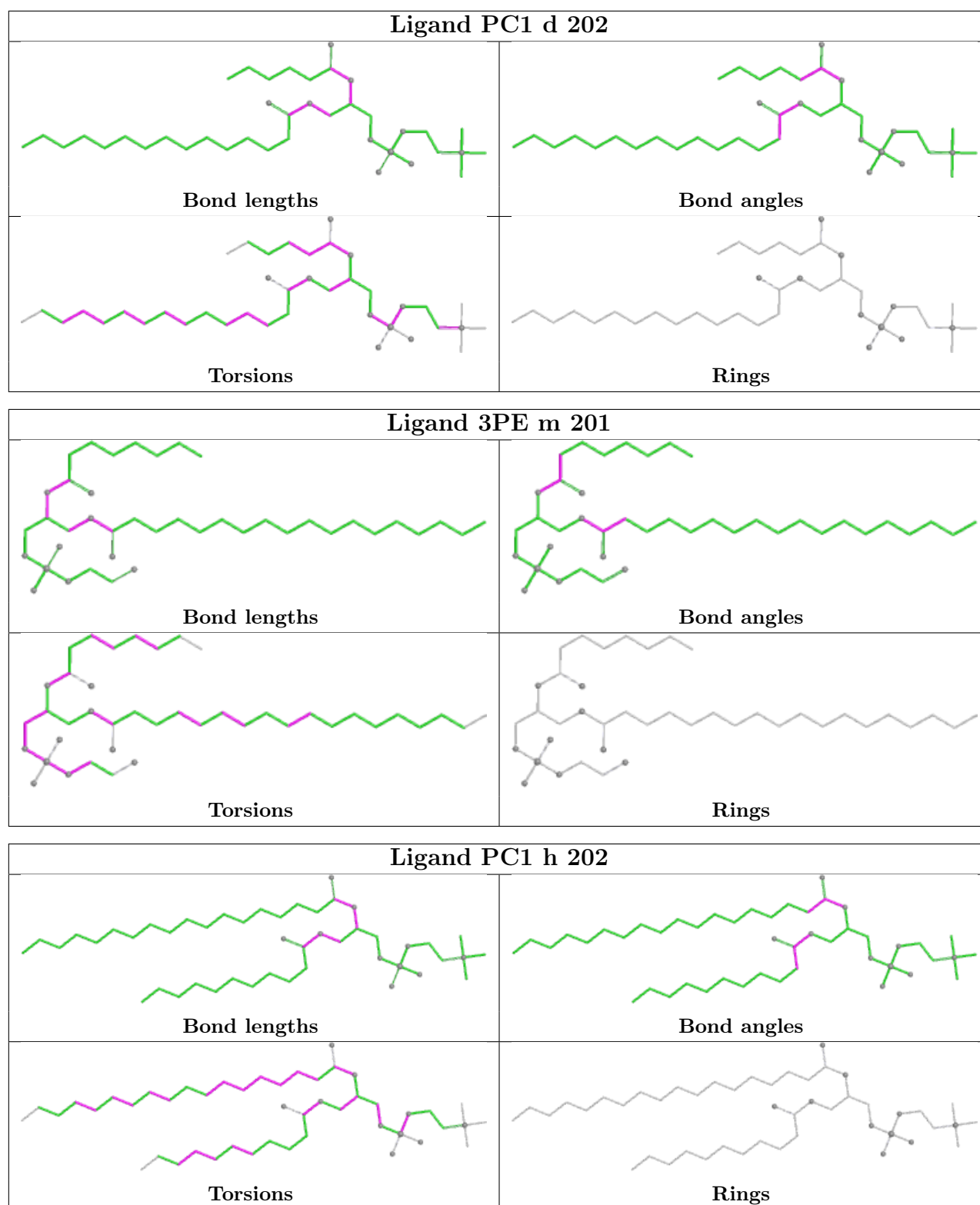


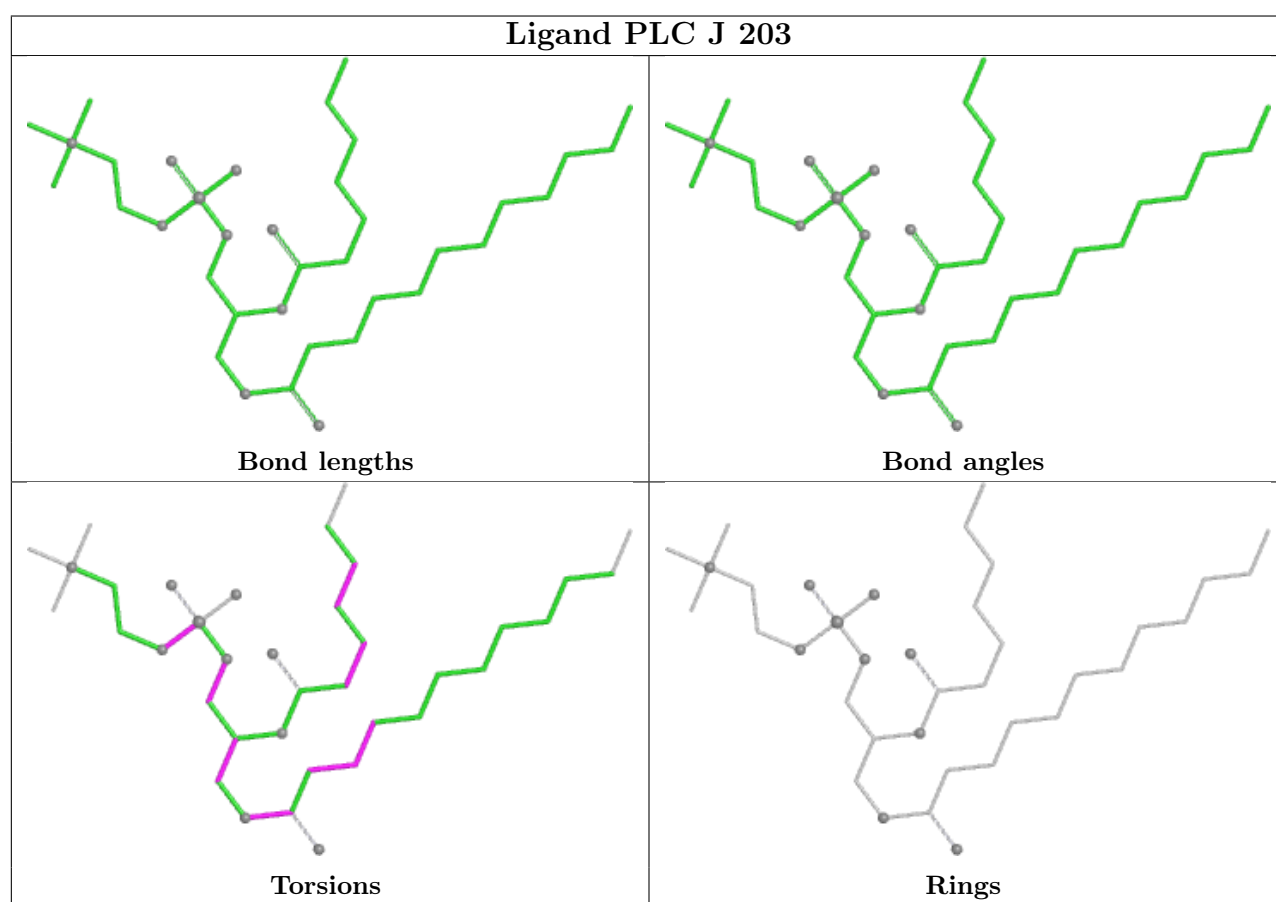
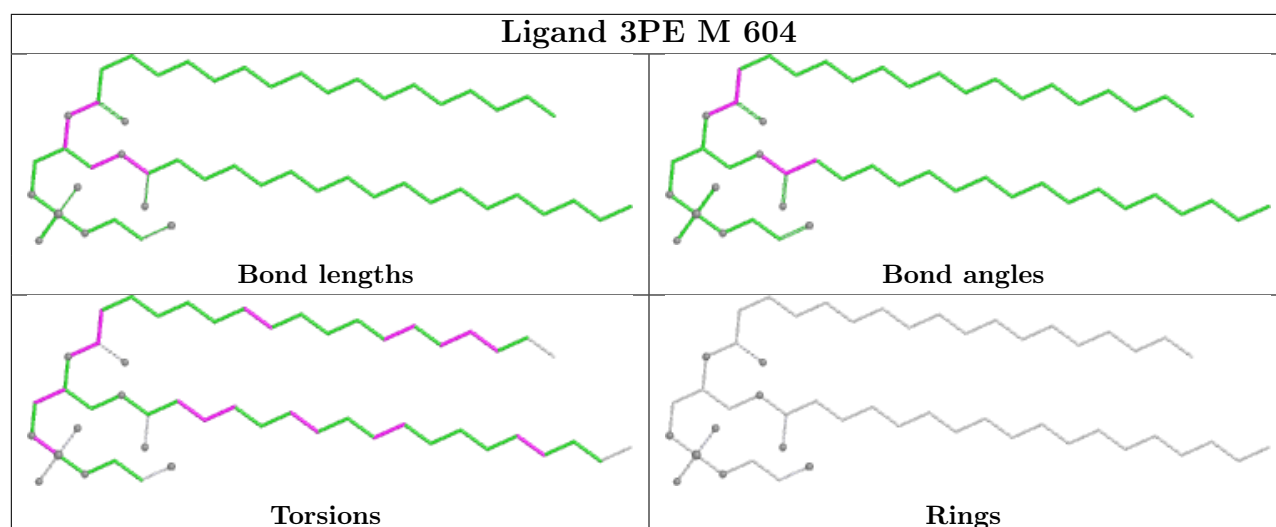
Ligand 3PE J 201

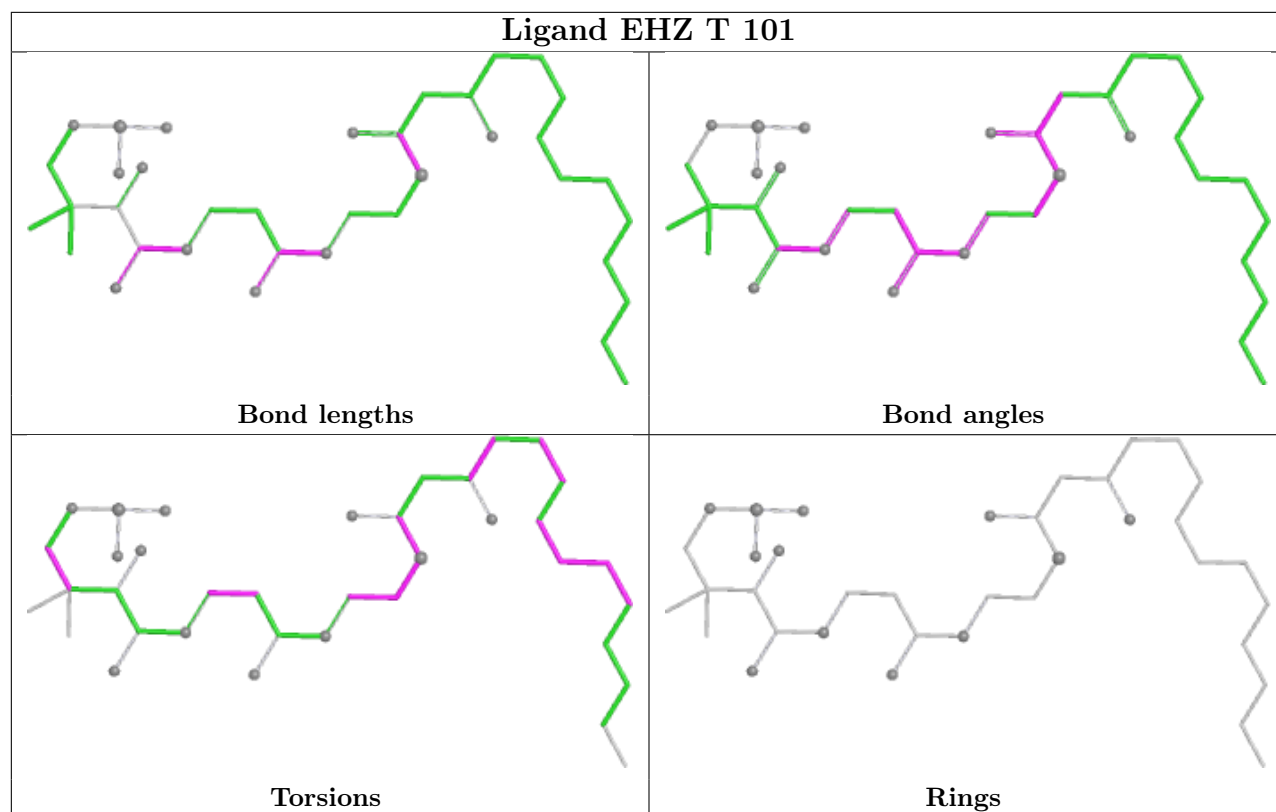
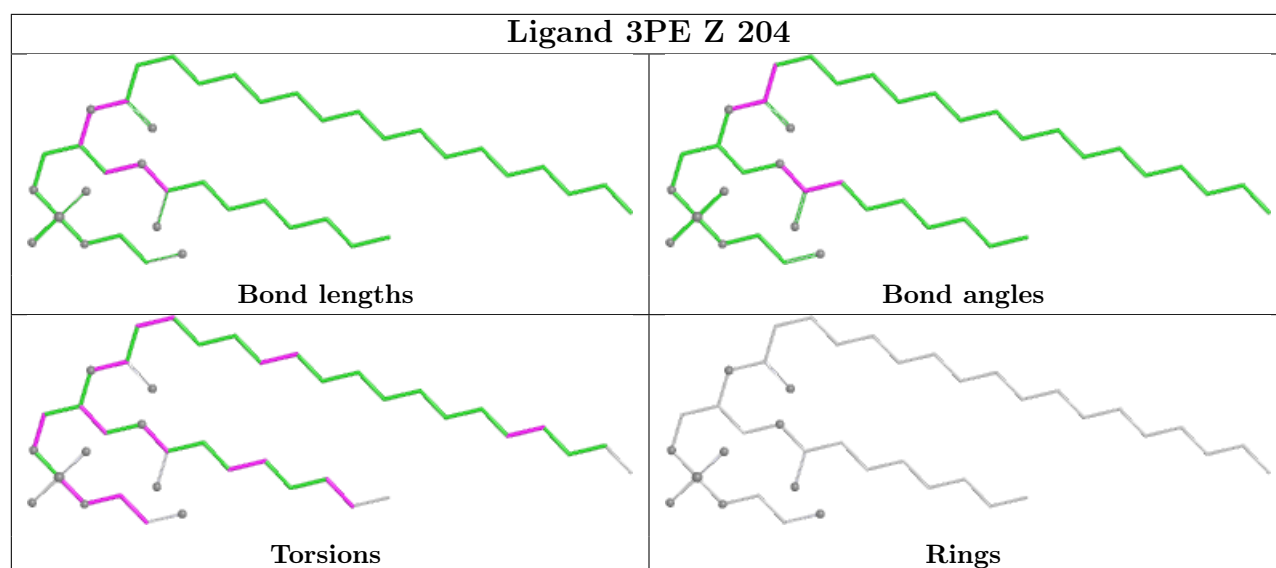


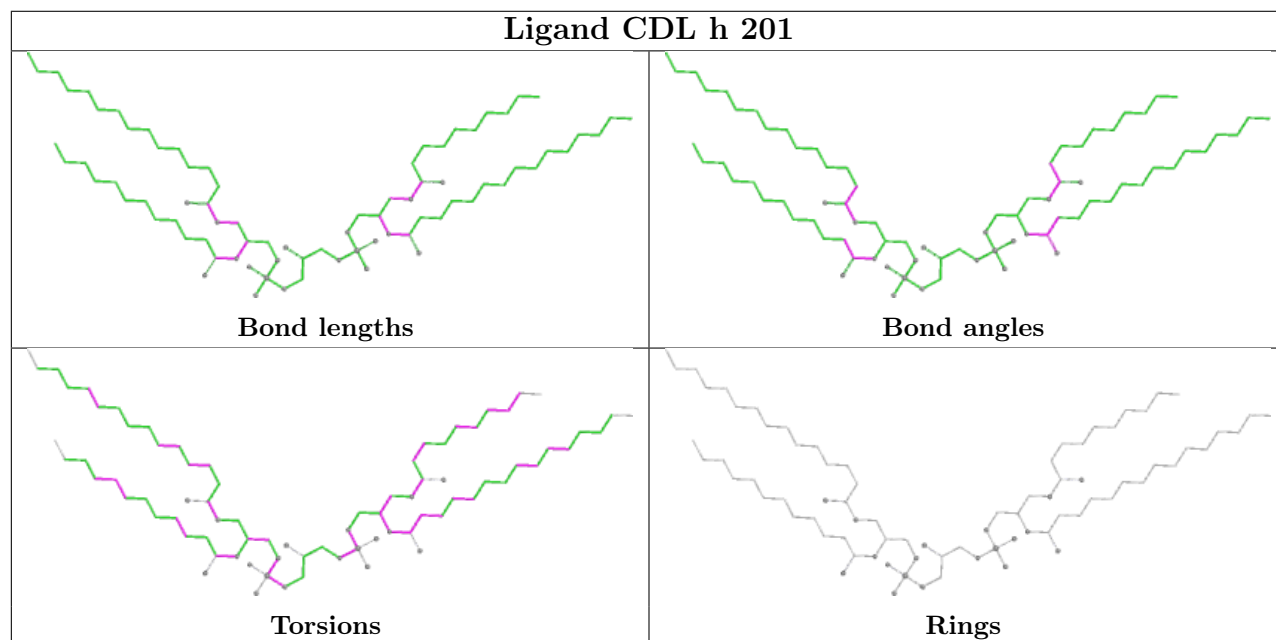
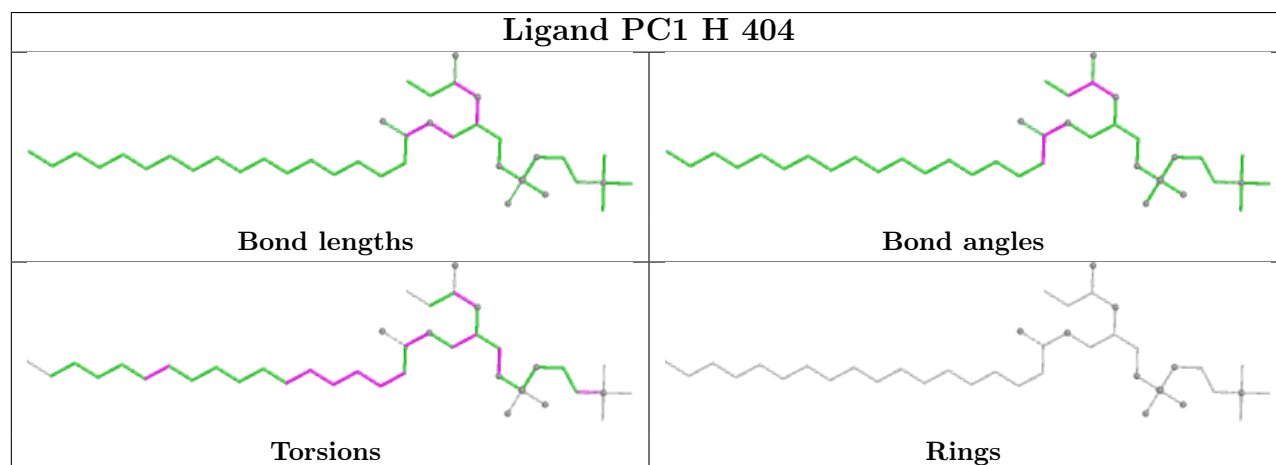
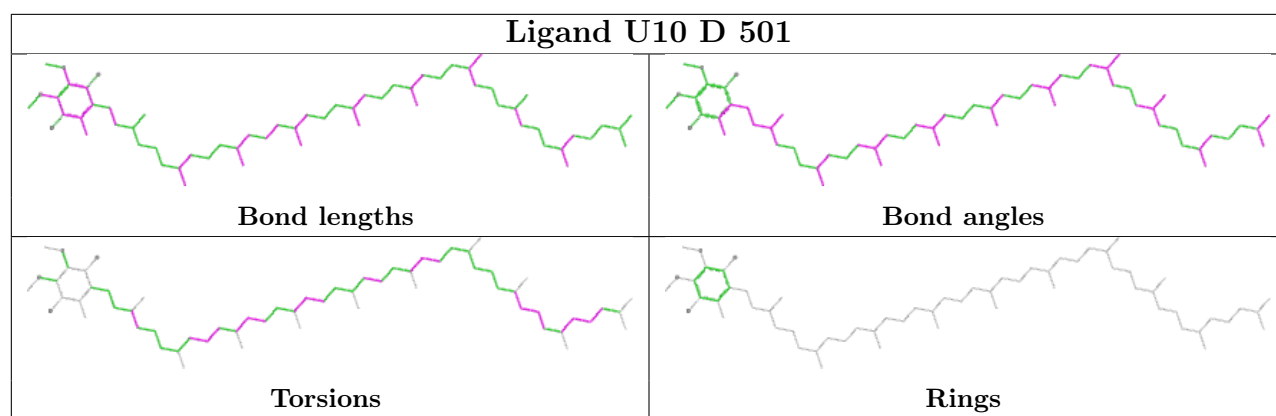
Ligand NDP P 501

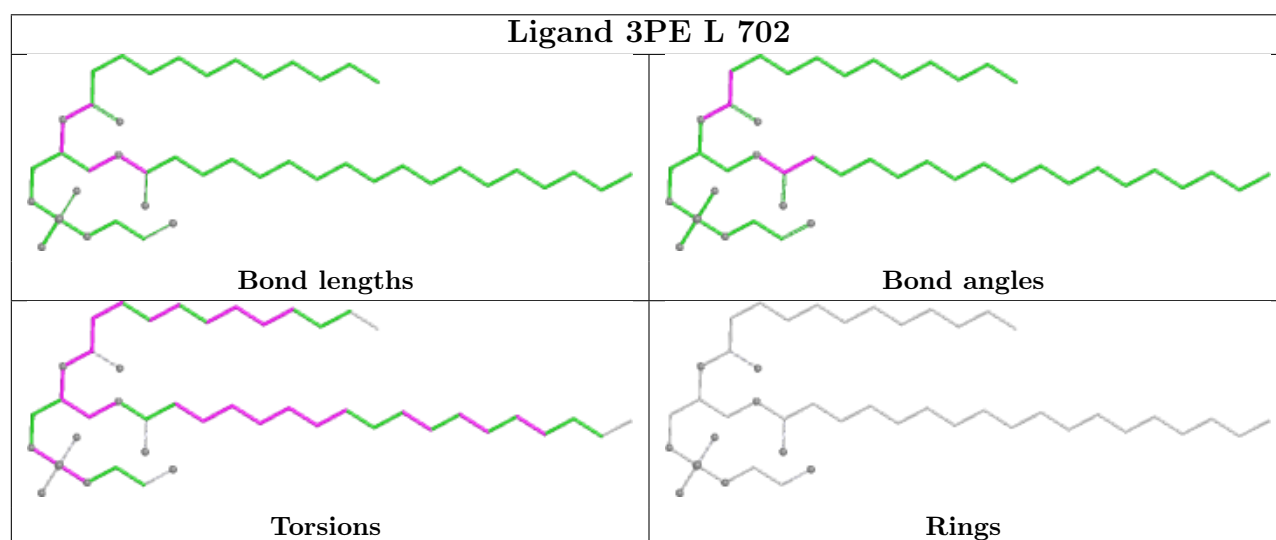
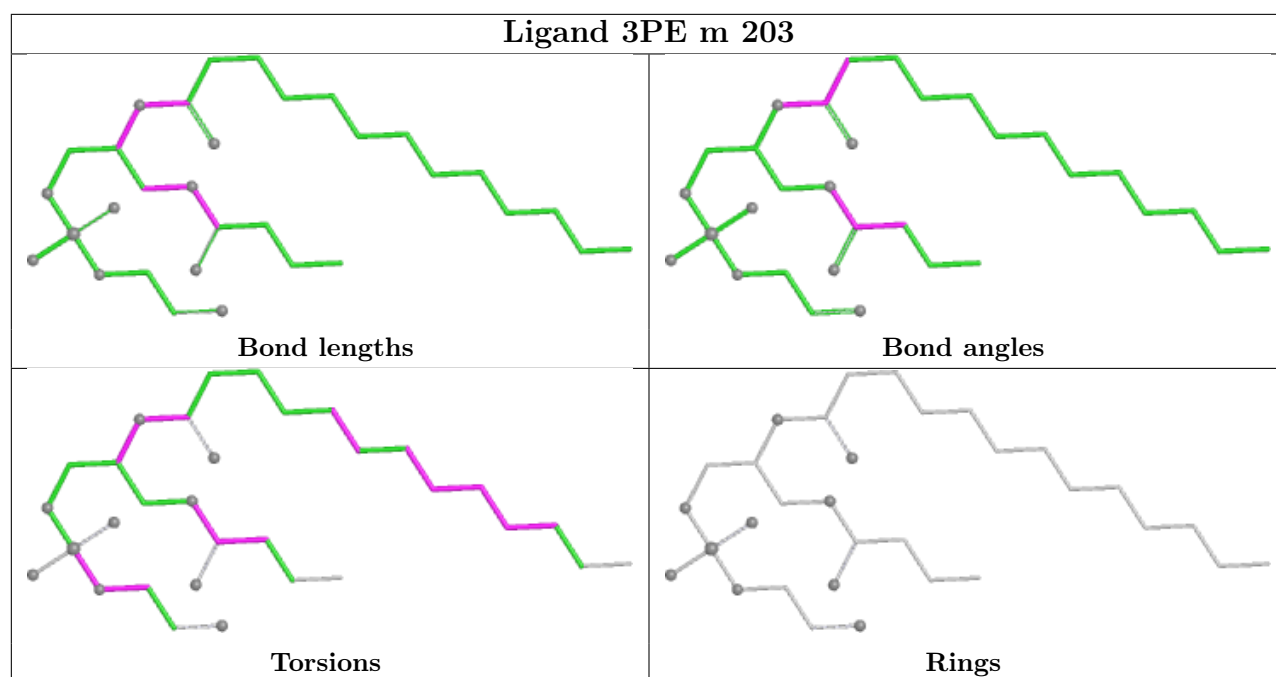


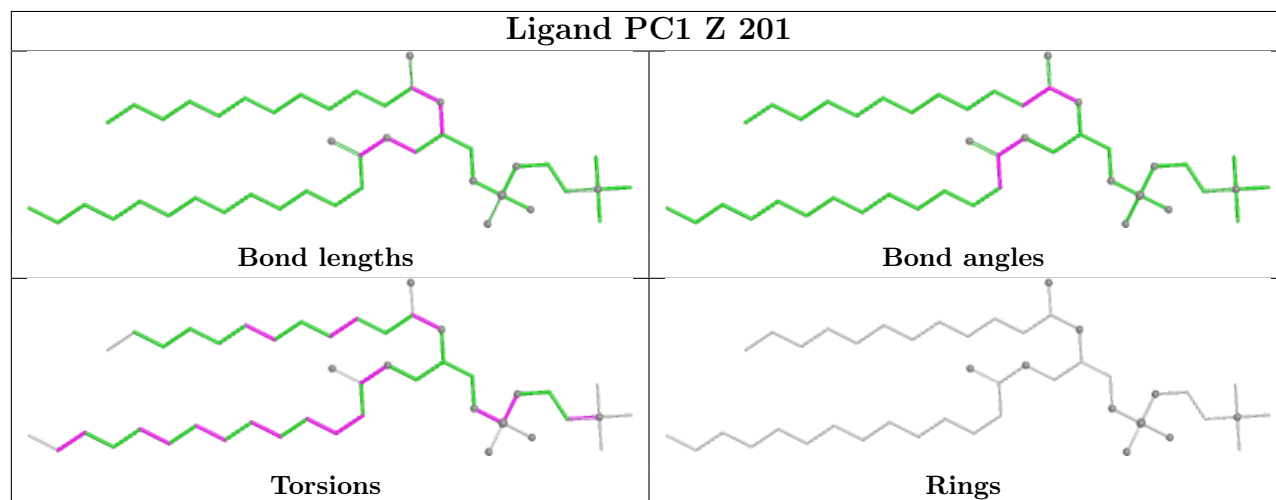
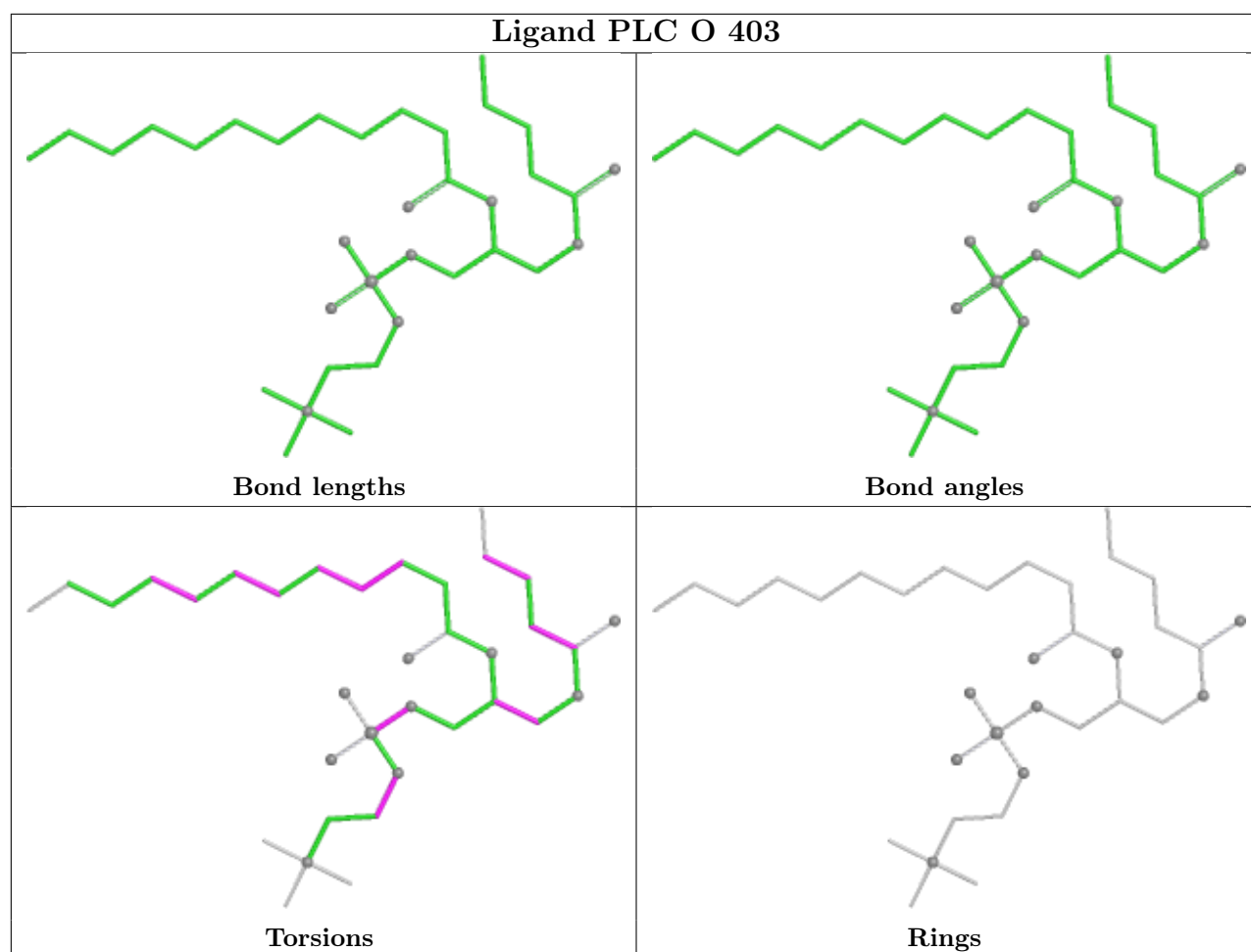


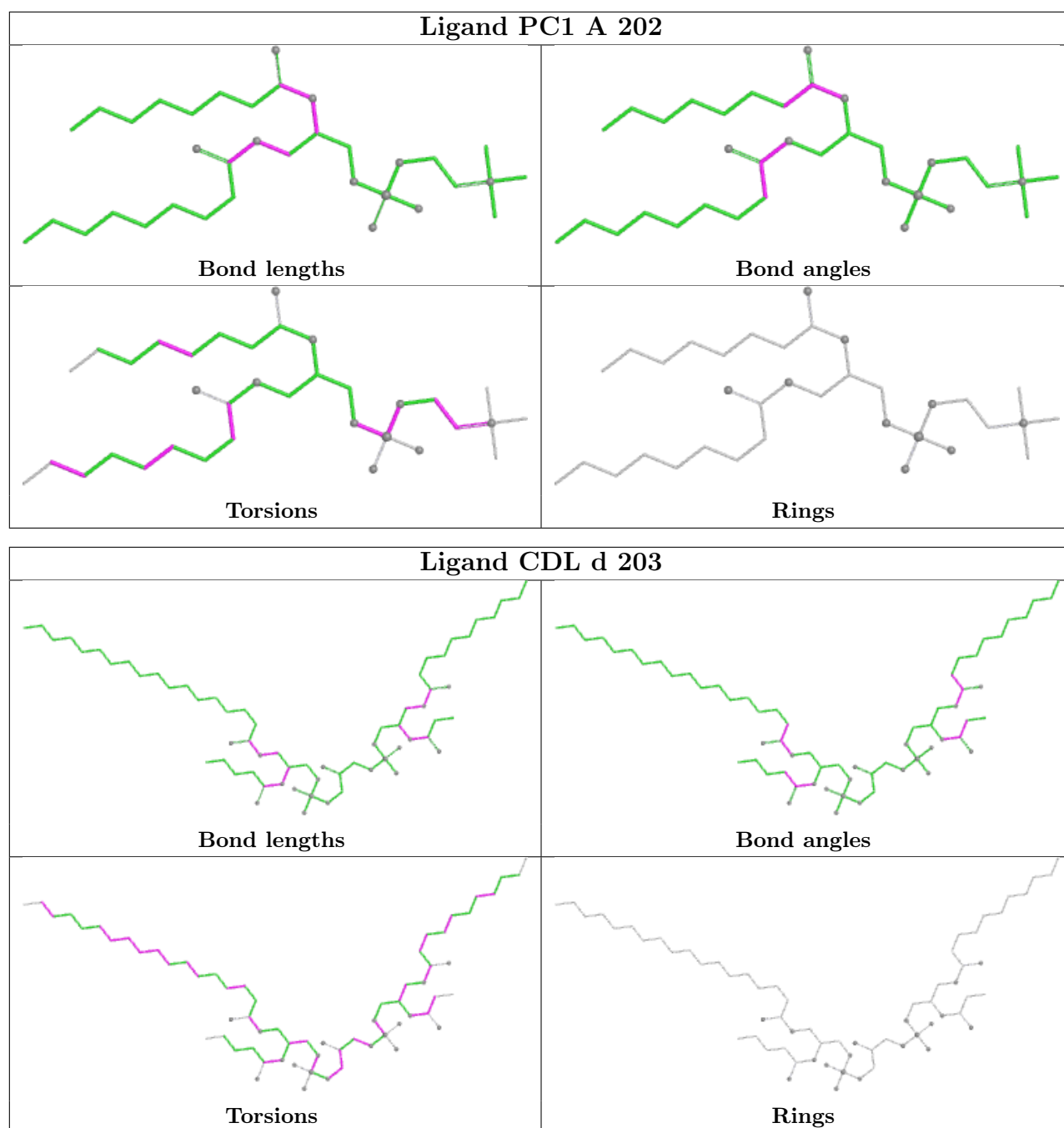


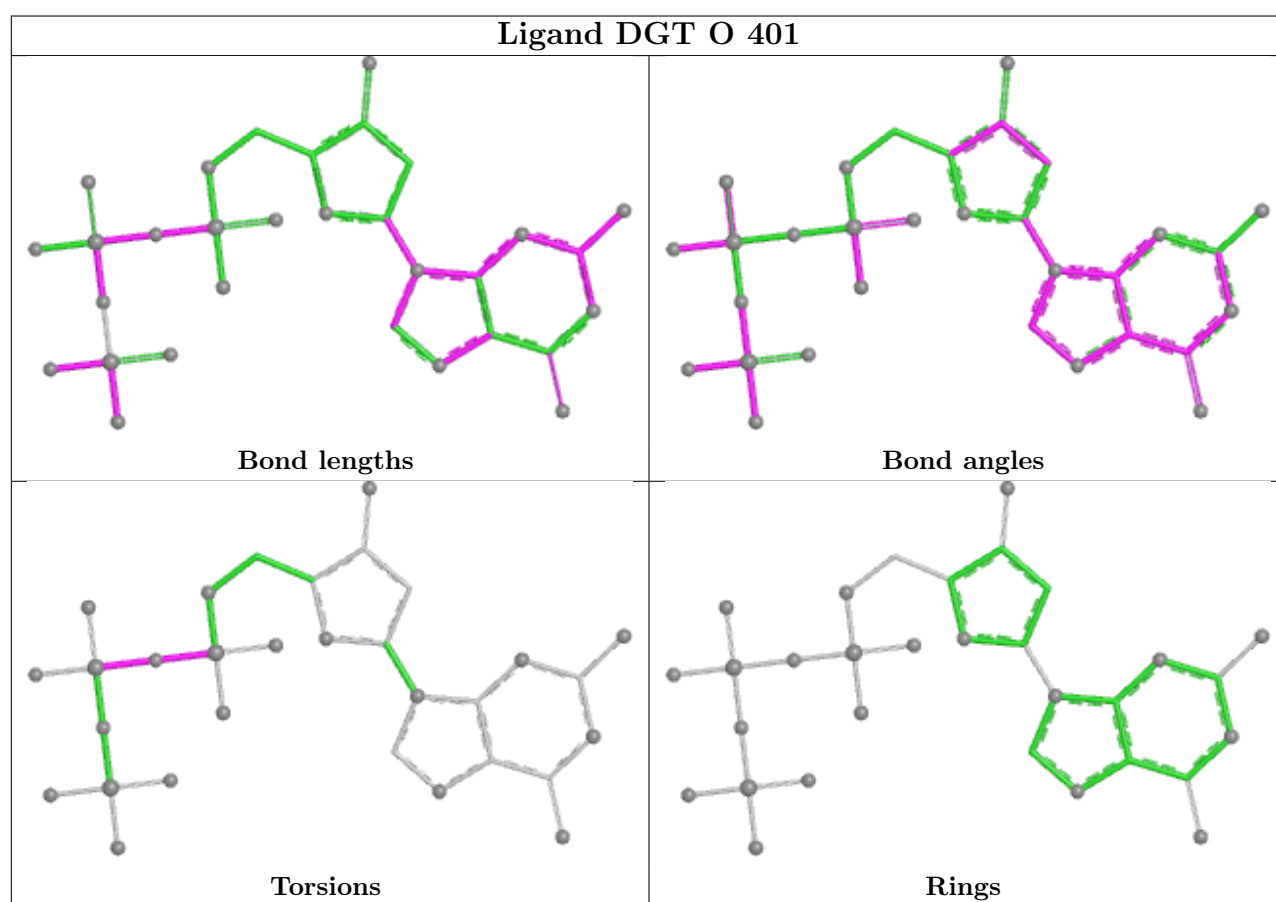
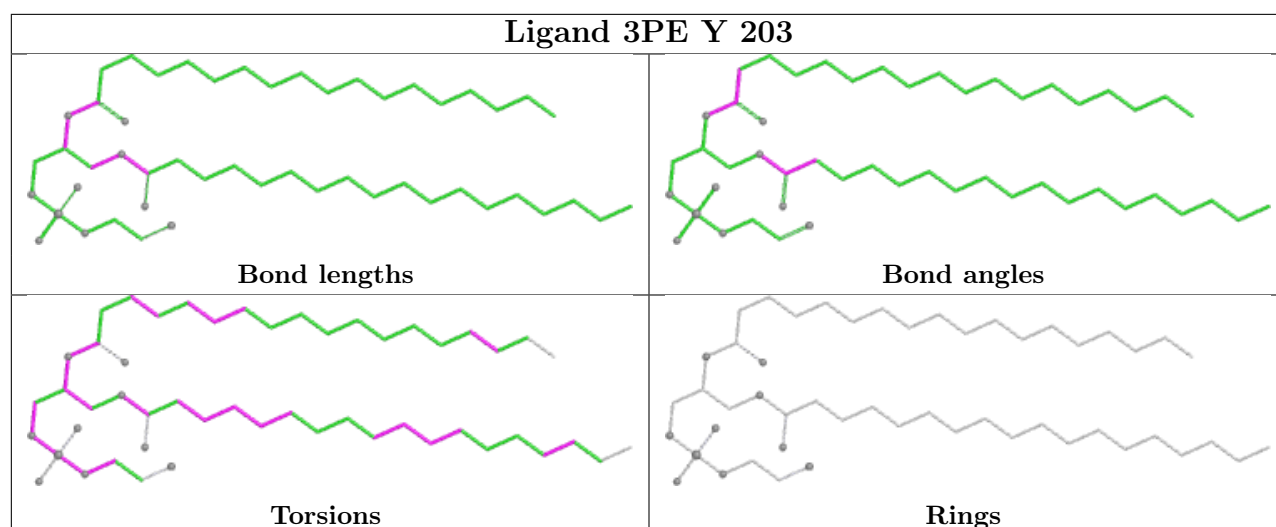


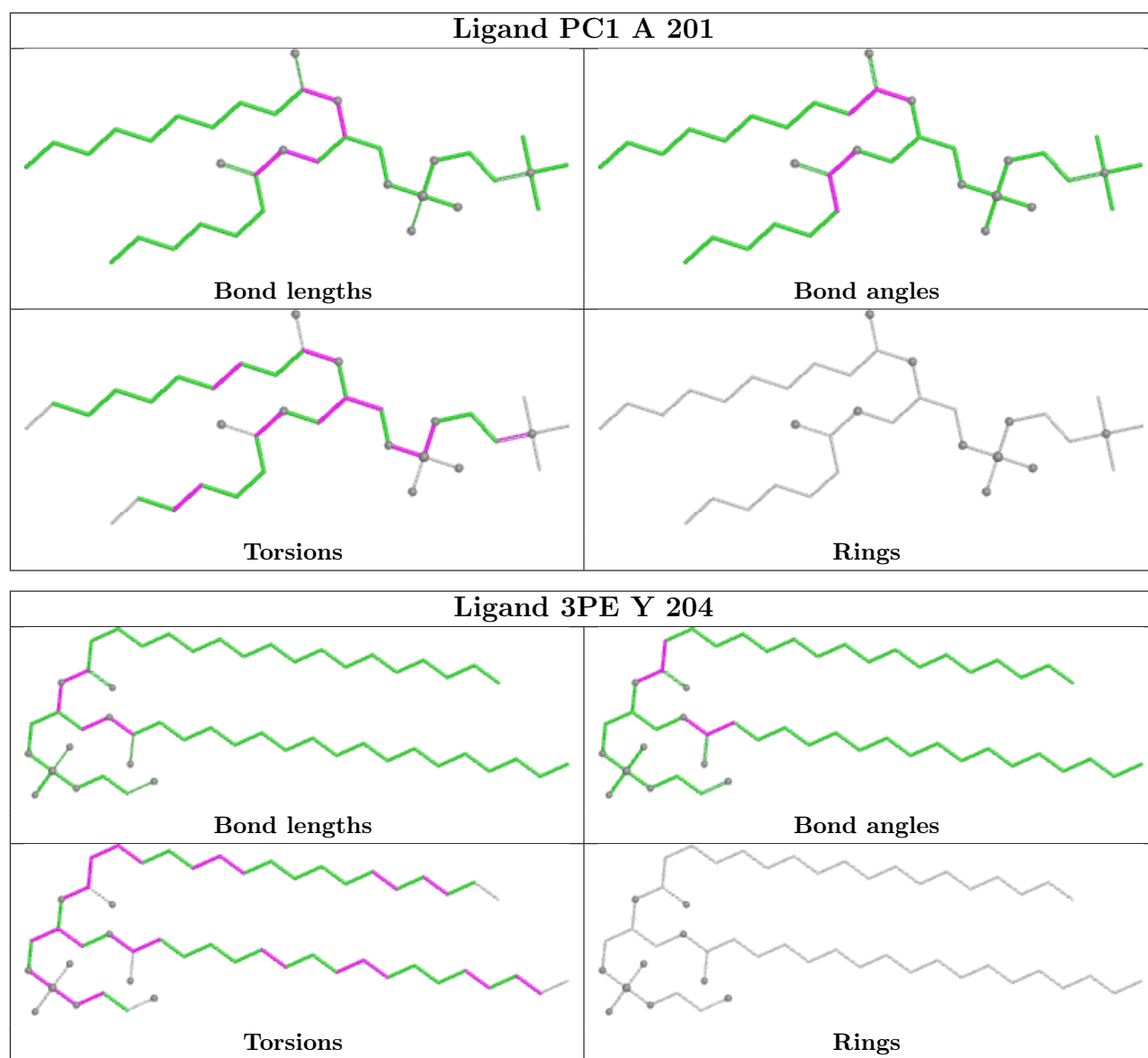


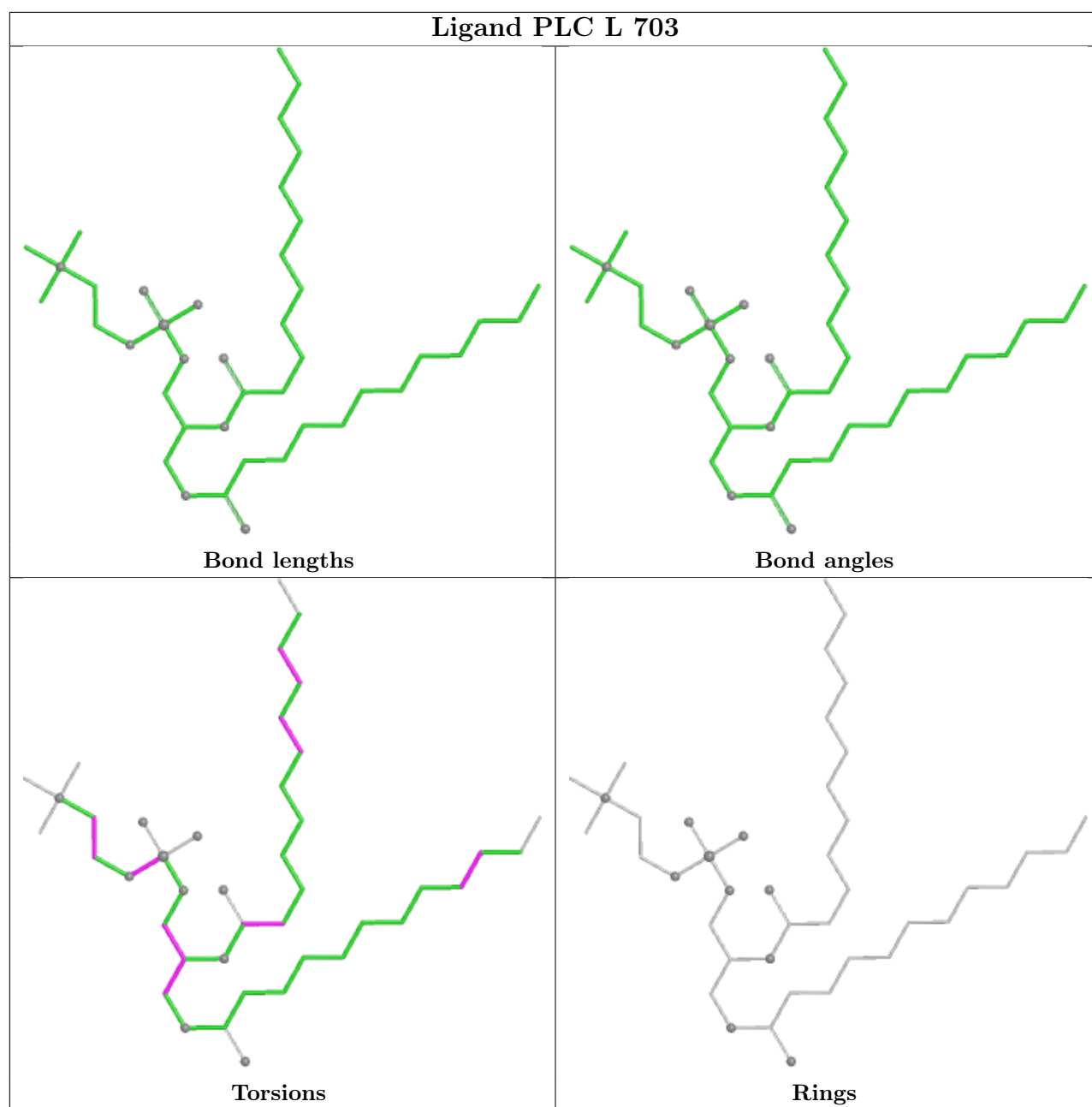




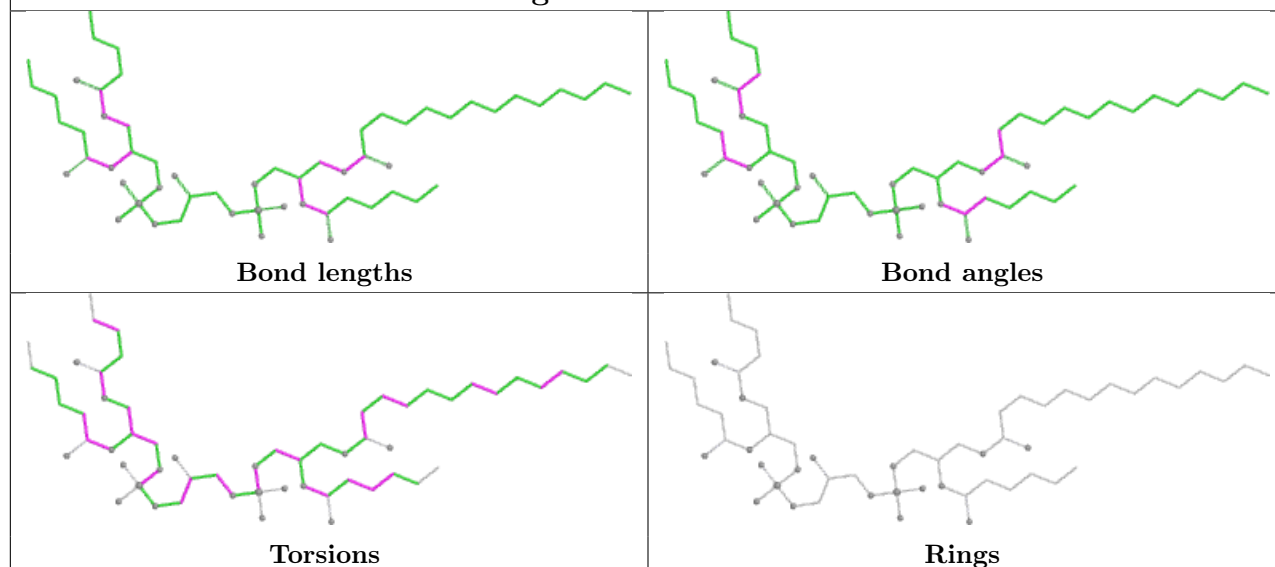




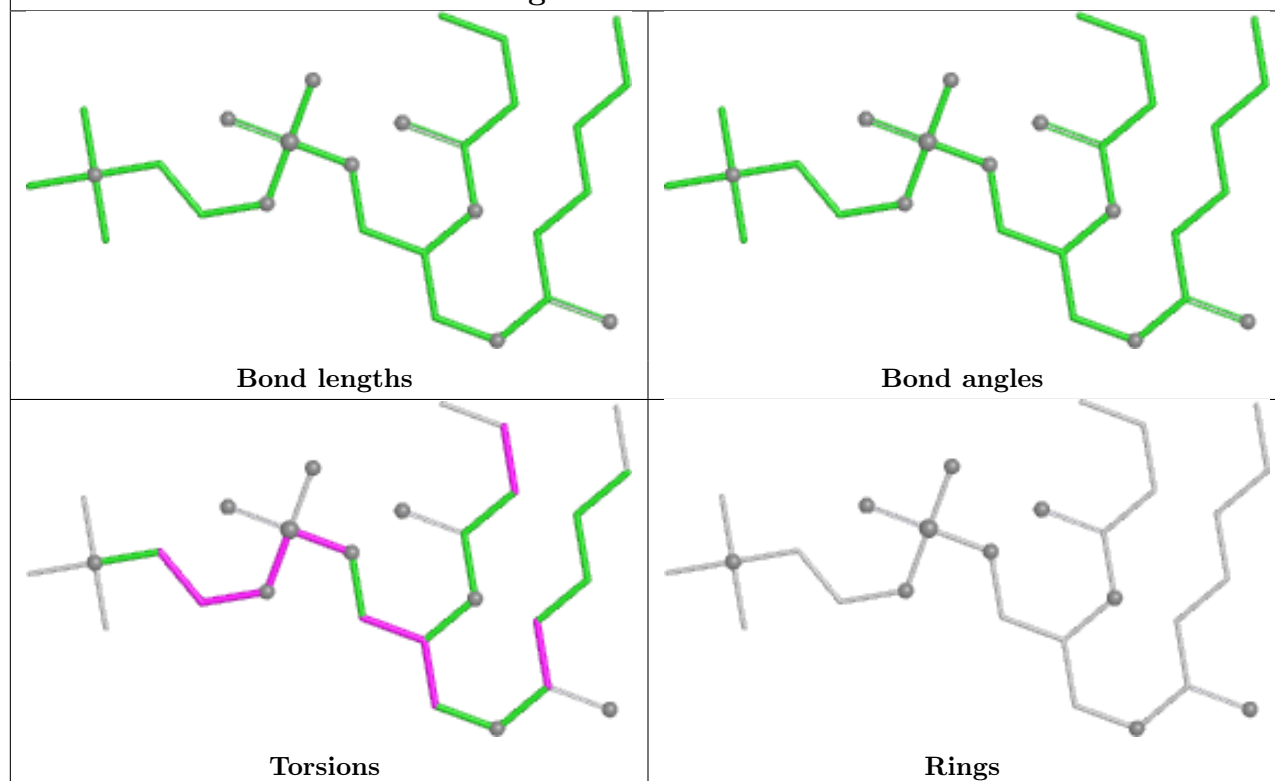


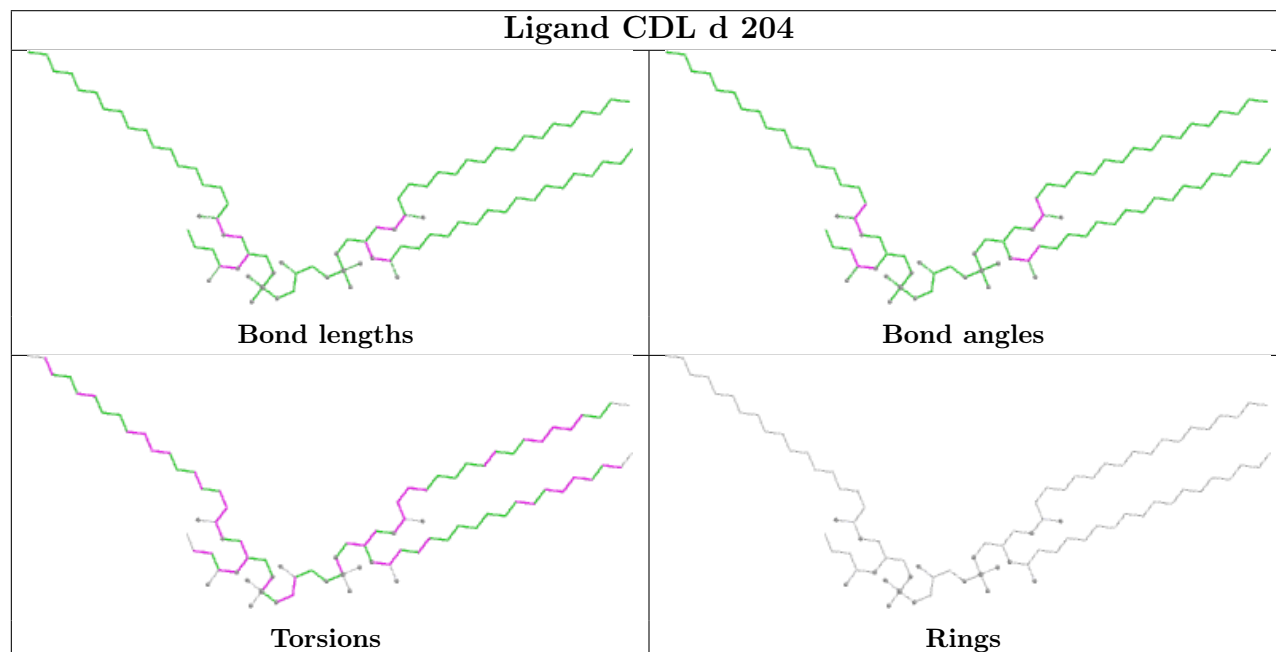
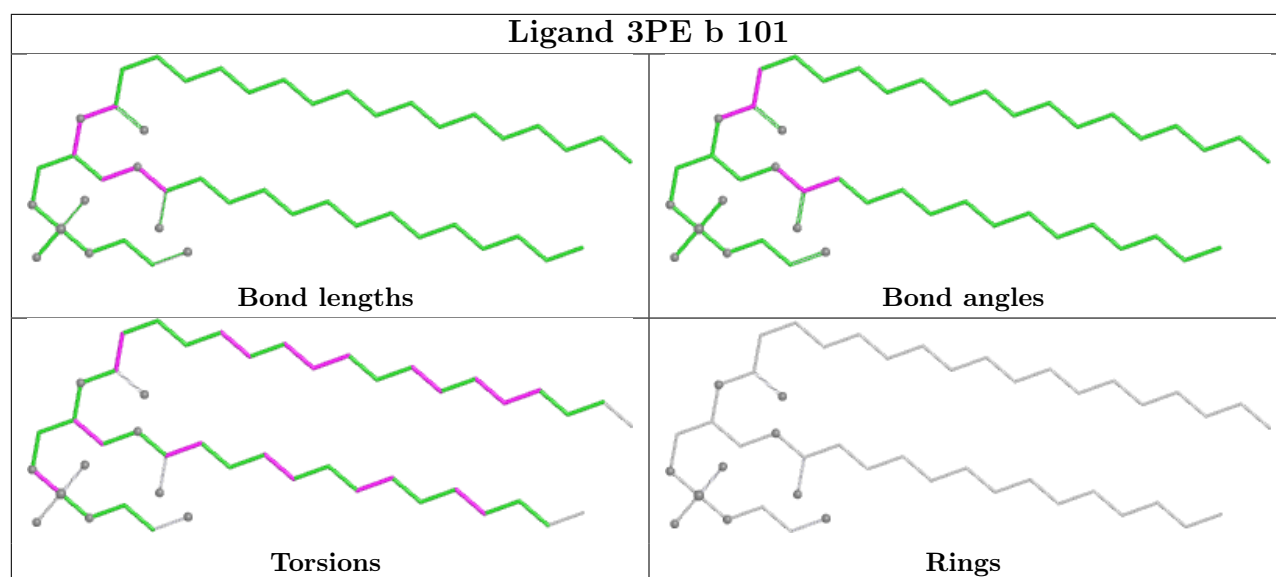


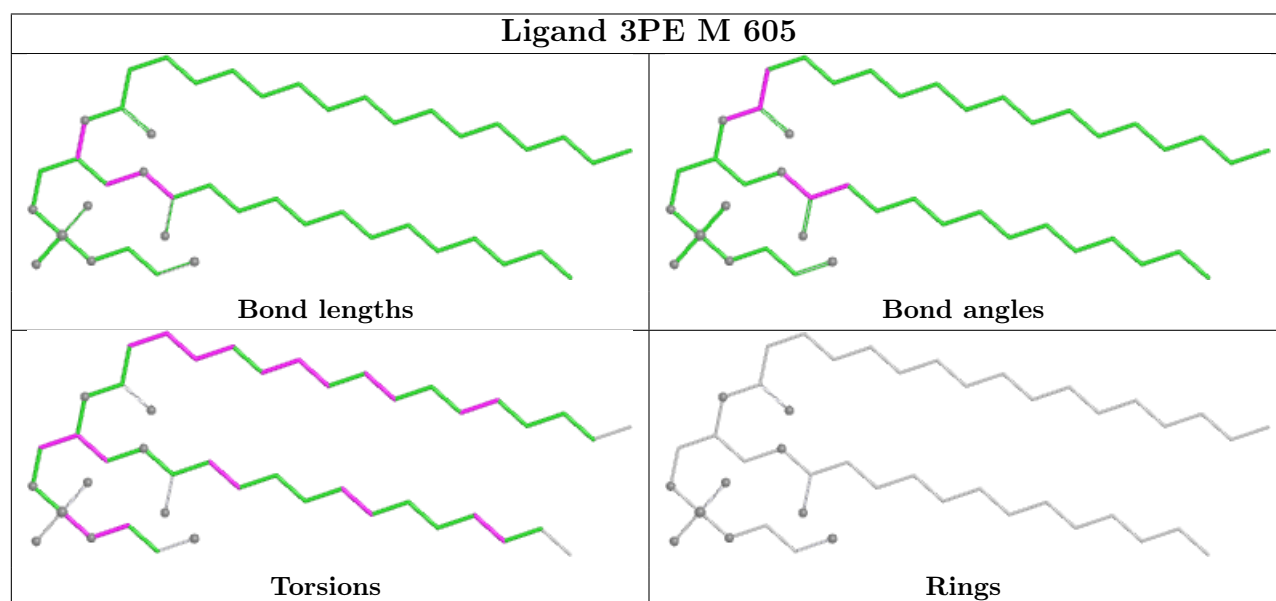
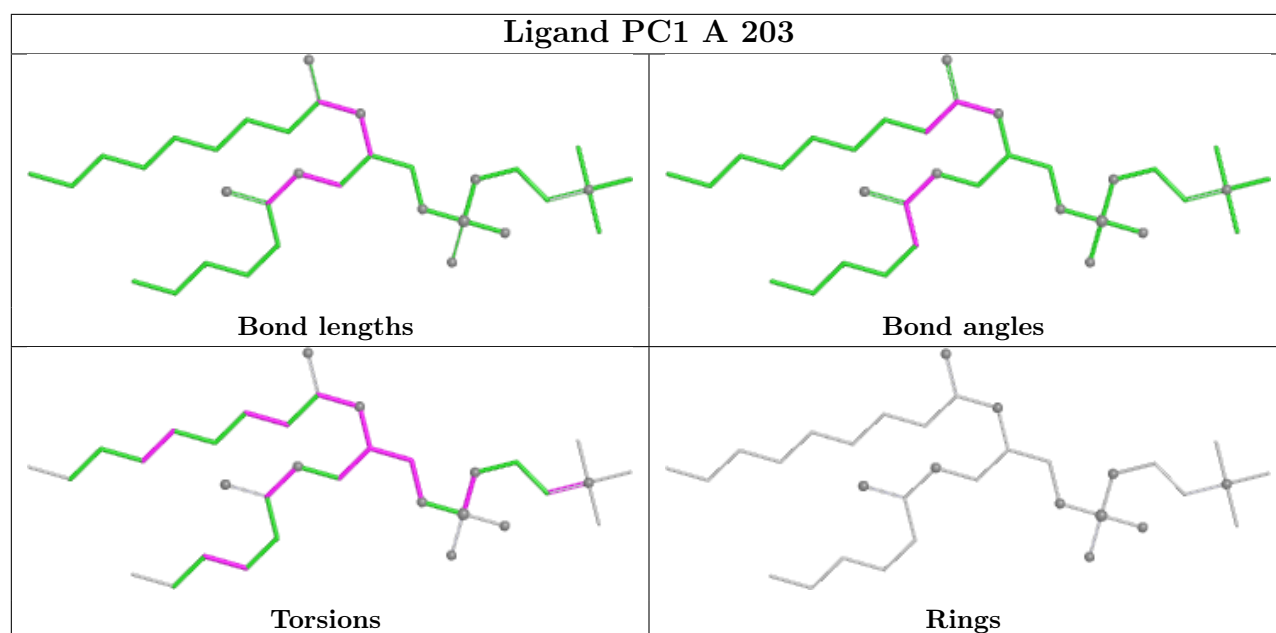
Ligand CDL P 503



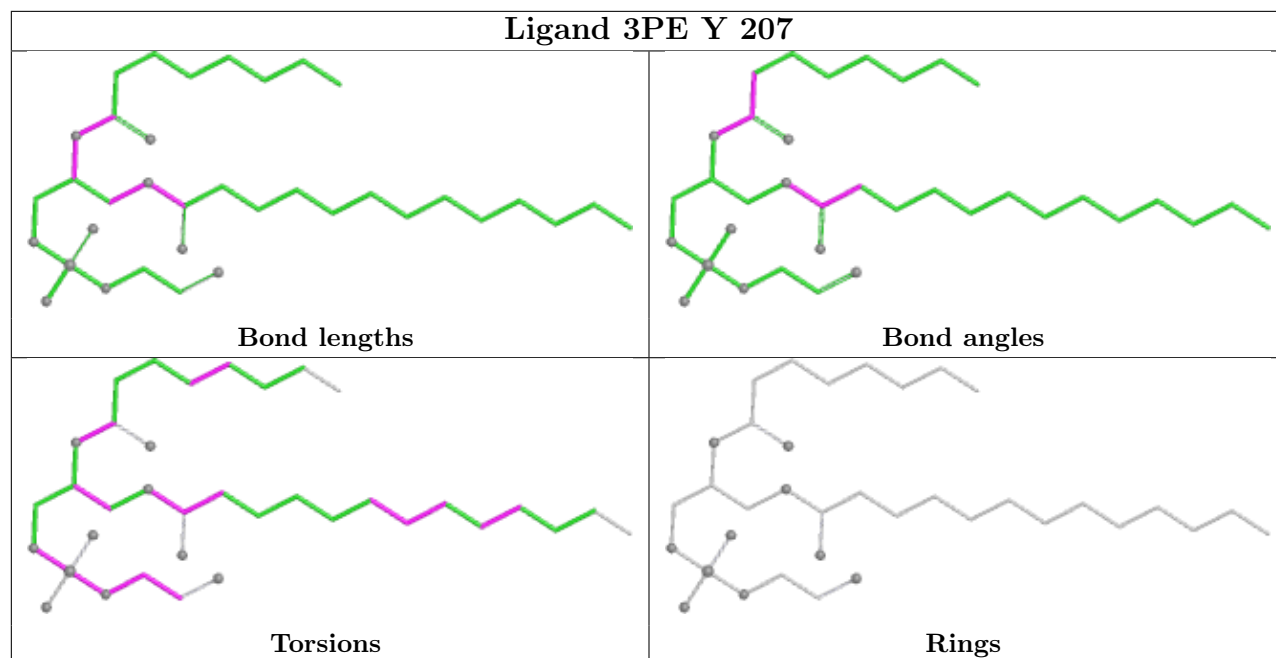
Ligand PLC M 608



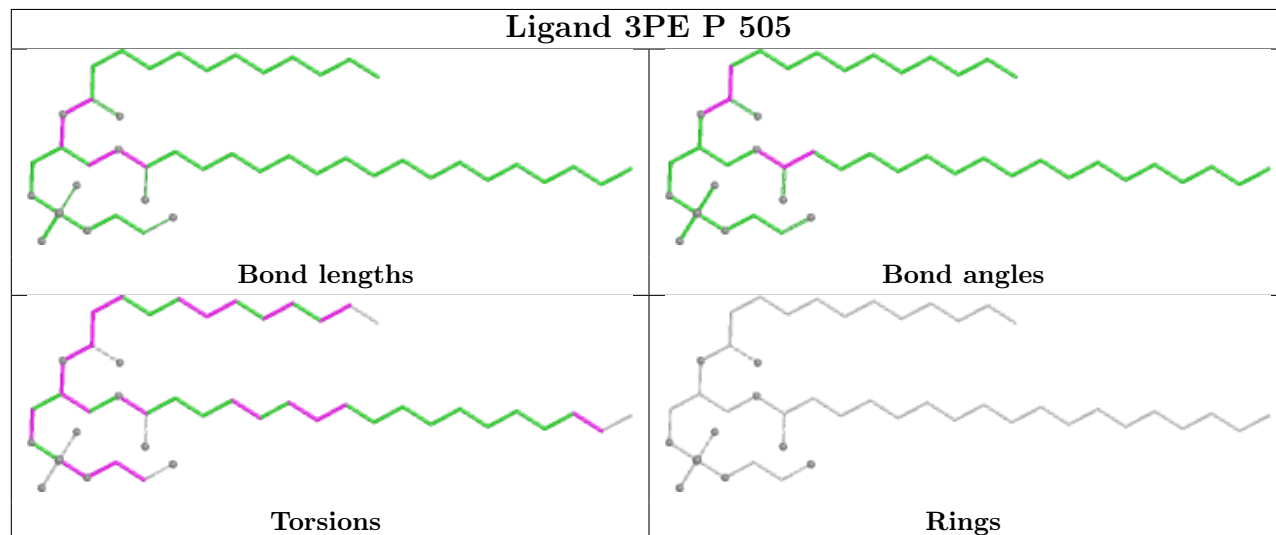




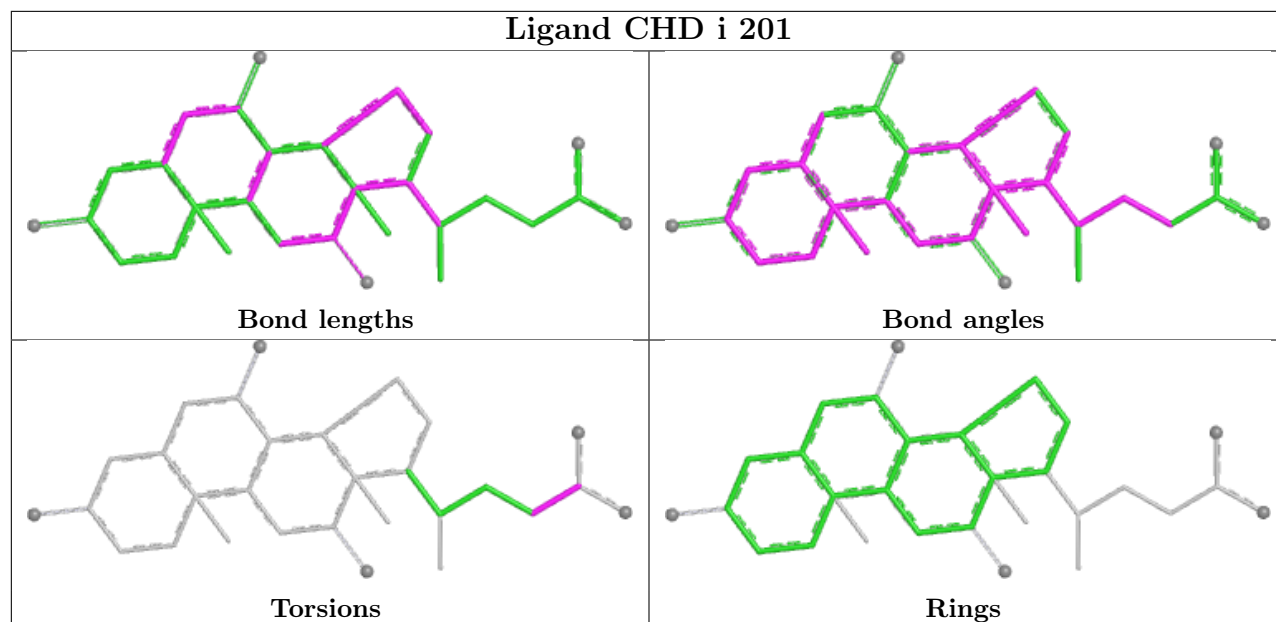
Ligand 3PE Y 207



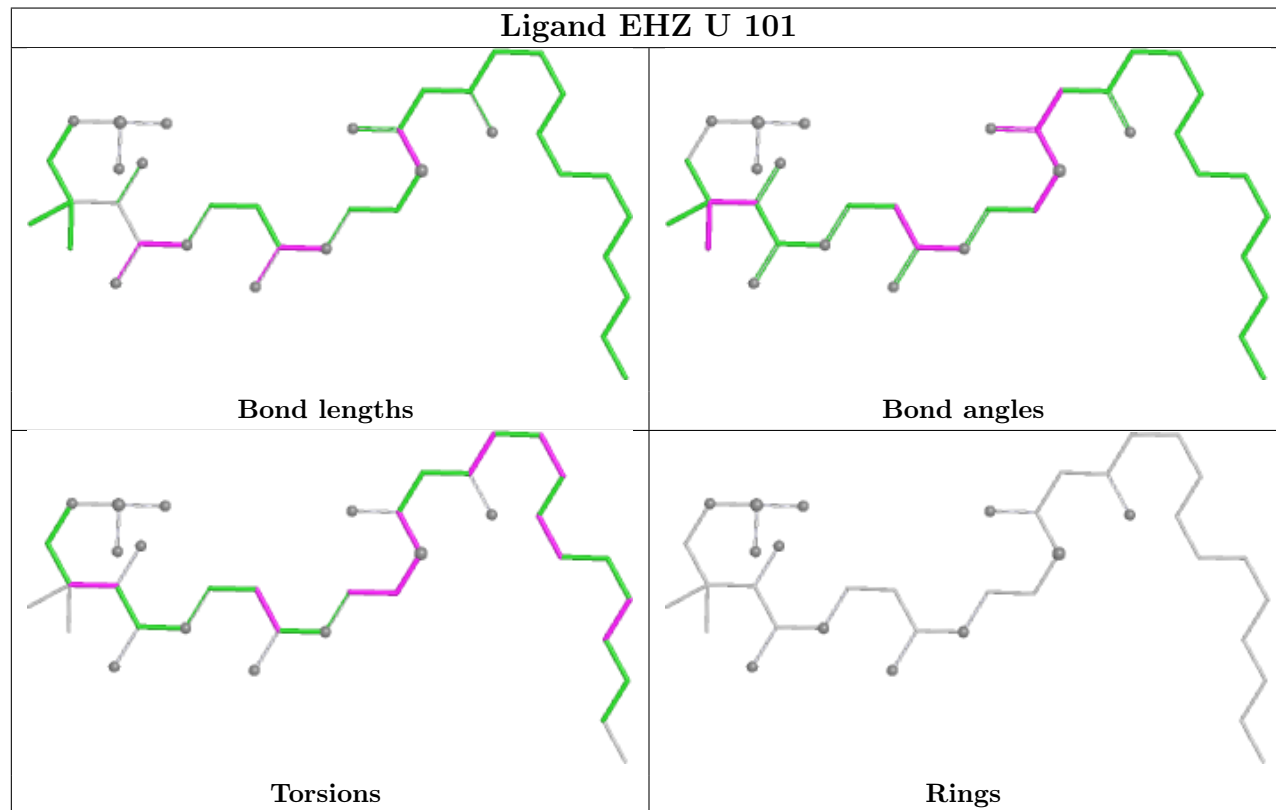
Ligand 3PE P 505

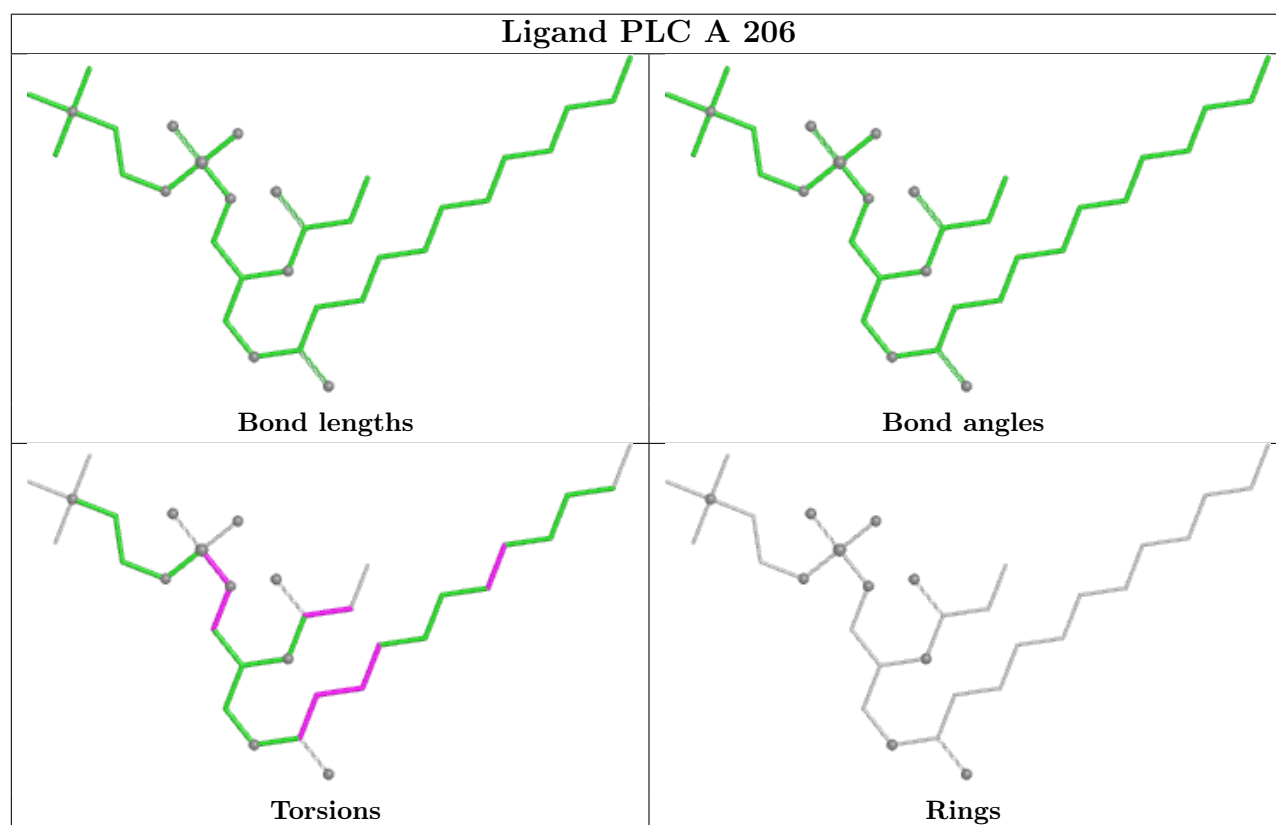
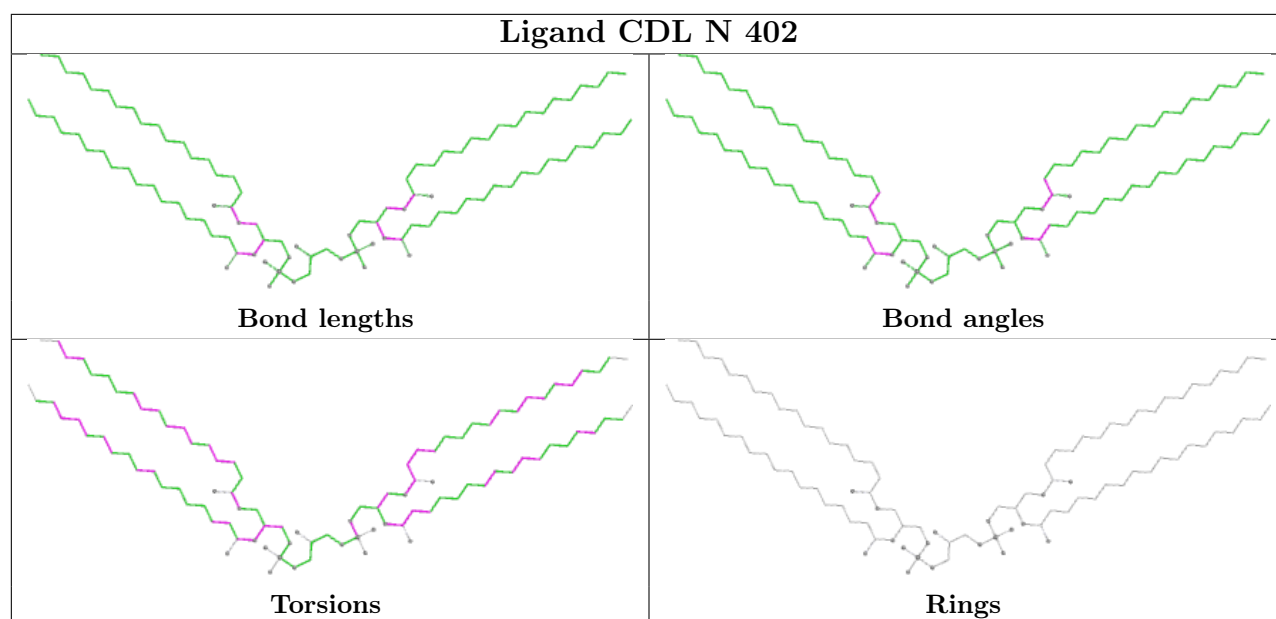


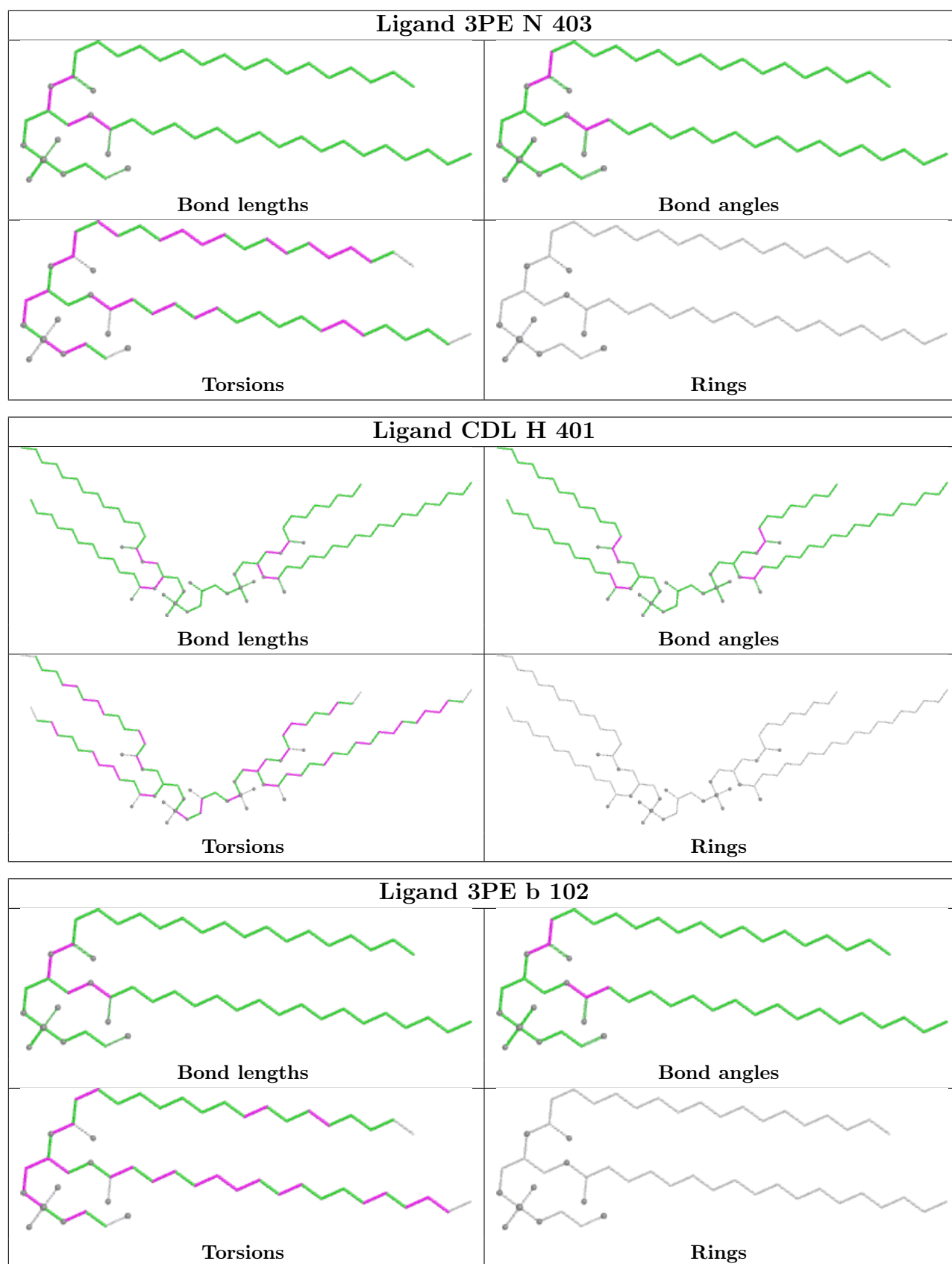
Ligand CHD i 201

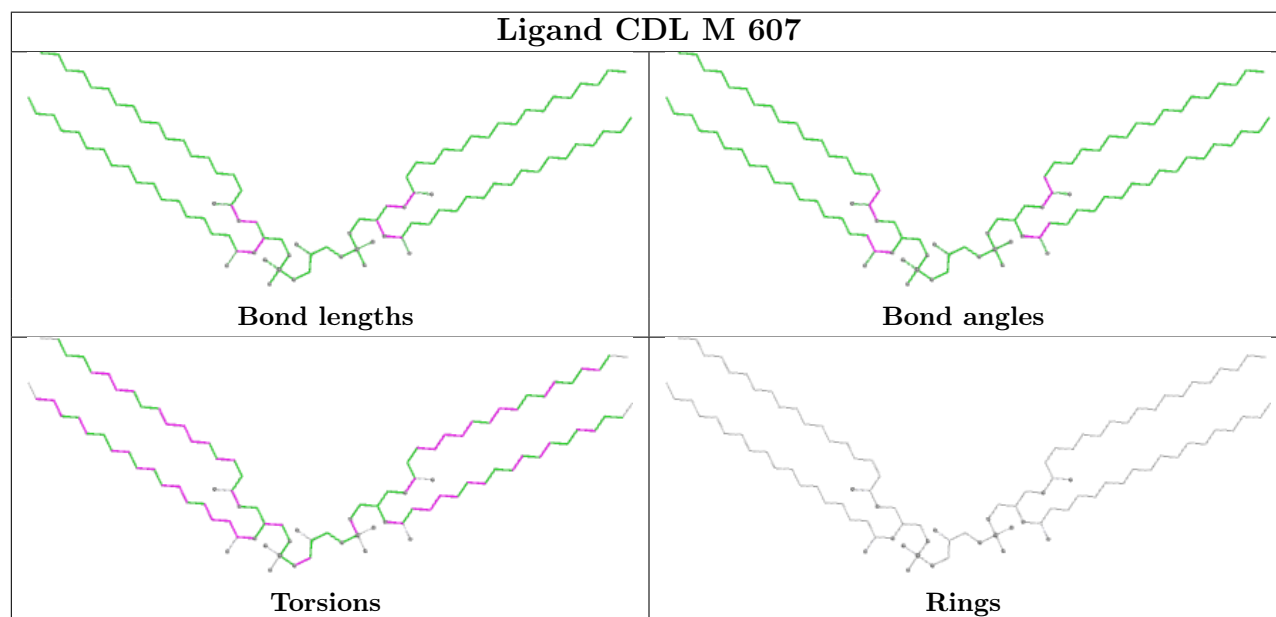
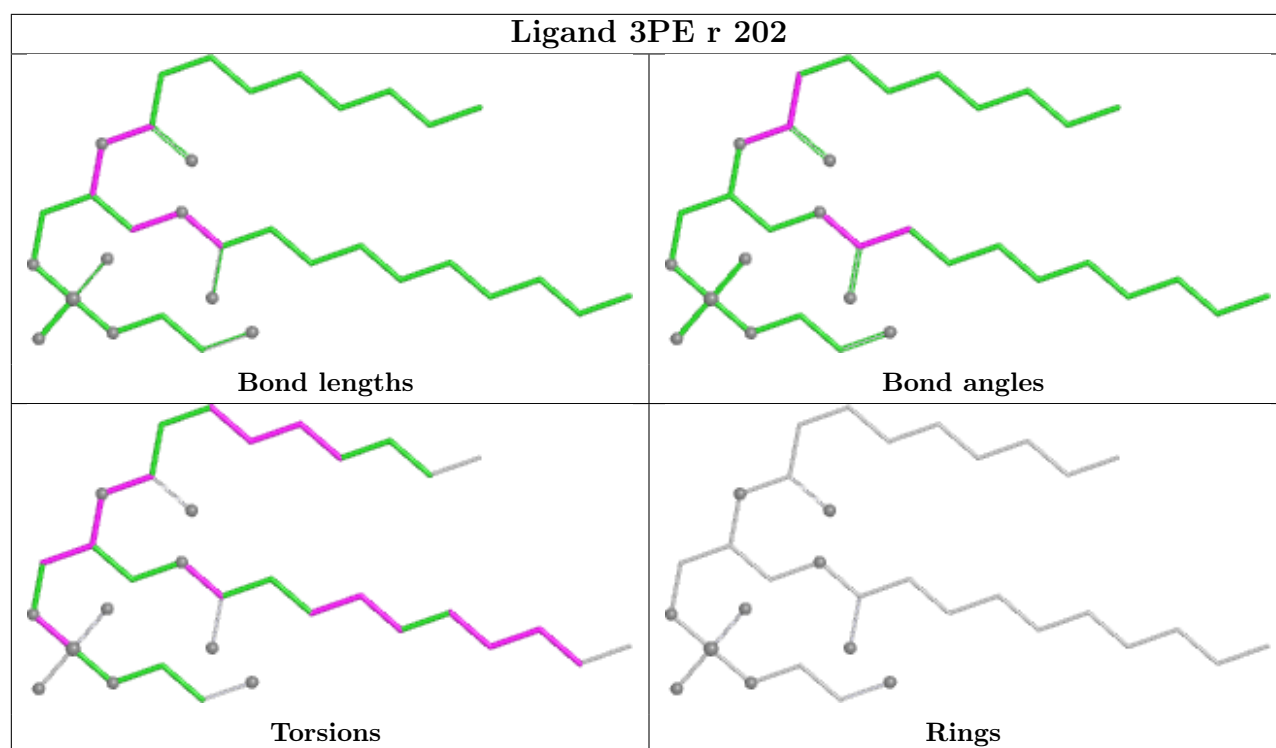


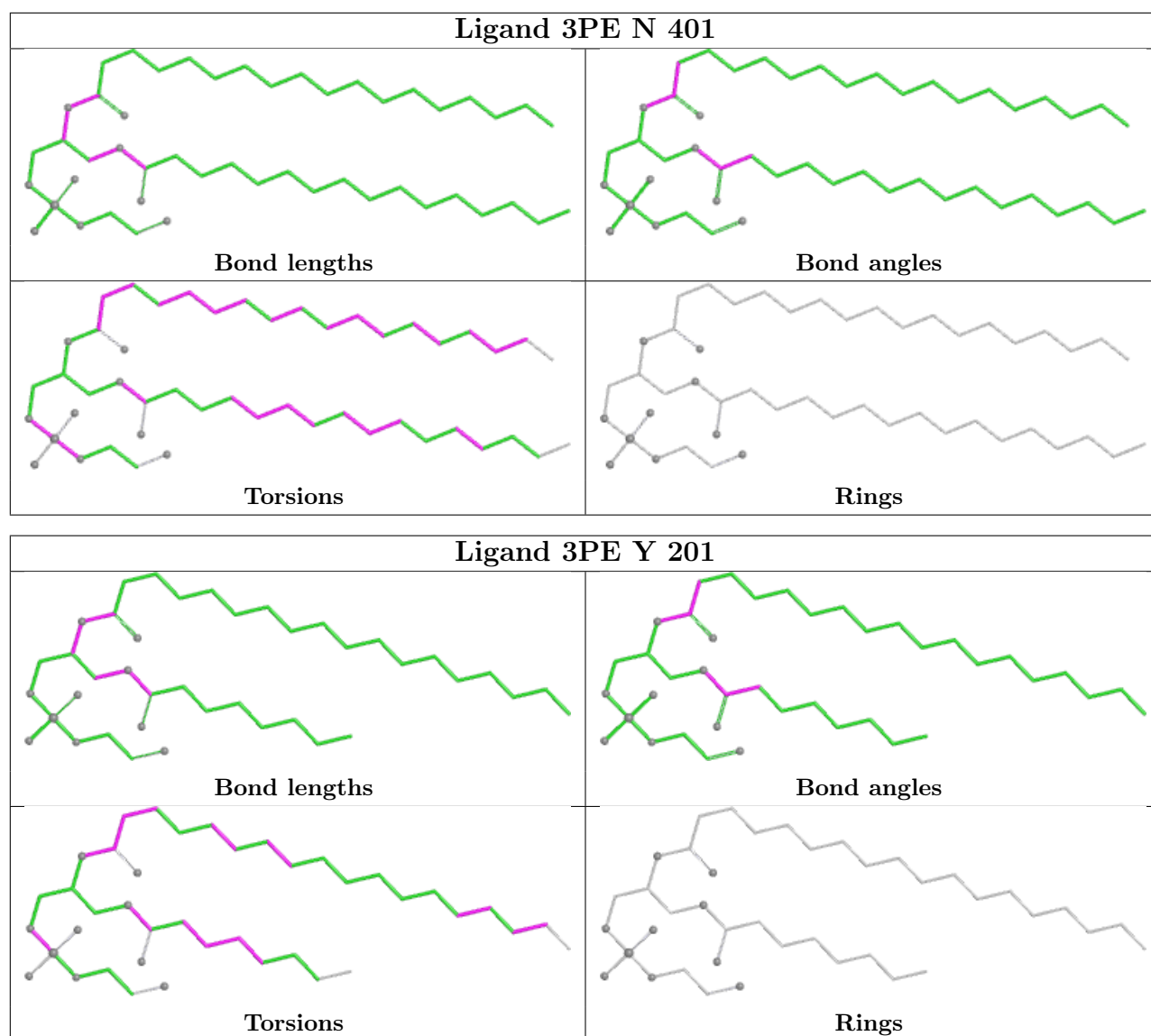
Ligand EHZ U 101

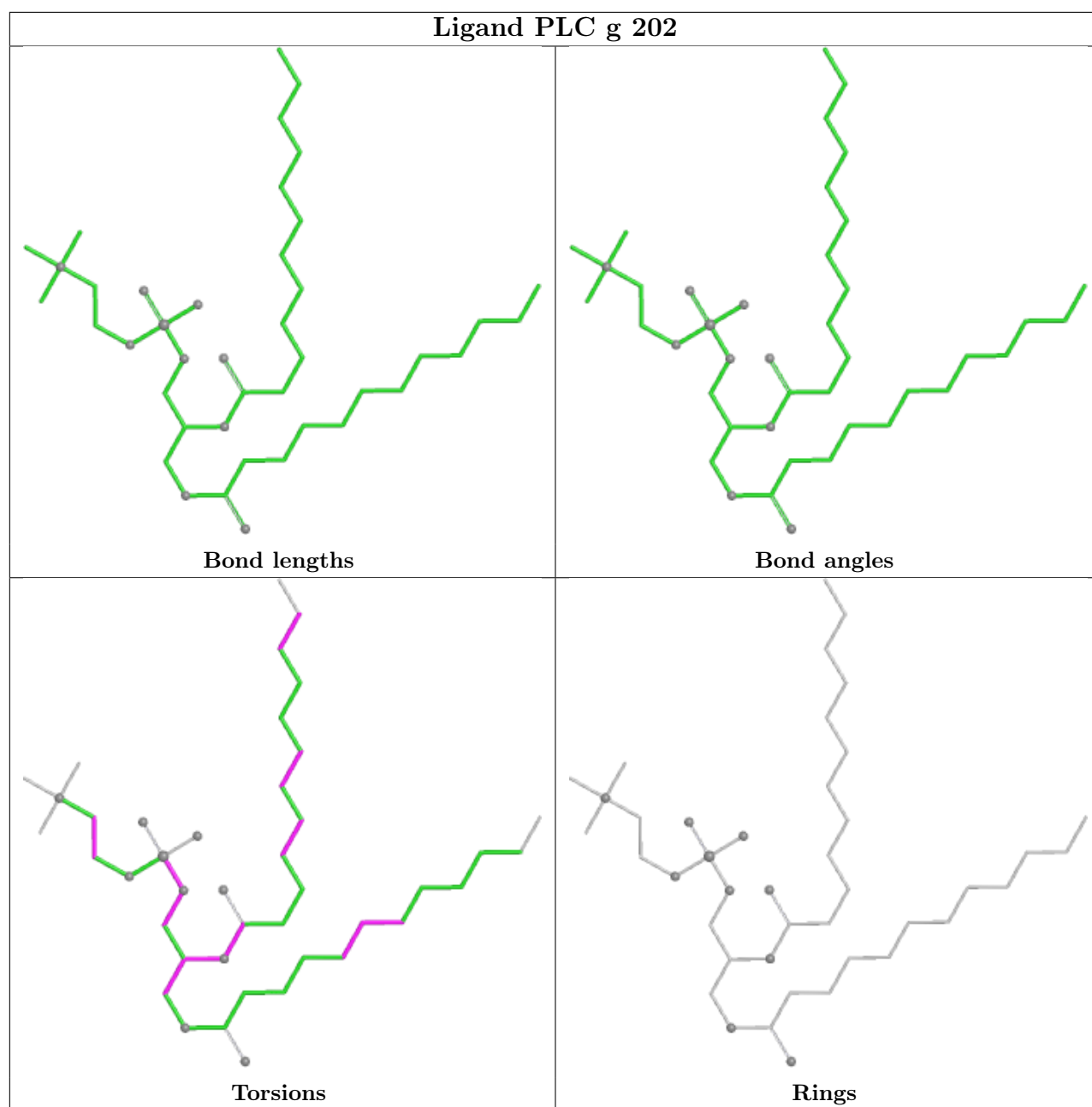


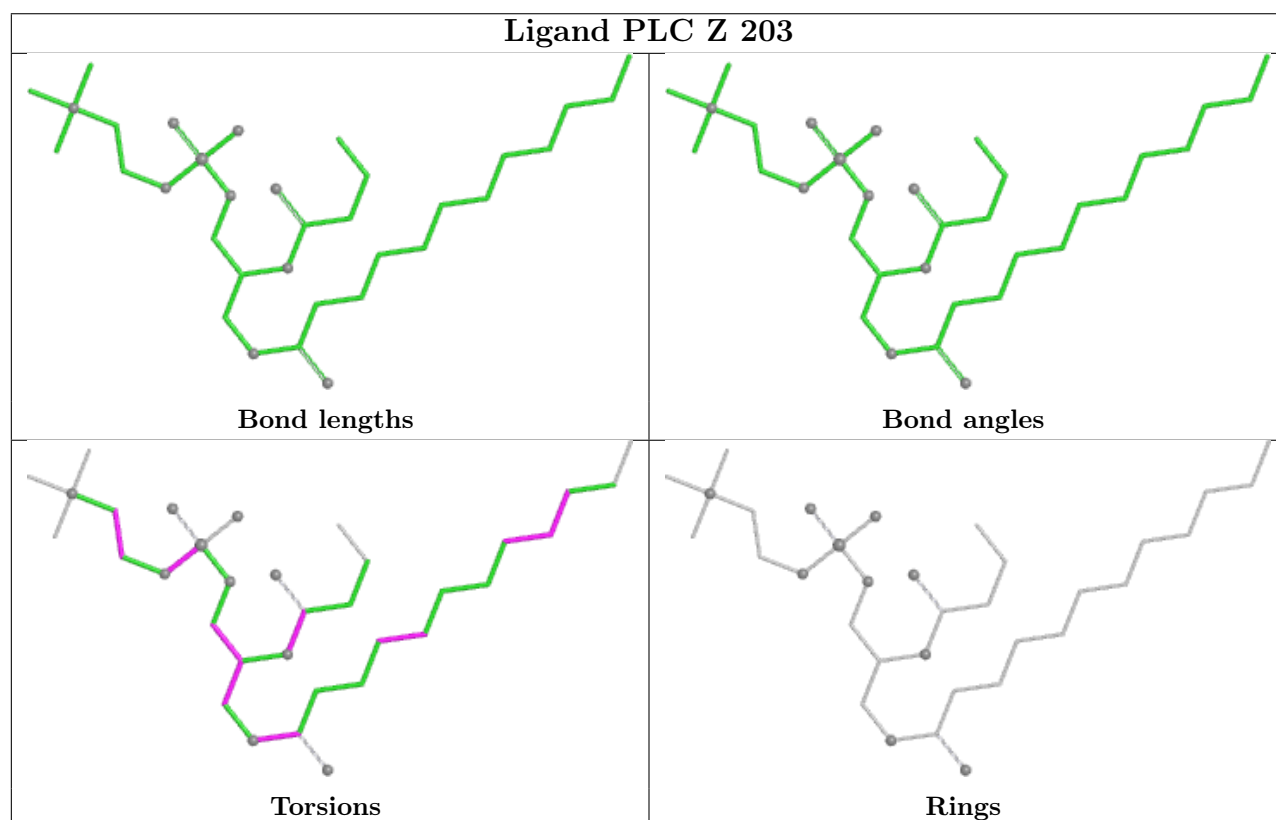
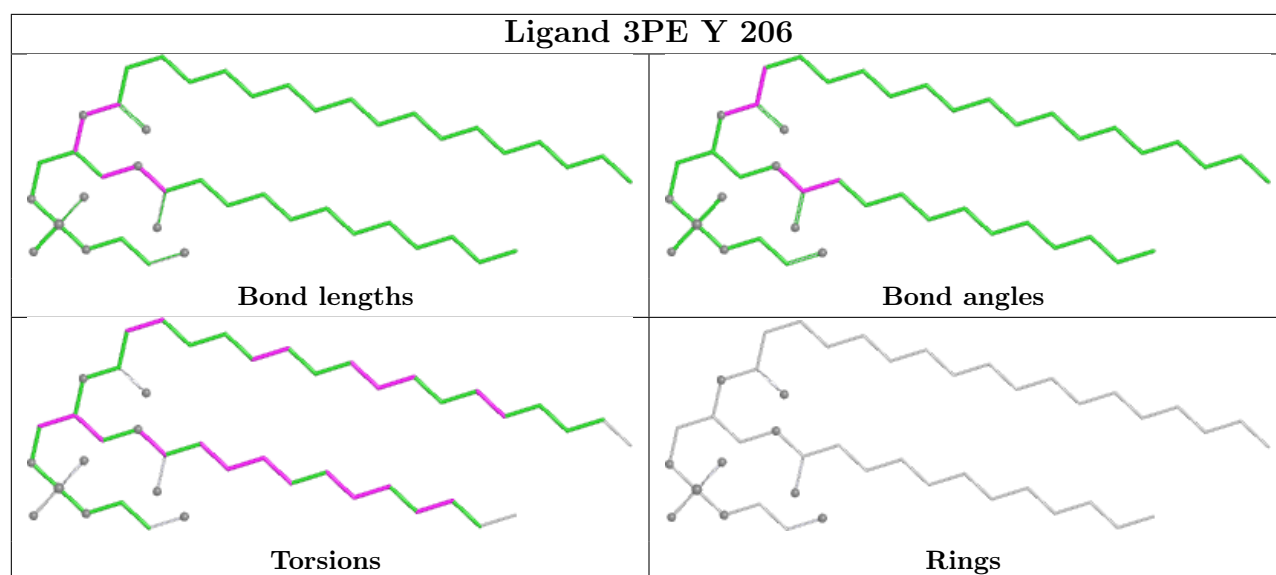


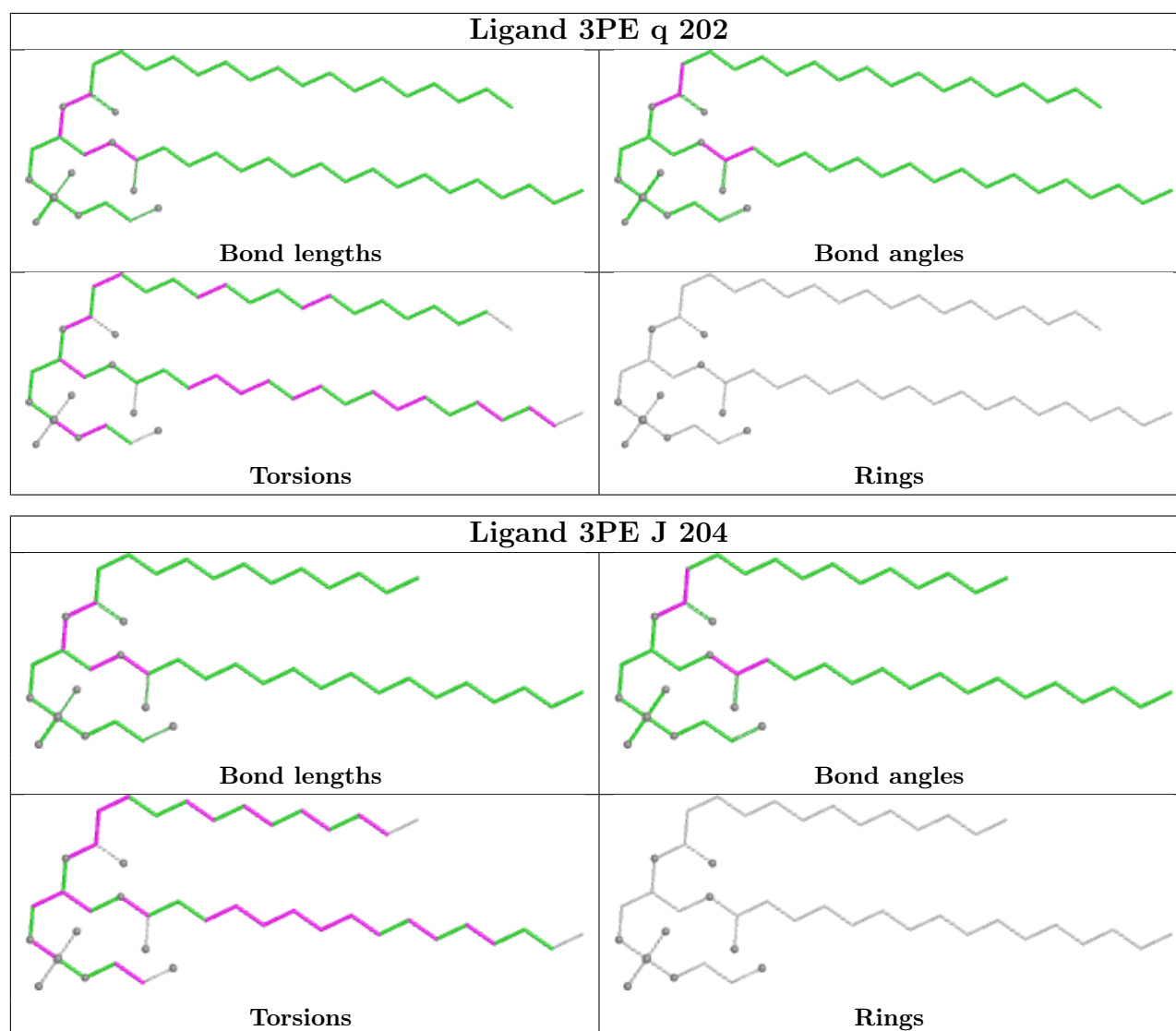












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

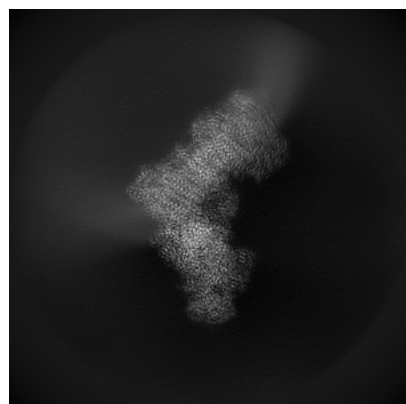
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18141. These allow visual inspection of the internal detail of the map and identification of artifacts.

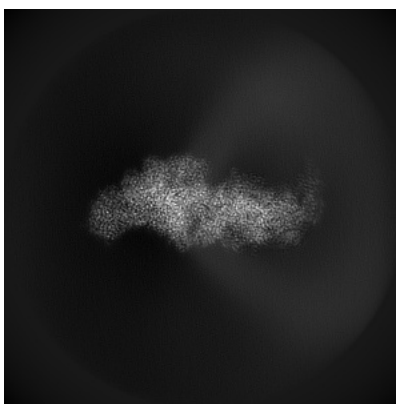
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

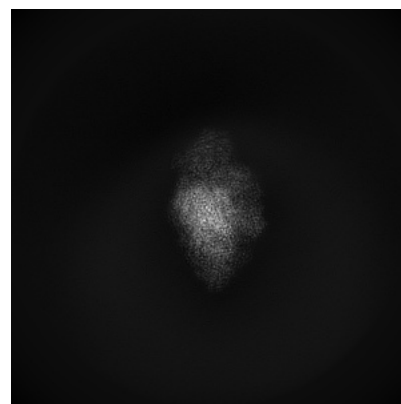
6.1.1 Primary map



X

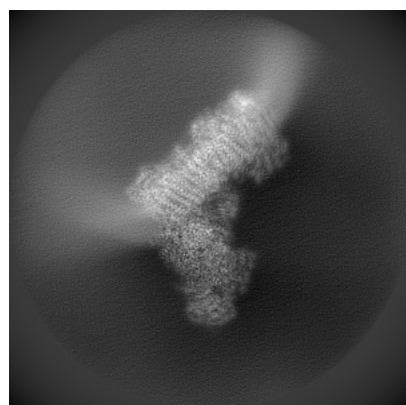


Y

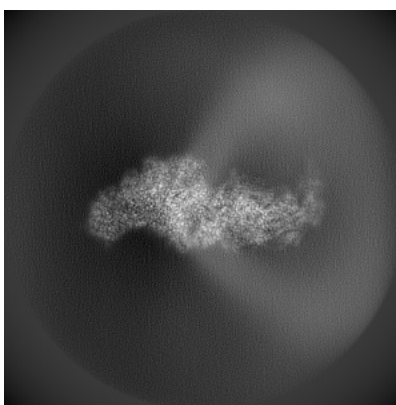


Z

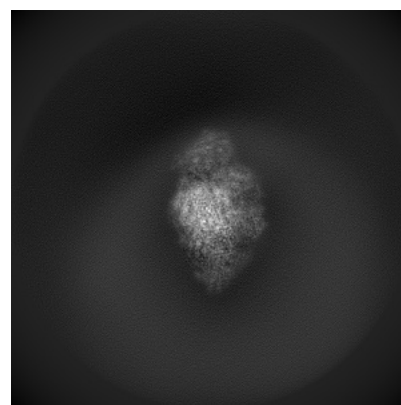
6.1.2 Raw map



X



Y

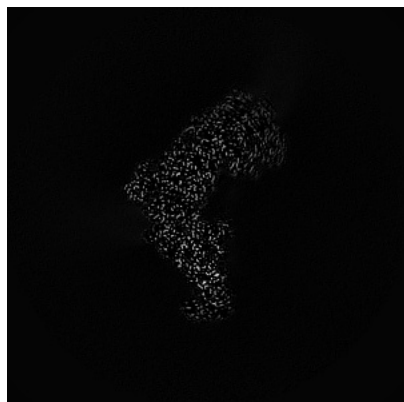


Z

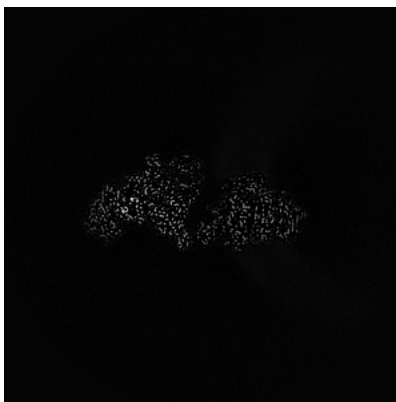
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225

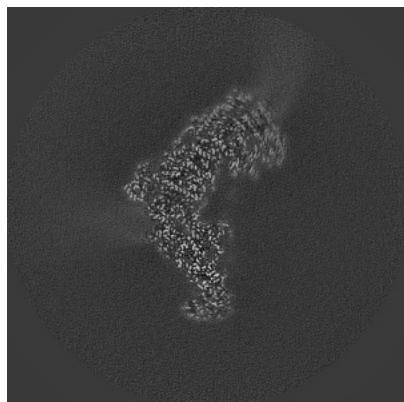


Y Index: 225

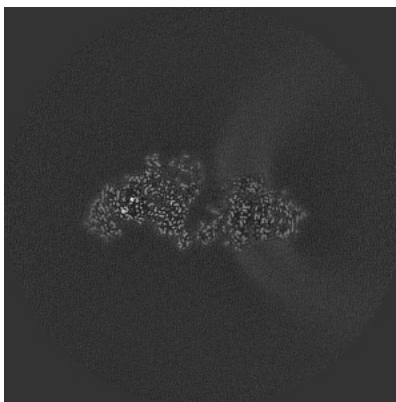


Z Index: 225

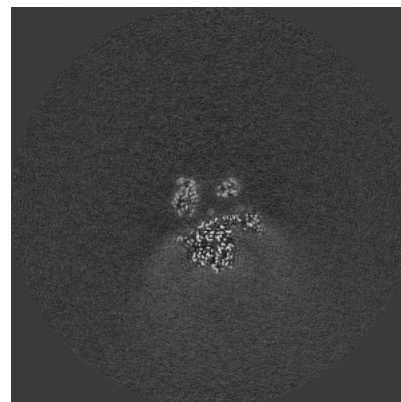
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

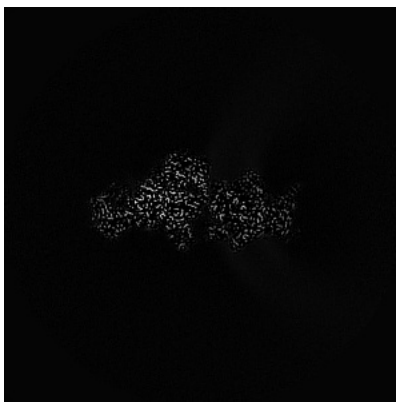
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 234

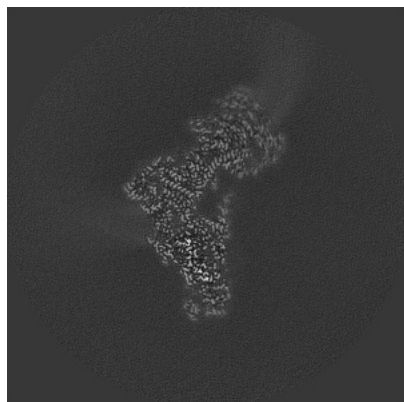


Y Index: 212

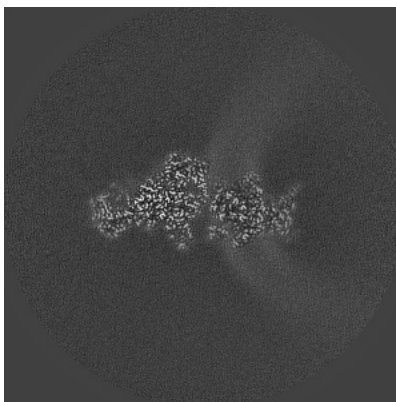


Z Index: 198

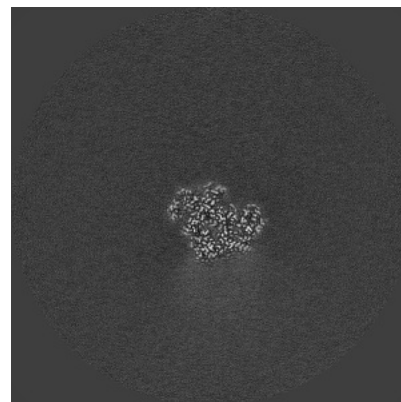
6.3.2 Raw map



X Index: 232



Y Index: 212

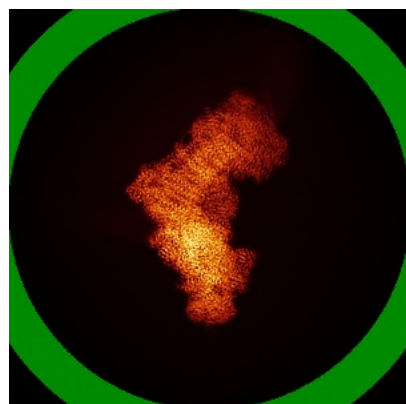


Z Index: 198

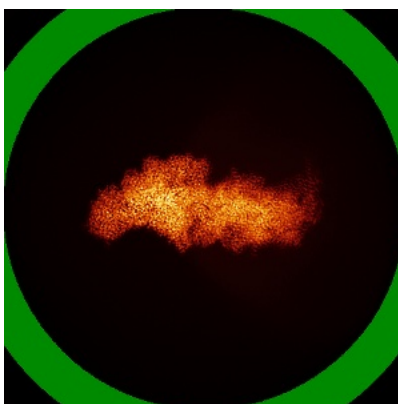
The images above show the largest variance slices of the map in three orthogonal directions.

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

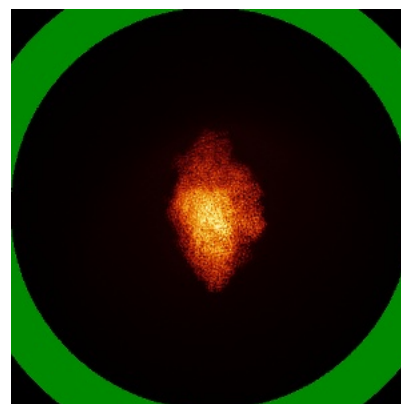
6.4.1 Primary map



X

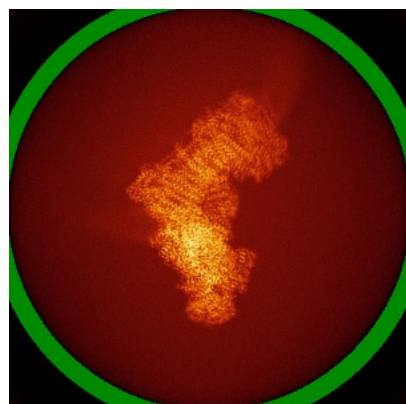


Y

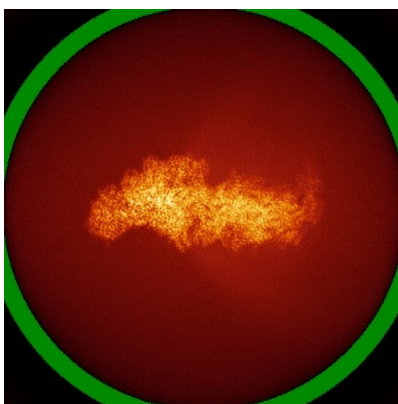


Z

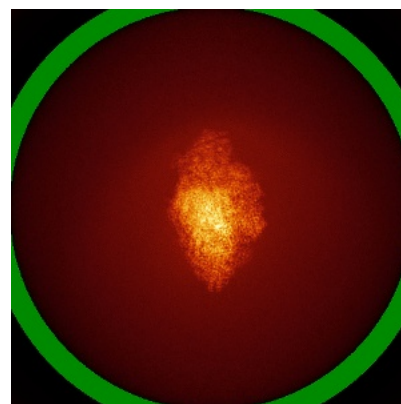
6.4.2 Raw map



X



Y

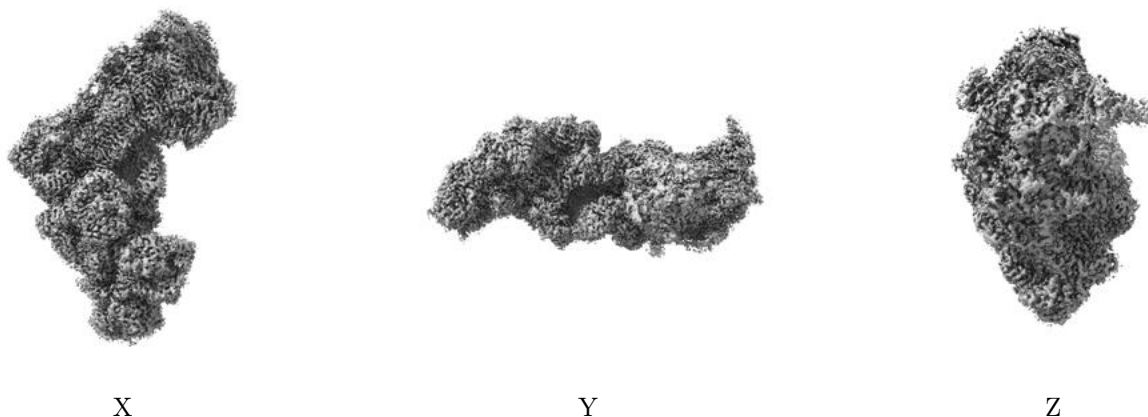


Z

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.

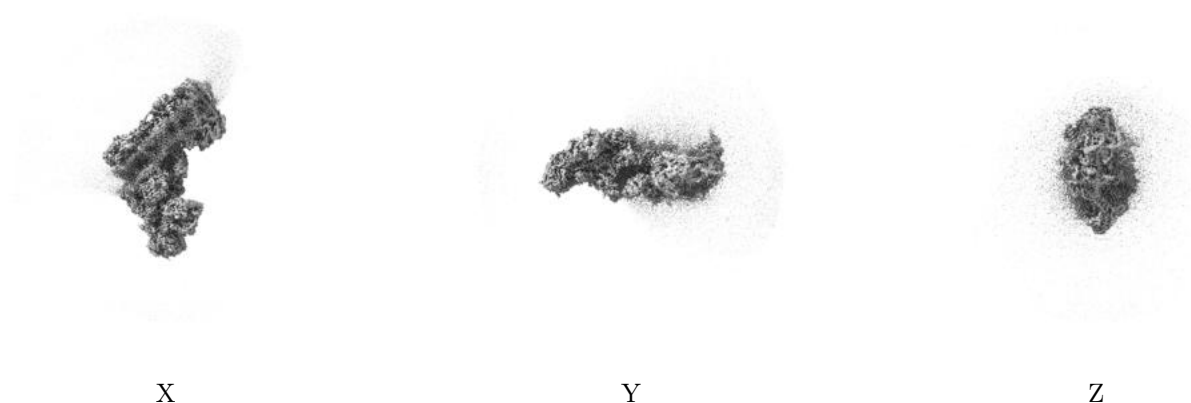
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

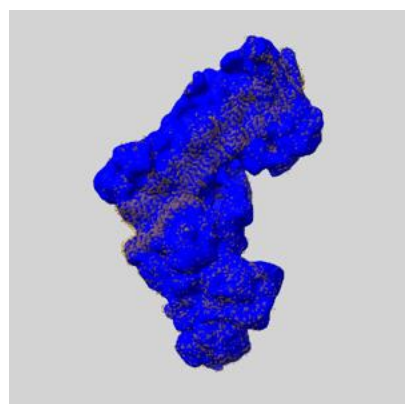
6.6 Mask visualisation [i](#)

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

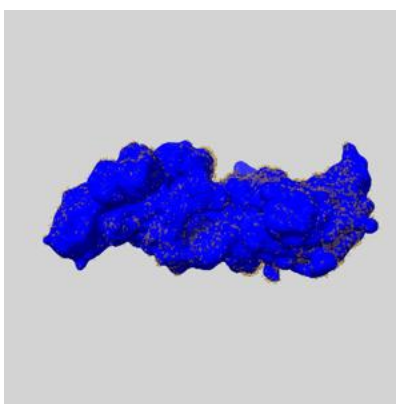
A mask typically either:

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

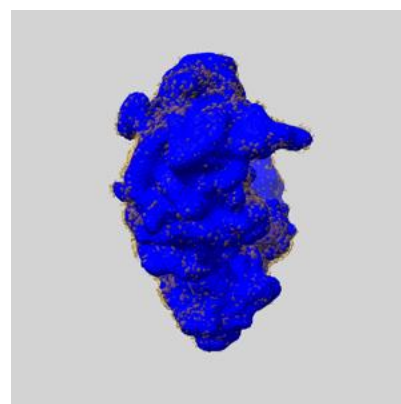
6.6.1 emd_18141_msk_1.map [i](#)



X



Y

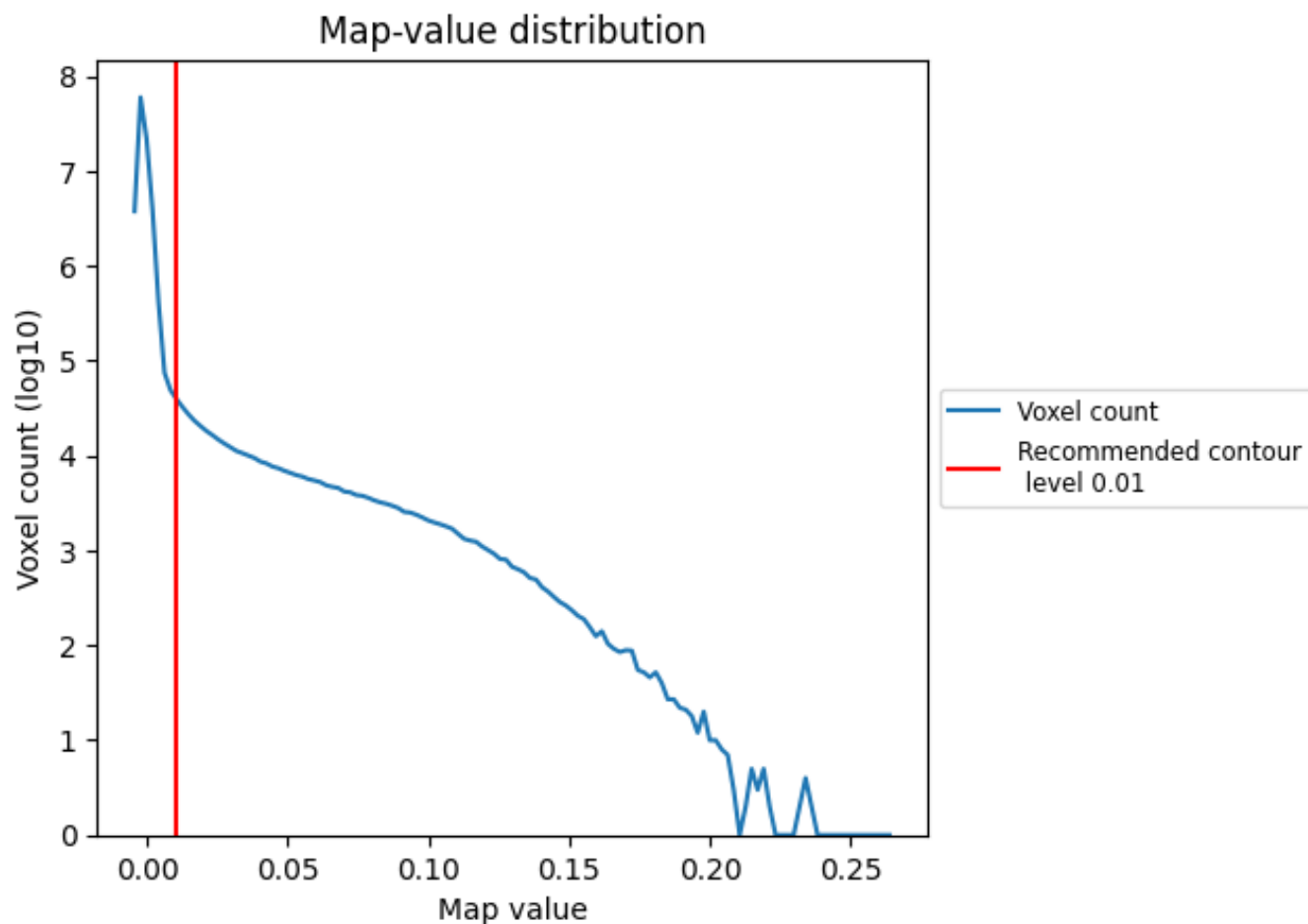


Z

7 Map analysis [i](#)

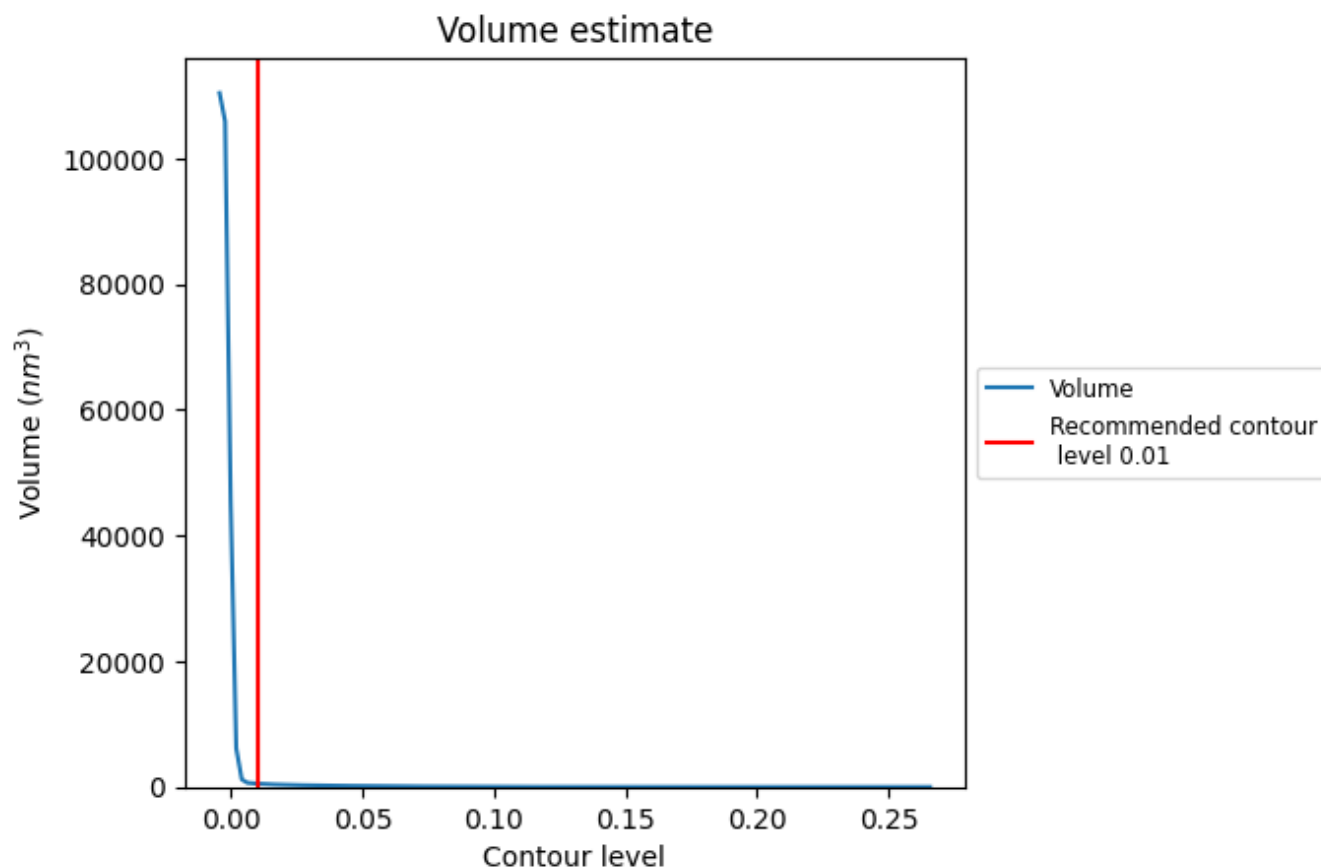
This section contains the results of statistical analysis of the map.

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.

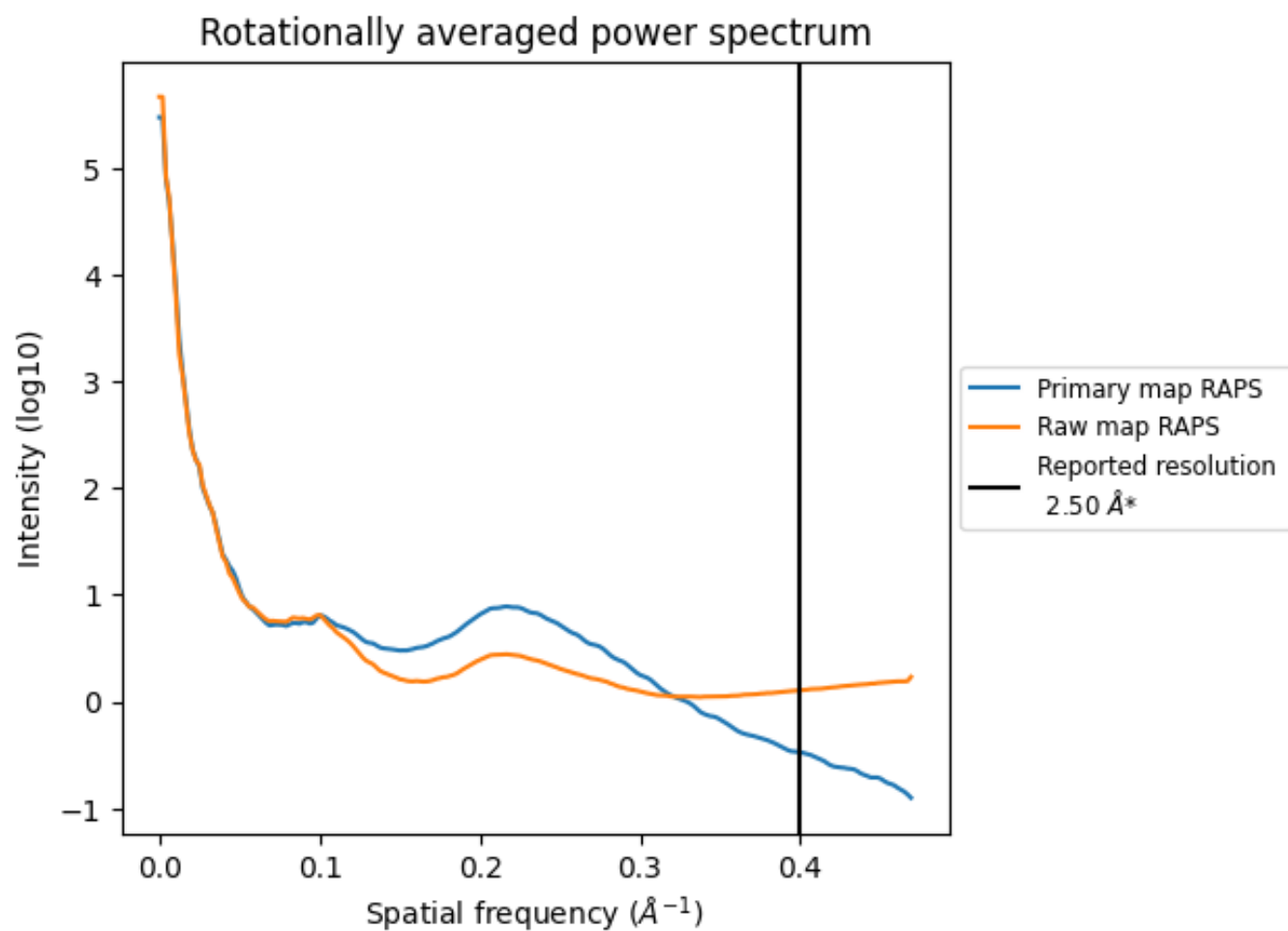
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 520 nm^3 ; this corresponds to an approximate mass of 470 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 ⓘ

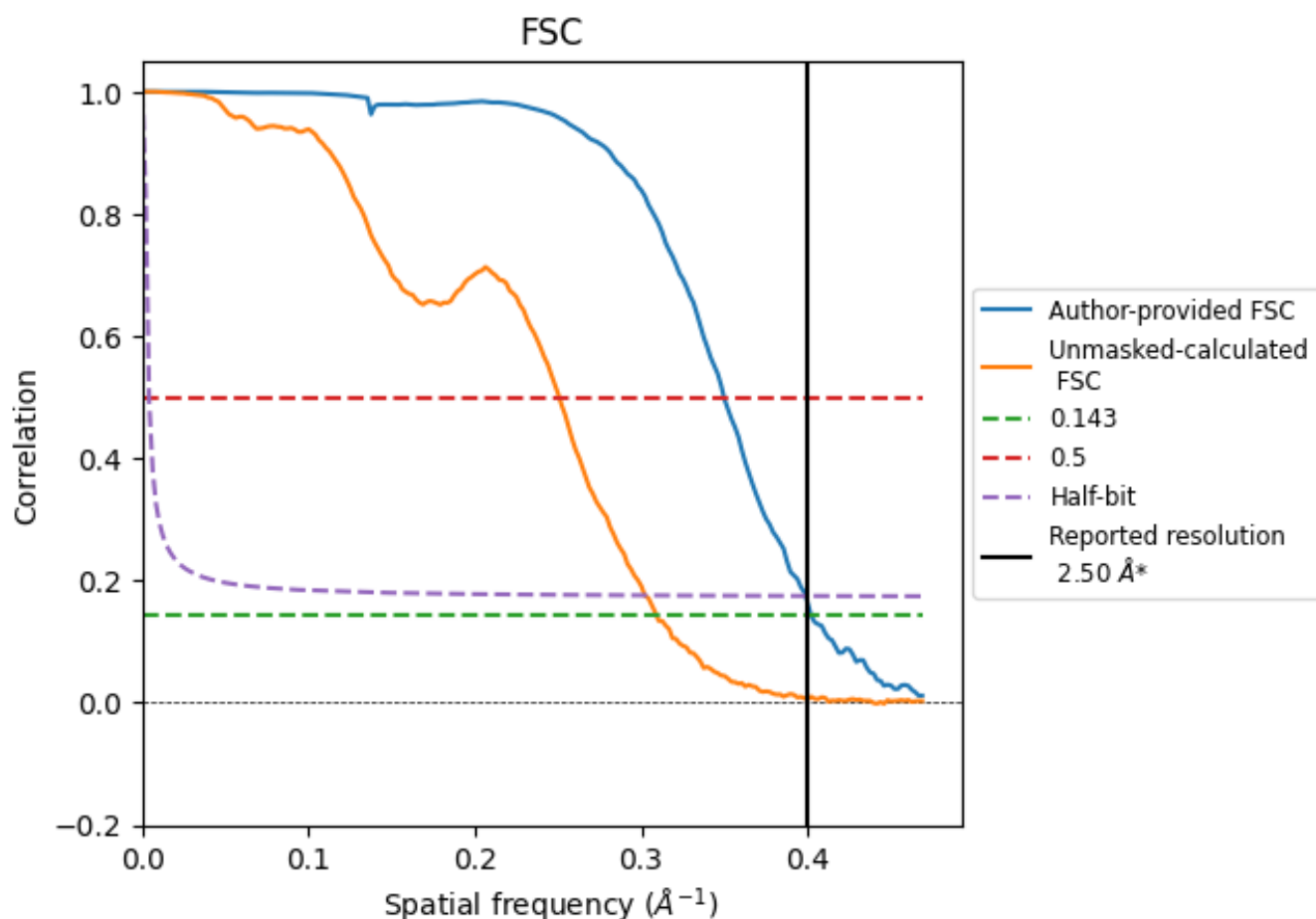


*Reported resolution corresponds to spatial frequency of $0.400 \text{ \AA}^{-1}$

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

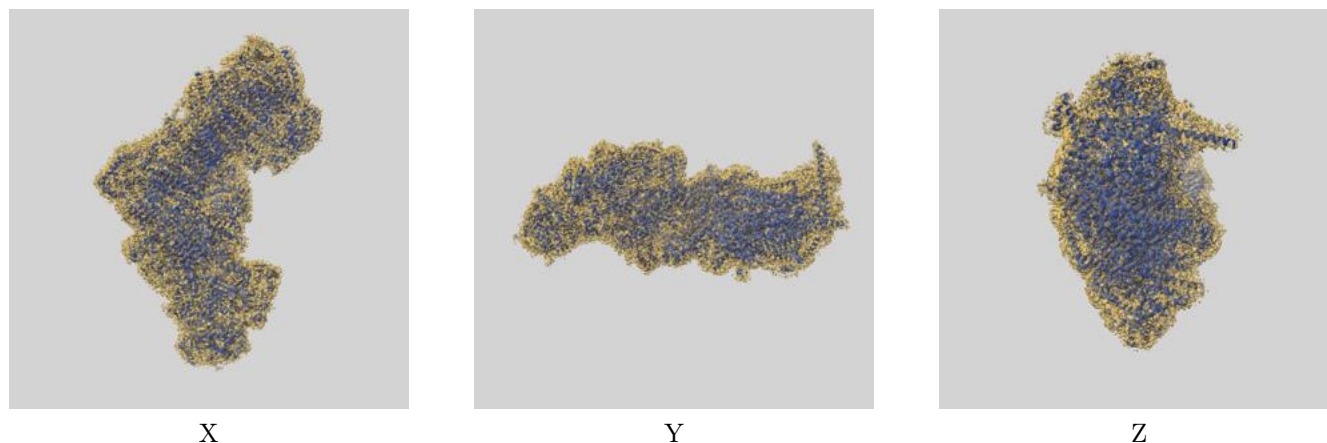
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.86	2.51
Unmasked-calculated*	3.23	3.99	3.31

*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 3.23 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

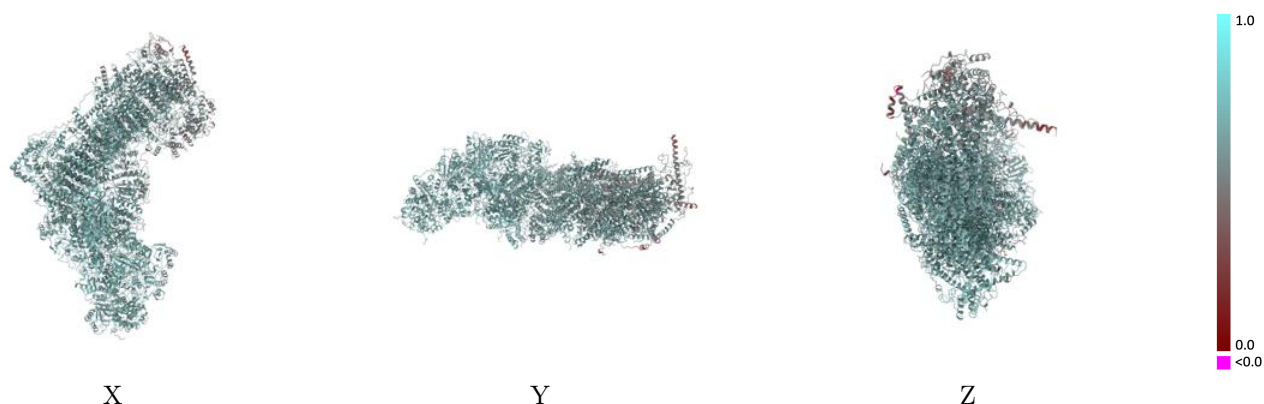
This section contains information regarding the fit between EMDB map EMD-18141 and PDB model 8Q48. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



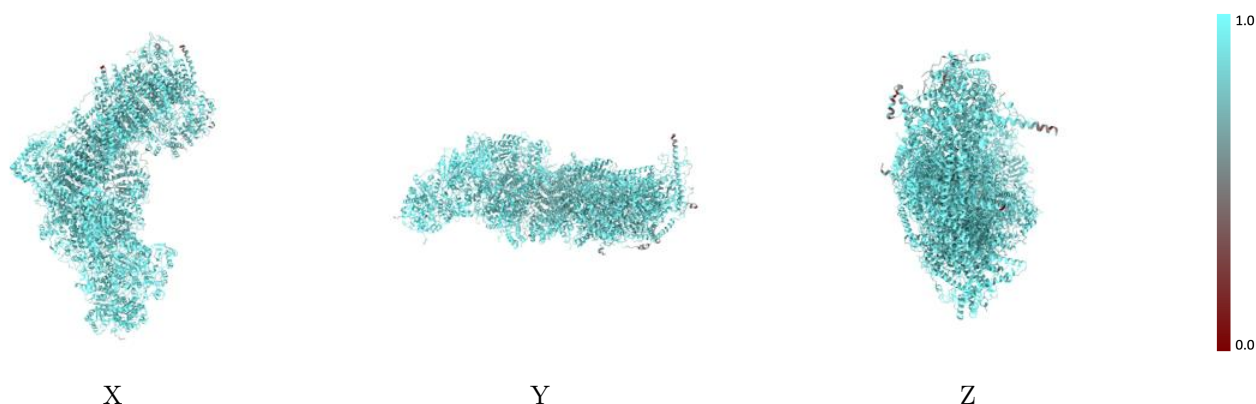
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



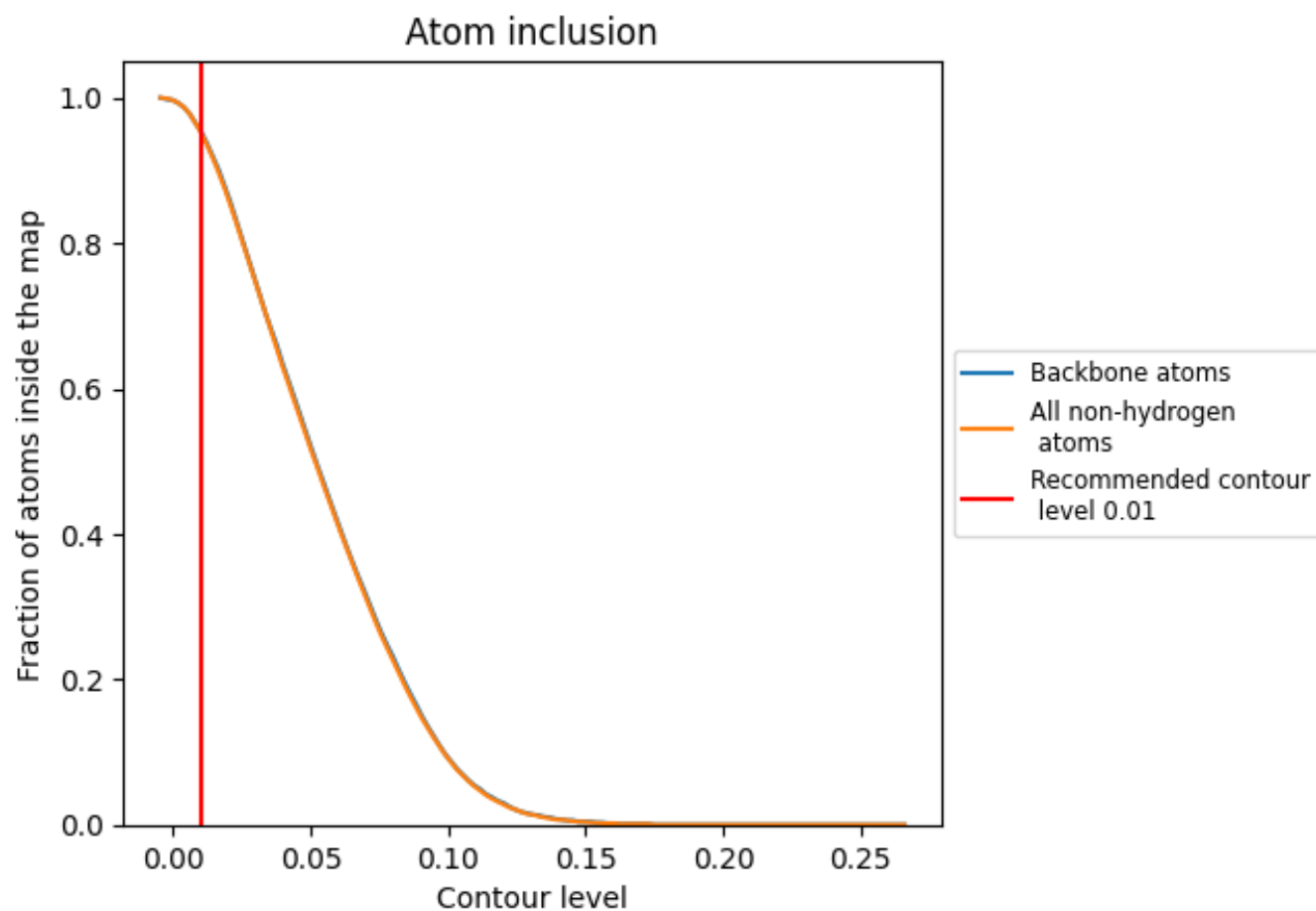
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9540	 0.6370
A	 0.9840	 0.6700
B	 0.9820	 0.6820
C	 0.9850	 0.6900
D	 0.9830	 0.6860
E	 0.9620	 0.6260
F	 0.9720	 0.6500
G	 0.9740	 0.6630
H	 0.9920	 0.6810
I	 0.9870	 0.6900
J	 0.9720	 0.6630
K	 0.9930	 0.6820
L	 0.9500	 0.6060
M	 0.9820	 0.6610
N	 0.9910	 0.6790
O	 0.9490	 0.6220
P	 0.9710	 0.6600
Q	 0.9660	 0.6660
R	 0.9720	 0.6680
S	 0.9290	 0.6030
T	 0.9120	 0.5900
U	 0.8420	 0.4890
V	 0.9700	 0.6600
W	 0.9730	 0.6660
X	 0.9620	 0.6500
Y	 0.9500	 0.6300
Z	 0.9740	 0.6540
a	 0.9760	 0.6670
b	 0.9570	 0.6440
c	 0.9480	 0.6310
d	 0.9550	 0.6440
e	 0.9500	 0.6450
f	 0.8680	 0.5830
g	 0.9200	 0.6050
h	 0.9660	 0.6450



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Chain	Atom inclusion	Q-score
i	 0.8200	 0.5070
j	 0.8450	 0.4960
k	 0.7720	 0.4500
l	 0.9130	 0.5770
m	 0.9090	 0.5860
n	 0.8950	 0.5360
o	 0.8210	 0.4860
p	 0.9040	 0.5880
q	 0.9700	 0.6660
r	 0.9740	 0.6650
s	 0.9080	 0.6040