



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:46 AM UTC

PDB ID : 8Q4A / pdb_00008q4a
EMDB ID : EMD-18143
Title : Outward-facing, open1 proteoliposome complex I at 2.6 Å. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-05
Resolution : 2.60 Å(reported)
Based on initial model : 7QSN

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

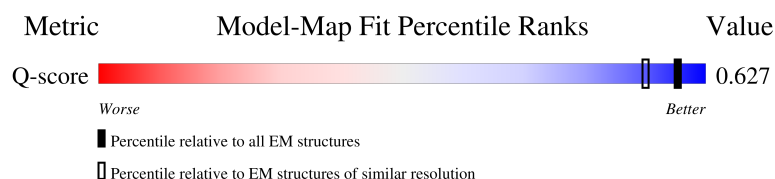
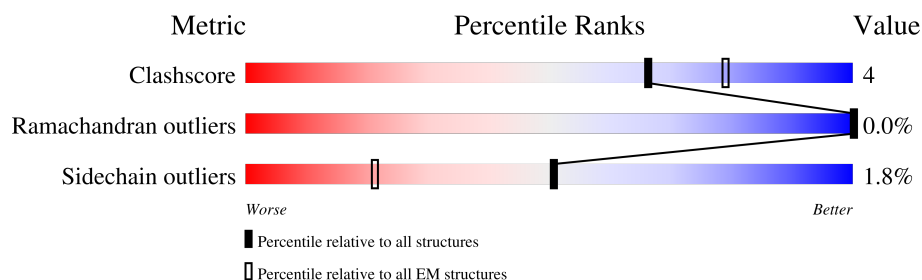
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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.



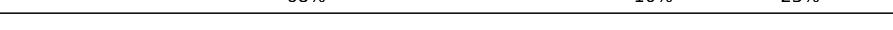
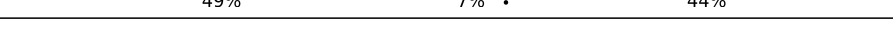
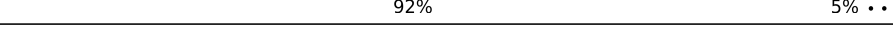
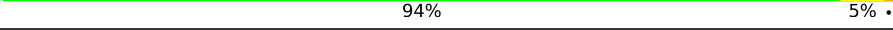
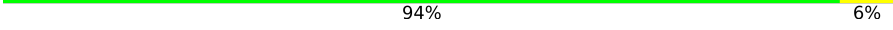
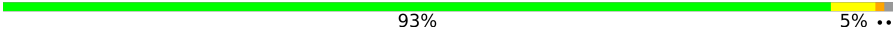
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	 89% 10% .
2	B	216	 61% 11% 28%
3	C	266	 73% 5% 22%
4	D	463	 80% 10% . 10%

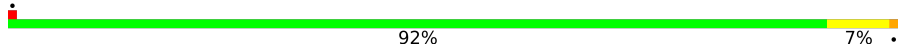
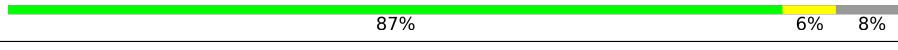
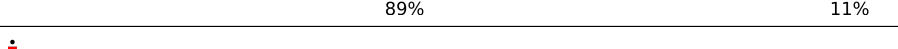
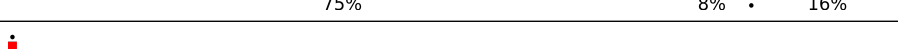
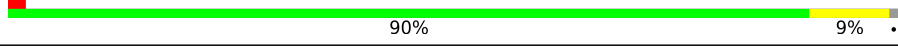
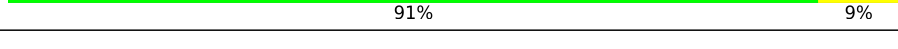
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	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 61 unique types of molecules in this entry. The entry contains 70646 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	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	419	Total	C	N	O	S	0	0
			3377	2159	580	613	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	691	Total	C	N	O	S	0	0
			5298	3318	925	1016	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	339	Total	C	N	O	S	0	0
			2728	1765	484	474	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	86	Total	C	N	O	S	0	0
			691	434	129	126	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	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	116	Total	C	N	O	S	0	0
			982	628	182	168	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	142	Total	C	N	O	S	0	0
			1157	743	202	203	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	98	Total	C	N	O	S	0	0
			825	521	157	141	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		

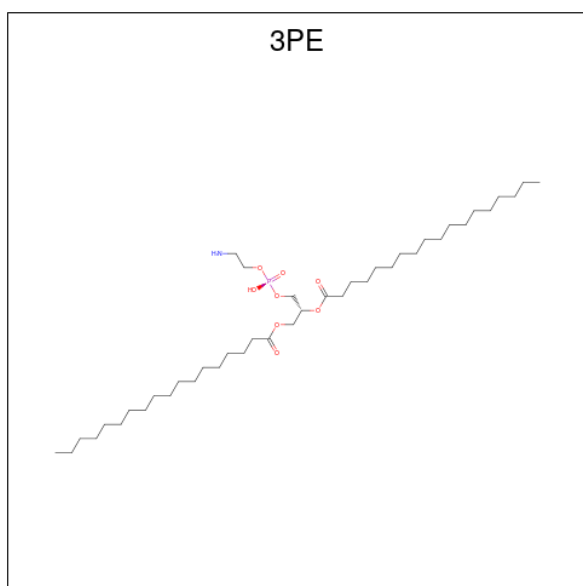
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



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
			40	30	1	8	1	
45	J	1	Total	C	N	O	P	0
			37	27	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
			34	24	1	8	1	
45	L	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	M	1	Total	C	N	O	P	0
			29	19	1	8	1	

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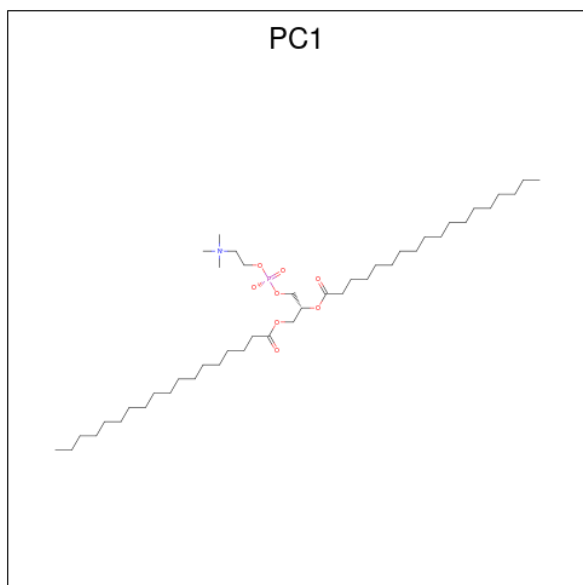
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	N	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	P	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	Y	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Z	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	Z	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	a	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	b	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	b	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	f	1	Total	C	N	O	P	0
			24	14	1	8	1	
45	i	1	Total	C	N	O	P	0
			45	35	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	

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Mol	Chain	Residues	Atoms					AltConf
45	r	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



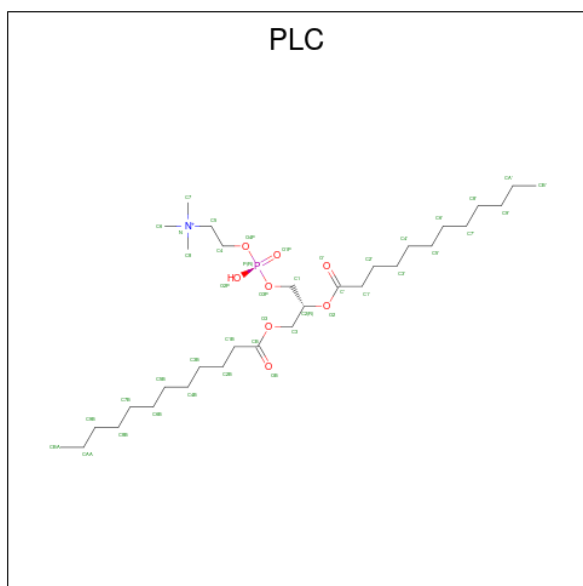
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
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
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	h	1	Total	C	N	O	P	0
			38	28	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
			41	31	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: $C_{32}H_{65}NO_8P$).



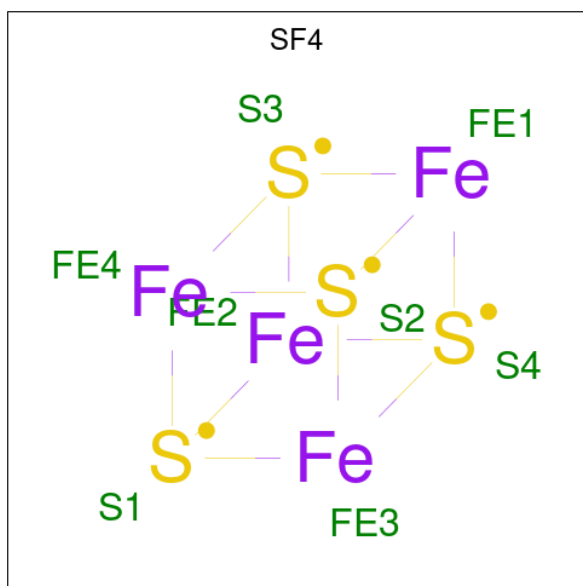
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
47	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	M	1	Total	C	N	O	P	0
			34	24	1	8	1	

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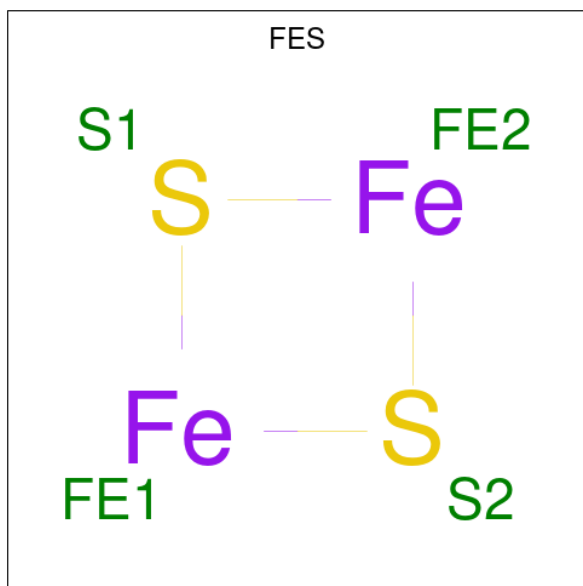
Mol	Chain	Residues	Atoms					AltConf
47	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	Z	1	Total	C	N	O	P	0
			36	26	1	8	1	
47	g	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



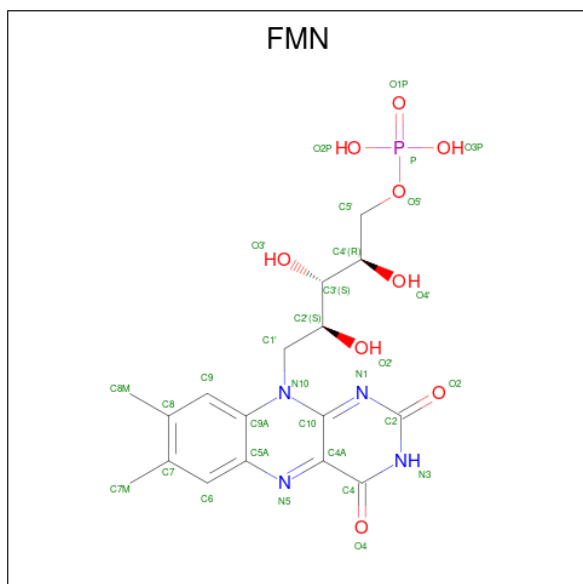
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

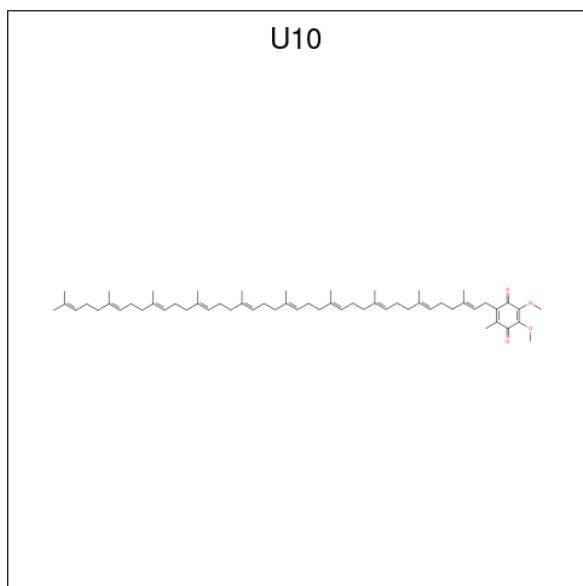


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

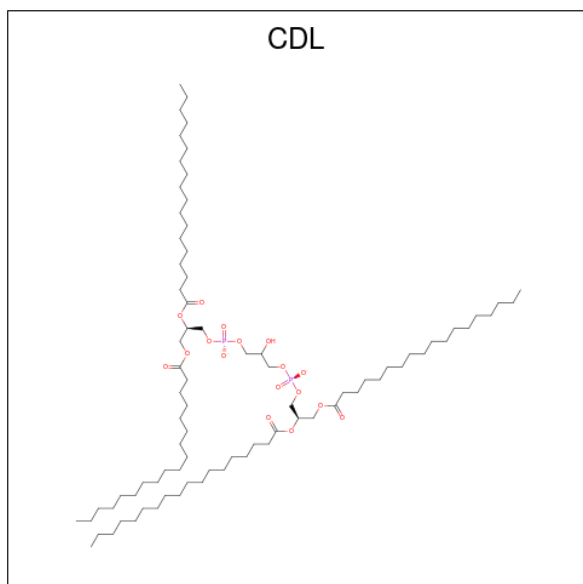
Mol	Chain	Residues	Atoms		AltConf
51	G	1	Total	K	0
			1	1	

- Molecule 52 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
52	H	1	Total	C	O	0
			34	30	4	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

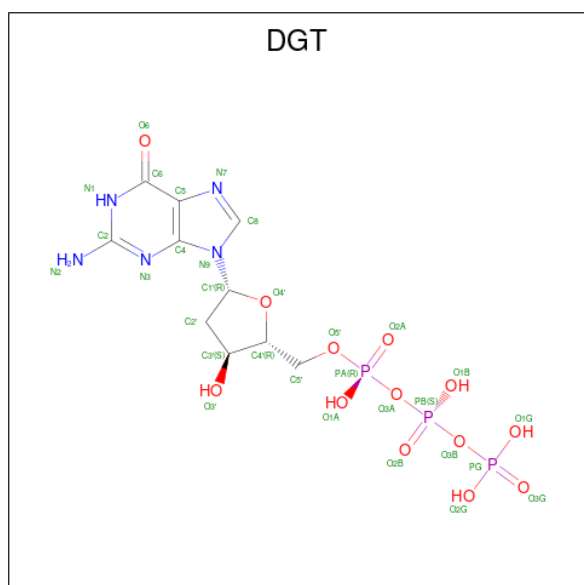


Mol	Chain	Residues	Atoms				AltConf
53	H	1	Total	C	O	P	0
			58	39	17	2	
53	L	1	Total	C	O	P	0
			100	81	17	2	
53	M	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			94	75	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	d	1	Total	C	O	P	0
			87	68	17	2	
53	h	1	Total	C	O	P	0
			76	57	17	2	
53	r	1	Total	C	O	P	0
			61	42	17	2	

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

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

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

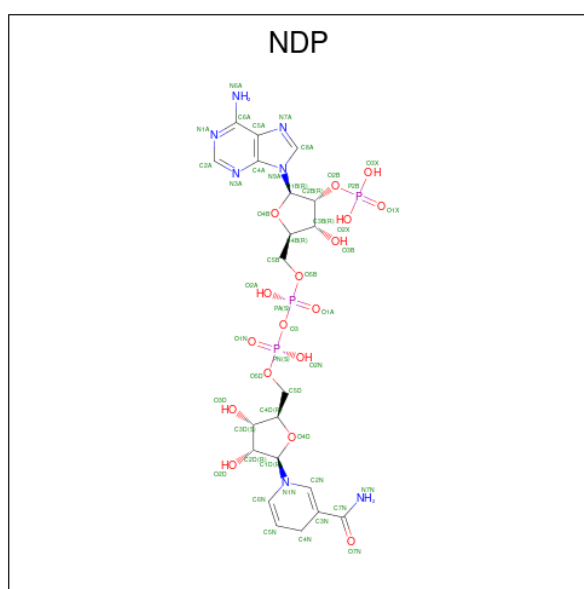


Mol	Chain	Residues	Atoms					AltConf
55	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

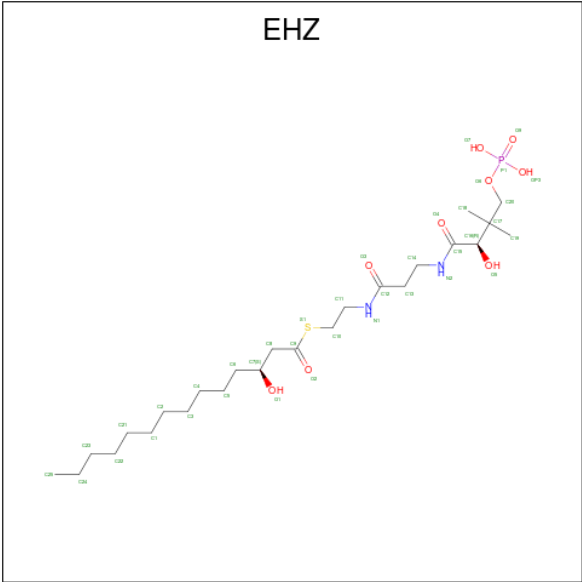
Mol	Chain	Residues	Atoms		AltConf
56	O	1	Total	Mg	0
			1	1	

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



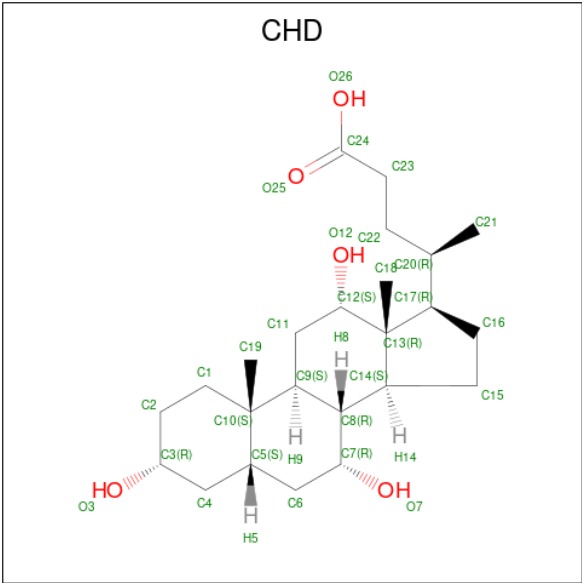
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



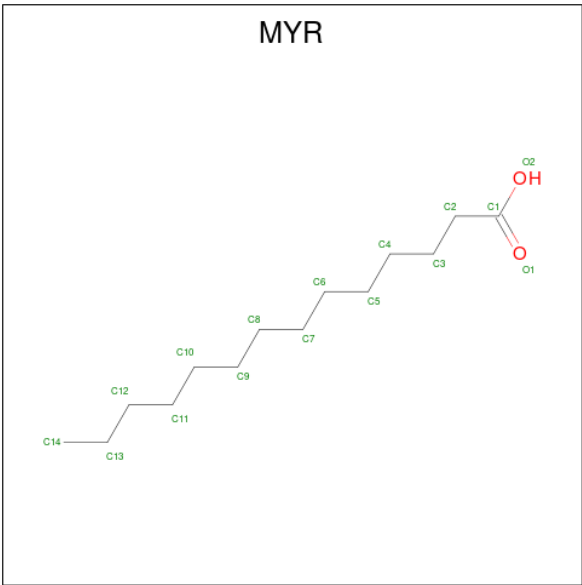
Mol	Chain	Residues	Atoms					AltConf
58	T	1	Total	C	N	O	P	S
			37	25	2	8	1	1
58	U	1	Total	C	N	O	P	S
			37	25	2	8	1	1

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



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

- Molecule 60 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	12	Total	O	0
			12	12	
61	B	56	Total	O	0
			56	56	
61	C	69	Total	O	0
			69	69	
61	D	137	Total	O	0
			137	137	
61	E	11	Total	O	0
			11	11	
61	F	31	Total	O	0
			31	31	
61	G	125	Total	O	0
			125	125	
61	H	29	Total	O	0
			29	29	
61	I	87	Total	O	0
			87	87	
61	J	7	Total	O	0
			7	7	
61	K	6	Total	O	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
61	L	8	Total 8	O 8	0
61	M	24	Total 24	O 24	0
61	N	31	Total 31	O 31	0
61	O	12	Total 12	O 12	0
61	P	26	Total 26	O 26	0
61	Q	55	Total 55	O 55	0
61	R	28	Total 28	O 28	0
61	S	1	Total 1	O 1	0
61	T	1	Total 1	O 1	0
61	U	1	Total 1	O 1	0
61	V	12	Total 12	O 12	0
61	W	14	Total 14	O 14	0
61	X	8	Total 8	O 8	0
61	Z	27	Total 27	O 27	0
61	a	11	Total 11	O 11	0
61	b	4	Total 4	O 4	0
61	d	6	Total 6	O 6	0
61	e	16	Total 16	O 16	0
61	g	1	Total 1	O 1	0
61	h	13	Total 13	O 13	0
61	l	5	Total 5	O 5	0

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Mol	Chain	Residues	Atoms		AltConf
61	m	3	Total 3	O 3	0
61	n	1	Total 1	O 1	0
61	o	1	Total 1	O 1	0
61	p	3	Total 3	O 3	0
61	q	33	Total 33	O 33	0
61	r	35	Total 35	O 35	0
61	s	3	Total 3	O 3	0

3 Residue-property plots [i](#)

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

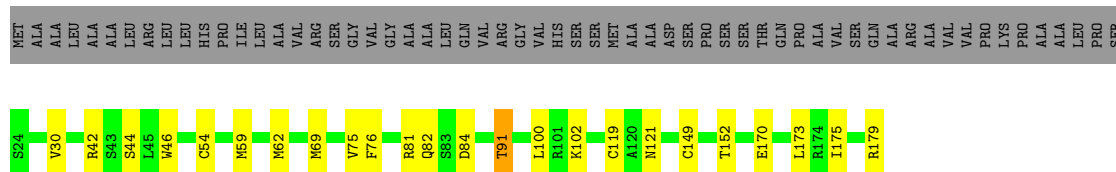
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



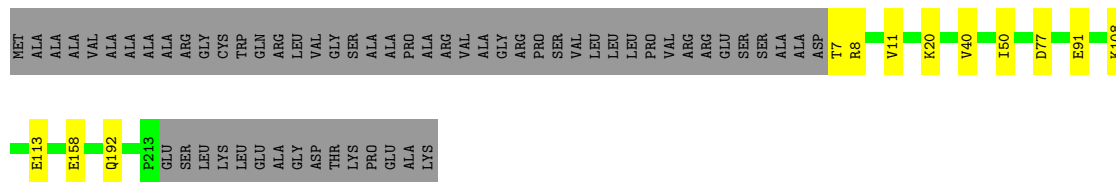
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



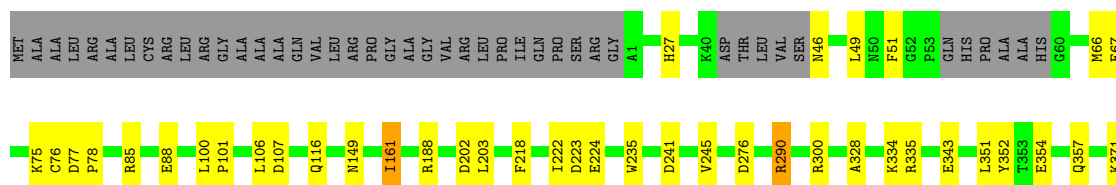
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

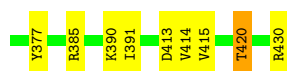
Chain C: 



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

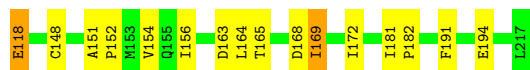
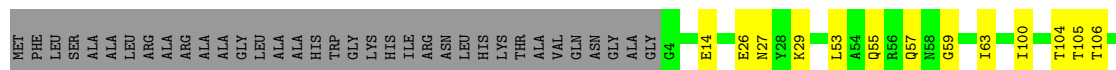
Chain D: 





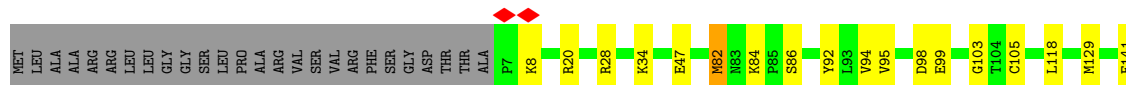
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 74% 11% 14%



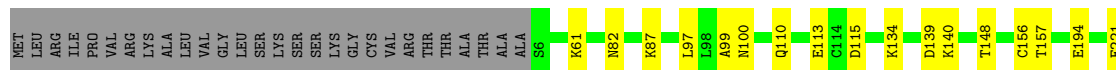
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 83% 10% 7%



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

Chain G: 85% 9% 5%



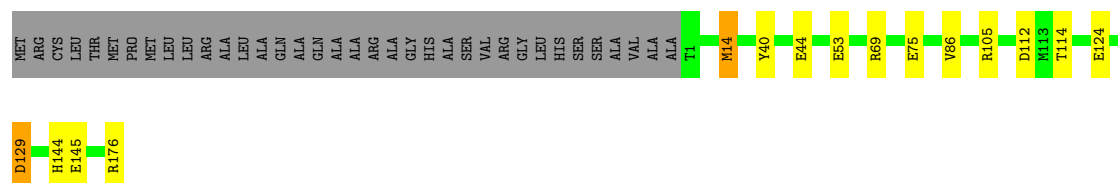
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 86% 14%



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

Chain I:  76% 6% 17%

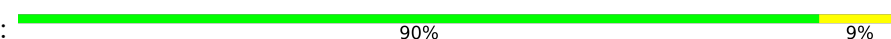


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  87% 12%



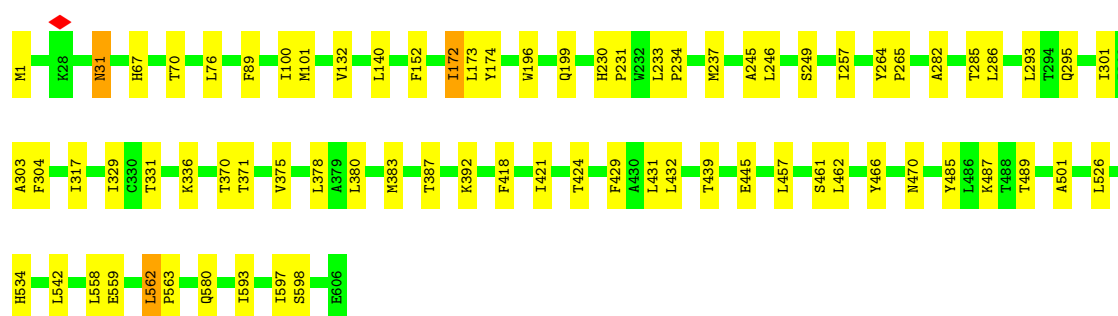
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  90% 9%

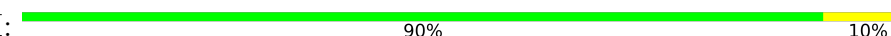


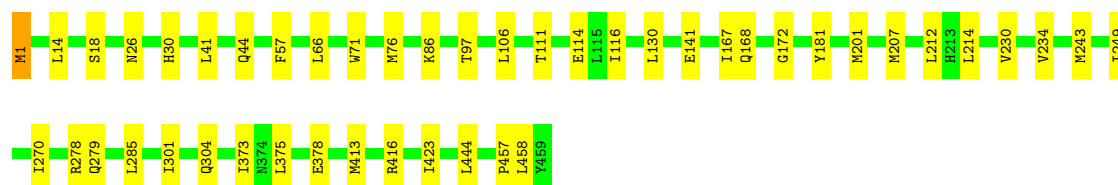
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  88% 12%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  90% 10%



- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

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

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

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

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

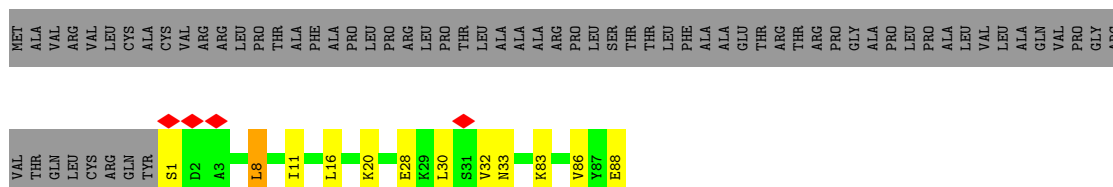
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:  78% 9% 13%



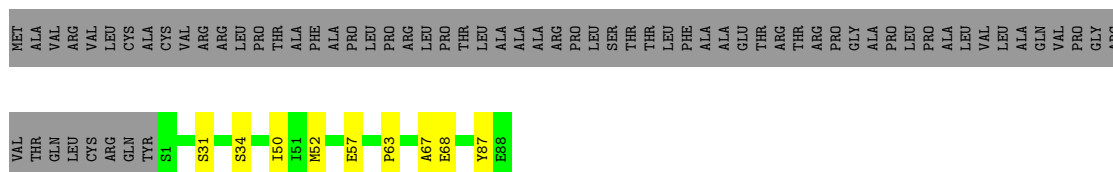
- Molecule 20: Acyl carrier protein, mitochondrial

Chain T:  49% 7% 44%



- Molecule 20: Acyl carrier protein, mitochondrial

Chain U:  51% 6% 44%



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

Chain V:  92% 5% ..



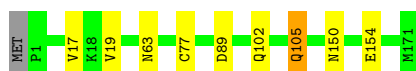
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  85% 5% 9%

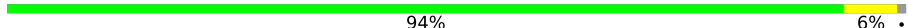


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  94% 5% ..

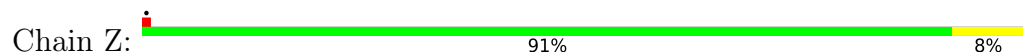


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

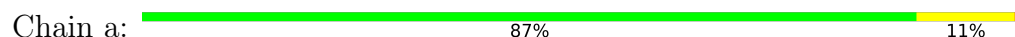
Chain Y:  94% 6% .



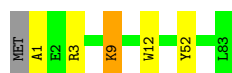
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



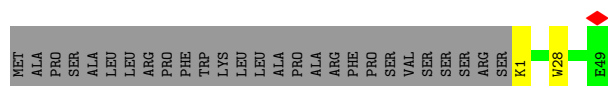
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



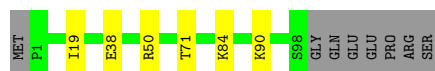
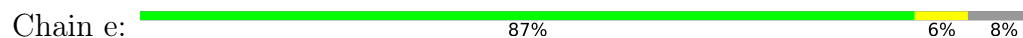
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



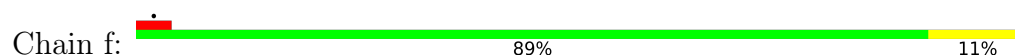
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

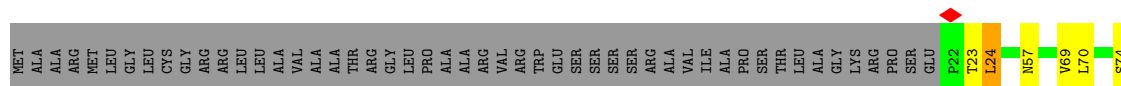


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

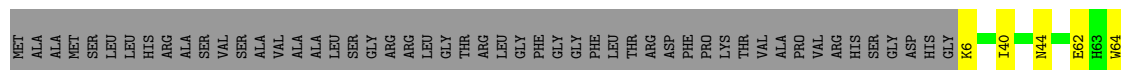




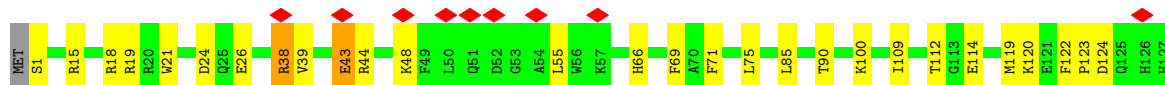
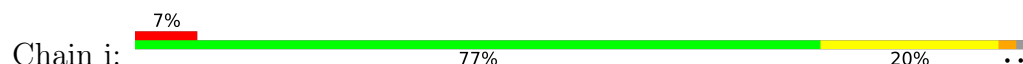
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



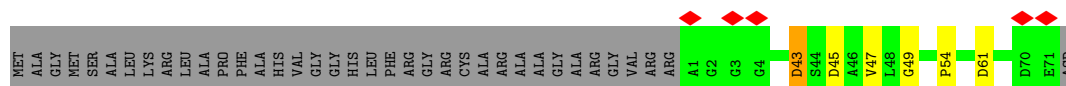
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



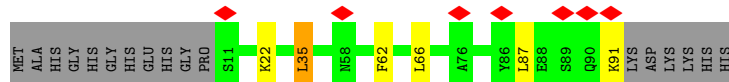
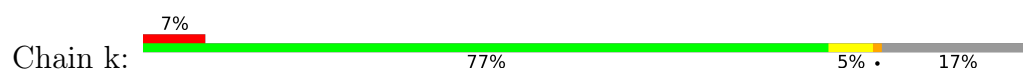
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



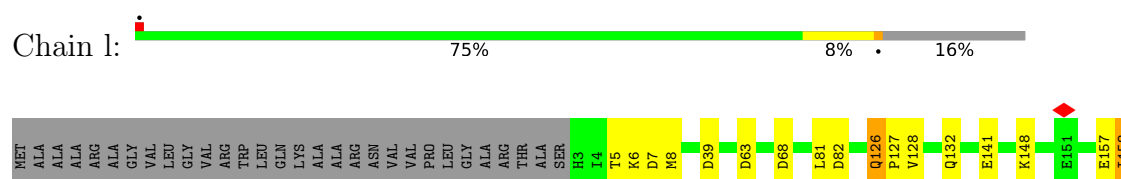
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



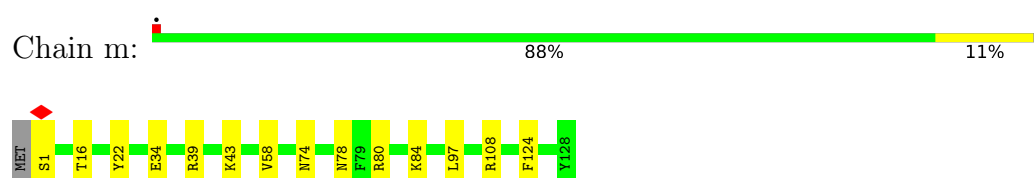
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



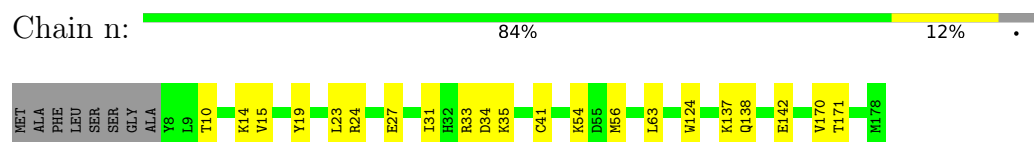
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



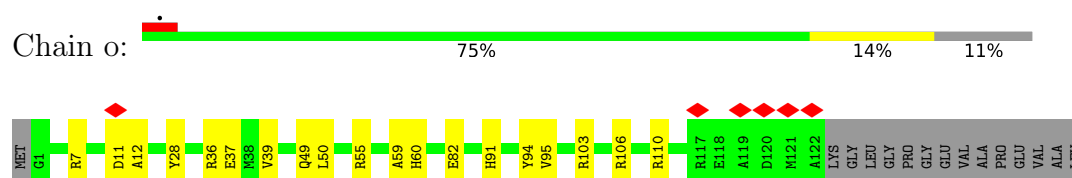
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



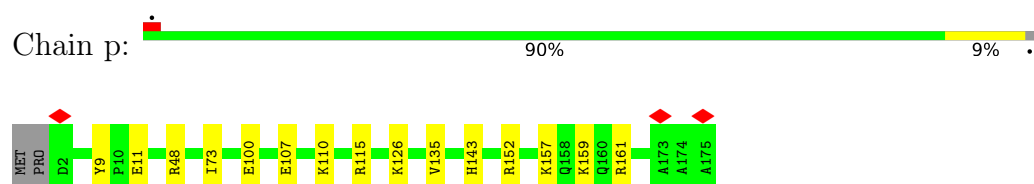
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



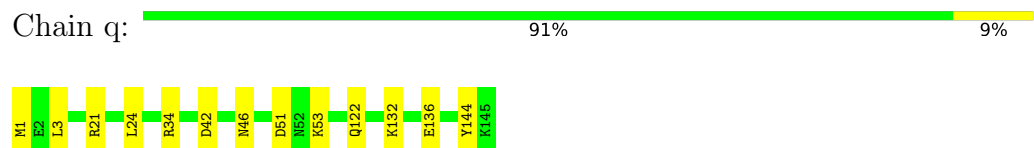
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



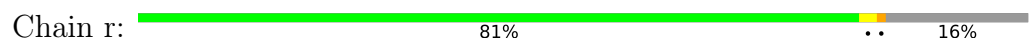
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

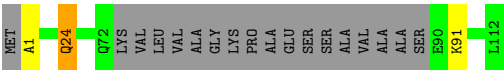


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

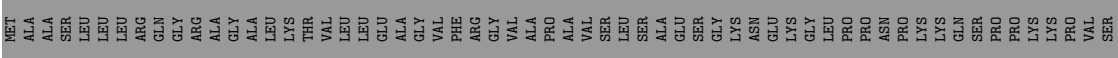


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	479.69998, 479.69998, 479.69998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.14	0/936	0.23	0/1281
2	B	0.21	0/1278	0.27	0/1728
3	C	0.19	0/1772	0.26	0/2413
4	D	0.20	0/3450	0.25	0/4670
5	E	0.14	0/1699	0.27	0/2312
6	F	0.14	0/3401	0.25	0/4595
7	G	0.17	0/5387	0.26	0/7301
8	H	0.18	0/2571	0.30	0/3513
9	I	0.22	0/1445	0.28	0/1956
10	J	0.16	0/1370	0.26	0/1859
11	K	0.16	0/745	0.22	0/1008
12	L	0.12	0/4920	0.24	0/6694
13	M	0.16	0/3738	0.24	0/5097
14	N	0.18	0/2792	0.25	0/3800
15	O	0.13	0/2651	0.21	0/3587
16	P	0.15	0/2804	0.24	0/3803
17	Q	0.17	0/1072	0.24	0/1449
18	R	0.18	0/753	0.23	0/1014
19	S	0.11	0/702	0.22	0/945
20	T	0.11	0/719	0.23	0/971
20	U	0.12	0/719	0.24	0/971
21	V	0.14	0/943	0.21	0/1277
22	W	0.14	0/1006	0.21	0/1352
23	X	0.14	0/1439	0.22	0/1942
24	Y	0.12	0/1042	0.19	0/1414
25	Z	0.15	0/1186	0.21	0/1599
26	a	0.17	0/584	0.22	0/786
27	b	0.13	0/667	0.22	0/916
28	c	0.14	0/427	0.18	0/579
29	d	0.15	0/1018	0.22	0/1375
30	e	0.15	0/846	0.24	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.13	0/505	0.21	0/681
32	g	0.12	0/873	0.27	0/1186
33	h	0.14	0/1188	0.22	0/1607
34	i	0.10	0/1127	0.23	0/1534
35	j	0.11	0/624	0.21	0/855
36	k	0.08	0/672	0.20	0/906
37	l	0.11	0/1369	0.23	0/1873
38	m	0.12	0/1088	0.20	0/1472
39	n	0.10	0/1540	0.21	0/2085
40	o	0.12	0/1073	0.23	0/1437
41	p	0.11	0/1491	0.19	0/2011
42	q	0.17	0/1242	0.25	0/1688
43	r	0.17	0/789	0.26	0/1068
44	s	0.10	0/383	0.20	0/518
All	All	0.15	0/68046	0.24	0/92259

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	10	0
2	B	1247	0	1256	18	0
3	C	1721	0	1675	8	0
4	D	3377	0	3327	35	0
5	E	1659	0	1664	20	0
6	F	3326	0	3282	33	0
7	G	5298	0	5316	47	0
8	H	2509	0	2621	31	0
9	I	1414	0	1370	18	0
10	J	1345	0	1352	17	0
11	K	745	0	785	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	54	0
13	M	3654	0	3852	36	0
14	N	2733	0	2912	28	0
15	O	2589	0	2566	23	0
16	P	2728	0	2749	25	0
17	Q	1049	0	1045	8	0
18	R	740	0	714	8	0
19	S	691	0	706	5	0
20	T	707	0	700	5	0
20	U	707	0	700	5	0
21	V	923	0	964	3	0
22	W	982	0	999	5	0
23	X	1402	0	1383	7	0
24	Y	1030	0	1039	3	0
25	Z	1157	0	1156	9	0
26	a	569	0	568	9	0
27	b	654	0	663	3	0
28	c	414	0	415	1	0
29	d	999	0	988	6	0
30	e	825	0	826	3	0
31	f	492	0	501	4	0
32	g	846	0	798	10	0
33	h	1154	0	1168	8	0
34	i	1097	0	1108	21	0
35	j	597	0	536	5	0
36	k	653	0	639	5	0
37	l	1314	0	1210	14	0
38	m	1070	0	1068	11	0
39	n	1487	0	1433	15	0
40	o	1048	0	1016	15	0
41	p	1458	0	1430	12	0
42	q	1212	0	1183	9	0
43	r	776	0	782	1	0
44	s	371	0	344	6	0
45	A	87	0	125	0	0
45	J	37	0	51	0	0
45	K	44	0	62	0	0
45	L	75	0	101	0	0
45	M	79	0	109	0	0
45	N	49	0	75	0	0
45	P	38	0	50	0	0
45	Y	347	0	513	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	78	0	104	1	0
45	a	36	0	49	1	0
45	b	79	0	112	2	0
45	d	49	0	75	0	0
45	f	24	0	22	0	0
45	i	45	0	67	0	0
45	m	41	0	59	0	0
45	q	51	0	82	1	0
45	r	30	0	34	0	0
46	A	103	0	128	2	0
46	B	94	0	136	1	0
46	H	88	0	130	0	0
46	I	98	0	150	0	0
46	J	48	0	73	2	0
46	L	44	0	65	2	0
46	M	35	0	44	0	0
46	d	39	0	52	0	0
46	h	38	0	53	0	0
46	l	47	0	71	0	0
46	m	41	0	56	0	0
46	q	49	0	75	2	0
47	A	38	0	53	0	0
47	J	35	0	47	0	0
47	L	36	0	49	0	0
47	M	34	0	45	0	0
47	O	62	0	77	0	0
47	Y	42	0	64	0	0
47	Z	36	0	49	0	0
47	g	42	0	64	0	0
48	B	8	0	0	0	0
48	F	8	0	0	0	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	1	0
51	G	1	0	0	0	0
52	H	34	0	41	17	0
53	H	58	0	63	0	0
53	L	100	0	156	0	0
53	M	100	0	156	3	0
53	N	94	0	141	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	d	152	0	204	1	0
53	h	76	0	96	2	0
53	r	61	0	66	0	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	31	0	12	3	0
56	O	1	0	0	0	0
57	P	48	0	26	2	0
58	T	37	0	0	0	0
58	U	37	0	0	1	0
59	i	29	0	38	6	0
60	o	15	0	27	0	0
61	A	12	0	0	0	0
61	B	56	0	0	2	0
61	C	69	0	0	3	0
61	D	137	0	0	10	0
61	E	11	0	0	0	0
61	F	31	0	0	2	0
61	G	125	0	0	8	0
61	H	29	0	0	0	0
61	I	87	0	0	2	0
61	J	7	0	0	1	0
61	K	6	0	0	0	0
61	L	8	0	0	0	0
61	M	24	0	0	3	0
61	N	31	0	0	2	0
61	O	12	0	0	1	0
61	P	26	0	0	3	0
61	Q	55	0	0	1	0
61	R	28	0	0	3	0
61	S	1	0	0	0	0
61	T	1	0	0	0	0
61	U	1	0	0	0	0
61	V	12	0	0	0	0
61	W	14	0	0	4	0
61	X	8	0	0	1	0
61	Z	27	0	0	1	0
61	a	11	0	0	2	0
61	b	4	0	0	1	0
61	d	6	0	0	0	0
61	e	16	0	0	0	0
61	g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	h	13	0	0	2	0
61	l	5	0	0	0	0
61	m	3	0	0	0	0
61	n	1	0	0	0	0
61	o	1	0	0	0	0
61	p	3	0	0	0	0
61	q	33	0	0	2	0
61	r	35	0	0	1	0
61	s	3	0	0	0	0
All	All	70646	0	70937	543	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 (543) 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)
52:H:401:U10:H201	52:H:401:U10:H253	1.55	0.86
13:M:457:PRO:O	32:g:84:ARG:NH2	2.09	0.86
15:O:94:TYR:HH	15:O:151:HIS:HD1	0.88	0.86
40:o:59:ALA:O	40:o:60:HIS:ND1	2.11	0.84
59:i:201:CHD:H212	59:i:201:CHD:H12	1.60	0.84
7:G:615:THR:OG1	7:G:617:ASP:OD1	1.98	0.82
3:C:91:GLU:OE2	3:C:108:LYS:NZ	2.13	0.81
7:G:139:ASP:OD2	61:G:901:HOH:O	1.98	0.81
14:N:263:LYS:NZ	61:N:501:HOH:O	2.13	0.81
4:D:343:GLU:OE2	61:D:501:HOH:O	1.98	0.81
7:G:260:GLU:OE2	7:G:397:LYS:NZ	2.15	0.80
7:G:366:THR:O	7:G:367:THR:OG1	2.00	0.80
4:D:46:ASN:ND2	4:D:67:GLU:OE2	2.15	0.80
33:h:107:GLU:OE1	61:h:301:HOH:O	1.99	0.80
22:W:29:ARG:NH1	22:W:33:GLU:OE2	2.16	0.79
32:g:86:GLN:NE2	41:p:100:GLU:OE2	2.15	0.79
7:G:113:GLU:OE2	61:G:902:HOH:O	2.00	0.79
6:F:428:GLU:OE2	6:F:432:GLN:NE2	2.16	0.79
23:X:154:GLU:N	23:X:154:GLU:OE1	2.16	0.79
13:M:278:ARG:NE	37:l:82:ASP:OD1	2.16	0.77
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.17	0.77
7:G:221:GLU:O	61:G:903:HOH:O	2.03	0.77
12:L:380:LEU:O	12:L:392:LYS:NZ	2.17	0.77
34:i:18:ARG:NH1	39:n:170:VAL:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:65:GLU:OE1	61:Z:301:HOH:O	2.03	0.77
7:G:232:ASP:OD2	61:G:904:HOH:O	2.03	0.76
42:q:122:GLN:OE1	61:q:301:HOH:O	2.02	0.76
9:I:124:GLU:OE2	61:I:301:HOH:O	2.03	0.76
3:C:192:GLN:OE1	61:C:302:HOH:O	2.04	0.76
6:F:224:ASN:ND2	50:F:502:FMN:O2	2.19	0.76
3:C:158:GLU:OE1	61:C:301:HOH:O	2.03	0.75
6:F:20:ARG:NH1	6:F:269:GLU:O	2.19	0.75
6:F:141:GLU:OE2	61:F:601:HOH:O	2.03	0.75
12:L:67:HIS:HE2	12:L:70:THR:HG1	1.33	0.75
3:C:7:THR:N	61:C:303:HOH:O	2.20	0.74
6:F:86:SER:OG	61:F:602:HOH:O	2.04	0.74
8:H:65:THR:HG21	16:P:325:ARG:HG2	1.69	0.74
14:N:47:ASN:O	14:N:49:ASN:ND2	2.20	0.74
17:Q:78:PRO:O	61:Q:201:HOH:O	2.06	0.74
26:a:25:ARG:NE	45:a:101:3PE:O14	2.20	0.74
7:G:475:GLN:OE1	61:G:906:HOH:O	2.04	0.74
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.67	0.74
15:O:32:CYS:SG	15:O:186:LYS:NZ	2.58	0.74
2:B:170:GLU:OE1	61:B:301:HOH:O	2.03	0.74
7:G:260:GLU:OE1	61:G:905:HOH:O	2.04	0.73
9:I:176:ARG:O	61:I:302:HOH:O	2.06	0.73
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.06	0.72
7:G:140:LYS:O	7:G:148:THR:OG1	2.07	0.72
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.23	0.72
13:M:416:ARG:NH2	61:M:703:HOH:O	2.21	0.72
4:D:88:GLU:O	61:D:503:HOH:O	2.07	0.72
23:X:89:ASP:OD2	61:X:201:HOH:O	2.08	0.72
12:L:31:ASN:OD1	12:L:31:ASN:N	2.23	0.71
33:h:111:ARG:NH2	61:h:302:HOH:O	2.22	0.71
22:W:98:GLN:OE1	61:W:201:HOH:O	2.09	0.71
4:D:66:MET:HE1	4:D:414:VAL:HG21	1.73	0.70
15:O:36:SER:OG	55:O:401:DGT:O1G	2.04	0.70
8:H:127:TYR:O	8:H:209:SER:OG	2.10	0.70
18:R:85:GLY:O	61:R:301:HOH:O	2.09	0.70
2:B:69:MET:HE2	2:B:76:PHE:HA	1.73	0.70
8:H:18:ALA:HB2	52:H:401:U10:H203	1.74	0.69
12:L:485:TYR:O	12:L:489:THR:OG1	2.10	0.69
18:R:92:ARG:NH1	61:R:302:HOH:O	2.22	0.69
31:f:53:GLU:N	31:f:53:GLU:OE1	2.25	0.69
13:M:378:GLU:OE2	61:M:701:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TRP:CZ2	52:H:401:U10:H1M2	2.28	0.69
15:O:216:GLU:N	15:O:216:GLU:OE1	2.25	0.69
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.25	0.69
37:l:5:THR:OG1	37:l:7:ASP:OD1	2.09	0.68
1:A:48:ARG:NH1	1:A:49:LEU:O	2.26	0.68
7:G:591:GLY:HA2	16:P:6:ILE:HG21	1.76	0.68
22:W:69:ASN:OD1	61:W:202:HOH:O	2.11	0.68
7:G:115:ASP:OD2	61:G:907:HOH:O	2.12	0.68
5:E:154:VAL:HG22	5:E:164:LEU:HD11	1.76	0.67
20:T:88:GLU:OE1	20:T:88:GLU:N	2.26	0.67
7:G:341:ASP:O	7:G:508:LYS:NZ	2.26	0.67
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.27	0.67
14:N:298:TYR:O	14:N:303:THR:OG1	2.08	0.67
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.27	0.67
13:M:279:GLN:OE1	61:M:702:HOH:O	2.13	0.67
10:J:78:GLN:OE1	10:J:78:GLN:N	2.28	0.66
19:S:82:SER:OG	19:S:84:ASP:OD1	2.05	0.66
4:D:77:ASP:OD1	61:D:504:HOH:O	2.14	0.66
1:A:115:GLU:N	1:A:115:GLU:OE1	2.29	0.66
37:l:157:GLU:OE1	37:l:158:ILE:N	2.29	0.65
26:a:4:GLU:OE1	61:a:201:HOH:O	2.13	0.65
4:D:107:ASP:OD2	61:D:505:HOH:O	2.14	0.65
15:O:281:GLU:N	15:O:281:GLU:OE1	2.30	0.65
38:m:16:THR:O	38:m:22:TYR:OH	2.08	0.65
5:E:164:LEU:HD13	5:E:169:ILE:HG12	1.77	0.65
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.29	0.65
40:o:82:GLU:N	40:o:82:GLU:OE1	2.30	0.65
52:H:401:U10:H101	52:H:401:U10:H13	1.78	0.65
7:G:339:ASP:OD1	19:S:16:ARG:NH1	2.29	0.64
15:O:307:GLY:O	15:O:320:LYS:NZ	2.22	0.64
12:L:152:PHE:HB2	12:L:172:ILE:HD13	1.79	0.64
12:L:245:ALA:O	12:L:249:SER:OG	2.14	0.64
12:L:293:LEU:HD11	12:L:418:PHE:CD2	2.32	0.64
37:l:141:GLU:N	37:l:141:GLU:OE1	2.29	0.64
40:o:28:TYR:O	40:o:103:ARG:NH2	2.29	0.64
18:R:70:ARG:NH1	61:R:303:HOH:O	2.29	0.64
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.31	0.64
8:H:135:ALA:HB2	8:H:201:THR:HG21	1.79	0.64
59:i:201:CHD:O3	59:i:201:CHD:H9	1.98	0.64
16:P:76:ARG:NH2	16:P:103:ASN:O	2.31	0.63
44:s:70:ARG:NH1	44:s:75:HIS:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:ALA:HB1	5:E:152:PRO:CD	2.28	0.63
8:H:224:PHE:CZ	52:H:401:U10:H72	2.34	0.63
31:f:4:LEU:HD13	31:f:4:LEU:O	1.99	0.63
6:F:364:PRO:HG2	6:F:403:THR:HG22	1.81	0.62
4:D:377:TYR:OH	61:D:502:HOH:O	2.04	0.62
40:o:11:ASP:OD1	40:o:12:ALA:N	2.32	0.62
25:Z:55:GLU:OE1	25:Z:58:ARG:NH2	2.33	0.62
9:I:145:GLU:OE1	9:I:145:GLU:N	2.30	0.62
14:N:72:MET:HE3	14:N:76:ILE:HD11	1.82	0.62
52:H:401:U10:C18	52:H:401:U10:H151	2.31	0.61
52:H:401:U10:H101	52:H:401:U10:C13	2.29	0.61
8:H:249:PRO:O	26:a:28:ARG:NH2	2.33	0.61
15:O:147:GLN:N	15:O:147:GLN:OE1	2.34	0.61
34:i:39:VAL:O	34:i:44:ARG:NH2	2.34	0.61
39:n:34:ASP:OD1	39:n:35:LYS:N	2.33	0.60
5:E:151:ALA:HB1	5:E:152:PRO:HD2	1.81	0.60
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.81	0.60
12:L:174:TYR:HH	12:L:534:HIS:HE2	1.42	0.60
40:o:50:LEU:O	40:o:55:ARG:NH1	2.34	0.60
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.36	0.60
29:d:112:VAL:O	41:p:159:LYS:NZ	2.35	0.60
4:D:218:PHE:CE2	4:D:222:ILE:HD11	2.37	0.59
8:H:111:LEU:HD11	10:J:57:PHE:CD1	2.36	0.59
1:A:71:LEU:O	10:J:147:TYR:OH	2.17	0.59
2:B:75:VAL:HG11	52:H:401:U10:H1M3	1.85	0.59
7:G:332:LYS:NZ	7:G:505:LEU:O	2.31	0.59
15:O:30:ASN:O	15:O:35:LYS:NZ	2.35	0.59
15:O:138:MET:CE	55:O:401:DGT:HN2	2.16	0.59
17:Q:15:GLU:OE1	17:Q:15:GLU:N	2.35	0.59
7:G:415:LEU:O	7:G:416:THR:OG1	2.12	0.59
12:L:378:LEU:HD22	12:L:383:MET:SD	2.42	0.59
35:j:54:PRO:HG2	40:o:95:VAL:HG22	1.85	0.59
7:G:558:ASP:OD1	42:q:144:TYR:OH	2.21	0.59
52:H:401:U10:C8	52:H:401:U10:H1M1	2.33	0.59
34:i:120:LYS:NZ	40:o:39:VAL:O	2.18	0.59
6:F:47:GLU:N	6:F:47:GLU:OE1	2.35	0.59
44:s:33:PHE:O	44:s:35:ASN:ND2	2.36	0.59
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.35	0.58
19:S:94:LEU:O	19:S:97:LYS:NZ	2.27	0.58
34:i:15:ARG:HD2	34:i:19:ARG:HH21	1.68	0.58
42:q:21:ARG:NH2	46:q:201:PC1:O14	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.36	0.58
34:i:43:GLU:N	34:i:43:GLU:OE1	2.37	0.58
34:i:66:HIS:CD2	59:i:201:CHD:H231	2.39	0.58
20:U:63:PRO:O	20:U:67:ALA:N	2.37	0.57
21:V:17:GLU:HG2	21:V:18:THR:HG23	1.85	0.57
8:H:24:GLU:OE2	8:H:274:ARG:NH2	2.37	0.57
25:Z:54:ARG:NH2	45:Z:202:3PE:O12	2.37	0.57
16:P:143:SER:OG	16:P:282:ASP:OD1	2.22	0.57
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.87	0.57
4:D:78:PRO:O	61:D:506:HOH:O	2.17	0.57
6:F:82:MET:HE3	6:F:129:MET:HB3	1.87	0.57
7:G:535:GLN:N	7:G:535:GLN:OE1	2.37	0.57
52:H:401:U10:H202	45:q:202:3PE:C3I	2.35	0.57
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.35	0.57
10:J:141:MET:HA	10:J:141:MET:HE2	1.85	0.57
16:P:60:ARG:NH2	61:P:603:HOH:O	2.32	0.57
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.22	0.56
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.09	0.56
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.38	0.56
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.40	0.56
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.85	0.56
32:g:90:ARG:NH2	41:p:107:GLU:OE2	2.39	0.56
6:F:194:GLU:OE2	6:F:204:ARG:NE	2.31	0.56
32:g:94:GLU:OE2	41:p:9:TYR:OH	2.14	0.56
4:D:430:ARG:NH1	61:D:514:HOH:O	2.38	0.56
22:W:91:GLU:OE2	61:W:203:HOH:O	2.17	0.56
39:n:10:THR:O	39:n:14:LYS:NZ	2.38	0.56
5:E:148:CYS:N	6:F:105:CYS:SG	2.79	0.56
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.87	0.56
9:I:112:ASP:OD1	9:I:114:THR:OG1	2.21	0.56
52:H:401:U10:O4	52:H:401:U10:H3M3	2.06	0.55
39:n:138:GLN:NE2	39:n:142:GLU:OE2	2.39	0.55
4:D:66:MET:HE3	4:D:76:CYS:SG	2.46	0.55
12:L:76:LEU:HD21	12:L:196:TRP:HE3	1.71	0.55
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.41	0.55
10:J:77:GLU:N	10:J:77:GLU:OE1	2.38	0.55
15:O:141:GLN:NE2	61:O:501:HOH:O	2.38	0.55
1:A:29:VAL:HG13	1:A:34:THR:HG21	1.88	0.55
8:H:99:ASN:N	46:J:203:PC1:O12	2.39	0.55
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.40	0.55
27:b:52:TYR:OH	61:b:201:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.88	0.55
2:B:42:ARG:NH1	46:B:203:PC1:O14	2.36	0.55
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.34	0.55
12:L:558:LEU:CB	13:M:214:LEU:HD11	2.36	0.55
14:N:269:GLU:O	14:N:273:ASN:ND2	2.37	0.54
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.40	0.54
10:J:133:SER:O	61:J:301:HOH:O	2.17	0.54
12:L:293:LEU:HD11	12:L:418:PHE:CE2	2.43	0.54
5:E:26:GLU:N	5:E:26:GLU:OE1	2.39	0.54
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.37	0.54
7:G:627:SER:OG	7:G:629:ASN:OD1	2.25	0.54
14:N:347:GLU:HB2	29:d:82:MET:HE2	1.90	0.54
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.23	0.54
10:J:124:ASP:OD1	11:K:2:SER:OG	2.24	0.54
41:p:11:GLU:OE1	41:p:115:ARG:NH2	2.40	0.54
2:B:149:CYS:O	61:B:302:HOH:O	2.18	0.54
7:G:338:VAL:HG13	7:G:609:MET:HE1	1.90	0.54
4:D:413:ASP:OD1	61:D:507:HOH:O	2.19	0.54
12:L:174:TYR:OH	12:L:534:HIS:NE2	2.32	0.54
23:X:150:ASN:OD1	30:e:50:ARG:NH1	2.40	0.54
25:Z:142:TYR:CE2	26:a:48:MET:HE1	2.43	0.54
16:P:293:ILE:C	16:P:294:LEU:HD12	2.33	0.53
7:G:366:THR:HB	7:G:450:MET:HE3	1.89	0.53
32:g:23:THR:HG22	32:g:24:LEU:HG	1.91	0.53
25:Z:128:ALA:O	25:Z:132:VAL:HG23	2.09	0.53
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.36	0.53
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.90	0.53
13:M:114:GLU:OE1	13:M:116:ILE:N	2.41	0.53
35:j:43:ASP:OD1	35:j:43:ASP:N	2.41	0.53
4:D:241:ASP:OD1	4:D:290:ARG:NH1	2.35	0.53
37:l:126:GLN:OE1	37:l:126:GLN:N	2.42	0.53
9:I:75:GLU:O	9:I:105:ARG:NH1	2.43	0.52
13:M:201:MET:HE1	13:M:212:LEU:HD11	1.92	0.52
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.43	0.52
15:O:205:ALA:O	15:O:209:THR:OG1	2.24	0.52
39:n:56:MET:HA	39:n:56:MET:HE2	1.92	0.52
10:J:173:ARG:NH2	10:J:175:ASN:O	2.43	0.52
37:l:8:MET:HE2	37:l:8:MET:HA	1.92	0.52
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.28	0.52
45:Y:201:3PE:H2I3	38:m:97:LEU:HD11	1.91	0.52
12:L:424:THR:HG23	36:k:62:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:542:LEU:O	13:M:278:ARG:NH1	2.41	0.52
2:B:179:ARG:NH1	57:P:501:NDP:O2X	2.41	0.52
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.92	0.52
7:G:82:ASN:O	7:G:87:LYS:NZ	2.43	0.52
12:L:439:THR:OG1	20:U:57:GLU:OE2	2.28	0.52
14:N:108:MET:SD	14:N:191:THR:HG21	2.50	0.52
29:d:120:ARG:O	38:m:108:ARG:NH2	2.43	0.52
6:F:438:GLN:N	6:F:438:GLN:OE1	2.43	0.51
15:O:30:ASN:OD1	15:O:31:ILE:N	2.40	0.51
18:R:2:VAL:HG21	18:R:37:GLU:OE1	2.10	0.51
7:G:324:ASP:OD1	7:G:324:ASP:N	2.43	0.51
52:H:401:U10:H201	52:H:401:U10:C25	2.35	0.51
52:H:401:U10:H151	52:H:401:U10:H18	1.92	0.51
12:L:67:HIS:CE1	12:L:70:THR:HG1	2.28	0.51
15:O:18:MET:HE3	15:O:116:LEU:HD23	1.91	0.51
5:E:104:THR:HG22	5:E:104:THR:O	2.10	0.51
20:T:32:VAL:HG13	20:T:33:ASN:OD1	2.10	0.51
32:g:110:SER:O	41:p:161:ARG:NH2	2.44	0.51
1:A:35:SER:O	2:B:81:ARG:NH2	2.43	0.51
2:B:44:SER:OG	8:H:51:ASP:OD1	2.17	0.51
12:L:295:GLN:O	12:L:301:ILE:HD11	2.11	0.51
12:L:76:LEU:HD21	12:L:196:TRP:CE3	2.45	0.51
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.45	0.51
34:i:100:LYS:O	40:o:49:GLN:NE2	2.44	0.51
12:L:466:TYR:O	12:L:470:ASN:ND2	2.38	0.50
5:E:172:ILE:HG23	5:E:182:PRO:HG2	1.92	0.50
40:o:91:HIS:O	40:o:95:VAL:HG23	2.12	0.50
16:P:14:SER:OG	61:P:601:HOH:O	2.16	0.50
3:C:77:ASP:OD1	4:D:390:LYS:NZ	2.34	0.50
14:N:342:MET:SD	53:d:201:CDL:H473	2.52	0.50
16:P:306:GLU:N	16:P:306:GLU:OE1	2.45	0.50
17:Q:89:LYS:NZ	17:Q:107:GLU:OE1	2.44	0.50
33:h:110:VAL:CG1	33:h:114:MET:HE3	2.41	0.50
2:B:62:MET:HE3	2:B:69:MET:SD	2.51	0.50
5:E:151:ALA:HB3	5:E:163:ASP:HA	1.94	0.50
13:M:423:ILE:HD11	38:m:58:VAL:HG13	1.93	0.50
8:H:225:MET:SD	52:H:401:U10:H211	2.51	0.50
4:D:161:ILE:HD11	4:D:235:TRP:HE3	1.76	0.49
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.43	0.49
26:a:37:ARG:NE	61:a:203:HOH:O	2.44	0.49
18:R:2:VAL:HG22	18:R:39:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:31:ILE:O	15:O:179:VAL:HG13	2.12	0.49
2:B:175:ILE:HD12	16:P:52:GLU:HG2	1.94	0.49
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.49
15:O:191:GLU:OE2	55:O:401:DGT:O3'	2.24	0.49
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.42	0.49
37:l:132:GLN:OE1	40:o:36:ARG:NH1	2.43	0.49
7:G:99:ALA:O	7:G:134:LYS:NZ	2.46	0.49
6:F:154:ARG:NH2	44:s:54:LEU:HD23	2.28	0.49
12:L:558:LEU:HB2	13:M:214:LEU:HD11	1.95	0.49
52:H:401:U10:C8	52:H:401:U10:C1M	2.91	0.48
5:E:105:THR:HG22	5:E:106:THR:H	1.78	0.48
4:D:223:ASP:OD2	61:D:508:HOH:O	2.20	0.48
7:G:156:CYS:O	7:G:157:THR:OG1	2.26	0.48
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.95	0.48
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.96	0.48
9:I:14:MET:HE1	27:b:12:TRP:CD1	2.48	0.48
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.96	0.48
12:L:375:VAL:HG13	12:L:462:LEU:HD21	1.95	0.48
15:O:128:ILE:HD12	15:O:160:ILE:HD12	1.95	0.48
6:F:84:LYS:NZ	6:F:212:ASP:OD1	2.47	0.48
6:F:234:ILE:O	6:F:238:GLY:N	2.47	0.48
40:o:37:GLU:N	40:o:37:GLU:OE1	2.45	0.48
26:a:67:GLU:N	26:a:67:GLU:OE1	2.42	0.48
12:L:432:LEU:HD11	36:k:62:PHE:HA	1.95	0.48
6:F:103:GLY:O	6:F:333:ALA:HB1	2.14	0.47
8:H:179:TRP:N	8:H:180:PRO:CD	2.77	0.47
44:s:42:GLN:OE1	44:s:42:GLN:N	2.42	0.47
3:C:113:GLU:OE2	17:Q:98:LYS:NZ	2.44	0.47
5:E:55:GLN:O	5:E:59:GLY:N	2.42	0.47
8:H:111:LEU:HD11	10:J:57:PHE:HD1	1.76	0.47
16:P:175:GLU:N	16:P:175:GLU:OE1	2.47	0.47
16:P:5:VAL:HG12	16:P:5:VAL:O	2.13	0.47
39:n:15:VAL:HG12	39:n:63:LEU:HD13	1.95	0.47
17:Q:27:GLU:OE1	17:Q:27:GLU:N	2.44	0.47
5:E:191:PHE:N	5:E:194:GLU:OE2	2.38	0.47
16:P:215:ILE:HG22	16:P:219:LYS:HE2	1.97	0.47
4:D:415:VAL:HG21	8:H:206:GLU:HB3	1.96	0.47
37:l:7:ASP:O	37:l:8:MET:HE2	2.15	0.47
13:M:285:LEU:HD23	13:M:285:LEU:C	2.39	0.47
14:N:313:MET:HE1	15:O:102:ALA:HB3	1.95	0.47
44:s:71:GLU:OE1	44:s:71:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:110:GLN:NE2	61:G:915:HOH:O	2.39	0.47
33:h:143:ASN:O	33:h:143:ASN:ND2	2.42	0.47
4:D:49:LEU:HD13	4:D:51:PHE:CZ	2.50	0.47
9:I:44:GLU:HA	26:a:1:MET:HE3	1.96	0.47
32:g:114:ASP:OD2	32:g:116:SER:OG	2.25	0.47
6:F:407:LEU:HD23	6:F:407:LEU:O	2.14	0.47
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.50	0.47
37:l:81:LEU:HD13	37:l:81:LEU:C	2.39	0.47
12:L:378:LEU:HD21	36:k:66:LEU:HD22	1.97	0.46
13:M:167:ILE:HD13	13:M:249:ILE:HD12	1.98	0.46
6:F:363:THR:HG21	7:G:97:LEU:HD13	1.97	0.46
13:M:423:ILE:CD1	38:m:58:VAL:HG13	2.45	0.46
16:P:183:ALA:O	16:P:186:ARG:NH1	2.48	0.46
12:L:199:GLN:NE2	41:p:110:LYS:O	2.49	0.46
14:N:272:LYS:HB3	24:Y:140:VAL:HG21	1.97	0.46
35:j:61:ASP:OD1	40:o:106:ARG:NH1	2.49	0.46
4:D:161:ILE:HD12	8:H:278:PRO:HB2	1.98	0.46
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.96	0.46
21:V:112:LYS:NZ	21:V:115:ILE:O	2.47	0.46
5:E:194:GLU:OE1	6:F:28:ARG:NH2	2.38	0.46
12:L:421:ILE:HA	12:L:501:ALA:HB2	1.97	0.46
38:m:34:GLU:N	38:m:34:GLU:OE1	2.49	0.46
13:M:41:LEU:O	13:M:44:GLN:NE2	2.47	0.46
36:k:87:LEU:O	36:k:87:LEU:HD23	2.16	0.46
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.97	0.45
5:E:151:ALA:O	5:E:152:PRO:C	2.57	0.45
8:H:146:LEU:HD11	8:H:192:GLU:HG3	1.97	0.45
9:I:14:MET:HE3	45:b:102:3PE:C27	2.46	0.45
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.47	0.45
40:o:59:ALA:O	40:o:60:HIS:CG	2.68	0.45
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.30	0.45
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.97	0.45
20:U:87:TYR:OH	34:i:26:GLU:OE2	2.24	0.45
6:F:407:LEU:HD23	6:F:407:LEU:C	2.42	0.45
12:L:371:THR:O	12:L:375:VAL:HG23	2.17	0.45
15:O:126:ARG:NE	15:O:206:TYR:OH	2.46	0.45
5:E:14:GLU:N	5:E:14:GLU:OE1	2.49	0.45
8:H:18:ALA:O	8:H:21:THR:OG1	2.33	0.45
20:U:52:MET:HE3	39:n:24:ARG:CD	2.46	0.45
7:G:422:LEU:O	7:G:428:ILE:HD13	2.16	0.45
33:h:40:ILE:O	33:h:44:ASN:ND2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:h:201:CDL:OB3	41:p:48:ARG:NH1	2.50	0.45
6:F:82:MET:HE1	6:F:92:TYR:O	2.16	0.45
2:B:59:MET:SD	2:B:62:MET:HE2	2.57	0.45
4:D:352:TYR:HD1	9:I:86:VAL:HG21	1.81	0.45
7:G:272:ASP:OD1	7:G:681:SER:OG	2.34	0.45
7:G:539:LYS:O	7:G:540:ASP:OD1	2.35	0.45
34:i:119:MET:HE3	34:i:122:PHE:CE1	2.51	0.45
7:G:684:MET:HA	7:G:684:MET:HE2	1.99	0.45
11:K:73:LEU:HD22	14:N:38:LEU:HD12	1.99	0.45
12:L:457:LEU:O	12:L:461:SER:N	2.40	0.45
12:L:598:SER:CB	14:N:100:MET:HE1	2.47	0.45
34:i:21:TRP:CZ3	39:n:171:THR:HG22	2.52	0.45
37:l:39:ASP:O	38:m:80:ARG:NH2	2.50	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.44
13:M:304:GLN:O	29:d:119:VAL:HG11	2.17	0.44
34:i:38:ARG:NE	34:i:38:ARG:O	2.49	0.44
7:G:460:ARG:NH2	7:G:462:ASP:OD2	2.51	0.44
13:M:141:GLU:N	13:M:141:GLU:OE1	2.50	0.44
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.99	0.44
13:M:76:MET:SD	13:M:230:VAL:HB	2.58	0.44
13:M:168:GLN:O	13:M:172:GLY:N	2.44	0.44
14:N:232:HIS:HB3	14:N:311:MET:HE3	2.00	0.44
16:P:103:ASN:OD1	16:P:103:ASN:N	2.50	0.44
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.53	0.44
34:i:69:PHE:HD2	59:i:201:CHD:H111	1.82	0.44
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.35	0.44
7:G:334:LEU:HD13	7:G:604:SER:HB3	1.99	0.44
37:l:128:VAL:HG11	40:o:94:TYR:CZ	2.53	0.44
42:q:3:LEU:HD13	42:q:3:LEU:C	2.42	0.44
4:D:224:GLU:OE1	9:I:40:TYR:OH	2.29	0.44
13:M:270:ILE:N	13:M:270:ILE:HD12	2.33	0.44
19:S:22:LEU:HD23	19:S:22:LEU:N	2.33	0.44
20:T:11:ILE:CD1	20:T:86:VAL:HG11	2.48	0.44
34:i:109:ILE:N	34:i:109:ILE:HD12	2.32	0.44
39:n:19:TYR:CZ	39:n:23:LEU:HD11	2.52	0.44
1:A:20:ILE:HG22	46:A:204:PC1:C29	2.48	0.44
8:H:28:LEU:HD13	8:H:275:ALA:HB2	1.99	0.44
12:L:257:ILE:HG23	12:L:317:ILE:HD11	1.98	0.44
20:U:31:SER:O	20:U:34:SER:OG	2.16	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.44
20:T:8:LEU:HD13	20:T:8:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASP:OD1	8:H:58:LYS:NZ	2.44	0.43
2:B:91:THR:HA	2:B:119:CYS:HB3	1.99	0.43
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.00	0.43
22:W:17:LYS:NZ	61:W:204:HOH:O	2.51	0.43
39:n:27:GLU:OE2	39:n:33:ARG:NH1	2.50	0.43
6:F:309:LYS:NZ	6:F:313:GLU:OE2	2.50	0.43
7:G:556:ILE:HD12	7:G:556:ILE:O	2.18	0.43
11:K:82:SER:O	11:K:86:GLY:N	2.46	0.43
14:N:324:THR:HG22	14:N:325:PHE:CD2	2.53	0.43
16:P:1:LEU:HD13	16:P:3:HIS:NE2	2.33	0.43
12:L:593:ILE:HG22	12:L:597:ILE:HD12	2.01	0.43
13:M:97:THR:HG21	53:M:602:CDL:H202	2.00	0.43
23:X:102:GLN:OE1	23:X:102:GLN:N	2.48	0.43
31:f:11:TRP:O	31:f:14:VAL:HG22	2.18	0.43
7:G:371:VAL:HG22	7:G:450:MET:HE1	2.01	0.43
10:J:23:LYS:NZ	11:K:18:GLY:O	2.49	0.43
12:L:140:LEU:O	12:L:140:LEU:HD23	2.19	0.43
12:L:257:ILE:HG22	12:L:329:ILE:HD11	2.00	0.43
13:M:18:SER:OG	13:M:26:ASN:OD1	2.19	0.43
53:M:602:CDL:H872	53:M:602:CDL:H232	2.00	0.43
59:i:201:CHD:H212	59:i:201:CHD:C12	2.37	0.43
6:F:306:LEU:C	6:F:306:LEU:HD12	2.43	0.43
7:G:293:HIS:ND1	16:P:1:LEU:HD12	2.33	0.43
9:I:129:ASP:OD1	9:I:129:ASP:N	2.50	0.43
46:L:702:PC1:O13	46:L:702:PC1:H132	2.18	0.43
15:O:22:SER:HB3	15:O:115:LEU:HD11	1.99	0.43
21:V:17:GLU:OE1	21:V:17:GLU:N	2.41	0.43
13:M:1:FME:SD	13:M:111:THR:HG21	2.58	0.43
13:M:181:TYR:O	41:p:152:ARG:NH1	2.51	0.43
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.53	0.43
38:m:124:PHE:HA	41:p:135:VAL:HG11	2.01	0.43
3:C:40:VAL:HG13	3:C:50:ILE:HD13	2.01	0.43
37:l:63:ASP:O	38:m:43:LYS:NZ	2.51	0.43
11:K:40:LEU:HD12	14:N:68:MET:HE3	2.00	0.43
41:p:143:HIS:O	41:p:157:LYS:NZ	2.50	0.43
7:G:651:LEU:HD21	19:S:45:LYS:HE2	2.00	0.43
10:J:171:ILE:HG23	14:N:45:MET:HE2	2.01	0.43
11:K:63:LEU:HD23	11:K:63:LEU:O	2.19	0.43
13:M:14:LEU:HD21	13:M:30:HIS:CD2	2.54	0.43
15:O:156:LYS:O	15:O:160:ILE:HG22	2.19	0.43
32:g:70:LEU:O	32:g:74:SER:OG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:55:LEU:HD13	34:i:55:LEU:C	2.43	0.43
1:A:27:LEU:CD1	46:A:202:PC1:H133	2.49	0.43
6:F:192:LEU:C	6:F:192:LEU:HD23	2.43	0.43
7:G:317:ALA:HB3	7:G:343:LEU:HD13	2.01	0.43
7:G:443:LEU:HD13	7:G:477:ILE:HD11	2.01	0.43
10:J:78:GLN:O	10:J:79:TYR:C	2.60	0.43
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.54	0.43
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.00	0.43
12:L:230:HIS:N	12:L:231:PRO:HD3	2.34	0.42
18:R:9:GLU:OE1	18:R:25:LYS:NZ	2.52	0.42
23:X:17:VAL:HG12	23:X:19:VAL:HG22	2.01	0.42
2:B:46:TRP:CH2	52:H:401:U10:H1M2	2.54	0.42
3:C:8:ARG:HB2	3:C:11:VAL:HG22	2.02	0.42
10:J:51:PHE:CE2	10:J:55:MET:HE3	2.54	0.42
35:j:47:VAL:HG22	35:j:47:VAL:O	2.17	0.42
2:B:30:VAL:HG13	2:B:173:LEU:HB3	2.01	0.42
8:H:195:ARG:HD3	8:H:231:ILE:HD11	2.02	0.42
16:P:253:PHE:C	16:P:254:LEU:HD22	2.44	0.42
8:H:289:LEU:C	8:H:289:LEU:HD13	2.44	0.42
46:L:702:PC1:H142	53:h:201:CDL:OA3	2.20	0.42
14:N:270:MET:CE	14:N:278:LEU:HD23	2.49	0.42
4:D:27:HIS:NE2	20:T:1:SER:O	2.52	0.42
16:P:145:TYR:N	16:P:282:ASP:OD2	2.51	0.42
14:N:105:LYS:NZ	61:N:507:HOH:O	2.53	0.42
14:N:115:VAL:HB	14:N:116:PRO:HD3	2.02	0.42
16:P:75:GLY:N	61:P:604:HOH:O	2.35	0.42
23:X:105:GLN:OE1	23:X:105:GLN:N	2.52	0.42
34:i:85:LEU:O	34:i:90:THR:HG23	2.20	0.42
2:B:121:ASN:HB3	9:I:114:THR:HG22	2.01	0.42
13:M:106:LEU:HD13	13:M:234:VAL:HG11	2.02	0.42
53:M:602:CDL:H872	53:M:602:CDL:C23	2.50	0.42
16:P:182:PHE:HZ	16:P:287:ILE:HG23	1.84	0.42
29:d:5:ARG:NH2	29:d:17:GLU:OE2	2.53	0.42
38:m:74:ASN:OD1	38:m:78:ASN:ND2	2.53	0.42
10:J:167:VAL:HG22	14:N:42:PRO:HG3	2.01	0.42
12:L:100:ILE:HG21	12:L:246:LEU:HB2	2.02	0.42
25:Z:142:TYR:CZ	26:a:48:MET:HE1	2.55	0.42
4:D:202:ASP:OD1	4:D:203:LEU:N	2.52	0.42
8:H:207:LEU:HD12	8:H:207:LEU:N	2.34	0.42
9:I:14:MET:HE2	27:b:9:LYS:HG2	2.02	0.42
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:146:PHE:N	14:N:147:PRO:CD	2.83	0.42
16:P:238:LEU:O	16:P:242:VAL:HG23	2.20	0.42
34:i:123:PRO:O	34:i:124:ASP:C	2.63	0.42
16:P:96:GLY:O	57:P:501:NDP:H8A	2.20	0.41
16:P:157:ARG:NH1	16:P:163:ALA:O	2.45	0.41
42:q:51:ASP:OD2	61:q:302:HOH:O	2.21	0.41
4:D:385:ARG:NE	61:D:516:HOH:O	2.41	0.41
12:L:237:MET:HE3	12:L:303:ALA:HB2	2.02	0.41
34:i:112:THR:HG23	34:i:114:GLU:H	1.84	0.41
14:N:19:ILE:O	14:N:23:SER:OG	2.31	0.41
4:D:328:ALA:O	4:D:351:LEU:HD11	2.21	0.41
7:G:194:GLU:OE1	7:G:194:GLU:N	2.40	0.41
7:G:331:LEU:HD22	7:G:525:LEU:HD22	2.02	0.41
12:L:331:THR:HB	12:L:387:THR:HG22	2.03	0.41
1:A:68:GLU:HG2	10:J:161:LEU:HD13	2.03	0.41
8:H:20:LEU:HD13	26:a:12:MET:HE1	2.03	0.41
12:L:257:ILE:CG2	12:L:329:ILE:HD11	2.50	0.41
12:L:286:LEU:C	12:L:286:LEU:HD13	2.45	0.41
13:M:373:ILE:HD11	13:M:444:LEU:HD12	2.01	0.41
45:Y:204:3PE:O12	45:Y:206:3PE:N	2.45	0.41
6:F:258:ILE:HD12	6:F:258:ILE:H	1.86	0.41
17:Q:89:LYS:HD2	17:Q:105:VAL:HG11	2.02	0.41
4:D:100:LEU:HB3	4:D:101:PRO:HD3	2.03	0.41
4:D:106:LEU:HD13	4:D:391:ILE:HG21	2.02	0.41
6:F:263:ASN:ND2	6:F:285:GLY:O	2.42	0.41
6:F:306:LEU:HD12	6:F:306:LEU:O	2.20	0.41
46:J:203:PC1:O13	46:J:203:PC1:H133	2.19	0.41
13:M:458:LEU:HD12	13:M:458:LEU:N	2.36	0.41
34:i:66:HIS:HD2	59:i:201:CHD:H231	1.82	0.41
35:j:45:ASP:O	35:j:49:GLY:N	2.48	0.41
16:P:201:VAL:HG13	16:P:340:ILE:HD12	2.02	0.41
42:q:3:LEU:HD13	42:q:3:LEU:O	2.21	0.41
5:E:118:GLU:N	5:E:118:GLU:OE1	2.54	0.41
12:L:173:LEU:HD23	12:L:173:LEU:C	2.46	0.41
12:L:282:ALA:HA	12:L:285:THR:HG22	2.02	0.41
12:L:429:PHE:CE1	39:n:31:ILE:HD13	2.56	0.41
24:Y:120:THR:O	24:Y:124:VAL:HG23	2.21	0.41
30:e:19:ILE:HG21	33:h:128:ILE:HG21	2.03	0.41
34:i:21:TRP:CE3	39:n:171:THR:HG22	2.56	0.41
4:D:100:LEU:C	4:D:100:LEU:HD13	2.46	0.41
12:L:429:PHE:HE1	39:n:31:ILE:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:559:GLU:HG2	13:M:214:LEU:HD13	2.03	0.41
12:L:562:LEU:CB	12:L:563:PRO:CD	2.98	0.41
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.02	0.41
43:r:24:GLN:NE2	61:r:303:HOH:O	2.38	0.41
12:L:89:PHE:CD2	12:L:132:VAL:HG21	2.56	0.40
34:i:71:PHE:CD1	34:i:75:LEU:HD23	2.56	0.40
42:q:42:ASP:OD1	42:q:46:ASN:N	2.54	0.40
6:F:98:ASP:O	6:F:99:GLU:C	2.65	0.40
8:H:224:PHE:CE2	52:H:401:U10:H72	2.56	0.40
13:M:375:LEU:C	13:M:375:LEU:HD13	2.46	0.40
18:R:1:GLY:N	18:R:42:ASP:OD2	2.38	0.40
25:Z:119:MET:HE2	30:e:71:THR:CG2	2.52	0.40
37:l:127:PRO:O	37:l:128:VAL:HG13	2.20	0.40
9:I:14:MET:HE3	45:b:102:3PE:H272	2.03	0.40
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.51	0.40
13:M:130:LEU:HD21	14:N:294:MET:CE	2.51	0.40
13:M:423:ILE:CD1	38:m:58:VAL:HG22	2.51	0.40
16:P:294:LEU:HD12	16:P:294:LEU:N	2.36	0.40
10:J:104:VAL:HA	10:J:107:VAL:HG12	2.03	0.40
12:L:558:LEU:HB3	13:M:214:LEU:HD11	2.04	0.40
36:k:35:LEU:HD11	39:n:41:CYS:SG	2.61	0.40
37:l:68:ASP:OD1	37:l:68:ASP:N	2.53	0.40
42:q:24:LEU:HD13	46:q:201:PC1:H221	2.04	0.40
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.03	0.40
4:D:300:ARG:NH2	4:D:420:THR:O	2.50	0.40
7:G:659:ASP:OD1	7:G:659:ASP:N	2.53	0.40
14:N:314:LYS:NZ	15:O:274:SER:OG	2.47	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%)	108 (96%)	5 (4%)	0	100	100
2	B	154/216 (71%)	149 (97%)	5 (3%)	0	100	100
3	C	205/266 (77%)	198 (97%)	7 (3%)	0	100	100
4	D	412/463 (89%)	397 (96%)	15 (4%)	0	100	100
5	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
6	F	430/464 (93%)	420 (98%)	10 (2%)	0	100	100
7	G	689/727 (95%)	669 (97%)	20 (3%)	0	100	100
8	H	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
11	K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	28
12	L	604/606 (100%)	578 (96%)	25 (4%)	1 (0%)	43	66
13	M	457/459 (100%)	449 (98%)	8 (2%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	312 (98%)	6 (2%)	0	100	100
16	P	335/380 (88%)	325 (97%)	10 (3%)	0	100	100
17	Q	127/175 (73%)	126 (99%)	1 (1%)	0	100	100
18	R	94/124 (76%)	88 (94%)	6 (6%)	0	100	100
19	S	84/99 (85%)	83 (99%)	1 (1%)	0	100	100
20	T	86/156 (55%)	79 (92%)	7 (8%)	0	100	100
20	U	86/156 (55%)	79 (92%)	7 (8%)	0	100	100
21	V	112/116 (97%)	109 (97%)	3 (3%)	0	100	100
22	W	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	140/144 (97%)	137 (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%)	45 (96%)	2 (4%)	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	i	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
35	j	69/108 (64%)	68 (99%)	1 (1%)	0	100	100
36	k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	m	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
39	n	169/179 (94%)	157 (93%)	12 (7%)	0	100	100
40	o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	p	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	87 (96%)	4 (4%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8173/9213 (89%)	7904 (97%)	267 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
11	K	2	SER

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%)	99 (99%)	1 (1%)	68	86
2	B	132/175 (75%)	127 (96%)	5 (4%)	29	56
3	C	188/228 (82%)	187 (100%)	1 (0%)	81	92
4	D	361/392 (92%)	355 (98%)	6 (2%)	53	78
5	E	183/205 (89%)	178 (97%)	5 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	346/368 (94%)	342 (99%)	4 (1%)	63	83
7	G	579/608 (95%)	571 (99%)	8 (1%)	59	81
8	H	274/274 (100%)	270 (98%)	4 (2%)	57	80
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	82
10	J	141/141 (100%)	138 (98%)	3 (2%)	47	73
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	70
12	L	533/533 (100%)	526 (99%)	7 (1%)	61	82
13	M	412/412 (100%)	408 (99%)	4 (1%)	68	86
14	N	315/315 (100%)	311 (99%)	4 (1%)	61	82
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	69
16	P	293/327 (90%)	286 (98%)	7 (2%)	43	70
17	Q	116/153 (76%)	115 (99%)	1 (1%)	70	87
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	82
19	S	76/82 (93%)	74 (97%)	2 (3%)	40	68
20	T	81/135 (60%)	75 (93%)	6 (7%)	13	29
20	U	81/135 (60%)	79 (98%)	2 (2%)	42	69
21	V	101/102 (99%)	97 (96%)	4 (4%)	28	55
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	87
23	X	154/155 (99%)	152 (99%)	2 (1%)	61	82
24	Y	101/102 (99%)	97 (96%)	4 (4%)	28	55
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	88
26	a	59/59 (100%)	57 (97%)	2 (3%)	32	60
27	b	71/72 (99%)	69 (97%)	2 (3%)	38	66
28	c	45/68 (66%)	44 (98%)	1 (2%)	45	72
29	d	105/105 (100%)	103 (98%)	2 (2%)	50	75
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	60
31	f	54/54 (100%)	54 (100%)	0	100	100
32	g	92/131 (70%)	88 (96%)	4 (4%)	26	51
33	h	121/158 (77%)	118 (98%)	3 (2%)	42	69
34	i	120/121 (99%)	117 (98%)	3 (2%)	42	69
35	j	61/84 (73%)	60 (98%)	1 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	63/76 (83%)	60 (95%)	3 (5%)	23	47
37	l	140/159 (88%)	136 (97%)	4 (3%)	37	65
38	m	113/114 (99%)	111 (98%)	2 (2%)	51	76
39	n	156/161 (97%)	154 (99%)	2 (1%)	61	82
40	o	110/120 (92%)	109 (99%)	1 (1%)	70	87
41	p	155/157 (99%)	154 (99%)	1 (1%)	78	91
42	q	130/130 (100%)	127 (98%)	3 (2%)	44	71
43	r	85/97 (88%)	83 (98%)	2 (2%)	43	70
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7205/7891 (91%)	7072 (98%)	133 (2%)	51	76

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
2	B	54	CYS
2	B	82	GLN
2	B	91	THR
2	B	100	LEU
2	B	102	LYS
3	C	20	LYS
4	D	75	LYS
4	D	161	ILE
4	D	245	VAL
4	D	290	ARG
4	D	334	LYS
4	D	420	THR
5	E	29	LYS
5	E	63	ILE
5	E	118	GLU
5	E	169	ILE
5	E	181	ILE
6	F	8	LYS
6	F	34	LYS
6	F	82	MET
6	F	438	GLN
7	G	61	LYS
7	G	224	LYS
7	G	475	GLN

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Mol	Chain	Res	Type
7	G	483	VAL
7	G	486	ASP
7	G	539	LYS
7	G	540	ASP
7	G	613	TYR
8	H	5	ASN
8	H	103	LEU
8	H	121	TRP
8	H	234	MET
9	I	14	MET
9	I	129	ASP
10	J	114	GLU
10	J	133	SER
10	J	135	PHE
11	K	34	GLU
11	K	37	MET
12	L	31	ASN
12	L	101	MET
12	L	172	ILE
12	L	336	LYS
12	L	445	GLU
12	L	487	LYS
12	L	580	GLN
13	M	57	PHE
13	M	86	LYS
13	M	207	MET
13	M	413	MET
14	N	40	ILE
14	N	46	LYS
14	N	236	LYS
14	N	263	LYS
15	O	40	LYS
15	O	79	LEU
15	O	81	LYS
15	O	126	ARG
15	O	157	LYS
15	O	186	LYS
15	O	242	LYS
16	P	52	GLU
16	P	122	LYS
16	P	139	ILE
16	P	199	LYS

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Mol	Chain	Res	Type
16	P	219	LYS
16	P	269	LEU
16	P	281	ARG
17	Q	16	LYS
18	R	77	LYS
19	S	38	LYS
19	S	47	ASN
20	T	8	LEU
20	T	16	LEU
20	T	20	LYS
20	T	28	GLU
20	T	30	LEU
20	T	83	LYS
20	U	50	ILE
20	U	68	GLU
21	V	39	LYS
21	V	66	LYS
21	V	92	LYS
21	V	115	ILE
22	W	40	ARG
23	X	77	CYS
23	X	105	GLN
24	Y	2	LYS
24	Y	49	LEU
24	Y	50	GLU
24	Y	114	CYS
25	Z	133	LEU
26	a	1	MET
26	a	69	ILE
27	b	3	ARG
27	b	9	LYS
28	c	1	LYS
29	d	5	ARG
29	d	8	ARG
30	e	38	GLU
30	e	84	LYS
30	e	90	LYS
32	g	24	LEU
32	g	57	ASN
32	g	98	LYS
32	g	117	LYS
33	h	6	LYS

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Mol	Chain	Res	Type
33	h	113	LEU
33	h	143	ASN
34	i	38	ARG
34	i	43	GLU
34	i	48	LYS
35	j	43	ASP
36	k	22	LYS
36	k	35	LEU
36	k	91	LYS
37	l	6	LYS
37	l	126	GLN
37	l	148	LYS
37	l	158	ILE
38	m	39	ARG
38	m	84	LYS
39	n	54	LYS
39	n	137	LYS
40	o	7	ARG
41	p	126	LYS
42	q	53	LYS
42	q	132	LYS
42	q	136	GLU
43	r	24	GLN
43	r	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
3	C	71	GLN
3	C	160	HIS
3	C	192	GLN
3	C	211	GLN
4	D	98	GLN
5	E	42	HIS
5	E	58	ASN
5	E	74	GLN
5	E	150	ASN
6	F	257	ASN
6	F	373	ASN
7	G	28	GLN
7	G	82	ASN

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Mol	Chain	Res	Type
7	G	141	ASN
7	G	155	GLN
7	G	402	ASN
8	H	99	ASN
8	H	317	GLN
12	L	170	GLN
13	M	81	GLN
13	M	88	ASN
13	M	139	GLN
13	M	220	HIS
13	M	338	HIS
15	O	114	HIS
15	O	190	HIS
16	P	44	GLN
17	Q	29	HIS
19	S	85	GLN
20	U	47	GLN
23	X	29	HIS
23	X	34	GLN
25	Z	75	GLN
29	d	79	GLN
30	e	26	HIS
32	g	57	ASN
33	h	63	HIS
36	k	20	GLN
38	m	78	ASN
40	o	46	ASN
40	o	109	GLN
42	q	59	HIS
42	q	112	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
1	FME	A	1	1	8,9,10	1.50	1 (12%)	8,9,11	1.35	1 (12%)
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.34	1 (16%)
43	AYA	r	1	43	6,7,8	1.89	2 (33%)	6,8,10	1.39	1 (16%)
8	FME	H	1	8	8,9,10	1.51	1 (12%)	8,9,11	1.46	2 (25%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	8,9,11	1.36	1 (12%)
27	AYA	b	1	27	6,7,8	1.91	2 (33%)	6,8,10	1.41	1 (16%)
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.25	1 (11%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	8,9,11	1.43	1 (12%)
4	2MR	D	85	4	10,12,13	2.48	2 (20%)	5,13,15	1.19	1 (20%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.34	1 (12%)
38	SAC	m	1	38	7,8,9	1.71	1 (14%)	7,9,11	1.28	1 (14%)
10	FME	J	1	10	8,9,10	1.50	1 (12%)	8,9,11	1.42	2 (25%)
42	AME	q	1	42	9,10,11	1.52	1 (11%)	9,11,13	1.36	2 (22%)
13	FME	M	1	13	8,9,10	1.50	1 (12%)	8,9,11	1.35	0
34	SAC	i	1	34	7,8,9	1.73	1 (14%)	7,9,11	1.56	1 (14%)

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
1	FME	A	1	1	-	1/7/9/11	-
24	AYA	Y	1	24	-	0/5/6/8	-
43	AYA	r	1	43	-	0/5/6/8	-
8	FME	H	1	8	-	1/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
27	AYA	b	1	27	-	1/5/6/8	-
29	AME	d	1	29	-	4/9/10/12	-
14	FME	N	1	14	-	2/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
12	FME	L	1	12	-	1/7/9/11	-
38	SAC	m	1	38	-	1/7/8/10	-
10	FME	J	1	10	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	AME	q	1	42	-	5/9/10/12	-
13	FME	M	1	13	-	0/7/9/11	-
34	SAC	i	1	34	-	4/7/8/10	-

All (19) 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	5.12	1.45	1.34
12	L	1	FME	CN-N	3.78	1.45	1.33
11	K	1	FME	CN-N	3.76	1.45	1.33
8	H	1	FME	CN-N	3.71	1.45	1.33
14	N	1	FME	CN-N	3.71	1.45	1.33
10	J	1	FME	CN-N	3.69	1.45	1.33
13	M	1	FME	CN-N	3.68	1.45	1.33
1	A	1	FME	CN-N	3.68	1.45	1.33
34	i	1	SAC	C1A-N	3.53	1.45	1.34
27	b	1	AYA	CT-N	3.50	1.45	1.34
29	d	1	AME	CT1-N	3.48	1.45	1.34
38	m	1	SAC	C1A-N	3.46	1.45	1.34
42	q	1	AME	CT1-N	3.45	1.45	1.34
43	r	1	AYA	CT-N	3.42	1.45	1.34
24	Y	1	AYA	CT-N	3.41	1.45	1.34
43	r	1	AYA	OT-CT	-2.10	1.18	1.23
27	b	1	AYA	OT-CT	-2.03	1.18	1.23
24	Y	1	AYA	OT-CT	-2.02	1.18	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.91	120.94	116.12
42	q	1	AME	CT2-CT1-N	2.44	120.17	116.12
43	r	1	AYA	CM-CT-N	2.43	120.16	116.12
27	b	1	AYA	CM-CT-N	2.42	120.13	116.12
24	Y	1	AYA	CM-CT-N	2.39	120.08	116.12
38	m	1	SAC	C2A-C1A-N	2.33	119.98	116.12
4	D	85	2MR	CD-NE-CZ	-2.18	119.28	123.36
1	A	1	FME	O1-CN-N	-2.17	119.71	125.32
10	J	1	FME	O1-CN-N	-2.12	119.84	125.32
29	d	1	AME	CT2-CT1-N	2.08	119.57	116.12
8	H	1	FME	CA-N-CN	-2.06	119.66	122.82
8	H	1	FME	O1-CN-N	-2.06	120.00	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	1	FME	O1-CN-N	-2.04	120.04	125.32
11	K	1	FME	O1-CN-N	-2.03	120.08	125.32
10	J	1	FME	CA-N-CN	-2.02	119.71	122.82
12	L	1	FME	O1-CN-N	-2.01	120.12	125.32
42	q	1	AME	CE-SD-CG	2.00	110.69	100.32

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 83 ligands modelled in this entry, 4 are monoatomic - leaving 79 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
55	DGT	O	401	56	32,33,33	3.31	14 (43%)	48,52,52	1.93	15 (31%)
48	SF4	B	201	2	0,12,12	-	-	-		
46	PC1	J	203	-	47,47,53	1.01	4 (8%)	53,55,61	1.05	2 (3%)
45	3PE	A	205	-	39,39,50	0.98	4 (10%)	42,44,55	1.08	2 (4%)
59	CHD	i	201	-	32,32,32	3.27	10 (31%)	51,51,51	2.40	17 (33%)
46	PC1	B	202	-	45,45,53	1.03	3 (6%)	51,53,61	1.06	2 (3%)
53	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.12	4 (5%)
46	PC1	I	204	-	43,43,53	1.05	4 (9%)	49,51,61	1.03	2 (4%)
45	3PE	Y	205	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
45	3PE	q	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.03	2 (3%)
45	3PE	Z	202	-	35,35,50	1.02	4 (11%)	38,40,55	1.13	2 (5%)
53	CDL	L	701	-	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
45	3PE	L	705	-	40,40,50	0.96	4 (10%)	43,45,55	1.17	2 (4%)
45	3PE	Y	203	-	26,26,50	1.19	4 (15%)	29,31,55	1.15	2 (6%)
45	3PE	Y	204	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)
45	3PE	b	102	-	36,36,50	1.02	4 (11%)	39,41,55	1.10	2 (5%)
47	PLC	A	206	-	37,37,41	0.55	0	43,45,49	0.53	0
47	PLC	L	703	-	35,35,41	0.55	0	41,43,49	0.53	0
46	PC1	A	202	-	34,34,53	1.17	4 (11%)	40,42,61	1.03	2 (5%)
46	PC1	H	404	-	46,46,53	1.01	4 (8%)	52,54,61	1.05	2 (3%)
53	CDL	M	602	-	99,99,99	0.88	8 (8%)	105,111,111	1.10	4 (3%)
45	3PE	M	604	-	49,49,50	0.88	4 (8%)	52,54,55	1.05	2 (3%)
49	FES	E	301	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	B	203	-	47,47,53	1.01	4 (8%)	53,55,61	1.09	2 (3%)
46	PC1	q	201	-	48,48,53	1.00	4 (8%)	54,56,61	1.02	2 (3%)
45	3PE	Y	207	-	44,44,50	0.93	4 (9%)	47,49,55	1.11	2 (4%)
46	PC1	H	403	-	40,40,53	1.10	4 (10%)	46,48,61	1.08	2 (4%)
46	PC1	h	202	-	37,37,53	1.07	3 (8%)	43,45,61	0.97	1 (2%)
45	3PE	M	603	-	28,28,50	1.14	4 (14%)	31,33,55	1.35	2 (6%)
48	SF4	I	202	9	0,12,12	-	-	-	-	-
58	EHZ	T	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.66	8 (22%)
47	PLC	J	202	-	34,34,41	0.55	0	40,42,49	0.55	0
46	PC1	I	203	-	53,53,53	0.94	4 (7%)	59,61,61	1.04	2 (3%)
45	3PE	Y	208	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
45	3PE	Y	202	-	44,44,50	0.93	4 (9%)	47,49,55	1.14	2 (4%)
45	3PE	K	101	-	43,43,50	0.94	4 (9%)	46,48,55	1.11	2 (4%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
47	PLC	Z	201	-	35,35,41	0.55	0	41,43,49	0.62	0
47	PLC	M	606	-	33,33,41	0.56	0	39,41,49	0.53	0
48	SF4	I	201	9	0,12,12	-	-	-	-	-
47	PLC	g	201	-	41,41,41	0.51	0	47,49,49	0.50	0
45	3PE	Y	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.11	2 (4%)
58	EHZ	U	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.63	5 (13%)
60	MYR	o	201	40	13,14,15	0.44	0	12,13,15	0.84	0
46	PC1	M	605	-	34,34,53	1.17	4 (11%)	40,42,61	1.08	2 (5%)
46	PC1	A	203	-	34,34,53	1.18	4 (11%)	40,42,61	1.11	2 (5%)
45	3PE	Z	203	-	41,41,50	0.96	4 (9%)	44,46,55	1.12	2 (4%)
53	CDL	h	201	-	75,75,99	1.01	8 (10%)	81,87,111	1.14	4 (4%)
53	CDL	d	202	-	86,86,99	0.94	7 (8%)	92,98,111	1.14	4 (4%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
57	NDP	P	501	-	51,52,52	3.99	27 (52%)	71,80,80	1.92	15 (21%)
53	CDL	H	402	-	57,57,99	1.11	7 (12%)	63,69,111	1.17	3 (4%)
48	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	A	201	-	46,46,50	0.89	4 (8%)	49,51,55	1.03	2 (4%)
45	3PE	L	704	-	33,33,50	1.06	4 (12%)	36,38,55	1.17	2 (5%)
46	PC1	l	701	-	46,46,53	1.02	4 (8%)	52,54,61	0.99	2 (3%)
45	3PE	i	202	-	44,44,50	0.91	4 (9%)	47,49,55	1.08	2 (4%)
52	U10	H	401	-	34,34,63	1.96	17 (50%)	42,44,79	1.49	5 (11%)
48	SF4	F	501	6	0,12,12	-	-	-	-	-
46	PC1	A	204	-	32,32,53	1.22	4 (12%)	38,40,61	1.05	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	PLC	O	403	-	30,30,41	0.55	0	34,37,49	0.61	0
50	FMN	F	502	-	33,33,33	2.71	10 (30%)	48,50,50	1.76	15 (31%)
53	CDL	N	401	-	93,93,99	0.91	8 (8%)	99,105,111	1.09	4 (4%)
45	3PE	f	101	-	23,23,50	1.25	4 (17%)	26,28,55	1.40	3 (11%)
47	PLC	Y	209	-	41,41,41	0.50	0	47,49,49	0.53	0
45	3PE	b	101	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	2 (4%)
46	PC1	L	702	-	43,43,53	1.05	4 (9%)	49,51,61	1.02	2 (4%)
46	PC1	d	204	-	38,38,53	1.13	4 (10%)	44,46,61	1.02	2 (4%)
45	3PE	r	202	-	29,29,50	1.13	4 (13%)	32,34,55	1.19	2 (6%)
45	3PE	d	203	-	48,48,50	0.89	4 (8%)	51,53,55	1.03	2 (3%)
45	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.12	2 (4%)
46	PC1	m	202	-	40,40,53	1.08	4 (10%)	46,48,61	1.04	2 (4%)
45	3PE	a	101	-	35,35,50	1.03	4 (11%)	38,40,55	1.03	2 (5%)
45	3PE	P	502	-	37,37,50	1.00	4 (10%)	40,42,55	1.14	2 (5%)
45	3PE	Y	206	-	50,50,50	0.87	4 (8%)	53,55,55	1.05	2 (3%)
47	PLC	O	404	-	30,30,41	0.59	0	36,38,49	0.60	0
45	3PE	J	201	-	36,36,50	1.02	4 (11%)	39,41,55	1.13	2 (5%)
53	CDL	r	201	-	60,60,99	1.13	7 (11%)	66,72,111	1.17	4 (6%)
45	3PE	N	402	-	48,48,50	0.89	4 (8%)	51,53,55	1.04	2 (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
55	DGT	O	401	56	-	9/22/34/34	0/3/3/3
48	SF4	B	201	2	-	-	0/6/5/5
46	PC1	J	203	-	-	23/51/51/57	-
45	3PE	A	205	-	-	15/43/43/54	-
59	CHD	i	201	-	-	4/9/74/74	0/4/4/4
46	PC1	B	202	-	-	21/49/49/57	-
53	CDL	d	201	-	-	36/75/75/110	-
46	PC1	I	204	-	-	14/47/47/57	-
45	3PE	Y	205	-	-	19/54/54/54	-
45	3PE	q	202	-	-	23/54/54/54	-
45	3PE	Z	202	-	-	14/39/39/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	CDL	L	701	-	-	41/110/110/110	-
45	3PE	L	705	-	-	23/44/44/54	-
45	3PE	Y	203	-	-	17/30/30/54	-
45	3PE	Y	204	-	-	16/54/54/54	-
45	3PE	b	102	-	-	18/40/40/54	-
47	PLC	A	206	-	-	10/41/41/45	-
47	PLC	L	703	-	-	16/39/39/45	-
46	PC1	A	202	-	-	15/38/38/57	-
46	PC1	H	404	-	-	25/50/50/57	-
53	CDL	M	602	-	-	47/110/110/110	-
45	3PE	M	604	-	-	22/53/53/54	-
49	FES	E	301	5	-	-	0/1/1/1
46	PC1	B	203	-	-	20/51/51/57	-
46	PC1	q	201	-	-	12/52/52/57	-
45	3PE	Y	207	-	-	29/48/48/54	-
46	PC1	H	403	-	-	11/44/44/57	-
46	PC1	h	202	-	-	17/40/40/57	-
45	3PE	M	603	-	-	13/31/31/54	-
48	SF4	I	202	9	-	-	0/6/5/5
58	EHZ	T	101	20	-	14/42/44/45	-
47	PLC	J	202	-	-	10/38/38/45	-
46	PC1	I	203	-	-	18/57/57/57	-
45	3PE	Y	208	-	-	17/39/39/54	-
45	3PE	Y	202	-	-	17/48/48/54	-
45	3PE	K	101	-	-	13/47/47/54	-
49	FES	G	803	7	-	-	0/1/1/1
47	PLC	Z	201	-	-	14/39/39/45	-
47	PLC	M	606	-	-	12/37/37/45	-
48	SF4	I	201	9	-	-	0/6/5/5
47	PLC	g	201	-	-	13/45/45/45	-
45	3PE	Y	201	-	-	16/44/44/54	-
58	EHZ	U	101	20	-	10/42/44/45	-
60	MYR	o	201	40	-	2/12/12/13	-
46	PC1	M	605	-	-	15/38/38/57	-
46	PC1	A	203	-	-	11/38/38/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Z	203	-	-	13/45/45/54	-
53	CDL	h	201	-	-	29/86/86/110	-
53	CDL	d	202	-	-	47/97/97/110	-
48	SF4	G	802	7	-	-	0/6/5/5
57	NDP	P	501	-	-	12/34/77/77	0/5/5/5
53	CDL	H	402	-	-	27/67/67/110	-
48	SF4	G	801	7	-	-	0/6/5/5
45	3PE	A	201	-	-	14/50/50/54	-
45	3PE	L	704	-	-	11/37/37/54	-
46	PC1	l	701	-	-	18/50/50/57	-
45	3PE	i	202	-	-	25/48/48/54	-
52	U10	H	401	-	-	10/29/53/87	0/1/1/1
48	SF4	F	501	6	-	-	0/6/5/5
46	PC1	A	204	-	-	17/36/36/57	-
47	PLC	O	403	-	-	6/33/33/45	-
50	FMN	F	502	-	-	6/18/18/18	0/3/3/3
53	CDL	N	401	-	-	35/104/104/110	-
45	3PE	f	101	-	-	12/26/26/54	-
47	PLC	Y	209	-	-	17/45/45/45	-
45	3PE	b	101	-	-	23/45/45/54	-
46	PC1	L	702	-	-	22/47/47/57	-
46	PC1	d	204	-	-	22/42/42/57	-
45	3PE	r	202	-	-	16/33/33/54	-
45	3PE	d	203	-	-	20/52/52/54	-
45	3PE	m	201	-	-	10/44/44/54	-
46	PC1	m	202	-	-	14/44/44/57	-
45	3PE	a	101	-	-	15/39/39/54	-
45	3PE	P	502	-	-	20/41/41/54	-
45	3PE	Y	206	-	-	24/54/54/54	-
47	PLC	O	404	-	-	14/34/34/45	-
45	3PE	J	201	-	-	22/40/40/54	-
53	CDL	r	201	-	-	30/71/71/110	-
45	3PE	N	402	-	-	28/52/52/54	-

All (331) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.23	1.70	1.59
57	P	501	NDP	C2B-C1B	-9.03	1.30	1.53
59	i	201	CHD	C11-C12	8.84	1.67	1.53
55	O	401	DGT	O6-C6	8.74	1.40	1.23
57	P	501	NDP	O4B-C1B	8.56	1.61	1.42
57	P	501	NDP	O4D-C1D	8.27	1.61	1.42
57	P	501	NDP	C7N-N7N	7.61	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.38	1.30	1.53
59	i	201	CHD	C16-C15	7.19	1.73	1.54
57	P	501	NDP	C6N-C5N	7.07	1.54	1.33
55	O	401	DGT	C5-N7	6.77	1.52	1.39
57	P	501	NDP	O4D-C4D	-6.54	1.30	1.45
50	F	502	FMN	C10-N1	6.45	1.46	1.33
50	F	502	FMN	C4A-N5	6.44	1.44	1.30
59	i	201	CHD	C20-C17	-6.23	1.43	1.54
57	P	501	NDP	P2B-O2B	5.49	1.69	1.59
50	F	502	FMN	C5A-N5	5.44	1.49	1.39
57	P	501	NDP	C6A-N6A	5.35	1.47	1.34
59	i	201	CHD	O12-C12	-5.35	1.34	1.43
59	i	201	CHD	C8-C9	5.31	1.64	1.53
59	i	201	CHD	C13-C17	5.28	1.64	1.55
57	P	501	NDP	O4B-C4B	-5.17	1.33	1.45
55	O	401	DGT	PB-O3B	5.13	1.65	1.59
55	O	401	DGT	PB-O3A	5.10	1.65	1.59
58	U	101	EHZ	C15-N2	5.06	1.45	1.33
55	O	401	DGT	PA-O3A	5.06	1.65	1.59
58	T	101	EHZ	C12-N1	5.04	1.45	1.33
58	U	101	EHZ	C12-N1	4.98	1.45	1.33
59	i	201	CHD	C6-C5	4.92	1.61	1.53
50	F	502	FMN	C2-N1	4.90	1.47	1.36
58	T	101	EHZ	C15-N2	4.89	1.45	1.33
50	F	502	FMN	C9A-N10	4.86	1.49	1.41
55	O	401	DGT	C2-N2	4.80	1.45	1.34
55	O	401	DGT	C2-N1	4.75	1.49	1.37
57	P	501	NDP	C2N-C3N	4.62	1.47	1.35
57	P	501	NDP	PN-O3	4.62	1.64	1.59
50	F	502	FMN	C2-N3	4.48	1.48	1.39
57	P	501	NDP	C5A-C4A	-4.42	1.31	1.39
55	O	401	DGT	C2-N3	4.35	1.43	1.33
55	O	401	DGT	C8-N9	-4.29	1.27	1.37
59	i	201	CHD	C15-C14	4.25	1.63	1.54
57	P	501	NDP	O7N-C7N	-4.12	1.14	1.24
57	P	501	NDP	C8A-N9A	-3.96	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	O	401	DGT	C4-N9	-3.94	1.28	1.38
57	P	501	NDP	O2D-C2D	3.71	1.52	1.43
50	F	502	FMN	C10-N10	3.66	1.45	1.37
50	F	502	FMN	C4-N3	3.54	1.45	1.38
59	i	201	CHD	C6-C7	3.44	1.59	1.52
52	H	401	U10	C4-C5	-3.34	1.39	1.48
57	P	501	NDP	C4N-C3N	3.21	1.56	1.50
52	H	401	U10	C3-C2	-3.05	1.40	1.48
50	F	502	FMN	O2-C2	-2.99	1.18	1.24
53	r	201	CDL	OB6-CB4	-2.91	1.39	1.46
52	H	401	U10	C7-C8	2.89	1.55	1.50
46	B	202	PC1	O21-C2	-2.87	1.39	1.46
53	r	201	CDL	OA6-CA4	-2.81	1.40	1.46
57	P	501	NDP	C5A-N7A	-2.80	1.34	1.39
46	L	702	PC1	O21-C2	-2.80	1.40	1.46
53	H	402	CDL	OA6-CA4	-2.79	1.40	1.46
53	H	402	CDL	OB6-CB4	-2.78	1.40	1.46
53	d	201	CDL	OA6-CA4	-2.78	1.40	1.46
53	d	202	CDL	OB6-CB4	-2.77	1.40	1.46
53	h	201	CDL	OA6-CA4	-2.77	1.40	1.46
53	h	201	CDL	OB6-CB4	-2.76	1.40	1.46
53	L	701	CDL	OA6-CA4	-2.76	1.40	1.46
52	H	401	U10	C6-C1	2.76	1.40	1.35
46	l	701	PC1	O21-C2	-2.75	1.40	1.46
53	M	602	CDL	OB6-CB4	-2.75	1.40	1.46
50	F	502	FMN	O4-C4	-2.74	1.18	1.23
46	I	203	PC1	O21-C2	-2.74	1.40	1.46
46	d	204	PC1	O21-C2	-2.74	1.40	1.46
45	b	102	3PE	O21-C2	-2.73	1.40	1.46
45	A	201	3PE	O21-C2	-2.73	1.40	1.46
45	Y	205	3PE	O21-C2	-2.73	1.40	1.46
45	N	402	3PE	O21-C2	-2.73	1.40	1.46
45	Y	202	3PE	O21-C2	-2.73	1.40	1.46
45	r	202	3PE	O21-C2	-2.72	1.40	1.46
45	K	101	3PE	O21-C2	-2.72	1.40	1.46
45	J	201	3PE	O21-C2	-2.71	1.40	1.46
46	I	204	PC1	O21-C2	-2.71	1.40	1.46
57	P	501	NDP	C4N-C5N	2.71	1.56	1.49
46	A	202	PC1	O21-C2	-2.71	1.40	1.46
45	M	603	3PE	O21-C2	-2.70	1.40	1.46
53	d	201	CDL	OB6-CB4	-2.70	1.40	1.46
45	Z	202	3PE	O21-C2	-2.70	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	208	3PE	O21-C2	-2.69	1.40	1.46
52	H	401	U10	C20-C19	2.69	1.57	1.50
46	A	204	PC1	O21-C2	-2.69	1.40	1.46
45	P	502	3PE	O21-C2	-2.68	1.40	1.46
46	H	404	PC1	O21-C2	-2.68	1.40	1.46
53	N	401	CDL	OB6-CB4	-2.68	1.40	1.46
45	Y	203	3PE	O21-C2	-2.67	1.40	1.46
45	a	101	3PE	O21-C2	-2.67	1.40	1.46
46	m	202	PC1	O21-C2	-2.67	1.40	1.46
46	h	202	PC1	O21-C2	-2.67	1.40	1.46
59	i	201	CHD	C13-C12	-2.66	1.50	1.54
53	M	602	CDL	OA6-CA4	-2.66	1.40	1.46
45	d	203	3PE	O21-C2	-2.66	1.40	1.46
53	L	701	CDL	OB6-CB4	-2.66	1.40	1.46
46	A	203	PC1	O21-C2	-2.64	1.40	1.46
45	m	201	3PE	O21-C2	-2.64	1.40	1.46
45	L	704	3PE	O21-C2	-2.64	1.40	1.46
46	J	203	PC1	O21-C2	-2.64	1.40	1.46
46	H	403	PC1	O21-C2	-2.64	1.40	1.46
46	q	201	PC1	O21-C2	-2.63	1.40	1.46
45	Y	207	3PE	O21-C2	-2.63	1.40	1.46
45	M	604	3PE	O21-C2	-2.63	1.40	1.46
46	M	605	PC1	O21-C2	-2.62	1.40	1.46
45	b	101	3PE	O21-C2	-2.61	1.40	1.46
55	O	401	DGT	C1'-N9	-2.61	1.41	1.48
45	A	205	3PE	O21-C2	-2.61	1.40	1.46
45	f	101	3PE	O21-C2	-2.59	1.40	1.46
45	Z	203	3PE	O21-C2	-2.58	1.40	1.46
45	Y	206	3PE	O21-C2	-2.56	1.40	1.46
46	B	203	PC1	O21-C2	-2.56	1.40	1.46
53	d	202	CDL	OA6-CA4	-2.56	1.40	1.46
45	Y	201	3PE	O21-C2	-2.55	1.40	1.46
45	Y	204	3PE	O21-C2	-2.55	1.40	1.46
53	N	401	CDL	OA6-CA4	-2.54	1.40	1.46
45	q	202	3PE	O21-C2	-2.54	1.40	1.46
53	d	202	CDL	OA8-CA7	2.53	1.40	1.33
45	L	705	3PE	O21-C2	-2.52	1.40	1.46
52	H	401	U10	C11-C9	2.50	1.56	1.51
53	H	402	CDL	OA8-CA7	2.50	1.40	1.33
52	H	401	U10	C15-C14	2.49	1.56	1.50
46	L	702	PC1	O31-C31	2.47	1.40	1.33
46	d	204	PC1	O31-C31	2.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	C6N-N1N	2.46	1.43	1.37
45	A	205	3PE	O31-C31	2.45	1.40	1.33
45	d	203	3PE	O31-C31	2.44	1.40	1.33
57	P	501	NDP	O3B-C3B	-2.44	1.36	1.43
53	h	201	CDL	OB8-CB7	2.44	1.40	1.33
45	Z	203	3PE	O31-C31	2.43	1.40	1.33
53	L	701	CDL	OB8-CB7	2.43	1.40	1.33
53	d	201	CDL	OB8-CB7	2.43	1.40	1.33
46	H	403	PC1	O31-C31	2.43	1.40	1.33
45	J	201	3PE	O31-C31	2.42	1.40	1.33
53	r	201	CDL	OB8-CB7	2.41	1.40	1.33
45	L	704	3PE	O31-C31	2.41	1.40	1.33
57	P	501	NDP	O3D-C3D	-2.41	1.37	1.43
53	N	401	CDL	OA8-CA7	2.41	1.40	1.33
46	M	605	PC1	O31-C31	2.41	1.40	1.33
53	M	602	CDL	OA8-CA7	2.41	1.40	1.33
46	q	201	PC1	O31-C31	2.40	1.40	1.33
46	H	404	PC1	O31-C31	2.40	1.40	1.33
45	i	202	3PE	O21-C2	-2.39	1.41	1.46
45	Y	208	3PE	O31-C31	2.39	1.40	1.33
46	B	203	PC1	O31-C31	2.39	1.40	1.33
45	q	202	3PE	O31-C31	2.39	1.40	1.33
46	I	204	PC1	O31-C31	2.39	1.40	1.33
46	m	202	PC1	O31-C31	2.39	1.40	1.33
58	T	101	EHZ	O4-C15	-2.38	1.18	1.23
45	m	201	3PE	O31-C31	2.38	1.40	1.33
53	M	602	CDL	OB8-CB7	2.38	1.40	1.33
53	d	201	CDL	OA8-CA6	-2.38	1.39	1.45
46	l	701	PC1	O31-C31	2.37	1.40	1.33
45	Y	201	3PE	O31-C31	2.37	1.40	1.33
46	A	203	PC1	O31-C31	2.36	1.40	1.33
46	A	204	PC1	O31-C31	2.36	1.40	1.33
53	h	201	CDL	OA8-CA7	2.36	1.40	1.33
46	A	202	PC1	O31-C31	2.36	1.40	1.33
45	f	101	3PE	O31-C31	2.36	1.40	1.33
46	I	203	PC1	O31-C31	2.36	1.40	1.33
53	d	202	CDL	OB8-CB6	-2.35	1.39	1.45
45	b	102	3PE	O31-C31	2.35	1.40	1.33
45	Y	203	3PE	O31-C31	2.35	1.40	1.33
45	K	101	3PE	O31-C3	-2.34	1.39	1.45
45	i	202	3PE	O31-C31	2.34	1.40	1.33
45	L	705	3PE	O31-C31	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	603	3PE	O31-C3	-2.34	1.39	1.45
53	N	401	CDL	OB8-CB7	2.33	1.40	1.33
58	U	101	EHZ	O4-C15	-2.33	1.18	1.23
53	N	401	CDL	OB8-CB6	-2.33	1.40	1.45
45	Y	205	3PE	O31-C3	-2.32	1.40	1.45
45	N	402	3PE	O31-C3	-2.32	1.40	1.45
53	h	201	CDL	OB8-CB6	-2.32	1.40	1.45
45	A	201	3PE	O31-C31	2.32	1.40	1.33
45	Y	206	3PE	O31-C31	2.31	1.40	1.33
45	Z	202	3PE	O31-C31	2.31	1.40	1.33
45	Y	204	3PE	O31-C31	2.31	1.40	1.33
45	b	101	3PE	O31-C31	2.31	1.40	1.33
45	N	402	3PE	O31-C31	2.31	1.40	1.33
58	T	101	EHZ	O3-C12	-2.30	1.18	1.23
58	U	101	EHZ	C9-S1	2.30	1.81	1.76
45	Y	207	3PE	O31-C31	2.30	1.40	1.33
45	P	502	3PE	O31-C31	2.30	1.40	1.33
53	r	201	CDL	OA8-CA6	-2.30	1.40	1.45
45	Y	202	3PE	O31-C31	2.30	1.40	1.33
52	H	401	U10	C7-C6	2.30	1.55	1.51
45	r	202	3PE	O31-C31	2.29	1.40	1.33
58	U	101	EHZ	O3-C12	-2.29	1.18	1.23
45	M	604	3PE	O31-C31	2.29	1.40	1.33
57	P	501	NDP	C7N-C3N	2.29	1.53	1.48
53	r	201	CDL	OA8-CA7	2.29	1.40	1.33
45	Y	207	3PE	O31-C3	-2.29	1.40	1.45
45	a	101	3PE	O31-C31	2.29	1.40	1.33
45	a	101	3PE	O31-C3	-2.29	1.40	1.45
46	J	203	PC1	O31-C31	2.28	1.40	1.33
52	H	401	U10	C16-C14	2.28	1.56	1.51
46	B	202	PC1	O31-C31	2.28	1.40	1.33
53	L	701	CDL	OA8-CA7	2.28	1.40	1.33
45	M	604	3PE	O31-C3	-2.28	1.40	1.45
45	f	101	3PE	O21-C21	2.27	1.40	1.35
45	r	202	3PE	O31-C3	-2.26	1.40	1.45
46	B	203	PC1	O31-C3	-2.26	1.40	1.45
46	B	202	PC1	O31-C3	-2.26	1.40	1.45
57	P	501	NDP	P2B-O1X	2.25	1.57	1.50
45	Y	205	3PE	O31-C31	2.25	1.39	1.33
45	Y	204	3PE	O31-C3	-2.25	1.40	1.45
55	O	401	DGT	PG-O1G	-2.25	1.46	1.54
58	T	101	EHZ	C9-S1	2.25	1.81	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	P	502	3PE	O31-C3	-2.25	1.40	1.45
45	M	603	3PE	O21-C21	2.24	1.40	1.35
46	J	203	PC1	O31-C3	-2.24	1.40	1.45
46	l	701	PC1	O31-C3	-2.24	1.40	1.45
53	d	201	CDL	OA8-CA7	2.24	1.39	1.33
55	O	401	DGT	PG-O2G	-2.23	1.46	1.54
53	L	701	CDL	OA8-CA6	-2.23	1.40	1.45
45	K	101	3PE	O31-C31	2.23	1.39	1.33
45	Y	202	3PE	O31-C3	-2.23	1.40	1.45
45	Z	202	3PE	O31-C3	-2.23	1.40	1.45
45	M	603	3PE	O31-C31	2.23	1.39	1.33
46	I	203	PC1	O31-C3	-2.23	1.40	1.45
46	h	202	PC1	O31-C3	-2.23	1.40	1.45
46	B	203	PC1	O21-C21	2.23	1.40	1.34
57	P	501	NDP	PA-O5B	2.22	1.68	1.59
45	i	202	3PE	O31-C3	-2.22	1.40	1.45
45	Y	208	3PE	O31-C3	-2.22	1.40	1.45
45	m	201	3PE	O31-C3	-2.22	1.40	1.45
46	A	204	PC1	O31-C3	-2.22	1.40	1.45
45	L	705	3PE	O31-C3	-2.22	1.40	1.45
53	r	201	CDL	OB8-CB6	-2.21	1.40	1.45
46	q	201	PC1	O21-C21	2.21	1.40	1.34
46	l	701	PC1	O21-C21	2.21	1.40	1.34
45	i	202	3PE	O21-C21	2.21	1.40	1.34
45	A	201	3PE	O31-C3	-2.21	1.40	1.45
45	b	101	3PE	O31-C3	-2.21	1.40	1.45
45	Y	206	3PE	O31-C3	-2.21	1.40	1.45
46	M	605	PC1	O21-C21	2.20	1.40	1.34
46	h	202	PC1	O21-C21	2.20	1.40	1.34
53	N	401	CDL	OB6-CB5	2.20	1.40	1.34
45	d	203	3PE	O31-C3	-2.20	1.40	1.45
46	I	204	PC1	O31-C3	-2.19	1.40	1.45
45	q	202	3PE	O31-C3	-2.19	1.40	1.45
52	H	401	U10	C1M-C1	2.19	1.55	1.50
46	A	203	PC1	O31-C3	-2.19	1.40	1.45
53	L	701	CDL	OB8-CB6	-2.19	1.40	1.45
45	f	101	3PE	O31-C3	-2.18	1.40	1.45
45	Y	203	3PE	O31-C3	-2.18	1.40	1.45
45	Y	201	3PE	O21-C21	2.18	1.40	1.34
53	M	602	CDL	OB8-CB6	-2.18	1.40	1.45
46	A	202	PC1	O21-C21	2.17	1.40	1.34
52	H	401	U10	O3-C3	2.17	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Z	203	3PE	O21-C21	2.17	1.40	1.34
45	Y	201	3PE	O31-C3	-2.17	1.40	1.45
53	M	602	CDL	OA6-CA5	2.17	1.40	1.34
46	H	404	PC1	O21-C21	2.17	1.40	1.34
46	d	204	PC1	O31-C3	-2.17	1.40	1.45
45	J	201	3PE	O31-C3	-2.16	1.40	1.45
46	J	203	PC1	O21-C21	2.16	1.40	1.34
46	H	403	PC1	O21-C21	2.16	1.40	1.34
55	O	401	DGT	C4-N3	2.16	1.39	1.34
45	d	203	3PE	O21-C21	2.16	1.40	1.34
46	A	202	PC1	O31-C3	-2.16	1.40	1.45
45	L	705	3PE	O21-C21	2.16	1.40	1.34
45	P	502	3PE	O21-C21	2.16	1.40	1.34
46	m	202	PC1	O31-C3	-2.16	1.40	1.45
45	M	604	3PE	O21-C21	2.16	1.40	1.34
46	m	202	PC1	O21-C21	2.15	1.40	1.34
46	A	203	PC1	O21-C21	2.15	1.40	1.34
52	H	401	U10	O4-C4	2.15	1.42	1.36
53	M	602	CDL	OA8-CA6	-2.15	1.40	1.45
45	q	202	3PE	O21-C21	2.15	1.40	1.34
46	A	204	PC1	O21-C21	2.15	1.40	1.34
45	Y	204	3PE	O21-C21	2.15	1.40	1.34
53	H	402	CDL	OB8-CB6	-2.14	1.40	1.45
53	d	201	CDL	OB6-CB5	2.14	1.40	1.34
53	d	201	CDL	OB8-CB6	-2.14	1.40	1.45
46	H	404	PC1	O31-C3	-2.13	1.40	1.45
45	b	101	3PE	O21-C21	2.13	1.40	1.34
53	N	401	CDL	OA6-CA5	2.13	1.40	1.34
45	b	102	3PE	O31-C3	-2.13	1.40	1.45
52	H	401	U10	C6-C5	-2.13	1.40	1.46
53	L	701	CDL	OB6-CB5	2.13	1.40	1.34
45	Y	207	3PE	O21-C21	2.13	1.40	1.34
46	I	204	PC1	O21-C21	2.13	1.40	1.34
45	a	101	3PE	O21-C21	2.13	1.40	1.34
52	H	401	U10	C25-C24	2.13	1.55	1.50
52	H	401	U10	C1-C2	-2.13	1.40	1.47
53	N	401	CDL	OA8-CA6	-2.13	1.40	1.45
45	m	201	3PE	O21-C21	2.12	1.40	1.34
53	d	202	CDL	OA6-CA5	2.12	1.40	1.34
46	q	201	PC1	O31-C3	-2.12	1.40	1.45
46	L	702	PC1	O31-C3	-2.12	1.40	1.45
45	Z	202	3PE	O21-C21	2.12	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	704	3PE	O31-C3	-2.12	1.40	1.45
46	d	204	PC1	O21-C21	2.11	1.40	1.34
53	d	202	CDL	OB8-CB7	2.11	1.39	1.33
53	h	201	CDL	OB6-CB5	2.11	1.40	1.34
53	r	201	CDL	OA6-CA5	2.11	1.40	1.34
45	J	201	3PE	O21-C21	2.11	1.40	1.34
45	L	704	3PE	O21-C21	2.11	1.40	1.34
53	h	201	CDL	OA8-CA6	-2.10	1.40	1.45
46	H	403	PC1	O31-C3	-2.10	1.40	1.45
52	H	401	U10	C22-C23	2.10	1.56	1.50
45	Y	206	3PE	O21-C21	2.10	1.40	1.34
46	M	605	PC1	O31-C3	-2.10	1.40	1.45
45	A	205	3PE	O21-C21	2.10	1.40	1.34
53	d	201	CDL	OA6-CA5	2.09	1.40	1.34
45	Y	208	3PE	O21-C21	2.09	1.40	1.34
45	Z	203	3PE	O31-C3	-2.09	1.40	1.45
46	I	203	PC1	O21-C21	2.09	1.40	1.34
45	A	205	3PE	O31-C3	-2.09	1.40	1.45
45	K	101	3PE	O21-C21	2.09	1.40	1.34
46	L	702	PC1	O21-C21	2.07	1.40	1.34
53	L	701	CDL	OA6-CA5	2.07	1.40	1.34
45	Y	205	3PE	O21-C21	2.07	1.40	1.34
57	P	501	NDP	C5B-C4B	2.07	1.57	1.51
45	Y	203	3PE	O21-C21	2.06	1.40	1.34
45	b	102	3PE	O21-C21	2.06	1.40	1.34
53	H	402	CDL	OB6-CB5	2.05	1.40	1.34
45	r	202	3PE	O21-C21	2.05	1.40	1.34
53	H	402	CDL	OA8-CA6	-2.05	1.40	1.45
53	d	202	CDL	OA8-CA6	-2.05	1.40	1.45
45	Y	202	3PE	O21-C21	2.05	1.40	1.34
45	A	201	3PE	O21-C21	2.04	1.40	1.34
52	H	401	U10	C10-C9	2.04	1.55	1.50
53	h	201	CDL	OA6-CA5	2.03	1.40	1.34
45	N	402	3PE	O21-C21	2.02	1.40	1.34
53	H	402	CDL	OA6-CA5	2.02	1.40	1.34
53	M	602	CDL	OB6-CB5	2.01	1.39	1.34

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	C8-N9-C4	7.38	119.86	106.03
59	i	201	CHD	C13-C17-C20	-6.94	111.08	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	i	201	CHD	C17-C13-C14	5.96	106.09	100.11
58	T	101	EHZ	C8-C9-S1	5.85	120.94	113.56
58	U	101	EHZ	C8-C9-S1	5.68	120.73	113.56
57	P	501	NDP	N6A-C6A-N1A	-5.62	105.86	118.38
57	P	501	NDP	N3A-C2A-N1A	-5.48	120.29	128.58
57	P	501	NDP	C4A-N9A-C1B	-5.30	114.24	126.63
57	P	501	NDP	C5A-C4A-N3A	-5.21	119.55	126.72
52	H	401	U10	C7-C8-C9	5.09	135.59	126.83
45	f	101	3PE	O21-C21-C22	5.08	120.15	111.09
59	i	201	CHD	C17-C13-C12	5.03	122.20	117.67
45	M	603	3PE	O21-C21-C22	4.91	119.85	111.09
57	P	501	NDP	C1B-N9A-C8A	4.81	137.78	127.09
59	i	201	CHD	C14-C13-C12	4.66	111.67	107.42
50	F	502	FMN	C7M-C7-C6	4.64	127.75	119.57
50	F	502	FMN	C9-C8-C7	4.55	126.36	119.69
45	L	705	3PE	O21-C21-C22	4.48	121.17	111.48
46	J	203	PC1	O21-C21-C22	4.24	120.65	111.48
46	H	404	PC1	O21-C21-C22	4.23	120.63	111.48
46	H	403	PC1	O21-C21-C22	4.23	120.63	111.48
46	I	203	PC1	O21-C21-C22	4.21	120.60	111.48
57	P	501	NDP	C5A-C6A-N6A	4.20	133.68	123.29
45	A	205	3PE	O21-C21-C22	4.20	120.56	111.48
45	r	202	3PE	O21-C21-C22	4.19	120.54	111.48
53	d	202	CDL	OB6-CB5-C51	4.18	120.53	111.48
59	i	201	CHD	C18-C13-C12	-4.16	104.89	109.06
45	b	101	3PE	O21-C21-C22	4.15	120.47	111.48
46	M	605	PC1	O21-C21-C22	4.13	120.42	111.48
45	Y	207	3PE	O21-C21-C22	4.12	120.39	111.48
53	h	201	CDL	OA6-CA5-C11	4.11	120.38	111.48
53	N	401	CDL	OB6-CB5-C51	4.10	120.34	111.48
46	q	201	PC1	O21-C21-C22	4.10	120.34	111.48
46	B	203	PC1	O21-C21-C22	4.09	120.34	111.48
45	K	101	3PE	O21-C21-C22	4.09	120.33	111.48
53	M	602	CDL	OB6-CB5-C51	4.09	120.32	111.48
53	r	201	CDL	OA6-CA5-C11	4.07	120.29	111.48
45	Y	201	3PE	O21-C21-C22	4.07	120.29	111.48
46	A	203	PC1	O21-C21-C22	4.06	120.25	111.48
45	Z	203	3PE	O21-C21-C22	4.04	120.22	111.48
45	m	201	3PE	O21-C21-C22	4.04	120.21	111.48
53	d	201	CDL	OA6-CA5-C11	4.03	120.20	111.48
45	Y	208	3PE	O21-C21-C22	4.03	120.20	111.48
45	L	704	3PE	O21-C21-C22	4.03	120.20	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	P	501	NDP	N9A-C8A-N7A	-4.03	108.22	113.94
45	Z	202	3PE	O21-C21-C22	4.02	120.18	111.48
45	Y	202	3PE	O21-C21-C22	4.01	120.16	111.48
53	H	402	CDL	OB6-CB5-C51	4.01	120.16	111.48
53	H	402	CDL	OA6-CA5-C11	3.97	120.07	111.48
53	h	201	CDL	OB6-CB5-C51	3.97	120.07	111.48
45	P	502	3PE	O21-C21-C22	3.97	120.06	111.48
46	I	204	PC1	O21-C21-C22	3.96	120.04	111.48
59	i	201	CHD	C18-C13-C17	-3.95	105.01	111.20
46	A	204	PC1	O21-C21-C22	3.94	120.00	111.48
53	r	201	CDL	OB6-CB5-C51	3.93	119.98	111.48
45	J	201	3PE	O21-C21-C22	3.91	119.93	111.48
53	d	202	CDL	OA6-CA5-C11	3.91	119.93	111.48
45	i	202	3PE	O21-C21-C22	3.90	119.91	111.48
45	Y	203	3PE	O21-C21-C22	3.89	119.90	111.48
53	M	602	CDL	OA6-CA5-C11	3.88	119.87	111.48
46	B	202	PC1	O21-C21-C22	3.85	119.80	111.48
45	Y	205	3PE	O21-C21-C22	3.81	119.73	111.48
45	Y	204	3PE	O21-C21-C22	3.81	119.72	111.48
53	L	701	CDL	OA6-CA5-C11	3.81	119.72	111.48
46	m	202	PC1	O21-C21-C22	3.81	119.71	111.48
46	A	202	PC1	O21-C21-C22	3.79	119.69	111.48
45	b	102	3PE	O21-C21-C22	3.78	119.66	111.48
59	i	201	CHD	C9-C10-C5	3.78	113.76	108.51
45	Y	206	3PE	O21-C21-C22	3.77	119.64	111.48
45	q	202	3PE	O21-C21-C22	3.76	119.61	111.48
46	h	202	PC1	O21-C21-C22	3.76	119.61	111.48
46	L	702	PC1	O21-C21-C22	3.74	119.58	111.48
53	L	701	CDL	OB6-CB5-C51	3.72	119.53	111.48
45	d	203	3PE	O21-C21-C22	3.72	119.52	111.48
45	M	604	3PE	O21-C21-C22	3.71	119.51	111.48
45	N	402	3PE	O21-C21-C22	3.62	119.30	111.48
46	d	204	PC1	O21-C21-C22	3.61	119.28	111.48
46	l	701	PC1	O21-C21-C22	3.59	119.25	111.48
50	F	502	FMN	C4-N3-C2	-3.55	119.33	125.64
52	H	401	U10	C8-C7-C6	3.55	120.82	112.08
59	i	201	CHD	C18-C13-C14	-3.53	105.67	111.20
53	N	401	CDL	OA6-CA5-C11	3.53	119.11	111.48
57	P	501	NDP	C2A-N3A-C4A	3.50	120.38	111.83
55	O	401	DGT	C1'-N9-C8	-3.48	120.10	127.91
45	A	201	3PE	O21-C21-C22	3.45	118.95	111.48
59	i	201	CHD	C4-C3-C2	3.42	114.80	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	d	202	CDL	OA8-CA7-C31	3.40	122.21	111.83
50	F	502	FMN	C8M-C8-C7	-3.31	114.00	120.76
57	P	501	NDP	N3A-C4A-N9A	3.21	132.62	127.17
55	O	401	DGT	C2-N1-C6	-3.18	119.34	125.11
55	O	401	DGT	C2'-C3'-C4'	3.18	109.25	102.80
45	Y	202	3PE	O31-C31-C32	3.09	121.26	111.83
45	Y	206	3PE	O31-C31-C32	3.00	120.97	111.83
46	A	203	PC1	O31-C31-C32	2.99	120.95	111.83
59	i	201	CHD	C23-C22-C20	-2.97	108.91	114.46
50	F	502	FMN	C4A-C10-N10	2.96	120.72	116.48
46	d	204	PC1	O31-C31-C32	2.96	120.86	111.83
52	H	401	U10	C10-C9-C11	2.96	120.36	115.23
46	B	203	PC1	O31-C31-C32	2.95	120.83	111.83
53	M	602	CDL	OB8-CB7-C71	2.93	120.75	111.83
53	H	402	CDL	OA8-CA7-C31	2.92	120.01	111.15
46	l	701	PC1	O31-C31-C32	2.91	120.72	111.83
46	J	203	PC1	O31-C31-C32	2.89	120.64	111.83
55	O	401	DGT	O2G-PG-O3B	2.87	114.28	104.64
45	Z	203	3PE	O31-C31-C32	2.86	120.57	111.83
45	Y	204	3PE	O31-C31-C32	2.86	120.54	111.83
58	T	101	EHZ	C13-C12-N1	2.85	121.54	116.34
45	Y	208	3PE	O31-C31-C32	2.83	119.75	111.15
45	N	402	3PE	O31-C31-C32	2.83	120.45	111.83
53	N	401	CDL	OA8-CA7-C31	2.82	120.45	111.83
57	P	501	NDP	C2B-C1B-N9A	-2.81	109.13	113.75
45	L	705	3PE	O31-C31-C32	2.80	120.38	111.83
53	h	201	CDL	OB8-CB7-C71	2.80	120.36	111.83
57	P	501	NDP	C5A-N7A-C8A	2.79	107.83	103.45
45	M	603	3PE	O31-C31-C32	2.79	120.33	111.83
53	d	201	CDL	OB8-CB7-C71	2.78	120.33	111.83
46	H	403	PC1	O31-C31-C32	2.78	120.30	111.83
45	J	201	3PE	O31-C31-C32	2.77	120.29	111.83
53	d	202	CDL	OB8-CB7-C71	2.77	120.29	111.83
46	H	404	PC1	O31-C31-C32	2.77	120.27	111.83
45	f	101	3PE	O31-C31-C32	2.76	120.25	111.83
45	M	604	3PE	O31-C31-C32	2.75	120.22	111.83
45	i	202	3PE	O31-C31-C32	2.75	120.22	111.83
45	Y	207	3PE	O31-C31-C32	2.75	120.21	111.83
59	i	201	CHD	C15-C14-C8	2.74	122.12	118.36
53	L	701	CDL	OA8-CA7-C31	2.74	120.18	111.83
46	A	202	PC1	O31-C31-C32	2.72	120.14	111.83
55	O	401	DGT	O1G-PG-O3B	2.72	113.77	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	a	101	3PE	O31-C31-C32	2.72	120.12	111.83
53	r	201	CDL	OB8-CB7-C71	2.71	120.10	111.83
46	m	202	PC1	O31-C31-C32	2.71	120.10	111.83
46	B	202	PC1	O31-C31-C32	2.71	120.09	111.83
53	N	401	CDL	OB8-CB7-C71	2.70	120.08	111.83
45	A	201	3PE	O31-C31-C32	2.70	120.07	111.83
46	L	702	PC1	O31-C31-C32	2.68	120.02	111.83
45	L	704	3PE	O31-C31-C32	2.68	120.01	111.83
46	A	204	PC1	O31-C31-C32	2.68	120.00	111.83
45	b	102	3PE	O31-C31-C32	2.67	119.98	111.83
45	r	202	3PE	O31-C31-C32	2.67	119.97	111.83
45	K	101	3PE	O31-C31-C32	2.67	119.97	111.83
45	b	101	3PE	O31-C31-C32	2.67	119.96	111.83
46	I	204	PC1	O31-C31-C32	2.65	119.93	111.83
53	M	602	CDL	OA8-CA7-C31	2.65	119.92	111.83
59	i	201	CHD	C11-C9-C10	-2.65	111.02	113.70
45	m	201	3PE	O31-C31-C32	2.64	119.89	111.83
45	Y	201	3PE	O31-C31-C32	2.64	119.88	111.83
58	T	101	EHZ	O2-C9-S1	-2.63	119.33	122.68
46	M	605	PC1	O31-C31-C32	2.63	119.86	111.83
53	h	201	CDL	OA8-CA7-C31	2.63	119.86	111.83
59	i	201	CHD	C1-C2-C3	2.63	113.97	110.48
53	r	201	CDL	OA8-CA7-C31	2.63	119.84	111.83
45	Y	203	3PE	O31-C31-C32	2.62	119.81	111.83
58	U	101	EHZ	O2-C9-C8	-2.62	119.62	123.74
53	d	201	CDL	OB6-CB5-C51	2.61	120.52	110.93
45	P	502	3PE	O31-C31-C32	2.60	119.78	111.83
53	L	701	CDL	OB8-CB7-C71	2.60	119.77	111.83
53	d	201	CDL	OA8-CA7-C31	2.60	119.76	111.83
45	A	205	3PE	O31-C31-C32	2.59	119.74	111.83
45	q	202	3PE	O31-C31-C32	2.59	119.72	111.83
58	U	101	EHZ	C7-C8-C9	-2.58	108.10	113.86
45	Y	205	3PE	O31-C31-C32	2.58	119.69	111.83
45	d	203	3PE	O31-C31-C32	2.57	119.68	111.83
50	F	502	FMN	C6-C7-C8	-2.56	115.93	119.69
58	T	101	EHZ	O2-C9-C8	-2.55	119.72	123.74
46	q	201	PC1	O31-C31-C32	2.54	119.58	111.83
50	F	502	FMN	C4A-C4-N3	2.53	119.69	113.25
52	H	401	U10	C10-C9-C8	-2.51	117.18	123.63
45	a	101	3PE	O21-C21-C22	2.49	120.08	110.93
58	T	101	EHZ	C10-S1-C9	2.46	109.12	101.84
55	O	401	DGT	C5-C6-N1	2.45	119.49	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	401	DGT	O1A-PA-O2A	-2.44	101.10	112.44
46	I	203	PC1	O31-C31-C32	2.43	119.25	111.83
50	F	502	FMN	O4-C4-C4A	-2.42	120.15	126.53
58	T	101	EHZ	C11-N1-C12	-2.39	118.36	122.82
58	U	101	EHZ	O2-C9-S1	-2.39	119.64	122.68
55	O	401	DGT	O1B-PB-O2B	-2.36	101.45	112.44
50	F	502	FMN	C5A-C9A-N10	2.36	120.10	117.97
45	Z	202	3PE	O31-C31-C32	2.35	119.02	111.83
55	O	401	DGT	O6-C6-C5	-2.35	120.32	126.53
52	H	401	U10	C15-C14-C16	2.32	119.26	115.23
50	F	502	FMN	C10-C4A-N5	-2.31	120.09	124.81
59	i	201	CHD	C19-C10-C9	-2.25	108.16	111.18
59	i	201	CHD	C9-C11-C12	-2.23	111.38	114.29
58	T	101	EHZ	C7-C8-C9	-2.22	108.90	113.86
59	i	201	CHD	C1-C10-C9	-2.19	107.93	111.34
50	F	502	FMN	C7M-C7-C8	-2.17	116.32	120.76
50	F	502	FMN	C6-C5A-C9A	2.17	122.03	119.05
50	F	502	FMN	C9A-C5A-N5	-2.14	120.18	122.45
57	P	501	NDP	C4A-C5A-N7A	-2.14	108.14	110.58
57	P	501	NDP	C4A-N9A-C8A	2.13	107.97	105.74
50	F	502	FMN	C4-C4A-C10	2.12	120.57	116.93
57	P	501	NDP	P2B-O2B-C2B	-2.10	117.83	123.43
45	f	101	3PE	C2-O21-C21	-2.09	114.16	117.85
59	i	201	CHD	C5-C4-C3	2.09	115.85	112.71
57	P	501	NDP	C6A-C5A-C4A	2.08	120.02	117.18
55	O	401	DGT	C6-C5-N7	2.07	134.06	130.29
55	O	401	DGT	C5-C4-N9	-2.06	101.96	105.66
58	T	101	EHZ	O3-C12-N1	-2.05	119.01	123.03
55	O	401	DGT	N9-C8-N7	-2.04	109.61	113.40
58	U	101	EHZ	C13-C12-N1	2.03	120.04	116.34
50	F	502	FMN	C4A-C10-N1	-2.03	119.62	124.59
55	O	401	DGT	C1'-N9-C4	-2.02	120.04	125.50
55	O	401	DGT	N9-C4-N3	2.00	129.96	125.95

There are no chirality outliers.

All (1291) 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-O12
45	A	205	3PE	C1-O11-P-O14
45	A	205	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	A	205	3PE	C11-O13-P-O12
45	J	201	3PE	C11-O13-P-O11
45	J	201	3PE	C11-O13-P-O14
45	L	704	3PE	O21-C2-C3-O31
45	L	704	3PE	C22-C21-O21-C2
45	L	705	3PE	C11-O13-P-O11
45	L	705	3PE	C11-O13-P-O14
45	L	705	3PE	C22-C21-O21-C2
45	M	604	3PE	C11-O13-P-O11
45	M	604	3PE	C11-O13-P-O12
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13
45	N	402	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	P	502	3PE	C1-O11-P-O12
45	P	502	3PE	C1-O11-P-O13
45	P	502	3PE	C1-O11-P-O14
45	P	502	3PE	C22-C21-O21-C2
45	Y	201	3PE	C1-O11-P-O12
45	Y	201	3PE	C1-O11-P-O13
45	Y	201	3PE	C1-O11-P-O14
45	Y	202	3PE	C1-O11-P-O13
45	Y	202	3PE	C1-O11-P-O14
45	Y	202	3PE	O13-C11-C12-N
45	Y	203	3PE	C1-O11-P-O12
45	Y	203	3PE	O13-C11-C12-N
45	Y	204	3PE	C11-O13-P-O14
45	Y	204	3PE	C22-C21-O21-C2
45	Y	206	3PE	C1-O11-P-O12
45	Y	206	3PE	C1-O11-P-O13
45	Y	206	3PE	C11-O13-P-O11
45	Y	206	3PE	C11-O13-P-O14
45	Y	206	3PE	C22-C21-O21-C2
45	Y	207	3PE	C1-O11-P-O12
45	Y	207	3PE	C1-O11-P-O13
45	Y	207	3PE	C1-O11-P-O14
45	Y	207	3PE	C11-O13-P-O14
45	Y	207	3PE	C12-C11-O13-P
45	Y	208	3PE	C1-O11-P-O13
45	Y	208	3PE	C1-O11-P-O14
45	Y	208	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	Y	208	3PE	C22-C21-O21-C2
45	Z	202	3PE	C12-C11-O13-P
45	Z	202	3PE	C22-C21-O21-C2
45	Z	203	3PE	C11-O13-P-O11
45	Z	203	3PE	C11-O13-P-O12
45	a	101	3PE	O22-C21-O21-C2
45	b	101	3PE	C1-O11-P-O13
45	b	101	3PE	C1-O11-P-O14
45	b	101	3PE	C11-O13-P-O11
45	b	101	3PE	C11-O13-P-O14
45	b	101	3PE	O22-C21-O21-C2
45	b	102	3PE	C1-O11-P-O12
45	b	102	3PE	C1-O11-P-O14
45	b	102	3PE	C11-O13-P-O11
45	b	102	3PE	C11-O13-P-O12
45	b	102	3PE	C11-O13-P-O14
45	d	203	3PE	C1-O11-P-O12
45	d	203	3PE	C1-O11-P-O13
45	d	203	3PE	C1-O11-P-O14
45	d	203	3PE	C11-O13-P-O11
45	d	203	3PE	C11-O13-P-O12
45	d	203	3PE	C11-O13-P-O14
45	d	203	3PE	O13-C11-C12-N
45	f	101	3PE	C1-O11-P-O12
45	f	101	3PE	C1-O11-P-O13
45	f	101	3PE	C1-O11-P-O14
45	f	101	3PE	O13-C11-C12-N
45	f	101	3PE	C22-C21-O21-C2
45	i	202	3PE	C1-O11-P-O12
45	i	202	3PE	C1-O11-P-O13
45	i	202	3PE	C1-O11-P-O14
45	i	202	3PE	C22-C21-O21-C2
45	m	201	3PE	O22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
45	q	202	3PE	C11-O13-P-O11
45	q	202	3PE	C11-O13-P-O12
45	r	202	3PE	O22-C21-O21-C2
45	r	202	3PE	C22-C21-O21-C2
46	A	202	PC1	C11-O13-P-O12
46	A	202	PC1	C11-O13-P-O14
46	A	202	PC1	C11-O13-P-O11
46	A	202	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	A	203	PC1	C1-O11-P-O12
46	A	203	PC1	C1-O11-P-O14
46	A	203	PC1	C1-O11-P-O13
46	A	203	PC1	O22-C21-O21-C2
46	A	204	PC1	C1-O11-P-O12
46	A	204	PC1	C1-O11-P-O13
46	A	204	PC1	C22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	202	PC1	O13-C11-C12-N
46	B	203	PC1	C11-O13-P-O12
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C1-O11-P-O14
46	B	203	PC1	C1-O11-P-O13
46	B	203	PC1	O22-C21-O21-C2
46	H	403	PC1	O21-C2-C3-O31
46	H	404	PC1	C11-O13-P-O12
46	H	404	PC1	C11-O13-P-O11
46	H	404	PC1	C1-O11-P-O12
46	H	404	PC1	C1-O11-P-O13
46	H	404	PC1	O22-C21-O21-C2
46	H	404	PC1	C22-C21-O21-C2
46	I	204	PC1	C1-O11-P-O12
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	J	203	PC1	O13-C11-C12-N
46	L	702	PC1	C11-O13-P-O12
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	M	605	PC1	C11-O13-P-O12
46	M	605	PC1	C11-O13-P-O11
46	M	605	PC1	O21-C2-C3-O31
46	M	605	PC1	C22-C21-O21-C2
46	d	204	PC1	C11-O13-P-O12
46	d	204	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	d	204	PC1	C11-O13-P-O11
46	d	204	PC1	C1-O11-P-O12
46	d	204	PC1	C1-O11-P-O14
46	d	204	PC1	C1-O11-P-O13
46	h	202	PC1	C2-C1-O11-P
46	l	701	PC1	C11-O13-P-O14
46	l	701	PC1	C11-O13-P-O11
46	m	202	PC1	C11-O13-P-O12
46	m	202	PC1	C11-O13-P-O14
46	q	201	PC1	C22-C21-O21-C2
47	A	206	PLC	O3P-C1-C2-O2
47	A	206	PLC	C1-O3P-P-O1P
47	A	206	PLC	C1-O3P-P-O2P
47	A	206	PLC	C1-O3P-P-O4P
47	J	202	PLC	O4P-C4-C5-N
47	J	202	PLC	C4-O4P-P-O1P
47	J	202	PLC	C4-O4P-P-O2P
47	J	202	PLC	C4-O4P-P-O3P
47	L	703	PLC	O4P-C4-C5-N
47	L	703	PLC	C1-O3P-P-O1P
47	L	703	PLC	C1-O3P-P-O4P
47	L	703	PLC	C4-O4P-P-O1P
47	L	703	PLC	C4-O4P-P-O2P
47	L	703	PLC	C4-O4P-P-O3P
47	M	606	PLC	C4-O4P-P-O3P
47	O	403	PLC	O2-C2-C3-O3
47	O	403	PLC	OB-CB-O3-C3
47	O	404	PLC	O'-C'-O2-C2
47	O	404	PLC	C4-O4P-P-O3P
47	Y	209	PLC	C1-O3P-P-O2P
47	Y	209	PLC	C1-O3P-P-O4P
47	Y	209	PLC	C4-O4P-P-O1P
47	Z	201	PLC	C1-O3P-P-O2P
47	Z	201	PLC	C1-O3P-P-O4P
47	Z	201	PLC	C4-O4P-P-O2P
47	Z	201	PLC	C4-O4P-P-O3P
47	g	201	PLC	C1-O3P-P-O1P
47	g	201	PLC	C1-O3P-P-O2P
47	g	201	PLC	C1-O3P-P-O4P
50	F	502	FMN	C1'-C2'-C3'-C4'
52	H	401	U10	C1-C6-C7-C8
52	H	401	U10	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
53	H	402	CDL	C1-CA2-OA2-PA1
53	H	402	CDL	CA2-OA2-PA1-OA4
53	H	402	CDL	CA3-OA5-PA1-OA2
53	H	402	CDL	CA3-OA5-PA1-OA3
53	H	402	CDL	C11-CA5-OA6-CA4
53	H	402	CDL	C51-CB5-OB6-CB4
53	M	602	CDL	CA3-OA5-PA1-OA2
53	M	602	CDL	CA3-OA5-PA1-OA3
53	M	602	CDL	CA3-OA5-PA1-OA4
53	M	602	CDL	CB2-OB2-PB2-OB5
53	N	401	CDL	OB7-CB5-OB6-CB4
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	C51-CB5-OB6-CB4
53	d	202	CDL	CA2-OA2-PA1-OA3
53	d	202	CDL	CA2-OA2-PA1-OA5
53	d	202	CDL	CB3-OB5-PB2-OB2
53	d	202	CDL	CB3-OB5-PB2-OB3
53	d	202	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	OB7-CB5-OB6-CB4
53	r	201	CDL	CA3-OA5-PA1-OA2
53	r	201	CDL	C11-CA5-OA6-CA4
53	r	201	CDL	CB2-OB2-PB2-OB3
53	r	201	CDL	CB2-OB2-PB2-OB4
53	r	201	CDL	CB2-OB2-PB2-OB5
53	r	201	CDL	C51-CB5-OB6-CB4
55	O	401	DGT	C5'-O5'-PA-O1A
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-O1N
57	P	501	NDP	C5D-O5D-PN-O2N
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	C12-C13-C14-N2
58	T	101	EHZ	O5-C16-C17-C20
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	O2-C9-S1-C10

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Mol	Chain	Res	Type	Atoms
58	U	101	EHZ	C8-C9-S1-C10
45	f	101	3PE	O22-C21-O21-C2
46	h	202	PC1	C32-C31-O31-C3
53	H	402	CDL	C71-CB7-OB8-CB6
45	Y	206	3PE	O32-C31-O31-C3
46	A	203	PC1	O32-C31-O31-C3
53	d	201	CDL	OB9-CB7-OB8-CB6
53	d	202	CDL	OA9-CA7-OA8-CA6
53	r	201	CDL	OB9-CB7-OB8-CB6
45	Y	206	3PE	C32-C31-O31-C3
45	Y	207	3PE	C32-C31-O31-C3
46	l	701	PC1	C32-C31-O31-C3
53	d	201	CDL	C71-CB7-OB8-CB6
53	d	202	CDL	C31-CA7-OA8-CA6
53	r	201	CDL	C71-CB7-OB8-CB6
46	h	202	PC1	O32-C31-O31-C3
45	J	201	3PE	O32-C31-O31-C3
45	Y	201	3PE	O32-C31-O31-C3
45	Y	207	3PE	O32-C31-O31-C3
45	Z	203	3PE	O32-C31-O31-C3
45	a	101	3PE	O32-C31-O31-C3
46	A	204	PC1	O32-C31-O31-C3
46	B	203	PC1	O32-C31-O31-C3
46	H	404	PC1	O32-C31-O31-C3
46	d	204	PC1	O32-C31-O31-C3
46	l	701	PC1	O32-C31-O31-C3
53	M	602	CDL	OB9-CB7-OB8-CB6
53	h	201	CDL	OB9-CB7-OB8-CB6
53	H	402	CDL	OB9-CB7-OB8-CB6
45	b	102	3PE	O32-C31-O31-C3
45	L	705	3PE	O22-C21-O21-C2
45	P	502	3PE	O22-C21-O21-C2
45	Y	206	3PE	O22-C21-O21-C2
45	i	202	3PE	O22-C21-O21-C2
46	A	204	PC1	O22-C21-O21-C2
46	M	605	PC1	O22-C21-O21-C2
46	q	201	PC1	O22-C21-O21-C2
53	H	402	CDL	OA7-CA5-OA6-CA4
53	H	402	CDL	OB7-CB5-OB6-CB4
53	M	602	CDL	OB7-CB5-OB6-CB4
53	d	201	CDL	OB7-CB5-OB6-CB4
53	d	202	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	OA7-CA5-OA6-CA4
53	r	201	CDL	OB7-CB5-OB6-CB4
45	J	201	3PE	C32-C31-O31-C3
45	L	705	3PE	C32-C31-O31-C3
45	N	402	3PE	C32-C31-O31-C3
45	Y	201	3PE	C32-C31-O31-C3
45	Z	203	3PE	C32-C31-O31-C3
45	a	101	3PE	C32-C31-O31-C3
46	A	203	PC1	C32-C31-O31-C3
46	A	204	PC1	C32-C31-O31-C3
46	B	203	PC1	C32-C31-O31-C3
46	d	204	PC1	C32-C31-O31-C3
45	a	101	3PE	C22-C21-O21-C2
45	b	101	3PE	C22-C21-O21-C2
46	A	203	PC1	C22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
47	O	404	PLC	C1'-C'-O2-C2
53	M	602	CDL	C51-CB5-OB6-CB4
53	N	401	CDL	C51-CB5-OB6-CB4
53	h	201	CDL	C11-CA5-OA6-CA4
53	h	201	CDL	C51-CB5-OB6-CB4
45	b	101	3PE	O32-C31-O31-C3
45	r	202	3PE	O32-C31-O31-C3
45	M	603	3PE	C32-C31-O31-C3
45	b	102	3PE	C32-C31-O31-C3
45	r	202	3PE	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
46	H	404	PC1	C32-C31-O31-C3
47	Z	201	PLC	C1B-CB-O3-C3
53	L	701	CDL	C31-CA7-OA8-CA6
53	M	602	CDL	C71-CB7-OB8-CB6
53	h	201	CDL	C71-CB7-OB8-CB6
45	L	705	3PE	O32-C31-O31-C3
45	M	603	3PE	O32-C31-O31-C3
45	N	402	3PE	O32-C31-O31-C3
53	L	701	CDL	OA9-CA7-OA8-CA6
45	L	704	3PE	O22-C21-O21-C2
45	Y	204	3PE	O22-C21-O21-C2
45	Z	202	3PE	O22-C21-O21-C2
53	r	201	CDL	OA7-CA5-OA6-CA4
53	d	201	CDL	O1-C1-CA2-OA2
45	b	101	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	f	101	3PE	C32-C31-O31-C3
47	Z	201	PLC	OB-CB-O3-C3
45	A	205	3PE	C22-C21-O21-C2
46	m	202	PC1	C22-C21-O21-C2
53	d	201	CDL	C11-CA5-OA6-CA4
52	H	401	U10	C20-C19-C21-C22
45	A	205	3PE	O22-C21-O21-C2
46	m	202	PC1	O22-C21-O21-C2
46	B	203	PC1	C2-C1-O11-P
47	L	703	PLC	C2-C1-O3P-P
45	f	101	3PE	O32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
59	i	201	CHD	C17-C20-C22-C23
53	d	202	CDL	C11-CA5-OA6-CA4
59	i	201	CHD	C21-C20-C22-C23
53	d	201	CDL	OA7-CA5-OA6-CA4
45	P	502	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
46	J	203	PC1	C32-C31-O31-C3
47	M	606	PLC	C1B-CB-O3-C3
47	g	201	PLC	C1B-CB-O3-C3
53	N	401	CDL	C31-CA7-OA8-CA6
52	H	401	U10	C18-C19-C21-C22
53	d	202	CDL	O1-C1-CB2-OB2
58	U	101	EHZ	C5-C6-C7-O1
45	P	502	3PE	O32-C31-O31-C3
46	J	203	PC1	O32-C31-O31-C3
47	M	606	PLC	OB-CB-O3-C3
45	b	102	3PE	O11-C1-C2-O21
46	q	201	PC1	C32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
45	Z	203	3PE	C31-C32-C33-C34
53	d	201	CDL	CB7-C71-C72-C73
45	q	202	3PE	C31-C32-C33-C34
46	J	203	PC1	C21-C22-C23-C24
52	H	401	U10	C19-C21-C22-C23
45	b	102	3PE	C21-C22-C23-C24
53	M	602	CDL	CB7-C71-C72-C73
45	d	203	3PE	C31-C32-C33-C34
46	B	203	PC1	C21-C22-C23-C24
46	J	203	PC1	C31-C32-C33-C34
53	M	602	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
47	g	201	PLC	OB-CB-O3-C3
53	N	401	CDL	OA9-CA7-OA8-CA6
53	H	402	CDL	O1-C1-CA2-OA2
53	r	201	CDL	O1-C1-CB2-OB2
45	A	201	3PE	C31-C32-C33-C34
45	K	101	3PE	C21-C22-C23-C24
53	d	202	CDL	OA7-CA5-OA6-CA4
45	i	202	3PE	C31-C32-C33-C34
45	d	203	3PE	C32-C31-O31-C3
53	N	401	CDL	C71-CB7-OB8-CB6
46	q	201	PC1	O32-C31-O31-C3
53	N	401	CDL	CA5-C11-C12-C13
53	H	402	CDL	CB2-C1-CA2-OA2
46	L	702	PC1	C32-C31-O31-C3
53	L	701	CDL	C71-CB7-OB8-CB6
53	d	201	CDL	C31-CA7-OA8-CA6
45	Y	202	3PE	C22-C21-O21-C2
46	I	203	PC1	C22-C21-O21-C2
46	h	202	PC1	C22-C21-O21-C2
47	Z	201	PLC	C1'-C'-O2-C2
47	g	201	PLC	C1'-C'-O2-C2
45	Y	202	3PE	O22-C21-O21-C2
46	I	203	PC1	O22-C21-O21-C2
46	h	202	PC1	O22-C21-O21-C2
47	Z	201	PLC	O'-C'-O2-C2
47	g	201	PLC	O'-C'-O2-C2
46	l	701	PC1	C21-C22-C23-C24
45	M	603	3PE	C22-C21-O21-C2
53	N	401	CDL	OB9-CB7-OB8-CB6
45	d	203	3PE	O32-C31-O31-C3
53	N	401	CDL	C11-CA5-OA6-CA4
46	I	204	PC1	C32-C31-O31-C3
46	H	403	PC1	C21-C22-C23-C24
53	H	402	CDL	CA5-C11-C12-C13
53	L	701	CDL	OB9-CB7-OB8-CB6
45	Y	202	3PE	C28-C29-C2A-C2B
53	H	402	CDL	C60-C61-C62-C63
45	b	102	3PE	C23-C24-C25-C26
45	f	101	3PE	C32-C33-C34-C35
45	i	202	3PE	C23-C24-C25-C26
46	A	204	PC1	C22-C23-C24-C25
46	B	203	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
53	d	202	CDL	C76-C77-C78-C79
45	Y	201	3PE	C31-C32-C33-C34
53	L	701	CDL	C20-C21-C22-C23
45	A	205	3PE	C35-C36-C37-C38
45	Y	202	3PE	C38-C39-C3A-C3B
45	Y	208	3PE	C2B-C2C-C2D-C2E
53	d	202	CDL	C62-C63-C64-C65
53	h	201	CDL	C37-C38-C39-C40
45	A	201	3PE	C33-C34-C35-C36
45	Y	205	3PE	C26-C27-C28-C29
46	B	202	PC1	C25-C26-C27-C28
53	H	402	CDL	C57-C58-C59-C60
53	d	202	CDL	C52-C53-C54-C55
58	U	101	EHZ	S1-C10-C11-N1
45	J	201	3PE	C27-C28-C29-C2A
45	Y	207	3PE	C33-C34-C35-C36
46	I	204	PC1	C32-C33-C34-C35
45	Y	206	3PE	C26-C27-C28-C29
53	M	602	CDL	C83-C84-C85-C86
45	A	205	3PE	C21-C22-C23-C24
45	Y	203	3PE	C21-C22-C23-C24
45	d	203	3PE	C22-C23-C24-C25
45	f	101	3PE	C33-C34-C35-C36
46	H	403	PC1	C2B-C2C-C2D-C2E
53	d	202	CDL	C61-C62-C63-C64
58	T	101	EHZ	C2-C3-C4-C5
46	L	702	PC1	C26-C27-C28-C29
45	J	201	3PE	C31-C32-C33-C34
46	L	702	PC1	O32-C31-O31-C3
45	Y	204	3PE	C2E-C2F-C2G-C2H
53	H	402	CDL	C11-C12-C13-C14
53	N	401	CDL	C38-C39-C40-C41
45	m	201	3PE	C32-C31-O31-C3
46	A	202	PC1	C32-C31-O31-C3
46	I	203	PC1	C23-C24-C25-C26
46	M	605	PC1	C33-C34-C35-C36
53	d	202	CDL	C58-C59-C60-C61
53	h	201	CDL	C51-C52-C53-C54
45	Y	202	3PE	C33-C34-C35-C36
45	Y	207	3PE	C28-C29-C2A-C2B
45	Z	203	3PE	C39-C3A-C3B-C3C
45	a	101	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
46	I	203	PC1	C36-C37-C38-C39
46	l	701	PC1	C32-C33-C34-C35
46	m	202	PC1	C25-C26-C27-C28
53	H	402	CDL	C55-C56-C57-C58
53	L	701	CDL	C17-C18-C19-C20
53	M	602	CDL	C74-C75-C76-C77
53	d	201	CDL	C34-C35-C36-C37
53	h	201	CDL	C74-C75-C76-C77
53	d	201	CDL	OA9-CA7-OA8-CA6
45	K	101	3PE	C35-C36-C37-C38
46	H	404	PC1	C25-C26-C27-C28
46	d	204	PC1	C34-C35-C36-C37
46	h	202	PC1	C22-C23-C24-C25
46	q	201	PC1	C28-C29-C2A-C2B
45	M	603	3PE	C35-C36-C37-C38
46	l	701	PC1	C23-C24-C25-C26
53	L	701	CDL	C74-C75-C76-C77
53	N	401	CDL	C22-C23-C24-C25
53	r	201	CDL	C71-C72-C73-C74
46	J	203	PC1	C37-C38-C39-C3A
45	b	102	3PE	C22-C21-O21-C2
45	P	502	3PE	C2-C1-O11-P
53	d	202	CDL	CB7-C71-C72-C73
45	Y	204	3PE	C35-C36-C37-C38
45	Y	205	3PE	C35-C36-C37-C38
45	Z	202	3PE	C22-C23-C24-C25
45	b	101	3PE	C33-C34-C35-C36
46	I	204	PC1	O32-C31-O31-C3
53	N	401	CDL	OA7-CA5-OA6-CA4
45	A	205	3PE	C23-C24-C25-C26
45	P	502	3PE	C35-C36-C37-C38
53	M	602	CDL	C32-C33-C34-C35
45	N	402	3PE	C35-C36-C37-C38
45	Y	204	3PE	C2A-C2B-C2C-C2D
45	Y	206	3PE	C33-C34-C35-C36
46	I	203	PC1	C28-C29-C2A-C2B
53	N	401	CDL	C35-C36-C37-C38
45	b	102	3PE	C25-C26-C27-C28
53	M	602	CDL	C73-C74-C75-C76
53	d	202	CDL	C81-C82-C83-C84
60	o	201	MYR	C3-C4-C5-C6
46	H	404	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
47	g	201	PLC	C1'-C2'-C3'-C4'
53	d	202	CDL	C37-C38-C39-C40
46	I	203	PC1	C32-C33-C34-C35
53	N	401	CDL	C57-C58-C59-C60
53	L	701	CDL	C53-C54-C55-C56
53	d	202	CDL	C54-C55-C56-C57
53	M	602	CDL	C62-C63-C64-C65
45	Y	203	3PE	C22-C21-O21-C2
46	L	702	PC1	C22-C21-O21-C2
53	d	202	CDL	CA7-C31-C32-C33
45	Y	203	3PE	O22-C21-O21-C2
45	N	402	3PE	C28-C29-C2A-C2B
47	g	201	PLC	C7'-C8'-C9'-CA'
53	d	201	CDL	C72-C73-C74-C75
53	d	202	CDL	C39-C40-C41-C42
47	J	202	PLC	C4B-C5B-C6B-C7B
45	d	203	3PE	C21-C22-C23-C24
45	d	203	3PE	C34-C35-C36-C37
45	i	202	3PE	C36-C37-C38-C39
47	Y	209	PLC	C3'-C4'-C5'-C6'
53	M	602	CDL	C38-C39-C40-C41
57	P	501	NDP	O4B-C4B-C5B-O5B
57	P	501	NDP	C3B-C4B-C5B-O5B
45	Y	203	3PE	C24-C25-C26-C27
46	A	202	PC1	C22-C23-C24-C25
45	Y	204	3PE	C33-C34-C35-C36
45	m	201	3PE	O32-C31-O31-C3
46	A	202	PC1	O32-C31-O31-C3
46	L	702	PC1	C29-C2A-C2B-C2C
53	M	602	CDL	C33-C34-C35-C36
53	M	602	CDL	C40-C41-C42-C43
45	J	201	3PE	C21-C22-C23-C24
45	a	101	3PE	C34-C35-C36-C37
47	M	606	PLC	C6B-C7B-C8B-C9B
45	Y	201	3PE	C22-C21-O21-C2
53	L	701	CDL	C15-C16-C17-C18
45	Y	207	3PE	C31-C32-C33-C34
45	A	201	3PE	O21-C2-C3-O31
45	M	603	3PE	O21-C2-C3-O31
45	d	203	3PE	O21-C2-C3-O31
46	l	701	PC1	O21-C2-C3-O31
45	M	604	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
53	H	402	CDL	C31-CA7-OA8-CA6
45	Y	201	3PE	C28-C29-C2A-C2B
46	H	403	PC1	C22-C23-C24-C25
46	I	701	PC1	C3B-C3C-C3D-C3E
46	L	702	PC1	C2E-C2F-C2G-C2H
53	M	602	CDL	C11-C12-C13-C14
53	d	201	CDL	C1-CB2-OB2-PB2
46	m	202	PC1	C24-C25-C26-C27
53	M	602	CDL	C31-C32-C33-C34
46	J	203	PC1	C24-C25-C26-C27
53	h	201	CDL	C32-C33-C34-C35
47	Z	201	PLC	C2-C3-O3-CB
45	a	101	3PE	C31-C32-C33-C34
45	N	402	3PE	C37-C38-C39-C3A
53	r	201	CDL	C53-C54-C55-C56
46	J	203	PC1	C33-C34-C35-C36
45	N	402	3PE	C2A-C2B-C2C-C2D
46	H	403	PC1	C26-C27-C28-C29
46	I	701	PC1	O11-C1-C2-C3
46	m	202	PC1	O11-C1-C2-C3
53	d	202	CDL	OA5-CA3-CA4-CA6
45	b	102	3PE	O22-C21-O21-C2
53	h	201	CDL	C15-C16-C17-C18
45	K	101	3PE	C22-C21-O21-C2
45	q	202	3PE	C22-C21-O21-C2
53	d	202	CDL	C35-C36-C37-C38
45	K	101	3PE	C32-C33-C34-C35
45	N	402	3PE	C33-C34-C35-C36
45	Y	201	3PE	C33-C34-C35-C36
46	I	204	PC1	C23-C24-C25-C26
45	Y	203	3PE	C1-C2-C3-O31
45	m	201	3PE	C1-C2-C3-O31
46	A	202	PC1	C1-C2-C3-O31
46	A	203	PC1	C1-C2-C3-O31
46	I	204	PC1	C1-C2-C3-O31
46	J	203	PC1	C1-C2-C3-O31
46	M	605	PC1	C1-C2-C3-O31
46	d	204	PC1	C1-C2-C3-O31
45	L	705	3PE	C29-C2A-C2B-C2C
46	d	204	PC1	C38-C39-C3A-C3B
46	m	202	PC1	C32-C31-O31-C3
45	A	201	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
45	Y	202	3PE	C34-C35-C36-C37
45	q	202	3PE	C3C-C3D-C3E-C3F
46	B	203	PC1	C36-C37-C38-C39
53	M	602	CDL	C18-C19-C20-C21
53	L	701	CDL	C40-C41-C42-C43
45	N	402	3PE	C22-C23-C24-C25
45	Y	201	3PE	O22-C21-O21-C2
53	d	201	CDL	C31-C32-C33-C34
53	d	202	CDL	C71-C72-C73-C74
53	H	402	CDL	OA9-CA7-OA8-CA6
46	l	701	PC1	C39-C3A-C3B-C3C
53	L	701	CDL	CA5-C11-C12-C13
45	M	604	3PE	C24-C25-C26-C27
45	Y	204	3PE	C38-C39-C3A-C3B
45	q	202	3PE	C33-C34-C35-C36
45	L	704	3PE	C33-C34-C35-C36
45	N	402	3PE	C2C-C2D-C2E-C2F
45	Y	201	3PE	C25-C26-C27-C28
45	a	101	3PE	C3C-C3D-C3E-C3F
53	h	201	CDL	C31-C32-C33-C34
45	Y	201	3PE	C22-C23-C24-C25
45	Z	203	3PE	C23-C24-C25-C26
53	N	401	CDL	C76-C77-C78-C79
45	Y	205	3PE	C2C-C2D-C2E-C2F
53	d	202	CDL	C32-C33-C34-C35
45	Y	208	3PE	O11-C1-C2-O21
45	f	101	3PE	O11-C1-C2-O21
53	d	201	CDL	OB5-CB3-CB4-OB6
45	Y	206	3PE	C34-C35-C36-C37
47	Y	209	PLC	C1B-CB-O3-C3
53	M	602	CDL	C31-CA7-OA8-CA6
45	Y	207	3PE	C22-C21-O21-C2
45	Y	207	3PE	C38-C39-C3A-C3B
53	L	701	CDL	C83-C84-C85-C86
53	d	202	CDL	C40-C41-C42-C43
46	I	203	PC1	C38-C39-C3A-C3B
46	m	202	PC1	C32-C33-C34-C35
45	N	402	3PE	O21-C2-C3-O31
45	i	202	3PE	O21-C2-C3-O31
46	I	204	PC1	O21-C2-C3-O31
46	h	202	PC1	O21-C2-C3-O31
53	d	202	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	C74-C75-C76-C77
53	r	201	CDL	C11-C12-C13-C14
45	i	202	3PE	C39-C3A-C3B-C3C
46	L	702	PC1	O22-C21-O21-C2
45	m	201	3PE	C35-C36-C37-C38
45	L	705	3PE	C21-C22-C23-C24
55	O	401	DGT	PA-O3A-PB-O2B
55	O	401	DGT	PB-O3A-PA-O2A
46	B	202	PC1	C22-C21-O21-C2
45	J	201	3PE	C2F-C2G-C2H-C2I
46	H	404	PC1	C36-C37-C38-C39
47	Y	209	PLC	CB-C1B-C2B-C3B
45	L	705	3PE	C28-C29-C2A-C2B
53	d	202	CDL	C44-C45-C46-C47
45	L	705	3PE	C27-C28-C29-C2A
53	N	401	CDL	C16-C17-C18-C19
46	q	201	PC1	C27-C28-C29-C2A
57	P	501	NDP	O4D-C1D-N1N-C6N
53	h	201	CDL	C54-C55-C56-C57
45	M	604	3PE	C3C-C3D-C3E-C3F
45	b	101	3PE	O11-C1-C2-C3
45	b	102	3PE	O11-C1-C2-C3
47	A	206	PLC	O3P-C1-C2-C3
47	Z	201	PLC	O3P-C1-C2-C3
53	d	201	CDL	OB5-CB3-CB4-CB6
45	r	202	3PE	C35-C36-C37-C38
45	N	402	3PE	C2F-C2G-C2H-C2I
46	q	201	PC1	C31-C32-C33-C34
46	m	202	PC1	O32-C31-O31-C3
53	d	202	CDL	C80-C81-C82-C83
45	Y	207	3PE	C22-C23-C24-C25
46	I	204	PC1	C25-C26-C27-C28
53	d	201	CDL	C39-C40-C41-C42
53	d	202	CDL	CA2-C1-CB2-OB2
53	d	202	CDL	C71-CB7-OB8-CB6
45	M	603	3PE	C33-C34-C35-C36
45	d	203	3PE	C28-C29-C2A-C2B
45	A	201	3PE	C1-C2-C3-O31
45	M	603	3PE	C1-C2-C3-O31
45	d	203	3PE	C1-C2-C3-O31
45	i	202	3PE	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	H	403	PC1	C1-C2-C3-O31
46	I	701	PC1	C1-C2-C3-O31
47	O	403	PLC	C1-C2-C3-O3
47	O	404	PLC	C1-C2-C3-O3
53	L	701	CDL	CB3-CB4-CB6-OB8
53	M	602	CDL	CB3-CB4-CB6-OB8
53	d	202	CDL	CB3-CB4-CB6-OB8
53	r	201	CDL	CA3-CA4-CA6-OA8
45	M	603	3PE	O22-C21-O21-C2
45	J	201	3PE	C29-C2A-C2B-C2C
45	a	101	3PE	C33-C34-C35-C36
45	d	203	3PE	C2B-C2C-C2D-C2E
46	H	404	PC1	C37-C38-C39-C3A
45	L	705	3PE	O11-C1-C2-O21
45	Y	203	3PE	O11-C1-C2-O21
46	m	202	PC1	O11-C1-C2-O21
47	Z	201	PLC	O3P-C1-C2-O2
53	d	202	CDL	OA5-CA3-CA4-OA6
46	I	203	PC1	C2B-C2C-C2D-C2E
46	L	702	PC1	C2A-C2B-C2C-C2D
45	A	201	3PE	O21-C21-C22-C23
45	Y	208	3PE	C2-C1-O11-P
53	M	602	CDL	C1-CA2-OA2-PA1
53	M	602	CDL	C1-CB2-OB2-PB2
53	h	201	CDL	C35-C36-C37-C38
58	T	101	EHZ	O1-C7-C8-C9
45	Y	208	3PE	C22-C23-C24-C25
45	r	202	3PE	O31-C31-C32-C33
47	J	202	PLC	C2B-C1B-CB-O3
45	b	101	3PE	O21-C2-C3-O31
45	m	201	3PE	O21-C2-C3-O31
46	A	202	PC1	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
46	H	404	PC1	O21-C2-C3-O31
46	J	203	PC1	O21-C2-C3-O31
47	L	703	PLC	O2-C2-C3-O3
53	d	201	CDL	OB6-CB4-CB6-OB8
53	h	201	CDL	OA6-CA4-CA6-OA8
53	d	201	CDL	C42-C43-C44-C45
46	H	404	PC1	C3C-C3D-C3E-C3F
53	r	201	CDL	C16-C17-C18-C19
45	r	202	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
53	L	701	CDL	C59-C60-C61-C62
57	P	501	NDP	PN-O3-PA-O5B
45	K	101	3PE	C39-C3A-C3B-C3C
46	q	201	PC1	C26-C27-C28-C29
45	Y	202	3PE	C26-C27-C28-C29
47	Y	209	PLC	OB-CB-O3-C3
45	Y	204	3PE	C21-C22-C23-C24
46	I	204	PC1	C31-C32-C33-C34
53	M	602	CDL	OA9-CA7-OA8-CA6
46	H	404	PC1	C24-C25-C26-C27
45	Y	205	3PE	O11-C1-C2-C3
47	Y	209	PLC	O3P-C1-C2-C3
53	M	602	CDL	OA5-CA3-CA4-CA6
45	Y	205	3PE	C31-C32-C33-C34
45	A	205	3PE	C38-C39-C3A-C3B
45	Y	205	3PE	C3D-C3E-C3F-C3G
45	K	101	3PE	O22-C21-O21-C2
45	q	202	3PE	O22-C21-O21-C2
53	M	602	CDL	C16-C17-C18-C19
45	Y	204	3PE	C32-C33-C34-C35
46	J	203	PC1	C2C-C2D-C2E-C2F
45	Y	206	3PE	C3-C2-O21-C21
45	q	202	3PE	C3-C2-O21-C21
55	O	401	DGT	PB-O3B-PG-O1G
47	A	206	PLC	C1'-C2'-C3'-C4'
53	M	602	CDL	C36-C37-C38-C39
45	r	202	3PE	C32-C33-C34-C35
45	P	502	3PE	C32-C33-C34-C35
46	B	202	PC1	O22-C21-O21-C2
45	b	101	3PE	O11-C1-C2-O21
47	Y	209	PLC	O3P-C1-C2-O2
53	M	602	CDL	OA5-CA3-CA4-OA6
45	q	202	3PE	C2D-C2E-C2F-C2G
53	L	701	CDL	C42-C43-C44-C45
45	K	101	3PE	C3C-C3D-C3E-C3F
45	L	704	3PE	C1-C2-C3-O31
46	H	404	PC1	C1-C2-C3-O31
47	J	202	PLC	C1-C2-C3-O3
53	h	201	CDL	CA3-CA4-CA6-OA8
53	L	701	CDL	C12-C13-C14-C15
53	N	401	CDL	C72-C73-C74-C75
45	m	201	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C12-C11-O13-P
45	A	205	3PE	C12-C11-O13-P
45	L	704	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	N	402	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	Y	203	3PE	C12-C11-O13-P
45	Y	204	3PE	C12-C11-O13-P
45	Y	206	3PE	C12-C11-O13-P
45	Y	208	3PE	C12-C11-O13-P
45	Z	203	3PE	C12-C11-O13-P
45	b	101	3PE	C12-C11-O13-P
45	b	102	3PE	C12-C11-O13-P
45	i	202	3PE	C12-C11-O13-P
47	L	703	PLC	C5-C4-O4P-P
47	M	606	PLC	C5-C4-O4P-P
46	A	203	PC1	O21-C2-C3-O31
47	O	404	PLC	O2-C2-C3-O3
53	M	602	CDL	OB6-CB4-CB6-OB8
53	r	201	CDL	OA6-CA4-CA6-OA8
45	Y	207	3PE	O22-C21-O21-C2
45	Y	206	3PE	C2B-C2C-C2D-C2E
46	H	403	PC1	C24-C25-C26-C27
53	L	701	CDL	C33-C34-C35-C36
53	d	202	CDL	OB9-CB7-OB8-CB6
45	Y	205	3PE	C22-C23-C24-C25
46	H	404	PC1	C3E-C3F-C3G-C3H
45	i	202	3PE	C25-C26-C27-C28
53	r	201	CDL	C52-C53-C54-C55
45	b	102	3PE	C28-C29-C2A-C2B
53	h	201	CDL	C11-C12-C13-C14
45	d	203	3PE	C39-C3A-C3B-C3C
47	L	703	PLC	C4B-C5B-C6B-C7B
46	I	204	PC1	C26-C27-C28-C29
45	L	705	3PE	C33-C34-C35-C36
46	d	204	PC1	O13-C11-C12-N
47	A	206	PLC	O4P-C4-C5-N
47	M	606	PLC	O4P-C4-C5-N
47	Y	209	PLC	O4P-C4-C5-N
53	d	202	CDL	C41-C42-C43-C44
46	L	702	PC1	C2C-C2D-C2E-C2F
45	q	202	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
47	O	404	PLC	C3B-C4B-C5B-C6B
47	Y	209	PLC	C2B-C3B-C4B-C5B
46	d	204	PC1	C36-C37-C38-C39
45	M	604	3PE	C3E-C3F-C3G-C3H
53	L	701	CDL	C16-C17-C18-C19
53	M	602	CDL	CA5-C11-C12-C13
45	L	705	3PE	O11-C1-C2-C3
45	Y	208	3PE	O11-C1-C2-C3
45	a	101	3PE	O11-C1-C2-C3
45	f	101	3PE	O11-C1-C2-C3
46	J	203	PC1	O11-C1-C2-C3
47	M	606	PLC	O3P-C1-C2-C3
53	N	401	CDL	OB5-CB3-CB4-CB6
53	d	201	CDL	OA5-CA3-CA4-CA6
46	J	203	PC1	C35-C36-C37-C38
50	F	502	FMN	N10-C1'-C2'-O2'
58	T	101	EHZ	C15-C16-C17-C20
58	T	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
45	P	502	3PE	C26-C27-C28-C29
45	K	101	3PE	C37-C38-C39-C3A
45	L	705	3PE	C32-C33-C34-C35
46	H	404	PC1	C33-C34-C35-C36
45	Y	202	3PE	O21-C21-C22-C23
45	P	502	3PE	C23-C24-C25-C26
45	N	402	3PE	C21-C22-C23-C24
45	q	202	3PE	C2-C1-O11-P
53	d	201	CDL	C36-C37-C38-C39
58	T	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	C11-C10-S1-C9
45	Y	205	3PE	C3F-C3G-C3H-C3I
45	Y	205	3PE	O11-C1-C2-O21
45	a	101	3PE	O11-C1-C2-O21
46	l	701	PC1	O11-C1-C2-O21
47	M	606	PLC	O3P-C1-C2-O2
53	d	201	CDL	OA5-CA3-CA4-OA6
45	M	604	3PE	C22-C23-C24-C25
45	Z	202	3PE	C33-C34-C35-C36
45	a	101	3PE	C32-C33-C34-C35
45	r	202	3PE	C22-C23-C24-C25
45	b	101	3PE	C34-C35-C36-C37
46	A	204	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
45	Y	205	3PE	C23-C24-C25-C26
45	P	502	3PE	O21-C2-C3-O31
45	r	202	3PE	O21-C2-C3-O31
53	L	701	CDL	OB6-CB4-CB6-OB8
53	d	202	CDL	OB6-CB4-CB6-OB8
45	i	202	3PE	C28-C29-C2A-C2B
46	I	203	PC1	C21-C22-C23-C24
45	L	705	3PE	C1-C2-C3-O31
45	Z	202	3PE	C1-C2-C3-O31
45	r	202	3PE	C1-C2-C3-O31
46	h	202	PC1	C1-C2-C3-O31
52	H	401	U10	C15-C14-C16-C17
53	M	602	CDL	C23-C24-C25-C26
45	q	202	3PE	O32-C31-O31-C3
53	h	201	CDL	C53-C54-C55-C56
45	Y	208	3PE	C2F-C2G-C2H-C2I
53	d	201	CDL	C77-C78-C79-C80
45	q	202	3PE	C32-C31-O31-C3
53	r	201	CDL	C31-C32-C33-C34
47	A	206	PLC	C2'-C3'-C4'-C5'
45	i	202	3PE	C3B-C3C-C3D-C3E
46	B	202	PC1	C23-C24-C25-C26
46	d	204	PC1	C32-C33-C34-C35
45	Y	208	3PE	C2E-C2F-C2G-C2H
45	q	202	3PE	C23-C24-C25-C26
45	A	205	3PE	C1-O11-P-O12
45	A	205	3PE	C1-O11-P-O13
45	A	205	3PE	C11-O13-P-O14
45	J	201	3PE	C11-O13-P-O12
45	L	704	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O12
45	L	704	3PE	C11-O13-P-O14
45	L	705	3PE	C11-O13-P-O12
45	M	603	3PE	O13-C11-C12-N
45	M	604	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O11
45	P	502	3PE	C11-O13-P-O11
45	P	502	3PE	C11-O13-P-O12
45	P	502	3PE	C11-O13-P-O14
45	Y	203	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O14
45	Y	206	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	Y	207	3PE	C11-O13-P-O11
45	Y	207	3PE	C11-O13-P-O12
45	Y	207	3PE	O13-C11-C12-N
45	Y	208	3PE	O13-C11-C12-N
45	Z	202	3PE	C11-O13-P-O14
45	Z	203	3PE	O13-C11-C12-N
45	b	101	3PE	C11-O13-P-O12
45	b	102	3PE	C1-O11-P-O13
45	i	202	3PE	C11-O13-P-O11
45	i	202	3PE	C11-O13-P-O14
45	m	201	3PE	O13-C11-C12-N
45	q	202	3PE	C1-O11-P-O12
45	q	202	3PE	C1-O11-P-O13
45	q	202	3PE	C1-O11-P-O14
45	r	202	3PE	C11-O13-P-O14
45	r	202	3PE	O13-C11-C12-N
46	A	203	PC1	C11-O13-P-O11
46	A	204	PC1	C11-O13-P-O11
46	A	204	PC1	C1-O11-P-O14
46	B	203	PC1	C11-O13-P-O11
46	J	203	PC1	C1-O11-P-O12
46	J	203	PC1	C1-O11-P-O13
46	L	702	PC1	C1-O11-P-O14
46	M	605	PC1	C11-O13-P-O14
46	M	605	PC1	C1-O11-P-O12
46	M	605	PC1	C1-O11-P-O14
46	M	605	PC1	C1-O11-P-O13
46	h	202	PC1	C11-O13-P-O14
46	h	202	PC1	C1-O11-P-O14
46	l	701	PC1	C11-O13-P-O12
46	m	202	PC1	C11-O13-P-O11
46	q	201	PC1	C11-O13-P-O14
47	L	703	PLC	C1-O3P-P-O2P
47	M	606	PLC	C4-O4P-P-O1P
47	O	404	PLC	C4-O4P-P-O1P
47	Z	201	PLC	C4-C5-N-C8
53	H	402	CDL	CA2-OA2-PA1-OA5
53	H	402	CDL	CA3-OA5-PA1-OA4
53	L	701	CDL	CA3-OA5-PA1-OA2
53	L	701	CDL	CA3-OA5-PA1-OA3
53	L	701	CDL	CA3-OA5-PA1-OA4
53	M	602	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
53	M	602	CDL	CB3-OB5-PB2-OB4
53	N	401	CDL	CA2-OA2-PA1-OA3
53	d	202	CDL	CB2-OB2-PB2-OB5
53	d	202	CDL	CB3-OB5-PB2-OB4
53	r	201	CDL	CA3-OA5-PA1-OA3
55	O	401	DGT	C5'-O5'-PA-O3A
55	O	401	DGT	C5'-O5'-PA-O2A
47	Y	209	PLC	C3B-C4B-C5B-C6B
47	g	201	PLC	C4'-C5'-C6'-C7'
50	F	502	FMN	O2'-C2'-C3'-C4'
45	M	603	3PE	C2-C1-O11-P
53	N	401	CDL	C44-C45-C46-C47
45	Y	202	3PE	C37-C38-C39-C3A
45	J	201	3PE	C3-C2-O21-C21
45	L	705	3PE	C3-C2-O21-C21
45	Y	204	3PE	C3-C2-O21-C21
45	i	202	3PE	C1-C2-O21-C21
47	Y	209	PLC	C1-C2-O2-C'
53	N	401	CDL	CA6-CA4-OA6-CA5
53	d	202	CDL	CA6-CA4-OA6-CA5
53	M	602	CDL	C52-C53-C54-C55
47	Y	209	PLC	C6'-C7'-C8'-C9'
46	A	204	PC1	C11-C12-N-C14
47	O	404	PLC	O3P-C1-C2-C3
46	A	202	PC1	C25-C26-C27-C28
53	M	602	CDL	OA7-CA5-OA6-CA4
46	J	203	PC1	O11-C1-C2-O21
45	A	201	3PE	C2C-C2D-C2E-C2F
45	Y	206	3PE	C39-C3A-C3B-C3C
60	o	201	MYR	C11-C12-C13-C14
45	Z	203	3PE	C34-C35-C36-C37
53	M	602	CDL	C77-C78-C79-C80
45	L	705	3PE	C31-C32-C33-C34
53	L	701	CDL	C36-C37-C38-C39
45	M	604	3PE	C3A-C3B-C3C-C3D
47	A	206	PLC	C2B-C3B-C4B-C5B
53	N	401	CDL	C19-C20-C21-C22
45	M	604	3PE	C3B-C3C-C3D-C3E
45	N	402	3PE	C2-C1-O11-P
45	Y	203	3PE	O21-C2-C3-O31
46	d	204	PC1	O21-C2-C3-O31
46	J	203	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	d	203	3PE	C2F-C2G-C2H-C2I
46	I	203	PC1	C3C-C3D-C3E-C3F
45	i	202	3PE	C2-C3-O31-C31
53	M	602	CDL	C11-CA5-OA6-CA4
45	Y	206	3PE	C31-C32-C33-C34
46	J	203	PC1	C34-C35-C36-C37
53	L	701	CDL	C32-C31-CA7-OA8
45	i	202	3PE	C3E-C3F-C3G-C3H
58	T	101	EHZ	O5-C16-C17-C18
58	T	101	EHZ	O5-C16-C17-C19
45	N	402	3PE	C1-C2-C3-O31
53	h	201	CDL	C36-C37-C38-C39
45	Y	201	3PE	C2D-C2E-C2F-C2G
45	Y	205	3PE	C33-C34-C35-C36
46	m	202	PC1	C38-C39-C3A-C3B
45	r	202	3PE	C23-C24-C25-C26
53	h	201	CDL	C39-C40-C41-C42
46	I	203	PC1	C11-C12-N-C14
45	Z	202	3PE	C25-C26-C27-C28
53	L	701	CDL	C38-C39-C40-C41
45	M	604	3PE	O22-C21-O21-C2
45	Y	202	3PE	C2D-C2E-C2F-C2G
53	H	402	CDL	C52-C53-C54-C55
45	Y	206	3PE	C36-C37-C38-C39
46	l	701	PC1	C37-C38-C39-C3A
46	M	605	PC1	C32-C31-O31-C3
45	Y	207	3PE	O11-C1-C2-O21
46	A	204	PC1	O11-C1-C2-O21
46	B	202	PC1	O11-C1-C2-O21
53	L	701	CDL	OA5-CA3-CA4-OA6
53	r	201	CDL	OB5-CB3-CB4-OB6
45	A	201	3PE	C26-C27-C28-C29
53	h	201	CDL	C76-C77-C78-C79
46	M	605	PC1	O32-C31-O31-C3
45	b	101	3PE	C3C-C3D-C3E-C3F
45	a	101	3PE	C3F-C3G-C3H-C3I
45	Y	201	3PE	C32-C33-C34-C35
53	M	602	CDL	C72-C73-C74-C75
53	N	401	CDL	C73-C74-C75-C76
46	d	204	PC1	C33-C34-C35-C36
45	A	201	3PE	C35-C36-C37-C38
45	Y	207	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C13-C14-C15-C16
45	Y	205	3PE	C27-C28-C29-C2A
45	i	202	3PE	C33-C34-C35-C36
46	B	203	PC1	C3C-C3D-C3E-C3F
46	A	204	PC1	C32-C33-C34-C35
46	d	204	PC1	C3B-C3C-C3D-C3E
46	I	203	PC1	C2C-C2D-C2E-C2F
53	r	201	CDL	C1-CB2-OB2-PB2
53	d	202	CDL	C34-C35-C36-C37
45	L	705	3PE	C35-C36-C37-C38
52	H	401	U10	C2-C3-O3-C3M
45	Y	202	3PE	C2A-C2B-C2C-C2D
45	i	202	3PE	C34-C35-C36-C37
46	l	701	PC1	C3D-C3E-C3F-C3G
46	A	204	PC1	C26-C27-C28-C29
45	i	202	3PE	C3D-C3E-C3F-C3G
46	H	404	PC1	C38-C39-C3A-C3B
45	M	604	3PE	O31-C31-C32-C33
45	Z	202	3PE	C1-C2-O21-C21
45	Z	202	3PE	C3-C2-O21-C21
47	L	703	PLC	C1-C2-O2-C'
53	H	402	CDL	CA6-CA4-OA6-CA5
46	H	404	PC1	C3B-C3C-C3D-C3E
53	H	402	CDL	C51-C52-C53-C54
53	h	201	CDL	C73-C74-C75-C76
53	h	201	CDL	C33-C34-C35-C36
46	B	202	PC1	C34-C35-C36-C37
46	h	202	PC1	C21-C22-C23-C24
45	Y	206	3PE	C2F-C2G-C2H-C2I
45	Y	204	3PE	O31-C31-C32-C33
45	Y	207	3PE	C2C-C2D-C2E-C2F
45	q	202	3PE	C25-C26-C27-C28
46	I	203	PC1	C27-C28-C29-C2A
45	Y	207	3PE	C29-C2A-C2B-C2C
45	M	603	3PE	C38-C39-C3A-C3B
53	L	701	CDL	C63-C64-C65-C66
47	g	201	PLC	CB-C1B-C2B-C3B
45	Y	204	3PE	O11-C1-C2-O21
46	h	202	PC1	O11-C1-C2-O21
53	N	401	CDL	OA5-CA3-CA4-OA6
53	N	401	CDL	OB5-CB3-CB4-OB6
45	Y	205	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
53	r	201	CDL	C13-C14-C15-C16
53	r	201	CDL	CB7-C71-C72-C73
47	Y	209	PLC	C6B-C7B-C8B-C9B
45	a	101	3PE	C2-C1-O11-P
45	b	101	3PE	C2-C1-O11-P
55	O	401	DGT	C4'-C5'-O5'-PA
45	b	101	3PE	C22-C23-C24-C25
50	F	502	FMN	O2'-C2'-C3'-O3'
45	L	705	3PE	O21-C2-C3-O31
45	Z	202	3PE	O21-C2-C3-O31
46	H	404	PC1	C32-C33-C34-C35
57	P	501	NDP	C2N-C3N-C7N-N7N
46	H	404	PC1	C34-C35-C36-C37
46	L	702	PC1	C32-C33-C34-C35
45	Y	208	3PE	C29-C2A-C2B-C2C
53	L	701	CDL	C64-C65-C66-C67
46	A	204	PC1	C11-C12-N-C15
46	I	203	PC1	C11-C12-N-C13
53	r	201	CDL	CA2-C1-CB2-OB2
45	P	502	3PE	C22-C23-C24-C25
45	Y	201	3PE	C29-C2A-C2B-C2C
58	U	101	EHZ	C21-C22-C23-C24
53	d	201	CDL	C71-C72-C73-C74
46	A	202	PC1	C24-C25-C26-C27
45	M	604	3PE	C23-C24-C25-C26
53	H	402	CDL	O1-C1-CB2-OB2
46	H	403	PC1	C2E-C2F-C2G-C2H
45	M	604	3PE	C22-C21-O21-C2
45	J	201	3PE	C23-C24-C25-C26
45	Z	202	3PE	C34-C35-C36-C37
46	B	203	PC1	C34-C35-C36-C37
55	O	401	DGT	PG-O3B-PB-O2B
53	L	701	CDL	C14-C15-C16-C17
45	Z	202	3PE	C28-C29-C2A-C2B
47	A	206	PLC	C2-C1-O3P-P
45	A	205	3PE	O31-C31-C32-C33
53	h	201	CDL	C16-C17-C18-C19
46	J	203	PC1	C11-C12-N-C15
53	d	202	CDL	C42-C43-C44-C45
46	I	204	PC1	C21-C22-C23-C24
45	b	101	3PE	C1-C2-C3-O31
47	L	703	PLC	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
53	d	201	CDL	CB3-CB4-CB6-OB8
53	r	201	CDL	CB3-CB4-CB6-OB8
45	Y	206	3PE	C3A-C3B-C3C-C3D
45	b	101	3PE	C37-C38-C39-C3A
59	i	201	CHD	C22-C23-C24-O26
45	J	201	3PE	C2C-C2D-C2E-C2F
45	K	101	3PE	C36-C37-C38-C39
47	O	404	PLC	C1B-C2B-C3B-C4B
45	Y	202	3PE	C39-C3A-C3B-C3C
46	H	403	PC1	O21-C21-C22-C23
53	M	602	CDL	C22-C23-C24-C25
45	J	201	3PE	O22-C21-O21-C2
45	q	202	3PE	C37-C38-C39-C3A
46	I	203	PC1	C3E-C3F-C3G-C3H
53	L	701	CDL	OB5-CB3-CB4-OB6
46	H	404	PC1	C28-C29-C2A-C2B
45	b	101	3PE	C3E-C3F-C3G-C3H
45	q	202	3PE	C34-C35-C36-C37
52	H	401	U10	C6-C7-C8-C9
53	M	602	CDL	C12-C11-CA5-OA6
53	d	201	CDL	C73-C74-C75-C76
46	A	204	PC1	C11-C12-N-C13
46	I	203	PC1	C11-C12-N-C15
45	Y	207	3PE	C36-C37-C38-C39
45	q	202	3PE	C39-C3A-C3B-C3C
50	F	502	FMN	C1'-C2'-C3'-O3'
45	Y	208	3PE	C25-C26-C27-C28
46	A	204	PC1	O21-C2-C3-O31
46	q	201	PC1	O21-C2-C3-O31
45	J	201	3PE	C22-C21-O21-C2
53	N	401	CDL	C18-C19-C20-C21
53	r	201	CDL	C18-C19-C20-C21
45	Z	203	3PE	C2-C1-O11-P
53	r	201	CDL	CB4-CB3-OB5-PB2
53	L	701	CDL	C58-C59-C60-C61
46	B	203	PC1	C25-C26-C27-C28
46	d	204	PC1	C35-C36-C37-C38
45	Y	205	3PE	C32-C33-C34-C35
46	B	203	PC1	C22-C23-C24-C25
45	Y	204	3PE	C31-C32-C33-C34
59	i	201	CHD	C22-C23-C24-O25
45	Y	204	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
50	F	502	FMN	C5'-O5'-P-O2P
46	L	702	PC1	C25-C26-C27-C28
46	J	203	PC1	C11-C12-N-C13
47	O	404	PLC	C4-C5-N-C8
45	A	201	3PE	O22-C21-C22-C23
53	h	201	CDL	C52-C53-C54-C55
45	Y	206	3PE	C32-C33-C34-C35
45	N	402	3PE	C23-C24-C25-C26
46	B	202	PC1	C31-C32-C33-C34
45	J	201	3PE	C1-C2-O21-C21
55	O	401	DGT	PB-O3B-PG-O2G
58	T	101	EHZ	O3-C12-C13-C14
45	N	402	3PE	C25-C26-C27-C28
58	U	101	EHZ	C3-C4-C5-C6
45	r	202	3PE	O32-C31-C32-C33
45	N	402	3PE	C24-C25-C26-C27
45	d	203	3PE	C3A-C3B-C3C-C3D
45	i	202	3PE	C32-C33-C34-C35
52	H	401	U10	C13-C14-C16-C17
53	L	701	CDL	C61-C62-C63-C64
46	L	702	PC1	C22-C23-C24-C25
47	M	606	PLC	C2B-C3B-C4B-C5B
47	O	404	PLC	C4-C5-N-C6
47	O	404	PLC	C4-C5-N-C7
46	h	202	PC1	C24-C25-C26-C27
47	O	403	PLC	C3'-C4'-C5'-C6'
45	K	101	3PE	C1-C2-C3-O31
45	P	502	3PE	C1-C2-C3-O31
46	q	201	PC1	C1-C2-C3-O31
58	T	101	EHZ	N1-C12-C13-C14
45	M	604	3PE	C28-C29-C2A-C2B
45	Y	208	3PE	C2D-C2E-C2F-C2G
45	L	705	3PE	C26-C27-C28-C29
45	M	604	3PE	C39-C3A-C3B-C3C
53	N	401	CDL	C37-C38-C39-C40
45	q	202	3PE	C12-C11-O13-P
47	O	403	PLC	C5-C4-O4P-P
47	Y	209	PLC	C5-C4-O4P-P
58	T	101	EHZ	C15-C16-C17-C19
45	M	603	3PE	C31-C32-C33-C34
46	H	404	PC1	C27-C28-C29-C2A
46	H	404	PC1	C3F-C3G-C3H-C3I

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Mol	Chain	Res	Type	Atoms
45	J	201	3PE	O21-C2-C3-O31
45	q	202	3PE	O21-C2-C3-O31
45	Y	205	3PE	C28-C29-C2A-C2B
53	M	602	CDL	C52-C51-CB5-OB6
47	J	202	PLC	C2B-C1B-CB-OB
45	Y	203	3PE	O11-C1-C2-C3
45	Y	207	3PE	O11-C1-C2-C3
45	L	704	3PE	C31-C32-C33-C34
46	L	702	PC1	C21-C22-C23-C24
53	r	201	CDL	CA7-C31-C32-C33
53	d	202	CDL	C77-C78-C79-C80
45	Y	206	3PE	C3D-C3E-C3F-C3G
46	J	203	PC1	C11-C12-N-C14
45	N	402	3PE	O31-C31-C32-C33
45	Y	201	3PE	O21-C21-C22-C23
47	O	404	PLC	C2B-C1B-CB-O3
53	d	201	CDL	C72-C71-CB7-OB8
47	Y	209	PLC	C7B-C8B-C9B-CAA
53	N	401	CDL	C41-C42-C43-C44
53	N	401	CDL	C43-C44-C45-C46
45	J	201	3PE	O31-C31-C32-C33
47	L	703	PLC	O'-C'-O2-C2
45	A	201	3PE	C25-C26-C27-C28
53	N	401	CDL	C23-C24-C25-C26
45	J	201	3PE	C2A-C2B-C2C-C2D
45	Y	207	3PE	C2A-C2B-C2C-C2D
45	Z	203	3PE	C27-C28-C29-C2A
46	h	202	PC1	C29-C2A-C2B-C2C
45	i	202	3PE	C27-C28-C29-C2A
46	I	203	PC1	O13-C11-C12-N
53	d	201	CDL	C43-C44-C45-C46
45	M	604	3PE	C29-C2A-C2B-C2C
45	Z	203	3PE	C26-C27-C28-C29
53	L	701	CDL	C44-C45-C46-C47
45	Y	205	3PE	O31-C31-C32-C33
46	B	203	PC1	O21-C21-C22-C23
47	J	202	PLC	O2-C'-C1'-C2'
53	L	701	CDL	C52-C51-CB5-OB6
47	O	403	PLC	C2'-C3'-C4'-C5'
53	N	401	CDL	C78-C79-C80-C81
45	m	201	3PE	C25-C26-C27-C28
47	g	201	PLC	C8'-C9'-CA'-CB'

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Mol	Chain	Res	Type	Atoms
46	H	403	PC1	O31-C31-C32-C33
46	L	702	PC1	O31-C31-C32-C33
46	q	201	PC1	C2F-C2G-C2H-C2I
47	L	703	PLC	C1'-C'-O2-C2
45	Y	206	3PE	C3C-C3D-C3E-C3F
45	M	604	3PE	C38-C39-C3A-C3B
46	A	202	PC1	O21-C21-C22-C23
45	Y	206	3PE	C2D-C2E-C2F-C2G
53	L	701	CDL	C35-C36-C37-C38
53	h	201	CDL	C40-C41-C42-C43
45	Y	202	3PE	C2C-C2D-C2E-C2F
46	d	204	PC1	C11-C12-N-C15
47	Z	201	PLC	C4-C5-N-C6
47	Z	201	PLC	C4-C5-N-C7
46	I	203	PC1	C25-C26-C27-C28
45	Y	205	3PE	O21-C21-C22-C23
53	H	402	CDL	C52-C51-CB5-OB6
53	N	401	CDL	C63-C64-C65-C66
46	m	202	PC1	O21-C2-C3-O31
53	d	202	CDL	OA6-CA4-CA6-OA8
53	N	401	CDL	C55-C56-C57-C58
45	Y	203	3PE	O21-C21-C22-C23
46	M	605	PC1	C32-C33-C34-C35
45	M	604	3PE	C32-C33-C34-C35
45	Y	207	3PE	O31-C31-C32-C33
52	H	401	U10	C23-C24-C26-C27
58	T	101	EHZ	C19-C17-C20-O6
53	d	202	CDL	C78-C79-C80-C81
45	J	201	3PE	C2B-C2C-C2D-C2E
47	g	201	PLC	C1-C2-O2-C'
45	K	101	3PE	C26-C27-C28-C29
46	B	202	PC1	C11-C12-N-C15
45	Y	207	3PE	O21-C21-C22-C23
53	M	602	CDL	C81-C82-C83-C84
53	L	701	CDL	OB7-CB5-OB6-CB4
53	M	602	CDL	C44-C45-C46-C47
45	J	201	3PE	C2D-C2E-C2F-C2G
45	A	205	3PE	C25-C26-C27-C28
45	N	402	3PE	C39-C3A-C3B-C3C
45	N	402	3PE	C26-C27-C28-C29
46	L	702	PC1	C2D-C2E-C2F-C2G
45	J	201	3PE	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
47	O	404	PLC	C2B-C1B-CB-OB
46	l	701	PC1	C22-C23-C24-C25
45	M	604	3PE	C35-C36-C37-C38
45	b	101	3PE	O31-C31-C32-C33
47	J	202	PLC	O'-C'-C1'-C2'
53	L	701	CDL	C52-C51-CB5-OB7
46	h	202	PC1	C28-C29-C2A-C2B
46	A	202	PC1	C11-C12-N-C14
46	A	202	PC1	C11-C12-N-C15
46	B	202	PC1	C11-C12-N-C14
46	d	204	PC1	C11-C12-N-C13
46	d	204	PC1	C11-C12-N-C14
45	P	502	3PE	O21-C21-C22-C23
46	I	204	PC1	C34-C35-C36-C37
53	N	401	CDL	C62-C63-C64-C65
53	d	201	CDL	C44-C45-C46-C47
53	L	701	CDL	O1-C1-CB2-OB2
53	H	402	CDL	C52-C51-CB5-OB7
53	M	602	CDL	C52-C51-CB5-OB7
46	A	203	PC1	C33-C34-C35-C36
46	h	202	PC1	C23-C24-C25-C26
46	h	202	PC1	C26-C27-C28-C29
45	L	704	3PE	C27-C28-C29-C2A
45	b	101	3PE	C3B-C3C-C3D-C3E
46	B	202	PC1	O21-C21-C22-C23
47	M	606	PLC	C2B-C1B-CB-O3
46	d	204	PC1	C23-C24-C25-C26
53	d	201	CDL	C72-C71-CB7-OB9
47	M	606	PLC	O'-C'-O2-C2
45	Z	202	3PE	C27-C28-C29-C2A
45	b	102	3PE	C29-C2A-C2B-C2C
53	L	701	CDL	CA2-C1-CB2-OB2
45	N	402	3PE	O32-C31-C32-C33
45	Y	205	3PE	O32-C31-C32-C33
45	Y	207	3PE	O32-C31-C32-C33
45	L	705	3PE	O31-C31-C32-C33
53	M	602	CDL	C32-C31-CA7-OA8
53	N	401	CDL	C72-C71-CB7-OB8
53	L	701	CDL	C41-C42-C43-C44
53	L	701	CDL	C37-C38-C39-C40
53	d	201	CDL	C32-C33-C34-C35
45	Y	207	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	Y	207	3PE	O22-C21-C22-C23
46	A	202	PC1	O22-C21-C22-C23
45	K	101	3PE	C2A-C2B-C2C-C2D
46	B	202	PC1	C11-C12-N-C13
46	H	403	PC1	O32-C31-C32-C33
45	K	101	3PE	O21-C21-C22-C23
53	h	201	CDL	C12-C11-CA5-OA6
45	Y	205	3PE	O22-C21-C22-C23
46	L	702	PC1	O32-C31-C32-C33
46	B	203	PC1	O22-C21-C22-C23
45	Y	208	3PE	C24-C25-C26-C27
45	Y	203	3PE	O22-C21-C22-C23
47	L	703	PLC	C'-C1'-C2'-C3'
45	M	604	3PE	O21-C21-C22-C23
45	P	502	3PE	O31-C31-C32-C33
46	J	203	PC1	O31-C31-C32-C33
53	d	202	CDL	C32-C31-CA7-OA8
57	P	501	NDP	PA-O3-PN-O2N
45	r	202	3PE	C34-C35-C36-C37
45	a	101	3PE	O31-C31-C32-C33
46	M	605	PC1	O21-C21-C22-C23
46	l	701	PC1	O21-C21-C22-C23
45	M	604	3PE	C33-C34-C35-C36
53	r	201	CDL	C54-C55-C56-C57
53	d	202	CDL	CA5-C11-C12-C13
45	L	705	3PE	O32-C31-C32-C33
53	N	401	CDL	C31-C32-C33-C34

There are no ring outliers.

22 monomers are involved in 50 short contacts:

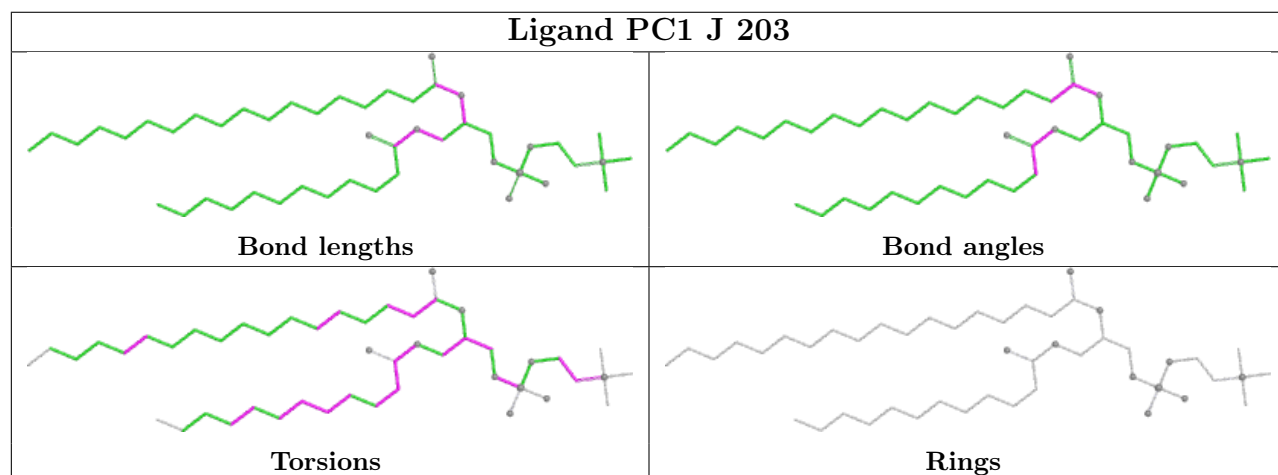
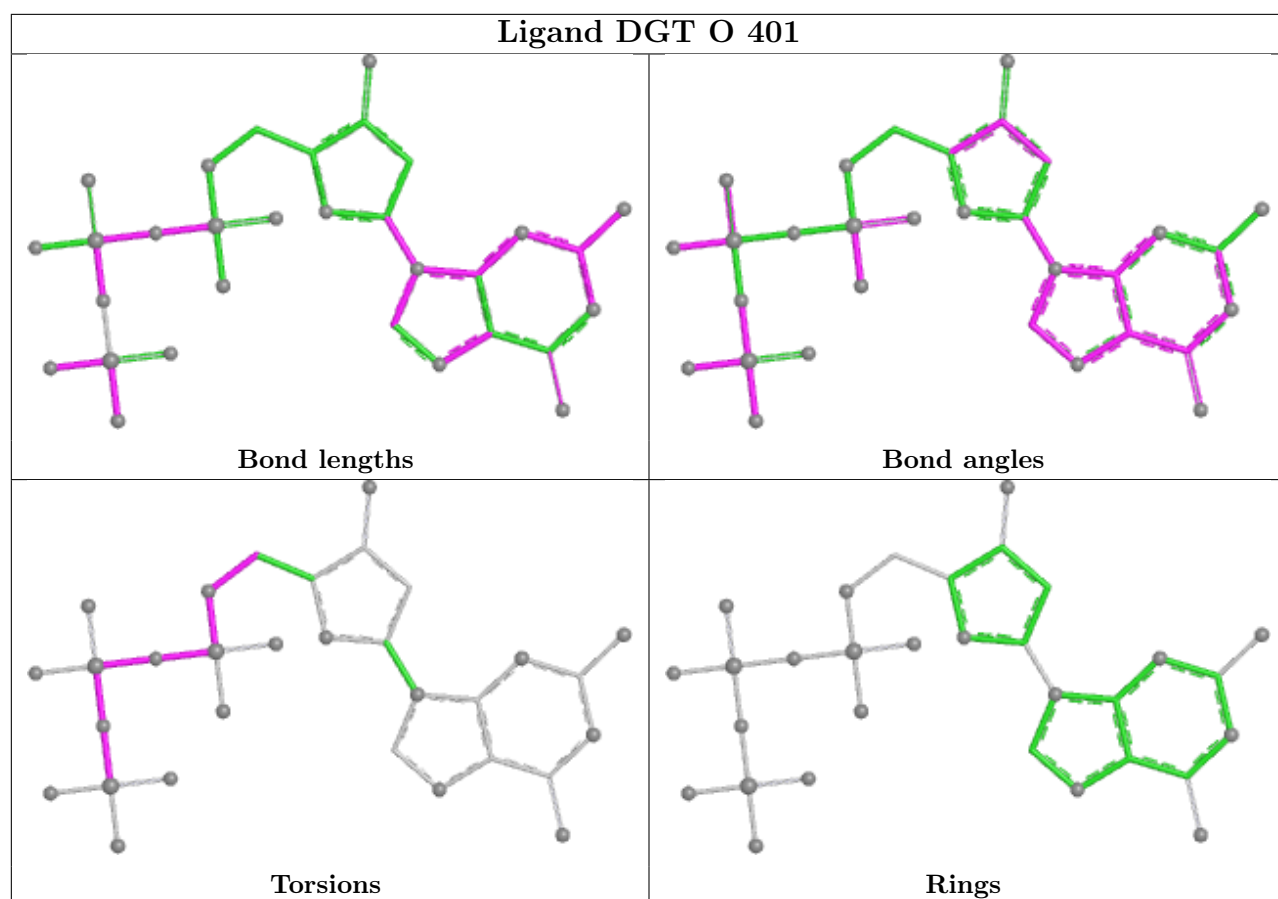
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	O	401	DGT	3	0
46	J	203	PC1	2	0
59	i	201	CHD	6	0
53	d	201	CDL	1	0
45	q	202	3PE	1	0
45	Z	202	3PE	1	0
45	Y	204	3PE	1	0
45	b	102	3PE	2	0
46	A	202	PC1	1	0
53	M	602	CDL	3	0

Continued on next page...

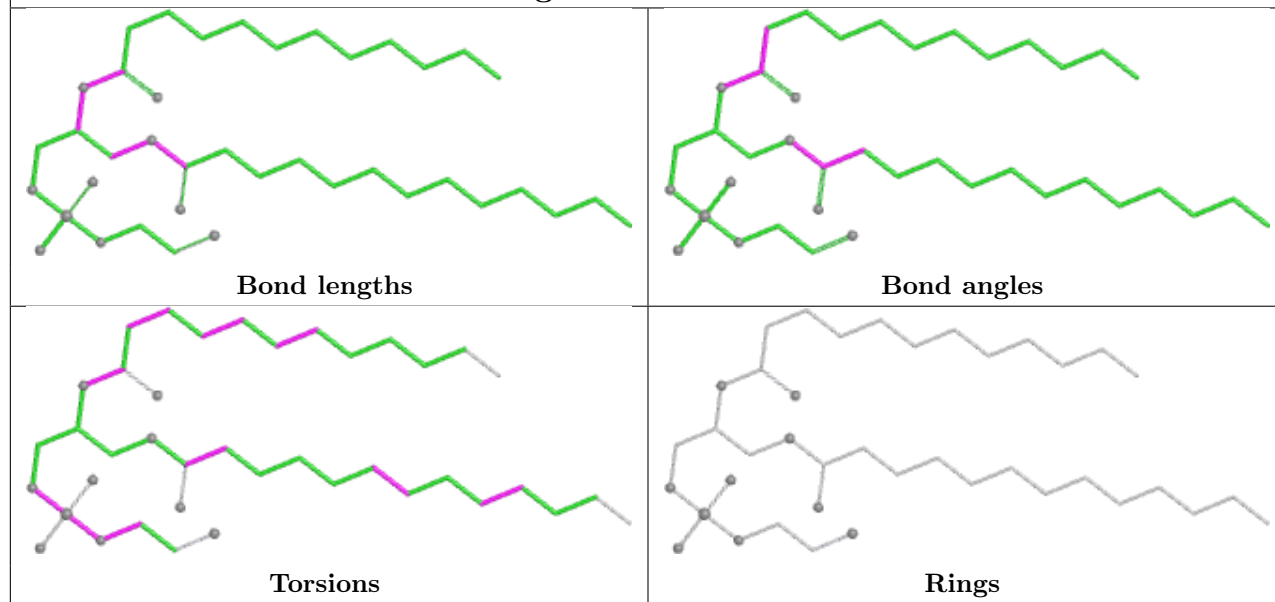
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	B	203	PC1	1	0
46	q	201	PC1	2	0
45	Y	201	3PE	1	0
58	U	101	EHZ	1	0
53	h	201	CDL	2	0
57	P	501	NDP	2	0
52	H	401	U10	17	0
46	A	204	PC1	1	0
50	F	502	FMN	1	0
46	L	702	PC1	2	0
45	a	101	3PE	1	0
45	Y	206	3PE	1	0

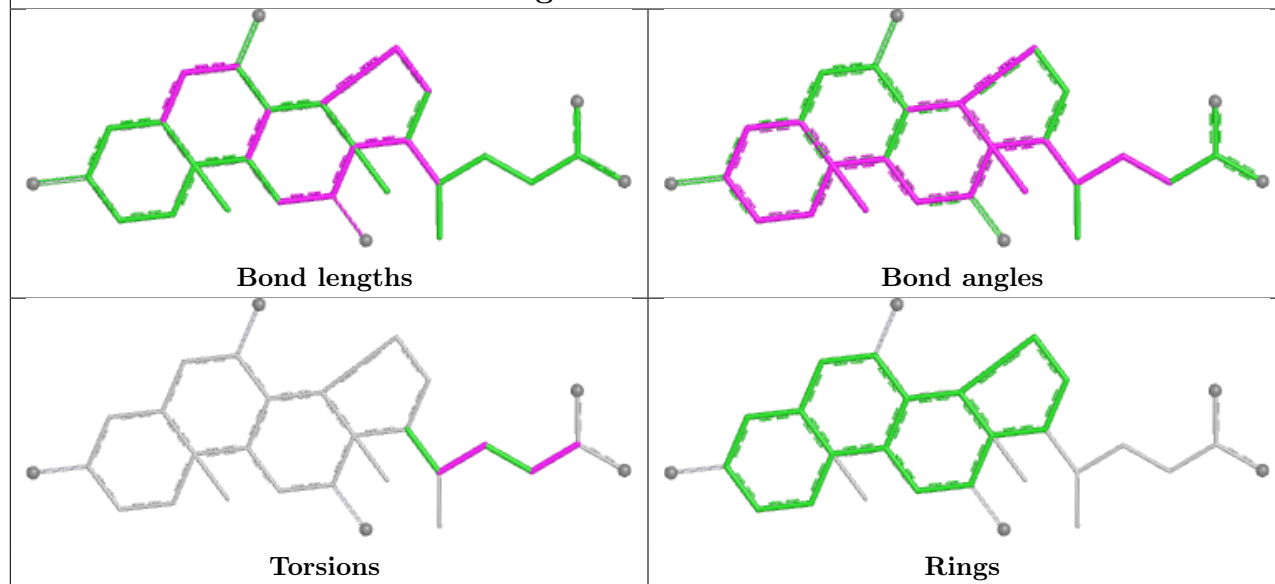
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



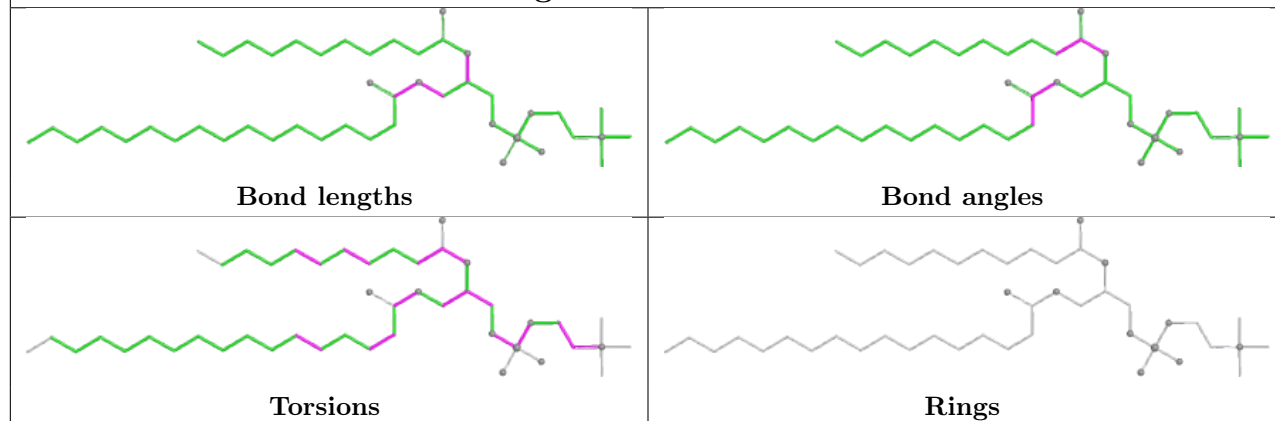
Ligand 3PE A 205

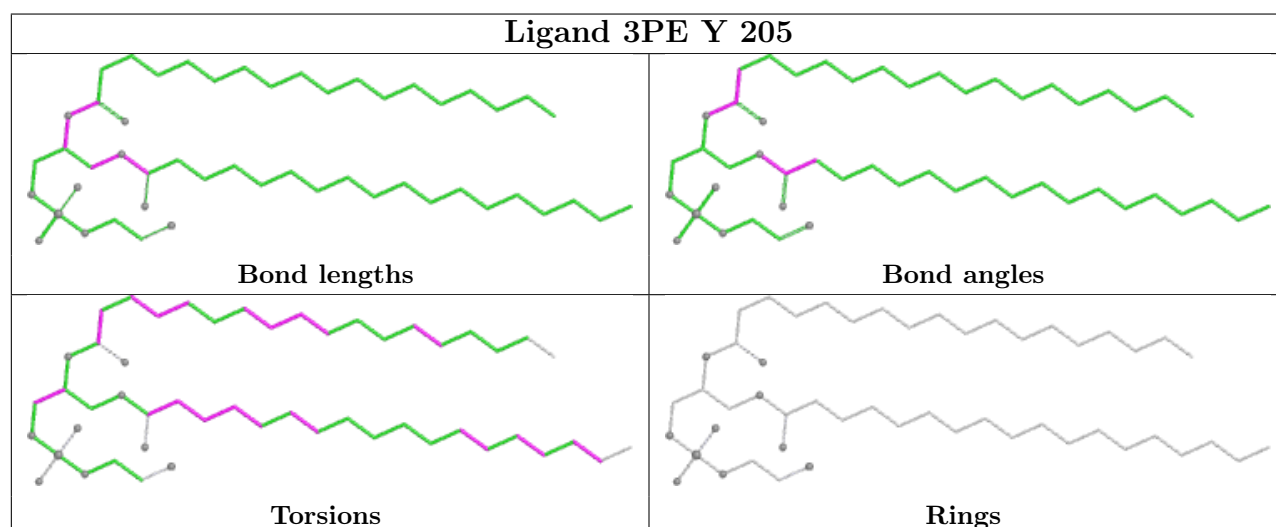
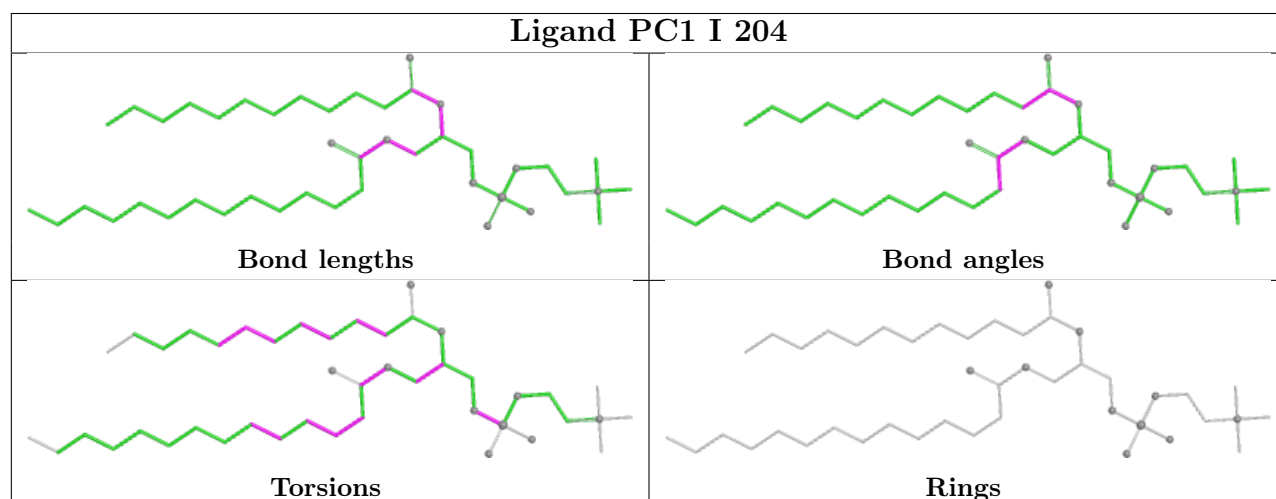
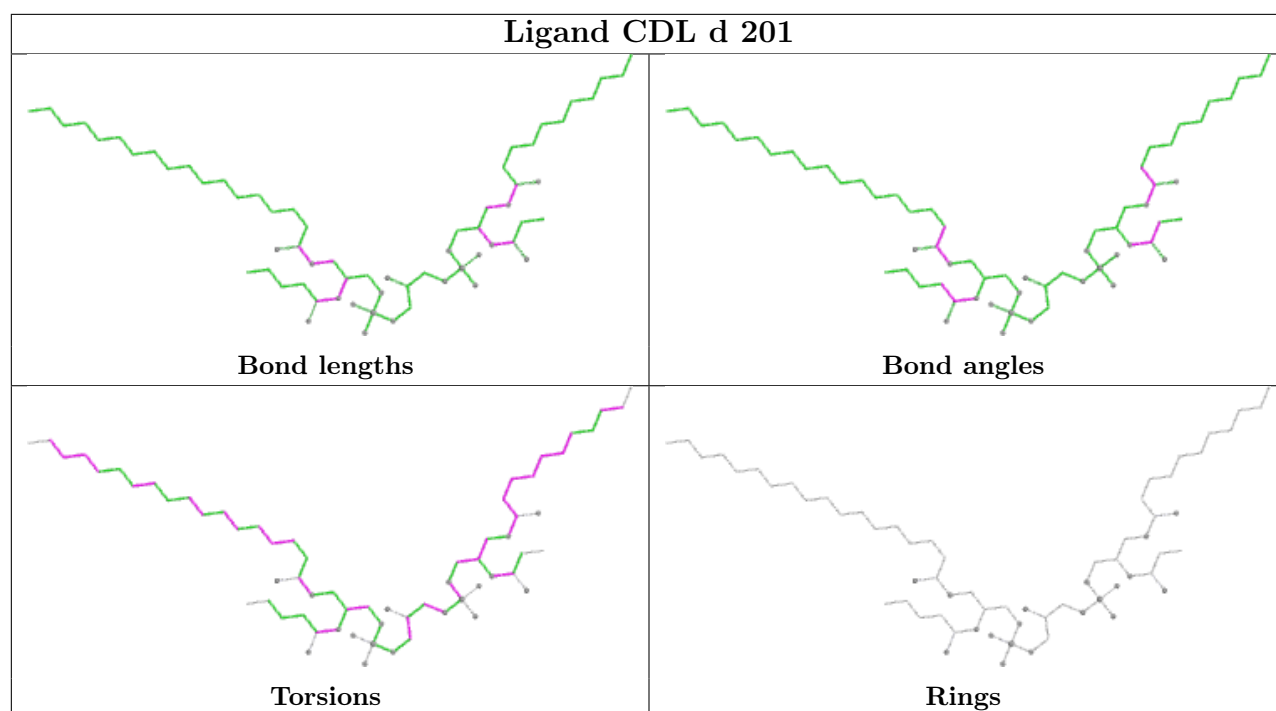


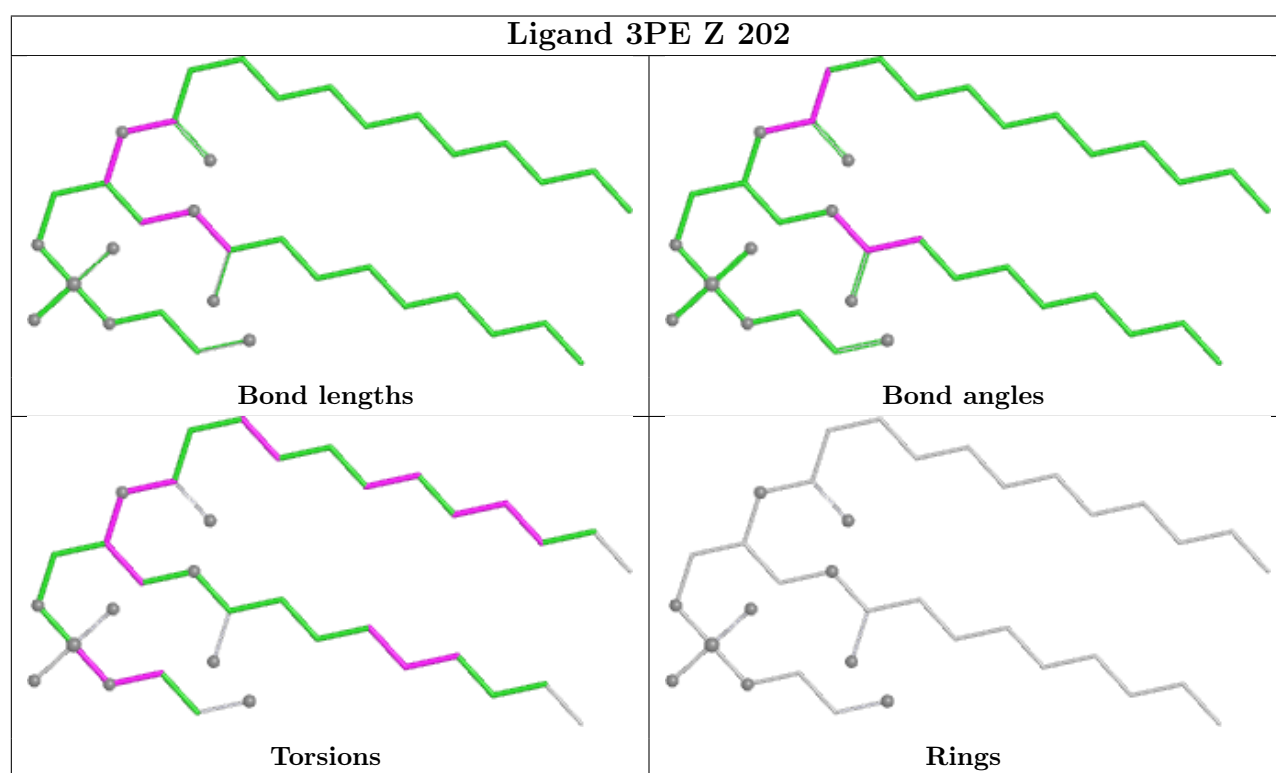
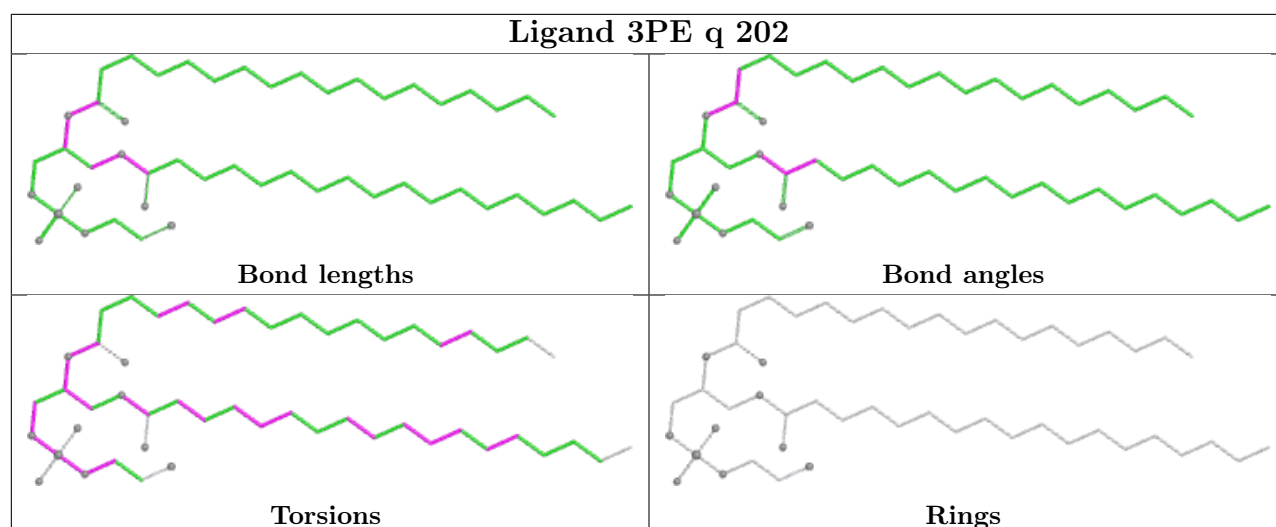
Ligand CHD i 201

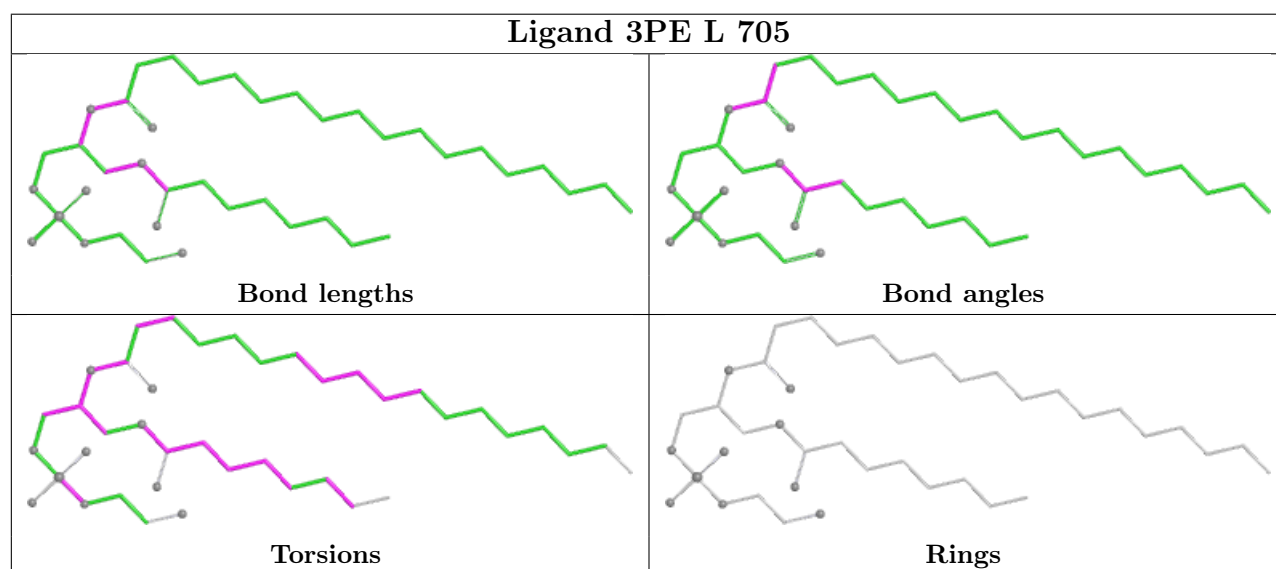
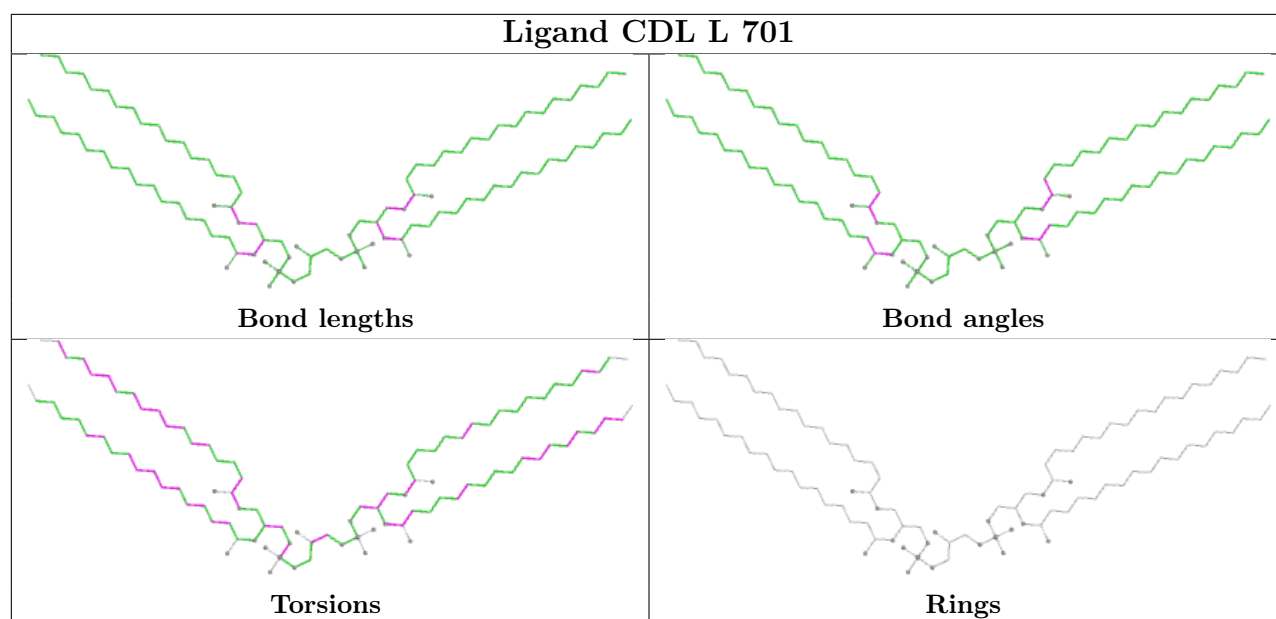


Ligand PC1 B 202

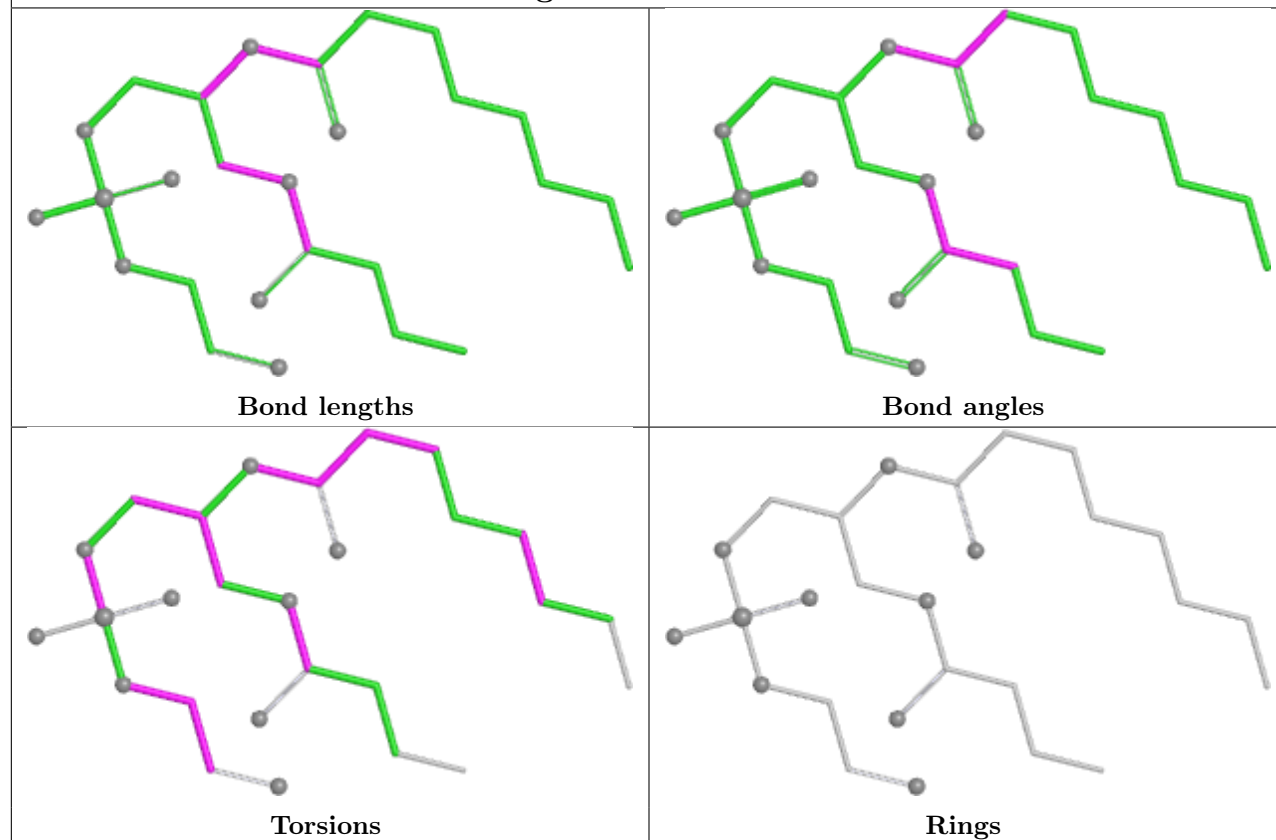




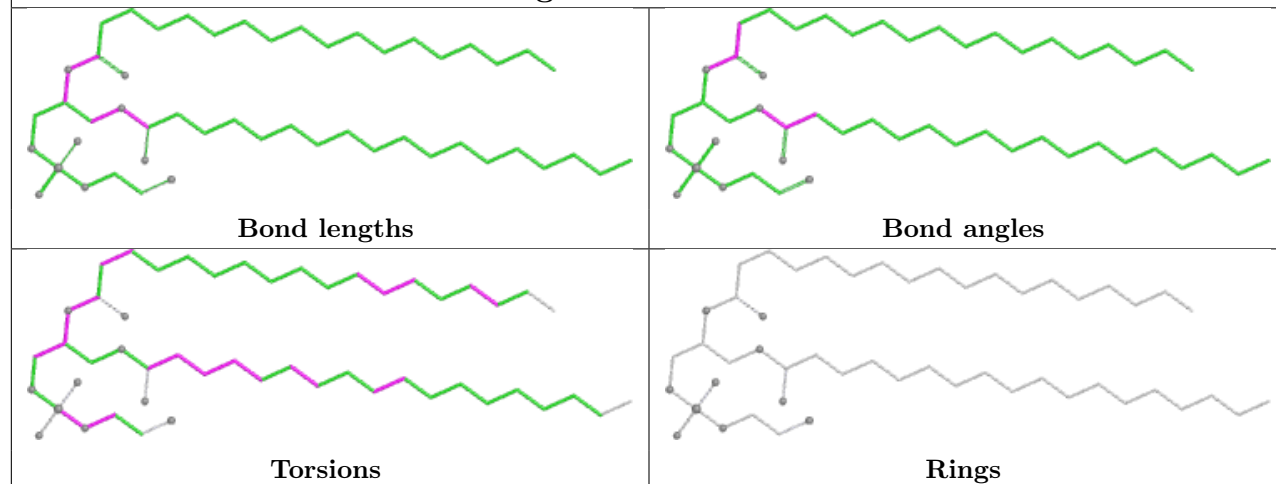


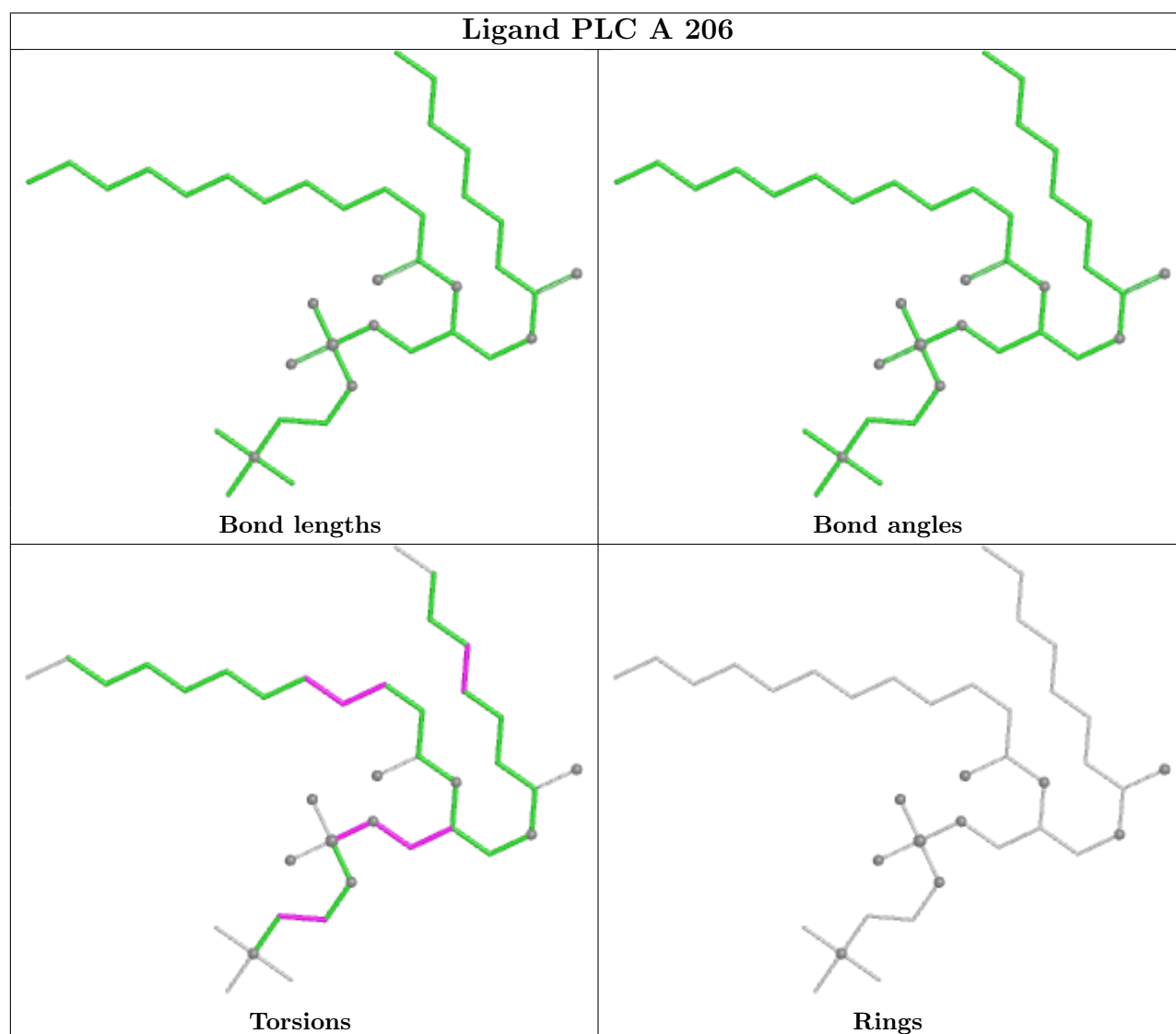
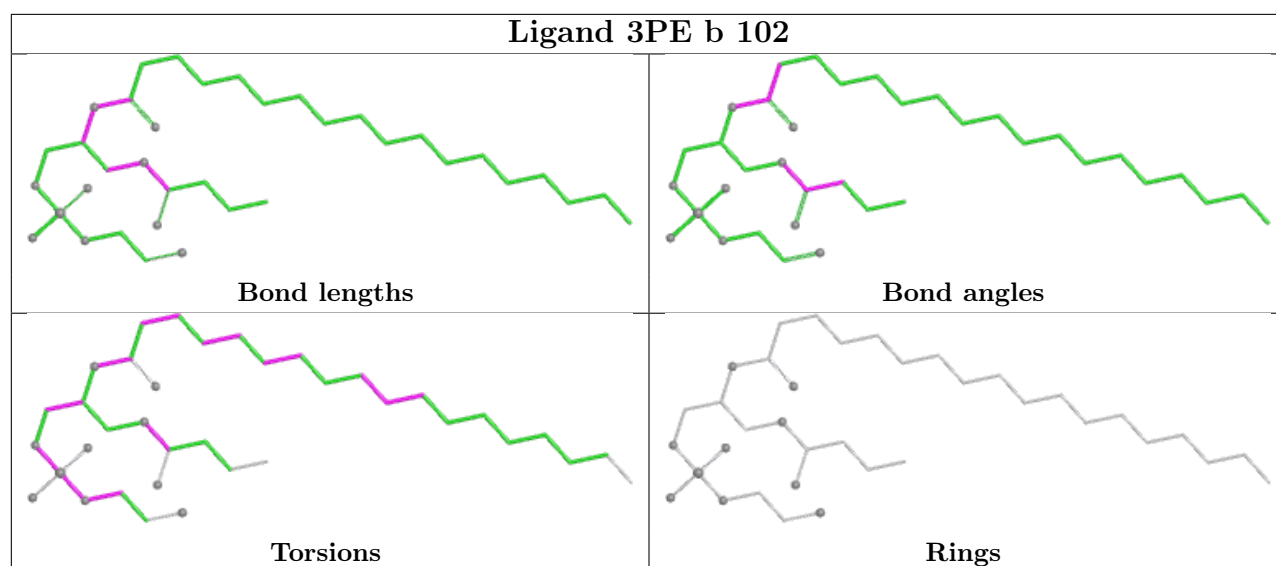


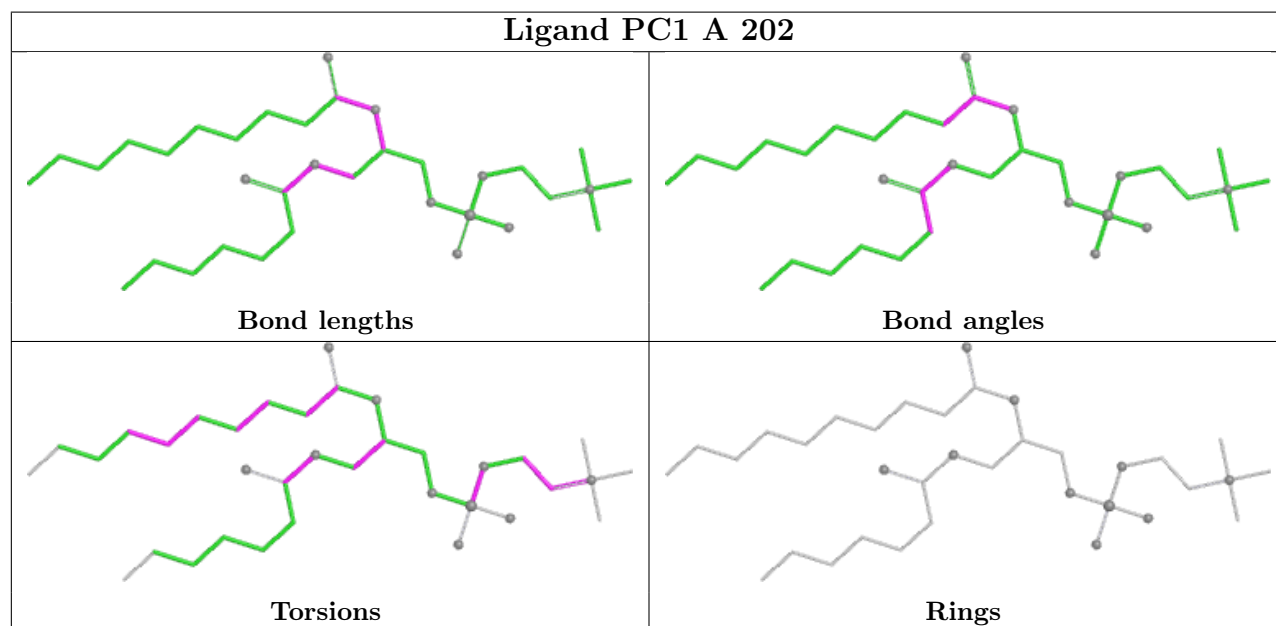
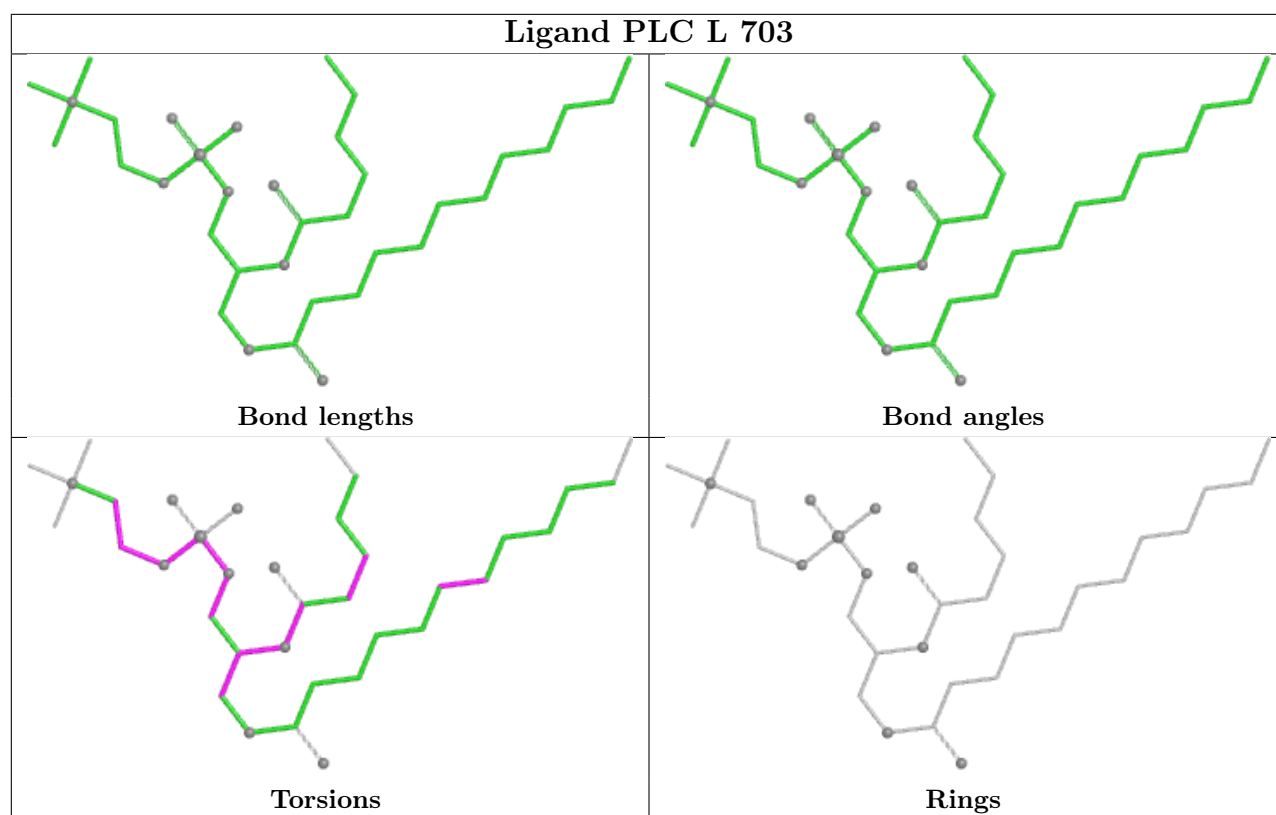
Ligand 3PE Y 203

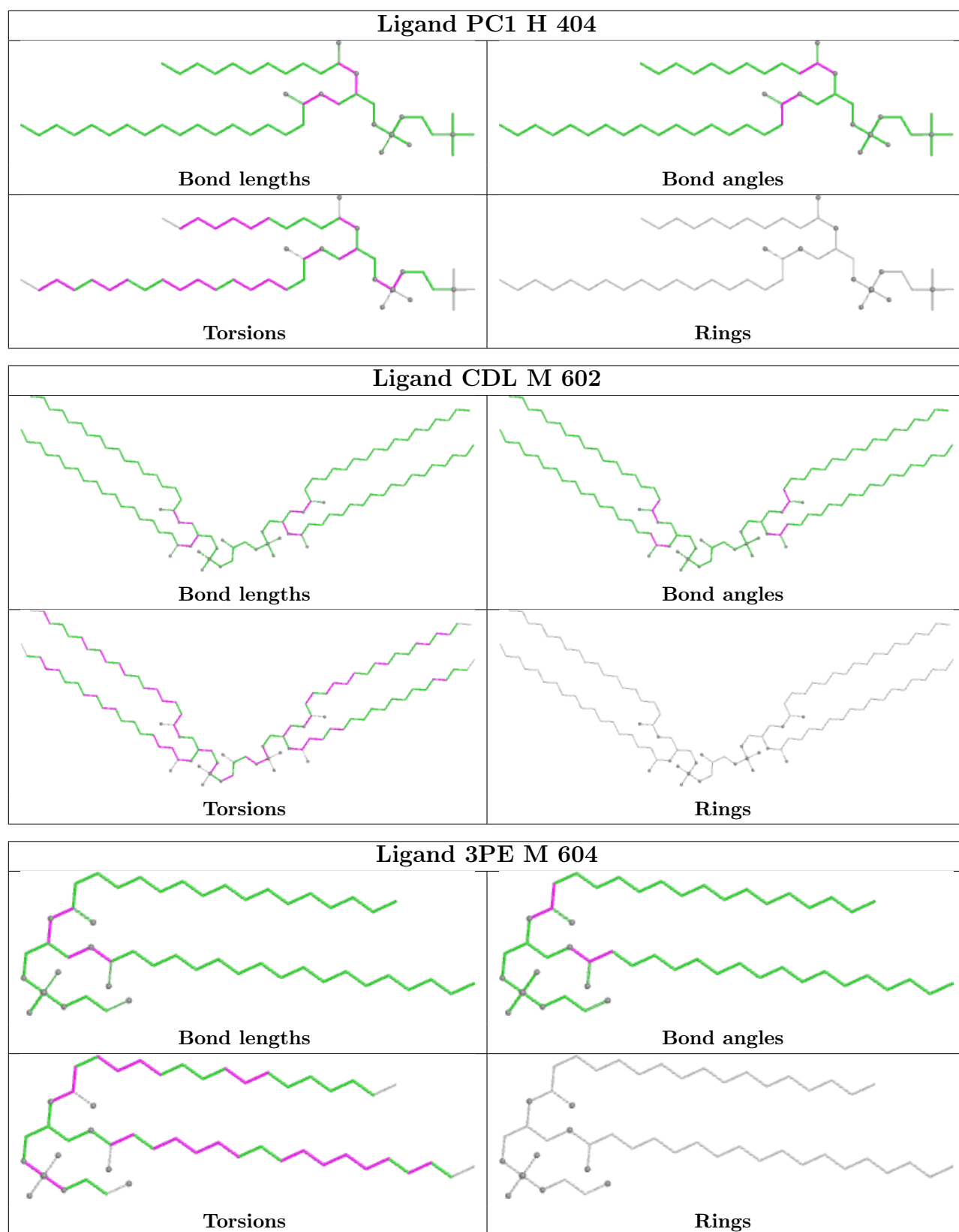


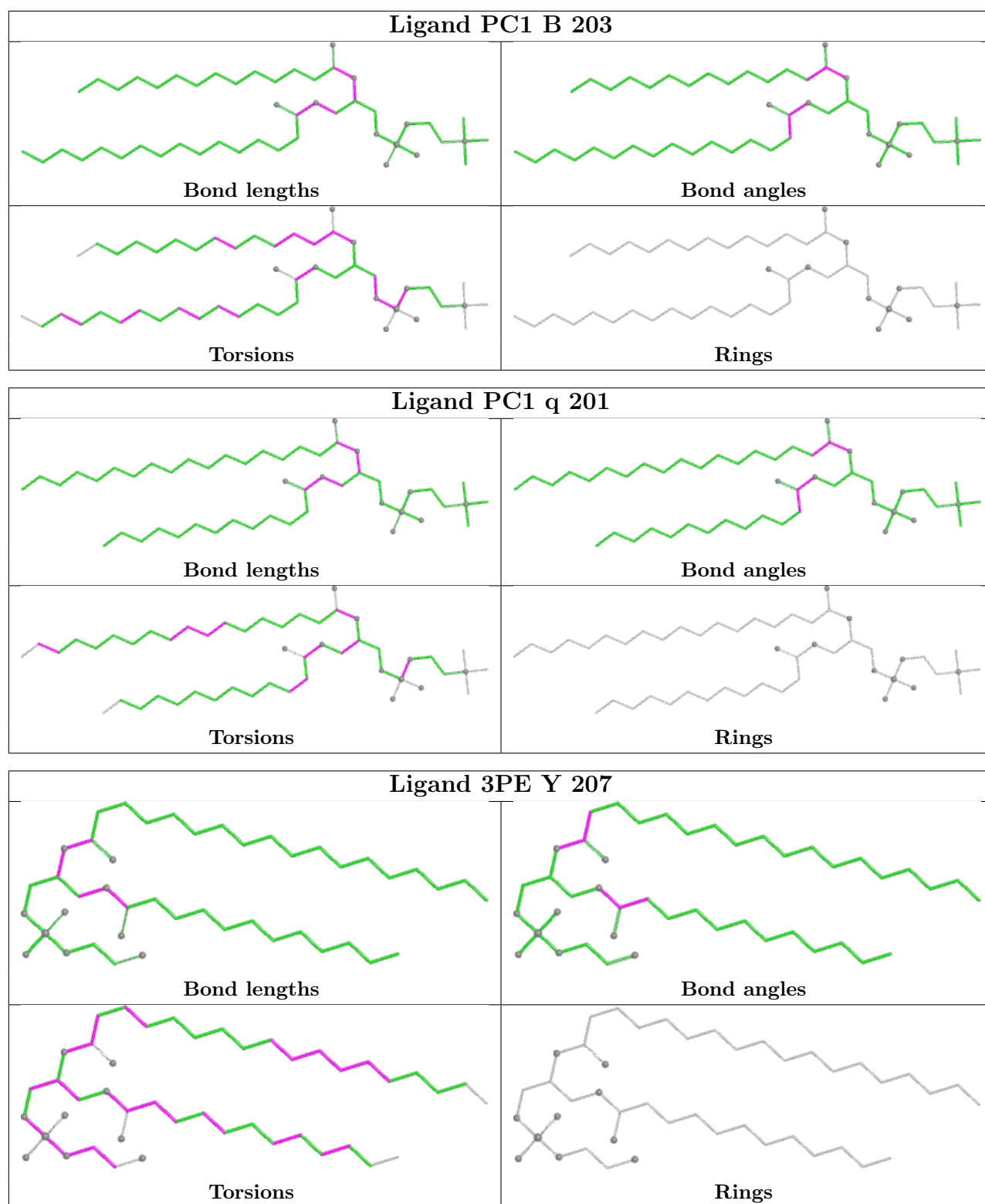
Ligand 3PE Y 204

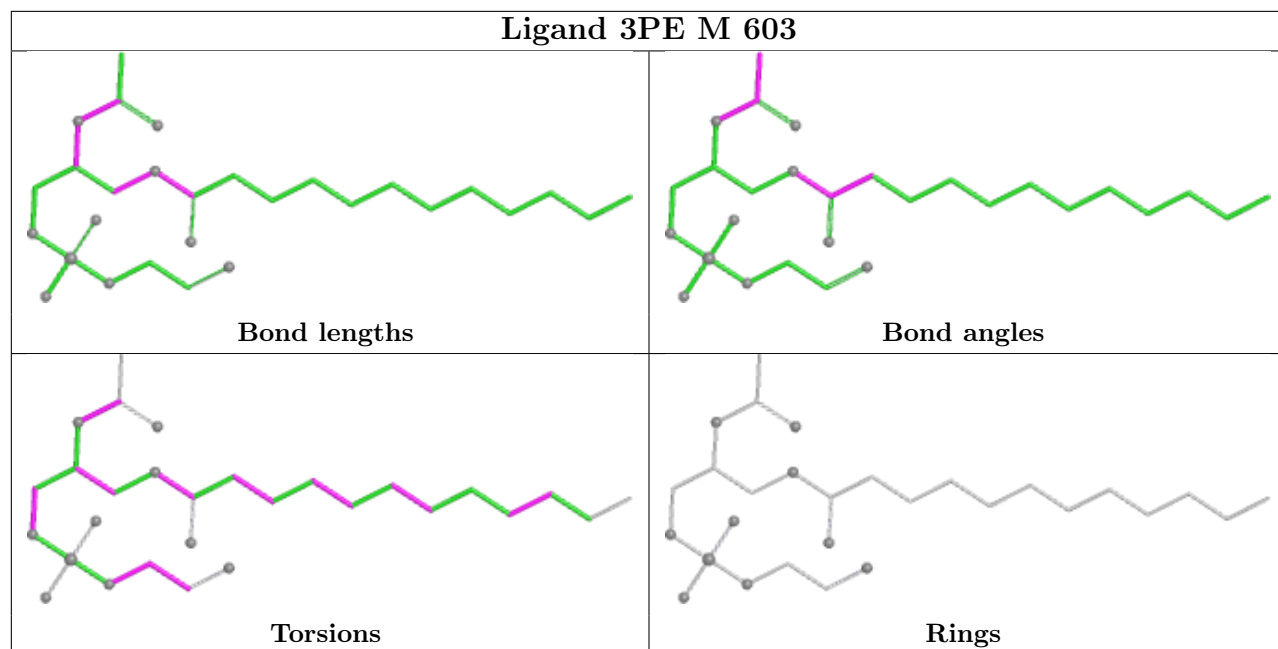
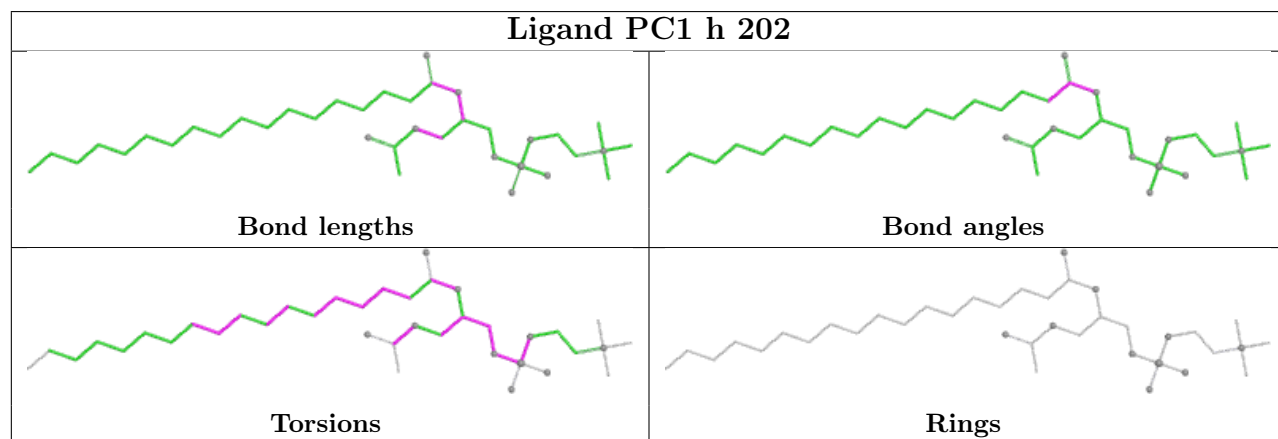
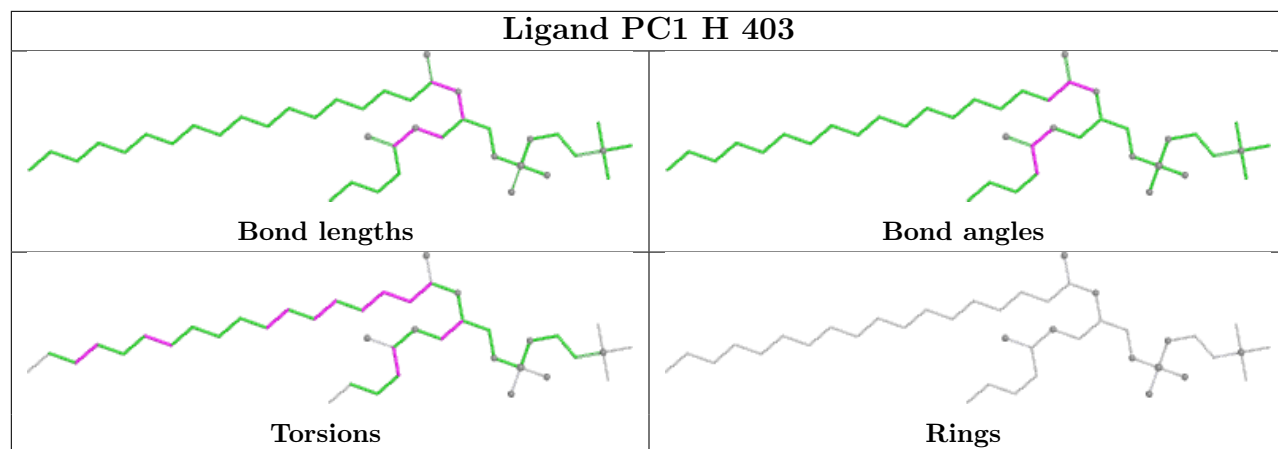


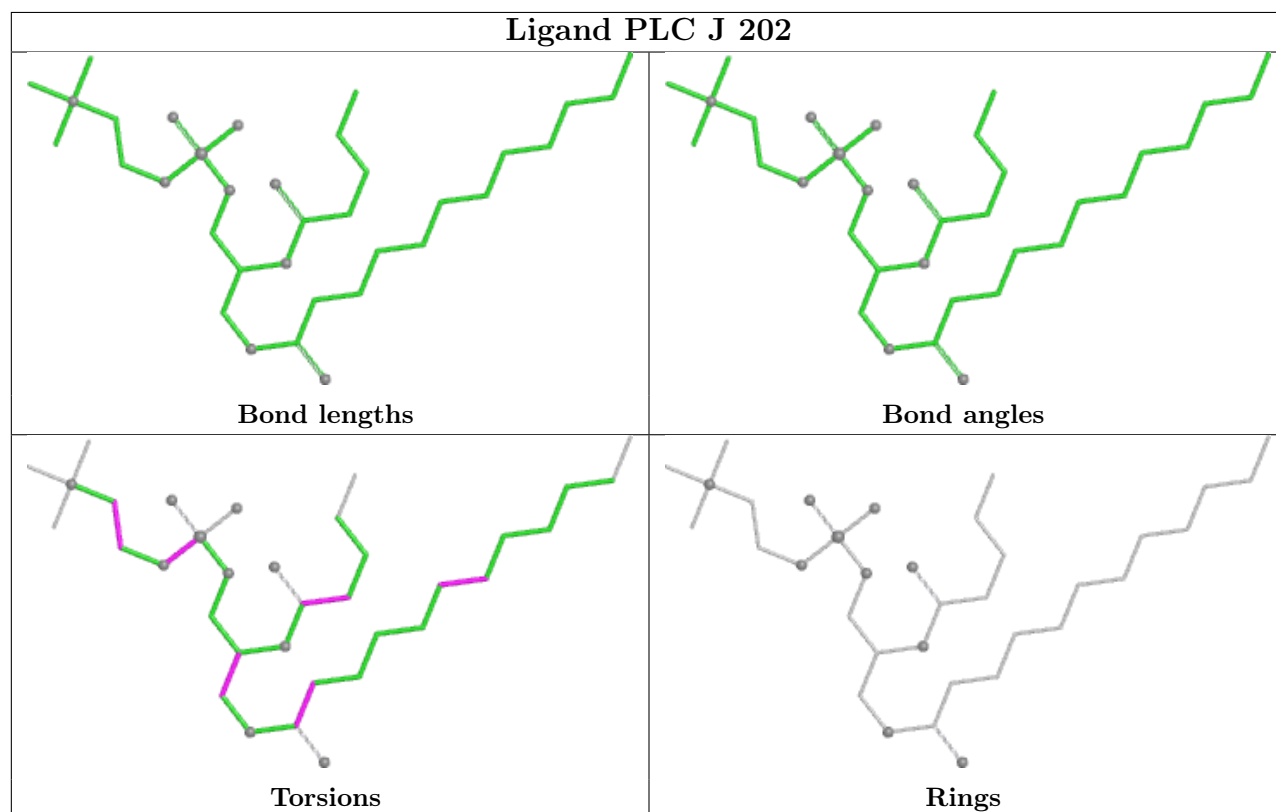
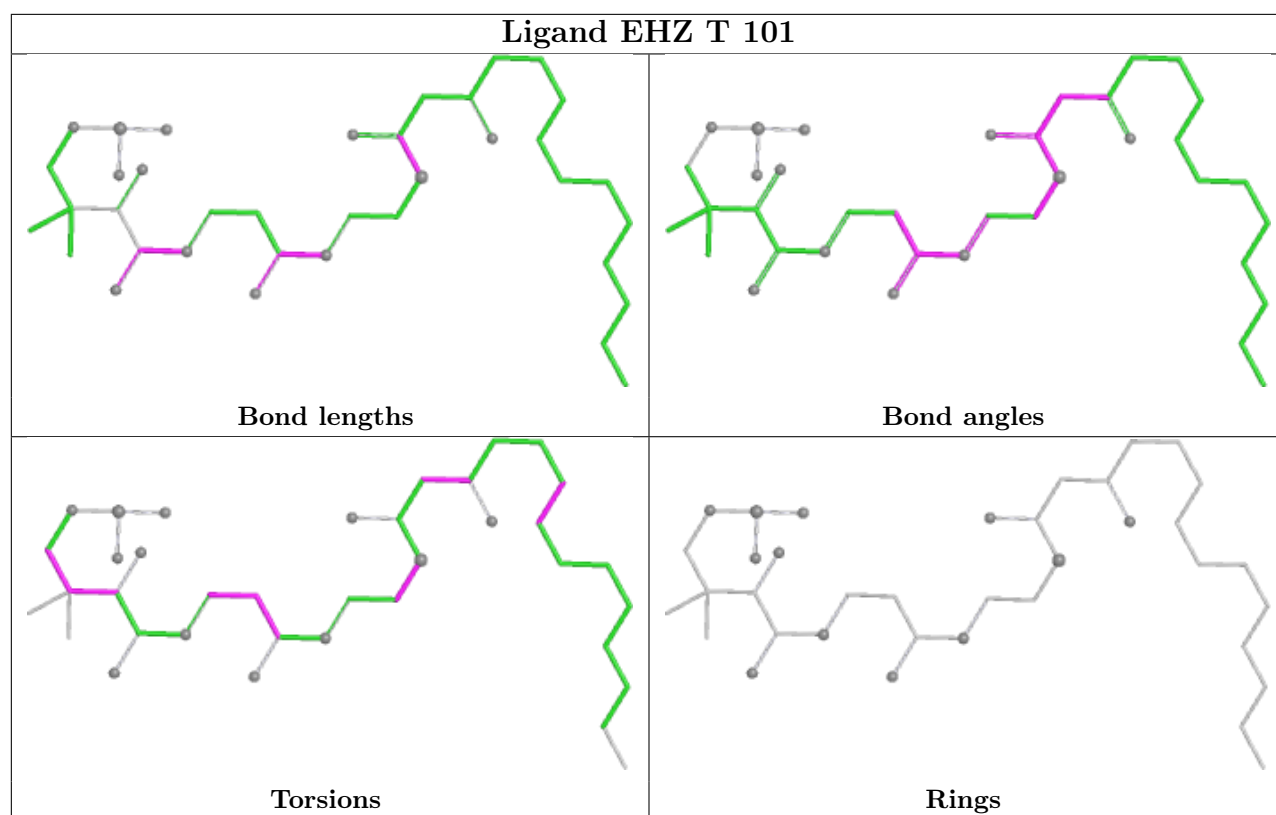


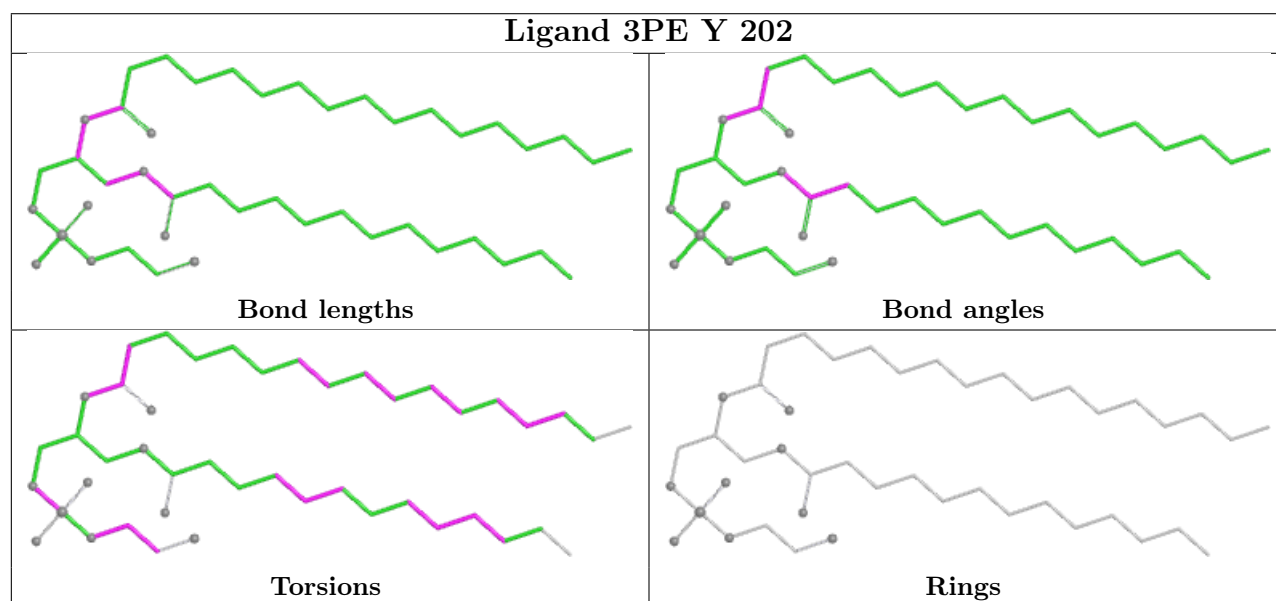
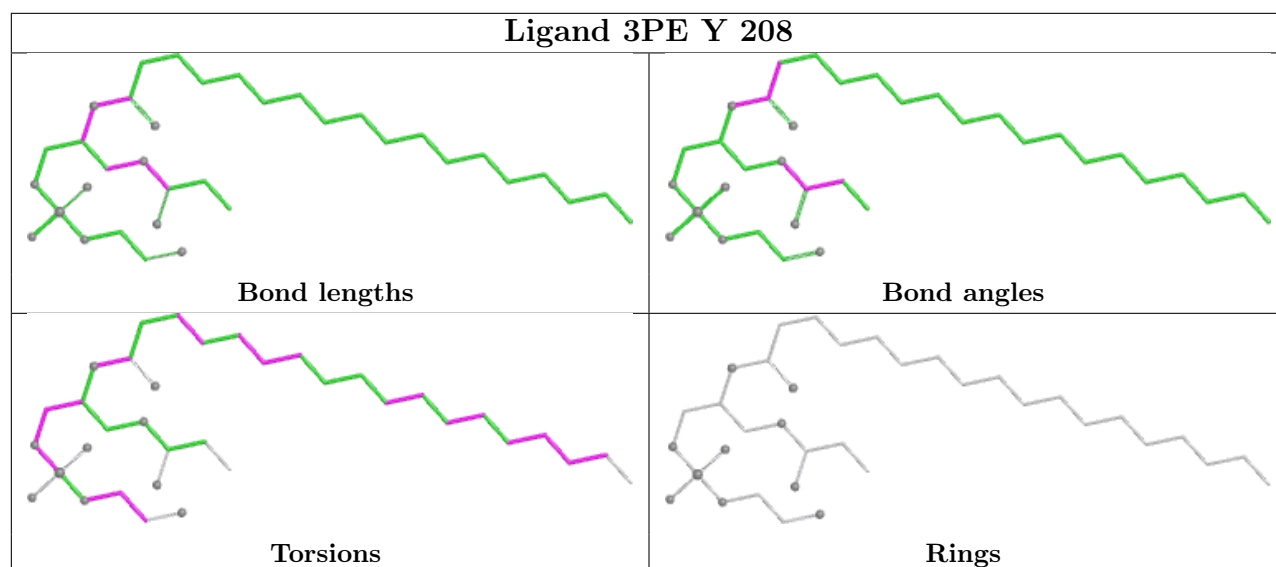
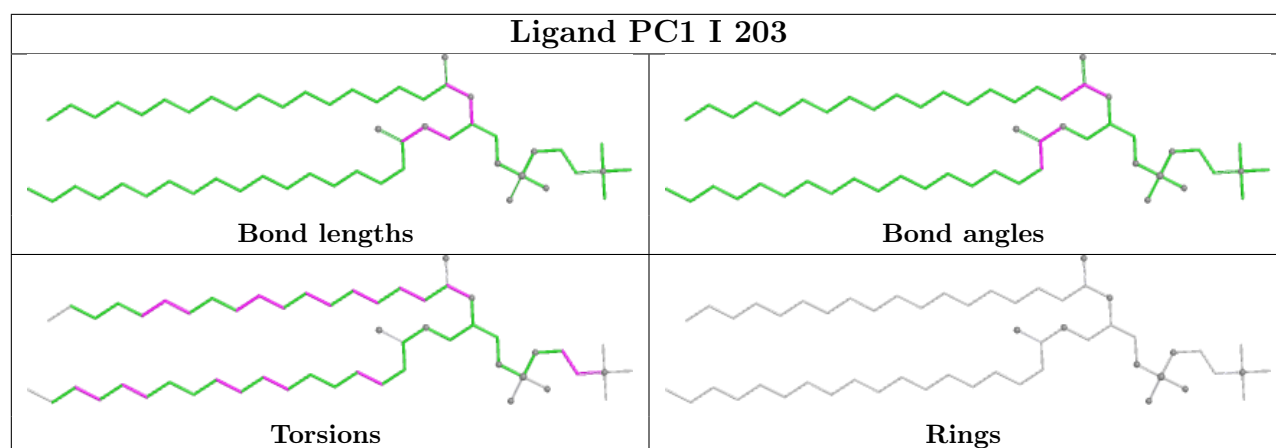


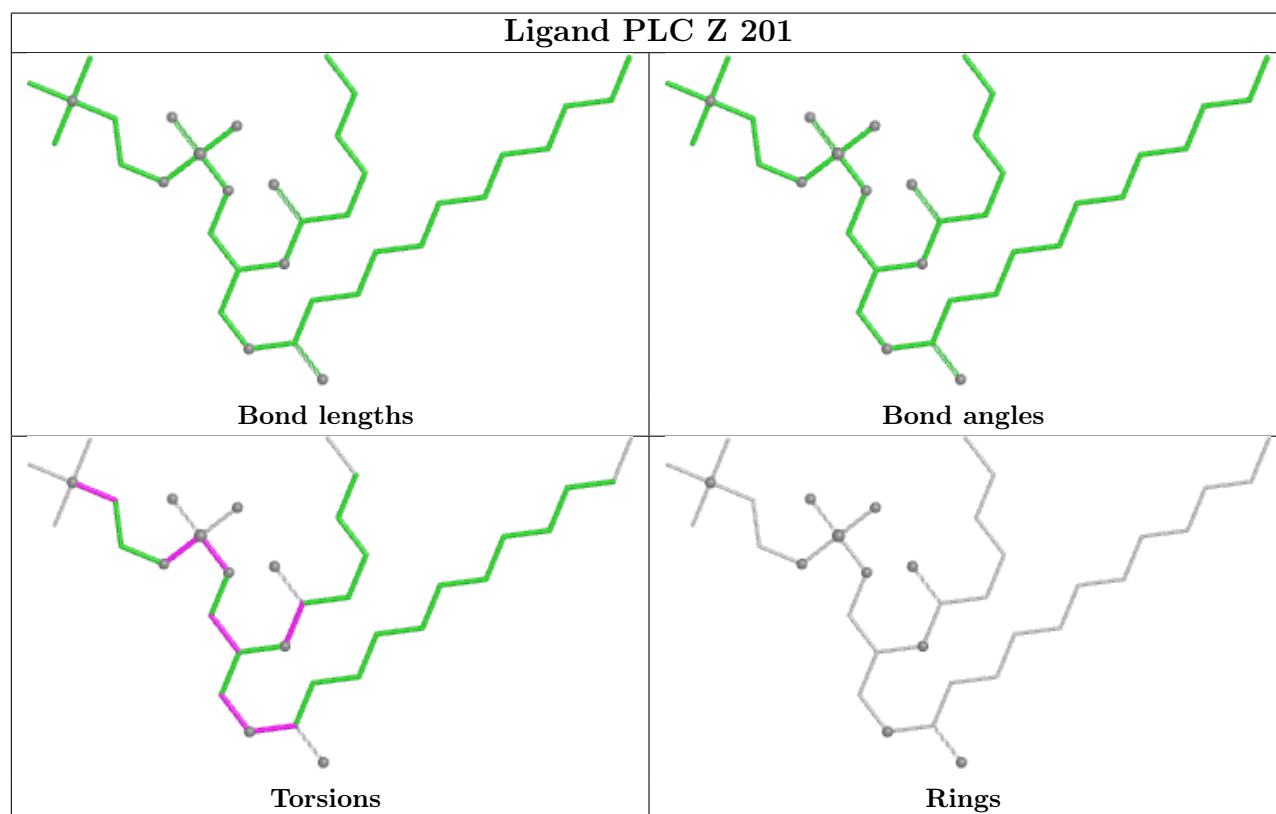
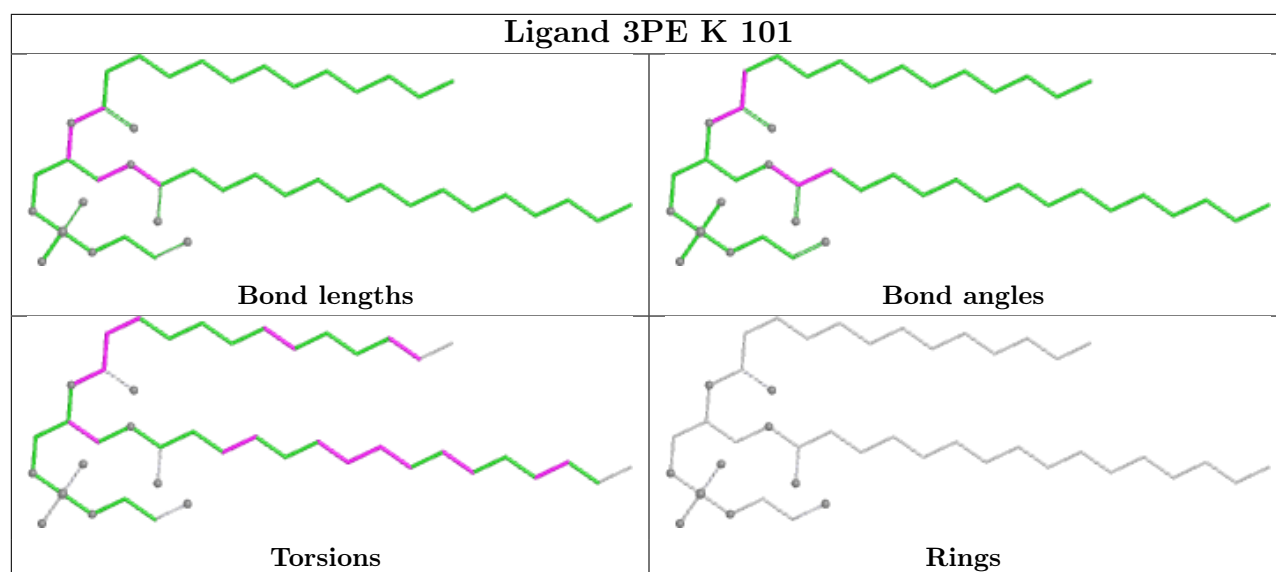


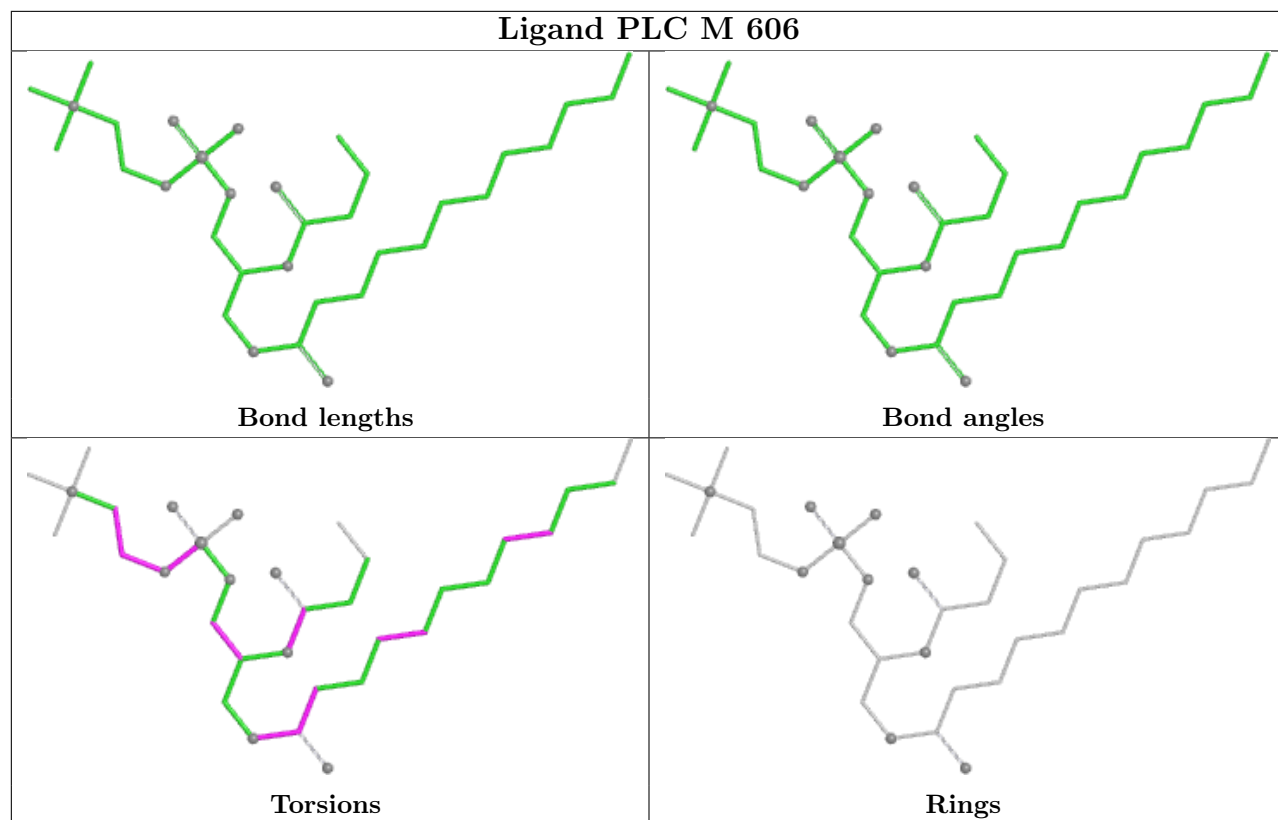


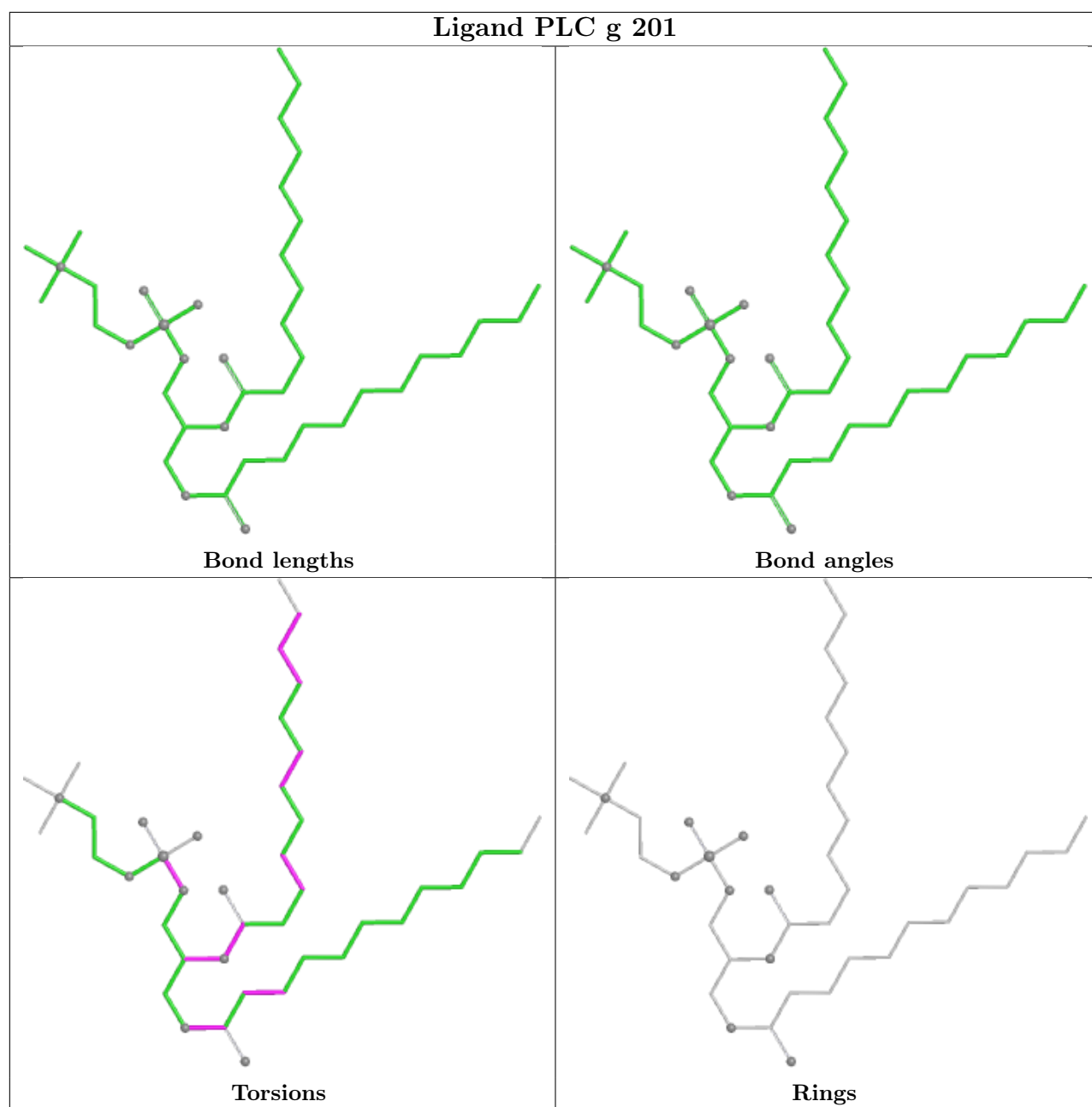


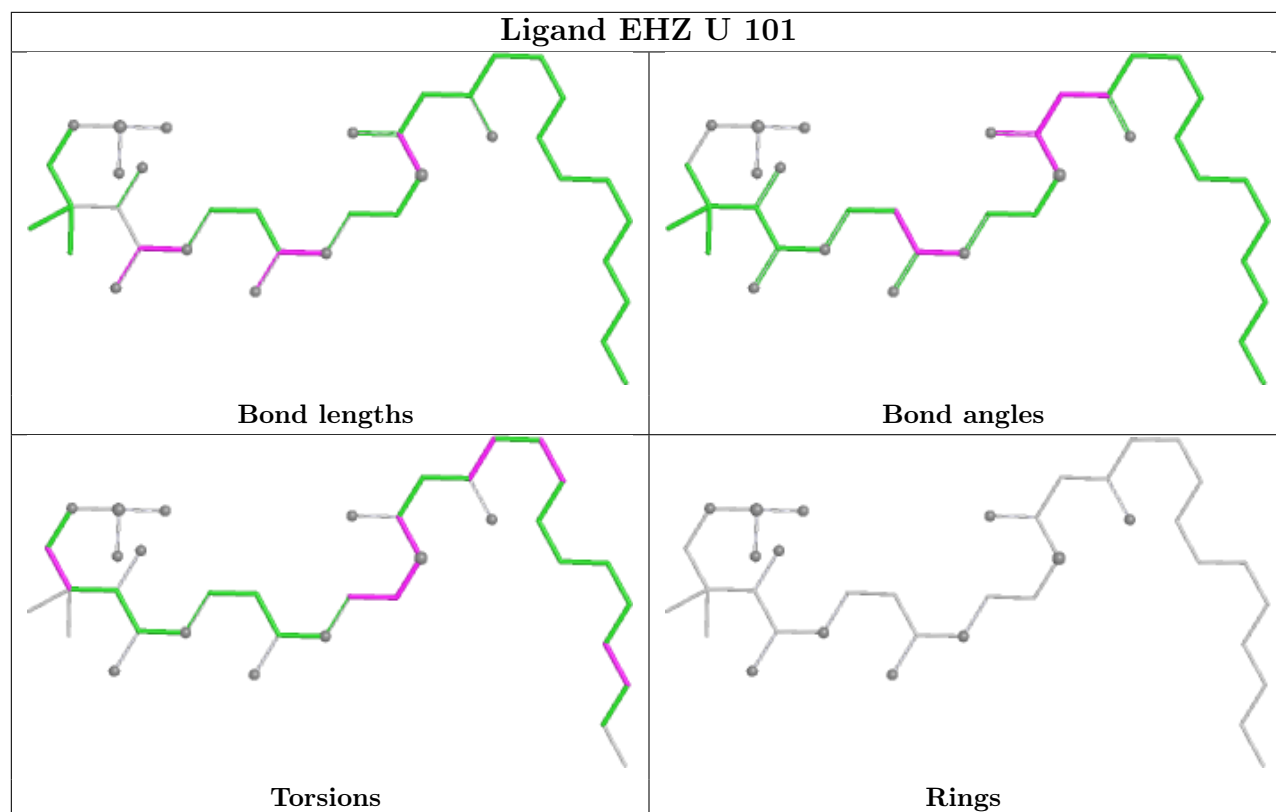
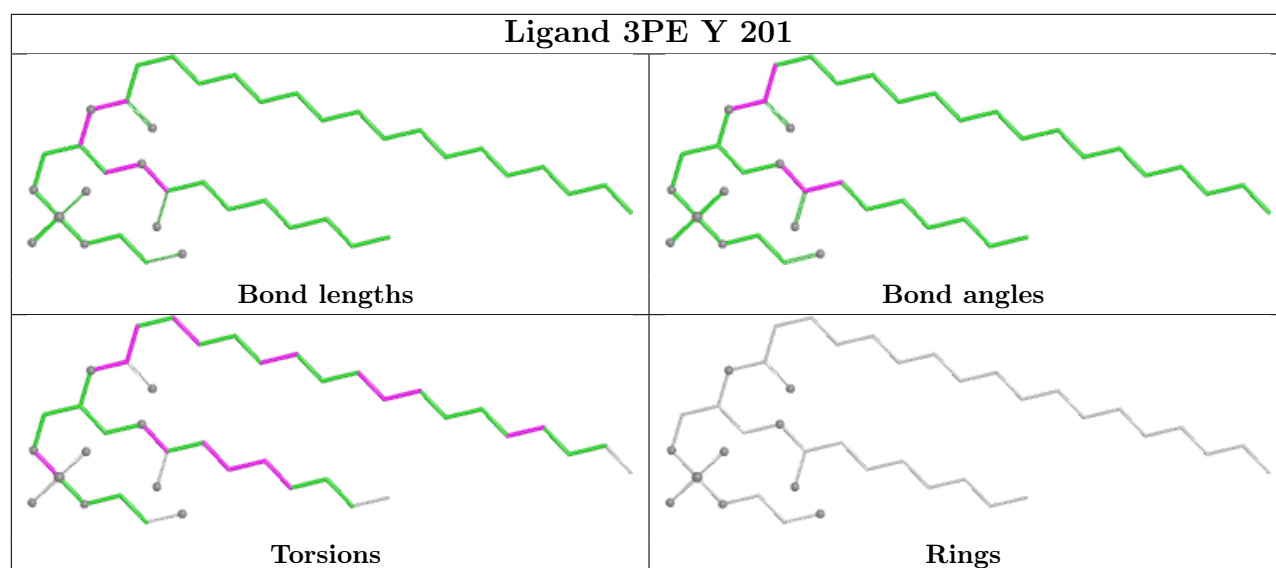


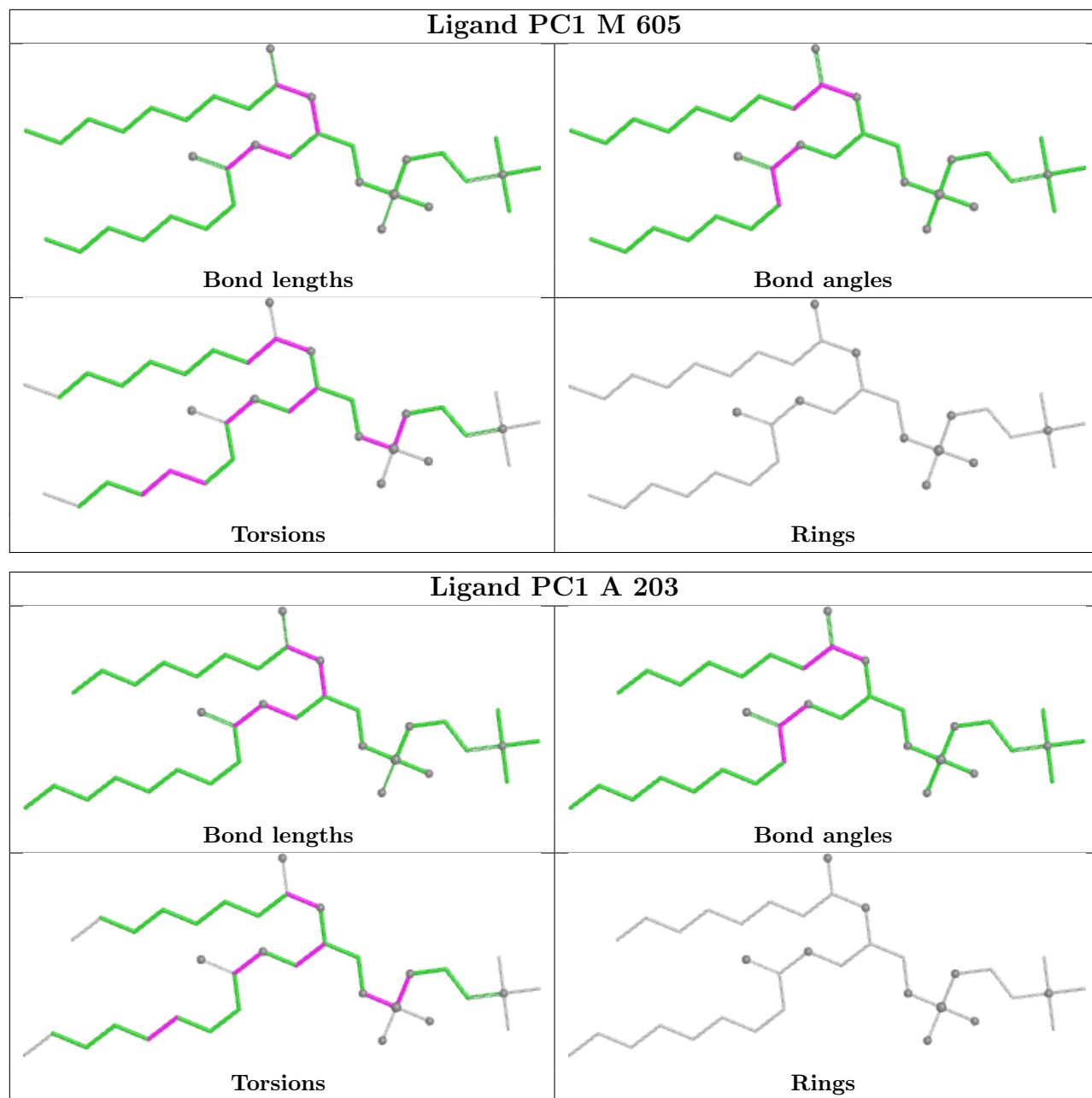


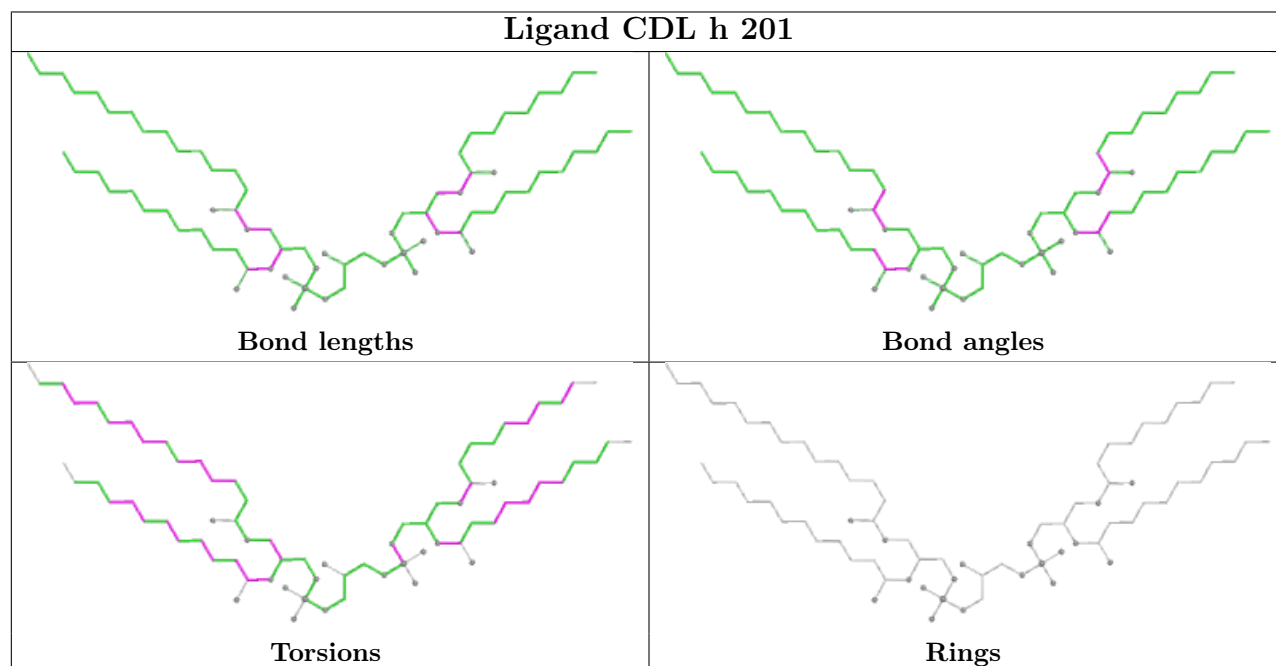
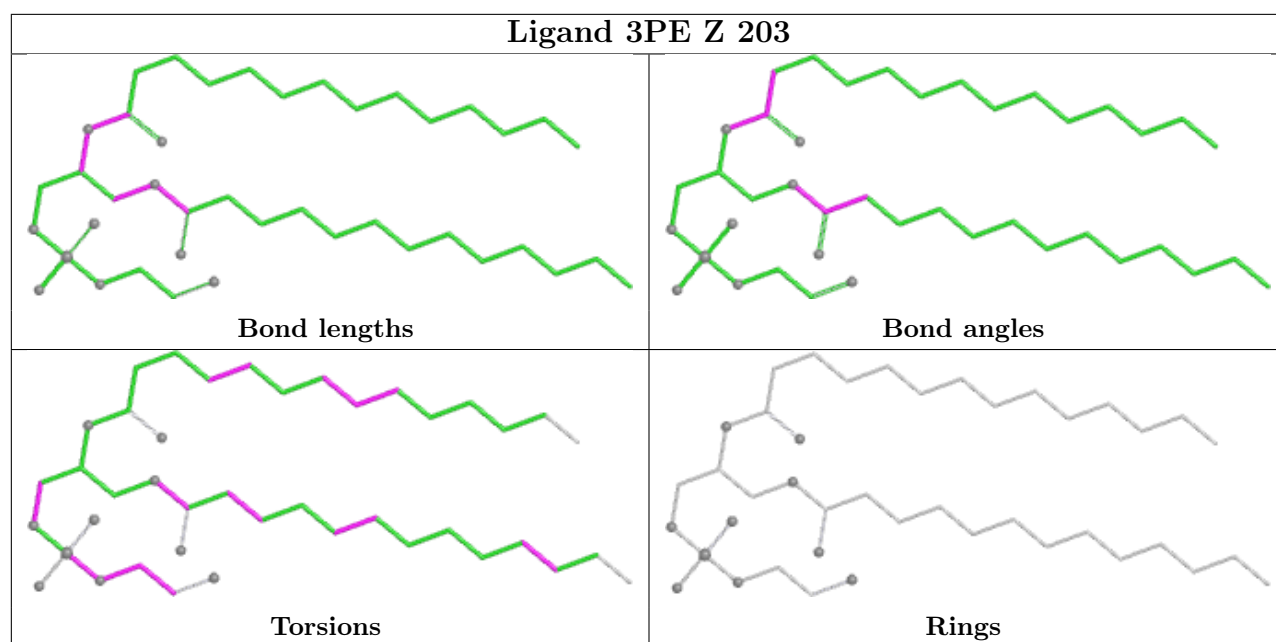


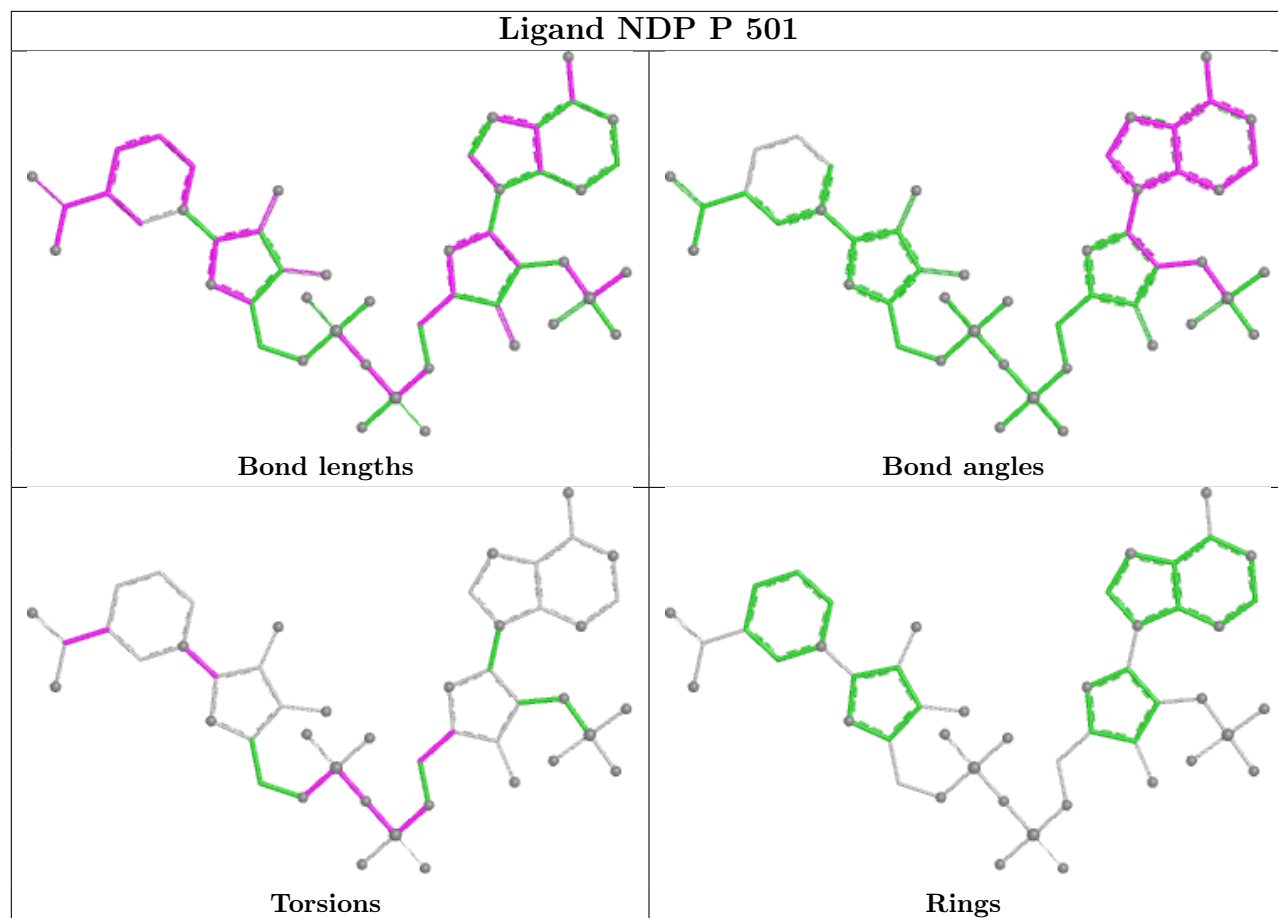
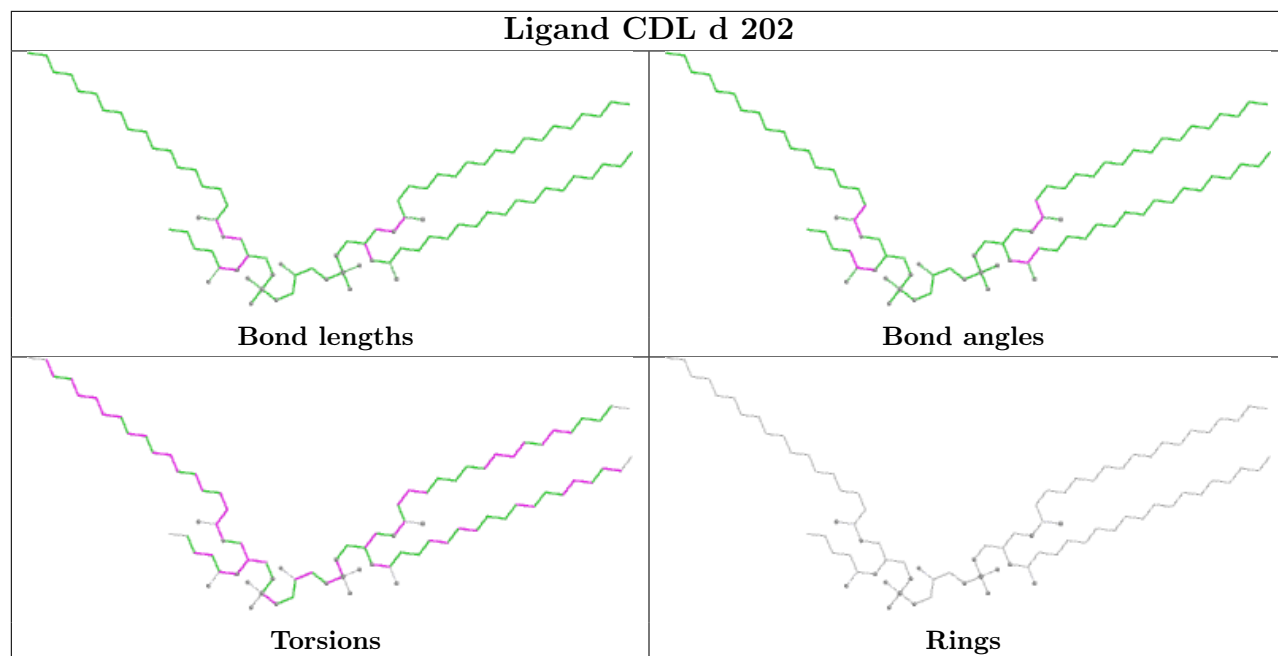


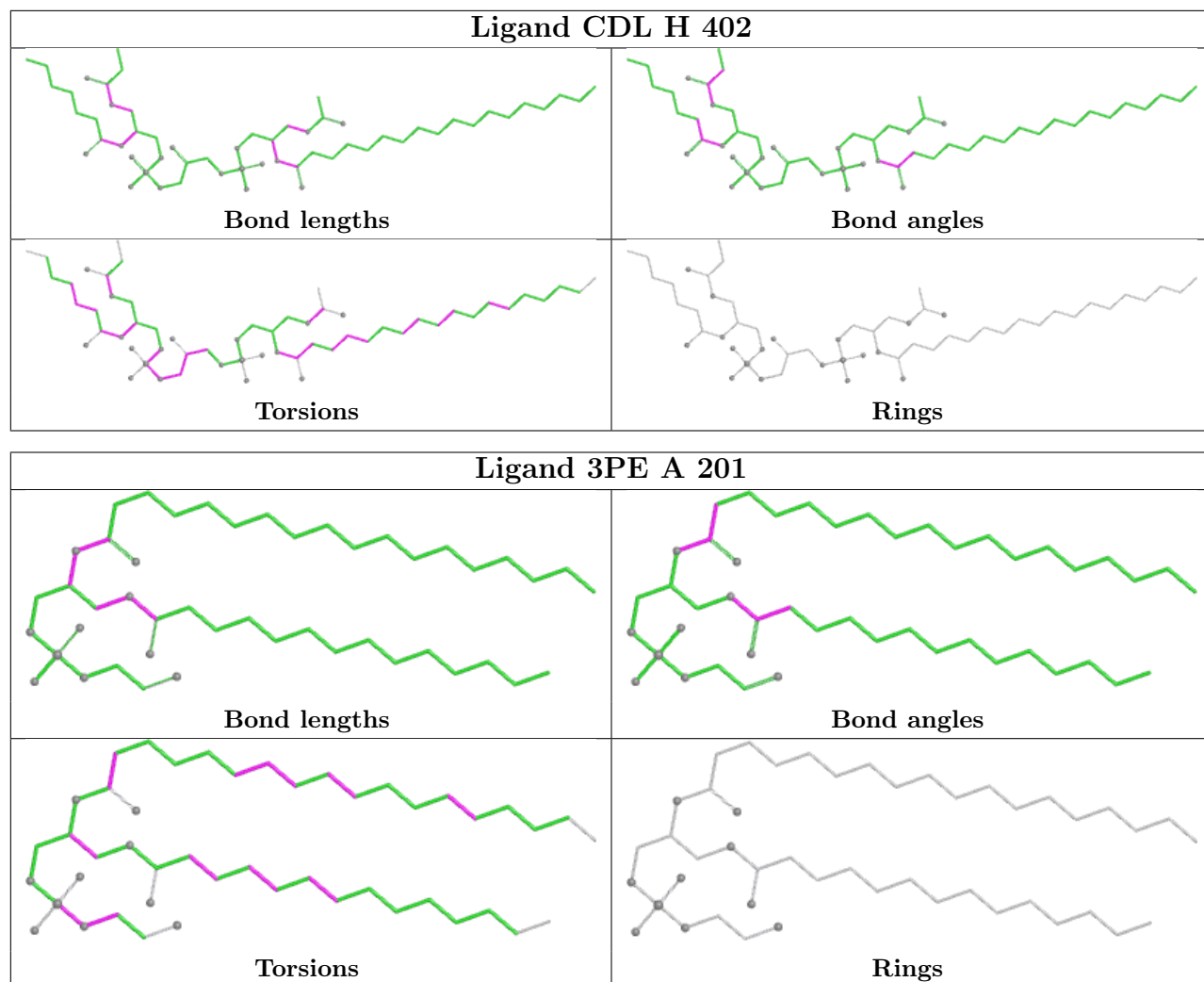


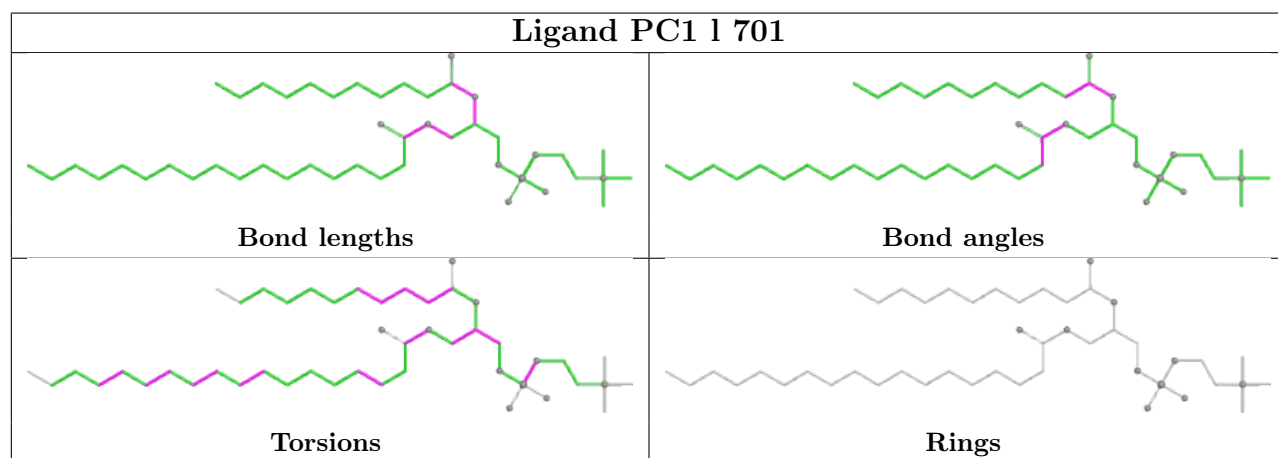
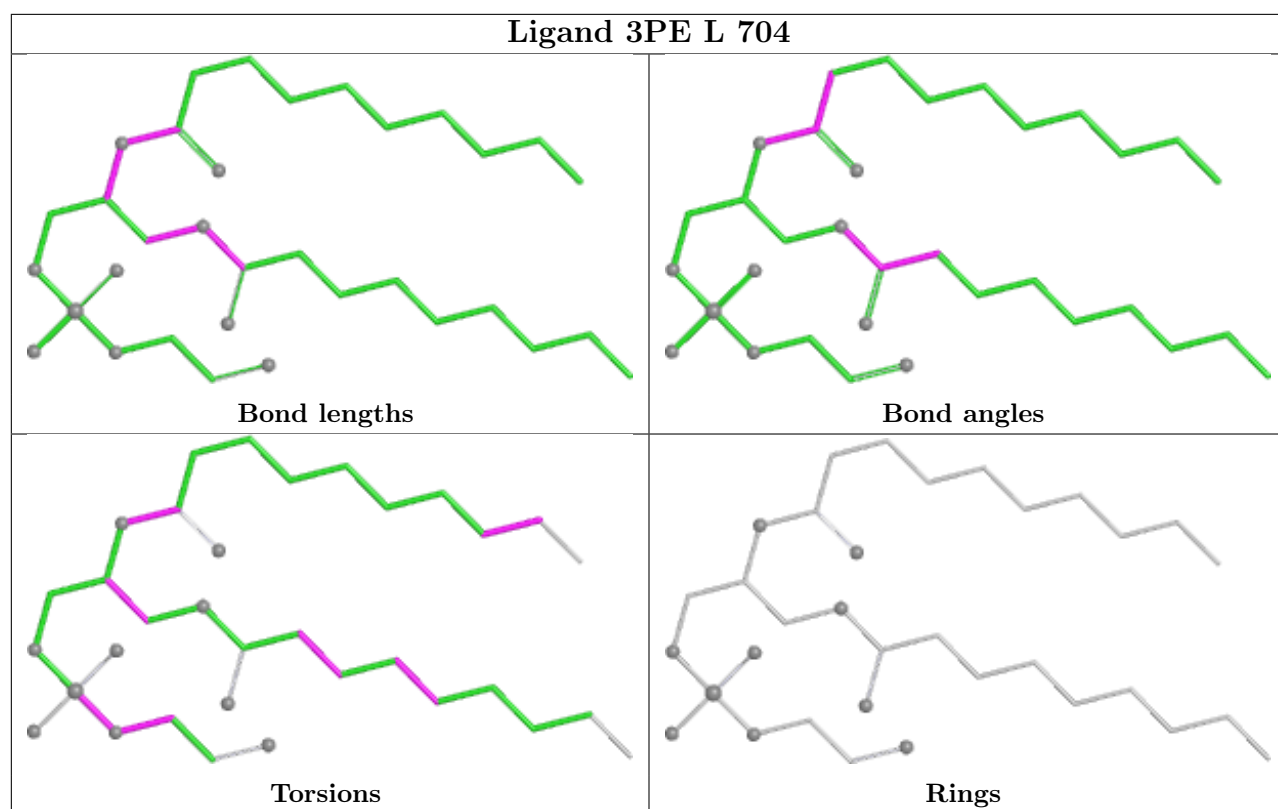




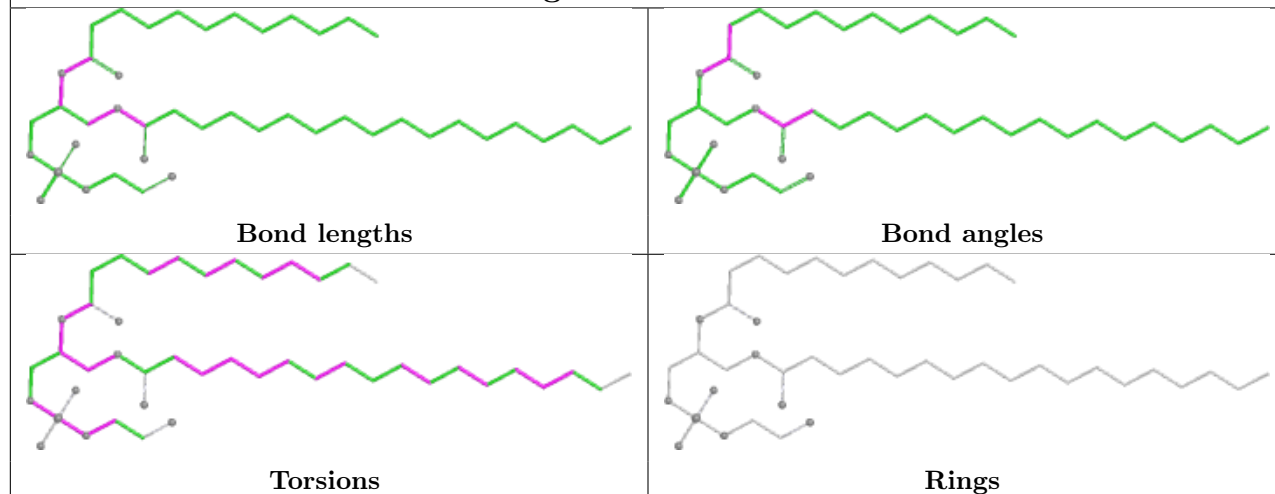




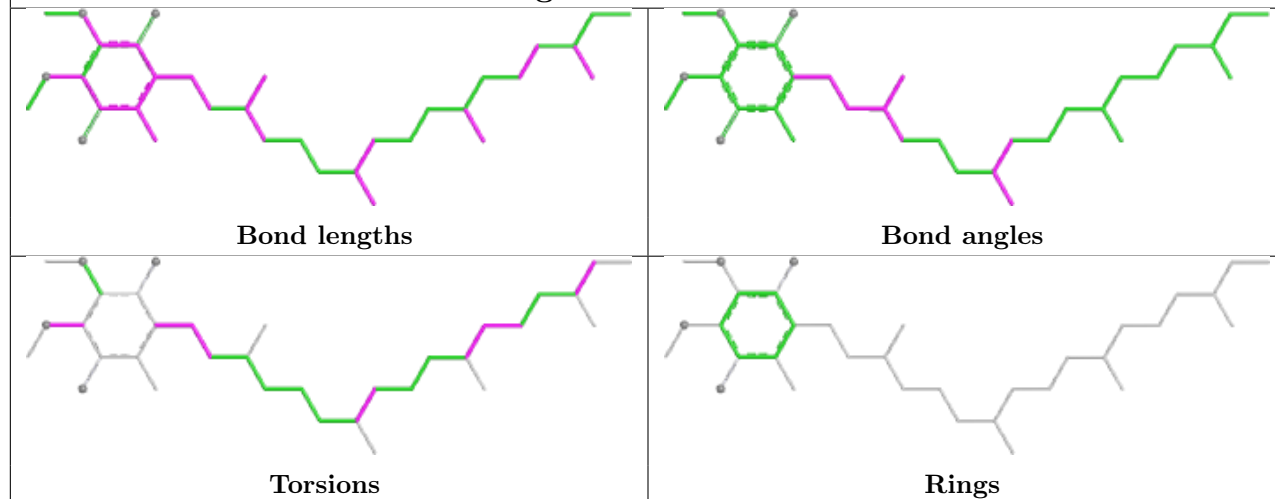




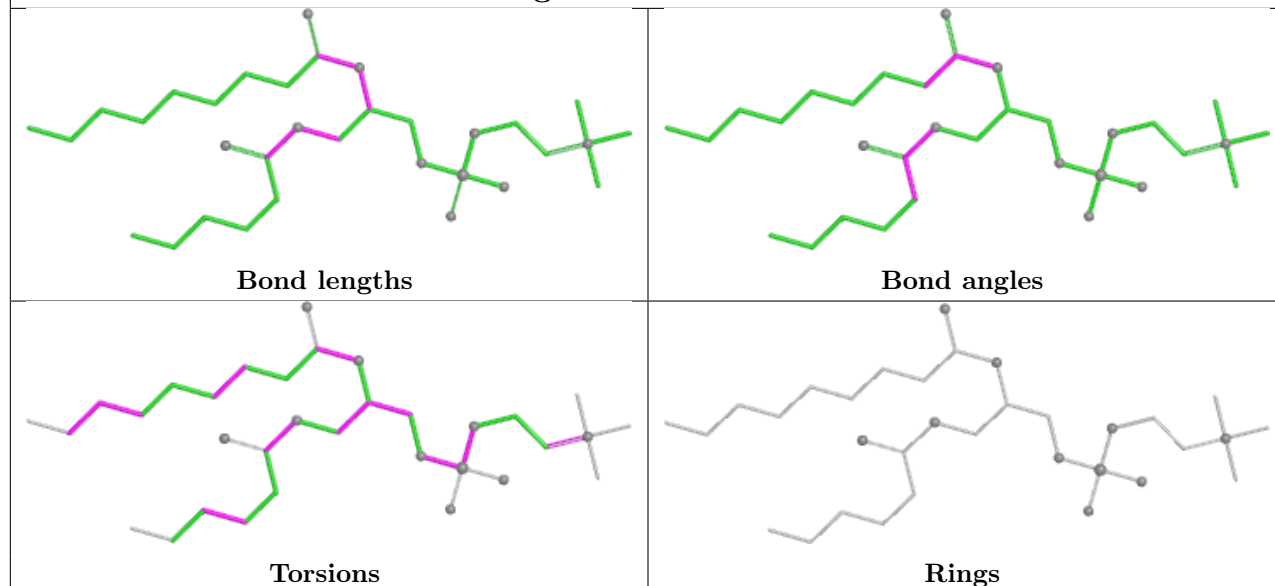
Ligand 3PE i 202

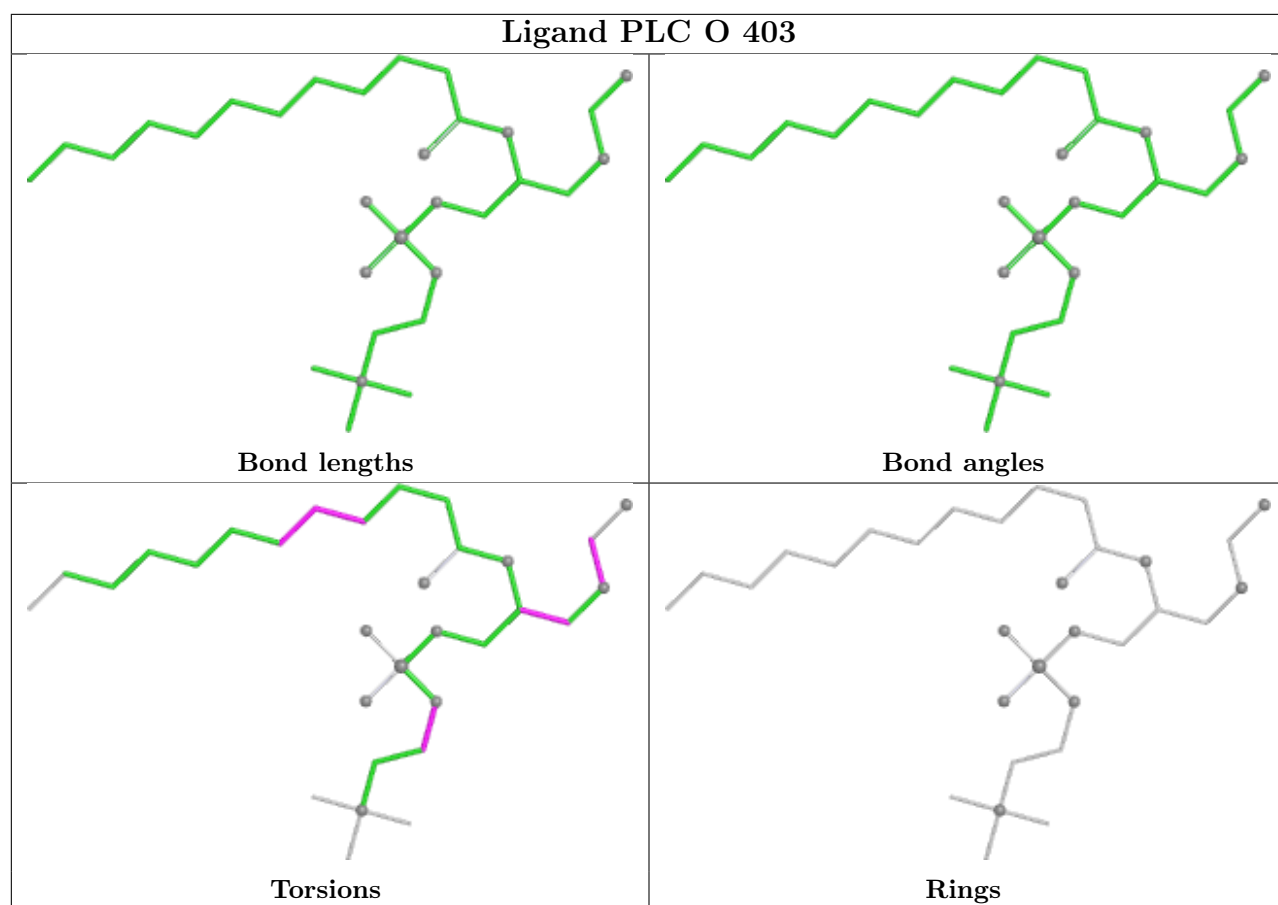


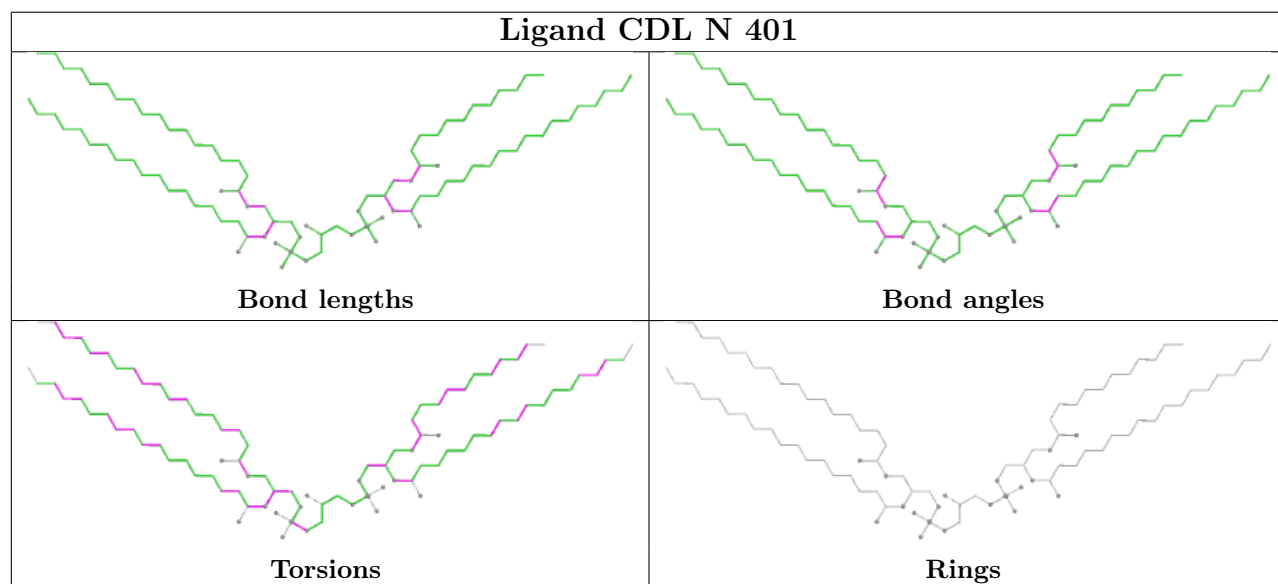
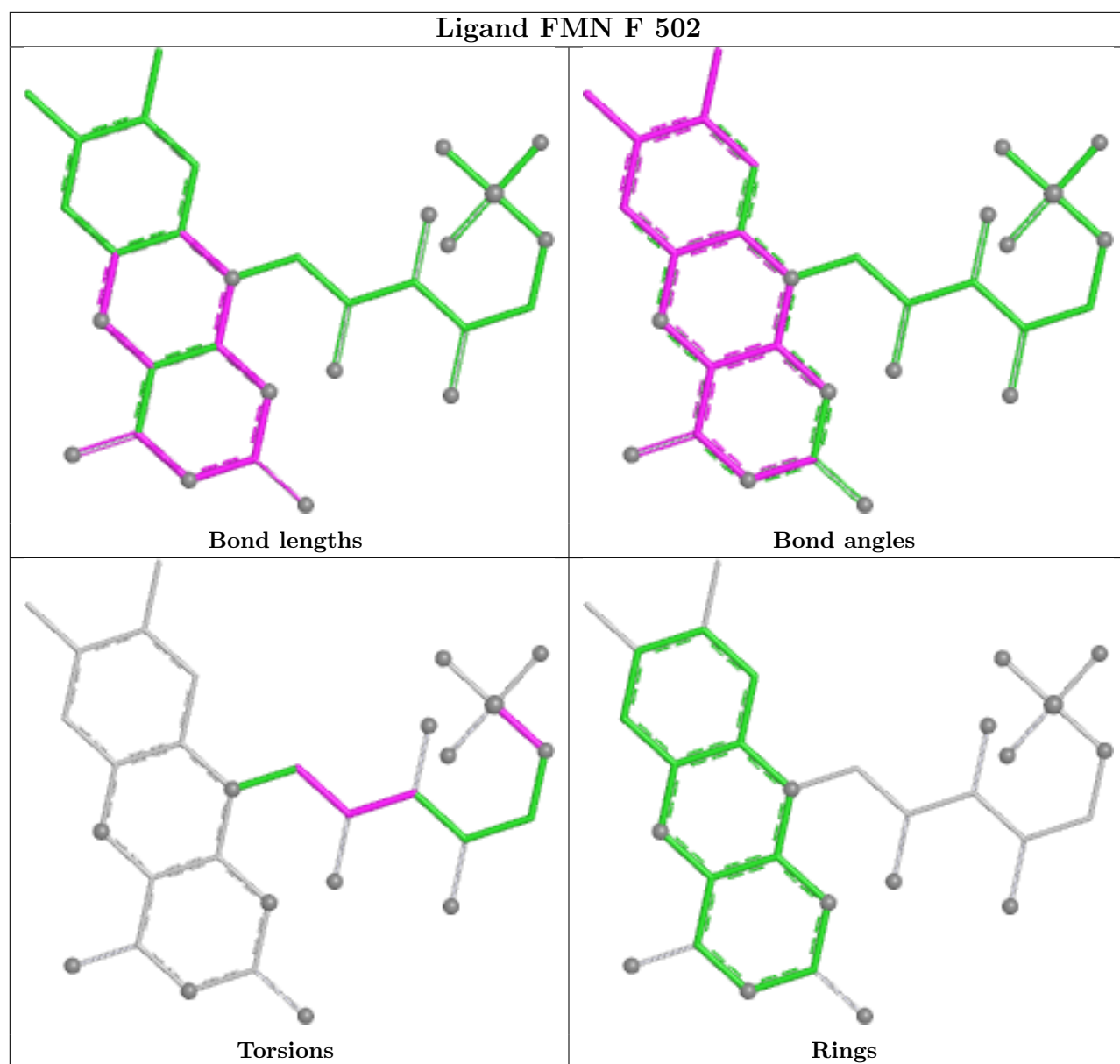
Ligand U10 H 401

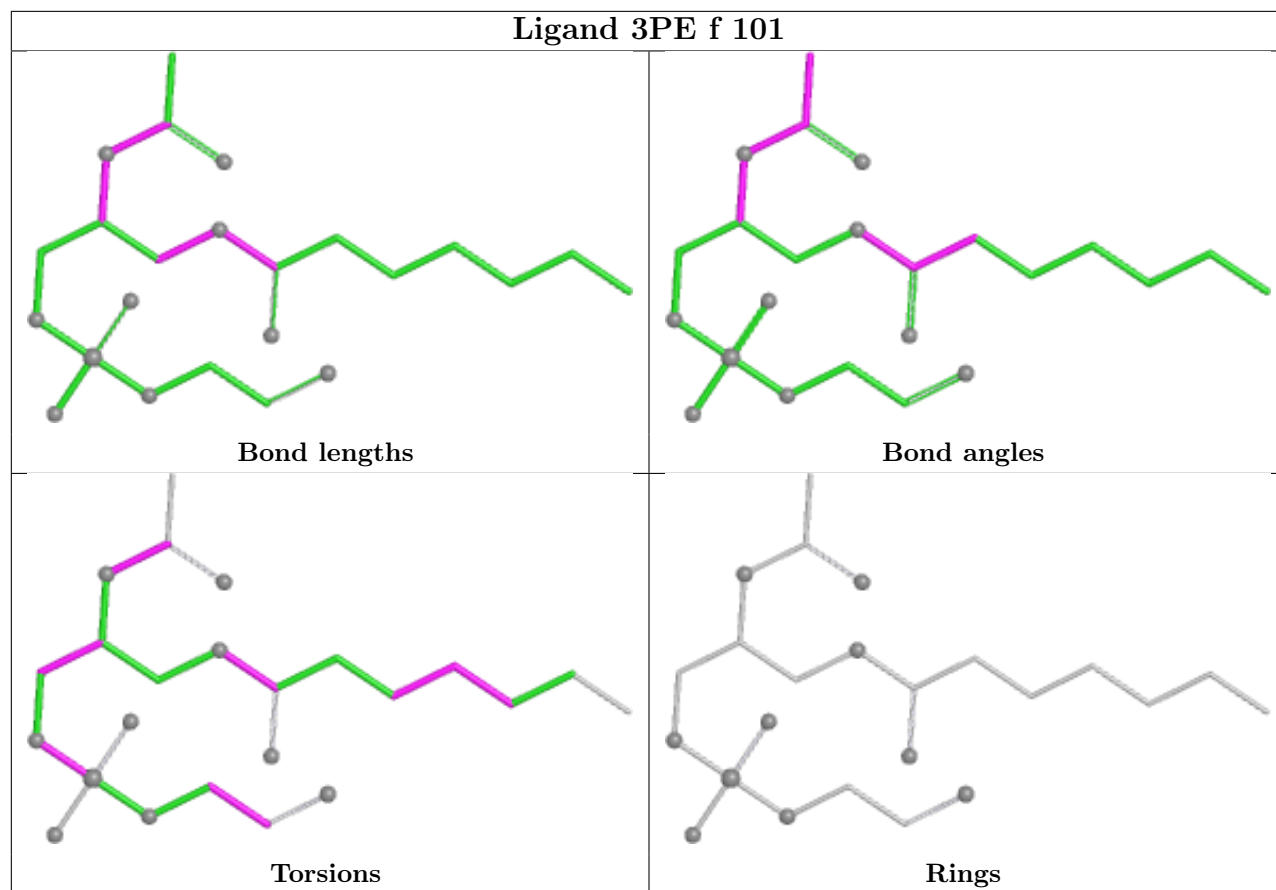


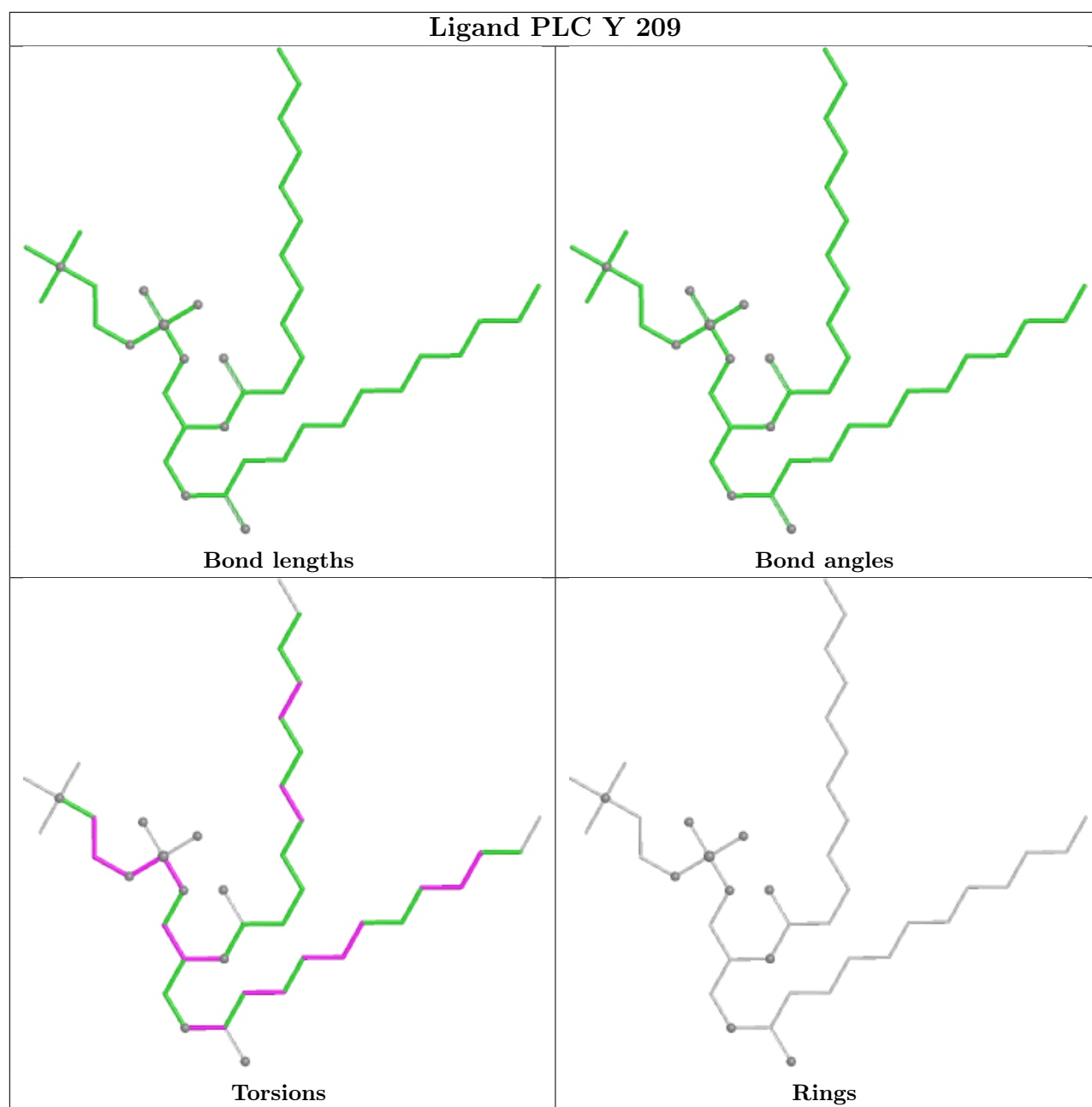
Ligand PC1 A 204

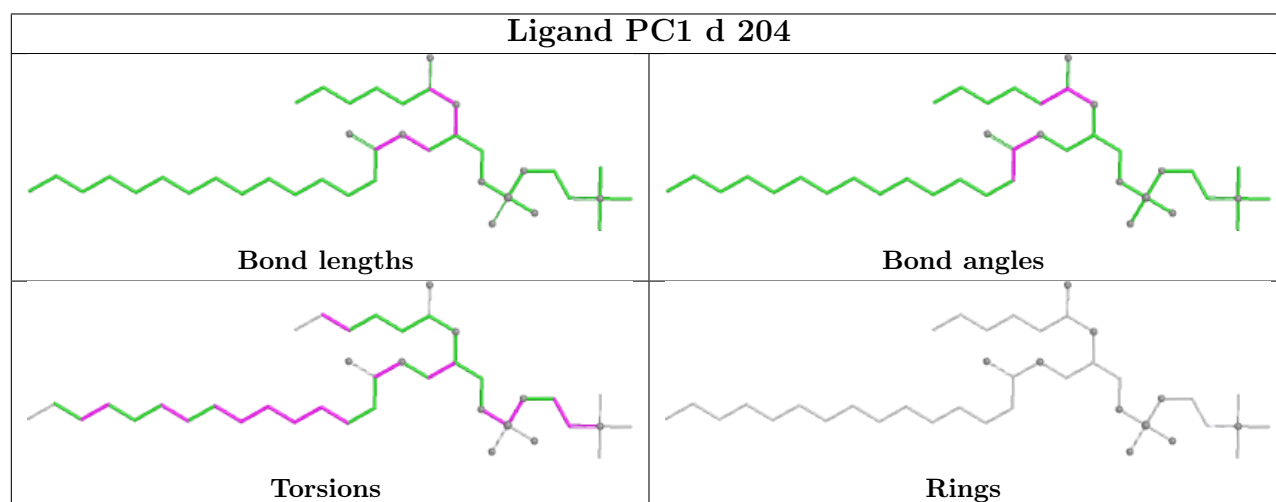
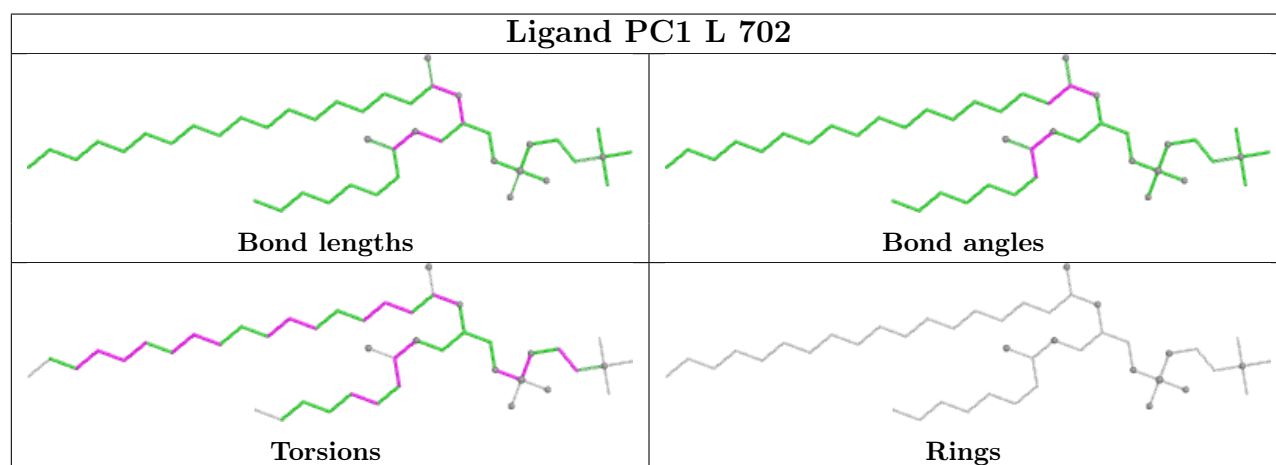
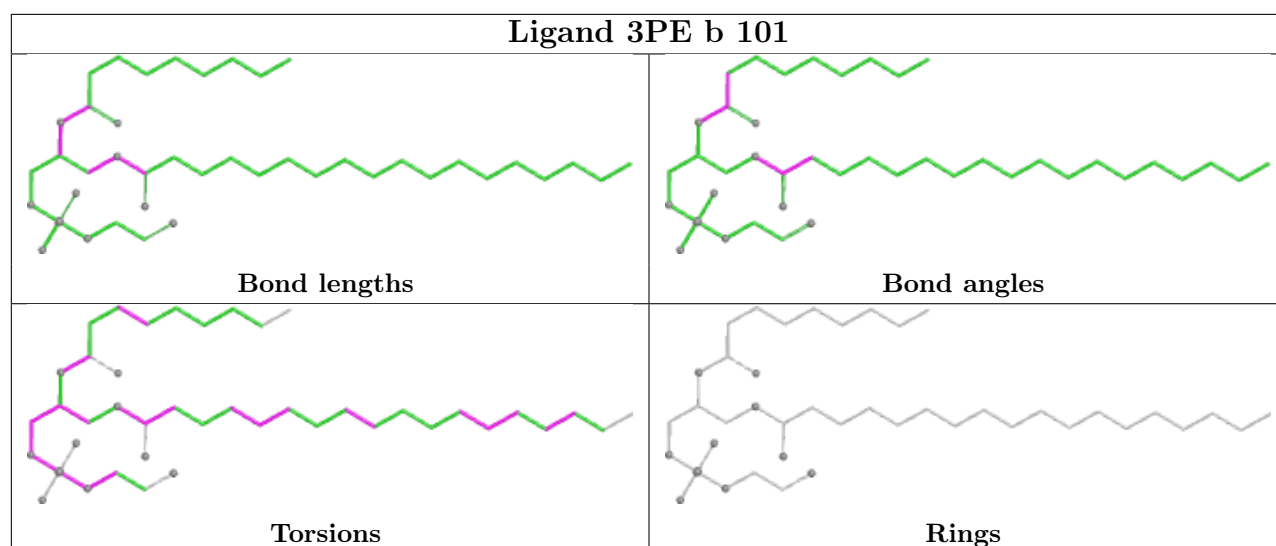


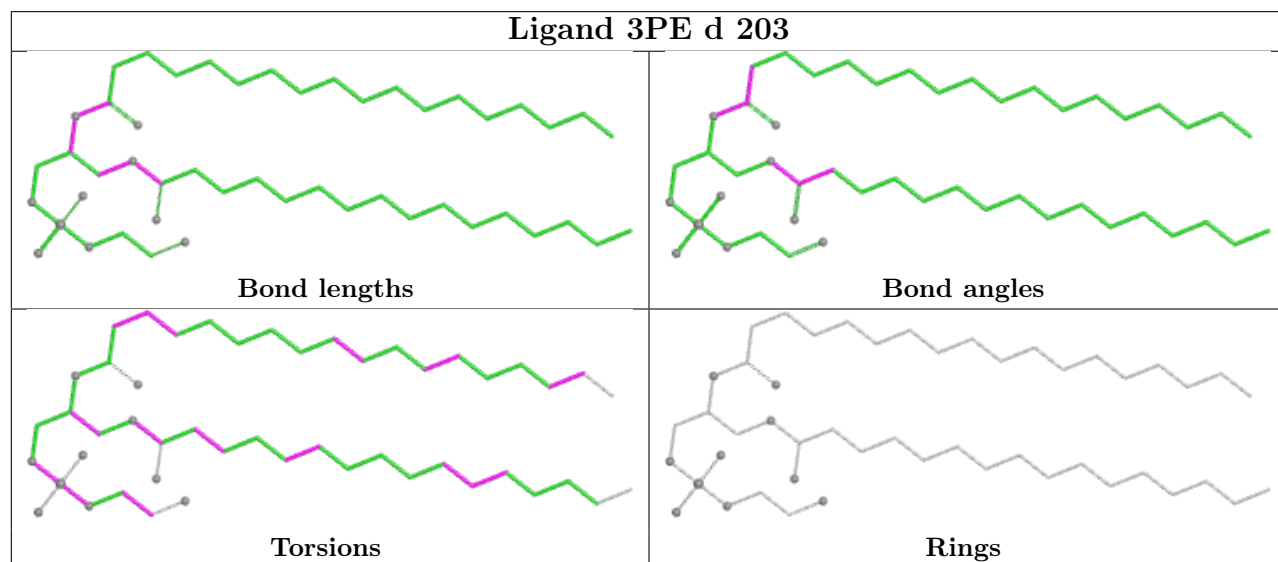
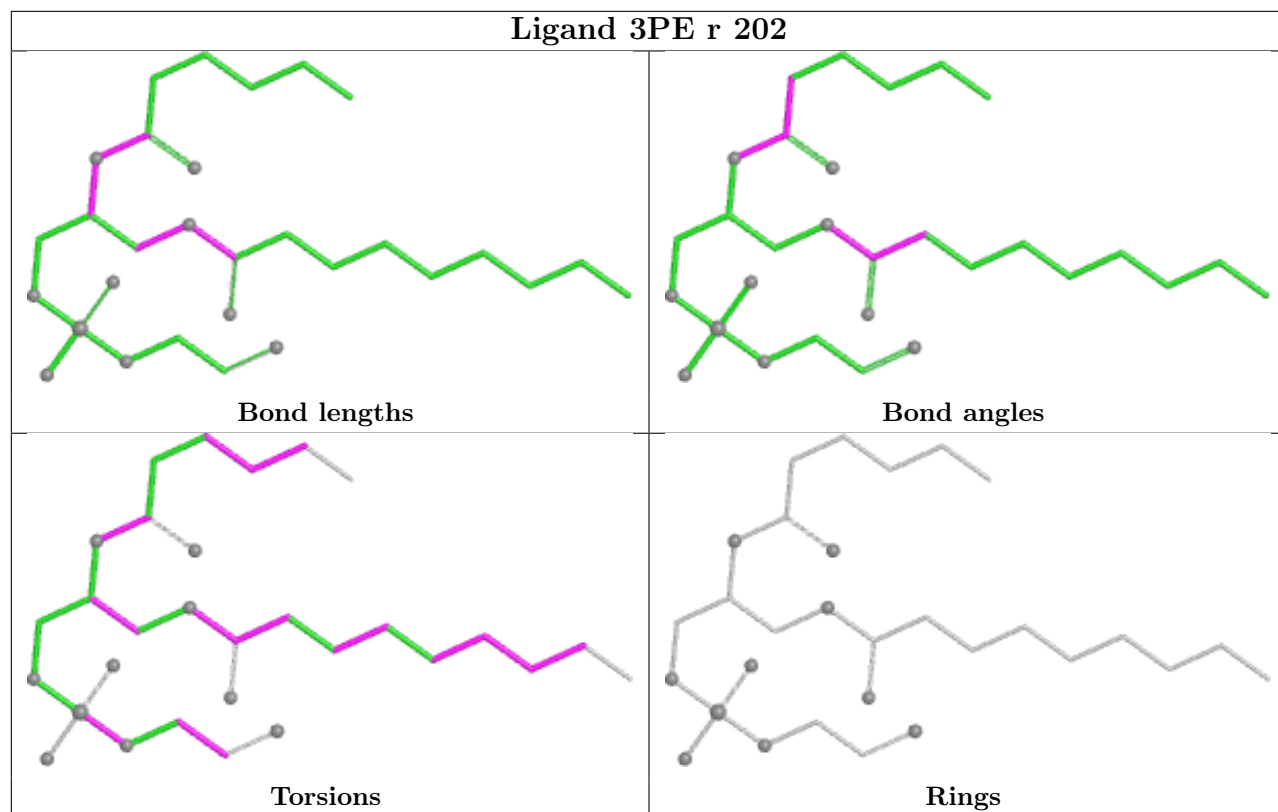


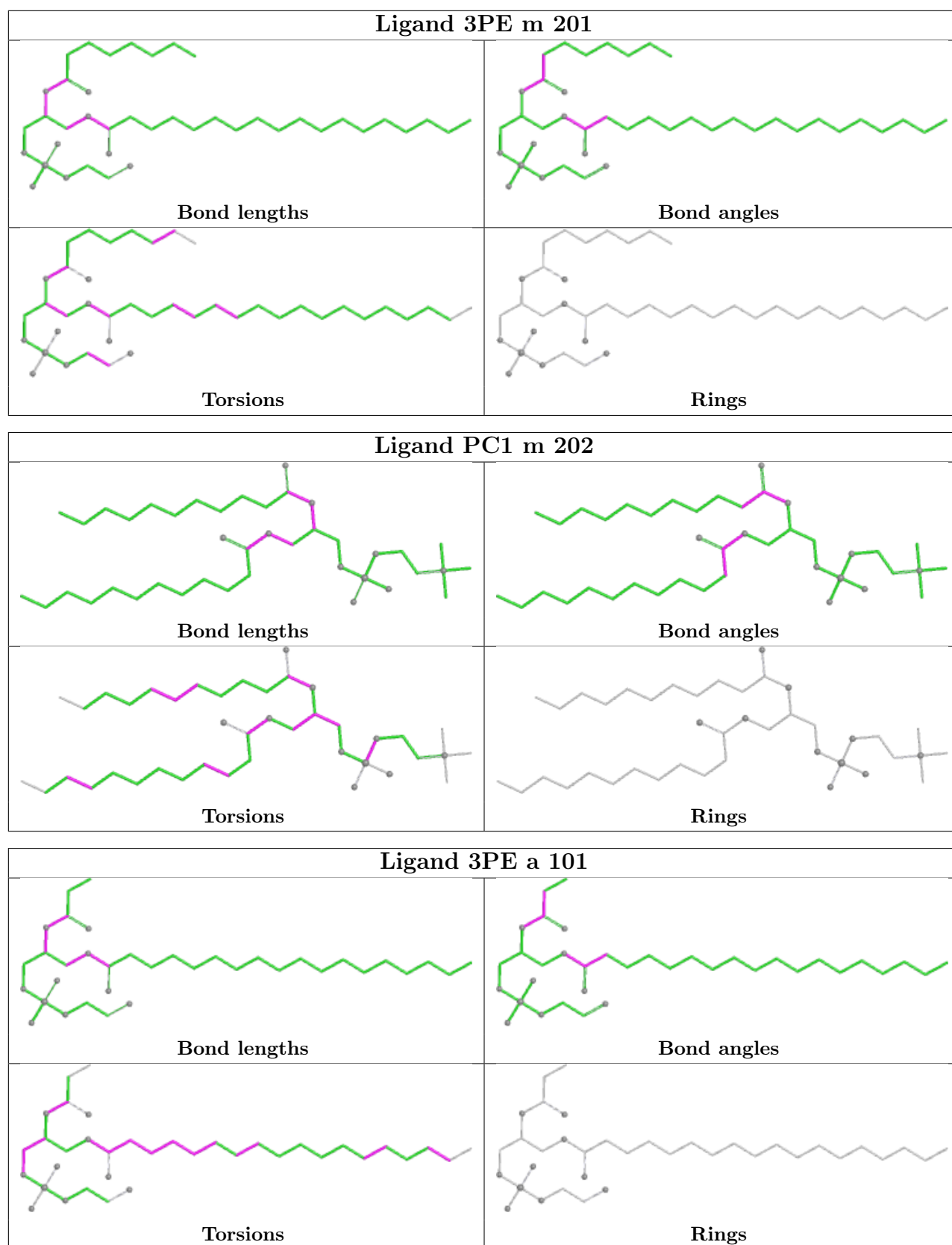


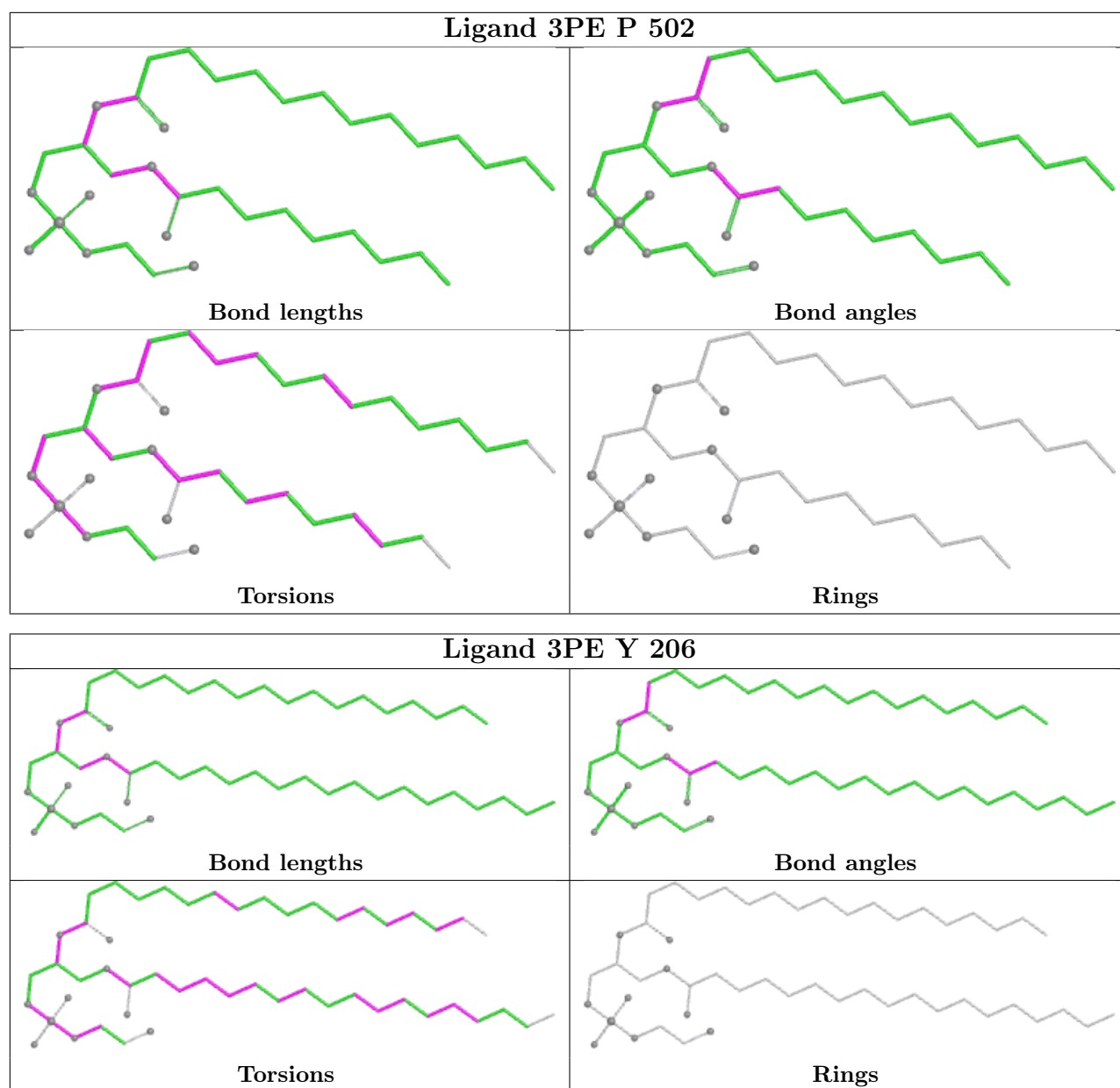




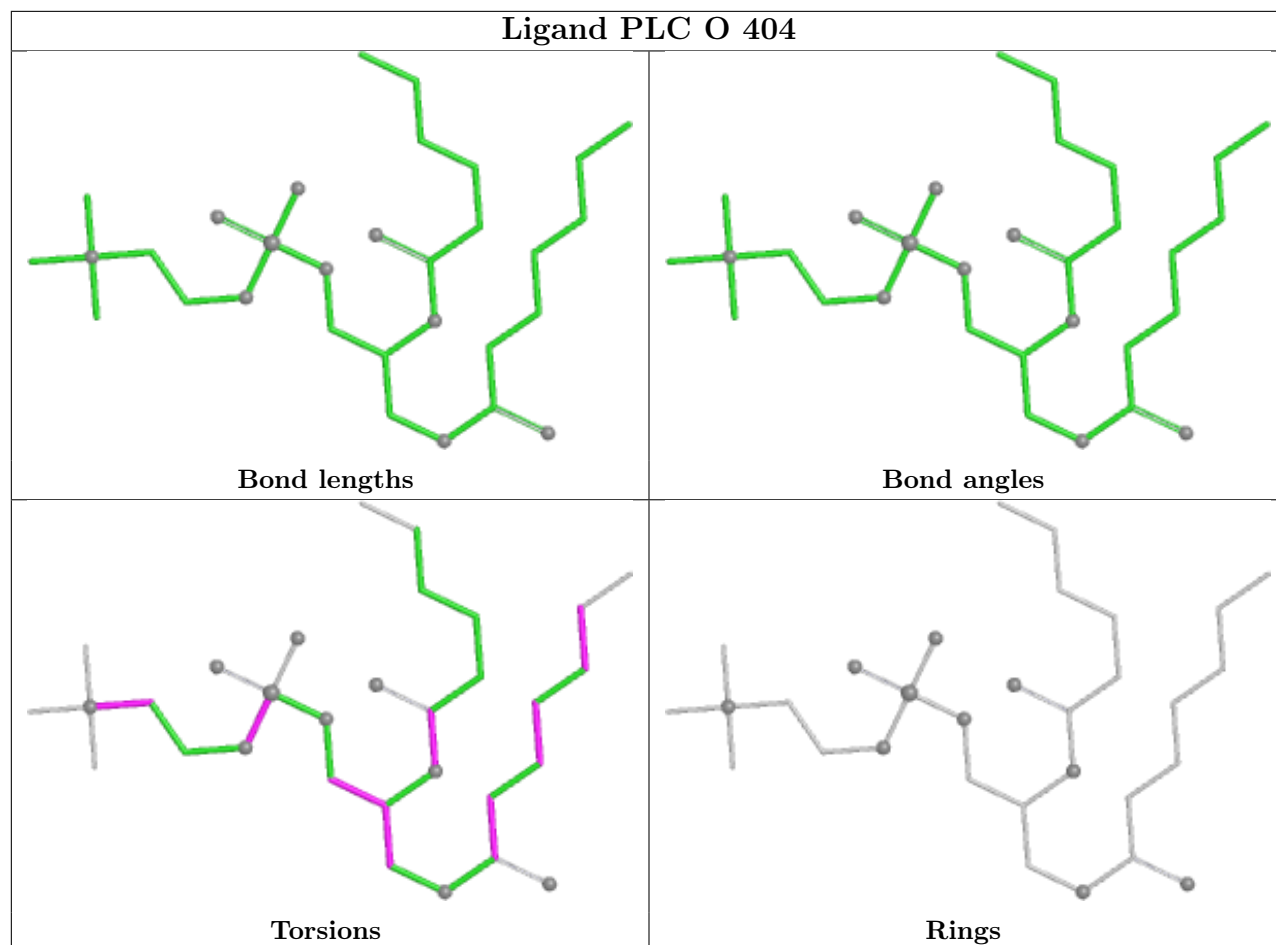




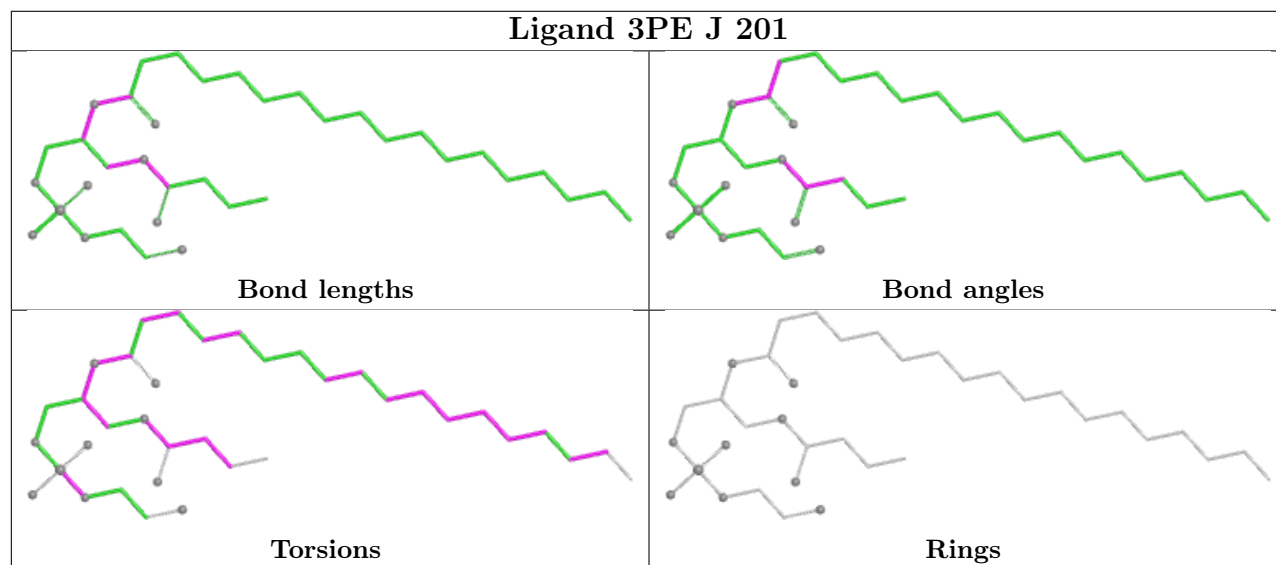


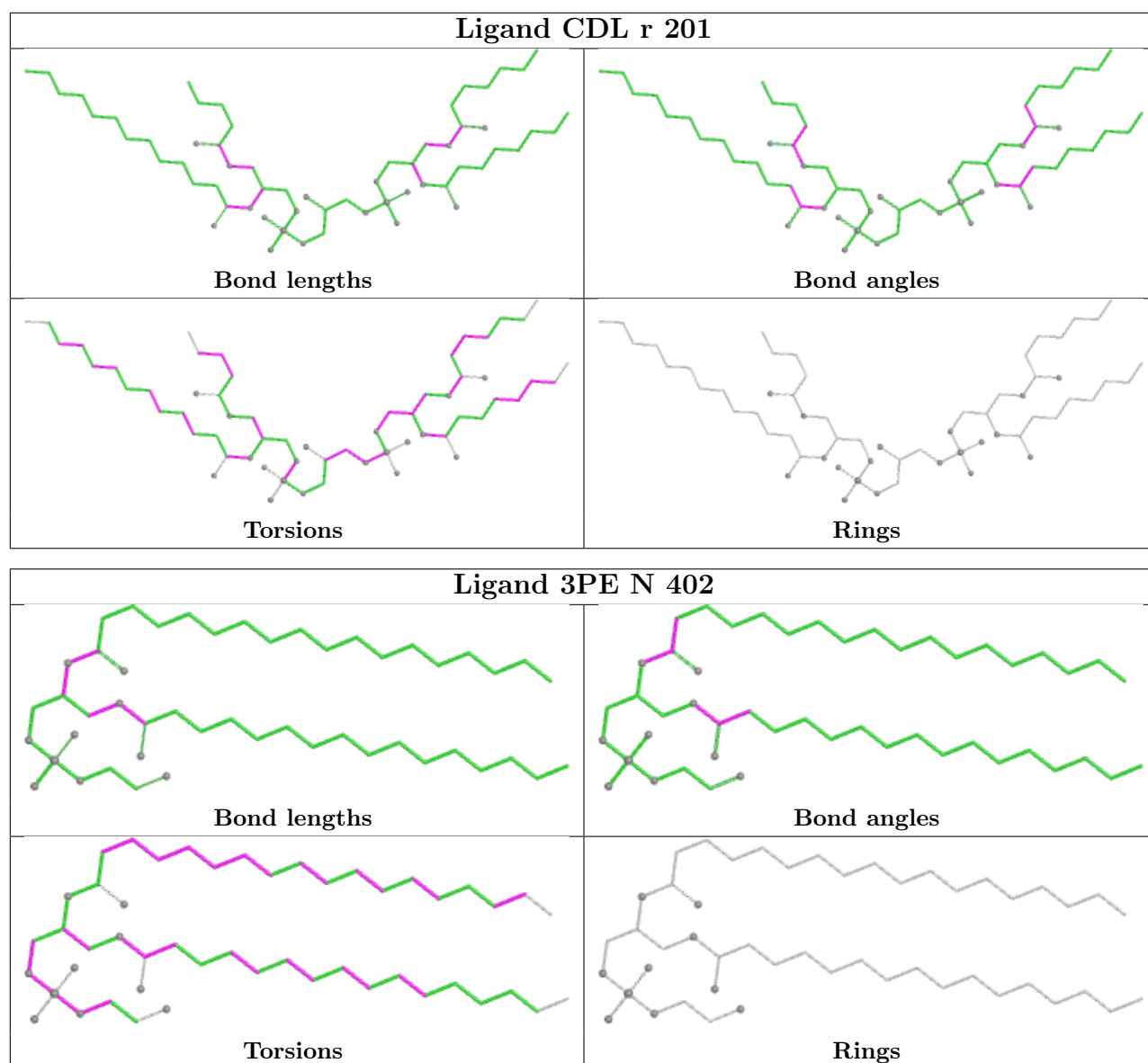


Ligand PLC O 404



Ligand 3PE J 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

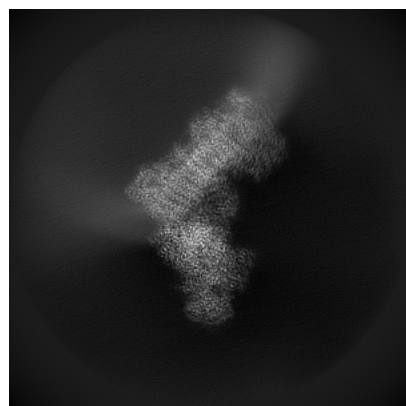
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18143. These allow visual inspection of the internal detail of the map and identification of artifacts.

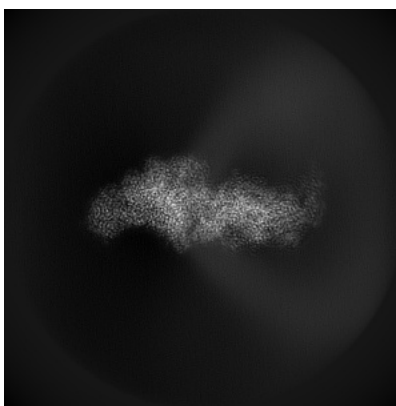
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

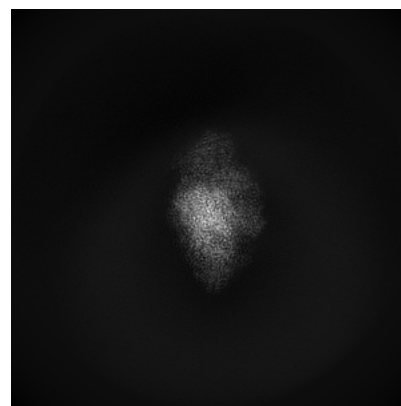
6.1.1 Primary map



X

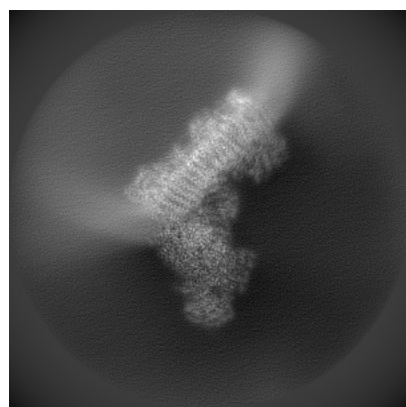


Y

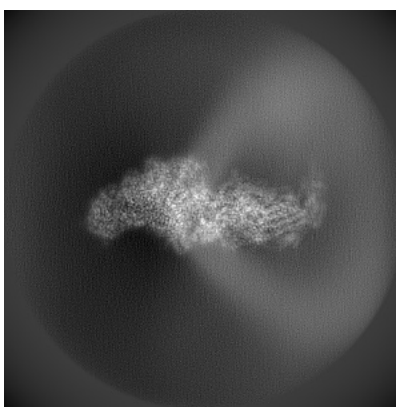


Z

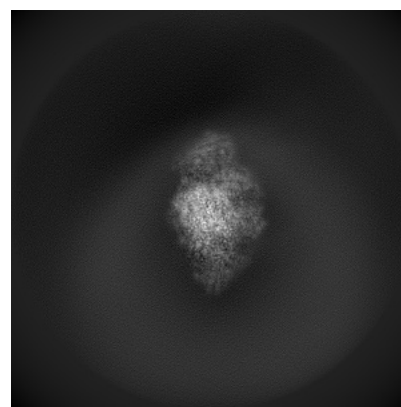
6.1.2 Raw map



X



Y

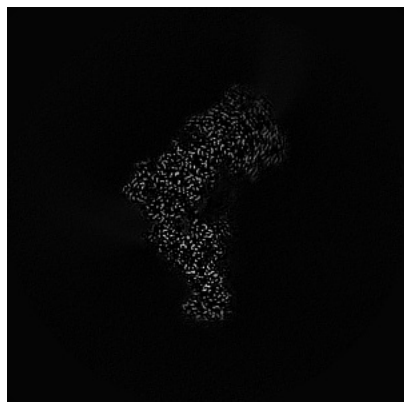


Z

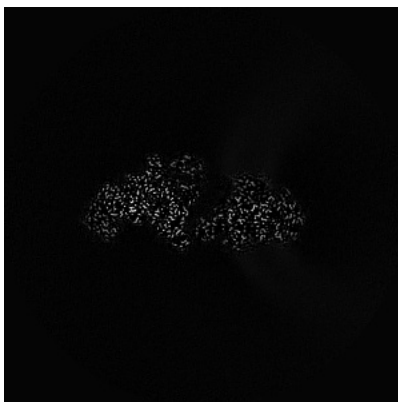
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

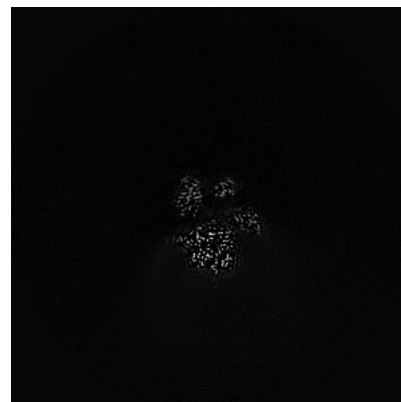
6.2.1 Primary map



X Index: 225

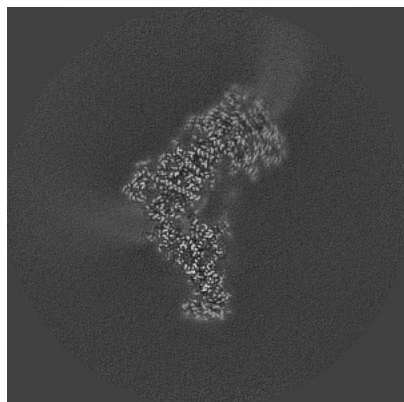


Y Index: 225

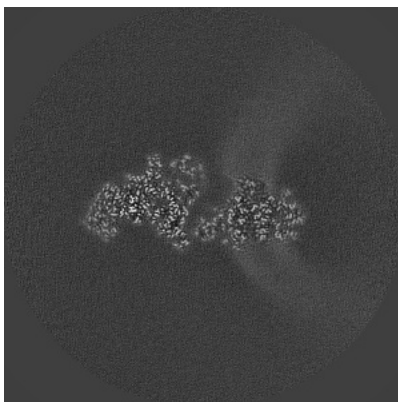


Z Index: 225

6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

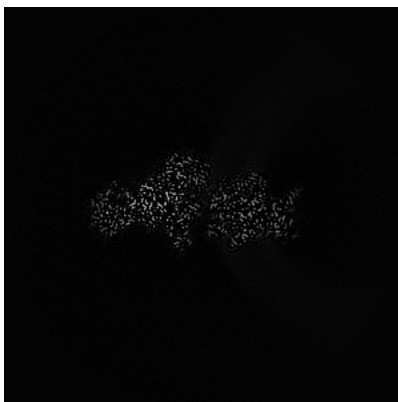
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 222

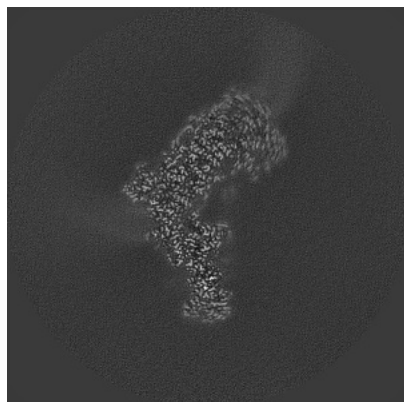


Y Index: 212

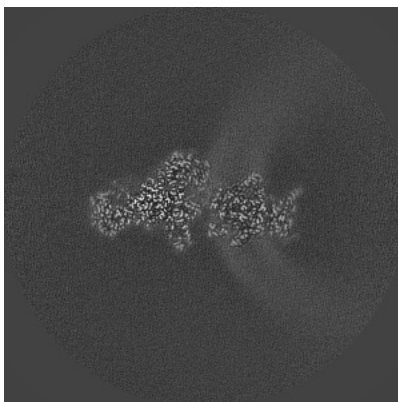


Z Index: 185

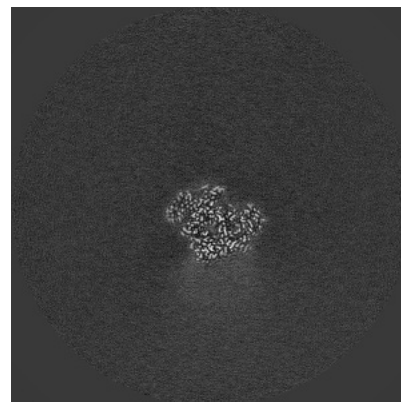
6.3.2 Raw map



X Index: 222



Y Index: 211

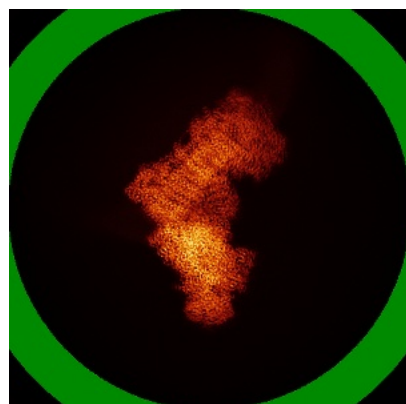


Z Index: 198

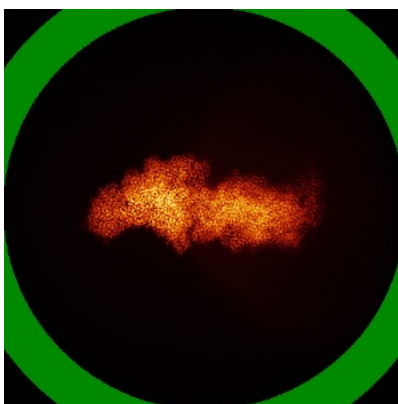
The images above show the largest variance slices of the map in three orthogonal directions.

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

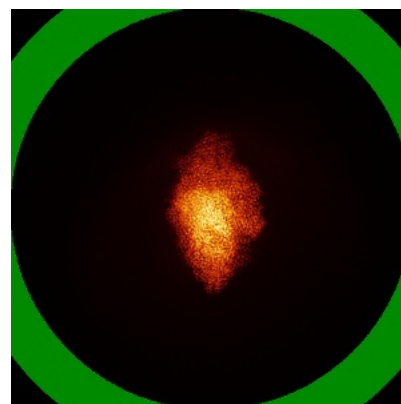
6.4.1 Primary map



X

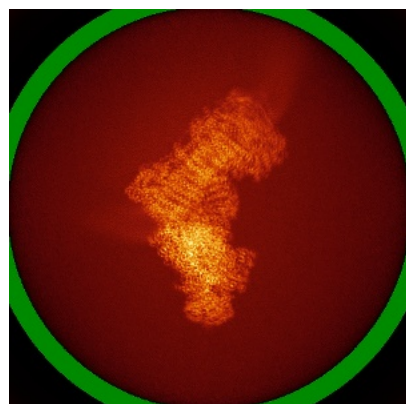


Y

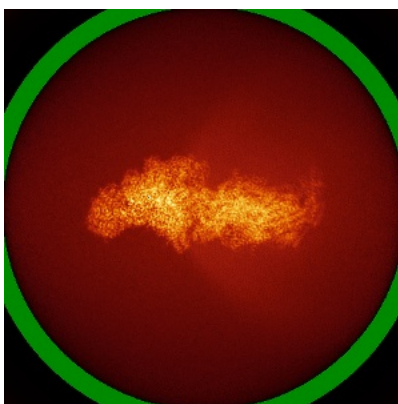


Z

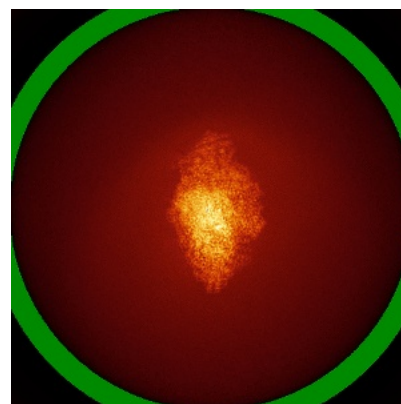
6.4.2 Raw map



X



Y

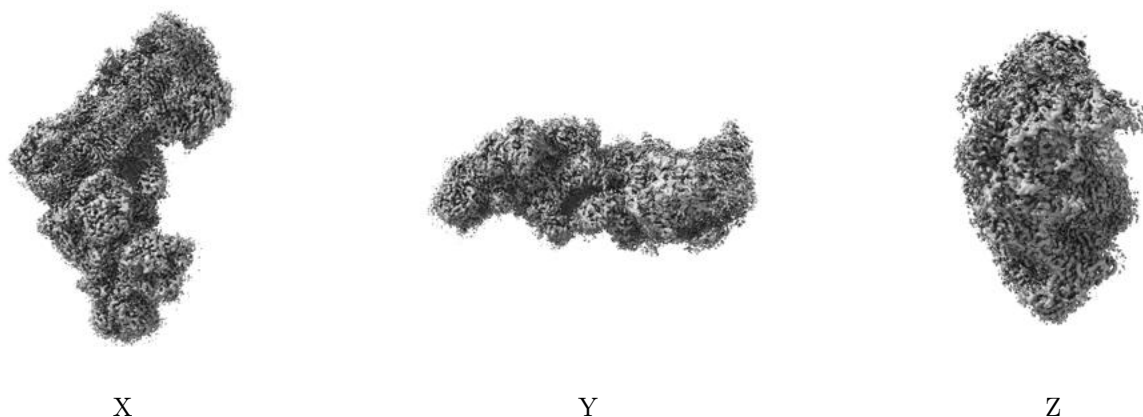


Z

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

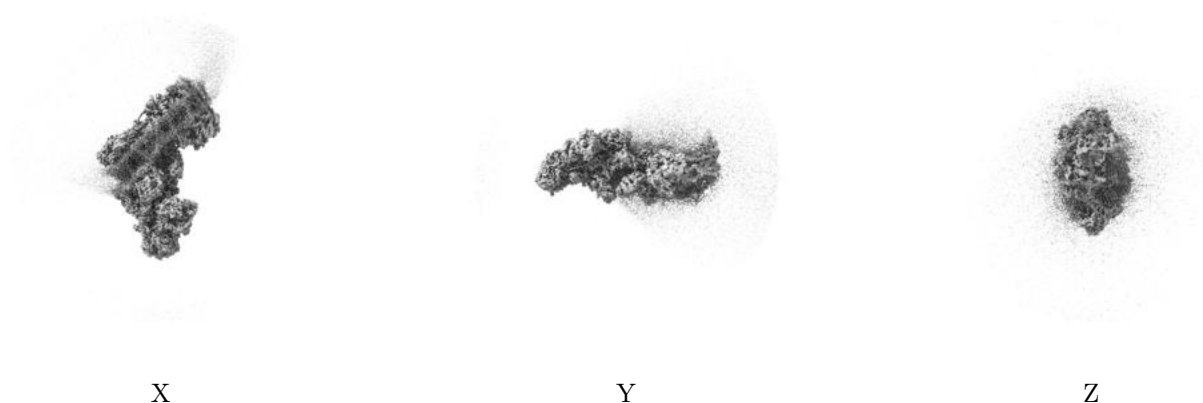
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

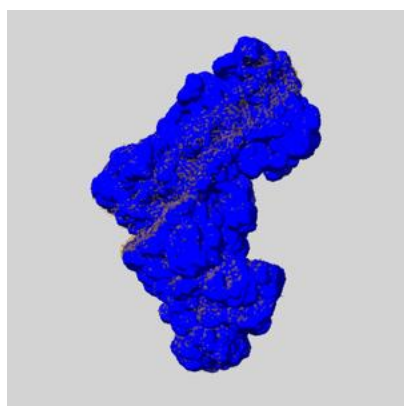
6.6 Mask visualisation [i](#)

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

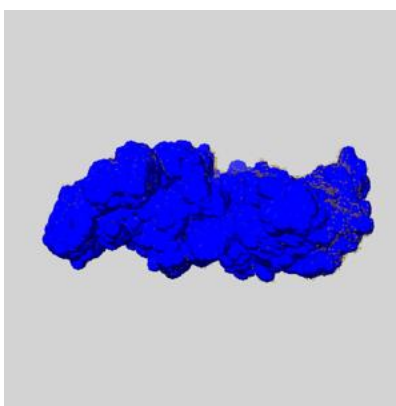
A mask typically either:

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

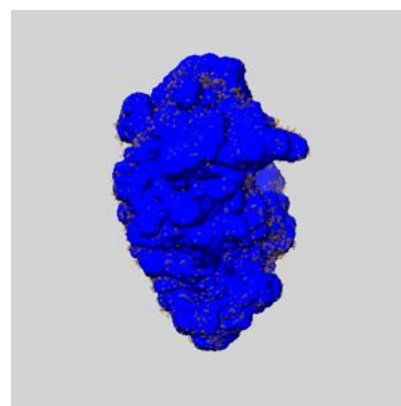
6.6.1 emd_18143_msk_1.map [i](#)



X



Y

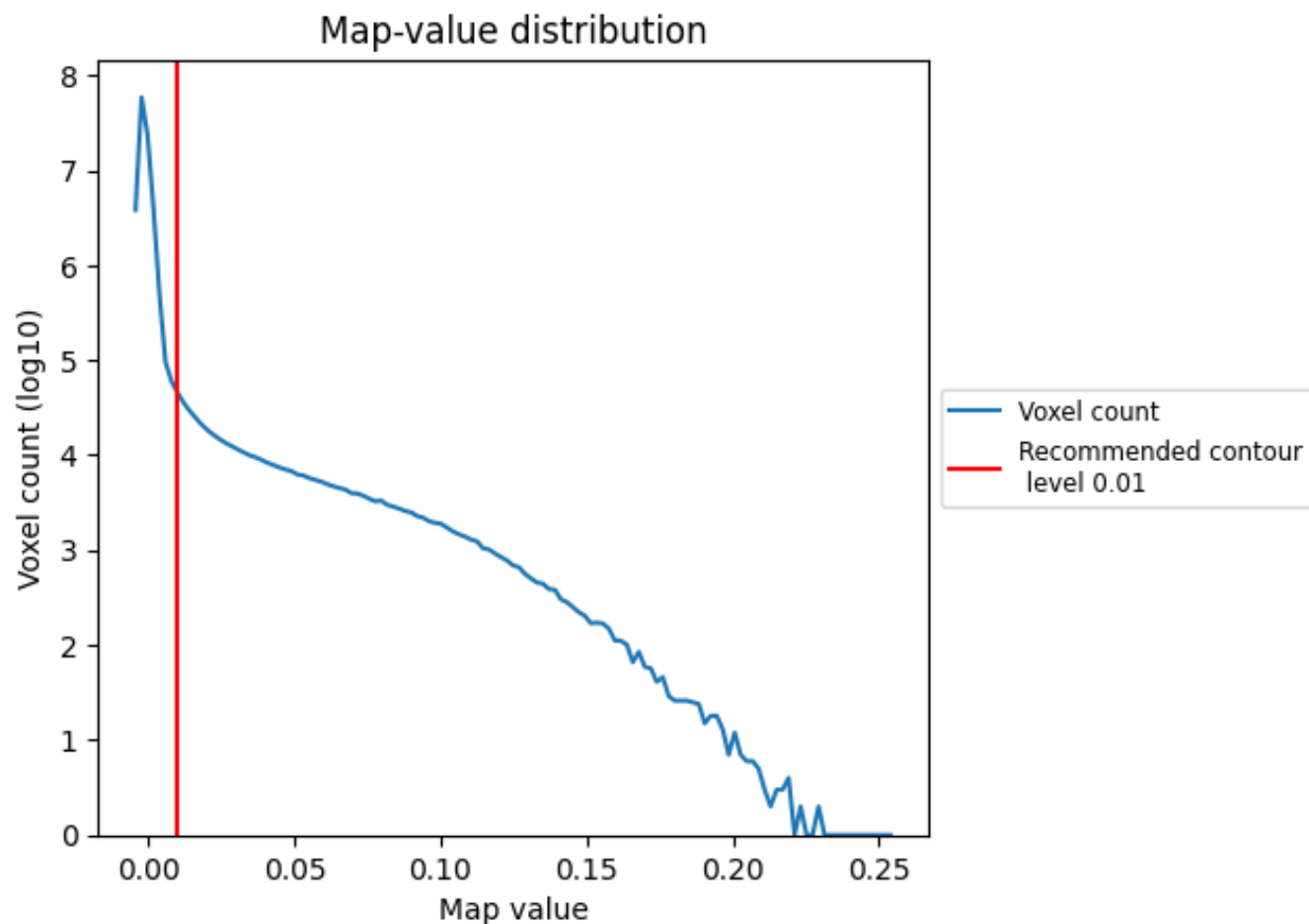


Z

7 Map analysis [i](#)

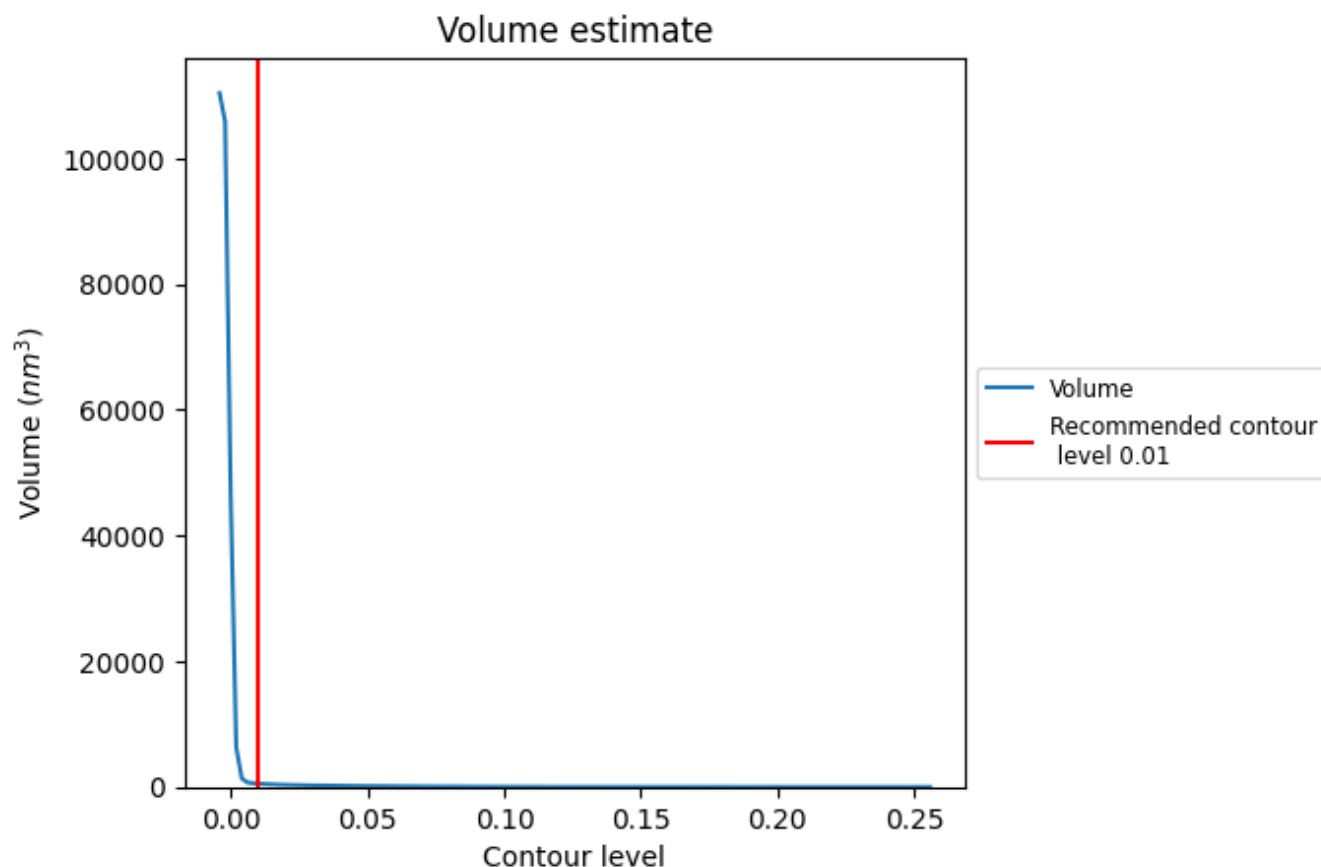
This section contains the results of statistical analysis of the map.

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.

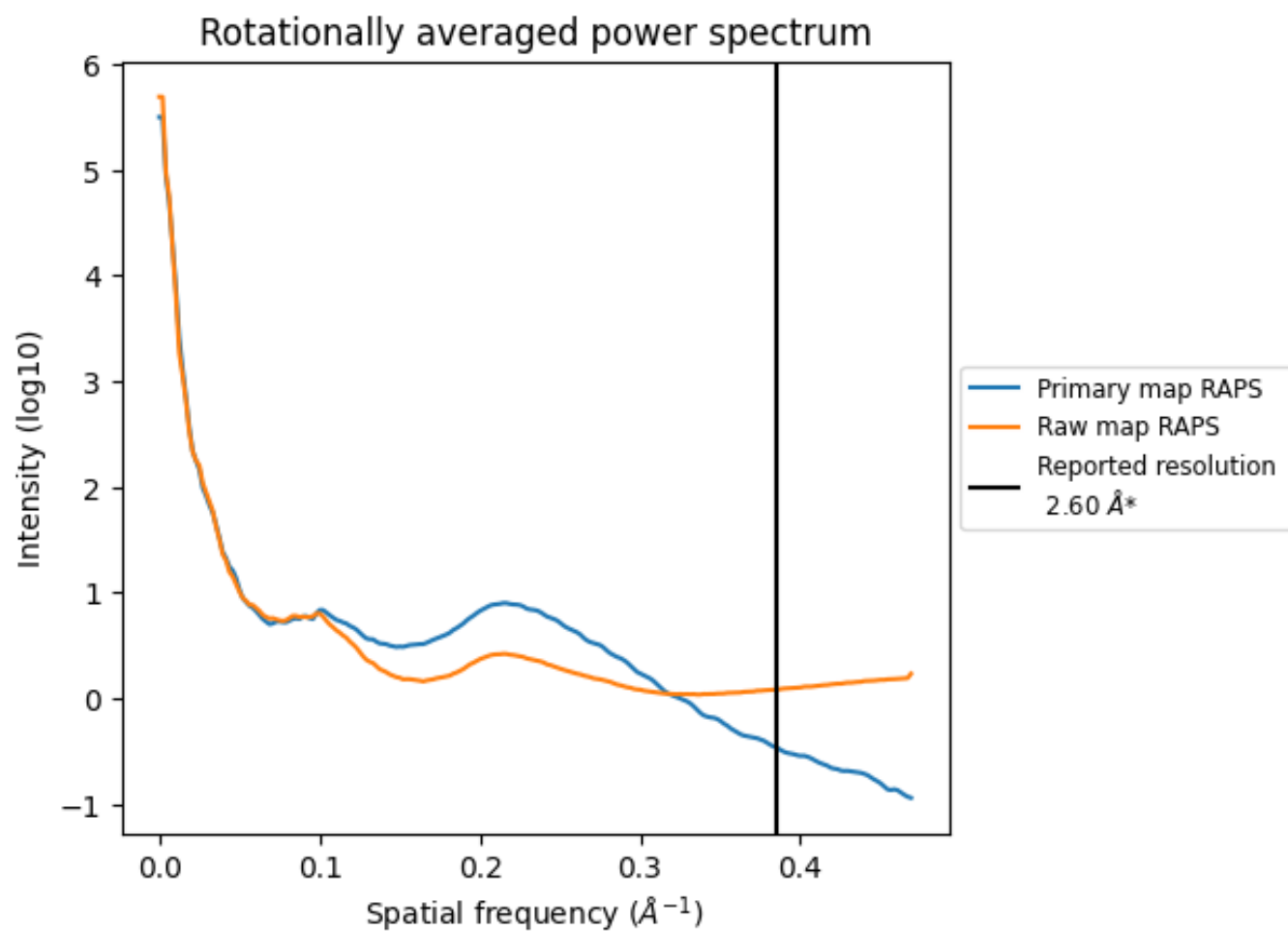
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 528 nm^3 ; this corresponds to an approximate mass of 477 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 ⓘ

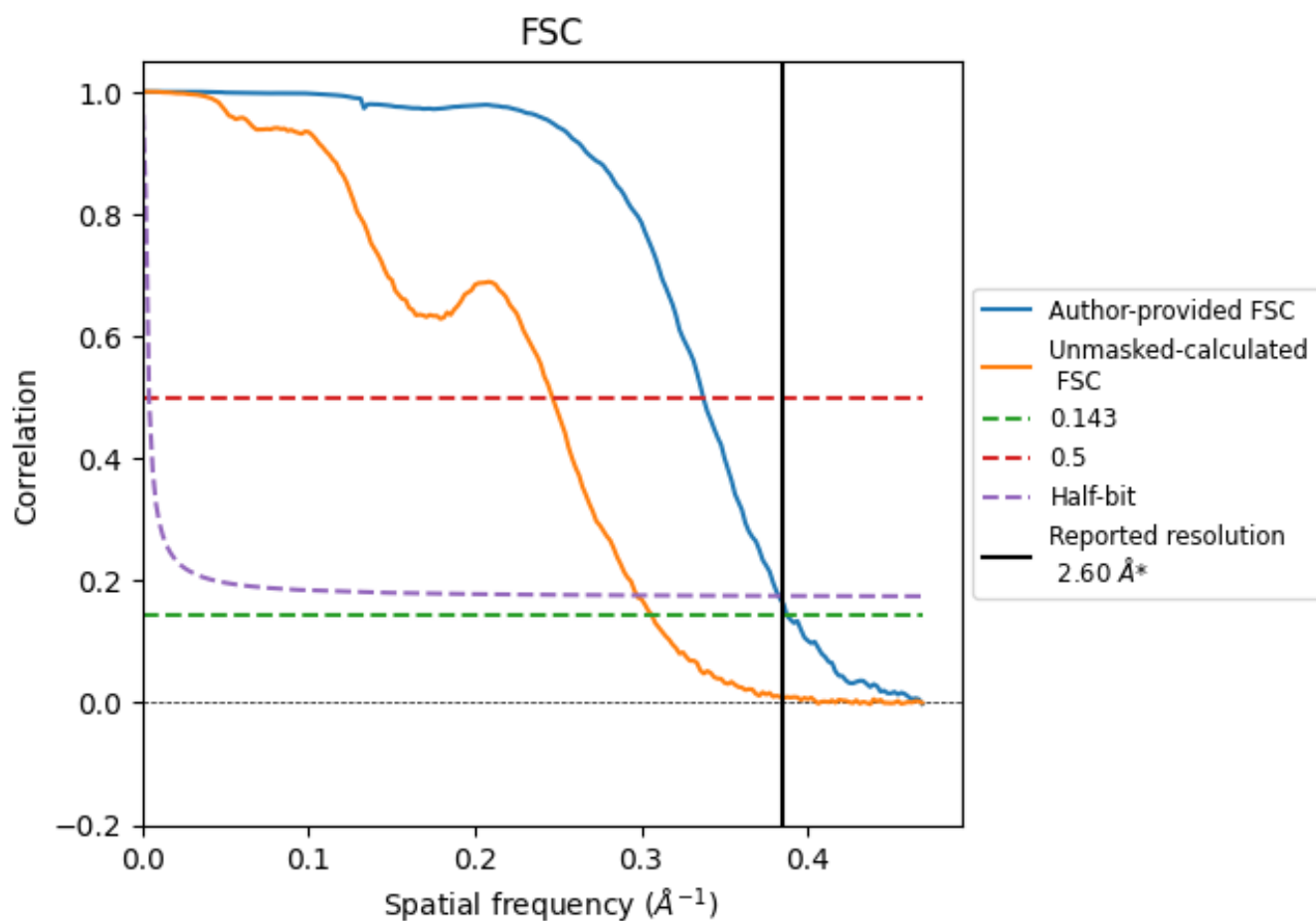


*Reported resolution corresponds to spatial frequency of $0.385 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

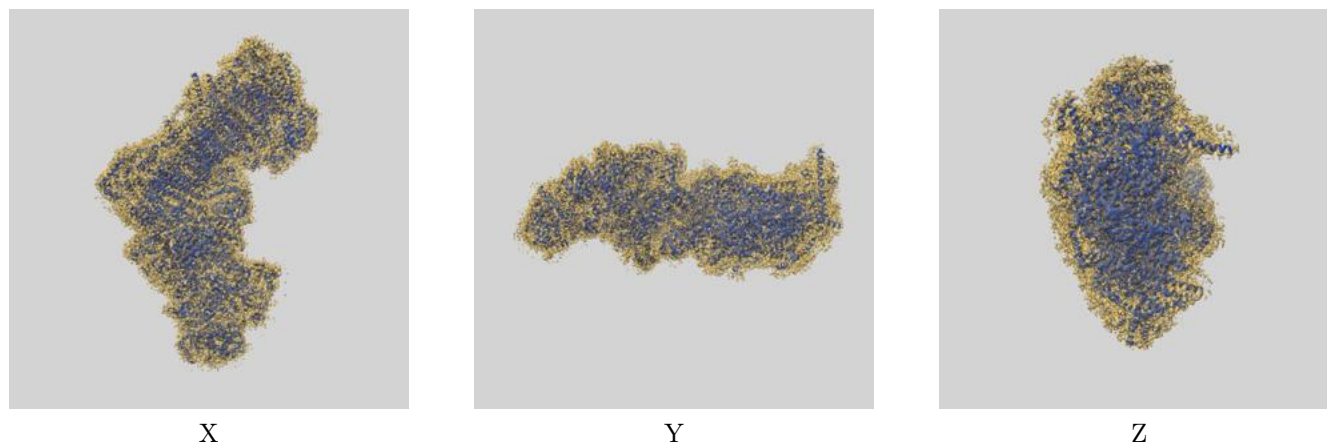
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.58	2.96	2.61
Unmasked-calculated*	3.26	4.06	3.36

*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 3.26 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

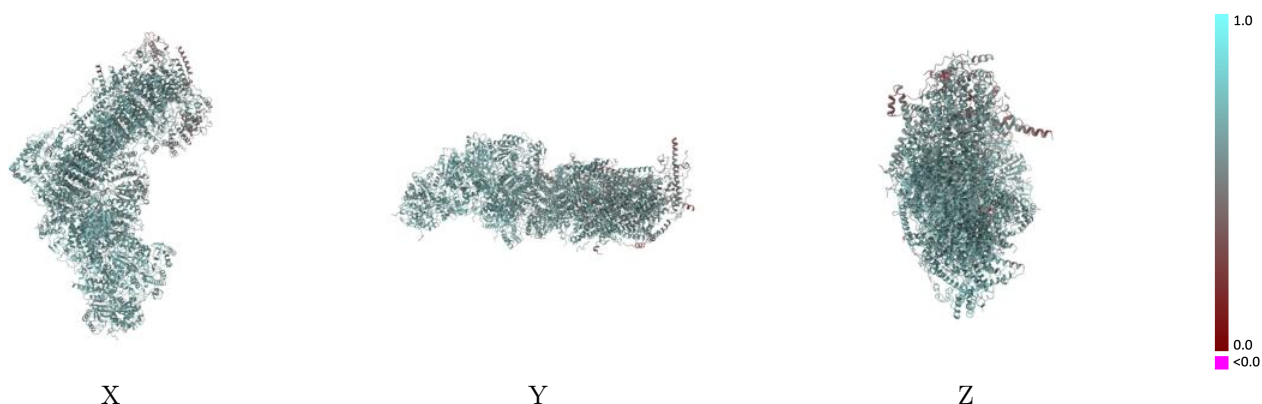
This section contains information regarding the fit between EMDB map EMD-18143 and PDB model 8Q4A. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



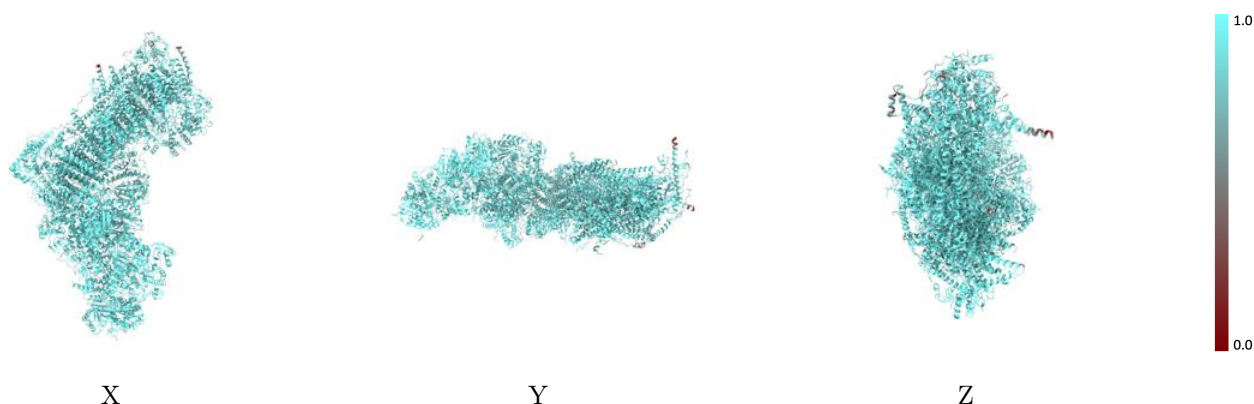
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



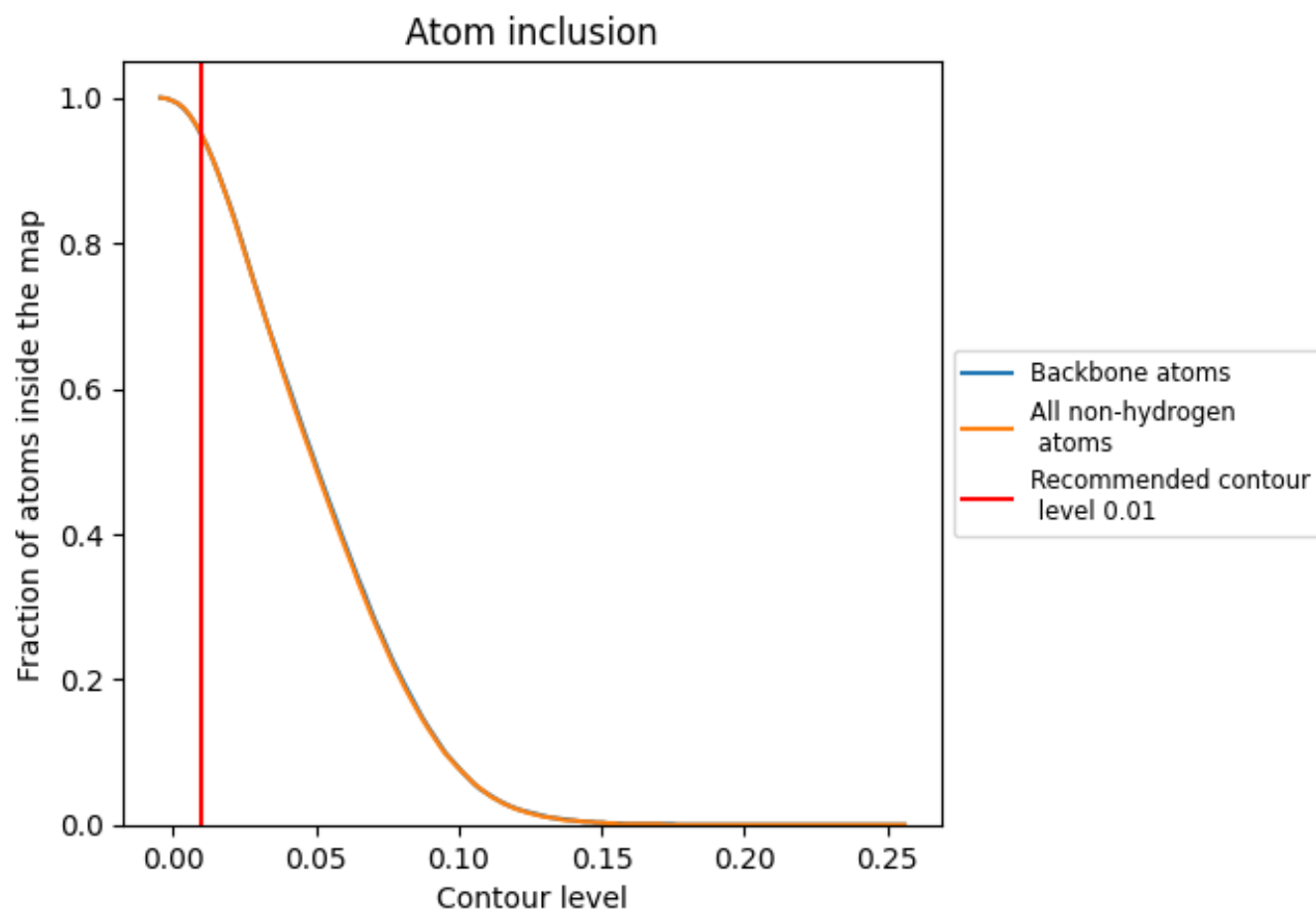
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.6270
A	 0.9660	 0.6380
B	 0.9830	 0.6720
C	 0.9910	 0.6830
D	 0.9870	 0.6770
E	 0.9520	 0.6140
F	 0.9650	 0.6350
G	 0.9720	 0.6530
H	 0.9780	 0.6560
I	 0.9920	 0.6850
J	 0.9450	 0.6300
K	 0.9920	 0.6660
L	 0.9490	 0.6080
M	 0.9850	 0.6570
N	 0.9910	 0.6710
O	 0.9440	 0.6120
P	 0.9540	 0.6250
Q	 0.9670	 0.6620
R	 0.9640	 0.6510
S	 0.9340	 0.6010
T	 0.8630	 0.5440
U	 0.8400	 0.4890
V	 0.9490	 0.6300
W	 0.9680	 0.6530
X	 0.9630	 0.6450
Y	 0.9460	 0.6210
Z	 0.9510	 0.6390
a	 0.9830	 0.6510
b	 0.9500	 0.6290
c	 0.9230	 0.6200
d	 0.9560	 0.6380
e	 0.9500	 0.6310
f	 0.8790	 0.5880
g	 0.9160	 0.5990
h	 0.9670	 0.6370



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Chain	Atom inclusion	Q-score
i	 0.8090	 0.5030
j	 0.8370	 0.4840
k	 0.7740	 0.4560
l	 0.9250	 0.5750
m	 0.9110	 0.5970
n	 0.8950	 0.5400
o	 0.8070	 0.4830
p	 0.9010	 0.5850
q	 0.9660	 0.6550
r	 0.9760	 0.6580
s	 0.9230	 0.5960