



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:58 PM UTC

PDB ID : 8Q0M / pdb_00008q0m
EMDB ID : EMD-18055
Title : Outward-facing, closed proteoliposome complex I at 3.1 Å. Initially purified in DDM.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-07-28
Resolution : 3.10 Å(reported)
Based on initial model : 7QSK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

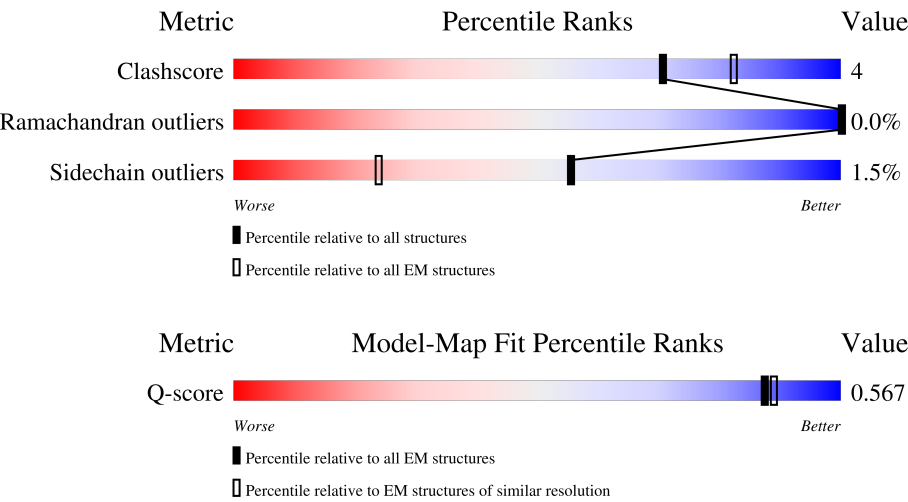
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.



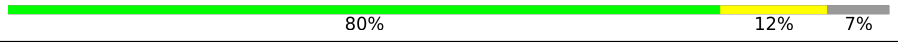
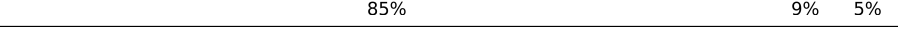
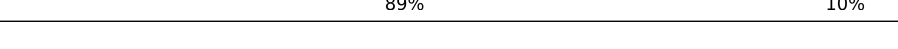
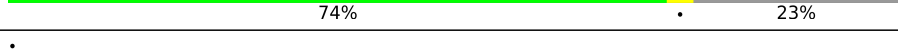
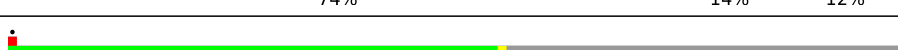
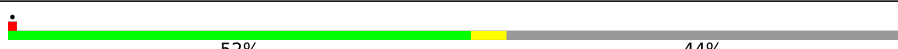
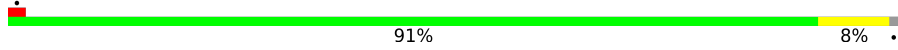
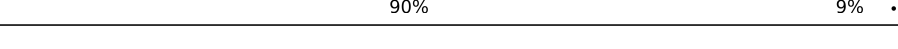
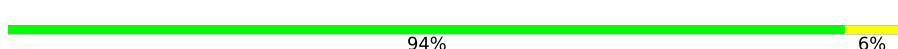
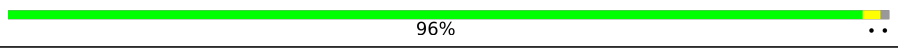
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	88%12%
2	B	216	62%9%28%
3	C	266	71%8%21%
4	D	463	85%7%7%

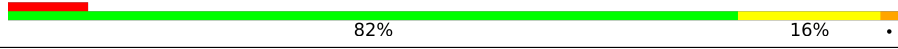
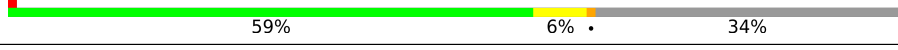
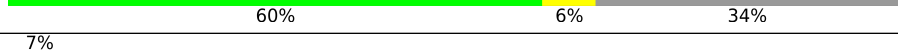
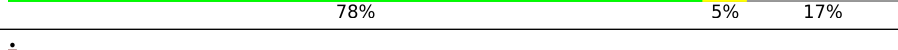
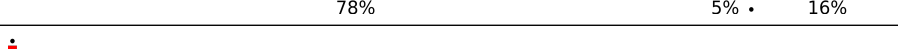
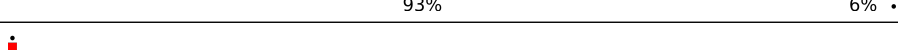
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 70158 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		

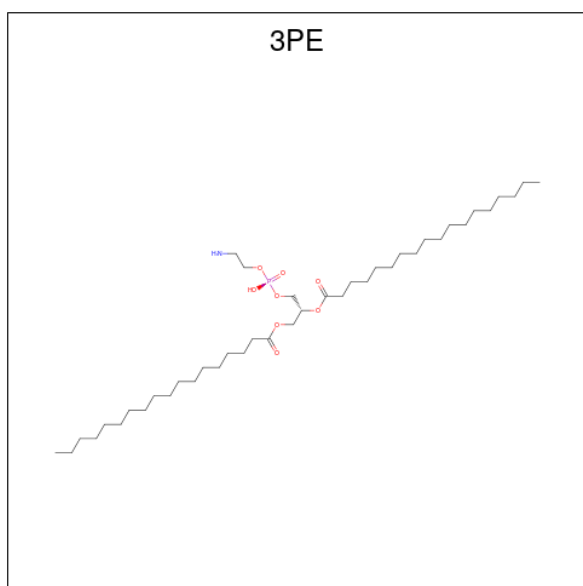
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
45	J	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	

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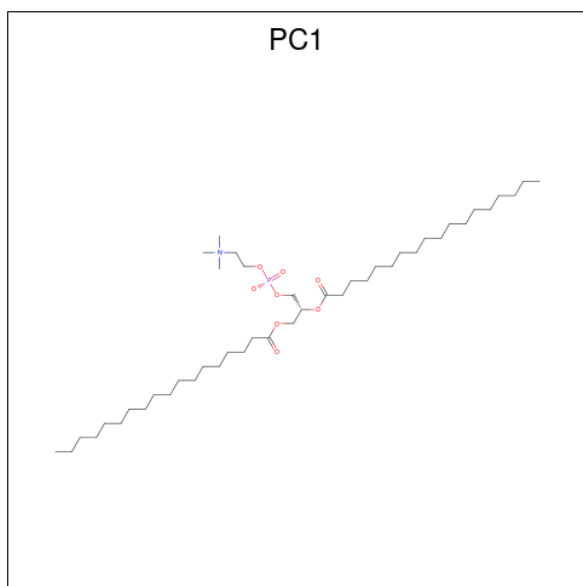
Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total 49	C 39	N 1	O 8	P 1	0
45	N	1	Total 45	C 35	N 1	O 8	P 1	0
45	N	1	Total 51	C 41	N 1	O 8	P 1	0
45	O	1	Total 45	C 35	N 1	O 8	P 1	0
45	P	1	Total 35	C 25	N 1	O 8	P 1	0
45	Y	1	Total 27	C 17	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 45	C 35	N 1	O 8	P 1	0
45	Y	1	Total 36	C 26	N 1	O 8	P 1	0
45	Y	1	Total 43	C 33	N 1	O 8	P 1	0
45	Z	1	Total 41	C 31	N 1	O 8	P 1	0
45	Z	1	Total 51	C 41	N 1	O 8	P 1	0
45	b	1	Total 51	C 41	N 1	O 8	P 1	0
45	e	1	Total 49	C 39	N 1	O 8	P 1	0
45	f	1	Total 34	C 24	N 1	O 8	P 1	0
45	f	1	Total 44	C 34	N 1	O 8	P 1	0
45	i	1	Total 45	C 35	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0
45	m	1	Total 32	C 22	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
45	m	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	q	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	r	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



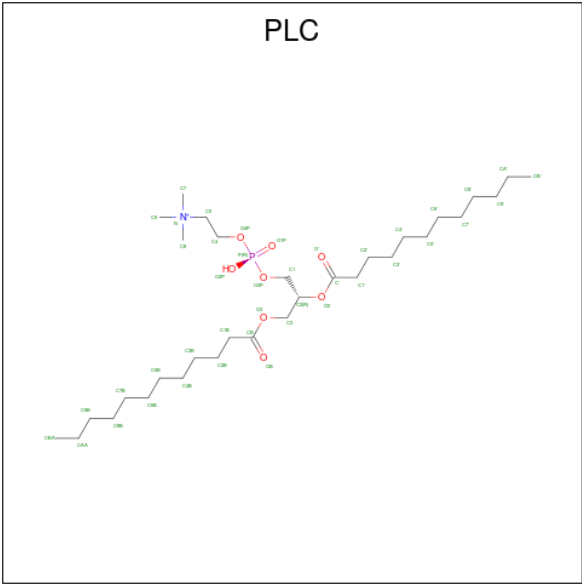
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	H	1	Total	C	N	O	P	0
			39	29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

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Mol	Chain	Residues	Atoms					AltConf
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	e	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	h	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 47 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



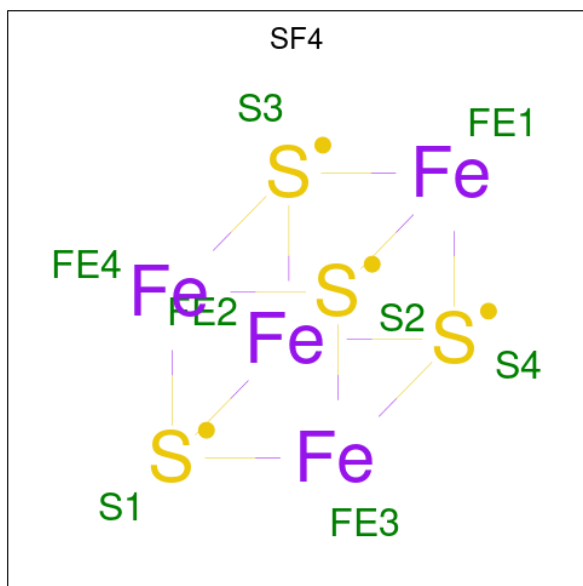
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			33	23	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
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
			42	32	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).



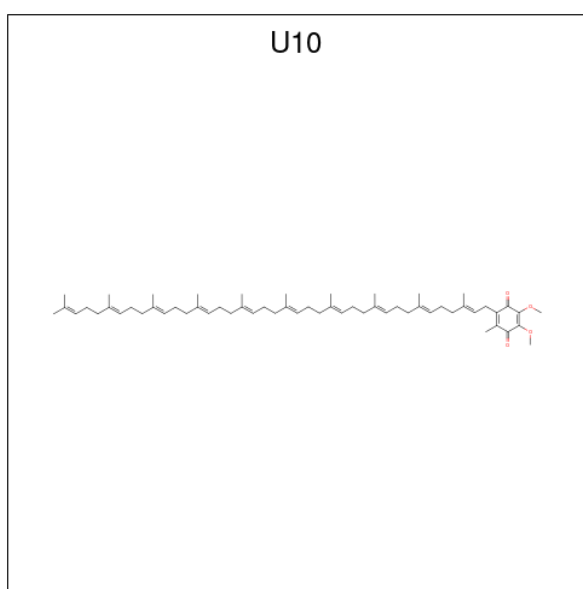
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	

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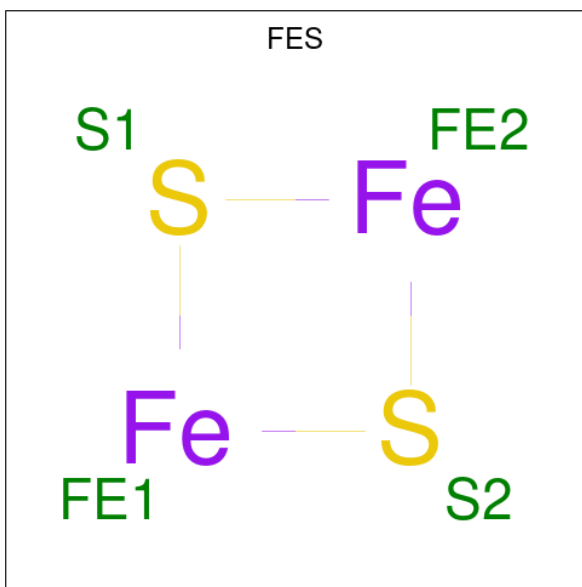
Mol	Chain	Residues	Atoms			AltConf
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



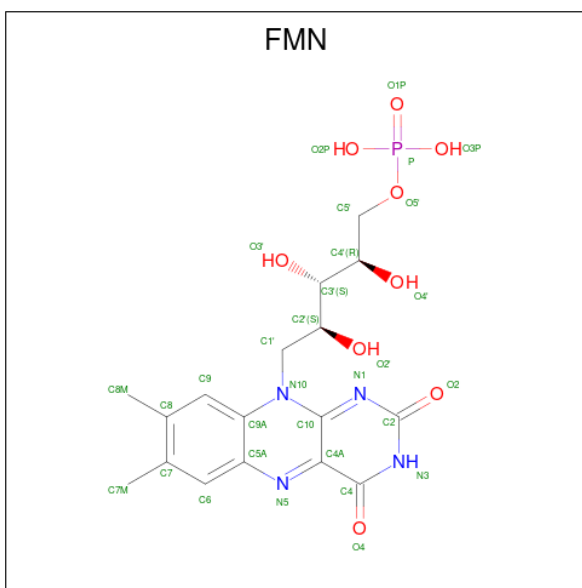
Mol	Chain	Residues	Atoms			AltConf
49	B	1	Total	C	O	0
			63	59	4	

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



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

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

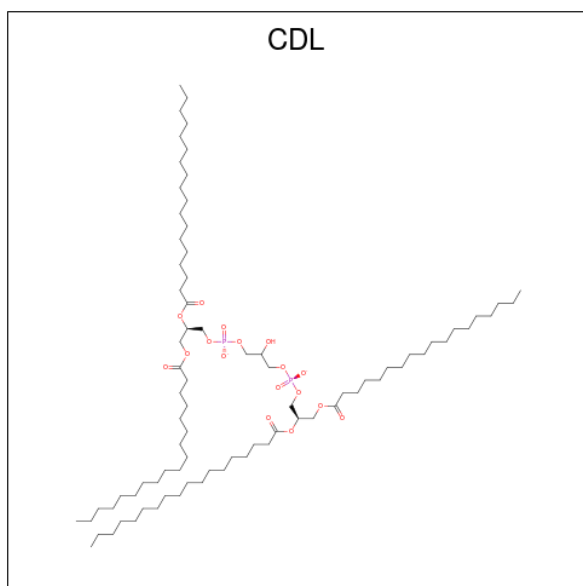


Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total 31	C 17	N 4	O 9	P 1	0

- 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: $C_{81}H_{156}O_{17}P_2$).

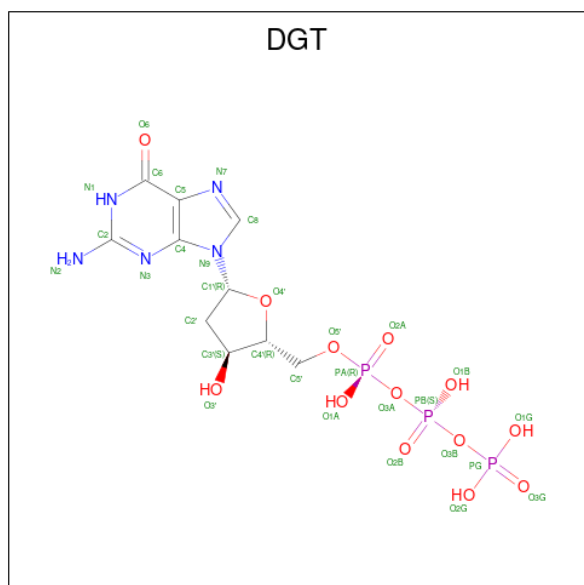


Mol	Chain	Residues	Atoms				AltConf
53	H	1	Total	C	O	P	0
			81	62	17	2	
53	L	1	Total	C	O	P	0
			76	57	17	2	
53	M	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			100	81	17	2	
53	P	1	Total	C	O	P	0
			59	40	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	d	1	Total	C	O	P	0
			86	67	17	2	
53	h	1	Total	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: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

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

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



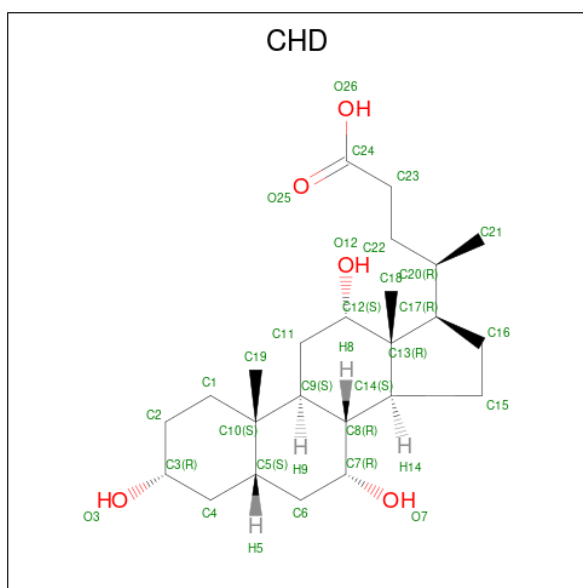
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total 48	C 21	N 7	O 17	P 3	0

- 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).



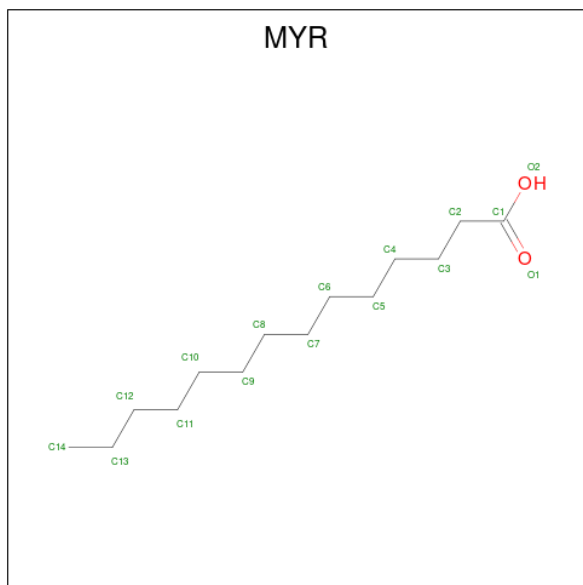
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
58	U	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

- Molecule 59 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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	

3 Residue-property plots [i](#)

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

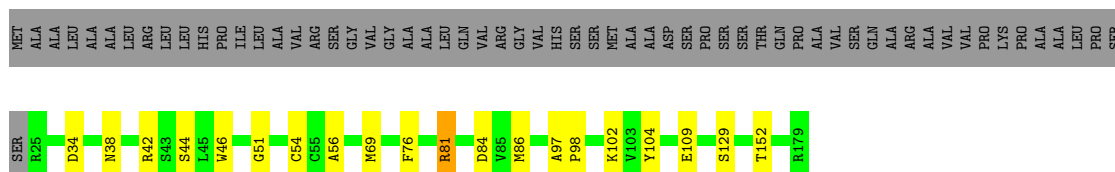
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



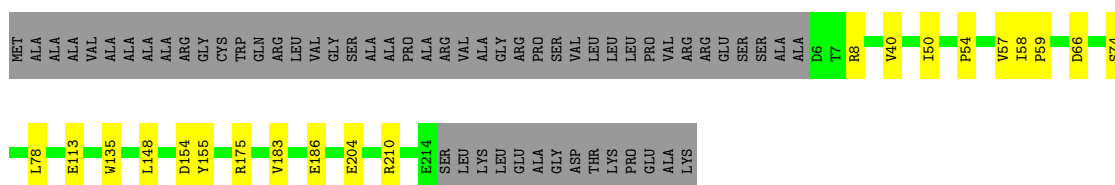
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



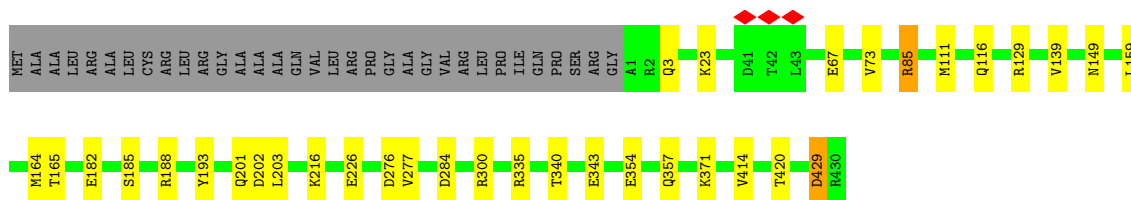
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



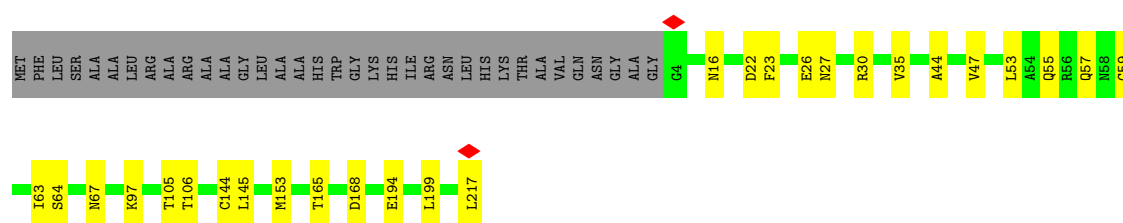
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 



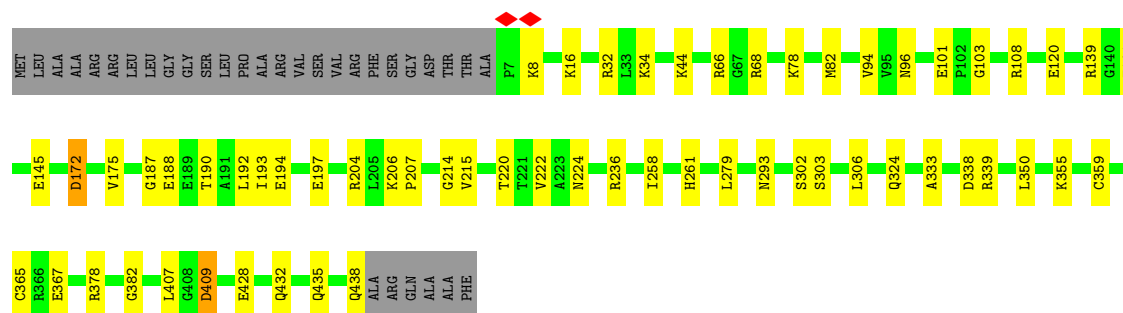
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 



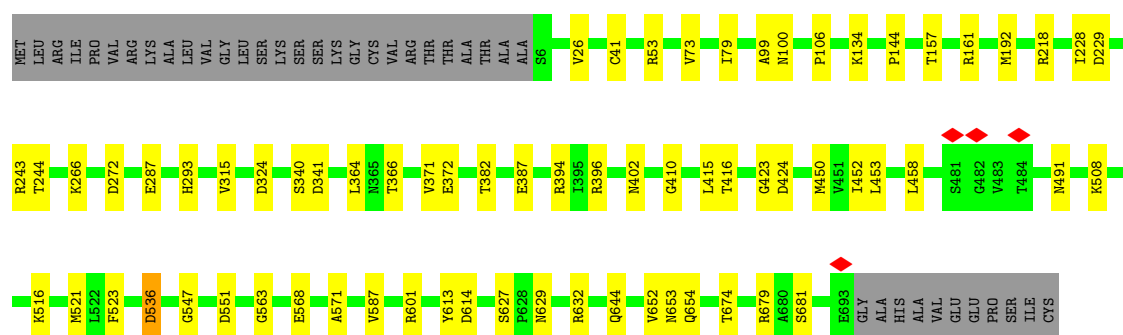
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 



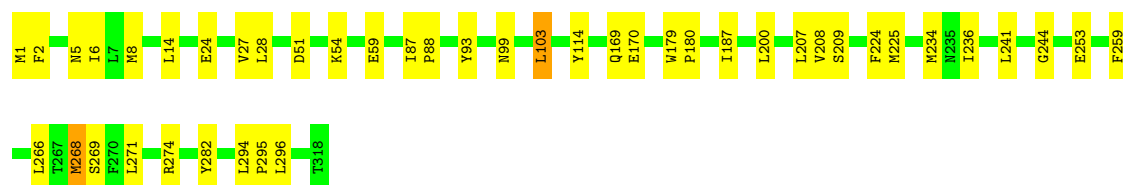
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 



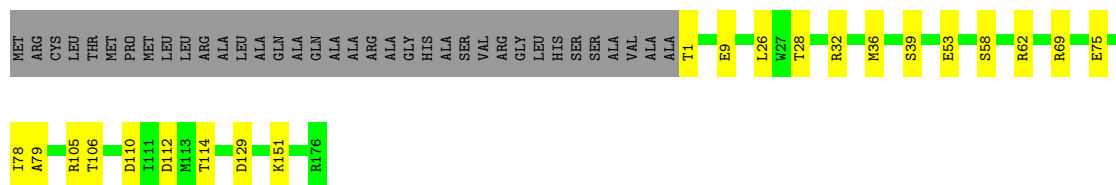
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 



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

Chain I:  73% 10% 17%

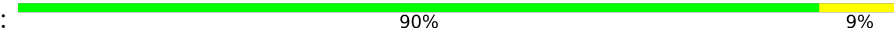


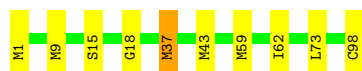
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  87% 12%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  90% 9%

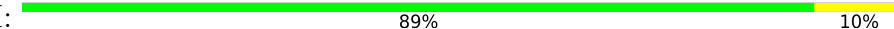


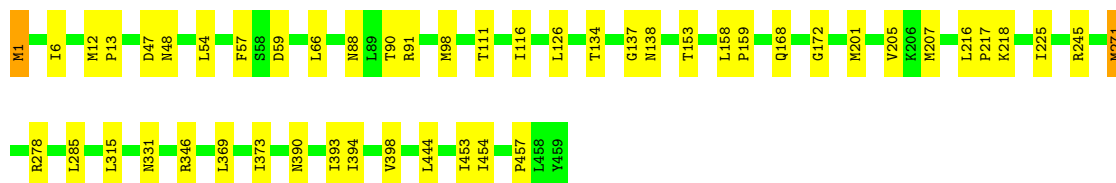
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  89% 11%



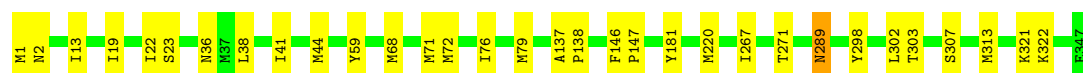
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  89% 10%



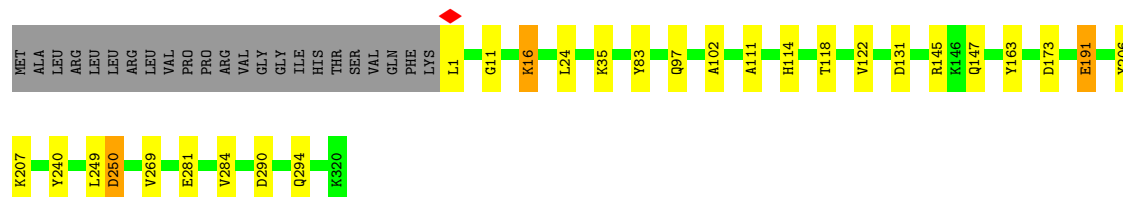
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 



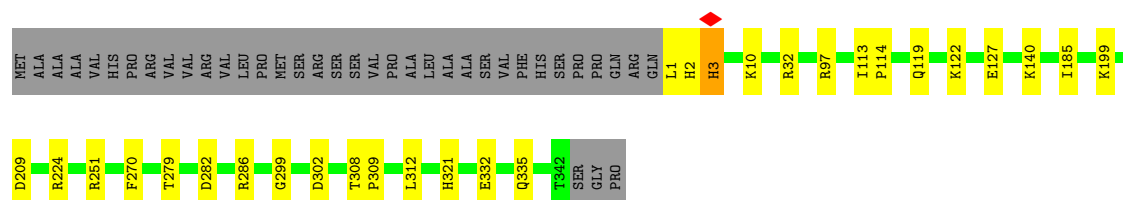
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 



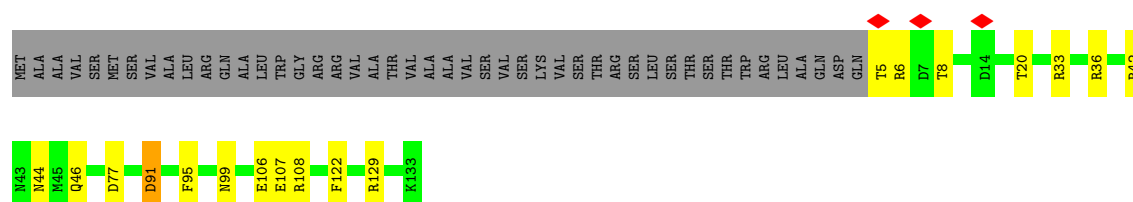
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 



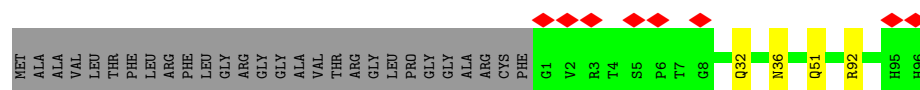
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 



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

Chain R: 

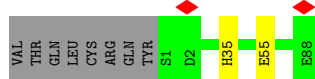


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

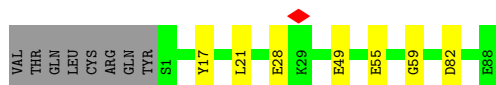
Chain S: 



- Molecule 20: Acyl carrier protein, mitochondrial



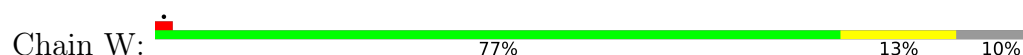
- Molecule 20: Acyl carrier protein, mitochondrial



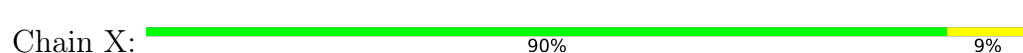
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



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



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

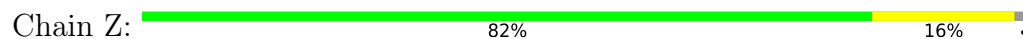


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





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



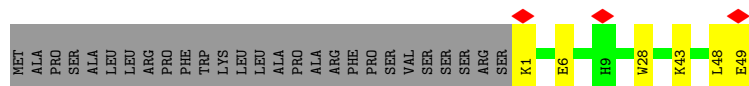
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



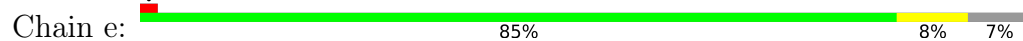
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



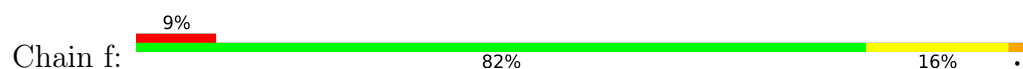
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

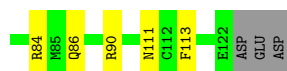
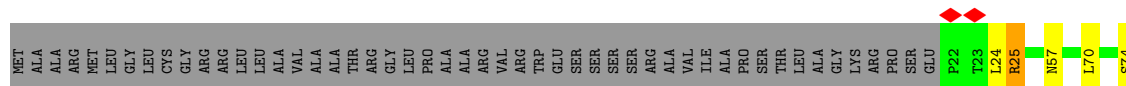


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

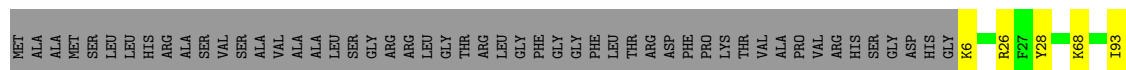




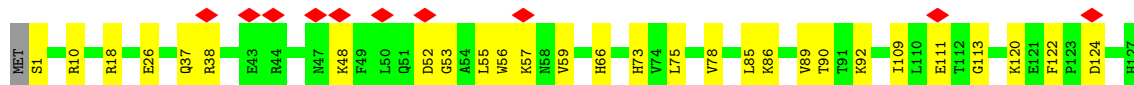
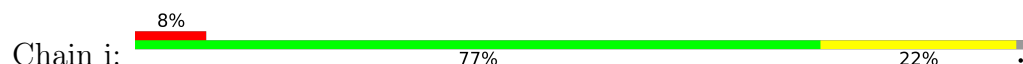
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



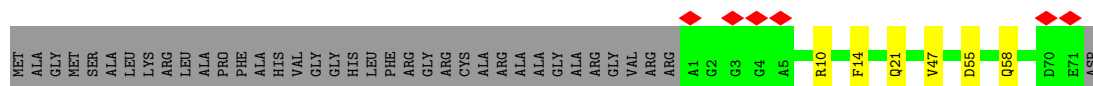
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



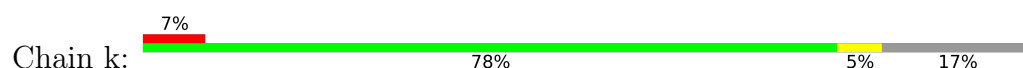
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



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

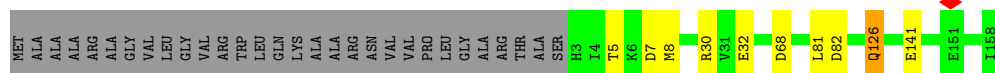


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

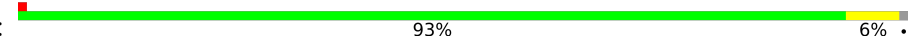


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:  78% 5% 16%



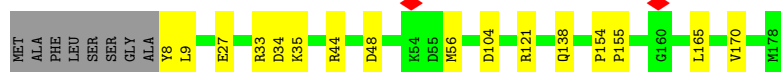
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:  93% 6%



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

Chain n:  87% 9%

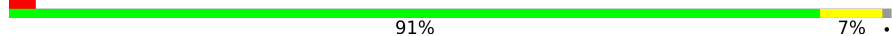


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  9% 80% 9% 11%



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

Chain p:  91% 7%



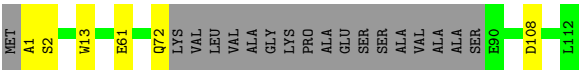
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  91% 9%

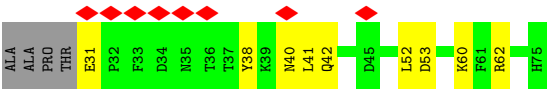
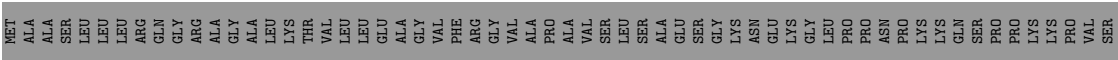


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  79% 5% 16%



● 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	81459	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 ($e^-/\text{\AA}^2$)	39.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/936	0.22	0/1281
2	B	0.16	0/1272	0.27	0/1720
3	C	0.15	0/1789	0.24	0/2436
4	D	0.15	0/3537	0.24	0/4794
5	E	0.11	0/1699	0.25	0/2312
6	F	0.11	0/3401	0.25	0/4595
7	G	0.13	0/5367	0.24	0/7274
8	H	0.14	0/2571	0.25	0/3513
9	I	0.16	0/1445	0.26	0/1956
10	J	0.13	0/1370	0.21	0/1859
11	K	0.13	0/745	0.22	0/1008
12	L	0.11	0/4920	0.23	0/6694
13	M	0.13	0/3738	0.22	0/5097
14	N	0.14	0/2792	0.24	0/3800
15	O	0.11	0/2651	0.21	0/3587
16	P	0.13	0/2831	0.22	0/3841
17	Q	0.13	0/1072	0.23	0/1449
18	R	0.14	0/753	0.20	0/1014
19	S	0.10	0/711	0.22	0/956
20	T	0.11	0/719	0.21	0/971
20	U	0.11	0/719	0.21	0/971
21	V	0.13	0/948	0.21	0/1284
22	W	0.12	0/1000	0.27	0/1344
23	X	0.11	0/1439	0.22	0/1942
24	Y	0.10	0/1042	0.19	0/1414
25	Z	0.12	0/1181	0.20	0/1592
26	a	0.14	0/584	0.21	0/786
27	b	0.10	0/667	0.21	0/916
28	c	0.12	0/427	0.18	0/579
29	d	0.12	0/1018	0.20	0/1375
30	e	0.12	0/850	0.22	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.12	0/505	0.22	0/681
32	g	0.11	0/873	0.23	0/1186
33	h	0.11	0/1188	0.21	0/1607
34	i	0.09	0/1127	0.23	0/1534
35	j	0.11	0/624	0.20	0/855
36	k	0.10	0/672	0.19	0/906
37	l	0.10	0/1369	0.22	0/1873
38	m	0.10	0/1088	0.21	0/1472
39	n	0.09	0/1540	0.21	0/2085
40	o	0.12	0/1073	0.22	0/1437
41	p	0.10	0/1491	0.21	0/2011
42	q	0.12	0/1242	0.21	0/1688
43	r	0.12	0/789	0.23	0/1068
44	s	0.08	0/392	0.21	0/531
All	All	0.12	0/68167	0.23	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	13	0
2	B	1241	0	1251	18	0
3	C	1738	0	1685	13	0
4	D	3459	0	3404	25	0
5	E	1659	0	1664	18	0
6	F	3326	0	3282	36	0
7	G	5279	0	5301	46	0
8	H	2509	0	2621	30	0
9	I	1414	0	1370	18	0
10	J	1345	0	1352	14	0
11	K	745	0	785	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	39	0
13	M	3654	0	3852	35	0
14	N	2733	0	2912	28	0
15	O	2589	0	2566	18	0
16	P	2754	0	2773	18	0
17	Q	1049	0	1045	11	0
18	R	740	0	714	2	0
19	S	700	0	719	9	0
20	T	707	0	700	1	0
20	U	707	0	700	5	0
21	V	928	0	972	5	0
22	W	976	0	991	11	0
23	X	1402	0	1381	9	0
24	Y	1030	0	1039	3	0
25	Z	1152	0	1151	23	0
26	a	569	0	568	3	0
27	b	654	0	663	2	0
28	c	414	0	415	6	0
29	d	999	0	988	6	0
30	e	829	0	829	8	0
31	f	492	0	501	6	0
32	g	846	0	798	7	0
33	h	1154	0	1168	7	0
34	i	1097	0	1108	17	0
35	j	597	0	536	3	0
36	k	653	0	642	3	0
37	l	1314	0	1210	10	0
38	m	1070	0	1068	4	0
39	n	1487	0	1433	11	0
40	o	1048	0	1016	9	0
41	p	1458	0	1430	9	0
42	q	1212	0	1183	7	0
43	r	776	0	782	5	0
44	s	380	0	349	9	0
45	A	135	0	201	0	0
45	J	65	0	81	0	0
45	K	44	0	62	0	0
45	L	51	0	82	1	0
45	N	145	0	221	2	0
45	O	45	0	67	2	0
45	P	35	0	44	0	0
45	Y	304	0	450	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	92	0	141	1	0
45	b	51	0	82	0	0
45	e	49	0	75	2	0
45	f	78	0	107	0	0
45	i	45	0	67	2	0
45	m	164	0	233	0	0
45	q	51	0	82	0	0
45	r	34	0	42	0	0
46	A	68	0	84	2	0
46	B	94	0	136	1	0
46	H	126	0	183	4	0
46	I	98	0	150	2	0
46	J	35	0	44	0	0
46	L	91	0	136	3	0
46	M	35	0	44	0	0
46	e	39	0	52	0	0
46	h	47	0	71	0	0
46	m	54	0	88	0	0
46	q	49	0	75	0	0
47	A	33	0	43	0	0
47	J	37	0	51	0	0
47	L	42	0	64	0	0
47	M	28	0	30	0	0
47	O	35	0	47	0	0
47	P	74	0	105	1	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	1	0
48	I	16	0	0	0	0
49	B	63	0	90	11	0
50	E	4	0	0	0	0
50	G	4	0	0	1	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	1	0
53	M	100	0	156	2	0
53	N	100	0	156	0	0
53	P	59	0	62	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	d	151	0	202	1	0
53	h	80	0	104	0	0
53	r	61	0	66	1	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	31	0	12	2	0
56	O	1	0	0	0	0
57	P	48	0	26	0	0
58	T	37	0	0	0	0
58	U	37	0	0	0	0
59	i	29	0	38	5	0
60	o	15	0	27	1	0
All	All	70158	0	71608	498	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 (498) 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)
12:L:67:HIS:HE2	12:L:70:THR:HG1	1.14	0.90
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.08	0.85
40:o:59:ALA:O	40:o:60:HIS:ND1	2.10	0.84
15:O:191:GLU:OE2	55:O:401:DGT:O3'	1.95	0.84
6:F:194:GLU:OE2	6:F:204:ARG:NH1	2.11	0.83
25:Z:92:GLU:OE2	30:e:91:TYR:OH	2.00	0.79
7:G:293:HIS:ND1	16:P:2:HIS:O	2.15	0.79
59:i:201:CHD:H212	59:i:201:CHD:H12	1.65	0.79
37:l:141:GLU:N	37:l:141:GLU:OE1	2.15	0.79
8:H:253:GLU:OE2	26:a:25:ARG:NH1	2.16	0.78
16:P:10:LYS:NZ	22:W:126:ASP:OD2	2.17	0.78
12:L:485:TYR:O	12:L:489:THR:OG1	2.03	0.78
12:L:35:TYR:HH	34:i:73:HIS:HE2	0.77	0.77
15:O:97:GLN:NE2	15:O:131:ASP:OD1	2.17	0.77
1:A:71:LEU:O	10:J:147:TYR:OH	2.04	0.76
3:C:8:ARG:NH1	43:r:61:GLU:OE2	2.19	0.76
15:O:83:TYR:OH	55:O:401:DGT:O3'	2.03	0.76
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.19	0.76
32:g:86:GLN:NE2	41:p:100:GLU:OE2	2.20	0.75
16:P:335:GLN:N	16:P:335:GLN:OE1	2.18	0.75
33:h:140:THR:O	33:h:143:ASN:ND2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:75:GLU:O	9:I:105:ARG:NH1	2.20	0.74
10:J:77:GLU:N	10:J:77:GLU:OE1	2.19	0.74
14:N:298:TYR:O	14:N:303:THR:OG1	2.03	0.74
28:c:1:LYS:NZ	28:c:6:GLU:OE1	2.19	0.74
1:A:33:LYS:O	2:B:81:ARG:NH2	2.21	0.74
41:p:143:HIS:O	41:p:157:LYS:NZ	2.19	0.74
7:G:632:ARG:NH2	19:S:58:SER:O	2.21	0.73
5:E:63:ILE:O	5:E:67:ASN:ND2	2.22	0.73
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.21	0.73
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.21	0.72
12:L:561:ILE:O	12:L:565:THR:OG1	2.06	0.72
11:K:73:LEU:HD21	14:N:41:ILE:HD12	1.70	0.72
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.20	0.71
7:G:644:GLN:N	7:G:644:GLN:OE1	2.23	0.71
4:D:226:GLU:OE1	25:Z:22:ARG:NH1	2.24	0.70
19:S:39:ARG:NH2	19:S:84:ASP:OD1	2.25	0.70
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.23	0.70
6:F:32:ARG:NH1	44:s:42:GLN:OE1	2.24	0.70
11:K:43:MET:SD	14:N:72:MET:HE1	2.32	0.69
19:S:23:CYS:O	19:S:33:ARG:NH1	2.25	0.69
4:D:182:GLU:OE1	9:I:58:SER:OG	2.05	0.69
9:I:28:THR:HG22	25:Z:34:MET:HE1	1.74	0.69
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.25	0.68
43:r:72:GLN:N	43:r:72:GLN:OE1	2.27	0.68
20:T:55:GLU:OE2	22:W:36:ARG:NH2	2.26	0.68
9:I:9:GLU:N	9:I:9:GLU:OE1	2.27	0.68
34:i:10:ARG:NH1	39:n:154:PRO:O	2.27	0.68
8:H:266:LEU:O	8:H:269:SER:OG	2.10	0.68
20:U:28:GLU:N	20:U:28:GLU:OE1	2.27	0.67
13:M:278:ARG:NE	37:l:82:ASP:OD2	2.24	0.67
30:e:58:GLU:N	30:e:58:GLU:OE1	2.27	0.67
39:n:34:ASP:OD1	39:n:35:LYS:N	2.26	0.67
40:o:23:THR:OG1	40:o:104:GLU:OE2	2.07	0.67
13:M:457:PRO:O	32:g:84:ARG:NH2	2.29	0.66
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.30	0.66
31:f:32:GLU:N	31:f:32:GLU:OE1	2.28	0.66
7:G:287:GLU:OE1	7:G:287:GLU:N	2.28	0.66
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.27	0.66
7:G:415:LEU:O	7:G:416:THR:OG1	2.10	0.65
14:N:19:ILE:O	14:N:23:SER:OG	2.07	0.65
2:B:44:SER:O	8:H:54:LYS:NZ	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:127:GLU:N	41:p:127:GLU:OE1	2.30	0.65
6:F:224:ASN:ND2	51:F:501:FMN:O2	2.30	0.65
6:F:66:ARG:O	6:F:68:ARG:NH1	2.30	0.65
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.15	0.64
13:M:66:LEU:HD11	13:M:111:THR:HG23	1.79	0.64
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.16	0.64
12:L:467:ILE:O	12:L:471:ASN:ND2	2.30	0.64
32:g:90:ARG:NH2	41:p:107:GLU:OE2	2.31	0.64
6:F:428:GLU:OE2	6:F:432:GLN:NE2	2.31	0.64
7:G:99:ALA:O	7:G:134:LYS:NZ	2.30	0.64
17:Q:33:ARG:NH1	17:Q:77:ASP:OD1	2.31	0.64
34:i:120:LYS:NZ	40:o:37:GLU:OE2	2.30	0.64
12:L:171:ALA:O	12:L:175:ASN:ND2	2.31	0.63
37:l:30:ARG:NH1	38:m:34:GLU:OE1	2.30	0.63
8:H:99:ASN:N	46:H:401:PC1:O12	2.31	0.63
5:E:22:ASP:OD1	5:E:23:PHE:N	2.30	0.63
6:F:96:ASN:ND2	6:F:187:GLY:O	2.29	0.63
3:C:113:GLU:N	3:C:113:GLU:OE1	2.32	0.62
5:E:30:ARG:NH2	44:s:53:ASP:OD1	2.32	0.62
34:i:37:GLN:NE2	34:i:38:ARG:O	2.32	0.62
17:Q:107:GLU:OE1	17:Q:108:ARG:N	2.32	0.62
44:s:31:GLU:N	44:s:31:GLU:OE1	2.33	0.62
13:M:394:ILE:O	13:M:398:VAL:HG23	2.00	0.62
2:B:76:PHE:CE2	49:B:202:U10:H152	2.34	0.62
7:G:272:ASP:OD1	7:G:681:SER:OG	2.16	0.62
5:E:26:GLU:OE1	5:E:26:GLU:N	2.31	0.62
12:L:560:ALA:O	12:L:565:THR:HG23	2.00	0.61
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.32	0.61
41:p:116:GLU:OE1	41:p:123:ASN:ND2	2.34	0.61
6:F:145:GLU:N	6:F:145:GLU:OE1	2.31	0.61
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.34	0.61
13:M:98:MET:HE1	53:M:604:CDL:C87	2.31	0.61
9:I:106:THR:O	9:I:151:LYS:NZ	2.31	0.61
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.33	0.61
20:U:21:LEU:HD13	36:k:37:ASN:HA	1.82	0.61
16:P:270:PHE:HD2	16:P:279:THR:HG22	1.66	0.61
3:C:183:VAL:O	22:W:100:THR:OG1	2.15	0.61
4:D:284:ASP:OD1	9:I:1:THR:OG1	2.15	0.61
34:i:92:LYS:NZ	45:i:202:3PE:O14	2.33	0.61
15:O:173:ASP:OD2	15:O:207:LYS:NZ	2.28	0.60
13:M:98:MET:HE2	13:M:98:MET:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:88:GLU:OE1	25:Z:127:ARG:NH2	2.34	0.60
6:F:407:LEU:HD23	6:F:407:LEU:O	2.00	0.60
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.84	0.60
14:N:220:MET:O	14:N:321:LYS:NZ	2.35	0.60
15:O:240:TYR:OH	21:V:21:GLU:OE1	2.18	0.60
10:J:168:ILE:O	10:J:172:THR:OG1	2.19	0.60
45:Y:202:3PE:O12	45:Y:204:3PE:N	2.22	0.60
9:I:28:THR:CG2	25:Z:34:MET:HE1	2.32	0.60
43:r:2:SER:O	53:r:202:CDL:O1	2.20	0.60
4:D:67:GLU:N	4:D:67:GLU:OE1	2.35	0.59
39:n:56:MET:HA	39:n:56:MET:HE2	1.84	0.59
25:Z:85:MET:HE1	25:Z:124:TYR:CE2	2.37	0.59
2:B:34:ASP:OD1	2:B:38:ASN:ND2	2.35	0.59
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.83	0.59
22:W:110:GLU:OE1	22:W:110:GLU:N	2.36	0.59
16:P:251:ARG:NH1	16:P:321:HIS:O	2.35	0.59
46:L:703:PC1:H3I3	13:M:398:VAL:HG22	1.84	0.58
1:A:115:GLU:N	1:A:115:GLU:OE1	2.35	0.58
34:i:111:GLU:OE1	34:i:111:GLU:N	2.36	0.58
2:B:69:MET:HE1	2:B:76:PHE:CD2	2.38	0.58
46:H:401:PC1:H142	25:Z:142:TYR:O	2.04	0.58
7:G:627:SER:OG	7:G:629:ASN:OD1	2.21	0.58
7:G:512:GLU:OE2	7:G:516:LYS:NZ	2.38	0.57
12:L:87:MET:HA	12:L:87:MET:HE2	1.85	0.57
5:E:144:CYS:O	6:F:139:ARG:NH2	2.36	0.57
33:h:6:LYS:NZ	34:i:26:GLU:OE2	2.33	0.57
10:J:33:LEU:HD23	10:J:64:MET:SD	2.44	0.57
15:O:281:GLU:N	15:O:281:GLU:OE1	2.36	0.57
7:G:654:GLN:OE1	7:G:654:GLN:N	2.38	0.57
10:J:2:MET:HA	10:J:2:MET:HE2	1.86	0.57
11:K:9:MET:HE3	14:N:79:MET:HE1	1.87	0.57
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.87	0.57
6:F:261:HIS:ND1	6:F:338:ASP:OD1	2.38	0.56
8:H:169:GLN:OE1	8:H:244:GLY:N	2.35	0.56
12:L:132:VAL:O	12:L:262:ARG:NH2	2.38	0.56
28:c:43:LYS:HG2	28:c:48:LEU:HD11	1.86	0.56
9:I:32:ARG:NH2	25:Z:25:PRO:O	2.36	0.56
7:G:341:ASP:O	7:G:508:LYS:NZ	2.35	0.56
25:Z:20:TYR:OH	43:r:108:ASP:OD2	2.22	0.56
8:H:207:LEU:O	8:H:209:SER:N	2.38	0.56
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:43:MET:HE1	14:N:72:MET:HE1	1.88	0.56
18:R:51:GLN:OE1	18:R:92:ARG:NH2	2.39	0.56
4:D:300:ARG:NH2	4:D:420:THR:O	2.38	0.55
3:C:148:LEU:O	22:W:87:MET:HE2	2.07	0.55
34:i:86:LYS:O	34:i:90:THR:OG1	2.24	0.55
42:q:32:ASP:OD2	42:q:58:ARG:NH2	2.40	0.55
7:G:372:GLU:OE2	7:G:394:ARG:NH1	2.39	0.55
7:G:547:GLY:O	7:G:563:GLY:N	2.36	0.55
17:Q:36:ARG:NH2	17:Q:106:GLU:OE1	2.40	0.55
2:B:46:TRP:CZ2	49:B:202:U10:H401	2.42	0.55
12:L:559:GLU:OE2	13:M:218:LYS:NZ	2.36	0.55
4:D:343:GLU:N	4:D:343:GLU:OE1	2.36	0.55
22:W:95:VAL:HG12	22:W:95:VAL:O	2.06	0.55
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.40	0.54
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.37	0.54
20:U:55:GLU:O	20:U:59:GLY:N	2.38	0.54
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.40	0.54
11:K:9:MET:CE	14:N:79:MET:HE1	2.37	0.54
15:O:147:GLN:OE1	15:O:147:GLN:N	2.36	0.54
5:E:55:GLN:O	5:E:59:GLY:N	2.36	0.54
11:K:43:MET:CE	14:N:72:MET:HE1	2.38	0.54
42:q:78:ASP:OD2	42:q:80:SER:OG	2.24	0.54
1:A:28:ASN:ND2	2:B:109:GLU:OE2	2.41	0.54
6:F:197:GLU:OE1	17:Q:129:ARG:NH1	2.36	0.54
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.90	0.53
42:q:114:LYS:HE2	42:q:117:LEU:HD11	1.89	0.53
7:G:568:GLU:HG2	7:G:587:VAL:HG23	1.90	0.53
3:C:204:GLU:OE1	3:C:210:ARG:NH1	2.42	0.53
59:i:201:CHD:H212	59:i:201:CHD:C12	2.38	0.53
12:L:54:PHE:O	12:L:58:GLY:N	2.34	0.52
39:n:44:ARG:NE	39:n:48:ASP:OD1	2.35	0.52
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.91	0.52
7:G:293:HIS:HD1	16:P:2:HIS:C	2.16	0.52
9:I:26:LEU:CD1	25:Z:34:MET:HE2	2.39	0.52
44:s:38:TYR:O	44:s:41:LEU:HD11	2.10	0.52
7:G:341:ASP:OD2	19:S:67:ARG:NH1	2.41	0.52
12:L:144:TRP:NE1	12:L:179:ASP:OD1	2.42	0.52
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.92	0.52
13:M:88:ASN:ND2	15:O:294:GLN:OE1	2.43	0.52
44:s:40:ASN:ND2	44:s:40:ASN:O	2.42	0.52
20:U:17:TYR:OH	36:k:11:TRP:NE1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:80:ARG:NH2	24:Y:85:ASP:OD2	2.42	0.52
3:C:154:ASP:OD1	3:C:155:TYR:N	2.42	0.52
10:J:141:MET:HA	10:J:141:MET:HE2	1.92	0.52
13:M:453:ILE:HG13	13:M:454:ILE:HG23	1.91	0.52
1:A:27:LEU:CD1	46:A:204:PC1:H133	2.40	0.51
23:X:109:CYS:SG	23:X:110:VAL:N	2.83	0.51
49:B:202:U10:H452	8:H:224:PHE:CG	2.46	0.51
12:L:587:TYR:O	12:L:590:SER:OG	2.20	0.51
15:O:145:ARG:NH1	15:O:281:GLU:OE2	2.44	0.51
7:G:382:THR:OG1	7:G:387:GLU:OE1	2.27	0.51
53:M:604:CDL:H401	53:d:202:CDL:H673	1.93	0.51
2:B:46:TRP:CE2	49:B:202:U10:H401	2.45	0.51
9:I:112:ASP:OD1	9:I:114:THR:OG1	2.24	0.51
38:m:36:LEU:O	38:m:40:SER:OG	2.23	0.51
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.93	0.51
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.46	0.51
19:S:18:ILE:CG2	19:S:64:LEU:HD11	2.41	0.51
13:M:91:ARG:NH2	15:O:290:ASP:OD2	2.44	0.50
16:P:282:ASP:OD2	16:P:286:ARG:NH1	2.38	0.50
12:L:446:ASN:ND2	35:j:21:GLN:OE1	2.43	0.50
16:P:127:GLU:OE1	16:P:127:GLU:N	2.44	0.50
7:G:266:LYS:NZ	7:G:674:THR:OG1	2.27	0.50
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.42	0.50
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.94	0.50
19:S:19:ARG:NH1	19:S:73:GLU:OE2	2.42	0.50
41:p:8:VAL:O	41:p:108:ARG:NH1	2.41	0.50
16:P:270:PHE:CD2	16:P:279:THR:HG22	2.46	0.50
22:W:123:VAL:HG23	22:W:124:GLY:N	2.26	0.50
3:C:175:ARG:NH2	3:C:186:GLU:OE2	2.43	0.50
12:L:534:HIS:ND1	46:L:703:PC1:O12	2.42	0.50
34:i:85:LEU:HD23	34:i:89:VAL:HG21	1.94	0.50
1:A:68:GLU:HG3	1:A:98:LEU:HD13	1.93	0.49
7:G:536:ASP:OD1	7:G:536:ASP:N	2.44	0.49
1:A:82:ALA:O	27:b:42:LEU:HD21	2.12	0.49
13:M:346:ARG:NE	37:l:68:ASP:OD2	2.44	0.49
23:X:1:PRO:N	25:Z:108:SER:O	2.45	0.49
40:o:11:ASP:OD1	40:o:12:ALA:N	2.45	0.49
2:B:86:MET:HE1	2:B:104:TYR:HB2	1.94	0.49
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.42	0.49
12:L:264:TYR:N	12:L:265:PRO:CD	2.75	0.49
5:E:16:ASN:O	5:E:64:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:366:THR:HB	7:G:450:MET:HE3	1.94	0.49
14:N:76:ILE:HA	14:N:79:MET:HE3	1.95	0.49
3:C:40:VAL:HG13	3:C:50:ILE:HD13	1.94	0.49
14:N:72:MET:HE2	14:N:76:ILE:HG13	1.93	0.49
49:B:202:U10:C19	49:B:202:U10:H151	2.42	0.49
31:f:53:GLU:N	31:f:53:GLU:OE1	2.46	0.49
1:A:100:VAL:HG13	45:O:403:3PE:H372	1.95	0.49
3:C:135:TRP:CE2	22:W:87:MET:HE1	2.48	0.49
11:K:37:MET:SD	14:N:68:MET:HE1	2.53	0.48
3:C:8:ARG:O	4:D:129:ARG:NH2	2.45	0.48
6:F:172:ASP:OD1	6:F:172:ASP:N	2.45	0.48
6:F:175:VAL:O	44:s:62:ARG:NH1	2.43	0.48
7:G:371:VAL:HG22	7:G:450:MET:HE1	1.94	0.48
15:O:250:ASP:OD1	15:O:250:ASP:N	2.46	0.48
40:o:59:ALA:O	40:o:60:HIS:CG	2.66	0.48
7:G:396:ARG:NH1	7:G:416:THR:O	2.47	0.48
17:Q:95:PHE:O	17:Q:99:ASN:ND2	2.44	0.48
37:l:126:GLN:NE2	60:o:201:MYR:O1	2.47	0.48
6:F:258:ILE:HD11	6:F:279:LEU:HG	1.96	0.48
6:F:306:LEU:C	6:F:306:LEU:HD12	2.39	0.48
13:M:1:FME:HE3	13:M:111:THR:HG21	1.96	0.48
1:A:27:LEU:HD12	46:A:204:PC1:H133	1.95	0.48
2:B:129:SER:OG	4:D:85:2MR:O	2.10	0.48
6:F:120:GLU:OE2	6:F:236:ARG:NH1	2.45	0.48
20:U:49:GLU:OE2	39:n:44:ARG:NH1	2.46	0.48
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.49	0.48
34:i:109:ILE:O	34:i:113:GLY:N	2.44	0.48
42:q:44:TYR:O	42:q:65:THR:HG21	2.13	0.48
9:I:26:LEU:HD13	25:Z:34:MET:HE2	1.95	0.48
29:d:6:GLN:O	29:d:8:ARG:NE	2.47	0.48
5:E:194:GLU:HB2	5:E:199:LEU:HD23	1.96	0.47
6:F:214:GLY:HA3	6:F:220:THR:HG22	1.96	0.47
12:L:479:GLN:NE2	12:L:481:THR:O	2.44	0.47
7:G:144:PRO:HD2	7:G:192:MET:HE1	1.96	0.47
7:G:324:ASP:OD1	7:G:324:ASP:N	2.47	0.47
8:H:2:PHE:HE2	8:H:6:ILE:HD11	1.77	0.47
12:L:81:LYS:C	12:L:82:MET:HE2	2.39	0.47
13:M:6:ILE:HD12	31:f:23:GLY:HA2	1.96	0.47
1:A:27:LEU:HD23	8:H:59:GLU:HG3	1.96	0.47
4:D:3:GLN:NE2	13:M:137:GLY:O	2.47	0.47
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:72:MET:HA	14:N:72:MET:HE3	1.95	0.47
14:N:298:TYR:CD1	14:N:302:LEU:HD12	2.48	0.47
7:G:424:ASP:N	7:G:424:ASP:OD1	2.47	0.47
10:J:129:ASP:OD1	10:J:130:THR:N	2.47	0.47
28:c:48:LEU:HD12	28:c:48:LEU:C	2.39	0.47
1:A:73:LEU:HD13	8:H:103:LEU:HD21	1.96	0.47
16:P:309:PRO:HD2	16:P:312:LEU:HD12	1.97	0.47
8:H:169:GLN:NE2	8:H:241:LEU:O	2.48	0.47
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.50	0.47
14:N:2:ASN:ND2	45:O:403:3PE:O22	2.47	0.47
17:Q:20:THR:HG22	17:Q:99:ASN:O	2.13	0.47
41:p:98:ASP:OD2	41:p:141:ARG:NH2	2.47	0.47
12:L:286:LEU:C	12:L:286:LEU:HD13	2.40	0.47
44:s:41:LEU:HD12	44:s:41:LEU:H	1.79	0.47
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.47
10:J:125:TRP:HB2	25:Z:136:THR:HG21	1.97	0.47
12:L:230:HIS:N	12:L:231:PRO:CD	2.78	0.47
2:B:42:ARG:NH1	46:B:204:PC1:O14	2.41	0.46
5:E:44:ALA:O	5:E:47:VAL:HG23	2.15	0.46
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.42	0.46
30:e:8:ARG:NH1	45:e:201:3PE:O12	2.46	0.46
3:C:54:PRO:O	3:C:57:VAL:HG23	2.16	0.46
6:F:139:ARG:NE	6:F:141:GLU:OE1	2.48	0.46
7:G:521:MET:HE2	7:G:523:PHE:CZ	2.51	0.46
8:H:14:LEU:HD22	8:H:225:MET:HE3	1.97	0.46
11:K:98:CYS:HG	14:N:181:TYR:HH	1.63	0.46
15:O:11:GLY:O	15:O:16:LYS:NZ	2.49	0.46
35:j:10:ARG:NH2	35:j:14:PHE:O	2.47	0.46
12:L:31:ASN:HD22	59:i:201:CHD:H151	1.80	0.46
34:i:52:ASP:OD1	34:i:53:GLY:N	2.49	0.46
34:i:66:HIS:CD2	59:i:201:CHD:H231	2.51	0.46
2:B:56:ALA:HB3	49:B:202:U10:H1M1	1.98	0.46
38:m:47:GLN:HB3	39:n:165:LEU:HD13	1.97	0.46
3:C:66:ASP:O	21:V:82:GLN:NE2	2.46	0.46
6:F:206:LYS:HB3	6:F:207:PRO:HA	1.97	0.46
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.98	0.46
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.47	0.46
39:n:138:GLN:NE2	39:n:155:PRO:O	2.48	0.46
7:G:53:ARG:N	50:G:803:FES:S1	2.83	0.46
16:P:119:GLN:O	16:P:119:GLN:NE2	2.49	0.46
4:D:193:TYR:OH	4:D:201:GLN:O	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:157:THR:N	48:G:802:SF4:S4	2.80	0.46
4:D:73:VAL:HG21	4:D:414:VAL:HG21	1.98	0.46
7:G:372:GLU:O	7:G:402:ASN:ND2	2.49	0.46
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.43	0.46
49:B:202:U10:H452	8:H:224:PHE:CD2	2.52	0.45
5:E:217:LEU:HD23	6:F:44:LYS:HD2	1.97	0.45
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.81	0.45
10:J:115:VAL:O	10:J:117:PHE:N	2.50	0.45
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.50	0.45
38:m:21:GLU:C	38:m:24:ILE:HD11	2.42	0.45
8:H:294:LEU:HB3	8:H:295:PRO:HD3	1.98	0.45
6:F:108:ARG:NE	6:F:145:GLU:OE2	2.50	0.45
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.98	0.45
13:M:373:ILE:HD11	13:M:444:LEU:CD1	2.47	0.45
19:S:57:CYS:O	19:S:60:VAL:HG22	2.17	0.45
24:Y:104:THR:HG22	24:Y:104:THR:O	2.17	0.45
2:B:76:PHE:CD2	49:B:202:U10:H152	2.51	0.45
37:l:32:GLU:OE1	37:l:32:GLU:N	2.50	0.45
7:G:26:VAL:HG22	7:G:73:VAL:HG12	1.99	0.45
7:G:243:ARG:O	7:G:244:THR:OG1	2.32	0.45
16:P:299:GLY:N	16:P:302:ASP:OD2	2.46	0.45
2:B:51:GLY:H	49:B:202:U10:H103	1.82	0.45
7:G:453:LEU:HD21	7:G:458:LEU:HD21	1.98	0.45
13:M:390:ASN:O	13:M:393:ILE:HG22	2.17	0.45
45:N:401:3PE:H2I1	45:Y:202:3PE:H2D2	1.98	0.45
6:F:293:ASN:O	6:F:339:ARG:N	2.48	0.45
13:M:90:THR:HG22	13:M:90:THR:O	2.17	0.45
29:d:13:PHE:O	29:d:78:ARG:NH1	2.48	0.45
49:B:202:U10:H222	49:B:202:U10:H201	1.86	0.44
53:L:705:CDL:OA9	33:h:26:ARG:NH1	2.50	0.44
10:J:23:LYS:NZ	11:K:18:GLY:O	2.50	0.44
26:a:34:LYS:NZ	26:a:61:TYR:O	2.47	0.44
7:G:551:ASP:OD2	7:G:679:ARG:NE	2.49	0.44
14:N:289:ASN:OD1	14:N:289:ASN:N	2.48	0.44
42:q:114:LYS:CE	42:q:117:LEU:HD11	2.47	0.44
13:M:271:MET:HE2	13:M:271:MET:HA	1.99	0.44
6:F:101:GLU:OE2	6:F:303:SER:OG	2.30	0.44
12:L:587:TYR:O	12:L:590:SER:N	2.48	0.44
14:N:22:ILE:HB	30:e:5:VAL:HG22	2.00	0.44
6:F:78:LYS:NZ	6:F:222:VAL:O	2.51	0.44
16:P:3:HIS:O	16:P:3:HIS:ND1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:88:GLU:OE1	22:W:97:LYS:NZ	2.31	0.44
15:O:249:LEU:HD12	15:O:249:LEU:N	2.33	0.44
1:A:42:ASP:OD1	2:B:102:LYS:NZ	2.49	0.44
49:B:202:U10:H252	4:D:159:LEU:HD11	1.99	0.44
4:D:164:MET:HE1	8:H:28:LEU:HD13	2.00	0.44
12:L:68:TRP:CE3	45:i:202:3PE:H3I3	2.53	0.44
17:Q:8:THR:O	17:Q:8:THR:HG22	2.17	0.44
39:n:104:ASP:OD1	39:n:121:ARG:NH2	2.48	0.44
16:P:332:GLU:OE2	22:W:55:VAL:N	2.38	0.44
23:X:102:GLN:OE1	23:X:102:GLN:N	2.49	0.44
40:o:36:ARG:NH1	40:o:93:ASP:OD1	2.46	0.44
25:Z:27:ARG:NH2	43:r:13:TRP:O	2.51	0.43
30:e:40:ILE:HG21	33:h:133:ILE:HD11	1.99	0.43
35:j:55:ASP:OD2	35:j:58:GLN:NE2	2.43	0.43
37:l:82:ASP:OD1	37:l:82:ASP:N	2.51	0.43
7:G:106:PRO:O	7:G:218:ARG:NH2	2.51	0.43
25:Z:97:MET:HE3	25:Z:100:VAL:HG21	2.00	0.43
42:q:46:ASN:OD1	42:q:65:THR:HG22	2.18	0.43
4:D:202:ASP:OD1	4:D:203:LEU:N	2.51	0.43
8:H:169:GLN:O	46:H:403:PC1:H153	2.18	0.43
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.46	0.43
7:G:315:VAL:O	7:G:340:SER:OG	2.34	0.43
7:G:652:VAL:O	7:G:653:ASN:C	2.61	0.43
29:d:5:ARG:NE	29:d:85:VAL:HG13	2.33	0.43
5:E:145:LEU:HD12	5:E:153:MET:SD	2.59	0.43
7:G:26:VAL:HG13	7:G:79:ILE:HD13	1.99	0.43
59:i:201:CHD:O7	59:i:201:CHD:H41	2.19	0.43
4:D:429:ASP:N	4:D:429:ASP:OD1	2.51	0.43
8:H:200:LEU:HD13	8:H:282:TYR:CB	2.49	0.43
12:L:14:LEU:HD23	12:L:14:LEU:O	2.18	0.43
12:L:421:ILE:HA	12:L:501:ALA:HB2	2.01	0.43
7:G:450:MET:HE2	7:G:452:ILE:HD11	2.00	0.43
16:P:185:ILE:HG22	16:P:185:ILE:O	2.17	0.43
17:Q:5:THR:OG1	17:Q:6:ARG:N	2.52	0.43
25:Z:119:MET:HE2	30:e:71:THR:HG21	2.01	0.43
36:k:25:LEU:O	36:k:30:LEU:N	2.51	0.43
5:E:105:THR:HG22	5:E:106:THR:N	2.34	0.42
7:G:41:CYS:O	7:G:161:ARG:NH2	2.38	0.42
12:L:71:ILE:N	12:L:71:ILE:HD12	2.34	0.42
39:n:8:TYR:C	39:n:9:LEU:HD12	2.44	0.42
5:E:35:VAL:O	5:E:35:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:THR:HG22	5:E:106:THR:H	1.83	0.42
8:H:268:MET:HE2	8:H:271:LEU:HD12	2.01	0.42
46:L:703:PC1:C3I	13:M:398:VAL:HG22	2.49	0.42
47:g:201:PLC:H63	33:h:28:TYR:OH	2.19	0.42
22:W:113:ARG:O	22:W:115:LYS:NZ	2.48	0.42
37:l:68:ASP:OD1	37:l:68:ASP:N	2.52	0.42
40:o:41:THR:N	40:o:44:GLU:OE1	2.47	0.42
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.01	0.42
46:I:203:PC1:O13	46:I:203:PC1:H132	2.20	0.42
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.01	0.42
4:D:139:VAL:HG21	4:D:277:VAL:CG2	2.49	0.42
14:N:313:MET:HE1	15:O:102:ALA:HB3	2.01	0.42
16:P:209:ASP:OD2	16:P:308:THR:N	2.42	0.42
40:o:39:VAL:HG12	40:o:39:VAL:O	2.18	0.42
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.02	0.42
12:L:2:ASN:OD1	12:L:3:MET:N	2.52	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.00	0.42
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	2.02	0.42
29:d:5:ARG:O	29:d:8:ARG:NH2	2.53	0.42
28:c:48:LEU:HD12	28:c:49:GLU:HB2	2.02	0.42
1:A:78:ALA:O	1:A:81:THR:HG22	2.20	0.42
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.42
34:i:56:TRP:O	34:i:59:VAL:HG12	2.19	0.42
10:J:100:GLU:O	10:J:104:VAL:HG23	2.19	0.42
14:N:44:MET:HE1	14:N:59:TYR:CG	2.55	0.42
17:Q:91:ASP:OD1	17:Q:91:ASP:N	2.51	0.42
30:e:8:ARG:NH2	45:e:201:3PE:O12	2.52	0.42
21:V:34:LEU:HD13	21:V:48:GLU:HG3	2.00	0.41
23:X:136:LEU:HD12	23:X:137:PRO:HD2	2.01	0.41
25:Z:55:GLU:OE1	25:Z:58:ARG:NH2	2.48	0.41
31:f:7:VAL:HG13	31:f:8:ARG:N	2.35	0.41
34:i:75:LEU:O	34:i:78:VAL:HG12	2.20	0.41
4:D:111:MET:SD	4:D:111:MET:N	2.91	0.41
6:F:188:GLU:OE1	6:F:190:THR:N	2.51	0.41
7:G:228:ILE:HG22	7:G:229:ASP:N	2.34	0.41
7:G:410:GLY:N	7:G:423:GLY:O	2.51	0.41
8:H:187:ILE:HD12	46:I:203:PC1:H262	2.02	0.41
12:L:230:HIS:N	12:L:231:PRO:HD3	2.35	0.41
47:P:503:PLC:O4P	47:P:503:PLC:H73	2.20	0.41
19:S:22:LEU:HD23	19:S:22:LEU:N	2.35	0.41
31:f:3:LEU:HD12	31:f:3:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:55:LEU:HD13	34:i:55:LEU:C	2.45	0.41
37:l:81:LEU:HD13	37:l:81:LEU:C	2.45	0.41
6:F:378:ARG:O	6:F:382:GLY:N	2.53	0.41
12:L:194:ASN:O	12:L:194:ASN:ND2	2.54	0.41
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.20	0.41
13:M:134:THR:OG1	14:N:302:LEU:HD13	2.21	0.41
15:O:114:HIS:O	15:O:118:THR:OG1	2.38	0.41
25:Z:119:MET:HE2	30:e:71:THR:CG2	2.50	0.41
27:b:42:LEU:O	27:b:42:LEU:HD23	2.20	0.41
6:F:103:GLY:O	6:F:333:ALA:HB1	2.21	0.41
12:L:355:ASP:OD2	12:L:357:ARG:NH2	2.53	0.41
13:M:47:ASP:OD1	13:M:48:ASN:N	2.54	0.41
13:M:201:MET:O	13:M:205:VAL:HG23	2.21	0.41
25:Z:84:GLN:NE2	25:Z:88:GLU:OE2	2.54	0.41
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.01	0.41
5:E:53:LEU:HD13	44:s:52:LEU:HD12	2.02	0.41
8:H:114:TYR:OH	10:J:65:MET:N	2.54	0.41
46:H:403:PC1:O13	46:H:403:PC1:H132	2.20	0.41
12:L:561:ILE:HG13	12:L:562:LEU:N	2.36	0.41
23:X:161:ARG:O	23:X:165:ARG:NH1	2.49	0.41
32:g:25:ARG:HE	32:g:25:ARG:HA	1.85	0.41
4:D:340:THR:O	4:D:340:THR:HG22	2.20	0.41
6:F:435:GLN:O	6:F:438:GLN:NE2	2.54	0.41
8:H:179:TRP:N	8:H:180:PRO:CD	2.84	0.41
14:N:298:TYR:HD1	14:N:302:LEU:HD12	1.85	0.41
21:V:5:LYS:NZ	21:V:75:GLN:OE1	2.37	0.41
32:g:70:LEU:O	32:g:74:SER:OG	2.28	0.41
34:i:18:ARG:NH1	39:n:170:VAL:O	2.43	0.41
4:D:139:VAL:HG21	4:D:277:VAL:HG22	2.03	0.41
4:D:185:SER:O	9:I:62:ARG:NH1	2.54	0.41
6:F:407:LEU:HD23	6:F:407:LEU:C	2.44	0.41
9:I:36:MET:O	9:I:39:SER:OG	2.31	0.41
9:I:79:ALA:HB2	9:I:106:THR:HG23	2.02	0.41
10:J:5:ILE:HG23	10:J:6:VAL:N	2.36	0.41
13:M:54:LEU:HD23	33:h:93:ILE:HG23	2.03	0.41
13:M:285:LEU:HD23	13:M:285:LEU:C	2.46	0.41
45:N:402:3PE:H351	24:Y:123:LEU:HD13	2.02	0.41
16:P:113:ILE:HB	16:P:114:PRO:HD3	2.02	0.41
16:P:127:GLU:O	16:P:224:ARG:NH1	2.54	0.41
25:Z:43:LEU:HD21	45:Z:202:3PE:H3C1	2.03	0.41
28:c:43:LYS:CG	28:c:48:LEU:HD11	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.03	0.41
6:F:409:ASP:N	6:F:409:ASP:OD1	2.52	0.41
11:K:73:LEU:HD22	14:N:38:LEU:HD12	2.02	0.41
13:M:225:ILE:HD13	13:M:331:ASN:HB2	2.02	0.41
14:N:307:SER:O	15:O:284:VAL:N	2.47	0.41
14:N:267:ILE:O	14:N:271:THR:HG23	2.21	0.40
23:X:79:GLU:HB3	23:X:80:PRO:HD3	2.03	0.40
2:B:44:SER:OG	8:H:51:ASP:OD1	2.28	0.40
6:F:101:GLU:CD	6:F:303:SER:HG	2.28	0.40
6:F:204:ARG:HD2	17:Q:122:PHE:CZ	2.56	0.40
8:H:27:VAL:HG21	8:H:268:MET:HE1	2.04	0.40
14:N:13:ILE:O	14:N:36:ASN:ND2	2.54	0.40
45:L:701:3PE:H3D1	13:M:398:VAL:HG21	2.04	0.40
13:M:158:LEU:HB2	13:M:159:PRO:HD3	2.04	0.40
13:M:168:GLN:O	13:M:172:GLY:N	2.53	0.40
13:M:373:ILE:HD11	13:M:444:LEU:HD12	2.03	0.40
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.40	0.40
2:B:97:ALA:HB3	2:B:98:PRO:HD3	2.03	0.40
9:I:26:LEU:HD12	25:Z:34:MET:HE2	2.03	0.40
19:S:94:LEU:HD12	19:S:94:LEU:N	2.36	0.40
29:d:56:ALA:O	29:d:61:GLN:NE2	2.53	0.40
34:i:122:PHE:CD1	40:o:39:VAL:HG11	2.57	0.40
8:H:24:GLU:HA	8:H:271:LEU:HD13	2.03	0.40
12:L:221:THR:HG23	12:L:226:GLN:HB2	2.04	0.40
13:M:59:ASP:OD1	13:M:245:ARG:NH2	2.52	0.40
15:O:111:ALA:HB1	15:O:122:VAL:HG21	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%)	109 (96%)	4 (4%)	0	100	100
2	B	153/216 (71%)	147 (96%)	6 (4%)	0	100	100
3	C	207/266 (78%)	203 (98%)	4 (2%)	0	100	100
4	D	427/463 (92%)	418 (98%)	9 (2%)	0	100	100
5	E	212/249 (85%)	200 (94%)	12 (6%)	0	100	100
6	F	430/464 (93%)	417 (97%)	13 (3%)	0	100	100
7	G	686/727 (94%)	658 (96%)	28 (4%)	0	100	100
8	H	316/318 (99%)	306 (97%)	9 (3%)	1 (0%)	36	67
9	I	174/212 (82%)	168 (97%)	6 (3%)	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%)	579 (96%)	25 (4%)	0	100	100
13	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	314 (99%)	4 (1%)	0	100	100
16	P	340/380 (90%)	332 (98%)	8 (2%)	0	100	100
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
18	R	94/124 (76%)	92 (98%)	2 (2%)	0	100	100
19	S	85/99 (86%)	83 (98%)	2 (2%)	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%)	162 (96%)	7 (4%)	0	100	100
24	Y	138/141 (98%)	138 (100%)	0	0	100	100
25	Z	139/144 (96%)	136 (98%)	3 (2%)	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%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	97/106 (92%)	97 (100%)	0	0	100	100
31	f	55/57 (96%)	55 (100%)	0	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%)	133 (98%)	3 (2%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	65 (94%)	4 (6%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	149 (97%)	5 (3%)	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%)	116 (97%)	4 (3%)	0	100	100
41	p	172/176 (98%)	172 (100%)	0	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	91/113 (80%)	86 (94%)	5 (6%)	0	100	100
44	s	43/109 (39%)	40 (93%)	3 (7%)	0	100	100
All	All	8193/9213 (89%)	7969 (97%)	223 (3%)	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%)	128 (98%)	3 (2%)	44	70
3	C	190/228 (83%)	188 (99%)	2 (1%)	65	78
4	D	370/392 (94%)	366 (99%)	4 (1%)	65	78
5	E	183/205 (89%)	182 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	346/368 (94%)	336 (97%)	10 (3%)	37	66
7	G	578/608 (95%)	576 (100%)	2 (0%)	86	87
8	H	274/274 (100%)	267 (97%)	7 (3%)	40	68
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	77
10	J	141/141 (100%)	139 (99%)	2 (1%)	59	76
11	K	85/85 (100%)	82 (96%)	3 (4%)	32	62
12	L	533/533 (100%)	523 (98%)	10 (2%)	50	73
13	M	412/412 (100%)	405 (98%)	7 (2%)	53	74
14	N	315/315 (100%)	312 (99%)	3 (1%)	68	79
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	69
16	P	296/327 (90%)	289 (98%)	7 (2%)	43	69
17	Q	116/153 (76%)	114 (98%)	2 (2%)	53	74
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	77
19	S	77/82 (94%)	77 (100%)	0	100	100
20	T	81/135 (60%)	80 (99%)	1 (1%)	63	78
20	U	81/135 (60%)	80 (99%)	1 (1%)	63	78
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	79
22	W	107/114 (94%)	103 (96%)	4 (4%)	30	61
23	X	154/155 (99%)	150 (97%)	4 (3%)	40	68
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	81
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%)	104 (99%)	1 (1%)	68	79
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	63
31	f	54/54 (100%)	51 (94%)	3 (6%)	19	49
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	63
33	h	121/158 (77%)	120 (99%)	1 (1%)	73	81
34	i	120/121 (99%)	117 (98%)	3 (2%)	42	69
35	j	61/84 (73%)	60 (98%)	1 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	75
37	l	140/159 (88%)	138 (99%)	2 (1%)	59	76
38	m	113/114 (99%)	112 (99%)	1 (1%)	70	80
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	109 (99%)	1 (1%)	70	80
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	130/130 (100%)	128 (98%)	2 (2%)	57	75
43	r	85/97 (88%)	85 (100%)	0	100	100
44	s	44/92 (48%)	43 (98%)	1 (2%)	44	70
All	All	7218/7891 (92%)	7110 (98%)	108 (2%)	55	75

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
2	B	81	ARG
2	B	84	ASP
3	C	74	SER
3	C	78	LEU
4	D	23	LYS
4	D	165	THR
4	D	216	LYS
4	D	429	ASP
5	E	97	LYS
6	F	8	LYS
6	F	16	LYS
6	F	34	LYS
6	F	82	MET
6	F	172	ASP
6	F	324	GLN
6	F	355	LYS
6	F	359	CYS
6	F	365	CYS
6	F	409	ASP
7	G	536	ASP
7	G	613	TYR
8	H	5	ASN
8	H	8	MET
8	H	103	LEU

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Mol	Chain	Res	Type
8	H	234	MET
8	H	268	MET
8	H	274	ARG
8	H	296	LEU
9	I	78	ILE
9	I	110	ASP
10	J	135	PHE
10	J	172	THR
11	K	15	SER
11	K	37	MET
11	K	59	MET
12	L	116	LYS
12	L	336	LYS
12	L	383	MET
12	L	394	LEU
12	L	487	LYS
12	L	503	GLU
12	L	509	LYS
12	L	514	HIS
12	L	580	GLN
12	L	601	LEU
13	M	57	PHE
13	M	116	ILE
13	M	138	ASN
13	M	207	MET
13	M	271	MET
13	M	315	LEU
13	M	369	LEU
14	N	71	MET
14	N	289	ASN
14	N	322	LYS
15	O	1	LEU
15	O	16	LYS
15	O	24	LEU
15	O	35	LYS
15	O	191	GLU
15	O	206	TYR
15	O	250	ASP
16	P	1	LEU
16	P	3	HIS
16	P	32	ARG
16	P	97	ARG

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Mol	Chain	Res	Type
16	P	122	LYS
16	P	140	LYS
16	P	199	LYS
17	Q	44	ASN
17	Q	91	ASP
18	R	32	GLN
20	T	35	HIS
20	U	82	ASP
21	V	6	LYS
22	W	47	HIS
22	W	56	LYS
22	W	69	ASN
22	W	98	GLN
23	X	15	GLN
23	X	43	MET
23	X	154	GLU
23	X	161	ARG
25	Z	4	LYS
29	d	106	LYS
30	e	53	LYS
30	e	90	LYS
30	e	97	HIS
31	f	4	LEU
31	f	32	GLU
31	f	33	LYS
32	g	24	LEU
32	g	25	ARG
32	g	57	ASN
33	h	68	LYS
34	i	48	LYS
34	i	57	LYS
34	i	124	ASP
35	j	47	VAL
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
44	s	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
3	C	88	ASN
3	C	211	GLN
4	D	190	HIS
4	D	316	ASN
6	F	324	GLN
7	G	7	ASN
7	G	237	ASN
8	H	5	ASN
8	H	317	GLN
12	L	269	ASN
13	M	83	HIS
13	M	88	ASN
13	M	188	ASN
13	M	293	HIS
13	M	304	GLN
13	M	331	ASN
13	M	338	HIS
13	M	399	ASN
14	N	134	GLN
15	O	2	GLN
15	O	120	GLN
15	O	180	GLN
15	O	190	HIS
16	P	2	HIS
16	P	180	ASN
17	Q	29	HIS
18	R	32	GLN
19	S	92	ASN
22	W	69	ASN
25	Z	111	HIS
29	d	61	GLN
29	d	79	GLN
31	f	13	HIS
37	l	87	ASN
37	l	132	GLN
38	m	47	GLN
39	n	77	GLN
40	o	53	GLN
43	r	12	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	1.74	1 (14%)	7,9,11	1.52	1 (14%)
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.37	1 (16%)
8	FME	H	1	8	8,9,10	1.51	1 (12%)	8,9,11	1.48	2 (25%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	8,9,11	1.43	2 (25%)
4	2MR	D	85	4	10,12,13	2.49	2 (20%)	5,13,15	1.31	1 (20%)
10	FME	J	1	10	8,9,10	1.53	1 (12%)	8,9,11	1.34	1 (12%)
38	SAC	m	1	38	7,8,9	1.74	1 (14%)	7,9,11	1.22	1 (14%)
42	AME	q	1	42	9,10,11	1.51	1 (11%)	9,11,13	1.27	1 (11%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	8,9,11	1.37	1 (12%)
29	AME	d	1	29	9,10,11	1.53	1 (11%)	9,11,13	1.26	1 (11%)
27	AYA	b	1	27	6,7,8	1.88	1 (16%)	6,8,10	1.32	1 (16%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.30	0
24	AYA	Y	1	24	6,7,8	1.88	2 (33%)	6,8,10	1.40	1 (16%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	8,9,11	1.45	2 (25%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	8,9,11	1.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SAC	i	1	34	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	AYA	r	1	43	-	0/5/6/8	-
8	FME	H	1	8	-	1/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
10	FME	J	1	10	-	2/7/9/11	-
38	SAC	m	1	38	-	1/7/8/10	-
42	AME	q	1	42	-	5/9/10/12	-
12	FME	L	1	12	-	1/7/9/11	-
29	AME	d	1	29	-	0/9/10/12	-
27	AYA	b	1	27	-	1/5/6/8	-
14	FME	N	1	14	-	3/7/9/11	-
24	AYA	Y	1	24	-	1/5/6/8	-
11	FME	K	1	11	-	3/7/9/11	-
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	5.56	1.45	1.33
4	D	85	2MR	CZ-NE	5.18	1.45	1.34
10	J	1	FME	CN-N	3.81	1.45	1.33
14	N	1	FME	CN-N	3.77	1.45	1.33
13	M	1	FME	CN-N	3.74	1.45	1.33
1	A	1	FME	CN-N	3.73	1.45	1.33
12	L	1	FME	CN-N	3.72	1.45	1.33
11	K	1	FME	CN-N	3.71	1.45	1.33
8	H	1	FME	CN-N	3.70	1.45	1.33
27	b	1	AYA	CT-N	3.55	1.45	1.34
38	m	1	SAC	C1A-N	3.53	1.45	1.34
34	i	1	SAC	C1A-N	3.51	1.45	1.34
29	d	1	AME	CT1-N	3.49	1.45	1.34
24	Y	1	AYA	CT-N	3.49	1.45	1.34
42	q	1	AME	CT1-N	3.46	1.45	1.34
43	r	1	AYA	CT-N	3.44	1.45	1.34
24	Y	1	AYA	OT-CT	-2.01	1.18	1.23
43	r	1	AYA	OT-CT	-2.00	1.18	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.89	120.91	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	1	AYA	CM-CT-N	2.43	120.15	116.12
43	r	1	AYA	CM-CT-N	2.39	120.09	116.12
27	b	1	AYA	CM-CT-N	2.38	120.07	116.12
8	H	1	FME	CA-N-CN	-2.37	119.17	122.82
29	d	1	AME	CT2-CT1-N	2.35	120.01	116.12
42	q	1	AME	CT2-CT1-N	2.16	119.70	116.12
11	K	1	FME	CA-N-CN	-2.14	119.53	122.82
38	m	1	SAC	C2A-C1A-N	2.14	119.67	116.12
11	K	1	FME	O1-CN-N	-2.13	119.82	125.32
1	A	1	FME	O1-CN-N	-2.08	119.94	125.32
8	H	1	FME	O1-CN-N	-2.05	120.02	125.32
10	J	1	FME	O1-CN-N	-2.04	120.04	125.32
12	L	1	FME	O1-CN-N	-2.04	120.04	125.32
4	D	85	2MR	CD-NE-CZ	-2.02	119.57	123.36
1	A	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

All (26) 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
11	K	1	FME	O-C-CA-CB
14	N	1	FME	CB-CA-N-CN
24	Y	1	AYA	O-C-CA-CB
27	b	1	AYA	O-C-CA-CB
34	i	1	SAC	C-CA-CB-OG
38	m	1	SAC	O-C-CA-CB
42	q	1	AME	C-CA-CB-CG
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CA-CB-CG-SD
42	q	1	AME	N-CA-CB-CG
11	K	1	FME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
42	q	1	AME	CB-CA-N-CT1
12	L	1	FME	CA-CB-CG-SD
42	q	1	AME	C-CA-N-CT1
8	H	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
13	M	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN
14	N	1	FME	CB-CG-SD-CE
14	N	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	85	2MR	1	0
13	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 4 are monoatomic - leaving 84 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	$\# Z > 2$
53	CDL	L	705	-	75,75,99	1.01	8 (10%)	81,87,111	1.10	4 (4%)
47	PLC	P	503	-	41,41,41	0.52	0	47,49,49	0.53	0
46	PC1	e	202	-	38,38,53	1.12	4 (10%)	44,46,61	1.05	2 (4%)
50	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	Y	205	-	44,44,50	0.92	4 (9%)	47,49,55	1.11	2 (4%)
45	3PE	f	102	-	43,43,50	0.94	4 (9%)	46,48,55	1.09	2 (4%)
47	PLC	O	404	-	34,34,41	0.56	0	40,42,49	0.56	0
47	PLC	P	504	-	31,31,41	0.57	0	37,39,49	0.58	0
46	PC1	B	204	-	47,47,53	1.01	4 (8%)	53,55,61	1.12	2 (3%)
46	PC1	L	702	-	43,43,53	1.05	4 (9%)	49,51,61	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	h	202	-	79,79,99	0.99	8 (10%)	85,91,111	1.15	4 (4%)
46	PC1	A	205	-	32,32,53	1.21	4 (12%)	38,40,61	1.10	2 (5%)
50	FES	G	803	7	0,4,4	-	-	-		
47	PLC	J	204	-	36,36,41	0.53	0	42,44,49	0.51	0
46	PC1	m	205	-	53,53,53	0.95	4 (7%)	59,61,61	1.04	2 (3%)
53	CDL	M	604	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	4 (3%)
46	PC1	A	204	-	34,34,53	1.18	4 (11%)	40,42,61	1.08	2 (5%)
47	PLC	Z	203	-	33,33,41	0.56	0	39,41,49	0.57	0
45	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
45	3PE	i	202	-	44,44,50	0.91	4 (9%)	47,49,55	1.07	2 (4%)
47	PLC	g	201	-	41,41,41	0.51	0	47,49,49	0.52	0
49	U10	B	202	-	63,63,63	1.88	26 (41%)	78,79,79	1.28	12 (15%)
48	SF4	G	802	7	0,12,12	-	-	-		
47	PLC	Y	208	-	41,41,41	0.51	0	47,49,49	0.50	0
58	EHZ	U	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.61	6 (16%)
45	3PE	Y	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.11	2 (3%)
45	3PE	J	201	-	28,28,50	1.14	4 (14%)	31,33,55	1.19	2 (6%)
48	SF4	B	201	2	0,12,12	-	-	-		
45	3PE	Y	206	-	35,35,50	1.04	4 (11%)	38,40,55	1.14	2 (5%)
46	PC1	M	602	-	34,34,53	1.18	4 (11%)	40,42,61	1.07	2 (5%)
45	3PE	Y	204	-	50,50,50	0.87	4 (8%)	53,55,55	1.02	2 (3%)
46	PC1	q	202	-	48,48,53	0.99	4 (8%)	54,56,61	0.97	2 (3%)
47	PLC	L	704	-	41,41,41	0.52	0	47,49,49	0.50	0
48	SF4	F	502	6	0,12,12	-	-	-		
45	3PE	Y	207	-	42,42,50	0.94	4 (9%)	45,47,55	1.06	2 (4%)
45	3PE	J	202	-	35,35,50	1.03	4 (11%)	38,40,55	1.13	2 (5%)
45	3PE	A	201	-	46,46,50	0.90	4 (8%)	49,51,55	1.07	2 (4%)
45	3PE	m	204	-	40,40,50	0.97	4 (10%)	43,45,55	1.11	2 (4%)
45	3PE	N	401	-	48,48,50	0.90	4 (8%)	51,53,55	1.09	2 (3%)
45	3PE	Z	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
51	FMN	F	501	-	33,33,33	2.75	10 (30%)	48,50,50	1.75	14 (29%)
59	CHD	i	201	-	32,32,32	3.26	10 (31%)	51,51,51	2.40	20 (39%)
53	CDL	H	404	-	80,80,99	0.98	8 (10%)	86,92,111	1.08	5 (5%)
46	PC1	H	402	-	38,38,53	1.11	4 (10%)	44,46,61	1.11	2 (4%)
45	3PE	Z	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.09	2 (4%)
45	3PE	O	403	-	44,44,50	0.93	4 (9%)	47,49,55	1.08	2 (4%)
47	PLC	M	603	-	27,27,41	0.62	0	33,35,49	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	SF4	I	202	9	0,12,12	-	-	-		
45	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.15	2 (4%)
53	CDL	d	202	-	85,85,99	0.95	8 (9%)	91,97,111	1.11	4 (4%)
47	PLC	A	206	-	32,32,41	0.57	0	38,40,49	0.57	0
45	3PE	N	402	-	44,44,50	0.94	4 (9%)	47,49,55	1.01	2 (4%)
45	3PE	A	202	-	36,36,50	1.02	4 (11%)	39,41,55	1.10	2 (5%)
53	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.10	4 (5%)
45	3PE	q	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
46	PC1	I	204	-	43,43,53	1.05	4 (9%)	49,51,61	1.04	2 (4%)
55	DGT	O	401	56	32,33,33	3.35	14 (43%)	48,52,52	1.96	13 (27%)
46	PC1	H	401	-	47,47,53	1.01	4 (8%)	53,55,61	1.05	2 (3%)
45	3PE	b	101	-	50,50,50	0.88	4 (8%)	53,55,55	1.07	2 (3%)
45	3PE	A	203	-	50,50,50	0.88	4 (8%)	53,55,55	1.05	2 (3%)
45	3PE	r	201	-	33,33,50	1.06	4 (12%)	36,38,55	1.05	2 (5%)
45	3PE	P	502	-	34,34,50	1.05	4 (11%)	37,39,55	1.10	2 (5%)
53	CDL	r	202	-	60,60,99	1.12	8 (13%)	66,72,111	1.14	4 (6%)
57	NDP	P	501	-	51,52,52	4.01	28 (54%)	71,80,80	1.92	14 (19%)
45	3PE	m	202	-	31,31,50	1.10	4 (12%)	34,36,55	1.18	2 (5%)
45	3PE	e	201	-	48,48,50	0.89	4 (8%)	51,53,55	1.06	2 (3%)
46	PC1	I	203	-	53,53,53	0.95	4 (7%)	59,61,61	1.01	2 (3%)
45	3PE	m	203	-	49,49,50	0.88	4 (8%)	52,54,55	1.02	2 (3%)
46	PC1	B	203	-	45,45,53	1.03	4 (8%)	51,53,61	1.00	2 (3%)
53	CDL	P	505	-	58,58,99	1.13	8 (13%)	64,70,111	1.16	4 (6%)
58	EHZ	T	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.53	5 (13%)
45	3PE	L	701	-	50,50,50	0.87	4 (8%)	53,55,55	1.05	2 (3%)
46	PC1	H	403	-	38,38,53	1.12	4 (10%)	44,46,61	0.96	2 (4%)
45	3PE	f	101	-	33,33,50	1.06	4 (12%)	36,38,55	1.14	2 (5%)
48	SF4	G	801	7	0,12,12	-	-	-		
46	PC1	h	201	-	46,46,53	1.02	4 (8%)	52,54,61	1.04	2 (3%)
45	3PE	Y	201	-	26,26,50	1.19	4 (15%)	29,31,55	1.20	2 (6%)
60	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.83	0
48	SF4	I	201	9	0,12,12	-	-	-		
46	PC1	L	703	-	46,46,53	1.02	4 (8%)	52,54,61	0.98	2 (3%)
46	PC1	J	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.04	2 (5%)
45	3PE	K	101	-	43,43,50	0.93	4 (9%)	46,48,55	1.07	2 (4%)
45	3PE	N	403	-	50,50,50	0.88	4 (8%)	53,55,55	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	CDL	N	404	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)

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
53	CDL	L	705	-	-	28/86/86/110	-
47	PLC	P	503	-	-	15/45/45/45	-
46	PC1	e	202	-	-	25/42/42/57	-
50	FES	E	301	5	-	-	0/1/1/1
45	3PE	Y	205	-	-	21/48/48/54	-
45	3PE	f	102	-	-	25/47/47/54	-
47	PLC	O	404	-	-	4/38/38/45	-
47	PLC	P	504	-	-	12/34/34/45	-
46	PC1	B	204	-	-	16/51/51/57	-
46	PC1	L	702	-	-	19/47/47/57	-
53	CDL	h	202	-	-	38/90/90/110	-
46	PC1	A	205	-	-	14/36/36/57	-
50	FES	G	803	7	-	-	0/1/1/1
47	PLC	J	204	-	-	14/40/40/45	-
46	PC1	m	205	-	-	15/57/57/57	-
53	CDL	M	604	-	-	48/110/110/110	-
46	PC1	A	204	-	-	19/38/38/57	-
47	PLC	Z	203	-	-	14/37/37/45	-
45	3PE	Y	203	-	-	23/54/54/54	-
45	3PE	i	202	-	-	24/48/48/54	-
47	PLC	g	201	-	-	11/45/45/45	-
49	U10	B	202	-	-	12/63/87/87	0/1/1/1
48	SF4	G	802	7	-	-	0/6/5/5
47	PLC	Y	208	-	-	14/45/45/45	-
58	EHZ	U	101	20	-	16/42/44/45	-
45	3PE	Y	202	-	-	27/54/54/54	-
45	3PE	J	201	-	-	13/32/32/54	-
48	SF4	B	201	2	-	-	0/6/5/5
45	3PE	Y	206	-	-	19/39/39/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	M	602	-	-	15/38/38/57	-
45	3PE	Y	204	-	-	23/54/54/54	-
46	PC1	q	202	-	-	25/52/52/57	-
47	PLC	L	704	-	-	11/45/45/45	-
48	SF4	F	502	6	-	-	0/6/5/5
45	3PE	Y	207	-	-	19/46/46/54	-
45	3PE	J	202	-	-	21/39/39/54	-
45	3PE	A	201	-	-	22/50/50/54	-
45	3PE	m	204	-	-	17/44/44/54	-
45	3PE	N	401	-	-	30/52/52/54	-
45	3PE	Z	202	-	-	28/54/54/54	-
51	FMN	F	501	-	-	5/18/18/18	0/3/3/3
59	CHD	i	201	-	-	4/9/74/74	0/4/4/4
53	CDL	H	404	-	-	32/91/91/110	-
46	PC1	H	402	-	-	14/42/42/57	-
45	3PE	Z	201	-	-	20/44/44/54	-
45	3PE	O	403	-	-	18/48/48/54	-
47	PLC	M	603	-	-	10/31/31/45	-
48	SF4	I	202	9	-	-	0/6/5/5
45	3PE	m	201	-	-	18/44/44/54	-
53	CDL	d	202	-	-	44/96/96/110	-
47	PLC	A	206	-	-	8/36/36/45	-
45	3PE	N	402	-	-	18/48/48/54	-
45	3PE	A	202	-	-	15/40/40/54	-
53	CDL	d	201	-	-	34/75/75/110	-
45	3PE	q	201	-	-	23/54/54/54	-
46	PC1	I	204	-	-	20/47/47/57	-
55	DGT	O	401	56	-	3/22/34/34	0/3/3/3
46	PC1	H	401	-	-	18/51/51/57	-
45	3PE	b	101	-	-	20/54/54/54	-
45	3PE	A	203	-	-	19/54/54/54	-
45	3PE	r	201	-	-	14/37/37/54	-
57	NDP	P	501	-	-	12/34/77/77	0/5/5/5
45	3PE	P	502	-	-	11/38/38/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	r	202	-	-	30/71/71/110	-
45	3PE	m	202	-	-	15/35/35/54	-
45	3PE	e	201	-	-	13/52/52/54	-
46	PC1	I	203	-	-	19/57/57/57	-
45	3PE	m	203	-	-	19/53/53/54	-
46	PC1	B	203	-	-	12/49/49/57	-
53	CDL	P	505	-	-	34/69/69/110	-
58	EHZ	T	101	20	-	14/42/44/45	-
45	3PE	L	701	-	-	25/54/54/54	-
46	PC1	H	403	-	-	15/42/42/57	-
45	3PE	f	101	-	-	22/37/37/54	-
48	SF4	G	801	7	-	-	0/6/5/5
46	PC1	h	201	-	-	23/50/50/57	-
45	3PE	Y	201	-	-	12/30/30/54	-
60	MYR	o	201	40	-	7/12/12/13	-
48	SF4	I	201	9	-	-	0/6/5/5
46	PC1	L	703	-	-	15/50/50/57	-
46	PC1	J	203	-	-	14/38/38/57	-
45	3PE	K	101	-	-	18/47/47/54	-
45	3PE	N	403	-	-	25/54/54/54	-
53	CDL	N	404	-	-	48/110/110/110	-

All (366) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.34	1.70	1.59
57	P	501	NDP	C2B-C1B	-9.07	1.30	1.53
59	i	201	CHD	C11-C12	9.04	1.68	1.53
55	O	401	DGT	O6-C6	8.85	1.40	1.23
57	P	501	NDP	O4B-C1B	8.64	1.62	1.42
57	P	501	NDP	O4D-C1D	8.17	1.60	1.42
57	P	501	NDP	C7N-N7N	7.66	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.31	1.30	1.53
59	i	201	CHD	C16-C15	7.18	1.73	1.54
57	P	501	NDP	C6N-C5N	7.09	1.54	1.33
55	O	401	DGT	C5-N7	6.71	1.52	1.39
57	P	501	NDP	O4D-C4D	-6.58	1.30	1.45
51	F	501	FMN	C10-N1	6.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	F	501	FMN	C4A-N5	6.46	1.44	1.30
59	i	201	CHD	C20-C17	-6.35	1.43	1.54
57	P	501	NDP	P2B-O2B	5.69	1.69	1.59
51	F	501	FMN	C5A-N5	5.51	1.49	1.39
57	P	501	NDP	C6A-N6A	5.37	1.47	1.34
55	O	401	DGT	PB-O3A	5.35	1.65	1.59
55	O	401	DGT	PA-O3A	5.30	1.65	1.59
59	i	201	CHD	O12-C12	-5.30	1.34	1.43
59	i	201	CHD	C13-C17	5.26	1.64	1.55
59	i	201	CHD	C8-C9	5.25	1.63	1.53
57	P	501	NDP	O4B-C4B	-5.24	1.33	1.45
55	O	401	DGT	PB-O3B	5.21	1.65	1.59
58	U	101	EHZ	C12-N1	5.12	1.45	1.33
58	T	101	EHZ	C12-N1	5.08	1.45	1.33
58	U	101	EHZ	C15-N2	5.03	1.45	1.33
51	F	501	FMN	C2-N1	4.98	1.47	1.36
51	F	501	FMN	C9A-N10	4.96	1.49	1.41
58	T	101	EHZ	C15-N2	4.93	1.45	1.33
55	O	401	DGT	C2-N2	4.86	1.45	1.34
55	O	401	DGT	C2-N1	4.77	1.49	1.37
57	P	501	NDP	PN-O3	4.72	1.64	1.59
57	P	501	NDP	C2N-C3N	4.65	1.48	1.35
59	i	201	CHD	C6-C5	4.61	1.61	1.53
51	F	501	FMN	C2-N3	4.51	1.48	1.39
55	O	401	DGT	C2-N3	4.44	1.43	1.33
55	O	401	DGT	C8-N9	-4.34	1.27	1.37
57	P	501	NDP	C5A-C4A	-4.17	1.31	1.39
57	P	501	NDP	O7N-C7N	-4.16	1.14	1.24
59	i	201	CHD	C15-C14	4.15	1.62	1.54
57	P	501	NDP	C8A-N9A	-3.86	1.31	1.37
55	O	401	DGT	C4-N9	-3.83	1.28	1.38
51	F	501	FMN	C4-N3	3.82	1.46	1.38
57	P	501	NDP	O2D-C2D	3.78	1.52	1.43
51	F	501	FMN	C10-N10	3.69	1.45	1.37
59	i	201	CHD	C6-C7	3.47	1.59	1.52
57	P	501	NDP	C4N-C3N	3.34	1.56	1.50
49	B	202	U10	C4-C5	-3.32	1.39	1.48
49	B	202	U10	C31-C29	3.07	1.57	1.51
49	B	202	U10	C51-C49	3.06	1.57	1.51
49	B	202	U10	C3-C2	-3.03	1.40	1.48
49	B	202	U10	C20-C19	2.92	1.57	1.50
51	F	501	FMN	O2-C2	-2.89	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	B	202	U10	C30-C29	2.83	1.57	1.50
49	B	202	U10	C6-C1	2.81	1.40	1.35
46	I	204	PC1	O21-C2	-2.81	1.40	1.46
53	H	404	CDL	OA6-CA4	-2.80	1.40	1.46
53	r	202	CDL	OB6-CB4	-2.80	1.40	1.46
45	N	402	3PE	O21-C2	-2.79	1.40	1.46
57	P	501	NDP	C4N-C5N	2.76	1.56	1.49
46	L	703	PC1	O21-C2	-2.76	1.40	1.46
53	d	202	CDL	OB6-CB4	-2.75	1.40	1.46
53	M	604	CDL	OB6-CB4	-2.75	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.74	1.40	1.46
53	r	202	CDL	OA6-CA4	-2.73	1.40	1.46
53	L	705	CDL	OB6-CB4	-2.73	1.40	1.46
46	L	702	PC1	O21-C2	-2.72	1.40	1.46
46	I	203	PC1	O21-C2	-2.72	1.40	1.46
45	Y	203	3PE	O21-C2	-2.72	1.40	1.46
46	e	202	PC1	O21-C2	-2.72	1.40	1.46
46	J	203	PC1	O21-C2	-2.72	1.40	1.46
53	L	705	CDL	OA6-CA4	-2.71	1.40	1.46
53	h	202	CDL	OA6-CA4	-2.71	1.40	1.46
53	P	505	CDL	OA6-CA4	-2.71	1.40	1.46
46	A	204	PC1	O21-C2	-2.71	1.40	1.46
55	O	401	DGT	C1'-N9	-2.70	1.41	1.48
53	H	404	CDL	OB6-CB4	-2.70	1.40	1.46
45	Y	206	3PE	O21-C2	-2.70	1.40	1.46
45	J	202	3PE	O21-C2	-2.70	1.40	1.46
45	e	201	3PE	O21-C2	-2.70	1.40	1.46
45	Z	201	3PE	O21-C2	-2.69	1.40	1.46
53	M	604	CDL	OA6-CA4	-2.69	1.40	1.46
46	m	205	PC1	O21-C2	-2.69	1.40	1.46
45	q	201	3PE	O21-C2	-2.68	1.40	1.46
49	B	202	U10	C35-C34	2.68	1.57	1.50
46	M	602	PC1	O21-C2	-2.68	1.40	1.46
46	h	201	PC1	O21-C2	-2.68	1.40	1.46
45	N	401	3PE	O21-C2	-2.68	1.40	1.46
57	P	501	NDP	C5A-N7A	-2.68	1.34	1.39
53	P	505	CDL	OB6-CB4	-2.67	1.40	1.46
45	O	403	3PE	O21-C2	-2.67	1.40	1.46
45	b	101	3PE	O21-C2	-2.67	1.40	1.46
46	H	401	PC1	O21-C2	-2.67	1.40	1.46
46	B	203	PC1	O21-C2	-2.67	1.40	1.46
53	N	404	CDL	OB6-CB4	-2.67	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	P	502	3PE	O21-C2	-2.66	1.40	1.46
46	A	205	PC1	O21-C2	-2.66	1.40	1.46
45	A	203	3PE	O21-C2	-2.66	1.40	1.46
45	Z	202	3PE	O21-C2	-2.65	1.40	1.46
46	B	204	PC1	O21-C2	-2.64	1.40	1.46
45	N	403	3PE	O21-C2	-2.64	1.40	1.46
45	Y	201	3PE	O21-C2	-2.64	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.64	1.40	1.46
53	h	202	CDL	OB6-CB4	-2.63	1.40	1.46
46	H	403	PC1	O21-C2	-2.63	1.40	1.46
51	F	501	FMN	O4-C4	-2.63	1.18	1.23
49	B	202	U10	C7-C8	2.63	1.54	1.50
49	B	202	U10	C15-C14	2.62	1.57	1.50
46	H	402	PC1	O21-C2	-2.62	1.40	1.46
45	f	102	3PE	O21-C2	-2.59	1.40	1.46
45	K	101	3PE	O21-C2	-2.59	1.40	1.46
45	f	101	3PE	O21-C2	-2.58	1.40	1.46
53	N	404	CDL	OA6-CA4	-2.58	1.40	1.46
45	Y	207	3PE	O21-C2	-2.58	1.40	1.46
45	m	202	3PE	O21-C2	-2.57	1.40	1.46
45	J	201	3PE	O21-C2	-2.57	1.40	1.46
45	A	201	3PE	O21-C2	-2.57	1.40	1.46
45	m	204	3PE	O21-C2	-2.56	1.40	1.46
45	A	202	3PE	O21-C2	-2.55	1.40	1.46
45	m	203	3PE	O21-C2	-2.54	1.40	1.46
45	L	701	3PE	O21-C2	-2.53	1.40	1.46
45	m	201	3PE	O21-C2	-2.52	1.40	1.46
57	P	501	NDP	C6N-N1N	2.51	1.43	1.37
45	Y	205	3PE	O21-C2	-2.50	1.40	1.46
45	r	201	3PE	O21-C2	-2.49	1.40	1.46
46	q	202	PC1	O21-C2	-2.47	1.40	1.46
49	B	202	U10	C1M-C1	2.47	1.55	1.50
53	H	404	CDL	OA8-CA7	2.47	1.40	1.33
45	i	202	3PE	O21-C2	-2.47	1.40	1.46
46	e	202	PC1	O31-C31	2.44	1.40	1.33
46	q	202	PC1	O31-C31	2.43	1.40	1.33
46	J	203	PC1	O31-C31	2.43	1.40	1.33
53	d	202	CDL	OA6-CA4	-2.43	1.40	1.46
53	d	202	CDL	OA8-CA7	2.43	1.40	1.33
57	P	501	NDP	O3B-C3B	-2.43	1.36	1.43
46	H	403	PC1	O31-C31	2.43	1.40	1.33
45	Y	202	3PE	O21-C2	-2.43	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	r	202	CDL	OB8-CB7	2.43	1.40	1.33
57	P	501	NDP	O3D-C3D	-2.43	1.36	1.43
53	P	505	CDL	OA8-CA7	2.43	1.40	1.33
53	L	705	CDL	OA8-CA7	2.42	1.40	1.33
58	T	101	EHZ	O4-C15	-2.42	1.18	1.23
45	J	202	3PE	O31-C31	2.42	1.40	1.33
46	h	201	PC1	O31-C31	2.42	1.40	1.33
45	K	101	3PE	O31-C3	-2.41	1.39	1.45
58	U	101	EHZ	C9-S1	2.41	1.81	1.76
45	N	402	3PE	O31-C31	2.41	1.40	1.33
53	H	404	CDL	OB8-CB7	2.41	1.40	1.33
53	N	404	CDL	OA8-CA7	2.41	1.40	1.33
46	I	204	PC1	O31-C31	2.40	1.40	1.33
53	P	505	CDL	OB8-CB7	2.40	1.40	1.33
49	B	202	U10	C50-C49	2.40	1.56	1.50
53	d	201	CDL	OB8-CB7	2.40	1.40	1.33
46	M	602	PC1	O31-C31	2.40	1.40	1.33
45	Y	204	3PE	O21-C2	-2.39	1.41	1.46
46	B	203	PC1	O31-C31	2.39	1.40	1.33
53	M	604	CDL	OA8-CA7	2.39	1.40	1.33
46	H	401	PC1	O31-C31	2.39	1.40	1.33
53	L	705	CDL	OB8-CB7	2.39	1.40	1.33
46	H	402	PC1	O31-C31	2.38	1.40	1.33
58	U	101	EHZ	O4-C15	-2.38	1.18	1.23
46	L	702	PC1	O31-C31	2.38	1.40	1.33
45	f	102	3PE	O31-C31	2.38	1.40	1.33
46	A	205	PC1	O31-C31	2.37	1.40	1.33
45	N	403	3PE	O31-C31	2.37	1.40	1.33
53	M	604	CDL	OB8-CB7	2.37	1.40	1.33
45	m	201	3PE	O31-C31	2.36	1.40	1.33
46	m	205	PC1	O31-C31	2.36	1.40	1.33
45	e	201	3PE	O31-C31	2.36	1.40	1.33
45	Y	203	3PE	O31-C3	-2.36	1.39	1.45
45	Y	206	3PE	O31-C31	2.36	1.40	1.33
45	A	202	3PE	O31-C31	2.36	1.40	1.33
45	N	401	3PE	O31-C31	2.36	1.40	1.33
45	Z	201	3PE	O31-C31	2.35	1.40	1.33
45	Y	205	3PE	O31-C31	2.35	1.40	1.33
45	f	101	3PE	O31-C31	2.35	1.40	1.33
46	I	203	PC1	O31-C31	2.35	1.40	1.33
49	B	202	U10	C40-C39	2.35	1.56	1.50
53	N	404	CDL	OB8-CB7	2.35	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	O	403	3PE	O31-C31	2.35	1.40	1.33
46	L	703	PC1	O31-C31	2.35	1.40	1.33
53	d	201	CDL	OA8-CA7	2.35	1.40	1.33
53	h	202	CDL	OA8-CA7	2.34	1.40	1.33
45	Y	207	3PE	O31-C31	2.34	1.40	1.33
57	P	501	NDP	C7N-C3N	2.34	1.53	1.48
45	L	701	3PE	O31-C31	2.34	1.40	1.33
53	h	202	CDL	OB8-CB7	2.34	1.40	1.33
45	m	202	3PE	O31-C31	2.34	1.40	1.33
46	A	204	PC1	O31-C31	2.34	1.40	1.33
45	m	203	3PE	O31-C31	2.34	1.40	1.33
45	A	201	3PE	O31-C31	2.33	1.40	1.33
45	r	201	3PE	O31-C31	2.33	1.40	1.33
58	U	101	EHZ	O3-C12	-2.33	1.18	1.23
57	P	501	NDP	P2B-O1X	2.33	1.57	1.50
45	i	202	3PE	O31-C31	2.33	1.40	1.33
49	B	202	U10	C41-C39	2.33	1.56	1.51
45	b	101	3PE	O31-C31	2.33	1.40	1.33
45	P	502	3PE	O31-C31	2.32	1.40	1.33
46	B	204	PC1	O31-C31	2.32	1.40	1.33
45	m	204	3PE	O31-C31	2.32	1.40	1.33
45	Y	204	3PE	O31-C31	2.32	1.40	1.33
53	d	202	CDL	OB8-CB7	2.31	1.40	1.33
45	Y	202	3PE	O31-C31	2.31	1.40	1.33
59	i	201	CHD	C13-C12	-2.31	1.51	1.54
45	Y	201	3PE	O31-C3	-2.31	1.40	1.45
53	h	202	CDL	OA8-CA6	-2.30	1.40	1.45
45	m	204	3PE	O31-C3	-2.29	1.40	1.45
45	J	201	3PE	O31-C3	-2.29	1.40	1.45
45	A	203	3PE	O31-C3	-2.29	1.40	1.45
58	T	101	EHZ	O3-C12	-2.29	1.18	1.23
45	A	203	3PE	O31-C31	2.29	1.40	1.33
45	q	201	3PE	O31-C31	2.29	1.40	1.33
53	r	202	CDL	OA8-CA7	2.29	1.40	1.33
53	h	202	CDL	OB8-CB6	-2.29	1.40	1.45
45	J	201	3PE	O31-C31	2.29	1.40	1.33
45	m	202	3PE	O31-C3	-2.29	1.40	1.45
46	q	202	PC1	O21-C21	2.29	1.40	1.34
45	Y	202	3PE	O31-C3	-2.28	1.40	1.45
57	P	501	NDP	PA-O5B	2.28	1.68	1.59
49	B	202	U10	C16-C14	2.28	1.56	1.51
53	d	201	CDL	OA8-CA6	-2.28	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	r	201	3PE	O31-C3	-2.27	1.40	1.45
55	O	401	DGT	C4-N3	2.27	1.39	1.34
45	Z	202	3PE	O31-C31	2.26	1.39	1.33
45	Y	204	3PE	O31-C3	-2.26	1.40	1.45
45	b	101	3PE	O31-C3	-2.26	1.40	1.45
55	O	401	DGT	PG-O2G	-2.25	1.46	1.54
45	Y	203	3PE	O31-C31	2.25	1.39	1.33
45	Y	206	3PE	O31-C3	-2.25	1.40	1.45
53	N	404	CDL	OB8-CB6	-2.25	1.40	1.45
46	L	703	PC1	O31-C3	-2.25	1.40	1.45
53	r	202	CDL	OA8-CA6	-2.25	1.40	1.45
45	Y	201	3PE	O31-C31	2.25	1.39	1.33
58	T	101	EHZ	C9-S1	2.25	1.81	1.76
46	A	204	PC1	O31-C3	-2.24	1.40	1.45
49	B	202	U10	C36-C34	2.24	1.55	1.51
49	B	202	U10	C46-C44	2.24	1.55	1.51
45	Z	202	3PE	O31-C3	-2.24	1.40	1.45
45	Z	201	3PE	O31-C3	-2.24	1.40	1.45
45	A	202	3PE	O31-C3	-2.23	1.40	1.45
45	N	403	3PE	O31-C3	-2.23	1.40	1.45
55	O	401	DGT	PG-O1G	-2.23	1.46	1.54
45	A	201	3PE	O31-C3	-2.23	1.40	1.45
45	P	502	3PE	O31-C3	-2.23	1.40	1.45
46	m	205	PC1	O31-C3	-2.23	1.40	1.45
53	N	404	CDL	OA6-CA5	2.23	1.40	1.34
45	m	203	3PE	O21-C21	2.22	1.40	1.34
45	N	401	3PE	O31-C3	-2.22	1.40	1.45
45	m	201	3PE	O31-C3	-2.22	1.40	1.45
45	L	701	3PE	O21-C21	2.22	1.40	1.34
45	K	101	3PE	O31-C31	2.22	1.39	1.33
49	B	202	U10	C26-C24	2.22	1.55	1.51
53	M	604	CDL	OA8-CA6	-2.22	1.40	1.45
53	d	201	CDL	OB6-CB5	2.21	1.40	1.34
53	d	202	CDL	OB8-CB6	-2.21	1.40	1.45
46	L	702	PC1	O31-C3	-2.21	1.40	1.45
53	H	404	CDL	OB8-CB6	-2.21	1.40	1.45
53	L	705	CDL	OB8-CB6	-2.21	1.40	1.45
45	O	403	3PE	O31-C3	-2.20	1.40	1.45
45	m	202	3PE	O21-C21	2.20	1.40	1.34
46	H	402	PC1	O21-C21	2.20	1.40	1.34
53	d	202	CDL	OA6-CA5	2.20	1.40	1.34
46	H	402	PC1	O31-C3	-2.20	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	m	201	3PE	O21-C21	2.20	1.40	1.34
45	f	101	3PE	O31-C3	-2.20	1.40	1.45
53	M	604	CDL	OB8-CB6	-2.20	1.40	1.45
45	Y	204	3PE	O21-C21	2.20	1.40	1.34
46	H	403	PC1	O31-C3	-2.19	1.40	1.45
45	Y	201	3PE	O21-C21	2.19	1.40	1.34
46	B	204	PC1	O31-C3	-2.19	1.40	1.45
45	f	101	3PE	O21-C21	2.19	1.40	1.34
45	J	202	3PE	O31-C3	-2.19	1.40	1.45
45	m	203	3PE	O31-C3	-2.19	1.40	1.45
45	N	402	3PE	O31-C3	-2.19	1.40	1.45
45	q	201	3PE	O31-C3	-2.19	1.40	1.45
45	A	201	3PE	O21-C21	2.18	1.40	1.34
53	d	201	CDL	OB8-CB6	-2.18	1.40	1.45
46	B	204	PC1	O21-C21	2.18	1.40	1.34
53	h	202	CDL	OB6-CB5	2.18	1.40	1.34
49	B	202	U10	C11-C9	2.18	1.55	1.51
46	H	401	PC1	O31-C3	-2.18	1.40	1.45
46	A	205	PC1	O31-C3	-2.18	1.40	1.45
53	d	202	CDL	OA8-CA6	-2.17	1.40	1.45
45	f	102	3PE	O21-C21	2.17	1.40	1.34
46	J	203	PC1	O21-C21	2.17	1.40	1.34
45	e	201	3PE	O31-C3	-2.17	1.40	1.45
45	A	202	3PE	O21-C21	2.17	1.40	1.34
45	i	202	3PE	O31-C3	-2.17	1.40	1.45
46	h	201	PC1	O31-C3	-2.17	1.40	1.45
46	m	205	PC1	O21-C21	2.17	1.40	1.34
45	K	101	3PE	O21-C21	2.16	1.40	1.34
46	M	602	PC1	O21-C21	2.16	1.40	1.34
45	J	201	3PE	O21-C21	2.16	1.40	1.34
46	e	202	PC1	O31-C3	-2.16	1.40	1.45
46	I	204	PC1	O31-C3	-2.16	1.40	1.45
46	A	205	PC1	O21-C21	2.16	1.40	1.34
46	B	203	PC1	O31-C3	-2.16	1.40	1.45
45	r	201	3PE	O21-C21	2.15	1.40	1.34
45	Y	202	3PE	O21-C21	2.15	1.40	1.34
45	f	102	3PE	O31-C3	-2.15	1.40	1.45
53	h	202	CDL	OA6-CA5	2.15	1.40	1.34
45	Y	207	3PE	O31-C3	-2.15	1.40	1.45
46	I	203	PC1	O21-C21	2.15	1.40	1.34
49	B	202	U10	C6-C5	-2.15	1.40	1.46
45	L	701	3PE	O31-C3	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	J	203	PC1	O31-C3	-2.15	1.40	1.45
49	B	202	U10	C1-C2	-2.15	1.39	1.47
45	Y	205	3PE	O21-C21	2.14	1.40	1.34
45	P	502	3PE	O21-C21	2.14	1.40	1.34
46	I	203	PC1	O31-C3	-2.14	1.40	1.45
45	i	202	3PE	O21-C21	2.14	1.40	1.34
46	M	602	PC1	O31-C3	-2.14	1.40	1.45
53	L	705	CDL	OA8-CA6	-2.14	1.40	1.45
53	M	604	CDL	OA6-CA5	2.14	1.40	1.34
45	b	101	3PE	O21-C21	2.14	1.40	1.34
57	P	501	NDP	C5B-C4B	2.13	1.58	1.51
53	r	202	CDL	OA6-CA5	2.13	1.40	1.34
46	H	401	PC1	O21-C21	2.13	1.40	1.34
45	N	403	3PE	O21-C21	2.13	1.40	1.34
45	Y	205	3PE	O31-C3	-2.13	1.40	1.45
45	m	204	3PE	O21-C21	2.13	1.40	1.34
46	H	403	PC1	O21-C21	2.13	1.40	1.34
53	H	404	CDL	OB6-CB5	2.13	1.40	1.34
45	A	203	3PE	O21-C21	2.13	1.40	1.34
53	P	505	CDL	OB8-CB6	-2.13	1.40	1.45
53	P	505	CDL	OA8-CA6	-2.13	1.40	1.45
45	Z	201	3PE	O21-C21	2.12	1.40	1.34
53	N	404	CDL	OB6-CB5	2.12	1.40	1.34
53	L	705	CDL	OB6-CB5	2.12	1.40	1.34
53	r	202	CDL	OB8-CB6	-2.12	1.40	1.45
46	q	202	PC1	O31-C3	-2.12	1.40	1.45
46	h	201	PC1	O21-C21	2.12	1.40	1.34
45	Y	207	3PE	O21-C21	2.12	1.40	1.34
53	d	201	CDL	OA6-CA5	2.11	1.40	1.34
49	B	202	U10	O4-C4	2.11	1.41	1.36
53	P	505	CDL	OA6-CA5	2.11	1.40	1.34
46	A	204	PC1	O21-C21	2.11	1.40	1.34
46	B	203	PC1	O21-C21	2.11	1.40	1.34
46	L	703	PC1	O21-C21	2.11	1.40	1.34
45	N	401	3PE	O21-C21	2.11	1.40	1.34
45	Z	202	3PE	O21-C21	2.10	1.40	1.34
45	q	201	3PE	O21-C21	2.10	1.40	1.34
53	N	404	CDL	OA8-CA6	-2.10	1.40	1.45
53	P	505	CDL	OB6-CB5	2.10	1.40	1.34
53	M	604	CDL	OB6-CB5	2.10	1.40	1.34
49	B	202	U10	O3-C3	2.09	1.41	1.36
45	e	201	3PE	O21-C21	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	H	404	CDL	OA8-CA6	-2.09	1.40	1.45
46	e	202	PC1	O21-C21	2.09	1.40	1.34
46	I	204	PC1	O21-C21	2.08	1.40	1.34
49	B	202	U10	C10-C9	2.08	1.55	1.50
53	H	404	CDL	OA6-CA5	2.08	1.40	1.34
53	r	202	CDL	OB6-CB5	2.08	1.40	1.34
45	O	403	3PE	O21-C21	2.07	1.40	1.34
45	J	202	3PE	O21-C21	2.07	1.40	1.34
45	N	402	3PE	O21-C21	2.07	1.40	1.34
45	Y	206	3PE	O21-C21	2.06	1.40	1.34
45	Y	203	3PE	O21-C21	2.05	1.40	1.34
53	L	705	CDL	OA6-CA5	2.05	1.40	1.34
46	L	702	PC1	O21-C21	2.05	1.40	1.34
49	B	202	U10	C25-C24	2.04	1.55	1.50
53	d	202	CDL	OB6-CB5	2.04	1.40	1.34
57	P	501	NDP	C5D-C4D	2.03	1.57	1.51
49	B	202	U10	C7-C6	2.02	1.55	1.51

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	C8-N9-C4	7.57	120.21	106.03
59	i	201	CHD	C13-C17-C20	-7.04	110.95	119.48
59	i	201	CHD	C14-C13-C12	5.67	112.60	107.42
57	P	501	NDP	N6A-C6A-N1A	-5.67	105.75	118.38
57	P	501	NDP	N3A-C2A-N1A	-5.56	120.16	128.58
57	P	501	NDP	C4A-N9A-C1B	-5.52	113.72	126.63
58	U	101	EHZ	C8-C9-S1	5.34	120.30	113.56
59	i	201	CHD	C17-C13-C14	5.25	105.38	100.11
57	P	501	NDP	C5A-C4A-N3A	-5.04	119.77	126.72
57	P	501	NDP	C1B-N9A-C8A	4.99	138.16	127.09
59	i	201	CHD	C17-C13-C12	4.81	122.00	117.67
58	T	101	EHZ	C8-C9-S1	4.80	119.62	113.56
53	h	202	CDL	OB6-CB5-C51	4.69	121.63	111.48
46	B	204	PC1	O21-C21-C22	4.67	121.59	111.48
51	F	501	FMN	C9-C8-C7	4.63	126.49	119.69
51	F	501	FMN	C7M-C7-C6	4.62	127.72	119.57
45	Y	202	3PE	O21-C21-C22	4.46	121.12	111.48
45	m	201	3PE	O21-C21-C22	4.42	121.04	111.48
45	Y	205	3PE	O21-C21-C22	4.41	121.01	111.48
46	H	402	PC1	O21-C21-C22	4.27	120.72	111.48
59	i	201	CHD	C18-C13-C12	-4.25	104.80	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	P	501	NDP	C5A-C6A-N6A	4.19	133.67	123.29
45	m	202	3PE	O21-C21-C22	4.18	120.52	111.48
45	m	204	3PE	O21-C21-C22	4.17	120.49	111.48
53	d	202	CDL	OB6-CB5-C51	4.14	120.44	111.48
53	M	604	CDL	OA6-CA5-C11	4.12	120.39	111.48
46	A	205	PC1	O21-C21-C22	4.12	120.39	111.48
46	I	203	PC1	O21-C21-C22	4.11	120.38	111.48
45	N	403	3PE	O21-C21-C22	4.09	120.33	111.48
46	H	401	PC1	O21-C21-C22	4.08	120.31	111.48
45	b	101	3PE	O21-C21-C22	4.07	120.29	111.48
45	Y	201	3PE	O21-C21-C22	4.07	120.28	111.48
45	O	403	3PE	O21-C21-C22	4.06	120.27	111.48
45	f	102	3PE	O21-C21-C22	4.06	120.25	111.48
53	N	404	CDL	OB6-CB5-C51	4.04	120.22	111.48
53	M	604	CDL	OB6-CB5-C51	4.02	120.19	111.48
45	J	201	3PE	O21-C21-C22	4.02	120.18	111.48
57	P	501	NDP	N9A-C8A-N7A	-4.02	108.24	113.94
45	Y	206	3PE	O21-C21-C22	4.01	120.16	111.48
53	h	202	CDL	OA6-CA5-C11	4.01	120.15	111.48
45	q	201	3PE	O21-C21-C22	4.00	120.13	111.48
45	N	401	3PE	O21-C21-C22	3.98	120.08	111.48
45	A	202	3PE	O21-C21-C22	3.97	120.06	111.48
53	H	404	CDL	OA6-CA5-C11	3.96	120.05	111.48
59	i	201	CHD	C18-C13-C17	-3.96	105.00	111.20
46	e	202	PC1	O21-C21-C22	3.96	120.05	111.48
53	d	201	CDL	OA6-CA5-C11	3.95	120.03	111.48
53	P	505	CDL	OB6-CB5-C51	3.95	120.02	111.48
45	Z	201	3PE	O21-C21-C22	3.94	120.01	111.48
46	M	602	PC1	O21-C21-C22	3.94	120.00	111.48
45	A	203	3PE	O21-C21-C22	3.93	119.99	111.48
53	P	505	CDL	OA6-CA5-C11	3.93	119.98	111.48
45	Z	202	3PE	O21-C21-C22	3.92	119.96	111.48
45	f	101	3PE	O21-C21-C22	3.92	119.95	111.48
45	K	101	3PE	O21-C21-C22	3.91	119.94	111.48
46	A	204	PC1	O21-C21-C22	3.91	119.93	111.48
55	O	401	DGT	C1'-N9-C8	-3.90	119.17	127.91
46	m	205	PC1	O21-C21-C22	3.90	119.91	111.48
45	L	701	3PE	O21-C21-C22	3.88	119.89	111.48
53	L	705	CDL	OA6-CA5-C11	3.88	119.88	111.48
53	L	705	CDL	OB6-CB5-C51	3.87	119.86	111.48
45	Y	203	3PE	O21-C21-C22	3.87	119.84	111.48
53	d	202	CDL	OA6-CA5-C11	3.86	119.84	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	Y	207	3PE	O21-C21-C22	3.84	119.80	111.48
45	i	202	3PE	O21-C21-C22	3.84	119.78	111.48
46	J	203	PC1	O21-C21-C22	3.82	119.75	111.48
45	J	202	3PE	O21-C21-C22	3.82	119.74	111.48
46	h	201	PC1	O21-C21-C22	3.81	119.73	111.48
46	L	702	PC1	O21-C21-C22	3.81	119.72	111.48
45	Y	204	3PE	O21-C21-C22	3.80	119.71	111.48
46	B	203	PC1	O21-C21-C22	3.80	119.70	111.48
53	H	404	CDL	OB6-CB5-C51	3.80	119.70	111.48
46	I	204	PC1	O21-C21-C22	3.77	119.64	111.48
45	A	201	3PE	O21-C21-C22	3.75	119.58	111.48
45	P	502	3PE	O21-C21-C22	3.75	119.58	111.48
45	e	201	3PE	O21-C21-C22	3.73	119.54	111.48
53	r	202	CDL	OB6-CB5-C51	3.72	119.53	111.48
53	r	202	CDL	OA6-CA5-C11	3.70	119.49	111.48
45	N	402	3PE	O21-C21-C22	3.69	119.46	111.48
45	m	203	3PE	O21-C21-C22	3.63	119.34	111.48
46	q	202	PC1	O21-C21-C22	3.61	119.30	111.48
45	r	201	3PE	O21-C21-C22	3.61	119.29	111.48
46	L	703	PC1	O21-C21-C22	3.58	119.23	111.48
53	N	404	CDL	OA6-CA5-C11	3.56	119.18	111.48
57	P	501	NDP	C2A-N3A-C4A	3.50	120.38	111.83
59	i	201	CHD	C18-C13-C14	-3.46	105.78	111.20
51	F	501	FMN	C4-N3-C2	-3.39	119.62	125.64
49	B	202	U10	C20-C19-C21	3.28	120.92	115.23
51	F	501	FMN	C8M-C8-C7	-3.27	114.07	120.76
49	B	202	U10	C7-C8-C9	3.21	132.36	126.83
55	O	401	DGT	C2-N1-C6	-3.17	119.37	125.11
59	i	201	CHD	C23-C22-C20	-3.11	108.66	114.46
57	P	501	NDP	N3A-C4A-N9A	3.09	132.41	127.17
49	B	202	U10	C15-C14-C16	3.08	120.58	115.23
53	M	604	CDL	OA8-CA7-C31	3.05	121.14	111.83
59	i	201	CHD	C1-C10-C5	2.99	112.04	107.75
55	O	401	DGT	C2'-C3'-C4'	2.98	108.85	102.80
46	B	204	PC1	O31-C31-C32	2.97	120.90	111.83
46	H	402	PC1	O31-C31-C32	2.97	120.16	111.15
55	O	401	DGT	O2G-PG-O3B	2.92	114.41	104.64
46	L	702	PC1	O31-C31-C32	2.91	120.72	111.83
53	d	201	CDL	OB6-CB5-C51	2.90	121.60	110.93
59	i	201	CHD	C1-C2-C3	2.90	114.33	110.48
45	N	401	3PE	O31-C31-C32	2.89	120.64	111.83
45	f	101	3PE	O31-C31-C32	2.88	120.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	J	202	3PE	O31-C31-C32	2.88	119.89	111.15
53	d	202	CDL	OA8-CA7-C31	2.88	120.61	111.83
53	d	202	CDL	OB8-CB7-C71	2.87	120.59	111.83
46	e	202	PC1	O31-C31-C32	2.87	120.58	111.83
51	F	501	FMN	C4A-C10-N10	2.86	120.57	116.48
45	N	402	3PE	O31-C31-C32	2.85	120.53	111.83
45	m	201	3PE	O31-C31-C32	2.83	120.47	111.83
46	m	205	PC1	O31-C31-C32	2.83	120.45	111.83
46	L	703	PC1	O31-C31-C32	2.82	120.44	111.83
46	H	403	PC1	O31-C31-C32	2.81	120.41	111.83
46	h	201	PC1	O31-C31-C32	2.81	120.41	111.83
45	L	701	3PE	O31-C31-C32	2.80	120.38	111.83
53	N	404	CDL	OA8-CA7-C31	2.79	120.34	111.83
45	Y	206	3PE	O31-C31-C32	2.79	120.34	111.83
46	A	204	PC1	O31-C31-C32	2.79	120.33	111.83
45	b	101	3PE	O31-C31-C32	2.79	120.33	111.83
53	r	202	CDL	OA8-CA7-C31	2.78	120.30	111.83
45	Y	202	3PE	O31-C31-C32	2.77	120.29	111.83
45	A	201	3PE	O31-C31-C32	2.76	120.25	111.83
49	B	202	U10	C50-C49-C51	2.76	120.02	115.23
45	q	201	3PE	O31-C31-C32	2.75	120.23	111.83
59	i	201	CHD	C15-C14-C8	2.75	122.13	118.36
58	T	101	EHZ	C13-C12-N1	2.75	121.36	116.34
53	r	202	CDL	OB8-CB7-C71	2.75	120.22	111.83
58	T	101	EHZ	C10-S1-C9	2.75	109.96	101.84
45	m	203	3PE	O31-C31-C32	2.73	120.16	111.83
45	f	102	3PE	O31-C31-C32	2.73	120.15	111.83
46	H	401	PC1	O31-C31-C32	2.73	120.14	111.83
53	L	705	CDL	OA8-CA7-C31	2.72	120.13	111.83
53	d	201	CDL	OA8-CA7-C31	2.71	120.11	111.83
57	P	501	NDP	C5A-N7A-C8A	2.71	107.71	103.45
45	J	201	3PE	O31-C31-C32	2.71	120.08	111.83
53	H	404	CDL	OA8-CA7-C31	2.70	120.08	111.83
53	M	604	CDL	OB8-CB7-C71	2.70	120.07	111.83
55	O	401	DGT	O1G-PG-O3B	2.70	113.68	104.64
45	Y	203	3PE	O31-C31-C32	2.70	120.06	111.83
45	r	201	3PE	O31-C31-C32	2.69	120.03	111.83
53	P	505	CDL	OB8-CB7-C71	2.68	120.01	111.83
46	I	204	PC1	O31-C31-C32	2.68	120.01	111.83
53	h	202	CDL	OA8-CA7-C31	2.67	119.98	111.83
45	Z	201	3PE	O31-C31-C32	2.67	119.96	111.83
53	h	202	CDL	OB8-CB7-C71	2.67	119.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	i	202	3PE	O31-C31-C32	2.67	119.96	111.83
46	M	602	PC1	O31-C31-C32	2.66	119.95	111.83
46	B	203	PC1	O31-C31-C32	2.66	119.94	111.83
46	A	205	PC1	O31-C31-C32	2.66	119.94	111.83
45	O	403	3PE	O31-C31-C32	2.66	119.93	111.83
51	F	501	FMN	C6-C7-C8	-2.66	115.79	119.69
45	Y	204	3PE	O31-C31-C32	2.65	119.93	111.83
45	Y	201	3PE	O31-C31-C32	2.64	119.89	111.83
45	P	502	3PE	O31-C31-C32	2.64	119.88	111.83
45	A	202	3PE	O31-C31-C32	2.63	119.86	111.83
45	m	202	3PE	O31-C31-C32	2.63	119.84	111.83
58	U	101	EHZ	C10-S1-C9	2.62	109.60	101.84
45	Y	205	3PE	O31-C31-C32	2.61	119.78	111.83
45	Y	207	3PE	O31-C31-C32	2.60	119.78	111.83
53	d	201	CDL	OB8-CB7-C71	2.60	119.76	111.83
45	m	204	3PE	O31-C31-C32	2.60	119.75	111.83
49	B	202	U10	C35-C34-C36	2.60	119.73	115.23
49	B	202	U10	C45-C44-C46	2.60	119.73	115.23
45	N	403	3PE	O31-C31-C32	2.59	119.74	111.83
46	J	203	PC1	O31-C31-C32	2.59	119.73	111.83
53	H	404	CDL	OB8-CB7-C71	2.59	119.73	111.83
53	L	705	CDL	OB8-CB7-C71	2.56	119.65	111.83
53	P	505	CDL	OA8-CA7-C31	2.56	119.65	111.83
59	i	201	CHD	C9-C10-C5	2.55	112.06	108.51
59	i	201	CHD	C6-C5-C4	-2.55	108.31	111.23
45	e	201	3PE	O31-C31-C32	2.54	119.58	111.83
45	K	101	3PE	O31-C31-C32	2.54	119.57	111.83
46	q	202	PC1	O31-C31-C32	2.53	119.55	111.83
49	B	202	U10	C40-C39-C41	2.52	119.61	115.23
45	Z	202	3PE	O31-C31-C32	2.52	119.51	111.83
45	A	203	3PE	O31-C31-C32	2.51	119.50	111.83
53	N	404	CDL	OB8-CB7-C71	2.50	119.46	111.83
51	F	501	FMN	C4A-C4-N3	2.47	119.55	113.25
51	F	501	FMN	O4-C4-C4A	-2.47	120.01	126.53
55	O	401	DGT	C5-C6-N1	2.47	119.53	113.25
46	H	403	PC1	O21-C21-C22	2.46	119.96	110.93
46	I	203	PC1	O31-C31-C32	2.46	119.33	111.83
49	B	202	U10	C10-C9-C11	2.45	119.48	115.23
55	O	401	DGT	O1B-PB-O2B	-2.41	101.22	112.44
58	U	101	EHZ	O2-C9-C8	-2.41	119.94	123.74
55	O	401	DGT	O6-C6-C5	-2.40	120.20	126.53
51	F	501	FMN	C9A-C5A-N5	-2.39	119.92	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	O1A-PA-O2A	-2.37	101.44	112.44
51	F	501	FMN	C10-C4A-N5	-2.36	119.98	124.81
55	O	401	DGT	C5-C4-N9	-2.33	101.48	105.66
59	i	201	CHD	C16-C17-C13	2.33	105.80	103.54
59	i	201	CHD	C1-C10-C9	-2.32	107.73	111.34
57	P	501	NDP	C2B-C1B-N9A	-2.31	109.95	113.75
55	O	401	DGT	N9-C4-N3	2.31	130.57	125.95
58	U	101	EHZ	O2-C9-S1	-2.30	119.76	122.68
58	T	101	EHZ	O2-C9-S1	-2.29	119.77	122.68
51	F	501	FMN	C5A-C9A-N10	2.28	120.03	117.97
59	i	201	CHD	C9-C11-C12	-2.28	111.32	114.29
49	B	202	U10	C25-C24-C23	-2.26	117.81	123.63
57	P	501	NDP	C4A-N9A-C8A	2.26	108.11	105.74
49	B	202	U10	C30-C29-C31	2.25	119.13	115.23
58	U	101	EHZ	C13-C12-N1	2.23	120.41	116.34
51	F	501	FMN	C6-C5A-C9A	2.23	122.11	119.05
59	i	201	CHD	C11-C9-C10	-2.15	111.52	113.70
57	P	501	NDP	C4A-C5A-N7A	-2.14	108.13	110.58
59	i	201	CHD	C15-C14-C13	2.13	105.61	103.54
55	O	401	DGT	N9-C8-N7	-2.11	109.48	113.40
59	i	201	CHD	C19-C10-C9	-2.10	108.35	111.18
51	F	501	FMN	C7M-C7-C8	-2.09	116.49	120.76
58	U	101	EHZ	C19-C17-C16	2.09	112.33	108.77
49	B	202	U10	C25-C24-C26	2.09	118.85	115.23
57	P	501	NDP	P2B-O2B-C2B	-2.07	117.89	123.43
58	T	101	EHZ	C11-N1-C12	-2.06	118.99	122.82
59	i	201	CHD	C16-C17-C20	-2.05	109.08	112.18
51	F	501	FMN	C5'-C4'-C3'	-2.05	108.36	112.22
49	B	202	U10	C20-C19-C18	-2.02	118.44	123.63
53	H	404	CDL	CA4-OA6-CA5	-2.00	113.00	117.80

There are no chirality outliers.

All (1457) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O14
45	A	201	3PE	O13-C11-C12-N
45	A	203	3PE	C1-O11-P-O14
45	A	203	3PE	C11-O13-P-O11
45	A	203	3PE	C11-O13-P-O12
45	A	203	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
45	A	203	3PE	O22-C21-O21-C2
45	J	201	3PE	C1-O11-P-O13
45	J	201	3PE	C1-O11-P-O14
45	J	201	3PE	O13-C11-C12-N
45	J	201	3PE	O22-C21-O21-C2
45	J	202	3PE	C11-O13-P-O11
45	J	202	3PE	C11-O13-P-O12
45	J	202	3PE	C11-O13-P-O14
45	K	101	3PE	C1-O11-P-O13
45	K	101	3PE	C1-O11-P-O14
45	L	701	3PE	C1-O11-P-O12
45	L	701	3PE	C1-O11-P-O14
45	L	701	3PE	C11-O13-P-O12
45	N	401	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O13
45	N	401	3PE	C1-O11-P-O14
45	N	401	3PE	C11-O13-P-O14
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C12-C11-O13-P
45	N	402	3PE	O13-C11-C12-N
45	N	403	3PE	C11-O13-P-O11
45	N	403	3PE	C12-C11-O13-P
45	N	403	3PE	C22-C21-O21-C2
45	O	403	3PE	O22-C21-O21-C2
45	P	502	3PE	C11-O13-P-O14
45	Y	201	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O12
45	Y	201	3PE	C22-C21-O21-C2
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C1-O11-P-O13
45	Y	202	3PE	C11-O13-P-O11
45	Y	202	3PE	C11-O13-P-O14
45	Y	202	3PE	C22-C21-O21-C2
45	Y	204	3PE	C1-O11-P-O12
45	Y	204	3PE	C1-O11-P-O13
45	Y	204	3PE	C1-O11-P-O14
45	Y	205	3PE	C11-O13-P-O11
45	Y	205	3PE	C11-O13-P-O12
45	Y	205	3PE	O13-C11-C12-N
45	Y	206	3PE	C11-O13-P-O11
45	Y	206	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	C11-O13-P-O14
45	Y	206	3PE	O22-C21-O21-C2
45	Y	207	3PE	C11-O13-P-O11
45	Y	207	3PE	C11-O13-P-O12
45	Y	207	3PE	C11-O13-P-O14
45	Y	207	3PE	C22-C21-O21-C2
45	Z	201	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O14
45	Z	201	3PE	C11-O13-P-O11
45	Z	201	3PE	C11-O13-P-O12
45	Z	201	3PE	O13-C11-C12-N
45	Z	202	3PE	C1-O11-P-O12
45	Z	202	3PE	C11-O13-P-O11
45	Z	202	3PE	C11-O13-P-O12
45	Z	202	3PE	C2-C1-O11-P
45	b	101	3PE	C1-O11-P-O12
45	b	101	3PE	C1-O11-P-O13
45	b	101	3PE	O11-C1-C2-O21
45	b	101	3PE	C22-C21-O21-C2
45	e	201	3PE	O32-C31-O31-C3
45	f	101	3PE	C11-O13-P-O11
45	f	101	3PE	C11-O13-P-O12
45	f	101	3PE	C11-O13-P-O14
45	f	101	3PE	O13-C11-C12-N
45	f	101	3PE	C22-C21-O21-C2
45	f	102	3PE	C1-O11-P-O12
45	f	102	3PE	C1-O11-P-O13
45	f	102	3PE	C1-O11-P-O14
45	f	102	3PE	C11-O13-P-O11
45	f	102	3PE	C11-O13-P-O12
45	i	202	3PE	C11-O13-P-O12
45	i	202	3PE	C11-O13-P-O14
45	i	202	3PE	C22-C21-O21-C2
45	m	201	3PE	C1-O11-P-O13
45	m	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O12
45	m	201	3PE	C11-O13-P-O14
45	m	201	3PE	O13-C11-C12-N
45	m	201	3PE	O22-C21-O21-C2
45	m	202	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O12
45	m	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	m	202	3PE	O22-C21-O21-C2
45	m	203	3PE	O13-C11-C12-N
45	q	201	3PE	C1-O11-P-O12
45	q	201	3PE	C1-O11-P-O13
45	q	201	3PE	C1-O11-P-O14
45	q	201	3PE	O21-C2-C3-O31
45	q	201	3PE	O22-C21-O21-C2
46	A	204	PC1	C1-O11-P-O14
46	A	204	PC1	C1-O11-P-O13
46	A	204	PC1	O13-C11-C12-N
46	A	204	PC1	O11-C1-C2-O21
46	A	205	PC1	O11-C1-C2-O21
46	A	205	PC1	O22-C21-O21-C2
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C11-O13-P-O11
46	B	204	PC1	O22-C21-O21-C2
46	H	401	PC1	C1-O11-P-O14
46	H	402	PC1	O13-C11-C12-N
46	H	402	PC1	C22-C21-O21-C2
46	I	203	PC1	O13-C11-C12-N
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	I	204	PC1	C11-O13-P-O11
46	I	204	PC1	C1-O11-P-O12
46	J	203	PC1	C11-O13-P-O12
46	J	203	PC1	C11-O13-P-O14
46	J	203	PC1	C11-O13-P-O11
46	L	702	PC1	C11-O13-P-O12
46	L	702	PC1	C11-O13-P-O14
46	L	702	PC1	C11-O13-P-O11
46	L	702	PC1	C1-O11-P-O12
46	L	702	PC1	C1-O11-P-O13
46	L	702	PC1	O13-C11-C12-N
46	L	703	PC1	C11-O13-P-O14
46	L	703	PC1	C11-O13-P-O11
46	L	703	PC1	O21-C2-C3-O31
46	M	602	PC1	O11-C1-C2-O21
46	M	602	PC1	O22-C21-O21-C2
46	M	602	PC1	C22-C21-O21-C2
46	e	202	PC1	C11-O13-P-O12
46	e	202	PC1	C11-O13-P-O14
46	e	202	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
46	e	202	PC1	C1-O11-P-O14
46	e	202	PC1	C1-O11-P-O13
46	h	201	PC1	C11-O13-P-O14
46	h	201	PC1	C11-O13-P-O11
46	h	201	PC1	C1-O11-P-O12
46	h	201	PC1	O11-C1-C2-O21
46	h	201	PC1	C22-C21-O21-C2
46	h	201	PC1	O32-C31-O31-C3
46	m	205	PC1	C11-O13-P-O12
46	m	205	PC1	C11-O13-P-O11
46	m	205	PC1	O22-C21-O21-C2
46	m	205	PC1	C22-C21-O21-C2
46	q	202	PC1	C11-O13-P-O12
46	q	202	PC1	C11-O13-P-O11
46	q	202	PC1	O13-C11-C12-N
47	A	206	PLC	C1-O3P-P-O4P
47	J	204	PLC	C4-O4P-P-O1P
47	J	204	PLC	C4-O4P-P-O2P
47	J	204	PLC	C4-O4P-P-O3P
47	L	704	PLC	C4-O4P-P-O1P
47	L	704	PLC	C4-O4P-P-O3P
47	M	603	PLC	C4-O4P-P-O1P
47	M	603	PLC	C4-O4P-P-O2P
47	M	603	PLC	C4-O4P-P-O3P
47	P	503	PLC	C1-O3P-P-O1P
47	P	503	PLC	C1-O3P-P-O2P
47	P	503	PLC	C1-O3P-P-O4P
47	P	503	PLC	C4-O4P-P-O1P
47	P	503	PLC	C4-O4P-P-O3P
47	P	504	PLC	C1-O3P-P-O1P
47	Y	208	PLC	O4P-C4-C5-N
47	Y	208	PLC	C4-O4P-P-O2P
47	Z	203	PLC	O4P-C4-C5-N
47	Z	203	PLC	C1'-C'-O2-C2
47	Z	203	PLC	C4-O4P-P-O2P
47	Z	203	PLC	C4-O4P-P-O3P
51	F	501	FMN	O3'-C3'-C4'-C5'
51	F	501	FMN	C4'-C5'-O5'-P
53	H	404	CDL	O1-C1-CA2-OA2
53	H	404	CDL	OA7-CA5-OA6-CA4
53	H	404	CDL	C11-CA5-OA6-CA4
53	H	404	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
53	H	404	CDL	CB2-OB2-PB2-OB5
53	H	404	CDL	OB5-CB3-CB4-OB6
53	L	705	CDL	CA2-OA2-PA1-OA4
53	L	705	CDL	CA2-OA2-PA1-OA5
53	L	705	CDL	CB2-OB2-PB2-OB3
53	M	604	CDL	O1-C1-CB2-OB2
53	M	604	CDL	C11-CA5-OA6-CA4
53	M	604	CDL	CB3-OB5-PB2-OB2
53	M	604	CDL	CB3-OB5-PB2-OB4
53	M	604	CDL	OB7-CB5-OB6-CB4
53	M	604	CDL	C51-CB5-OB6-CB4
53	N	404	CDL	CB3-OB5-PB2-OB3
53	N	404	CDL	OB6-CB4-CB6-OB8
53	N	404	CDL	C51-CB5-OB6-CB4
53	P	505	CDL	C11-CA5-OA6-CA4
53	P	505	CDL	CB3-OB5-PB2-OB2
53	P	505	CDL	CB3-OB5-PB2-OB3
53	P	505	CDL	CB3-OB5-PB2-OB4
53	d	201	CDL	O1-C1-CA2-OA2
53	d	201	CDL	CB2-C1-CA2-OA2
53	d	201	CDL	CB3-OB5-PB2-OB2
53	d	201	CDL	CB3-OB5-PB2-OB3
53	d	201	CDL	CB3-OB5-PB2-OB4
53	d	201	CDL	OB7-CB5-OB6-CB4
53	d	201	CDL	C51-CB5-OB6-CB4
53	d	202	CDL	CA3-OA5-PA1-OA2
53	d	202	CDL	OA7-CA5-OA6-CA4
53	d	202	CDL	C11-CA5-OA6-CA4
53	d	202	CDL	CB2-OB2-PB2-OB3
53	d	202	CDL	CB3-OB5-PB2-OB2
53	d	202	CDL	CB3-OB5-PB2-OB3
53	d	202	CDL	CB3-OB5-PB2-OB4
53	d	202	CDL	C51-CB5-OB6-CB4
53	h	202	CDL	CA2-OA2-PA1-OA4
53	h	202	CDL	CA2-OA2-PA1-OA5
53	h	202	CDL	CB2-OB2-PB2-OB3
53	h	202	CDL	CB2-OB2-PB2-OB4
53	h	202	CDL	CB2-OB2-PB2-OB5
53	h	202	CDL	CB3-OB5-PB2-OB2
53	h	202	CDL	CB3-OB5-PB2-OB3
53	h	202	CDL	CB3-OB5-PB2-OB4
53	h	202	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
53	h	202	CDL	C51-CB5-OB6-CB4
53	r	202	CDL	CA3-OA5-PA1-OA2
53	r	202	CDL	CA3-OA5-PA1-OA4
53	r	202	CDL	C11-CA5-OA6-CA4
53	r	202	CDL	CB2-OB2-PB2-OB3
53	r	202	CDL	CB2-OB2-PB2-OB5
53	r	202	CDL	CB3-OB5-PB2-OB3
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	C12-C13-C14-N2
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	C18-C17-C20-O6
58	T	101	EHZ	C19-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
58	U	101	EHZ	C8-C9-S1-C10
45	O	403	3PE	O32-C31-O31-C3
46	L	702	PC1	O32-C31-O31-C3
53	N	404	CDL	OB9-CB7-OB8-CB6
46	H	403	PC1	C32-C31-O31-C3
46	L	702	PC1	C32-C31-O31-C3
45	P	502	3PE	O32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
45	Y	204	3PE	O32-C31-O31-C3
45	Y	206	3PE	O32-C31-O31-C3
45	Y	207	3PE	O32-C31-O31-C3
45	b	101	3PE	O32-C31-O31-C3
45	f	101	3PE	O32-C31-O31-C3
45	m	201	3PE	O32-C31-O31-C3
46	H	403	PC1	O32-C31-O31-C3
46	e	202	PC1	O32-C31-O31-C3
46	m	205	PC1	O32-C31-O31-C3
53	M	604	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	OA9-CA7-OA8-CA6
53	r	202	CDL	OA9-CA7-OA8-CA6
45	N	403	3PE	O22-C21-O21-C2
45	Y	201	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
45	Z	201	3PE	O22-C21-O21-C2
45	b	101	3PE	O22-C21-O21-C2
45	f	101	3PE	O22-C21-O21-C2
45	i	202	3PE	O22-C21-O21-C2
46	A	204	PC1	O22-C21-O21-C2
46	h	201	PC1	O22-C21-O21-C2
47	Z	203	PLC	O'-C'-O2-C2
47	g	201	PLC	O'-C'-O2-C2
53	M	604	CDL	OA7-CA5-OA6-CA4
53	N	404	CDL	OB7-CB5-OB6-CB4
53	P	505	CDL	OA7-CA5-OA6-CA4
53	d	202	CDL	OB7-CB5-OB6-CB4
53	r	202	CDL	OA7-CA5-OA6-CA4
45	J	201	3PE	C32-C31-O31-C3
45	O	403	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
45	Y	204	3PE	C32-C31-O31-C3
45	b	101	3PE	C32-C31-O31-C3
45	e	201	3PE	C32-C31-O31-C3
46	e	202	PC1	C32-C31-O31-C3
46	h	201	PC1	C32-C31-O31-C3
53	M	604	CDL	C31-CA7-OA8-CA6
53	N	404	CDL	C71-CB7-OB8-CB6
53	d	201	CDL	C31-CA7-OA8-CA6
53	r	202	CDL	C31-CA7-OA8-CA6
45	A	203	3PE	C22-C21-O21-C2
45	J	201	3PE	C22-C21-O21-C2
45	O	403	3PE	C22-C21-O21-C2
45	Y	206	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
45	q	201	3PE	C22-C21-O21-C2
46	A	204	PC1	C22-C21-O21-C2
46	A	205	PC1	C22-C21-O21-C2
46	B	204	PC1	C22-C21-O21-C2
47	g	201	PLC	C1'-C'-O2-C2
49	B	202	U10	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
49	B	202	U10	C18-C19-C21-C22
53	h	202	CDL	OB9-CB7-OB8-CB6
45	N	401	3PE	C32-C31-O31-C3
45	P	502	3PE	C32-C31-O31-C3
45	Y	206	3PE	C32-C31-O31-C3
45	Y	207	3PE	C32-C31-O31-C3
45	f	101	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
45	m	204	3PE	C32-C31-O31-C3
46	B	204	PC1	C32-C31-O31-C3
46	m	205	PC1	C32-C31-O31-C3
53	N	404	CDL	C31-CA7-OA8-CA6
53	h	202	CDL	C71-CB7-OB8-CB6
45	J	201	3PE	O32-C31-O31-C3
46	B	204	PC1	O32-C31-O31-C3
46	H	402	PC1	O32-C31-O31-C3
46	L	703	PC1	O32-C31-O31-C3
53	h	202	CDL	OA9-CA7-OA8-CA6
45	Y	207	3PE	O22-C21-O21-C2
46	H	402	PC1	O22-C21-O21-C2
53	P	505	CDL	O1-C1-CB2-OB2
46	H	402	PC1	C32-C31-O31-C3
53	h	202	CDL	C31-CA7-OA8-CA6
45	m	204	3PE	O32-C31-O31-C3
53	N	404	CDL	OA9-CA7-OA8-CA6
45	Z	201	3PE	C22-C21-O21-C2
45	Z	202	3PE	C22-C21-O21-C2
51	F	501	FMN	C2'-C3'-C4'-O4'
46	L	703	PC1	C32-C31-O31-C3
45	N	401	3PE	O32-C31-O31-C3
45	Z	202	3PE	O22-C21-O21-C2
49	B	202	U10	C34-C36-C37-C38
49	B	202	U10	C44-C46-C47-C48
49	B	202	U10	C49-C51-C52-C53
51	F	501	FMN	C2'-C3'-C4'-C5'
59	i	201	CHD	C21-C20-C22-C23
49	B	202	U10	C16-C17-C18-C19
45	m	202	3PE	C32-C31-O31-C3
53	L	705	CDL	C71-CB7-OB8-CB6
53	d	202	CDL	C31-CA7-OA8-CA6
59	i	201	CHD	C17-C20-C22-C23
53	H	404	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
53	M	604	CDL	CA2-C1-CB2-OB2
53	d	202	CDL	CB2-C1-CA2-OA2
45	Y	205	3PE	C32-C31-O31-C3
45	Z	202	3PE	C32-C31-O31-C3
45	f	102	3PE	C32-C31-O31-C3
45	r	201	3PE	C32-C31-O31-C3
46	I	204	PC1	C32-C31-O31-C3
53	d	201	CDL	C71-CB7-OB8-CB6
53	L	705	CDL	OB9-CB7-OB8-CB6
53	d	202	CDL	OA9-CA7-OA8-CA6
53	H	404	CDL	CB5-C51-C52-C53
53	L	705	CDL	O1-C1-CB2-OB2
45	Y	205	3PE	O32-C31-O31-C3
53	d	201	CDL	OB9-CB7-OB8-CB6
51	F	501	FMN	O3'-C3'-C4'-O4'
45	Y	206	3PE	C31-C32-C33-C34
46	e	202	PC1	C21-C22-C23-C24
58	T	101	EHZ	C5-C6-C7-O1
46	I	204	PC1	O32-C31-O31-C3
47	J	204	PLC	C'-C1'-C2'-C3'
49	B	202	U10	C24-C26-C27-C28
45	e	201	3PE	C31-C32-C33-C34
45	i	202	3PE	C31-C32-C33-C34
46	H	403	PC1	C31-C32-C33-C34
46	L	703	PC1	C21-C22-C23-C24
47	P	504	PLC	C'-C1'-C2'-C3'
53	N	404	CDL	CB5-C51-C52-C53
45	Z	202	3PE	O32-C31-O31-C3
45	r	201	3PE	O32-C31-O31-C3
45	N	402	3PE	C21-C22-C23-C24
46	I	203	PC1	C21-C22-C23-C24
46	q	202	PC1	C31-C32-C33-C34
53	h	202	CDL	CB5-C51-C52-C53
45	f	102	3PE	O32-C31-O31-C3
45	m	202	3PE	O32-C31-O31-C3
53	H	404	CDL	CB7-C71-C72-C73
53	r	202	CDL	CA5-C11-C12-C13
46	B	203	PC1	C32-C31-O31-C3
47	P	503	PLC	C1'-C'-O2-C2
47	P	503	PLC	O'-C'-O2-C2
53	L	705	CDL	CA2-C1-CB2-OB2
47	P	504	PLC	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
47	P	504	PLC	C4-C5-N-C8
57	P	501	NDP	C3B-C4B-C5B-O5B
45	Y	203	3PE	C22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
53	d	202	CDL	CB7-C71-C72-C73
53	d	202	CDL	O1-C1-CA2-OA2
45	O	403	3PE	C2-C1-O11-P
46	H	402	PC1	C2-C1-O11-P
53	M	604	CDL	C1-CA2-OA2-PA1
53	P	505	CDL	C1-CB2-OB2-PB2
53	d	202	CDL	CA3-CA4-OA6-CA5
46	B	203	PC1	O32-C31-O31-C3
45	A	202	3PE	C22-C21-O21-C2
46	I	203	PC1	C22-C21-O21-C2
53	P	505	CDL	C51-CB5-OB6-CB4
46	I	203	PC1	C32-C31-O31-C3
47	P	504	PLC	C4-C5-N-C6
45	Y	203	3PE	C21-C22-C23-C24
45	m	204	3PE	C31-C32-C33-C34
45	q	201	3PE	C21-C22-C23-C24
45	N	401	3PE	C2E-C2F-C2G-C2H
45	O	403	3PE	C34-C35-C36-C37
45	f	102	3PE	C23-C24-C25-C26
46	I	203	PC1	C38-C39-C3A-C3B
53	N	404	CDL	C79-C80-C81-C82
45	A	203	3PE	C2C-C2D-C2E-C2F
45	J	201	3PE	C33-C34-C35-C36
45	N	402	3PE	C35-C36-C37-C38
45	N	403	3PE	C3A-C3B-C3C-C3D
45	Z	202	3PE	C39-C3A-C3B-C3C
45	i	202	3PE	C36-C37-C38-C39
46	B	203	PC1	C33-C34-C35-C36
46	H	401	PC1	C2B-C2C-C2D-C2E
46	I	204	PC1	C32-C33-C34-C35
46	L	703	PC1	C32-C33-C34-C35
53	d	201	CDL	C38-C39-C40-C41
53	d	202	CDL	C41-C42-C43-C44
53	d	202	CDL	C79-C80-C81-C82
45	Y	204	3PE	C31-C32-C33-C34
45	A	202	3PE	C24-C25-C26-C27
45	N	403	3PE	C32-C33-C34-C35
45	Y	205	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
45	Y	207	3PE	C2E-C2F-C2G-C2H
45	q	201	3PE	C36-C37-C38-C39
46	B	204	PC1	C3B-C3C-C3D-C3E
46	H	401	PC1	C24-C25-C26-C27
46	I	203	PC1	C25-C26-C27-C28
53	M	604	CDL	C83-C84-C85-C86
60	o	201	MYR	C7-C8-C9-C10
45	N	401	3PE	C38-C39-C3A-C3B
45	Y	203	3PE	C25-C26-C27-C28
45	Z	201	3PE	C2D-C2E-C2F-C2G
45	f	101	3PE	C35-C36-C37-C38
45	m	201	3PE	C35-C36-C37-C38
46	I	203	PC1	C22-C23-C24-C25
53	L	705	CDL	C36-C37-C38-C39
53	d	201	CDL	C72-C73-C74-C75
45	K	101	3PE	C28-C29-C2A-C2B
45	L	701	3PE	C2B-C2C-C2D-C2E
45	Z	202	3PE	C2A-C2B-C2C-C2D
46	L	703	PC1	C23-C24-C25-C26
53	H	404	CDL	CA7-C31-C32-C33
53	d	201	CDL	CB7-C71-C72-C73
45	A	203	3PE	C32-C33-C34-C35
53	H	404	CDL	C56-C57-C58-C59
53	N	404	CDL	C81-C82-C83-C84
45	A	201	3PE	C3A-C3B-C3C-C3D
45	N	401	3PE	C3B-C3C-C3D-C3E
45	f	101	3PE	C33-C34-C35-C36
45	m	203	3PE	C32-C33-C34-C35
46	I	204	PC1	C22-C21-O21-C2
53	L	705	CDL	C11-CA5-OA6-CA4
45	Y	206	3PE	C38-C39-C3A-C3B
53	N	404	CDL	C16-C17-C18-C19
53	d	201	CDL	C36-C37-C38-C39
58	U	101	EHZ	C5-C6-C7-C8
45	b	101	3PE	C37-C38-C39-C3A
45	m	203	3PE	C34-C35-C36-C37
57	P	501	NDP	O4B-C4B-C5B-O5B
45	A	201	3PE	C27-C28-C29-C2A
46	m	205	PC1	C2D-C2E-C2F-C2G
53	M	604	CDL	C57-C58-C59-C60
45	b	101	3PE	C28-C29-C2A-C2B
45	f	102	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	I	204	PC1	C25-C26-C27-C28
45	N	401	3PE	C33-C34-C35-C36
45	Z	202	3PE	C2D-C2E-C2F-C2G
53	P	505	CDL	OB7-CB5-OB6-CB4
45	Y	204	3PE	C28-C29-C2A-C2B
46	e	202	PC1	C38-C39-C3A-C3B
47	Z	203	PLC	C2B-C3B-C4B-C5B
46	A	205	PC1	C32-C31-O31-C3
46	H	401	PC1	C32-C31-O31-C3
53	r	202	CDL	CA3-CA4-CA6-OA8
45	N	401	3PE	C25-C26-C27-C28
53	M	604	CDL	C14-C15-C16-C17
53	d	202	CDL	C37-C38-C39-C40
45	m	204	3PE	C21-C22-C23-C24
46	q	202	PC1	C21-C22-C23-C24
53	N	404	CDL	CB7-C71-C72-C73
45	J	202	3PE	C27-C28-C29-C2A
45	K	101	3PE	C36-C37-C38-C39
45	K	101	3PE	C24-C25-C26-C27
45	L	701	3PE	C26-C27-C28-C29
45	Y	202	3PE	C2E-C2F-C2G-C2H
45	m	201	3PE	C22-C23-C24-C25
46	B	204	PC1	C28-C29-C2A-C2B
53	N	404	CDL	C35-C36-C37-C38
53	d	201	CDL	C75-C76-C77-C78
53	d	202	CDL	C58-C59-C60-C61
53	h	202	CDL	C58-C59-C60-C61
46	I	203	PC1	O32-C31-O31-C3
53	H	404	CDL	C12-C13-C14-C15
53	M	604	CDL	C40-C41-C42-C43
53	M	604	CDL	C62-C63-C64-C65
53	N	404	CDL	C22-C23-C24-C25
53	d	202	CDL	C81-C82-C83-C84
45	Y	205	3PE	C2C-C2D-C2E-C2F
46	M	602	PC1	C32-C33-C34-C35
53	L	705	CDL	CA5-C11-C12-C13
45	K	101	3PE	C3B-C3C-C3D-C3E
45	Y	204	3PE	C32-C33-C34-C35
46	H	403	PC1	C32-C33-C34-C35
53	N	404	CDL	C76-C77-C78-C79
46	L	703	PC1	C39-C3A-C3B-C3C
53	M	604	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	C34-C35-C36-C37
45	m	203	3PE	C38-C39-C3A-C3B
46	M	602	PC1	C21-C22-C23-C24
46	M	602	PC1	C31-C32-C33-C34
46	A	205	PC1	C24-C25-C26-C27
46	B	203	PC1	C38-C39-C3A-C3B
45	A	203	3PE	C36-C37-C38-C39
45	N	402	3PE	C23-C24-C25-C26
45	Y	205	3PE	C32-C33-C34-C35
45	q	201	3PE	C32-C33-C34-C35
46	q	202	PC1	C27-C28-C29-C2A
53	M	604	CDL	C13-C14-C15-C16
45	A	202	3PE	O22-C21-O21-C2
46	I	203	PC1	O22-C21-O21-C2
53	L	705	CDL	OA7-CA5-OA6-CA4
45	A	201	3PE	C24-C25-C26-C27
45	N	401	3PE	C36-C37-C38-C39
53	M	604	CDL	C72-C73-C74-C75
45	J	202	3PE	C2E-C2F-C2G-C2H
47	Y	208	PLC	C3B-C4B-C5B-C6B
53	H	404	CDL	C53-C54-C55-C56
53	N	404	CDL	C58-C59-C60-C61
53	M	604	CDL	CA5-C11-C12-C13
53	r	202	CDL	CB7-C71-C72-C73
45	O	403	3PE	C2B-C2C-C2D-C2E
45	Z	202	3PE	C22-C23-C24-C25
45	r	201	3PE	C22-C23-C24-C25
46	B	204	PC1	C32-C33-C34-C35
53	M	604	CDL	C51-C52-C53-C54
53	d	202	CDL	C62-C63-C64-C65
45	N	401	3PE	C34-C35-C36-C37
45	r	201	3PE	C33-C34-C35-C36
46	B	204	PC1	C36-C37-C38-C39
47	L	704	PLC	C7B-C8B-C9B-CAA
47	P	503	PLC	C1'-C2'-C3'-C4'
47	Y	208	PLC	C4'-C5'-C6'-C7'
53	M	604	CDL	C31-C32-C33-C34
57	P	501	NDP	O4D-C1D-N1N-C6N
46	L	702	PC1	C32-C33-C34-C35
53	M	604	CDL	CB5-C51-C52-C53
53	P	505	CDL	CA5-C11-C12-C13
45	N	403	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
46	L	703	PC1	C3B-C3C-C3D-C3E
53	d	202	CDL	C35-C36-C37-C38
60	o	201	MYR	C2-C3-C4-C5
46	M	602	PC1	C33-C34-C35-C36
45	J	202	3PE	C22-C21-O21-C2
45	f	102	3PE	C22-C21-O21-C2
46	L	702	PC1	C22-C21-O21-C2
46	e	202	PC1	C22-C21-O21-C2
53	N	404	CDL	C11-CA5-OA6-CA4
53	r	202	CDL	C51-CB5-OB6-CB4
45	L	701	3PE	C35-C36-C37-C38
53	r	202	CDL	OB7-CB5-OB6-CB4
46	I	203	PC1	C26-C27-C28-C29
46	h	201	PC1	C29-C2A-C2B-C2C
47	g	201	PLC	C4B-C5B-C6B-C7B
53	M	604	CDL	C59-C60-C61-C62
45	f	102	3PE	C27-C28-C29-C2A
45	Y	202	3PE	C39-C3A-C3B-C3C
45	m	202	3PE	C22-C23-C24-C25
45	N	402	3PE	C28-C29-C2A-C2B
46	M	602	PC1	C23-C24-C25-C26
53	H	404	CDL	C74-C75-C76-C77
45	A	201	3PE	C33-C34-C35-C36
47	g	201	PLC	C2'-C3'-C4'-C5'
53	d	202	CDL	C32-C33-C34-C35
53	r	202	CDL	C17-C18-C19-C20
45	e	201	3PE	C28-C29-C2A-C2B
53	P	505	CDL	C71-C72-C73-C74
53	r	202	CDL	C51-C52-C53-C54
58	U	101	EHZ	C5-C6-C7-O1
45	Y	202	3PE	C33-C34-C35-C36
58	T	101	EHZ	C1-C2-C3-C4
46	A	205	PC1	O32-C31-O31-C3
46	H	401	PC1	O32-C31-O31-C3
53	N	404	CDL	C55-C56-C57-C58
45	J	202	3PE	O22-C21-O21-C2
45	K	101	3PE	O11-C1-C2-O21
45	O	403	3PE	O11-C1-C2-O21
45	e	201	3PE	O11-C1-C2-O21
53	M	604	CDL	OA5-CA3-CA4-OA6
53	r	202	CDL	OB5-CB3-CB4-OB6
53	d	202	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
46	B	203	PC1	C3C-C3D-C3E-C3F
47	P	503	PLC	C1B-C2B-C3B-C4B
45	Y	205	3PE	C21-C22-C23-C24
45	Y	206	3PE	C23-C24-C25-C26
45	A	201	3PE	O21-C2-C3-O31
45	N	401	3PE	O21-C2-C3-O31
53	h	202	CDL	OB6-CB4-CB6-OB8
53	r	202	CDL	OA6-CA4-CA6-OA8
45	A	202	3PE	C33-C34-C35-C36
45	b	101	3PE	C22-C23-C24-C25
53	N	404	CDL	C23-C24-C25-C26
45	A	203	3PE	C2A-C2B-C2C-C2D
53	P	505	CDL	C78-C79-C80-C81
47	L	704	PLC	C7'-C8'-C9'-CA'
53	M	604	CDL	C18-C19-C20-C21
53	P	505	CDL	C75-C76-C77-C78
45	Y	207	3PE	C36-C37-C38-C39
45	f	101	3PE	C2-C1-O11-P
47	J	204	PLC	C2-C1-O3P-P
45	N	401	3PE	C2C-C2D-C2E-C2F
45	Y	203	3PE	C2E-C2F-C2G-C2H
46	I	203	PC1	C3B-C3C-C3D-C3E
46	L	702	PC1	C26-C27-C28-C29
53	N	404	CDL	C38-C39-C40-C41
45	f	102	3PE	O22-C21-O21-C2
46	I	204	PC1	O22-C21-O21-C2
53	P	505	CDL	CA2-C1-CB2-OB2
45	m	202	3PE	C26-C27-C28-C29
46	e	202	PC1	C32-C33-C34-C35
46	e	202	PC1	C3B-C3C-C3D-C3E
53	h	202	CDL	C31-C32-C33-C34
45	N	401	3PE	C27-C28-C29-C2A
53	M	604	CDL	C34-C35-C36-C37
53	N	404	CDL	C72-C73-C74-C75
53	P	505	CDL	C51-C52-C53-C54
46	H	401	PC1	C21-C22-C23-C24
45	f	102	3PE	C22-C23-C24-C25
47	O	404	PLC	C1'-C2'-C3'-C4'
47	J	204	PLC	C1'-C'-O2-C2
53	h	202	CDL	C11-CA5-OA6-CA4
45	m	201	3PE	C33-C34-C35-C36
46	J	203	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	d	202	CDL	C71-C72-C73-C74
46	H	403	PC1	C33-C34-C35-C36
45	i	202	3PE	C39-C3A-C3B-C3C
46	H	403	PC1	C35-C36-C37-C38
46	m	205	PC1	C3A-C3B-C3C-C3D
46	H	402	PC1	C22-C23-C24-C25
45	Y	207	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
45	m	201	3PE	O11-C1-C2-C3
45	m	203	3PE	O11-C1-C2-C3
46	A	205	PC1	O11-C1-C2-C3
46	H	401	PC1	O11-C1-C2-C3
46	M	602	PC1	O11-C1-C2-C3
53	d	201	CDL	OA5-CA3-CA4-CA6
53	r	202	CDL	OB5-CB3-CB4-CB6
53	N	404	CDL	OA7-CA5-OA6-CA4
45	Z	201	3PE	C24-C25-C26-C27
45	b	101	3PE	C34-C35-C36-C37
46	I	203	PC1	C37-C38-C39-C3A
46	h	201	PC1	C22-C23-C24-C25
53	H	404	CDL	C51-CB5-OB6-CB4
45	Y	207	3PE	C27-C28-C29-C2A
53	h	202	CDL	C72-C73-C74-C75
53	N	404	CDL	C31-C32-C33-C34
46	e	202	PC1	O22-C21-O21-C2
46	L	702	PC1	C21-C22-C23-C24
45	Y	206	3PE	C1-C2-C3-O31
45	f	102	3PE	C1-C2-C3-O31
45	q	201	3PE	C1-C2-C3-O31
46	B	203	PC1	C1-C2-C3-O31
46	I	204	PC1	C1-C2-C3-O31
47	P	503	PLC	C1-C2-C3-O3
53	H	404	CDL	CB3-CB4-CB6-OB8
53	H	404	CDL	C37-C38-C39-C40
53	d	201	CDL	C31-C32-C33-C34
47	J	204	PLC	C5B-C6B-C7B-C8B
47	Y	208	PLC	C2'-C3'-C4'-C5'
46	A	204	PC1	C32-C31-O31-C3
45	Y	207	3PE	C33-C34-C35-C36
53	N	404	CDL	C11-C12-C13-C14
53	N	404	CDL	C71-C72-C73-C74
53	h	202	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
45	q	201	3PE	C33-C34-C35-C36
45	Y	203	3PE	C2C-C2D-C2E-C2F
45	Y	205	3PE	C36-C37-C38-C39
46	q	202	PC1	C2C-C2D-C2E-C2F
46	m	205	PC1	C23-C24-C25-C26
45	m	204	3PE	C26-C27-C28-C29
45	i	202	3PE	C26-C27-C28-C29
45	P	502	3PE	C36-C37-C38-C39
46	L	703	PC1	C37-C38-C39-C3A
46	h	201	PC1	C24-C25-C26-C27
45	Z	201	3PE	C32-C31-O31-C3
53	P	505	CDL	C31-CA7-OA8-CA6
45	A	201	3PE	C2D-C2E-C2F-C2G
45	A	202	3PE	C27-C28-C29-C2A
45	N	403	3PE	C24-C25-C26-C27
53	r	202	CDL	C31-C32-C33-C34
45	O	403	3PE	C2E-C2F-C2G-C2H
45	N	401	3PE	O11-C1-C2-O21
46	B	204	PC1	O11-C1-C2-O21
53	N	404	CDL	OA5-CA3-CA4-OA6
45	Z	201	3PE	C34-C35-C36-C37
45	b	101	3PE	C36-C37-C38-C39
45	Y	202	3PE	C32-C31-O31-C3
45	A	201	3PE	C2A-C2B-C2C-C2D
45	Z	202	3PE	C2F-C2G-C2H-C2I
53	M	604	CDL	C33-C34-C35-C36
45	Z	202	3PE	C3C-C3D-C3E-C3F
53	H	404	CDL	C34-C35-C36-C37
45	A	202	3PE	C26-C27-C28-C29
45	N	402	3PE	C39-C3A-C3B-C3C
47	J	204	PLC	C2'-C3'-C4'-C5'
46	I	203	PC1	C3F-C3G-C3H-C3I
45	f	102	3PE	C33-C34-C35-C36
45	J	201	3PE	O21-C2-C3-O31
46	A	204	PC1	O21-C2-C3-O31
46	I	204	PC1	O21-C2-C3-O31
46	J	203	PC1	O21-C2-C3-O31
53	H	404	CDL	OB6-CB4-CB6-OB8
45	N	403	3PE	C3B-C3C-C3D-C3E
45	m	203	3PE	C27-C28-C29-C2A
46	M	602	PC1	C24-C25-C26-C27
53	M	604	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
53	d	202	CDL	C76-C77-C78-C79
46	A	205	PC1	C26-C27-C28-C29
58	U	101	EHZ	O5-C16-C17-C18
58	U	101	EHZ	O5-C16-C17-C19
53	H	404	CDL	C17-C18-C19-C20
45	L	701	3PE	C3F-C3G-C3H-C3I
45	O	403	3PE	C38-C39-C3A-C3B
45	A	202	3PE	C32-C31-O31-C3
45	Y	204	3PE	C22-C21-O21-C2
45	A	203	3PE	C26-C27-C28-C29
45	J	202	3PE	C21-C22-C23-C24
45	A	202	3PE	C22-C23-C24-C25
45	Y	203	3PE	C3F-C3G-C3H-C3I
53	d	202	CDL	C64-C65-C66-C67
53	L	705	CDL	C34-C35-C36-C37
46	L	702	PC1	O22-C21-O21-C2
53	L	705	CDL	C35-C36-C37-C38
53	L	705	CDL	C58-C59-C60-C61
45	N	403	3PE	C2-C1-O11-P
53	d	201	CDL	C1-CB2-OB2-PB2
46	I	204	PC1	C39-C3A-C3B-C3C
53	d	202	CDL	C61-C62-C63-C64
47	Z	203	PLC	C4B-C5B-C6B-C7B
46	M	602	PC1	C26-C27-C28-C29
53	M	604	CDL	C41-C42-C43-C44
53	d	202	CDL	C82-C83-C84-C85
53	N	404	CDL	C44-C45-C46-C47
53	d	202	CDL	C44-C45-C46-C47
45	K	101	3PE	O11-C1-C2-C3
45	L	701	3PE	O11-C1-C2-C3
45	N	401	3PE	O11-C1-C2-C3
45	O	403	3PE	O11-C1-C2-C3
46	B	204	PC1	O11-C1-C2-C3
46	q	202	PC1	O11-C1-C2-C3
47	M	603	PLC	O3P-C1-C2-C3
47	Y	208	PLC	O3P-C1-C2-C3
53	H	404	CDL	OB5-CB3-CB4-CB6
53	N	404	CDL	OA5-CA3-CA4-CA6
53	M	604	CDL	C72-C71-CB7-OB8
45	K	101	3PE	C21-C22-C23-C24
46	I	204	PC1	C22-C23-C24-C25
45	Y	203	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
45	q	201	3PE	C29-C2A-C2B-C2C
46	A	204	PC1	O32-C31-O31-C3
47	M	603	PLC	C'-C1'-C2'-C3'
46	H	401	PC1	C36-C37-C38-C39
45	Y	203	3PE	C35-C36-C37-C38
46	B	204	PC1	C2B-C2C-C2D-C2E
53	N	404	CDL	C78-C79-C80-C81
53	r	202	CDL	C18-C19-C20-C21
45	b	101	3PE	C25-C26-C27-C28
45	A	201	3PE	C1-C2-C3-O31
45	Y	205	3PE	C1-C2-C3-O31
45	i	202	3PE	C1-C2-C3-O31
46	J	203	PC1	C1-C2-C3-O31
46	L	703	PC1	C1-C2-C3-O31
53	L	705	CDL	CA3-CA4-CA6-OA8
53	N	404	CDL	CB3-CB4-CB6-OB8
53	h	202	CDL	CB3-CB4-CB6-OB8
46	q	202	PC1	C32-C33-C34-C35
45	q	201	3PE	C2B-C2C-C2D-C2E
53	d	201	CDL	C40-C41-C42-C43
45	N	401	3PE	C35-C36-C37-C38
45	Y	206	3PE	C35-C36-C37-C38
46	L	702	PC1	C22-C23-C24-C25
45	f	102	3PE	C21-C22-C23-C24
45	Z	201	3PE	O32-C31-O31-C3
46	J	203	PC1	C22-C23-C24-C25
46	H	401	PC1	C39-C3A-C3B-C3C
46	L	702	PC1	C2B-C2C-C2D-C2E
47	P	503	PLC	C2B-C3B-C4B-C5B
45	Y	207	3PE	O11-C1-C2-O21
45	m	203	3PE	O11-C1-C2-O21
53	P	505	CDL	OA5-CA3-CA4-OA6
46	B	203	PC1	C24-C25-C26-C27
45	m	201	3PE	C2-C1-O11-P
45	m	204	3PE	C24-C25-C26-C27
58	U	101	EHZ	C1-C2-C3-C4
58	U	101	EHZ	O2-C9-S1-C10
45	Y	203	3PE	C32-C33-C34-C35
45	Y	204	3PE	C2D-C2E-C2F-C2G
53	L	705	CDL	C13-C14-C15-C16
45	N	402	3PE	C38-C39-C3A-C3B
45	m	203	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
45	P	502	3PE	O21-C2-C3-O31
45	Y	205	3PE	O21-C2-C3-O31
45	f	101	3PE	O21-C2-C3-O31
46	I	203	PC1	O21-C2-C3-O31
47	P	504	PLC	O2-C2-C3-O3
46	e	202	PC1	C33-C34-C35-C36
45	Y	201	3PE	C24-C25-C26-C27
47	J	204	PLC	O'-C'-O2-C2
53	h	202	CDL	OA7-CA5-OA6-CA4
46	H	403	PC1	C3B-C3C-C3D-C3E
45	Y	205	3PE	C31-C32-C33-C34
53	P	505	CDL	OA9-CA7-OA8-CA6
45	J	202	3PE	C29-C2A-C2B-C2C
45	Y	203	3PE	C39-C3A-C3B-C3C
46	I	203	PC1	C2F-C2G-C2H-C2I
45	J	202	3PE	C22-C23-C24-C25
45	m	204	3PE	C2D-C2E-C2F-C2G
53	H	404	CDL	C61-C62-C63-C64
53	M	604	CDL	C16-C17-C18-C19
45	A	203	3PE	C3C-C3D-C3E-C3F
58	U	101	EHZ	C3-C4-C5-C6
53	d	201	CDL	CA5-C11-C12-C13
46	q	202	PC1	C32-C31-O31-C3
53	N	404	CDL	C19-C20-C21-C22
46	q	202	PC1	C23-C24-C25-C26
45	m	203	3PE	C3B-C3C-C3D-C3E
57	P	501	NDP	PN-O3-PA-O5B
45	A	203	3PE	C29-C2A-C2B-C2C
53	M	604	CDL	C39-C40-C41-C42
45	N	402	3PE	C25-C26-C27-C28
45	Y	207	3PE	C29-C2A-C2B-C2C
46	H	402	PC1	C24-C25-C26-C27
46	H	402	PC1	C29-C2A-C2B-C2C
45	f	101	3PE	C39-C3A-C3B-C3C
53	N	404	CDL	O1-C1-CA2-OA2
45	Z	202	3PE	C26-C27-C28-C29
45	L	701	3PE	C22-C21-O21-C2
47	P	504	PLC	C1'-C'-O2-C2
53	N	404	CDL	CB2-C1-CA2-OA2
45	A	202	3PE	C35-C36-C37-C38
45	L	701	3PE	C24-C25-C26-C27
46	m	205	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
53	N	404	CDL	C40-C41-C42-C43
45	Y	205	3PE	C37-C38-C39-C3A
45	N	402	3PE	O11-C1-C2-C3
45	N	403	3PE	O11-C1-C2-C3
45	e	201	3PE	O11-C1-C2-C3
46	A	204	PC1	O11-C1-C2-C3
46	L	703	PC1	O11-C1-C2-C3
46	h	201	PC1	O11-C1-C2-C3
47	L	704	PLC	O3P-C1-C2-C3
53	M	604	CDL	OA5-CA3-CA4-CA6
53	N	404	CDL	C64-C65-C66-C67
45	Z	202	3PE	C34-C35-C36-C37
45	i	202	3PE	C3D-C3E-C3F-C3G
45	N	401	3PE	C29-C2A-C2B-C2C
45	A	202	3PE	O32-C31-O31-C3
45	q	201	3PE	C3F-C3G-C3H-C3I
45	Z	202	3PE	C3E-C3F-C3G-C3H
46	q	202	PC1	C28-C29-C2A-C2B
45	Y	204	3PE	O22-C21-O21-C2
53	H	404	CDL	OB7-CB5-OB6-CB4
45	m	203	3PE	C28-C29-C2A-C2B
53	L	705	CDL	C62-C63-C64-C65
45	Y	204	3PE	C3-C2-O21-C21
45	r	201	3PE	C1-C2-O21-C21
47	g	201	PLC	C1-C2-O2-C'
53	N	404	CDL	CA6-CA4-OA6-CA5
45	Y	202	3PE	O32-C31-O31-C3
53	h	202	CDL	O1-C1-CA2-OA2
45	m	201	3PE	O11-C1-C2-O21
45	r	201	3PE	O11-C1-C2-O21
46	H	401	PC1	O11-C1-C2-O21
46	q	202	PC1	O11-C1-C2-O21
47	M	603	PLC	O3P-C1-C2-O2
47	Z	203	PLC	O3P-C1-C2-O2
53	h	202	CDL	OA5-CA3-CA4-OA6
45	K	101	3PE	C32-C33-C34-C35
45	L	701	3PE	C32-C33-C34-C35
45	A	203	3PE	C1-C2-C3-O31
45	N	401	3PE	C1-C2-C3-O31
45	O	403	3PE	C1-C2-C3-O31
45	r	201	3PE	C1-C2-C3-O31
46	I	203	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
47	Z	203	PLC	C1-C2-C3-O3
53	M	604	CDL	CB3-CB4-CB6-OB8
53	P	505	CDL	CB3-CB4-CB6-OB8
53	d	202	CDL	CA3-CA4-CA6-OA8
45	N	402	3PE	C31-C32-C33-C34
46	e	202	PC1	C23-C24-C25-C26
45	Y	204	3PE	C36-C37-C38-C39
46	m	205	PC1	C36-C37-C38-C39
53	r	202	CDL	C13-C14-C15-C16
45	A	201	3PE	C12-C11-O13-P
45	J	201	3PE	C12-C11-O13-P
45	J	202	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	Y	203	3PE	C12-C11-O13-P
45	Y	205	3PE	C12-C11-O13-P
45	Y	206	3PE	C12-C11-O13-P
45	Y	207	3PE	C12-C11-O13-P
45	Z	202	3PE	C12-C11-O13-P
45	f	101	3PE	C12-C11-O13-P
45	m	201	3PE	C12-C11-O13-P
45	m	202	3PE	C12-C11-O13-P
45	m	204	3PE	C12-C11-O13-P
45	r	201	3PE	C12-C11-O13-P
47	A	206	PLC	C5-C4-O4P-P
47	O	404	PLC	C5-C4-O4P-P
45	f	101	3PE	C38-C39-C3A-C3B
45	Y	205	3PE	C25-C26-C27-C28
45	A	203	3PE	O21-C2-C3-O31
45	Y	203	3PE	O21-C2-C3-O31
45	Y	206	3PE	O21-C2-C3-O31
45	f	102	3PE	O21-C2-C3-O31
45	i	202	3PE	O21-C2-C3-O31
46	B	203	PC1	O21-C2-C3-O31
46	H	401	PC1	O21-C2-C3-O31
46	L	702	PC1	O21-C2-C3-O31
53	L	705	CDL	OA6-CA4-CA6-OA8
53	M	604	CDL	OB6-CB4-CB6-OB8
53	P	505	CDL	OB6-CB4-CB6-OB8
45	Y	204	3PE	C3D-C3E-C3F-C3G
46	q	202	PC1	O32-C31-O31-C3
45	Y	202	3PE	C37-C38-C39-C3A
45	Y	203	3PE	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
53	M	604	CDL	C11-C12-C13-C14
46	H	402	PC1	C21-C22-C23-C24
45	J	202	3PE	C32-C31-O31-C3
45	Y	202	3PE	C24-C25-C26-C27
45	m	203	3PE	C22-C23-C24-C25
46	m	205	PC1	C37-C38-C39-C3A
46	I	204	PC1	C38-C39-C3A-C3B
47	L	704	PLC	O4P-C4-C5-N
47	M	603	PLC	O4P-C4-C5-N
47	g	201	PLC	O4P-C4-C5-N
55	O	401	DGT	PA-O3A-PB-O1B
57	P	501	NDP	PN-O3-PA-O1A
45	q	201	3PE	C3A-C3B-C3C-C3D
53	M	604	CDL	C74-C75-C76-C77
46	M	602	PC1	C32-C31-O31-C3
47	g	201	PLC	C8'-C9'-CA'-CB'
45	Y	205	3PE	C29-C2A-C2B-C2C
46	h	201	PC1	C2B-C2C-C2D-C2E
45	m	201	3PE	C24-C25-C26-C27
45	L	701	3PE	O22-C21-O21-C2
45	L	701	3PE	C29-C2A-C2B-C2C
47	L	704	PLC	C5'-C6'-C7'-C8'
45	K	101	3PE	C38-C39-C3A-C3B
46	h	201	PC1	C34-C35-C36-C37
45	i	202	3PE	C25-C26-C27-C28
45	q	201	3PE	C39-C3A-C3B-C3C
45	m	204	3PE	O11-C1-C2-C3
53	P	505	CDL	OA5-CA3-CA4-CA6
53	h	202	CDL	OA5-CA3-CA4-CA6
46	J	203	PC1	C33-C34-C35-C36
47	P	504	PLC	O'-C'-O2-C2
53	d	201	CDL	C44-C45-C46-C47
45	Z	201	3PE	C35-C36-C37-C38
45	Y	204	3PE	C22-C23-C24-C25
45	b	101	3PE	C26-C27-C28-C29
45	Z	202	3PE	C25-C26-C27-C28
53	h	202	CDL	C33-C34-C35-C36
46	M	602	PC1	O32-C31-O31-C3
45	m	202	3PE	C2-C1-O11-P
47	Y	208	PLC	C2-C1-O3P-P
45	e	201	3PE	C39-C3A-C3B-C3C
46	B	204	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
47	J	204	PLC	C8B-C9B-CAA-CBA
45	L	701	3PE	O11-C1-C2-O21
45	N	402	3PE	O11-C1-C2-O21
45	N	403	3PE	O11-C1-C2-O21
45	Y	206	3PE	O11-C1-C2-O21
45	m	204	3PE	O11-C1-C2-O21
46	L	703	PC1	O11-C1-C2-O21
47	L	704	PLC	O3P-C1-C2-O2
47	Y	208	PLC	O3P-C1-C2-O2
53	d	201	CDL	OA5-CA3-CA4-OA6
45	J	202	3PE	O32-C31-O31-C3
46	H	403	PC1	C11-C12-N-C13
46	H	403	PC1	C11-C12-N-C15
47	Z	203	PLC	C4-C5-N-C8
45	L	701	3PE	C3B-C3C-C3D-C3E
53	M	604	CDL	C35-C36-C37-C38
45	Y	203	3PE	C26-C27-C28-C29
45	O	403	3PE	O21-C2-C3-O31
45	Z	202	3PE	O21-C2-C3-O31
45	r	201	3PE	O21-C2-C3-O31
46	e	202	PC1	O21-C2-C3-O31
47	P	503	PLC	O2-C2-C3-O3
47	A	206	PLC	C2B-C3B-C4B-C5B
47	P	504	PLC	C8'-C9'-CA'-CB'
45	J	202	3PE	C1-C2-C3-O31
45	Y	203	3PE	C1-C2-C3-O31
45	Z	202	3PE	C1-C2-C3-O31
46	A	204	PC1	C1-C2-C3-O31
46	L	702	PC1	C1-C2-C3-O31
46	e	202	PC1	C1-C2-C3-O31
47	J	204	PLC	C1-C2-C3-O3
47	L	704	PLC	C1-C2-C3-O3
47	P	504	PLC	C1-C2-C3-O3
53	L	705	CDL	CB3-CB4-CB6-OB8
53	d	202	CDL	CB3-CB4-CB6-OB8
45	N	403	3PE	C21-C22-C23-C24
45	q	201	3PE	C34-C35-C36-C37
45	b	101	3PE	C3B-C3C-C3D-C3E
45	K	101	3PE	C31-C32-C33-C34
60	o	201	MYR	C6-C7-C8-C9
46	I	203	PC1	C2D-C2E-C2F-C2G
45	A	202	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	A	202	3PE	O13-C11-C12-N
45	J	201	3PE	C1-O11-P-O12
45	J	202	3PE	C1-O11-P-O12
45	J	202	3PE	C1-O11-P-O13
45	J	202	3PE	C1-O11-P-O14
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	O13-C11-C12-N
45	L	701	3PE	C1-O11-P-O13
45	L	701	3PE	C11-O13-P-O11
45	L	701	3PE	C11-O13-P-O14
45	N	401	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O14
45	N	403	3PE	O13-C11-C12-N
45	P	502	3PE	C11-O13-P-O11
45	Y	201	3PE	C1-O11-P-O14
45	Y	201	3PE	C11-O13-P-O14
45	Y	202	3PE	C1-O11-P-O14
45	Y	202	3PE	C11-O13-P-O12
45	Y	202	3PE	O13-C11-C12-N
45	Y	203	3PE	C1-O11-P-O14
45	Z	201	3PE	C11-O13-P-O14
45	Z	202	3PE	C1-O11-P-O13
45	Z	202	3PE	C1-O11-P-O14
45	Z	202	3PE	C11-O13-P-O14
45	e	201	3PE	C11-O13-P-O14
45	f	101	3PE	C1-O11-P-O12
45	f	101	3PE	C1-O11-P-O13
45	f	102	3PE	C11-O13-P-O14
45	i	202	3PE	C11-O13-P-O11
45	i	202	3PE	O13-C11-C12-N
45	m	203	3PE	C11-O13-P-O11
45	m	203	3PE	C11-O13-P-O12
45	m	204	3PE	C11-O13-P-O11
45	m	204	3PE	C11-O13-P-O12
45	q	201	3PE	C11-O13-P-O14
45	r	201	3PE	C1-O11-P-O14
46	A	204	PC1	C11-O13-P-O12
46	A	204	PC1	C11-O13-P-O14
46	A	204	PC1	C11-O13-P-O11
46	A	204	PC1	C1-O11-P-O12
46	A	205	PC1	C11-O13-P-O12
46	A	205	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	B	203	PC1	C11-O13-P-O12
46	B	204	PC1	C11-O13-P-O14
46	H	401	PC1	C1-O11-P-O12
46	H	401	PC1	C1-O11-P-O13
46	H	402	PC1	C11-O13-P-O14
46	H	403	PC1	C11-O13-P-O12
46	H	403	PC1	C11-O13-P-O14
46	H	403	PC1	C11-O13-P-O11
46	H	403	PC1	C11-C12-N-C14
46	I	204	PC1	C1-O11-P-O14
46	I	204	PC1	C1-O11-P-O13
46	J	203	PC1	C1-O11-P-O14
46	L	702	PC1	C1-O11-P-O14
46	e	202	PC1	C11-O13-P-O11
46	h	201	PC1	C1-O11-P-O14
46	h	201	PC1	C1-O11-P-O13
46	q	202	PC1	C11-O13-P-O14
46	q	202	PC1	C1-O11-P-O14
47	A	206	PLC	C1-O3P-P-O1P
47	A	206	PLC	C4-O4P-P-O1P
47	L	704	PLC	C4-O4P-P-O2P
47	P	503	PLC	C4-O4P-P-O2P
47	P	504	PLC	C4-O4P-P-O3P
47	Z	203	PLC	C1-O3P-P-O1P
53	L	705	CDL	CA2-OA2-PA1-OA3
53	M	604	CDL	CB3-OB5-PB2-OB3
53	P	505	CDL	CA2-OA2-PA1-OA3
53	d	201	CDL	CA3-OA5-PA1-OA3
53	d	201	CDL	CB2-OB2-PB2-OB3
53	d	202	CDL	CA3-OA5-PA1-OA3
53	h	202	CDL	CA3-OA5-PA1-OA3
53	r	202	CDL	CA3-OA5-PA1-OA3
53	r	202	CDL	CB3-OB5-PB2-OB2
58	U	101	EHZ	O5-C16-C17-C20
46	h	201	PC1	C36-C37-C38-C39
53	N	404	CDL	C18-C19-C20-C21
45	Y	207	3PE	C2-C1-O11-P
45	Z	201	3PE	C2-C1-O11-P
46	H	403	PC1	C2-C1-O11-P
47	g	201	PLC	C2-C1-O3P-P
53	d	201	CDL	CA4-CA3-OA5-PA1
53	r	202	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
60	o	201	MYR	C11-C10-C9-C8
45	K	101	3PE	O22-C21-O21-C2
53	H	404	CDL	C71-C72-C73-C74
53	N	404	CDL	C62-C63-C64-C65
45	N	401	3PE	C21-C22-C23-C24
45	N	403	3PE	C35-C36-C37-C38
53	H	404	CDL	C11-C12-C13-C14
58	T	101	EHZ	C3-C4-C5-C6
46	q	202	PC1	C1-C2-O21-C21
47	Y	208	PLC	C1-C2-O2-C'
47	Y	208	PLC	C3-C2-O2-C'
53	d	202	CDL	CB6-CB4-OB6-CB5
45	Z	201	3PE	C25-C26-C27-C28
53	H	404	CDL	C31-C32-C33-C34
45	Y	206	3PE	C36-C37-C38-C39
46	e	202	PC1	C11-C12-N-C15
45	r	201	3PE	O11-C1-C2-C3
53	d	201	CDL	OB5-CB3-CB4-CB6
45	i	202	3PE	C33-C34-C35-C36
45	O	403	3PE	C35-C36-C37-C38
46	H	401	PC1	C32-C33-C34-C35
53	d	201	CDL	OB5-CB3-CB4-OB6
45	m	203	3PE	C23-C24-C25-C26
46	L	703	PC1	C25-C26-C27-C28
53	H	404	CDL	C63-C64-C65-C66
53	L	705	CDL	C14-C15-C16-C17
45	Y	201	3PE	C31-C32-C33-C34
45	m	202	3PE	O21-C2-C3-O31
53	d	202	CDL	OA6-CA4-CA6-OA8
45	N	403	3PE	C22-C23-C24-C25
47	P	504	PLC	C7'-C8'-C9'-CA'
45	K	101	3PE	C22-C21-O21-C2
53	L	705	CDL	C32-C31-CA7-OA8
53	H	404	CDL	C72-C73-C74-C75
46	h	201	PC1	C2F-C2G-C2H-C2I
45	r	201	3PE	C36-C37-C38-C39
45	J	201	3PE	C1-C2-C3-O31
46	e	202	PC1	C35-C36-C37-C38
46	B	203	PC1	C36-C37-C38-C39
45	J	201	3PE	C37-C38-C39-C3A
45	Y	207	3PE	C34-C35-C36-C37
58	U	101	EHZ	C1-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	O	403	3PE	C27-C28-C29-C2A
53	d	202	CDL	C32-C31-CA7-OA8
45	e	201	3PE	C22-C23-C24-C25
45	m	204	3PE	C34-C35-C36-C37
45	Y	202	3PE	C27-C28-C29-C2A
45	L	701	3PE	C2F-C2G-C2H-C2I
53	h	202	CDL	C53-C54-C55-C56
53	P	505	CDL	C71-CB7-OB8-CB6
45	b	101	3PE	C2-C1-O11-P
45	f	101	3PE	C3A-C3B-C3C-C3D
45	f	101	3PE	C34-C35-C36-C37
45	N	401	3PE	C37-C38-C39-C3A
45	f	102	3PE	C3D-C3E-C3F-C3G
46	h	201	PC1	C26-C27-C28-C29
45	N	403	3PE	C2C-C2D-C2E-C2F
53	P	505	CDL	OB9-CB7-OB8-CB6
60	o	201	MYR	C4-C5-C6-C7
46	J	203	PC1	C11-C12-N-C14
53	P	505	CDL	C76-C77-C78-C79
45	q	201	3PE	C32-C31-O31-C3
46	e	202	PC1	C3A-C3B-C3C-C3D
45	m	203	3PE	C29-C2A-C2B-C2C
53	h	202	CDL	C11-C12-C13-C14
46	h	201	PC1	C37-C38-C39-C3A
45	m	203	3PE	C31-C32-C33-C34
46	m	205	PC1	C2A-C2B-C2C-C2D
45	A	203	3PE	C3E-C3F-C3G-C3H
45	Z	201	3PE	C28-C29-C2A-C2B
46	I	203	PC1	C23-C24-C25-C26
45	e	201	3PE	C2A-C2B-C2C-C2D
45	N	402	3PE	C2A-C2B-C2C-C2D
45	Y	202	3PE	C3F-C3G-C3H-C3I
45	A	201	3PE	C2-C1-O11-P
45	f	102	3PE	C2-C1-O11-P
45	K	101	3PE	C27-C28-C29-C2A
45	i	202	3PE	C21-C22-C23-C24
45	q	201	3PE	C3D-C3E-C3F-C3G
53	h	202	CDL	CB2-C1-CA2-OA2
53	d	202	CDL	C80-C81-C82-C83
53	N	404	CDL	C14-C15-C16-C17
45	J	202	3PE	C2D-C2E-C2F-C2G
46	A	205	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
53	L	705	CDL	C71-C72-C73-C74
45	i	202	3PE	C3E-C3F-C3G-C3H
45	Y	206	3PE	C34-C35-C36-C37
45	Y	205	3PE	C22-C23-C24-C25
53	L	705	CDL	C64-C65-C66-C67
45	J	202	3PE	C3-C2-O21-C21
45	Y	202	3PE	C1-C2-O21-C21
45	i	202	3PE	C3-C2-O21-C21
45	Y	204	3PE	C3A-C3B-C3C-C3D
45	N	403	3PE	C2D-C2E-C2F-C2G
53	P	505	CDL	C74-C75-C76-C77
53	r	202	CDL	C71-C72-C73-C74
53	M	604	CDL	C71-CB7-OB8-CB6
60	o	201	MYR	C11-C12-C13-C14
53	h	202	CDL	OB5-CB3-CB4-OB6
47	P	503	PLC	C3'-C4'-C5'-C6'
47	A	206	PLC	O2-C'-C1'-C2'
53	h	202	CDL	C73-C74-C75-C76
45	A	201	3PE	C2C-C2D-C2E-C2F
49	B	202	U10	C45-C44-C46-C47
46	q	202	PC1	C25-C26-C27-C28
45	Y	206	3PE	O11-C1-C2-C3
53	h	202	CDL	OB5-CB3-CB4-CB6
45	J	202	3PE	O21-C2-C3-O31
47	O	404	PLC	O2-C2-C3-O3
53	d	202	CDL	OB6-CB4-CB6-OB8
53	r	202	CDL	OB6-CB4-CB6-OB8
45	N	403	3PE	C25-C26-C27-C28
46	H	402	PC1	C27-C28-C29-C2A
53	d	202	CDL	C56-C57-C58-C59
46	q	202	PC1	C3A-C3B-C3C-C3D
46	J	203	PC1	C11-C12-N-C15
46	e	202	PC1	C11-C12-N-C14
45	N	403	3PE	C28-C29-C2A-C2B
49	B	202	U10	C35-C34-C36-C37
57	P	501	NDP	C2B-O2B-P2B-O1X
53	N	404	CDL	C17-C18-C19-C20
53	d	202	CDL	O1-C1-CB2-OB2
45	L	701	3PE	C3D-C3E-C3F-C3G
46	B	204	PC1	C34-C35-C36-C37
53	d	202	CDL	CA5-C11-C12-C13
45	q	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	P	503	PLC	C6B-C7B-C8B-C9B
55	O	401	DGT	PB-O3A-PA-O2A
45	Y	203	3PE	C22-C23-C24-C25
45	i	202	3PE	C27-C28-C29-C2A
53	d	202	CDL	C42-C43-C44-C45
45	m	201	3PE	C38-C39-C3A-C3B
53	N	404	CDL	C43-C44-C45-C46
53	M	604	CDL	C36-C37-C38-C39
49	B	202	U10	C40-C39-C41-C42
46	h	201	PC1	C2-C1-O11-P
46	h	201	PC1	C2D-C2E-C2F-C2G
45	f	102	3PE	C3F-C3G-C3H-C3I
53	M	604	CDL	OB9-CB7-OB8-CB6
45	L	701	3PE	C37-C38-C39-C3A
45	A	201	3PE	C31-C32-C33-C34
45	L	701	3PE	C31-C32-C33-C34
45	L	701	3PE	C38-C39-C3A-C3B
45	Y	205	3PE	C33-C34-C35-C36
45	Y	201	3PE	C1-C2-C3-O31
58	U	101	EHZ	O3-C12-C13-C14
53	h	202	CDL	C40-C41-C42-C43
45	m	204	3PE	O21-C21-C22-C23
46	B	204	PC1	C27-C28-C29-C2A
45	K	101	3PE	C26-C27-C28-C29
45	Z	201	3PE	C29-C2A-C2B-C2C
45	Z	202	3PE	O11-C1-C2-O21
53	M	604	CDL	C72-C71-CB7-OB9
45	A	201	3PE	O21-C21-C22-C23
45	A	201	3PE	C29-C2A-C2B-C2C
45	Y	201	3PE	C23-C24-C25-C26
45	Z	202	3PE	C33-C34-C35-C36
45	r	201	3PE	C24-C25-C26-C27
46	J	203	PC1	C11-C12-N-C13
46	e	202	PC1	C11-C12-N-C13
53	M	604	CDL	C24-C25-C26-C27
47	Z	203	PLC	O3P-C1-C2-C3
45	A	203	3PE	C3F-C3G-C3H-C3I
45	b	101	3PE	C33-C34-C35-C36
45	f	102	3PE	C35-C36-C37-C38
45	Z	201	3PE	O21-C2-C3-O31
53	d	201	CDL	OB6-CB4-CB6-OB8
45	Y	206	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
45	Y	204	3PE	C2A-C2B-C2C-C2D
45	m	204	3PE	C2F-C2G-C2H-C2I
47	g	201	PLC	C1B-C2B-C3B-C4B
53	h	202	CDL	C52-C53-C54-C55
46	I	203	PC1	C31-C32-C33-C34
45	Y	204	3PE	C37-C38-C39-C3A
45	q	201	3PE	C24-C25-C26-C27
45	P	502	3PE	C39-C3A-C3B-C3C
46	H	402	PC1	C2A-C2B-C2C-C2D
53	N	404	CDL	C61-C62-C63-C64
45	O	403	3PE	C28-C29-C2A-C2B
46	I	204	PC1	C11-C12-N-C15
59	i	201	CHD	C22-C23-C24-O26
45	i	202	3PE	C1-C2-O21-C21
45	m	202	3PE	C1-C2-O21-C21
45	m	202	3PE	C3-C2-O21-C21
47	J	204	PLC	OB-CB-O3-C3
45	Y	202	3PE	C35-C36-C37-C38
45	Y	205	3PE	C35-C36-C37-C38
45	N	403	3PE	C2A-C2B-C2C-C2D
45	P	502	3PE	C33-C34-C35-C36
53	d	201	CDL	C39-C40-C41-C42
45	i	202	3PE	C3B-C3C-C3D-C3E
46	H	401	PC1	C28-C29-C2A-C2B
59	i	201	CHD	C22-C23-C24-O25
53	d	201	CDL	C1-CA2-OA2-PA1
45	N	403	3PE	C29-C2A-C2B-C2C
46	I	204	PC1	C11-C12-N-C14
47	Z	203	PLC	C4-C5-N-C6
45	P	502	3PE	C1-C2-C3-O31
45	m	202	3PE	C1-C2-C3-O31
46	A	205	PC1	C1-C2-C3-O31
46	H	401	PC1	C1-C2-C3-O31
47	O	404	PLC	C1-C2-C3-O3
49	B	202	U10	C19-C21-C22-C23
58	U	101	EHZ	N1-C12-C13-C14
53	M	604	CDL	CA7-C31-C32-C33
46	A	204	PC1	C25-C26-C27-C28
53	N	404	CDL	C42-C43-C44-C45
45	A	201	3PE	O31-C31-C32-C33
58	U	101	EHZ	C15-C16-C17-C18
46	q	202	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
45	m	204	3PE	C32-C33-C34-C35
53	L	705	CDL	C37-C38-C39-C40
45	O	403	3PE	C24-C25-C26-C27
45	e	201	3PE	C3A-C3B-C3C-C3D
53	M	604	CDL	C80-C81-C82-C83
46	A	205	PC1	O21-C2-C3-O31
45	J	202	3PE	C2C-C2D-C2E-C2F
45	Z	202	3PE	C35-C36-C37-C38
53	L	705	CDL	C38-C39-C40-C41
45	m	203	3PE	O21-C21-C22-C23
45	Y	203	3PE	O11-C1-C2-C3
45	Y	205	3PE	C2E-C2F-C2G-C2H
53	H	404	CDL	C58-C59-C60-C61
47	Z	203	PLC	C4-C5-N-C7
45	Y	207	3PE	C28-C29-C2A-C2B
47	Y	208	PLC	C2B-C1B-CB-O3
45	Y	202	3PE	C3C-C3D-C3E-C3F
47	A	206	PLC	C2-C1-O3P-P
45	A	202	3PE	C29-C2A-C2B-C2C
45	P	502	3PE	C21-C22-C23-C24
45	N	403	3PE	O21-C21-C22-C23
53	h	202	CDL	C56-C57-C58-C59
46	H	403	PC1	O13-C11-C12-N
46	J	203	PC1	O13-C11-C12-N
45	Y	202	3PE	C28-C29-C2A-C2B
53	N	404	CDL	C32-C33-C34-C35
45	Z	201	3PE	C32-C33-C34-C35
45	N	401	3PE	O31-C31-C32-C33
45	f	101	3PE	O31-C31-C32-C33
45	Y	207	3PE	C2C-C2D-C2E-C2F
47	Y	208	PLC	C4B-C5B-C6B-C7B
53	L	705	CDL	C53-C54-C55-C56
45	L	701	3PE	O21-C21-C22-C23
45	P	502	3PE	C22-C23-C24-C25
53	P	505	CDL	C52-C53-C54-C55
60	o	201	MYR	C1-C2-C3-C4
45	i	202	3PE	C34-C35-C36-C37
45	e	201	3PE	C21-C22-C23-C24
45	i	202	3PE	O21-C21-C22-C23
46	q	202	PC1	O31-C31-C32-C33
53	N	404	CDL	C72-C71-CB7-OB8
47	J	204	PLC	C1B-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
45	Y	202	3PE	C38-C39-C3A-C3B
53	P	505	CDL	C12-C11-CA5-OA6
45	Z	202	3PE	C24-C25-C26-C27
46	H	401	PC1	C26-C27-C28-C29
46	q	202	PC1	C22-C23-C24-C25
45	Y	204	3PE	O31-C31-C32-C33
53	d	202	CDL	C52-C51-CB5-OB6
53	r	202	CDL	C32-C31-CA7-OA8
45	A	201	3PE	C34-C35-C36-C37
45	f	101	3PE	C1-C2-C3-O31
53	d	201	CDL	CB3-CB4-CB6-OB8
45	Y	204	3PE	C3C-C3D-C3E-C3F
46	I	204	PC1	C11-C12-N-C13
47	L	704	PLC	C8'-C9'-CA'-CB'
45	f	102	3PE	O21-C21-C22-C23
46	M	602	PC1	O31-C31-C32-C33
49	B	202	U10	C43-C44-C46-C47
58	T	101	EHZ	O3-C12-C13-C14
46	m	205	PC1	C39-C3A-C3B-C3C
46	q	202	PC1	C2E-C2F-C2G-C2H
45	Y	203	3PE	O21-C21-C22-C23
45	b	101	3PE	O21-C21-C22-C23
47	M	603	PLC	O2-C'-C1'-C2'
47	J	204	PLC	C3B-C4B-C5B-C6B
45	Y	204	3PE	C2B-C2C-C2D-C2E
46	J	203	PC1	O31-C31-C32-C33
53	P	505	CDL	C72-C71-CB7-OB8
45	f	102	3PE	C32-C33-C34-C35
53	H	404	CDL	C54-C55-C56-C57
45	A	201	3PE	C26-C27-C28-C29
45	N	401	3PE	C2F-C2G-C2H-C2I
53	h	202	CDL	CB3-CB4-OB6-CB5
45	e	201	3PE	C34-C35-C36-C37
46	B	204	PC1	C26-C27-C28-C29
53	P	505	CDL	C72-C73-C74-C75
45	Y	202	3PE	O31-C31-C32-C33
57	P	501	NDP	C3D-C4D-C5D-O5D
53	N	404	CDL	C34-C35-C36-C37
45	r	201	3PE	O22-C21-O21-C2
58	T	101	EHZ	N1-C12-C13-C14
45	m	204	3PE	C33-C34-C35-C36
45	N	401	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	N	403	3PE	O32-C31-O31-C3
46	e	202	PC1	O21-C21-C22-C23
46	A	204	PC1	C22-C23-C24-C25
53	r	202	CDL	C32-C31-CA7-OA9
53	P	505	CDL	C32-C31-CA7-OA8
45	m	203	3PE	O22-C21-C22-C23
46	A	204	PC1	C11-C12-N-C14
46	L	702	PC1	C11-C12-N-C14
53	P	505	CDL	C11-C12-C13-C14
53	H	404	CDL	C73-C74-C75-C76
45	A	201	3PE	O32-C31-C32-C33
45	L	701	3PE	O22-C21-C22-C23
45	f	101	3PE	O32-C31-C32-C33
45	N	403	3PE	C32-C31-O31-C3
45	N	401	3PE	C31-C32-C33-C34
45	Y	204	3PE	O32-C31-C32-C33
45	N	402	3PE	C26-C27-C28-C29
47	A	206	PLC	O'-C'-C1'-C2'
45	A	201	3PE	C36-C37-C38-C39
53	L	705	CDL	OB6-CB4-CB6-OB8
53	N	404	CDL	C72-C71-CB7-OB9
45	q	201	3PE	O31-C31-C32-C33
53	r	202	CDL	C52-C51-CB5-OB6
45	Y	202	3PE	C22-C23-C24-C25
45	A	203	3PE	C35-C36-C37-C38
45	b	101	3PE	O22-C21-C22-C23
45	i	202	3PE	O22-C21-C22-C23
47	Y	208	PLC	C2B-C1B-CB-OB
53	H	404	CDL	C59-C60-C61-C62
45	Y	202	3PE	C2-C1-O11-P
46	M	602	PC1	C2-C1-O11-P
45	A	203	3PE	O31-C31-C32-C33
45	Y	201	3PE	O31-C31-C32-C33
53	M	604	CDL	C12-C11-CA5-OA6
46	A	204	PC1	C11-C12-N-C15
46	q	202	PC1	O32-C31-C32-C33
45	Y	204	3PE	O21-C21-C22-C23
46	H	401	PC1	O21-C21-C22-C23
45	Y	201	3PE	O11-C1-C2-C3
46	m	205	PC1	C28-C29-C2A-C2B
47	M	603	PLC	O'-C'-C1'-C2'
53	d	202	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	O21-C21-C22-C23
47	Y	208	PLC	O2-C'-C1'-C2'
45	N	401	3PE	C22-C23-C24-C25
45	N	401	3PE	C24-C25-C26-C27
53	d	201	CDL	C37-C38-C39-C40
47	g	201	PLC	C3B-C4B-C5B-C6B
46	H	402	PC1	C23-C24-C25-C26
46	h	201	PC1	C21-C22-C23-C24
45	A	202	3PE	O21-C21-C22-C23
45	O	403	3PE	O21-C21-C22-C23
55	O	401	DGT	PA-O3A-PB-O2B
45	A	202	3PE	O22-C21-C22-C23
53	P	505	CDL	C12-C11-CA5-OA7
46	q	202	PC1	C29-C2A-C2B-C2C
45	Y	203	3PE	O31-C31-C32-C33
46	A	205	PC1	O21-C21-C22-C23
47	M	603	PLC	C2B-C1B-CB-O3
47	g	201	PLC	O2-C'-C1'-C2'
45	f	102	3PE	O22-C21-C22-C23
46	e	202	PC1	O22-C21-C22-C23
53	P	505	CDL	C72-C71-CB7-OB9
45	m	203	3PE	C39-C3A-C3B-C3C

There are no ring outliers.

28 monomers are involved in 51 short contacts:

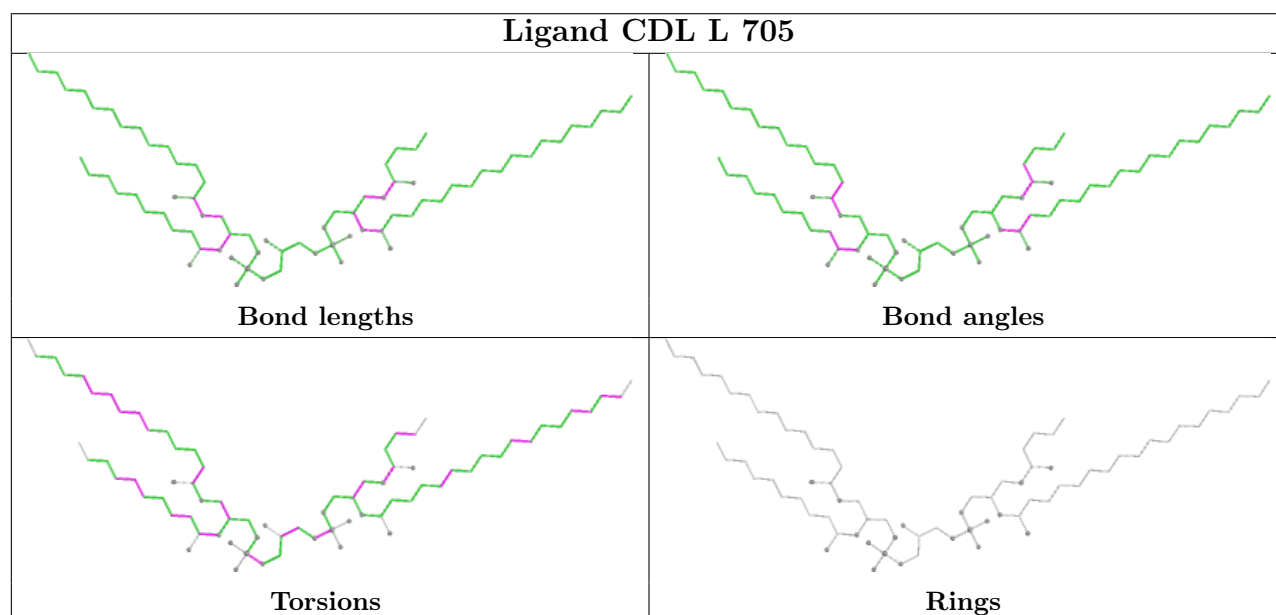
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	L	705	CDL	1	0
47	P	503	PLC	1	0
46	B	204	PC1	1	0
50	G	803	FES	1	0
53	M	604	CDL	2	0
46	A	204	PC1	2	0
45	i	202	3PE	2	0
47	g	201	PLC	1	0
49	B	202	U10	11	0
48	G	802	SF4	1	0
45	Y	202	3PE	2	0
45	Y	204	3PE	1	0
45	N	401	3PE	1	0
45	Z	202	3PE	1	0
51	F	501	FMN	1	0

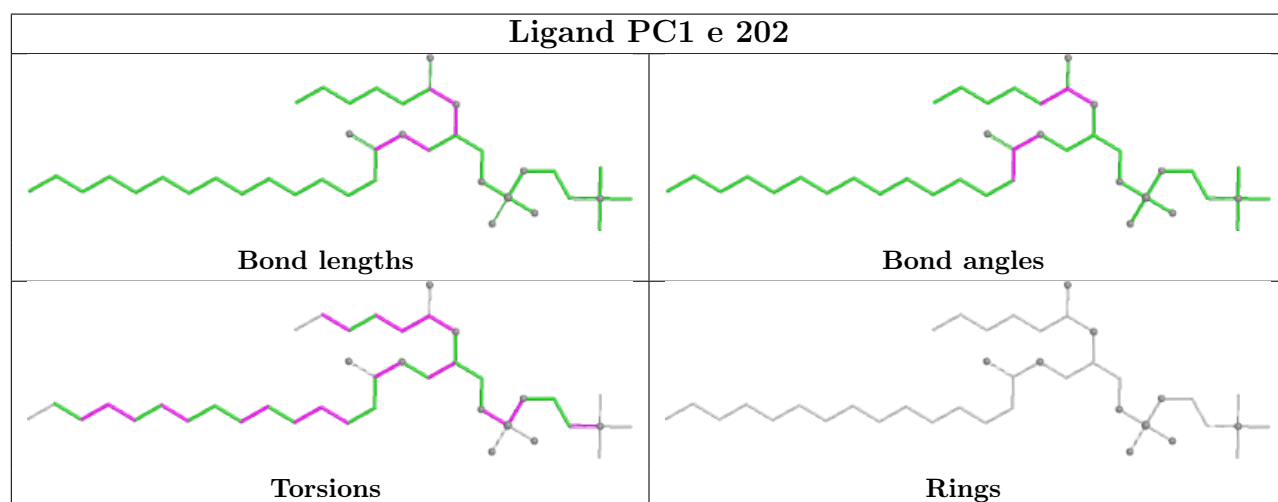
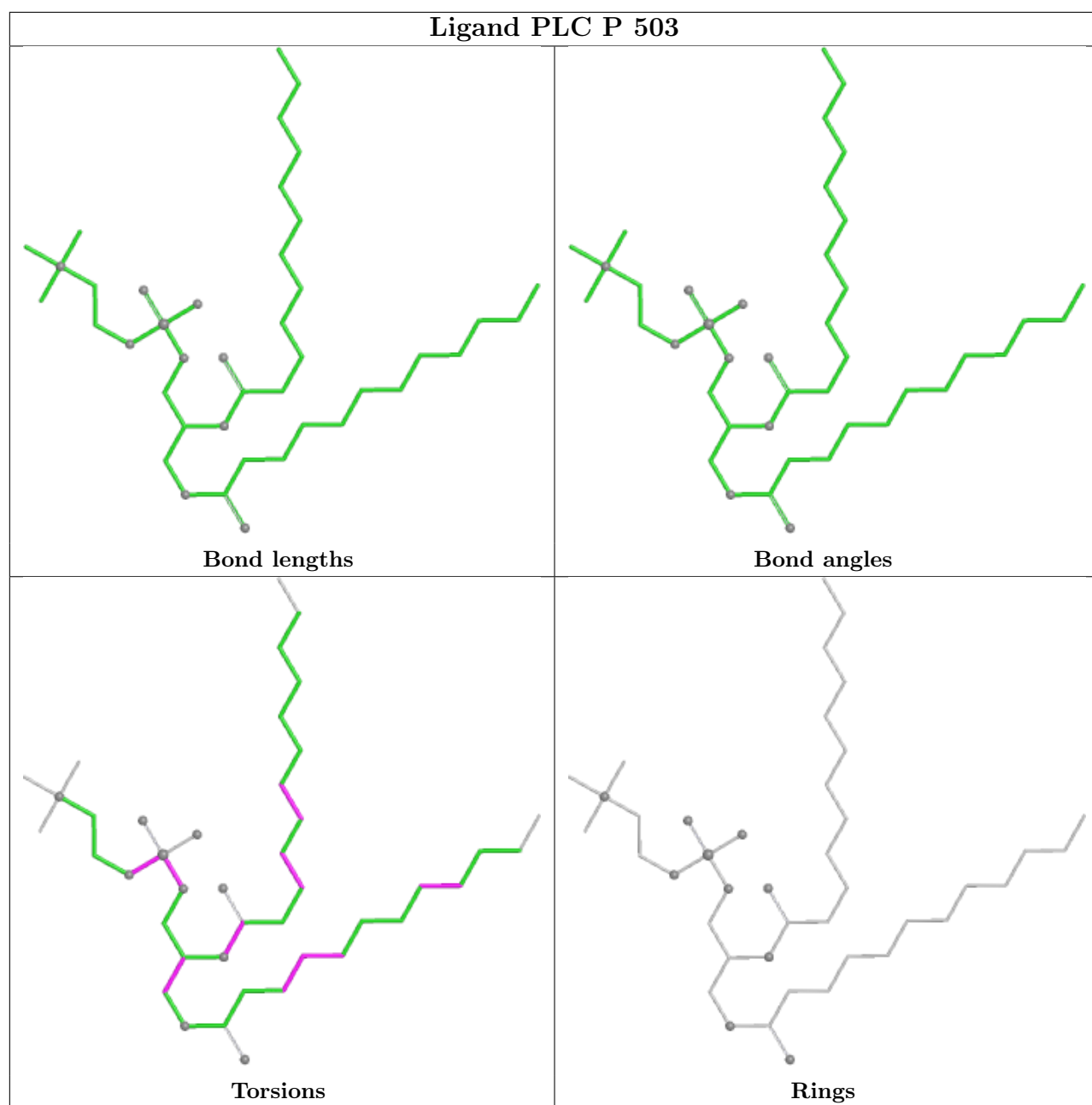
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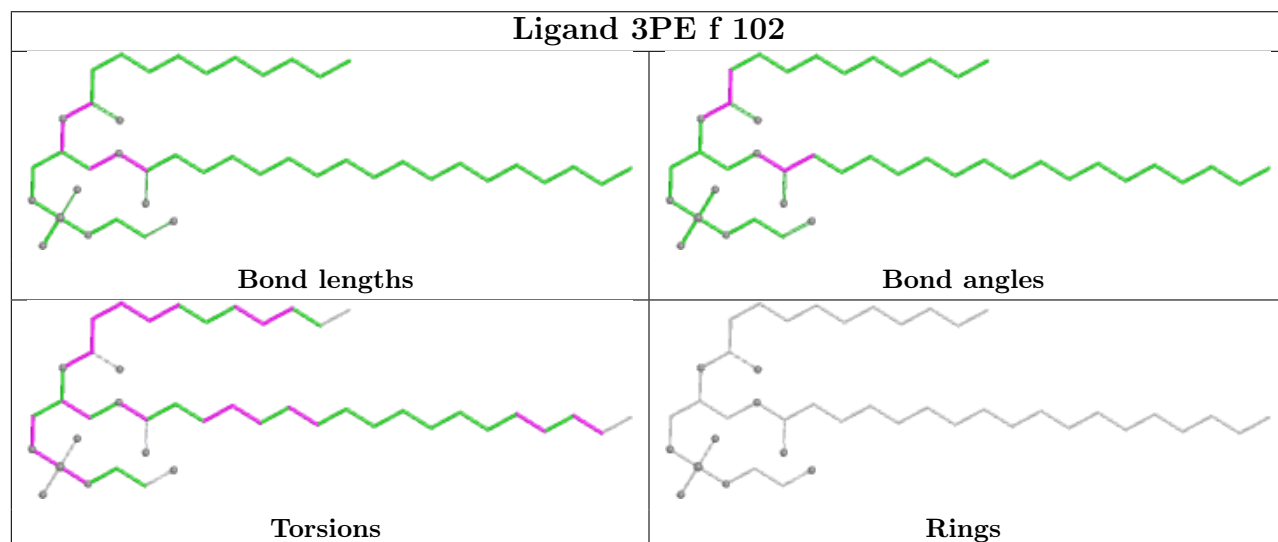
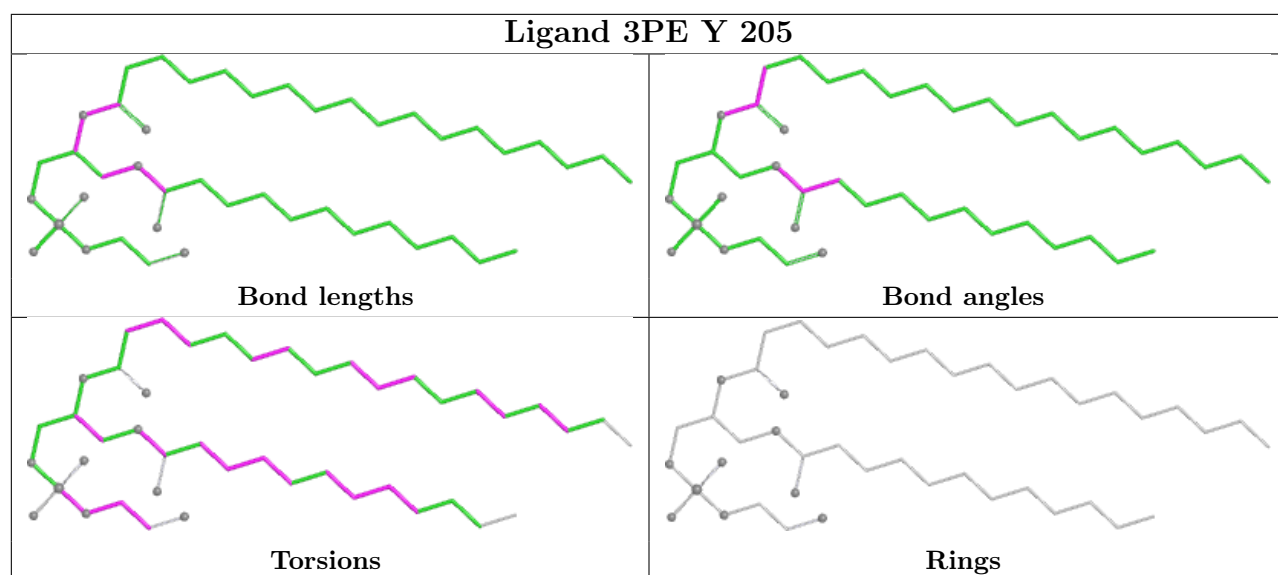
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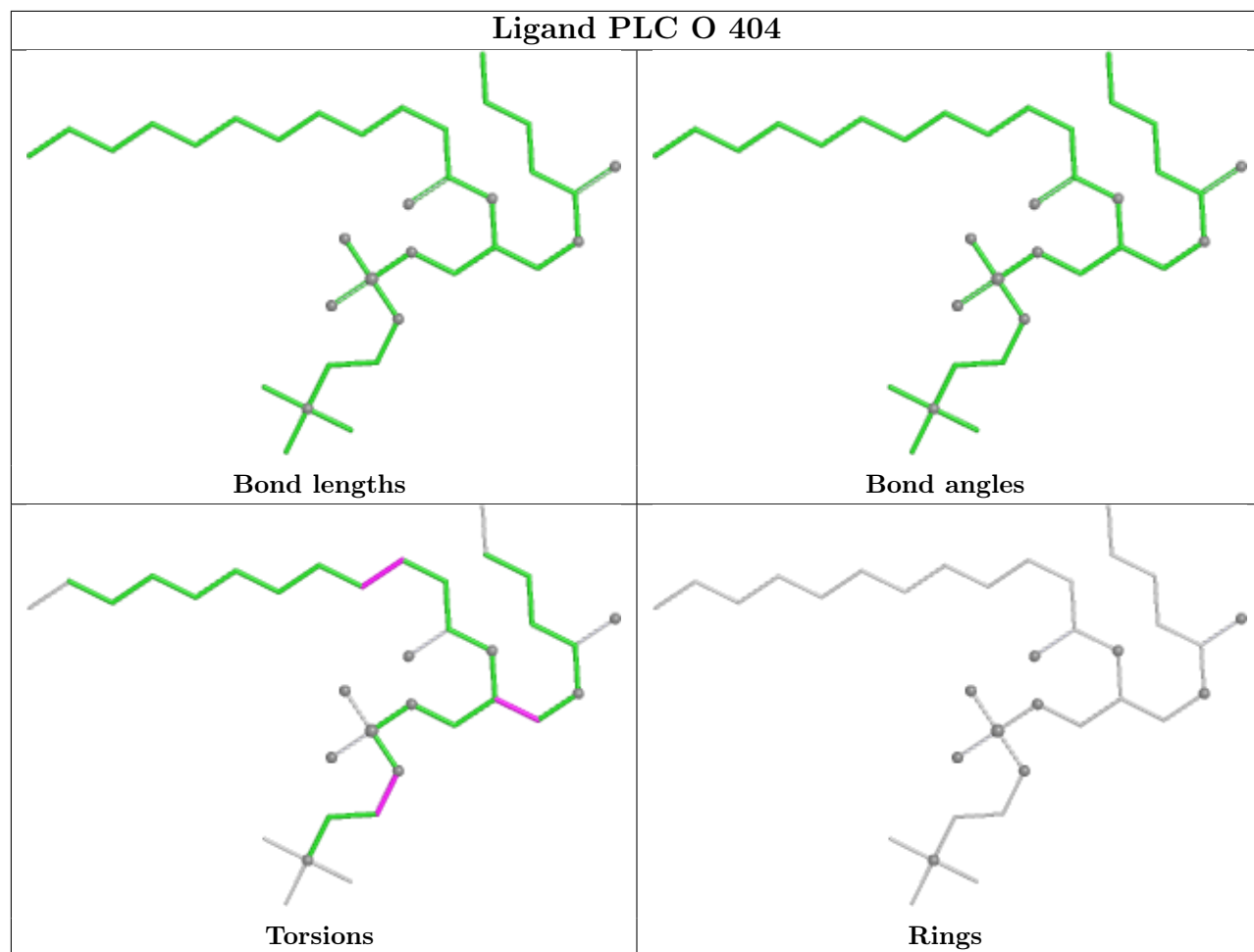
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	i	201	CHD	5	0
45	O	403	3PE	2	0
53	d	202	CDL	1	0
45	N	402	3PE	1	0
55	O	401	DGT	2	0
46	H	401	PC1	2	0
53	r	202	CDL	1	0
45	e	201	3PE	2	0
46	I	203	PC1	2	0
45	L	701	3PE	1	0
46	H	403	PC1	2	0
60	o	201	MYR	1	0
46	L	703	PC1	3	0

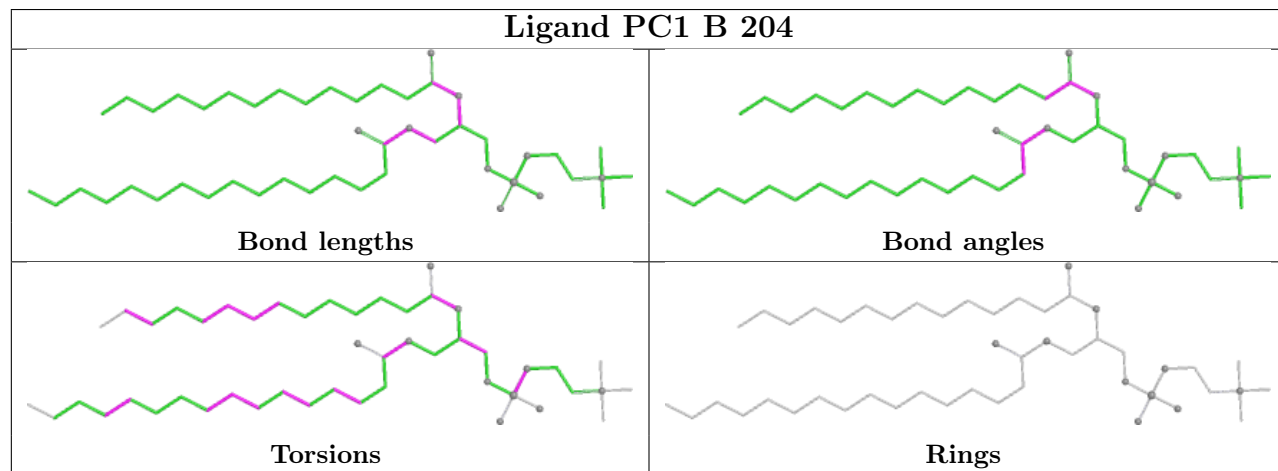
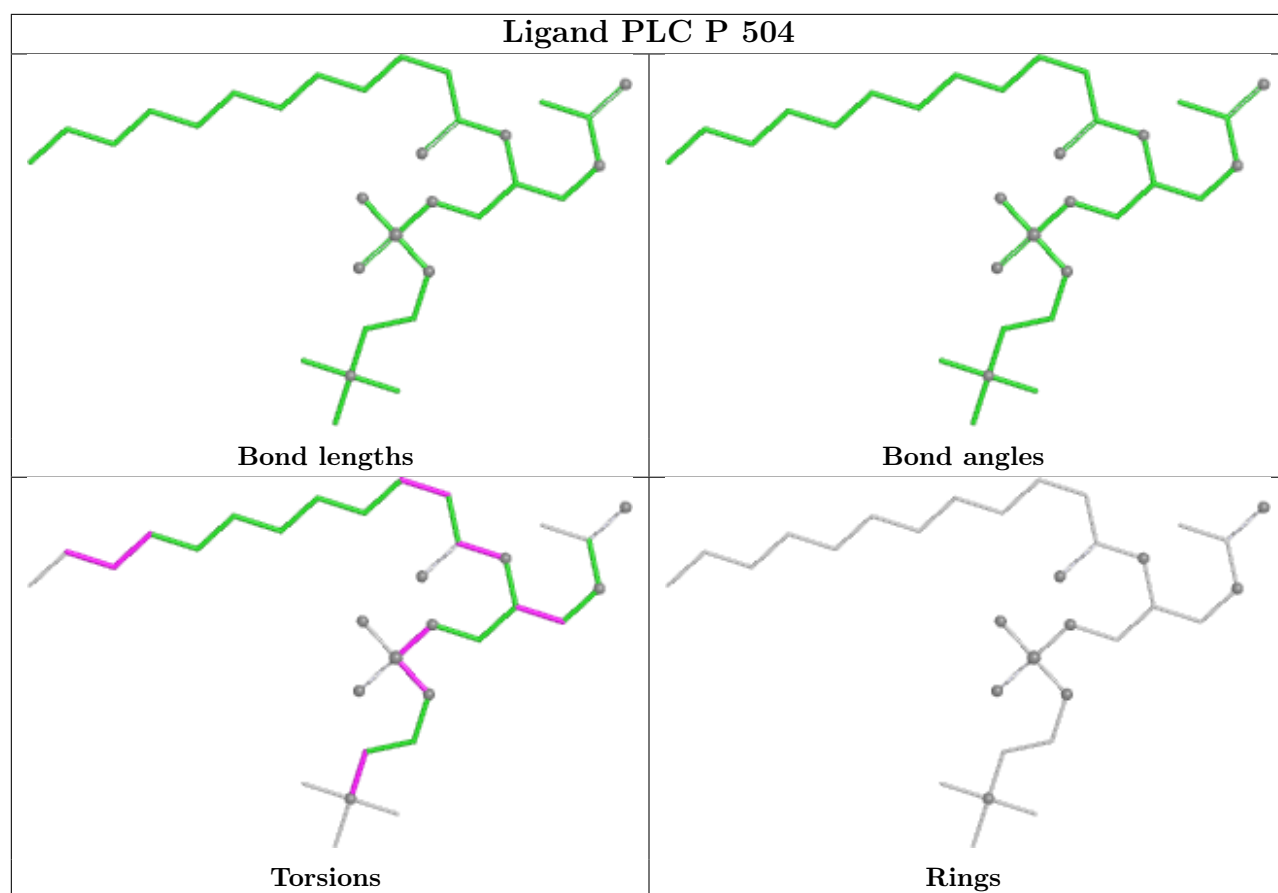
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

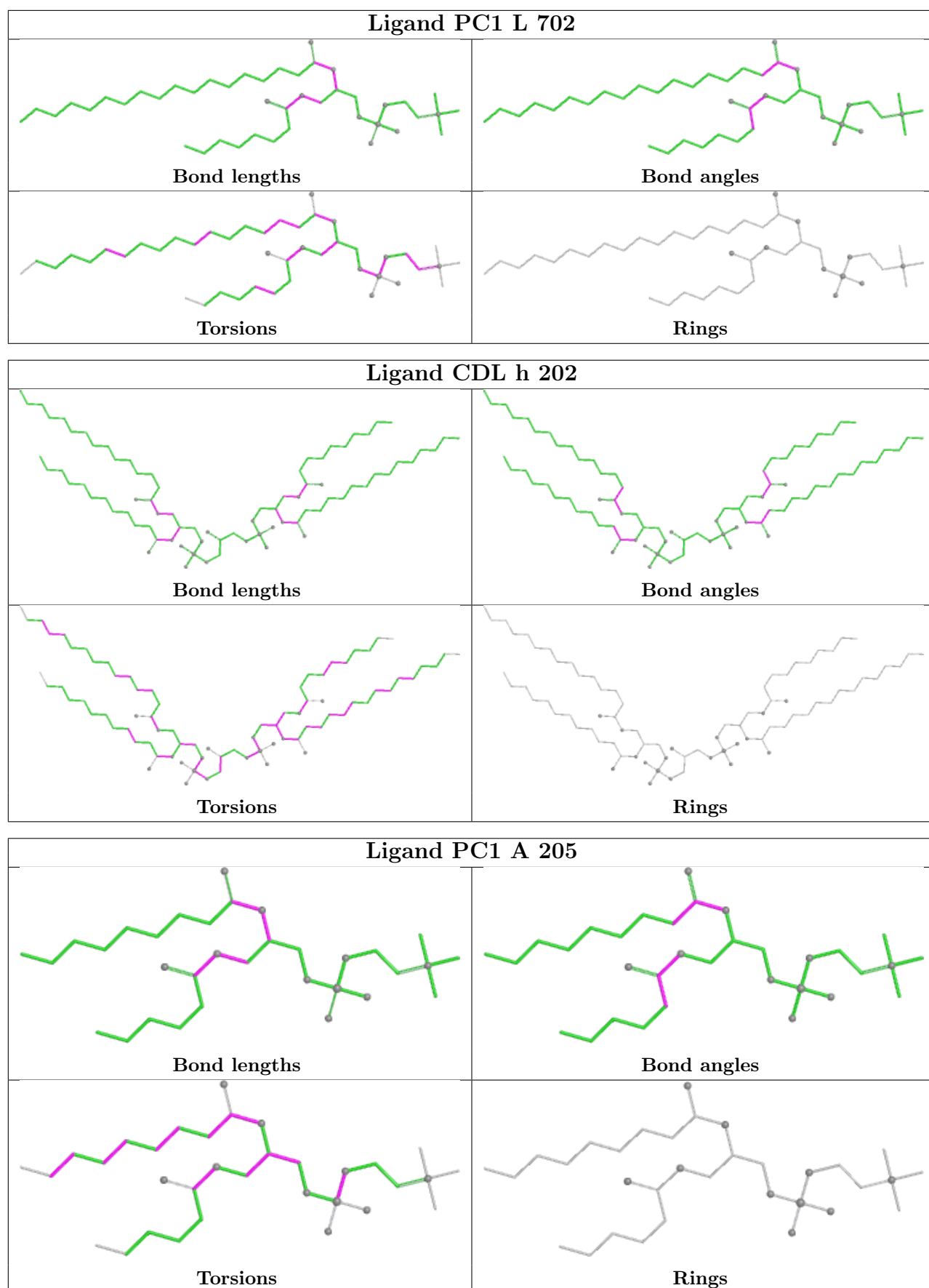


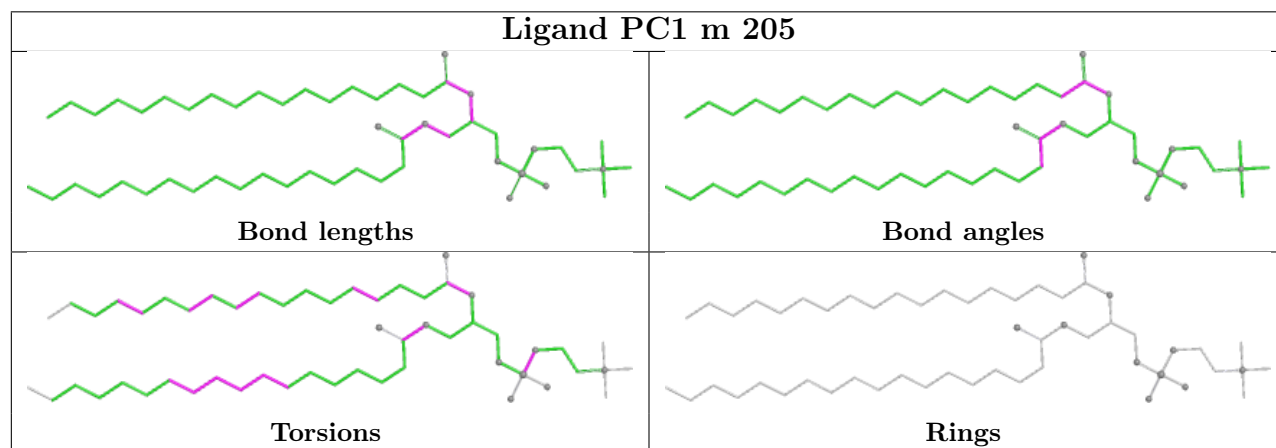
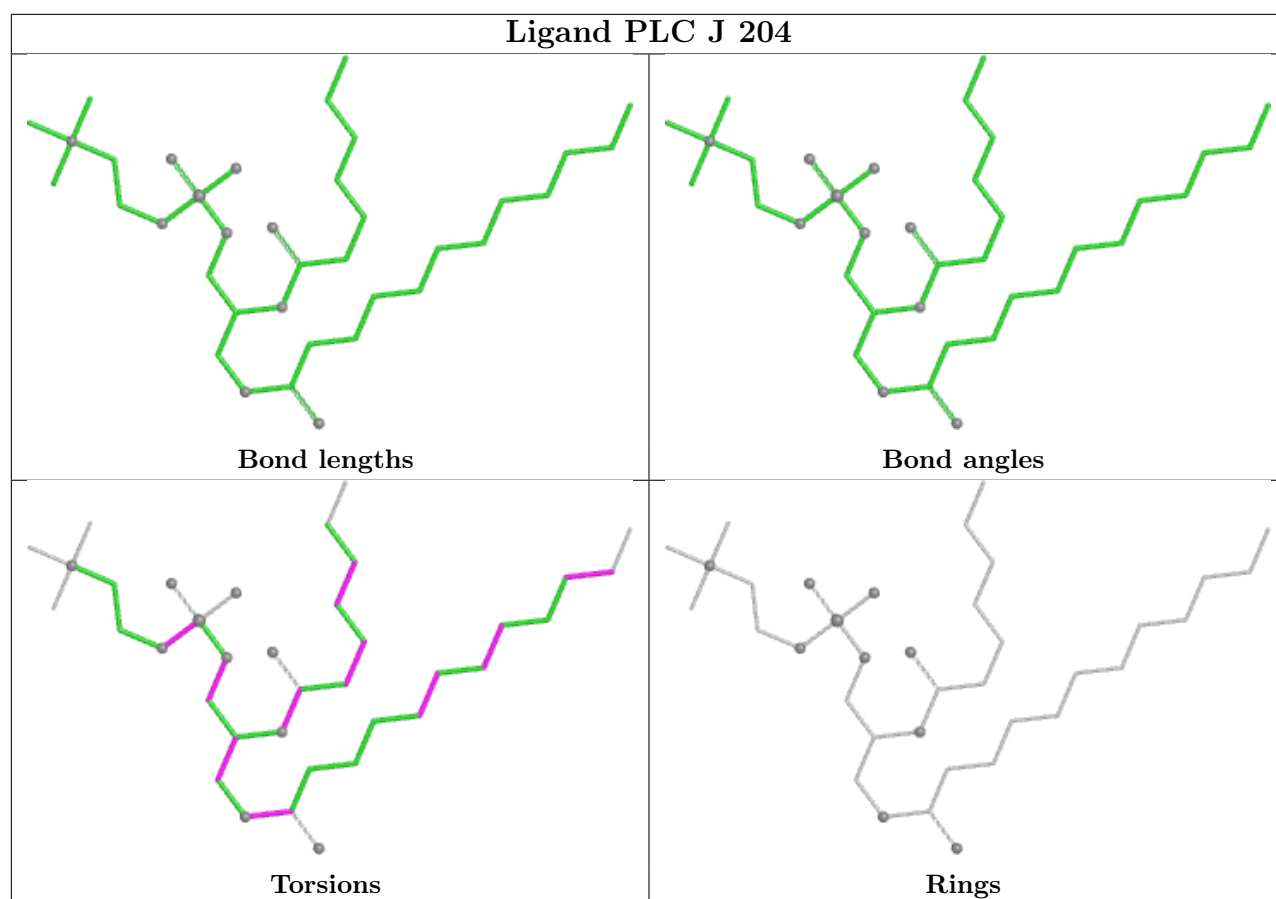


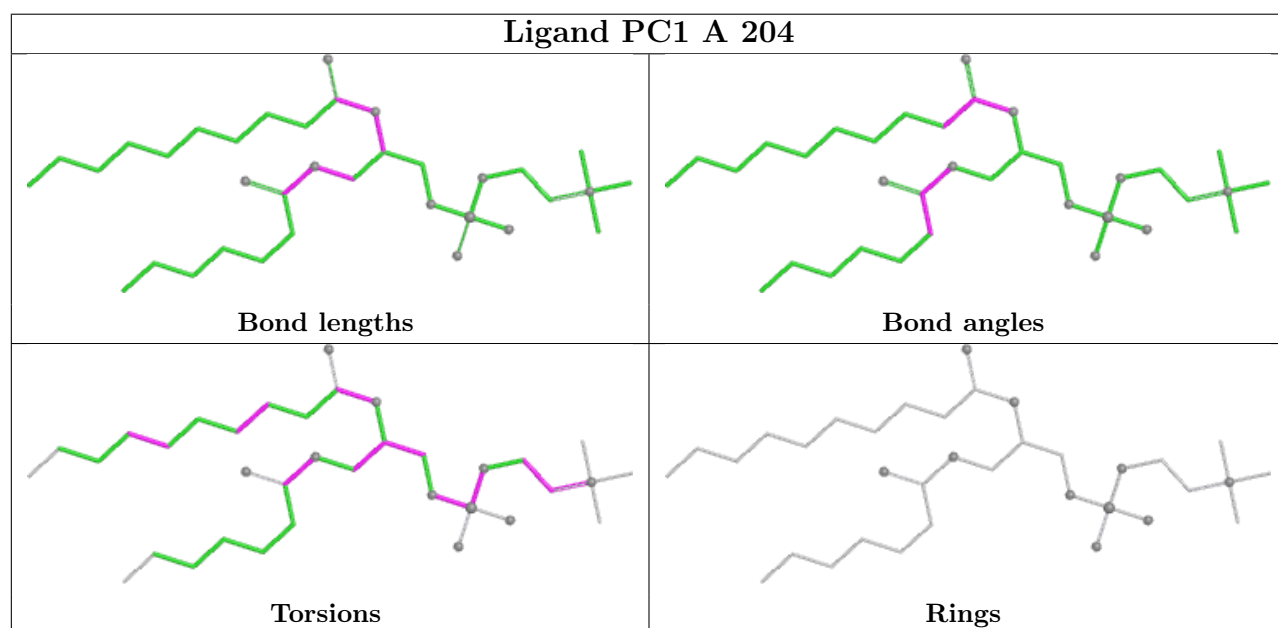
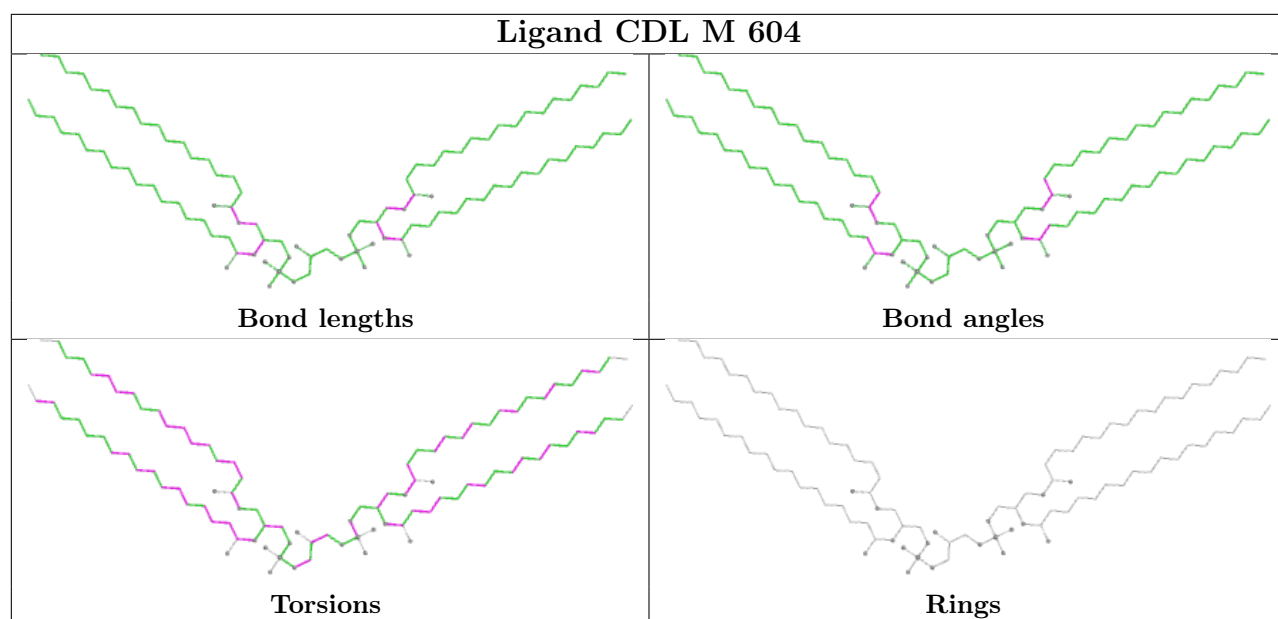




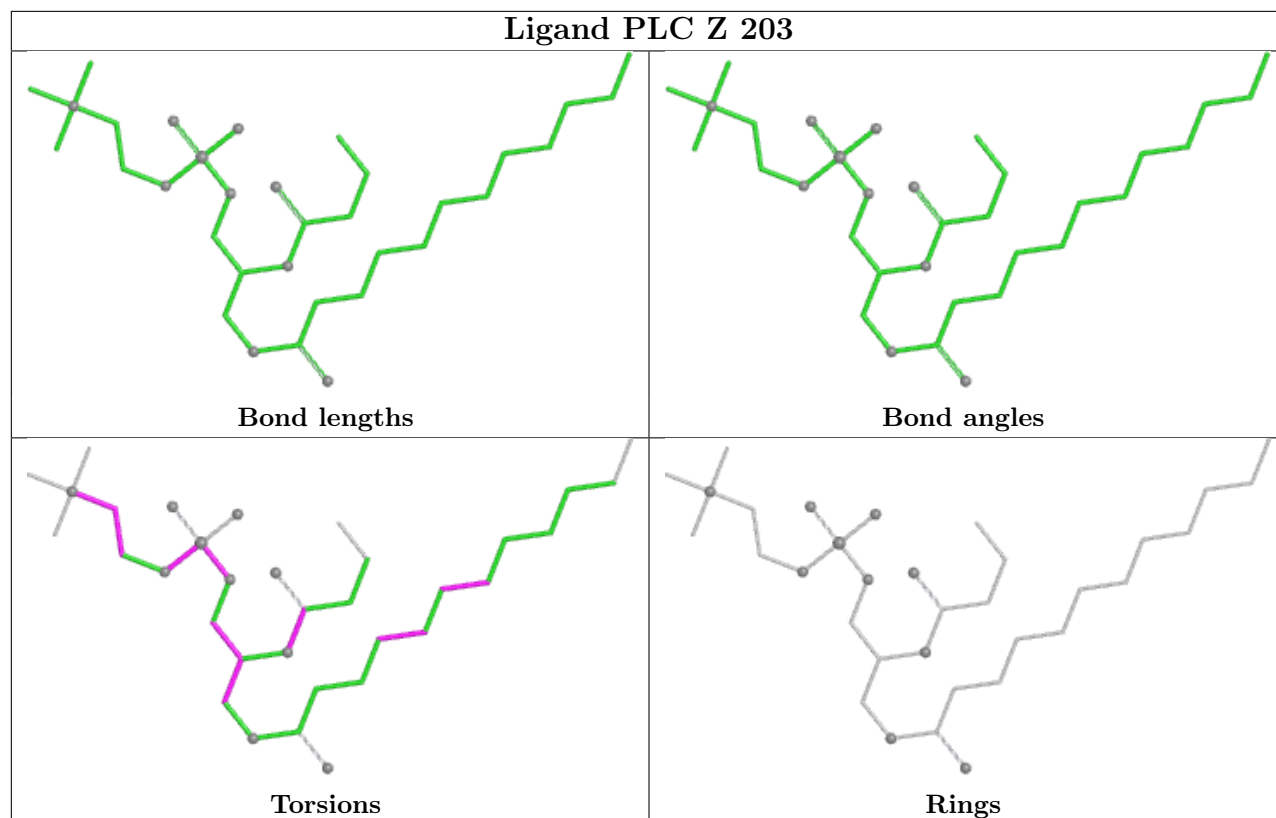




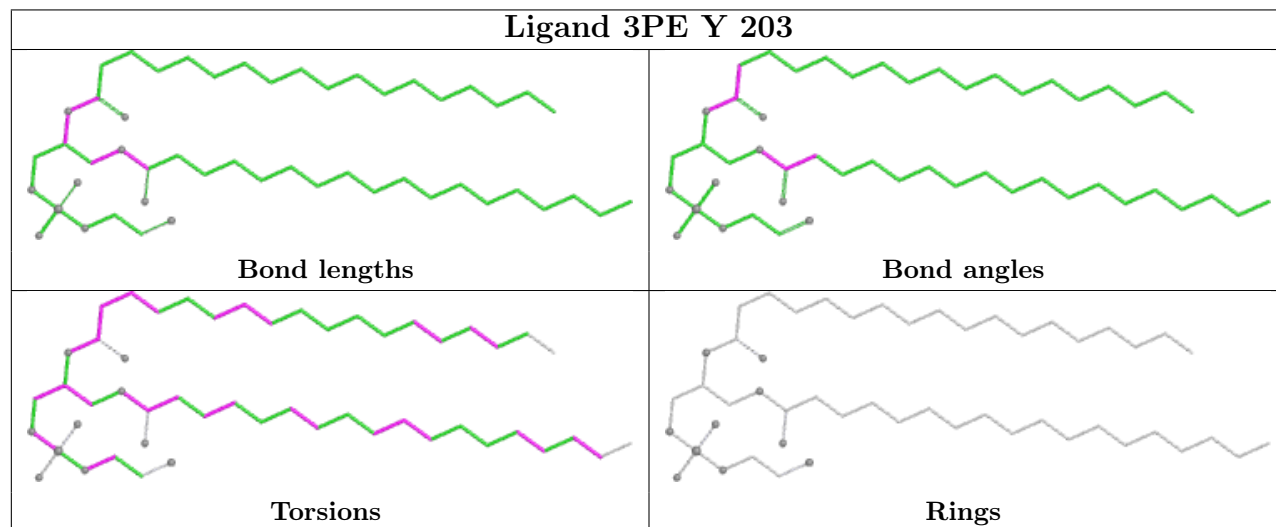


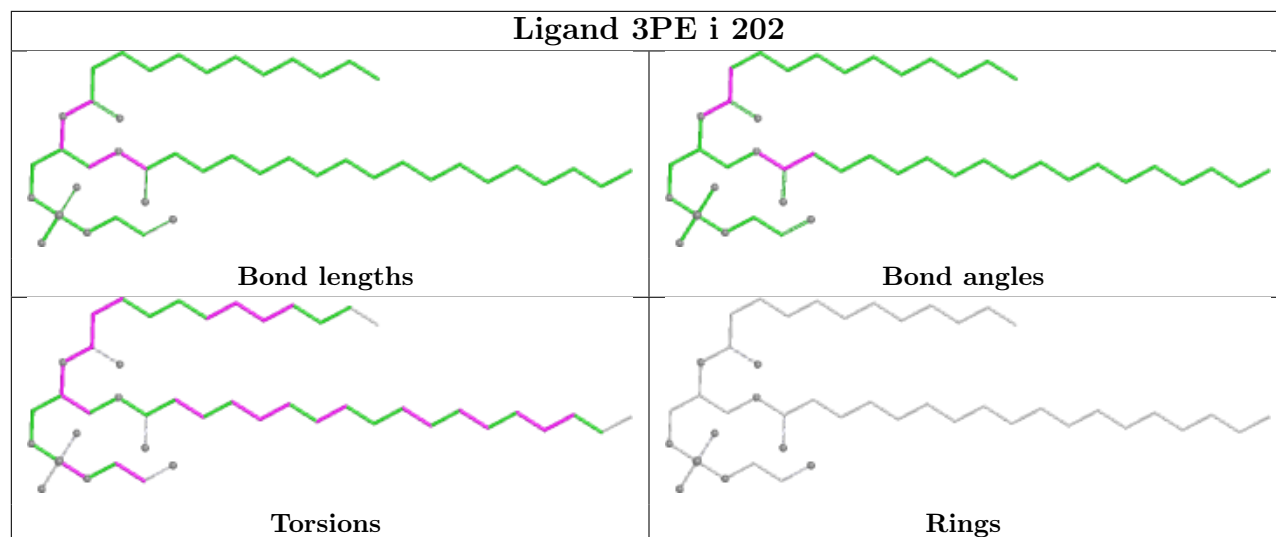


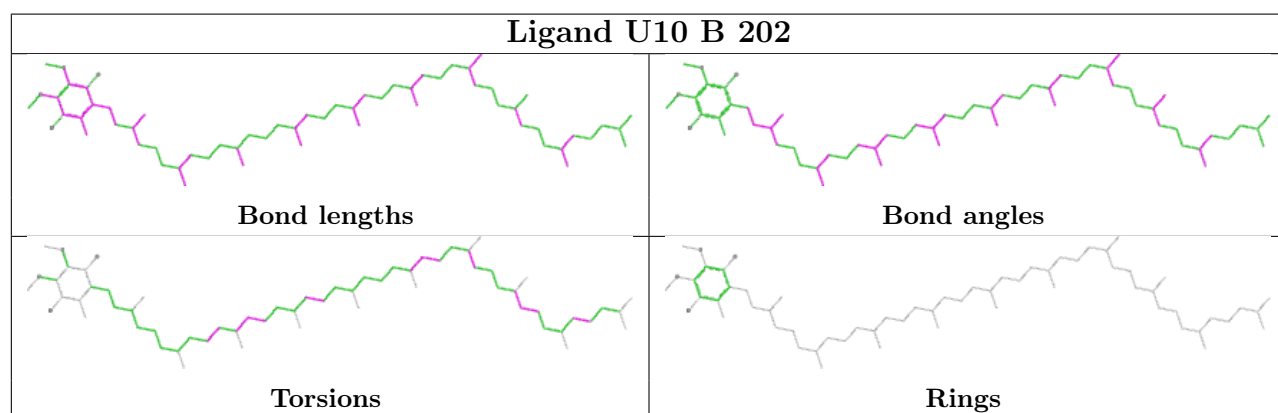
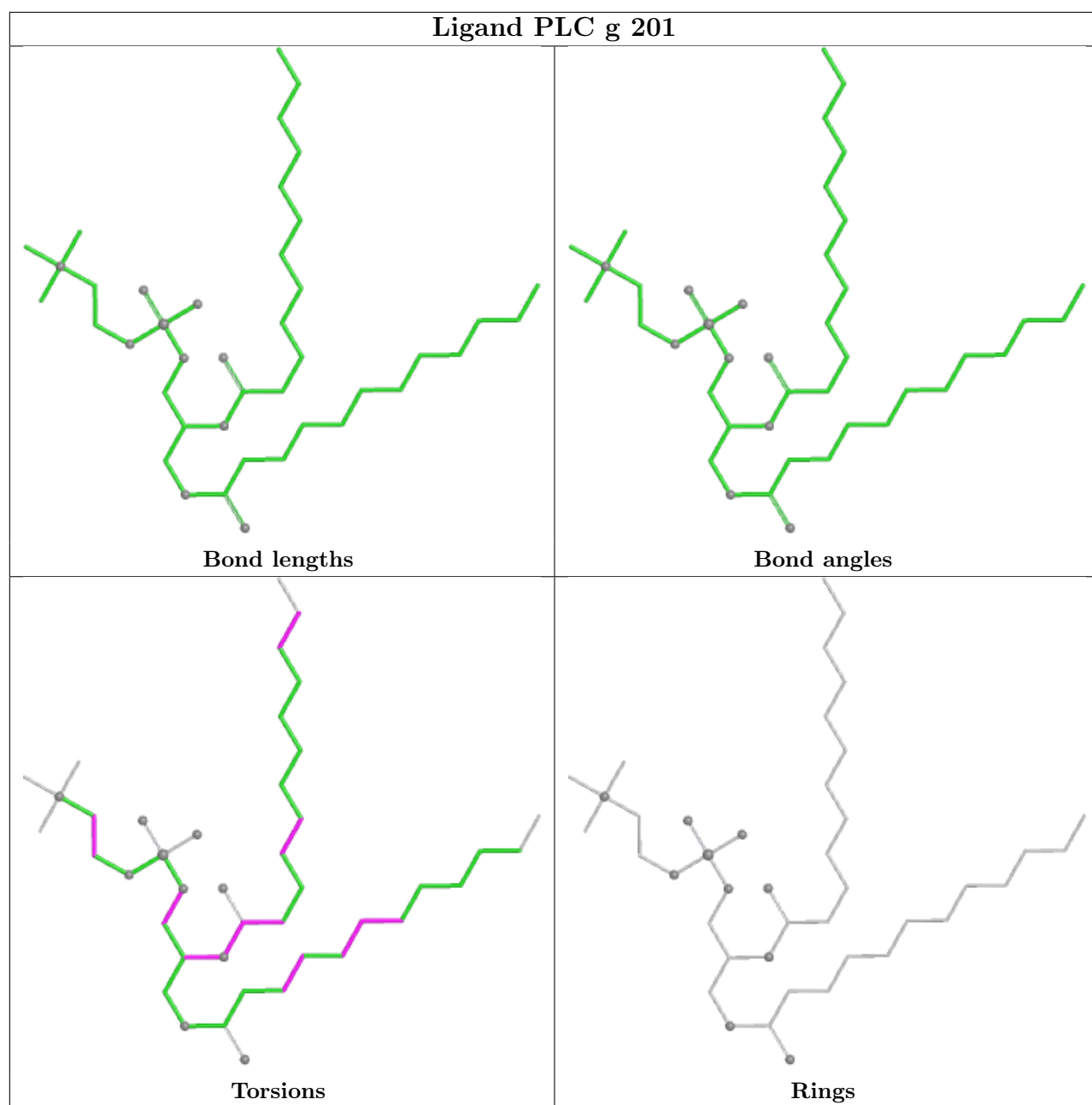
Ligand PLC Z 203

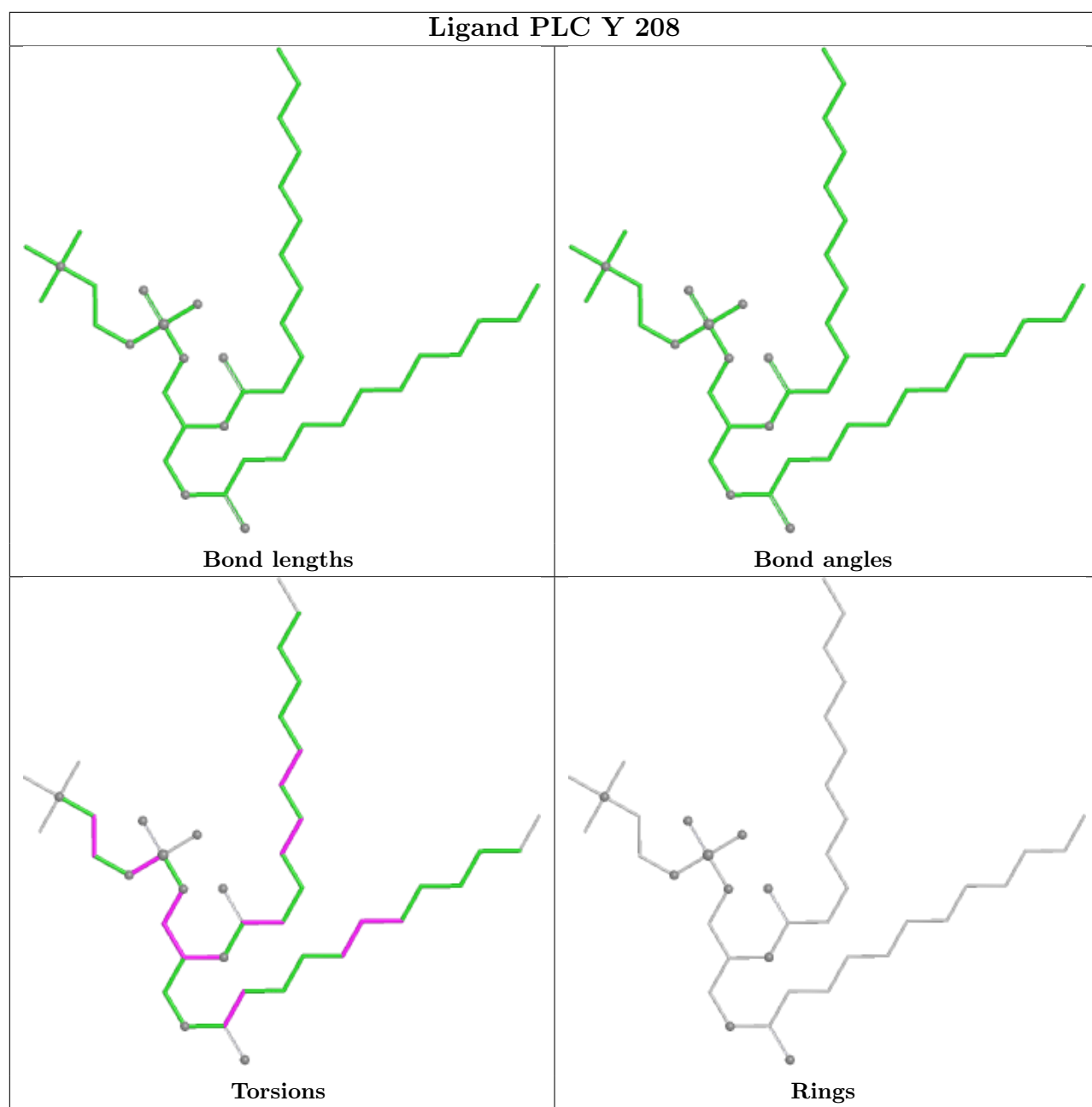


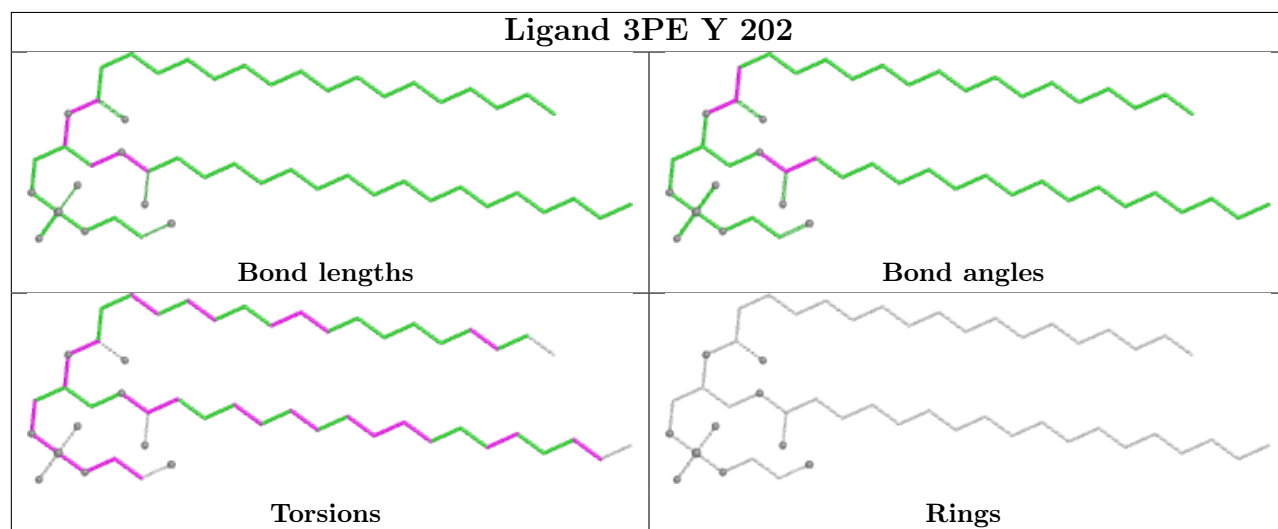
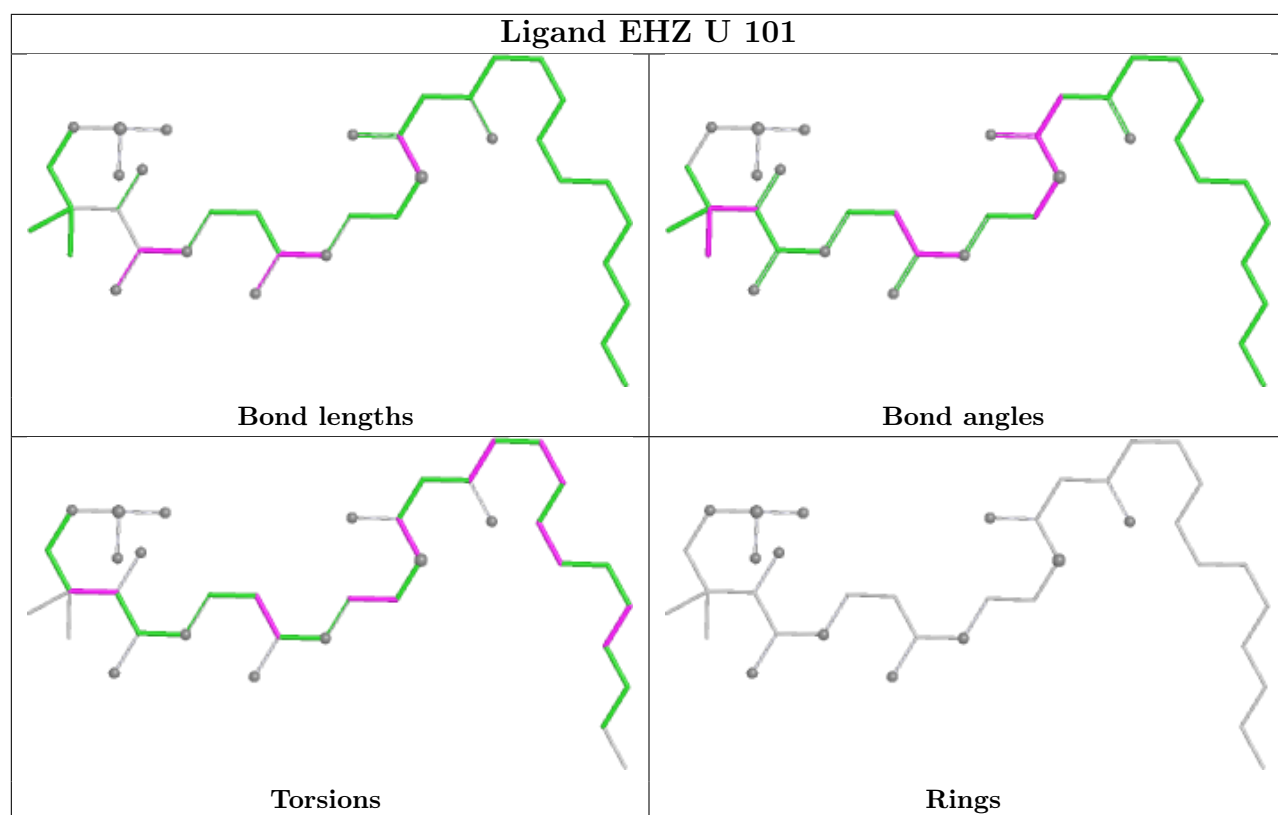
Ligand 3PE Y 203



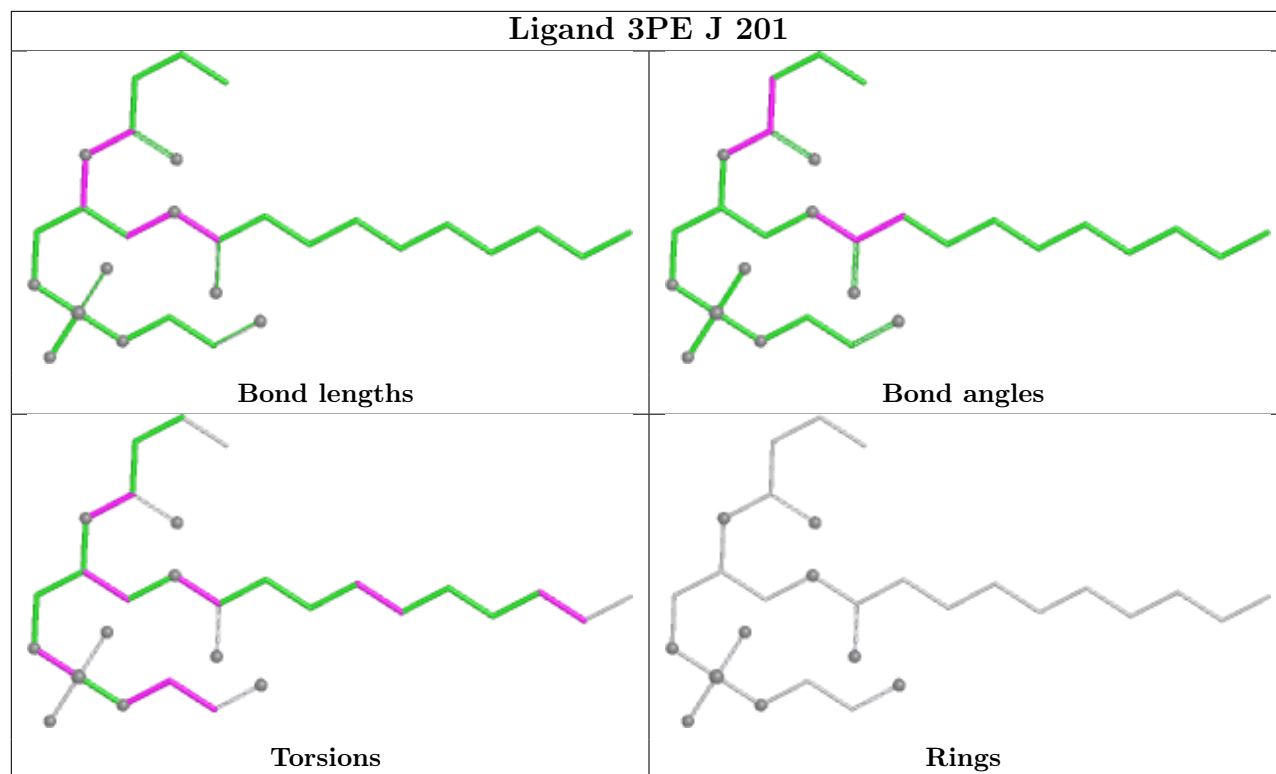




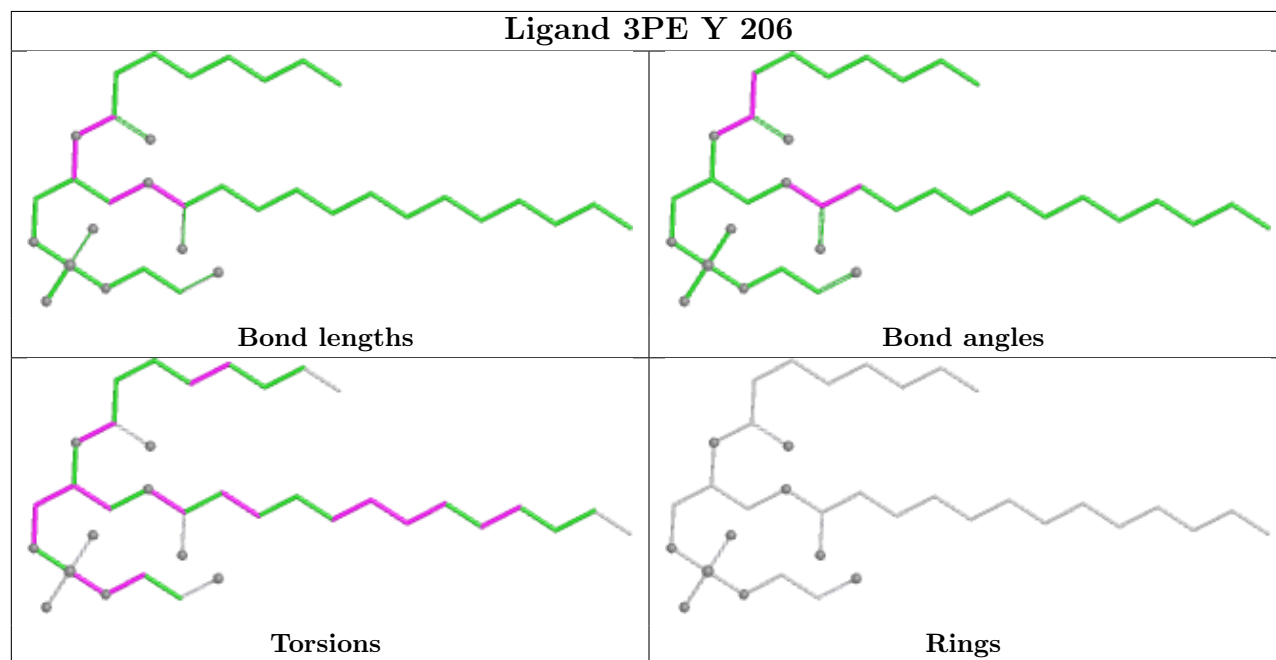


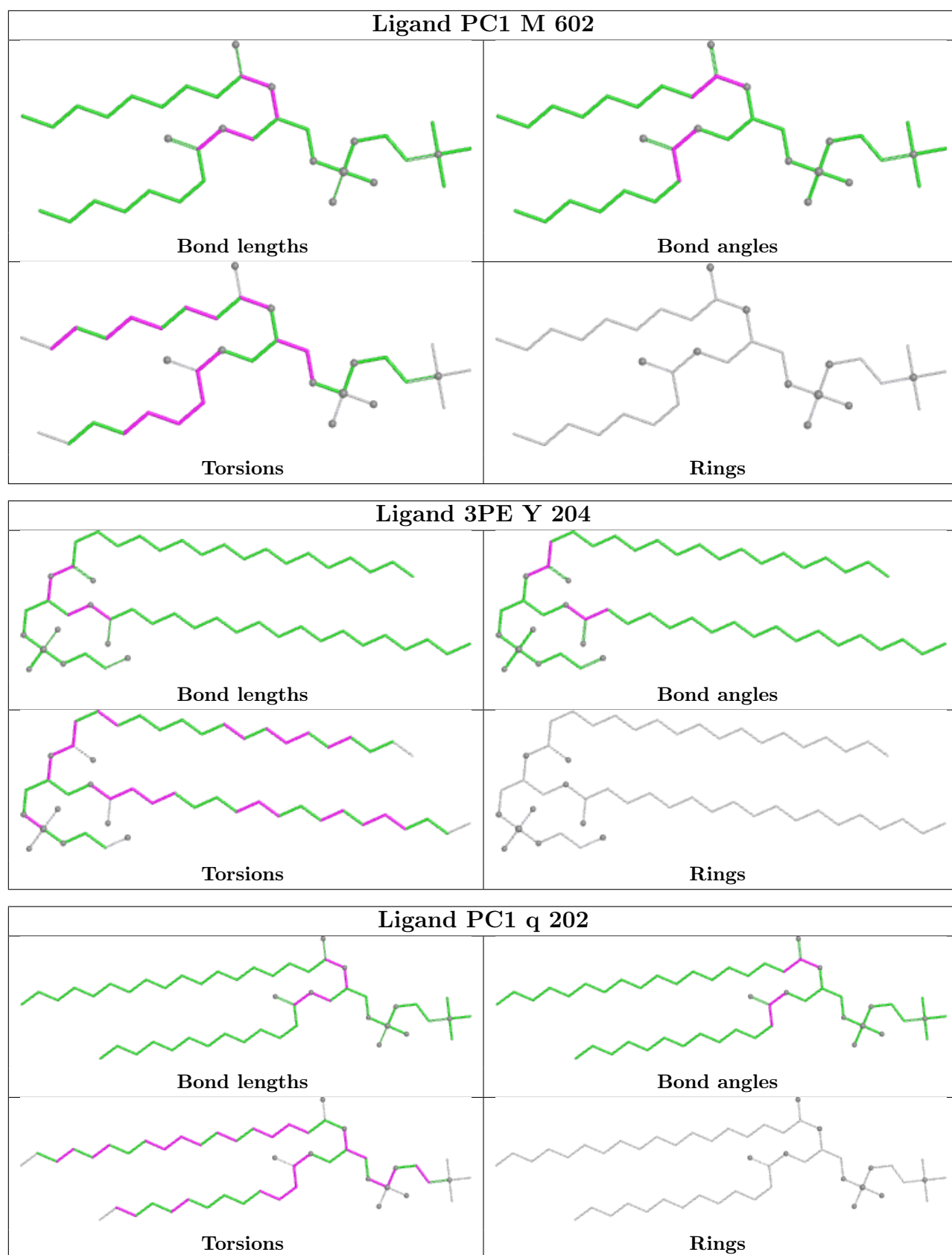


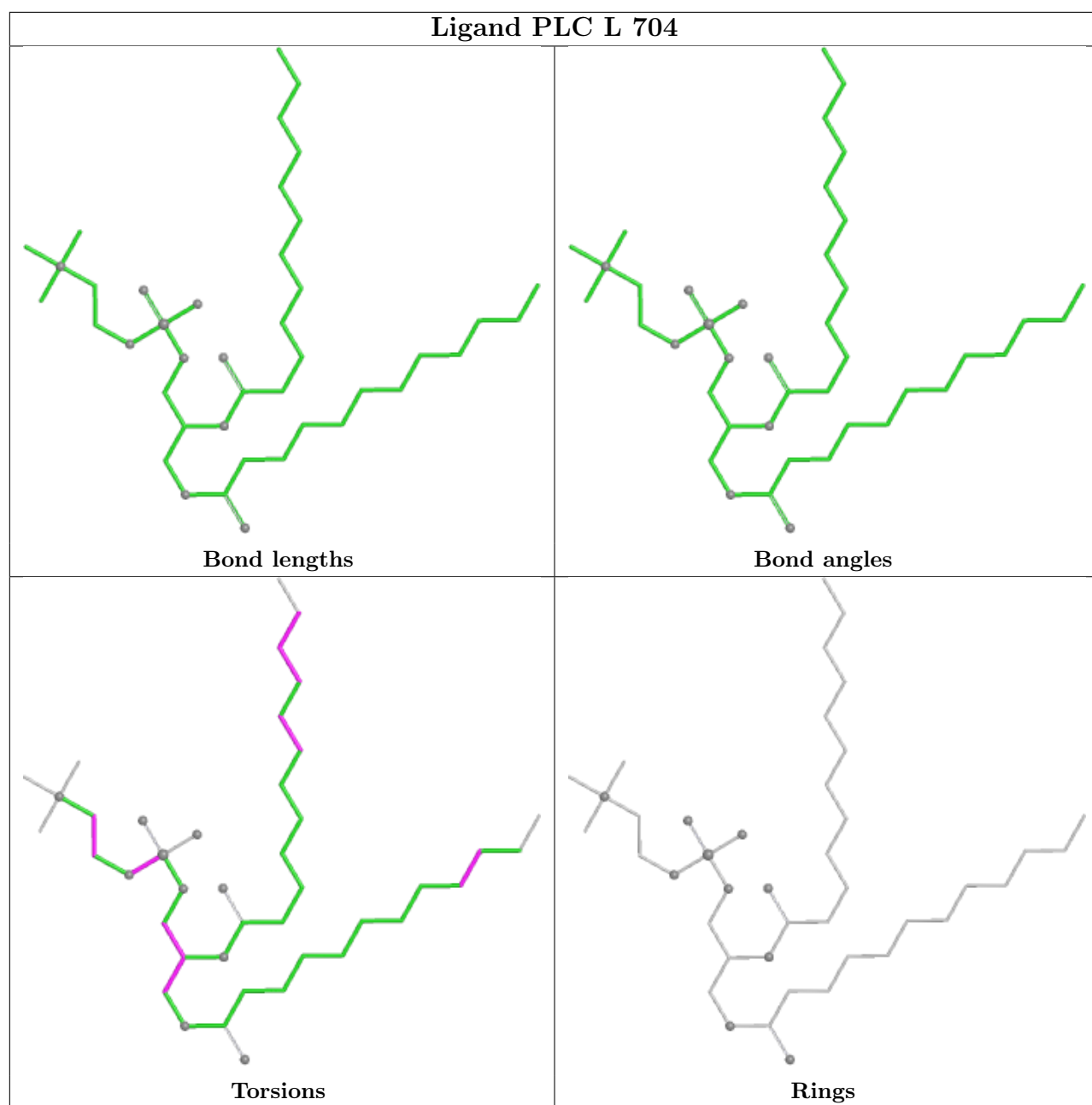
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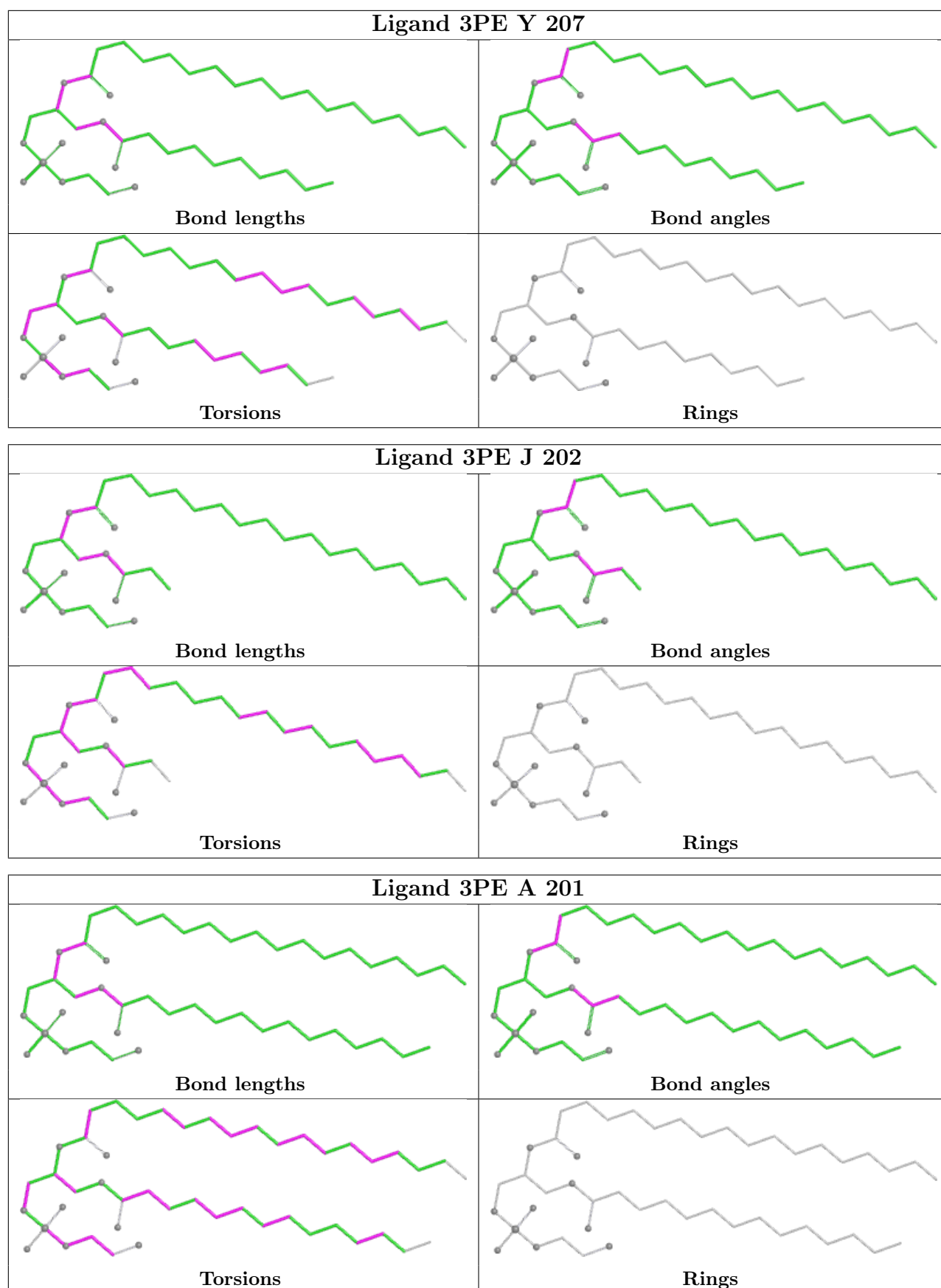


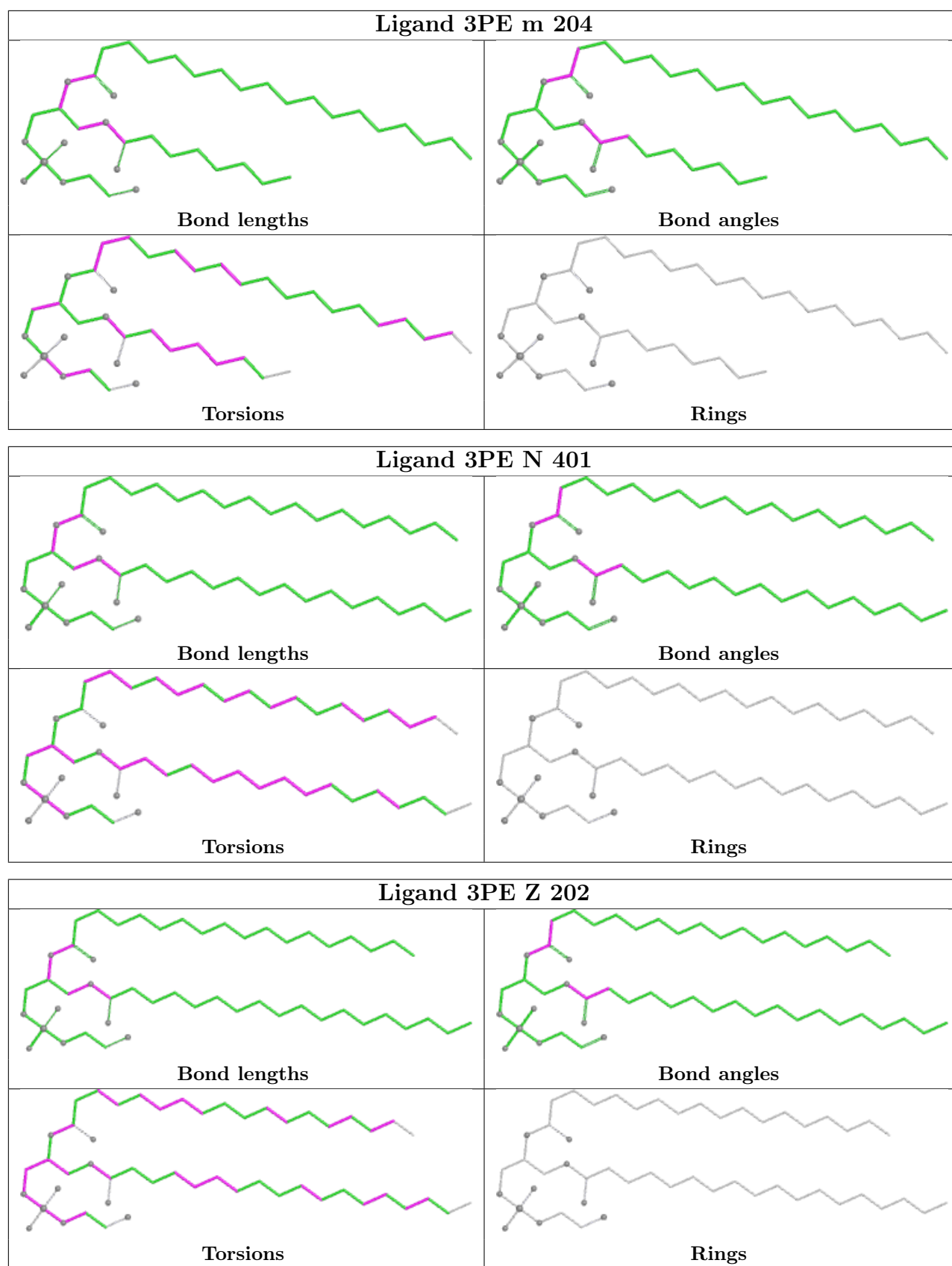
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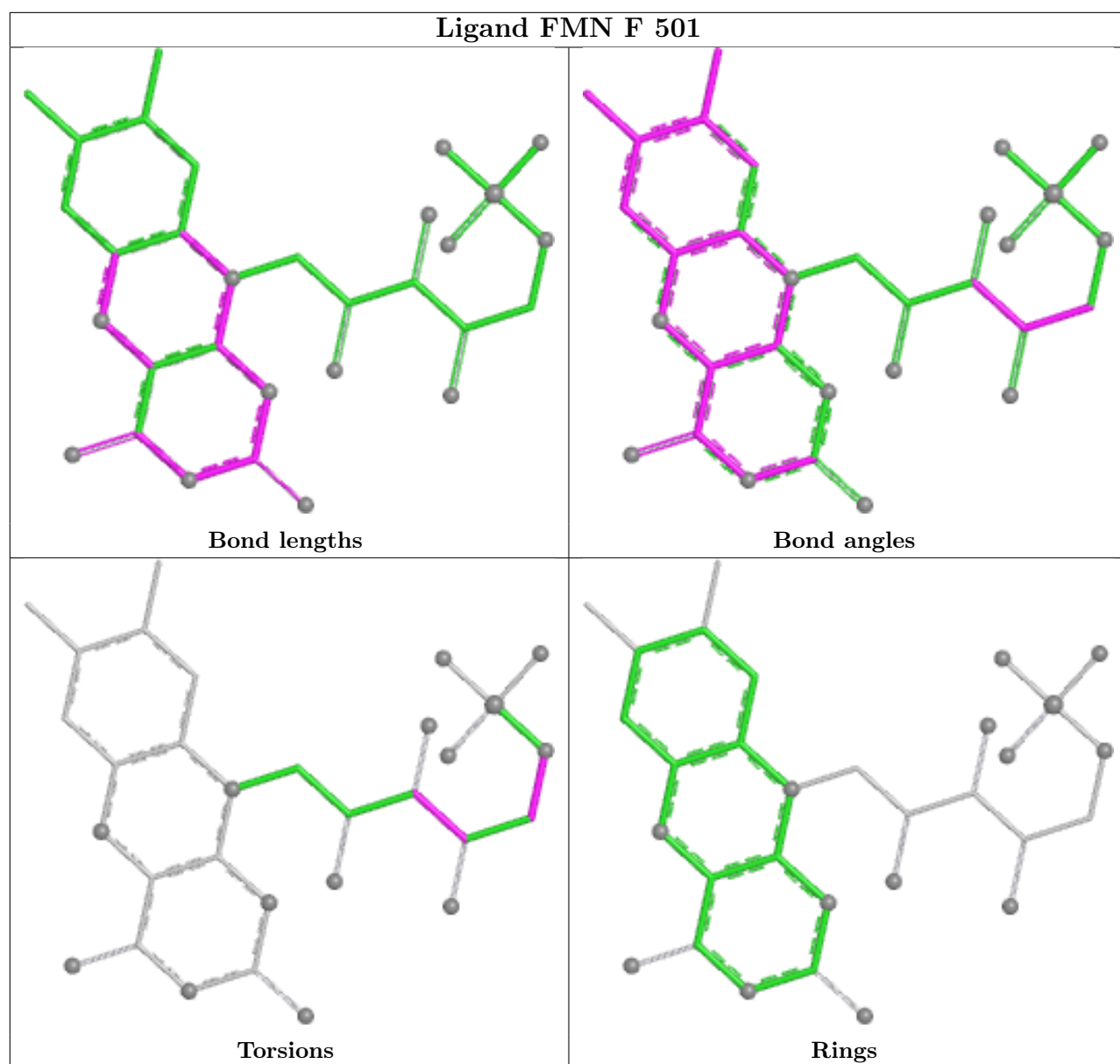


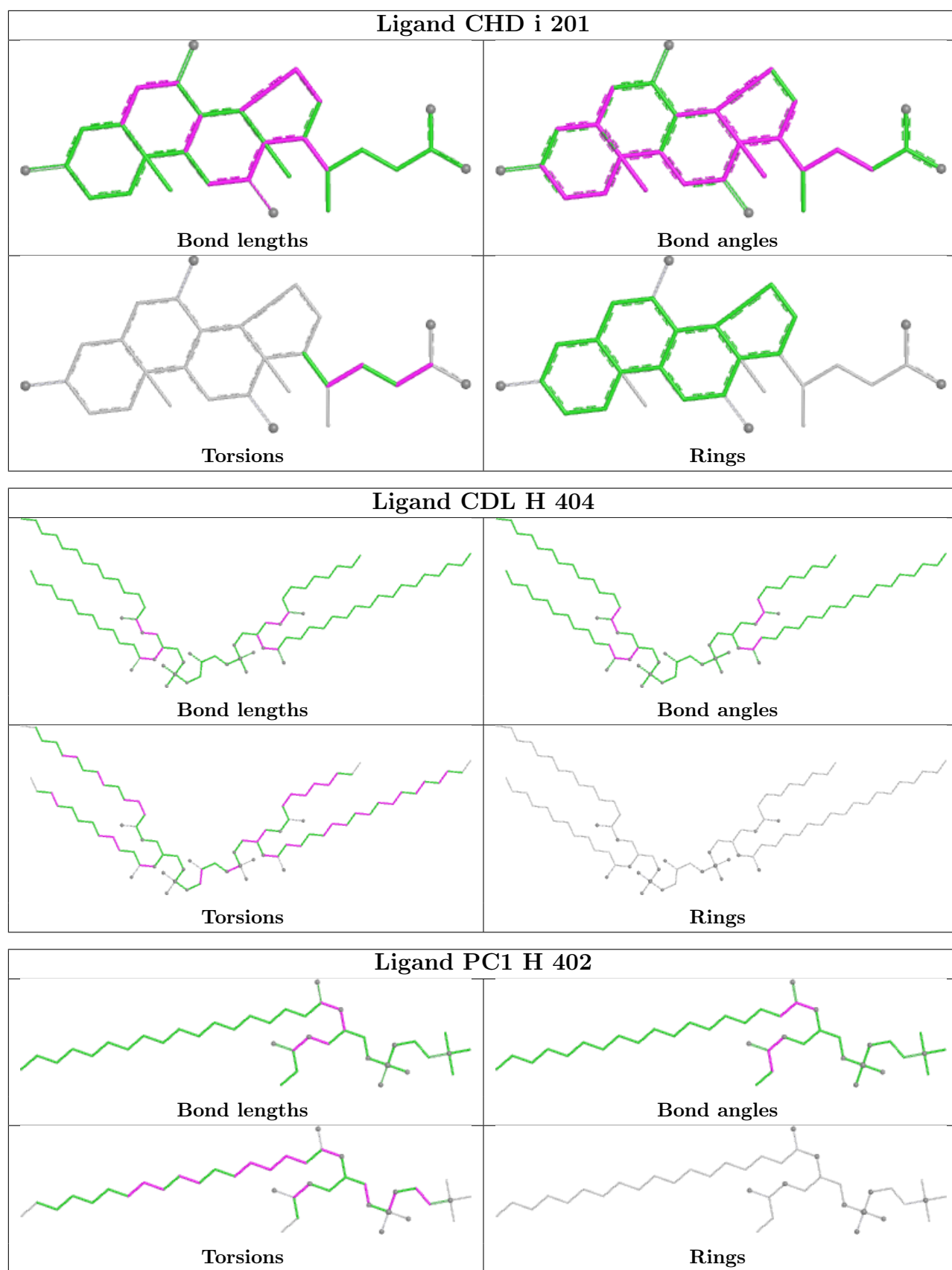


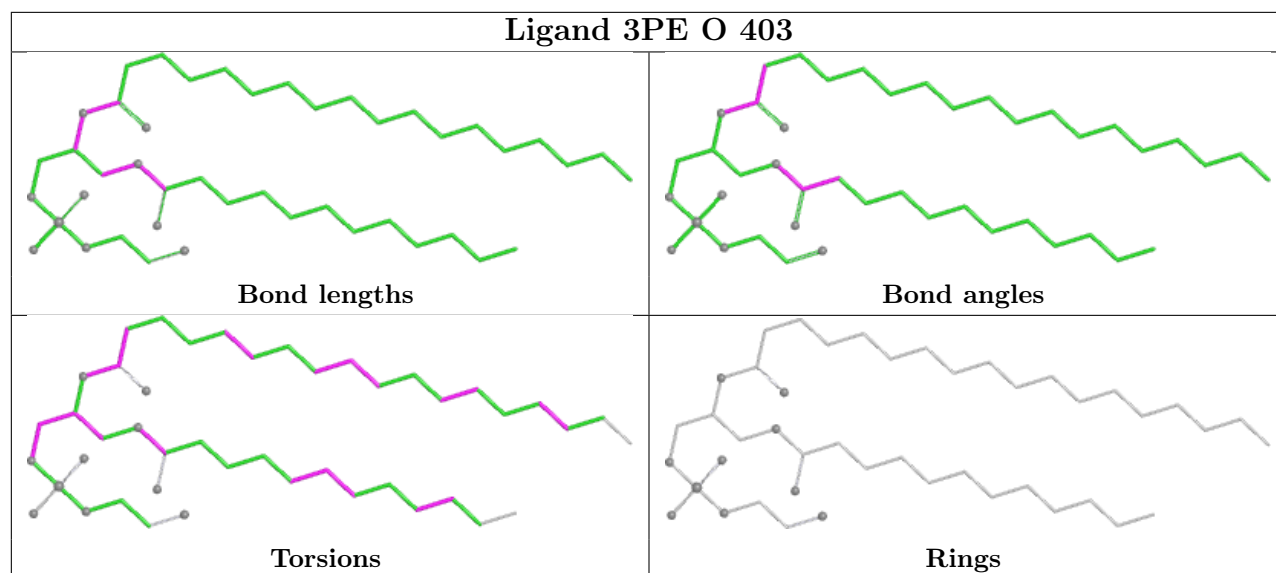
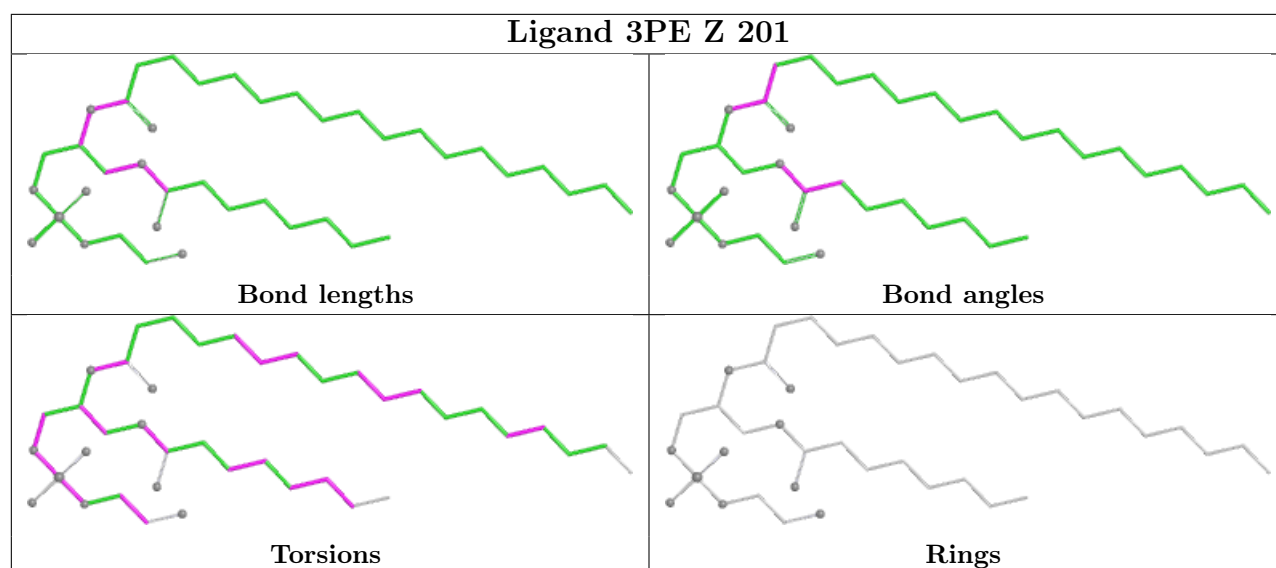


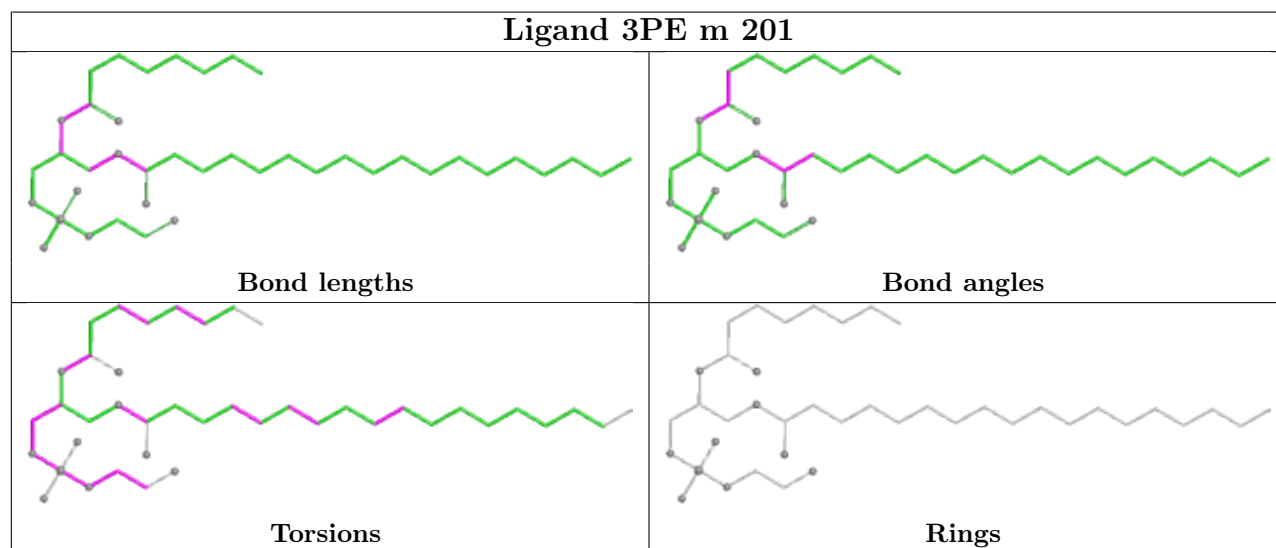
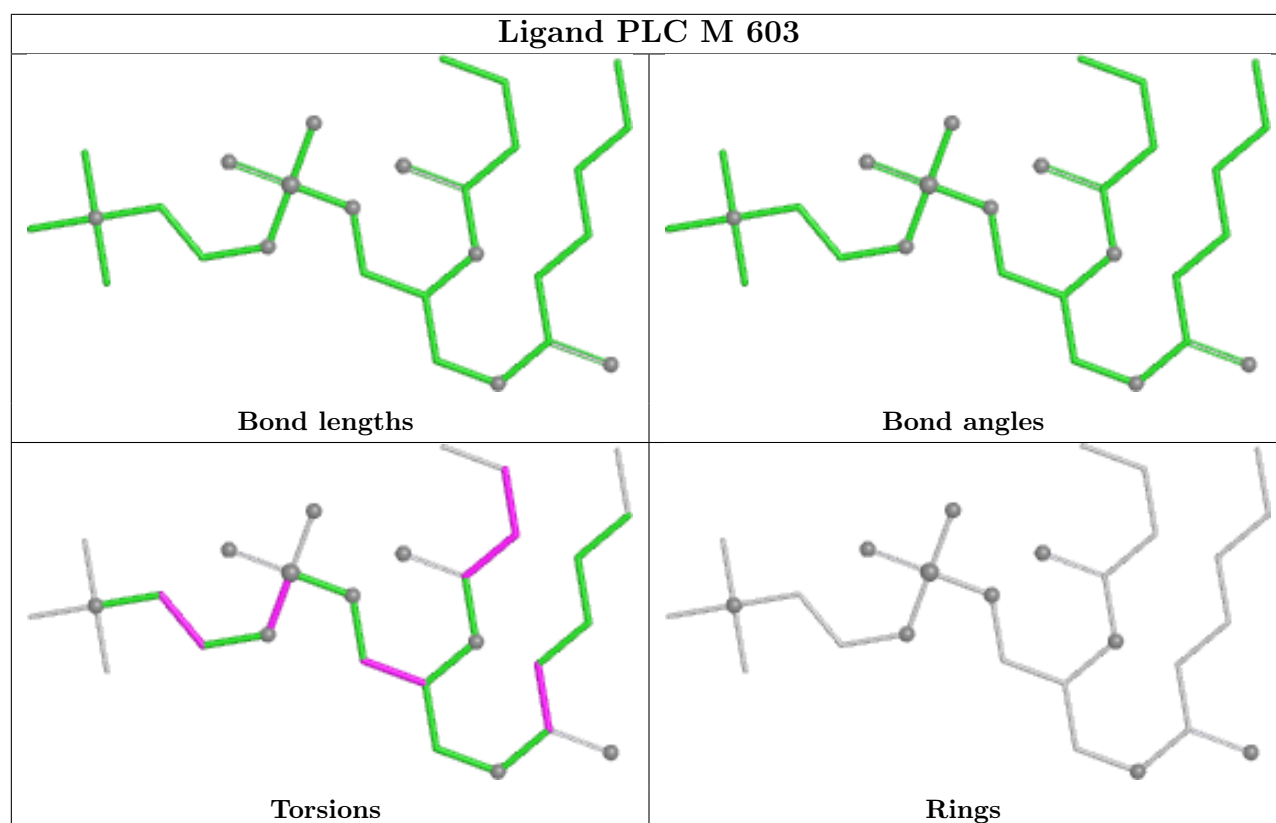


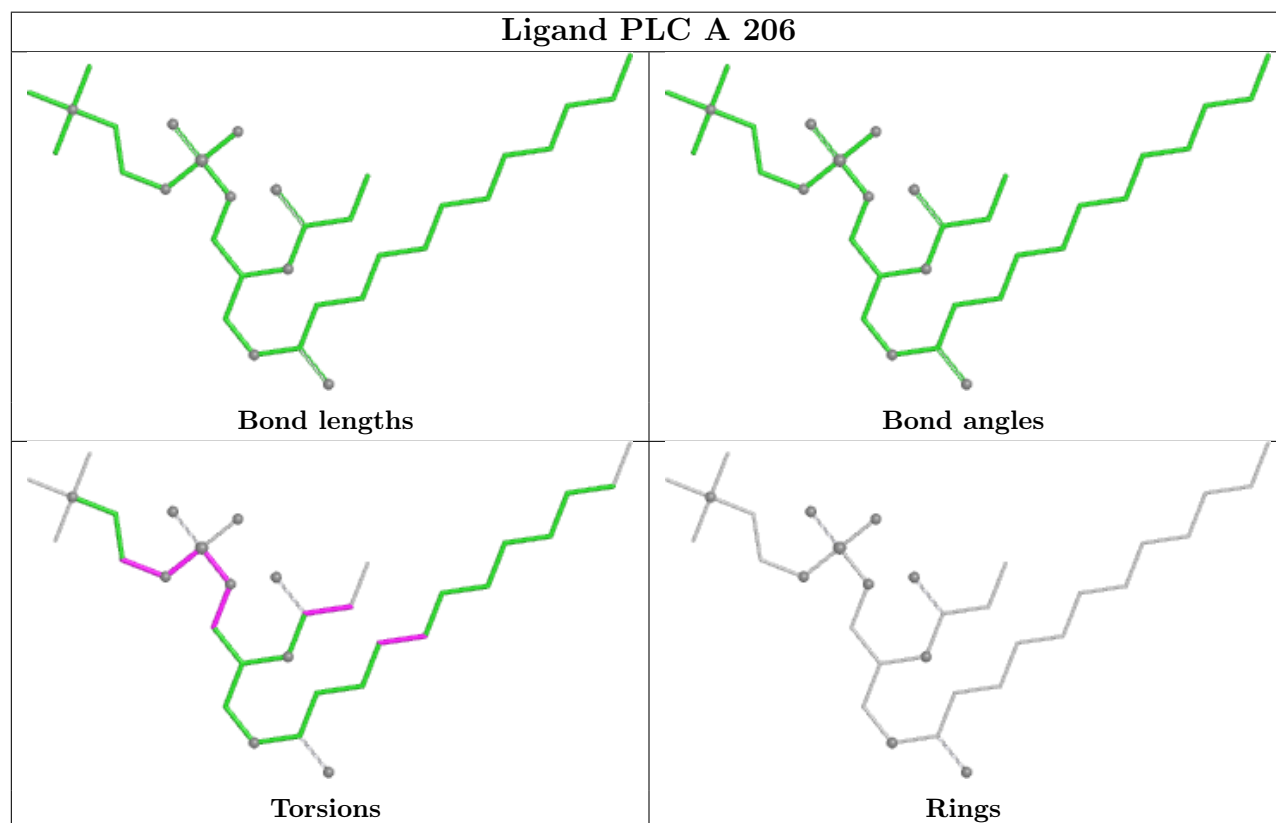
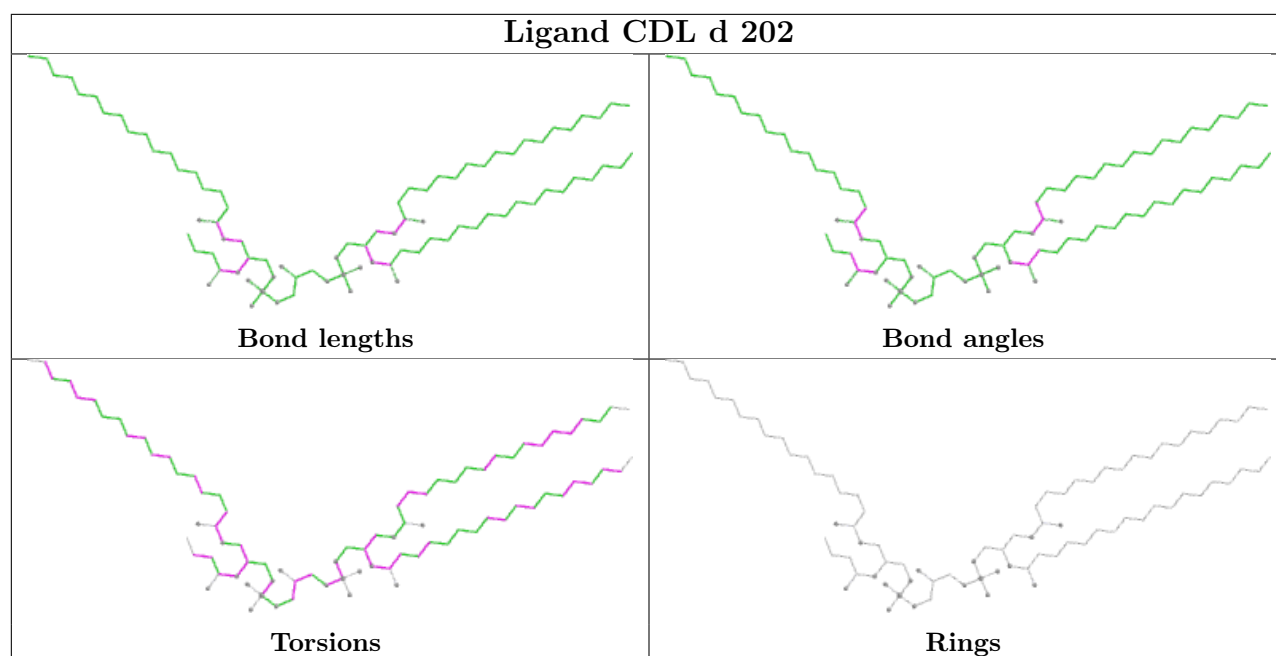


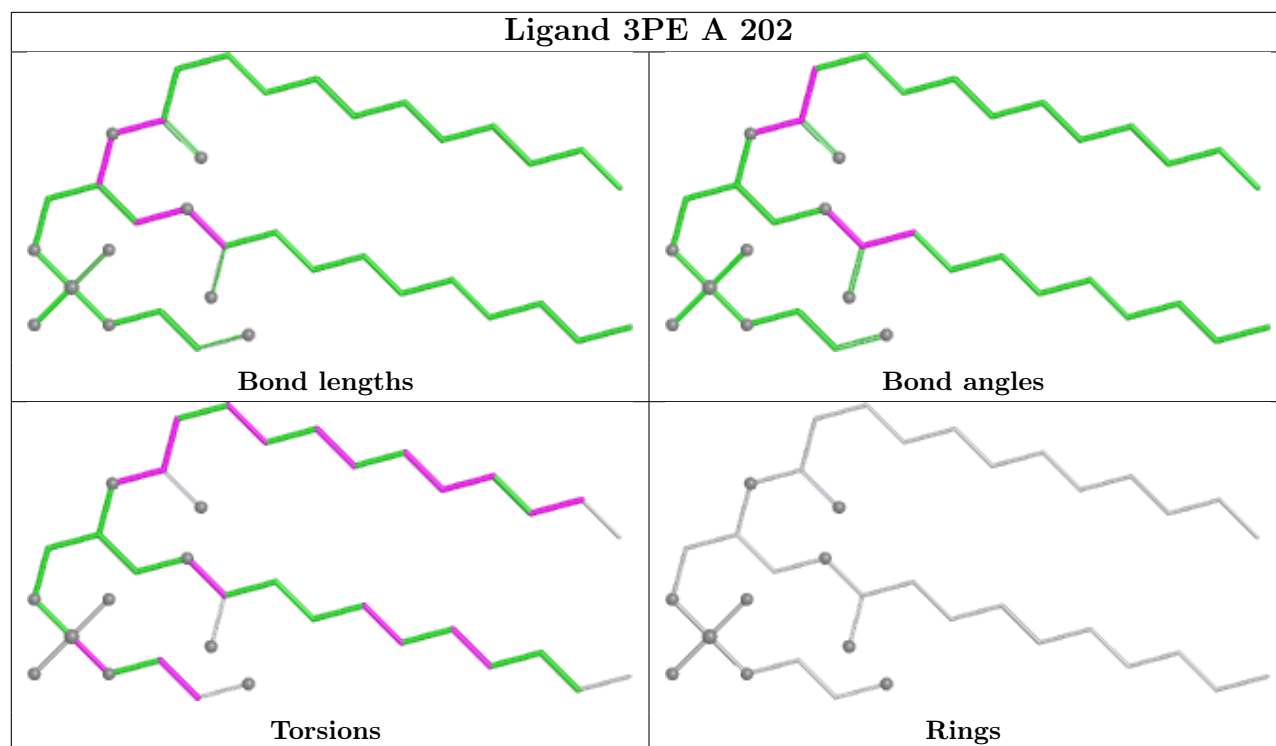
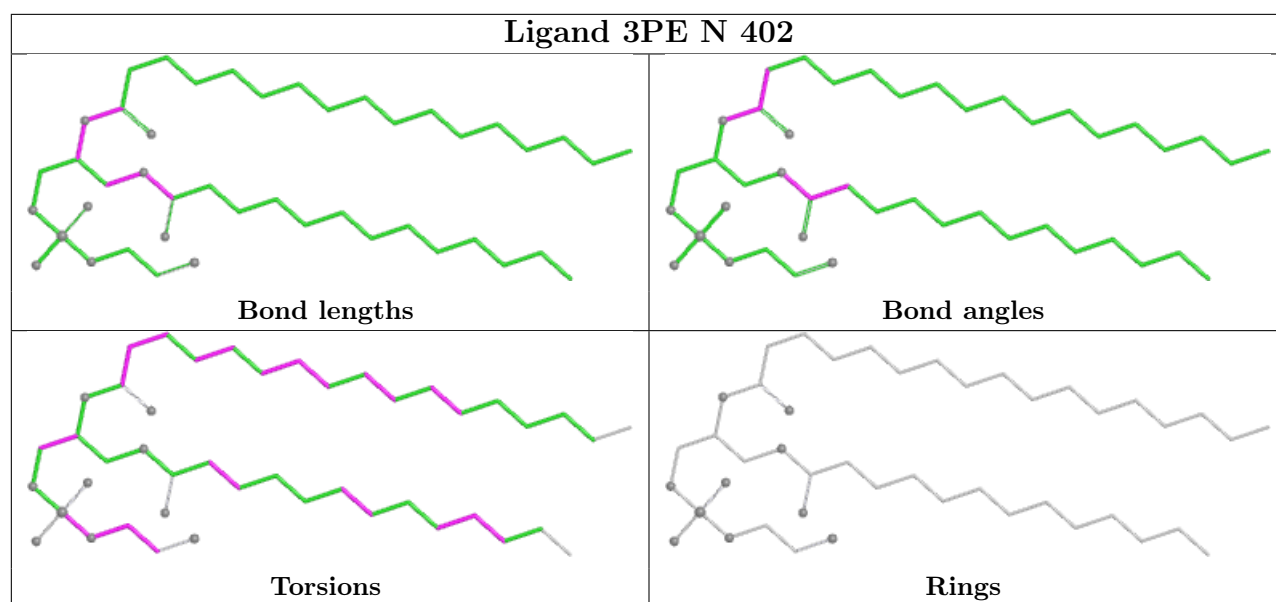


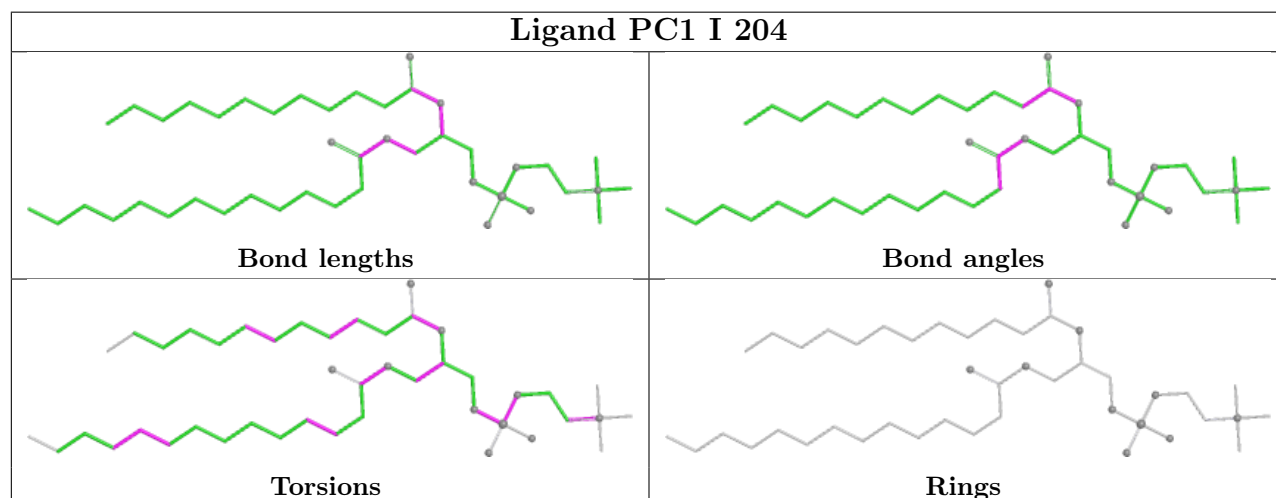
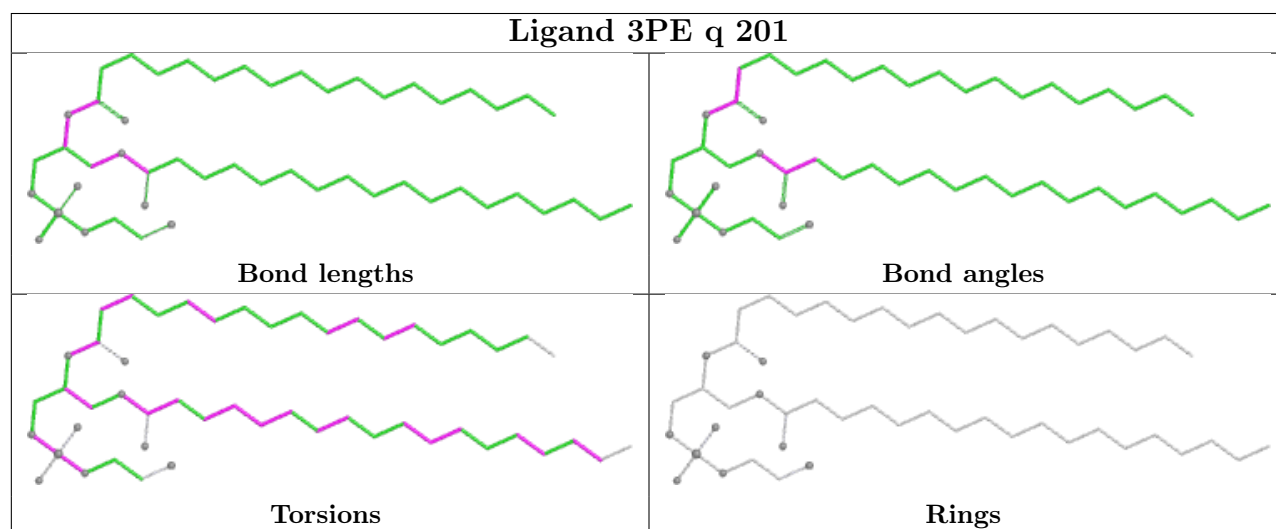
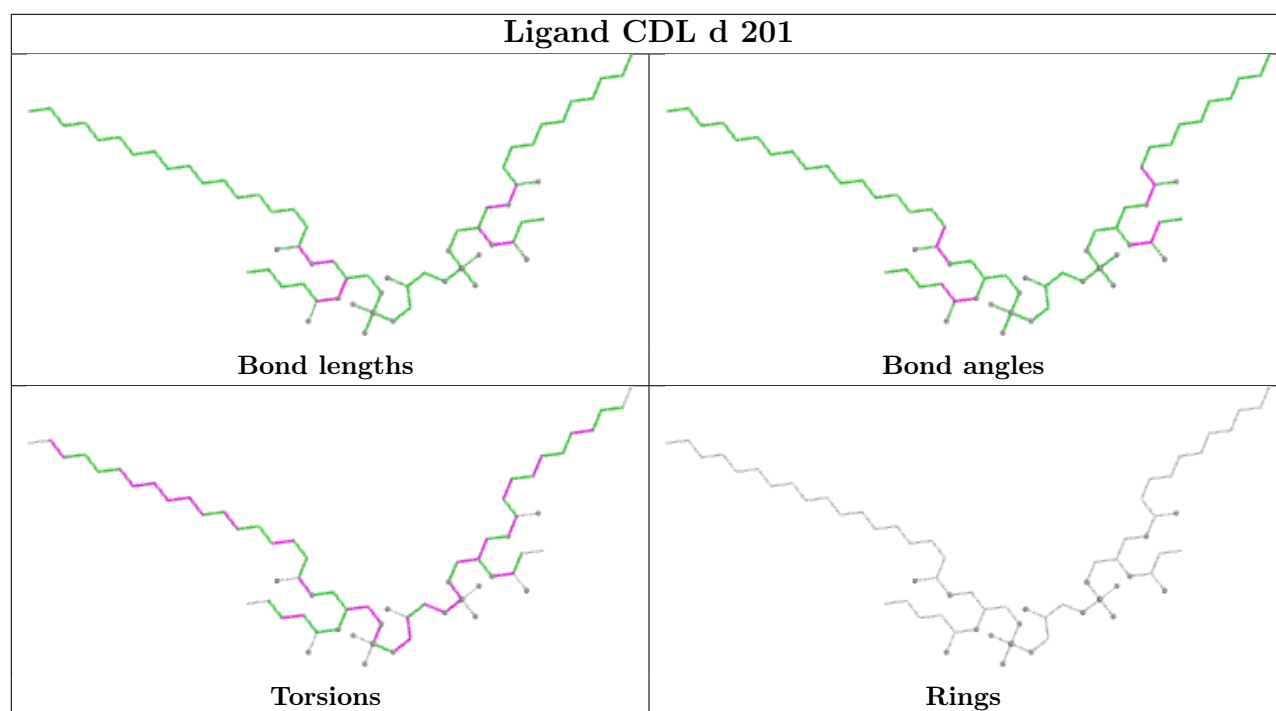


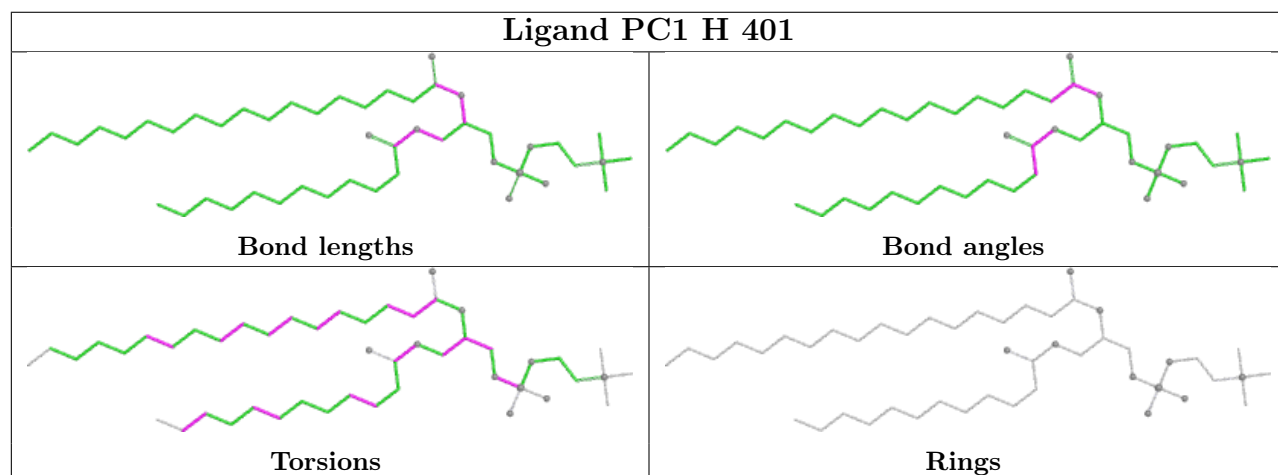
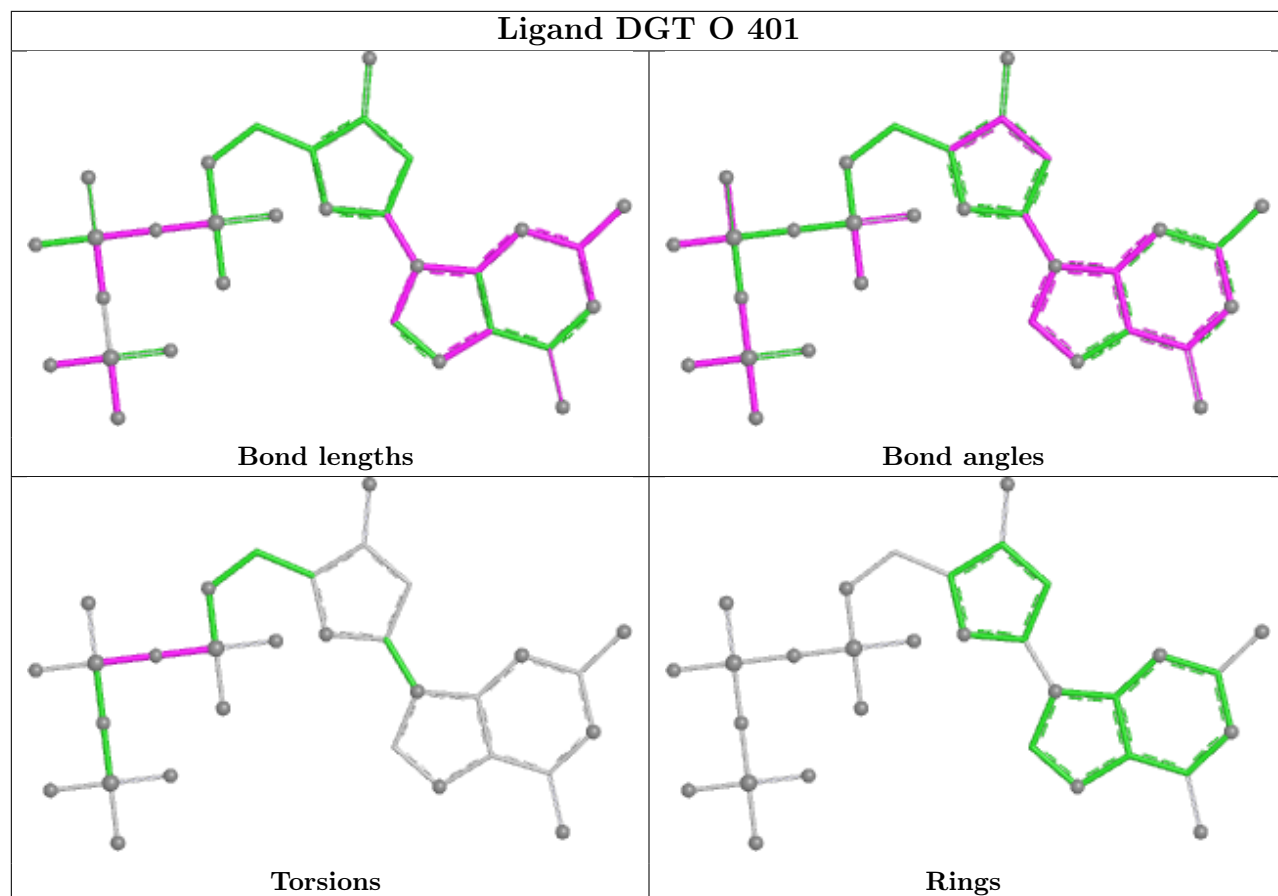


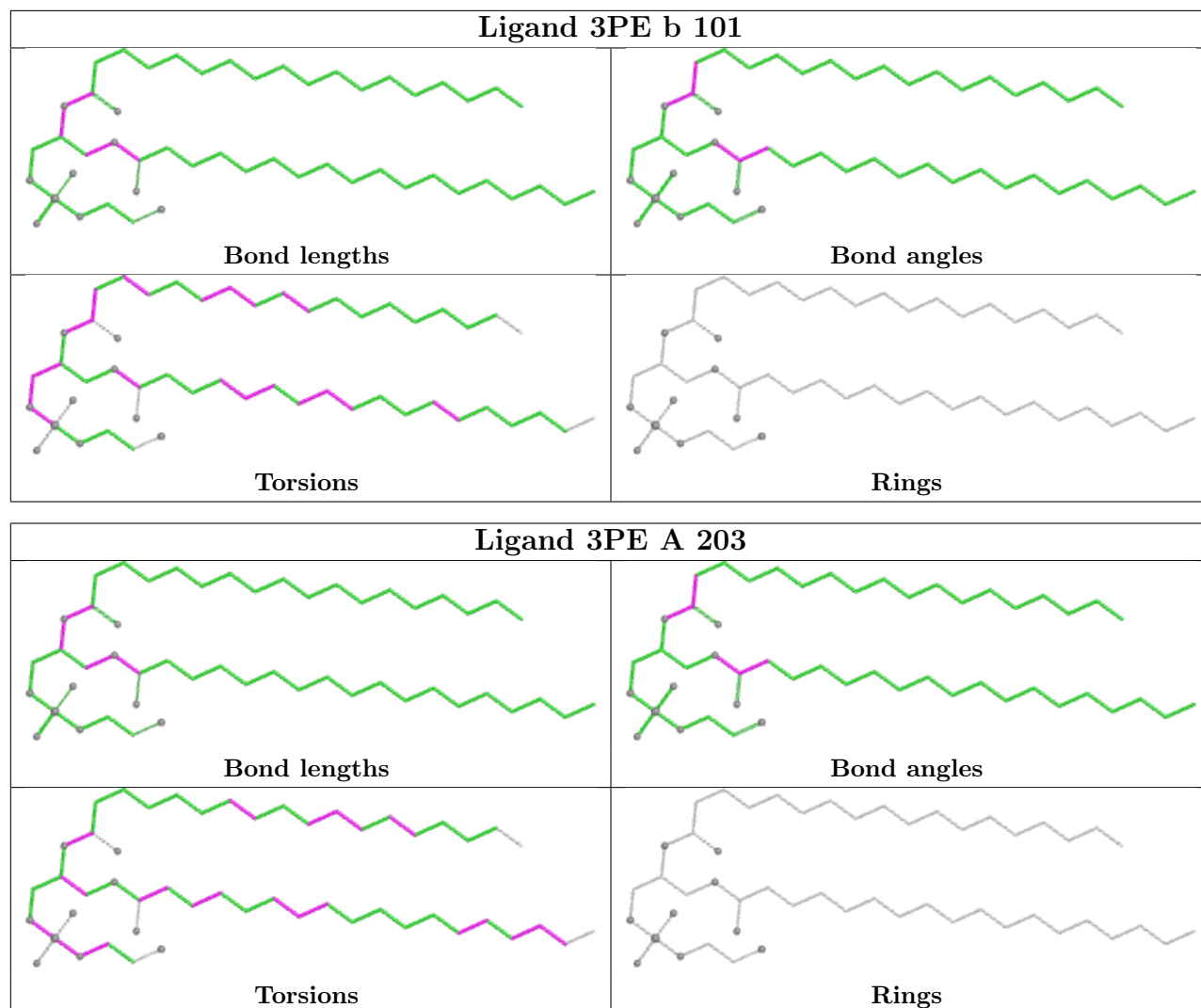


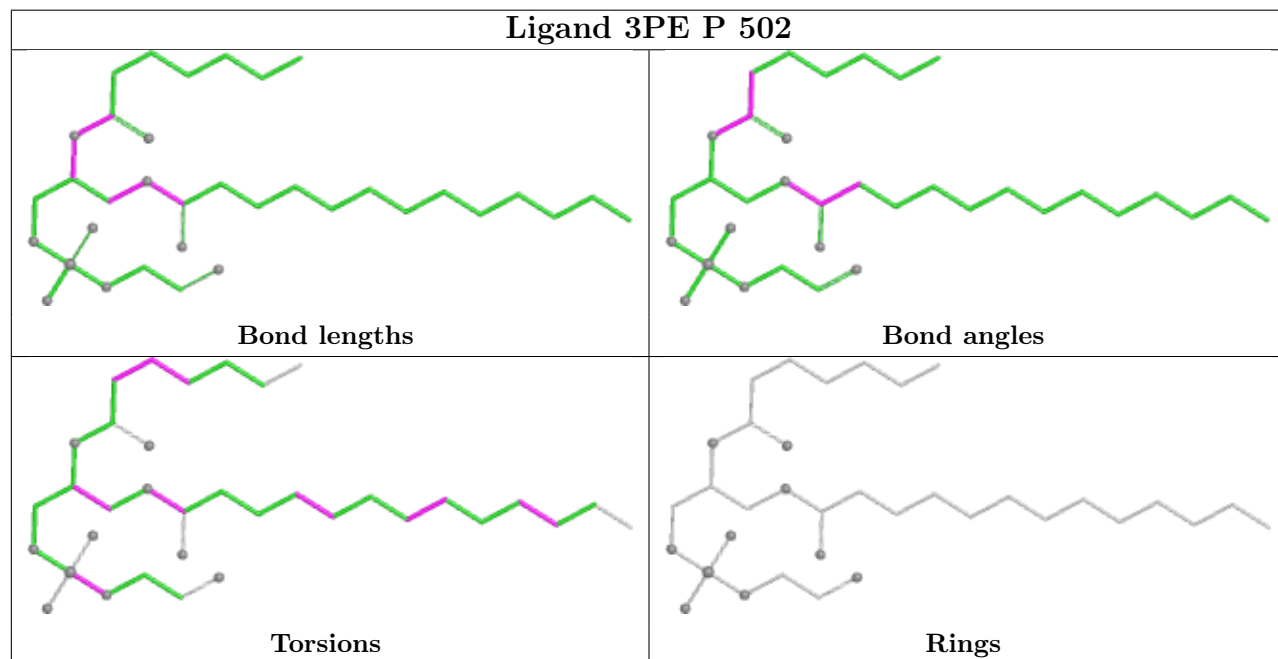
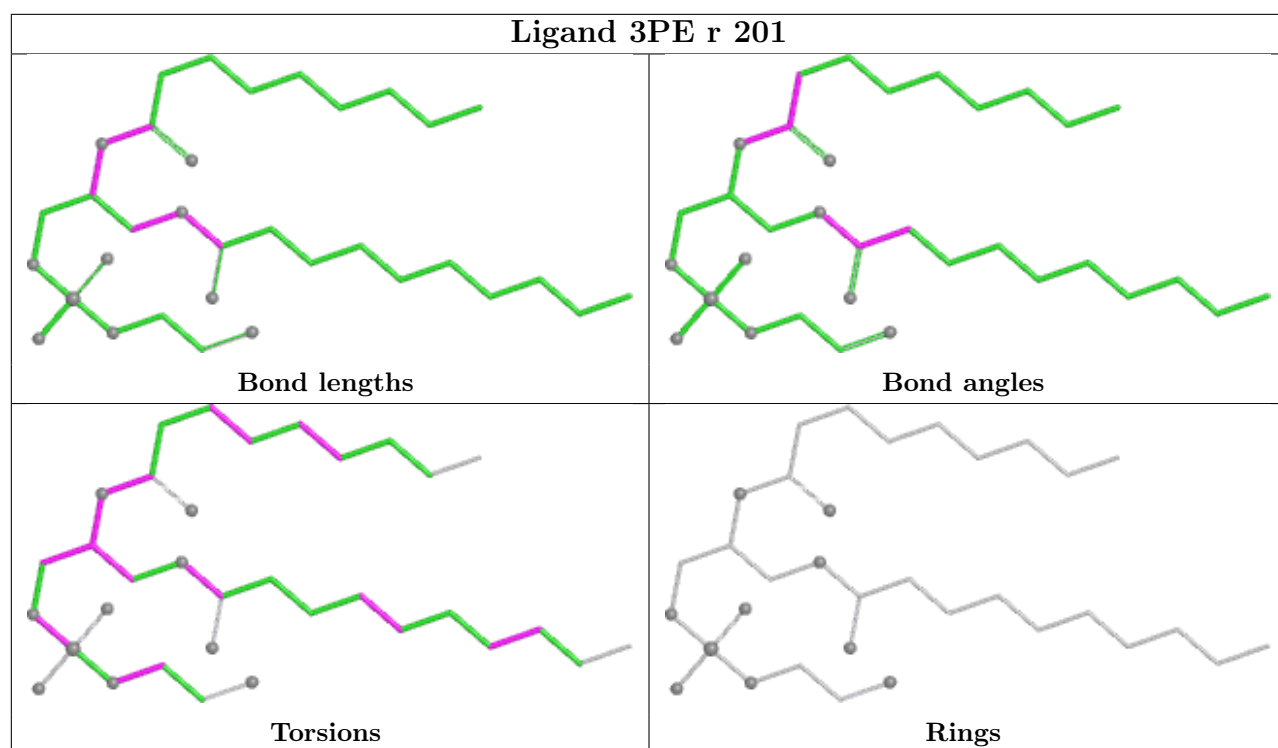


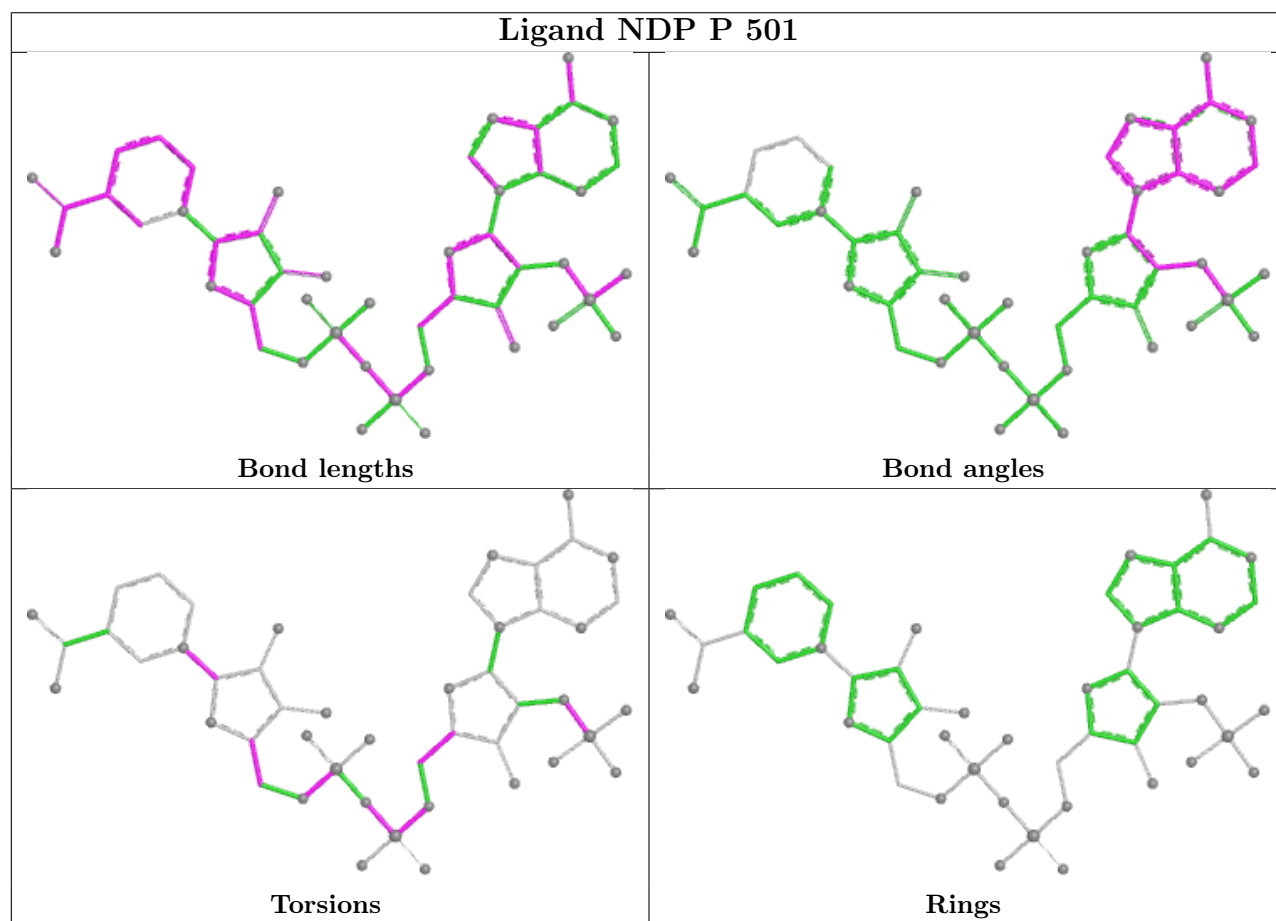
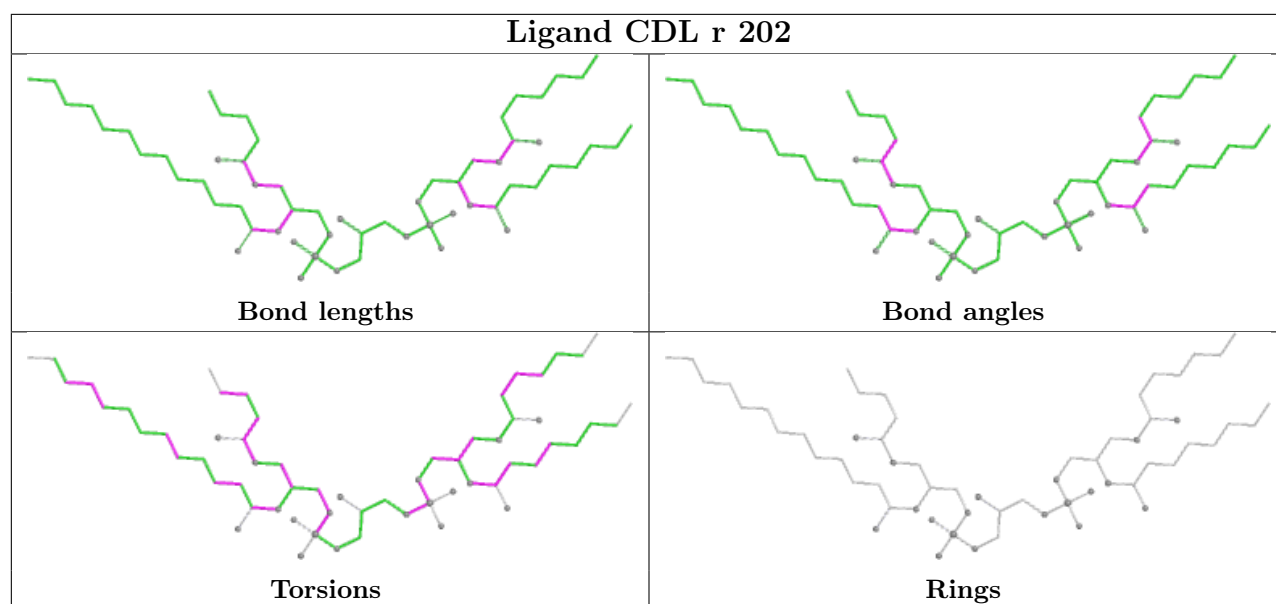


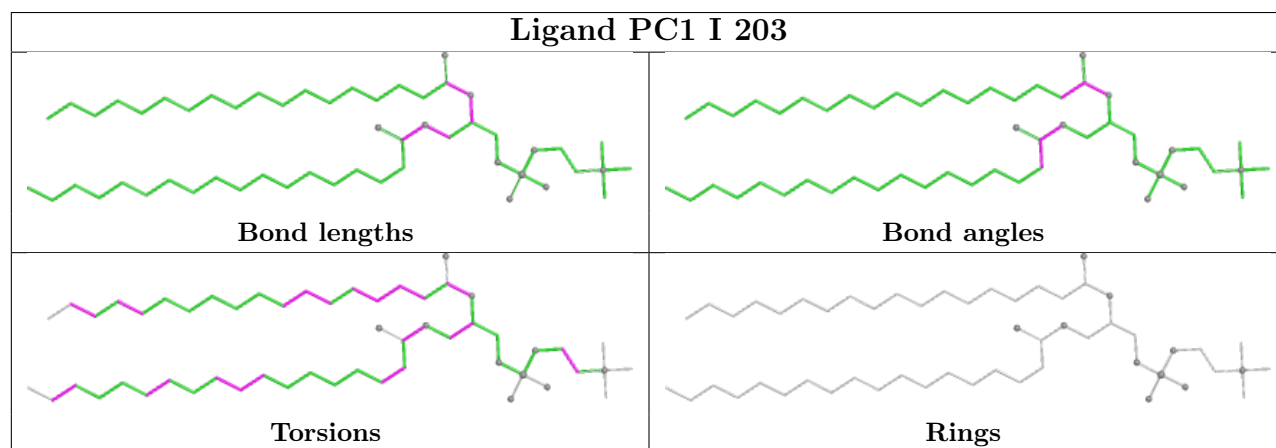
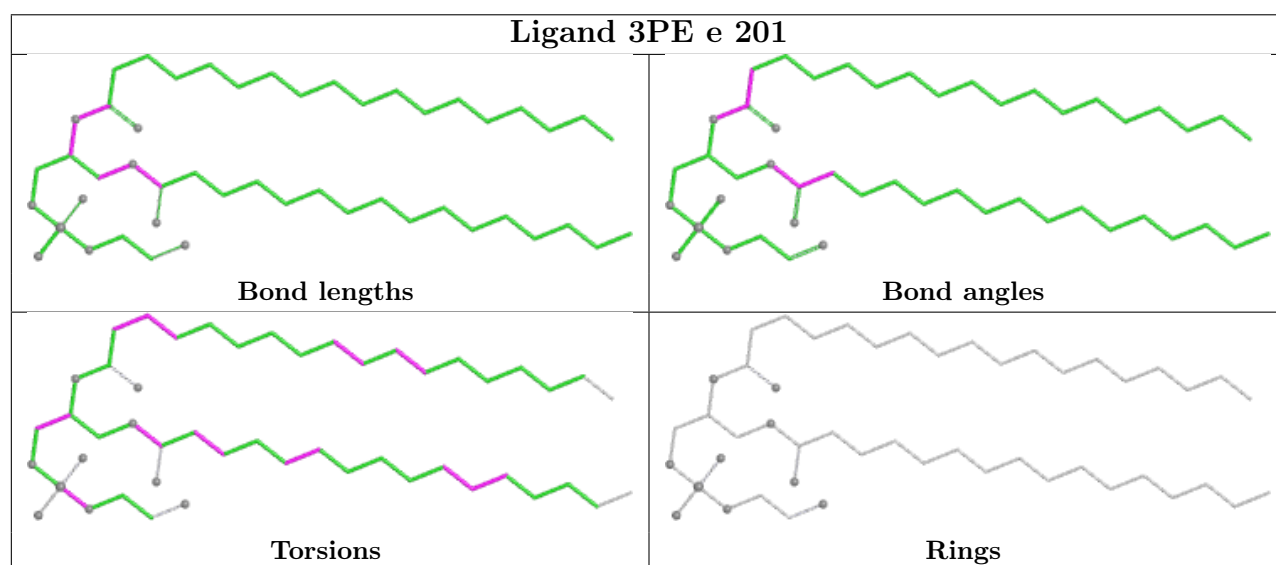
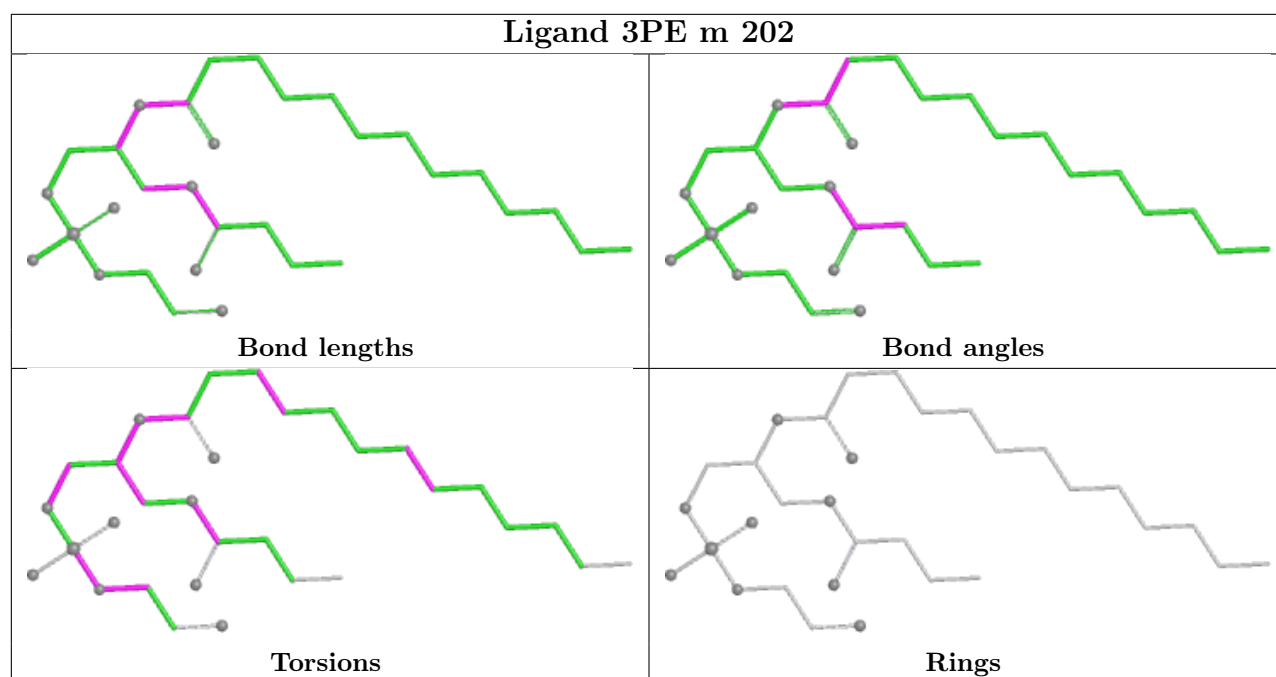


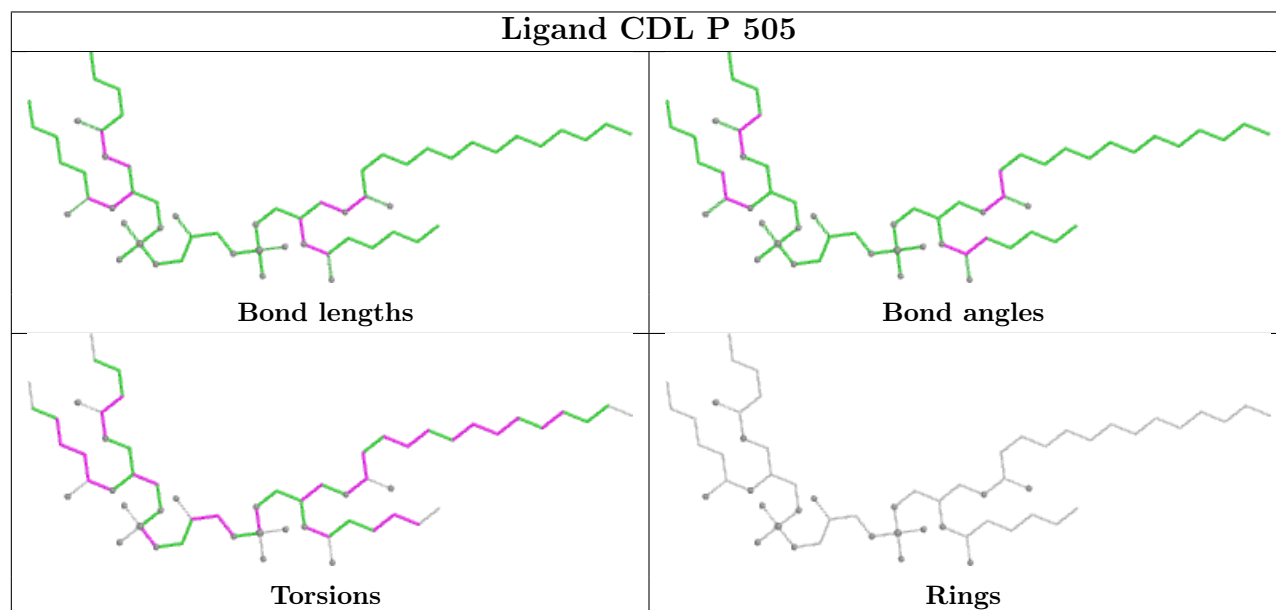
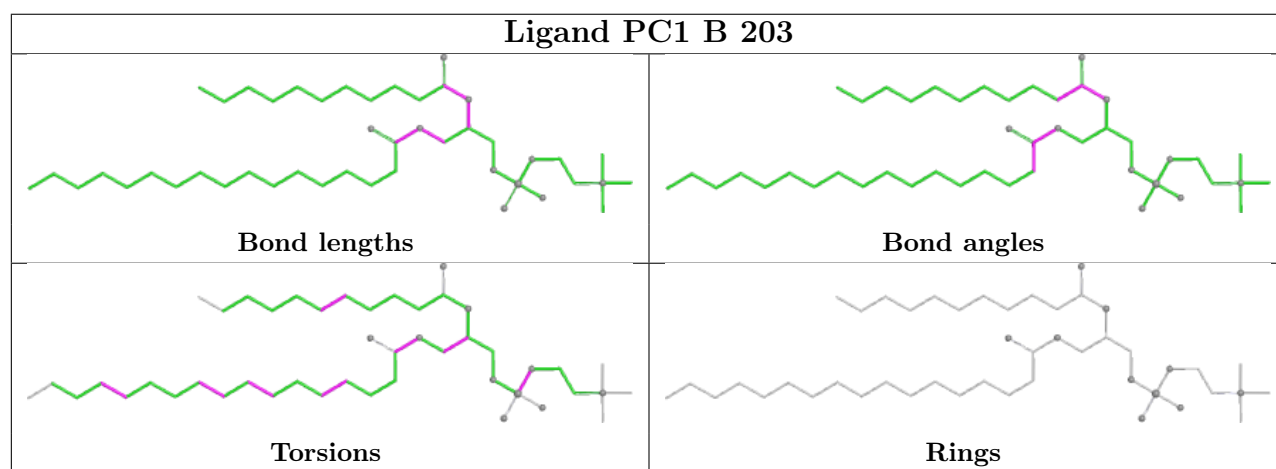
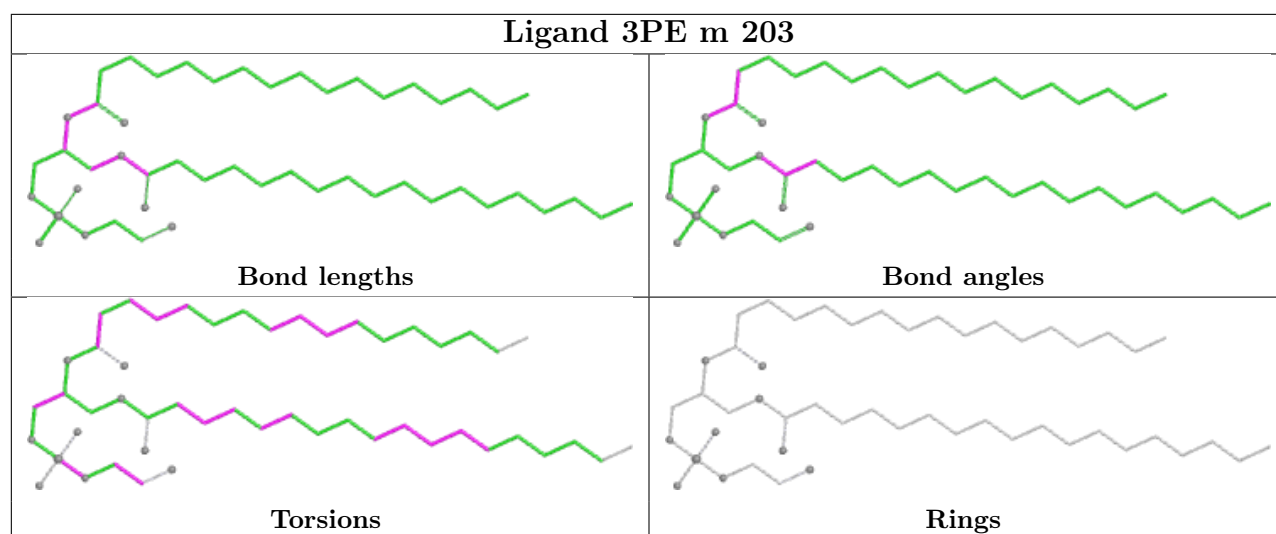


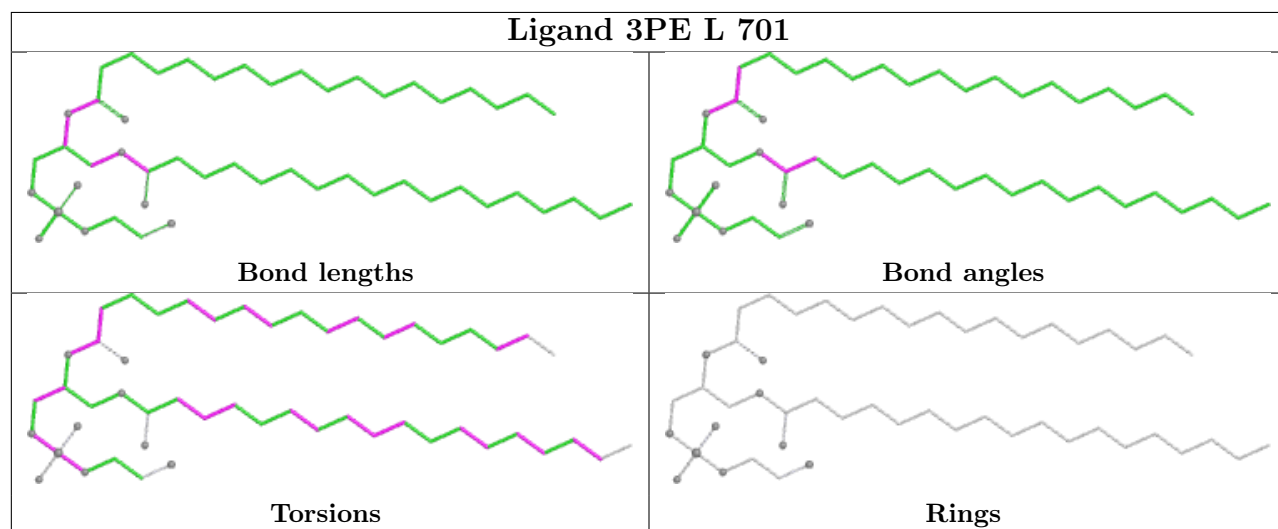
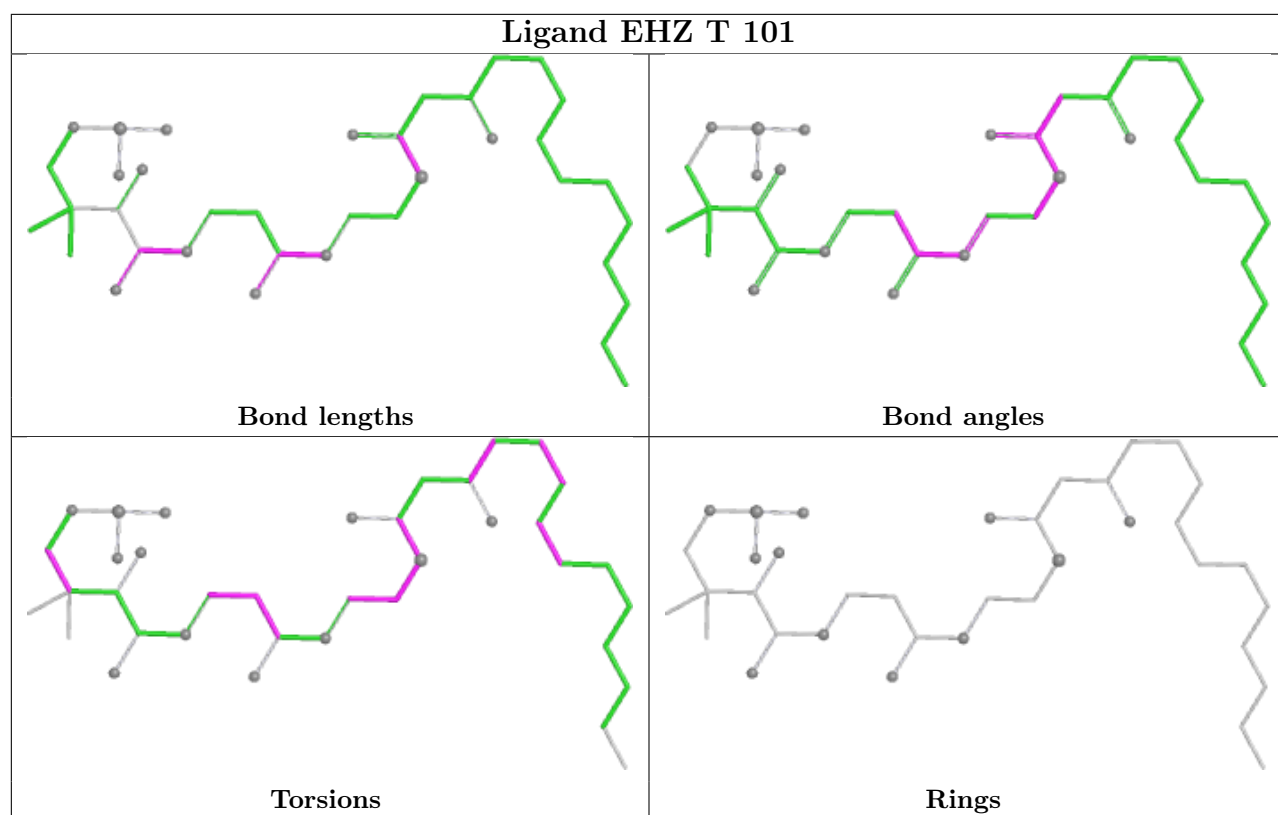


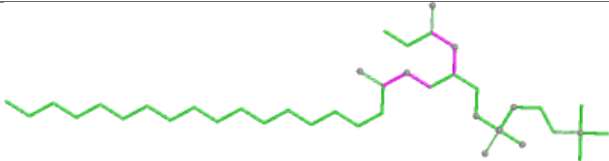
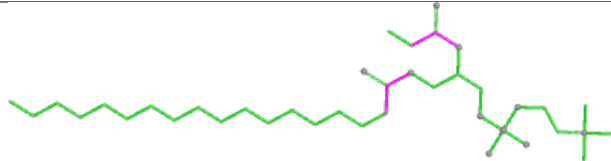
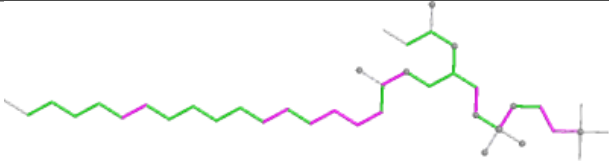
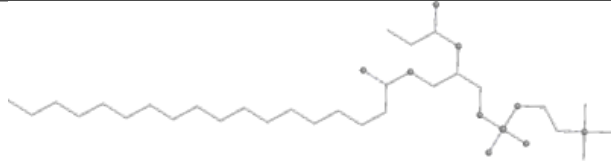


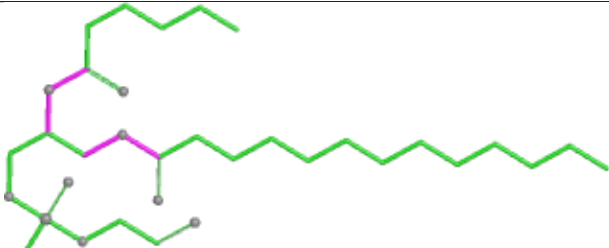
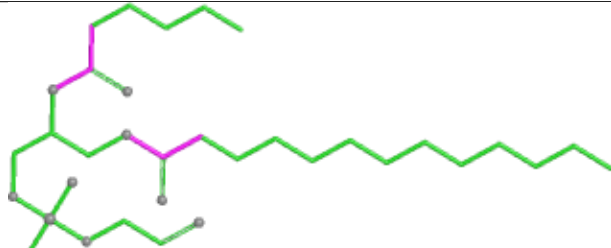
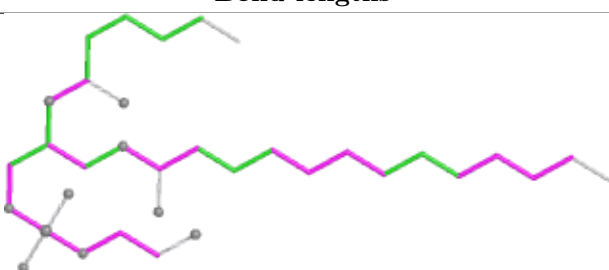
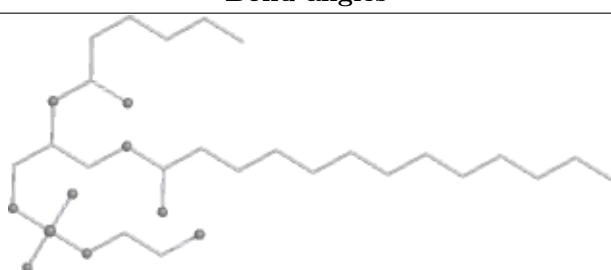


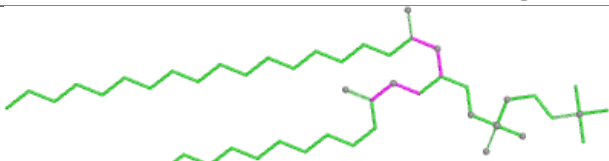
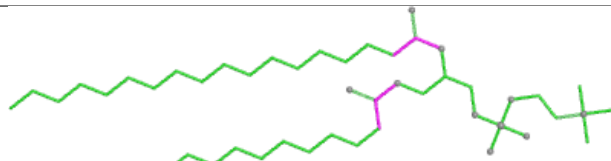
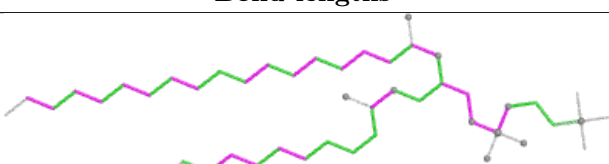
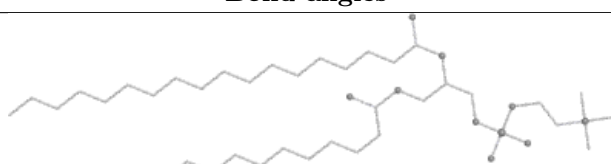




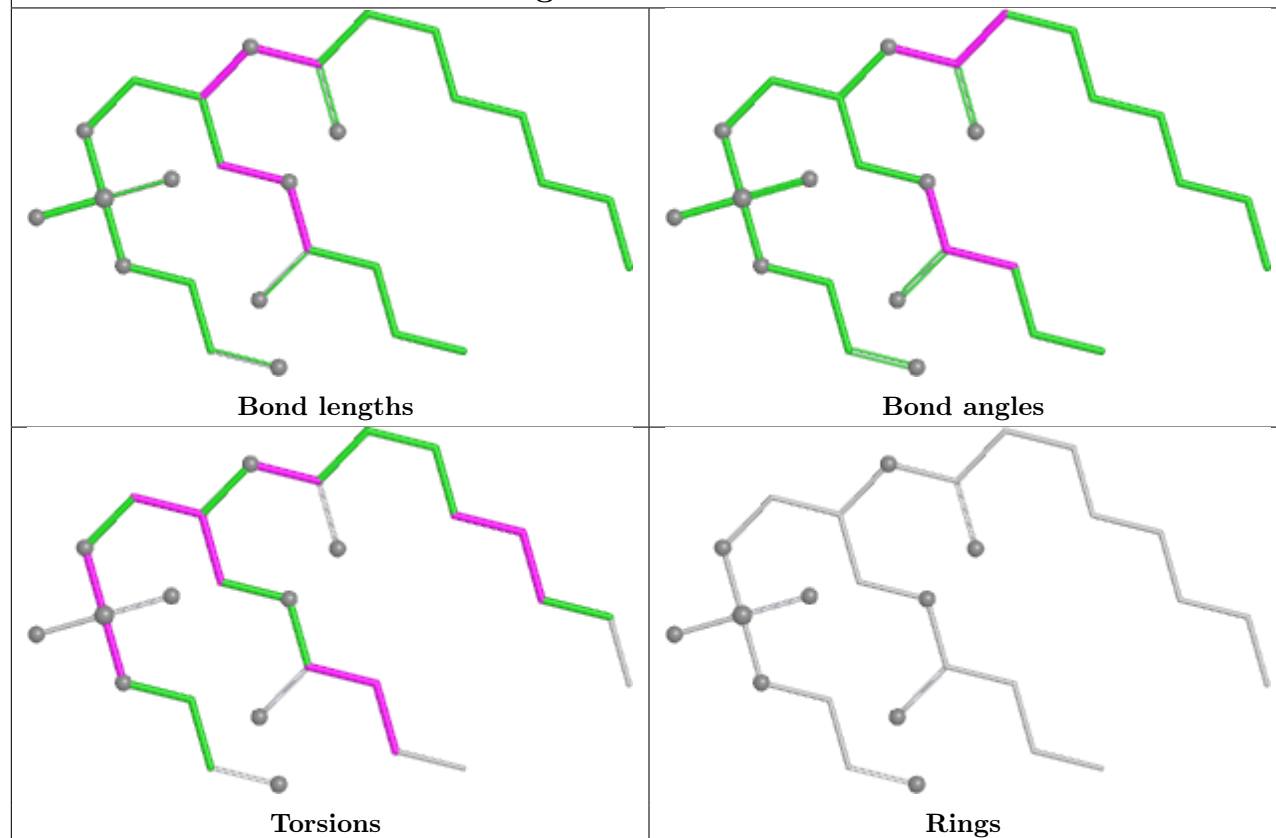


Ligand PC1 H 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

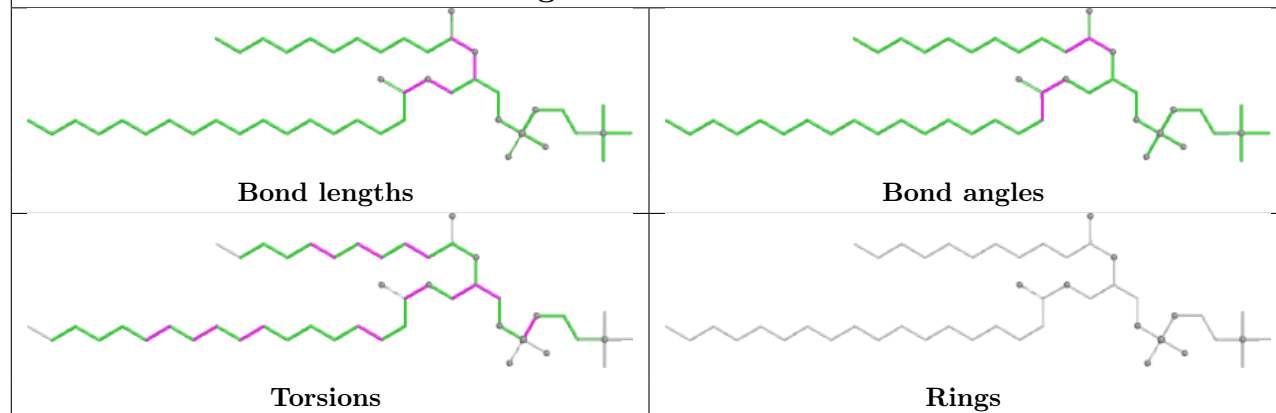
Ligand 3PE f 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

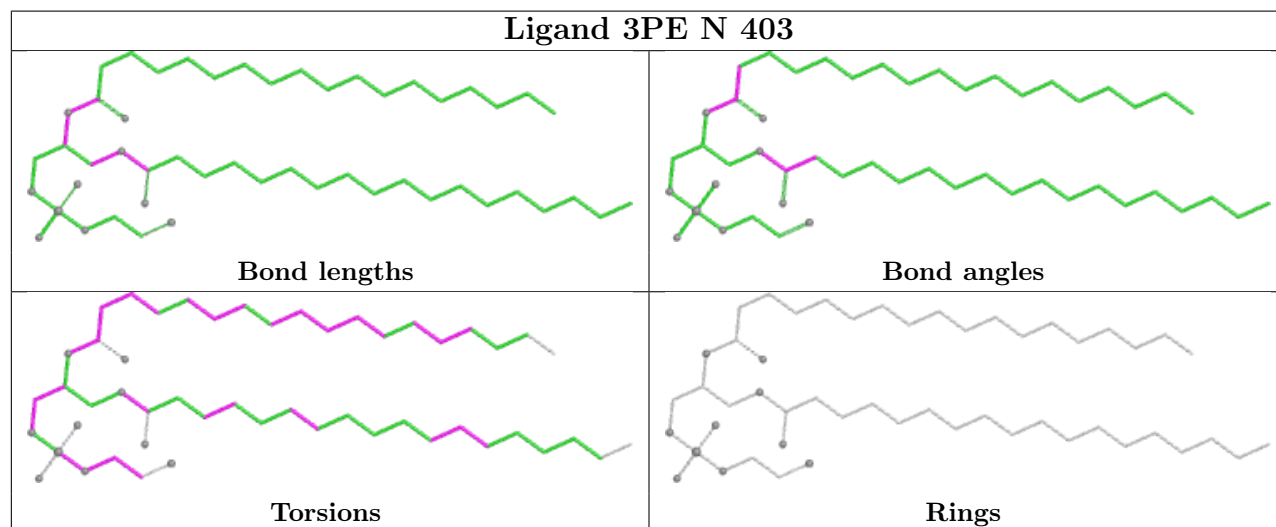
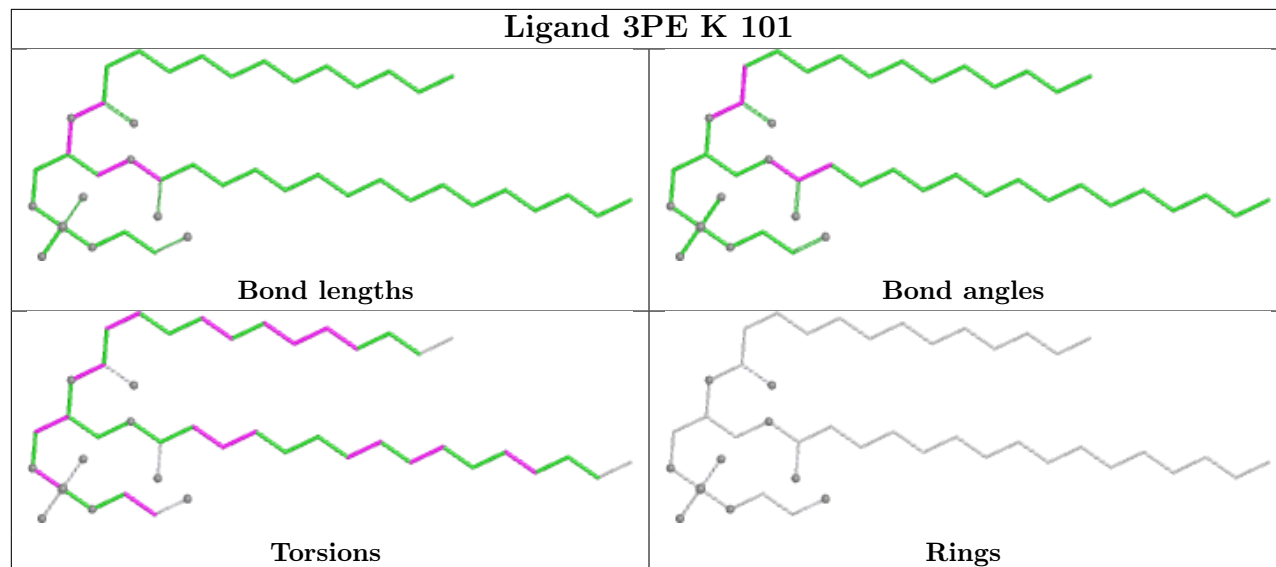
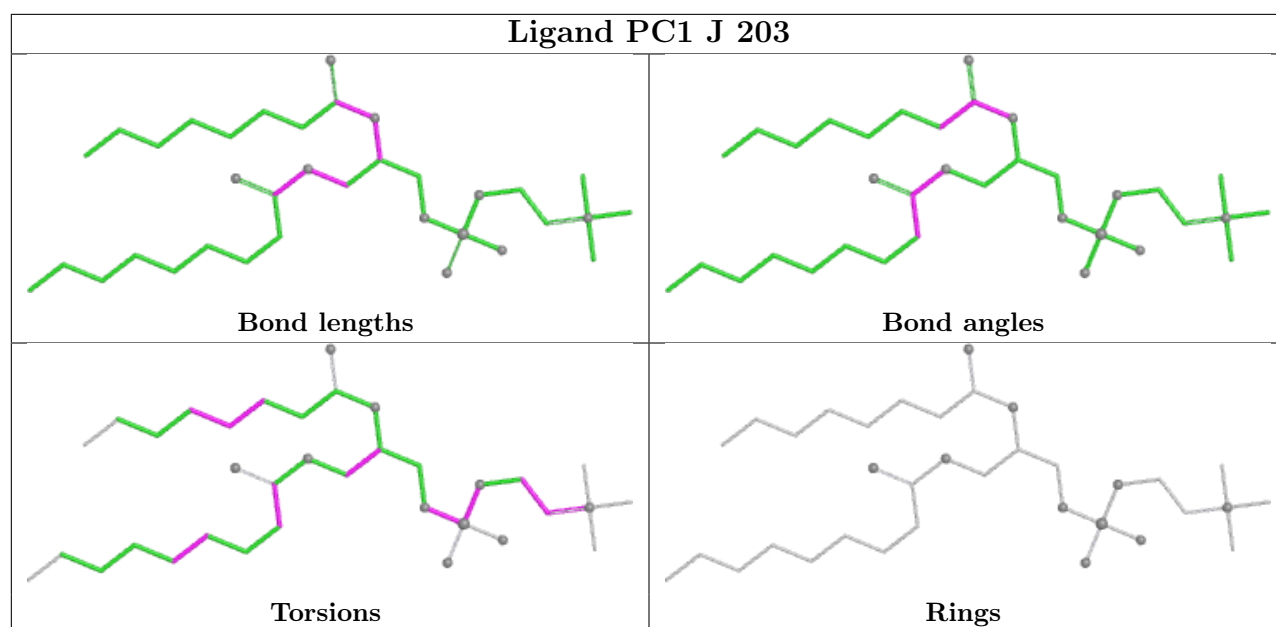
Ligand PC1 h 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

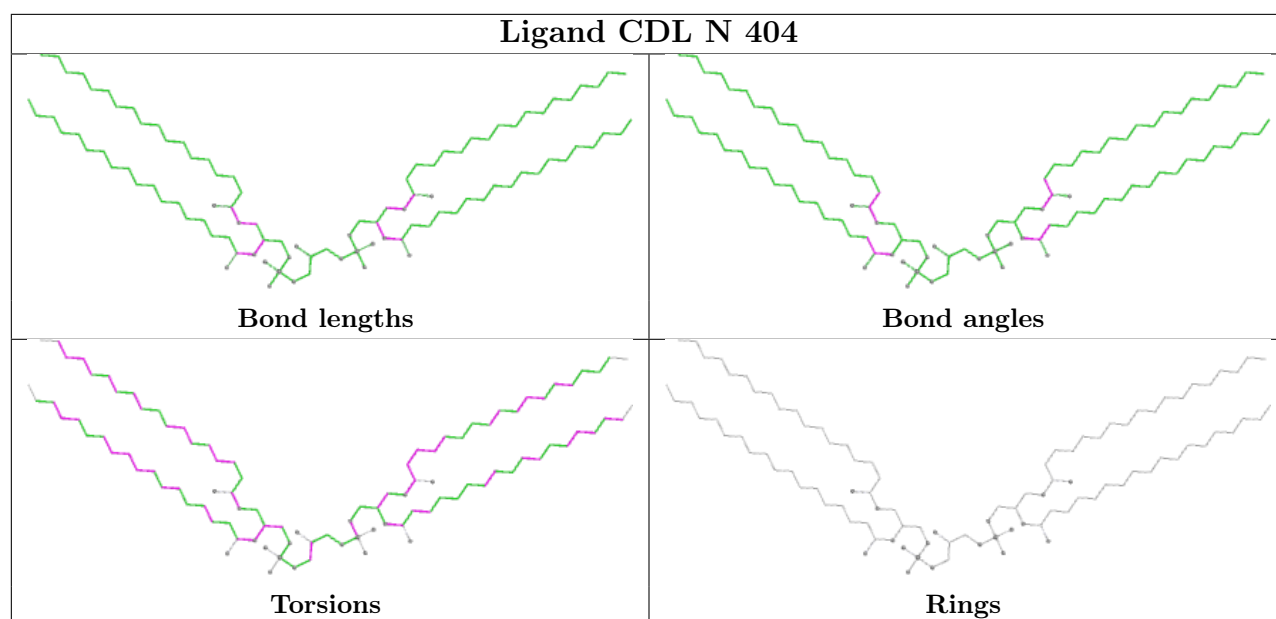
Ligand 3PE Y 201



Ligand PC1 L 703







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.

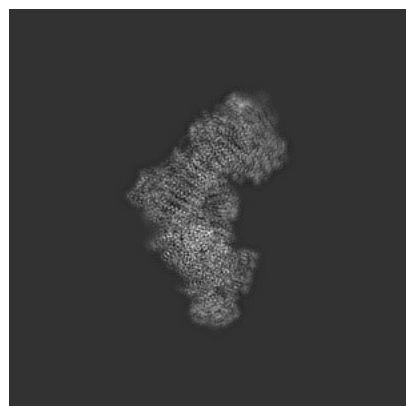
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18055. These allow visual inspection of the internal detail of the map and identification of artifacts.

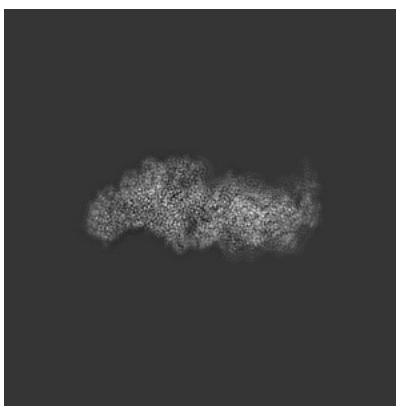
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

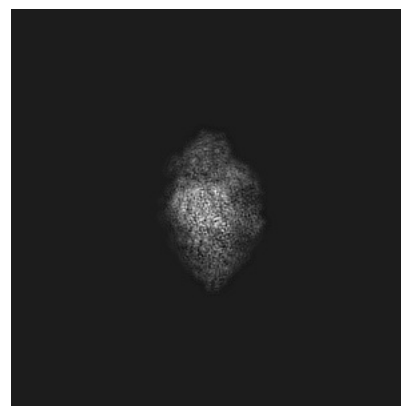
6.1.1 Primary map



X

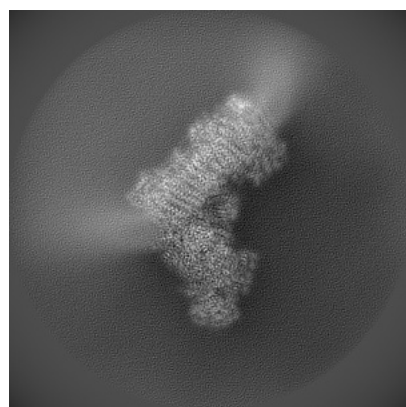


Y

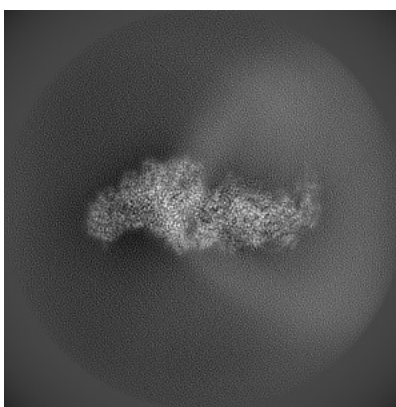


Z

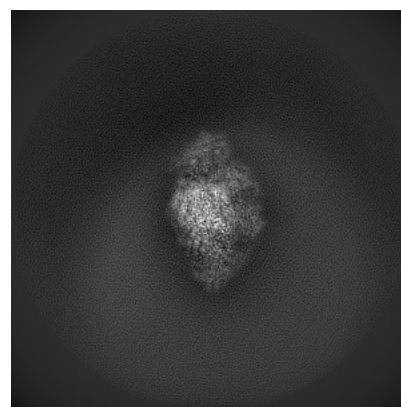
6.1.2 Raw map



X



Y



Z

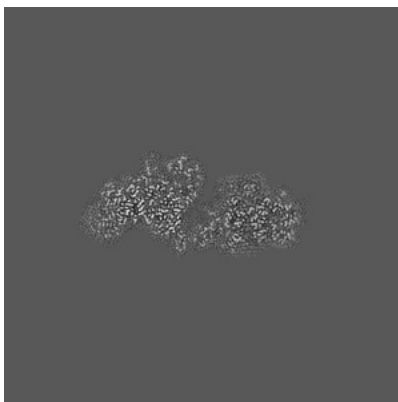
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

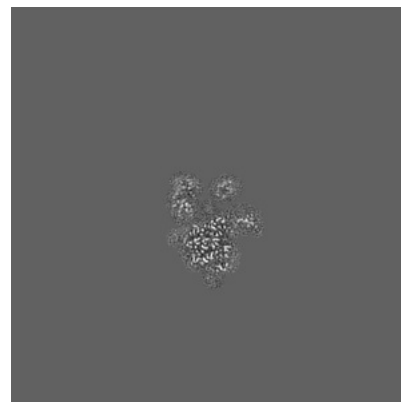
6.2.1 Primary map



X Index: 180

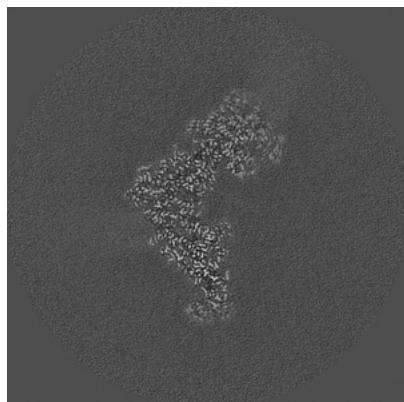


Y Index: 180

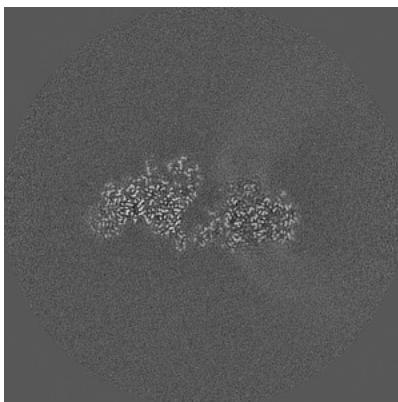


Z Index: 180

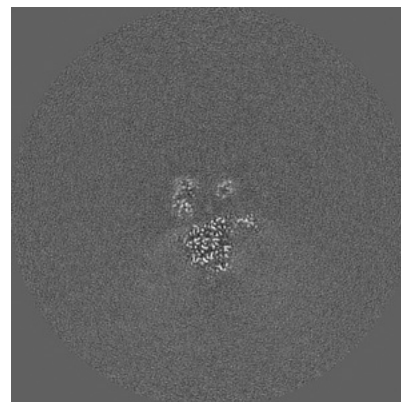
6.2.2 Raw map



X Index: 180



Y Index: 180

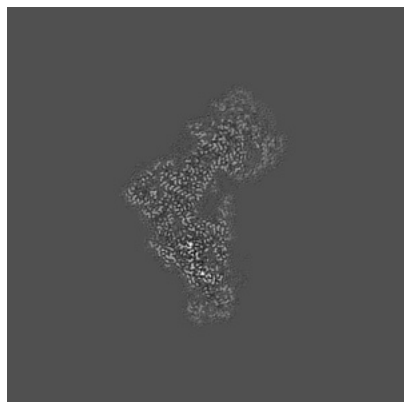


Z Index: 180

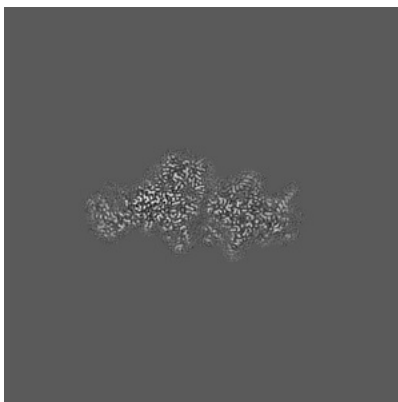
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

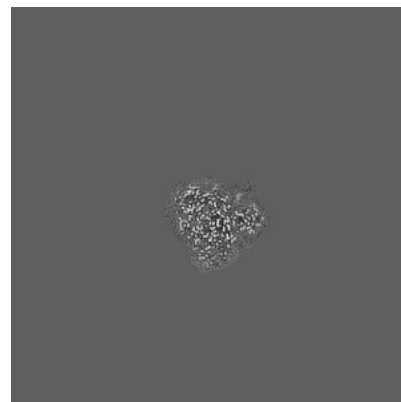
6.3.1 Primary map



X Index: 184

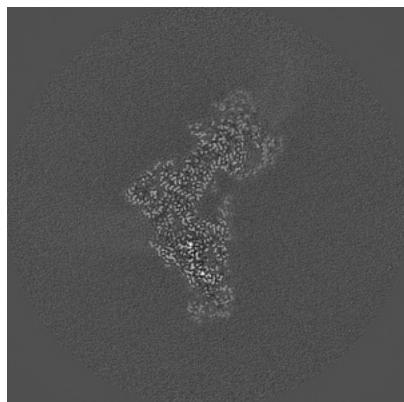


Y Index: 171

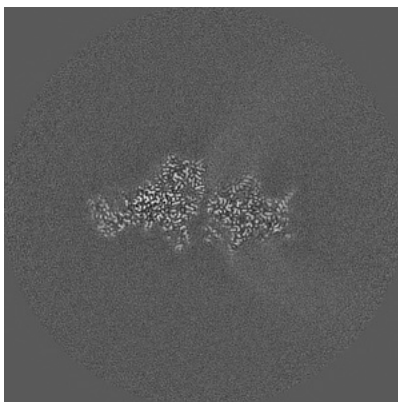


Z Index: 150

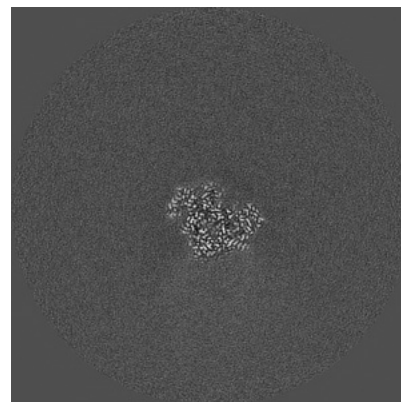
6.3.2 Raw map



X Index: 184



Y Index: 171

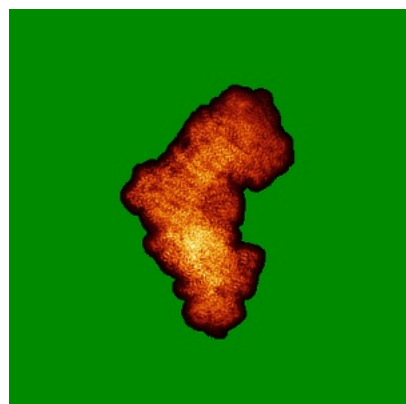


Z Index: 155

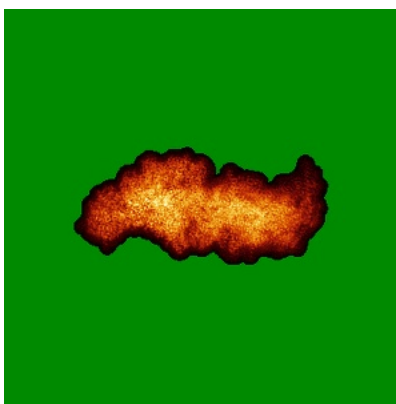
The images above show the largest variance slices of the map in three orthogonal directions.

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

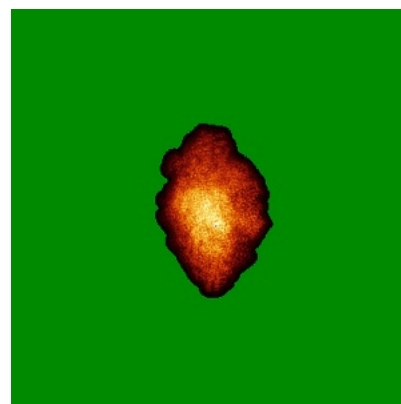
6.4.1 Primary map



X

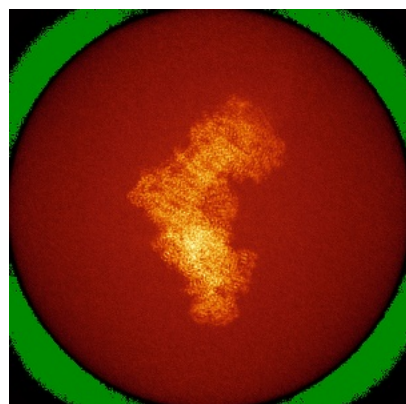


Y

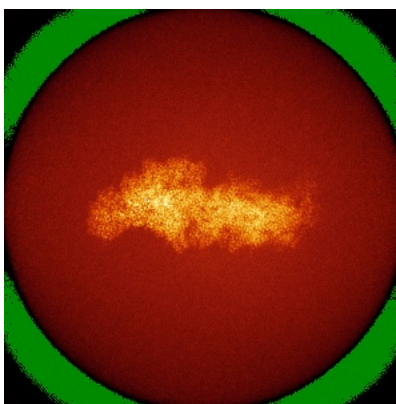


Z

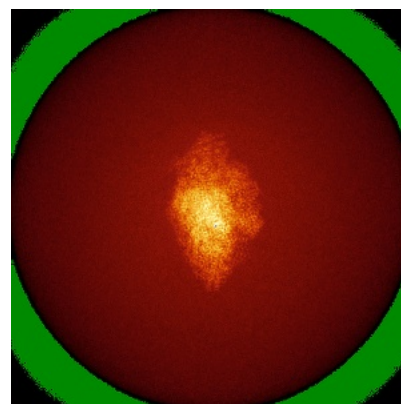
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

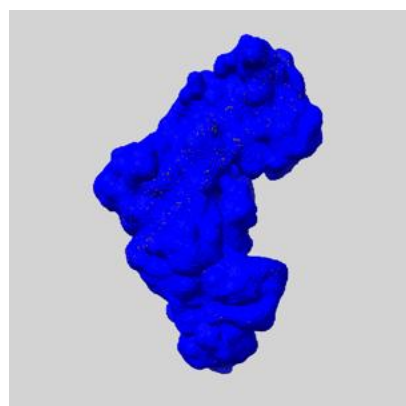
6.6 Mask visualisation [i](#)

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

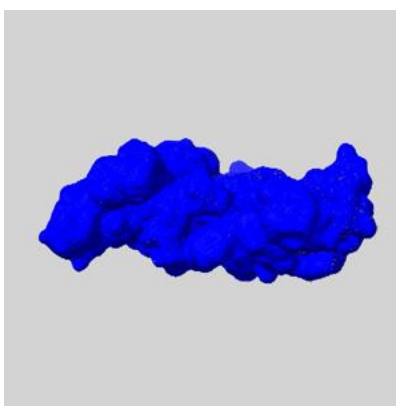
A mask typically either:

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

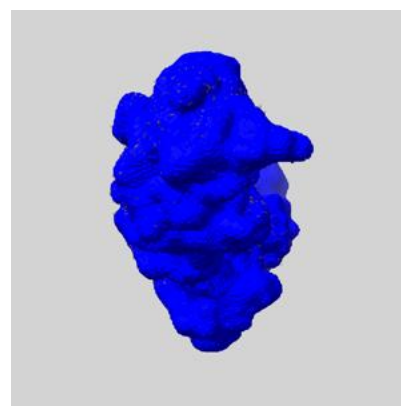
6.6.1 emd_18055_msk_1.map [i](#)



X



Y

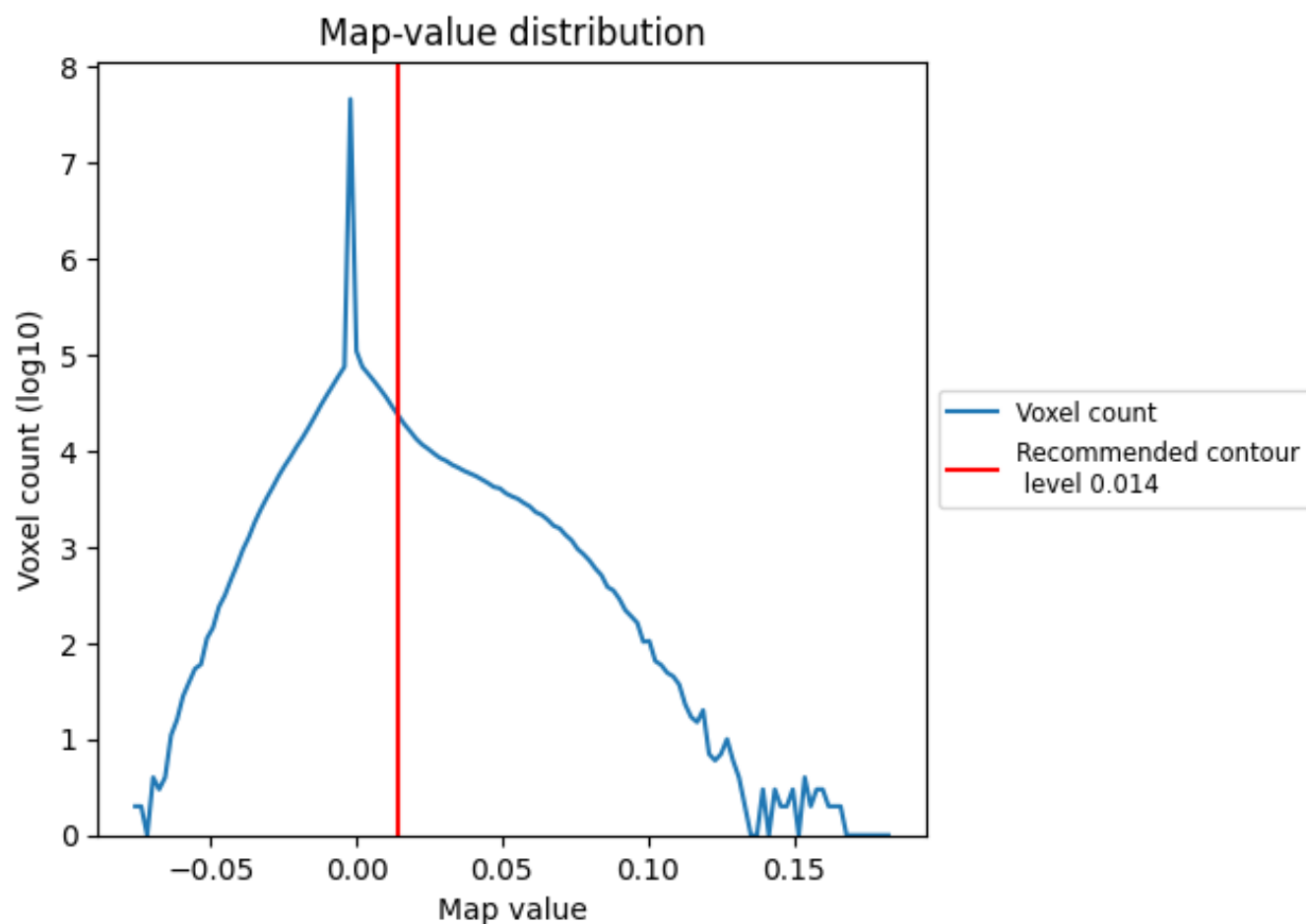


Z

7 Map analysis [i](#)

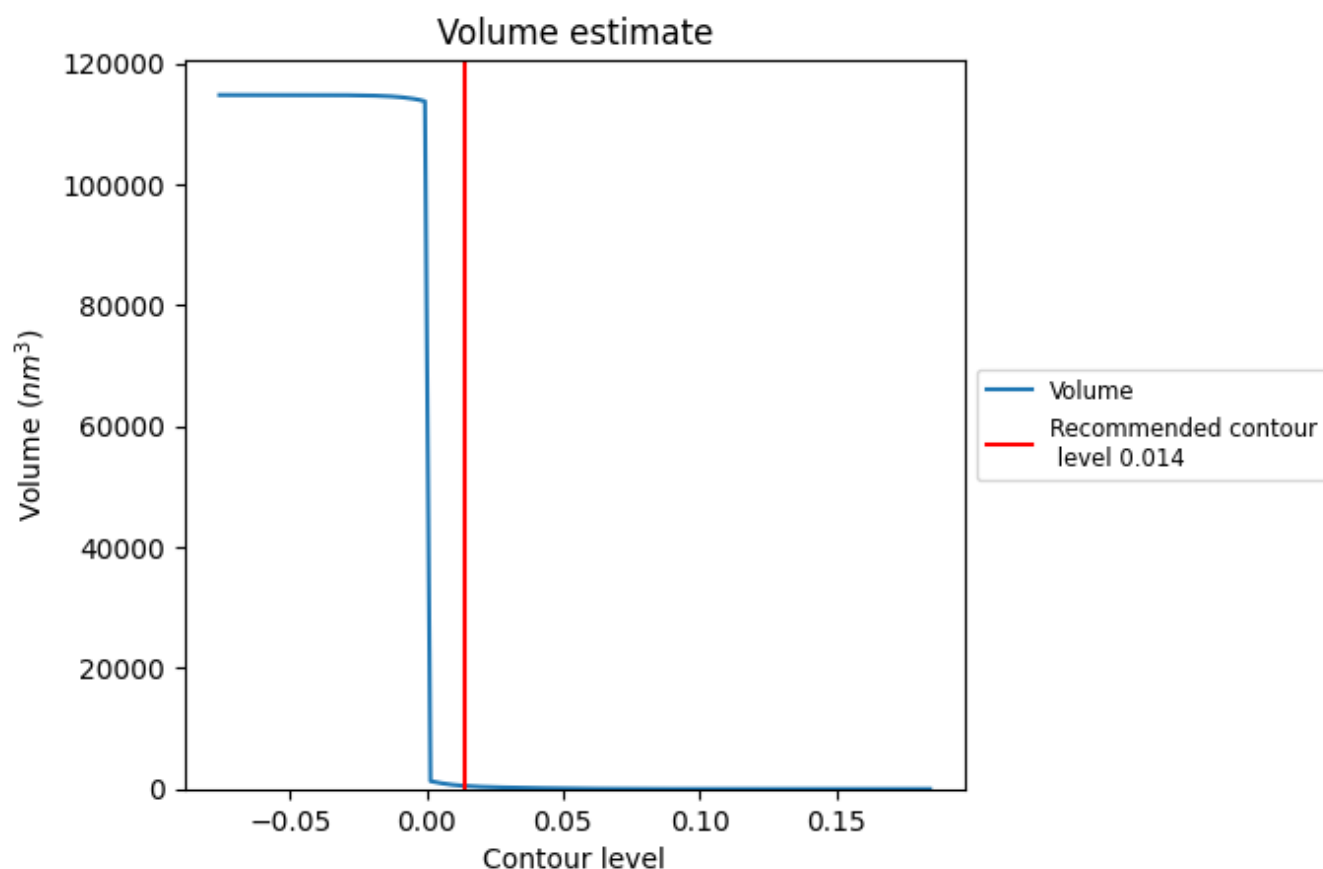
This section contains the results of statistical analysis of the map.

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.

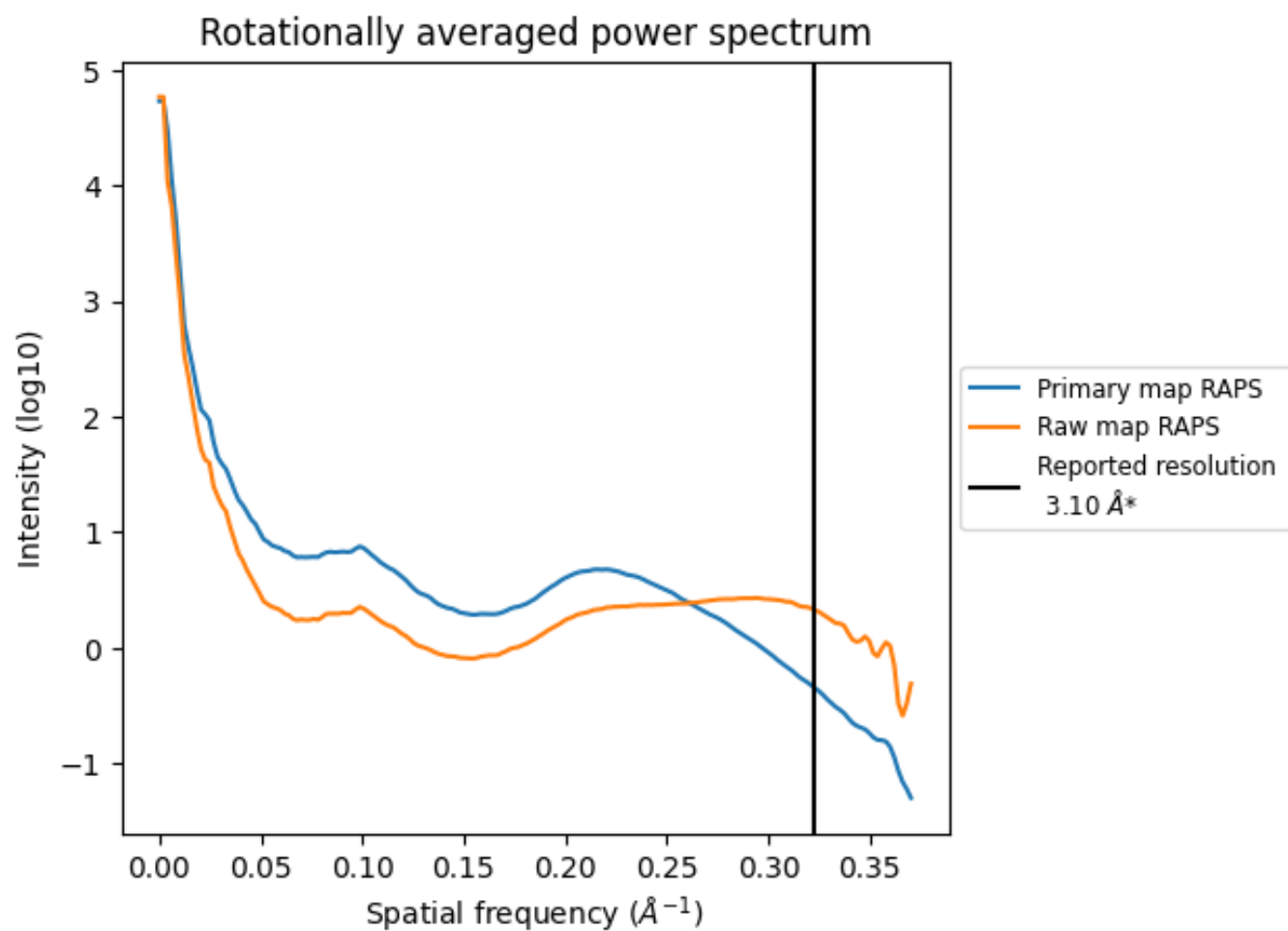
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm³; this corresponds to an approximate mass of 461 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 ⓘ

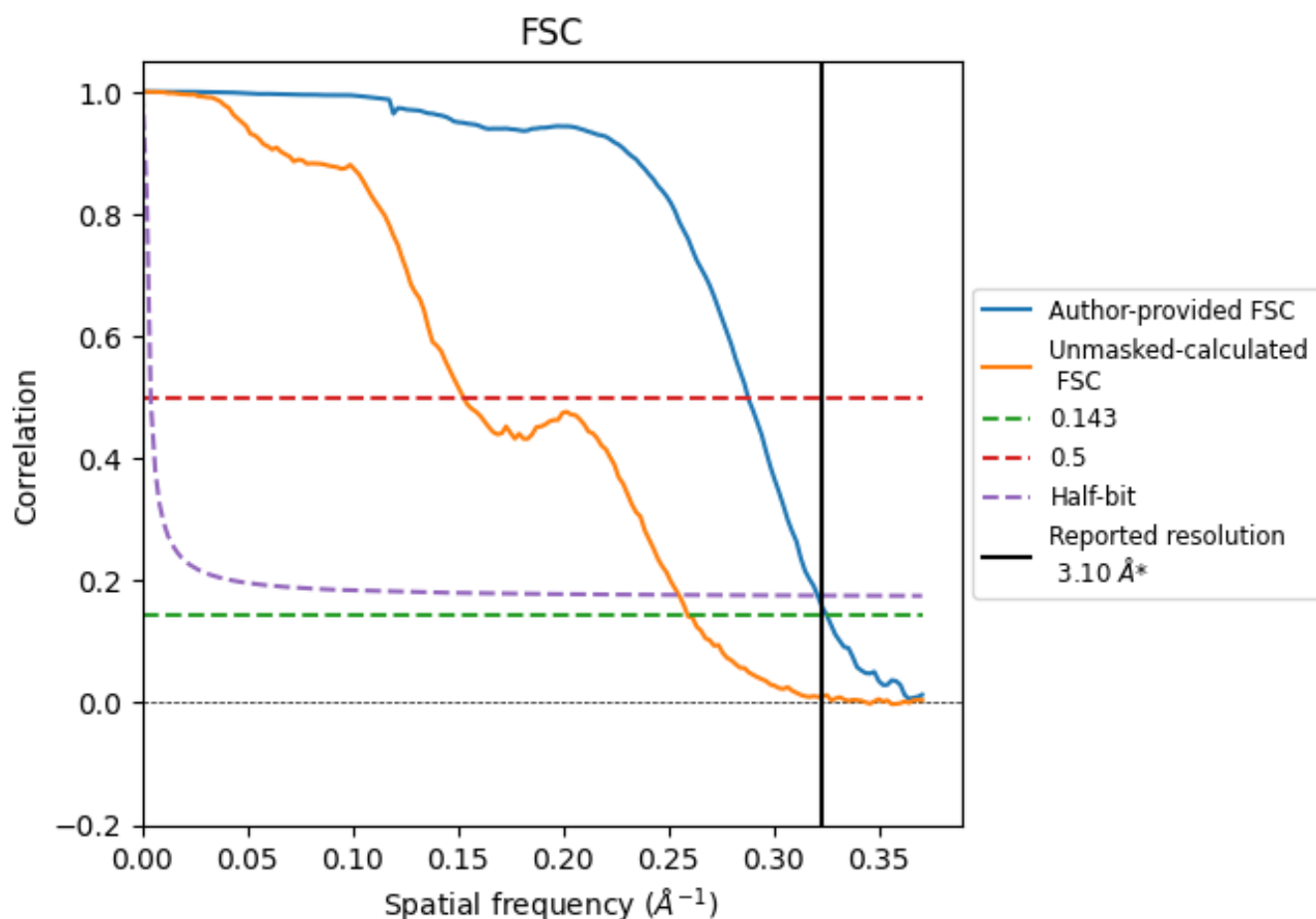


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

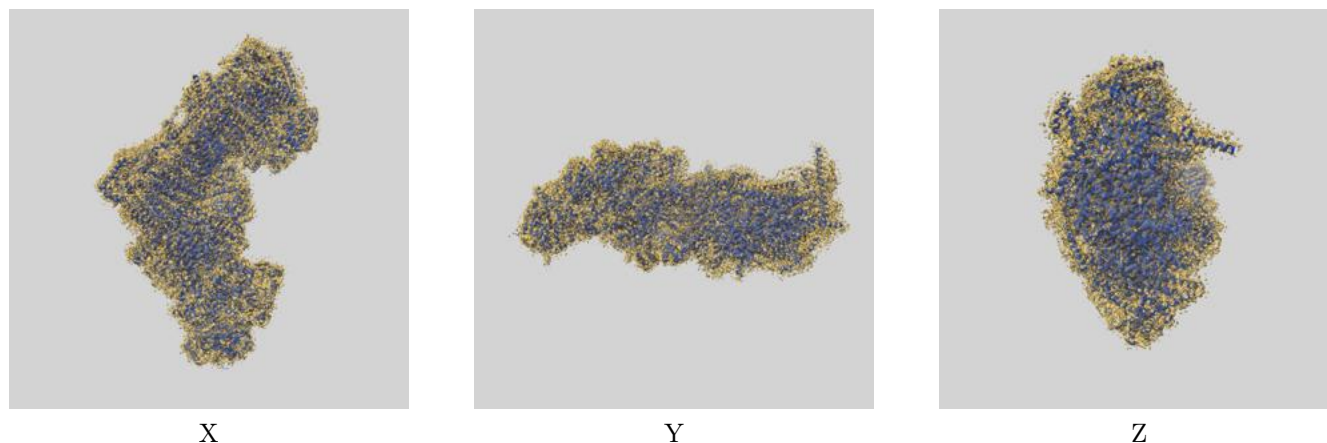
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.48	3.12
Unmasked-calculated*	3.86	6.56	3.92

*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 3.86 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

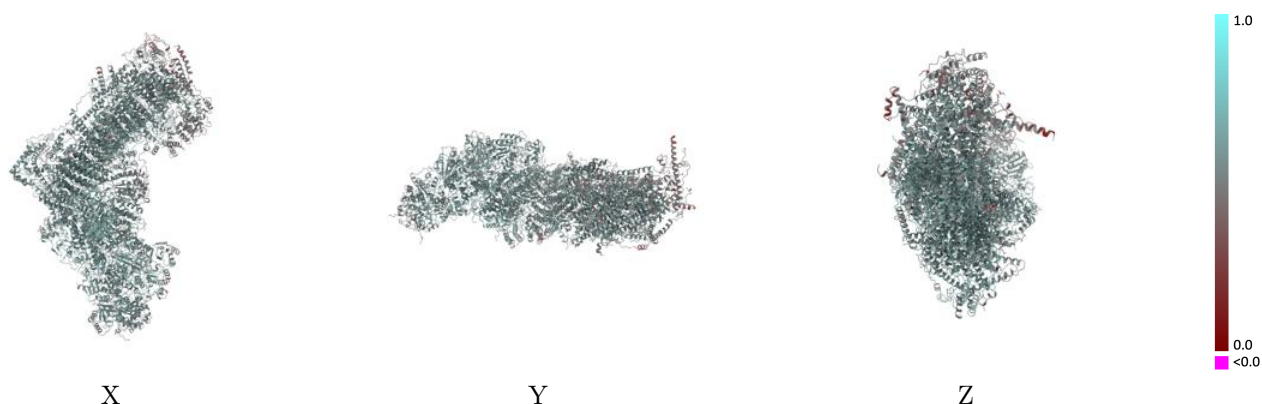
This section contains information regarding the fit between EMDB map EMD-18055 and PDB model 8Q0M. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



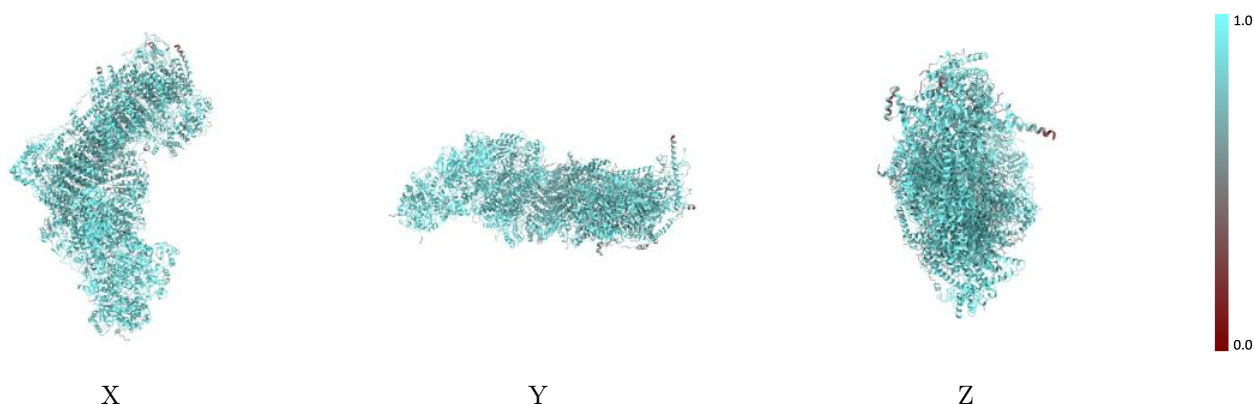
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



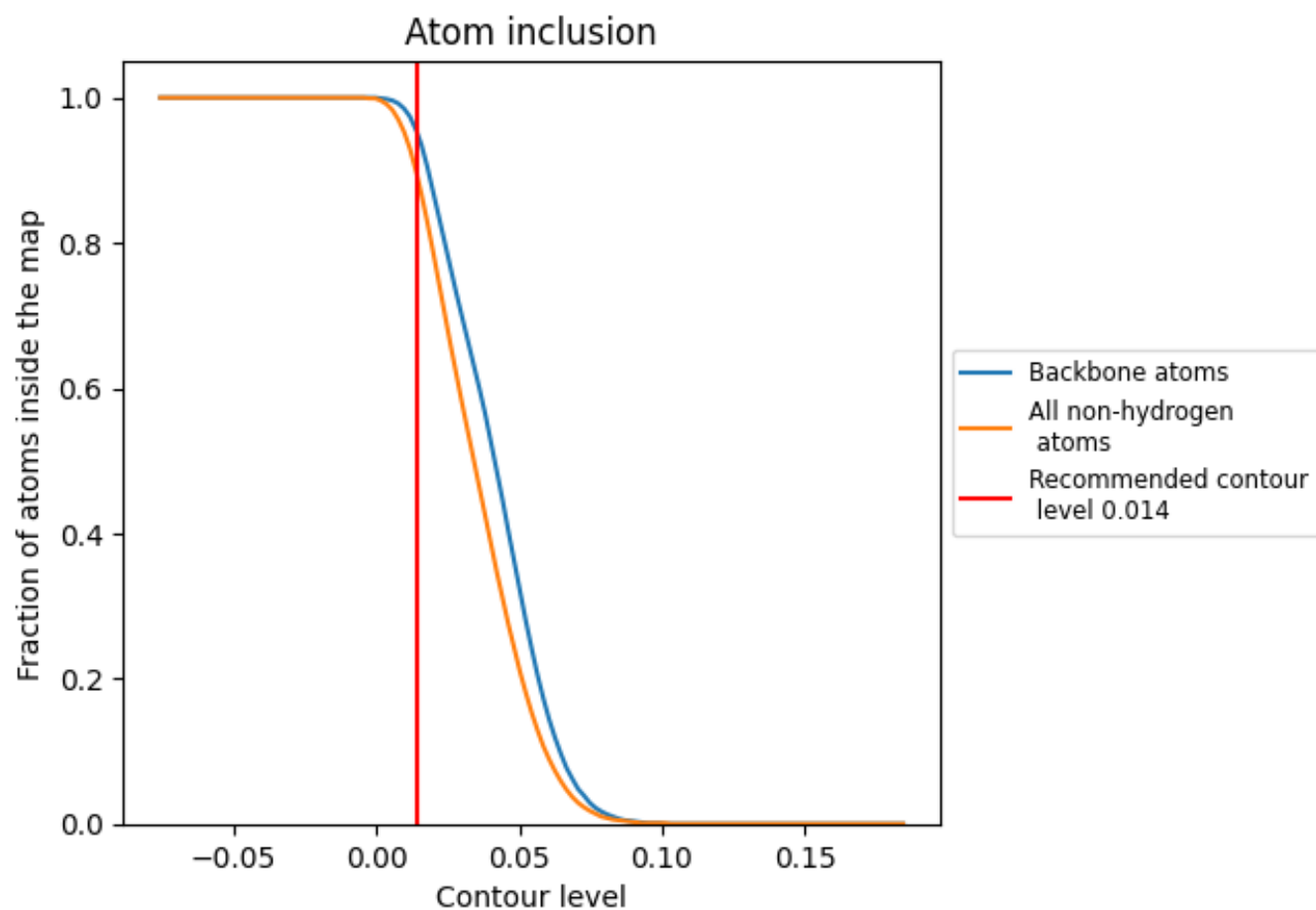
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5670
A	 0.8830	 0.5900
B	 0.9270	 0.6060
C	 0.9530	 0.6130
D	 0.9500	 0.6060
E	 0.9000	 0.5430
F	 0.9250	 0.5630
G	 0.9340	 0.5810
H	 0.9380	 0.6030
I	 0.9620	 0.6140
J	 0.8870	 0.5780
K	 0.9450	 0.6030
L	 0.8730	 0.5580
M	 0.9470	 0.6020
N	 0.9350	 0.6010
O	 0.8970	 0.5510
P	 0.9140	 0.5840
Q	 0.9030	 0.5840
R	 0.8400	 0.5610
S	 0.8650	 0.5180
T	 0.8460	 0.5100
U	 0.8050	 0.4910
V	 0.9050	 0.5700
W	 0.9220	 0.5830
X	 0.9160	 0.5770
Y	 0.8250	 0.5550
Z	 0.8920	 0.5710
a	 0.9510	 0.5950
b	 0.8750	 0.5620
c	 0.7800	 0.5130
d	 0.8940	 0.5730
e	 0.8690	 0.5580
f	 0.7430	 0.5130
g	 0.8440	 0.5440
h	 0.8950	 0.5760



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7690	 0.4730
j	 0.7770	 0.4610
k	 0.7350	 0.4410
l	 0.8780	 0.5310
m	 0.8440	 0.5490
n	 0.8730	 0.5120
o	 0.7620	 0.4490
p	 0.8550	 0.5320
q	 0.9100	 0.5910
r	 0.9050	 0.5800
s	 0.7220	 0.4720