



Full wwPDB EM Validation Report ⓘ

Jun 17, 2024 – 09:11 am BST

PDB ID : 8Q1P
EMDB ID : EMD-18066
Title : Inward-facing, open2 proteoliposome complex I at 2.9 Å, after deactivation treatment. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-01
Resolution : 2.90 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

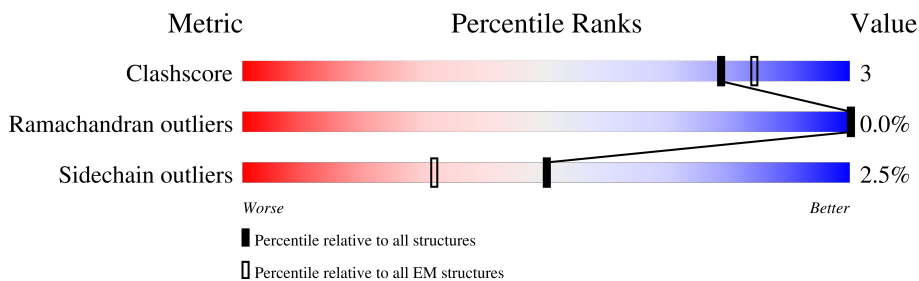
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	115	
2	B	216	
3	C	266	
4	D	463	
5	E	249	
6	F	464	
7	G	727	
8	H	318	


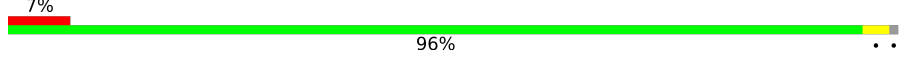








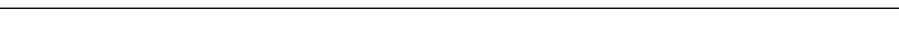

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Mol	Chain	Length	Quality of chain
9	I	212	77% 5% 17%
10	J	175	83% 11%
11	K	98	90% 8%
12	L	606	92% 8%
13	M	459	96%
14	N	347	93% 7%
15	O	343	80% 13% 7%
16	P	380	79% 8% 12%
17	Q	175	69% 5% 26%
18	R	124	73% 5% 23%
19	S	99	80% 6% 13%
20	T	156	45% 11% 44%
20	U	156	53% 44%
21	V	116	94%
22	W	128	84% 6% 9%
23	X	172	92% 7%
24	Y	141	92% 7%
25	Z	144	90% 8%
26	a	70	96%
27	b	84	96%
28	c	76	62% 36%
29	d	120	97%
30	e	106	92% 8%
31	f	57	95% 5%
32	g	154	62% 34%

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Mol	Chain	Length	Quality of chain
33	h	189	 72% 27%
34	i	128	 7% 96%
35	j	108	 63% 34%
36	k	98	 82% 17%
37	l	186	 83% 16%
38	m	129	 97%
39	n	179	 94%
40	o	137	 85% 11%
41	p	176	 97%
42	q	145	 97%
43	r	113	 82% 16%
44	s	109	 39% 60%

2 Entry composition i

There are 59 unique types of molecules in this entry. The entry contains 68995 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
			Total	C	N	O	S		
1	A	102	823	561	117	140	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	156	1247	795	225	213	14	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	418	3373	2157	579	612	25	0	0

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
			Total	C	N	O	S		
5	E	214	1659	1059	278	312	10	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	691	5298	3318	925	1016	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	315	2488	1667	382	416	23	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	168	1281	861	183	225	12	0	0

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
16	P	334	2677	1730	475	467	5	0	0

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

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

- 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 subunit 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 subunit 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 subunit 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 subunit 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 subunit 11.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	142	1157	743	202	203	9	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	98	825	521	157	141	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

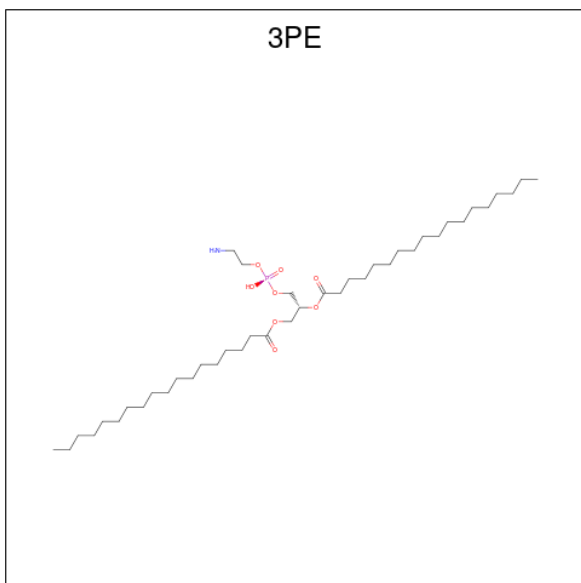
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	44	371	233	66	71	1	0	0

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	A	1	47	37	1	8	1	0
45	A	1	44	34	1	8	1	0
45	H	1	39	29	1	8	1	0
45	I	1	36	26	1	8	1	0
45	J	1	36	26	1	8	1	0
45	J	1	44	34	1	8	1	0
45	L	1	45	35	1	8	1	0

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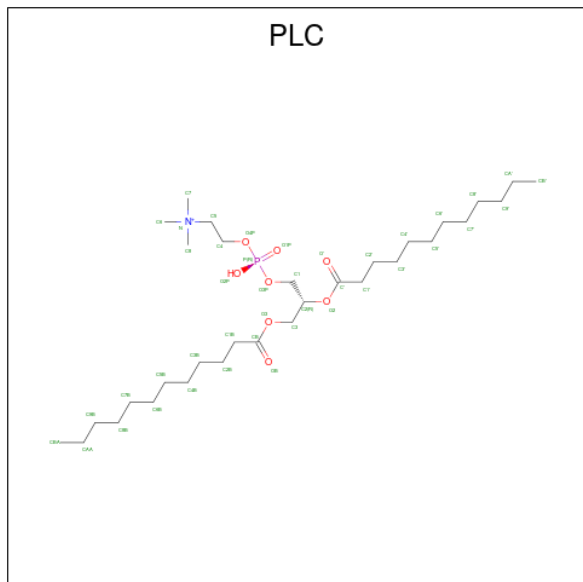
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	L	1	Total 35	C 25	N 1	O 8	P 1	0
45	M	1	Total 50	C 40	N 1	O 8	P 1	0
45	M	1	Total 45	C 35	N 1	O 8	P 1	0
45	N	1	Total 49	C 39	N 1	O 8	P 1	0
45	Y	1	Total 27	C 17	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 47	C 37	N 1	O 8	P 1	0
45	Y	1	Total 37	C 27	N 1	O 8	P 1	0
45	Z	1	Total 41	C 31	N 1	O 8	P 1	0
45	Z	1	Total 35	C 25	N 1	O 8	P 1	0
45	d	1	Total 49	C 39	N 1	O 8	P 1	0
45	f	1	Total 30	C 20	N 1	O 8	P 1	0
45	f	1	Total 32	C 22	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



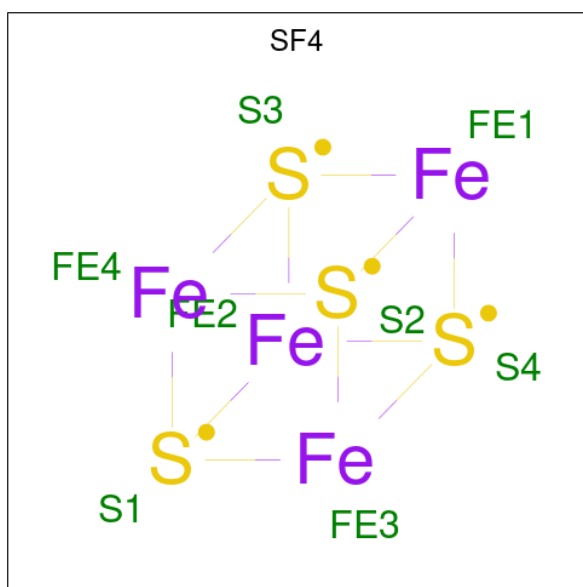
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	Total 35	C 25	N 1	O 8	P 1	0
46	A	1	Total 46	C 36	N 1	O 8	P 1	0
46	B	1	Total 48	C 38	N 1	O 8	P 1	0
46	H	1	Total 48	C 38	N 1	O 8	P 1	0
46	H	1	Total 42	C 32	N 1	O 8	P 1	0
46	I	1	Total 54	C 44	N 1	O 8	P 1	0
46	L	1	Total 54	C 44	N 1	O 8	P 1	0
46	M	1	Total 35	C 25	N 1	O 8	P 1	0
46	Z	1	Total 44	C 34	N 1	O 8	P 1	0
46	d	1	Total 39	C 29	N 1	O 8	P 1	0
46	g	1	Total 44	C 34	N 1	O 8	P 1	0
46	h	1	Total 36	C 26	N 1	O 8	P 1	0
46	m	1	Total 54	C 44	N 1	O 8	P 1	0
46	q	1	Total 34	C 24	N 1	O 8	P 1	0

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



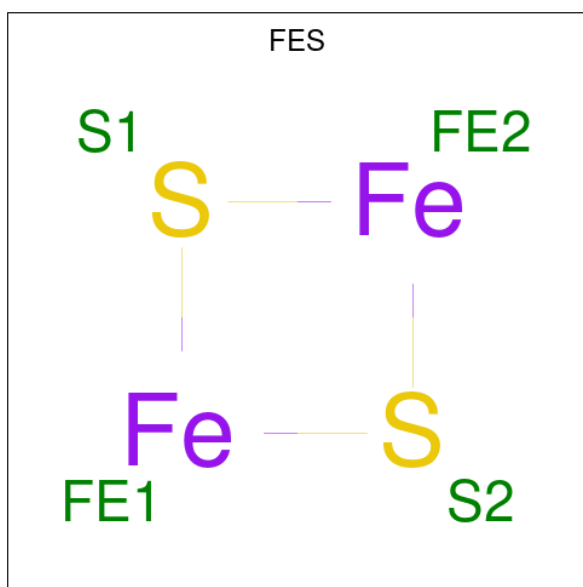
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	Total 42	32	1	8	1	0
47	B	1	Total 42	32	1	8	1	0
47	L	1	Total 31	21	1	8	1	0
47	M	1	Total 34	24	1	8	1	0
47	Y	1	Total 32	22	1	8	1	0
47	Z	1	Total 36	26	1	8	1	0
47	g	1	Total 29	19	1	8	1	0

- Molecule 48 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



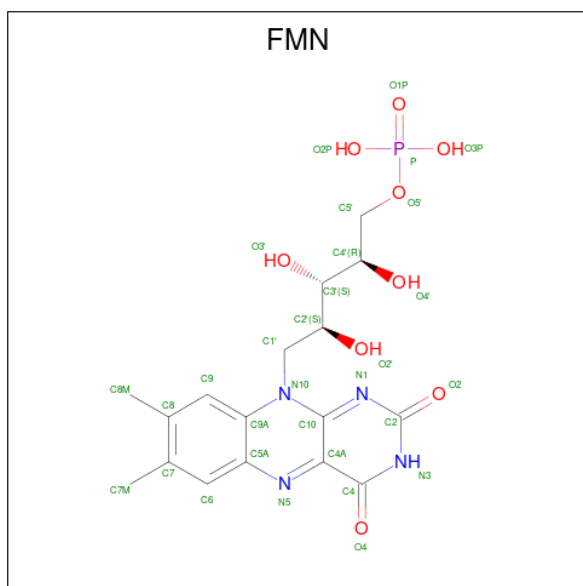
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	B	1	8	4	4	0
48	F	1	8	4	4	0
48	G	1	8	4	4	0
48	G	1	8	4	4	0
48	I	1	8	4	4	0
48	I	1	8	4	4	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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 (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

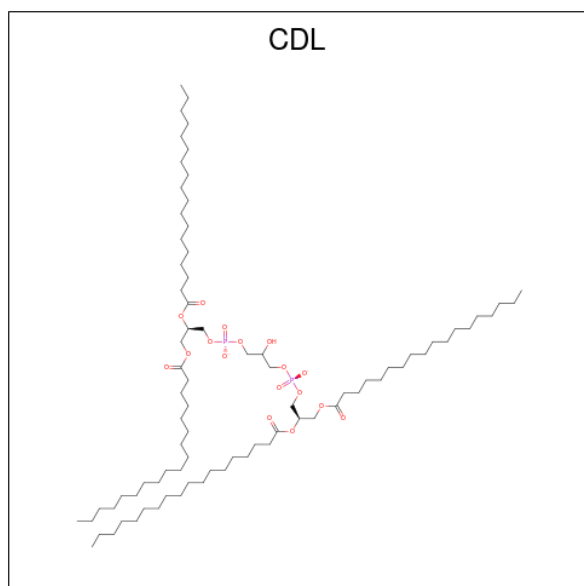


Mol	Chain	Residues	Atoms				AltConf	
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

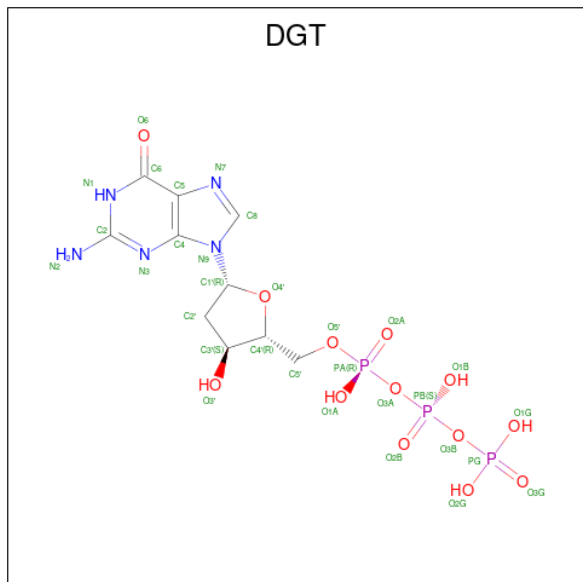


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	L	1	100	81	17	2	0
52	M	1	100	81	17	2	0
52	O	1	85	66	17	2	0
52	X	1	100	81	17	2	0
52	d	1	65	46	17	2	0
52	h	1	80	61	17	2	0
52	r	1	61	42	17	2	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



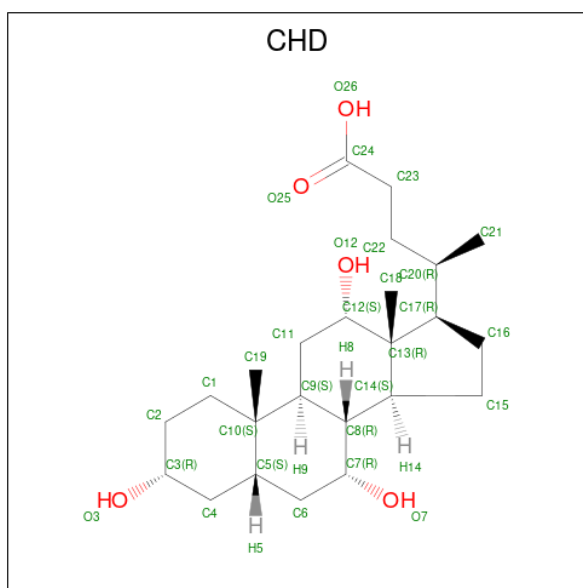
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	O	1	31	10	5	13	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

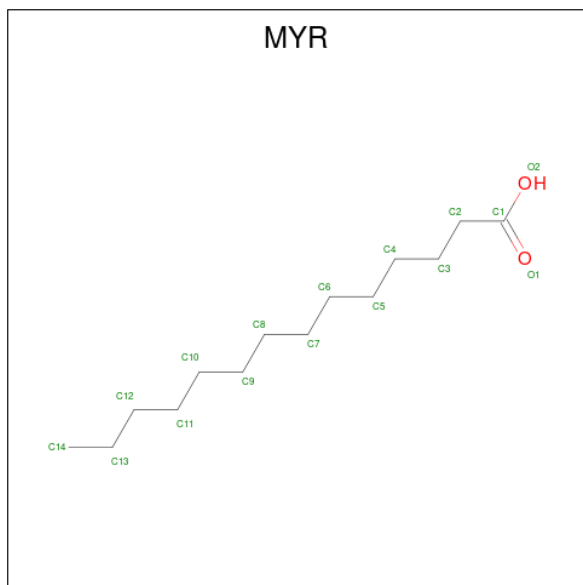
- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

- Molecule 58 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).




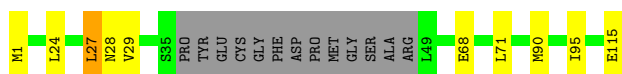
Mol	Chain	Residues	Atoms		AltConf	
59	o	1	Total	C	O	0
			15	14	1	

3 Residue-property plots [i](#)

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

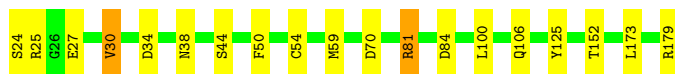
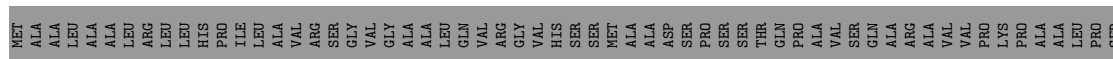
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



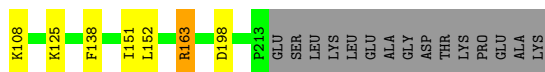
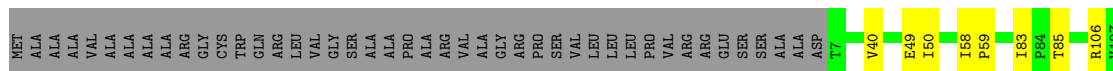
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 




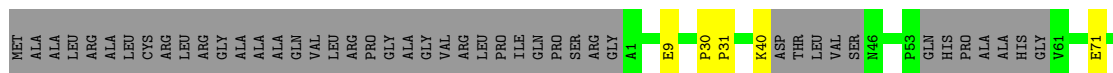
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



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

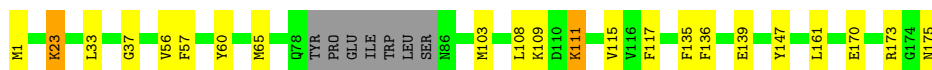
Chain D: 





- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 83% 11%



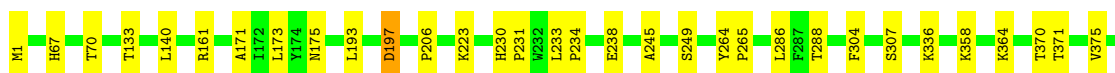
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 90% 8%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 92% 8%



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 96%



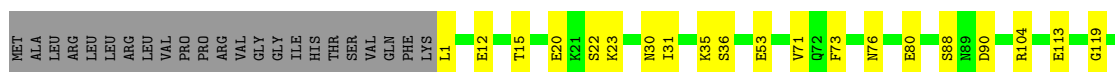
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

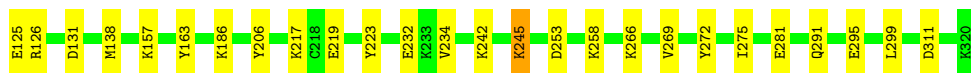
Chain N: 93% 7%



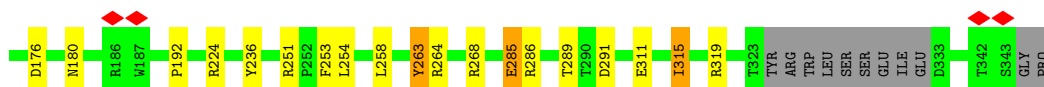
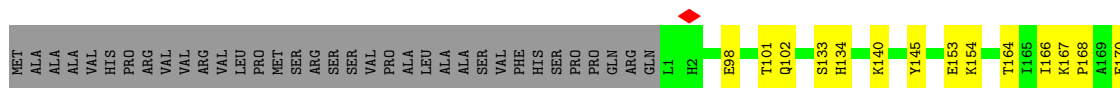
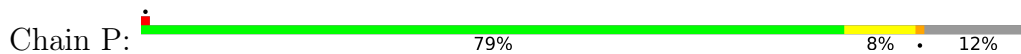
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 80% 13% 7%

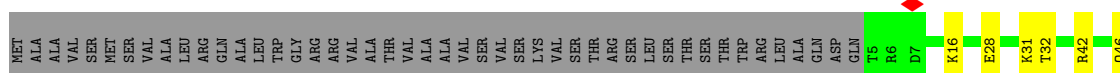




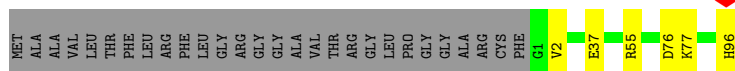
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



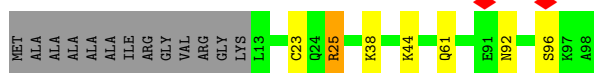
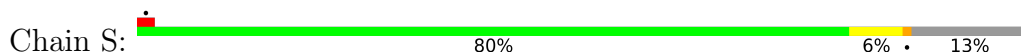
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



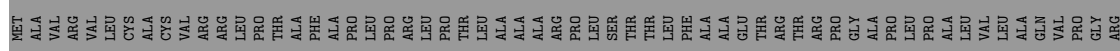
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



- Molecule 20: Acyl carrier protein, mitochondrial





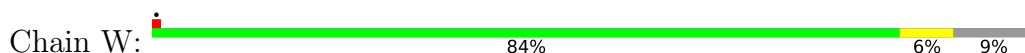
- Molecule 20: Acyl carrier protein, mitochondrial



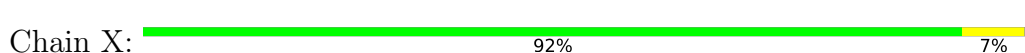
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



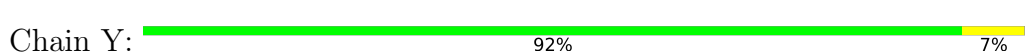
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



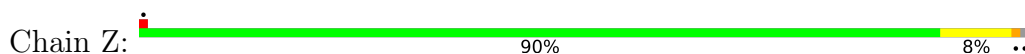
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



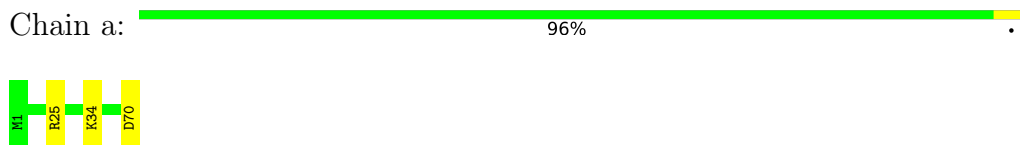
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



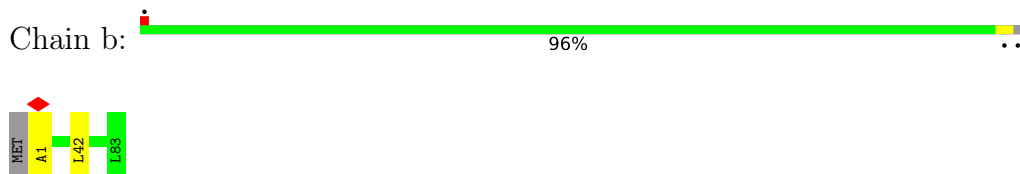
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



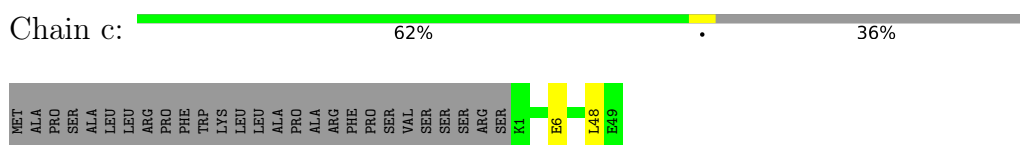
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



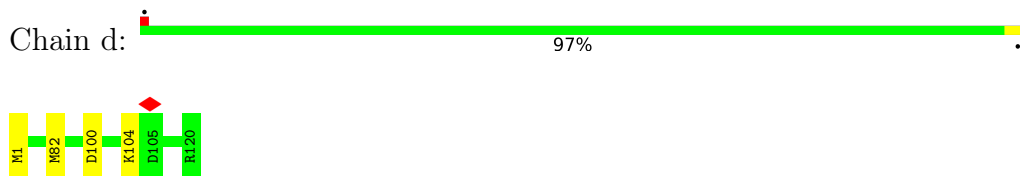
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



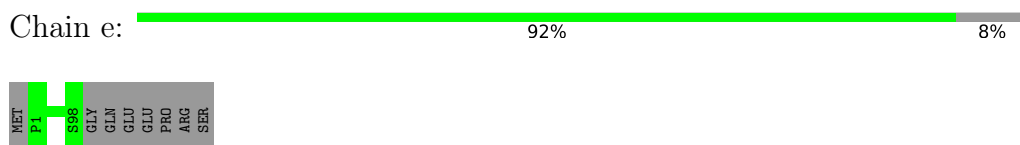
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



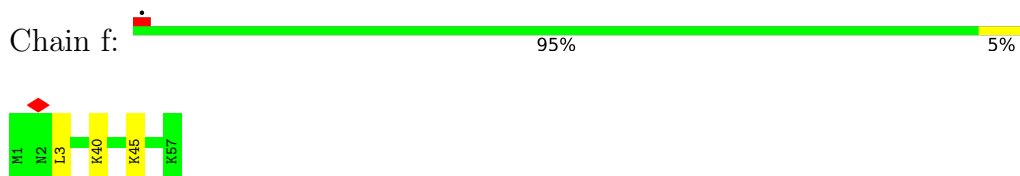
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

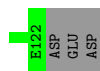
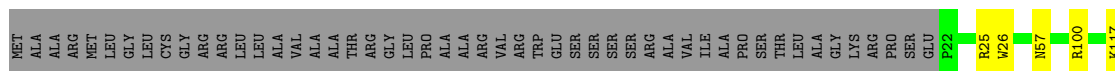


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

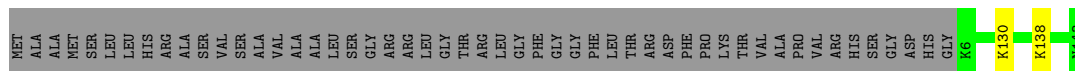


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

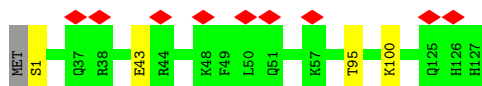




- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



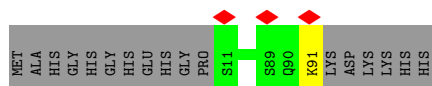
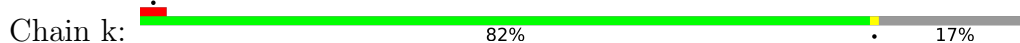
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



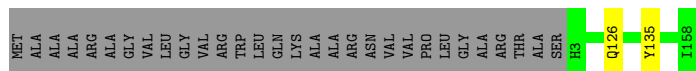
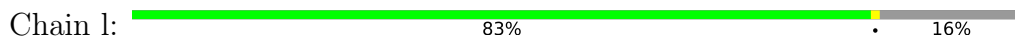
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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

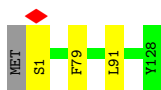


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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





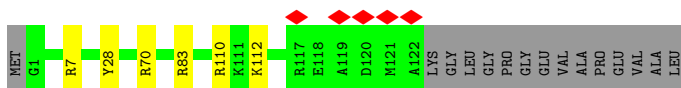
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 94%



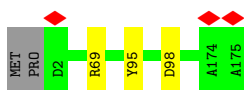
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 85%



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

Chain p: 97%



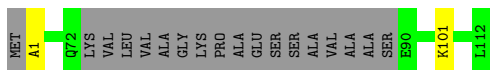
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 97%



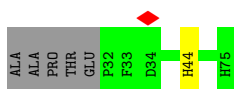
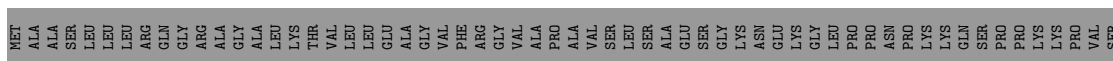
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r: 82%



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

Chain s: 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58386	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 ($e^-/\text{\AA}^2$)	40, 40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.388	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.072, 1.072, 1.072	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/833	0.38	0/1140
2	B	0.28	0/1278	0.52	0/1728
3	C	0.28	0/1772	0.51	0/2413
4	D	0.28	0/3446	0.48	0/4665
5	E	0.26	0/1699	0.46	0/2312
6	F	0.25	0/3401	0.50	0/4595
7	G	0.25	0/5387	0.50	0/7301
8	H	0.26	0/2549	0.43	0/3481
9	I	0.29	0/1445	0.52	0/1956
10	J	0.27	0/1301	0.41	0/1761
11	K	0.24	0/745	0.40	0/1008
12	L	0.25	0/4920	0.41	0/6694
13	M	0.24	0/3738	0.42	0/5097
14	N	0.25	0/2792	0.42	0/3800
15	O	0.26	0/2651	0.43	0/3587
16	P	0.25	0/2750	0.50	0/3729
17	Q	0.25	0/1072	0.51	0/1449
18	R	0.27	0/753	0.50	0/1014
19	S	0.23	0/702	0.50	0/945
20	T	0.24	0/719	0.40	0/971
20	U	0.25	0/719	0.39	0/971
21	V	0.24	0/943	0.41	0/1277
22	W	0.24	0/1006	0.49	0/1352
23	X	0.25	0/1439	0.47	0/1942
24	Y	0.24	0/1042	0.46	0/1414
25	Z	0.26	0/1186	0.51	0/1599
26	a	0.26	0/584	0.50	0/786
27	b	0.25	0/667	0.44	0/916
28	c	0.26	0/427	0.41	0/579
29	d	0.27	0/1018	0.49	0/1375
30	e	0.24	0/846	0.49	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.25	0/505	0.49	0/681
32	g	0.26	0/873	0.45	0/1186
33	h	0.26	0/1188	0.47	0/1607
34	i	0.24	0/1127	0.46	0/1534
35	j	0.25	0/624	0.43	0/855
36	k	0.24	0/672	0.44	0/906
37	l	0.25	0/1369	0.44	0/1873
38	m	0.26	0/1088	0.51	0/1472
39	n	0.25	0/1540	0.48	0/2085
40	o	0.25	0/1073	0.51	0/1437
41	p	0.24	0/1491	0.49	0/2011
42	q	0.27	0/1242	0.49	0/1688
43	r	0.27	0/789	0.50	0/1068
44	s	0.24	0/383	0.48	0/518
All	All	0.26	0/67794	0.47	0/91909

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	823	0	866	9	0
2	B	1247	0	1256	13	0
3	C	1721	0	1675	9	0
4	D	3373	0	3324	18	0
5	E	1659	0	1664	6	0
6	F	3326	0	3282	20	0
7	G	5298	0	5316	43	0
8	H	2488	0	2595	35	0
9	I	1414	0	1370	10	0
10	J	1281	0	1292	11	0
11	K	745	0	785	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	25	0
13	M	3654	0	3852	10	0
14	N	2733	0	2912	13	0
15	O	2589	0	2566	25	0
16	P	2677	0	2701	20	0
17	Q	1049	0	1045	3	0
18	R	740	0	714	3	0
19	S	691	0	706	2	0
20	T	707	0	700	7	0
20	U	707	0	700	1	0
21	V	923	0	964	2	0
22	W	982	0	999	4	0
23	X	1402	0	1381	8	0
24	Y	1030	0	1039	5	0
25	Z	1157	0	1156	6	0
26	a	569	0	568	0	0
27	b	654	0	663	0	0
28	c	414	0	415	0	0
29	d	999	0	988	0	0
30	e	825	0	826	0	0
31	f	492	0	501	0	0
32	g	846	0	798	0	0
33	h	1154	0	1168	0	0
34	i	1097	0	1108	0	0
35	j	597	0	536	0	0
36	k	653	0	639	0	0
37	l	1314	0	1210	0	0
38	m	1070	0	1068	0	0
39	n	1487	0	1433	0	0
40	o	1048	0	1018	0	0
41	p	1458	0	1430	0	0
42	q	1212	0	1183	0	0
43	r	776	0	782	0	0
44	s	371	0	344	0	0
45	A	91	0	136	0	0
45	H	39	0	52	0	0
45	I	36	0	49	0	0
45	J	80	0	111	0	0
45	L	80	0	114	0	0
45	M	95	0	141	0	0
45	N	49	0	75	0	0
45	Y	264	0	396	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	76	0	103	0	0
45	d	49	0	75	0	0
45	f	62	0	72	0	0
45	m	82	0	118	0	0
46	A	81	0	110	2	0
46	B	48	0	70	0	0
46	H	90	0	134	1	0
46	I	54	0	88	0	0
46	L	54	0	88	1	0
46	M	35	0	44	0	0
46	Z	44	0	62	1	0
46	d	39	0	52	0	0
46	g	44	0	65	0	0
46	h	36	0	46	0	0
46	m	54	0	88	0	0
46	q	34	0	42	0	0
47	A	42	0	64	0	0
47	B	42	0	64	0	0
47	L	31	0	36	0	0
47	M	34	0	45	0	0
47	Y	32	0	41	0	0
47	Z	36	0	49	0	0
47	g	29	0	32	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	1	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	0	0
51	G	1	0	0	0	0
52	L	100	0	156	0	0
52	M	100	0	156	4	0
52	O	85	0	117	0	0
52	X	100	0	156	2	0
52	d	65	0	77	0	0
52	h	80	0	104	0	0
52	r	61	0	66	0	0
53	M	1	0	0	0	0
53	R	1	0	0	0	0
54	O	31	0	12	4	0
55	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	P	48	0	26	3	0
57	T	37	0	0	1	0
57	U	37	0	0	0	0
58	i	29	0	38	0	0
59	o	15	0	27	0	0
All	All	68995	0	70114	287	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 3.

All (287) 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)
19:S:92:ASN:O	19:S:96:SER:OG	1.95	0.85
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.11	0.84
14:N:298:TYR:O	14:N:303:THR:OG1	1.94	0.84
4:D:165:THR:OG1	8:H:275:ALA:O	1.93	0.83
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.14	0.80
12:L:161:ARG:NH1	12:L:238:GLU:OE1	2.15	0.80
6:F:131:ALA:O	6:F:171:TYR:OH	1.99	0.79
1:A:71:LEU:O	10:J:147:TYR:OH	2.01	0.78
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.65	0.78
1:A:28:ASN:ND2	46:A:204:PC1:O32	2.17	0.78
7:G:366:THR:O	7:G:367:THR:OG1	2.00	0.77
7:G:140:LYS:O	7:G:148:THR:OG1	2.02	0.77
25:Z:89:ASN:ND2	25:Z:122:GLU:O	2.18	0.76
7:G:601:ARG:NH2	7:G:605:GLU:OE1	2.19	0.76
10:J:108:LEU:O	10:J:111:LYS:NZ	2.18	0.76
15:O:53:GLU:OE2	15:O:126:ARG:NH1	2.20	0.75
4:D:226:GLU:O	4:D:230:THR:OG1	2.06	0.74
13:M:43:ASN:O	13:M:50:LEU:HD11	1.87	0.74
3:C:49:GLU:OE2	3:C:106:ARG:NH2	2.21	0.72
4:D:149:ASN:OD1	4:D:371:LYS:NZ	2.22	0.72
3:C:198:ASP:OD2	7:G:224:LYS:NZ	2.20	0.72
16:P:164:THR:OG1	16:P:224:ARG:NH2	2.23	0.72
52:M:602:CDL:H272	52:X:201:CDL:H671	1.72	0.71
8:H:61:LEU:O	8:H:61:LEU:HD13	1.91	0.71
15:O:113:GLU:OE1	15:O:266:LYS:NZ	2.24	0.70
57:T:101:EHZ:O1	57:T:101:EHZ:O2	2.08	0.70
15:O:73:PHE:CE2	15:O:299:LEU:HD11	2.26	0.70
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:M:602:CDL:OA4	52:M:602:CDL:O1	2.08	0.69
24:Y:6:ARG:NH1	24:Y:10:ASP:OD1	2.26	0.68
20:T:61:GLU:N	20:T:61:GLU:OE1	2.26	0.68
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.27	0.68
8:H:67:SER:O	8:H:70:MET:N	2.26	0.68
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.26	0.67
2:B:81:ARG:CZ	8:H:61:LEU:HD11	2.24	0.67
2:B:27:GLU:N	2:B:27:GLU:OE1	2.28	0.67
7:G:415:LEU:O	7:G:416:THR:OG1	2.14	0.66
16:P:285:GLU:N	16:P:285:GLU:OE1	2.28	0.66
9:I:65:HIS:CE1	9:I:116:CYS:SG	2.89	0.66
15:O:138:MET:CE	54:O:401:DGT:HN2	2.09	0.65
1:A:24:LEU:O	1:A:27:LEU:HD22	1.96	0.65
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.77	0.65
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.09	0.65
7:G:693:GLU:OE1	7:G:693:GLU:N	2.30	0.64
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.29	0.64
15:O:22:SER:OG	15:O:119:GLY:O	2.12	0.64
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.80	0.63
12:L:245:ALA:O	12:L:249:SER:OG	2.16	0.63
23:X:102:GLN:N	23:X:102:GLN:OE1	2.31	0.63
15:O:272:TYR:O	15:O:275:ILE:HG23	1.98	0.63
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.14	0.62
5:E:105:THR:HG22	5:E:106:THR:H	1.64	0.62
15:O:88:SER:OG	15:O:90:ASP:OD1	2.12	0.62
2:B:44:SER:OG	8:H:51:ASP:OD1	2.05	0.62
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.34	0.62
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.32	0.62
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.35	0.61
23:X:154:GLU:N	23:X:154:GLU:OE1	2.34	0.61
6:F:141:GLU:OE1	6:F:141:GLU:N	2.34	0.60
13:M:141:GLU:N	13:M:141:GLU:OE1	2.34	0.60
15:O:291:GLN:NE2	15:O:295:GLU:OE2	2.34	0.60
15:O:281:GLU:N	15:O:281:GLU:OE1	2.35	0.59
2:B:70:ASP:OD2	8:H:34:ARG:NH2	2.35	0.59
10:J:170:GLU:OE1	10:J:173:ARG:NH2	2.36	0.58
20:T:55:GLU:OE2	22:W:36:ARG:NH2	2.35	0.58
13:M:47:ASP:OD1	13:M:48:ASN:N	2.36	0.58
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.84	0.58
2:B:34:ASP:OD1	2:B:38:ASN:ND2	2.36	0.58
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:97:ARG:HD2	25:Z:59:LEU:HD13	1.86	0.58
7:G:460:ARG:NH2	7:G:659:ASP:OD1	2.37	0.57
15:O:219:GLU:OE2	15:O:245:LYS:NZ	2.35	0.57
16:P:98:GLU:OE1	16:P:286:ARG:NH2	2.38	0.57
4:D:71:GLU:OE2	8:H:134:ARG:NH1	2.36	0.57
4:D:227:GLU:OE2	9:I:32:ARG:NH2	2.37	0.57
12:L:173:LEU:HD11	46:L:704:PC1:H381	1.87	0.57
14:N:40:ILE:HD12	14:N:43:ILE:HD11	1.87	0.56
7:G:259:ASN:HB2	7:G:390:LEU:HD13	1.88	0.56
24:Y:81:GLU:OE1	24:Y:81:GLU:N	2.39	0.56
7:G:460:ARG:NE	7:G:462:ASP:OD1	2.39	0.56
18:R:2:VAL:HG21	18:R:37:GLU:OE1	2.06	0.55
2:B:84:ASP:OD1	8:H:58:LYS:NZ	2.37	0.55
7:G:259:ASN:CB	7:G:390:LEU:HD13	2.37	0.55
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.88	0.55
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.89	0.55
9:I:65:HIS:CD2	48:I:201:SF4:S1	3.00	0.54
9:I:144:HIS:O	9:I:144:HIS:ND1	2.40	0.54
15:O:138:MET:HE3	54:O:401:DGT:HN2	1.72	0.54
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.88	0.54
12:L:445:GLU:O	12:L:451:ILE:HD11	2.07	0.54
5:E:68:LYS:NZ	5:E:71:GLU:OE2	2.23	0.54
15:O:104:ARG:NE	15:O:131:ASP:OD1	2.39	0.54
4:D:241:ASP:OD1	4:D:290:ARG:NH1	2.38	0.53
15:O:30:ASN:OD1	15:O:31:ILE:N	2.37	0.53
6:F:270:GLU:OE1	6:F:271:GLU:N	2.37	0.53
13:M:187:HIS:O	13:M:192:ASN:ND2	2.37	0.53
20:T:22:TYR:O	20:T:24:LYS:N	2.41	0.53
6:F:358:SER:OG	6:F:365:CYS:SG	2.54	0.53
3:C:49:GLU:OE1	3:C:108:LYS:NZ	2.41	0.53
7:G:475:GLN:NE2	7:G:643:GLN:OE1	2.42	0.53
1:A:27:LEU:HD23	1:A:28:ASN:N	2.24	0.53
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.90	0.52
2:B:81:ARG:NH2	8:H:61:LEU:HD21	2.24	0.52
7:G:375:ASP:OD1	7:G:375:ASP:N	2.41	0.52
16:P:264:ARG:NE	16:P:285:GLU:OE2	2.39	0.52
23:X:57:GLU:OE1	23:X:60:LYS:NZ	2.41	0.52
2:B:81:ARG:NH2	2:B:106:GLN:O	2.40	0.52
15:O:80:GLU:N	15:O:80:GLU:OE1	2.42	0.52
14:N:270:MET:CE	14:N:278:LEU:HD23	2.39	0.52
15:O:232:GLU:OE1	15:O:232:GLU:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:407:LEU:HD23	6:F:407:LEU:O	2.10	0.52
15:O:30:ASN:O	15:O:35:LYS:NZ	2.43	0.52
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.75	0.51
6:F:101:GLU:OE1	6:F:184:TYR:OH	2.15	0.51
8:H:32:GLN:OE1	8:H:34:ARG:NH1	2.42	0.51
16:P:101:THR:HG22	16:P:102:GLN:H	1.74	0.51
6:F:99:GLU:OE2	6:F:107:ASP:N	2.44	0.51
6:F:224:ASN:OD1	6:F:225:VAL:N	2.42	0.51
12:L:562:LEU:CB	12:L:563:PRO:HD3	2.41	0.51
21:V:17:GLU:OE1	21:V:17:GLU:N	2.39	0.51
3:C:151:ILE:HG23	3:C:152:LEU:HG	1.93	0.51
7:G:480:SER:O	7:G:481:SER:OG	2.21	0.50
12:L:197:ASP:OD1	12:L:197:ASP:N	2.45	0.50
1:A:115:GLU:OE1	1:A:115:GLU:N	2.39	0.50
13:M:133:ILE:HD11	13:M:231:LEU:HD11	1.94	0.50
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.11	0.50
16:P:253:PHE:C	16:P:254:LEU:HD22	2.32	0.50
7:G:535:GLN:N	7:G:535:GLN:OE1	2.44	0.50
5:E:104:THR:HG22	5:E:104:THR:O	2.10	0.50
8:H:102:VAL:CG1	8:H:150:LEU:HD21	2.40	0.50
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.93	0.49
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.94	0.49
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.20	0.49
12:L:264:TYR:N	12:L:265:PRO:CD	2.75	0.49
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.45	0.49
5:E:18:GLU:N	5:E:18:GLU:OE1	2.44	0.49
4:D:9:GLU:OE1	4:D:9:GLU:N	2.43	0.49
16:P:153:GLU:OE1	16:P:167:LYS:NZ	2.31	0.49
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.48	0.49
7:G:615:THR:OG1	7:G:617:ASP:OD1	2.23	0.49
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.95	0.49
52:M:602:CDL:H381	52:X:201:CDL:H673	1.93	0.49
2:B:179:ARG:O	16:P:101:THR:HG21	2.12	0.48
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.95	0.48
12:L:193:LEU:HD11	12:L:206:PRO:HG3	1.95	0.48
13:M:418:LYS:NZ	13:M:421:TYR:OH	2.32	0.48
8:H:99:ASN:N	46:H:402:PC1:O12	2.42	0.48
7:G:347:GLU:OE2	7:G:495:ARG:NE	2.41	0.48
8:H:74:ALA:HB3	8:H:75:PRO:HD3	1.96	0.48
10:J:37:GLY:HA2	11:K:38:LEU:HD21	1.96	0.48
16:P:145:TYR:OH	56:P:501:NDP:O2D	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:16:LEU:O	20:T:20:LYS:NZ	2.44	0.48
13:M:143:LEU:HD11	14:N:303:THR:HG21	1.94	0.48
23:X:120:ASP:N	23:X:123:ASP:OD2	2.46	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.94	0.48
15:O:223:TYR:CE2	15:O:234:VAL:HG22	2.49	0.48
15:O:186:LYS:NZ	54:O:401:DGT:O2B	2.47	0.48
16:P:315:ILE:HD13	16:P:315:ILE:O	2.14	0.48
12:L:193:LEU:HD11	12:L:206:PRO:CG	2.43	0.48
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.96	0.48
10:J:173:ARG:NH1	10:J:175:ASN:O	2.46	0.48
9:I:75:GLU:O	9:I:105:ARG:NH1	2.47	0.47
9:I:77:CYS:O	9:I:105:ARG:NH1	2.46	0.47
2:B:152:THR:HG22	4:D:188:ARG:HD3	1.97	0.47
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.48	0.47
12:L:371:THR:O	12:L:375:VAL:HG23	2.14	0.47
23:X:79:GLU:N	23:X:79:GLU:OE1	2.48	0.47
7:G:60:GLU:OE1	7:G:78:ASN:ND2	2.41	0.47
7:G:318:ILE:HD11	7:G:532:ILE:HD12	1.97	0.47
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.50	0.47
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.45	0.47
8:H:179:TRP:N	8:H:180:PRO:CD	2.78	0.47
14:N:146:PHE:N	14:N:147:PRO:CD	2.77	0.47
7:G:148:THR:HG22	7:G:208:LEU:CD2	2.45	0.47
21:V:29:LYS:HD2	21:V:87:LEU:HD21	1.97	0.47
8:H:66:SER:OG	8:H:124:ASN:OD1	2.08	0.47
12:L:288:THR:HG21	12:L:307:SER:HB3	1.97	0.47
7:G:285:ARG:NH1	7:G:557:ALA:O	2.45	0.46
15:O:20:GLU:O	15:O:23:LYS:NZ	2.28	0.46
16:P:166:ILE:HG22	16:P:168:PRO:HD3	1.97	0.46
20:U:20:LYS:HD3	20:U:30:LEU:HD23	1.97	0.46
6:F:165:ASN:OD1	6:F:170:GLY:N	2.44	0.46
12:L:171:ALA:O	12:L:175:ASN:ND2	2.37	0.46
15:O:36:SER:OG	54:O:401:DGT:O2G	2.27	0.46
12:L:140:LEU:O	12:L:140:LEU:HD23	2.15	0.46
7:G:514:ILE:HG21	7:G:532:ILE:HD13	1.96	0.46
11:K:40:LEU:HD13	14:N:71:MET:HB3	1.96	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.78	0.46
12:L:286:LEU:C	12:L:286:LEU:HD13	2.36	0.46
6:F:268:VAL:HG21	6:F:283:HIS:ND1	2.31	0.46
15:O:311:ASP:OD1	15:O:311:ASP:N	2.48	0.46
17:Q:88:THR:OG1	17:Q:91:ASP:OD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:ARG:NH1	7:G:138:GLU:OE2	2.49	0.46
15:O:223:TYR:HE2	15:O:234:VAL:HG13	1.79	0.46
12:L:562:LEU:HB2	12:L:563:PRO:HD3	1.97	0.46
7:G:272:ASP:OD1	7:G:681:SER:OG	2.24	0.45
4:D:111:MET:SD	4:D:111:MET:N	2.90	0.45
7:G:138:GLU:OE2	18:R:77:LYS:NZ	2.45	0.45
7:G:644:GLN:OE1	7:G:644:GLN:N	2.45	0.45
22:W:23:ASP:N	22:W:23:ASP:OD1	2.50	0.45
24:Y:109:ILE:HD11	45:Y:202:3PE:H2	1.99	0.45
1:A:27:LEU:HD21	46:A:204:PC1:C34	2.47	0.45
1:A:29:VAL:O	1:A:29:VAL:HG22	2.17	0.45
6:F:380:VAL:O	6:F:429:ARG:NH1	2.50	0.45
13:M:120:ILE:HD11	14:N:264:TRP:CH2	2.52	0.45
8:H:103:LEU:HD13	8:H:160:PHE:CD1	2.52	0.45
12:L:133:THR:HG22	12:L:133:THR:O	2.17	0.44
7:G:324:ASP:OD1	7:G:324:ASP:N	2.50	0.44
8:H:202:GLU:N	8:H:202:GLU:OE1	2.49	0.44
2:B:179:ARG:NH2	56:P:501:NDP:O2X	2.50	0.44
4:D:161:ILE:HD12	8:H:278:PRO:CB	2.47	0.44
7:G:255:HIS:CD2	7:G:258:ILE:HD12	2.52	0.44
9:I:86:VAL:HG22	9:I:86:VAL:O	2.17	0.44
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.00	0.44
4:D:161:ILE:HD12	8:H:278:PRO:HB2	1.97	0.44
6:F:306:LEU:C	6:F:306:LEU:HD12	2.38	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.80	0.44
16:P:170:GLU:OE1	16:P:170:GLU:N	2.51	0.44
25:Z:126:LEU:N	25:Z:126:LEU:HD23	2.32	0.44
16:P:192:PRO:HB3	16:P:258:LEU:HD22	2.00	0.44
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.00	0.44
3:C:83:ILE:HD12	3:C:83:ILE:N	2.33	0.44
22:W:116:ASP:OD1	22:W:116:ASP:N	2.50	0.44
25:Z:90:LEU:HD11	25:Z:105:VAL:HG12	1.99	0.44
16:P:192:PRO:O	16:P:263:TYR:OH	2.33	0.43
20:T:36:PHE:HD1	20:T:40:LEU:HD12	1.83	0.43
14:N:261:MET:HG3	14:N:340:THR:HG23	2.01	0.43
8:H:49:ILE:N	8:H:49:ILE:HD12	2.33	0.43
23:X:79:GLU:HB2	23:X:80:PRO:HD3	2.01	0.43
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.43
4:D:145:THR:OG1	4:D:181:TYR:OH	2.29	0.43
6:F:407:LEU:HD23	6:F:407:LEU:C	2.39	0.43
14:N:182:SER:OG	14:N:293:TYR:OH	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:160:ILE:CD1	7:G:174:THR:HG23	2.49	0.43
8:H:111:LEU:HD11	10:J:57:PHE:HD1	1.84	0.42
6:F:120:GLU:OE2	6:F:236:ARG:NH1	2.51	0.42
16:P:285:GLU:O	16:P:289:THR:OG1	2.22	0.42
7:G:148:THR:HG22	7:G:208:LEU:HD23	2.01	0.42
7:G:479:THR:HG22	7:G:479:THR:O	2.20	0.42
12:L:467:ILE:O	12:L:471:ASN:ND2	2.41	0.42
8:H:97:ASN:H	25:Z:143:THR:HG22	1.85	0.42
15:O:15:THR:OG1	15:O:253:ASP:OD1	2.26	0.42
15:O:71:VAL:HG22	15:O:76:ASN:HA	2.02	0.42
12:L:577:VAL:HG13	12:L:578:THR:HG23	2.00	0.42
16:P:133:SER:O	16:P:168:PRO:HD2	2.20	0.42
16:P:166:ILE:N	16:P:166:ILE:HD12	2.34	0.42
2:B:24:SER:OG	2:B:25:ARG:N	2.52	0.42
11:K:1:FME:O	11:K:2:SER:HB2	2.20	0.42
14:N:340:THR:N	14:N:341:PRO:HD2	2.35	0.42
3:C:40:VAL:HG13	3:C:50:ILE:HD13	2.00	0.41
10:J:33:LEU:HD23	10:J:65:MET:SD	2.60	0.41
11:K:82:SER:O	11:K:86:GLY:N	2.48	0.41
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.03	0.41
46:Z:203:PC1:O13	46:Z:203:PC1:H132	2.19	0.41
7:G:147:LYS:HD3	7:G:149:ILE:HD11	2.02	0.41
8:H:277:TYR:OH	9:I:30:LEU:O	2.26	0.41
24:Y:90:LEU:HD23	24:Y:90:LEU:O	2.20	0.41
6:F:114:ASP:N	6:F:115:PRO:HD3	2.36	0.41
8:H:310:LEU:HD12	8:H:310:LEU:O	2.20	0.41
14:N:41:ILE:N	14:N:42:PRO:HD2	2.35	0.41
2:B:30:VAL:HG22	2:B:173:LEU:HB3	2.01	0.41
6:F:96:ASN:ND2	6:F:187:GLY:O	2.48	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.01	0.41
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.02	0.41
3:C:138:PHE:O	3:C:163:ARG:NH1	2.47	0.41
52:M:602:CDL:C54	14:N:242:VAL:HG11	2.51	0.41
4:D:148:LEU:O	4:D:174:ARG:NH1	2.54	0.41
6:F:103:GLY:O	6:F:333:ALA:HB1	2.21	0.41
6:F:129:MET:CE	6:F:221:THR:HG21	2.51	0.41
7:G:147:LYS:CD	7:G:149:ILE:HD11	2.51	0.41
7:G:149:ILE:HD12	7:G:149:ILE:N	2.35	0.41
7:G:185:THR:O	7:G:187:ILE:N	2.51	0.41
10:J:56:VAL:O	10:J:60:TYR:HB3	2.21	0.41
56:P:501:NDP:O2N	56:P:501:NDP:N7N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:43:LYS:O	24:Y:54:ARG:NH1	2.47	0.41
7:G:321:GLY:HA2	7:G:496:ILE:HG23	2.02	0.41
7:G:326:GLU:OE1	7:G:326:GLU:N	2.47	0.41
10:J:23:LYS:NZ	11:K:21:MET:O	2.47	0.41
4:D:30:PRO:HA	4:D:31:PRO:HD3	1.98	0.40
10:J:115:VAL:O	10:J:117:PHE:N	2.48	0.40
8:H:20:LEU:HD23	8:H:228:TYR:HD2	1.85	0.40
7:G:323:VAL:HG12	7:G:324:ASP:N	2.36	0.40
7:G:365:ASN:ND2	7:G:490:MET:O	2.40	0.40
16:P:133:SER:OG	16:P:134:HIS:N	2.54	0.40
19:S:23:CYS:SG	19:S:25:ARG:NH2	2.93	0.40
20:T:21:LEU:HD12	20:T:21:LEU:C	2.42	0.40
18:R:55:ARG:NH2	18:R:76:ASP:OD2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	98/115 (85%)	94 (96%)	4 (4%)	0	100	100
2	B	154/216 (71%)	151 (98%)	3 (2%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100
4	D	411/463 (89%)	398 (97%)	13 (3%)	0	100	100
5	E	212/249 (85%)	200 (94%)	12 (6%)	0	100	100
6	F	430/464 (93%)	418 (97%)	12 (3%)	0	100	100
7	G	689/727 (95%)	668 (97%)	21 (3%)	0	100	100
8	H	311/318 (98%)	297 (96%)	14 (4%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	164/175 (94%)	158 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	15	45
12	L	604/606 (100%)	580 (96%)	23 (4%)	1 (0%)	47	78
13	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	330/380 (87%)	319 (97%)	11 (3%)	0	100	100
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	84 (98%)	1 (1%)	1 (1%)	13	40
20	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
21	V	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
22	W	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
23	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
24	Y	138/141 (98%)	138 (100%)	0	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	96/106 (91%)	96 (100%)	0	0	100	100
31	f	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
32	g	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	69 (100%)	0	0	100	100
36	k	79/98 (81%)	77 (98%)	2 (2%)	0	100	100
37	l	154/186 (83%)	147 (96%)	7 (4%)	0	100	100
38	m	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
39	n	169/179 (94%)	166 (98%)	3 (2%)	0	100	100
40	o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
43	r	91/113 (80%)	88 (97%)	3 (3%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8138/9213 (88%)	7920 (97%)	215 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	T	23	ASP
11	K	2	SER
12	L	562	LEU

5.3.2 Protein sidechains [i](#)

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	90/100 (90%)	88 (98%)	2 (2%)	52	81
2	B	132/175 (75%)	125 (95%)	7 (5%)	22	54
3	C	188/228 (82%)	186 (99%)	2 (1%)	73	92
4	D	361/392 (92%)	356 (99%)	5 (1%)	67	89
5	E	183/205 (89%)	179 (98%)	4 (2%)	52	81
6	F	346/368 (94%)	336 (97%)	10 (3%)	42	76
7	G	579/608 (95%)	566 (98%)	13 (2%)	52	81
8	H	271/274 (99%)	264 (97%)	7 (3%)	46	77
9	I	151/175 (86%)	148 (98%)	3 (2%)	55	82
10	J	134/141 (95%)	127 (95%)	7 (5%)	23	55
11	K	85/85 (100%)	82 (96%)	3 (4%)	36	70
12	L	533/533 (100%)	524 (98%)	9 (2%)	60	86
13	M	412/412 (100%)	411 (100%)	1 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	315/315 (100%)	311 (99%)	4 (1%)	69	90
15	O	283/303 (93%)	274 (97%)	9 (3%)	39	73
16	P	288/327 (88%)	279 (97%)	9 (3%)	40	74
17	Q	116/153 (76%)	112 (97%)	4 (3%)	37	71
18	R	79/97 (81%)	78 (99%)	1 (1%)	69	90
19	S	76/82 (93%)	72 (95%)	4 (5%)	22	54
20	T	81/135 (60%)	73 (90%)	8 (10%)	8	24
20	U	81/135 (60%)	77 (95%)	4 (5%)	25	57
21	V	101/102 (99%)	99 (98%)	2 (2%)	55	82
22	W	108/114 (95%)	104 (96%)	4 (4%)	34	68
23	X	154/155 (99%)	151 (98%)	3 (2%)	57	84
24	Y	101/102 (99%)	99 (98%)	2 (2%)	55	82
25	Z	120/121 (99%)	116 (97%)	4 (3%)	38	72
26	a	59/59 (100%)	56 (95%)	3 (5%)	24	56
27	b	71/72 (99%)	70 (99%)	1 (1%)	67	89
28	c	45/68 (66%)	43 (96%)	2 (4%)	28	61
29	d	105/105 (100%)	102 (97%)	3 (3%)	42	76
30	e	89/96 (93%)	89 (100%)	0	100	100
31	f	54/54 (100%)	51 (94%)	3 (6%)	21	52
32	g	92/131 (70%)	87 (95%)	5 (5%)	22	54
33	h	121/158 (77%)	119 (98%)	2 (2%)	60	86
34	i	120/121 (99%)	117 (98%)	3 (2%)	47	78
35	j	61/84 (73%)	58 (95%)	3 (5%)	25	57
36	k	63/76 (83%)	62 (98%)	1 (2%)	62	86
37	l	140/159 (88%)	138 (99%)	2 (1%)	67	89
38	m	113/114 (99%)	111 (98%)	2 (2%)	59	85
39	n	156/161 (97%)	153 (98%)	3 (2%)	57	84
40	o	110/120 (92%)	104 (94%)	6 (6%)	21	53
41	p	155/157 (99%)	152 (98%)	3 (2%)	57	84
42	q	130/130 (100%)	126 (97%)	4 (3%)	40	74
43	r	85/97 (88%)	84 (99%)	1 (1%)	71	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	s	43/92 (47%)	42 (98%)	1 (2%)	50	80
All	All	7180/7891 (91%)	7001 (98%)	179 (2%)	50	78

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	90	MET
2	B	30	VAL
2	B	50	PHE
2	B	54	CYS
2	B	59	MET
2	B	81	ARG
2	B	100	LEU
2	B	125	TYR
3	C	125	LYS
3	C	163	ARG
4	D	40	LYS
4	D	230	THR
4	D	290	ARG
4	D	404	LYS
4	D	410	MET
5	E	48	LEU
5	E	68	LYS
5	E	183	LYS
5	E	217	LEU
6	F	8	LYS
6	F	44	LYS
6	F	132	ARG
6	F	206	LYS
6	F	249	ARG
6	F	270	GLU
6	F	324	GLN
6	F	359	CYS
6	F	365	CYS
6	F	405	CYS
7	G	35	MET
7	G	39	ARG
7	G	75	LYS
7	G	129	ARG
7	G	236	SER
7	G	275	LYS

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Mol	Chain	Res	Type
7	G	306	MET
7	G	476	LYS
7	G	495	ARG
7	G	499	GLN
7	G	601	ARG
7	G	613	TYR
7	G	650	LYS
8	H	5	ASN
8	H	54	LYS
8	H	70	MET
8	H	73	LEU
8	H	121	TRP
8	H	237	PHE
8	H	254	LEU
9	I	14	MET
9	I	65	HIS
9	I	144	HIS
10	J	23	LYS
10	J	103	MET
10	J	109	LYS
10	J	111	LYS
10	J	135	PHE
10	J	136	PHE
10	J	139	GLU
11	K	34	GLU
11	K	53	PHE
11	K	73	LEU
12	L	197	ASP
12	L	223	LYS
12	L	336	LYS
12	L	358	LYS
12	L	364	LYS
12	L	481	THR
12	L	554	ASP
12	L	580	GLN
12	L	581	LYS
13	M	207	MET
14	N	46	LYS
14	N	71	MET
14	N	117	GLU
14	N	187	MET
15	O	1	LEU

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Mol	Chain	Res	Type
15	O	12	GLU
15	O	125	GLU
15	O	157	LYS
15	O	206	TYR
15	O	217	LYS
15	O	242	LYS
15	O	245	LYS
15	O	258	LYS
16	P	140	LYS
16	P	154	LYS
16	P	251	ARG
16	P	263	TYR
16	P	268	ARG
16	P	285	GLU
16	P	291	ASP
16	P	315	ILE
16	P	319	ARG
17	Q	16	LYS
17	Q	31	LYS
17	Q	70	MET
17	Q	91	ASP
18	R	96	HIS
19	S	25	ARG
19	S	38	LYS
19	S	44	LYS
19	S	61	GLN
20	T	12	LYS
20	T	16	LEU
20	T	44	SER
20	T	60	PHE
20	T	69	LYS
20	T	71	MET
20	T	72	CYS
20	T	83	LYS
20	U	20	LYS
20	U	71	MET
20	U	72	CYS
20	U	83	LYS
21	V	44	ARG
21	V	65	LYS
22	W	40	ARG
22	W	56	LYS

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Mol	Chain	Res	Type
22	W	60	ASP
22	W	68	LYS
23	X	5	GLU
23	X	13	LYS
23	X	47	TRP
24	Y	114	CYS
24	Y	119	LEU
25	Z	21	LYS
25	Z	98	LYS
25	Z	133	LEU
25	Z	143	THR
26	a	25	ARG
26	a	34	LYS
26	a	70	ASP
27	b	42	LEU
28	c	6	GLU
28	c	48	LEU
29	d	82	MET
29	d	100	ASP
29	d	104	LYS
31	f	3	LEU
31	f	40	LYS
31	f	45	LYS
32	g	25	ARG
32	g	26	TRP
32	g	57	ASN
32	g	100	ARG
32	g	117	LYS
33	h	130	LYS
33	h	138	LYS
34	i	43	GLU
34	i	95	THR
34	i	100	LYS
35	j	39	ARG
35	j	40	PHE
35	j	58	GLN
36	k	91	LYS
37	l	126	GLN
37	l	135	TYR
38	m	79	PHE
38	m	91	LEU
39	n	8	TYR

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Mol	Chain	Res	Type
39	n	54	LYS
39	n	97	LYS
40	o	7	ARG
40	o	28	TYR
40	o	70	ARG
40	o	83	ARG
40	o	110	ARG
40	o	112	LYS
41	p	69	ARG
41	p	95	TYR
41	p	98	ASP
42	q	53	LYS
42	q	59	HIS
42	q	107	LYS
42	q	136	GLU
43	r	101	LYS
44	s	44	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
13	M	338	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
42	AME	q	1	42	9,10,11	1.45	1 (11%)	9,11,13	1.62	2 (22%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	7,9,11	1.64	1 (14%)
29	AME	d	1	29	9,10,11	1.46	1 (11%)	9,11,13	1.66	2 (22%)
34	SAC	i	1	34	7,8,9	1.67	1 (14%)	8,9,11	1.49	1 (12%)
24	AYA	Y	1	24	6,7,8	1.81	1 (16%)	5,8,10	1.41	1 (20%)
4	2MR	D	85	4	10,12,13	2.36	2 (20%)	5,13,15	1.41	1 (20%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.25	1 (20%)
27	AYA	b	1	27	6,7,8	1.81	1 (16%)	5,8,10	1.33	1 (20%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	7,9,11	1.61	1 (14%)
13	FME	M	1	13	8,9,10	1.50	1 (12%)	7,9,11	1.60	1 (14%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	7,9,11	1.71	3 (42%)
38	SAC	m	1	38	7,8,9	1.66	1 (14%)	8,9,11	1.24	1 (12%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	7,9,11	1.72	3 (42%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	7,9,11	1.58	1 (14%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	7,9,11	1.63	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
42	AME	q	1	42	-	5/9/10/12	-
14	FME	N	1	14	-	3/7/9/11	-
29	AME	d	1	29	-	3/9/10/12	-
34	SAC	i	1	34	-	5/7/8/10	-
24	AYA	Y	1	24	-	0/4/6/8	-
4	2MR	D	85	4	-	0/10/13/15	-
43	AYA	r	1	43	-	0/4/6/8	-
27	AYA	b	1	27	-	1/4/6/8	-
11	FME	K	1	11	-	3/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
8	FME	H	1	8	-	3/7/9/11	-
38	SAC	m	1	38	-	2/7/8/10	-
1	FME	A	1	1	-	2/7/9/11	-
10	FME	J	1	10	-	3/7/9/11	-
12	FME	L	1	12	-	2/7/9/11	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.12	1.44	1.33
4	D	85	2MR	CZ-NE	5.07	1.45	1.34
12	L	1	FME	CN-N	3.69	1.45	1.33
11	K	1	FME	CN-N	3.67	1.45	1.33
14	N	1	FME	CN-N	3.67	1.45	1.33
10	J	1	FME	CN-N	3.66	1.45	1.33
13	M	1	FME	CN-N	3.65	1.45	1.33
1	A	1	FME	CN-N	3.63	1.45	1.33
8	H	1	FME	CN-N	3.62	1.45	1.33
38	m	1	SAC	C1A-N	3.36	1.45	1.34
34	i	1	SAC	C1A-N	3.36	1.45	1.34
27	b	1	AYA	CT-N	3.32	1.45	1.34
29	d	1	AME	CT1-N	3.28	1.45	1.34
24	Y	1	AYA	CT-N	3.24	1.45	1.34
42	q	1	AME	CT1-N	3.22	1.45	1.34
43	r	1	AYA	CT-N	3.20	1.45	1.34
43	r	1	AYA	OT-CT	-2.02	1.18	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	3.01	121.19	116.10
42	q	1	AME	CE-SD-CG	2.92	110.42	100.40
29	d	1	AME	CE-SD-CG	2.83	110.11	100.40
13	M	1	FME	CE-SD-CG	2.73	109.79	100.40
1	A	1	FME	CE-SD-CG	2.73	109.77	100.40
10	J	1	FME	CE-SD-CG	2.73	109.77	100.40
12	L	1	FME	CE-SD-CG	2.69	109.65	100.40
14	N	1	FME	CE-SD-CG	2.66	109.54	100.40
8	H	1	FME	CE-SD-CG	2.60	109.33	100.40
11	K	1	FME	CE-SD-CG	2.56	109.21	100.40
24	Y	1	AYA	CM-CT-N	2.40	120.17	116.10
29	d	1	AME	CT2-CT1-N	2.30	120.00	116.10
27	b	1	AYA	CM-CT-N	2.26	119.93	116.10
38	m	1	SAC	C2A-C1A-N	2.25	119.91	116.10
42	q	1	AME	CT2-CT1-N	2.20	119.83	116.10
43	r	1	AYA	CM-CT-N	2.17	119.78	116.10
4	D	85	2MR	CQ2-NH2-CZ	-2.12	119.18	123.86
1	A	1	FME	CA-N-CN	-2.10	119.59	122.82
1	A	1	FME	O1-CN-N	-2.08	119.78	125.27
8	H	1	FME	CA-N-CN	-2.07	119.64	122.82
8	H	1	FME	O1-CN-N	-2.05	119.88	125.27

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
12	L	1	FME	O-C-CA-CB
13	M	1	FME	O-C-CA-CB
14	N	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	C-CA-CB-CG
34	i	1	SAC	O-C-CA-CB
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
42	q	1	AME	N-CA-CB-CG
10	J	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
10	J	1	FME	CB-CG-SD-CE
42	q	1	AME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
11	K	1	FME	N-CA-CB-CG
42	q	1	AME	C-CA-N-CT1
11	K	1	FME	CB-CA-N-CN
29	d	1	AME	CB-CA-N-CT1
42	q	1	AME	CB-CA-N-CT1
29	d	1	AME	N-CA-CB-CG
42	q	1	AME	C-CA-CB-CG
11	K	1	FME	C-CA-CB-CG
13	M	1	FME	C-CA-CB-CG
27	b	1	AYA	C-CA-N-CT
29	d	1	AME	C-CA-N-CT1
38	m	1	SAC	C-CA-N-C1A
38	m	1	SAC	CB-CA-N-C1A
8	H	1	FME	CB-CA-N-CN
10	J	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
11	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 4 are monoatomic - leaving 67 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	Y	201	-	26,26,50	1.17	4 (15%)	29,31,55	1.15	2 (6%)
47	PLC	g	202	-	28,28,41	0.59	0	34,36,49	0.62	0
49	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	L	702	-	44,44,50	0.91	4 (9%)	47,49,55	1.08	2 (4%)
46	PC1	g	201	-	43,43,53	1.02	4 (9%)	49,51,61	1.05	2 (4%)
47	PLC	B	203	-	41,41,41	0.50	0	47,49,49	0.51	0
48	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	N	401	-	48,48,50	0.87	4 (8%)	51,53,55	0.99	2 (3%)
46	PC1	I	204	-	53,53,53	0.93	4 (7%)	59,61,61	0.99	2 (3%)
45	3PE	M	604	-	44,44,50	0.91	4 (9%)	47,49,55	1.02	2 (4%)
45	3PE	A	201	-	46,46,50	0.90	4 (8%)	49,51,55	1.01	2 (4%)
52	CDL	L	701	-	99,99,99	0.87	8 (8%)	105,111,111	1.06	4 (3%)
52	CDL	X	201	-	99,99,99	0.87	8 (8%)	105,111,111	1.06	4 (3%)
45	3PE	M	603	-	49,49,50	0.87	4 (8%)	52,54,55	1.04	2 (3%)
46	PC1	h	202	-	35,35,53	1.13	4 (11%)	41,43,61	1.09	2 (4%)
48	SF4	F	502	6	0,12,12	-	-	-	-	-
54	DGT	O	401	55	26,33,33	2.65	8 (30%)	32,52,52	1.70	10 (31%)
45	3PE	Y	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
46	PC1	H	402	-	47,47,53	1.00	4 (8%)	53,55,61	1.01	2 (3%)
45	3PE	A	202	-	43,43,50	0.93	4 (9%)	46,48,55	1.09	2 (4%)
45	3PE	f	102	-	31,31,50	1.08	4 (12%)	34,36,55	1.13	2 (5%)
45	3PE	m	202	-	40,40,50	0.96	4 (10%)	43,45,55	1.08	2 (4%)
46	PC1	d	203	-	38,38,53	1.10	4 (10%)	44,46,61	1.09	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	L	703	-	34,34,50	0.95	3 (8%)	37,39,55	1.12	1 (2%)
45	3PE	Y	205	-	46,46,50	0.90	4 (8%)	49,51,55	1.03	2 (4%)
45	3PE	Y	204	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)
46	PC1	m	203	-	53,53,53	0.94	4 (7%)	59,61,61	0.99	2 (3%)
52	CDL	O	403	-	84,84,99	0.94	8 (9%)	90,96,111	1.09	4 (4%)
45	3PE	J	201	-	35,35,50	1.02	4 (11%)	38,40,55	1.13	2 (5%)
45	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)
46	PC1	Z	203	-	43,43,53	1.03	4 (9%)	49,51,61	0.98	2 (4%)
46	PC1	q	201	-	33,33,53	1.16	4 (12%)	39,41,61	1.03	2 (5%)
52	CDL	h	201	-	79,79,99	0.98	8 (10%)	85,91,111	1.10	4 (4%)
45	3PE	Z	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.07	2 (4%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
46	PC1	A	204	-	45,45,53	1.02	4 (8%)	51,53,61	1.03	2 (3%)
45	3PE	H	401	-	38,38,50	0.98	4 (10%)	41,43,55	1.07	2 (4%)
45	3PE	m	201	-	40,40,50	0.96	4 (10%)	43,45,55	1.13	2 (4%)
47	PLC	L	705	-	30,30,41	0.59	0	36,38,49	0.58	0
57	EHZ	T	101	20	29,36,37	1.74	5 (17%)	35,44,47	1.54	4 (11%)
46	PC1	L	704	-	53,53,53	0.93	4 (7%)	59,61,61	0.97	2 (3%)
46	PC1	H	403	-	41,41,53	1.06	4 (9%)	47,49,61	1.08	2 (4%)
47	PLC	A	205	-	41,41,41	0.50	0	47,49,49	0.51	0
52	CDL	d	201	-	64,64,99	1.06	8 (12%)	70,76,111	1.12	4 (5%)
45	3PE	d	202	-	48,48,50	0.88	4 (8%)	51,53,55	1.04	2 (3%)
57	EHZ	U	101	20	29,36,37	1.68	5 (17%)	35,44,47	1.63	7 (20%)
59	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.91	0
47	PLC	Y	207	-	31,31,41	0.56	0	37,39,49	0.58	0
46	PC1	B	202	-	47,47,53	0.98	3 (6%)	53,55,61	1.04	2 (3%)
58	CHD	i	201	-	32,32,32	3.21	10 (31%)	51,51,51	2.33	16 (31%)
45	3PE	I	203	-	35,35,50	1.01	4 (11%)	38,40,55	1.18	2 (5%)
46	PC1	M	605	-	34,34,53	1.16	3 (8%)	40,42,61	1.03	2 (5%)
48	SF4	I	202	9	0,12,12	-	-	-	-	-
45	3PE	Y	206	-	36,36,50	1.00	4 (11%)	39,41,55	1.11	2 (5%)
47	PLC	Z	204	-	35,35,41	0.54	0	41,43,49	0.53	0
52	CDL	M	602	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)
45	3PE	f	101	-	29,29,50	1.09	4 (13%)	32,34,55	1.27	2 (6%)
52	CDL	r	201	-	60,60,99	1.10	7 (11%)	66,72,111	1.12	4 (6%)
50	FMN	F	501	-	33,33,33	2.78	10 (30%)	48,50,50	1.74	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	A	203	-	34,34,53	1.16	4 (11%)	40,42,61	1.05	2 (5%)
47	PLC	M	606	-	33,33,41	0.57	0	39,41,49	0.52	0
49	FES	G	803	7	0,4,4	-	-	-	-	-
45	3PE	J	202	-	43,43,50	0.92	4 (9%)	46,48,55	1.02	2 (4%)
48	SF4	B	201	2	0,12,12	-	-	-	-	-
48	SF4	I	201	9	0,12,12	-	-	-	-	-
56	NDP	P	501	-	45,52,52	4.27	23 (51%)	53,80,80	2.07	5 (9%)
45	3PE	Z	202	-	34,34,50	1.02	4 (11%)	37,39,55	1.14	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Y	201	-	-	12/30/30/54	-
47	PLC	g	202	-	-	14/31/31/45	-
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	L	702	-	-	16/48/48/54	-
46	PC1	g	201	-	-	23/47/47/57	-
47	PLC	B	203	-	-	16/45/45/45	-
48	SF4	G	801	7	-	-	0/6/5/5
45	3PE	N	401	-	-	25/52/52/54	-
46	PC1	I	204	-	-	17/57/57/57	-
45	3PE	M	604	-	-	28/48/48/54	-
45	3PE	A	201	-	-	28/50/50/54	-
52	CDL	L	701	-	-	41/110/110/110	-
52	CDL	X	201	-	-	48/110/110/110	-
45	3PE	M	603	-	-	21/53/53/54	-
46	PC1	h	202	-	-	22/39/39/57	-
54	DGT	O	401	55	-	4/18/34/34	0/3/3/3
48	SF4	F	502	6	-	-	0/6/5/5
45	3PE	Y	202	-	-	22/54/54/54	-
46	PC1	H	402	-	-	28/51/51/57	-
45	3PE	A	202	-	-	25/47/47/54	-
45	3PE	f	102	-	-	19/35/35/54	-
45	3PE	m	202	-	-	18/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	d	203	-	-	19/42/42/57	-
45	3PE	L	703	-	-	17/37/37/54	-
45	3PE	Y	205	-	-	24/50/50/54	-
45	3PE	Y	204	-	-	22/54/54/54	-
46	PC1	m	203	-	-	29/57/57/57	-
52	CDL	O	403	-	-	49/95/95/110	-
45	3PE	J	201	-	-	15/39/39/54	-
45	3PE	Y	203	-	-	26/54/54/54	-
46	PC1	Z	203	-	-	18/47/47/57	-
46	PC1	q	201	-	-	17/37/37/57	-
52	CDL	h	201	-	-	25/90/90/110	-
45	3PE	Z	201	-	-	19/44/44/54	-
48	SF4	G	802	7	-	-	0/6/5/5
46	PC1	A	204	-	-	19/49/49/57	-
45	3PE	H	401	-	-	19/42/42/54	-
45	3PE	m	201	-	-	14/44/44/54	-
47	PLC	L	705	-	-	10/34/34/45	-
57	EHZ	T	101	20	-	11/42/44/45	-
46	PC1	L	704	-	-	23/57/57/57	-
46	PC1	H	403	-	-	22/45/45/57	-
47	PLC	A	205	-	-	18/45/45/45	-
52	CDL	d	201	-	-	27/75/75/110	-
45	3PE	d	202	-	-	17/52/52/54	-
57	EHZ	U	101	20	-	7/42/44/45	-
59	MYR	o	201	40	-	3/11/12/13	-
47	PLC	Y	207	-	-	10/34/34/45	-
46	PC1	B	202	-	-	21/51/51/57	-
58	CHD	i	201	-	-	2/9/74/74	1/4/4/4
45	3PE	I	203	-	-	22/39/39/54	-
46	PC1	M	605	-	-	14/38/38/57	-
48	SF4	I	202	9	-	-	0/6/5/5
45	3PE	Y	206	-	-	11/40/40/54	-
47	PLC	Z	204	-	-	14/39/39/45	-
52	CDL	M	602	-	-	47/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	f	101	-	-	13/32/32/54	-
52	CDL	r	201	-	-	25/71/71/110	-
50	FMN	F	501	-	-	3/18/18/18	0/3/3/3
46	PC1	A	203	-	-	14/38/38/57	-
47	PLC	M	606	-	-	11/37/37/45	-
56	NDP	P	501	-	-	6/30/77/77	0/5/5/5
45	3PE	J	202	-	-	16/47/47/54	-
48	SF4	B	201	2	-	-	0/6/5/5
48	SF4	I	201	9	-	-	0/6/5/5
49	FES	G	803	7	-	-	0/1/1/1
45	3PE	Z	202	-	-	13/38/38/54	-

All (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O4B-C1B	14.99	1.62	1.41
56	P	501	NDP	C6N-C5N	12.10	1.54	1.33
58	i	201	CHD	C11-C12	8.59	1.67	1.53
54	O	401	DGT	O6-C6	8.37	1.40	1.23
56	P	501	NDP	C7N-N7N	8.29	1.55	1.33
56	P	501	NDP	O4D-C1D	8.15	1.61	1.42
50	F	501	FMN	C4A-N5	7.25	1.44	1.30
56	P	501	NDP	C2D-C1D	-7.20	1.30	1.53
58	i	201	CHD	C16-C15	7.15	1.73	1.54
50	F	501	FMN	C10-N1	6.57	1.46	1.33
56	P	501	NDP	O4D-C4D	-6.47	1.30	1.45
58	i	201	CHD	C20-C17	-6.15	1.43	1.54
57	T	101	EHZ	C12-N1	5.47	1.45	1.33
57	T	101	EHZ	C15-N2	5.44	1.45	1.33
56	P	501	NDP	P2B-O2B	5.35	1.69	1.59
57	U	101	EHZ	C15-N2	5.30	1.45	1.33
57	U	101	EHZ	C12-N1	5.29	1.45	1.33
58	i	201	CHD	C8-C9	5.26	1.64	1.53
58	i	201	CHD	O12-C12	-5.23	1.34	1.43
50	F	501	FMN	C5A-N5	5.17	1.49	1.39
58	i	201	CHD	C13-C17	5.14	1.64	1.55
56	P	501	NDP	O4B-C4B	-5.12	1.33	1.45
50	F	501	FMN	C9A-N10	5.06	1.50	1.41
50	F	501	FMN	C2-N1	4.80	1.48	1.36
54	O	401	DGT	C2-N2	4.72	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	O	401	DGT	C2-N1	4.68	1.49	1.37
56	P	501	NDP	C2N-C3N	4.61	1.47	1.34
58	i	201	CHD	C6-C5	4.56	1.61	1.53
54	O	401	DGT	C2-N3	4.26	1.43	1.33
50	F	501	FMN	C2-N3	4.25	1.48	1.39
58	i	201	CHD	C15-C14	4.15	1.63	1.54
56	P	501	NDP	O7N-C7N	-4.06	1.14	1.24
56	P	501	NDP	O2D-C2D	3.99	1.52	1.43
58	i	201	CHD	C6-C7	3.85	1.59	1.52
50	F	501	FMN	C10-N10	3.84	1.45	1.37
56	P	501	NDP	C6A-N6A	3.78	1.47	1.34
50	F	501	FMN	C4-N3	3.76	1.45	1.38
56	P	501	NDP	C5A-C4A	-3.58	1.31	1.40
56	P	501	NDP	C4N-C3N	3.26	1.56	1.49
50	F	501	FMN	O2-C2	-2.95	1.18	1.24
56	P	501	NDP	C2A-N3A	2.83	1.36	1.32
56	P	501	NDP	C4N-C5N	2.77	1.56	1.48
54	O	401	DGT	C5-C6	-2.75	1.41	1.47
46	A	204	PC1	O21-C2	-2.69	1.39	1.46
58	i	201	CHD	C13-C12	-2.67	1.50	1.54
54	O	401	DGT	C1'-N9	-2.67	1.41	1.49
52	r	201	CDL	OA6-CA4	-2.65	1.40	1.46
50	F	501	FMN	O4-C4	-2.65	1.18	1.23
52	r	201	CDL	OB6-CB4	-2.65	1.40	1.46
46	d	203	PC1	O21-C2	-2.64	1.40	1.46
52	M	602	CDL	OB6-CB4	-2.62	1.40	1.46
52	O	403	CDL	OB6-CB4	-2.61	1.40	1.46
46	H	402	PC1	O21-C2	-2.59	1.40	1.46
52	h	201	CDL	OB6-CB4	-2.58	1.40	1.46
46	I	204	PC1	O21-C2	-2.57	1.40	1.46
46	L	704	PC1	O21-C2	-2.56	1.40	1.46
52	L	701	CDL	OA6-CA4	-2.56	1.40	1.46
46	h	202	PC1	O21-C2	-2.55	1.40	1.46
52	X	201	CDL	OB6-CB4	-2.53	1.40	1.46
52	h	201	CDL	OA6-CA4	-2.53	1.40	1.46
45	m	201	3PE	O21-C2	-2.53	1.40	1.46
52	M	602	CDL	OA6-CA4	-2.53	1.40	1.46
46	M	605	PC1	O21-C2	-2.52	1.40	1.46
52	L	701	CDL	OB6-CB4	-2.52	1.40	1.46
45	Y	201	3PE	O21-C2	-2.52	1.40	1.46
45	Z	201	3PE	O21-C2	-2.52	1.40	1.46
56	P	501	NDP	O3D-C3D	-2.52	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O3B-C3B	-2.52	1.37	1.43
52	d	201	CDL	OA6-CA4	-2.52	1.40	1.46
46	g	201	PC1	O21-C2	-2.51	1.40	1.46
46	M	605	PC1	O31-C31	2.51	1.40	1.33
45	A	201	3PE	O21-C2	-2.51	1.40	1.46
45	J	201	3PE	O21-C2	-2.51	1.40	1.46
45	Y	206	3PE	O21-C2	-2.50	1.40	1.46
45	d	202	3PE	O21-C2	-2.50	1.40	1.46
45	Y	203	3PE	O21-C2	-2.50	1.40	1.46
46	q	201	PC1	O21-C2	-2.49	1.40	1.46
46	Z	203	PC1	O21-C2	-2.49	1.40	1.46
45	f	101	3PE	O21-C2	-2.49	1.40	1.46
46	A	203	PC1	O21-C2	-2.48	1.40	1.46
46	H	403	PC1	O21-C2	-2.48	1.40	1.46
45	f	102	3PE	O21-C2	-2.48	1.40	1.46
45	m	202	3PE	O21-C2	-2.48	1.40	1.46
45	I	203	3PE	O21-C2	-2.48	1.40	1.46
52	d	201	CDL	OB8-CB7	2.48	1.40	1.33
45	J	202	3PE	O21-C2	-2.48	1.40	1.46
52	X	201	CDL	OA8-CA7	2.47	1.40	1.33
45	L	702	3PE	O21-C2	-2.47	1.40	1.46
57	T	101	EHZ	C9-S1	2.47	1.82	1.76
45	M	604	3PE	O21-C2	-2.47	1.40	1.46
45	N	401	3PE	O21-C2	-2.47	1.40	1.46
45	m	202	3PE	O31-C31	2.46	1.40	1.33
52	r	201	CDL	OB8-CB7	2.46	1.40	1.33
46	m	203	PC1	O21-C2	-2.46	1.40	1.46
52	d	201	CDL	OB6-CB4	-2.46	1.40	1.46
52	M	602	CDL	OA8-CA7	2.45	1.40	1.33
46	A	204	PC1	O31-C31	2.44	1.40	1.33
45	Z	202	3PE	O21-C2	-2.43	1.40	1.46
45	H	401	3PE	O21-C2	-2.43	1.40	1.46
52	h	201	CDL	OA8-CA7	2.43	1.40	1.33
46	B	202	PC1	O21-C2	-2.43	1.40	1.46
46	m	203	PC1	O31-C31	2.42	1.40	1.33
45	J	201	3PE	O31-C31	2.42	1.40	1.33
52	L	701	CDL	OB8-CB7	2.42	1.40	1.33
46	B	202	PC1	O31-C31	2.41	1.40	1.33
45	M	603	3PE	O21-C2	-2.41	1.40	1.46
46	h	202	PC1	O31-C31	2.40	1.40	1.33
46	L	704	PC1	O31-C31	2.40	1.40	1.33
45	d	202	3PE	O31-C31	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	203	PC1	O31-C31	2.40	1.40	1.33
45	A	202	3PE	O21-C2	-2.39	1.40	1.46
45	Z	201	3PE	O31-C31	2.39	1.40	1.33
46	Z	203	PC1	O31-C31	2.39	1.40	1.33
52	h	201	CDL	OB8-CB7	2.38	1.40	1.33
45	L	702	3PE	O31-C31	2.38	1.40	1.33
52	O	403	CDL	OA6-CA4	-2.38	1.40	1.46
45	Y	205	3PE	O21-C2	-2.38	1.40	1.46
45	M	603	3PE	O31-C31	2.38	1.40	1.33
45	Y	201	3PE	O31-C31	2.38	1.40	1.33
46	q	201	PC1	O31-C31	2.38	1.40	1.33
56	P	501	NDP	C6N-N1N	2.37	1.43	1.37
46	g	201	PC1	O31-C31	2.37	1.40	1.33
46	d	203	PC1	O31-C31	2.37	1.40	1.33
45	L	703	3PE	O21-C2	-2.37	1.40	1.46
45	Y	202	3PE	O21-C2	-2.37	1.40	1.46
52	O	403	CDL	OA8-CA7	2.37	1.40	1.33
52	r	201	CDL	OA8-CA7	2.37	1.40	1.33
45	Y	205	3PE	O31-C31	2.37	1.40	1.33
57	U	101	EHZ	O3-C12	-2.36	1.18	1.23
45	Y	204	3PE	O21-C2	-2.36	1.40	1.46
45	A	201	3PE	O31-C31	2.36	1.40	1.33
46	I	204	PC1	O31-C31	2.36	1.40	1.33
45	m	201	3PE	O31-C31	2.36	1.40	1.33
52	O	403	CDL	OB8-CB7	2.36	1.40	1.33
45	H	401	3PE	O31-C31	2.36	1.40	1.33
57	U	101	EHZ	C9-S1	2.36	1.81	1.76
52	M	602	CDL	OB8-CB7	2.35	1.40	1.33
45	A	202	3PE	O31-C31	2.35	1.40	1.33
45	Y	206	3PE	O31-C31	2.35	1.40	1.33
45	Y	203	3PE	O31-C31	2.34	1.40	1.33
46	H	403	PC1	O31-C31	2.34	1.40	1.33
45	Y	202	3PE	O31-C31	2.34	1.40	1.33
56	P	501	NDP	C7N-C3N	2.34	1.53	1.48
46	H	402	PC1	O31-C31	2.33	1.40	1.33
52	X	201	CDL	OA6-CA4	-2.33	1.40	1.46
45	f	101	3PE	O31-C31	2.33	1.40	1.33
45	Z	202	3PE	O31-C31	2.33	1.40	1.33
52	d	201	CDL	OA8-CA7	2.33	1.40	1.33
45	Y	204	3PE	O31-C31	2.33	1.40	1.33
57	T	101	EHZ	O3-C12	-2.32	1.18	1.23
45	f	102	3PE	O31-C31	2.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	T	101	EHZ	O4-C15	-2.32	1.18	1.23
45	I	203	3PE	O31-C31	2.31	1.40	1.33
45	N	401	3PE	O31-C31	2.31	1.40	1.33
52	L	701	CDL	OA8-CA7	2.31	1.40	1.33
52	X	201	CDL	OB8-CB6	-2.31	1.39	1.45
56	P	501	NDP	PA-O5B	2.29	1.68	1.59
45	f	101	3PE	O21-C21	2.27	1.40	1.35
45	M	604	3PE	O31-C31	2.27	1.40	1.33
46	H	402	PC1	O31-C3	-2.27	1.40	1.45
45	J	202	3PE	O31-C31	2.26	1.39	1.33
52	X	201	CDL	OB8-CB7	2.25	1.39	1.33
52	d	201	CDL	OA8-CA6	-2.23	1.40	1.45
45	A	201	3PE	O31-C3	-2.23	1.40	1.45
57	U	101	EHZ	O4-C15	-2.23	1.19	1.23
52	M	602	CDL	OB8-CB6	-2.23	1.40	1.45
45	Y	205	3PE	O21-C21	2.22	1.40	1.34
45	M	604	3PE	O31-C3	-2.22	1.40	1.45
45	A	202	3PE	O21-C21	2.21	1.40	1.34
52	O	403	CDL	OB8-CB6	-2.21	1.40	1.45
52	h	201	CDL	OB8-CB6	-2.21	1.40	1.45
52	L	701	CDL	OA8-CA6	-2.21	1.40	1.45
45	d	202	3PE	O31-C3	-2.21	1.40	1.45
45	J	202	3PE	O31-C3	-2.21	1.40	1.45
45	Y	204	3PE	O21-C21	2.20	1.40	1.34
52	O	403	CDL	OA6-CA5	2.20	1.40	1.34
45	M	603	3PE	O21-C21	2.20	1.40	1.34
45	f	102	3PE	O21-C21	2.19	1.40	1.34
56	P	501	NDP	P2B-O1X	2.19	1.57	1.50
52	d	201	CDL	OB6-CB5	2.19	1.40	1.34
45	Y	206	3PE	O31-C3	-2.19	1.40	1.45
45	Y	202	3PE	O31-C3	-2.19	1.40	1.45
45	Y	203	3PE	O31-C3	-2.19	1.40	1.45
45	Y	204	3PE	O31-C3	-2.19	1.40	1.45
46	q	201	PC1	O21-C21	2.18	1.40	1.34
52	d	201	CDL	OA6-CA5	2.18	1.40	1.34
46	Z	203	PC1	O21-C21	2.18	1.40	1.34
45	N	401	3PE	O31-C3	-2.18	1.40	1.45
45	f	102	3PE	O31-C3	-2.18	1.40	1.45
45	d	202	3PE	O21-C21	2.18	1.40	1.34
46	h	202	PC1	O31-C3	-2.18	1.40	1.45
46	H	403	PC1	O21-C21	2.18	1.40	1.34
45	m	201	3PE	O31-C3	-2.18	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	J	202	3PE	O21-C21	2.18	1.40	1.34
52	h	201	CDL	OA6-CA5	2.18	1.40	1.34
46	B	202	PC1	O21-C21	2.18	1.40	1.34
54	O	401	DGT	PG-O1G	-2.18	1.46	1.54
46	d	203	PC1	O31-C3	-2.17	1.40	1.45
46	q	201	PC1	O31-C3	-2.17	1.40	1.45
46	A	203	PC1	O21-C21	2.17	1.40	1.34
45	Y	205	3PE	O31-C3	-2.17	1.40	1.45
45	I	203	3PE	O31-C3	-2.17	1.40	1.45
45	M	604	3PE	O21-C21	2.17	1.40	1.34
46	m	203	PC1	O21-C21	2.16	1.40	1.34
52	X	201	CDL	OA6-CA5	2.16	1.40	1.34
54	O	401	DGT	PG-O2G	-2.16	1.46	1.54
45	Y	203	3PE	O21-C21	2.16	1.40	1.34
45	H	401	3PE	O21-C21	2.16	1.40	1.34
45	A	201	3PE	O21-C21	2.16	1.40	1.34
52	O	403	CDL	OA8-CA6	-2.16	1.40	1.45
45	Y	201	3PE	O31-C3	-2.16	1.40	1.45
46	g	201	PC1	O31-C3	-2.15	1.40	1.45
45	H	401	3PE	O31-C3	-2.15	1.40	1.45
52	r	201	CDL	OA8-CA6	-2.15	1.40	1.45
45	Z	201	3PE	O31-C3	-2.15	1.40	1.45
45	I	203	3PE	O21-C21	2.15	1.40	1.34
46	I	204	PC1	O21-C21	2.15	1.40	1.34
46	Z	203	PC1	O31-C3	-2.15	1.40	1.45
46	H	403	PC1	O31-C3	-2.14	1.40	1.45
52	L	701	CDL	OB8-CB6	-2.14	1.40	1.45
52	X	201	CDL	OB6-CB5	2.14	1.40	1.34
45	J	201	3PE	O21-C21	2.14	1.40	1.34
45	Z	201	3PE	O21-C21	2.14	1.40	1.34
45	L	703	3PE	O21-C21	2.14	1.40	1.34
45	Z	202	3PE	O21-C21	2.14	1.40	1.34
52	L	701	CDL	OB6-CB5	2.13	1.40	1.34
46	M	605	PC1	O21-C21	2.13	1.40	1.34
45	Y	202	3PE	O21-C21	2.13	1.40	1.34
46	I	204	PC1	O31-C3	-2.12	1.40	1.45
45	Y	206	3PE	O21-C21	2.11	1.40	1.34
45	L	703	3PE	O31-C3	-2.11	1.40	1.45
45	L	702	3PE	O21-C21	2.11	1.40	1.34
45	m	202	3PE	O21-C21	2.11	1.40	1.34
45	M	603	3PE	O31-C3	-2.11	1.40	1.45
45	Y	201	3PE	O21-C21	2.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	f	101	3PE	O31-C3	-2.10	1.40	1.45
52	X	201	CDL	OA8-CA6	-2.10	1.40	1.45
46	h	202	PC1	O21-C21	2.10	1.40	1.34
46	A	203	PC1	O31-C3	-2.10	1.40	1.45
52	h	201	CDL	OA8-CA6	-2.10	1.40	1.45
52	M	602	CDL	OA8-CA6	-2.10	1.40	1.45
56	P	501	NDP	C5B-C4B	2.10	1.58	1.51
52	h	201	CDL	OB6-CB5	2.10	1.40	1.34
45	m	201	3PE	O21-C21	2.09	1.40	1.34
52	M	602	CDL	OA6-CA5	2.09	1.40	1.34
45	L	702	3PE	O31-C3	-2.09	1.40	1.45
45	N	401	3PE	O21-C21	2.09	1.40	1.34
45	A	202	3PE	O31-C3	-2.09	1.40	1.45
46	L	704	PC1	O31-C3	-2.09	1.40	1.45
45	J	201	3PE	O31-C3	-2.09	1.40	1.45
46	A	204	PC1	O31-C3	-2.08	1.40	1.45
46	m	203	PC1	O31-C3	-2.08	1.40	1.45
52	r	201	CDL	OB8-CB6	-2.07	1.40	1.45
46	H	402	PC1	O21-C21	2.07	1.40	1.34
52	d	201	CDL	OB8-CB6	-2.07	1.40	1.45
52	O	403	CDL	OB6-CB5	2.06	1.40	1.34
45	m	202	3PE	O31-C3	-2.06	1.40	1.45
46	g	201	PC1	O21-C21	2.06	1.40	1.34
46	L	704	PC1	O21-C21	2.06	1.40	1.34
45	Z	202	3PE	O31-C3	-2.06	1.40	1.45
52	M	602	CDL	OB6-CB5	2.05	1.40	1.34
46	A	204	PC1	O21-C21	2.04	1.40	1.34
52	L	701	CDL	OA6-CA5	2.03	1.40	1.34
46	d	203	PC1	O21-C21	2.02	1.40	1.34
52	r	201	CDL	OA6-CA5	2.01	1.40	1.34

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	C5A-C6A-N6A	8.74	133.63	120.35
58	i	201	CHD	C13-C17-C20	-7.10	111.02	119.50
56	P	501	NDP	C1B-N9A-C4A	-7.10	114.17	126.64
56	P	501	NDP	N6A-C6A-N1A	-6.20	105.71	118.57
57	T	101	EHZ	C8-C9-S1	5.87	120.89	113.63
58	i	201	CHD	C17-C13-C14	5.49	105.63	100.09
56	P	501	NDP	N3A-C2A-N1A	-5.38	120.27	128.68
58	i	201	CHD	C14-C13-C12	5.37	112.40	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	U	101	EHZ	C8-C9-S1	5.34	120.24	113.63
45	f	101	3PE	O21-C21-C22	4.85	120.02	111.09
50	F	501	FMN	C9-C8-C7	4.69	126.39	119.67
58	i	201	CHD	C17-C13-C12	4.62	121.89	117.67
50	F	501	FMN	C7M-C7-C6	4.52	127.85	119.49
45	L	703	3PE	O21-C21-C22	4.32	120.82	111.50
45	A	202	3PE	O21-C21-C22	4.30	120.76	111.50
45	m	201	3PE	O21-C21-C22	4.30	120.76	111.50
58	i	201	CHD	C18-C13-C12	-4.28	104.71	109.07
52	M	602	CDL	OB6-CB5-C51	4.23	120.63	111.50
52	X	201	CDL	OB6-CB5-C51	4.22	120.61	111.50
46	B	202	PC1	O21-C21-C22	4.21	120.57	111.50
52	r	201	CDL	OB6-CB5-C51	4.11	120.37	111.50
46	d	203	PC1	O21-C21-C22	4.11	120.36	111.50
45	I	203	3PE	O21-C21-C22	4.10	120.35	111.50
45	Z	202	3PE	O21-C21-C22	4.10	120.33	111.50
45	L	702	3PE	O21-C21-C22	4.08	120.29	111.50
46	g	201	PC1	O21-C21-C22	4.05	120.24	111.50
45	Y	202	3PE	O21-C21-C22	4.05	120.23	111.50
45	m	202	3PE	O21-C21-C22	4.05	120.23	111.50
52	M	602	CDL	OA6-CA5-C11	4.04	120.21	111.50
45	f	102	3PE	O21-C21-C22	4.04	120.21	111.50
46	H	403	PC1	O21-C21-C22	4.03	120.18	111.50
52	L	701	CDL	OA6-CA5-C11	4.01	120.14	111.50
52	O	403	CDL	OB6-CB5-C51	3.99	120.10	111.50
46	h	202	PC1	O21-C21-C22	3.97	120.06	111.50
45	H	401	3PE	O21-C21-C22	3.95	120.01	111.50
46	M	605	PC1	O21-C21-C22	3.95	120.00	111.50
46	A	203	PC1	O21-C21-C22	3.94	119.99	111.50
45	Y	206	3PE	O21-C21-C22	3.93	119.98	111.50
52	h	201	CDL	OB6-CB5-C51	3.93	119.98	111.50
45	M	603	3PE	O21-C21-C22	3.92	119.96	111.50
52	d	201	CDL	OA6-CA5-C11	3.91	119.94	111.50
45	Y	201	3PE	O21-C21-C22	3.91	119.92	111.50
45	Y	203	3PE	O21-C21-C22	3.90	119.91	111.50
46	A	204	PC1	O21-C21-C22	3.90	119.90	111.50
46	H	402	PC1	O21-C21-C22	3.88	119.87	111.50
52	L	701	CDL	OB6-CB5-C51	3.87	119.84	111.50
45	Y	204	3PE	O21-C21-C22	3.85	119.81	111.50
45	Y	205	3PE	O21-C21-C22	3.82	119.74	111.50
45	Z	201	3PE	O21-C21-C22	3.82	119.74	111.50
52	X	201	CDL	OA6-CA5-C11	3.81	119.71	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	I	204	PC1	O21-C21-C22	3.79	119.68	111.50
45	J	201	3PE	O21-C21-C22	3.77	119.62	111.50
52	r	201	CDL	OA6-CA5-C11	3.77	119.62	111.50
45	d	202	3PE	O21-C21-C22	3.76	119.61	111.50
46	L	704	PC1	O21-C21-C22	3.76	119.60	111.50
52	O	403	CDL	OA6-CA5-C11	3.75	119.58	111.50
46	Z	203	PC1	O21-C21-C22	3.74	119.57	111.50
46	m	203	PC1	O21-C21-C22	3.74	119.56	111.50
58	i	201	CHD	C18-C13-C17	-3.73	105.37	111.21
52	h	201	CDL	OA6-CA5-C11	3.72	119.52	111.50
45	M	604	3PE	O21-C21-C22	3.64	119.35	111.50
58	i	201	CHD	C18-C13-C14	-3.62	105.55	111.21
45	J	202	3PE	O21-C21-C22	3.59	119.23	111.50
45	N	401	3PE	O21-C21-C22	3.57	119.19	111.50
45	A	201	3PE	O21-C21-C22	3.56	119.17	111.50
58	i	201	CHD	C1-C10-C5	3.55	113.02	107.77
52	d	201	CDL	OB6-CB5-C51	3.55	120.69	110.80
46	q	201	PC1	O21-C21-C22	3.43	120.37	110.80
45	I	203	3PE	O31-C31-C32	3.34	120.15	111.38
50	F	501	FMN	C4-N3-C2	-3.32	119.51	125.64
45	J	201	3PE	O31-C31-C32	3.28	119.99	111.38
50	F	501	FMN	C8M-C8-C7	-3.28	114.01	120.74
54	O	401	DGT	C5-C6-N1	3.12	119.46	113.95
54	O	401	DGT	C2-N1-C6	-3.10	119.39	125.10
52	d	201	CDL	OB8-CB7-C71	2.93	121.12	111.91
54	O	401	DGT	PB-O3B-PG	-2.92	122.81	132.83
54	O	401	DGT	O2G-PG-O3B	2.89	114.34	104.64
52	h	201	CDL	OA8-CA7-C31	2.86	120.88	111.91
58	i	201	CHD	C23-C22-C20	-2.85	109.31	114.52
57	U	101	EHZ	C13-C12-N1	2.81	121.16	116.42
54	O	401	DGT	C2'-C3'-C4'	2.81	108.62	102.76
52	X	201	CDL	OA8-CA7-C31	2.80	120.70	111.91
45	Y	202	3PE	O31-C31-C32	2.80	120.68	111.91
45	Y	203	3PE	O31-C31-C32	2.79	120.65	111.91
45	Y	205	3PE	O31-C31-C32	2.76	120.58	111.91
52	M	602	CDL	OA8-CA7-C31	2.76	120.58	111.91
58	i	201	CHD	C6-C5-C4	-2.74	108.03	111.19
58	i	201	CHD	C15-C14-C8	2.74	122.17	118.33
45	M	604	3PE	O31-C31-C32	2.74	120.51	111.91
46	H	403	PC1	O31-C31-C32	2.74	120.49	111.91
57	U	101	EHZ	C14-C13-C12	-2.73	107.81	112.36
54	O	401	DGT	O1G-PG-O3B	2.71	113.72	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	h	201	CDL	OB8-CB7-C71	2.71	120.41	111.91
46	g	201	PC1	O31-C31-C32	2.70	120.38	111.91
46	d	203	PC1	O31-C31-C32	2.69	120.36	111.91
45	Y	204	3PE	O31-C31-C32	2.69	120.34	111.91
50	F	501	FMN	C6-C7-C8	-2.69	115.82	119.67
46	H	402	PC1	O31-C31-C32	2.67	120.28	111.91
56	P	501	NDP	PN-O3-PA	-2.67	123.68	132.83
54	O	401	DGT	PA-O3A-PB	-2.66	123.70	132.83
45	A	201	3PE	O31-C31-C32	2.66	120.25	111.91
50	F	501	FMN	C4A-C10-N10	2.65	120.35	116.48
45	m	201	3PE	O31-C31-C32	2.64	120.19	111.91
46	B	202	PC1	O31-C31-C32	2.62	120.12	111.91
52	O	403	CDL	OB8-CB7-C71	2.61	120.11	111.91
46	L	704	PC1	O31-C31-C32	2.61	120.08	111.91
46	h	202	PC1	O31-C31-C32	2.60	120.07	111.91
45	Z	202	3PE	O31-C31-C32	2.60	120.06	111.91
45	J	202	3PE	O31-C31-C32	2.60	120.06	111.91
52	M	602	CDL	OB8-CB7-C71	2.60	120.06	111.91
45	f	102	3PE	O31-C31-C32	2.59	120.05	111.91
46	q	201	PC1	O31-C31-C32	2.59	120.03	111.91
45	L	702	3PE	O31-C31-C32	2.59	120.03	111.91
50	F	501	FMN	C4A-C4-N3	2.58	119.75	113.19
52	O	403	CDL	OA8-CA7-C31	2.56	119.94	111.91
46	A	203	PC1	O31-C31-C32	2.55	119.92	111.91
52	L	701	CDL	OA8-CA7-C31	2.52	119.83	111.91
46	m	203	PC1	O31-C31-C32	2.52	119.82	111.91
52	L	701	CDL	OB8-CB7-C71	2.52	119.81	111.91
50	F	501	FMN	O4-C4-C4A	-2.51	119.93	126.60
45	Y	206	3PE	O31-C31-C32	2.51	119.78	111.91
52	r	201	CDL	OA8-CA7-C31	2.51	119.77	111.91
46	A	204	PC1	O31-C31-C32	2.48	119.70	111.91
45	Z	201	3PE	O31-C31-C32	2.48	119.70	111.91
45	A	202	3PE	O31-C31-C32	2.47	119.66	111.91
52	d	201	CDL	OA8-CA7-C31	2.47	119.65	111.91
45	m	202	3PE	O31-C31-C32	2.46	119.64	111.91
58	i	201	CHD	C19-C10-C9	-2.46	107.79	111.18
45	M	603	3PE	O31-C31-C32	2.46	119.63	111.91
46	I	204	PC1	O31-C31-C32	2.45	119.61	111.91
58	i	201	CHD	C9-C11-C12	-2.45	111.06	114.30
45	f	101	3PE	O31-C31-C32	2.45	119.59	111.91
45	H	401	3PE	O31-C31-C32	2.44	119.56	111.91
45	Y	201	3PE	O31-C31-C32	2.43	119.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	N	401	3PE	O31-C31-C32	2.43	119.53	111.91
57	U	101	EHZ	C5-C6-C7	-2.42	107.89	114.85
57	T	101	EHZ	C13-C12-N1	2.38	120.44	116.42
46	M	605	PC1	O31-C31-C32	2.38	119.39	111.91
45	d	202	3PE	O31-C31-C32	2.37	119.33	111.91
46	Z	203	PC1	O31-C31-C32	2.35	119.30	111.91
50	F	501	FMN	C5A-C9A-N10	2.33	120.36	117.95
57	U	101	EHZ	C13-C14-N2	-2.32	107.21	111.90
52	X	201	CDL	OB8-CB7-C71	2.32	119.19	111.91
50	F	501	FMN	C9A-C5A-N5	-2.31	119.93	122.43
52	r	201	CDL	OB8-CB7-C71	2.31	119.14	111.91
57	T	101	EHZ	O2-C9-S1	-2.30	119.62	122.61
50	F	501	FMN	C6-C5A-C9A	2.28	122.17	118.94
57	T	101	EHZ	C10-S1-C9	2.23	108.82	101.87
54	O	401	DGT	O1B-PB-O2B	-2.19	101.39	112.24
50	F	501	FMN	C4A-C10-N1	-2.18	119.66	124.73
57	U	101	EHZ	O2-C9-S1	-2.18	119.78	122.61
58	i	201	CHD	C21-C20-C17	-2.18	109.58	112.92
50	F	501	FMN	C4-C4A-C10	2.18	120.45	116.79
54	O	401	DGT	O1A-PA-O2A	-2.18	101.47	112.24
50	F	501	FMN	C7M-C7-C8	-2.15	116.33	120.74
50	F	501	FMN	C10-C4A-N5	-2.12	120.36	124.86
58	i	201	CHD	C11-C9-C10	-2.10	111.56	113.73
54	O	401	DGT	O6-C6-C5	-2.08	120.30	124.37
58	i	201	CHD	C4-C3-C2	2.03	112.97	110.55
57	U	101	EHZ	C11-N1-C12	-2.02	119.09	122.84

There are no chirality outliers.

All (1139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C11-O13-P-O14
45	A	202	3PE	C1-O11-P-O14
45	A	202	3PE	C11-O13-P-O14
45	A	202	3PE	O22-C21-O21-C2
45	H	401	3PE	C1-O11-P-O12
45	H	401	3PE	C1-O11-P-O13
45	H	401	3PE	C1-O11-P-O14
45	I	203	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C1-O11-P-O14
45	I	203	3PE	C11-O13-P-O11
45	I	203	3PE	C11-O13-P-O12
45	I	203	3PE	C11-O13-P-O14
45	I	203	3PE	O11-C1-C2-O21
45	I	203	3PE	C22-C21-O21-C2
45	J	202	3PE	C1-O11-P-O12
45	J	202	3PE	C1-O11-P-O13
45	J	202	3PE	C1-O11-P-O14
45	J	202	3PE	O11-C1-C2-O21
45	L	702	3PE	O11-C1-C2-O21
45	L	702	3PE	O22-C21-O21-C2
45	L	702	3PE	C22-C21-O21-C2
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	703	3PE	O22-C21-O21-C2
45	M	603	3PE	C11-O13-P-O12
45	M	603	3PE	O11-C1-C2-O21
45	M	604	3PE	C1-O11-P-O12
45	M	604	3PE	C1-O11-P-O13
45	M	604	3PE	C1-O11-P-O14
45	M	604	3PE	C11-O13-P-O14
45	M	604	3PE	C2-C1-O11-P
45	M	604	3PE	C12-C11-O13-P
45	N	401	3PE	C1-O11-P-O12
45	N	401	3PE	C1-O11-P-O14
45	N	401	3PE	C11-O13-P-O12
45	N	401	3PE	C11-O13-P-O14
45	N	401	3PE	O11-C1-C2-O21
45	Y	201	3PE	C1-O11-P-O12
45	Y	201	3PE	C1-O11-P-O14
45	Y	201	3PE	C11-O13-P-O12
45	Y	202	3PE	C22-C21-O21-C2
45	Y	203	3PE	C1-O11-P-O12
45	Y	203	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O14
45	Y	203	3PE	C11-O13-P-O11
45	Y	203	3PE	O13-C11-C12-N
45	Y	204	3PE	C1-O11-P-O12
45	Y	204	3PE	C11-O13-P-O12
45	Y	205	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
45	Y	205	3PE	C1-O11-P-O14
45	Y	206	3PE	C11-O13-P-O11
45	Y	206	3PE	C11-O13-P-O12
45	Y	206	3PE	C11-O13-P-O14
45	Y	206	3PE	C22-C21-O21-C2
45	Z	201	3PE	C12-C11-O13-P
45	Z	201	3PE	O21-C2-C3-O31
45	Z	202	3PE	C1-O11-P-O12
45	Z	202	3PE	C1-O11-P-O14
45	Z	202	3PE	O22-C21-O21-C2
45	f	102	3PE	C1-O11-P-O12
45	f	102	3PE	C1-O11-P-O13
45	f	102	3PE	C1-O11-P-O14
45	f	102	3PE	C11-O13-P-O12
45	m	201	3PE	O13-C11-C12-N
45	m	201	3PE	O22-C21-O21-C2
45	m	202	3PE	C11-O13-P-O14
45	m	202	3PE	O22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
46	A	203	PC1	C11-O13-P-O12
46	A	203	PC1	C11-O13-P-O11
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	H	402	PC1	C1-O11-P-O12
46	H	402	PC1	C1-O11-P-O14
46	H	402	PC1	O13-C11-C12-N
46	H	403	PC1	C11-O13-P-O11
46	H	403	PC1	C1-O11-P-O12
46	H	403	PC1	C1-O11-P-O14
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	O13-C11-C12-N
46	L	704	PC1	C1-O11-P-O14
46	M	605	PC1	C11-O13-P-O14
46	M	605	PC1	C12-C11-O13-P
46	M	605	PC1	O13-C11-C12-N
46	M	605	PC1	O21-C2-C3-O31
46	M	605	PC1	O22-C21-O21-C2
46	Z	203	PC1	O13-C11-C12-N
46	g	201	PC1	C1-O11-P-O12
46	g	201	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	g	201	PC1	O13-C11-C12-N
46	h	202	PC1	C11-O13-P-O12
46	h	202	PC1	C11-O13-P-O14
46	h	202	PC1	C11-O13-P-O11
46	h	202	PC1	C1-O11-P-O12
46	h	202	PC1	C1-O11-P-O14
46	h	202	PC1	C1-O11-P-O13
46	h	202	PC1	C22-C21-O21-C2
46	m	203	PC1	C11-O13-P-O12
46	m	203	PC1	C11-O13-P-O14
46	m	203	PC1	C1-O11-P-O12
46	m	203	PC1	C1-O11-P-O14
46	m	203	PC1	C1-O11-P-O13
46	m	203	PC1	C22-C21-O21-C2
46	q	201	PC1	C11-O13-P-O12
46	q	201	PC1	C11-O13-P-O14
46	q	201	PC1	C11-O13-P-O11
46	q	201	PC1	O13-C11-C12-N
46	q	201	PC1	O22-C21-O21-C2
46	q	201	PC1	C22-C21-O21-C2
47	A	205	PLC	O2-C2-C3-O3
47	A	205	PLC	C4-O4P-P-O1P
47	A	205	PLC	C4-O4P-P-O2P
47	B	203	PLC	C1'-C'-O2-C2
47	B	203	PLC	O'-C'-O2-C2
47	B	203	PLC	C4-O4P-P-O2P
47	L	705	PLC	C1'-C'-O2-C2
47	L	705	PLC	C4-O4P-P-O2P
47	M	606	PLC	C4-O4P-P-O1P
47	M	606	PLC	C4-O4P-P-O3P
47	Y	207	PLC	C4-O4P-P-O1P
47	g	202	PLC	O2-C2-C3-O3
47	g	202	PLC	C1-O3P-P-O1P
50	F	501	FMN	N10-C1'-C2'-O2'
52	L	701	CDL	CB2-OB2-PB2-OB4
52	M	602	CDL	C1-CA2-OA2-PA1
52	M	602	CDL	OB7-CB5-OB6-CB4
52	O	403	CDL	CA2-OA2-PA1-OA3
52	O	403	CDL	CB2-OB2-PB2-OB3
52	O	403	CDL	CB2-OB2-PB2-OB4
52	O	403	CDL	CB2-OB2-PB2-OB5
52	O	403	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
52	X	201	CDL	C1-CA2-OA2-PA1
52	X	201	CDL	C11-CA5-OA6-CA4
52	X	201	CDL	C51-CB5-OB6-CB4
52	d	201	CDL	OB7-CB5-OB6-CB4
52	h	201	CDL	CA2-OA2-PA1-OA3
52	h	201	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	O1-C1-CB2-OB2
52	r	201	CDL	CA3-OA5-PA1-OA2
52	r	201	CDL	CA3-OA5-PA1-OA4
54	O	401	DGT	PB-O3B-PG-O1G
56	P	501	NDP	C5B-O5B-PA-O1A
57	T	101	EHZ	C6-C7-C8-C9
57	T	101	EHZ	S1-C10-C11-N1
57	T	101	EHZ	C12-C13-C14-N2
57	U	101	EHZ	S1-C10-C11-N1
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
45	J	201	3PE	O32-C31-O31-C3
46	d	203	PC1	O32-C31-O31-C3
46	g	201	PC1	O32-C31-O31-C3
52	d	201	CDL	OB9-CB7-OB8-CB6
46	g	201	PC1	C32-C31-O31-C3
52	d	201	CDL	C71-CB7-OB8-CB6
45	Y	203	3PE	O32-C31-O31-C3
45	Y	205	3PE	O32-C31-O31-C3
45	m	201	3PE	O32-C31-O31-C3
46	H	402	PC1	O32-C31-O31-C3
46	H	403	PC1	O32-C31-O31-C3
46	m	203	PC1	O32-C31-O31-C3
46	q	201	PC1	O32-C31-O31-C3
52	L	701	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OB9-CB7-OB8-CB6
52	X	201	CDL	OA9-CA7-OA8-CA6
52	h	201	CDL	OB9-CB7-OB8-CB6
45	I	203	3PE	O22-C21-O21-C2
45	Y	202	3PE	O22-C21-O21-C2
45	Y	206	3PE	O22-C21-O21-C2
46	h	202	PC1	O22-C21-O21-C2
46	m	203	PC1	O22-C21-O21-C2
47	L	705	PLC	O'-C'-O2-C2
52	X	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
52	X	201	CDL	OB7-CB5-OB6-CB4
45	J	201	3PE	C32-C31-O31-C3
45	M	604	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
45	Y	205	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
46	H	403	PC1	C32-C31-O31-C3
46	d	203	PC1	C32-C31-O31-C3
46	m	203	PC1	C32-C31-O31-C3
46	q	201	PC1	C32-C31-O31-C3
52	M	602	CDL	C31-CA7-OA8-CA6
52	M	602	CDL	C71-CB7-OB8-CB6
52	X	201	CDL	C31-CA7-OA8-CA6
52	h	201	CDL	C31-CA7-OA8-CA6
52	h	201	CDL	C71-CB7-OB8-CB6
45	A	202	3PE	C22-C21-O21-C2
45	L	703	3PE	C22-C21-O21-C2
45	Z	202	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
46	M	605	PC1	C22-C21-O21-C2
52	M	602	CDL	C51-CB5-OB6-CB4
52	d	201	CDL	C51-CB5-OB6-CB4
52	h	201	CDL	C51-CB5-OB6-CB4
45	d	202	3PE	O32-C31-O31-C3
45	A	202	3PE	C32-C31-O31-C3
45	d	202	3PE	C32-C31-O31-C3
46	H	402	PC1	C32-C31-O31-C3
47	Z	204	PLC	C1B-CB-O3-C3
52	L	701	CDL	C31-CA7-OA8-CA6
52	O	403	CDL	C71-CB7-OB8-CB6
52	O	403	CDL	OB7-CB5-OB6-CB4
45	M	604	3PE	O32-C31-O31-C3
52	h	201	CDL	OA9-CA7-OA8-CA6
45	f	102	3PE	C32-C31-O31-C3
47	A	205	PLC	C1B-CB-O3-C3
52	O	403	CDL	C31-CA7-OA8-CA6
52	O	403	CDL	OB9-CB7-OB8-CB6
45	Y	203	3PE	C22-C21-O21-C2
52	M	602	CDL	C11-CA5-OA6-CA4
46	h	202	PC1	C2-C1-O11-P
47	Z	204	PLC	OB-CB-O3-C3
45	A	202	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	A	205	PLC	OB-CB-O3-C3
52	O	403	CDL	OA9-CA7-OA8-CA6
46	A	203	PC1	C32-C31-O31-C3
45	f	102	3PE	O32-C31-O31-C3
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CA2-C1-CB2-OB2
45	Y	203	3PE	O22-C21-O21-C2
45	Y	204	3PE	C32-C31-O31-C3
47	L	705	PLC	C'-C1'-C2'-C3'
47	B	203	PLC	CB-C1B-C2B-C3B
52	O	403	CDL	CB7-C71-C72-C73
45	f	101	3PE	O21-C2-C3-O31
45	Y	204	3PE	O32-C31-O31-C3
52	M	602	CDL	OA7-CA5-OA6-CA4
45	Y	201	3PE	C22-C21-O21-C2
45	Y	204	3PE	C22-C21-O21-C2
47	M	606	PLC	C1'-C'-O2-C2
47	B	203	PLC	C'-C1'-C2'-C3'
46	A	203	PC1	C21-C22-C23-C24
46	m	203	PC1	C31-C32-C33-C34
45	L	702	3PE	C31-C32-C33-C34
45	Y	203	3PE	C31-C32-C33-C34
45	Y	205	3PE	C31-C32-C33-C34
46	Z	203	PC1	C21-C22-C23-C24
52	M	602	CDL	CA5-C11-C12-C13
52	r	201	CDL	CA5-C11-C12-C13
52	r	201	CDL	CA7-C31-C32-C33
52	r	201	CDL	OA7-CA5-OA6-CA4
45	J	202	3PE	C21-C22-C23-C24
45	N	401	3PE	C31-C32-C33-C34
45	f	101	3PE	C31-C32-C33-C34
52	L	701	CDL	C11-CA5-OA6-CA4
45	Y	203	3PE	C21-C22-C23-C24
45	Z	201	3PE	C21-C22-C23-C24
46	A	203	PC1	O32-C31-O31-C3
45	J	201	3PE	C22-C21-O21-C2
47	g	202	PLC	C1'-C'-O2-C2
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C11-O13-P-O11
45	A	202	3PE	C1-O11-P-O13
45	A	202	3PE	C11-O13-P-O11
45	H	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	M	603	3PE	C1-O11-P-O13
45	M	604	3PE	C11-O13-P-O11
45	N	401	3PE	C1-O11-P-O13
45	N	401	3PE	C11-O13-P-O11
45	Y	201	3PE	C1-O11-P-O13
45	Y	201	3PE	C11-O13-P-O11
45	Y	204	3PE	C1-O11-P-O13
45	Y	204	3PE	C11-O13-P-O11
45	Y	205	3PE	C1-O11-P-O13
45	Y	205	3PE	C11-O13-P-O11
45	Z	201	3PE	C11-O13-P-O11
45	Z	202	3PE	C1-O11-P-O13
45	f	102	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O11
46	H	402	PC1	C1-O11-P-O13
46	H	403	PC1	C1-O11-P-O13
46	I	204	PC1	C11-O13-P-O11
46	L	704	PC1	C1-O11-P-O13
46	Z	203	PC1	C11-O13-P-O11
46	m	203	PC1	C11-O13-P-O11
47	A	205	PLC	C4-O4P-P-O3P
47	B	203	PLC	C4-O4P-P-O3P
47	L	705	PLC	C4-O4P-P-O3P
47	Y	207	PLC	C4-O4P-P-O3P
47	Z	204	PLC	C4-O4P-P-O3P
47	g	202	PLC	C1-O3P-P-O4P
52	L	701	CDL	CB2-OB2-PB2-OB5
52	M	602	CDL	CB3-OB5-PB2-OB2
52	O	403	CDL	CA2-OA2-PA1-OA5
52	h	201	CDL	CB3-OB5-PB2-OB2
52	r	201	CDL	CB3-OB5-PB2-OB2
52	d	201	CDL	CB7-C71-C72-C73
45	J	201	3PE	O22-C21-O21-C2
45	Y	201	3PE	O22-C21-O21-C2
45	Y	204	3PE	O22-C21-O21-C2
47	M	606	PLC	O'-C'-O2-C2
47	g	202	PLC	O'-C'-O2-C2
52	L	701	CDL	OA7-CA5-OA6-CA4
45	I	203	3PE	C32-C31-O31-C3
45	H	401	3PE	C36-C37-C38-C39
46	L	704	PC1	C23-C24-C25-C26
45	f	102	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
52	O	403	CDL	C11-CA5-OA6-CA4
45	H	401	3PE	C33-C34-C35-C36
45	J	201	3PE	C29-C2A-C2B-C2C
45	J	202	3PE	C33-C34-C35-C36
45	L	702	3PE	C32-C33-C34-C35
45	L	702	3PE	C22-C23-C24-C25
45	N	401	3PE	C24-C25-C26-C27
45	Z	201	3PE	C27-C28-C29-C2A
45	d	202	3PE	C24-C25-C26-C27
46	A	204	PC1	C23-C24-C25-C26
46	H	402	PC1	C25-C26-C27-C28
46	H	403	PC1	C3A-C3B-C3C-C3D
46	m	203	PC1	C3B-C3C-C3D-C3E
47	B	203	PLC	C2B-C3B-C4B-C5B
52	X	201	CDL	C16-C17-C18-C19
45	A	201	3PE	C33-C34-C35-C36
45	f	101	3PE	C37-C38-C39-C3A
46	L	704	PC1	C2B-C2C-C2D-C2E
47	B	203	PLC	C6'-C7'-C8'-C9'
47	M	606	PLC	C1B-C2B-C3B-C4B
52	X	201	CDL	C52-C53-C54-C55
45	f	102	3PE	O22-C21-O21-C2
52	O	403	CDL	OA7-CA5-OA6-CA4
46	m	203	PC1	C21-C22-C23-C24
45	H	401	3PE	C3A-C3B-C3C-C3D
45	f	101	3PE	C22-C21-O21-C2
46	L	704	PC1	C2E-C2F-C2G-C2H
46	d	203	PC1	C35-C36-C37-C38
52	h	201	CDL	C34-C35-C36-C37
46	g	201	PC1	C28-C29-C2A-C2B
52	X	201	CDL	C32-C33-C34-C35
52	r	201	CDL	C53-C54-C55-C56
52	d	201	CDL	O1-C1-CA2-OA2
45	I	203	3PE	C22-C23-C24-C25
45	I	203	3PE	C27-C28-C29-C2A
45	Z	202	3PE	C34-C35-C36-C37
45	m	202	3PE	C33-C34-C35-C36
46	g	201	PC1	C32-C33-C34-C35
47	g	202	PLC	C1'-C2'-C3'-C4'
45	Y	202	3PE	C31-C32-C33-C34
46	A	204	PC1	C32-C31-O31-C3
45	A	202	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
45	J	201	3PE	C27-C28-C29-C2A
46	B	202	PC1	C32-C33-C34-C35
46	I	204	PC1	C37-C38-C39-C3A
47	Z	204	PLC	C1B-C2B-C3B-C4B
52	L	701	CDL	C83-C84-C85-C86
52	M	602	CDL	C40-C41-C42-C43
52	M	602	CDL	C83-C84-C85-C86
52	X	201	CDL	C61-C62-C63-C64
59	o	201	MYR	C4-C5-C6-C7
45	I	203	3PE	O32-C31-O31-C3
45	m	201	3PE	C28-C29-C2A-C2B
46	d	203	PC1	C39-C3A-C3B-C3C
52	X	201	CDL	C78-C79-C80-C81
57	U	101	EHZ	C3-C4-C5-C6
45	J	201	3PE	C25-C26-C27-C28
45	Y	202	3PE	C25-C26-C27-C28
46	B	202	PC1	C3C-C3D-C3E-C3F
46	L	704	PC1	C3E-C3F-C3G-C3H
46	h	202	PC1	C25-C26-C27-C28
52	r	201	CDL	C72-C73-C74-C75
45	M	604	3PE	C32-C33-C34-C35
46	A	204	PC1	C26-C27-C28-C29
46	B	202	PC1	C3A-C3B-C3C-C3D
47	A	205	PLC	C6'-C7'-C8'-C9'
45	A	201	3PE	C2B-C2C-C2D-C2E
52	O	403	CDL	C72-C73-C74-C75
45	N	401	3PE	C2C-C2D-C2E-C2F
45	Y	203	3PE	C35-C36-C37-C38
45	Y	203	3PE	C27-C28-C29-C2A
45	Y	203	3PE	C2E-C2F-C2G-C2H
45	f	102	3PE	C32-C33-C34-C35
46	B	202	PC1	C27-C28-C29-C2A
46	g	201	PC1	C2A-C2B-C2C-C2D
52	O	403	CDL	C17-C18-C19-C20
52	X	201	CDL	C37-C38-C39-C40
45	A	201	3PE	C25-C26-C27-C28
46	B	202	PC1	C34-C35-C36-C37
46	M	605	PC1	C32-C33-C34-C35
52	O	403	CDL	C36-C37-C38-C39
52	X	201	CDL	C22-C23-C24-C25
52	h	201	CDL	C15-C16-C17-C18
45	A	201	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
45	M	604	3PE	O13-C11-C12-N
45	Z	201	3PE	O13-C11-C12-N
45	J	202	3PE	C3C-C3D-C3E-C3F
45	Y	204	3PE	C26-C27-C28-C29
45	Y	205	3PE	C33-C34-C35-C36
45	Z	202	3PE	C32-C33-C34-C35
45	f	102	3PE	C22-C23-C24-C25
46	H	402	PC1	C37-C38-C39-C3A
45	M	603	3PE	C3C-C3D-C3E-C3F
45	Y	201	3PE	C22-C23-C24-C25
46	H	403	PC1	C36-C37-C38-C39
52	X	201	CDL	C58-C59-C60-C61
46	d	203	PC1	C34-C35-C36-C37
52	X	201	CDL	CB3-CB4-CB6-OB8
45	m	201	3PE	C2A-C2B-C2C-C2D
46	H	402	PC1	C23-C24-C25-C26
46	H	402	PC1	C21-C22-C23-C24
45	f	101	3PE	C33-C34-C35-C36
45	Y	204	3PE	C3B-C3C-C3D-C3E
46	L	704	PC1	C3B-C3C-C3D-C3E
52	L	701	CDL	C33-C34-C35-C36
52	d	201	CDL	C42-C43-C44-C45
46	h	202	PC1	C31-C32-C33-C34
45	L	703	3PE	C27-C28-C29-C2A
52	X	201	CDL	C54-C55-C56-C57
46	g	201	PC1	C26-C27-C28-C29
52	X	201	CDL	C81-C82-C83-C84
45	J	202	3PE	C34-C35-C36-C37
46	m	203	PC1	C37-C38-C39-C3A
52	M	602	CDL	C63-C64-C65-C66
46	A	204	PC1	O32-C31-O31-C3
46	L	704	PC1	C39-C3A-C3B-C3C
46	g	201	PC1	C2C-C2D-C2E-C2F
52	O	403	CDL	C59-C60-C61-C62
46	L	704	PC1	C32-C31-O31-C3
46	d	203	PC1	C22-C21-O21-C2
52	d	201	CDL	C11-CA5-OA6-CA4
45	Y	202	3PE	C35-C36-C37-C38
47	M	606	PLC	C7B-C8B-C9B-CAA
52	X	201	CDL	C35-C36-C37-C38
52	O	403	CDL	C55-C56-C57-C58
52	X	201	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
52	r	201	CDL	C15-C16-C17-C18
47	A	205	PLC	C3'-C4'-C5'-C6'
52	O	403	CDL	C18-C19-C20-C21
46	L	704	PC1	O32-C31-O31-C3
46	H	403	PC1	O22-C21-O21-C2
46	L	704	PC1	O22-C21-O21-C2
52	L	701	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	OB7-CB5-OB6-CB4
45	M	604	3PE	C31-C32-C33-C34
45	Y	202	3PE	C21-C22-C23-C24
45	m	202	3PE	C21-C22-C23-C24
45	f	101	3PE	C32-C31-O31-C3
45	L	702	3PE	C39-C3A-C3B-C3C
45	Y	204	3PE	C38-C39-C3A-C3B
52	M	602	CDL	C62-C63-C64-C65
45	A	202	3PE	C31-C32-C33-C34
45	M	604	3PE	C21-C22-C23-C24
45	N	401	3PE	C21-C22-C23-C24
45	Y	205	3PE	C21-C22-C23-C24
45	N	401	3PE	C38-C39-C3A-C3B
45	Y	204	3PE	C32-C33-C34-C35
46	I	204	PC1	C36-C37-C38-C39
52	M	602	CDL	C11-C12-C13-C14
52	O	403	CDL	C22-C23-C24-C25
45	A	201	3PE	C31-C32-C33-C34
52	O	403	CDL	CA5-C11-C12-C13
45	M	604	3PE	C22-C21-O21-C2
46	A	204	PC1	C22-C21-O21-C2
46	H	402	PC1	C22-C21-O21-C2
46	H	403	PC1	C22-C21-O21-C2
46	L	704	PC1	C22-C21-O21-C2
52	L	701	CDL	C51-CB5-OB6-CB4
52	h	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	C51-CB5-OB6-CB4
45	L	702	3PE	C3D-C3E-C3F-C3G
46	H	402	PC1	C36-C37-C38-C39
46	Z	203	PC1	C24-C25-C26-C27
47	A	205	PLC	C4B-C5B-C6B-C7B
46	A	204	PC1	O22-C21-O21-C2
46	H	402	PC1	O22-C21-O21-C2
46	d	203	PC1	O22-C21-O21-C2
45	H	401	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	M	603	3PE	C33-C34-C35-C36
46	m	203	PC1	C35-C36-C37-C38
45	A	202	3PE	C28-C29-C2A-C2B
46	m	203	PC1	C2E-C2F-C2G-C2H
52	O	403	CDL	C20-C21-C22-C23
45	M	604	3PE	O22-C21-O21-C2
52	d	201	CDL	OA7-CA5-OA6-CA4
52	h	201	CDL	OA7-CA5-OA6-CA4
45	Z	201	3PE	C22-C21-O21-C2
45	H	401	3PE	C38-C39-C3A-C3B
45	Y	205	3PE	C2C-C2D-C2E-C2F
46	m	203	PC1	C24-C25-C26-C27
52	O	403	CDL	C56-C57-C58-C59
45	M	603	3PE	C11-O13-P-O11
46	H	402	PC1	C11-O13-P-O11
46	g	201	PC1	C11-O13-P-O11
46	g	201	PC1	C1-O11-P-O13
52	O	403	CDL	CA3-OA5-PA1-OA2
52	h	201	CDL	C72-C73-C74-C75
57	T	101	EHZ	C22-C23-C24-C25
52	O	403	CDL	C19-C20-C21-C22
45	J	202	3PE	O11-C1-C2-C3
45	M	603	3PE	O11-C1-C2-C3
46	H	403	PC1	O11-C1-C2-C3
47	L	705	PLC	O3P-C1-C2-C3
47	Y	207	PLC	O3P-C1-C2-C3
46	A	203	PC1	C24-C25-C26-C27
47	M	606	PLC	CB-C1B-C2B-C3B
45	Y	204	3PE	C35-C36-C37-C38
52	L	701	CDL	C36-C37-C38-C39
45	m	201	3PE	C2B-C2C-C2D-C2E
52	L	701	CDL	C61-C62-C63-C64
45	Z	201	3PE	C32-C33-C34-C35
46	q	201	PC1	C35-C36-C37-C38
45	m	201	3PE	C32-C33-C34-C35
46	I	204	PC1	C2D-C2E-C2F-C2G
47	g	202	PLC	C1B-CB-O3-C3
45	A	201	3PE	C23-C24-C25-C26
45	H	401	3PE	C34-C35-C36-C37
45	H	401	3PE	C1-C2-C3-O31
45	L	703	3PE	C1-C2-C3-O31
45	Y	202	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	f	101	3PE	C1-C2-C3-O31
45	f	102	3PE	C1-C2-C3-O31
45	m	202	3PE	C1-C2-C3-O31
47	g	202	PLC	C1-C2-C3-O3
52	r	201	CDL	CA3-CA4-CA6-OA8
52	M	602	CDL	CA7-C31-C32-C33
52	d	201	CDL	C72-C73-C74-C75
45	A	202	3PE	C36-C37-C38-C39
46	H	402	PC1	C29-C2A-C2B-C2C
52	X	201	CDL	C84-C85-C86-C87
45	M	603	3PE	C35-C36-C37-C38
46	M	605	PC1	C35-C36-C37-C38
45	A	202	3PE	C38-C39-C3A-C3B
46	B	202	PC1	C38-C39-C3A-C3B
46	h	202	PC1	C26-C27-C28-C29
52	O	403	CDL	C58-C59-C60-C61
52	X	201	CDL	C44-C45-C46-C47
45	f	101	3PE	O32-C31-O31-C3
46	m	203	PC1	C38-C39-C3A-C3B
47	A	205	PLC	C2B-C3B-C4B-C5B
47	B	203	PLC	C8B-C9B-CAA-CBA
52	d	201	CDL	C11-C12-C13-C14
45	A	201	3PE	C21-C22-C23-C24
47	Z	204	PLC	CB-C1B-C2B-C3B
45	Z	201	3PE	C32-C31-O31-C3
45	Y	202	3PE	C37-C38-C39-C3A
52	O	403	CDL	CA6-CA4-OA6-CA5
52	h	201	CDL	C76-C77-C78-C79
45	Y	202	3PE	C3A-C3B-C3C-C3D
52	d	201	CDL	C36-C37-C38-C39
52	O	403	CDL	C11-C12-C13-C14
45	Y	204	3PE	C29-C2A-C2B-C2C
46	h	202	PC1	C2B-C2C-C2D-C2E
46	A	204	PC1	C21-C22-C23-C24
45	N	401	3PE	C35-C36-C37-C38
52	M	602	CDL	C74-C75-C76-C77
52	X	201	CDL	C71-C72-C73-C74
52	d	201	CDL	C31-C32-C33-C34
52	L	701	CDL	C57-C58-C59-C60
45	J	201	3PE	C23-C24-C25-C26
46	A	204	PC1	C22-C23-C24-C25
46	I	204	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
47	Y	207	PLC	C1'-C2'-C3'-C4'
45	Z	201	3PE	O32-C31-O31-C3
45	A	201	3PE	C32-C33-C34-C35
59	o	201	MYR	C9-C10-C11-C12
52	X	201	CDL	CB2-C1-CA2-OA2
45	I	203	3PE	C28-C29-C2A-C2B
46	Z	203	PC1	C22-C23-C24-C25
46	B	202	PC1	C32-C31-O31-C3
45	A	202	3PE	C2F-C2G-C2H-C2I
52	r	201	CDL	C17-C18-C19-C20
45	N	401	3PE	C27-C28-C29-C2A
52	M	602	CDL	C51-C52-C53-C54
45	I	203	3PE	O11-C1-C2-C3
45	L	702	3PE	O11-C1-C2-C3
45	M	604	3PE	O11-C1-C2-C3
45	N	401	3PE	O11-C1-C2-C3
52	O	403	CDL	OB5-CB3-CB4-CB6
52	X	201	CDL	OA5-CA3-CA4-CA6
52	d	201	CDL	OA5-CA3-CA4-CA6
52	r	201	CDL	OB5-CB3-CB4-CB6
47	B	203	PLC	C6B-C7B-C8B-C9B
45	Y	201	3PE	C21-C22-C23-C24
46	H	402	PC1	C33-C34-C35-C36
46	Z	203	PC1	C25-C26-C27-C28
52	M	602	CDL	C14-C15-C16-C17
46	g	201	PC1	C33-C34-C35-C36
45	Z	201	3PE	O22-C21-O21-C2
45	I	203	3PE	C24-C25-C26-C27
45	f	101	3PE	O22-C21-O21-C2
46	d	203	PC1	C3B-C3C-C3D-C3E
52	M	602	CDL	C16-C17-C18-C19
45	A	202	3PE	C32-C33-C34-C35
45	d	202	3PE	C3D-C3E-C3F-C3G
52	M	602	CDL	C41-C42-C43-C44
45	M	603	3PE	C38-C39-C3A-C3B
45	I	203	3PE	C1-C2-C3-O31
45	Y	206	3PE	C1-C2-C3-O31
45	Z	201	3PE	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31
46	H	402	PC1	C1-C2-C3-O31
47	B	203	PLC	C1-C2-C3-O3
45	A	201	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
45	m	202	3PE	C32-C31-O31-C3
45	Y	202	3PE	C1-O11-P-O13
46	M	605	PC1	C11-O13-P-O11
52	M	602	CDL	CA3-OA5-PA1-OA2
52	X	201	CDL	CA2-OA2-PA1-OA5
52	h	201	CDL	CA2-OA2-PA1-OA5
52	O	403	CDL	CB5-C51-C52-C53
52	X	201	CDL	CB7-C71-C72-C73
46	h	202	PC1	C23-C24-C25-C26
52	d	201	CDL	C34-C35-C36-C37
45	L	703	3PE	O11-C1-C2-O21
45	M	604	3PE	O11-C1-C2-O21
46	B	202	PC1	O11-C1-C2-O21
46	g	201	PC1	O11-C1-C2-O21
47	L	705	PLC	O3P-C1-C2-O2
52	O	403	CDL	OB5-CB3-CB4-OB6
52	X	201	CDL	OA5-CA3-CA4-OA6
52	d	201	CDL	OA5-CA3-CA4-OA6
52	d	201	CDL	OB5-CB3-CB4-OB6
45	d	202	3PE	C31-C32-C33-C34
45	N	401	3PE	C33-C34-C35-C36
46	d	203	PC1	C31-C32-C33-C34
52	d	201	CDL	CA5-C11-C12-C13
57	T	101	EHZ	C5-C6-C7-O1
45	d	202	3PE	C28-C29-C2A-C2B
52	L	701	CDL	C23-C24-C25-C26
45	A	201	3PE	O21-C2-C3-O31
45	d	202	3PE	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
46	H	402	PC1	O21-C2-C3-O31
52	r	201	CDL	OA6-CA4-CA6-OA8
45	A	201	3PE	C36-C37-C38-C39
52	L	701	CDL	C58-C59-C60-C61
59	o	201	MYR	C6-C7-C8-C9
46	I	204	PC1	C22-C21-O21-C2
52	M	602	CDL	C44-C45-C46-C47
45	Z	201	3PE	C29-C2A-C2B-C2C
45	Y	202	3PE	C2B-C2C-C2D-C2E
45	L	703	3PE	C23-C24-C25-C26
45	Z	202	3PE	C24-C25-C26-C27
45	Z	202	3PE	C2-C1-O11-P
47	Z	204	PLC	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
50	F	501	FMN	C4'-C5'-O5'-P
52	L	701	CDL	CB4-CB3-OB5-PB2
46	B	202	PC1	O32-C31-O31-C3
57	T	101	EHZ	O2-C9-S1-C10
45	A	201	3PE	C35-C36-C37-C38
46	H	402	PC1	C32-C33-C34-C35
52	M	602	CDL	C31-C32-C33-C34
46	I	204	PC1	O22-C21-O21-C2
45	Z	201	3PE	C2B-C2C-C2D-C2E
46	A	204	PC1	C3A-C3B-C3C-C3D
52	O	403	CDL	C14-C15-C16-C17
45	A	201	3PE	O11-C1-C2-C3
45	L	703	3PE	O11-C1-C2-C3
45	Y	203	3PE	O11-C1-C2-C3
46	g	201	PC1	O11-C1-C2-C3
52	d	201	CDL	OB5-CB3-CB4-CB6
45	A	201	3PE	C3A-C3B-C3C-C3D
56	P	501	NDP	O4D-C1D-N1N-C6N
52	d	201	CDL	C31-CA7-OA8-CA6
45	N	401	3PE	C28-C29-C2A-C2B
52	L	701	CDL	C52-C53-C54-C55
45	M	604	3PE	C23-C24-C25-C26
45	d	202	3PE	C39-C3A-C3B-C3C
46	Z	203	PC1	C22-C21-O21-C2
47	Z	204	PLC	C6B-C7B-C8B-C9B
52	r	201	CDL	C71-CB7-OB8-CB6
46	H	403	PC1	C32-C33-C34-C35
46	m	203	PC1	C26-C27-C28-C29
45	Y	204	3PE	C3-C2-O21-C21
46	Z	203	PC1	C32-C31-O31-C3
52	L	701	CDL	C71-CB7-OB8-CB6
45	Z	201	3PE	C25-C26-C27-C28
45	A	201	3PE	C1-C2-C3-O31
46	d	203	PC1	C1-C2-C3-O31
46	h	202	PC1	C1-C2-C3-O31
46	m	203	PC1	C2-C1-O11-P
47	A	205	PLC	C1-C2-C3-O3
52	X	201	CDL	C1-CB2-OB2-PB2
52	d	201	CDL	OA9-CA7-OA8-CA6
52	X	201	CDL	C11-C12-C13-C14
45	A	201	3PE	O11-C1-C2-O21
52	L	701	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
52	O	403	CDL	C57-C58-C59-C60
46	g	201	PC1	C2E-C2F-C2G-C2H
45	A	202	3PE	C22-C23-C24-C25
45	Y	205	3PE	C29-C2A-C2B-C2C
57	T	101	EHZ	O1-C7-C8-C9
45	M	604	3PE	C33-C34-C35-C36
45	Y	206	3PE	O21-C2-C3-O31
45	m	202	3PE	O21-C2-C3-O31
46	A	203	PC1	O21-C2-C3-O31
46	d	203	PC1	O21-C2-C3-O31
47	B	203	PLC	O2-C2-C3-O3
52	X	201	CDL	OB6-CB4-CB6-OB8
45	A	202	3PE	C2A-C2B-C2C-C2D
45	N	401	3PE	C2D-C2E-C2F-C2G
45	Y	205	3PE	C28-C29-C2A-C2B
56	P	501	NDP	C5B-O5B-PA-O3
45	L	703	3PE	C2D-C2E-C2F-C2G
45	m	202	3PE	O32-C31-O31-C3
52	M	602	CDL	CB5-C51-C52-C53
52	L	701	CDL	C75-C76-C77-C78
46	Z	203	PC1	O22-C21-O21-C2
56	P	501	NDP	O4B-C4B-C5B-O5B
52	L	701	CDL	C31-C32-C33-C34
46	d	203	PC1	C38-C39-C3A-C3B
46	Z	203	PC1	O32-C31-O31-C3
52	r	201	CDL	OB9-CB7-OB8-CB6
45	Y	205	3PE	C38-C39-C3A-C3B
45	H	401	3PE	C21-C22-C23-C24
45	A	202	3PE	C34-C35-C36-C37
45	L	702	3PE	C11-O13-P-O11
47	A	205	PLC	C1-O3P-P-O4P
52	X	201	CDL	CA3-OA5-PA1-OA2
52	d	201	CDL	CB2-OB2-PB2-OB5
46	d	203	PC1	C37-C38-C39-C3A
52	h	201	CDL	C73-C74-C75-C76
57	U	101	EHZ	C1-C2-C3-C4
52	X	201	CDL	O1-C1-CA2-OA2
52	L	701	CDL	C16-C17-C18-C19
52	r	201	CDL	C71-C72-C73-C74
57	T	101	EHZ	C2-C1-C21-C22
45	M	603	3PE	C2-C1-O11-P
46	A	203	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
52	X	201	CDL	C63-C64-C65-C66
45	H	401	3PE	C11-O13-P-O12
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	C11-O13-P-O14
45	Y	204	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O14
45	Y	205	3PE	C11-O13-P-O14
45	Z	201	3PE	C11-O13-P-O14
45	f	102	3PE	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O14
46	H	402	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	L	704	PC1	C1-O11-P-O12
46	Z	203	PC1	C11-O13-P-O12
46	Z	203	PC1	C11-O13-P-O14
46	d	203	PC1	C1-O11-P-O12
46	g	201	PC1	C11-O13-P-O12
46	q	201	PC1	C1-O11-P-O14
47	L	705	PLC	C4-O4P-P-O1P
47	Z	204	PLC	C4-O4P-P-O1P
47	g	202	PLC	C1-O3P-P-O2P
52	L	701	CDL	CB2-OB2-PB2-OB3
52	M	602	CDL	CB3-OB5-PB2-OB3
52	O	403	CDL	CA2-OA2-PA1-OA4
52	O	403	CDL	CA3-OA5-PA1-OA3
52	h	201	CDL	CA2-OA2-PA1-OA4
52	h	201	CDL	CB3-OB5-PB2-OB3
52	h	201	CDL	CB3-OB5-PB2-OB4
52	r	201	CDL	CA3-OA5-PA1-OA3
52	r	201	CDL	CB3-OB5-PB2-OB3
56	P	501	NDP	C5B-O5B-PA-O2A
52	X	201	CDL	C17-C18-C19-C20
45	A	202	3PE	O11-C1-C2-C3
45	L	702	3PE	C3C-C3D-C3E-C3F
45	f	101	3PE	O13-C11-C12-N
52	M	602	CDL	C52-C53-C54-C55
52	L	701	CDL	C79-C80-C81-C82
45	J	201	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	N	401	3PE	C12-C11-O13-P
45	Y	203	3PE	C12-C11-O13-P
45	Y	205	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	C12-C11-O13-P
45	f	101	3PE	C12-C11-O13-P
45	m	202	3PE	C12-C11-O13-P
47	Z	204	PLC	C5-C4-O4P-P
52	r	201	CDL	C52-C51-CB5-OB6
47	g	202	PLC	OB-CB-O3-C3
46	L	704	PC1	C21-C22-C23-C24
45	A	202	3PE	C33-C34-C35-C36
45	J	202	3PE	C35-C36-C37-C38
45	Y	203	3PE	C29-C2A-C2B-C2C
52	O	403	CDL	C76-C77-C78-C79
52	M	602	CDL	C18-C19-C20-C21
45	A	202	3PE	O11-C1-C2-O21
45	Y	203	3PE	O11-C1-C2-O21
47	Y	207	PLC	O3P-C1-C2-O2
50	F	501	FMN	N10-C1'-C2'-C3'
52	r	201	CDL	OB5-CB3-CB4-OB6
45	Z	201	3PE	C22-C23-C24-C25
46	A	203	PC1	C22-C21-O21-C2
52	L	701	CDL	OB9-CB7-OB8-CB6
45	J	202	3PE	C38-C39-C3A-C3B
46	H	403	PC1	O13-C11-C12-N
46	M	605	PC1	C1-C2-C3-O31
46	Z	203	PC1	C34-C35-C36-C37
47	A	205	PLC	O4P-C4-C5-N
47	M	606	PLC	O4P-C4-C5-N
47	Y	207	PLC	O4P-C4-C5-N
47	Z	204	PLC	O4P-C4-C5-N
46	A	203	PC1	O22-C21-O21-C2
45	L	703	3PE	O21-C2-C3-O31
45	f	102	3PE	O21-C2-C3-O31
52	L	701	CDL	OA6-CA4-CA6-OA8
45	J	201	3PE	C2D-C2E-C2F-C2G
45	M	604	3PE	C2B-C2C-C2D-C2E
46	q	201	PC1	C37-C38-C39-C3A
52	M	602	CDL	C60-C61-C62-C63
52	h	201	CDL	C74-C75-C76-C77
47	B	203	PLC	C1B-C2B-C3B-C4B
45	M	603	3PE	C3E-C3F-C3G-C3H
47	A	205	PLC	C2'-C3'-C4'-C5'
45	M	603	3PE	C36-C37-C38-C39
45	N	401	3PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
45	Y	202	3PE	C38-C39-C3A-C3B
45	Y	204	3PE	C24-C25-C26-C27
45	L	702	3PE	C23-C24-C25-C26
46	H	403	PC1	C3E-C3F-C3G-C3H
45	f	102	3PE	C25-C26-C27-C28
52	M	602	CDL	C72-C73-C74-C75
46	Z	203	PC1	C29-C2A-C2B-C2C
45	Y	202	3PE	C39-C3A-C3B-C3C
45	m	202	3PE	C37-C38-C39-C3A
52	O	403	CDL	C75-C76-C77-C78
45	M	603	3PE	C39-C3A-C3B-C3C
45	Y	202	3PE	C1-C2-O21-C21
45	Z	202	3PE	C3-C2-O21-C21
46	m	203	PC1	C1-C2-O21-C21
47	Y	207	PLC	C1-C2-O2-C'
47	Y	207	PLC	C3-C2-O2-C'
47	g	202	PLC	C1-C2-O2-C'
47	g	202	PLC	C3-C2-O2-C'
52	L	701	CDL	CA6-CA4-OA6-CA5
52	X	201	CDL	CA6-CA4-OA6-CA5
52	X	201	CDL	CB3-CB4-OB6-CB5
46	L	704	PC1	C37-C38-C39-C3A
45	J	202	3PE	C37-C38-C39-C3A
45	N	401	3PE	C2E-C2F-C2G-C2H
46	m	203	PC1	C28-C29-C2A-C2B
45	f	102	3PE	C35-C36-C37-C38
46	H	403	PC1	C22-C23-C24-C25
46	L	704	PC1	C32-C33-C34-C35
52	M	602	CDL	C81-C82-C83-C84
52	M	602	CDL	C78-C79-C80-C81
45	H	401	3PE	C2-C1-O11-P
47	M	606	PLC	C2-C1-O3P-P
46	H	403	PC1	O11-C1-C2-O21
52	L	701	CDL	C76-C77-C78-C79
45	I	203	3PE	O21-C2-C3-O31
45	J	201	3PE	C11-O13-P-O11
45	Y	206	3PE	C1-O11-P-O13
45	d	202	3PE	C11-O13-P-O11
46	A	204	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O13
47	B	203	PLC	C1-O3P-P-O4P
52	X	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
52	d	201	CDL	CB3-OB5-PB2-OB2
45	m	201	3PE	C25-C26-C27-C28
45	Y	202	3PE	C26-C27-C28-C29
46	A	204	PC1	C35-C36-C37-C38
46	L	704	PC1	C36-C37-C38-C39
52	h	201	CDL	CB7-C71-C72-C73
45	N	401	3PE	C39-C3A-C3B-C3C
52	X	201	CDL	C42-C43-C44-C45
52	M	602	CDL	C15-C16-C17-C18
46	d	203	PC1	C3A-C3B-C3C-C3D
45	J	201	3PE	O31-C31-C32-C33
46	g	201	PC1	C22-C21-O21-C2
46	g	201	PC1	O22-C21-O21-C2
54	O	401	DGT	PB-O3A-PA-O1A
45	M	604	3PE	C28-C29-C2A-C2B
52	O	403	CDL	C12-C13-C14-C15
46	m	203	PC1	C2D-C2E-C2F-C2G
45	N	401	3PE	C2-C1-O11-P
52	X	201	CDL	C62-C63-C64-C65
45	Y	203	3PE	C37-C38-C39-C3A
45	M	603	3PE	C28-C29-C2A-C2B
45	J	202	3PE	C28-C29-C2A-C2B
45	A	201	3PE	C2D-C2E-C2F-C2G
47	g	202	PLC	C2'-C3'-C4'-C5'
46	H	402	PC1	O21-C21-C22-C23
46	A	203	PC1	C32-C33-C34-C35
47	Z	204	PLC	O3P-C1-C2-C3
46	q	201	PC1	C32-C33-C34-C35
45	Z	202	3PE	O11-C1-C2-O21
46	m	203	PC1	C29-C2A-C2B-C2C
45	f	102	3PE	C24-C25-C26-C27
46	I	204	PC1	C29-C2A-C2B-C2C
45	Y	205	3PE	C2D-C2E-C2F-C2G
45	d	202	3PE	C32-C33-C34-C35
46	g	201	PC1	C22-C23-C24-C25
45	m	201	3PE	C21-C22-C23-C24
45	A	202	3PE	C35-C36-C37-C38
45	J	201	3PE	O32-C31-C32-C33
46	H	403	PC1	C3D-C3E-C3F-C3G
52	h	201	CDL	C32-C31-CA7-OA8
46	I	204	PC1	C35-C36-C37-C38
52	M	602	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
47	Y	207	PLC	C5'-C6'-C7'-C8'
45	Z	202	3PE	C1-C2-C3-O31
46	A	203	PC1	C1-C2-C3-O31
45	J	202	3PE	C29-C2A-C2B-C2C
46	Z	203	PC1	C27-C28-C29-C2A
46	B	202	PC1	C36-C37-C38-C39
47	A	205	PLC	C6B-C7B-C8B-C9B
46	L	704	PC1	C34-C35-C36-C37
46	m	203	PC1	C3-C2-O21-C21
52	X	201	CDL	CB6-CB4-OB6-CB5
46	L	704	PC1	C27-C28-C29-C2A
46	q	201	PC1	C1-O11-P-O13
45	M	604	3PE	C29-C2A-C2B-C2C
52	M	602	CDL	C77-C78-C79-C80
46	m	203	PC1	C3D-C3E-C3F-C3G
45	J	202	3PE	C27-C28-C29-C2A
45	f	101	3PE	C35-C36-C37-C38
57	T	101	EHZ	C5-C6-C7-C8
45	m	202	3PE	C3E-C3F-C3G-C3H
46	L	704	PC1	C22-C23-C24-C25
45	L	703	3PE	C28-C29-C2A-C2B
52	M	602	CDL	C56-C57-C58-C59
52	L	701	CDL	O1-C1-CB2-OB2
45	Y	203	3PE	C32-C33-C34-C35
46	Z	203	PC1	C38-C39-C3A-C3B
52	M	602	CDL	C34-C35-C36-C37
45	M	603	3PE	C31-C32-C33-C34
58	i	201	CHD	C13-C17-C20-C21
45	M	604	3PE	C25-C26-C27-C28
57	T	101	EHZ	C11-C10-S1-C9
57	U	101	EHZ	C11-C10-S1-C9
45	Y	202	3PE	C3E-C3F-C3G-C3H
46	q	201	PC1	C31-C32-C33-C34
45	A	201	3PE	C2A-C2B-C2C-C2D
52	L	701	CDL	C14-C15-C16-C17
46	L	704	PC1	C33-C34-C35-C36
46	Z	203	PC1	C3A-C3B-C3C-C3D
45	f	101	3PE	C34-C35-C36-C37
46	H	402	PC1	C27-C28-C29-C2A
52	X	201	CDL	C72-C71-CB7-OB8
52	L	701	CDL	CA2-C1-CB2-OB2
52	X	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C2B-C2C-C2D-C2E
52	L	701	CDL	C18-C19-C20-C21
52	O	403	CDL	C24-C25-C26-C27
45	Y	201	3PE	C23-C24-C25-C26
46	m	203	PC1	C3E-C3F-C3G-C3H
45	Y	205	3PE	C27-C28-C29-C2A
45	Y	205	3PE	C2A-C2B-C2C-C2D
46	h	202	PC1	C22-C23-C24-C25
52	M	602	CDL	C75-C76-C77-C78
54	O	401	DGT	PA-O3A-PB-O1B
46	H	402	PC1	C11-C12-N-C13
46	I	204	PC1	C11-C12-N-C14
45	L	702	3PE	C27-C28-C29-C2A
52	L	701	CDL	C54-C55-C56-C57
45	m	201	3PE	O21-C21-C22-C23
52	L	701	CDL	CA3-CA4-CA6-OA8
45	Y	203	3PE	C33-C34-C35-C36
45	M	604	3PE	C22-C23-C24-C25
52	L	701	CDL	C19-C20-C21-C22
46	A	204	PC1	C3D-C3E-C3F-C3G
46	A	204	PC1	O11-C1-C2-O21
52	M	602	CDL	OB5-CB3-CB4-OB6
45	M	603	3PE	C3A-C3B-C3C-C3D
52	h	201	CDL	C39-C40-C41-C42
45	J	201	3PE	C2C-C2D-C2E-C2F
45	Y	202	3PE	C34-C35-C36-C37
46	g	201	PC1	C11-C12-N-C13
46	B	202	PC1	O11-C1-C2-C3
46	H	402	PC1	C22-C23-C24-C25
45	Z	201	3PE	O21-C21-C22-C23
45	A	202	3PE	C2-C1-O11-P
46	M	605	PC1	C2-C1-O11-P
52	M	602	CDL	CB2-C1-CA2-OA2
52	d	201	CDL	CB2-C1-CA2-OA2
46	H	403	PC1	C3F-C3G-C3H-C3I
52	L	701	CDL	C73-C74-C75-C76
46	M	605	PC1	C24-C25-C26-C27
52	M	602	CDL	C80-C81-C82-C83
56	P	501	NDP	C3B-C4B-C5B-O5B
47	L	705	PLC	C2B-C1B-CB-O3
52	O	403	CDL	C16-C17-C18-C19
47	Z	204	PLC	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
45	H	401	3PE	O22-C21-O21-C2
45	d	202	3PE	C3A-C3B-C3C-C3D
46	g	201	PC1	C11-C12-N-C14
45	m	201	3PE	C35-C36-C37-C38
52	X	201	CDL	C40-C41-C42-C43
52	h	201	CDL	C56-C57-C58-C59
45	I	203	3PE	C26-C27-C28-C29
45	A	201	3PE	O31-C31-C32-C33
57	T	101	EHZ	C8-C9-S1-C10
45	Z	202	3PE	C21-C22-C23-C24
52	L	701	CDL	C59-C60-C61-C62
57	U	101	EHZ	C2-C1-C21-C22
45	Y	204	3PE	C2E-C2F-C2G-C2H
45	m	201	3PE	C2D-C2E-C2F-C2G
46	h	202	PC1	O31-C31-C32-C33
47	M	606	PLC	C2B-C1B-CB-O3
45	m	202	3PE	C34-C35-C36-C37
45	Y	205	3PE	O31-C31-C32-C33
46	I	204	PC1	O31-C31-C32-C33
47	A	205	PLC	C2B-C1B-CB-O3
52	O	403	CDL	C74-C75-C76-C77
45	J	202	3PE	C26-C27-C28-C29
46	A	203	PC1	O11-C1-C2-O21
46	H	402	PC1	O31-C31-C32-C33
52	O	403	CDL	C52-C51-CB5-OB6
46	H	402	PC1	C11-C12-N-C15
46	I	204	PC1	C11-C12-N-C13
46	A	204	PC1	C37-C38-C39-C3A
45	M	603	3PE	O21-C21-C22-C23
45	m	202	3PE	C38-C39-C3A-C3B
54	O	401	DGT	PB-O3B-PG-O2G
45	m	202	3PE	C31-C32-C33-C34
46	H	403	PC1	C3B-C3C-C3D-C3E
52	O	403	CDL	C72-C71-CB7-OB8
45	I	203	3PE	C2F-C2G-C2H-C2I
45	M	604	3PE	C38-C39-C3A-C3B
45	M	604	3PE	O21-C2-C3-O31
52	M	602	CDL	C64-C65-C66-C67
52	L	701	CDL	C78-C79-C80-C81
45	L	702	3PE	O31-C31-C32-C33
45	M	604	3PE	O31-C31-C32-C33
45	Y	203	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C39-C3A-C3B-C3C
45	A	201	3PE	C37-C38-C39-C3A
45	Y	203	3PE	C3B-C3C-C3D-C3E
52	L	701	CDL	C24-C25-C26-C27
45	H	401	3PE	C22-C21-O21-C2
45	A	202	3PE	O21-C21-C22-C23
45	Y	203	3PE	O21-C21-C22-C23
46	d	203	PC1	C3C-C3D-C3E-C3F
52	M	602	CDL	C12-C13-C14-C15
58	i	201	CHD	C17-C20-C22-C23
46	A	204	PC1	C3C-C3D-C3E-C3F
46	m	203	PC1	C3F-C3G-C3H-C3I
45	d	202	3PE	C21-C22-C23-C24
45	L	702	3PE	C3F-C3G-C3H-C3I
45	d	202	3PE	C26-C27-C28-C29
52	M	602	CDL	C72-C71-CB7-OB8
47	A	205	PLC	C3B-C4B-C5B-C6B
45	Y	205	3PE	O32-C31-C32-C33
52	O	403	CDL	C15-C16-C17-C18
45	L	703	3PE	C26-C27-C28-C29
46	h	202	PC1	O32-C31-C32-C33
52	L	701	CDL	C43-C44-C45-C46
45	I	203	3PE	C29-C2A-C2B-C2C
45	N	401	3PE	C25-C26-C27-C28
52	X	201	CDL	C13-C14-C15-C16
45	A	201	3PE	O32-C31-C32-C33
45	Z	201	3PE	O22-C21-C22-C23
52	M	602	CDL	C37-C38-C39-C40
45	Y	205	3PE	C1-C2-C3-O31
45	d	202	3PE	C1-C2-C3-O31
46	Z	203	PC1	C23-C24-C25-C26
45	Y	204	3PE	C28-C29-C2A-C2B
46	A	204	PC1	C32-C33-C34-C35
47	L	705	PLC	C2B-C1B-CB-OB
52	L	701	CDL	C11-C12-C13-C14
52	X	201	CDL	C73-C74-C75-C76
45	H	401	3PE	C11-O13-P-O14
45	L	703	3PE	C1-O11-P-O14
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C11-O13-P-O14
45	d	202	3PE	C1-O11-P-O14
46	A	204	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	H	402	PC1	C11-C12-N-C14
46	M	605	PC1	C1-O11-P-O14
46	g	201	PC1	C11-C12-N-C15
52	O	403	CDL	CA3-OA5-PA1-OA4
52	O	403	CDL	CB3-OB5-PB2-OB3
52	X	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	CB2-OB2-PB2-OB3
52	d	201	CDL	CB3-OB5-PB2-OB3
45	M	604	3PE	O32-C31-C32-C33
46	H	403	PC1	C2-C3-O31-C31
45	Y	202	3PE	O11-C1-C2-C3
46	h	202	PC1	C27-C28-C29-C2A
45	Y	204	3PE	O13-C11-C12-N
45	m	202	3PE	O13-C11-C12-N
45	L	702	3PE	O32-C31-C32-C33
45	M	603	3PE	O22-C21-C22-C23
46	I	204	PC1	O32-C31-C32-C33
52	O	403	CDL	C72-C71-CB7-OB9
45	L	703	3PE	O21-C21-C22-C23
45	Y	205	3PE	C37-C38-C39-C3A
47	Y	207	PLC	C7'-C8'-C9'-CA'
45	Y	203	3PE	O22-C21-C22-C23
46	A	204	PC1	C38-C39-C3A-C3B
46	d	203	PC1	C23-C24-C25-C26
45	Y	202	3PE	C3F-C3G-C3H-C3I
45	A	202	3PE	O22-C21-C22-C23
46	H	402	PC1	O32-C31-C32-C33
52	O	403	CDL	C52-C51-CB5-OB7
45	I	203	3PE	C12-C11-O13-P
46	H	403	PC1	C12-C11-O13-P
46	h	202	PC1	C12-C11-O13-P
47	g	202	PLC	C5-C4-O4P-P
47	A	205	PLC	C2B-C1B-CB-OB
47	M	606	PLC	C2B-C1B-CB-OB
45	d	202	3PE	C35-C36-C37-C38
45	f	102	3PE	C33-C34-C35-C36
46	I	204	PC1	C11-C12-N-C15
47	Z	204	PLC	C4-C5-N-C8
46	A	204	PC1	O21-C21-C22-C23
46	h	202	PC1	O21-C21-C22-C23
45	H	401	3PE	O21-C21-C22-C23
45	Y	205	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	f	102	3PE	O21-C21-C22-C23
46	d	203	PC1	O21-C21-C22-C23
47	B	203	PLC	O2-C'-C1'-C2'
45	m	202	3PE	C23-C24-C25-C26
46	B	202	PC1	C29-C2A-C2B-C2C
45	Y	203	3PE	O32-C31-C32-C33
52	M	602	CDL	C72-C71-CB7-OB9
52	d	201	CDL	C1-CA2-OA2-PA1
45	A	201	3PE	C22-C23-C24-C25
45	Y	204	3PE	C39-C3A-C3B-C3C
52	h	201	CDL	C71-C72-C73-C74
45	J	201	3PE	O11-C1-C2-O21
45	Y	206	3PE	O11-C1-C2-O21
45	Y	201	3PE	O31-C31-C32-C33
46	q	201	PC1	O31-C31-C32-C33
46	m	203	PC1	C2B-C2C-C2D-C2E
45	Y	201	3PE	O32-C31-C32-C33
45	Y	205	3PE	O22-C21-C22-C23
46	d	203	PC1	O22-C21-C22-C23
46	h	202	PC1	O22-C21-C22-C23
46	B	202	PC1	O31-C31-C32-C33
46	q	201	PC1	C38-C39-C3A-C3B
45	L	703	3PE	O22-C21-C22-C23
46	L	704	PC1	C3A-C3B-C3C-C3D
45	N	401	3PE	O21-C21-C22-C23
47	Z	204	PLC	O2-C'-C1'-C2'
52	X	201	CDL	C33-C34-C35-C36
45	H	401	3PE	O22-C21-C22-C23
45	d	202	3PE	C2F-C2G-C2H-C2I
46	M	605	PC1	C25-C26-C27-C28
46	q	201	PC1	O32-C31-C32-C33
47	B	203	PLC	O'-C'-C1'-C2'
45	Y	202	3PE	O31-C31-C32-C33
45	Y	206	3PE	O31-C31-C32-C33
46	H	403	PC1	O31-C31-C32-C33
46	L	704	PC1	O21-C21-C22-C23

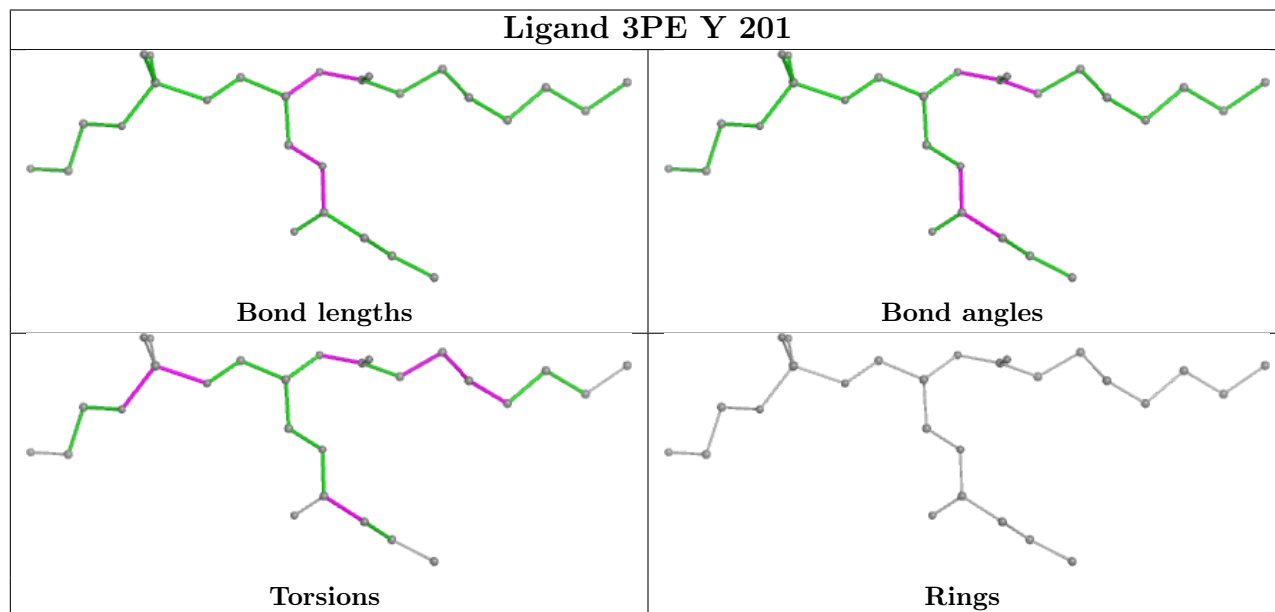
All (1) ring outliers are listed below:

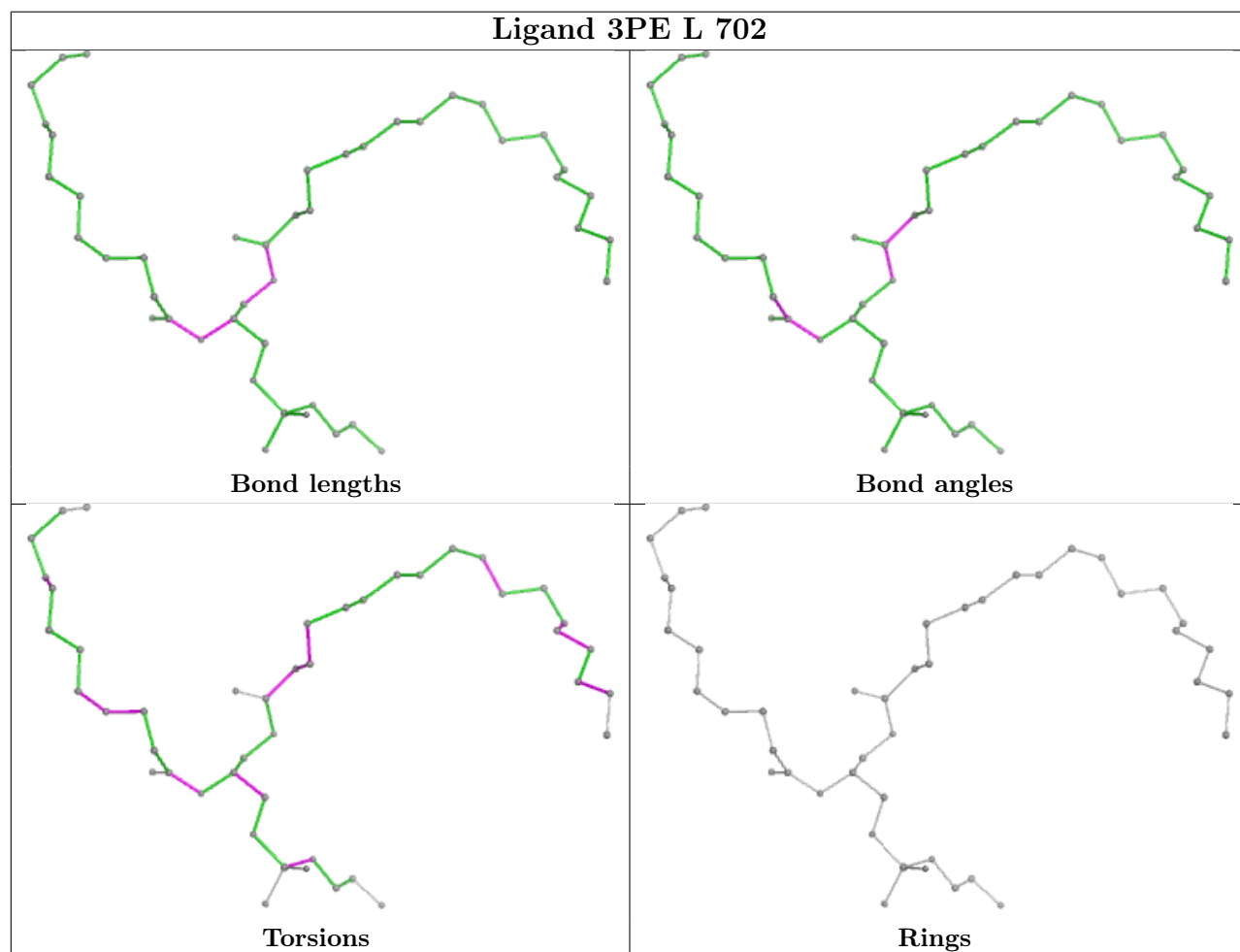
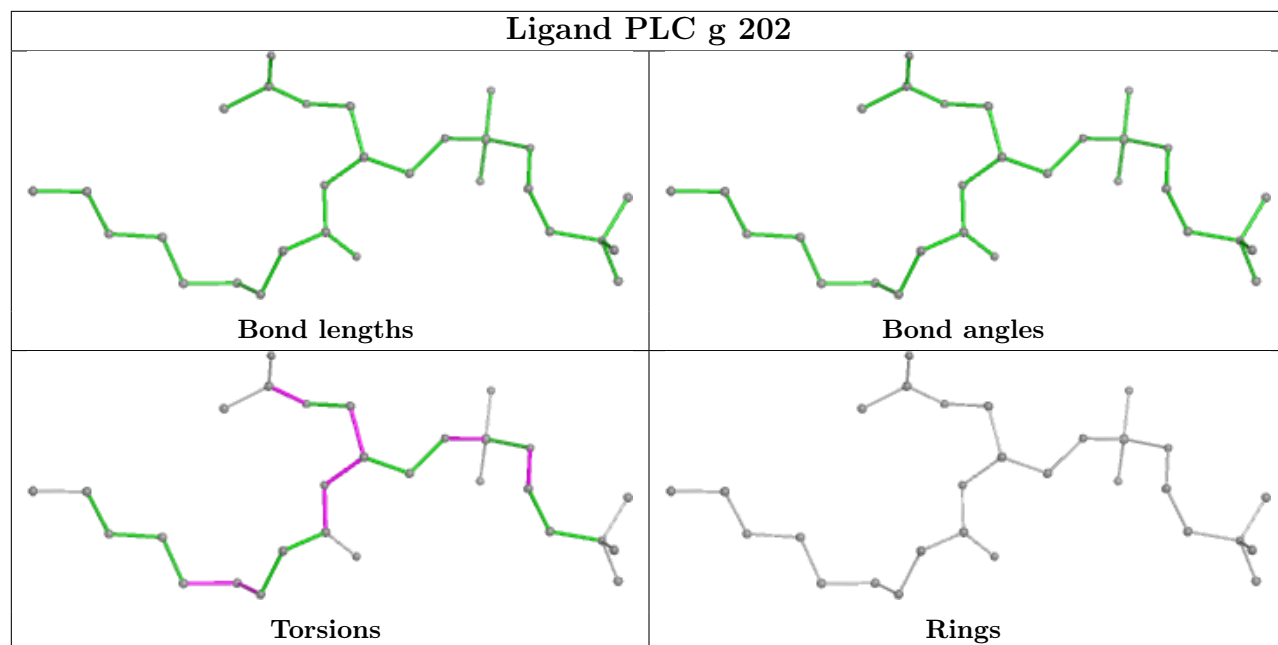
Mol	Chain	Res	Type	Atoms
58	i	201	CHD	C1-C10-C2-C3-C4-C5

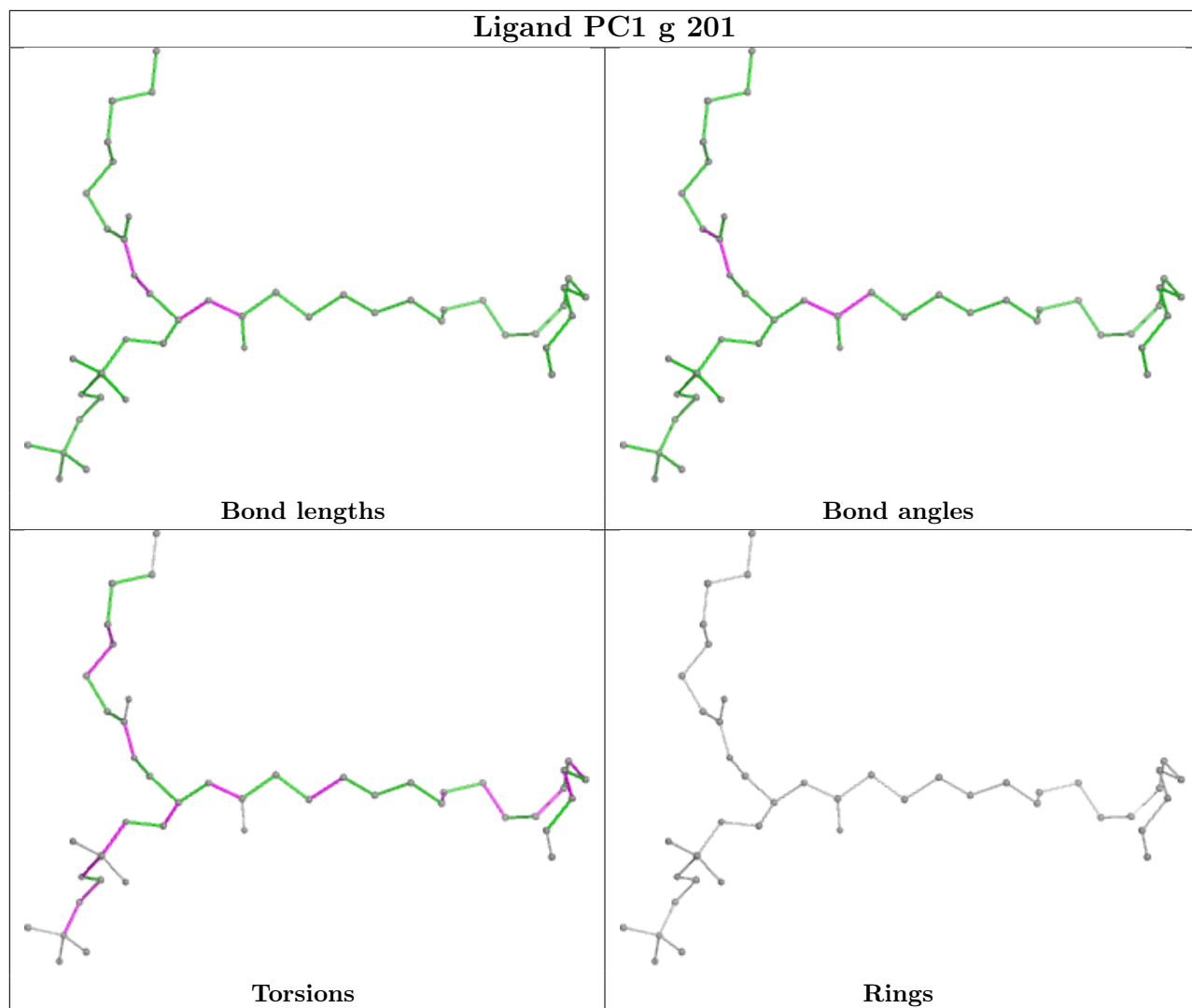
11 monomers are involved in 19 short contacts:

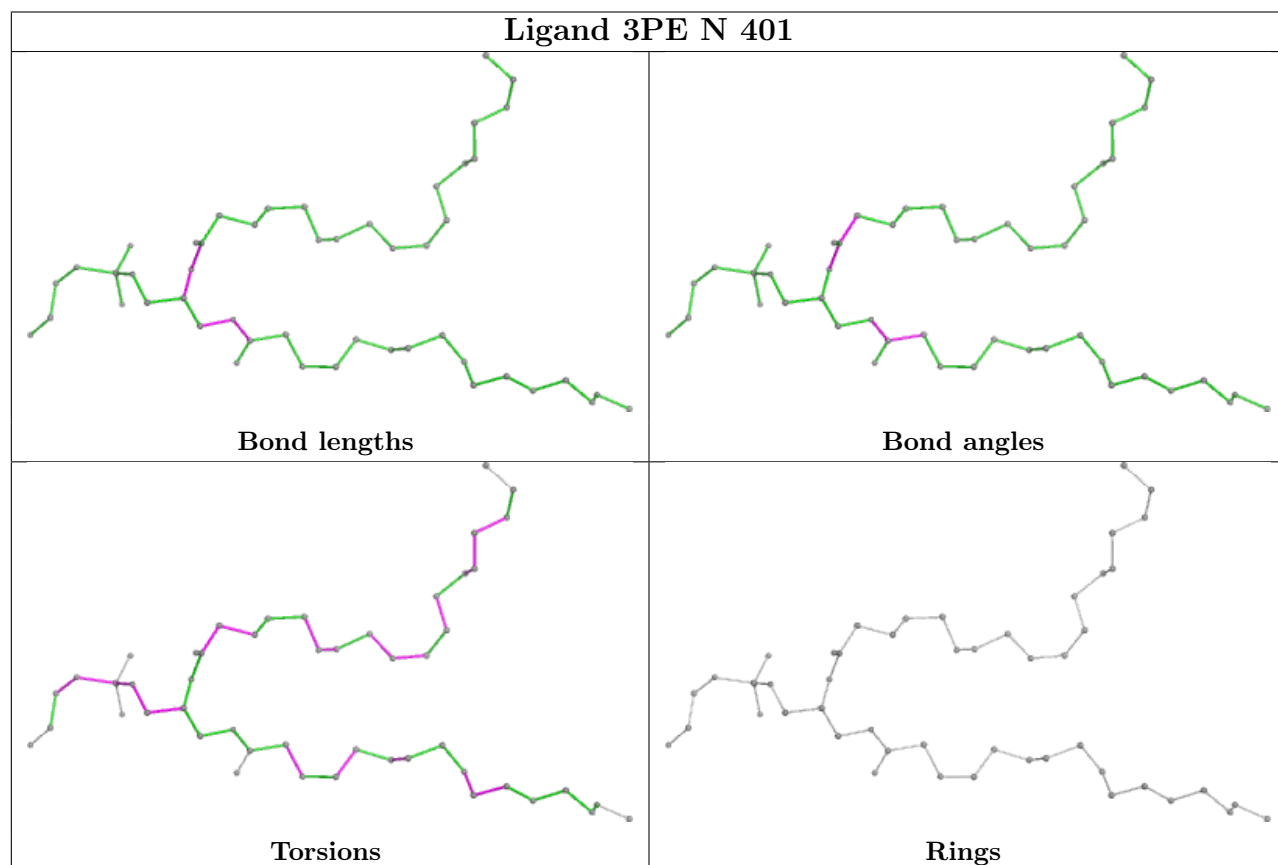
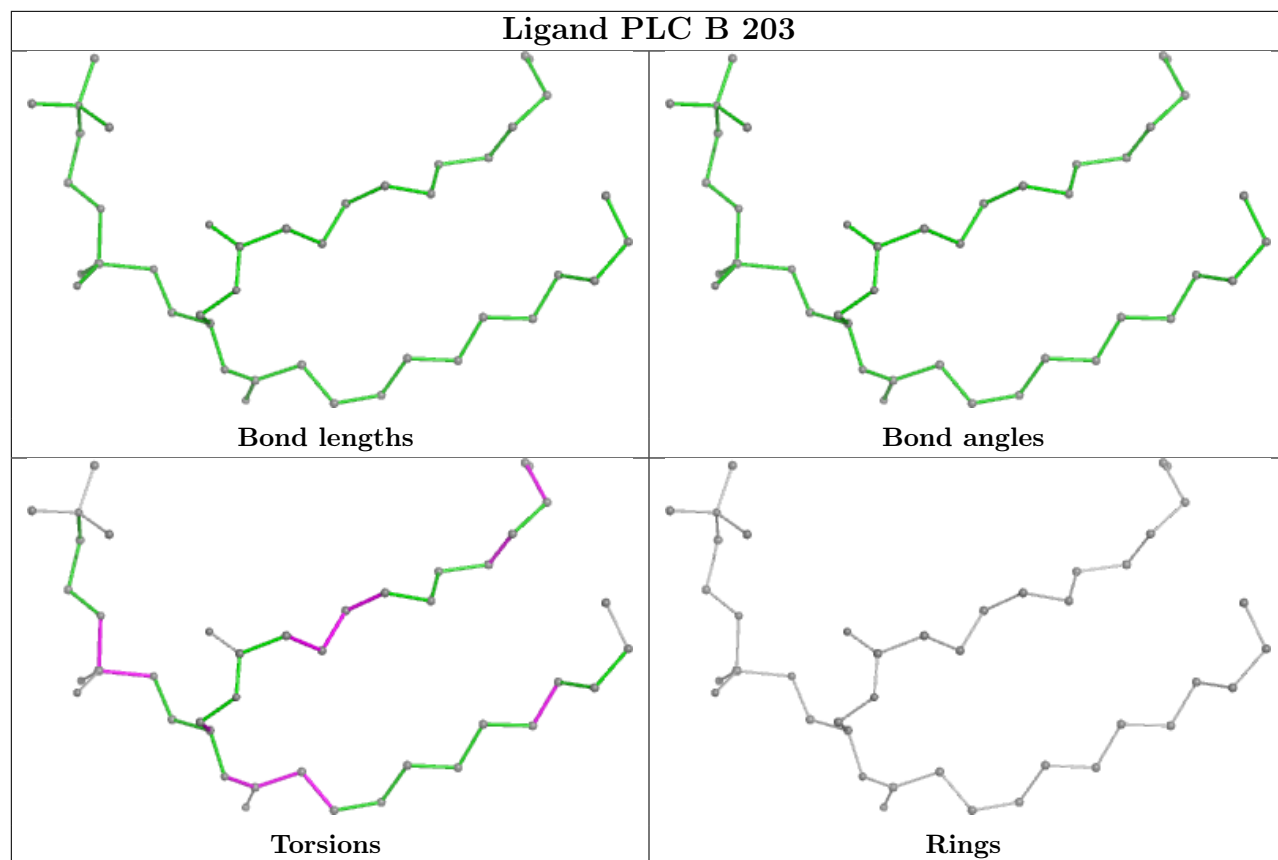
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	X	201	CDL	2	0
54	O	401	DGT	4	0
45	Y	202	3PE	1	0
46	H	402	PC1	1	0
46	Z	203	PC1	1	0
46	A	204	PC1	2	0
57	T	101	EHZ	1	0
46	L	704	PC1	1	0
52	M	602	CDL	4	0
48	I	201	SF4	1	0
56	P	501	NDP	3	0

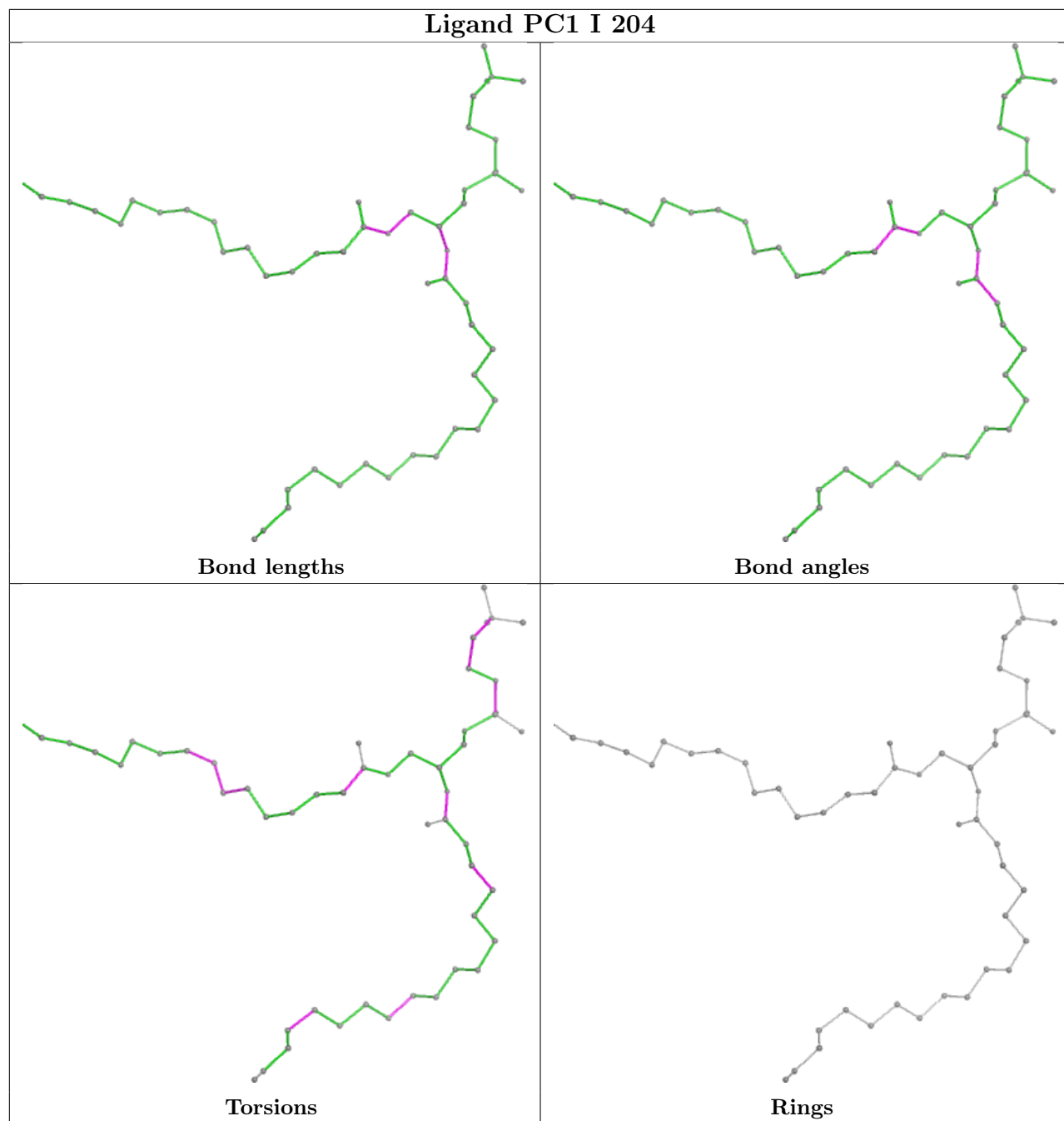
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

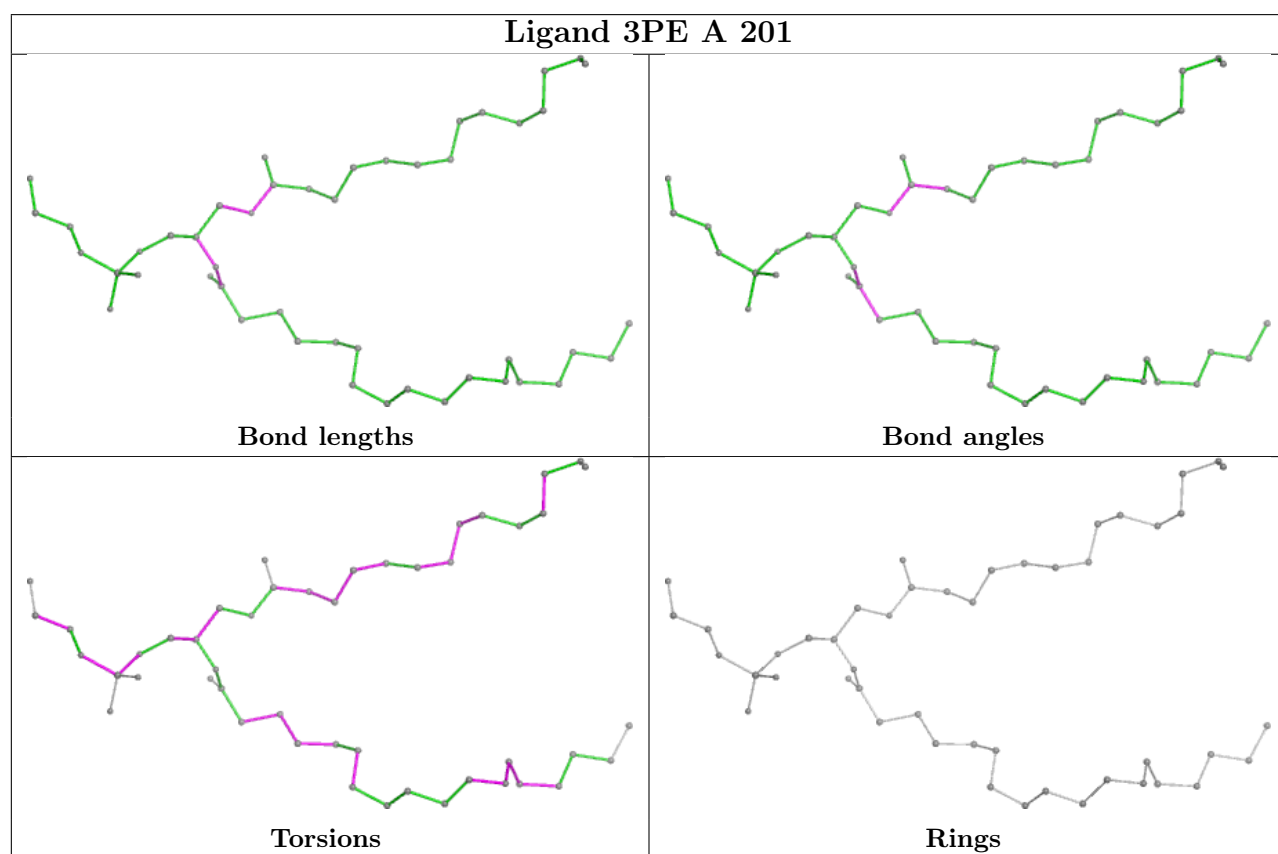
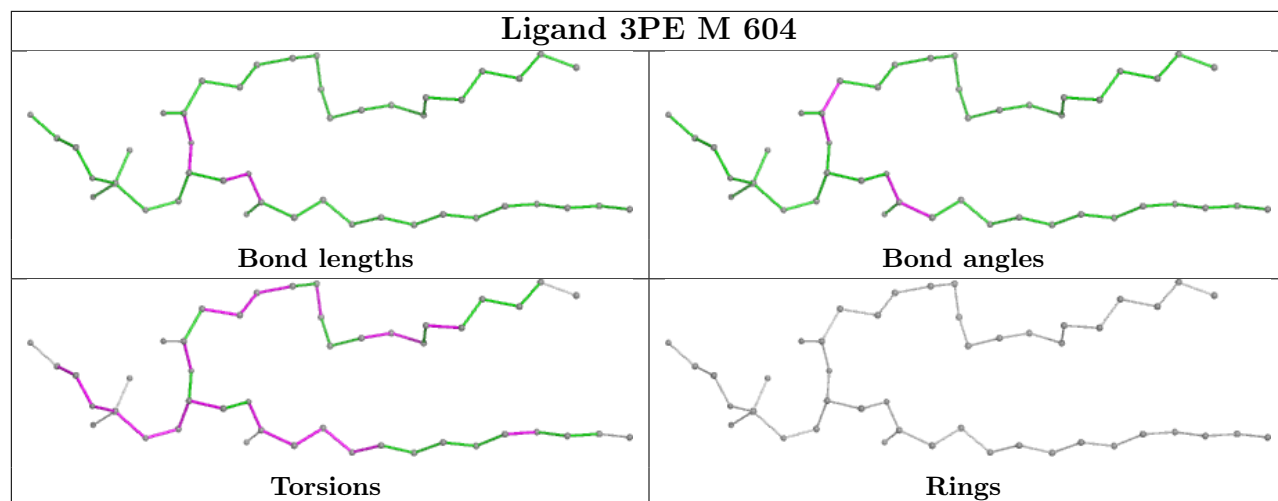


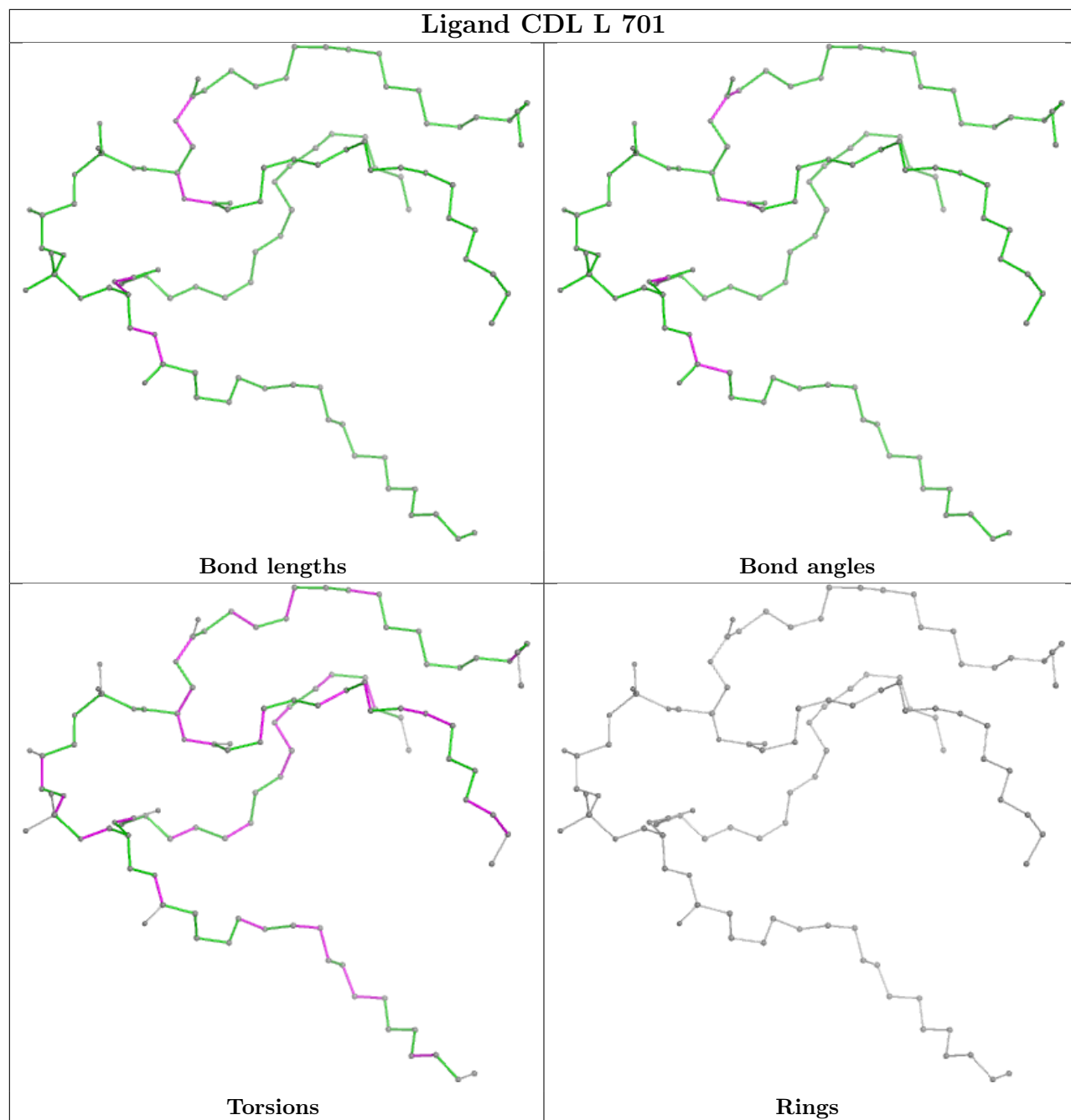


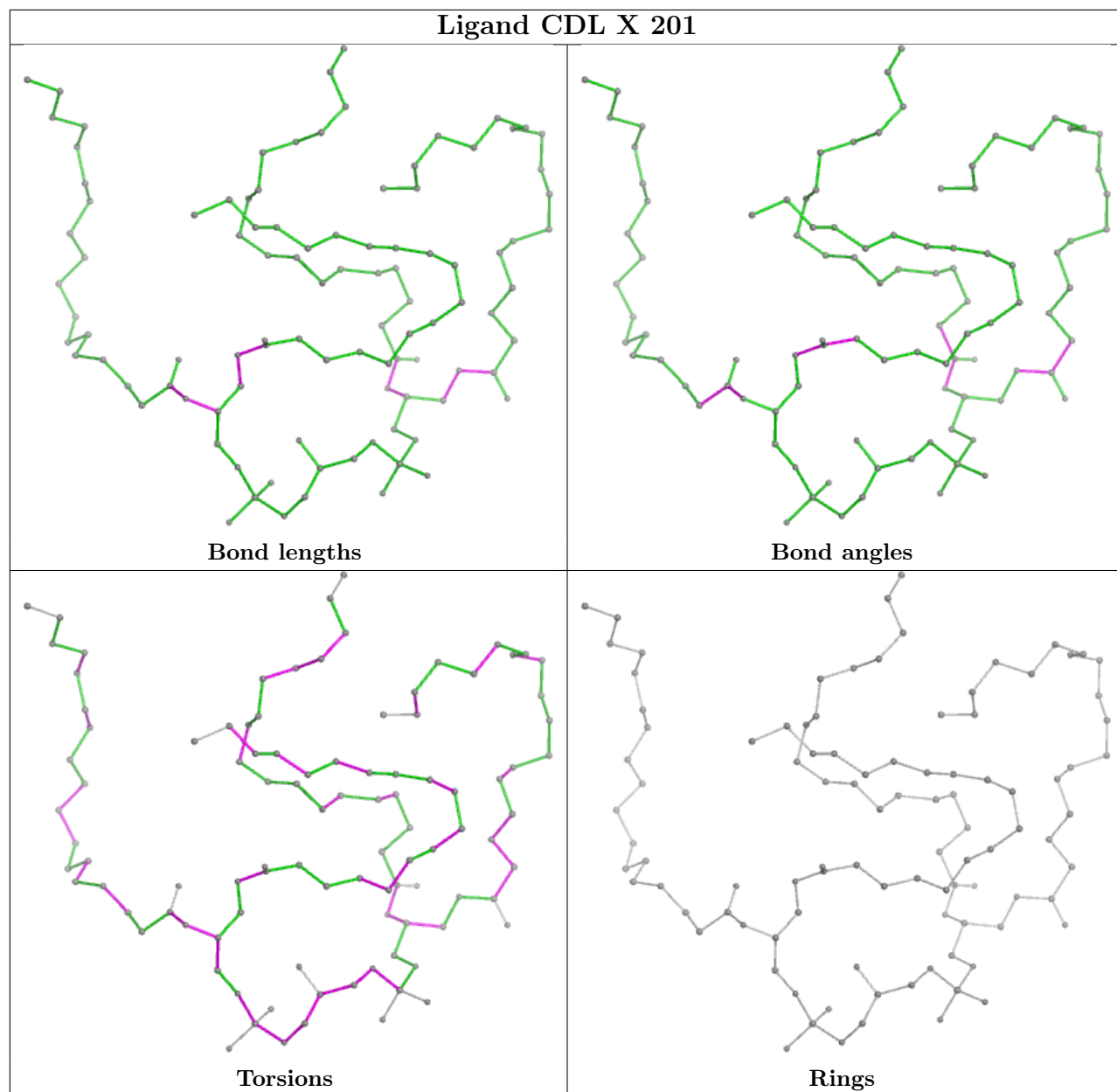


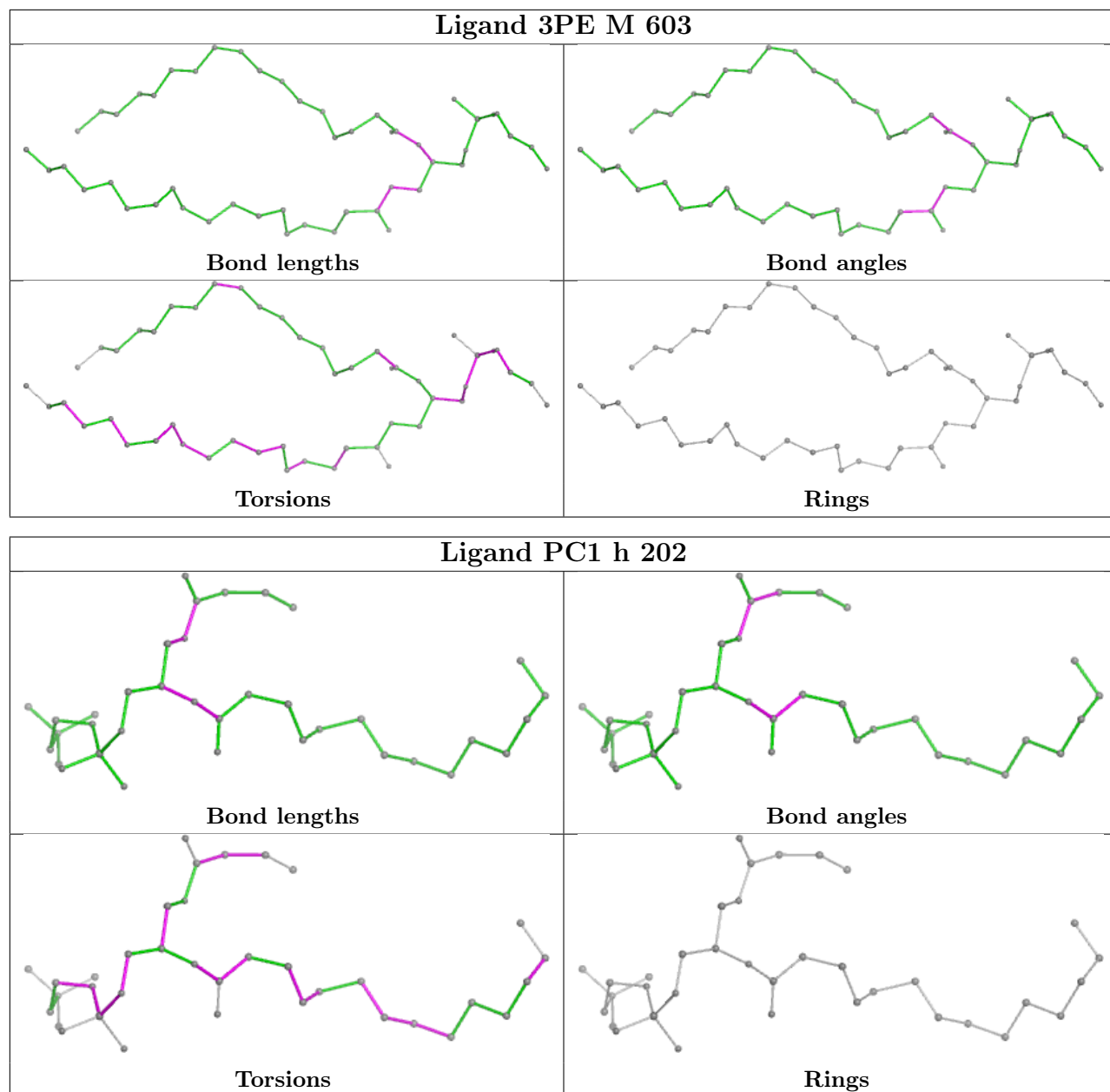


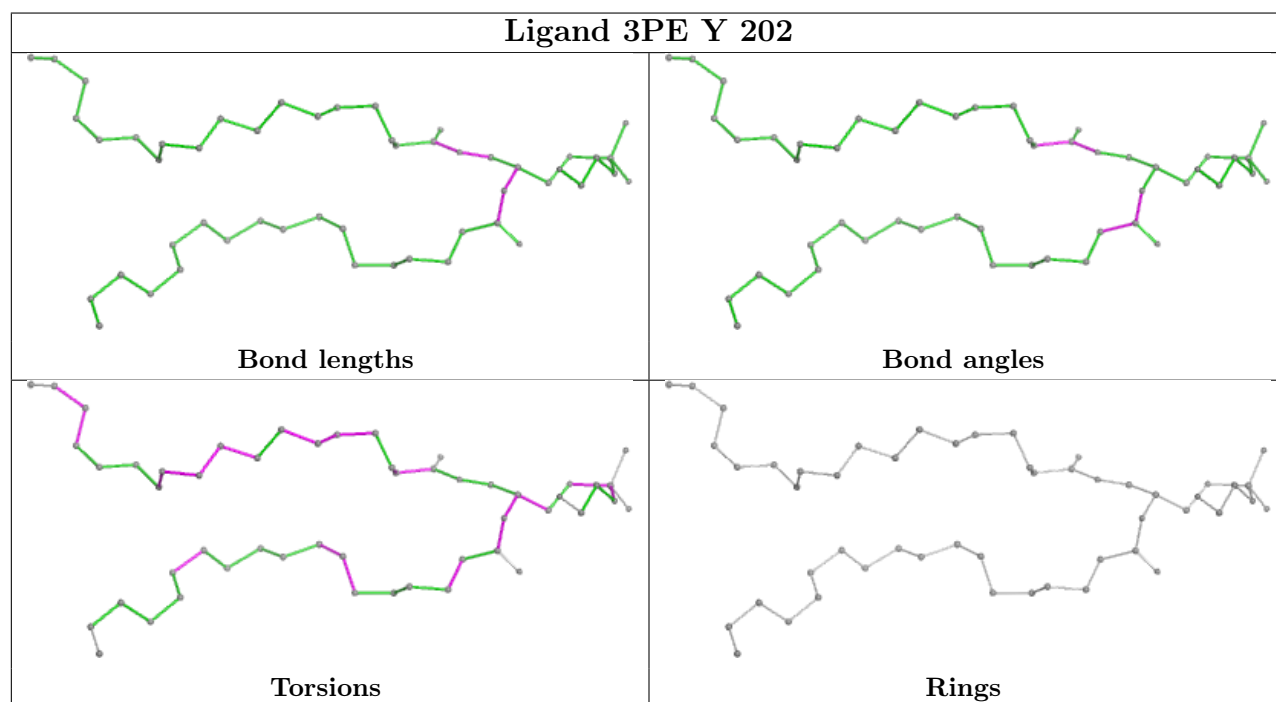
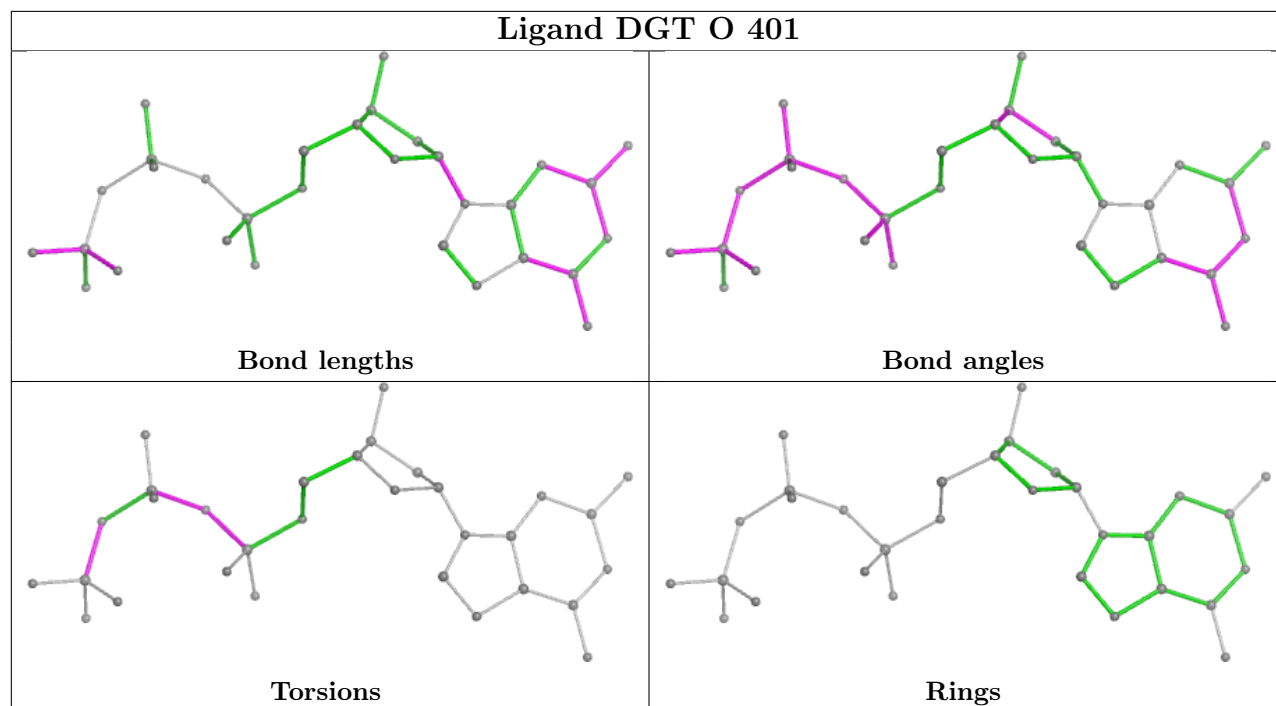


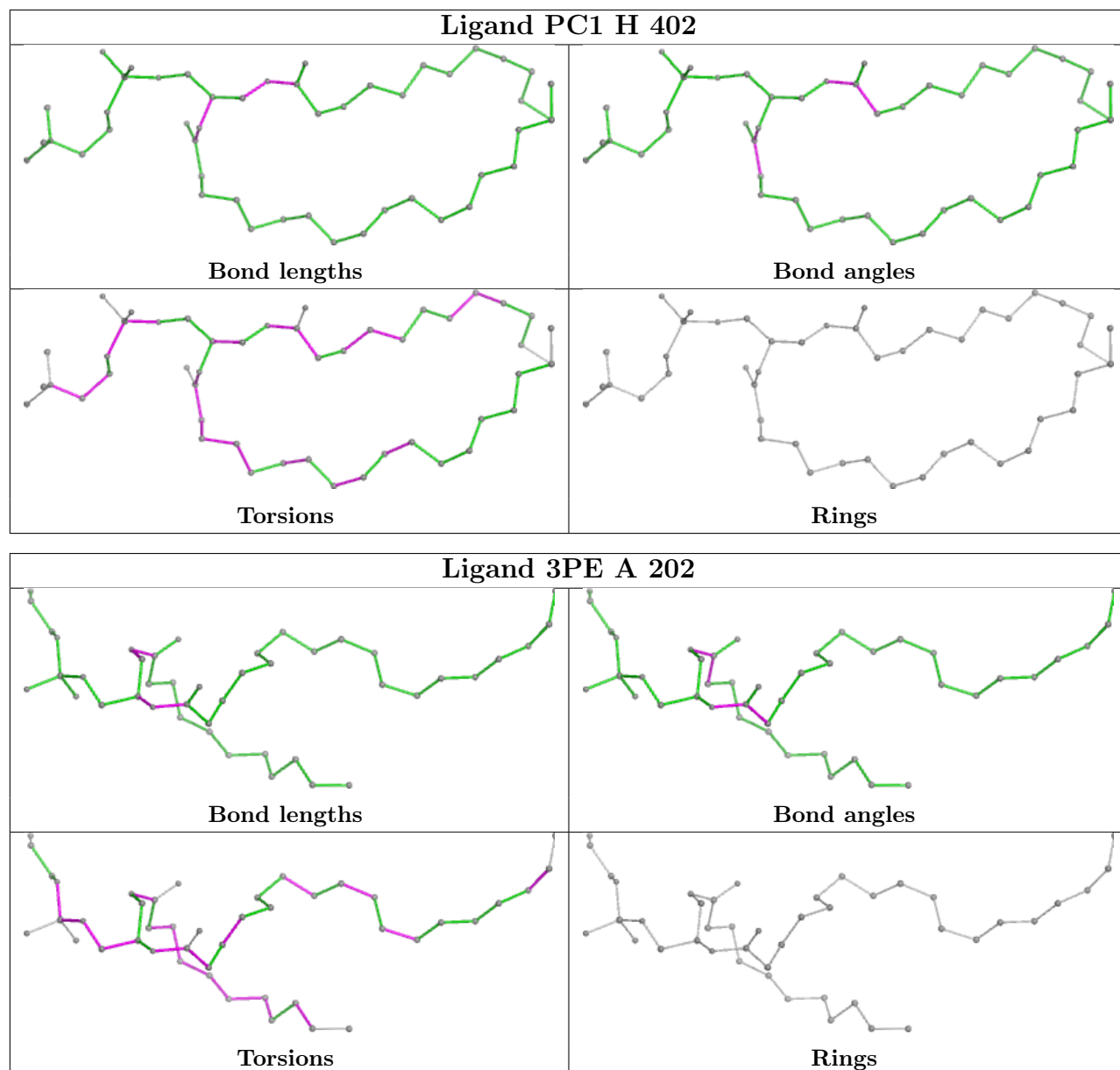


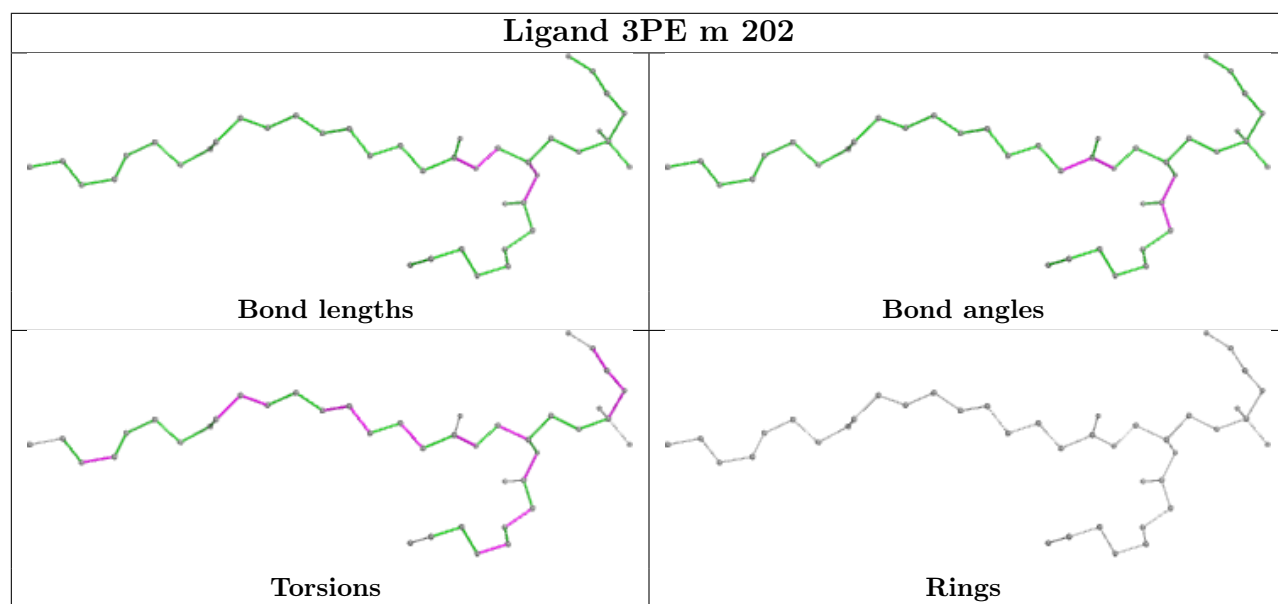
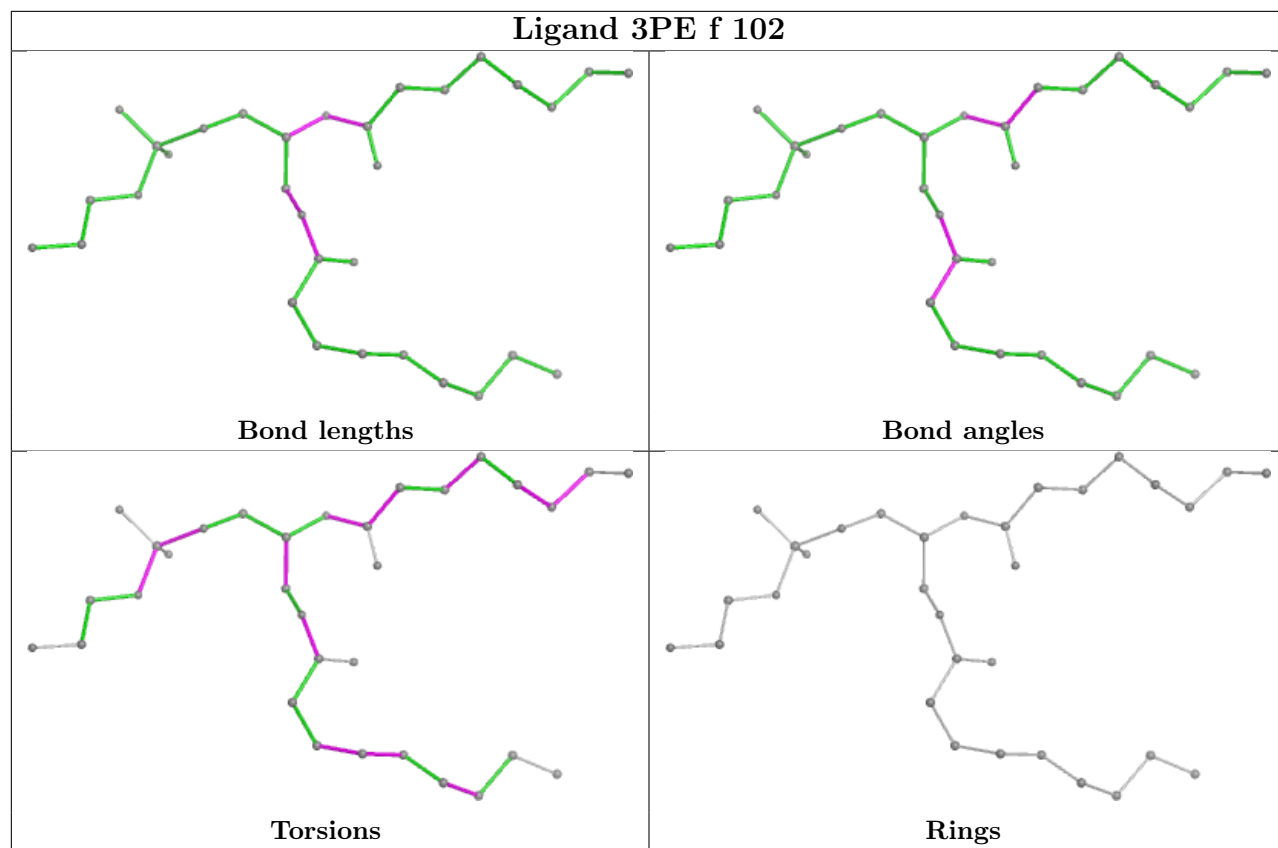


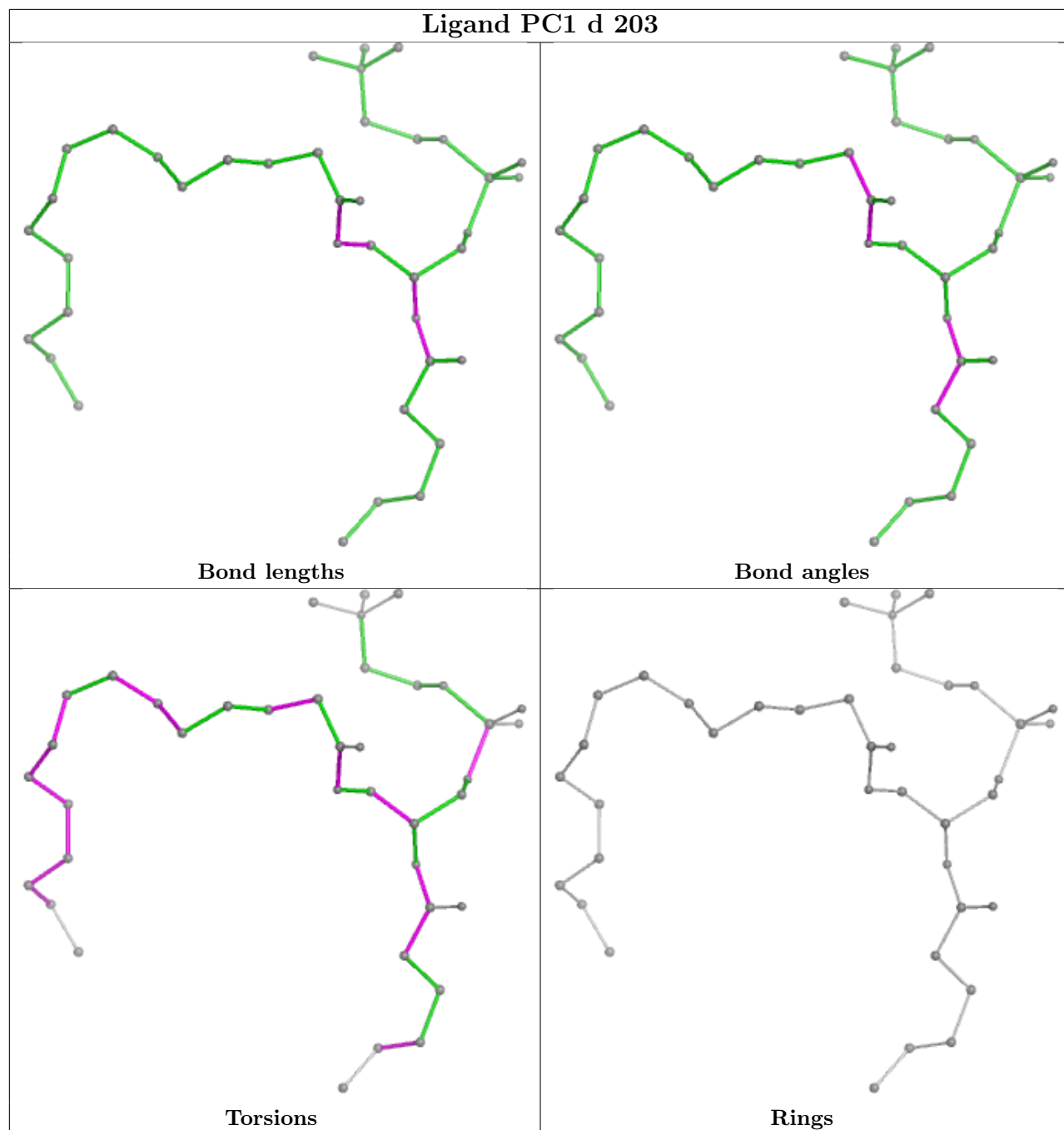


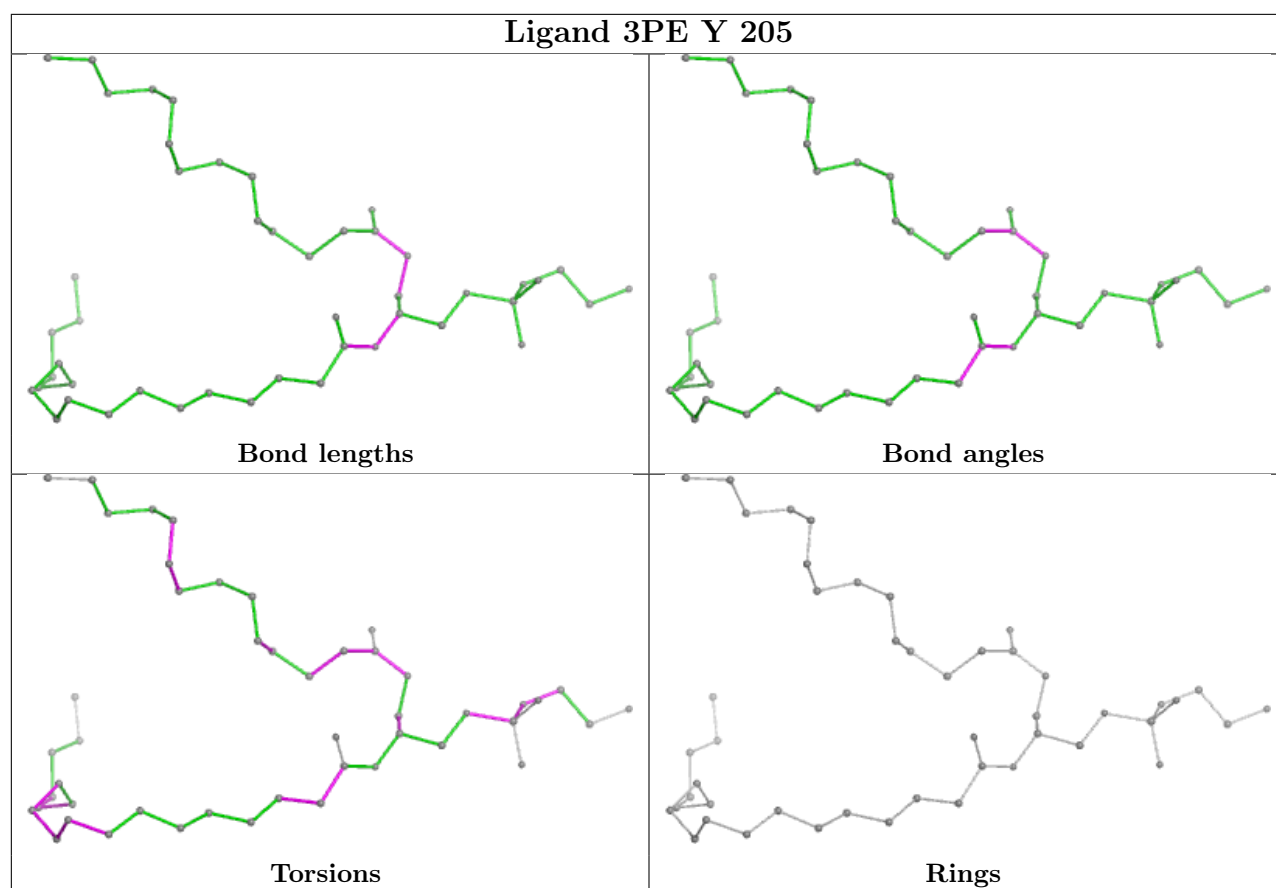
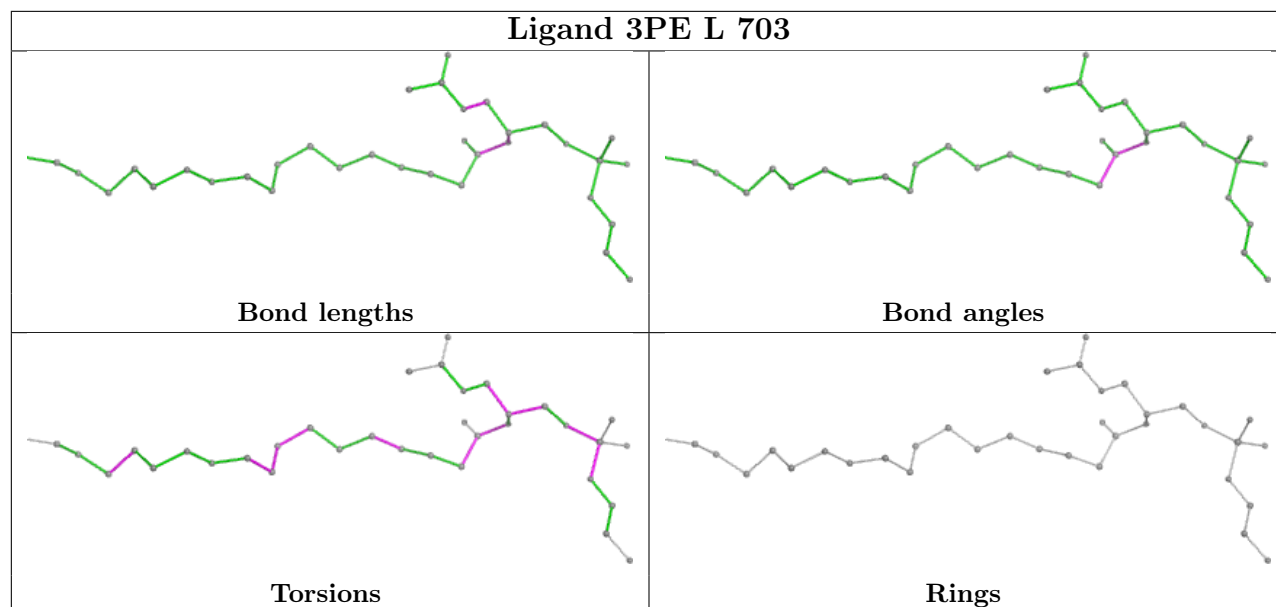


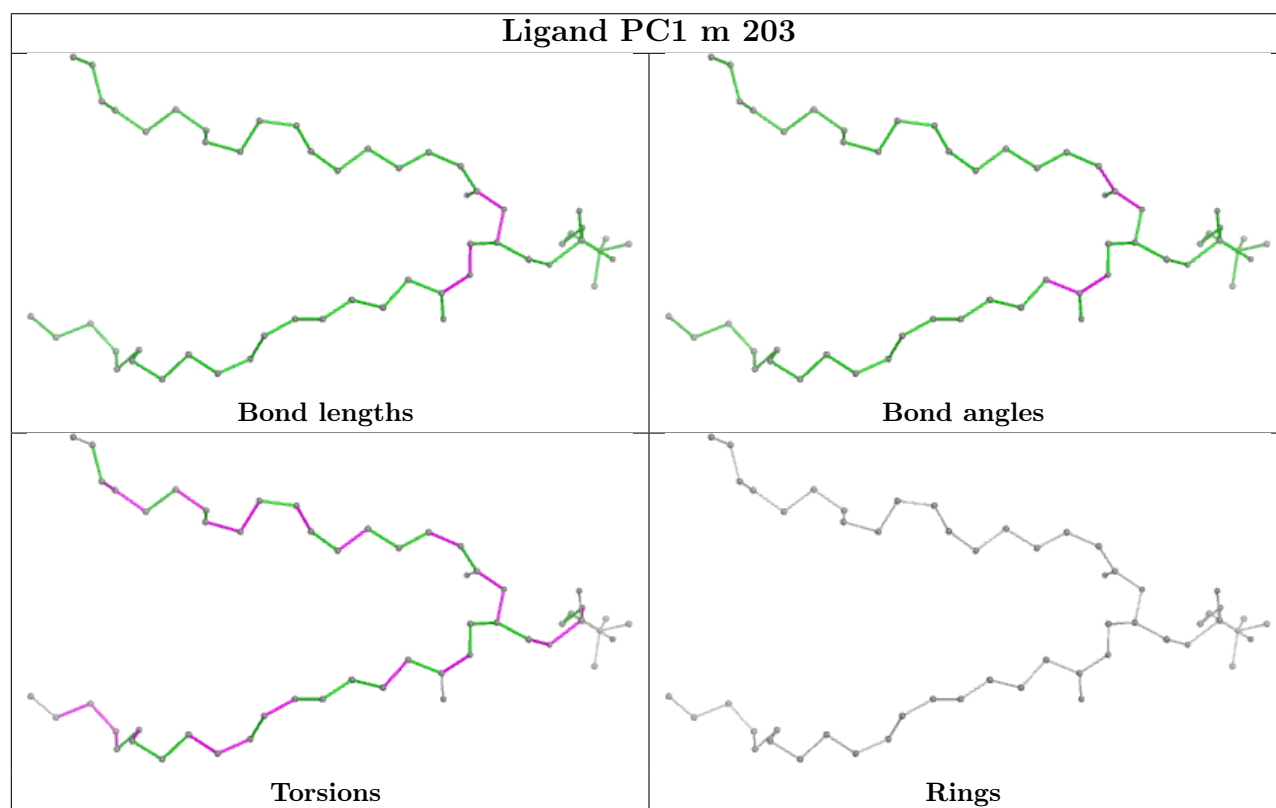
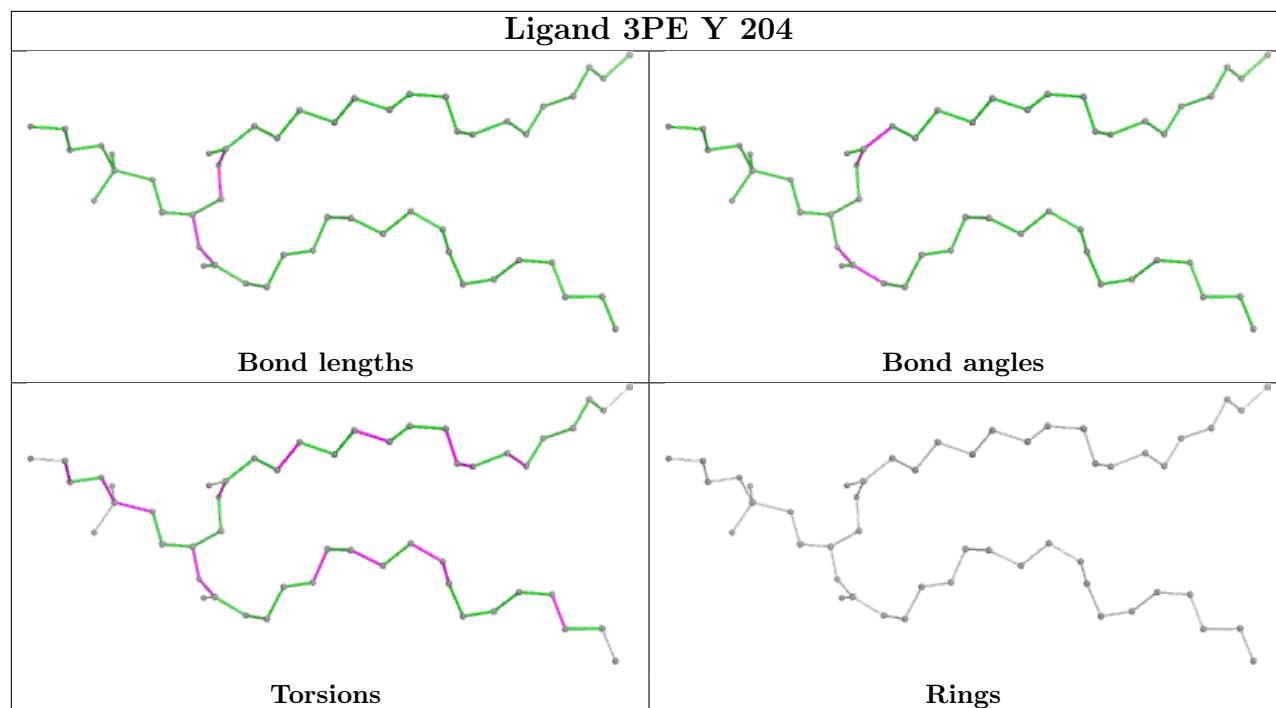


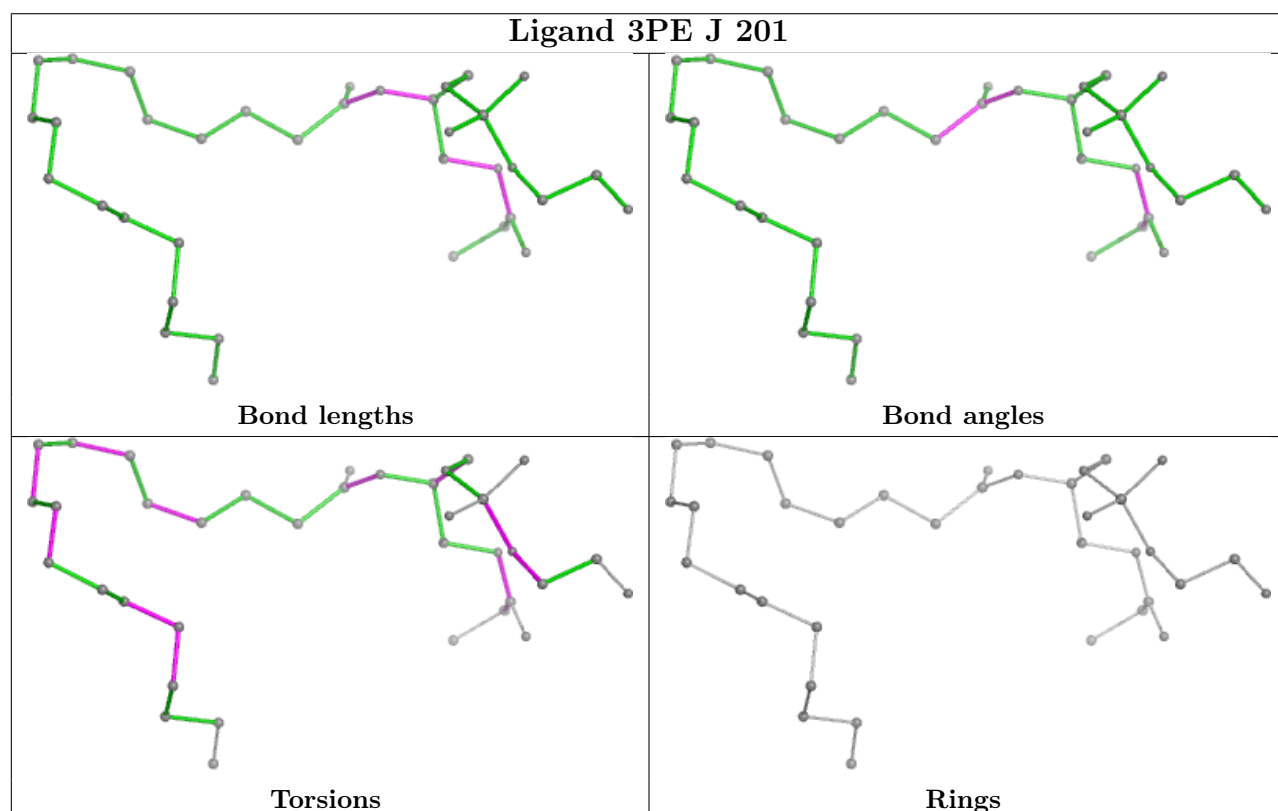
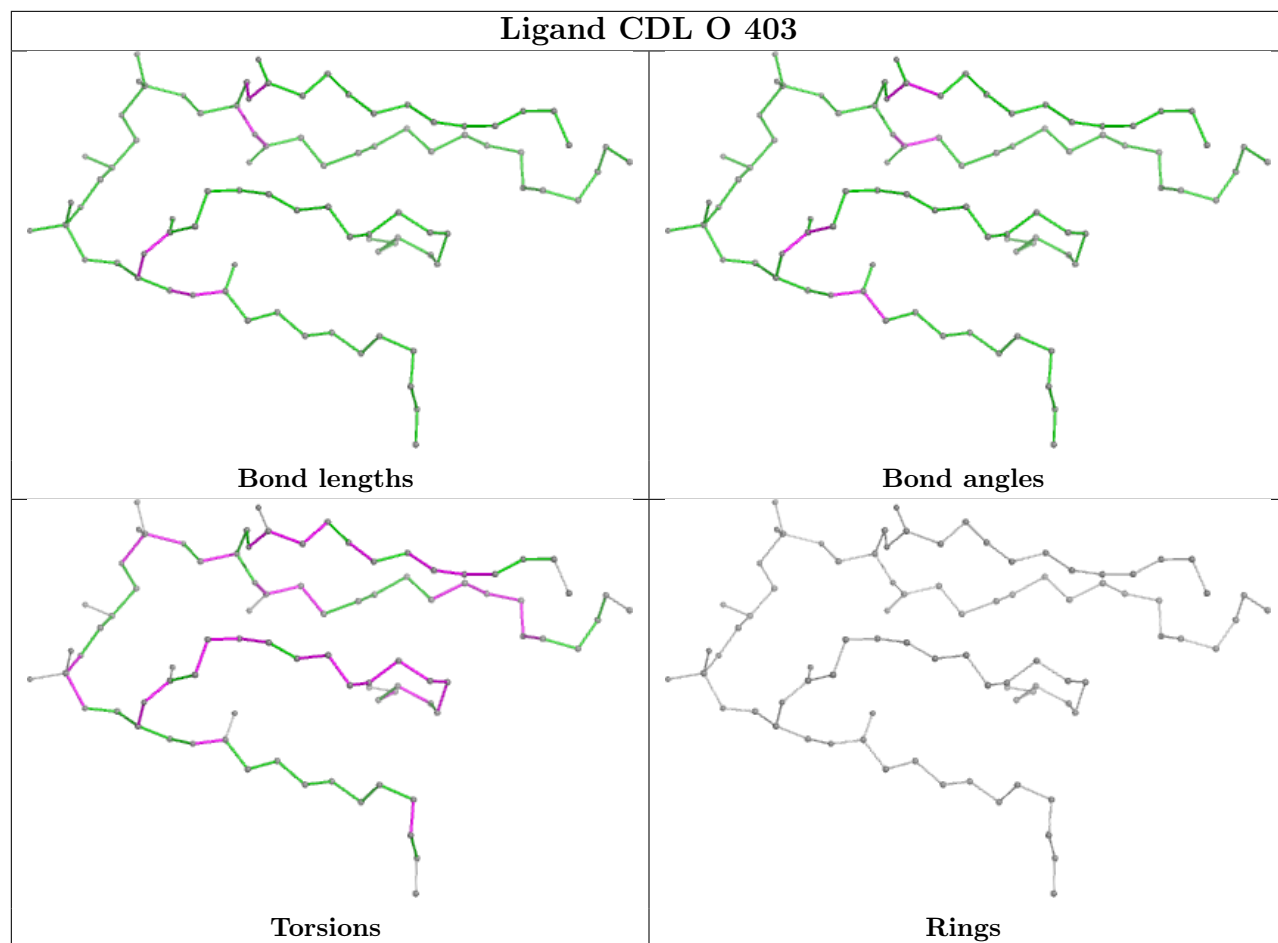


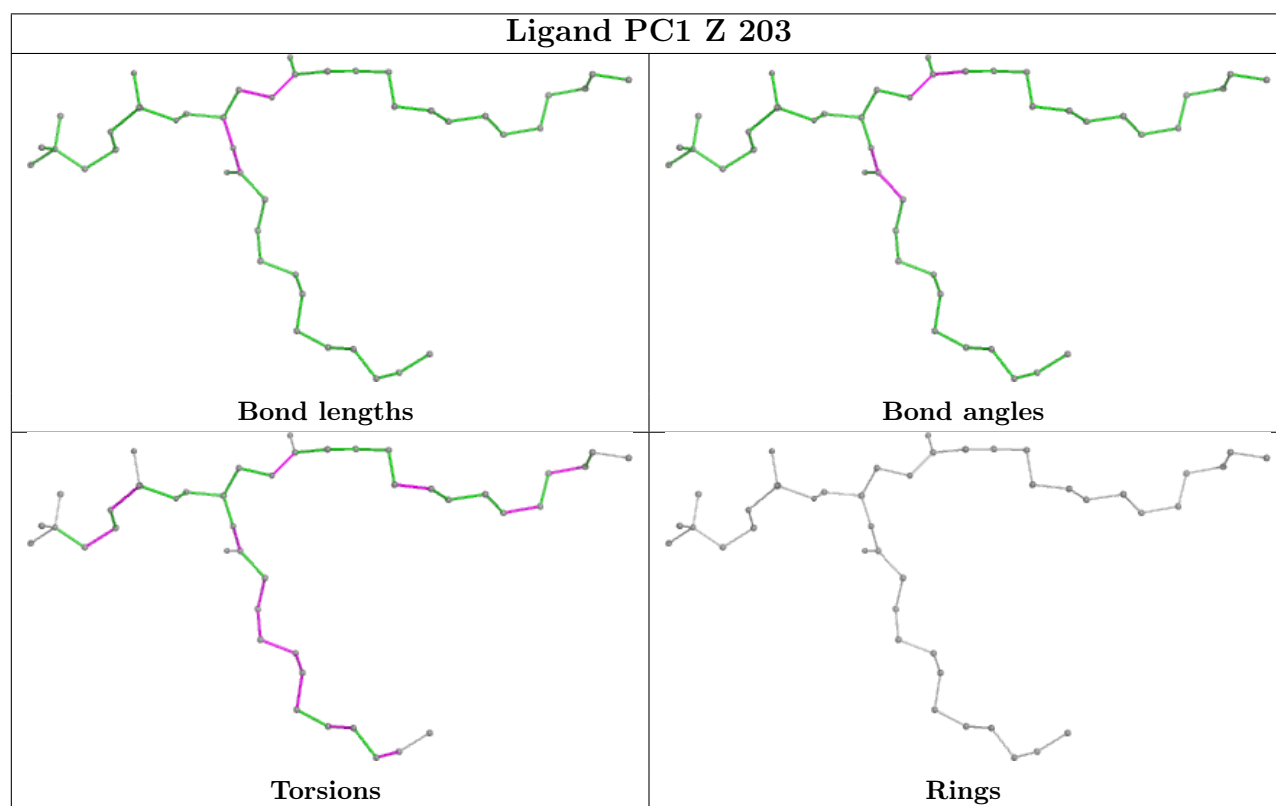
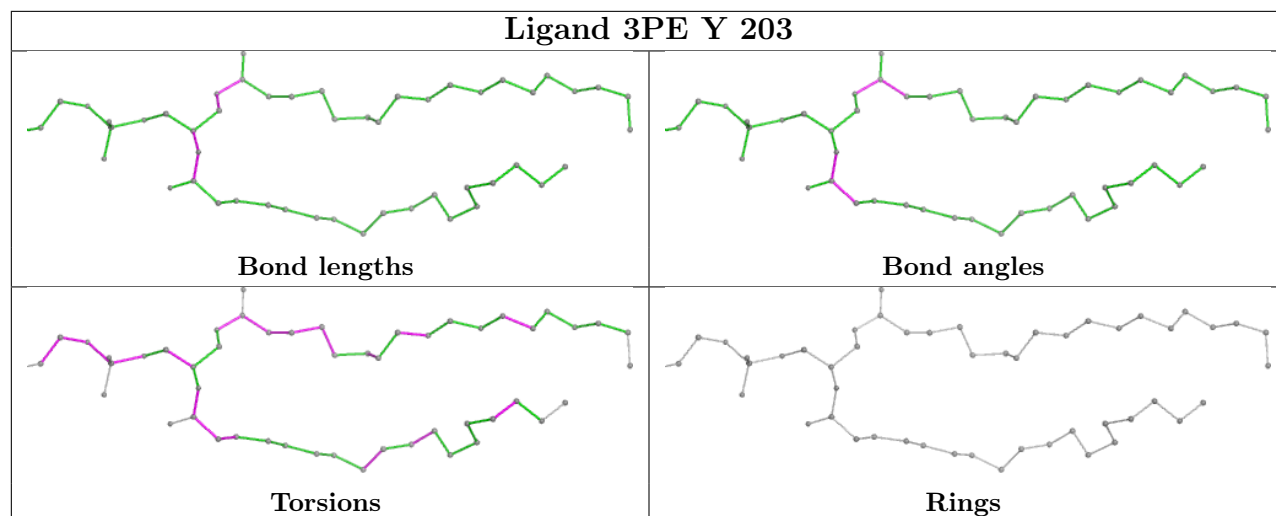


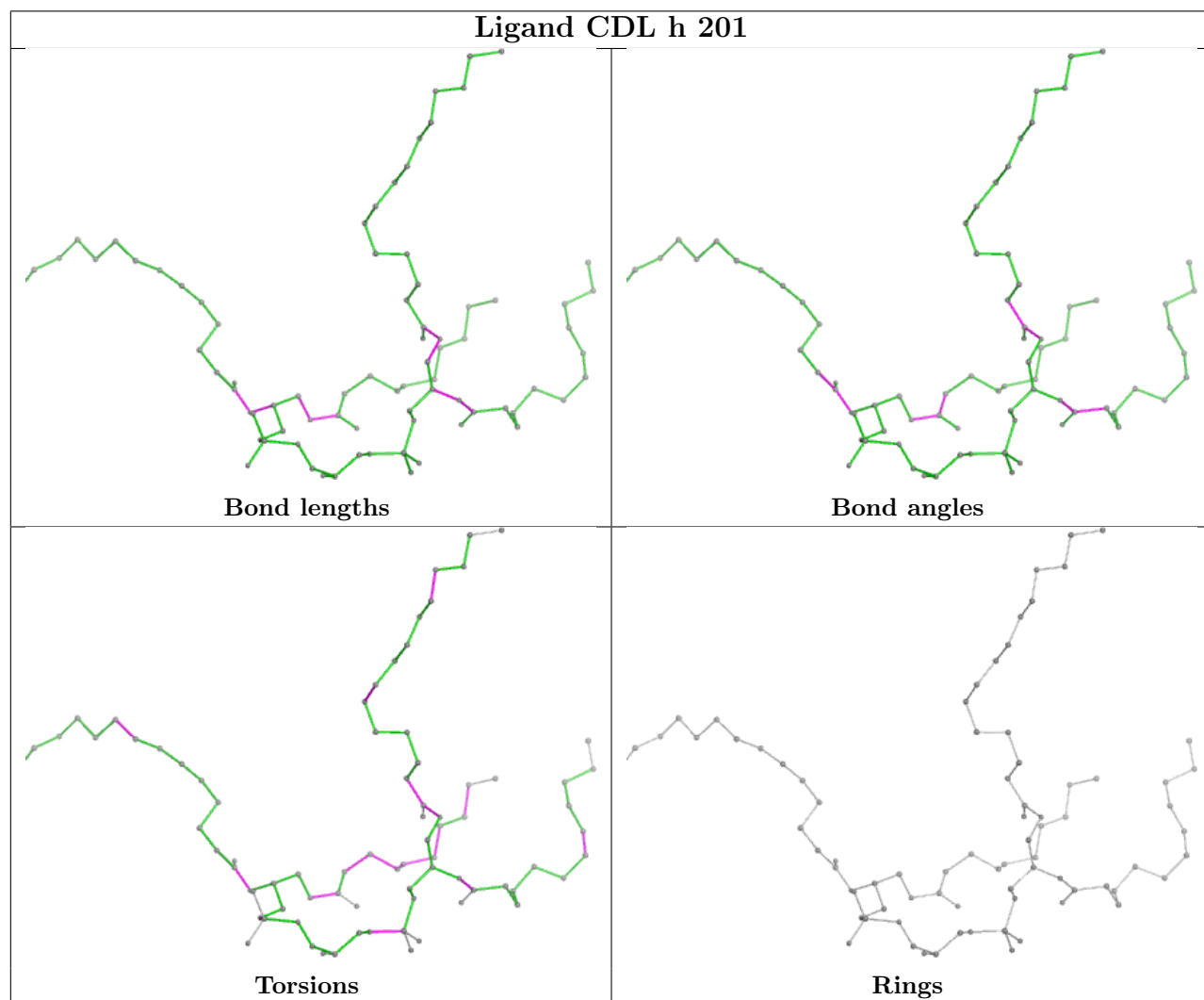
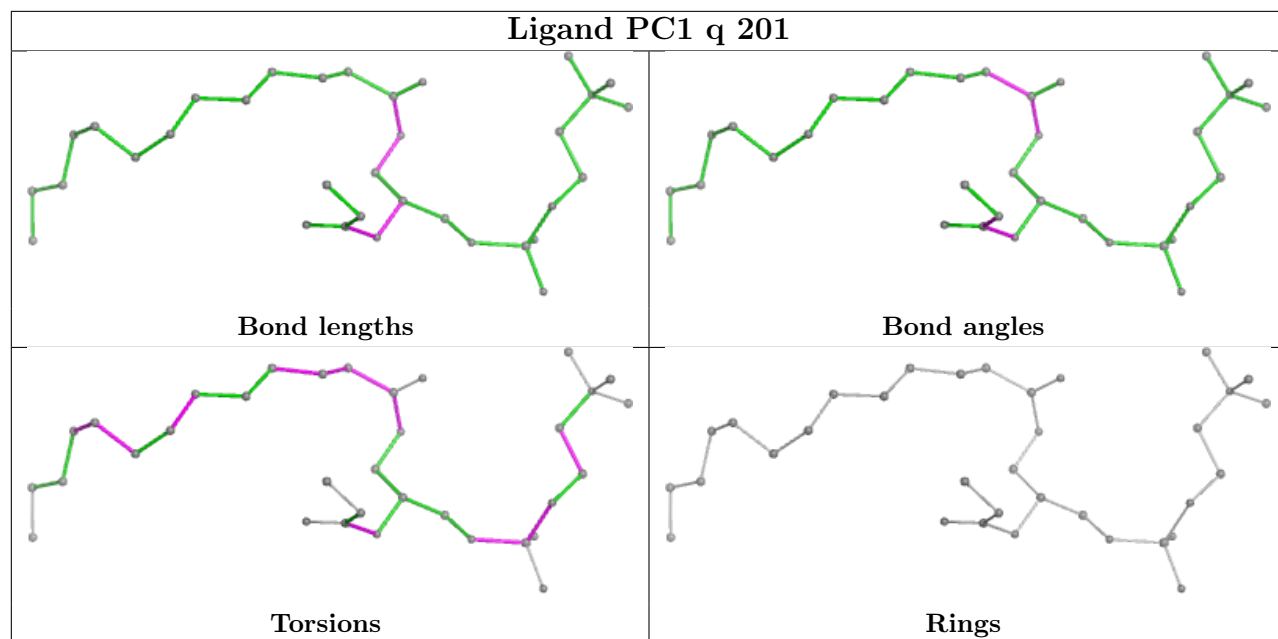


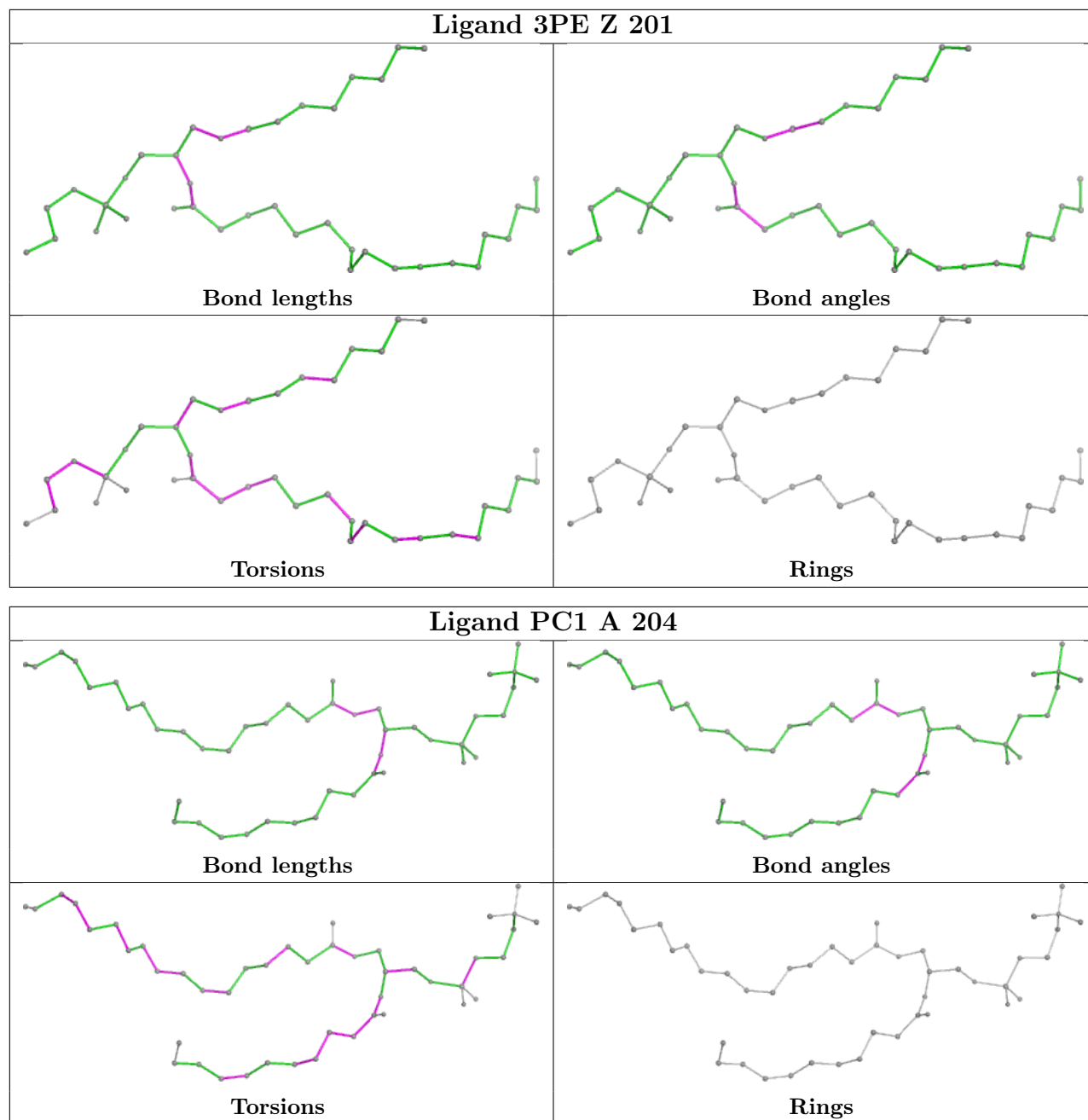


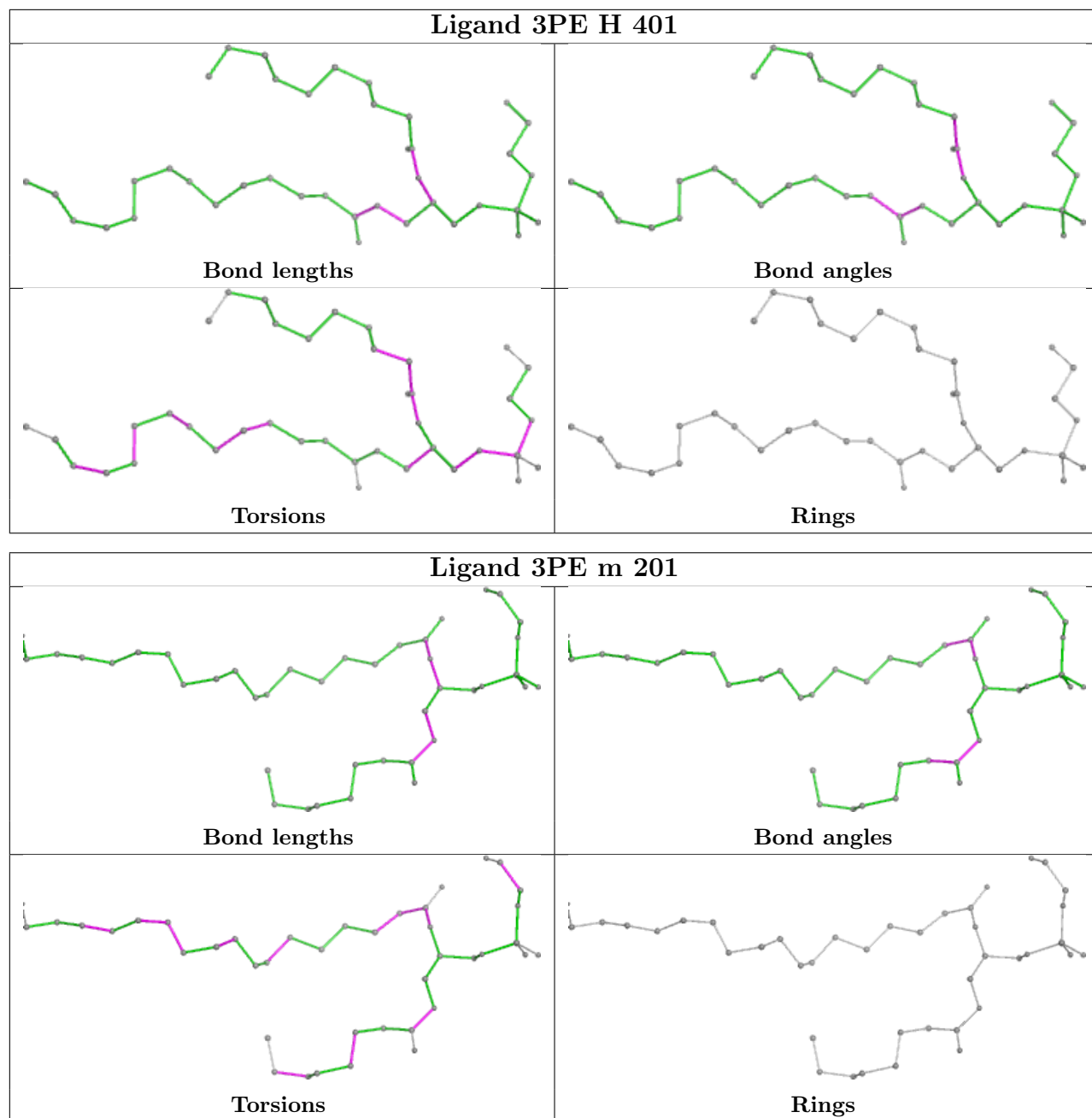


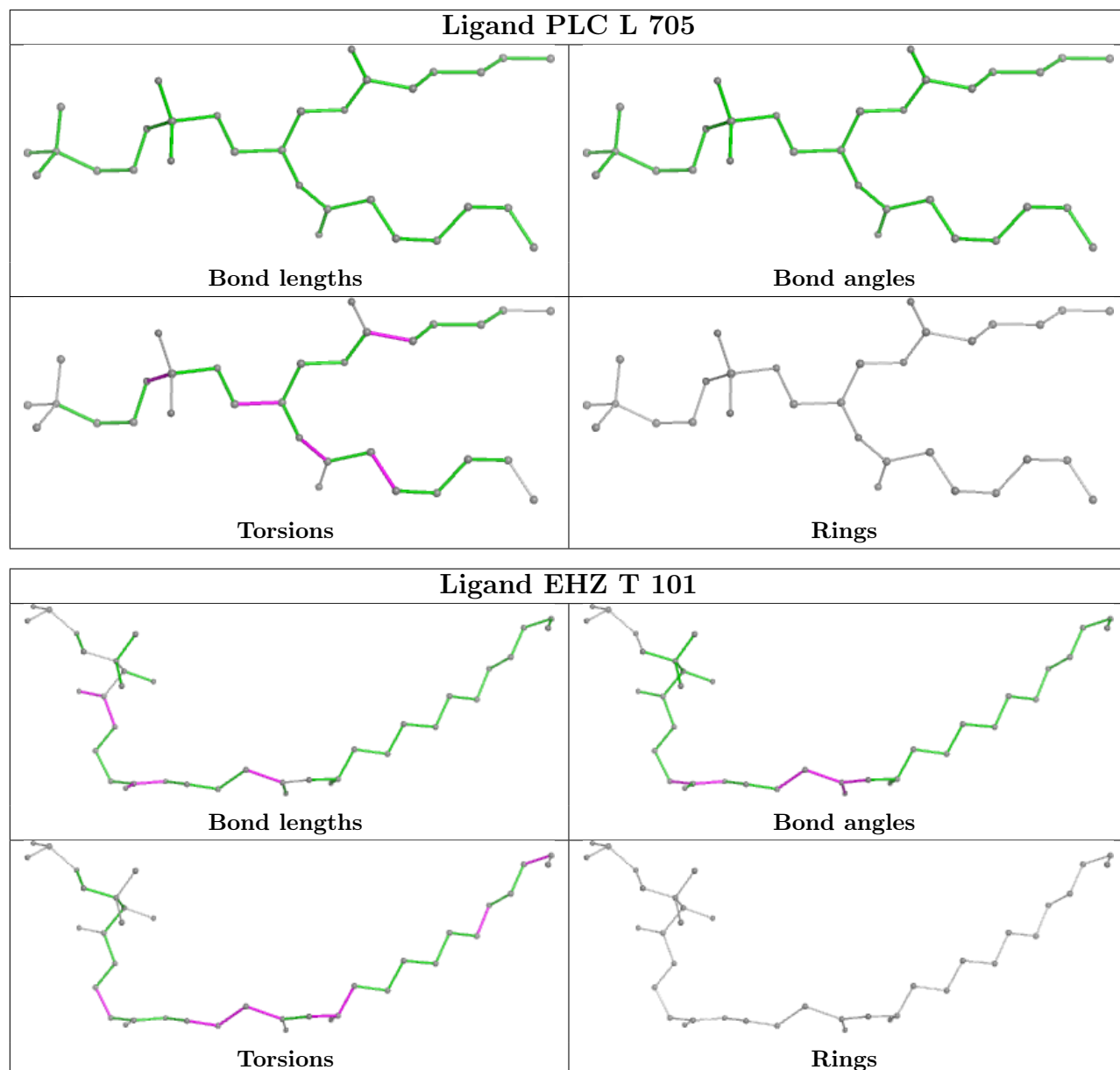


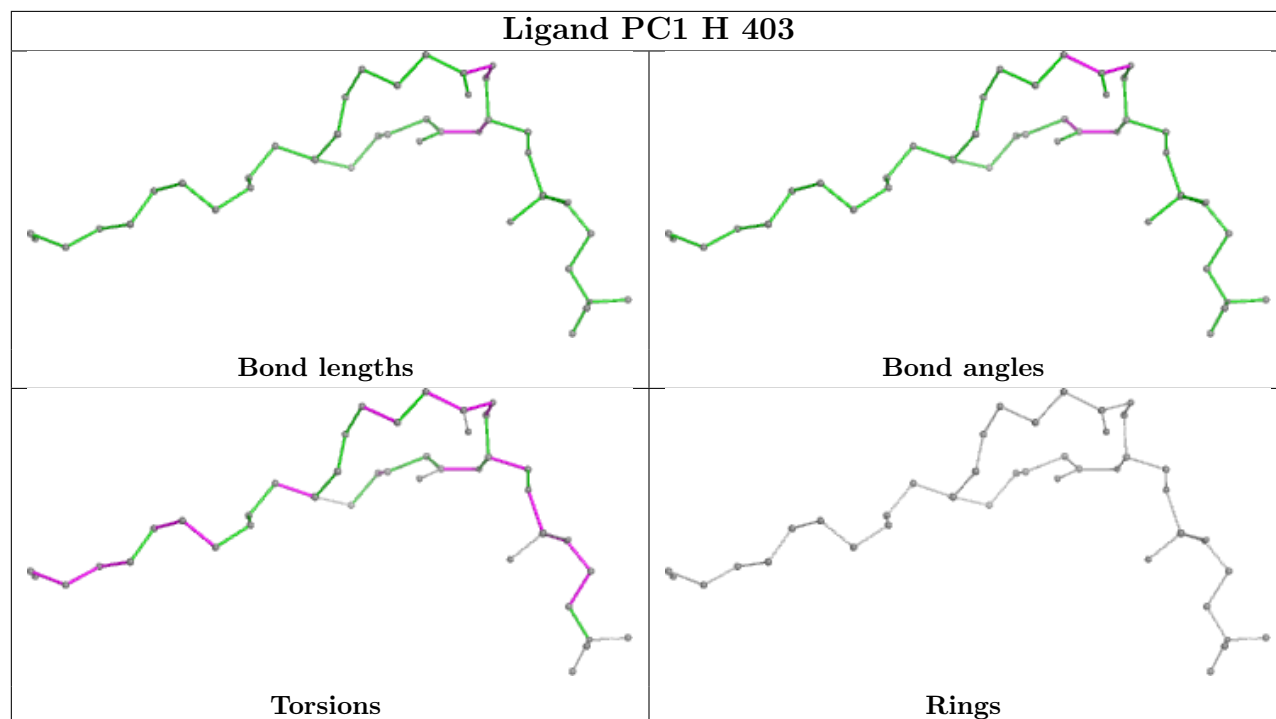
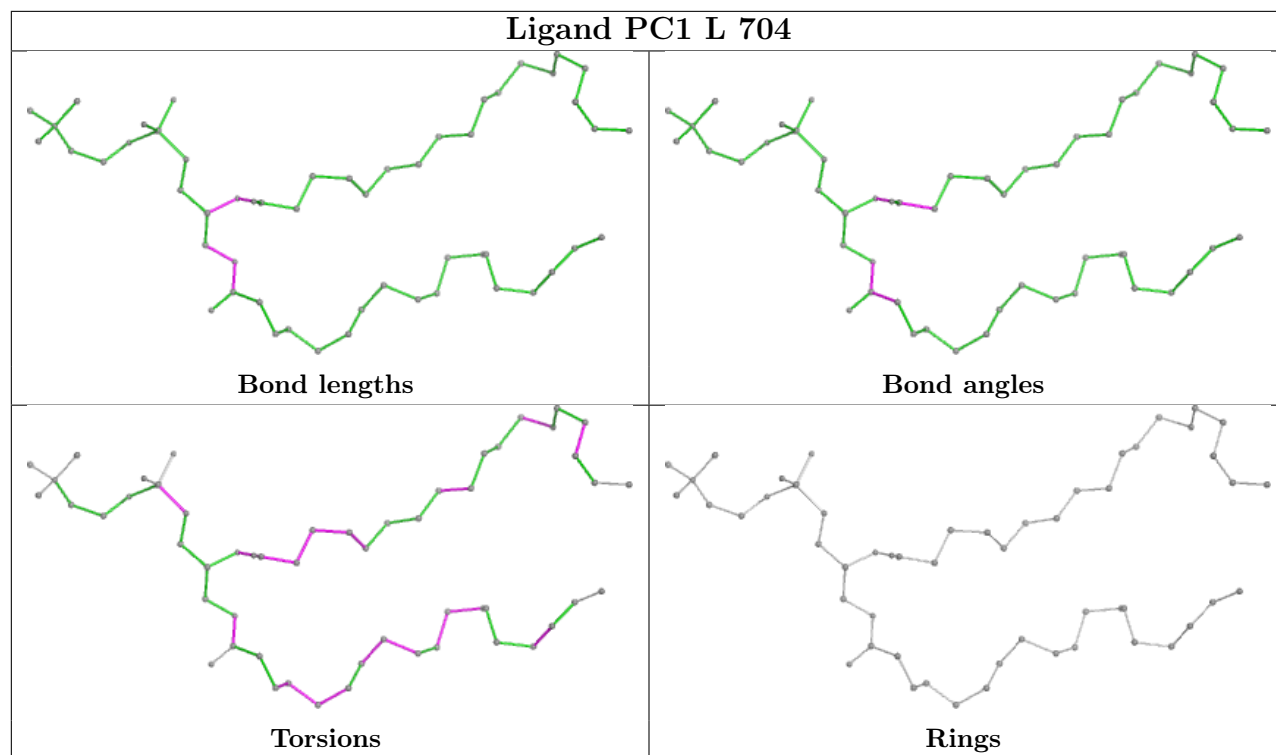


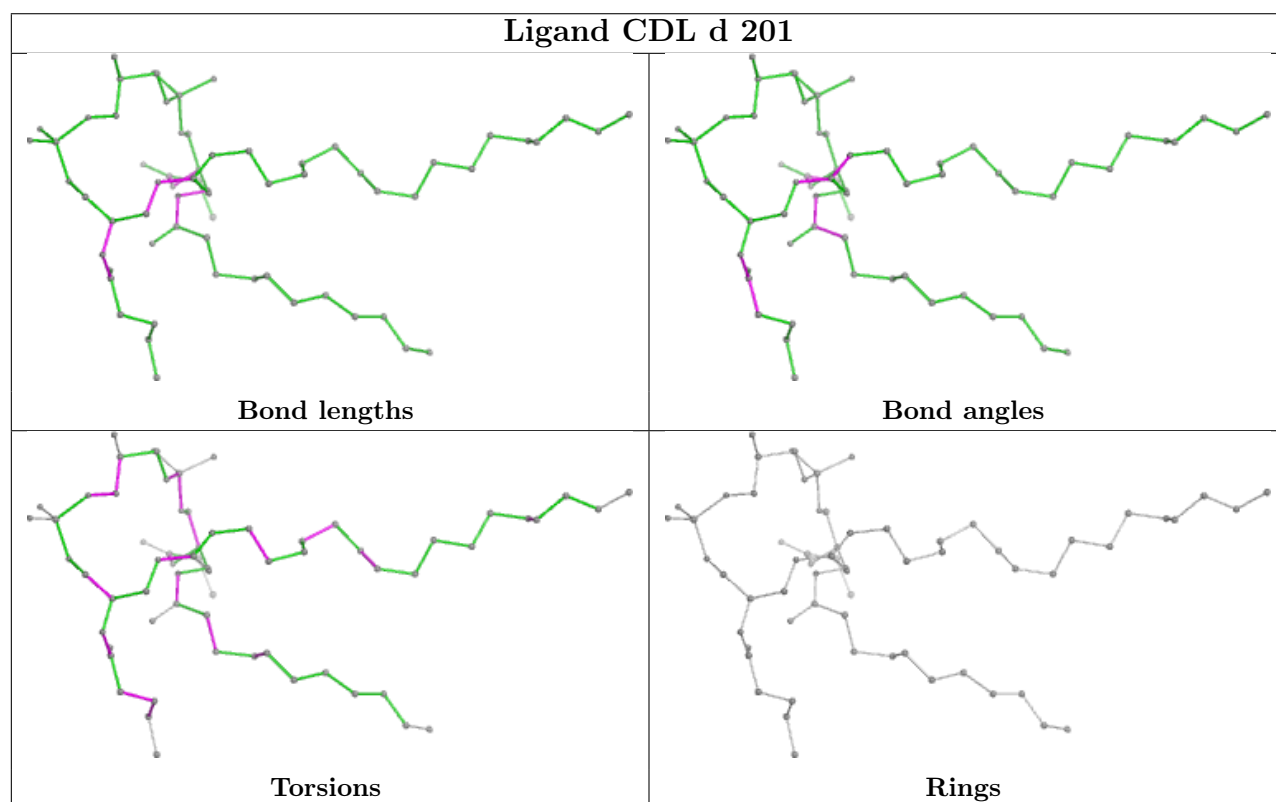
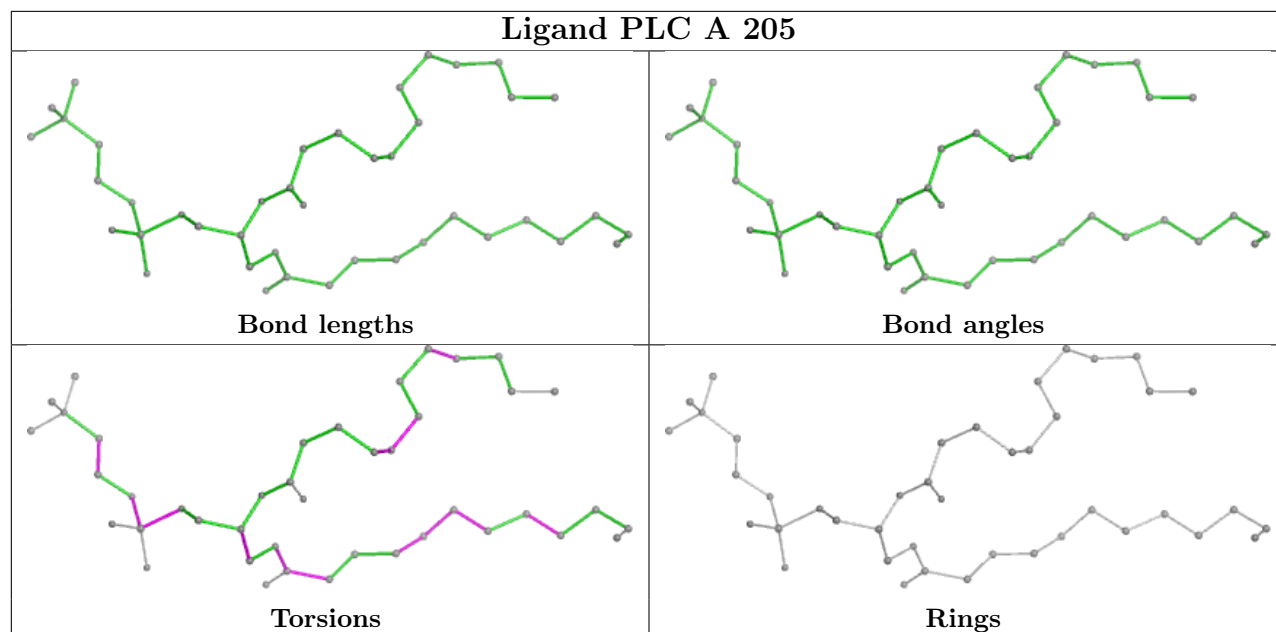


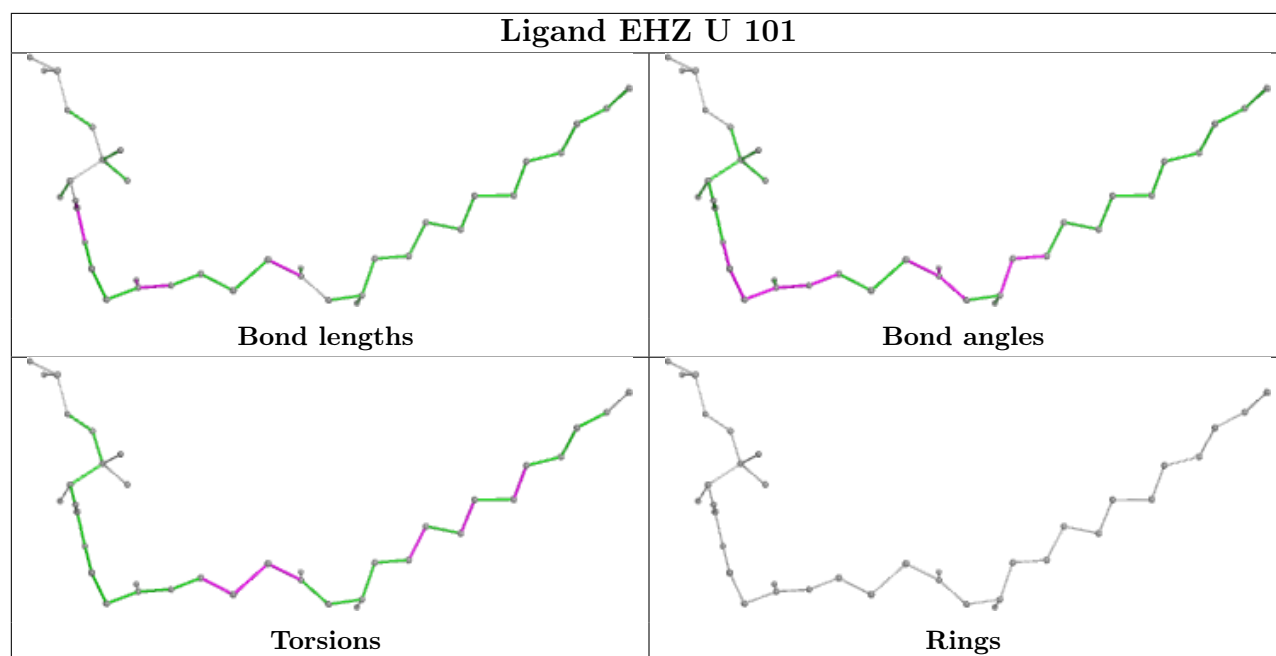
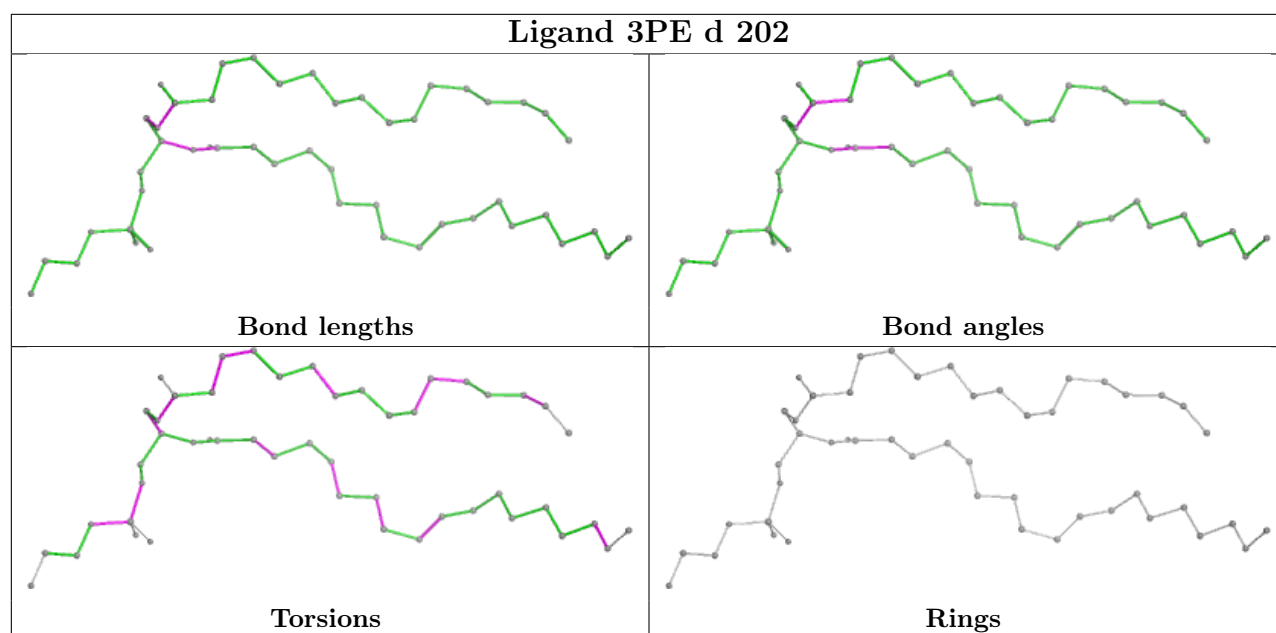


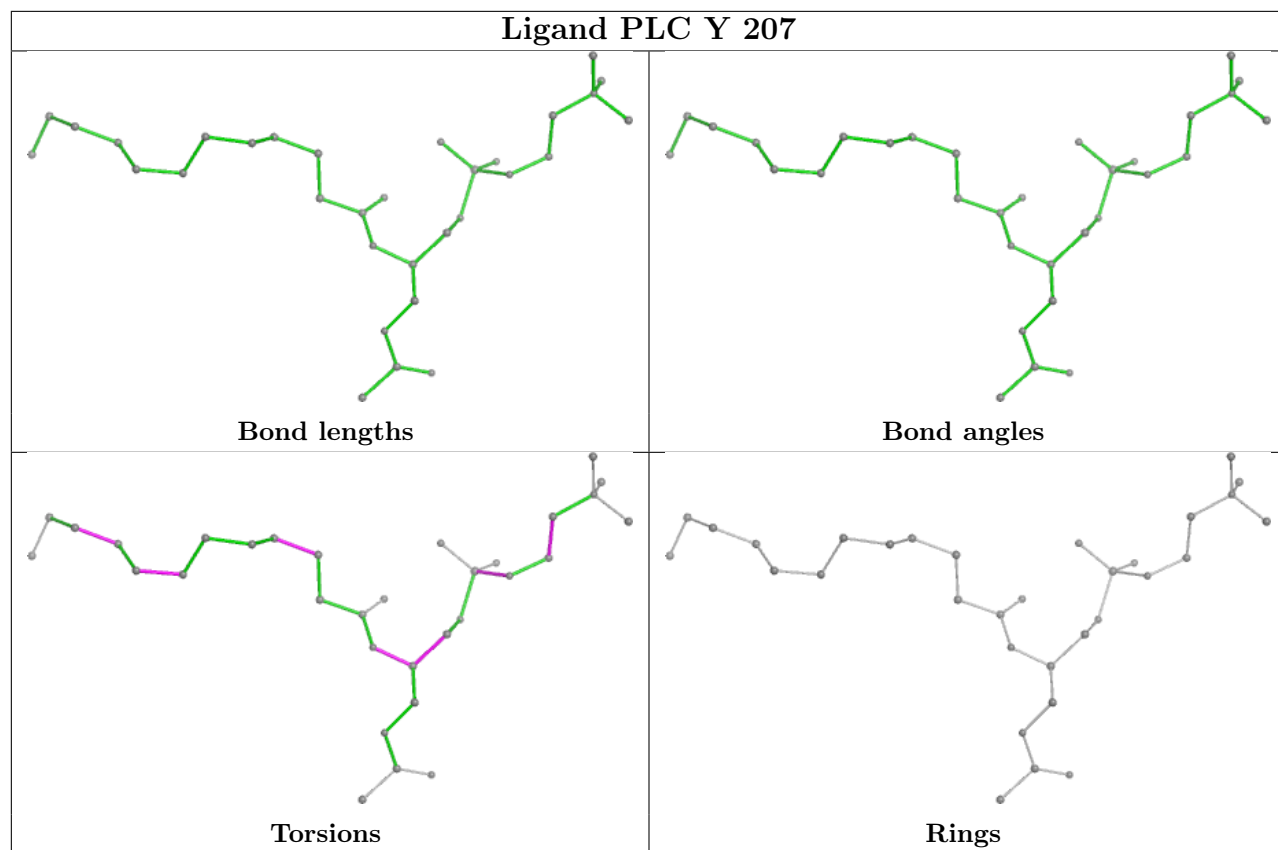


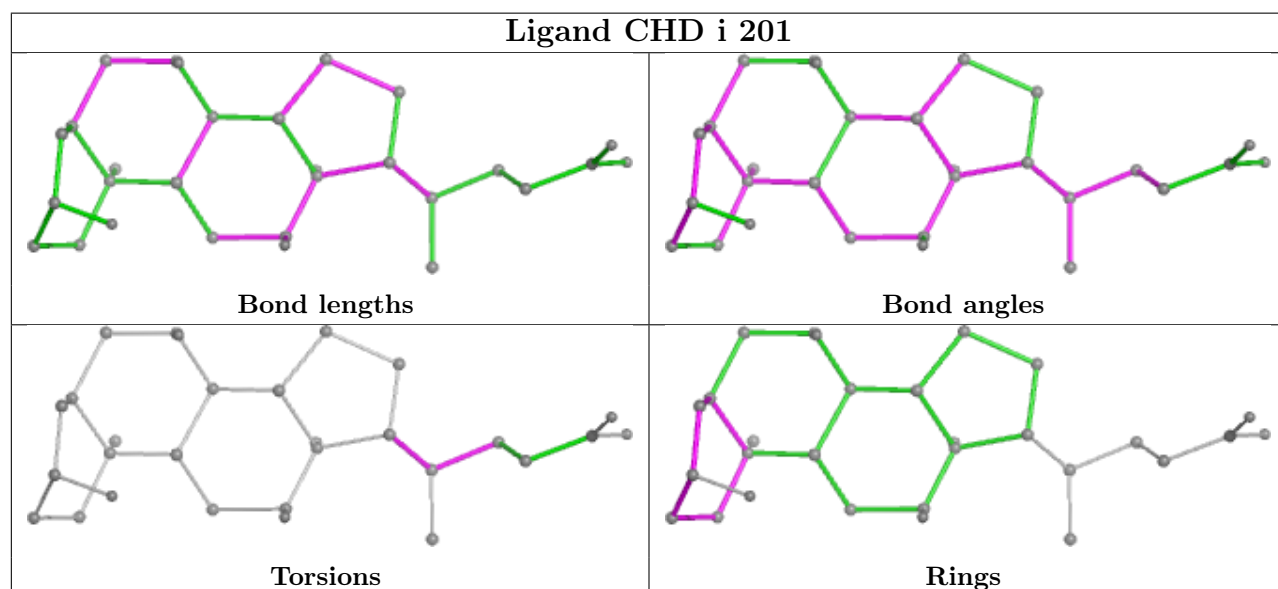
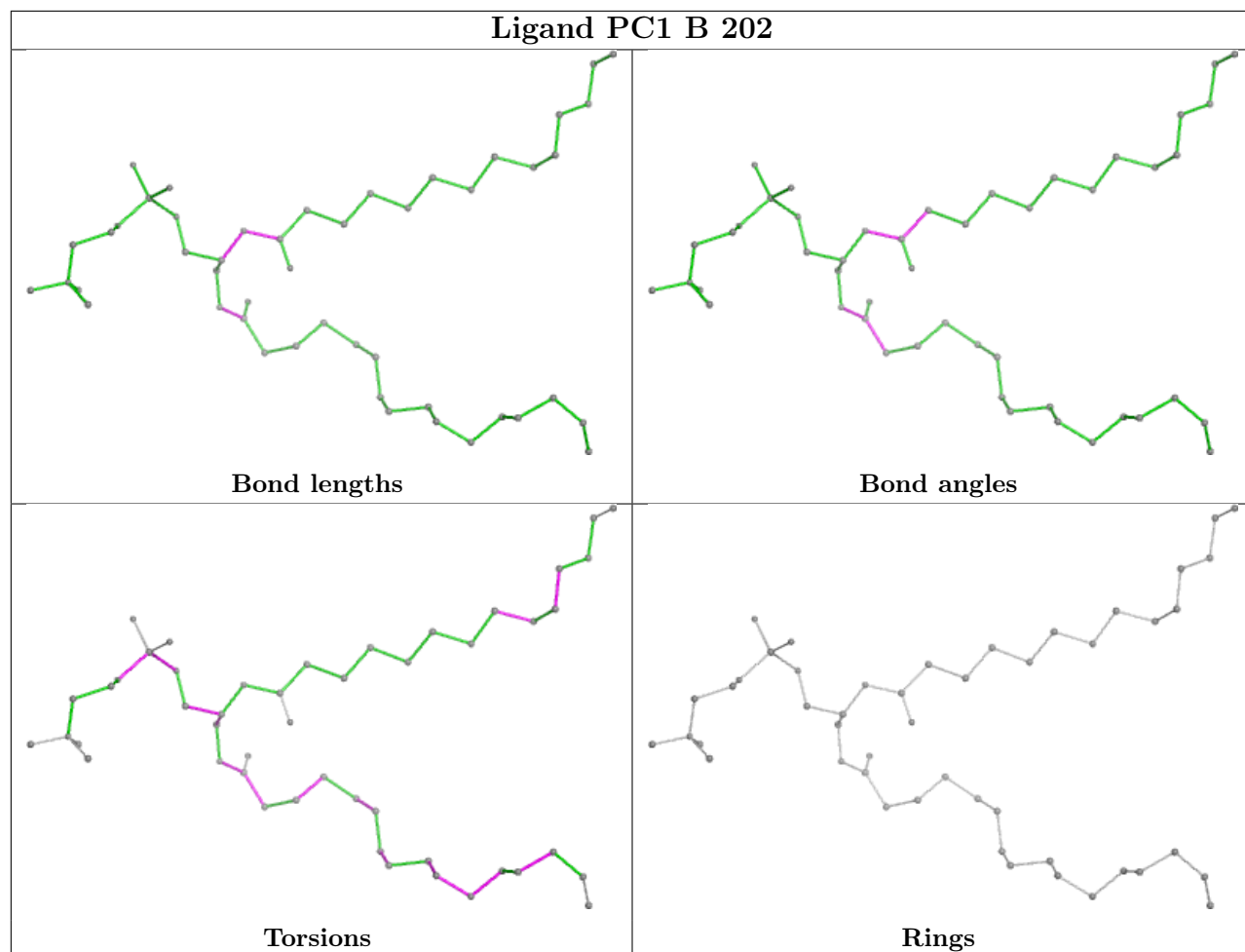


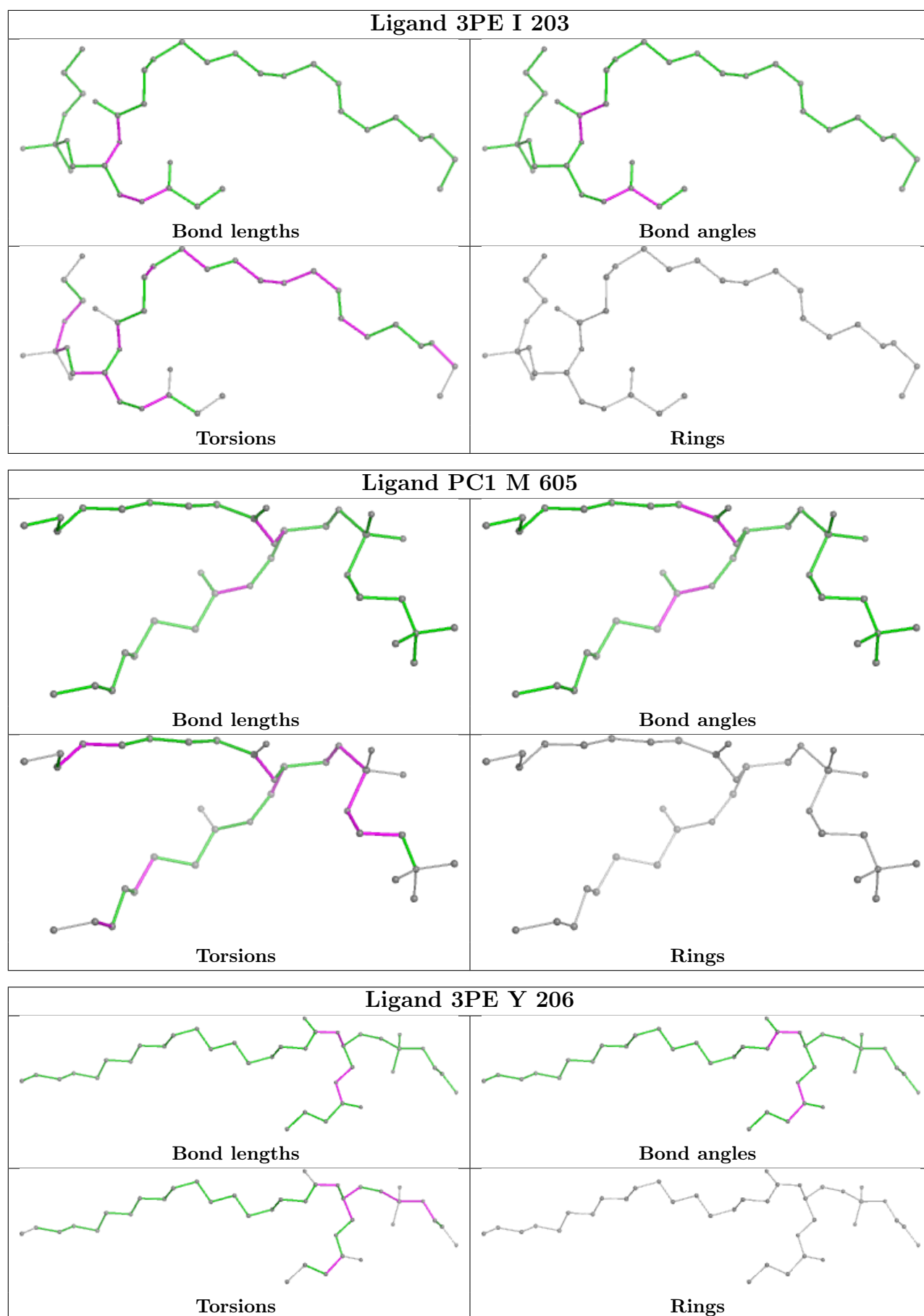


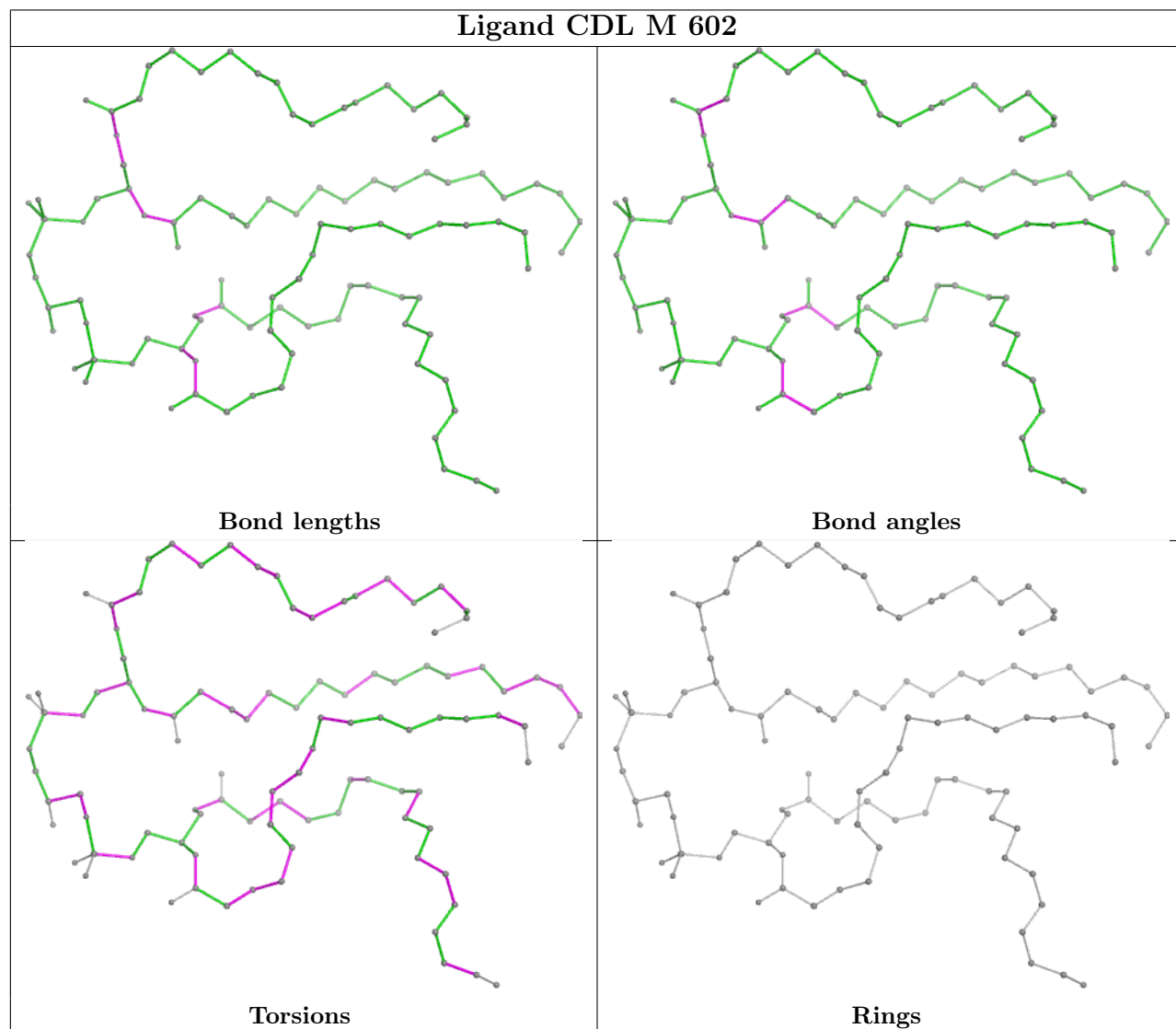
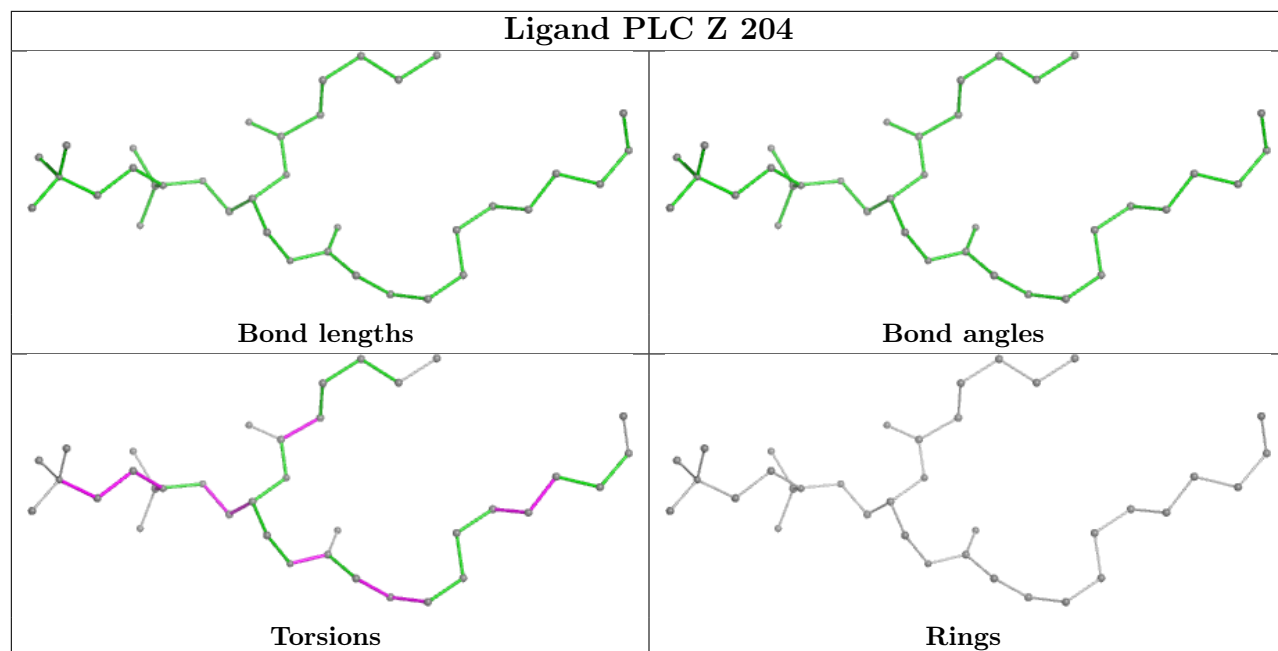


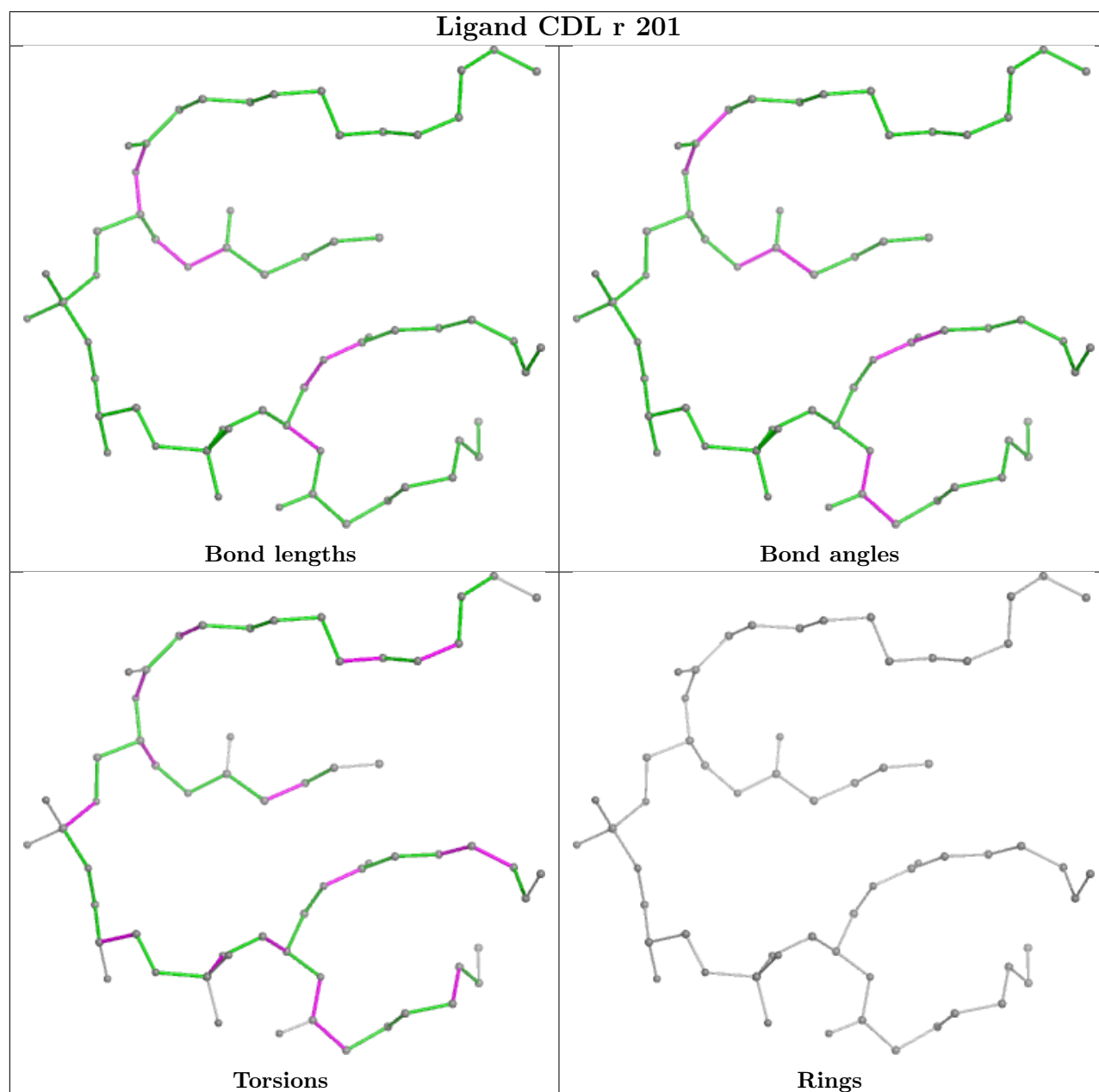
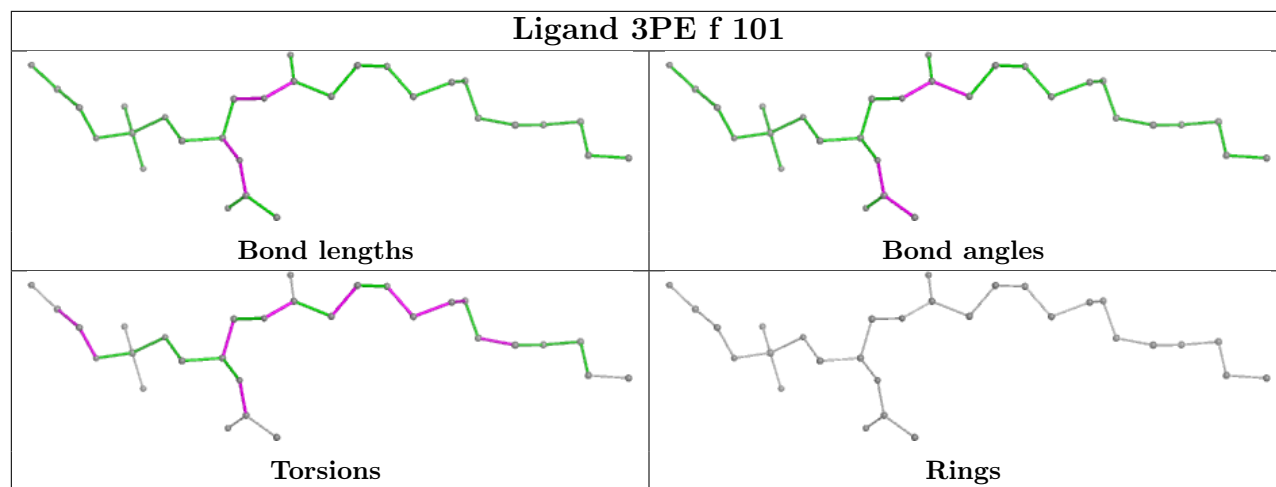


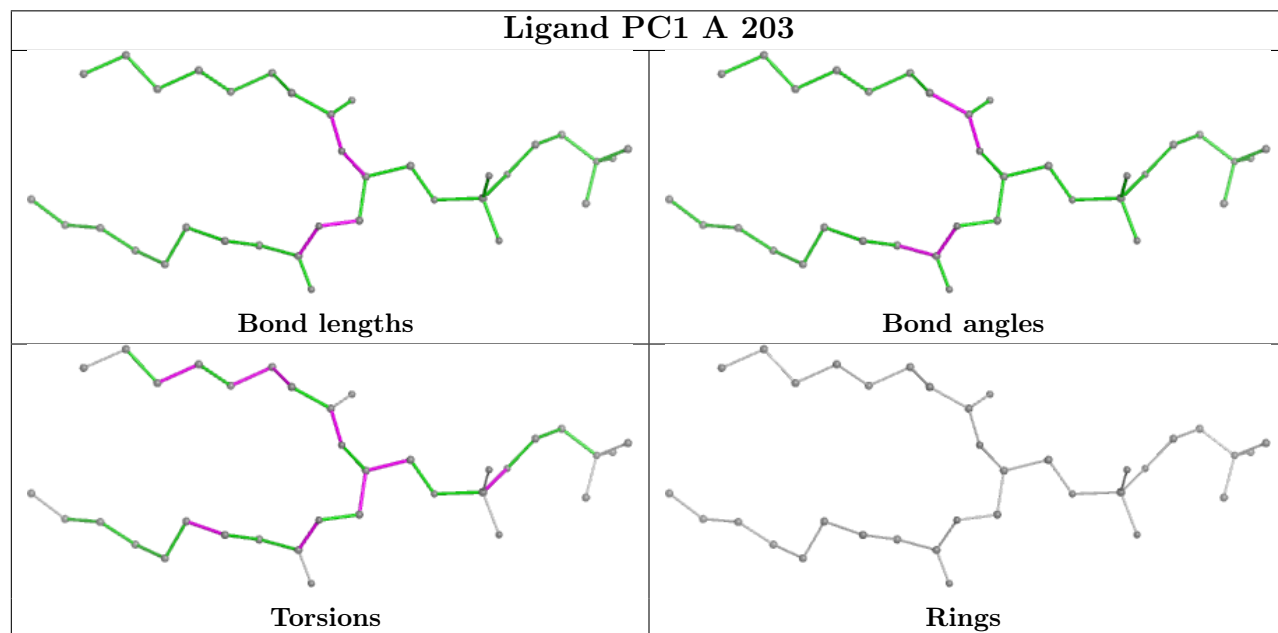
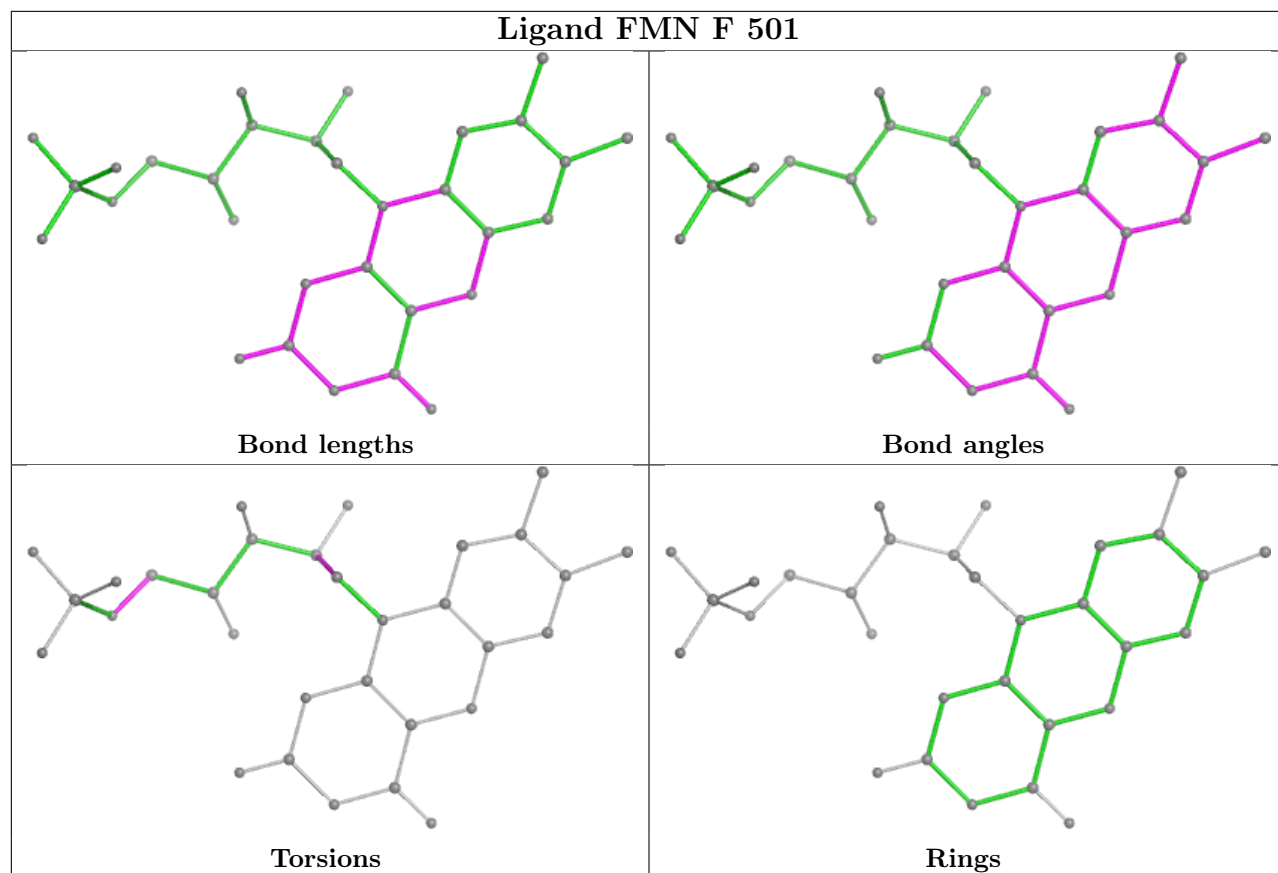


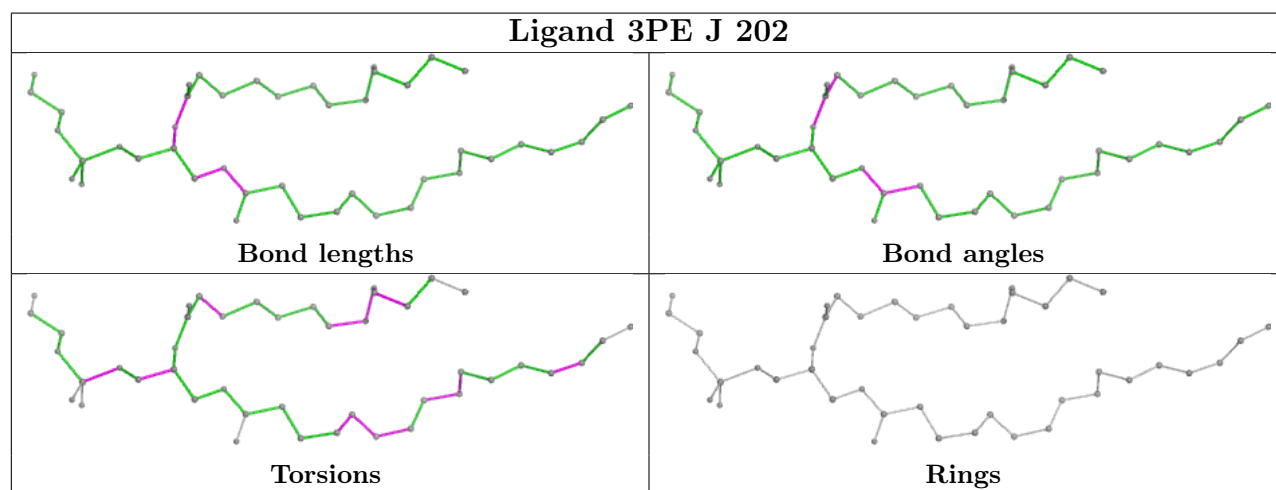
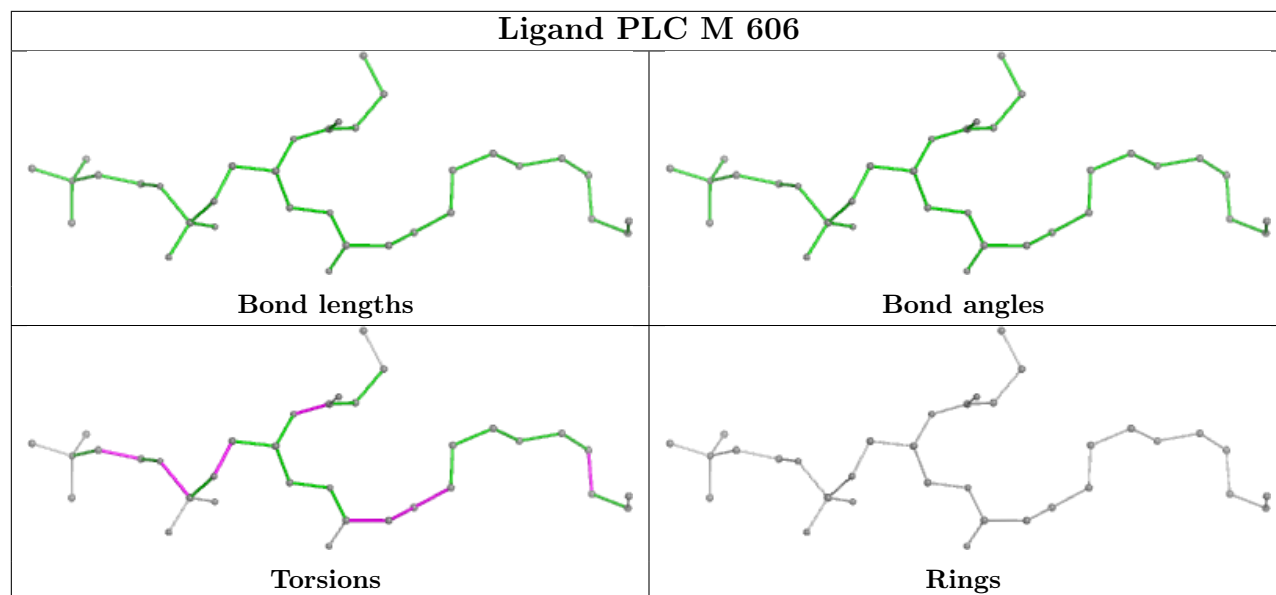


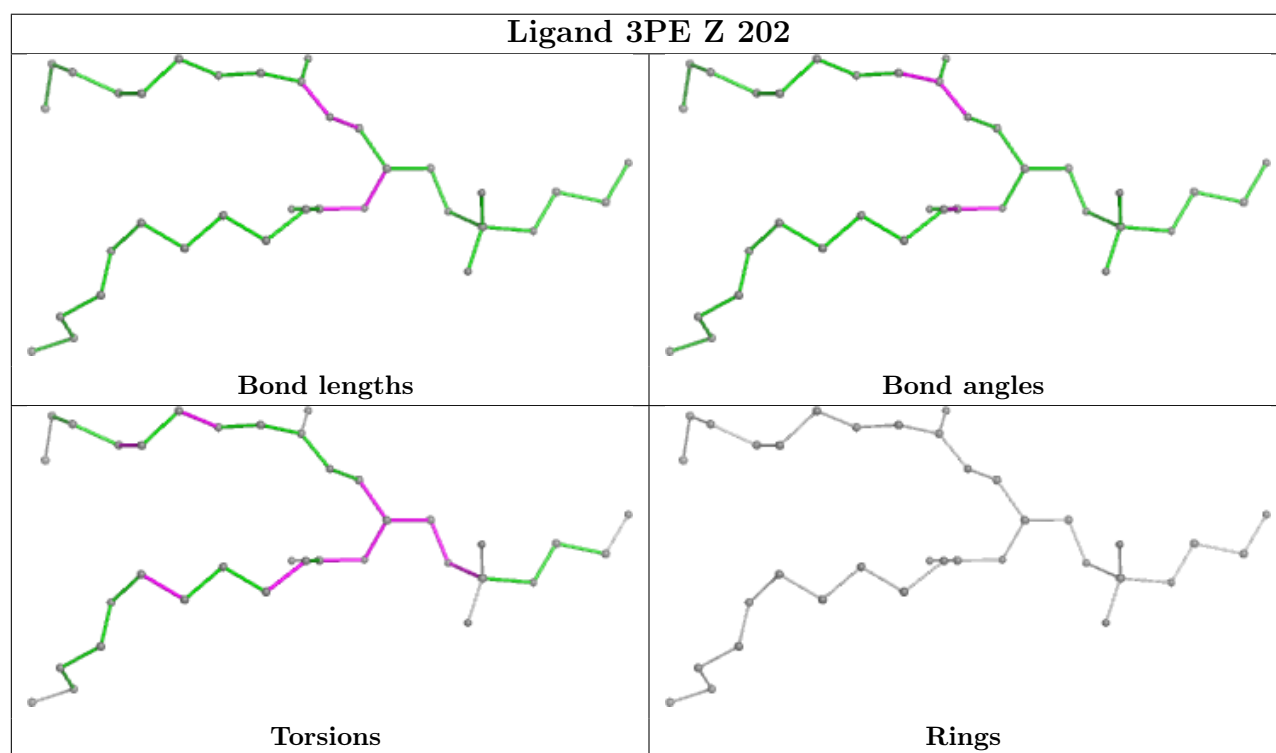
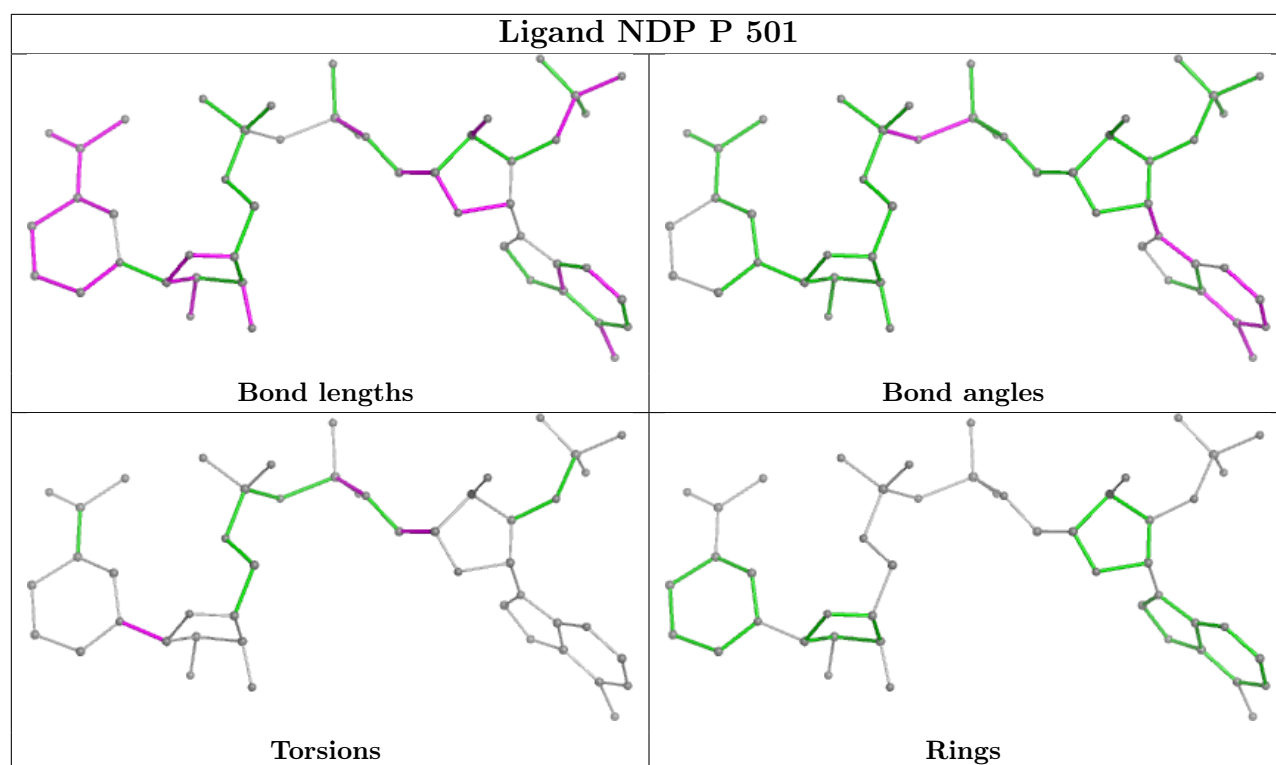












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

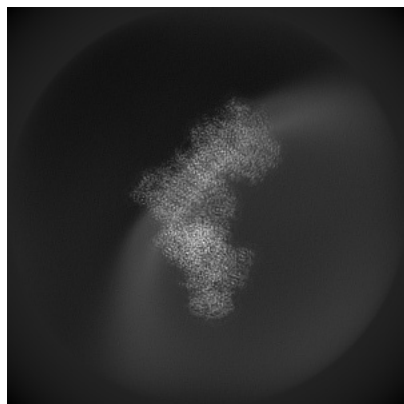
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18066. These allow visual inspection of the internal detail of the map and identification of artifacts.

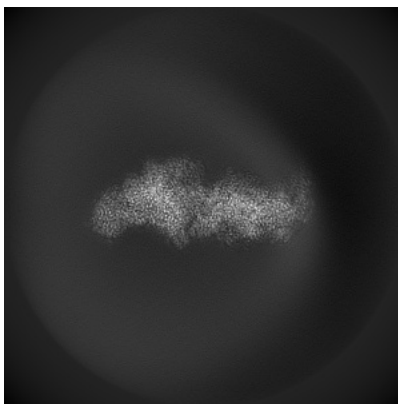
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

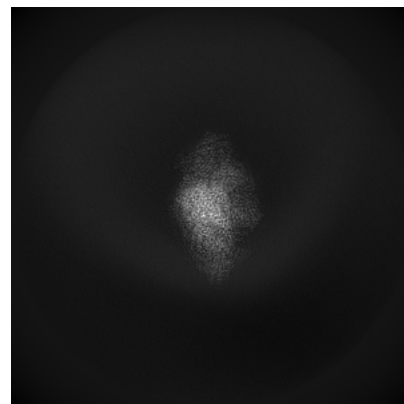
6.1.1 Primary map



X

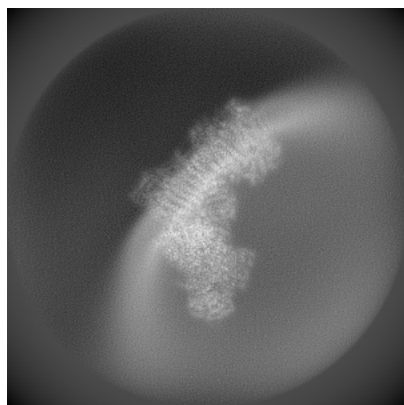


Y

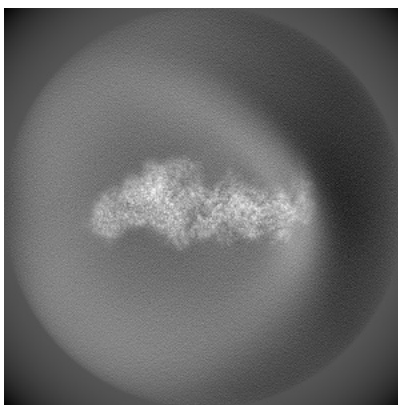


Z

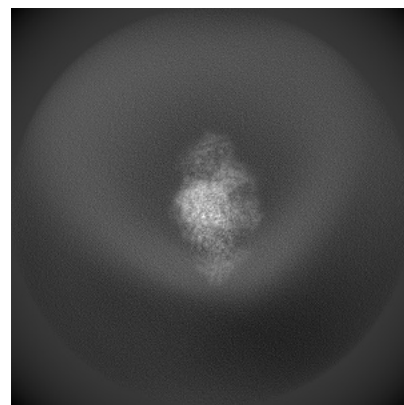
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

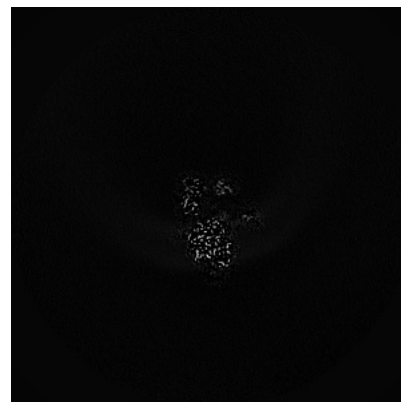
6.2.1 Primary map



X Index: 240

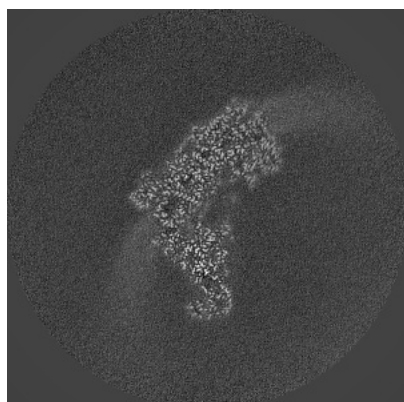


Y Index: 240

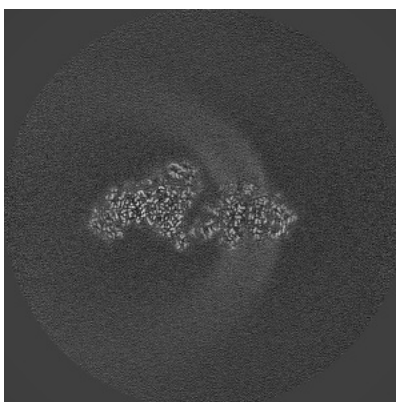


Z Index: 240

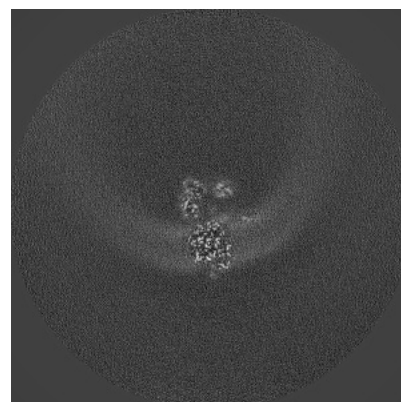
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

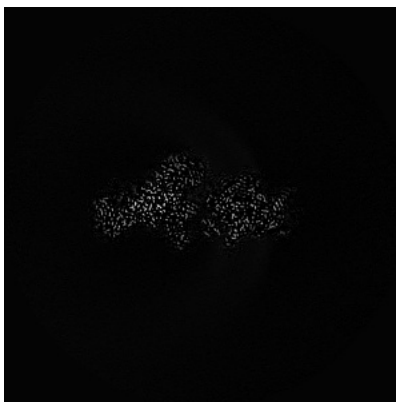
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 243

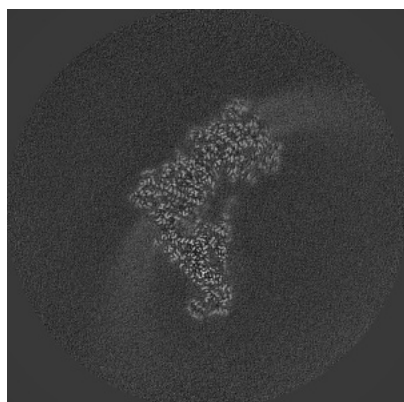


Y Index: 231

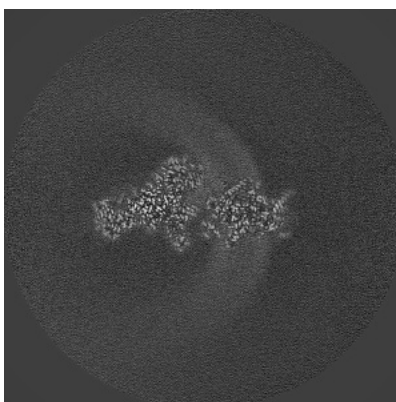


Z Index: 185

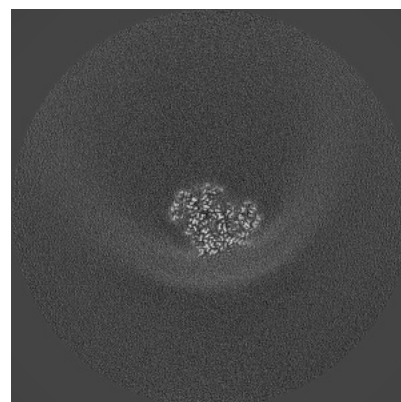
6.3.2 Raw map



X Index: 243



Y Index: 231

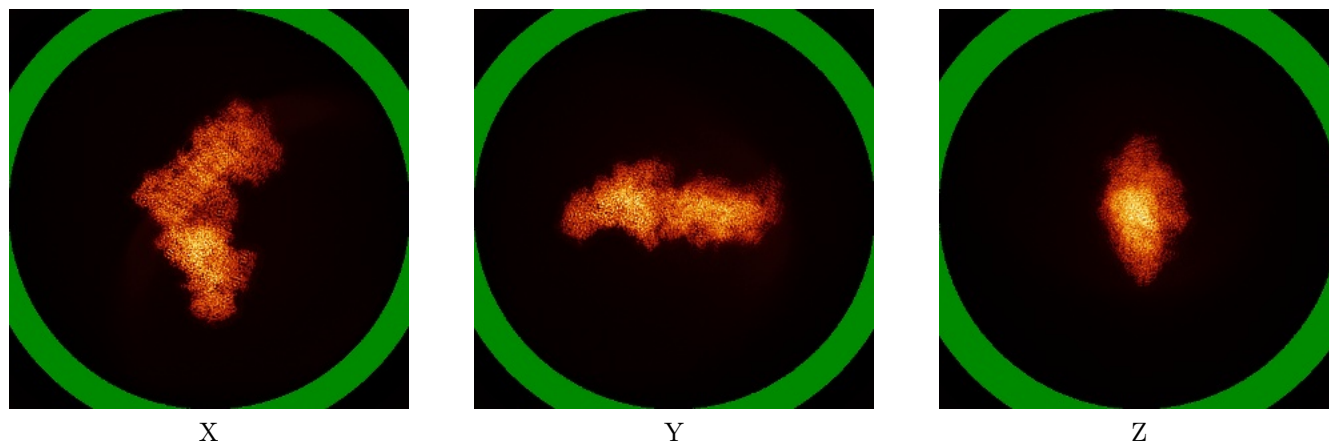


Z Index: 208

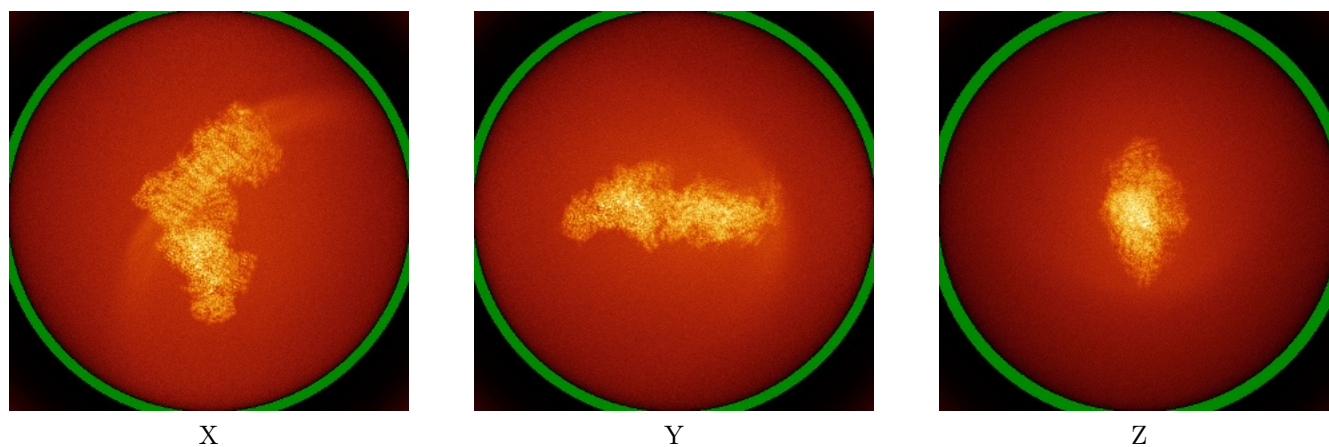
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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



X



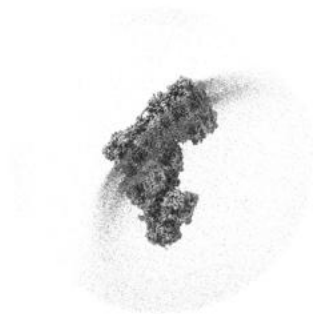
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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



X



Y



Z

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.

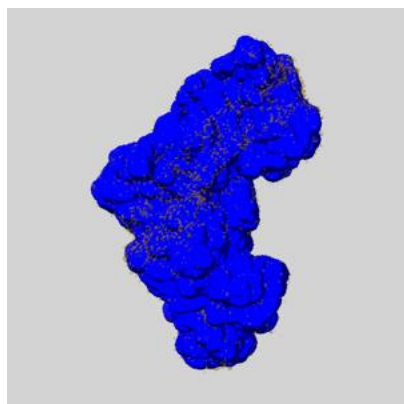
6.6 Mask visualisation [i](#)

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

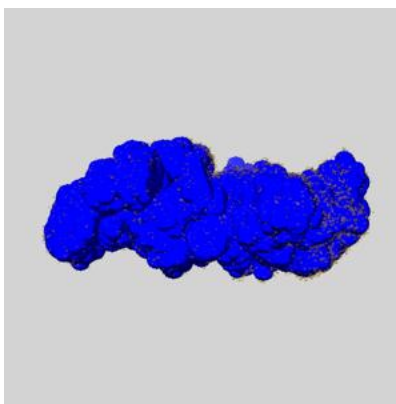
A mask typically either:

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

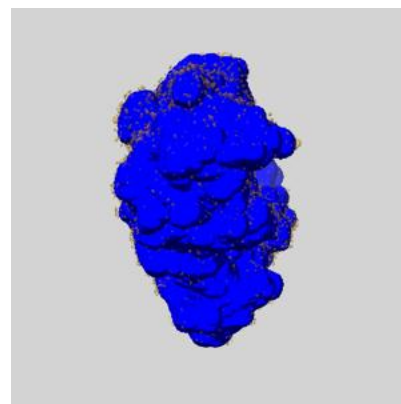
6.6.1 emd_18066_msk_1.map [i](#)



X



Y

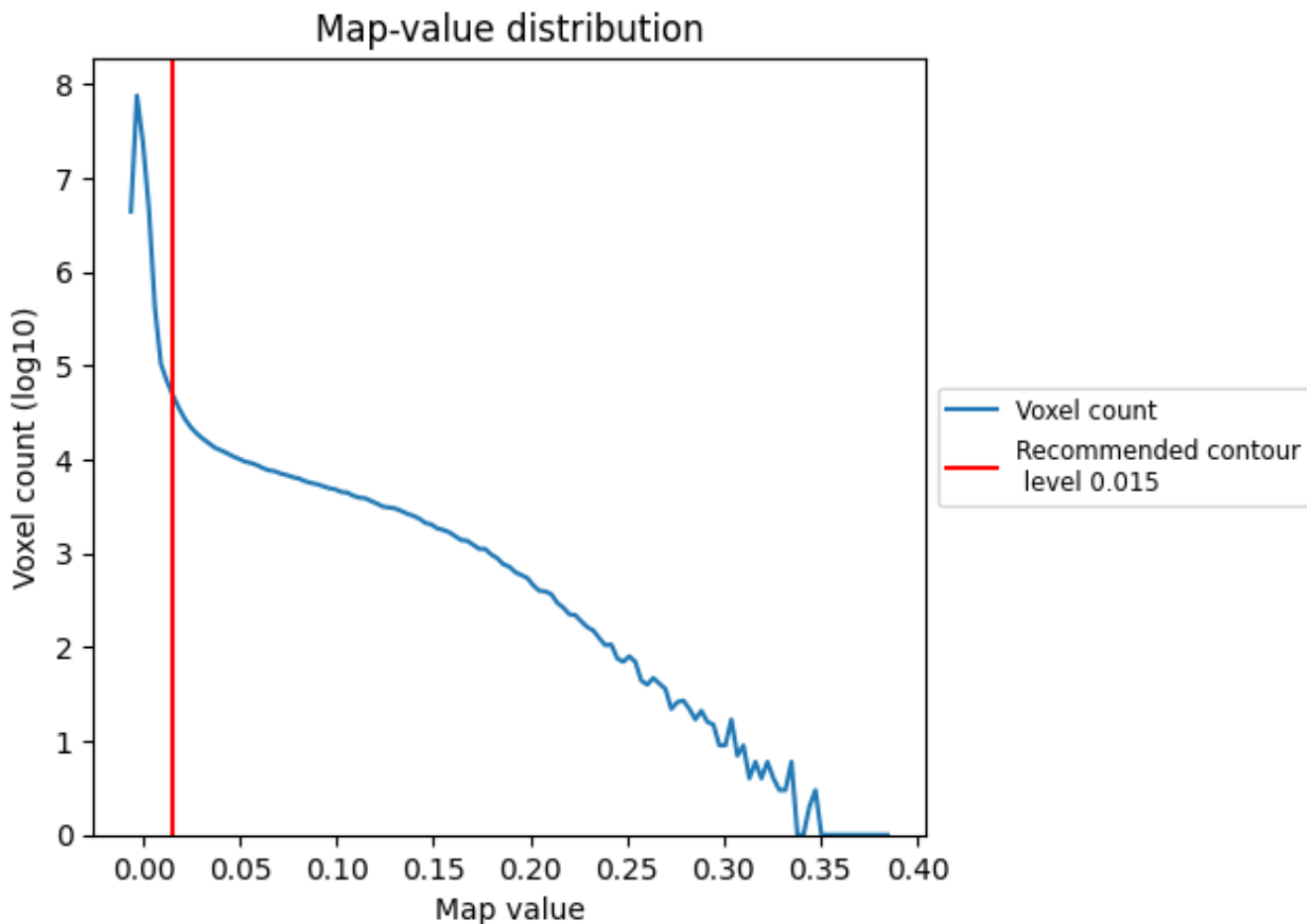


Z

7 Map analysis [i](#)

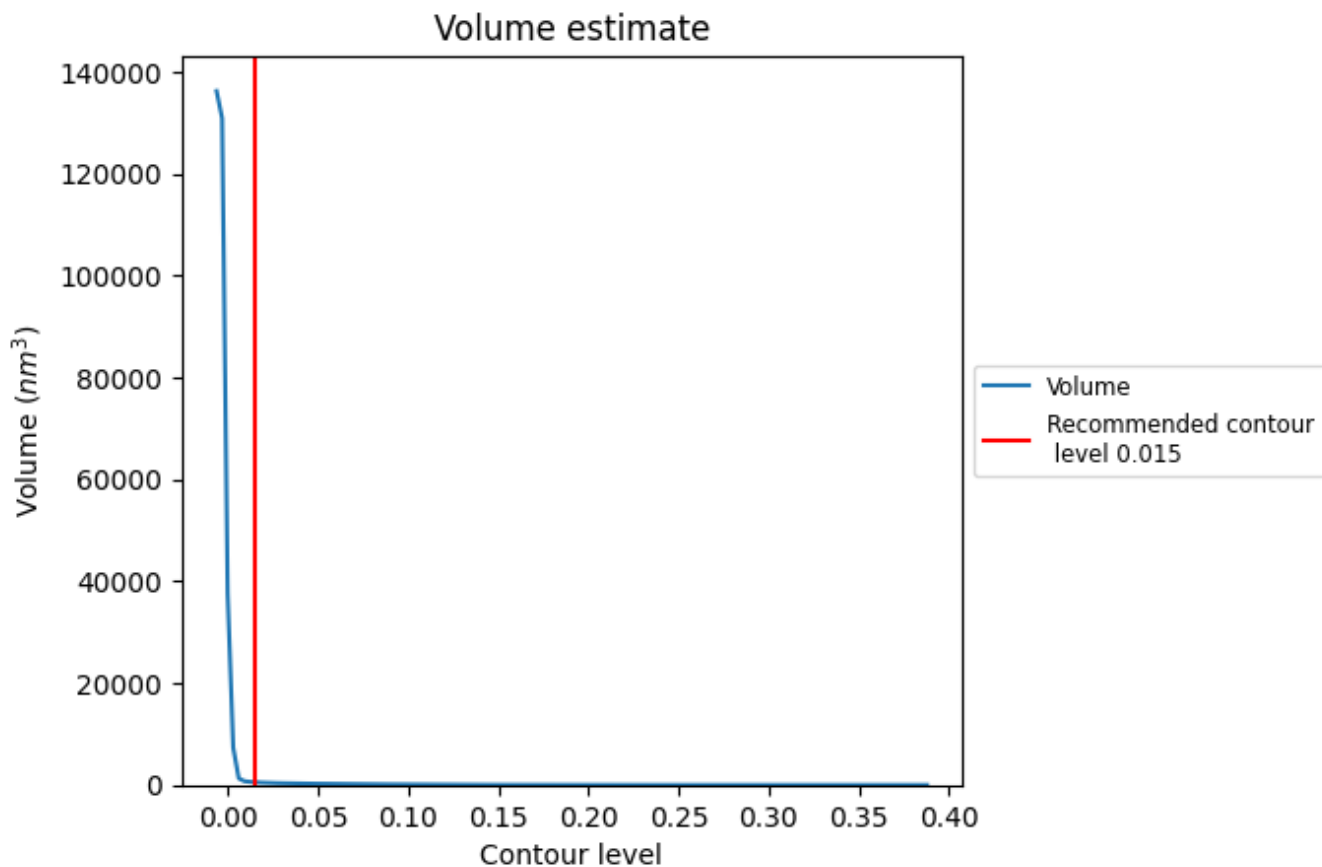
This section contains the results of statistical analysis of the map.

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.

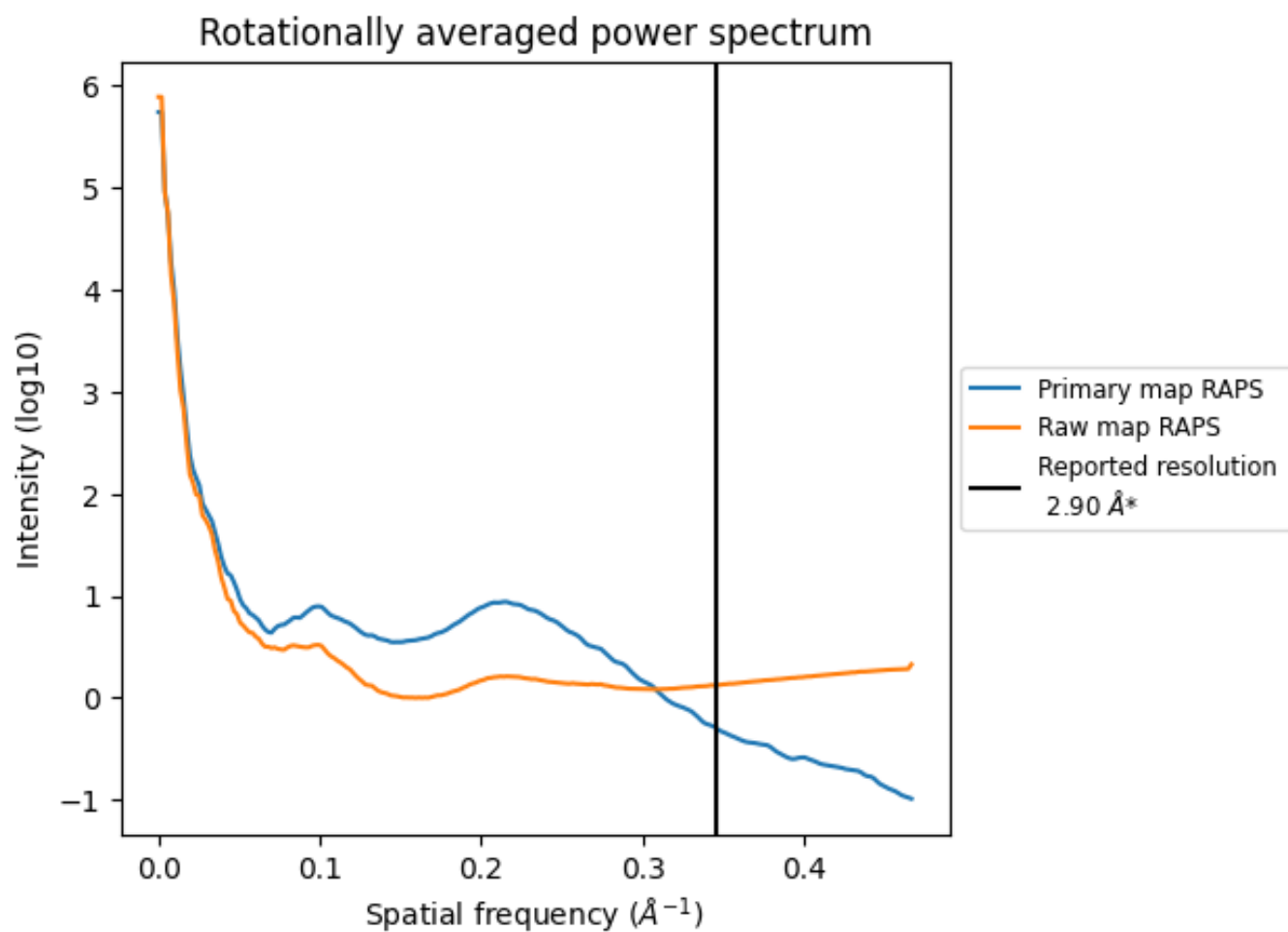
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 533 nm^3 ; this corresponds to an approximate mass of 482 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 i

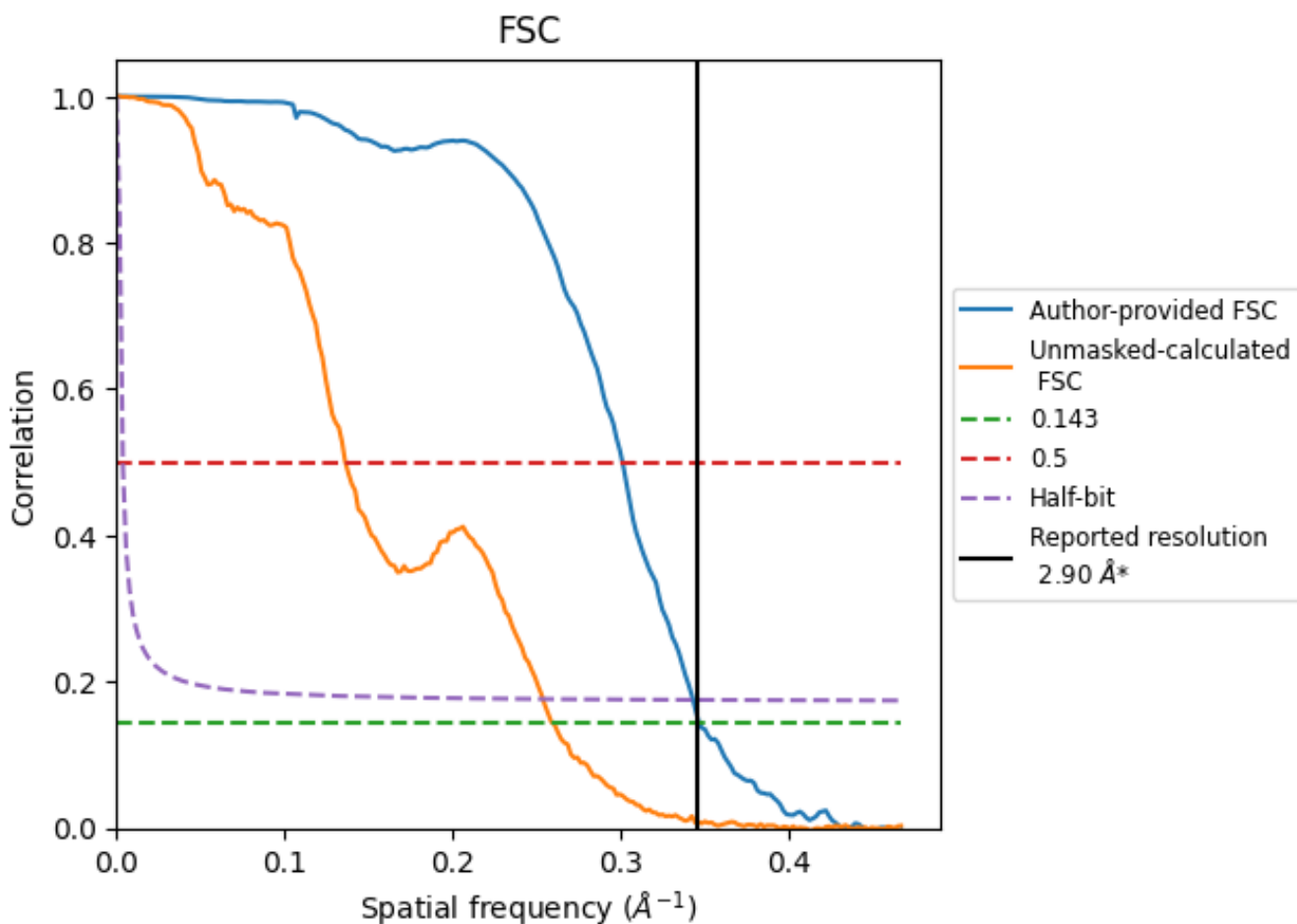


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

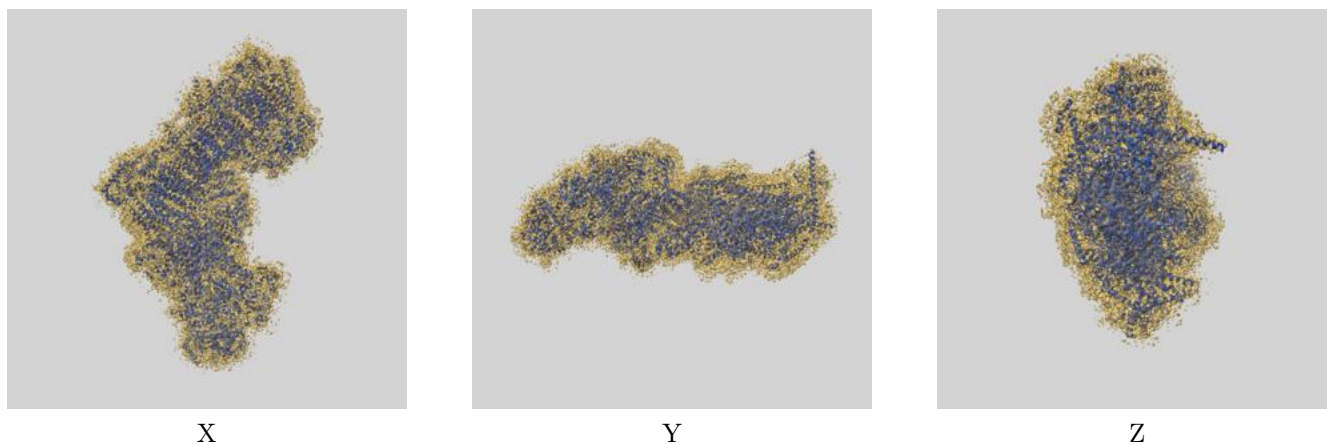
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.89	3.32	2.92
Unmasked-calculated*	3.86	7.35	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

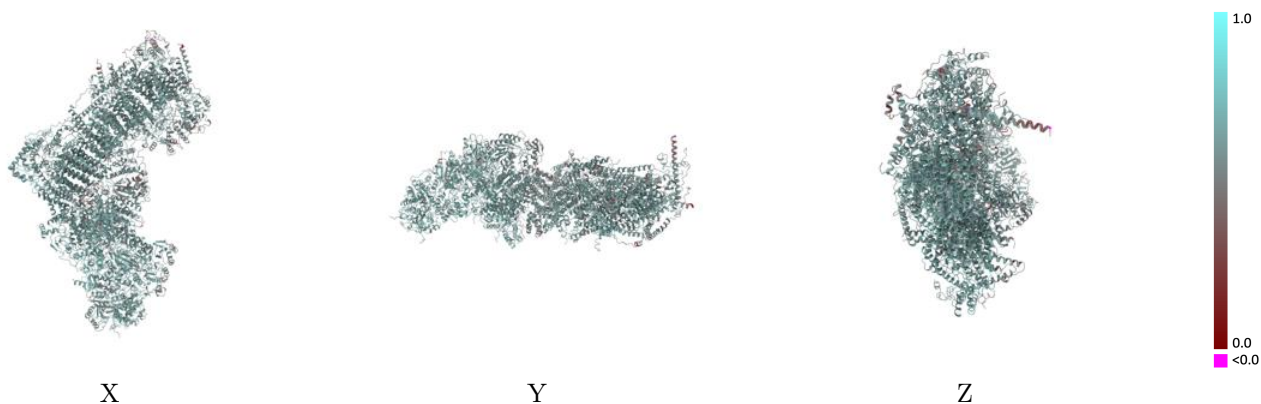
This section contains information regarding the fit between EMDB map EMD-18066 and PDB model 8Q1P. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



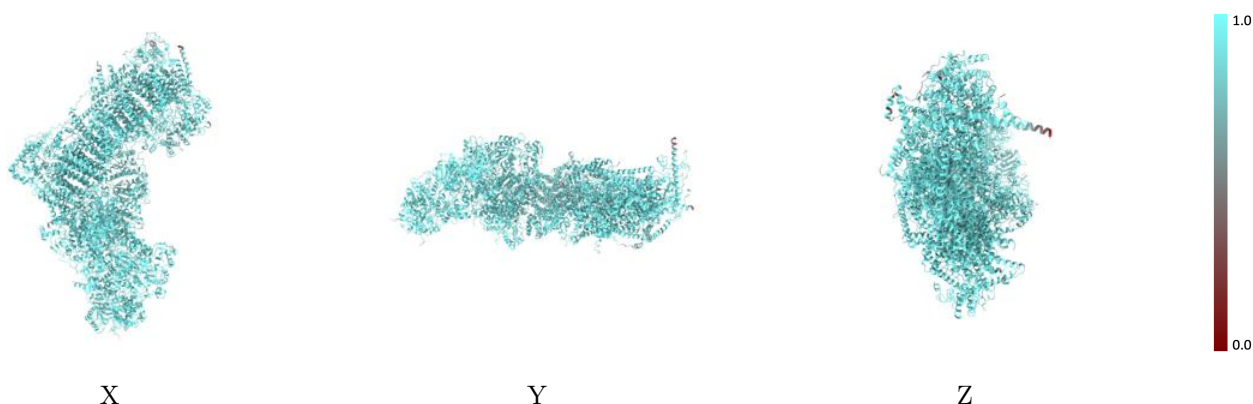
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



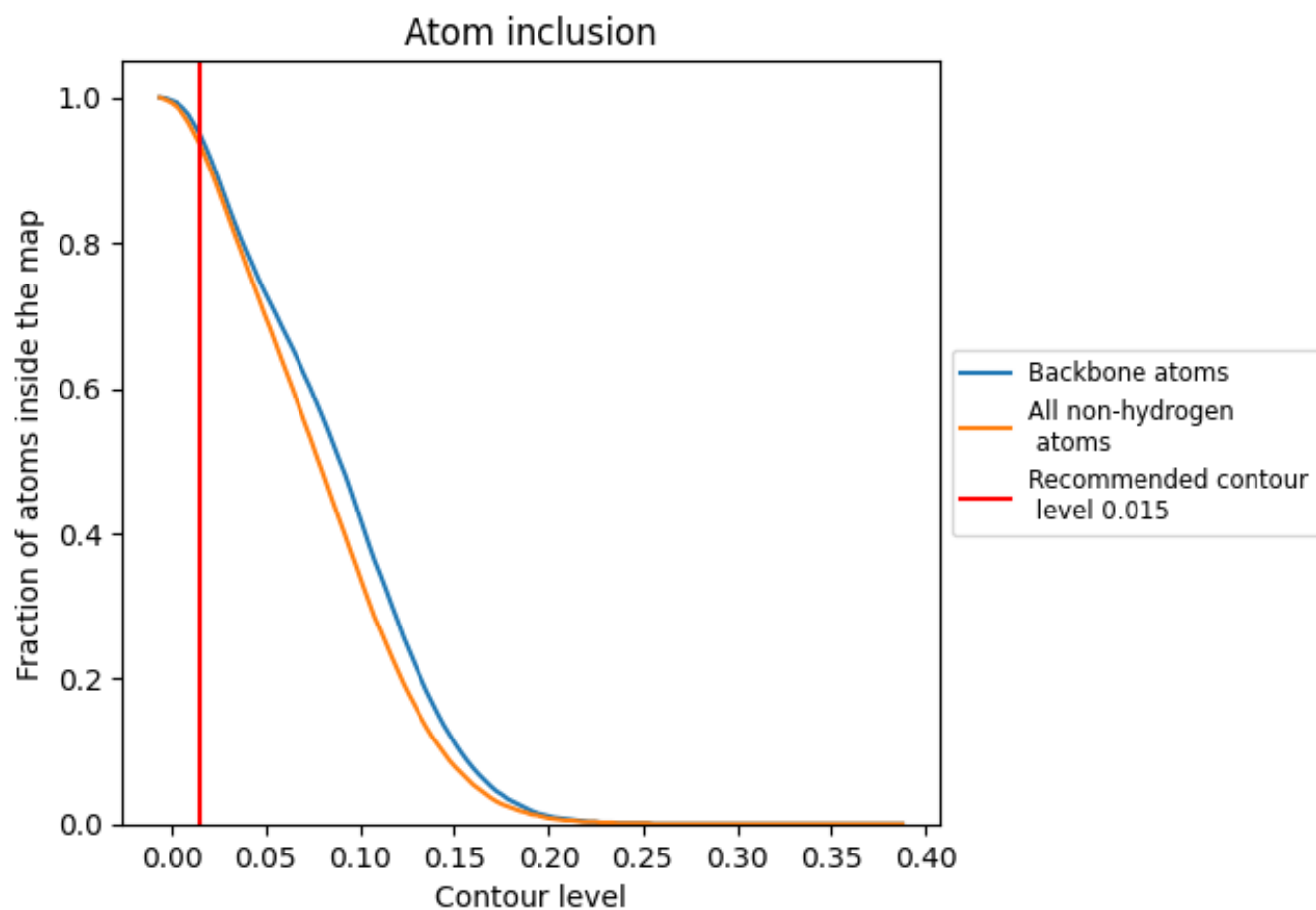
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.6040
A	 0.9420	 0.6000
B	 0.9650	 0.6360
C	 0.9760	 0.6520
D	 0.9690	 0.6420
E	 0.9410	 0.6010
F	 0.9550	 0.6190
G	 0.9500	 0.6190
H	 0.9550	 0.6160
I	 0.9780	 0.6510
J	 0.9440	 0.6040
K	 0.9700	 0.6260
L	 0.9430	 0.6030
M	 0.9700	 0.6310
N	 0.9750	 0.6390
O	 0.9290	 0.5890
P	 0.9080	 0.5680
Q	 0.9550	 0.6310
R	 0.9520	 0.6260
S	 0.9090	 0.5690
T	 0.8100	 0.4900
U	 0.8660	 0.5340
V	 0.9430	 0.6130
W	 0.9250	 0.6010
X	 0.9270	 0.6050
Y	 0.9080	 0.5750
Z	 0.9270	 0.6000
a	 0.9510	 0.6280
b	 0.9230	 0.5940
c	 0.9090	 0.5870
d	 0.9410	 0.6090
e	 0.9200	 0.5860
f	 0.8650	 0.5550
g	 0.9230	 0.5840
h	 0.9560	 0.6170



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.8370	 0.5240
j	 0.8750	 0.5550
k	 0.8460	 0.5210
l	 0.9180	 0.5750
m	 0.9010	 0.5850
n	 0.9120	 0.5650
o	 0.8340	 0.5160
p	 0.9010	 0.5690
q	 0.9580	 0.6230
r	 0.9700	 0.6340
s	 0.9230	 0.5920