



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:00 PM UTC

PDB ID : 8Q1Y / pdb_00008q1y
EMDB ID : EMD-18068
Title : Outward-facing, open2 proteoliposome complex I at 2.6 Å, after deactivation treatment. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-01
Resolution : 2.60 Å(reported)
Based on initial model : 7QSN

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

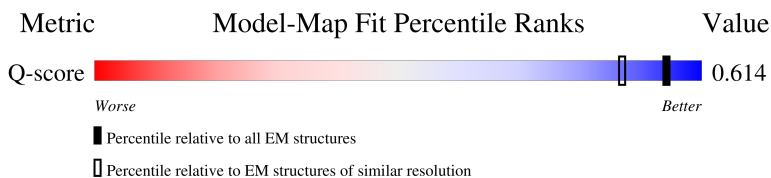
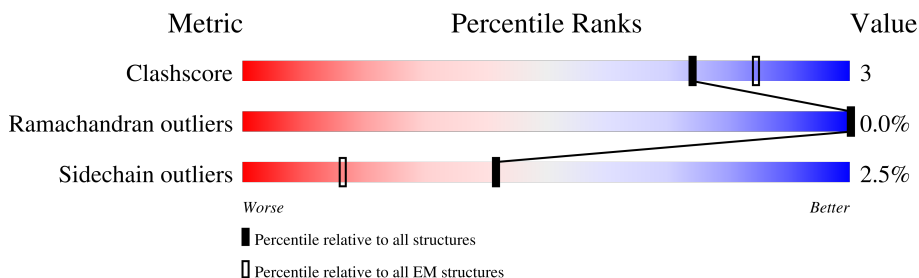
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

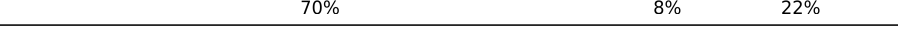
The reported resolution of this entry is 2.60 Å.

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



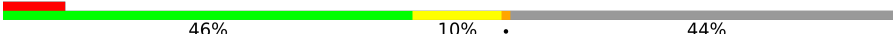
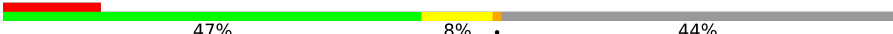
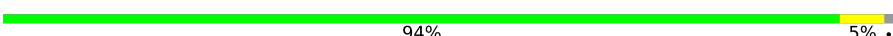
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

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

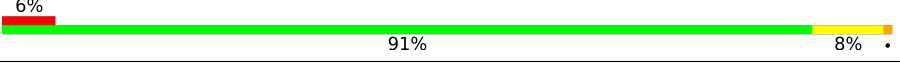
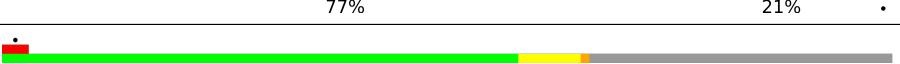
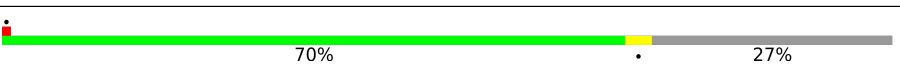
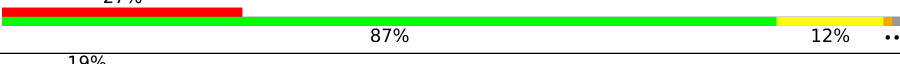
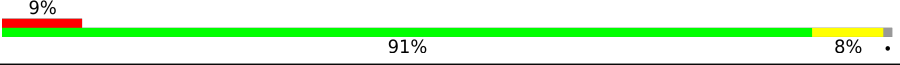
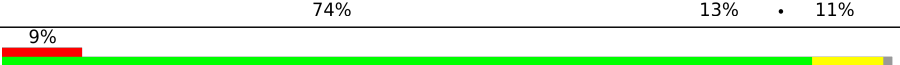
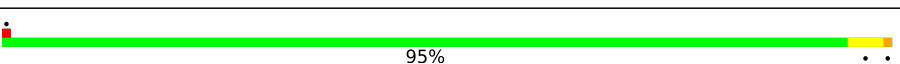
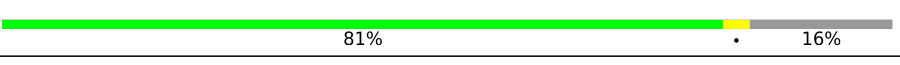
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

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

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 69324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	101	Total	C	N	O	S	0	0
			815	555	116	139	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	417	Total	C	N	O	S	0	0
			3364	2151	577	611	25		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	316	Total	C	N	O	S	0	0
			2496	1673	383	417	23		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	335	Total	C	N	O	S	0	0
			2689	1739	476	469	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	114	Total	C	N	O	S	0	0
			923	597	156	167	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	116	Total	C	N	O	S	0	0
			982	628	182	168	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

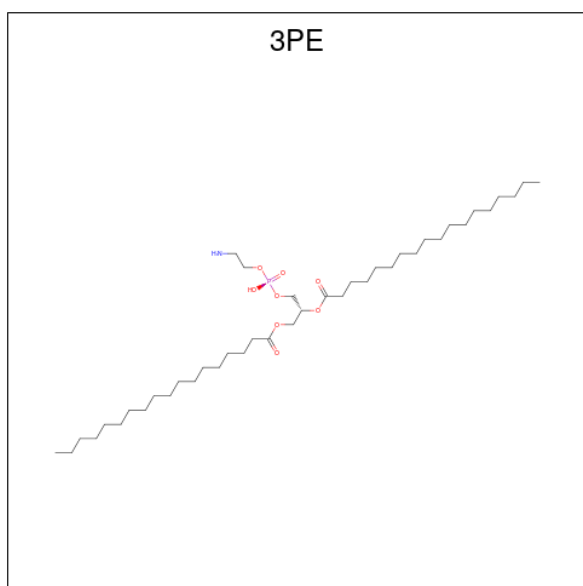
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

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



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	H	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	J	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	J	1	Total	C	N	O	P	0
			36	26	1	8	1	
45	K	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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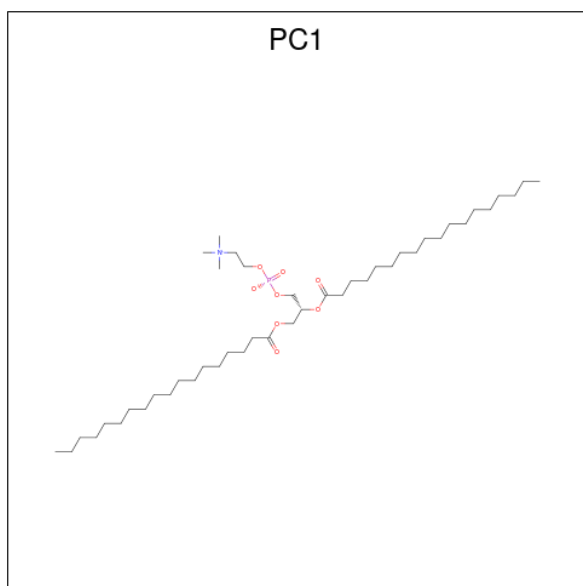
Mol	Chain	Residues	Atoms					AltConf
45	M	1	Total	C	N	O	P	0
			30	20	1	8	1	
45	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
45	M	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	N	1	Total	C	N	O	P	0
			45	35	1	8	1	
45	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	N	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	Y	1	Total	C	N	O	P	0
			34	24	1	8	1	
45	Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	Z	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	b	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	f	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	h	1	Total	C	N	O	P	0
			32	22	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
45	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	m	1	Total	C	N	O	P	0
			30	20	1	8	1	
45	q	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	r	1	Total	C	N	O	P	0
			28	18	1	8	1	

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



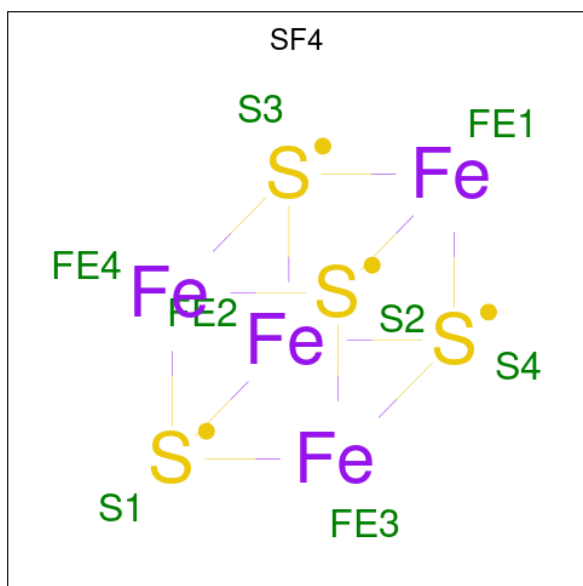
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	L	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	g	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	h	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	m	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	q	1	Total	C	N	O	P	0
			23	13	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



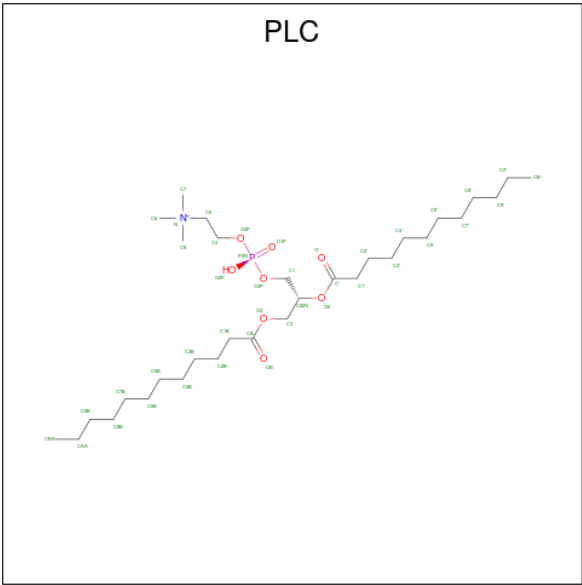
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	

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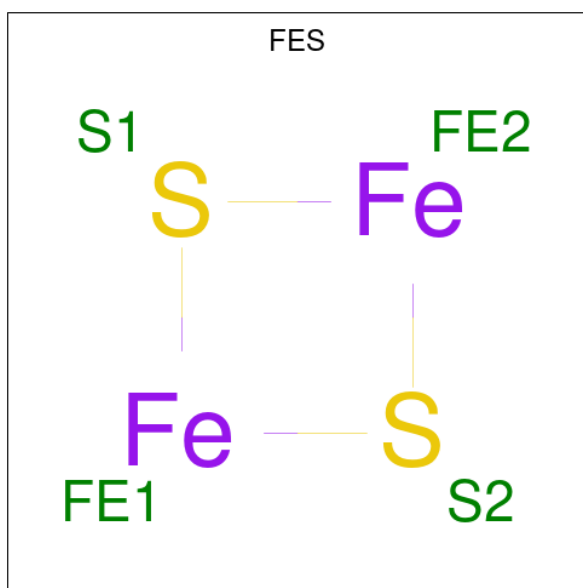
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



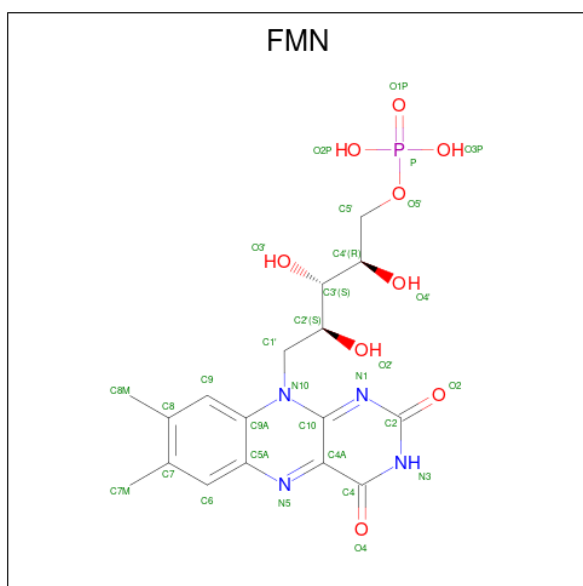
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			28	18	1	8	1	
48	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
48	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	O	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	Y	1	Total	C	N	O	P	0
			37	27	1	8	1	
48	Z	1	Total	C	N	O	P	0
			34	24	1	8	1	
48	b	1	Total	C	N	O	P	0
			38	28	1	8	1	
48	d	1	Total	C	N	O	P	0
			32	22	1	8	1	
48	g	1	Total	C	N	O	P	0
			28	18	1	8	1	

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



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

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



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

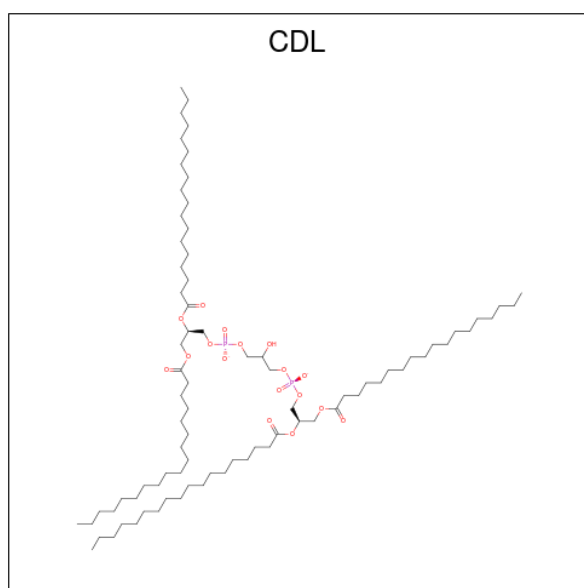
- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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



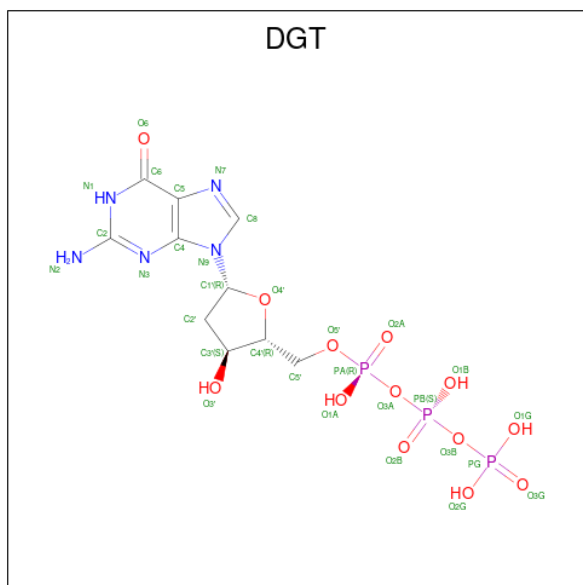
Mol	Chain	Residues	Atoms				AltConf
53	M	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			84	65	17	2	
53	X	1	Total	C	O	P	0
			86	67	17	2	
53	d	1	Total	C	O	P	0
			65	46	17	2	
53	h	1	Total	C	O	P	0
			70	51	17	2	
53	i	1	Total	C	O	P	0
			72	53	17	2	

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Mol	Chain	Residues	Atoms				AltConf
53	r	1	Total	C	O	P	0
			58	39	17	2	

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



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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



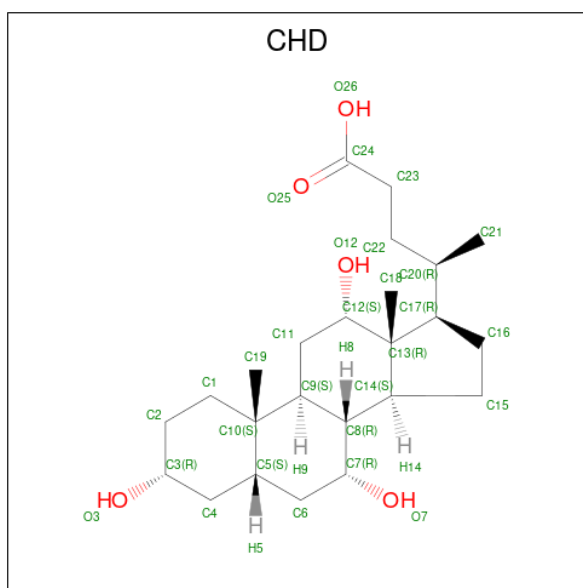
Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



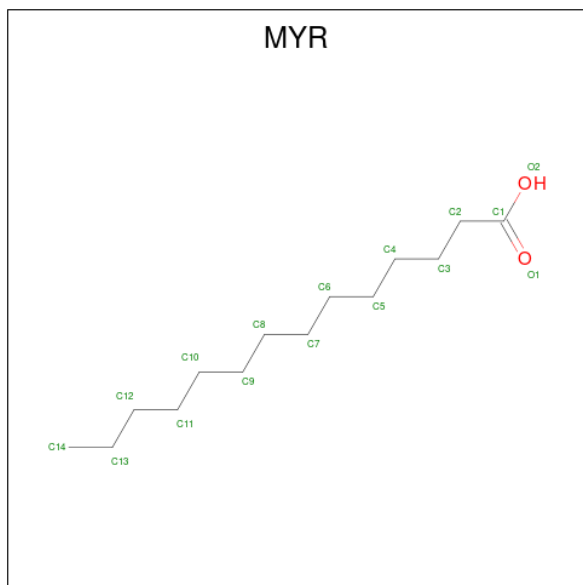
Mol	Chain	Residues	Atoms						AltConf
57	T	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
57	U	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

- Molecule 58 is CHOLIC ACID (CCD ID: 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 (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

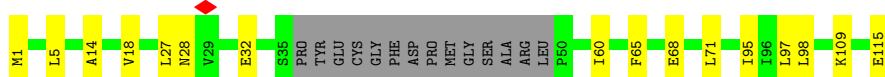
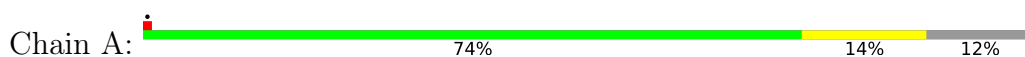


Mol	Chain	Residues	Atoms			AltConf
59	o	1	Total	C	O	0
			15	14	1	

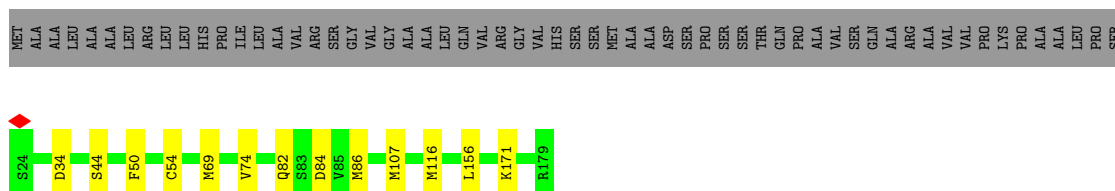
3 Residue-property plots [i](#)

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.

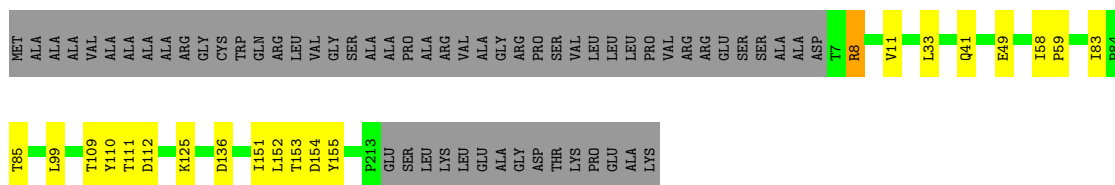
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



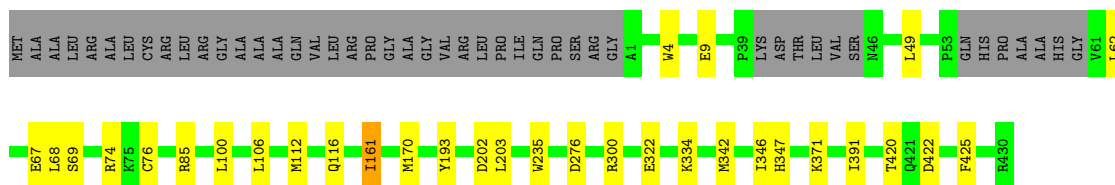
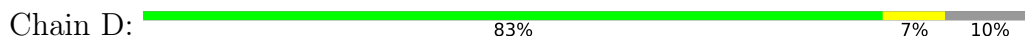
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

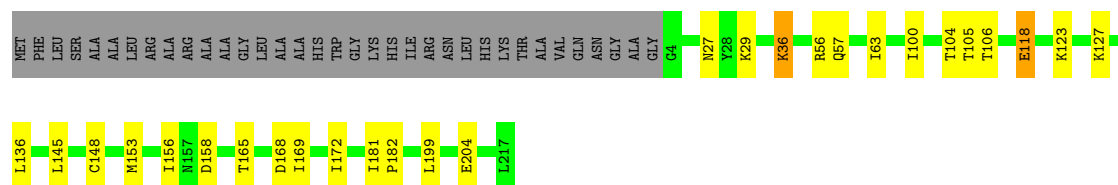


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



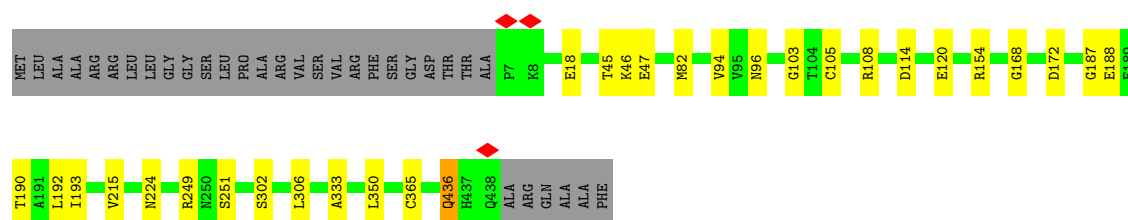
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  75% 10% 14%



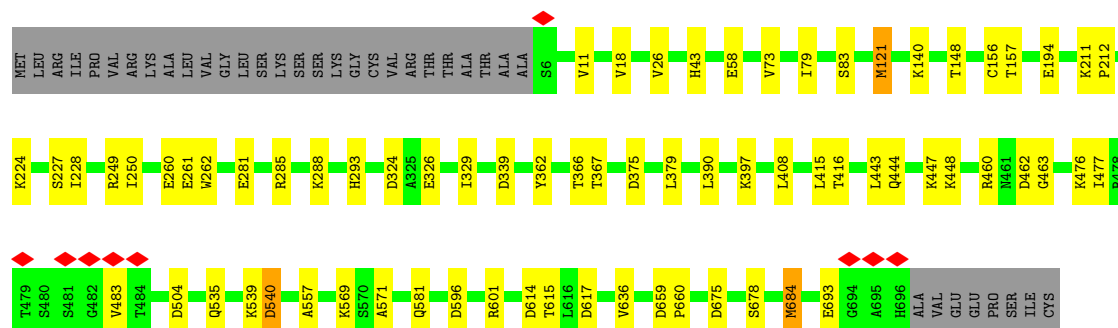
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  87% 6% 7%



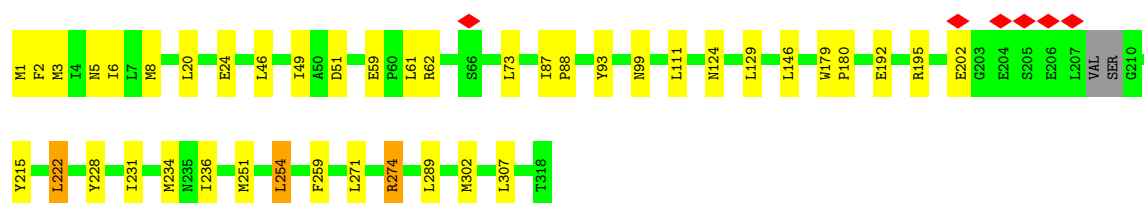
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  85% 9% 5%



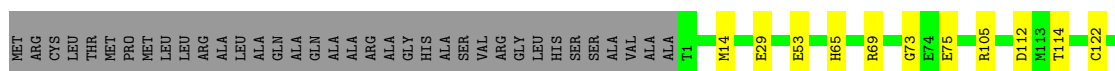
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  86% 12% 2%



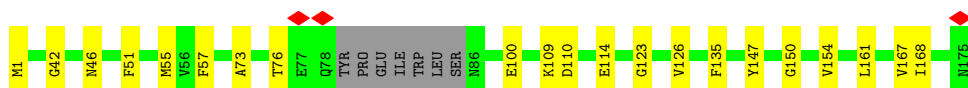
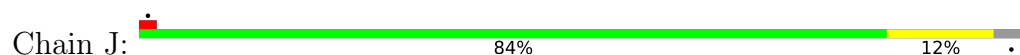
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  78% 5% 17%



R176

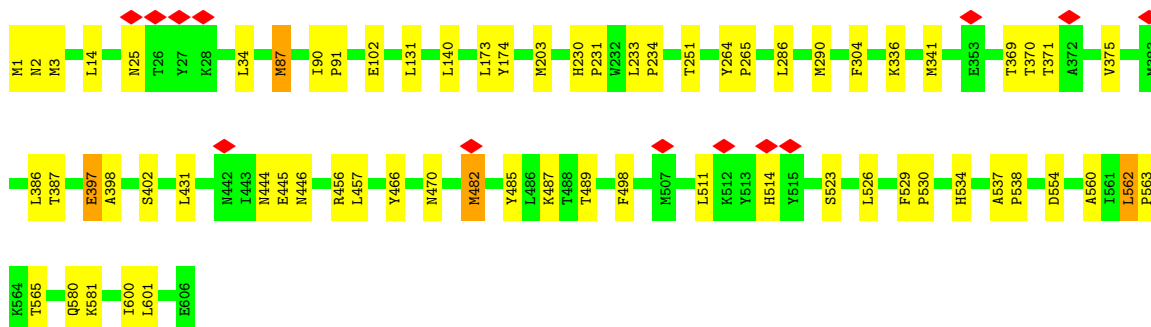
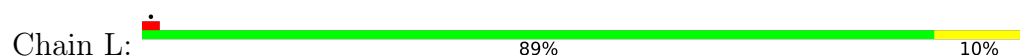
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

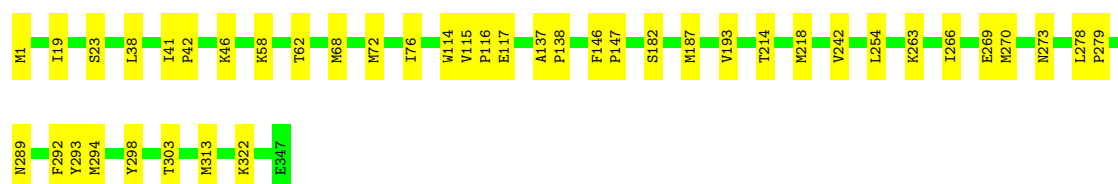


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



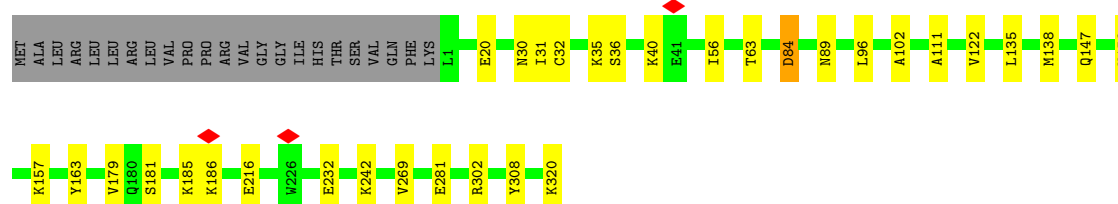
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2





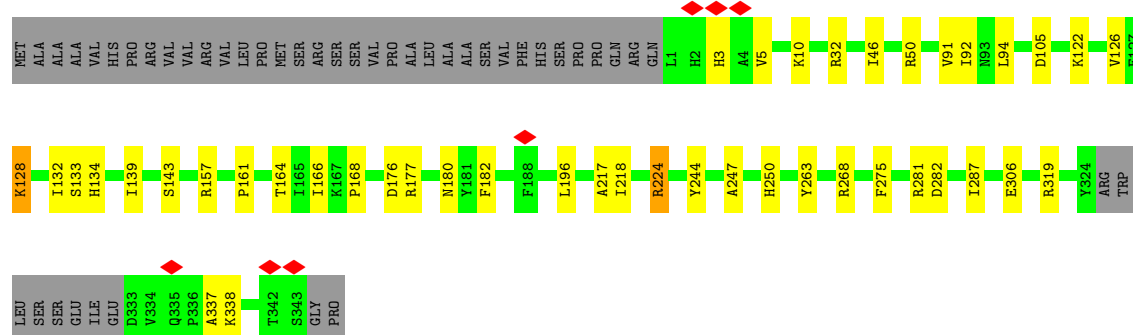
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 84% 9% 7%



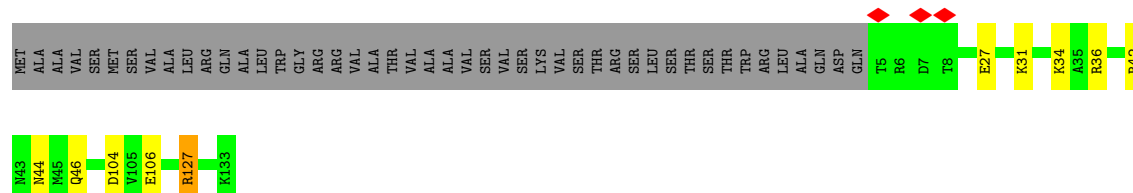
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 77% 11% 12%



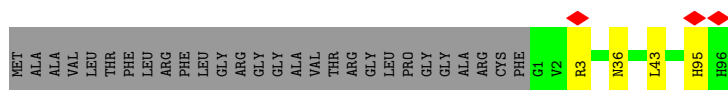
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 68% 5% 26%

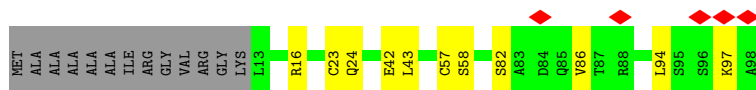
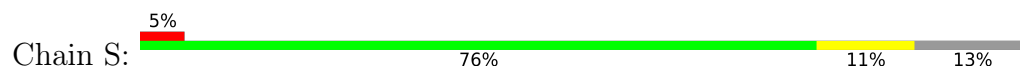


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R: 74% 23%



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



- Molecule 20: Acyl carrier protein, mitochondrial



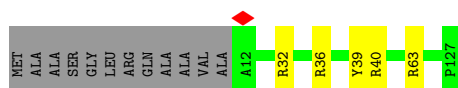
- Molecule 20: Acyl carrier protein, mitochondrial



- 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

Chain Y: 94% 5%



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

Chain Z: 89% 10%



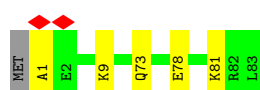
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a: 90% 10%



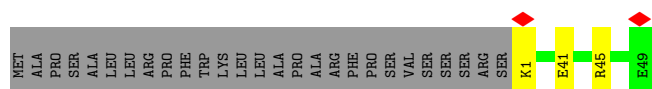
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b: 93% 6%



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

Chain c: 61% 36%



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

Chain d: 6% 91% 8%



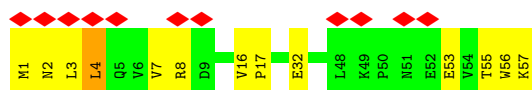
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 



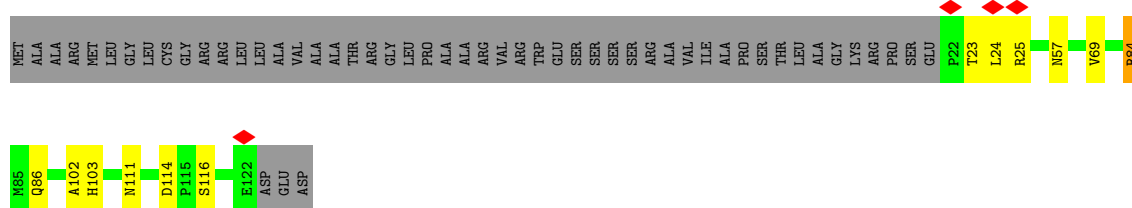
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 



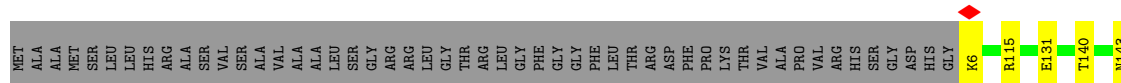
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 



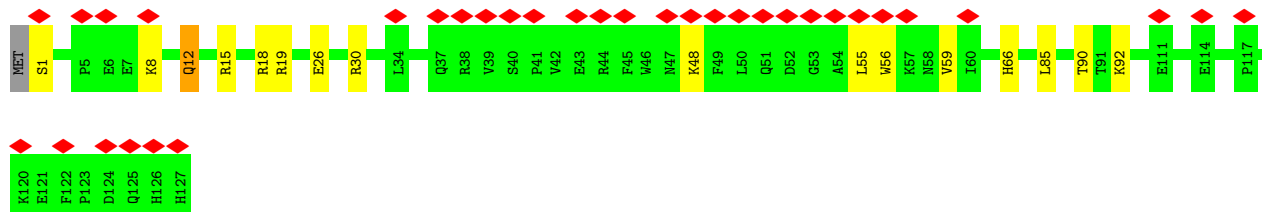
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 



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

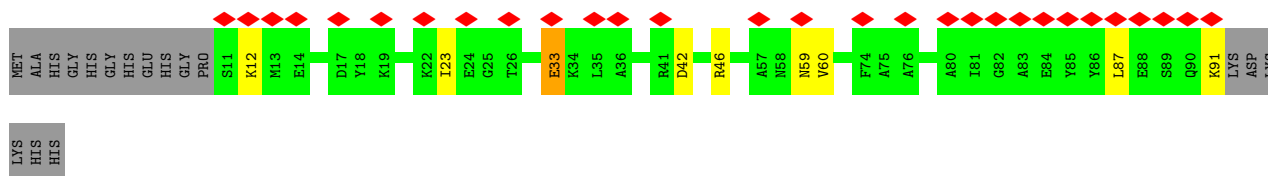
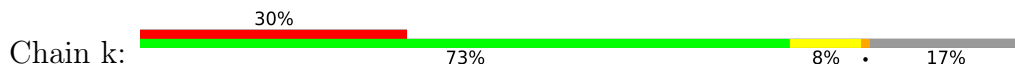
Chain i: 



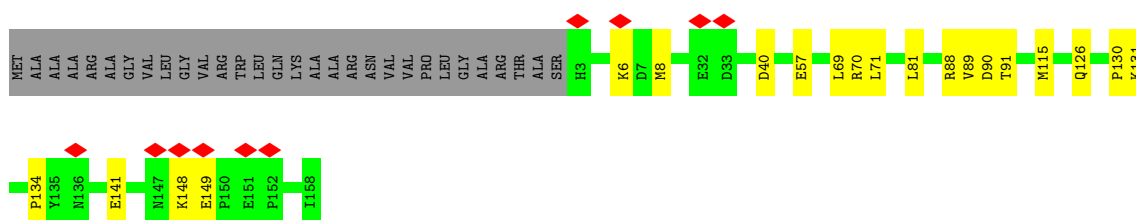
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j: 

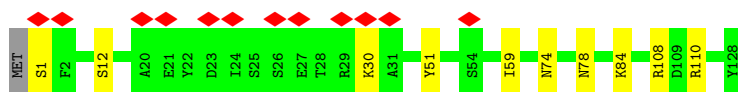
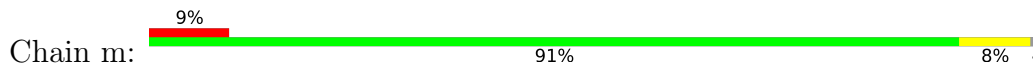
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



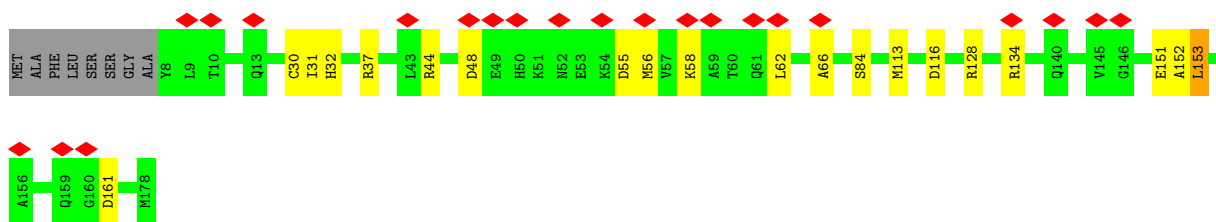
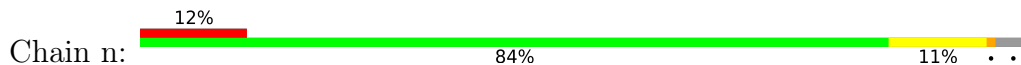
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



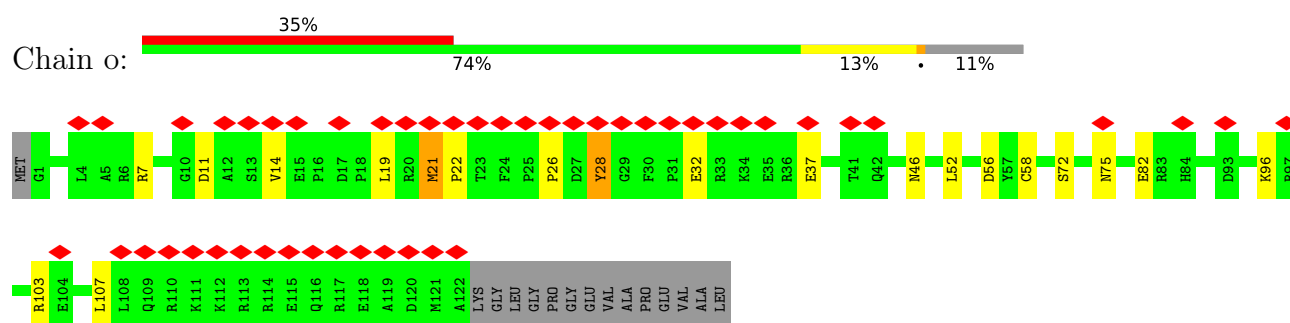
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



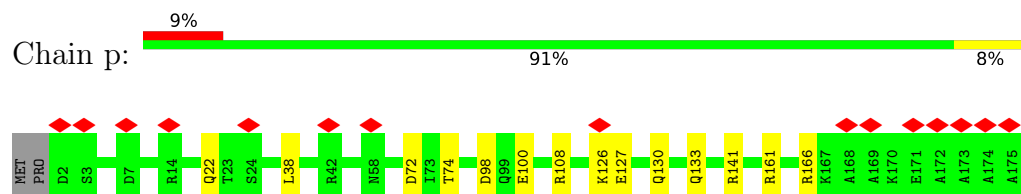
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



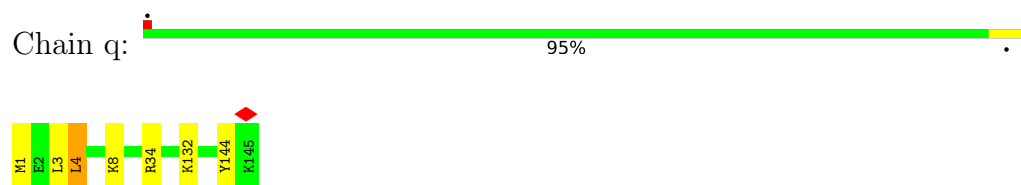
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



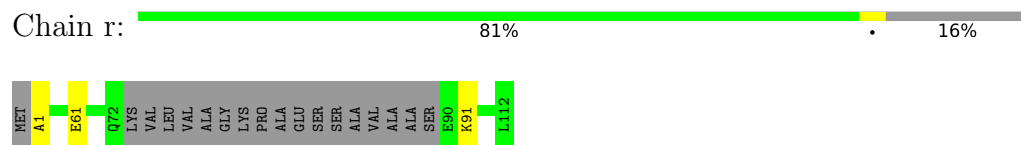
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



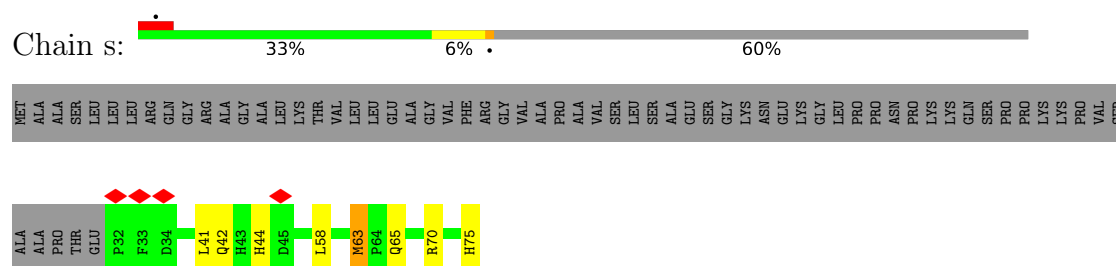
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93255	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	0.355	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.11	0/825	0.21	0/1128
2	B	0.14	0/1278	0.25	0/1728
3	C	0.13	0/1772	0.26	0/2413
4	D	0.14	0/3437	0.24	0/4654
5	E	0.11	0/1699	0.27	0/2312
6	F	0.11	0/3401	0.23	0/4595
7	G	0.12	0/5387	0.25	0/7301
8	H	0.13	0/2557	0.28	0/3492
9	I	0.16	0/1445	0.27	0/1956
10	J	0.11	0/1301	0.22	0/1761
11	K	0.11	0/745	0.24	0/1008
12	L	0.09	0/4920	0.23	0/6694
13	M	0.11	0/3738	0.23	0/5097
14	N	0.12	0/2792	0.25	0/3800
15	O	0.09	0/2651	0.21	0/3587
16	P	0.11	0/2763	0.23	0/3747
17	Q	0.11	0/1072	0.23	0/1449
18	R	0.14	0/753	0.22	0/1014
19	S	0.08	0/702	0.22	0/945
20	T	0.10	0/719	0.22	0/971
20	U	0.11	0/719	0.24	0/971
21	V	0.09	0/943	0.21	0/1277
22	W	0.10	0/1006	0.22	0/1352
23	X	0.10	0/1439	0.22	0/1942
24	Y	0.09	0/1042	0.19	0/1414
25	Z	0.11	0/1186	0.21	0/1599
26	a	0.13	0/584	0.22	0/786
27	b	0.09	0/667	0.21	0/916
28	c	0.12	0/427	0.17	0/579
29	d	0.10	0/1018	0.21	0/1375
30	e	0.10	0/846	0.22	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.12	0/505	0.23	0/681
32	g	0.10	0/873	0.25	0/1186
33	h	0.09	0/1188	0.20	0/1607
34	i	0.08	0/1127	0.22	0/1534
35	j	0.10	0/624	0.22	0/855
36	k	0.07	0/672	0.20	0/906
37	l	0.09	0/1369	0.24	0/1873
38	m	0.08	0/1088	0.21	0/1472
39	n	0.08	0/1540	0.22	0/2085
40	o	0.11	0/1073	0.24	0/1437
41	p	0.08	0/1491	0.19	0/2011
42	q	0.12	0/1242	0.23	0/1688
43	r	0.11	0/789	0.24	0/1068
44	s	0.09	0/383	0.22	0/518
All	All	0.11	0/67798	0.23	0/91915

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	815	0	856	12	0
2	B	1247	0	1256	5	0
3	C	1721	0	1675	11	0
4	D	3364	0	3311	19	0
5	E	1659	0	1664	14	0
6	F	3326	0	3282	19	0
7	G	5298	0	5316	38	0
8	H	2496	0	2606	29	0
9	I	1414	0	1370	8	0
10	J	1281	0	1292	14	0
11	K	745	0	785	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	45	0
13	M	3654	0	3852	20	0
14	N	2733	0	2912	28	0
15	O	2589	0	2566	22	0
16	P	2689	0	2710	22	0
17	Q	1049	0	1045	6	0
18	R	740	0	714	3	0
19	S	691	0	706	6	0
20	T	707	0	700	11	0
20	U	707	0	700	11	0
21	V	923	0	964	3	0
22	W	982	0	999	6	0
23	X	1402	0	1383	6	0
24	Y	1030	0	1039	2	0
25	Z	1157	0	1156	10	0
26	a	569	0	568	5	0
27	b	654	0	663	1	0
28	c	414	0	415	1	0
29	d	999	0	988	7	0
30	e	825	0	826	9	0
31	f	492	0	501	6	0
32	g	846	0	798	9	0
33	h	1154	0	1168	4	0
34	i	1097	0	1108	11	0
35	j	597	0	536	4	0
36	k	653	0	639	6	0
37	l	1314	0	1210	12	0
38	m	1070	0	1068	6	0
39	n	1487	0	1433	13	0
40	o	1048	0	1016	11	0
41	p	1458	0	1430	7	0
42	q	1212	0	1183	2	0
43	r	776	0	782	1	0
44	s	371	0	344	6	0
45	A	43	0	63	0	0
45	H	36	0	49	0	0
45	I	37	0	51	0	0
45	J	67	0	85	0	0
45	K	44	0	62	0	0
45	L	45	0	67	1	0
45	M	159	0	217	1	0
45	N	134	0	199	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Y	311	0	467	3	0
45	Z	88	0	133	1	0
45	b	98	0	153	0	0
45	d	49	0	75	1	0
45	f	51	0	82	1	0
45	h	32	0	38	0	0
45	m	71	0	93	0	0
45	q	51	0	82	0	0
45	r	28	0	30	0	0
46	A	76	0	100	0	0
46	B	48	0	70	0	0
46	H	87	0	128	2	0
46	I	54	0	88	1	0
46	L	54	0	88	1	0
46	M	35	0	44	0	0
46	Z	44	0	62	0	0
46	d	39	0	52	0	0
46	g	44	0	65	1	0
46	h	40	0	54	0	0
46	m	40	0	54	0	0
46	q	23	0	20	0	0
47	B	8	0	0	0	0
47	F	8	0	0	0	0
47	G	16	0	0	0	0
47	I	16	0	0	1	0
48	B	28	0	30	0	0
48	J	35	0	47	0	0
48	L	42	0	64	0	0
48	O	42	0	64	0	0
48	Y	37	0	51	0	0
48	Z	34	0	45	0	0
48	b	38	0	53	0	0
48	d	32	0	41	0	0
48	g	28	0	30	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	1	0
51	G	1	0	0	0	0
52	M	1	0	0	0	0
52	R	1	0	0	0	0
53	M	100	0	156	3	0
53	N	84	0	115	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	X	86	0	125	3	0
53	d	65	0	77	0	0
53	h	70	0	87	0	0
53	i	72	0	88	0	0
53	r	58	0	60	1	0
54	O	31	0	12	2	0
55	O	1	0	0	0	0
56	P	48	0	26	2	0
57	T	37	0	0	1	0
57	U	37	0	0	0	0
58	i	29	0	38	4	0
59	o	15	0	27	0	0
All	All	69324	0	70521	440	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 (440) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:487:LYS:NZ	35:j:46:ALA:O	2.08	0.86
32:g:102:ALA:O	32:g:103:HIS:ND1	2.11	0.84
11:K:73:LEU:HD21	14:N:41:ILE:HD12	1.61	0.83
45:L:702:3PE:O14	34:i:92:LYS:NZ	2.14	0.81
7:G:675:ASP:OD1	7:G:678:SER:OG	1.98	0.81
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.14	0.80
2:B:82:GLN:NE2	8:H:215:TYR:O	2.15	0.80
29:d:5:ARG:NH1	29:d:7:GLY:O	2.15	0.79
7:G:615:THR:OG1	7:G:617:ASP:OD1	2.01	0.79
7:G:260:GLU:OE2	7:G:397:LYS:NZ	2.16	0.78
1:A:71:LEU:O	10:J:147:TYR:OH	2.01	0.78
12:L:485:TYR:O	12:L:489:THR:OG1	2.02	0.77
7:G:140:LYS:O	7:G:148:THR:OG1	2.02	0.76
7:G:569:LYS:NZ	7:G:596:ASP:OD2	2.17	0.76
29:d:6:GLN:N	29:d:6:GLN:OE1	2.19	0.75
38:m:74:ASN:OD1	38:m:78:ASN:ND2	2.20	0.75
7:G:460:ARG:NH2	7:G:659:ASP:OD1	2.21	0.74
30:e:83:GLU:OE1	30:e:87:LYS:NZ	2.20	0.73
39:n:44:ARG:NH2	39:n:48:ASP:OD1	2.21	0.73
15:O:308:TYR:OH	15:O:320:LYS:O	2.06	0.73
20:T:55:GLU:OE2	22:W:36:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:98:ASP:OD2	41:p:141:ARG:NH2	2.22	0.72
36:k:42:ASP:OD1	39:n:37:ARG:NH2	2.22	0.72
8:H:24:GLU:OE2	8:H:274:ARG:NH2	2.23	0.72
15:O:216:GLU:N	15:O:216:GLU:OE1	2.23	0.71
20:U:85:ASP:OD2	34:i:18:ARG:NH2	2.23	0.71
23:X:154:GLU:N	23:X:154:GLU:OE1	2.24	0.70
20:T:88:GLU:OE1	20:T:88:GLU:N	2.23	0.70
41:p:72:ASP:OD2	41:p:74:THR:OG1	2.09	0.70
1:A:18:VAL:HG22	8:H:222:LEU:HD23	1.74	0.70
25:Z:130:GLU:N	25:Z:130:GLU:OE1	2.25	0.69
34:i:30:ARG:NH2	39:n:116:ASP:OD1	2.25	0.69
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.25	0.69
53:M:607:CDL:H272	53:X:201:CDL:H671	1.74	0.69
12:L:601:LEU:HD11	45:Y:207:3PE:H222	1.75	0.68
20:U:87:TYR:OH	34:i:26:GLU:OE2	2.10	0.68
15:O:32:CYS:SG	15:O:186:LYS:NZ	2.66	0.68
40:o:46:ASN:ND2	40:o:46:ASN:O	2.26	0.68
5:E:204:GLU:N	5:E:204:GLU:OE1	2.27	0.67
26:a:55:SER:OG	26:a:57:VAL:O	2.06	0.67
37:l:40:ASP:OD2	38:m:84:LYS:NZ	2.27	0.67
7:G:366:THR:O	7:G:367:THR:OG1	2.12	0.66
6:F:224:ASN:ND2	50:F:502:FMN:O2	2.28	0.66
15:O:232:GLU:OE1	15:O:232:GLU:N	2.28	0.66
37:l:57:GLU:OE2	38:m:12:SER:OG	2.12	0.66
58:i:201:CHD:H212	58:i:201:CHD:H12	1.78	0.66
6:F:18:GLU:N	6:F:18:GLU:OE1	2.29	0.66
15:O:281:GLU:N	15:O:281:GLU:OE1	2.28	0.66
16:P:306:GLU:N	16:P:306:GLU:OE1	2.29	0.66
20:U:36:PHE:O	20:U:42:LEU:N	2.29	0.66
12:L:369:THR:N	12:L:445:GLU:OE2	2.29	0.65
34:i:12:GLN:OE1	34:i:15:ARG:NH2	2.30	0.64
44:s:42:GLN:OE1	44:s:42:GLN:N	2.30	0.64
20:T:28:GLU:N	20:T:28:GLU:OE1	2.31	0.64
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.11	0.63
15:O:147:GLN:N	15:O:147:GLN:OE1	2.31	0.63
13:M:457:PRO:O	32:g:84:ARG:NH2	2.31	0.63
17:Q:127:ARG:NH1	44:s:75:HIS:O	2.30	0.63
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.80	0.63
39:n:55:ASP:OD2	39:n:58:LYS:N	2.31	0.63
20:U:23:ASP:OD1	36:k:46:ARG:NH2	2.32	0.62
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:56:ARG:NH2	5:E:158:ASP:OD2	2.33	0.62
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.82	0.62
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.17	0.62
36:k:33:GLU:N	36:k:33:GLU:OE1	2.33	0.62
8:H:146:LEU:HD11	8:H:192:GLU:HG3	1.82	0.62
7:G:249:ARG:C	7:G:250:ILE:HD12	2.25	0.62
20:U:71:MET:SD	20:U:71:MET:N	2.73	0.62
19:S:42:GLU:N	19:S:42:GLU:OE1	2.32	0.61
5:E:148:CYS:N	6:F:105:CYS:SG	2.73	0.61
14:N:298:TYR:O	14:N:303:THR:OG1	2.15	0.61
21:V:21:GLU:OE1	21:V:21:GLU:N	2.33	0.61
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.83	0.61
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.36	0.61
12:L:397:GLU:N	12:L:397:GLU:OE1	2.34	0.61
7:G:261:GLU:OE1	17:Q:42:ARG:NH2	2.34	0.61
7:G:339:ASP:OD1	19:S:16:ARG:NH1	2.34	0.61
15:O:36:SER:OG	54:O:401:DGT:O1G	2.19	0.61
20:U:87:TYR:OH	33:h:6:LYS:NZ	2.32	0.61
5:E:36:LYS:O	44:s:65:GLN:NE2	2.34	0.60
40:o:37:GLU:OE1	40:o:37:GLU:N	2.33	0.60
9:I:65:HIS:CE1	47:I:201:SF4:S2	2.95	0.60
14:N:214:THR:HG22	14:N:218:MET:HE2	1.83	0.60
20:T:49:GLU:OE2	22:W:63:ARG:NH1	2.35	0.60
41:p:108:ARG:NH2	41:p:130:GLN:OE1	2.35	0.60
12:L:341:MET:CE	12:L:457:LEU:HD12	2.32	0.59
53:X:201:CDL:OA4	53:X:201:CDL:O1	2.19	0.59
8:H:124:ASN:O	8:H:124:ASN:ND2	2.35	0.59
6:F:436:GLN:N	6:F:436:GLN:OE1	2.35	0.59
7:G:285:ARG:NH1	7:G:557:ALA:O	2.35	0.59
32:g:86:GLN:NE2	41:p:100:GLU:OE2	2.36	0.59
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.83	0.58
36:k:87:LEU:H	36:k:87:LEU:HD23	1.67	0.58
1:A:32:GLU:N	1:A:32:GLU:OE1	2.36	0.58
25:Z:125:GLY:C	25:Z:126:LEU:HD12	2.28	0.58
57:T:101:EHZ:O1	57:T:101:EHZ:O2	2.19	0.58
7:G:156:CYS:O	7:G:157:THR:OG1	2.18	0.58
31:f:53:GLU:N	31:f:53:GLU:OE1	2.36	0.58
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.35	0.58
7:G:443:LEU:HD13	7:G:477:ILE:HD11	1.86	0.58
12:L:34:LEU:HD21	58:i:201:CHD:H221	1.85	0.58
7:G:693:GLU:OE1	7:G:693:GLU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:58:GLU:N	30:e:58:GLU:OE1	2.36	0.57
4:D:62:LEU:HD13	4:D:425:PHE:CE1	2.39	0.57
14:N:269:GLU:O	14:N:273:ASN:ND2	2.38	0.57
4:D:62:LEU:HD13	4:D:425:PHE:CZ	2.39	0.57
16:P:217:ALA:O	16:P:224:ARG:NH2	2.36	0.57
25:Z:119:MET:HE2	30:e:71:THR:HG21	1.86	0.57
5:E:104:THR:HG22	5:E:104:THR:O	2.04	0.57
20:U:72:CYS:O	20:U:75:GLU:N	2.36	0.57
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.35	0.56
15:O:63:THR:OG1	15:O:302:ARG:NH2	2.39	0.56
40:o:82:GLU:N	40:o:82:GLU:OE1	2.35	0.56
14:N:19:ILE:O	14:N:23:SER:OG	2.16	0.56
32:g:114:ASP:OD2	32:g:116:SER:OG	2.18	0.56
7:G:415:LEU:O	7:G:416:THR:OG1	2.23	0.56
20:U:28:GLU:N	20:U:28:GLU:OE1	2.39	0.56
1:A:65:PHE:CD2	1:A:98:LEU:HD11	2.40	0.56
8:H:111:LEU:HD11	10:J:57:PHE:CD1	2.40	0.56
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.37	0.56
5:E:165:THR:OG1	5:E:168:ASP:OD1	2.25	0.55
35:j:10:ARG:NH2	35:j:14:PHE:O	2.36	0.55
7:G:462:ASP:OD1	7:G:463:GLY:N	2.39	0.55
45:M:602:3PE:O22	45:f:101:3PE:N	2.39	0.55
6:F:45:THR:OG1	6:F:120:GLU:OE2	2.25	0.55
13:M:271:MET:HE2	13:M:271:MET:HA	1.88	0.55
12:L:290:MET:O	12:L:523:SER:OG	2.23	0.55
2:B:44:SER:OG	8:H:51:ASP:OD1	2.19	0.55
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.88	0.55
23:X:102:GLN:N	23:X:102:GLN:OE1	2.40	0.55
12:L:398:ALA:O	12:L:402:SER:OG	2.16	0.54
4:D:322:GLU:OE1	4:D:322:GLU:N	2.39	0.54
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.43	0.54
20:T:25:ILE:HD11	20:T:42:LEU:HD11	1.90	0.54
12:L:600:ILE:HG22	12:L:601:LEU:HD12	1.89	0.54
6:F:46:LYS:NZ	6:F:168:GLY:O	2.41	0.53
15:O:30:ASN:O	15:O:35:LYS:NZ	2.40	0.53
14:N:182:SER:OG	14:N:293:TYR:OH	2.11	0.53
32:g:23:THR:HG22	32:g:24:LEU:HD12	1.91	0.53
39:n:62:LEU:O	39:n:66:ALA:N	2.40	0.53
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.39	0.53
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.92	0.52
37:l:149:GLU:OE1	37:l:149:GLU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:94:LEU:HD23	16:P:132:ILE:HG13	1.91	0.52
4:D:371:LYS:NZ	4:D:422:ASP:OD1	2.42	0.52
9:I:112:ASP:OD1	9:I:114:THR:OG1	2.27	0.52
12:L:174:TYR:OH	12:L:534:HIS:NE2	2.33	0.52
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.44	0.52
16:P:128:LYS:NZ	16:P:218:ILE:O	2.42	0.52
44:s:41:LEU:O	44:s:44:HIS:NE2	2.43	0.52
1:A:14:ALA:O	1:A:18:VAL:HG23	2.10	0.52
11:K:73:LEU:HD21	14:N:41:ILE:CD1	2.37	0.52
14:N:313:MET:HE1	15:O:102:ALA:HB3	1.92	0.52
34:i:55:LEU:HD13	34:i:55:LEU:O	2.09	0.52
5:E:105:THR:HG22	5:E:106:THR:H	1.75	0.52
15:O:181:SER:OG	15:O:185:LYS:NZ	2.43	0.52
1:A:115:GLU:N	1:A:115:GLU:OE1	2.43	0.51
40:o:21:MET:HB3	40:o:22:PRO:HD2	1.92	0.51
44:s:63:MET:HE2	44:s:63:MET:HA	1.93	0.51
6:F:96:ASN:ND2	6:F:187:GLY:O	2.41	0.51
6:F:302:SER:HB2	6:F:350:LEU:HD22	1.92	0.51
36:k:59:ASN:OD1	36:k:60:VAL:N	2.44	0.51
39:n:30:CYS:O	39:n:32:HIS:N	2.44	0.51
16:P:247:ALA:O	16:P:250:HIS:ND1	2.41	0.51
37:l:90:ASP:OD1	37:l:91:THR:N	2.44	0.51
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.93	0.51
4:D:67:GLU:C	4:D:68:LEU:HD12	2.36	0.51
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.93	0.51
8:H:111:LEU:HD11	10:J:57:PHE:HD1	1.76	0.51
19:S:23:CYS:SG	19:S:24:GLN:N	2.83	0.51
20:T:16:LEU:HD13	20:T:16:LEU:O	2.10	0.50
58:i:201:CHD:O7	58:i:201:CHD:H41	2.11	0.50
37:l:115:MET:HE3	37:l:115:MET:HA	1.93	0.50
6:F:306:LEU:C	6:F:306:LEU:HD12	2.37	0.50
25:Z:119:MET:HE2	30:e:71:THR:CG2	2.42	0.50
20:U:40:LEU:O	20:U:40:LEU:HD12	2.12	0.50
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.93	0.50
13:M:385:THR:HG21	13:M:396:MET:HE1	1.94	0.50
38:m:51:TYR:O	39:n:128:ARG:NH2	2.43	0.50
24:Y:140:VAL:O	33:h:115:ARG:NH1	2.45	0.50
31:f:55:THR:HG1	31:f:56:TRP:CD1	2.29	0.50
12:L:264:TYR:N	12:L:265:PRO:CD	2.75	0.50
12:L:341:MET:HE1	12:L:457:LEU:HD12	1.93	0.50
29:d:109:TYR:HA	29:d:112:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:47:GLU:N	6:F:47:GLU:OE1	2.45	0.49
37:l:141:GLU:OE1	37:l:141:GLU:N	2.41	0.49
2:B:116:MET:SD	2:B:156:LEU:HD22	2.52	0.49
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.47	0.49
12:L:2:ASN:OD1	12:L:3:MET:N	2.44	0.49
12:L:87:MET:HA	12:L:87:MET:HE2	1.94	0.49
12:L:534:HIS:ND1	46:L:701:PC1:O12	2.43	0.49
36:k:87:LEU:O	36:k:91:LYS:NZ	2.46	0.49
7:G:444:GLN:OE1	7:G:476:LYS:NZ	2.31	0.49
19:S:82:SER:O	19:S:86:VAL:N	2.45	0.49
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.39	0.49
39:n:153:LEU:N	39:n:153:LEU:HD22	2.27	0.49
7:G:43:HIS:NE2	7:G:261:GLU:OE2	2.42	0.49
11:K:63:LEU:HD23	11:K:63:LEU:O	2.13	0.49
12:L:446:ASN:ND2	35:j:21:GLN:OE1	2.46	0.49
14:N:193:VAL:HB	14:N:266:ILE:HG23	1.95	0.49
37:l:134:PRO:HD3	40:o:56:ASP:O	2.13	0.49
15:O:20:GLU:OE1	15:O:20:GLU:N	2.39	0.48
15:O:111:ALA:HB1	15:O:122:VAL:HG21	1.94	0.48
6:F:103:GLY:O	6:F:333:ALA:HB1	2.13	0.48
35:j:11:TYR:O	35:j:12:ARG:C	2.56	0.48
41:p:127:GLU:N	41:p:127:GLU:OE1	2.46	0.48
14:N:146:PHE:N	14:N:147:PRO:CD	2.76	0.48
58:i:201:CHD:H212	58:i:201:CHD:C12	2.43	0.48
11:K:73:LEU:HD22	14:N:38:LEU:HD12	1.96	0.48
29:d:11:PHE:O	30:e:8:ARG:NH1	2.42	0.48
16:P:139:ILE:C	16:P:139:ILE:HD12	2.39	0.48
16:P:164:THR:OG1	16:P:224:ARG:NH1	2.46	0.48
3:C:8:ARG:NH2	43:r:61:GLU:OE2	2.46	0.48
39:n:31:ILE:N	39:n:31:ILE:HD12	2.29	0.48
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.94	0.48
11:K:43:MET:HE1	14:N:72:MET:HE1	1.96	0.47
4:D:49:LEU:CD1	4:D:68:LEU:HD13	2.44	0.47
3:C:58:ILE:HB	3:C:59:PRO:HD3	1.96	0.47
4:D:4:TRP:CG	13:M:140:THR:HG1	2.32	0.47
4:D:202:ASP:OD1	4:D:203:LEU:N	2.47	0.47
10:J:150:GLY:O	10:J:154:VAL:HG23	2.14	0.47
16:P:182:PHE:HZ	16:P:287:ILE:HG23	1.79	0.47
39:n:56:MET:HA	39:n:56:MET:HE2	1.95	0.47
3:C:151:ILE:HG23	3:C:152:LEU:HG	1.96	0.47
40:o:72:SER:O	40:o:75:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9:GLU:OE1	4:D:9:GLU:N	2.46	0.47
19:S:57:CYS:SG	19:S:58:SER:N	2.85	0.47
12:L:230:HIS:N	12:L:231:PRO:CD	2.77	0.47
4:D:49:LEU:HD13	4:D:68:LEU:HD13	1.97	0.47
4:D:106:LEU:HD11	4:D:391:ILE:HD13	1.96	0.47
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.97	0.47
16:P:157:ARG:NH1	16:P:161:PRO:O	2.47	0.47
16:P:177:ARG:NH2	56:P:501:NDP:O3	2.47	0.47
41:p:38:LEU:HD23	41:p:38:LEU:O	2.14	0.47
5:E:145:LEU:HD12	5:E:153:MET:SD	2.55	0.47
7:G:227:SER:OG	7:G:228:ILE:N	2.48	0.47
12:L:466:TYR:O	12:L:470:ASN:ND2	2.41	0.47
15:O:135:LEU:HD22	15:O:152:TYR:CD1	2.50	0.47
16:P:46:ILE:N	16:P:46:ILE:HD12	2.30	0.47
15:O:308:TYR:HH	15:O:320:LYS:C	2.17	0.47
53:X:201:CDL:H873	53:X:201:CDL:H542	1.97	0.47
45:d:201:3PE:O12	30:e:8:ARG:NH2	2.42	0.47
16:P:133:SER:OG	16:P:134:HIS:N	2.48	0.46
12:L:371:THR:O	12:L:375:VAL:HG23	2.16	0.46
5:E:172:ILE:HG23	5:E:182:PRO:HG2	1.97	0.46
39:n:151:GLU:OE1	39:n:151:GLU:N	2.48	0.46
3:C:111:THR:OG1	3:C:112:ASP:N	2.48	0.46
10:J:167:VAL:HG22	14:N:42:PRO:HG3	1.98	0.46
16:P:5:VAL:HG12	16:P:5:VAL:O	2.15	0.46
12:L:482:MET:HE3	12:L:487:LYS:CG	2.45	0.46
15:O:89:ASN:O	32:g:23:THR:HG21	2.15	0.46
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.14	0.46
34:i:55:LEU:HD13	34:i:55:LEU:C	2.41	0.46
8:H:2:PHE:HE2	8:H:6:ILE:HD11	1.78	0.46
8:H:99:ASN:N	46:H:402:PC1:O12	2.44	0.46
12:L:286:LEU:C	12:L:286:LEU:HD13	2.41	0.46
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.46	0.46
46:g:201:PC1:O13	46:g:201:PC1:H132	2.16	0.46
9:I:75:GLU:O	9:I:105:ARG:NH1	2.48	0.46
8:H:251:MET:HE2	8:H:254:LEU:HD23	1.97	0.46
7:G:535:GLN:N	7:G:535:GLN:OE1	2.50	0.45
5:E:199:LEU:HD12	5:E:199:LEU:N	2.32	0.45
37:l:88:ARG:O	37:l:89:VAL:C	2.59	0.45
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.33	0.45
12:L:560:ALA:O	12:L:565:THR:HG23	2.16	0.45
53:M:607:CDL:H541	14:N:242:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:21:MET:HB3	40:o:22:PRO:CD	2.46	0.45
46:I:204:PC1:H3I1	45:Z:202:3PE:H381	1.99	0.45
17:Q:27:GLU:OE1	17:Q:27:GLU:N	2.42	0.45
8:H:179:TRP:N	8:H:180:PRO:CD	2.78	0.45
8:H:202:GLU:OE1	8:H:202:GLU:N	2.45	0.45
13:M:116:ILE:HG12	13:M:174:LEU:HD13	1.98	0.45
3:C:154:ASP:OD1	3:C:155:TYR:N	2.49	0.45
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.98	0.45
12:L:526:LEU:HD12	12:L:530:PRO:HG2	1.99	0.45
45:N:402:3PE:H272	45:Y:205:3PE:H2I2	1.98	0.45
45:Y:202:3PE:N	45:Y:203:3PE:O13	2.50	0.45
31:f:3:LEU:O	31:f:7:VAL:HG12	2.17	0.45
37:l:81:LEU:HD13	37:l:81:LEU:C	2.42	0.45
14:N:72:MET:HE3	14:N:76:ILE:HD11	2.00	0.45
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.99	0.44
8:H:46:LEU:HD23	8:H:49:ILE:HD12	1.98	0.44
15:O:138:MET:CE	54:O:401:DGT:HN2	2.30	0.44
21:V:61:GLU:OE2	21:V:66:LYS:NZ	2.47	0.44
13:M:130:LEU:HD21	14:N:294:MET:CE	2.47	0.44
16:P:143:SER:OG	16:P:282:ASP:OD1	2.35	0.44
40:o:21:MET:HE2	40:o:21:MET:HA	1.99	0.44
7:G:58:GLU:OE1	7:G:83:SER:OG	2.29	0.44
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.98	0.44
8:H:87:ILE:N	8:H:88:PRO:CD	2.80	0.44
14:N:193:VAL:O	14:N:193:VAL:HG22	2.17	0.44
15:O:31:ILE:O	15:O:179:VAL:HG13	2.17	0.44
3:C:41:GLN:NE2	3:C:49:GLU:OE1	2.42	0.44
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.35	0.44
27:b:78:GLU:OE1	27:b:81:LYS:NZ	2.47	0.44
32:g:23:THR:HG22	32:g:24:LEU:CD1	2.47	0.44
7:G:194:GLU:OE1	7:G:194:GLU:N	2.41	0.44
53:r:202:CDL:OB3	53:r:202:CDL:O1	2.32	0.44
1:A:27:LEU:HD12	16:P:275:PHE:CZ	2.52	0.44
12:L:562:LEU:CB	12:L:563:PRO:CD	2.96	0.44
17:Q:36:ARG:NH2	17:Q:106:GLU:OE1	2.50	0.44
4:D:347:HIS:CD2	7:G:121:MET:HE3	2.53	0.44
7:G:483:VAL:O	7:G:483:VAL:HG23	2.18	0.44
5:E:105:THR:HG22	5:E:106:THR:N	2.32	0.43
29:d:5:ARG:NE	29:d:85:VAL:HG13	2.32	0.43
3:C:109:THR:OG1	3:C:110:TYR:N	2.50	0.43
8:H:20:LEU:HD13	26:a:12:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:GLU:OE1	8:H:228:TYR:OH	2.30	0.43
12:L:482:MET:SD	12:L:482:MET:N	2.92	0.43
5:E:100:ILE:HG12	5:E:156:ILE:HD12	2.01	0.43
6:F:94:VAL:HG11	6:F:192:LEU:HD22	2.01	0.43
13:M:114:GLU:OE1	13:M:116:ILE:N	2.51	0.43
1:A:60:ILE:HG21	10:J:168:ILE:HG21	2.00	0.43
4:D:69:SER:OG	4:D:74:ARG:NE	2.51	0.43
8:H:289:LEU:C	8:H:289:LEU:HD13	2.43	0.43
13:M:47:ASP:OD1	13:M:48:ASN:N	2.50	0.43
13:M:154:LEU:HD11	14:N:254:LEU:HD21	2.00	0.43
14:N:270:MET:CE	14:N:278:LEU:HD23	2.48	0.43
10:J:110:ASP:OD1	10:J:110:ASP:N	2.50	0.43
12:L:482:MET:HE2	12:L:482:MET:O	2.18	0.43
20:U:40:LEU:HD12	20:U:40:LEU:C	2.43	0.43
33:h:140:THR:O	33:h:143:ASN:ND2	2.44	0.43
12:L:90:ILE:HB	12:L:91:PRO:HD3	2.00	0.43
15:O:56:ILE:HD11	15:O:96:LEU:HD11	2.00	0.43
18:R:95:HIS:O	18:R:95:HIS:ND1	2.49	0.43
26:a:37:ARG:HG2	26:a:48:MET:HE2	2.00	0.43
37:l:69:LEU:HB3	37:l:71:LEU:HD13	1.99	0.43
3:C:136:ASP:OD1	3:C:153:THR:OG1	2.33	0.43
12:L:131:LEU:HD23	12:L:131:LEU:O	2.18	0.43
12:L:140:LEU:O	12:L:140:LEU:HD23	2.19	0.43
17:Q:34:LYS:NZ	17:Q:104:ASP:OD1	2.52	0.43
4:D:68:LEU:HD12	4:D:68:LEU:N	2.33	0.43
8:H:307:LEU:HD21	25:Z:46:TYR:CD1	2.54	0.43
15:O:84:ASP:N	15:O:84:ASP:OD1	2.51	0.43
23:X:11:ASP:N	23:X:11:ASP:OD1	2.52	0.43
25:Z:97:MET:HE2	25:Z:100:VAL:HG21	2.01	0.43
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.51	0.43
25:Z:104:LYS:O	30:e:74:ARG:NH2	2.51	0.43
5:E:118:GLU:N	5:E:118:GLU:OE1	2.52	0.42
6:F:192:LEU:C	6:F:192:LEU:HD23	2.44	0.42
7:G:684:MET:HA	7:G:684:MET:HE2	2.01	0.42
10:J:42:GLY:O	10:J:46:ASN:ND2	2.49	0.42
10:J:51:PHE:CE2	10:J:55:MET:HE3	2.54	0.42
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.01	0.42
14:N:115:VAL:HB	14:N:116:PRO:HD3	2.02	0.42
34:i:56:TRP:O	34:i:59:VAL:HG12	2.19	0.42
7:G:281:GLU:OE1	7:G:293:HIS:ND1	2.52	0.42
9:I:29:GLU:OE1	9:I:29:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:GLY:HA3	18:R:43:LEU:HD13	2.00	0.42
7:G:326:GLU:OE1	7:G:326:GLU:N	2.49	0.42
16:P:91:VAL:HG23	16:P:126:VAL:HG11	2.00	0.42
37:l:130:PRO:O	37:l:131:LYS:C	2.62	0.42
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.00	0.42
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.41	0.42
13:M:130:LEU:HD21	14:N:294:MET:HE1	2.00	0.42
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.54	0.42
40:o:11:ASP:OD2	40:o:14:VAL:HG13	2.18	0.42
1:A:18:VAL:HG22	8:H:222:LEU:CD2	2.48	0.42
10:J:100:GLU:OE1	11:K:10:MET:HE3	2.20	0.42
13:M:97:THR:HG21	53:M:607:CDL:H202	2.01	0.42
13:M:285:LEU:HD23	13:M:285:LEU:C	2.44	0.42
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.01	0.42
15:O:56:ILE:HD11	15:O:96:LEU:CD1	2.49	0.42
23:X:44:LEU:HD22	23:X:130:VAL:HG13	2.01	0.42
30:e:21:SER:N	30:e:36:GLU:OE1	2.53	0.42
39:n:151:GLU:O	39:n:152:ALA:HB3	2.20	0.42
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.43	0.42
12:L:386:LEU:HD23	12:L:387:THR:N	2.35	0.42
13:M:231:LEU:HD23	13:M:235:LEU:HD12	2.01	0.42
34:i:12:GLN:HG2	34:i:15:ARG:HH22	1.84	0.42
37:l:70:ARG:C	37:l:71:LEU:HD12	2.45	0.42
9:I:65:HIS:CD2	9:I:122:CYS:SG	3.12	0.42
12:L:173:LEU:C	12:L:173:LEU:HD23	2.45	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.02	0.42
16:P:166:ILE:HG22	16:P:168:PRO:HD3	2.02	0.42
39:n:134:ARG:NH2	39:n:161:ASP:OD1	2.46	0.42
2:B:86:MET:HE3	2:B:107:MET:HE2	2.02	0.41
7:G:460:ARG:NH2	7:G:660:PRO:O	2.53	0.41
12:L:203:MET:HE3	12:L:203:MET:O	2.20	0.41
16:P:244:TYR:HB2	16:P:337:ALA:HB2	2.02	0.41
4:D:300:ARG:NH2	4:D:420:THR:O	2.48	0.41
4:D:342:MET:HE3	4:D:346:ILE:HG13	2.03	0.41
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.53	0.41
14:N:289:ASN:HA	14:N:292:PHE:CE2	2.55	0.41
19:S:43:LEU:HD11	19:S:94:LEU:HD11	2.02	0.41
6:F:192:LEU:HD23	6:F:192:LEU:O	2.20	0.41
12:L:14:LEU:HD23	12:L:14:LEU:O	2.20	0.41
24:Y:68:ILE:HD12	24:Y:99:ILE:HG13	2.01	0.41
7:G:539:LYS:O	7:G:540:ASP:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:444:ASN:OD1	12:L:445:GLU:N	2.53	0.41
16:P:105:ASP:OD1	16:P:105:ASP:N	2.54	0.41
34:i:85:LEU:O	34:i:90:THR:HG23	2.20	0.41
40:o:26:PRO:O	40:o:28:TYR:N	2.53	0.41
7:G:379:LEU:HB2	7:G:408:LEU:HD12	2.02	0.41
10:J:123:GLY:O	10:J:126:VAL:HG22	2.21	0.41
1:A:5:LEU:HD22	8:H:3:MET:HE1	2.03	0.41
1:A:95:ILE:HG21	8:H:302:MET:HG3	2.02	0.41
3:C:8:ARG:CB	3:C:11:VAL:HG22	2.50	0.41
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.55	0.41
6:F:188:GLU:OE1	6:F:190:THR:N	2.54	0.41
12:L:102:GLU:OE1	12:L:456:ARG:NH2	2.44	0.41
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.50	0.41
31:f:3:LEU:C	31:f:3:LEU:HD12	2.46	0.41
11:K:36:MET:HE2	14:N:68:MET:HB3	2.02	0.41
46:H:402:PC1:O13	46:H:402:PC1:H133	2.20	0.41
11:K:55:LEU:HD21	30:e:25:PRO:HD3	2.03	0.41
12:L:482:MET:HE2	12:L:482:MET:H	1.86	0.41
13:M:403:THR:HA	13:M:406:TYR:CE2	2.56	0.41
2:B:69:MET:HE2	2:B:74:VAL:HG12	2.03	0.41
3:C:99:LEU:N	3:C:99:LEU:HD12	2.36	0.41
12:L:511:LEU:HD12	12:L:511:LEU:N	2.36	0.41
14:N:41:ILE:N	14:N:42:PRO:HD2	2.35	0.41
29:d:99:GLU:OE1	29:d:99:GLU:N	2.41	0.41
29:d:120:ARG:O	38:m:108:ARG:NH2	2.54	0.41
4:D:112:MET:HE2	4:D:193:TYR:HB3	2.03	0.41
6:F:172:ASP:OD1	6:F:172:ASP:N	2.54	0.41
10:J:51:PHE:CZ	10:J:55:MET:HE3	2.56	0.41
16:P:50:ARG:NH2	56:P:501:NDP:O2X	2.46	0.41
20:T:56:ASP:OD1	22:W:40:ARG:NH2	2.50	0.41
20:T:64:ASP:OD2	22:W:32:ARG:NH1	2.54	0.41
42:q:4:LEU:HD12	42:q:8:LYS:HE3	2.02	0.41
7:G:11:VAL:HG11	7:G:73:VAL:HG22	2.02	0.40
8:H:129:LEU:HD21	10:J:73:ALA:O	2.21	0.40
14:N:278:LEU:HB3	14:N:279:PRO:HD3	2.03	0.40
8:H:61:LEU:N	8:H:61:LEU:HD22	2.36	0.40
20:T:35:HIS:N	20:T:39:ASP:OD2	2.42	0.40
6:F:154:ARG:HA	44:s:58:LEU:HD21	2.04	0.40
13:M:254:THR:O	13:M:254:THR:HG22	2.20	0.40
13:M:422:HIS:HB2	38:m:59:ILE:HD12	2.02	0.40
31:f:2:ASN:OD1	31:f:4:LEU:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:131:GLU:N	33:h:131:GLU:OE1	2.55	0.40
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.03	0.40
20:T:52:MET:HE1	22:W:39:TYR:CG	2.57	0.40
25:Z:142:TYR:CE2	26:a:48:MET:HE1	2.57	0.40
7:G:26:VAL:HG13	7:G:79:ILE:HD13	2.02	0.40
7:G:211:LYS:HB3	7:G:212:PRO:HD3	2.03	0.40
20:U:8:LEU:HD11	34:i:19:ARG:NH1	2.36	0.40
23:X:3:ILE:HD13	25:Z:107:GLU:HA	2.03	0.40
40:o:32:GLU:OE1	40:o:32:GLU:N	2.55	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	97/115 (84%)	94 (97%)	3 (3%)	0	100	100
2	B	154/216 (71%)	151 (98%)	3 (2%)	0	100	100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	410/463 (89%)	399 (97%)	11 (3%)	0	100	100
5	E	212/249 (85%)	205 (97%)	7 (3%)	0	100	100
6	F	430/464 (93%)	419 (97%)	11 (3%)	0	100	100
7	G	689/727 (95%)	664 (96%)	25 (4%)	0	100	100
8	H	312/318 (98%)	300 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	170 (98%)	4 (2%)	0	100	100
10	J	164/175 (94%)	156 (95%)	8 (5%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	585 (97%)	18 (3%)	1 (0%)	43	66
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
15	O	318/343 (93%)	310 (98%)	8 (2%)	0	100	100
16	P	331/380 (87%)	322 (97%)	9 (3%)	0	100	100
17	Q	127/175 (73%)	124 (98%)	3 (2%)	0	100	100
18	R	94/124 (76%)	93 (99%)	1 (1%)	0	100	100
19	S	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	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%)	167 (99%)	2 (1%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	96/106 (91%)	94 (98%)	2 (2%)	0	100	100
31	f	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
32	g	99/154 (64%)	91 (92%)	8 (8%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
35	j	69/108 (64%)	64 (93%)	5 (7%)	0	100	100
36	k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
37	l	154/186 (83%)	141 (92%)	13 (8%)	0	100	100
38	m	126/129 (98%)	123 (98%)	3 (2%)	0	100	100
39	n	169/179 (94%)	160 (95%)	9 (5%)	0	100	100
40	o	120/137 (88%)	108 (90%)	12 (10%)	0	100	100
41	p	172/176 (98%)	171 (99%)	1 (1%)	0	100	100
42	q	143/145 (99%)	143 (100%)	0	0	100	100
43	r	91/113 (80%)	88 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8138/9213 (88%)	7896 (97%)	241 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/100 (89%)	86 (97%)	3 (3%)	32	60
2	B	132/175 (75%)	127 (96%)	5 (4%)	29	56
3	C	188/228 (82%)	185 (98%)	3 (2%)	55	79
4	D	360/392 (92%)	355 (99%)	5 (1%)	59	81
5	E	183/205 (89%)	174 (95%)	9 (5%)	22	47
6	F	346/368 (94%)	339 (98%)	7 (2%)	48	74
7	G	579/608 (95%)	567 (98%)	12 (2%)	47	73
8	H	272/274 (99%)	263 (97%)	9 (3%)	33	61
9	I	151/175 (86%)	150 (99%)	1 (1%)	76	89
10	J	134/141 (95%)	130 (97%)	4 (3%)	36	64
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	83
12	L	533/533 (100%)	522 (98%)	11 (2%)	47	73
13	M	412/412 (100%)	403 (98%)	9 (2%)	45	72
14	N	315/315 (100%)	311 (99%)	4 (1%)	61	82
15	O	283/303 (93%)	279 (99%)	4 (1%)	59	81
16	P	289/327 (88%)	277 (96%)	12 (4%)	26	52
17	Q	116/153 (76%)	113 (97%)	3 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	82
19	S	76/82 (93%)	75 (99%)	1 (1%)	61	82
20	T	81/135 (60%)	77 (95%)	4 (5%)	22	47
20	U	81/135 (60%)	77 (95%)	4 (5%)	22	47
21	V	101/102 (99%)	98 (97%)	3 (3%)	36	64
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	148 (96%)	6 (4%)	28	55
24	Y	101/102 (99%)	98 (97%)	3 (3%)	36	64
25	Z	120/121 (99%)	118 (98%)	2 (2%)	53	78
26	a	59/59 (100%)	58 (98%)	1 (2%)	53	78
27	b	71/72 (99%)	69 (97%)	2 (3%)	38	66
28	c	45/68 (66%)	44 (98%)	1 (2%)	45	72
29	d	105/105 (100%)	103 (98%)	2 (2%)	50	75
30	e	89/96 (93%)	85 (96%)	4 (4%)	24	50
31	f	54/54 (100%)	49 (91%)	5 (9%)	8	18
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	61
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	120/121 (99%)	116 (97%)	4 (3%)	33	61
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	63/76 (83%)	60 (95%)	3 (5%)	23	47
37	l	140/159 (88%)	136 (97%)	4 (3%)	37	65
38	m	113/114 (99%)	111 (98%)	2 (2%)	51	76
39	n	156/161 (97%)	153 (98%)	3 (2%)	50	75
40	o	110/120 (92%)	101 (92%)	9 (8%)	10	24
41	p	155/157 (99%)	151 (97%)	4 (3%)	40	68
42	q	130/130 (100%)	126 (97%)	4 (3%)	35	63
43	r	85/97 (88%)	84 (99%)	1 (1%)	63	83
44	s	43/92 (47%)	41 (95%)	2 (5%)	23	48
All	All	7180/7891 (91%)	7000 (98%)	180 (2%)	42	69

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	97	LEU
1	A	109	LYS
2	B	34	ASP
2	B	50	PHE
2	B	54	CYS
2	B	84	ASP
2	B	171	LYS
3	C	8	ARG
3	C	33	LEU
3	C	125	LYS
4	D	76	CYS
4	D	100	LEU
4	D	161	ILE
4	D	170	MET
4	D	334	LYS
5	E	29	LYS
5	E	36	LYS
5	E	63	ILE
5	E	118	GLU
5	E	123	LYS
5	E	127	LYS
5	E	136	LEU
5	E	169	ILE
5	E	181	ILE
6	F	82	MET
6	F	108	ARG
6	F	114	ASP
6	F	249	ARG
6	F	251	SER
6	F	365	CYS
6	F	436	GLN
7	G	18	VAL
7	G	121	MET
7	G	224	LYS
7	G	288	LYS
7	G	329	ILE
7	G	375	ASP
7	G	447	LYS
7	G	448	LYS
7	G	540	ASP
7	G	581	GLN
7	G	636	VAL

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Mol	Chain	Res	Type
7	G	684	MET
8	H	5	ASN
8	H	8	MET
8	H	59	GLU
8	H	62	ARG
8	H	73	LEU
8	H	222	LEU
8	H	234	MET
8	H	254	LEU
8	H	274	ARG
9	I	14	MET
10	J	76	THR
10	J	109	LYS
10	J	114	GLU
10	J	135	PHE
11	K	37	MET
12	L	25	ASN
12	L	87	MET
12	L	251	THR
12	L	336	LYS
12	L	397	GLU
12	L	482	MET
12	L	498	PHE
12	L	514	HIS
12	L	554	ASP
12	L	580	GLN
12	L	581	LYS
13	M	3	LYS
13	M	72	LEU
13	M	207	MET
13	M	315	LEU
13	M	340	ARG
13	M	355	MET
13	M	413	MET
13	M	416	ARG
13	M	418	LYS
14	N	46	LYS
14	N	187	MET
14	N	263	LYS
14	N	322	LYS
15	O	40	LYS
15	O	84	ASP

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Mol	Chain	Res	Type
15	O	157	LYS
15	O	242	LYS
16	P	3	HIS
16	P	10	LYS
16	P	32	ARG
16	P	122	LYS
16	P	128	LYS
16	P	196	LEU
16	P	224	ARG
16	P	263	TYR
16	P	268	ARG
16	P	281	ARG
16	P	319	ARG
16	P	338	LYS
17	Q	31	LYS
17	Q	44	ASN
17	Q	127	ARG
18	R	3	ARG
19	S	97	LYS
20	T	12	LYS
20	T	16	LEU
20	T	20	LYS
20	T	86	VAL
20	U	20	LYS
20	U	38	LYS
20	U	42	LEU
20	U	61	GLU
21	V	6	LYS
21	V	59	LYS
21	V	65	LYS
23	X	11	ASP
23	X	74	LYS
23	X	76	HIS
23	X	77	CYS
23	X	100	ARG
23	X	133	ASP
24	Y	49	LEU
24	Y	114	CYS
24	Y	119	LEU
25	Z	54	ARG
25	Z	133	LEU
26	a	69	ILE

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Mol	Chain	Res	Type
27	b	9	LYS
27	b	73	GLN
28	c	1	LYS
29	d	6	GLN
29	d	50	ARG
30	e	4	ASP
30	e	52	GLU
30	e	84	LYS
30	e	96	HIS
31	f	1	MET
31	f	4	LEU
31	f	8	ARG
31	f	32	GLU
31	f	57	LYS
32	g	25	ARG
32	g	57	ASN
32	g	84	ARG
34	i	8	LYS
34	i	12	GLN
34	i	48	LYS
34	i	66	HIS
36	k	12	LYS
36	k	23	ILE
36	k	33	GLU
37	l	6	LYS
37	l	8	MET
37	l	126	GLN
37	l	148	LYS
38	m	30	LYS
38	m	110	ARG
39	n	84	SER
39	n	113	MET
39	n	153	LEU
40	o	7	ARG
40	o	19	LEU
40	o	21	MET
40	o	28	TYR
40	o	52	LEU
40	o	58	CYS
40	o	96	LYS
40	o	103	ARG
40	o	107	LEU

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Mol	Chain	Res	Type
41	p	22	GLN
41	p	126	LYS
41	p	133	GLN
41	p	166	ARG
42	q	3	LEU
42	q	4	LEU
42	q	132	LYS
42	q	144	TYR
43	r	91	LYS
44	s	63	MET
44	s	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	95	ASN
3	C	160	HIS
4	D	46	ASN
4	D	190	HIS
4	D	200	HIS
4	D	201	GLN
5	E	58	ASN
6	F	200	GLN
7	G	237	ASN
7	G	392	ASN
7	G	402	ASN
7	G	546	GLN
7	G	581	GLN
7	G	644	GLN
7	G	665	GLN
8	H	5	ASN
8	H	235	ASN
8	H	248	ASN
11	K	7	ASN
11	K	83	ASN
12	L	31	ASN
12	L	295	GLN
12	L	309	GLN
13	M	144	ASN
13	M	293	HIS
13	M	331	ASN
13	M	338	HIS

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Mol	Chain	Res	Type
13	M	374	ASN
14	N	48	HIS
15	O	114	HIS
15	O	271	ASN
16	P	87	HIS
16	P	260	HIS
17	Q	29	HIS
19	S	47	ASN
19	S	72	GLN
20	T	74	GLN
23	X	29	HIS
28	c	9	HIS
29	d	117	HIS
30	e	6	GLN
32	g	57	ASN
34	i	82	HIS
37	l	99	ASN
38	m	116	GLN
39	n	77	GLN
40	o	60	HIS
41	p	27	ASN
41	p	103	ASN
41	p	160	GLN
42	q	123	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	AME	q	1	42	9,10,11	1.53	1 (11%)	9,11,13	1.59	2 (22%)
13	FME	M	1	13	8,9,10	1.49	1 (12%)	8,9,11	1.39	1 (12%)
27	AYA	b	1	27	6,7,8	1.88	1 (16%)	6,8,10	1.26	1 (16%)
34	SAC	i	1	34	7,8,9	1.76	1 (14%)	7,9,11	1.63	1 (14%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.47	2 (25%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.39	1 (12%)
43	AYA	r	1	43	6,7,8	1.86	2 (33%)	6,8,10	1.39	1 (16%)
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.30	1 (11%)
11	FME	K	1	11	8,9,10	1.52	1 (12%)	8,9,11	1.37	1 (12%)
4	2MR	D	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.36	1 (20%)
8	FME	H	1	8	8,9,10	1.51	1 (12%)	8,9,11	1.48	2 (25%)
38	SAC	m	1	38	7,8,9	1.74	1 (14%)	7,9,11	1.23	1 (14%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	8,9,11	1.37	1 (12%)
24	AYA	Y	1	24	6,7,8	1.88	2 (33%)	6,8,10	1.50	1 (16%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	8,9,11	1.41	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	AME	q	1	42	-	5/9/10/12	-
13	FME	M	1	13	-	2/7/9/11	-
27	AYA	b	1	27	-	1/5/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
12	FME	L	1	12	-	2/7/9/11	-
14	FME	N	1	14	-	2/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
29	AME	d	1	29	-	0/9/10/12	-
11	FME	K	1	11	-	2/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
8	FME	H	1	8	-	1/7/9/11	-
38	SAC	m	1	38	-	0/7/8/10	-
1	FME	A	1	1	-	1/7/9/11	-
24	AYA	Y	1	24	-	0/5/6/8	-
10	FME	J	1	10	-	2/7/9/11	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.51	1.45	1.33
4	D	85	2MR	CZ-NE	5.08	1.45	1.34
11	K	1	FME	CN-N	3.77	1.45	1.33
12	L	1	FME	CN-N	3.74	1.45	1.33
10	J	1	FME	CN-N	3.74	1.45	1.33
1	A	1	FME	CN-N	3.74	1.45	1.33
14	N	1	FME	CN-N	3.73	1.45	1.33
8	H	1	FME	CN-N	3.71	1.45	1.33
13	M	1	FME	CN-N	3.70	1.45	1.33
34	i	1	SAC	C1A-N	3.62	1.46	1.34
27	b	1	AYA	CT-N	3.53	1.45	1.34
38	m	1	SAC	C1A-N	3.52	1.45	1.34
42	q	1	AME	CT1-N	3.48	1.45	1.34
29	d	1	AME	CT1-N	3.48	1.45	1.34
43	r	1	AYA	CT-N	3.42	1.45	1.34
24	Y	1	AYA	CT-N	3.37	1.45	1.34
24	Y	1	AYA	OT-CT	-2.09	1.18	1.23
43	r	1	AYA	OT-CT	-2.06	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	3.21	121.45	116.12
42	q	1	AME	CT2-CT1-N	2.67	120.55	116.12
42	q	1	AME	CE-SD-CG	2.66	114.08	100.32
24	Y	1	AYA	CM-CT-N	2.53	120.31	116.12
43	r	1	AYA	CM-CT-N	2.47	120.21	116.12
29	d	1	AME	CT2-CT1-N	2.40	120.10	116.12
38	m	1	SAC	C2A-C1A-N	2.24	119.83	116.12
27	b	1	AYA	CM-CT-N	2.19	119.76	116.12
12	L	1	FME	O1-CN-N	-2.17	119.71	125.32
8	H	1	FME	O1-CN-N	-2.13	119.82	125.32
12	L	1	FME	CA-N-CN	-2.13	119.55	122.82
8	H	1	FME	CA-N-CN	-2.11	119.58	122.82
10	J	1	FME	O1-CN-N	-2.10	119.89	125.32
4	D	85	2MR	CD-NE-CZ	-2.08	119.46	123.36
1	A	1	FME	O1-CN-N	-2.08	119.95	125.32
14	N	1	FME	O1-CN-N	-2.06	119.99	125.32
11	K	1	FME	O1-CN-N	-2.06	120.01	125.32
13	M	1	FME	O1-CN-N	-2.05	120.03	125.32

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 81 ligands modelled in this entry, 4 are monoatomic - leaving 77 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
48	PLC	d	203	-	31,31,41	0.58	0	37,39,49	0.60	0
53	CDL	d	204	-	64,64,99	1.08	8 (12%)	70,76,111	1.12	4 (5%)
53	CDL	i	202	-	71,71,99	1.04	8 (11%)	77,83,111	1.14	4 (5%)
58	CHD	i	201	-	32,32,32	3.27	10 (31%)	51,51,51	2.42	17 (33%)
53	CDL	M	607	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	4 (3%)
50	FMN	F	502	-	33,33,33	2.77	10 (30%)	48,50,50	1.77	13 (27%)
53	CDL	N	404	-	83,83,99	0.96	8 (9%)	89,95,111	1.06	4 (4%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
45	3PE	f	101	-	50,50,50	0.88	4 (8%)	53,55,55	1.07	2 (3%)
46	PC1	B	202	-	47,47,53	1.02	4 (8%)	53,55,61	1.10	2 (3%)
45	3PE	Y	201	-	26,26,50	1.19	4 (15%)	29,31,55	1.14	2 (6%)
45	3PE	M	605	-	44,44,50	0.92	4 (9%)	47,49,55	1.14	2 (4%)
45	3PE	Y	203	-	50,50,50	0.88	4 (8%)	53,55,55	1.08	2 (3%)
45	3PE	q	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)
45	3PE	m	202	-	29,29,50	1.12	4 (13%)	32,34,55	1.19	2 (6%)
45	3PE	Z	202	-	50,50,50	0.88	4 (8%)	53,55,55	1.03	2 (3%)
45	3PE	Y	207	-	50,50,50	0.88	4 (8%)	53,55,55	1.05	2 (3%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	b	101	-	46,46,50	0.90	4 (8%)	49,51,55	1.01	2 (4%)
46	PC1	A	203	-	40,40,53	1.09	4 (10%)	46,48,61	1.05	2 (4%)
46	PC1	h	202	-	39,39,53	1.09	4 (10%)	45,47,61	1.08	2 (4%)
46	PC1	H	403	-	38,38,53	1.11	4 (10%)	44,46,61	0.98	2 (4%)
45	3PE	Y	206	-	33,33,50	1.06	4 (12%)	36,38,55	1.14	2 (5%)
45	3PE	N	401	-	44,44,50	0.93	4 (9%)	47,49,55	1.09	2 (4%)
45	3PE	M	603	-	49,49,50	0.88	4 (8%)	52,54,55	1.04	2 (3%)
45	3PE	I	203	-	36,36,50	1.02	4 (11%)	39,41,55	1.14	2 (5%)
46	PC1	M	606	-	34,34,53	1.17	4 (11%)	40,42,61	1.10	2 (5%)
45	3PE	A	201	-	42,42,50	0.95	4 (9%)	45,47,55	1.07	2 (4%)
45	3PE	H	401	-	35,35,50	1.02	4 (11%)	38,40,55	1.00	2 (5%)
56	NDP	P	501	-	51,52,52	4.01	28 (54%)	71,80,80	1.92	13 (18%)
48	PLC	B	203	-	27,27,41	0.62	0	33,35,49	0.59	0
57	EHZ	T	101	20	31,36,37	1.61	5 (16%)	36,44,47	1.68	6 (16%)
46	PC1	L	701	-	53,53,53	0.95	4 (7%)	59,61,61	0.96	2 (3%)
53	CDL	r	202	-	57,57,99	1.15	8 (14%)	63,69,111	1.12	4 (6%)
48	PLC	J	203	-	34,34,41	0.55	0	40,42,49	0.53	0
57	EHZ	U	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.58	7 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	m	201	-	40,40,50	0.98	4 (10%)	43,45,55	1.12	2 (4%)
45	3PE	Z	201	-	36,36,50	1.02	4 (11%)	39,41,55	1.04	2 (5%)
45	3PE	h	201	-	31,31,50	1.10	4 (12%)	34,36,55	1.17	2 (5%)
45	3PE	M	604	-	33,33,50	1.06	4 (12%)	36,38,55	1.16	2 (5%)
46	PC1	g	201	-	43,43,53	1.05	4 (9%)	49,51,61	1.02	2 (4%)
45	3PE	N	402	-	39,39,50	0.98	4 (10%)	42,44,55	1.13	2 (4%)
48	PLC	b	103	-	37,37,41	0.53	0	43,45,49	0.54	0
48	PLC	L	703	-	41,41,41	0.51	0	47,49,49	0.51	0
46	PC1	A	202	-	34,34,53	1.18	4 (11%)	40,42,61	1.09	2 (5%)
45	3PE	J	201	-	30,30,50	1.10	4 (13%)	33,35,55	1.16	2 (6%)
48	PLC	Y	208	-	36,36,41	0.54	0	42,44,49	0.57	1 (2%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
59	MYR	o	201	40	13,14,15	0.41	0	12,13,15	0.90	0
46	PC1	Z	203	-	43,43,53	1.05	4 (9%)	49,51,61	1.03	2 (4%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
45	3PE	J	202	-	35,35,50	1.03	4 (11%)	38,40,55	1.14	2 (5%)
45	3PE	b	102	-	50,50,50	0.88	4 (8%)	53,55,55	1.10	2 (3%)
45	3PE	d	201	-	48,48,50	0.89	4 (8%)	51,53,55	1.06	2 (3%)
45	3PE	Y	204	-	50,50,50	0.88	4 (8%)	53,55,55	1.05	2 (3%)
46	PC1	I	204	-	53,53,53	0.94	4 (7%)	59,61,61	1.06	2 (3%)
53	CDL	h	203	-	69,69,99	1.05	8 (11%)	75,81,111	1.09	4 (5%)
53	CDL	X	201	-	85,85,99	0.95	8 (9%)	91,97,111	1.10	4 (4%)
47	SF4	I	201	9	0,12,12	-	-	-	-	-
47	SF4	F	501	6	0,12,12	-	-	-	-	-
48	PLC	Z	204	-	33,33,41	0.57	0	39,41,49	0.59	0
45	3PE	Y	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
54	DGT	O	401	55	32,33,33	3.32	14 (43%)	48,52,52	1.90	14 (29%)
45	3PE	K	101	-	43,43,50	0.95	4 (9%)	46,48,55	1.04	2 (4%)
46	PC1	H	402	-	47,47,53	1.02	4 (8%)	53,55,61	1.02	2 (3%)
45	3PE	Y	205	-	45,45,50	0.92	4 (8%)	48,50,55	1.10	2 (4%)
46	PC1	q	202	-	22,22,53	1.36	3 (13%)	28,30,61	0.81	1 (3%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
45	3PE	L	702	-	44,44,50	0.92	4 (9%)	47,49,55	1.07	2 (4%)
46	PC1	d	202	-	38,38,53	1.12	4 (10%)	44,46,61	0.99	2 (4%)
45	3PE	M	602	-	29,29,50	1.12	4 (13%)	32,34,55	1.00	2 (6%)
46	PC1	m	203	-	39,39,53	1.09	4 (10%)	45,47,61	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	N	403	-	48,48,50	0.89	4 (8%)	51,53,55	1.07	2 (3%)
48	PLC	O	403	-	41,41,41	0.51	0	47,49,49	0.56	0
45	3PE	r	201	-	27,27,50	1.17	4 (14%)	30,32,55	1.20	2 (6%)
48	PLC	g	202	-	27,27,41	0.61	0	33,35,49	0.66	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLC	d	203	-	-	8/34/34/45	-
53	CDL	d	204	-	-	29/75/75/110	-
53	CDL	i	202	-	-	33/82/82/110	-
58	CHD	i	201	-	-	3/9/74/74	0/4/4/4
53	CDL	M	607	-	-	51/110/110/110	-
50	FMN	F	502	-	-	2/18/18/18	0/3/3/3
53	CDL	N	404	-	-	44/94/94/110	-
49	FES	G	803	7	-	-	0/1/1/1
45	3PE	f	101	-	-	23/54/54/54	-
46	PC1	B	202	-	-	22/51/51/57	-
45	3PE	Y	201	-	-	12/30/30/54	-
45	3PE	M	605	-	-	11/48/48/54	-
45	3PE	Y	203	-	-	27/54/54/54	-
45	3PE	q	201	-	-	23/54/54/54	-
45	3PE	m	202	-	-	16/33/33/54	-
45	3PE	Z	202	-	-	22/54/54/54	-
45	3PE	Y	207	-	-	25/54/54/54	-
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	b	101	-	-	26/50/50/54	-
46	PC1	A	203	-	-	14/44/44/57	-
46	PC1	h	202	-	-	15/43/43/57	-
46	PC1	H	403	-	-	17/42/42/57	-
45	3PE	Y	206	-	-	14/37/37/54	-
45	3PE	N	401	-	-	21/48/48/54	-
45	3PE	M	603	-	-	21/53/53/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	I	203	-	-	17/40/40/54	-
46	PC1	M	606	-	-	15/38/38/57	-
45	3PE	A	201	-	-	21/46/46/54	-
45	3PE	H	401	-	-	15/39/39/54	-
56	NDP	P	501	-	-	12/34/77/77	0/5/5/5
48	PLC	B	203	-	-	10/31/31/45	-
57	EHZ	T	101	20	-	13/42/44/45	-
46	PC1	L	701	-	-	23/57/57/57	-
53	CDL	r	202	-	-	23/68/68/110	-
48	PLC	J	203	-	-	12/38/38/45	-
57	EHZ	U	101	20	-	20/42/44/45	-
45	3PE	m	201	-	-	20/44/44/54	-
45	3PE	Z	201	-	-	17/40/40/54	-
45	3PE	h	201	-	-	17/35/35/54	-
45	3PE	M	604	-	-	10/37/37/54	-
46	PC1	g	201	-	-	17/47/47/57	-
45	3PE	N	402	-	-	22/43/43/54	-
48	PLC	b	103	-	-	16/41/41/45	-
48	PLC	L	703	-	-	17/45/45/45	-
46	PC1	A	202	-	-	17/38/38/57	-
45	3PE	J	201	-	-	18/34/34/54	-
48	PLC	Y	208	-	-	13/40/40/45	-
47	SF4	G	801	7	-	-	0/6/5/5
59	MYR	o	201	40	-	4/12/12/13	-
46	PC1	Z	203	-	-	17/47/47/57	-
47	SF4	B	201	2	-	-	0/6/5/5
45	3PE	J	202	-	-	13/39/39/54	-
45	3PE	b	102	-	-	21/54/54/54	-
45	3PE	d	201	-	-	22/52/52/54	-
45	3PE	Y	204	-	-	25/54/54/54	-
46	PC1	I	204	-	-	23/57/57/57	-
53	CDL	h	203	-	-	30/80/80/110	-
53	CDL	X	201	-	-	46/96/96/110	-
47	SF4	I	201	9	-	-	0/6/5/5
47	SF4	F	501	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLC	Z	204	-	-	11/37/37/45	-
45	3PE	Y	202	-	-	19/54/54/54	-
47	SF4	I	202	9	-	-	0/6/5/5
54	DGT	O	401	55	-	5/22/34/34	0/3/3/3
45	3PE	K	101	-	-	20/47/47/54	-
46	PC1	H	402	-	-	23/51/51/57	-
45	3PE	Y	205	-	-	25/49/49/54	-
46	PC1	q	202	-	-	10/25/25/57	-
47	SF4	G	802	7	-	-	0/6/5/5
45	3PE	L	702	-	-	21/48/48/54	-
46	PC1	d	202	-	-	18/42/42/57	-
45	3PE	M	602	-	-	12/33/33/54	-
46	PC1	m	203	-	-	16/43/43/57	-
45	3PE	N	403	-	-	22/52/52/54	-
48	PLC	O	403	-	-	15/45/45/45	-
45	3PE	r	201	-	-	14/31/31/54	-
48	PLC	g	202	-	-	8/30/30/45	-

All (311) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	PA-O3	10.41	1.70	1.59
58	i	201	CHD	C11-C12	9.11	1.68	1.53
56	P	501	NDP	C2B-C1B	-8.95	1.31	1.53
54	O	401	DGT	O6-C6	8.84	1.40	1.23
56	P	501	NDP	O4B-C1B	8.63	1.61	1.42
56	P	501	NDP	O4D-C1D	8.27	1.61	1.42
56	P	501	NDP	C7N-N7N	7.66	1.55	1.33
56	P	501	NDP	C2D-C1D	-7.25	1.30	1.53
58	i	201	CHD	C16-C15	7.22	1.73	1.54
56	P	501	NDP	C6N-C5N	7.18	1.55	1.33
54	O	401	DGT	C5-N7	6.74	1.52	1.39
50	F	502	FMN	C10-N1	6.60	1.46	1.33
50	F	502	FMN	C4A-N5	6.52	1.44	1.30
56	P	501	NDP	O4D-C4D	-6.49	1.30	1.45
58	i	201	CHD	C20-C17	-6.19	1.43	1.54
56	P	501	NDP	P2B-O2B	5.72	1.69	1.59
50	F	502	FMN	C5A-N5	5.45	1.49	1.39
56	P	501	NDP	C6A-N6A	5.37	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	i	201	CHD	C13-C17	5.35	1.64	1.55
58	i	201	CHD	C8-C9	5.31	1.64	1.53
57	T	101	EHZ	C12-N1	5.20	1.45	1.33
58	i	201	CHD	O12-C12	-5.19	1.35	1.43
54	O	401	DGT	PA-O3A	5.18	1.65	1.59
54	O	401	DGT	PB-O3A	5.15	1.65	1.59
57	U	101	EHZ	C12-N1	5.14	1.45	1.33
50	F	502	FMN	C9A-N10	5.08	1.50	1.41
57	U	101	EHZ	C15-N2	5.07	1.45	1.33
54	O	401	DGT	PB-O3B	5.05	1.65	1.59
50	F	502	FMN	C2-N1	5.04	1.48	1.36
56	P	501	NDP	O4B-C4B	-5.04	1.33	1.45
57	T	101	EHZ	C15-N2	4.99	1.45	1.33
56	P	501	NDP	PN-O3	4.93	1.64	1.59
54	O	401	DGT	C2-N2	4.85	1.45	1.34
54	O	401	DGT	C2-N1	4.79	1.49	1.37
58	i	201	CHD	C6-C5	4.58	1.61	1.53
56	P	501	NDP	C2N-C3N	4.57	1.47	1.35
50	F	502	FMN	C2-N3	4.56	1.49	1.39
54	O	401	DGT	C2-N3	4.34	1.43	1.33
56	P	501	NDP	C5A-C4A	-4.22	1.31	1.39
54	O	401	DGT	C8-N9	-4.21	1.28	1.37
58	i	201	CHD	C15-C14	4.21	1.63	1.54
56	P	501	NDP	O7N-C7N	-4.10	1.14	1.24
54	O	401	DGT	C4-N9	-3.95	1.28	1.38
50	F	502	FMN	C10-N10	3.83	1.45	1.37
56	P	501	NDP	C8A-N9A	-3.81	1.31	1.37
56	P	501	NDP	O2D-C2D	3.80	1.52	1.43
50	F	502	FMN	C4-N3	3.76	1.45	1.38
58	i	201	CHD	C6-C7	3.54	1.59	1.52
56	P	501	NDP	C4N-C3N	3.24	1.56	1.50
50	F	502	FMN	O2-C2	-2.87	1.18	1.24
53	r	202	CDL	OB6-CB4	-2.79	1.40	1.46
53	M	607	CDL	OB6-CB4	-2.78	1.40	1.46
56	P	501	NDP	C4N-C5N	2.78	1.56	1.49
53	r	202	CDL	OA6-CA4	-2.77	1.40	1.46
45	Z	201	3PE	O21-C2	-2.76	1.40	1.46
53	X	201	CDL	OB6-CB4	-2.76	1.40	1.46
45	J	202	3PE	O21-C2	-2.75	1.40	1.46
53	d	204	CDL	OA6-CA4	-2.75	1.40	1.46
53	N	404	CDL	OB6-CB4	-2.74	1.40	1.46
53	d	204	CDL	OB6-CB4	-2.73	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	402	PC1	O21-C2	-2.73	1.40	1.46
45	q	201	3PE	O21-C2	-2.72	1.40	1.46
46	A	203	PC1	O21-C2	-2.72	1.40	1.46
45	N	403	3PE	O21-C2	-2.72	1.40	1.46
46	L	701	PC1	O21-C2	-2.71	1.40	1.46
45	h	201	3PE	O21-C2	-2.71	1.40	1.46
45	K	101	3PE	O21-C2	-2.70	1.40	1.46
56	P	501	NDP	C5A-N7A	-2.70	1.34	1.39
45	r	201	3PE	O21-C2	-2.70	1.40	1.46
53	i	202	CDL	OA6-CA4	-2.69	1.40	1.46
46	M	606	PC1	O21-C2	-2.68	1.40	1.46
45	d	201	3PE	O21-C2	-2.68	1.40	1.46
53	h	203	CDL	OA6-CA4	-2.68	1.40	1.46
45	Z	202	3PE	O21-C2	-2.68	1.40	1.46
46	I	204	PC1	O21-C2	-2.67	1.40	1.46
53	i	202	CDL	OB6-CB4	-2.67	1.40	1.46
45	m	201	3PE	O21-C2	-2.67	1.40	1.46
46	Z	203	PC1	O21-C2	-2.67	1.40	1.46
46	q	202	PC1	O21-C2	-2.67	1.40	1.46
46	A	202	PC1	O21-C2	-2.66	1.40	1.46
45	N	402	3PE	O21-C2	-2.66	1.40	1.46
46	d	202	PC1	O21-C2	-2.65	1.40	1.46
45	M	604	3PE	O21-C2	-2.65	1.40	1.46
45	Y	203	3PE	O21-C2	-2.65	1.40	1.46
53	M	607	CDL	OA6-CA4	-2.65	1.40	1.46
45	b	101	3PE	O21-C2	-2.64	1.40	1.46
45	I	203	3PE	O21-C2	-2.64	1.40	1.46
45	H	401	3PE	O21-C2	-2.63	1.40	1.46
53	h	203	CDL	OB6-CB4	-2.63	1.40	1.46
45	Y	207	3PE	O21-C2	-2.63	1.40	1.46
45	Y	201	3PE	O21-C2	-2.63	1.40	1.46
45	Y	205	3PE	O21-C2	-2.62	1.40	1.46
45	m	202	3PE	O21-C2	-2.62	1.40	1.46
56	P	501	NDP	C6N-N1N	2.61	1.43	1.37
45	Y	204	3PE	O21-C2	-2.61	1.40	1.46
45	Y	206	3PE	O21-C2	-2.61	1.40	1.46
46	H	403	PC1	O21-C2	-2.61	1.40	1.46
45	A	201	3PE	O21-C2	-2.61	1.40	1.46
46	B	202	PC1	O21-C2	-2.61	1.40	1.46
46	m	203	PC1	O21-C2	-2.60	1.40	1.46
45	M	602	3PE	O21-C2	-2.59	1.40	1.46
46	g	201	PC1	O21-C2	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	603	3PE	O21-C2	-2.59	1.40	1.46
45	b	102	3PE	O21-C2	-2.59	1.40	1.46
46	h	202	PC1	O21-C2	-2.59	1.40	1.46
45	J	201	3PE	O21-C2	-2.58	1.40	1.46
50	F	502	FMN	O4-C4	-2.58	1.18	1.23
45	f	101	3PE	O21-C2	-2.57	1.40	1.46
45	M	605	3PE	O21-C2	-2.57	1.40	1.46
53	N	404	CDL	OA6-CA4	-2.56	1.40	1.46
54	O	401	DGT	C1'-N9	-2.54	1.41	1.48
45	Y	202	3PE	O21-C2	-2.50	1.40	1.46
57	T	101	EHZ	C9-S1	2.49	1.82	1.76
53	h	203	CDL	OB8-CB7	2.48	1.40	1.33
53	i	202	CDL	OB8-CB7	2.48	1.40	1.33
46	g	201	PC1	O31-C31	2.47	1.40	1.33
53	X	201	CDL	OA6-CA4	-2.46	1.40	1.46
45	N	401	3PE	O31-C31	2.46	1.40	1.33
53	r	202	CDL	OA8-CA7	2.46	1.40	1.33
45	N	401	3PE	O21-C2	-2.44	1.40	1.46
53	r	202	CDL	OB8-CB7	2.43	1.40	1.33
57	T	101	EHZ	O3-C12	-2.43	1.18	1.23
45	L	702	3PE	O21-C2	-2.42	1.40	1.46
53	M	607	CDL	OA8-CA7	2.42	1.40	1.33
53	N	404	CDL	OB8-CB7	2.41	1.40	1.33
53	X	201	CDL	OA8-CA7	2.41	1.40	1.33
46	H	402	PC1	O31-C31	2.41	1.40	1.33
46	A	203	PC1	O31-C31	2.41	1.40	1.33
53	d	204	CDL	OB8-CB7	2.41	1.40	1.33
45	J	202	3PE	O31-C31	2.40	1.40	1.33
45	N	402	3PE	O31-C31	2.40	1.40	1.33
45	I	203	3PE	O31-C31	2.40	1.40	1.33
45	m	201	3PE	O31-C31	2.40	1.40	1.33
53	d	204	CDL	OA8-CA6	-2.40	1.39	1.45
46	h	202	PC1	O31-C31	2.40	1.40	1.33
56	P	501	NDP	O3D-C3D	-2.40	1.37	1.43
46	M	606	PC1	O31-C31	2.40	1.40	1.33
53	N	404	CDL	OA8-CA7	2.39	1.40	1.33
53	X	201	CDL	OB8-CB7	2.39	1.40	1.33
45	Y	207	3PE	O31-C31	2.39	1.40	1.33
58	i	201	CHD	C13-C12	-2.39	1.50	1.54
56	P	501	NDP	O3B-C3B	-2.39	1.37	1.43
45	d	201	3PE	O31-C31	2.39	1.40	1.33
56	P	501	NDP	PA-O5B	2.38	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	B	202	PC1	O31-C3	-2.38	1.39	1.45
45	M	604	3PE	O31-C31	2.38	1.40	1.33
46	d	202	PC1	O31-C31	2.38	1.40	1.33
57	T	101	EHZ	O4-C15	-2.38	1.18	1.23
45	K	101	3PE	O31-C31	2.38	1.40	1.33
45	Y	202	3PE	O31-C31	2.38	1.40	1.33
45	Y	201	3PE	O31-C31	2.38	1.40	1.33
53	M	607	CDL	OB8-CB7	2.38	1.40	1.33
57	U	101	EHZ	C9-S1	2.38	1.81	1.76
46	H	403	PC1	O31-C31	2.37	1.40	1.33
45	r	201	3PE	O31-C31	2.37	1.40	1.33
46	A	202	PC1	O31-C31	2.36	1.40	1.33
45	Y	204	3PE	O31-C31	2.36	1.40	1.33
45	Z	201	3PE	O31-C31	2.36	1.40	1.33
45	H	401	3PE	O31-C31	2.36	1.40	1.33
45	f	101	3PE	O31-C31	2.36	1.40	1.33
45	h	201	3PE	O31-C31	2.36	1.40	1.33
45	J	201	3PE	O31-C31	2.36	1.40	1.33
45	A	201	3PE	O31-C31	2.35	1.40	1.33
46	m	203	PC1	O31-C31	2.35	1.40	1.33
45	Y	205	3PE	O31-C31	2.34	1.40	1.33
45	m	202	3PE	O31-C31	2.34	1.40	1.33
45	Y	206	3PE	O31-C31	2.34	1.40	1.33
45	M	602	3PE	O31-C31	2.34	1.40	1.33
46	I	204	PC1	O31-C31	2.34	1.40	1.33
57	U	101	EHZ	O4-C15	-2.34	1.18	1.23
45	M	603	3PE	O31-C31	2.33	1.40	1.33
46	L	701	PC1	O31-C31	2.33	1.40	1.33
45	L	702	3PE	O31-C31	2.33	1.40	1.33
56	P	501	NDP	P2B-O1X	2.33	1.57	1.50
53	i	202	CDL	OA8-CA7	2.33	1.40	1.33
45	N	403	3PE	O31-C31	2.32	1.40	1.33
45	b	101	3PE	O31-C31	2.32	1.40	1.33
46	Z	203	PC1	O31-C31	2.32	1.40	1.33
45	b	102	3PE	O31-C31	2.32	1.40	1.33
45	Z	202	3PE	O31-C31	2.32	1.40	1.33
57	U	101	EHZ	O3-C12	-2.31	1.18	1.23
53	h	203	CDL	OA8-CA7	2.31	1.40	1.33
56	P	501	NDP	C7N-C3N	2.30	1.53	1.48
45	Y	203	3PE	O31-C31	2.30	1.40	1.33
45	M	605	3PE	O31-C31	2.29	1.40	1.33
45	K	101	3PE	O31-C3	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	B	202	PC1	O31-C31	2.29	1.40	1.33
45	m	201	3PE	O31-C3	-2.28	1.40	1.45
45	q	201	3PE	O31-C31	2.27	1.40	1.33
45	b	102	3PE	O31-C3	-2.27	1.40	1.45
45	M	603	3PE	O31-C3	-2.26	1.40	1.45
45	b	101	3PE	O31-C3	-2.26	1.40	1.45
45	N	401	3PE	O21-C21	2.26	1.40	1.34
53	d	204	CDL	OA8-CA7	2.26	1.39	1.33
45	m	202	3PE	O31-C3	-2.25	1.40	1.45
46	Z	203	PC1	O31-C3	-2.25	1.40	1.45
45	h	201	3PE	O31-C3	-2.25	1.40	1.45
46	L	701	PC1	O31-C3	-2.25	1.40	1.45
45	Y	204	3PE	O31-C3	-2.24	1.40	1.45
45	f	101	3PE	O31-C3	-2.24	1.40	1.45
46	A	203	PC1	O31-C3	-2.24	1.40	1.45
45	q	201	3PE	O31-C3	-2.24	1.40	1.45
53	X	201	CDL	OB8-CB6	-2.24	1.40	1.45
45	H	401	3PE	O31-C3	-2.24	1.40	1.45
45	Y	203	3PE	O31-C3	-2.24	1.40	1.45
46	B	202	PC1	O21-C21	2.24	1.40	1.34
56	P	501	NDP	C5B-C4B	2.23	1.58	1.51
54	O	401	DGT	PG-O2G	-2.23	1.46	1.54
45	I	203	3PE	O31-C3	-2.23	1.40	1.45
45	M	602	3PE	O31-C3	-2.23	1.40	1.45
45	A	201	3PE	O31-C3	-2.22	1.40	1.45
46	H	403	PC1	O31-C3	-2.22	1.40	1.45
45	L	702	3PE	O31-C3	-2.22	1.40	1.45
45	N	403	3PE	O31-C3	-2.22	1.40	1.45
54	O	401	DGT	PG-O1G	-2.22	1.46	1.54
45	Y	205	3PE	O31-C3	-2.22	1.40	1.45
46	d	202	PC1	O21-C21	2.22	1.40	1.34
45	Y	206	3PE	O31-C3	-2.22	1.40	1.45
53	i	202	CDL	OA8-CA6	-2.21	1.40	1.45
53	h	203	CDL	OA8-CA6	-2.20	1.40	1.45
46	d	202	PC1	O31-C3	-2.20	1.40	1.45
45	M	604	3PE	O31-C3	-2.20	1.40	1.45
45	Y	203	3PE	O21-C21	2.20	1.40	1.34
45	Z	202	3PE	O31-C3	-2.19	1.40	1.45
45	r	201	3PE	O31-C3	-2.19	1.40	1.45
45	f	101	3PE	O21-C21	2.19	1.40	1.34
46	h	202	PC1	O21-C21	2.19	1.40	1.34
45	b	102	3PE	O21-C21	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A	202	PC1	O21-C21	2.19	1.40	1.34
45	N	401	3PE	O31-C3	-2.19	1.40	1.45
45	M	602	3PE	O21-C21	2.19	1.40	1.34
53	N	404	CDL	OA6-CA5	2.19	1.40	1.34
45	Z	201	3PE	O31-C3	-2.18	1.40	1.45
53	M	607	CDL	OB8-CB6	-2.18	1.40	1.45
45	b	101	3PE	O21-C21	2.18	1.40	1.34
46	m	203	PC1	O21-C21	2.18	1.40	1.34
46	M	606	PC1	O31-C3	-2.18	1.40	1.45
46	L	701	PC1	O21-C21	2.18	1.40	1.34
54	O	401	DGT	C4-N3	2.18	1.39	1.34
53	r	202	CDL	OB8-CB6	-2.18	1.40	1.45
46	H	402	PC1	O21-C21	2.17	1.40	1.34
45	A	201	3PE	O21-C21	2.17	1.40	1.34
46	A	202	PC1	O31-C3	-2.17	1.40	1.45
45	Y	205	3PE	O21-C21	2.17	1.40	1.34
45	Z	202	3PE	O21-C21	2.17	1.40	1.34
53	h	203	CDL	OB6-CB5	2.17	1.40	1.34
53	i	202	CDL	OB8-CB6	-2.17	1.40	1.45
45	Y	207	3PE	O31-C3	-2.17	1.40	1.45
45	J	201	3PE	O21-C21	2.17	1.40	1.34
45	M	605	3PE	O31-C3	-2.16	1.40	1.45
53	M	607	CDL	OA8-CA6	-2.16	1.40	1.45
46	H	403	PC1	O21-C21	2.16	1.40	1.34
46	h	202	PC1	O31-C3	-2.16	1.40	1.45
53	h	203	CDL	OA6-CA5	2.16	1.40	1.34
45	m	202	3PE	O21-C21	2.16	1.40	1.34
53	N	404	CDL	OB8-CB6	-2.16	1.40	1.45
46	Z	203	PC1	O21-C21	2.16	1.40	1.34
53	d	204	CDL	OB8-CB6	-2.16	1.40	1.45
53	X	201	CDL	OA6-CA5	2.16	1.40	1.34
45	L	702	3PE	O21-C21	2.16	1.40	1.34
53	i	202	CDL	OB6-CB5	2.15	1.40	1.34
45	d	201	3PE	O31-C3	-2.15	1.40	1.45
53	M	607	CDL	OA6-CA5	2.15	1.40	1.34
46	g	201	PC1	O21-C21	2.15	1.40	1.34
45	Y	207	3PE	O21-C21	2.15	1.40	1.34
45	M	603	3PE	O21-C21	2.15	1.40	1.34
45	Y	202	3PE	O21-C21	2.15	1.40	1.34
45	I	203	3PE	O21-C21	2.14	1.40	1.34
53	h	203	CDL	OB8-CB6	-2.14	1.40	1.45
45	M	604	3PE	O21-C21	2.14	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	J	202	3PE	O31-C3	-2.14	1.40	1.45
46	m	203	PC1	O31-C3	-2.14	1.40	1.45
46	q	202	PC1	O31-C3	-2.13	1.40	1.45
53	d	204	CDL	OB6-CB5	2.13	1.40	1.34
45	Y	201	3PE	O21-C21	2.13	1.40	1.34
46	I	204	PC1	O31-C3	-2.13	1.40	1.45
56	P	501	NDP	C5D-C4D	2.13	1.58	1.51
46	M	606	PC1	O21-C21	2.13	1.40	1.34
53	r	202	CDL	OA8-CA6	-2.13	1.40	1.45
53	N	404	CDL	OA8-CA6	-2.12	1.40	1.45
53	i	202	CDL	OA6-CA5	2.12	1.40	1.34
45	K	101	3PE	O21-C21	2.12	1.40	1.34
45	Y	202	3PE	O31-C3	-2.12	1.40	1.45
45	H	401	3PE	O21-C21	2.12	1.40	1.34
45	Y	204	3PE	O21-C21	2.12	1.40	1.34
46	H	402	PC1	O31-C3	-2.11	1.40	1.45
46	q	202	PC1	O21-C21	2.11	1.40	1.34
53	X	201	CDL	OB6-CB5	2.11	1.40	1.34
46	g	201	PC1	O31-C3	-2.11	1.40	1.45
45	Y	201	3PE	O31-C3	-2.11	1.40	1.45
45	J	201	3PE	O31-C3	-2.11	1.40	1.45
45	r	201	3PE	O21-C21	2.10	1.40	1.34
45	Y	206	3PE	O21-C21	2.10	1.40	1.34
45	J	202	3PE	O21-C21	2.10	1.40	1.34
45	N	402	3PE	O21-C21	2.10	1.40	1.34
45	m	201	3PE	O21-C21	2.09	1.40	1.34
45	M	605	3PE	O21-C21	2.09	1.40	1.34
53	M	607	CDL	OB6-CB5	2.09	1.40	1.34
46	A	203	PC1	O21-C21	2.08	1.40	1.34
45	h	201	3PE	O21-C21	2.08	1.40	1.34
45	Z	201	3PE	O21-C21	2.08	1.40	1.34
53	N	404	CDL	OB6-CB5	2.07	1.40	1.34
45	N	402	3PE	O31-C3	-2.07	1.40	1.45
53	d	204	CDL	OA6-CA5	2.07	1.40	1.34
45	d	201	3PE	O21-C21	2.07	1.40	1.34
53	X	201	CDL	OA8-CA6	-2.07	1.40	1.45
46	I	204	PC1	O21-C21	2.06	1.40	1.34
45	N	403	3PE	O21-C21	2.06	1.40	1.34
45	q	201	3PE	O21-C21	2.05	1.40	1.34
53	r	202	CDL	OA6-CA5	2.04	1.40	1.34
53	r	202	CDL	OB6-CB5	2.04	1.40	1.34

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	i	201	CHD	C13-C17-C20	-7.39	110.53	119.48
54	O	401	DGT	C8-N9-C4	7.38	119.86	106.03
58	i	201	CHD	C14-C13-C12	6.17	113.06	107.42
57	T	101	EHZ	C8-C9-S1	5.84	120.92	113.56
56	P	501	NDP	N6A-C6A-N1A	-5.71	105.66	118.38
56	P	501	NDP	N3A-C2A-N1A	-5.59	120.12	128.58
58	i	201	CHD	C17-C13-C14	5.41	105.54	100.11
56	P	501	NDP	C4A-N9A-C1B	-5.36	114.09	126.63
56	P	501	NDP	C5A-C4A-N3A	-5.00	119.83	126.72
57	U	101	EHZ	C8-C9-S1	4.92	119.77	113.56
56	P	501	NDP	C1B-N9A-C8A	4.89	137.94	127.09
50	F	502	FMN	C9-C8-C7	4.72	126.62	119.69
50	F	502	FMN	C7M-C7-C6	4.72	127.89	119.57
45	M	605	3PE	O21-C21-C22	4.54	121.31	111.48
46	B	202	PC1	O21-C21-C22	4.40	120.99	111.48
45	m	201	3PE	O21-C21-C22	4.29	120.77	111.48
58	i	201	CHD	C18-C13-C12	-4.29	104.77	109.06
53	M	607	CDL	OA6-CA5-C11	4.28	120.75	111.48
46	h	202	PC1	O21-C21-C22	4.26	120.70	111.48
56	P	501	NDP	C5A-C6A-N6A	4.25	133.82	123.29
45	b	102	3PE	O21-C21-C22	4.22	120.61	111.48
46	H	402	PC1	O21-C21-C22	4.22	120.61	111.48
45	f	101	3PE	O21-C21-C22	4.22	120.60	111.48
58	i	201	CHD	C17-C13-C12	4.21	121.46	117.67
45	N	402	3PE	O21-C21-C22	4.17	120.50	111.48
45	J	201	3PE	O21-C21-C22	4.16	120.49	111.48
46	I	204	PC1	O21-C21-C22	4.14	120.43	111.48
46	m	203	PC1	O21-C21-C22	4.10	120.36	111.48
45	M	604	3PE	O21-C21-C22	4.10	120.35	111.48
45	m	202	3PE	O21-C21-C22	4.09	120.33	111.48
53	M	607	CDL	OB6-CB5-C51	4.09	120.32	111.48
45	N	403	3PE	O21-C21-C22	4.08	120.31	111.48
53	X	201	CDL	OB6-CB5-C51	4.08	120.31	111.48
53	i	202	CDL	OA6-CA5-C11	4.07	120.29	111.48
45	Y	205	3PE	O21-C21-C22	4.06	120.27	111.48
45	q	201	3PE	O21-C21-C22	4.05	120.25	111.48
45	Y	206	3PE	O21-C21-C22	4.04	120.21	111.48
56	P	501	NDP	N9A-C8A-N7A	-4.02	108.23	113.94
45	I	203	3PE	O21-C21-C22	4.01	120.16	111.48
45	h	201	3PE	O21-C21-C22	3.99	120.12	111.48
45	Y	207	3PE	O21-C21-C22	3.99	120.11	111.48
45	Y	204	3PE	O21-C21-C22	3.96	120.05	111.48
45	N	401	3PE	O21-C21-C22	3.95	120.03	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Z	203	PC1	O21-C21-C22	3.95	120.02	111.48
45	Y	203	3PE	O21-C21-C22	3.94	120.01	111.48
53	h	203	CDL	OB6-CB5-C51	3.94	120.01	111.48
46	g	201	PC1	O21-C21-C22	3.94	120.00	111.48
46	A	202	PC1	O21-C21-C22	3.94	120.00	111.48
46	M	606	PC1	O21-C21-C22	3.93	119.98	111.48
53	d	204	CDL	OA6-CA5-C11	3.92	119.95	111.48
53	r	202	CDL	OA6-CA5-C11	3.91	119.94	111.48
45	r	201	3PE	O21-C21-C22	3.91	119.94	111.48
46	A	203	PC1	O21-C21-C22	3.90	119.91	111.48
53	N	404	CDL	OB6-CB5-C51	3.89	119.89	111.48
45	J	202	3PE	O21-C21-C22	3.89	119.89	111.48
53	i	202	CDL	OB6-CB5-C51	3.88	119.88	111.48
45	M	603	3PE	O21-C21-C22	3.86	119.84	111.48
45	A	201	3PE	O21-C21-C22	3.85	119.82	111.48
58	i	201	CHD	C18-C13-C17	-3.84	105.19	111.20
45	Z	202	3PE	O21-C21-C22	3.83	119.77	111.48
45	Y	201	3PE	O21-C21-C22	3.80	119.71	111.48
45	L	702	3PE	O21-C21-C22	3.80	119.70	111.48
45	Y	202	3PE	O21-C21-C22	3.80	119.70	111.48
45	d	201	3PE	O21-C21-C22	3.79	119.68	111.48
45	K	101	3PE	O21-C21-C22	3.77	119.63	111.48
53	X	201	CDL	OA6-CA5-C11	3.72	119.52	111.48
46	d	202	PC1	O21-C21-C22	3.71	119.51	111.48
53	N	404	CDL	OA6-CA5-C11	3.67	119.42	111.48
53	h	203	CDL	OA6-CA5-C11	3.67	119.41	111.48
58	i	201	CHD	C18-C13-C14	-3.63	105.52	111.20
53	r	202	CDL	OB6-CB5-C51	3.60	119.27	111.48
45	b	101	3PE	O21-C21-C22	3.58	119.23	111.48
56	P	501	NDP	C2A-N3A-C4A	3.49	120.36	111.83
46	L	701	PC1	O21-C21-C22	3.45	118.95	111.48
45	Z	201	3PE	O21-C21-C22	3.43	118.91	111.48
50	F	502	FMN	C4-N3-C2	-3.38	119.64	125.64
54	O	401	DGT	C1'-N9-C8	-3.36	120.37	127.91
50	F	502	FMN	C8M-C8-C7	-3.34	113.93	120.76
57	T	101	EHZ	C13-C12-N1	3.24	122.25	116.34
54	O	401	DGT	C2-N1-C6	-3.19	119.32	125.11
53	X	201	CDL	OB8-CB7-C71	3.14	121.41	111.83
58	i	201	CHD	C1-C10-C5	3.13	112.25	107.75
58	i	201	CHD	C15-C14-C8	3.06	122.56	118.36
45	Y	202	3PE	O31-C31-C32	3.04	121.11	111.83
56	P	501	NDP	N3A-C4A-N9A	3.01	132.29	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	N	401	3PE	O31-C31-C32	3.00	120.97	111.83
54	O	401	DGT	O2G-PG-O3B	2.97	114.60	104.64
46	I	204	PC1	O31-C31-C32	2.95	120.84	111.83
45	J	202	3PE	O31-C31-C32	2.91	119.98	111.15
46	A	203	PC1	O31-C31-C32	2.88	120.61	111.83
46	B	202	PC1	O31-C31-C32	2.85	120.52	111.83
57	U	101	EHZ	C10-S1-C9	2.85	110.26	101.84
57	T	101	EHZ	C10-S1-C9	2.84	110.25	101.84
46	H	403	PC1	O31-C31-C32	2.82	120.44	111.83
46	A	202	PC1	O31-C31-C32	2.82	120.44	111.83
45	r	201	3PE	O31-C31-C32	2.82	120.44	111.83
53	M	607	CDL	OB8-CB7-C71	2.82	120.43	111.83
45	m	201	3PE	O31-C31-C32	2.82	120.43	111.83
56	P	501	NDP	C5A-N7A-C8A	2.81	107.86	103.45
58	i	201	CHD	C6-C5-C4	-2.81	108.02	111.23
46	m	203	PC1	O31-C31-C32	2.80	120.37	111.83
45	I	203	3PE	O31-C31-C32	2.79	120.33	111.83
53	M	607	CDL	OA8-CA7-C31	2.78	120.31	111.83
45	Y	203	3PE	O31-C31-C32	2.77	120.30	111.83
45	N	402	3PE	O31-C31-C32	2.77	120.28	111.83
53	i	202	CDL	OA8-CA7-C31	2.77	120.27	111.83
50	F	502	FMN	C6-C7-C8	-2.76	115.63	119.69
56	P	501	NDP	C2B-C1B-N9A	-2.76	109.21	113.75
45	M	602	3PE	O31-C31-C32	2.76	120.24	111.83
46	M	606	PC1	O31-C31-C32	2.76	120.24	111.83
46	H	402	PC1	O31-C31-C32	2.76	120.24	111.83
45	Y	204	3PE	O31-C31-C32	2.75	120.21	111.83
46	h	202	PC1	O31-C31-C32	2.75	120.21	111.83
53	d	204	CDL	OB8-CB7-C71	2.74	120.20	111.83
58	i	201	CHD	C9-C10-C5	2.74	112.33	108.51
45	H	401	3PE	O31-C31-C32	2.73	120.16	111.83
53	h	203	CDL	OA8-CA7-C31	2.73	120.16	111.83
53	N	404	CDL	OA8-CA7-C31	2.73	120.15	111.83
54	O	401	DGT	O1G-PG-O3B	2.73	113.78	104.64
45	h	201	3PE	O31-C31-C32	2.73	120.14	111.83
45	f	101	3PE	O31-C31-C32	2.72	120.12	111.83
53	i	202	CDL	OB8-CB7-C71	2.71	120.09	111.83
45	Y	205	3PE	O31-C31-C32	2.71	120.09	111.83
45	b	102	3PE	O31-C31-C32	2.71	120.08	111.83
46	g	201	PC1	O31-C31-C32	2.70	120.07	111.83
45	Y	206	3PE	O31-C31-C32	2.69	120.03	111.83
50	F	502	FMN	C4A-C10-N10	2.69	120.33	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	q	201	3PE	O31-C31-C32	2.69	120.03	111.83
45	A	201	3PE	O31-C31-C32	2.69	120.02	111.83
45	N	403	3PE	O31-C31-C32	2.68	120.02	111.83
45	M	605	3PE	O31-C31-C32	2.68	119.99	111.83
45	Y	207	3PE	O31-C31-C32	2.68	119.99	111.83
53	d	204	CDL	OA8-CA7-C31	2.67	119.98	111.83
50	F	502	FMN	C5A-C9A-N10	2.67	120.38	117.97
46	L	701	PC1	O31-C31-C32	2.67	119.97	111.83
45	L	702	3PE	O31-C31-C32	2.67	119.96	111.83
45	Y	201	3PE	O31-C31-C32	2.66	119.95	111.83
45	Z	201	3PE	O31-C31-C32	2.65	119.93	111.83
45	M	604	3PE	O31-C31-C32	2.65	119.90	111.83
45	m	202	3PE	O31-C31-C32	2.64	119.89	111.83
53	d	204	CDL	OB6-CB5-C51	2.64	120.62	110.93
57	T	101	EHZ	O2-C9-C8	-2.63	119.60	123.74
53	X	201	CDL	OA8-CA7-C31	2.63	119.86	111.83
45	d	201	3PE	O31-C31-C32	2.60	119.76	111.83
46	d	202	PC1	O31-C31-C32	2.60	119.75	111.83
53	N	404	CDL	OB8-CB7-C71	2.59	119.74	111.83
53	r	202	CDL	OB8-CB7-C71	2.59	119.73	111.83
45	J	201	3PE	O31-C31-C32	2.59	119.73	111.83
45	K	101	3PE	O31-C31-C32	2.59	119.72	111.83
45	Z	202	3PE	O31-C31-C32	2.58	119.69	111.83
53	h	203	CDL	OB8-CB7-C71	2.58	119.69	111.83
46	Z	203	PC1	O31-C31-C32	2.55	119.61	111.83
57	T	101	EHZ	O2-C9-S1	-2.52	119.48	122.68
45	b	101	3PE	O31-C31-C32	2.52	119.51	111.83
45	H	401	3PE	O21-C21-C22	2.50	120.12	110.93
45	M	603	3PE	O31-C31-C32	2.49	119.44	111.83
50	F	502	FMN	C9A-C5A-N5	-2.49	119.81	122.45
50	F	502	FMN	C4A-C4-N3	2.48	119.58	113.25
54	O	401	DGT	C5-C6-N1	2.48	119.57	113.25
53	r	202	CDL	OA8-CA7-C31	2.47	119.37	111.83
50	F	502	FMN	O4-C4-C4A	-2.45	120.08	126.53
45	M	602	3PE	O21-C21-C22	2.42	119.81	110.93
58	i	201	CHD	C19-C10-C9	-2.40	107.95	111.18
54	O	401	DGT	O1A-PA-O2A	-2.39	101.35	112.44
46	H	403	PC1	O21-C21-C22	2.38	119.68	110.93
54	O	401	DGT	O6-C6-C5	-2.37	120.28	126.53
50	F	502	FMN	C6-C5A-C9A	2.35	122.28	119.05
54	O	401	DGT	O1B-PB-O2B	-2.33	101.59	112.44
54	O	401	DGT	C2'-C3'-C4'	2.32	107.51	102.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	i	201	CHD	C1-C2-C3	2.31	113.54	110.48
46	q	202	PC1	O21-C21-C22	2.29	119.35	110.93
57	U	101	EHZ	C13-C12-N1	2.28	120.50	116.34
57	U	101	EHZ	C16-C15-N2	2.25	120.76	116.48
57	U	101	EHZ	O2-C9-C8	-2.23	120.23	123.74
58	i	201	CHD	C1-C10-C9	-2.21	107.91	111.34
50	F	502	FMN	C10-C4A-N5	-2.20	120.31	124.81
56	P	501	NDP	C4A-C5A-N7A	-2.20	108.07	110.58
54	O	401	DGT	C5-C4-N9	-2.17	101.77	105.66
58	i	201	CHD	C13-C14-C8	-2.15	112.00	114.72
54	O	401	DGT	C1'-N9-C4	-2.12	119.77	125.50
58	i	201	CHD	C11-C9-C10	-2.12	111.55	113.70
56	P	501	NDP	C4A-N9A-C8A	2.12	107.97	105.74
57	U	101	EHZ	O2-C9-S1	-2.12	119.99	122.68
48	g	202	PLC	C3-C2-C1	2.10	116.69	111.78
50	F	502	FMN	C7M-C7-C8	-2.10	116.48	120.76
57	T	101	EHZ	O3-C12-N1	-2.08	118.94	123.03
54	O	401	DGT	N9-C4-N3	2.08	130.11	125.95
57	U	101	EHZ	C14-N2-C15	-2.05	118.87	122.55
48	Y	208	PLC	C3-C2-C1	2.03	116.52	111.78
54	O	401	DGT	C8-N7-C5	-2.02	100.66	104.26
58	i	201	CHD	C16-C17-C13	2.01	105.50	103.54

There are no chirality outliers.

All (1284) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C11-O13-P-O14
45	H	401	3PE	C11-O13-P-O11
45	H	401	3PE	C11-O13-P-O12
45	H	401	3PE	C22-C21-O21-C2
45	I	203	3PE	C11-O13-P-O11
45	I	203	3PE	C11-O13-P-O14
45	I	203	3PE	O13-C11-C12-N
45	I	203	3PE	O22-C21-O21-C2
45	I	203	3PE	C22-C21-O21-C2
45	J	201	3PE	C11-O13-P-O11
45	J	201	3PE	C11-O13-P-O14
45	J	201	3PE	C12-C11-O13-P
45	J	201	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	J	202	3PE	C11-O13-P-O11
45	J	202	3PE	C11-O13-P-O12
45	K	101	3PE	C1-O11-P-O12
45	K	101	3PE	C1-O11-P-O13
45	K	101	3PE	C11-O13-P-O12
45	K	101	3PE	O11-C1-C2-O21
45	L	702	3PE	C1-O11-P-O12
45	L	702	3PE	C1-O11-P-O13
45	L	702	3PE	C11-O13-P-O11
45	L	702	3PE	C11-O13-P-O12
45	L	702	3PE	C11-O13-P-O14
45	L	702	3PE	C22-C21-O21-C2
45	M	602	3PE	C11-O13-P-O14
45	M	602	3PE	C12-C11-O13-P
45	M	603	3PE	C1-O11-P-O13
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	C12-C11-O13-P
45	M	604	3PE	O22-C21-O21-C2
45	M	604	3PE	C22-C21-O21-C2
45	M	605	3PE	C1-O11-P-O14
45	N	401	3PE	C11-O13-P-O11
45	N	401	3PE	C11-O13-P-O14
45	N	401	3PE	C12-C11-O13-P
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	N	402	3PE	O22-C21-O21-C2
45	Y	201	3PE	C1-O11-P-O13
45	Y	201	3PE	C1-O11-P-O14
45	Y	201	3PE	O13-C11-C12-N
45	Y	202	3PE	C1-O11-P-O14
45	Y	202	3PE	C11-O13-P-O11
45	Y	202	3PE	C11-O13-P-O14
45	Y	202	3PE	C22-C21-O21-C2
45	Y	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	C11-O13-P-O12
45	Y	203	3PE	C11-O13-P-O14
45	Y	203	3PE	C22-C21-O21-C2
45	Y	204	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	Y	204	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O11
45	Y	204	3PE	C11-O13-P-O14
45	Y	204	3PE	C22-C21-O21-C2
45	Y	205	3PE	C11-O13-P-O11
45	Y	205	3PE	C11-O13-P-O12
45	Y	205	3PE	C11-O13-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	O22-C21-O21-C2
45	Y	207	3PE	C1-O11-P-O12
45	Y	207	3PE	C11-O13-P-O11
45	Y	207	3PE	C11-O13-P-O12
45	Y	207	3PE	O22-C21-O21-C2
45	Y	207	3PE	C22-C21-O21-C2
45	Z	201	3PE	C1-O11-P-O12
45	Z	201	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O14
45	Z	201	3PE	C11-O13-P-O14
45	Z	201	3PE	O13-C11-C12-N
45	Z	202	3PE	C1-O11-P-O12
45	Z	202	3PE	C1-O11-P-O13
45	Z	202	3PE	C1-O11-P-O14
45	b	101	3PE	C1-O11-P-O13
45	b	101	3PE	C1-O11-P-O14
45	b	102	3PE	C1-O11-P-O12
45	b	102	3PE	C1-O11-P-O13
45	b	102	3PE	C12-C11-O13-P
45	b	102	3PE	O22-C21-O21-C2
45	d	201	3PE	C11-O13-P-O11
45	d	201	3PE	C11-O13-P-O12
45	d	201	3PE	C11-O13-P-O14
45	d	201	3PE	C22-C21-O21-C2
45	f	101	3PE	C1-O11-P-O13
45	f	101	3PE	C11-O13-P-O11
45	f	101	3PE	C11-O13-P-O12
45	f	101	3PE	C22-C21-O21-C2
45	h	201	3PE	C1-O11-P-O14
45	h	201	3PE	C11-O13-P-O11
45	h	201	3PE	C11-O13-P-O12
45	h	201	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	h	201	3PE	O11-C1-C2-O21
45	h	201	3PE	C22-C21-O21-C2
45	m	201	3PE	C11-O13-P-O12
45	m	201	3PE	O13-C11-C12-N
45	m	201	3PE	O32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
45	m	201	3PE	O22-C21-O21-C2
45	m	202	3PE	C1-O11-P-O13
45	m	202	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O12
45	m	202	3PE	C11-O13-P-O14
45	m	202	3PE	O13-C11-C12-N
45	m	202	3PE	O22-C21-O21-C2
45	q	201	3PE	C11-O13-P-O11
45	q	201	3PE	C11-O13-P-O12
45	q	201	3PE	C11-O13-P-O14
45	q	201	3PE	O22-C21-O21-C2
45	r	201	3PE	C1-O11-P-O12
45	r	201	3PE	C1-O11-P-O13
45	r	201	3PE	C1-O11-P-O14
45	r	201	3PE	C11-O13-P-O11
45	r	201	3PE	C11-O13-P-O12
45	r	201	3PE	C11-O13-P-O14
45	r	201	3PE	O32-C31-O31-C3
45	r	201	3PE	C22-C21-O21-C2
46	A	202	PC1	C11-O13-P-O12
46	A	202	PC1	C11-O13-P-O11
46	A	202	PC1	O13-C11-C12-N
46	A	203	PC1	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O11
46	A	203	PC1	C22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O12
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	202	PC1	C2-C1-O11-P
46	B	202	PC1	O22-C21-O21-C2
46	H	402	PC1	C1-O11-P-O12
46	H	402	PC1	C1-O11-P-O14
46	H	402	PC1	C1-O11-P-O13
46	H	402	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
46	H	403	PC1	C1-O11-P-O12
46	H	403	PC1	C1-O11-P-O13
46	H	403	PC1	O13-C11-C12-N
46	I	204	PC1	C1-O11-P-O12
46	I	204	PC1	C1-O11-P-O14
46	I	204	PC1	C1-O11-P-O13
46	I	204	PC1	O13-C11-C12-N
46	L	701	PC1	C11-O13-P-O12
46	L	701	PC1	C11-O13-P-O14
46	L	701	PC1	C11-O13-P-O11
46	L	701	PC1	O21-C2-C3-O31
46	L	701	PC1	O32-C31-O31-C3
46	M	606	PC1	C1-O11-P-O14
46	Z	203	PC1	C11-O13-P-O14
46	Z	203	PC1	C11-O13-P-O11
46	Z	203	PC1	C1-O11-P-O12
46	d	202	PC1	C11-O13-P-O12
46	d	202	PC1	C1-O11-P-O12
46	d	202	PC1	C1-O11-P-O14
46	d	202	PC1	C1-O11-P-O13
46	d	202	PC1	O32-C31-O31-C3
46	g	201	PC1	C11-O13-P-O12
46	g	201	PC1	C1-O11-P-O12
46	g	201	PC1	C1-O11-P-O14
46	g	201	PC1	C1-O11-P-O13
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	m	203	PC1	C11-O13-P-O12
46	m	203	PC1	C11-O13-P-O14
46	m	203	PC1	C11-O13-P-O11
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	202	PC1	C11-O13-P-O14
46	q	202	PC1	C11-O13-P-O11
46	q	202	PC1	O11-C1-C2-O21
48	B	203	PLC	C4-O4P-P-O1P
48	B	203	PLC	C4-O4P-P-O3P
48	J	203	PLC	C4-O4P-P-O1P
48	J	203	PLC	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	J	203	PLC	C4-O4P-P-O3P
48	L	703	PLC	C2-C1-O3P-P
48	L	703	PLC	C1-O3P-P-O1P
48	L	703	PLC	C1-O3P-P-O2P
48	L	703	PLC	C1-O3P-P-O4P
48	Y	208	PLC	C1-O3P-P-O2P
48	Y	208	PLC	C1-O3P-P-O4P
48	Y	208	PLC	C4-O4P-P-O1P
48	Z	204	PLC	C1'-C'-O2-C2
48	Z	204	PLC	C1-O3P-P-O1P
48	b	103	PLC	C1-O3P-P-O2P
48	b	103	PLC	C1-O3P-P-O4P
48	b	103	PLC	C4-O4P-P-O1P
48	d	203	PLC	C1-O3P-P-O2P
48	d	203	PLC	C4-O4P-P-O3P
48	g	202	PLC	C1-O3P-P-O2P
48	g	202	PLC	C1-O3P-P-O4P
50	F	502	FMN	N10-C1'-C2'-O2'
53	M	607	CDL	CA2-OA2-PA1-OA3
53	M	607	CDL	CA2-OA2-PA1-OA4
53	M	607	CDL	CA2-OA2-PA1-OA5
53	M	607	CDL	CA3-OA5-PA1-OA2
53	M	607	CDL	CA3-OA5-PA1-OA3
53	M	607	CDL	CA3-OA5-PA1-OA4
53	M	607	CDL	CB2-OB2-PB2-OB4
53	M	607	CDL	CB2-OB2-PB2-OB5
53	M	607	CDL	CB3-OB5-PB2-OB2
53	M	607	CDL	OB7-CB5-OB6-CB4
53	N	404	CDL	CB2-OB2-PB2-OB3
53	N	404	CDL	C51-CB5-OB6-CB4
53	X	201	CDL	C1-CA2-OA2-PA1
53	X	201	CDL	CA2-OA2-PA1-OA5
53	X	201	CDL	CB3-OB5-PB2-OB2
53	X	201	CDL	CB3-OB5-PB2-OB3
53	X	201	CDL	CB3-OB5-PB2-OB4
53	X	201	CDL	C51-CB5-OB6-CB4
53	d	204	CDL	CB2-OB2-PB2-OB3
53	d	204	CDL	CB2-OB2-PB2-OB5
53	d	204	CDL	CB3-OB5-PB2-OB3
53	d	204	CDL	OB7-CB5-OB6-CB4
53	i	202	CDL	CB2-OB2-PB2-OB3
53	i	202	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
53	i	202	CDL	CB2-OB2-PB2-OB5
53	r	202	CDL	CA3-OA5-PA1-OA2
53	r	202	CDL	CA3-OA5-PA1-OA3
53	r	202	CDL	C11-CA5-OA6-CA4
53	r	202	CDL	OB5-CB3-CB4-OB6
54	O	401	DGT	C5'-O5'-PA-O2A
56	P	501	NDP	C5B-O5B-PA-O1A
56	P	501	NDP	C5B-O5B-PA-O2A
56	P	501	NDP	C5B-O5B-PA-O3
56	P	501	NDP	C5D-O5D-PN-O3
56	P	501	NDP	C5D-O5D-PN-O2N
57	T	101	EHZ	C6-C7-C8-C9
57	T	101	EHZ	C11-C10-S1-C9
57	T	101	EHZ	C16-C17-C20-O6
57	U	101	EHZ	O1-C7-C8-C9
57	U	101	EHZ	S1-C10-C11-N1
57	U	101	EHZ	C15-C16-C17-C19
57	U	101	EHZ	C15-C16-C17-C20
57	U	101	EHZ	C16-C17-C20-O6
57	U	101	EHZ	C18-C17-C20-O6
57	U	101	EHZ	C19-C17-C20-O6
57	U	101	EHZ	O2-C9-S1-C10
57	U	101	EHZ	C8-C9-S1-C10
45	A	201	3PE	O32-C31-O31-C3
45	N	403	3PE	O32-C31-O31-C3
45	Y	204	3PE	O32-C31-O31-C3
53	X	201	CDL	OA9-CA7-OA8-CA6
53	X	201	CDL	OB9-CB7-OB8-CB6
53	d	204	CDL	OB9-CB7-OB8-CB6
45	N	403	3PE	C32-C31-O31-C3
45	Y	204	3PE	C32-C31-O31-C3
46	L	701	PC1	C32-C31-O31-C3
53	X	201	CDL	C31-CA7-OA8-CA6
53	X	201	CDL	C71-CB7-OB8-CB6
53	d	204	CDL	C71-CB7-OB8-CB6
45	H	401	3PE	O32-C31-O31-C3
45	I	203	3PE	O32-C31-O31-C3
45	J	201	3PE	O32-C31-O31-C3
45	M	604	3PE	O32-C31-O31-C3
45	N	401	3PE	O32-C31-O31-C3
45	Y	203	3PE	O32-C31-O31-C3
45	Y	205	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	O32-C31-O31-C3
45	h	201	3PE	O32-C31-O31-C3
46	A	203	PC1	O32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
46	H	403	PC1	O32-C31-O31-C3
46	h	202	PC1	O32-C31-O31-C3
53	M	607	CDL	OA9-CA7-OA8-CA6
53	M	607	CDL	OB9-CB7-OB8-CB6
53	h	203	CDL	OA9-CA7-OA8-CA6
53	h	203	CDL	OB9-CB7-OB8-CB6
45	H	401	3PE	O22-C21-O21-C2
45	L	702	3PE	O22-C21-O21-C2
45	Y	204	3PE	O22-C21-O21-C2
45	d	201	3PE	O22-C21-O21-C2
45	f	101	3PE	O22-C21-O21-C2
45	h	201	3PE	O22-C21-O21-C2
45	r	201	3PE	O22-C21-O21-C2
46	A	203	PC1	O22-C21-O21-C2
46	I	204	PC1	O22-C21-O21-C2
46	m	203	PC1	O22-C21-O21-C2
53	N	404	CDL	OB7-CB5-OB6-CB4
53	X	201	CDL	OB7-CB5-OB6-CB4
45	A	201	3PE	C32-C31-O31-C3
45	H	401	3PE	C32-C31-O31-C3
45	J	201	3PE	C32-C31-O31-C3
45	M	604	3PE	C32-C31-O31-C3
45	N	401	3PE	C32-C31-O31-C3
45	Y	203	3PE	C32-C31-O31-C3
45	Y	205	3PE	C32-C31-O31-C3
45	Y	206	3PE	C32-C31-O31-C3
45	b	102	3PE	C32-C31-O31-C3
45	h	201	3PE	C32-C31-O31-C3
45	r	201	3PE	C32-C31-O31-C3
46	A	203	PC1	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
46	H	403	PC1	C32-C31-O31-C3
46	M	606	PC1	C32-C31-O31-C3
46	d	202	PC1	C32-C31-O31-C3
46	h	202	PC1	C32-C31-O31-C3
53	M	607	CDL	C31-CA7-OA8-CA6
53	M	607	CDL	C71-CB7-OB8-CB6
53	h	203	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
45	J	201	3PE	C22-C21-O21-C2
45	N	402	3PE	C22-C21-O21-C2
45	Y	206	3PE	C22-C21-O21-C2
45	b	102	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
45	m	202	3PE	C22-C21-O21-C2
45	q	201	3PE	C22-C21-O21-C2
46	B	202	PC1	C22-C21-O21-C2
46	I	204	PC1	C22-C21-O21-C2
53	M	607	CDL	C51-CB5-OB6-CB4
53	d	204	CDL	C51-CB5-OB6-CB4
46	m	203	PC1	O32-C31-O31-C3
53	d	204	CDL	OA9-CA7-OA8-CA6
46	q	202	PC1	O32-C31-O31-C3
45	d	201	3PE	O32-C31-O31-C3
45	I	203	3PE	C32-C31-O31-C3
45	d	201	3PE	C32-C31-O31-C3
46	m	203	PC1	C32-C31-O31-C3
53	N	404	CDL	C71-CB7-OB8-CB6
53	h	203	CDL	C71-CB7-OB8-CB6
46	M	606	PC1	O32-C31-O31-C3
53	i	202	CDL	OA9-CA7-OA8-CA6
45	Y	202	3PE	O22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
48	Z	204	PLC	O'-C'-O2-C2
53	r	202	CDL	OA7-CA5-OA6-CA4
46	q	202	PC1	C32-C31-O31-C3
53	M	607	CDL	O1-C1-CA2-OA2
53	N	404	CDL	O1-C1-CA2-OA2
53	d	204	CDL	O1-C1-CA2-OA2
46	A	202	PC1	C32-C31-O31-C3
53	d	204	CDL	C31-CA7-OA8-CA6
45	b	102	3PE	O32-C31-O31-C3
46	A	202	PC1	O32-C31-O31-C3
53	N	404	CDL	OB9-CB7-OB8-CB6
46	M	606	PC1	C22-C21-O21-C2
46	h	202	PC1	C22-C21-O21-C2
53	X	201	CDL	C11-CA5-OA6-CA4
53	i	202	CDL	C31-CA7-OA8-CA6
53	X	201	CDL	OA7-CA5-OA6-CA4
45	Y	207	3PE	C32-C31-O31-C3
53	i	202	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
45	Y	207	3PE	O32-C31-O31-C3
53	i	202	CDL	OB9-CB7-OB8-CB6
46	H	403	PC1	C22-C21-O21-C2
46	h	202	PC1	O22-C21-O21-C2
45	Z	201	3PE	C32-C31-O31-C3
45	f	101	3PE	C32-C31-O31-C3
45	m	202	3PE	C32-C31-O31-C3
46	Z	203	PC1	C32-C31-O31-C3
53	N	404	CDL	C31-CA7-OA8-CA6
48	O	403	PLC	C4-C5-N-C8
45	m	202	3PE	O32-C31-O31-C3
53	N	404	CDL	OA9-CA7-OA8-CA6
53	d	204	CDL	CB7-C71-C72-C73
45	f	101	3PE	O32-C31-O31-C3
53	M	607	CDL	OB5-CB3-CB4-OB6
46	M	606	PC1	O21-C2-C3-O31
48	O	403	PLC	O2-C2-C3-O3
53	M	607	CDL	CB7-C71-C72-C73
45	Y	204	3PE	C21-C22-C23-C24
53	r	202	CDL	CB5-C51-C52-C53
46	B	202	PC1	C21-C22-C23-C24
48	O	403	PLC	CB-C1B-C2B-C3B
46	M	606	PC1	O22-C21-O21-C2
45	N	401	3PE	C31-C32-C33-C34
45	Z	201	3PE	C21-C22-C23-C24
46	H	402	PC1	C21-C22-C23-C24
46	Z	203	PC1	C31-C32-C33-C34
46	d	202	PC1	C31-C32-C33-C34
45	Z	201	3PE	O32-C31-O31-C3
45	A	201	3PE	C31-C32-C33-C34
45	b	102	3PE	C21-C22-C23-C24
45	f	101	3PE	C21-C22-C23-C24
46	A	202	PC1	C21-C22-C23-C24
46	Z	203	PC1	O32-C31-O31-C3
45	Y	201	3PE	C32-C31-O31-C3
48	b	103	PLC	C1B-CB-O3-C3
53	M	607	CDL	CB5-C51-C52-C53
46	H	403	PC1	O22-C21-O21-C2
45	J	202	3PE	C21-C22-C23-C24
45	d	201	3PE	C31-C32-C33-C34
45	Z	202	3PE	C32-C31-O31-C3
45	Y	203	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
53	r	202	CDL	CA5-C11-C12-C13
53	N	404	CDL	CB2-C1-CA2-OA2
48	O	403	PLC	C4-C5-N-C7
46	g	201	PC1	C32-C31-O31-C3
46	d	202	PC1	C21-C22-C23-C24
53	M	607	CDL	C11-CA5-OA6-CA4
53	d	204	CDL	C11-CA5-OA6-CA4
53	M	607	CDL	OA7-CA5-OA6-CA4
53	d	204	CDL	OA7-CA5-OA6-CA4
46	I	204	PC1	C21-C22-C23-C24
45	M	603	3PE	C2-C1-O11-P
45	Z	202	3PE	C31-C32-C33-C34
45	Y	201	3PE	O32-C31-O31-C3
45	K	101	3PE	C22-C21-O21-C2
45	M	603	3PE	C22-C21-O21-C2
45	M	605	3PE	C22-C21-O21-C2
45	N	401	3PE	C22-C21-O21-C2
53	i	202	CDL	C11-CA5-OA6-CA4
48	O	403	PLC	C4-C5-N-C6
45	K	101	3PE	C35-C36-C37-C38
45	Y	204	3PE	C39-C3A-C3B-C3C
45	Y	206	3PE	C36-C37-C38-C39
45	Z	202	3PE	C38-C39-C3A-C3B
46	L	701	PC1	C3B-C3C-C3D-C3E
53	X	201	CDL	C35-C36-C37-C38
45	M	605	3PE	C35-C36-C37-C38
45	Y	203	3PE	C26-C27-C28-C29
45	Y	205	3PE	C2A-C2B-C2C-C2D
45	b	102	3PE	C28-C29-C2A-C2B
46	L	701	PC1	C29-C2A-C2B-C2C
53	M	607	CDL	C37-C38-C39-C40
53	d	204	CDL	C72-C73-C74-C75
45	Y	204	3PE	C25-C26-C27-C28
45	Y	207	3PE	C2C-C2D-C2E-C2F
46	L	701	PC1	C32-C33-C34-C35
53	M	607	CDL	C13-C14-C15-C16
59	o	201	MYR	C2-C3-C4-C5
45	Z	202	3PE	O32-C31-O31-C3
48	b	103	PLC	OB-CB-O3-C3
45	A	201	3PE	C24-C25-C26-C27
45	M	605	3PE	C33-C34-C35-C36
45	N	403	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
45	Y	202	3PE	C2C-C2D-C2E-C2F
45	Y	207	3PE	C3B-C3C-C3D-C3E
45	Z	202	3PE	C29-C2A-C2B-C2C
45	h	201	3PE	C33-C34-C35-C36
46	H	403	PC1	C36-C37-C38-C39
53	M	607	CDL	C18-C19-C20-C21
53	X	201	CDL	C82-C83-C84-C85
57	T	101	EHZ	C2-C3-C4-C5
45	M	603	3PE	C2D-C2E-C2F-C2G
45	Y	206	3PE	C33-C34-C35-C36
45	Z	202	3PE	C2B-C2C-C2D-C2E
53	X	201	CDL	C37-C38-C39-C40
45	q	201	3PE	C21-C22-C23-C24
46	M	606	PC1	C31-C32-C33-C34
45	N	402	3PE	C2C-C2D-C2E-C2F
53	h	203	CDL	C60-C61-C62-C63
45	K	101	3PE	C22-C23-C24-C25
45	Z	202	3PE	C35-C36-C37-C38
45	f	101	3PE	C24-C25-C26-C27
45	J	202	3PE	C22-C21-O21-C2
53	r	202	CDL	C51-CB5-OB6-CB4
45	H	401	3PE	C3E-C3F-C3G-C3H
45	J	202	3PE	C27-C28-C29-C2A
45	Y	202	3PE	C2B-C2C-C2D-C2E
57	U	101	EHZ	C5-C6-C7-C8
45	N	403	3PE	C2A-C2B-C2C-C2D
45	Y	204	3PE	C33-C34-C35-C36
53	N	404	CDL	C17-C18-C19-C20
48	b	103	PLC	C'-C1'-C2'-C3'
45	L	702	3PE	C3A-C3B-C3C-C3D
46	d	202	PC1	C36-C37-C38-C39
53	N	404	CDL	C78-C79-C80-C81
53	X	201	CDL	C58-C59-C60-C61
53	i	202	CDL	C16-C17-C18-C19
45	b	101	3PE	C26-C27-C28-C29
45	q	201	3PE	C27-C28-C29-C2A
48	L	703	PLC	C3'-C4'-C5'-C6'
53	X	201	CDL	C61-C62-C63-C64
46	I	204	PC1	C36-C37-C38-C39
53	M	607	CDL	C32-C33-C34-C35
45	M	603	3PE	C3A-C3B-C3C-C3D
45	Y	205	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	Y	207	3PE	C39-C3A-C3B-C3C
46	L	701	PC1	C39-C3A-C3B-C3C
57	T	101	EHZ	C1-C2-C3-C4
45	K	101	3PE	O22-C21-O21-C2
45	M	605	3PE	O22-C21-O21-C2
45	q	201	3PE	C25-C26-C27-C28
45	A	201	3PE	C3C-C3D-C3E-C3F
45	N	401	3PE	C24-C25-C26-C27
46	H	403	PC1	C3A-C3B-C3C-C3D
46	I	204	PC1	C35-C36-C37-C38
53	h	203	CDL	C34-C35-C36-C37
45	N	403	3PE	C31-C32-C33-C34
45	Y	207	3PE	C21-C22-C23-C24
45	A	201	3PE	C36-C37-C38-C39
45	A	201	3PE	C3E-C3F-C3G-C3H
45	M	604	3PE	C35-C36-C37-C38
45	M	605	3PE	C2A-C2B-C2C-C2D
45	N	403	3PE	C2D-C2E-C2F-C2G
45	Y	201	3PE	C22-C23-C24-C25
45	m	202	3PE	C35-C36-C37-C38
46	B	202	PC1	C38-C39-C3A-C3B
48	b	103	PLC	C4'-C5'-C6'-C7'
53	M	607	CDL	C57-C58-C59-C60
53	N	404	CDL	C22-C23-C24-C25
53	X	201	CDL	C51-C52-C53-C54
45	N	403	3PE	C28-C29-C2A-C2B
45	Y	207	3PE	C33-C34-C35-C36
48	O	403	PLC	C2'-C3'-C4'-C5'
45	f	101	3PE	C34-C35-C36-C37
45	m	202	3PE	C33-C34-C35-C36
45	A	201	3PE	C34-C35-C36-C37
45	Y	205	3PE	C38-C39-C3A-C3B
45	q	201	3PE	C3B-C3C-C3D-C3E
46	H	402	PC1	C24-C25-C26-C27
46	H	402	PC1	C33-C34-C35-C36
53	N	404	CDL	CA5-C11-C12-C13
53	N	404	CDL	CB7-C71-C72-C73
46	g	201	PC1	O32-C31-O31-C3
46	d	202	PC1	C33-C34-C35-C36
46	L	701	PC1	C35-C36-C37-C38
45	K	101	3PE	C32-C33-C34-C35
45	N	401	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
46	H	402	PC1	C34-C35-C36-C37
46	M	606	PC1	C25-C26-C27-C28
53	N	404	CDL	C12-C13-C14-C15
45	Z	202	3PE	C21-C22-C23-C24
53	i	202	CDL	C12-C13-C14-C15
53	M	607	CDL	C83-C84-C85-C86
53	X	201	CDL	C77-C78-C79-C80
53	i	202	CDL	C32-C33-C34-C35
45	J	202	3PE	O22-C21-O21-C2
45	M	603	3PE	O22-C21-O21-C2
45	N	401	3PE	O22-C21-O21-C2
53	i	202	CDL	OA7-CA5-OA6-CA4
53	r	202	CDL	OB7-CB5-OB6-CB4
45	b	101	3PE	C34-C35-C36-C37
46	A	202	PC1	C23-C24-C25-C26
45	N	401	3PE	C32-C33-C34-C35
45	Y	203	3PE	C29-C2A-C2B-C2C
45	Y	205	3PE	C25-C26-C27-C28
46	H	402	PC1	C29-C2A-C2B-C2C
45	M	602	3PE	C32-C31-O31-C3
46	g	201	PC1	C26-C27-C28-C29
53	N	404	CDL	C51-C52-C53-C54
45	Y	203	3PE	C2D-C2E-C2F-C2G
45	b	102	3PE	C23-C24-C25-C26
45	M	602	3PE	C33-C34-C35-C36
45	Y	207	3PE	C35-C36-C37-C38
53	M	607	CDL	C23-C24-C25-C26
45	r	201	3PE	C31-C32-C33-C34
53	M	607	CDL	CA5-C11-C12-C13
45	M	603	3PE	C35-C36-C37-C38
45	N	402	3PE	C26-C27-C28-C29
53	d	204	CDL	C35-C36-C37-C38
45	J	202	3PE	C29-C2A-C2B-C2C
45	N	401	3PE	C27-C28-C29-C2A
46	m	203	PC1	C24-C25-C26-C27
45	N	402	3PE	C32-C31-O31-C3
45	M	602	3PE	C22-C21-O21-C2
45	Z	201	3PE	C22-C21-O21-C2
57	T	101	EHZ	C12-C13-C14-N2
46	h	202	PC1	C29-C2A-C2B-C2C
48	L	703	PLC	C5B-C6B-C7B-C8B
45	Z	201	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	C38-C39-C3A-C3B
48	L	703	PLC	C7'-C8'-C9'-CA'
45	N	402	3PE	C33-C34-C35-C36
46	H	402	PC1	C32-C33-C34-C35
45	Y	203	3PE	C31-C32-C33-C34
45	q	201	3PE	C32-C33-C34-C35
45	q	201	3PE	C35-C36-C37-C38
53	M	607	CDL	C14-C15-C16-C17
53	h	203	CDL	C72-C73-C74-C75
53	r	202	CDL	C71-C72-C73-C74
57	U	101	EHZ	C5-C6-C7-O1
45	b	102	3PE	C33-C34-C35-C36
45	M	602	3PE	C31-C32-C33-C34
45	b	102	3PE	C2D-C2E-C2F-C2G
46	H	402	PC1	C28-C29-C2A-C2B
45	H	401	3PE	O11-C1-C2-O21
45	N	403	3PE	O11-C1-C2-O21
53	N	404	CDL	OA5-CA3-CA4-OA6
46	Z	203	PC1	C22-C21-O21-C2
45	A	201	3PE	C3A-C3B-C3C-C3D
45	Y	203	3PE	C3B-C3C-C3D-C3E
53	N	404	CDL	C55-C56-C57-C58
45	f	101	3PE	C32-C33-C34-C35
45	M	603	3PE	C31-C32-C33-C34
45	L	702	3PE	C35-C36-C37-C38
46	A	203	PC1	C3C-C3D-C3E-C3F
46	H	402	PC1	O21-C2-C3-O31
46	m	203	PC1	O21-C2-C3-O31
45	N	401	3PE	C2E-C2F-C2G-C2H
48	g	202	PLC	C1'-C2'-C3'-C4'
45	K	101	3PE	C3A-C3B-C3C-C3D
56	P	501	NDP	O4D-C1D-N1N-C6N
45	Y	207	3PE	C38-C39-C3A-C3B
46	A	203	PC1	C34-C35-C36-C37
45	Z	202	3PE	C2-C1-O11-P
45	M	605	3PE	C27-C28-C29-C2A
46	H	403	PC1	C3E-C3F-C3G-C3H
45	N	401	3PE	C22-C23-C24-C25
45	Y	204	3PE	C34-C35-C36-C37
48	J	203	PLC	C2B-C3B-C4B-C5B
53	d	204	CDL	C74-C75-C76-C77
45	d	201	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
57	U	101	EHZ	C22-C23-C24-C25
57	T	101	EHZ	C22-C23-C24-C25
53	N	404	CDL	C71-C72-C73-C74
45	K	101	3PE	O11-C1-C2-C3
45	N	403	3PE	O11-C1-C2-C3
45	Y	202	3PE	O11-C1-C2-C3
45	Y	204	3PE	O11-C1-C2-C3
45	h	201	3PE	O11-C1-C2-C3
45	r	201	3PE	O11-C1-C2-C3
53	M	607	CDL	OB5-CB3-CB4-CB6
53	N	404	CDL	OA5-CA3-CA4-CA6
53	X	201	CDL	OA5-CA3-CA4-CA6
53	i	202	CDL	OB5-CB3-CB4-CB6
53	N	404	CDL	C72-C73-C74-C75
53	i	202	CDL	CA5-C11-C12-C13
53	M	607	CDL	C73-C74-C75-C76
45	M	602	3PE	O32-C31-O31-C3
45	Y	204	3PE	C29-C2A-C2B-C2C
46	d	202	PC1	C34-C35-C36-C37
45	Y	203	3PE	C34-C35-C36-C37
48	B	203	PLC	C'-C1'-C2'-C3'
48	B	203	PLC	C1'-C'-O2-C2
46	L	701	PC1	C27-C28-C29-C2A
45	N	401	3PE	C28-C29-C2A-C2B
45	q	201	3PE	C1-C2-C3-O31
46	H	402	PC1	C1-C2-C3-O31
46	M	606	PC1	C1-C2-C3-O31
46	h	202	PC1	C1-C2-C3-O31
48	O	403	PLC	C1-C2-C3-O3
48	Z	204	PLC	C1-C2-C3-O3
53	h	203	CDL	CB3-CB4-CB6-OB8
45	Y	202	3PE	C35-C36-C37-C38
46	Z	203	PC1	C37-C38-C39-C3A
45	M	605	3PE	C23-C24-C25-C26
46	H	403	PC1	C3B-C3C-C3D-C3E
45	N	403	3PE	C23-C24-C25-C26
53	h	203	CDL	C35-C36-C37-C38
45	Y	203	3PE	C38-C39-C3A-C3B
45	b	101	3PE	C38-C39-C3A-C3B
53	h	203	CDL	C33-C34-C35-C36
53	h	203	CDL	CA5-C11-C12-C13
45	N	402	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	I	204	PC1	C25-C26-C27-C28
48	J	203	PLC	C6B-C7B-C8B-C9B
45	N	403	3PE	C34-C35-C36-C37
45	Y	207	3PE	C28-C29-C2A-C2B
45	f	101	3PE	C2E-C2F-C2G-C2H
48	Z	204	PLC	CB-C1B-C2B-C3B
45	Y	204	3PE	C3-C2-O21-C21
45	A	201	3PE	C38-C39-C3A-C3B
45	M	603	3PE	C2A-C2B-C2C-C2D
45	m	201	3PE	C22-C23-C24-C25
45	I	203	3PE	C24-C25-C26-C27
45	Z	202	3PE	C3B-C3C-C3D-C3E
53	M	607	CDL	CB2-C1-CA2-OA2
48	L	703	PLC	O3P-C1-C2-O2
48	d	203	PLC	O3P-C1-C2-O2
45	N	401	3PE	C34-C35-C36-C37
48	Z	204	PLC	C1B-CB-O3-C3
53	X	201	CDL	C44-C45-C46-C47
53	i	202	CDL	C72-C73-C74-C75
45	I	203	3PE	C22-C23-C24-C25
45	M	602	3PE	C35-C36-C37-C38
45	M	603	3PE	C23-C24-C25-C26
46	L	701	PC1	C3E-C3F-C3G-C3H
46	g	201	PC1	C2F-C2G-C2H-C2I
48	g	202	PLC	C'-C1'-C2'-C3'
45	M	603	3PE	C3C-C3D-C3E-C3F
53	X	201	CDL	C71-C72-C73-C74
45	A	201	3PE	O21-C2-C3-O31
45	q	201	3PE	O21-C2-C3-O31
46	d	202	PC1	O21-C2-C3-O31
53	r	202	CDL	OA6-CA4-CA6-OA8
45	Z	201	3PE	C24-C25-C26-C27
53	i	202	CDL	C39-C40-C41-C42
46	H	402	PC1	C2F-C2G-C2H-C2I
45	b	102	3PE	C35-C36-C37-C38
46	Z	203	PC1	C26-C27-C28-C29
53	M	607	CDL	C42-C43-C44-C45
45	q	201	3PE	C2F-C2G-C2H-C2I
58	i	201	CHD	C20-C22-C23-C24
45	Y	207	3PE	C3E-C3F-C3G-C3H
53	N	404	CDL	C35-C36-C37-C38
45	Y	205	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
57	U	101	EHZ	O5-C16-C17-C18
57	U	101	EHZ	O5-C16-C17-C19
45	Z	201	3PE	C25-C26-C27-C28
46	M	606	PC1	C23-C24-C25-C26
45	Y	205	3PE	C26-C27-C28-C29
56	P	501	NDP	PN-O3-PA-O1A
46	B	202	PC1	C33-C34-C35-C36
53	N	404	CDL	C11-CA5-OA6-CA4
53	h	203	CDL	C38-C39-C40-C41
45	J	202	3PE	C2F-C2G-C2H-C2I
48	b	103	PLC	C4B-C5B-C6B-C7B
53	N	404	CDL	C60-C61-C62-C63
46	m	203	PC1	C21-C22-C23-C24
45	b	101	3PE	C29-C2A-C2B-C2C
53	i	202	CDL	C41-C42-C43-C44
45	M	602	3PE	O22-C21-O21-C2
53	r	202	CDL	C1-CB2-OB2-PB2
57	T	101	EHZ	S1-C10-C11-N1
45	K	101	3PE	C25-C26-C27-C28
45	L	702	3PE	C32-C33-C34-C35
45	N	402	3PE	C21-C22-C23-C24
45	H	401	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
46	L	701	PC1	O11-C1-C2-C3
48	O	403	PLC	O3P-C1-C2-C3
53	d	204	CDL	OA5-CA3-CA4-CA6
53	r	202	CDL	OB5-CB3-CB4-CB6
53	i	202	CDL	C51-CB5-OB6-CB4
46	B	202	PC1	C39-C3A-C3B-C3C
45	N	403	3PE	O21-C21-C22-C23
45	b	102	3PE	C37-C38-C39-C3A
45	M	603	3PE	C39-C3A-C3B-C3C
45	Y	203	3PE	C24-C25-C26-C27
53	r	202	CDL	C16-C17-C18-C19
45	q	201	3PE	C3F-C3G-C3H-C3I
48	J	203	PLC	C5B-C6B-C7B-C8B
45	K	101	3PE	C23-C24-C25-C26
45	Y	207	3PE	C2E-C2F-C2G-C2H
45	Z	201	3PE	C27-C28-C29-C2A
45	q	201	3PE	C3D-C3E-C3F-C3G
53	N	404	CDL	C31-C32-C33-C34
45	H	401	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	m	201	3PE	C29-C2A-C2B-C2C
45	J	202	3PE	C1-C2-C3-O31
45	L	702	3PE	C1-C2-C3-O31
45	M	603	3PE	C1-C2-C3-O31
45	Z	202	3PE	C1-C2-C3-O31
46	A	202	PC1	C1-C2-C3-O31
46	m	203	PC1	C1-C2-C3-O31
48	L	703	PLC	C1-C2-C3-O3
53	M	607	CDL	CA3-CA4-CA6-OA8
53	i	202	CDL	CA3-CA4-CA6-OA8
53	i	202	CDL	C36-C37-C38-C39
45	Y	203	3PE	C2C-C2D-C2E-C2F
45	Y	202	3PE	C33-C34-C35-C36
53	h	203	CDL	C31-C32-C33-C34
45	Y	205	3PE	C28-C29-C2A-C2B
45	b	101	3PE	C36-C37-C38-C39
53	N	404	CDL	C20-C21-C22-C23
46	h	202	PC1	C31-C32-C33-C34
45	I	203	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
45	Y	204	3PE	O11-C1-C2-O21
45	d	201	3PE	O11-C1-C2-O21
48	O	403	PLC	O3P-C1-C2-O2
53	i	202	CDL	OB5-CB3-CB4-OB6
45	L	702	3PE	C38-C39-C3A-C3B
46	A	203	PC1	C32-C33-C34-C35
48	O	403	PLC	C6B-C7B-C8B-C9B
53	X	201	CDL	C41-C42-C43-C44
45	J	201	3PE	C2-C1-O11-P
57	T	101	EHZ	O1-C7-C8-C9
45	d	201	3PE	C39-C3A-C3B-C3C
45	J	201	3PE	C32-C33-C34-C35
45	K	101	3PE	C37-C38-C39-C3A
46	H	403	PC1	C32-C33-C34-C35
46	L	701	PC1	C26-C27-C28-C29
45	Y	203	3PE	C28-C29-C2A-C2B
46	L	701	PC1	C23-C24-C25-C26
45	M	603	3PE	O21-C2-C3-O31
45	N	403	3PE	O21-C2-C3-O31
45	Z	202	3PE	O21-C2-C3-O31
45	b	102	3PE	O21-C2-C3-O31
46	A	202	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
48	Z	204	PLC	O2-C2-C3-O3
48	g	202	PLC	O2-C2-C3-O3
53	M	607	CDL	OA6-CA4-CA6-OA8
48	L	703	PLC	C6B-C7B-C8B-C9B
54	O	401	DGT	O4'-C4'-C5'-O5'
56	P	501	NDP	C3B-C4B-C5B-O5B
45	J	201	3PE	C35-C36-C37-C38
45	Y	202	3PE	C3A-C3B-C3C-C3D
45	Y	203	3PE	C3F-C3G-C3H-C3I
45	b	101	3PE	C37-C38-C39-C3A
45	J	201	3PE	C36-C37-C38-C39
45	b	101	3PE	C2A-C2B-C2C-C2D
45	H	401	3PE	C36-C37-C38-C39
53	M	607	CDL	C75-C76-C77-C78
53	i	202	CDL	CA7-C31-C32-C33
53	M	607	CDL	C78-C79-C80-C81
56	P	501	NDP	PN-O3-PA-O5B
46	M	606	PC1	C32-C33-C34-C35
45	d	201	3PE	C22-C23-C24-C25
53	M	607	CDL	C62-C63-C64-C65
57	U	101	EHZ	C6-C7-C8-C9
53	M	607	CDL	C35-C36-C37-C38
48	J	203	PLC	C1B-C2B-C3B-C4B
45	Z	201	3PE	C2F-C2G-C2H-C2I
45	Y	204	3PE	C36-C37-C38-C39
46	H	403	PC1	C3D-C3E-C3F-C3G
45	Y	204	3PE	C28-C29-C2A-C2B
53	d	204	CDL	C11-C12-C13-C14
53	d	204	CDL	CB2-C1-CA2-OA2
45	b	101	3PE	C2C-C2D-C2E-C2F
48	Z	204	PLC	OB-CB-O3-C3
45	b	101	3PE	O21-C21-C22-C23
46	H	402	PC1	C32-C31-O31-C3
45	Y	201	3PE	O11-C1-C2-C3
45	Y	205	3PE	O11-C1-C2-C3
45	Z	201	3PE	O11-C1-C2-C3
45	d	201	3PE	O11-C1-C2-C3
46	B	202	PC1	O11-C1-C2-C3
46	q	202	PC1	O11-C1-C2-C3
48	B	203	PLC	O3P-C1-C2-C3
48	d	203	PLC	O3P-C1-C2-C3
53	h	203	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	C23-C24-C25-C26
46	Z	203	PC1	C34-C35-C36-C37
45	I	203	3PE	C28-C29-C2A-C2B
45	M	603	3PE	C36-C37-C38-C39
48	L	703	PLC	C2B-C3B-C4B-C5B
53	M	607	CDL	C17-C18-C19-C20
53	d	204	CDL	C76-C77-C78-C79
46	m	203	PC1	C39-C3A-C3B-C3C
46	Z	203	PC1	O22-C21-O21-C2
48	B	203	PLC	O'-C'-O2-C2
53	N	404	CDL	OA7-CA5-OA6-CA4
46	g	201	PC1	C2C-C2D-C2E-C2F
45	N	403	3PE	C2B-C2C-C2D-C2E
45	N	401	3PE	C3-C2-O21-C21
53	N	404	CDL	CA6-CA4-OA6-CA5
53	X	201	CDL	CA5-C11-C12-C13
45	b	101	3PE	C27-C28-C29-C2A
53	i	202	CDL	OB7-CB5-OB6-CB4
45	Y	201	3PE	O11-C1-C2-O21
45	Y	205	3PE	O11-C1-C2-O21
45	Z	201	3PE	O11-C1-C2-O21
45	b	101	3PE	O11-C1-C2-O21
45	f	101	3PE	O11-C1-C2-O21
45	r	201	3PE	O11-C1-C2-O21
46	I	204	PC1	O11-C1-C2-O21
48	Y	208	PLC	O3P-C1-C2-O2
53	N	404	CDL	C74-C75-C76-C77
45	N	402	3PE	C1-C2-C3-O31
45	b	102	3PE	C1-C2-C3-O31
45	m	202	3PE	C1-C2-C3-O31
48	b	103	PLC	C1-C2-C3-O3
48	g	202	PLC	C1-C2-C3-O3
45	K	101	3PE	C12-C11-O13-P
45	N	402	3PE	C12-C11-O13-P
45	Y	202	3PE	C12-C11-O13-P
45	Y	204	3PE	C12-C11-O13-P
45	Y	205	3PE	C12-C11-O13-P
45	Y	206	3PE	C12-C11-O13-P
45	h	201	3PE	C12-C11-O13-P
45	m	201	3PE	C12-C11-O13-P
45	m	202	3PE	C12-C11-O13-P
48	Y	208	PLC	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
53	i	202	CDL	CB7-C71-C72-C73
45	L	702	3PE	O21-C2-C3-O31
45	Y	207	3PE	O21-C2-C3-O31
45	b	101	3PE	O21-C2-C3-O31
45	m	202	3PE	O21-C2-C3-O31
48	L	703	PLC	O2-C2-C3-O3
45	Z	202	3PE	C26-C27-C28-C29
45	J	201	3PE	C33-C34-C35-C36
45	Y	206	3PE	C22-C23-C24-C25
45	b	102	3PE	C3C-C3D-C3E-C3F
46	H	402	PC1	C2D-C2E-C2F-C2G
45	b	102	3PE	C34-C35-C36-C37
53	r	202	CDL	C12-C13-C14-C15
54	O	401	DGT	C3'-C4'-C5'-O5'
56	P	501	NDP	O4B-C4B-C5B-O5B
45	I	203	3PE	C2-C1-O11-P
45	N	401	3PE	C2-C1-O11-P
48	Y	208	PLC	O4P-C4-C5-N
48	b	103	PLC	O4P-C4-C5-N
45	J	201	3PE	C2-C3-O31-C31
45	N	402	3PE	C32-C33-C34-C35
46	g	201	PC1	C22-C23-C24-C25
53	r	202	CDL	CA7-C31-C32-C33
46	H	402	PC1	O32-C31-O31-C3
53	N	404	CDL	C56-C57-C58-C59
59	o	201	MYR	C4-C5-C6-C7
45	m	201	3PE	C26-C27-C28-C29
45	Y	204	3PE	C2B-C2C-C2D-C2E
45	N	403	3PE	C38-C39-C3A-C3B
45	h	201	3PE	C26-C27-C28-C29
53	r	202	CDL	CB7-C71-C72-C73
53	h	203	CDL	C37-C38-C39-C40
45	J	201	3PE	O11-C1-C2-C3
45	f	101	3PE	O11-C1-C2-C3
46	I	204	PC1	O11-C1-C2-C3
48	J	203	PLC	O3P-C1-C2-C3
48	L	703	PLC	O3P-C1-C2-C3
48	Y	208	PLC	O3P-C1-C2-C3
45	Y	203	3PE	C35-C36-C37-C38
57	T	101	EHZ	C18-C17-C20-O6
57	T	101	EHZ	C19-C17-C20-O6
46	g	201	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	Z	203	PC1	C23-C24-C25-C26
46	H	402	PC1	C26-C27-C28-C29
48	d	203	PLC	C2-C1-O3P-P
57	U	101	EHZ	C11-C10-S1-C9
48	b	103	PLC	C1'-C2'-C3'-C4'
48	Z	204	PLC	C8B-C9B-CAA-CBA
45	J	201	3PE	O11-C1-C2-O21
45	m	201	3PE	O11-C1-C2-O21
46	B	202	PC1	O11-C1-C2-O21
46	L	701	PC1	O11-C1-C2-O21
48	B	203	PLC	O3P-C1-C2-O2
53	X	201	CDL	OA5-CA3-CA4-OA6
53	d	204	CDL	OA5-CA3-CA4-OA6
53	h	203	CDL	OA5-CA3-CA4-OA6
53	i	202	CDL	C54-C55-C56-C57
46	H	402	PC1	O21-C21-C22-C23
53	X	201	CDL	C63-C64-C65-C66
46	H	402	PC1	C35-C36-C37-C38
46	I	204	PC1	C22-C23-C24-C25
45	J	202	3PE	O21-C2-C3-O31
48	b	103	PLC	O2-C2-C3-O3
53	h	203	CDL	OB6-CB4-CB6-OB8
53	i	202	CDL	OA6-CA4-CA6-OA8
45	q	201	3PE	C23-C24-C25-C26
48	Y	208	PLC	C'-C1'-C2'-C3'
45	A	201	3PE	C1-C2-C3-O31
45	Y	207	3PE	C1-C2-C3-O31
45	b	101	3PE	C1-C2-C3-O31
46	L	701	PC1	C1-C2-C3-O31
46	d	202	PC1	C1-C2-C3-O31
53	r	202	CDL	CA3-CA4-CA6-OA8
45	I	203	3PE	C2F-C2G-C2H-C2I
53	M	607	CDL	C44-C45-C46-C47
46	h	202	PC1	C2B-C2C-C2D-C2E
45	b	101	3PE	C31-C32-C33-C34
46	h	202	PC1	C22-C23-C24-C25
46	H	403	PC1	C31-C32-C33-C34
46	I	204	PC1	C28-C29-C2A-C2B
53	X	201	CDL	C31-C32-C33-C34
45	H	401	3PE	C11-O13-P-O14
45	I	203	3PE	C11-O13-P-O12
45	J	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	J	201	3PE	O13-C11-C12-N
45	K	101	3PE	C11-O13-P-O11
45	K	101	3PE	C11-O13-P-O14
45	L	702	3PE	O13-C11-C12-N
45	M	603	3PE	C11-O13-P-O14
45	M	603	3PE	O13-C11-C12-N
45	M	604	3PE	O13-C11-C12-N
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13
45	N	402	3PE	C1-O11-P-O14
45	Y	202	3PE	C11-O13-P-O12
45	Y	204	3PE	C1-O11-P-O12
45	Y	207	3PE	C1-O11-P-O13
45	Y	207	3PE	C1-O11-P-O14
45	Y	207	3PE	C11-O13-P-O14
45	Y	207	3PE	O13-C11-C12-N
45	Z	202	3PE	O13-C11-C12-N
45	b	101	3PE	C1-O11-P-O12
45	b	101	3PE	O13-C11-C12-N
45	b	102	3PE	O13-C11-C12-N
45	f	101	3PE	C1-O11-P-O14
45	h	201	3PE	C1-O11-P-O13
45	m	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O14
45	m	202	3PE	C1-O11-P-O12
46	A	202	PC1	C1-O11-P-O14
46	A	202	PC1	C1-O11-P-O13
46	A	203	PC1	C11-C12-N-C15
46	B	202	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	I	204	PC1	C11-O13-P-O11
46	M	606	PC1	C1-O11-P-O13
46	Z	203	PC1	C1-O11-P-O14
46	Z	203	PC1	C1-O11-P-O13
46	d	202	PC1	C11-O13-P-O14
46	d	202	PC1	C11-O13-P-O11
46	g	201	PC1	C11-O13-P-O14
46	g	201	PC1	C11-O13-P-O11
46	m	203	PC1	C1-O11-P-O12
46	q	202	PC1	C1-O11-P-O14
48	B	203	PLC	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
48	Z	204	PLC	C1-O3P-P-O4P
48	b	103	PLC	C4-O4P-P-O3P
48	d	203	PLC	C1-O3P-P-O4P
48	d	203	PLC	C4-O4P-P-O1P
53	N	404	CDL	CB2-OB2-PB2-OB4
53	N	404	CDL	CB2-OB2-PB2-OB5
53	N	404	CDL	CB3-OB5-PB2-OB2
53	N	404	CDL	CB3-OB5-PB2-OB3
53	N	404	CDL	CB3-OB5-PB2-OB4
53	X	201	CDL	CA2-OA2-PA1-OA3
53	X	201	CDL	CB2-OB2-PB2-OB3
53	d	204	CDL	CA3-OA5-PA1-OA3
53	d	204	CDL	CB3-OB5-PB2-OB2
53	d	204	CDL	CB3-OB5-PB2-OB4
53	h	203	CDL	CA2-OA2-PA1-OA5
53	r	202	CDL	CB2-OB2-PB2-OB3
54	O	401	DGT	C5'-O5'-PA-O3A
57	U	101	EHZ	O5-C16-C17-C20
45	N	401	3PE	C38-C39-C3A-C3B
46	q	202	PC1	O21-C21-C22-C23
48	O	403	PLC	C2-C1-O3P-P
50	F	502	FMN	C4'-C5'-O5'-P
53	d	204	CDL	C1-CB2-OB2-PB2
46	Z	203	PC1	C29-C2A-C2B-C2C
45	Y	203	3PE	C22-C23-C24-C25
45	f	101	3PE	C23-C24-C25-C26
45	b	102	3PE	C2B-C2C-C2D-C2E
45	N	403	3PE	C22-C23-C24-C25
45	Y	202	3PE	C22-C23-C24-C25
48	L	703	PLC	CB-C1B-C2B-C3B
53	i	202	CDL	C52-C53-C54-C55
45	d	201	3PE	C34-C35-C36-C37
45	Y	202	3PE	C3-C2-O21-C21
45	d	201	3PE	C1-C2-O21-C21
45	M	602	3PE	C34-C35-C36-C37
45	m	201	3PE	O11-C1-C2-C3
46	g	201	PC1	C25-C26-C27-C28
48	J	203	PLC	C1'-C2'-C3'-C4'
46	A	203	PC1	O11-C1-C2-O21
48	L	703	PLC	C1B-C2B-C3B-C4B
45	Y	203	3PE	C23-C24-C25-C26
53	h	203	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C27-C28-C29-C2A
46	L	701	PC1	C36-C37-C38-C39
46	H	403	PC1	C2-C1-O11-P
45	N	402	3PE	O21-C2-C3-O31
46	h	202	PC1	O21-C2-C3-O31
46	q	202	PC1	O21-C2-C3-O31
53	d	204	CDL	OB6-CB4-CB6-OB8
48	L	703	PLC	C4B-C5B-C6B-C7B
45	r	201	3PE	C36-C37-C38-C39
45	A	201	3PE	C23-C24-C25-C26
59	o	201	MYR	C10-C11-C12-C13
54	O	401	DGT	PA-O3A-PB-O1B
45	b	101	3PE	C2B-C2C-C2D-C2E
53	M	607	CDL	C59-C60-C61-C62
56	P	501	NDP	C3D-C4D-C5D-O5D
45	Z	202	3PE	C24-C25-C26-C27
46	A	203	PC1	C11-C12-N-C13
46	H	402	PC1	C11-C12-N-C13
53	d	204	CDL	C31-C32-C33-C34
53	X	201	CDL	CB2-C1-CA2-OA2
57	T	101	EHZ	C5-C6-C7-O1
53	r	202	CDL	C18-C19-C20-C21
48	g	202	PLC	C2-C1-O3P-P
53	h	203	CDL	C32-C33-C34-C35
45	Y	204	3PE	C3D-C3E-C3F-C3G
53	M	607	CDL	C74-C75-C76-C77
45	M	605	3PE	O21-C21-C22-C23
53	r	202	CDL	C17-C18-C19-C20
59	o	201	MYR	C9-C10-C11-C12
46	d	202	PC1	C23-C24-C25-C26
45	q	201	3PE	C2A-C2B-C2C-C2D
45	h	201	3PE	C23-C24-C25-C26
53	N	404	CDL	C14-C15-C16-C17
53	M	607	CDL	C34-C35-C36-C37
45	L	702	3PE	C3F-C3G-C3H-C3I
46	B	202	PC1	C3D-C3E-C3F-C3G
45	h	201	3PE	C32-C33-C34-C35
45	Z	201	3PE	C2A-C2B-C2C-C2D
46	I	204	PC1	C26-C27-C28-C29
46	d	202	PC1	C3B-C3C-C3D-C3E
46	A	203	PC1	C11-C12-N-C14
48	L	703	PLC	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C22-C23-C24-C25
45	Y	205	3PE	C2C-C2D-C2E-C2F
45	d	201	3PE	C3-C2-O21-C21
46	H	403	PC1	C3-C2-O21-C21
53	X	201	CDL	CA3-CA4-OA6-CA5
46	I	204	PC1	C33-C34-C35-C36
45	b	101	3PE	C3A-C3B-C3C-C3D
46	M	606	PC1	C34-C35-C36-C37
48	b	103	PLC	C2-C3-O3-CB
45	N	403	3PE	C35-C36-C37-C38
53	M	607	CDL	C40-C41-C42-C43
46	H	402	PC1	C11-C12-N-C15
45	h	201	3PE	C22-C23-C24-C25
53	N	404	CDL	C24-C25-C26-C27
45	M	602	3PE	C37-C38-C39-C3A
48	O	403	PLC	C1B-CB-O3-C3
46	g	201	PC1	C34-C35-C36-C37
45	b	101	3PE	C39-C3A-C3B-C3C
45	M	604	3PE	O21-C2-C3-O31
45	N	403	3PE	C26-C27-C28-C29
45	Z	202	3PE	C27-C28-C29-C2A
53	X	201	CDL	C36-C37-C38-C39
46	H	402	PC1	C11-C12-N-C14
45	N	401	3PE	C37-C38-C39-C3A
58	i	201	CHD	C22-C23-C24-O26
45	K	101	3PE	C36-C37-C38-C39
46	L	701	PC1	C37-C38-C39-C3A
45	L	702	3PE	C36-C37-C38-C39
48	O	403	PLC	OB-CB-O3-C3
46	B	202	PC1	C28-C29-C2A-C2B
53	h	203	CDL	C56-C57-C58-C59
46	B	202	PC1	C3B-C3C-C3D-C3E
45	d	201	3PE	C3A-C3B-C3C-C3D
53	X	201	CDL	C62-C63-C64-C65
45	d	201	3PE	C2F-C2G-C2H-C2I
58	i	201	CHD	C22-C23-C24-O25
45	m	202	3PE	C2-C1-O11-P
46	q	202	PC1	O22-C21-C22-C23
46	L	701	PC1	O22-C21-O21-C2
45	N	403	3PE	O22-C21-C22-C23
45	N	401	3PE	C33-C34-C35-C36
46	I	204	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
57	U	101	EHZ	O3-C12-C13-C14
46	Z	203	PC1	C3B-C3C-C3D-C3E
53	N	404	CDL	C57-C58-C59-C60
45	A	201	3PE	O11-C1-C2-O21
45	Y	206	3PE	O11-C1-C2-O21
45	Y	203	3PE	C39-C3A-C3B-C3C
48	Y	208	PLC	C7'-C8'-C9'-CA'
53	h	203	CDL	C63-C64-C65-C66
45	M	604	3PE	C31-C32-C33-C34
45	d	201	3PE	C26-C27-C28-C29
45	K	101	3PE	C38-C39-C3A-C3B
45	I	203	3PE	O11-C1-C2-C3
46	A	203	PC1	O11-C1-C2-C3
45	f	101	3PE	C2D-C2E-C2F-C2G
45	Y	205	3PE	C21-C22-C23-C24
45	N	402	3PE	O31-C31-C32-C33
53	M	607	CDL	C12-C11-CA5-OA6
46	Z	203	PC1	C27-C28-C29-C2A
48	b	103	PLC	C2B-C3B-C4B-C5B
53	N	404	CDL	C75-C76-C77-C78
56	P	501	NDP	O4D-C4D-C5D-O5D
45	Z	202	3PE	C33-C34-C35-C36
48	d	203	PLC	C2B-C1B-CB-O3
45	K	101	3PE	C3D-C3E-C3F-C3G
46	M	606	PC1	C24-C25-C26-C27
45	L	702	3PE	C34-C35-C36-C37
46	g	201	PC1	C27-C28-C29-C2A
53	i	202	CDL	C56-C57-C58-C59
45	N	402	3PE	O21-C21-C22-C23
48	J	203	PLC	C4-C5-N-C8
45	L	702	3PE	C1-C2-O21-C21
45	L	702	3PE	C3-C2-O21-C21
46	H	403	PC1	C1-C2-O21-C21
53	N	404	CDL	C34-C35-C36-C37
46	M	606	PC1	C33-C34-C35-C36
45	q	201	3PE	C2B-C2C-C2D-C2E
45	Y	202	3PE	C3E-C3F-C3G-C3H
45	f	101	3PE	C26-C27-C28-C29
53	i	202	CDL	C35-C36-C37-C38
45	m	201	3PE	C28-C29-C2A-C2B
45	M	605	3PE	C2-C1-O11-P
45	Y	202	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
53	h	203	CDL	OB5-CB3-CB4-OB6
45	q	201	3PE	C39-C3A-C3B-C3C
48	Y	208	PLC	C2'-C3'-C4'-C5'
57	U	101	EHZ	N1-C12-C13-C14
45	m	201	3PE	C2B-C2C-C2D-C2E
53	M	607	CDL	C24-C25-C26-C27
57	U	101	EHZ	C15-C16-C17-C18
48	B	203	PLC	OB-CB-O3-C3
45	H	401	3PE	C38-C39-C3A-C3B
53	X	201	CDL	OA6-CA4-CA6-OA8
53	i	202	CDL	OB6-CB4-CB6-OB8
53	X	201	CDL	C72-C71-CB7-OB8
53	h	203	CDL	OB7-CB5-OB6-CB4
45	Y	204	3PE	C2A-C2B-C2C-C2D
45	A	201	3PE	O11-C1-C2-C3
53	M	607	CDL	C16-C17-C18-C19
46	A	202	PC1	C11-C12-N-C14
46	I	204	PC1	C11-C12-N-C13
46	I	204	PC1	C11-C12-N-C14
53	N	404	CDL	C18-C19-C20-C21
53	i	202	CDL	C12-C11-CA5-OA6
53	M	607	CDL	C15-C16-C17-C18
45	Y	207	3PE	C2F-C2G-C2H-C2I
46	h	202	PC1	C23-C24-C25-C26
45	J	202	3PE	O31-C31-C32-C33
53	N	404	CDL	C36-C37-C38-C39
46	L	701	PC1	C22-C21-O21-C2
48	O	403	PLC	O'-C'-O2-C2
45	f	101	3PE	C33-C34-C35-C36
45	q	201	3PE	C2C-C2D-C2E-C2F
53	h	203	CDL	C54-C55-C56-C57
45	q	201	3PE	C37-C38-C39-C3A
53	h	203	CDL	C52-C51-CB5-OB6
48	B	203	PLC	C1B-CB-O3-C3
45	N	403	3PE	C21-C22-C23-C24
53	X	201	CDL	C84-C85-C86-C87
45	L	702	3PE	O21-C21-C22-C23
45	Y	201	3PE	O31-C31-C32-C33
45	Y	205	3PE	C27-C28-C29-C2A
45	m	201	3PE	C2A-C2B-C2C-C2D
46	A	202	PC1	C11-C12-N-C13
45	b	101	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	b	101	3PE	O31-C31-C32-C33
45	f	101	3PE	O21-C21-C22-C23
45	M	604	3PE	O11-C1-C2-O21
45	b	102	3PE	C36-C37-C38-C39
45	f	101	3PE	C2A-C2B-C2C-C2D
53	X	201	CDL	C60-C61-C62-C63
45	Y	205	3PE	C2B-C2C-C2D-C2E
53	h	203	CDL	C51-CB5-OB6-CB4
48	J	203	PLC	C3B-C4B-C5B-C6B
53	i	202	CDL	C11-C12-C13-C14
45	Y	205	3PE	C36-C37-C38-C39
45	Y	205	3PE	C2-C1-O11-P
53	h	203	CDL	C1-CB2-OB2-PB2
45	m	201	3PE	O21-C21-C22-C23
48	Y	208	PLC	O2-C'-C1'-C2'
53	X	201	CDL	C52-C51-CB5-OB6
53	d	204	CDL	C72-C71-CB7-OB8
45	N	402	3PE	C29-C2A-C2B-C2C
53	X	201	CDL	C74-C75-C76-C77
45	N	403	3PE	C1-C2-C3-O31
48	Y	208	PLC	C1-C2-C3-O3
46	I	204	PC1	C11-C12-N-C15
45	J	202	3PE	C23-C24-C25-C26
53	N	404	CDL	OA6-CA4-CA6-OA8
53	r	202	CDL	OB6-CB4-CB6-OB8
45	Y	207	3PE	C3F-C3G-C3H-C3I
45	Y	202	3PE	C32-C33-C34-C35
48	g	202	PLC	C2'-C3'-C4'-C5'
45	A	201	3PE	O31-C31-C32-C33
45	Y	201	3PE	O21-C21-C22-C23
45	Y	205	3PE	O31-C31-C32-C33
53	X	201	CDL	CA7-C31-C32-C33
53	M	607	CDL	C41-C42-C43-C44
46	h	202	PC1	C27-C28-C29-C2A
53	X	201	CDL	C73-C74-C75-C76
45	M	603	3PE	C27-C28-C29-C2A
45	f	101	3PE	C35-C36-C37-C38
46	L	701	PC1	C3A-C3B-C3C-C3D
46	A	202	PC1	C11-C12-N-C15
46	m	203	PC1	C23-C24-C25-C26
45	M	603	3PE	C22-C23-C24-C25
45	Y	203	3PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
53	X	201	CDL	C75-C76-C77-C78
46	A	202	PC1	O21-C21-C22-C23
45	Y	204	3PE	C3B-C3C-C3D-C3E
53	N	404	CDL	CB4-CB3-OB5-PB2
53	h	203	CDL	C52-C51-CB5-OB7
48	J	203	PLC	O2-C'-C1'-C2'
45	N	403	3PE	C32-C33-C34-C35
45	Y	205	3PE	C39-C3A-C3B-C3C
45	L	702	3PE	O22-C21-C22-C23
53	X	201	CDL	C72-C71-CB7-OB9
45	M	605	3PE	C2D-C2E-C2F-C2G
45	b	101	3PE	O32-C31-C32-C33
45	f	101	3PE	O22-C21-C22-C23
53	d	204	CDL	C72-C71-CB7-OB9
48	b	103	PLC	C7'-C8'-C9'-CA'
45	H	401	3PE	C3C-C3D-C3E-C3F
48	O	403	PLC	C1'-C'-O2-C2
48	Z	204	PLC	C2B-C1B-CB-O3
45	q	201	3PE	C3E-C3F-C3G-C3H
53	h	203	CDL	C55-C56-C57-C58
45	Y	201	3PE	O32-C31-C32-C33
45	Y	205	3PE	O32-C31-C32-C33
45	m	201	3PE	O22-C21-C22-C23
46	A	202	PC1	O22-C21-O21-C2
53	X	201	CDL	C52-C51-CB5-OB7
45	M	602	3PE	O31-C31-C32-C33
45	Z	202	3PE	C37-C38-C39-C3A
45	d	201	3PE	C23-C24-C25-C26
53	i	202	CDL	C12-C11-CA5-OA7
45	Y	205	3PE	C24-C25-C26-C27
45	H	401	3PE	C39-C3A-C3B-C3C
45	A	201	3PE	O32-C31-C32-C33
45	J	202	3PE	C2B-C2C-C2D-C2E
45	Z	202	3PE	O31-C31-C32-C33
45	Y	206	3PE	O11-C1-C2-C3
53	r	202	CDL	C72-C73-C74-C75
45	J	201	3PE	O21-C21-C22-C23
45	m	201	3PE	C21-C22-C23-C24
46	d	202	PC1	C38-C39-C3A-C3B
46	B	202	PC1	C2A-C2B-C2C-C2D
53	X	201	CDL	C56-C57-C58-C59
45	I	203	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
57	T	101	EHZ	C5-C6-C7-C8
46	A	202	PC1	O22-C21-C22-C23
45	d	201	3PE	C21-C22-C23-C24
45	b	101	3PE	C35-C36-C37-C38
45	M	604	3PE	C34-C35-C36-C37
45	d	201	3PE	O21-C21-C22-C23
46	B	202	PC1	O21-C21-C22-C23
45	Y	201	3PE	O22-C21-C22-C23
48	Y	208	PLC	O'-C'-C1'-C2'

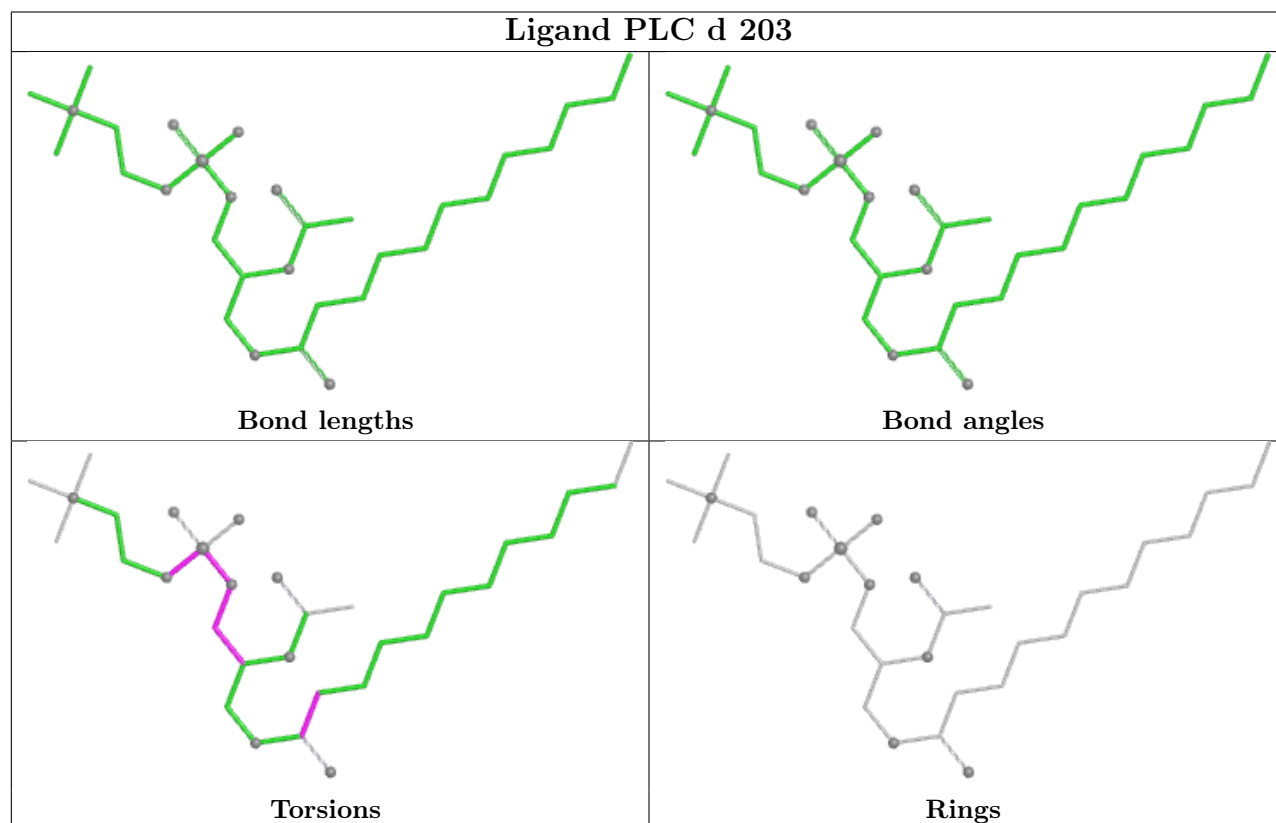
There are no ring outliers.

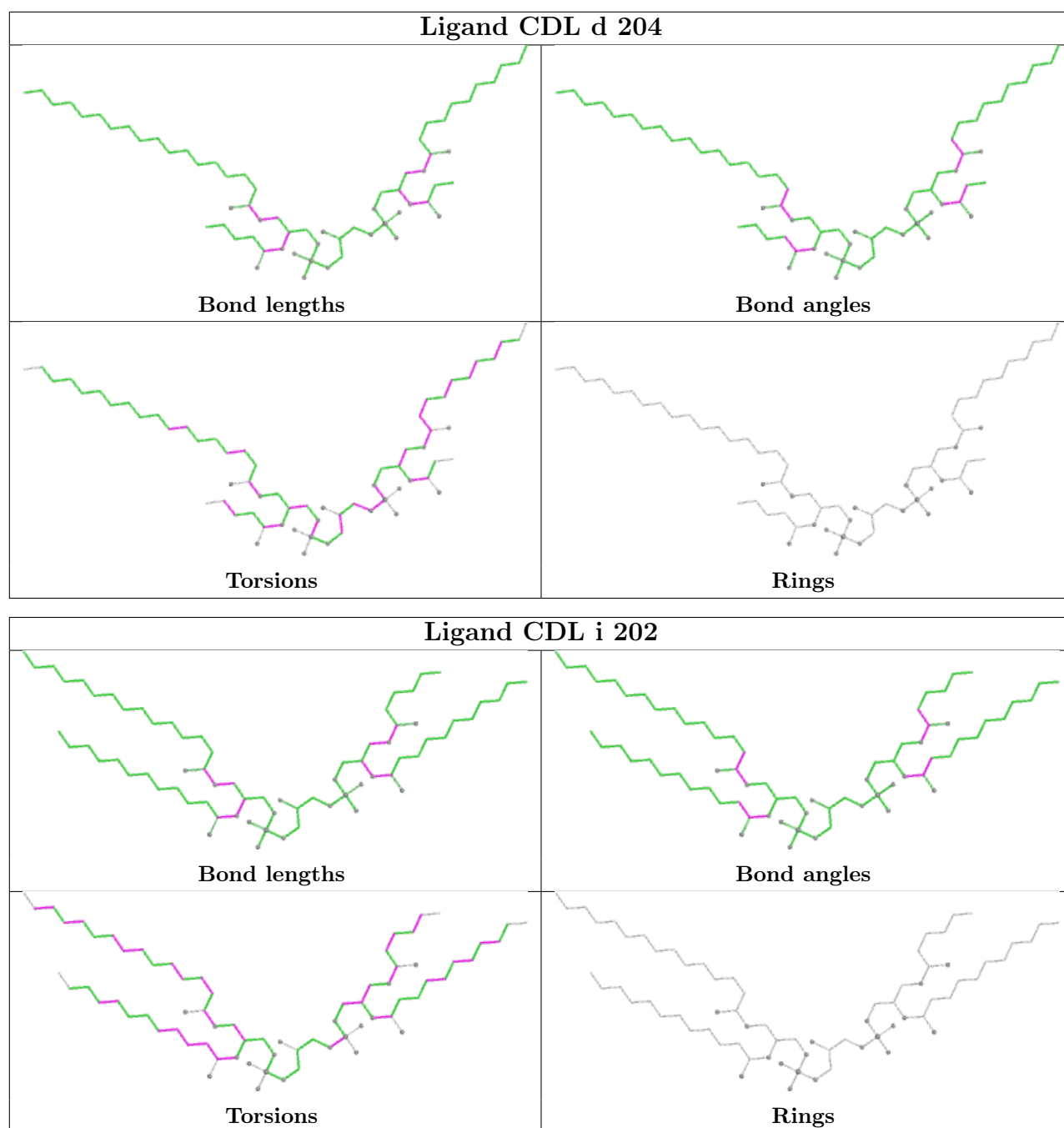
23 monomers are involved in 28 short contacts:

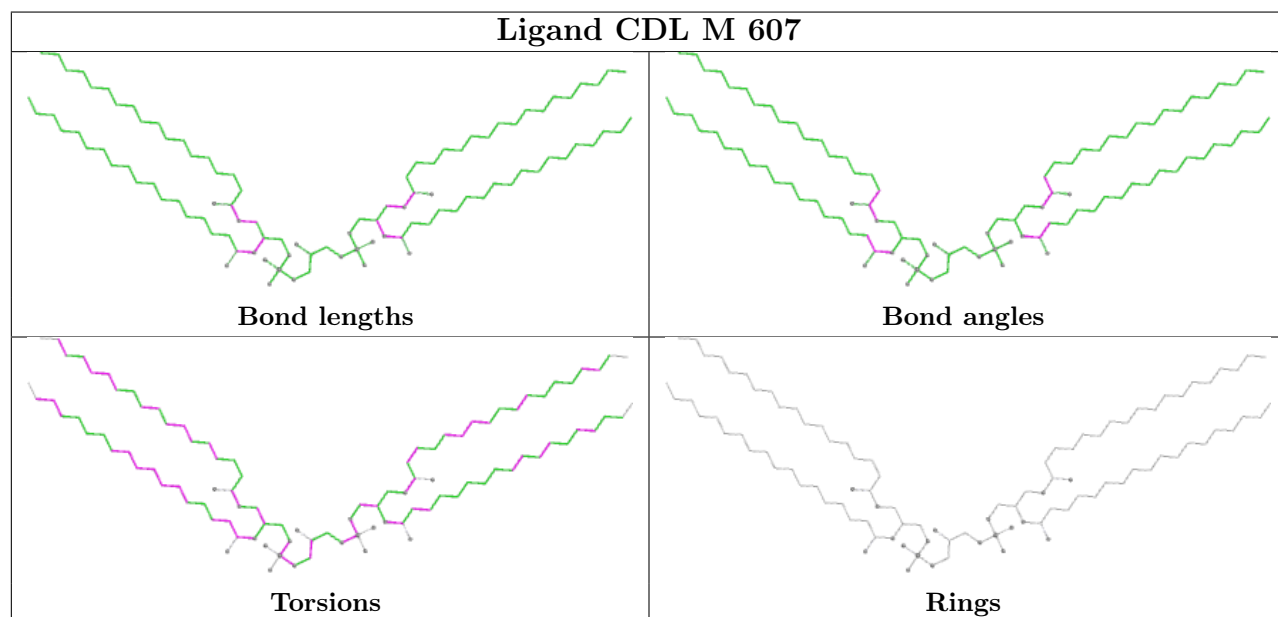
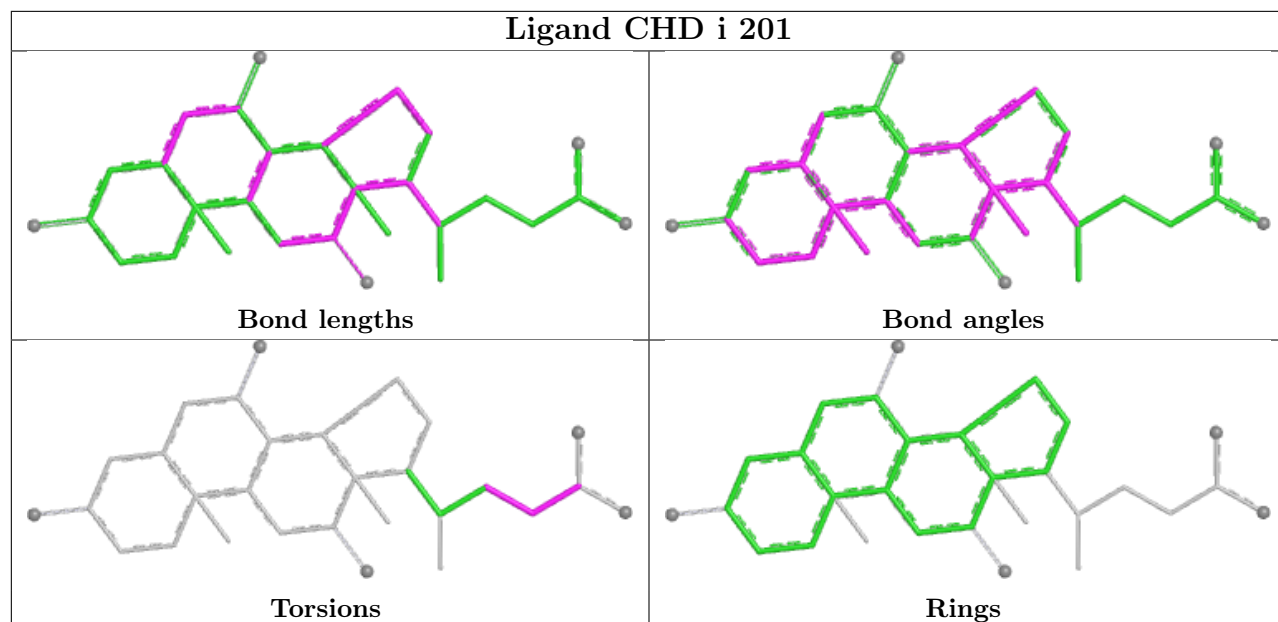
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	i	201	CHD	4	0
53	M	607	CDL	3	0
50	F	502	FMN	1	0
45	f	101	3PE	1	0
45	Y	203	3PE	1	0
45	Z	202	3PE	1	0
45	Y	207	3PE	1	0
56	P	501	NDP	2	0
57	T	101	EHZ	1	0
46	L	701	PC1	1	0
53	r	202	CDL	1	0
46	g	201	PC1	1	0
45	N	402	3PE	1	0
45	d	201	3PE	1	0
46	I	204	PC1	1	0
53	X	201	CDL	3	0
47	I	201	SF4	1	0
45	Y	202	3PE	1	0
54	O	401	DGT	2	0
46	H	402	PC1	2	0
45	Y	205	3PE	1	0
45	L	702	3PE	1	0
45	M	602	3PE	1	0

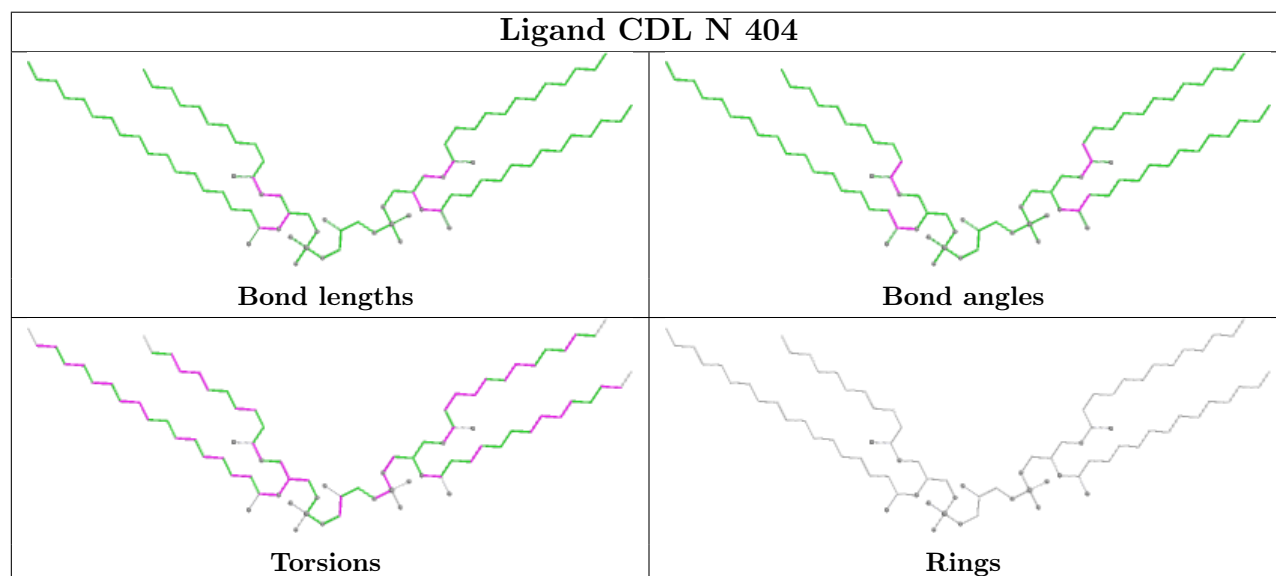
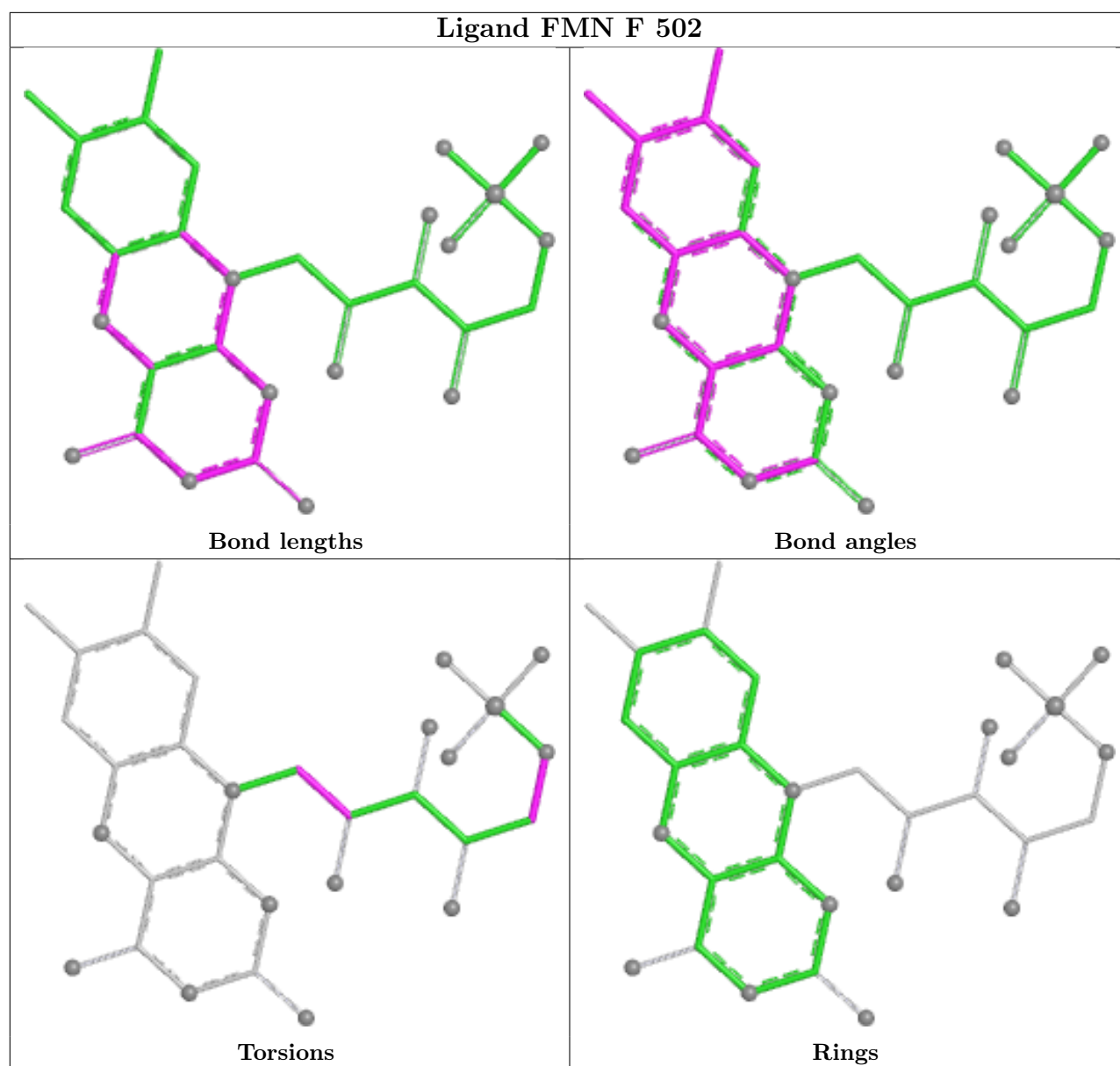
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

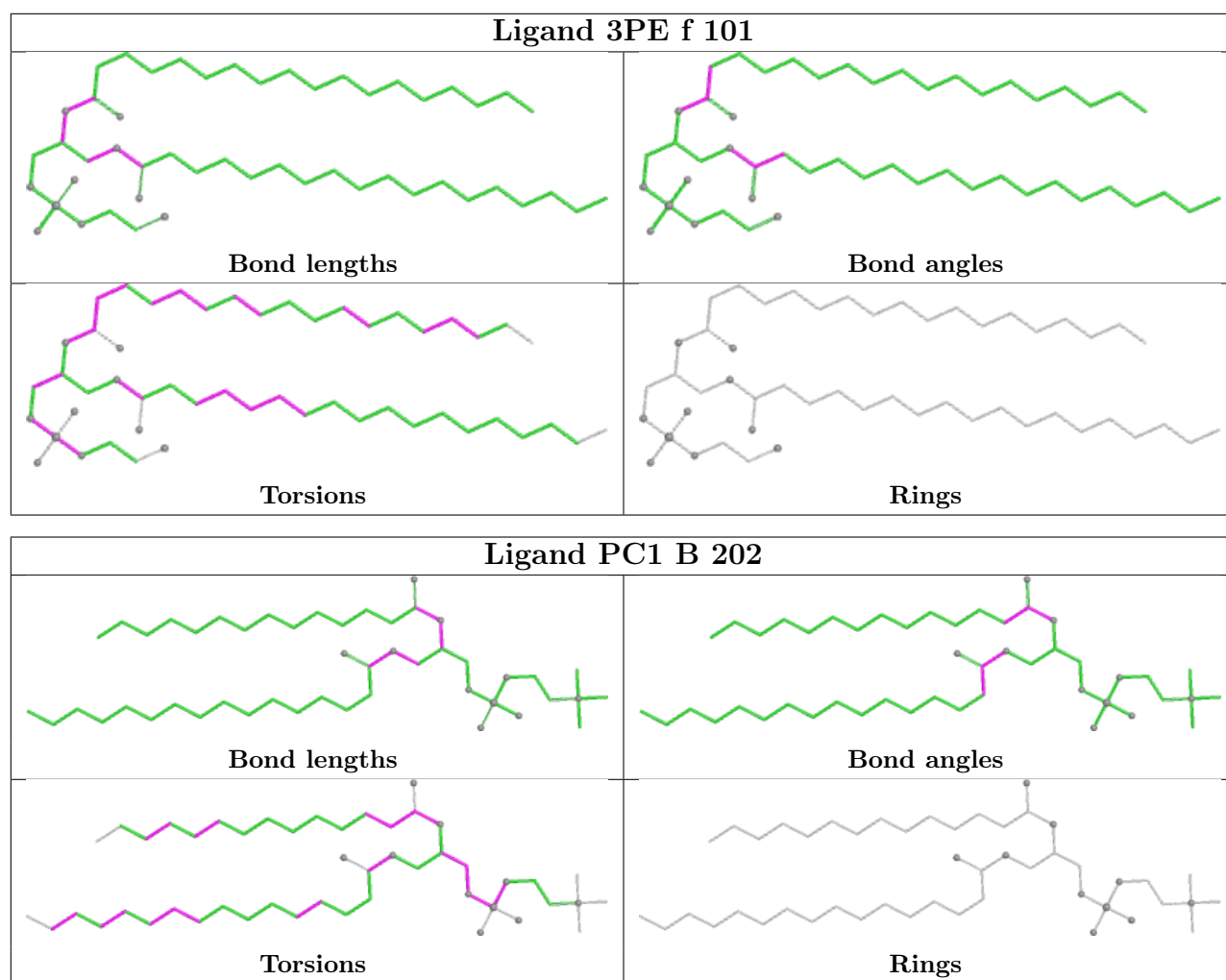
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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



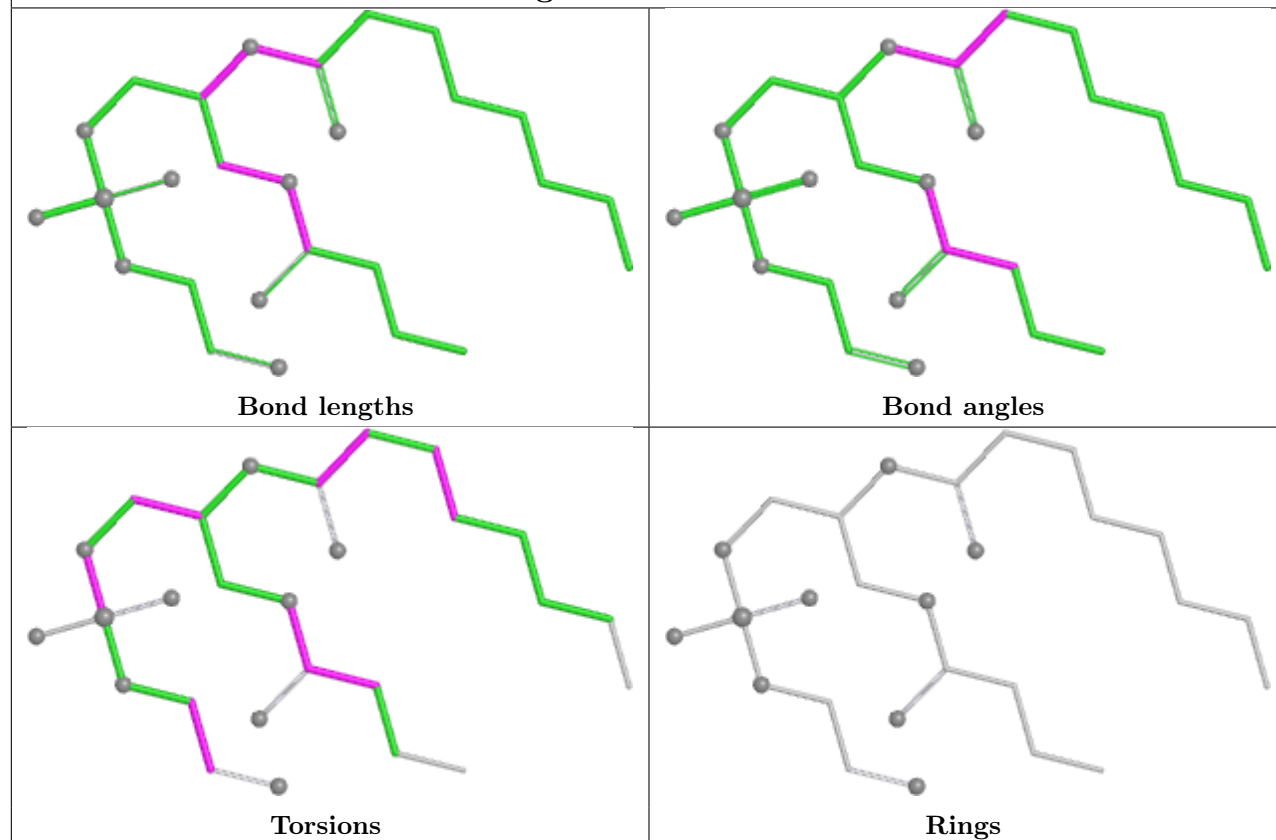




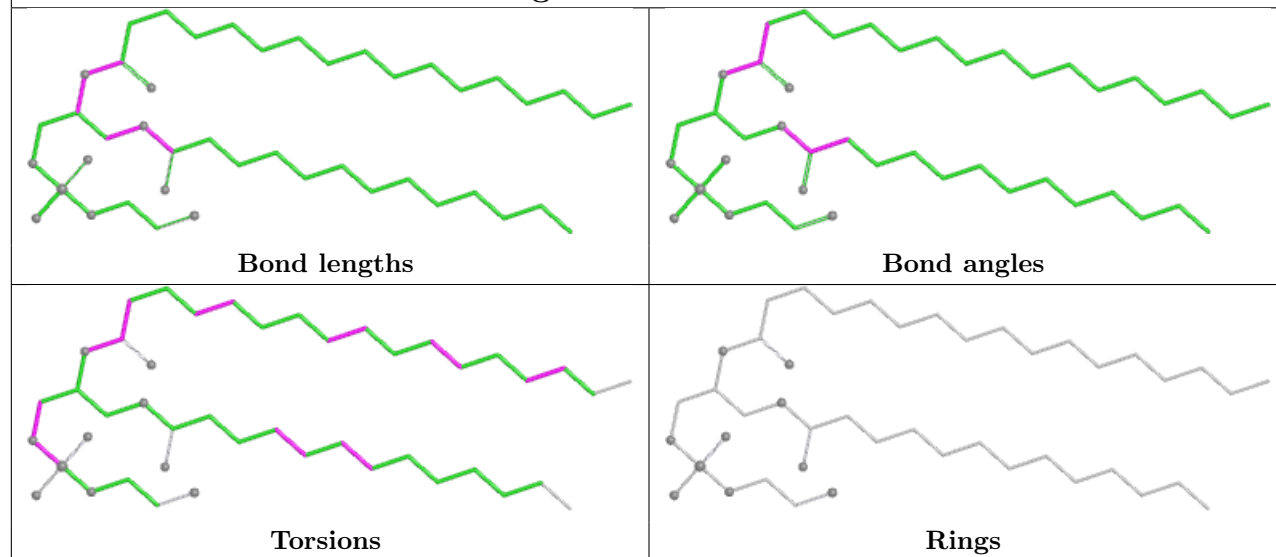


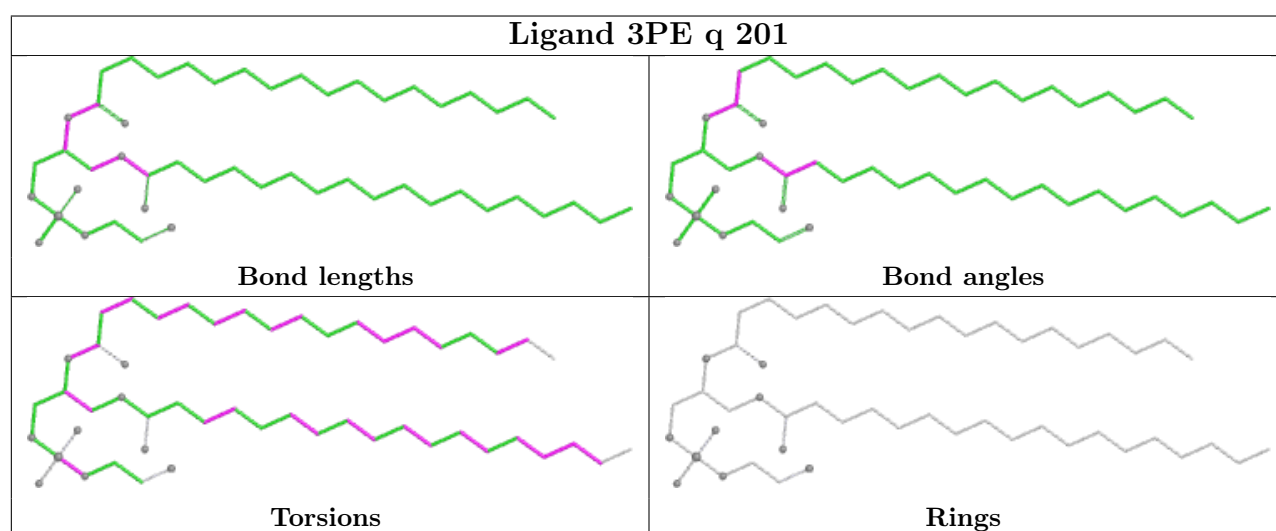
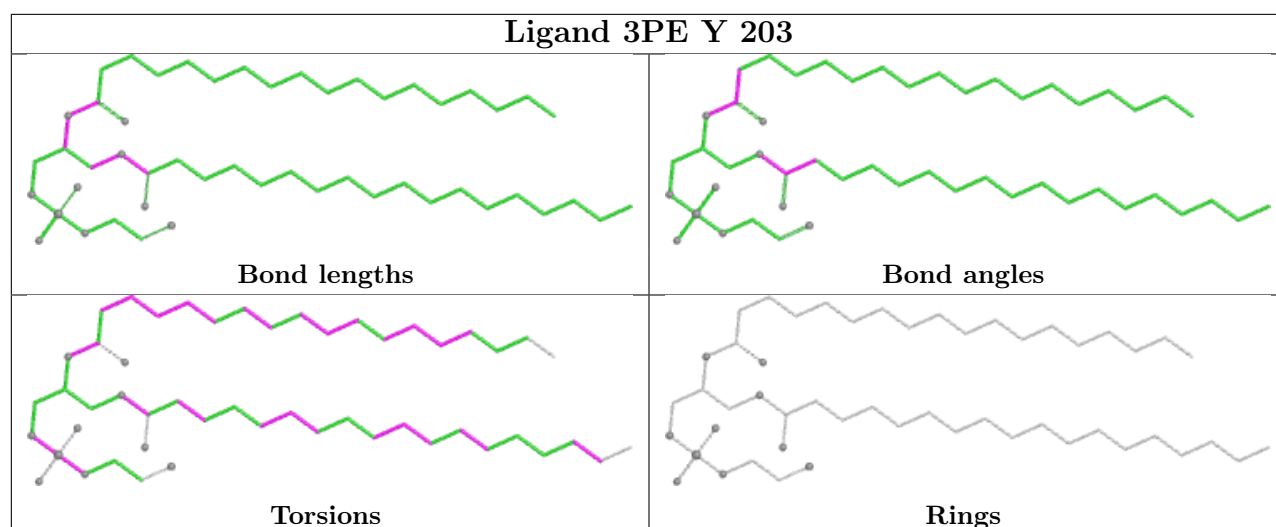


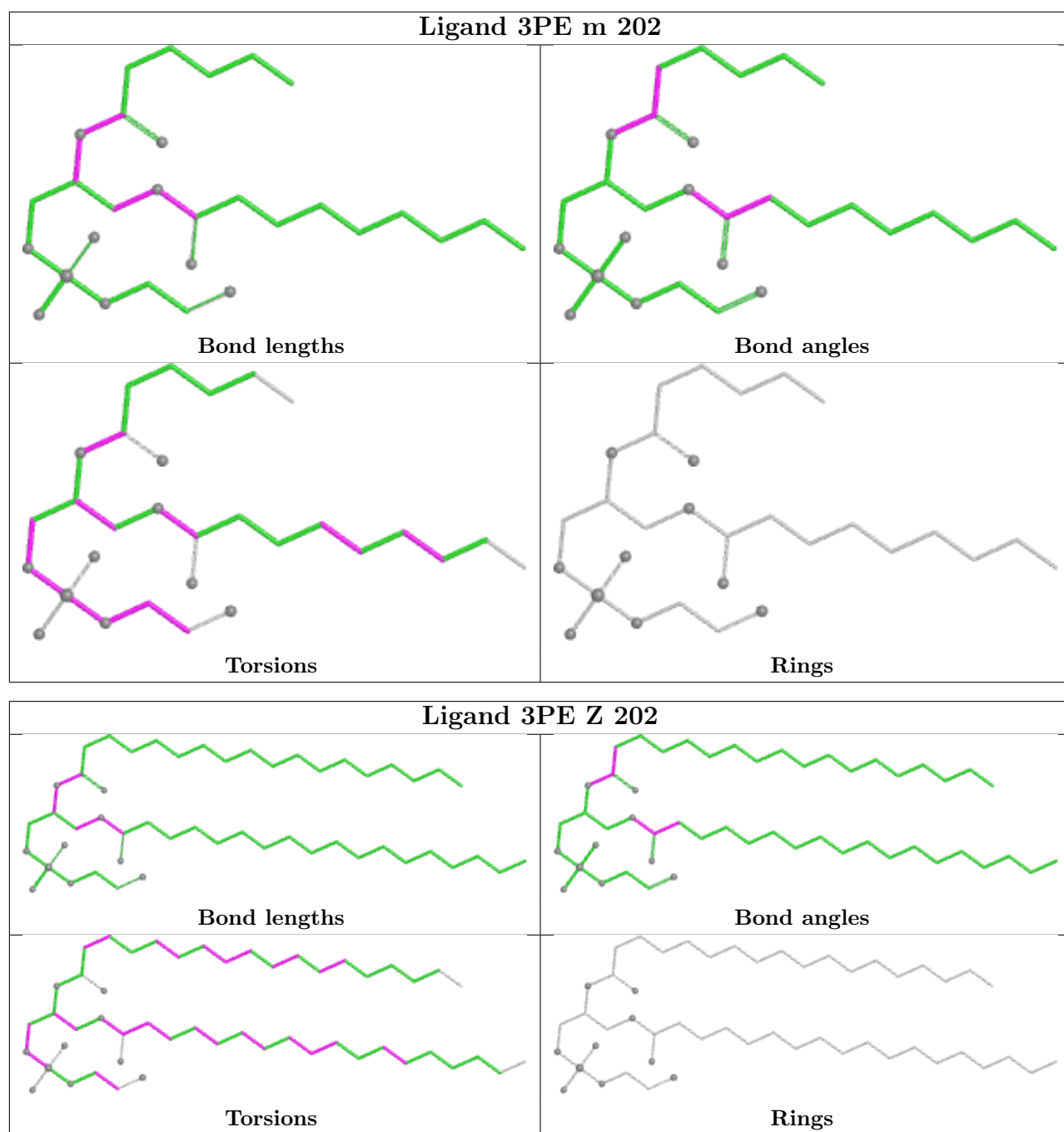
Ligand 3PE Y 201

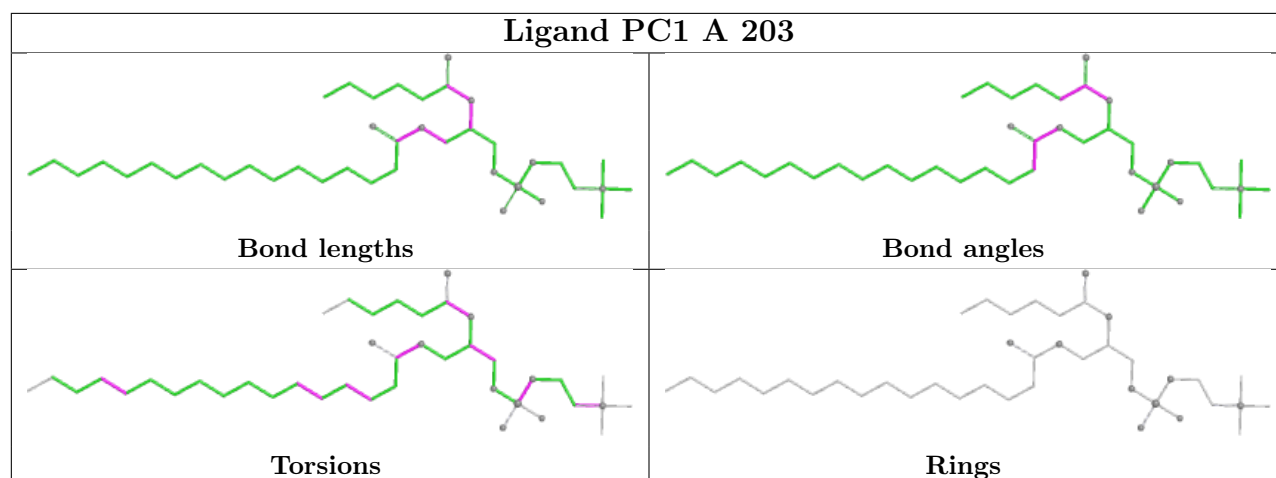
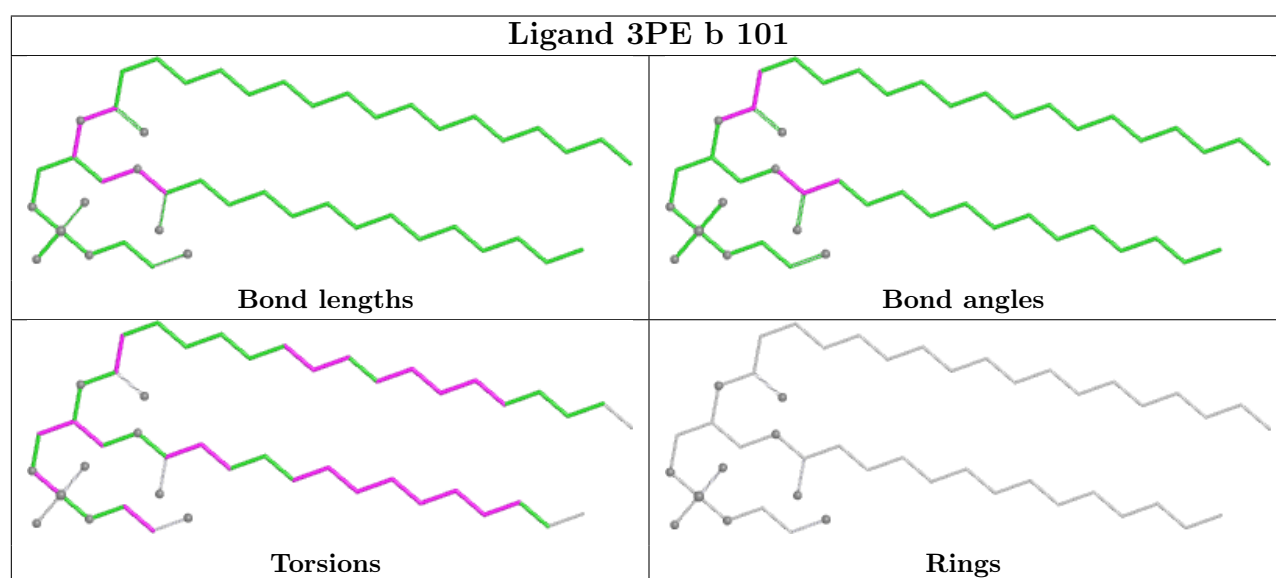
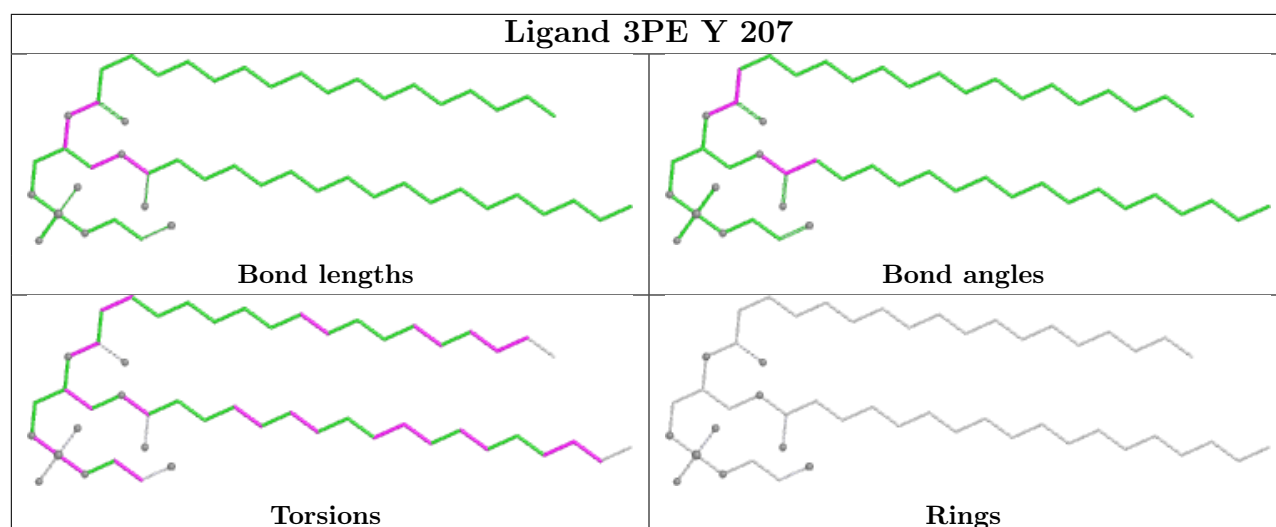


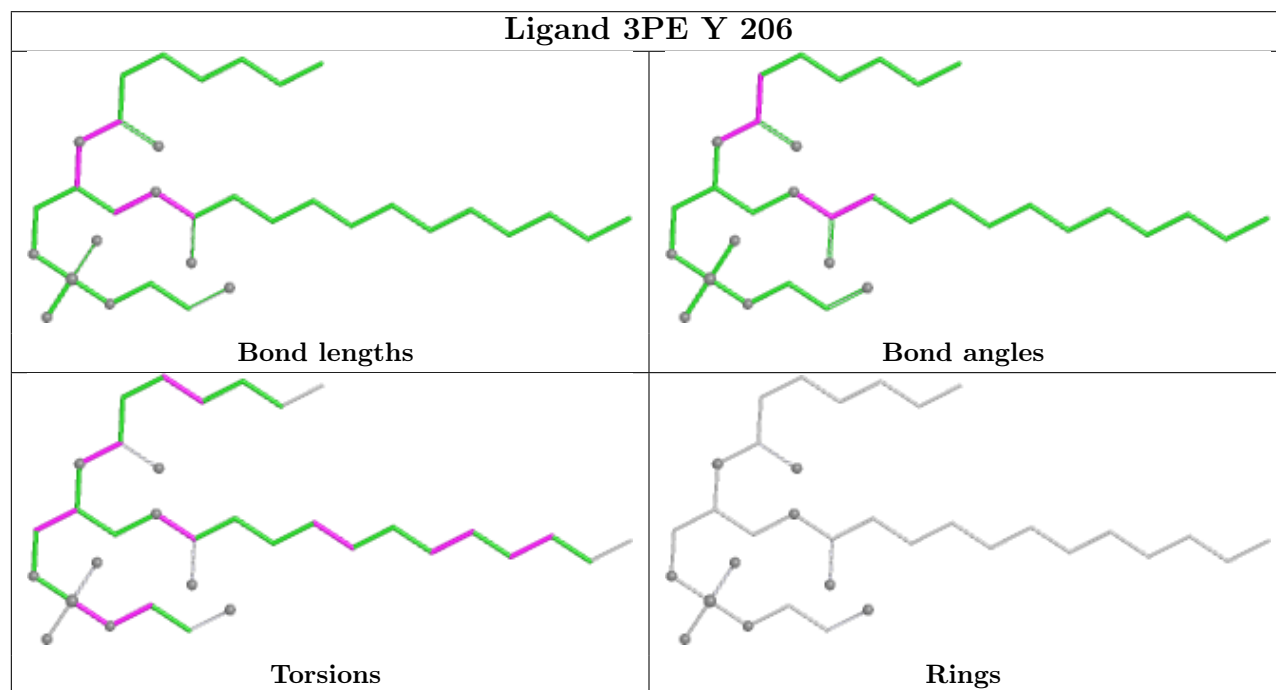
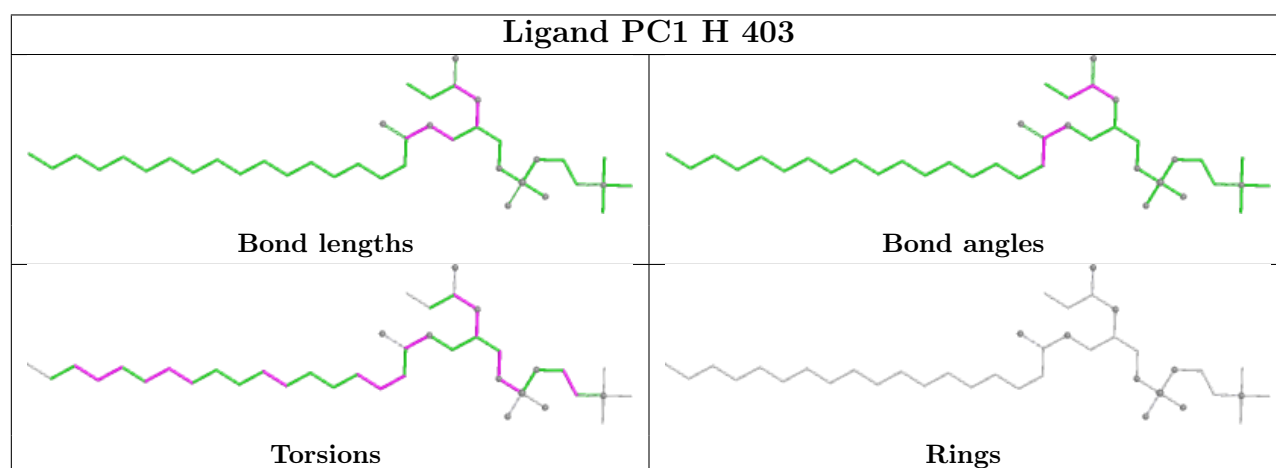
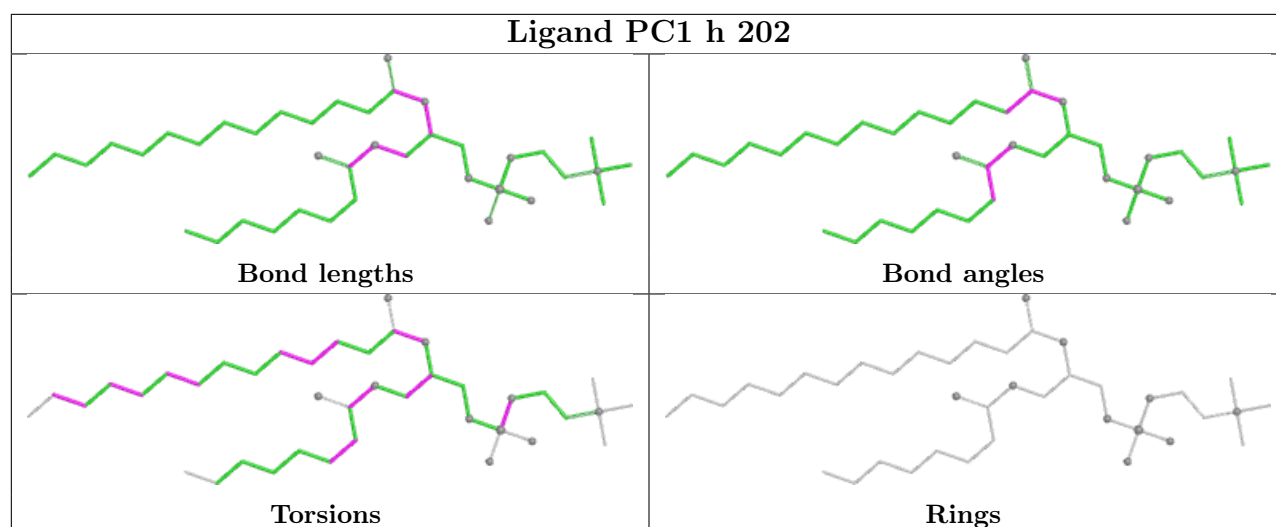
Ligand 3PE M 605

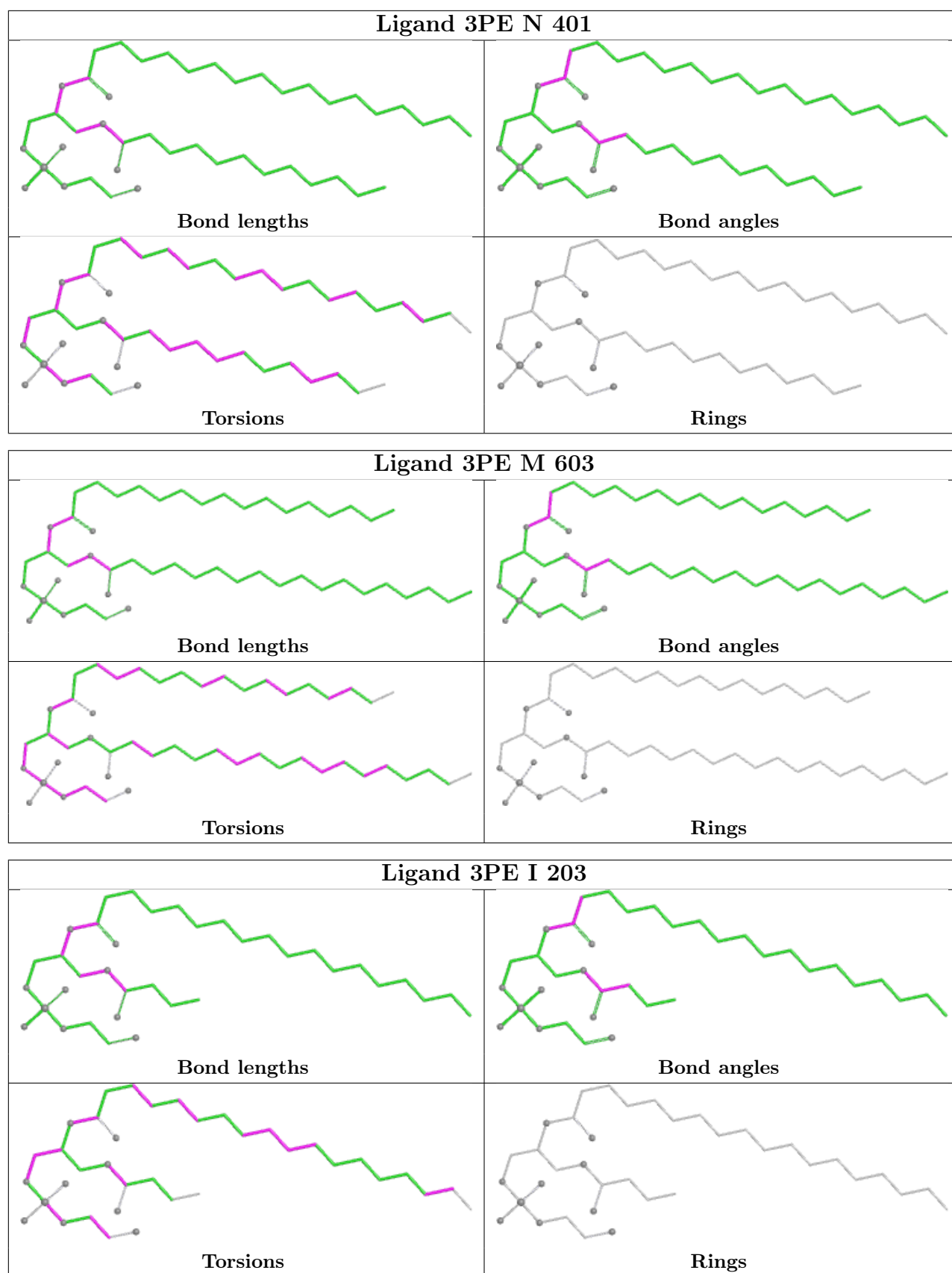


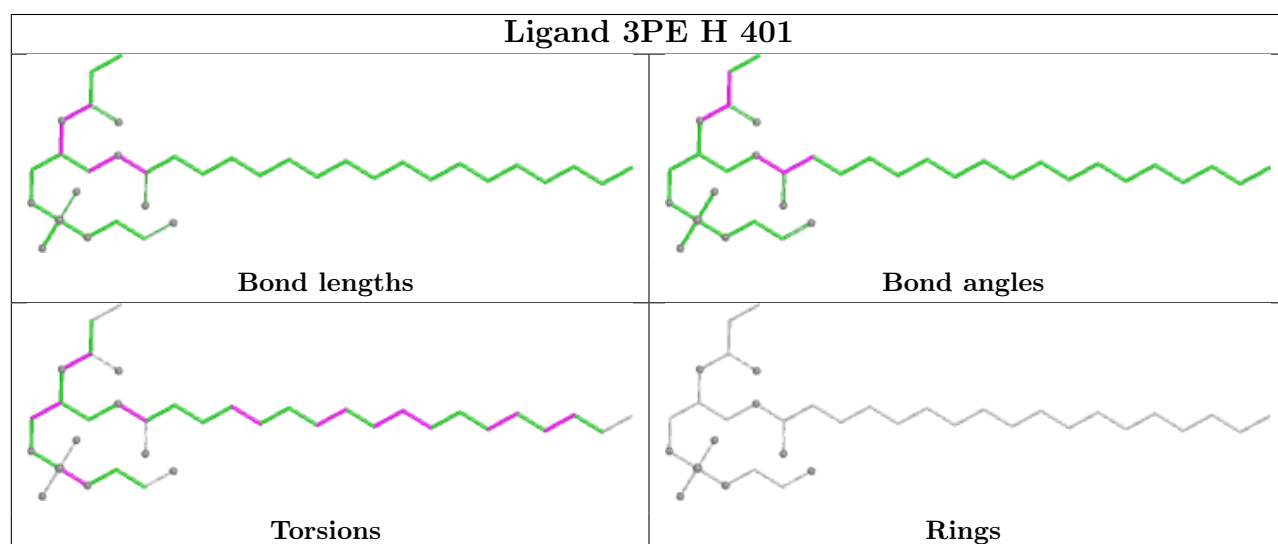
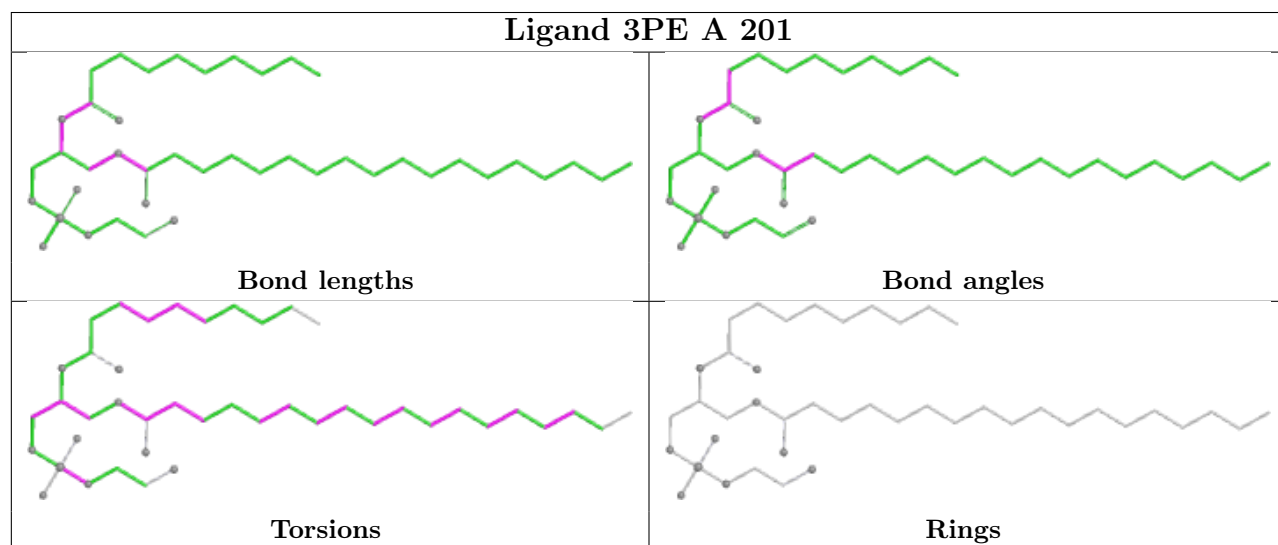
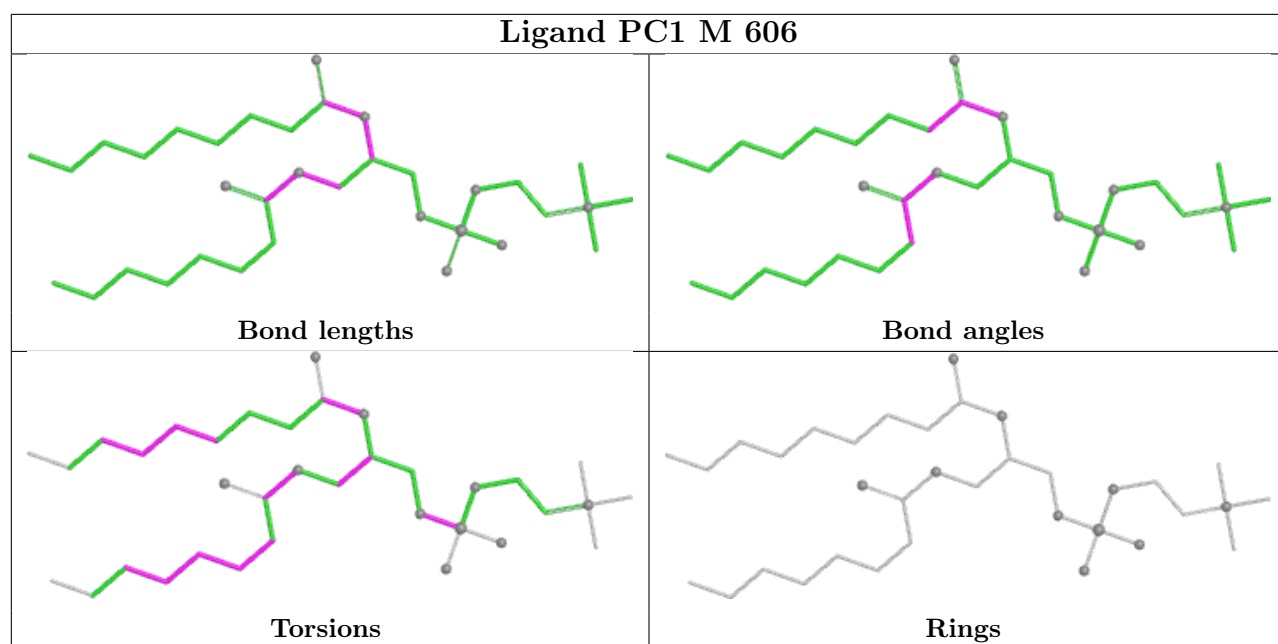


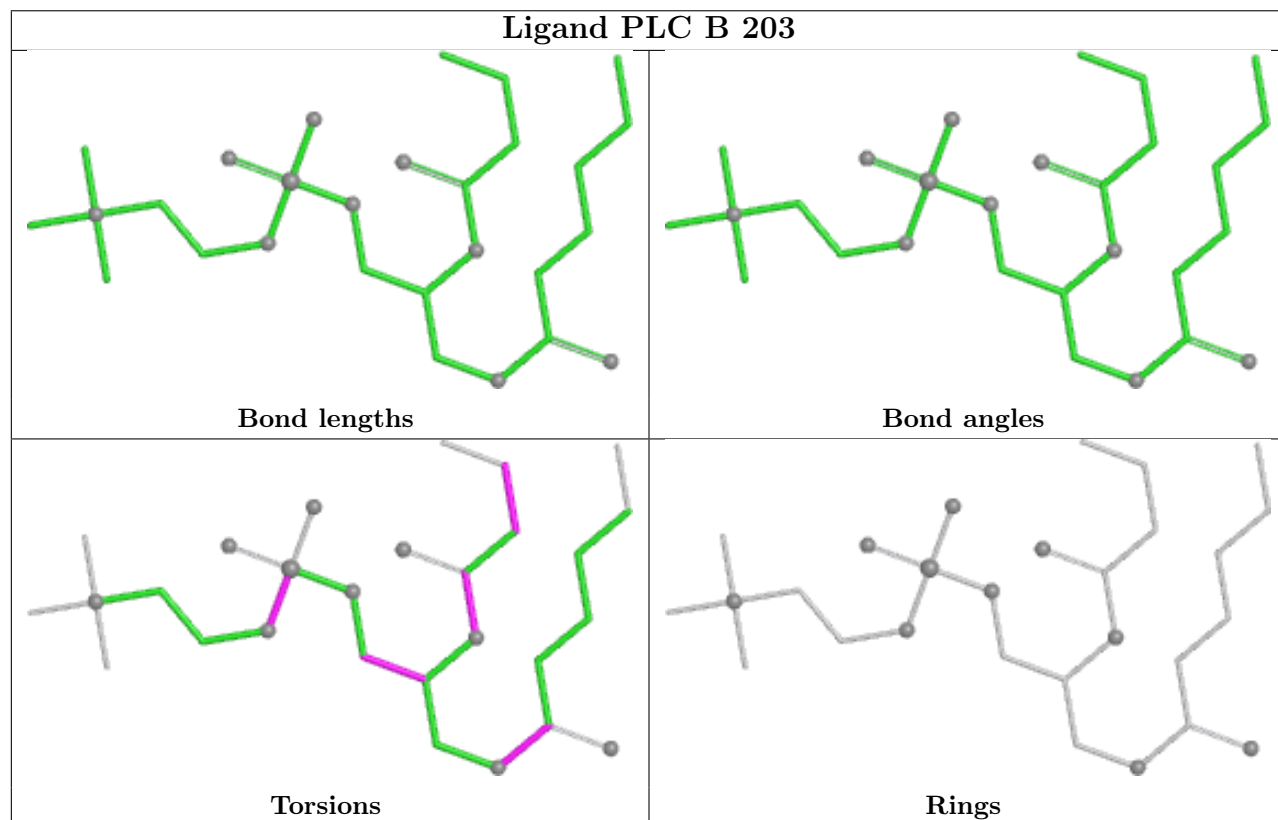
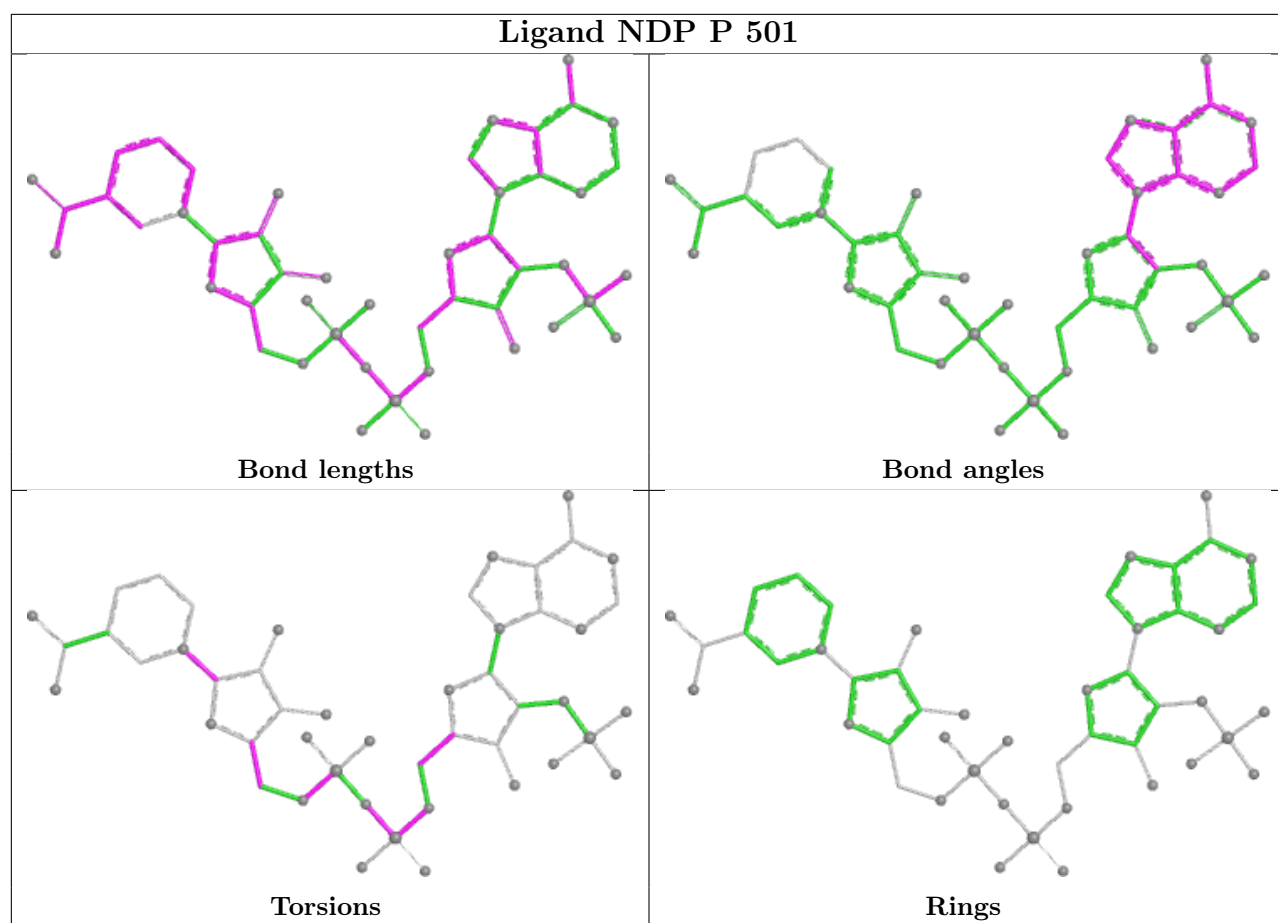


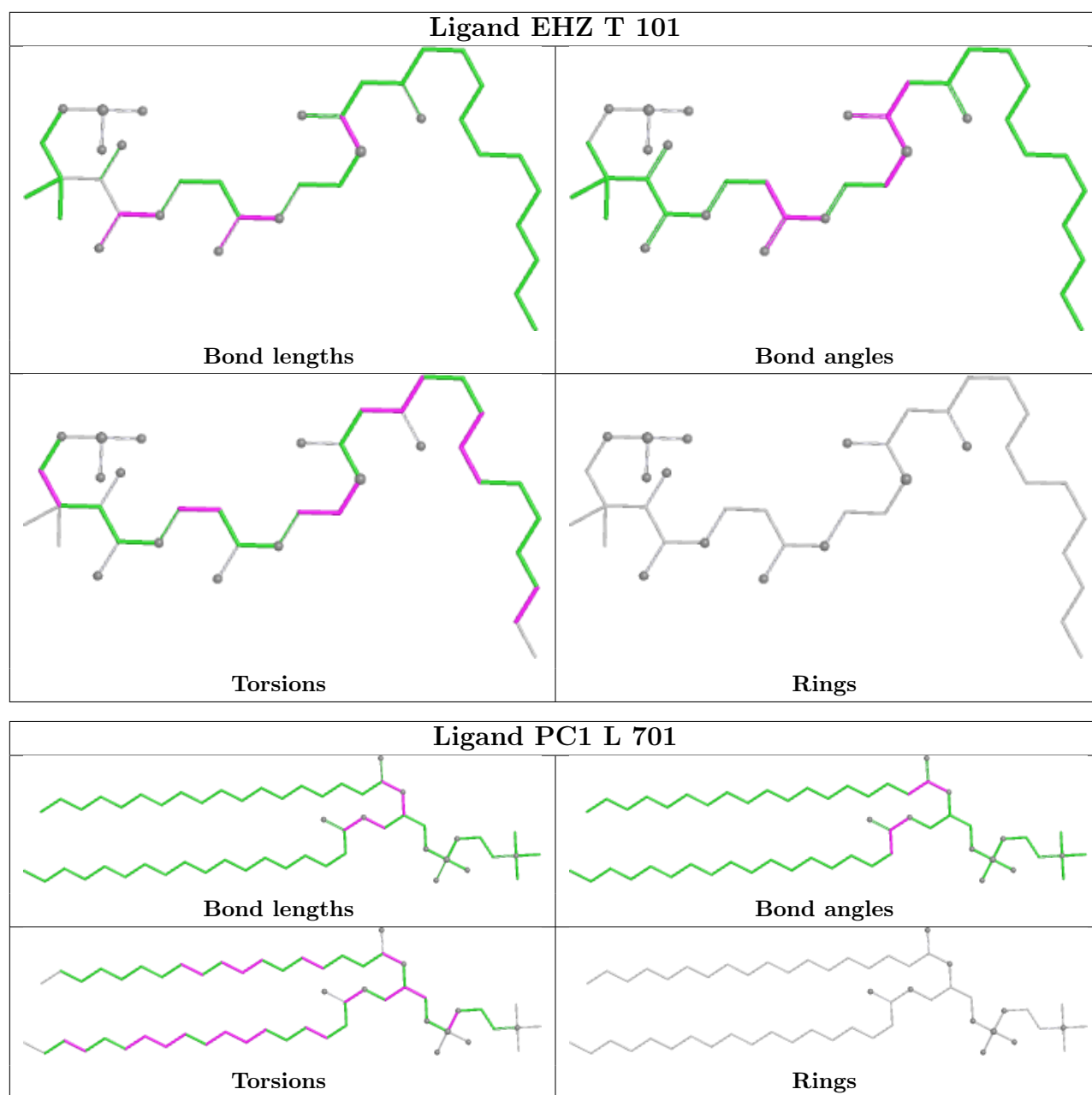


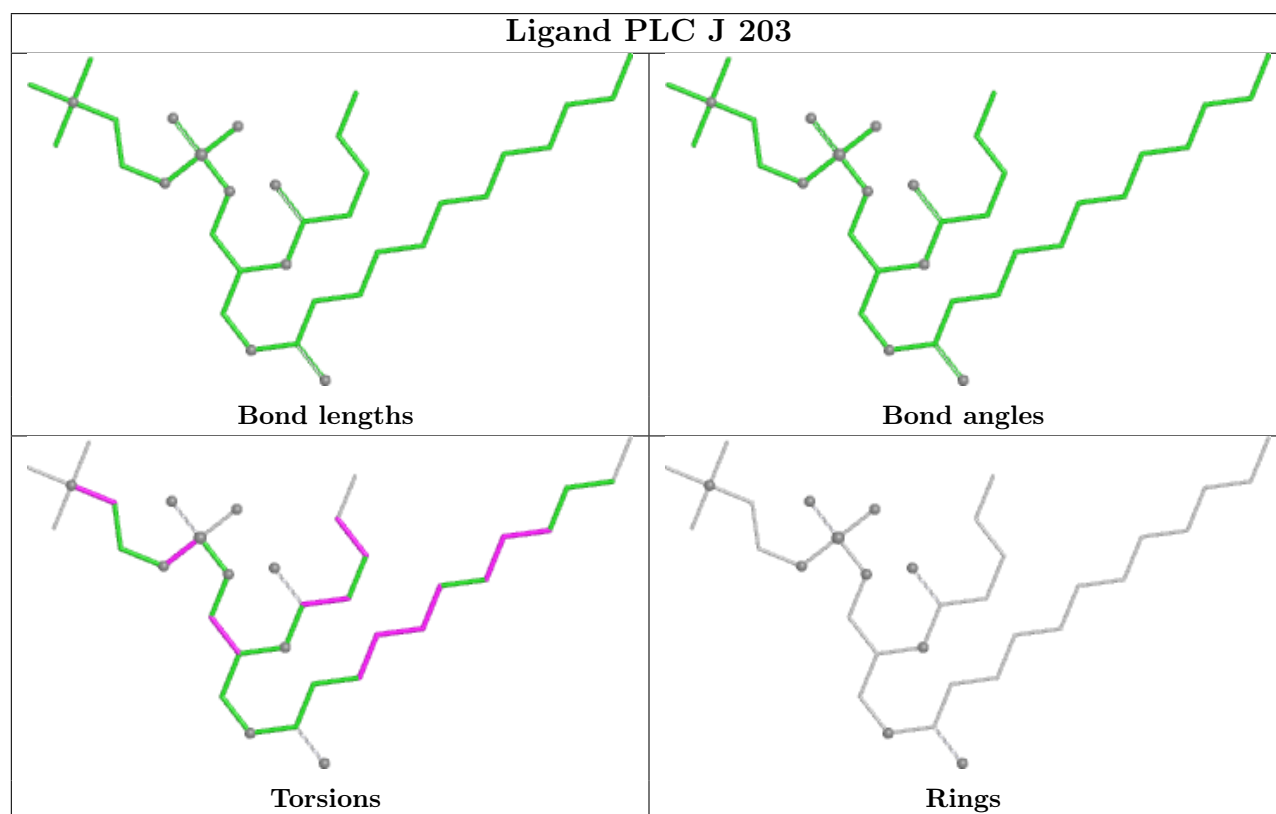
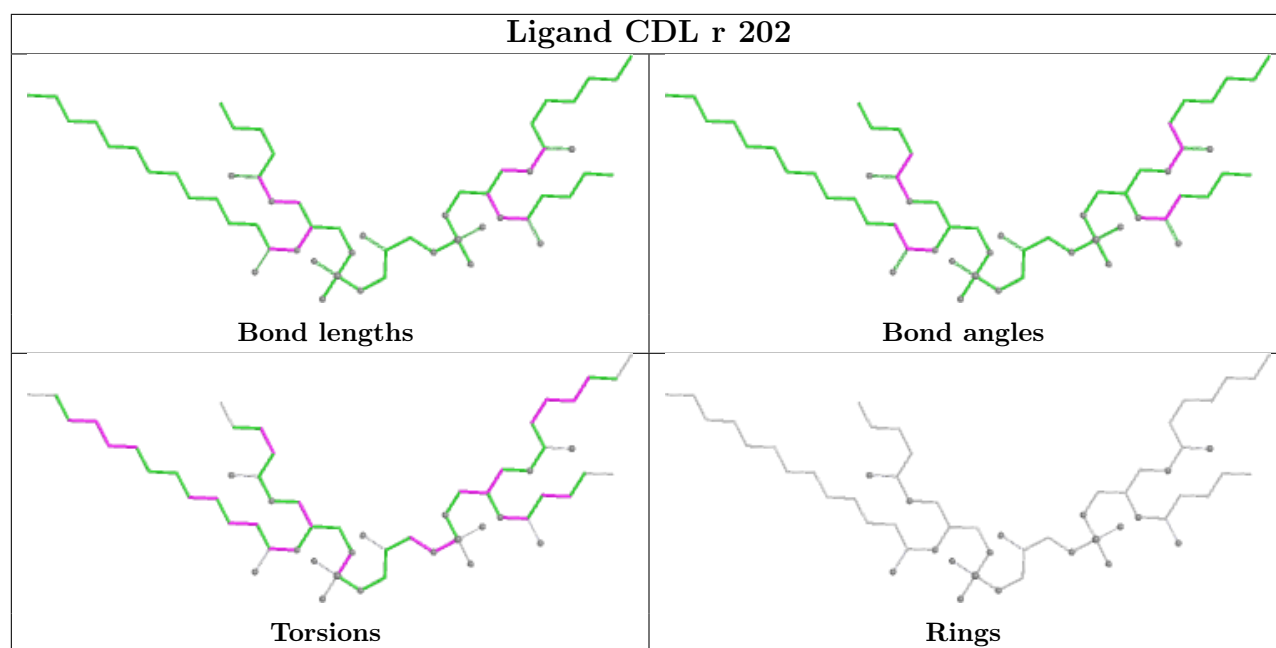


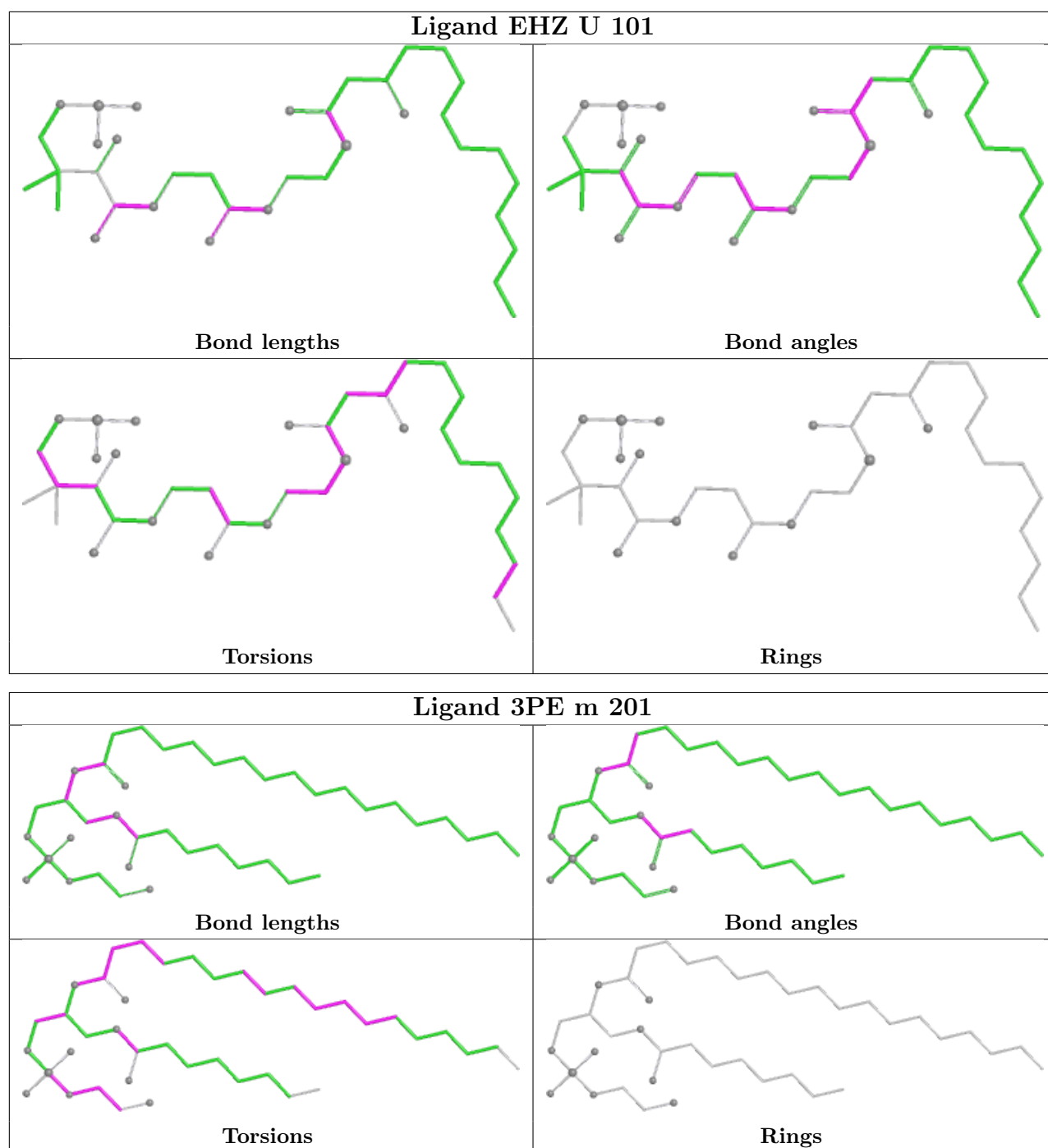


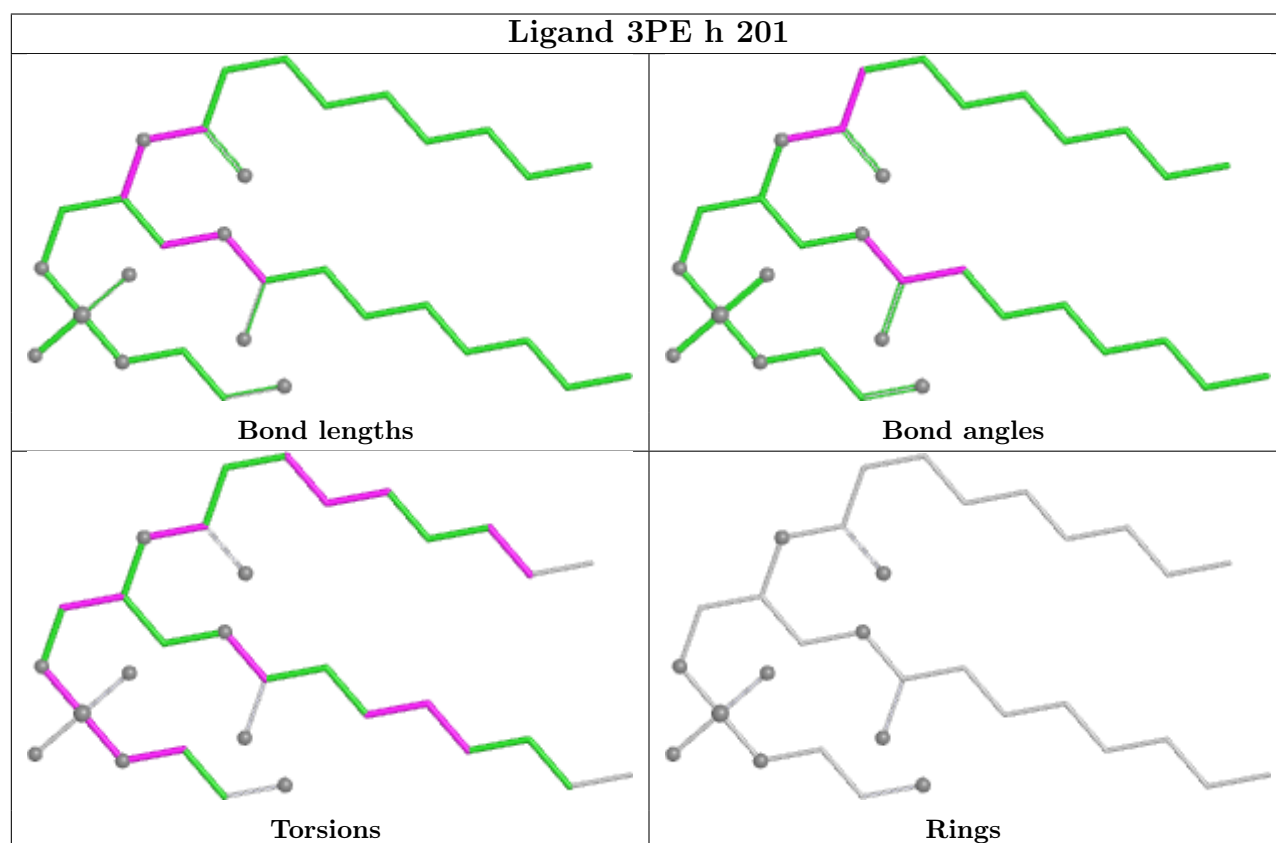
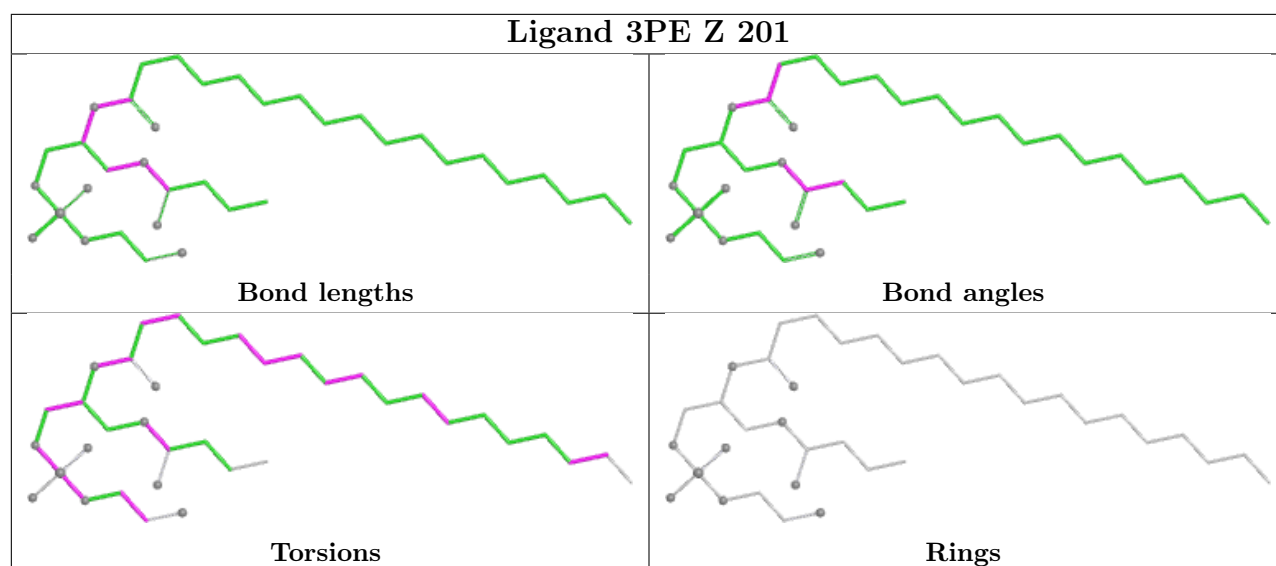


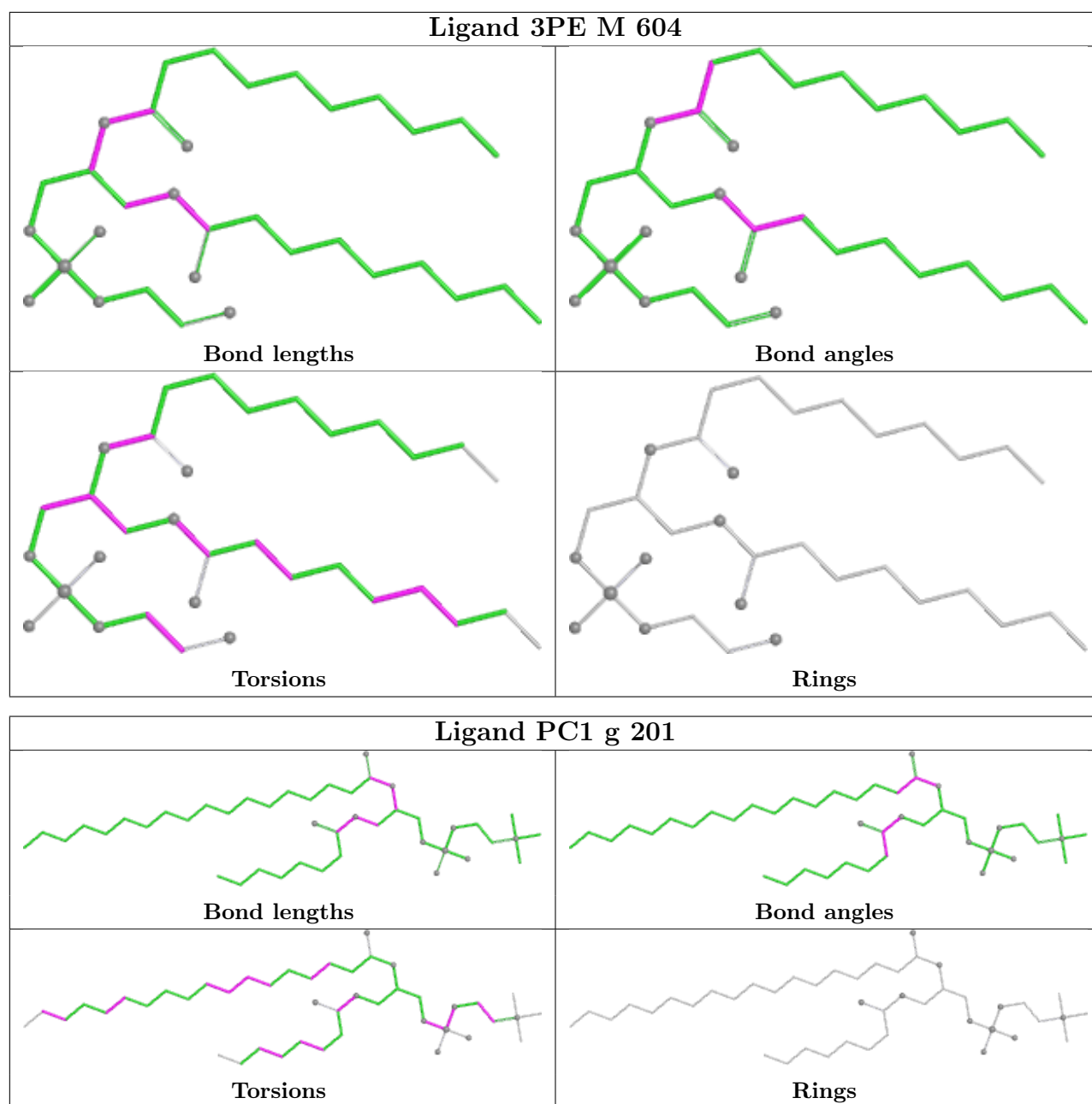


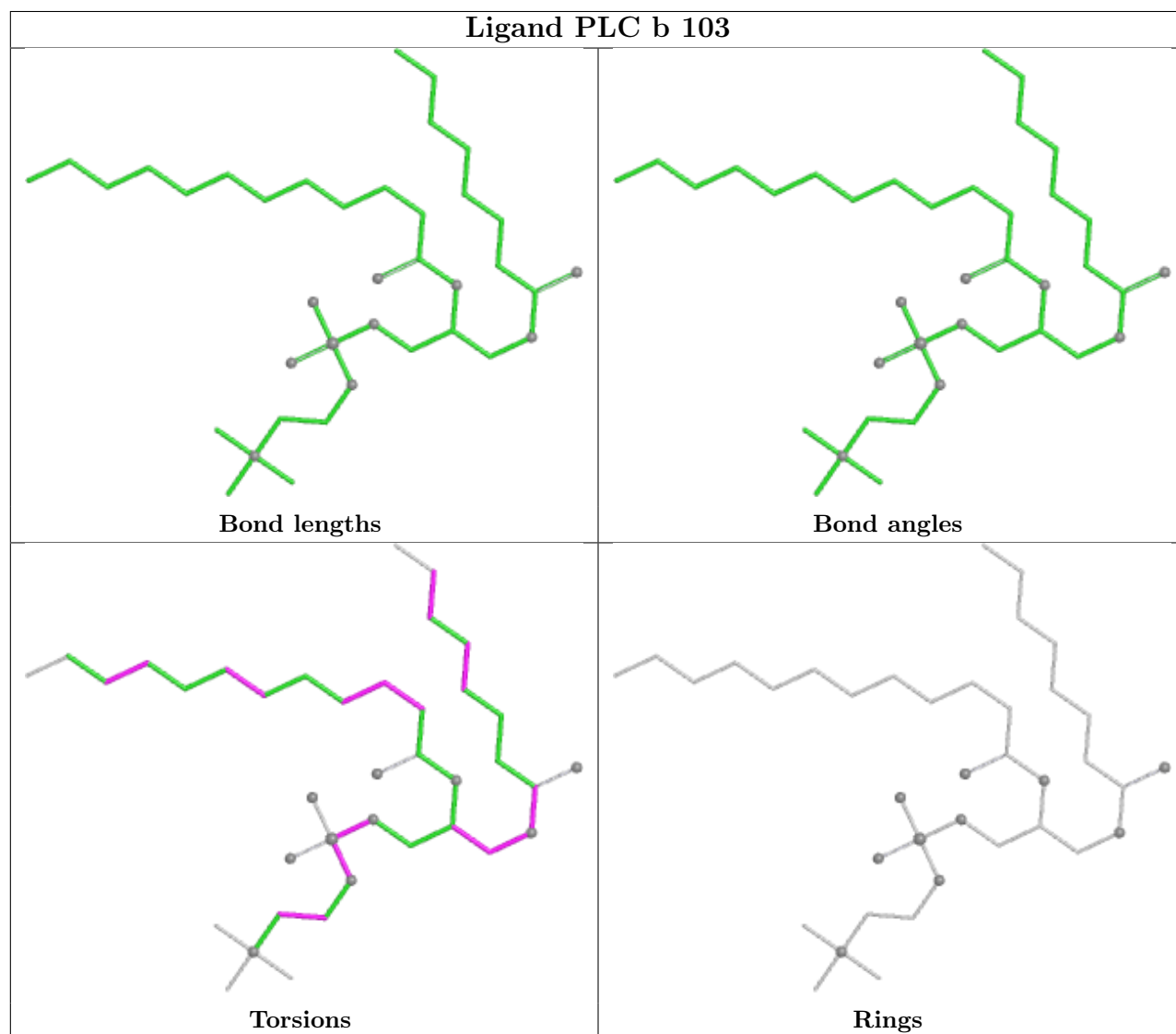
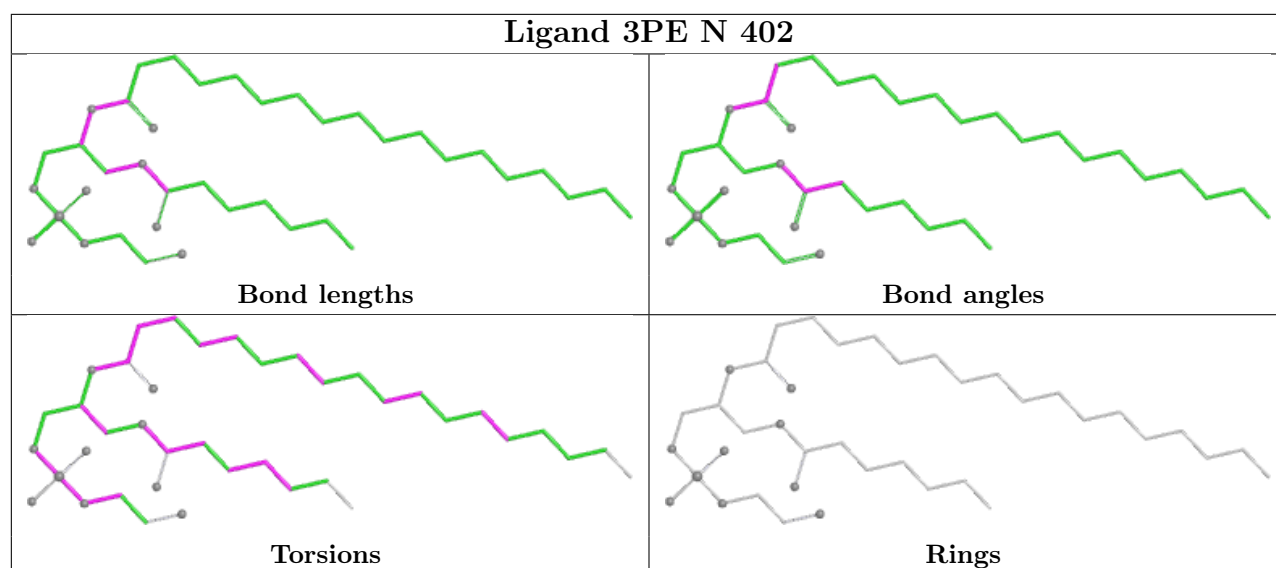


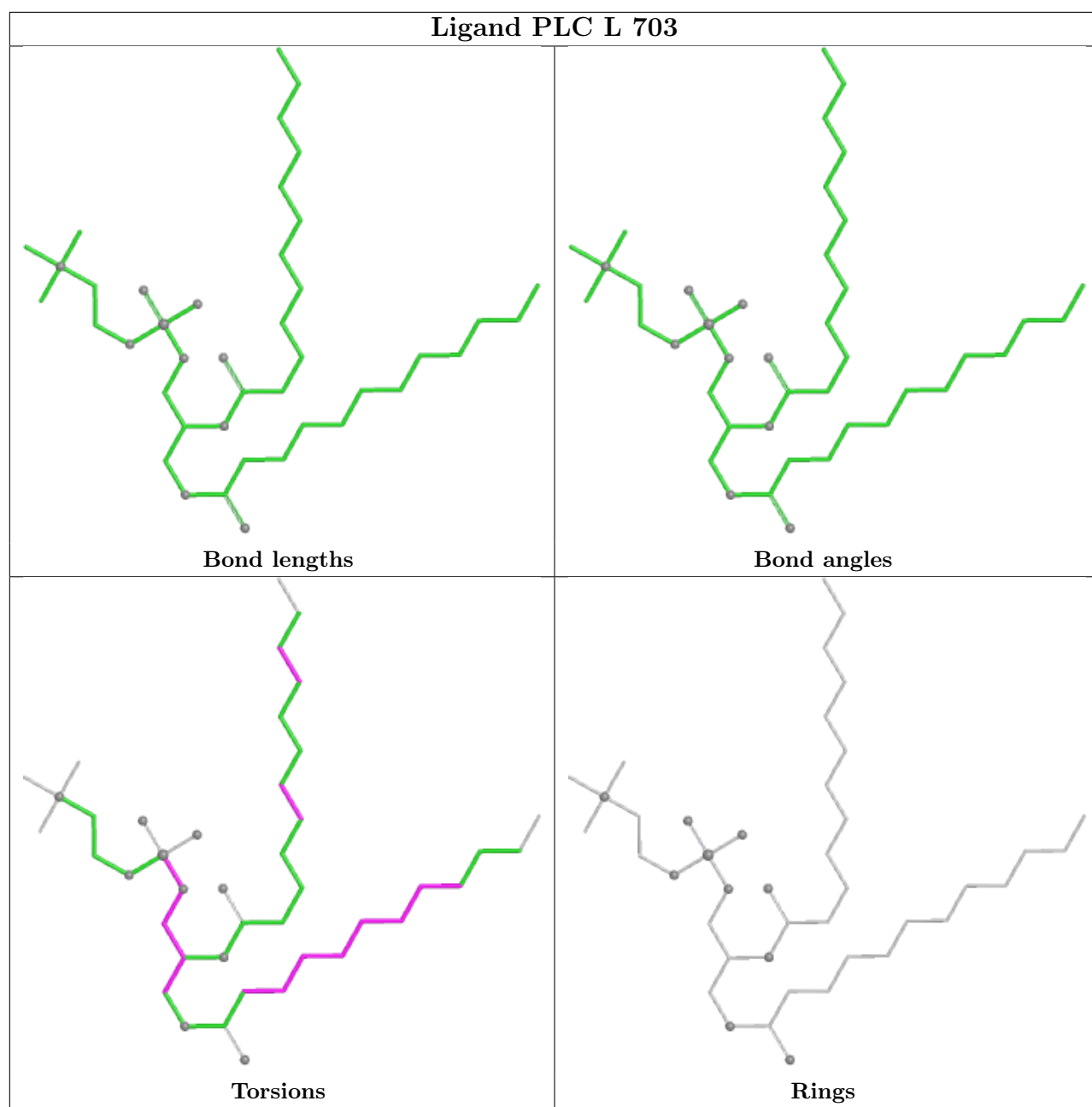




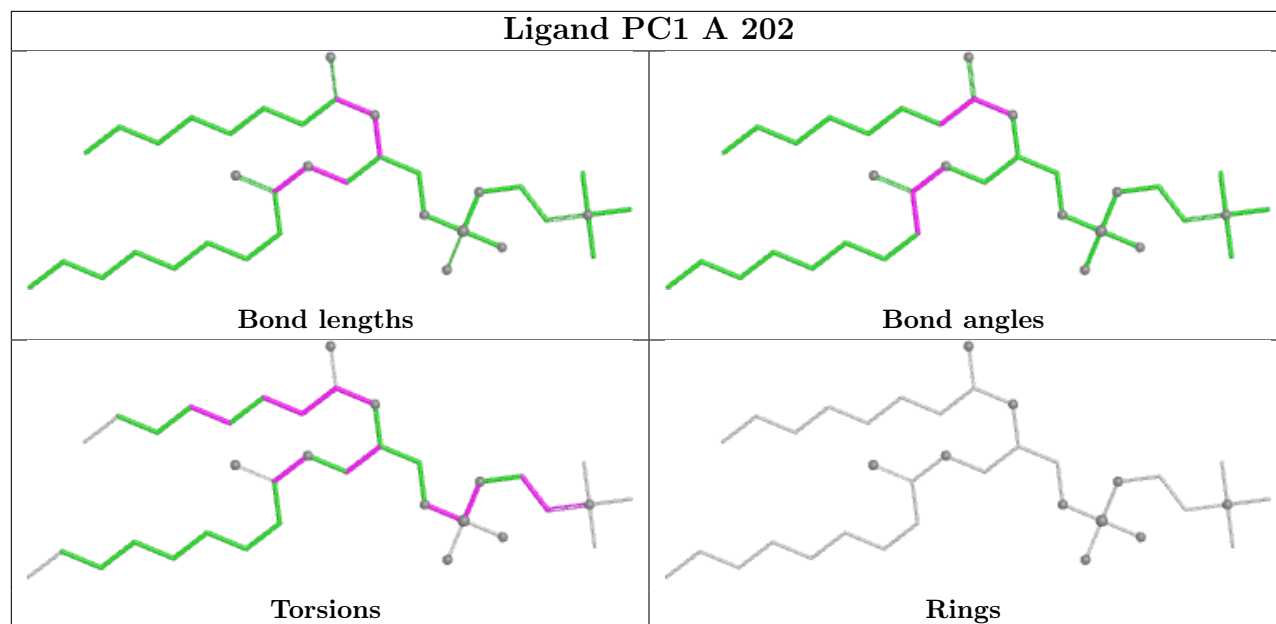




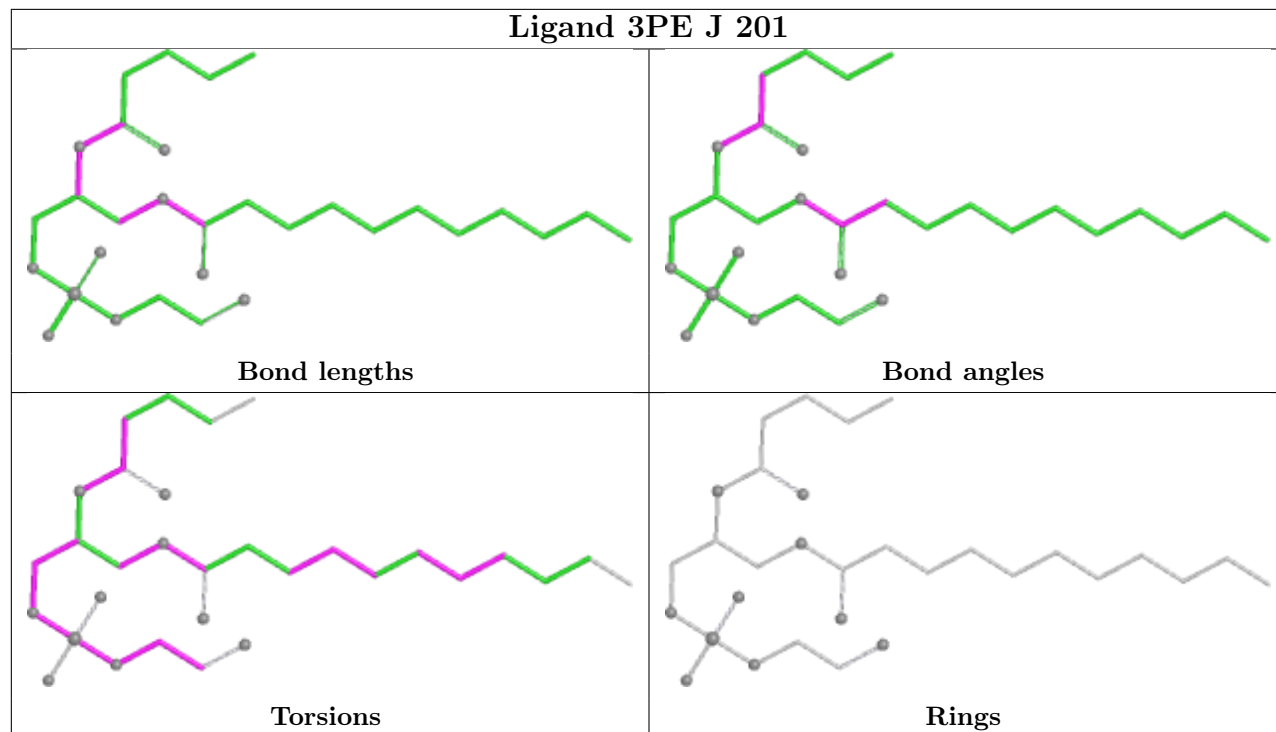




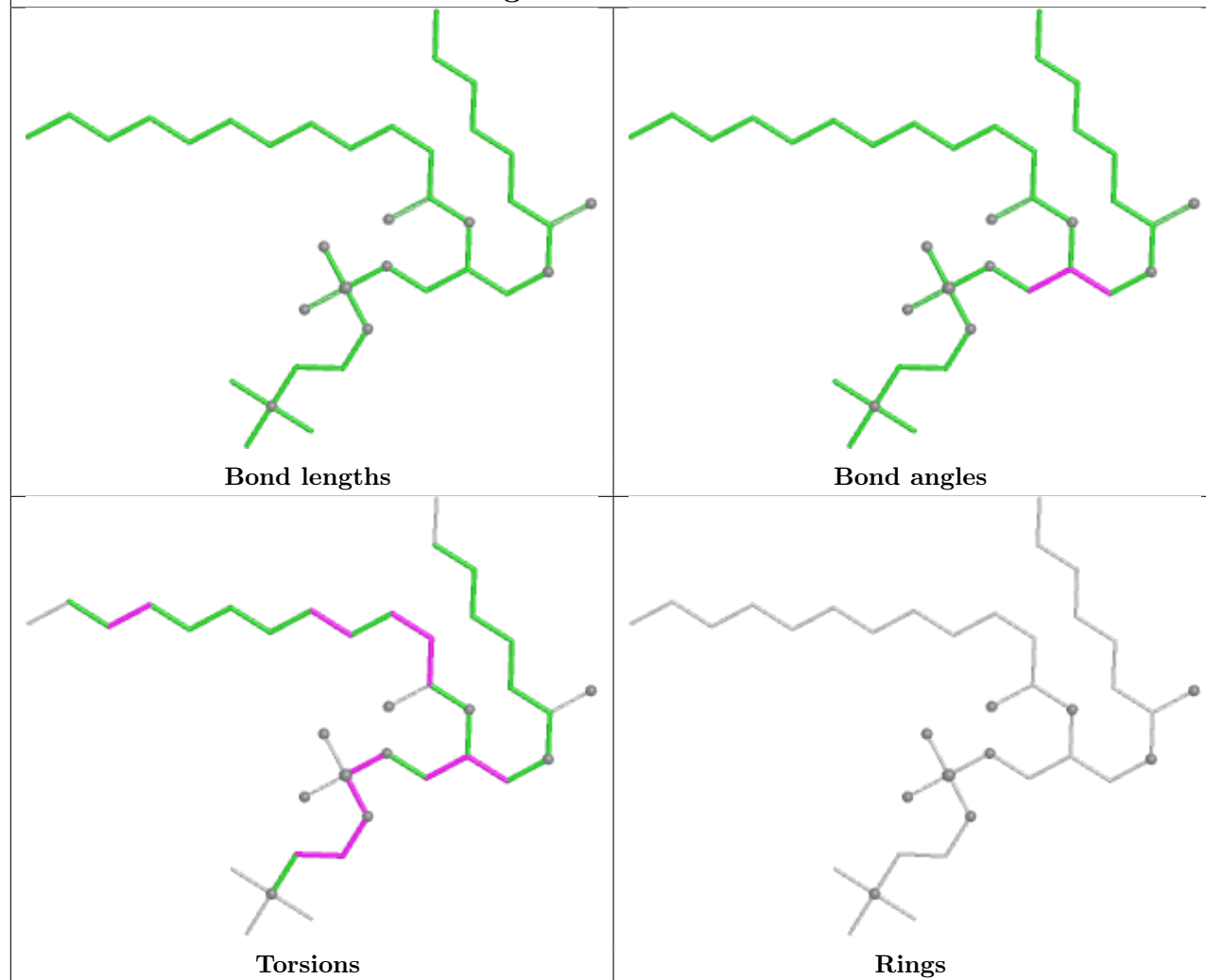
Ligand PC1 A 202



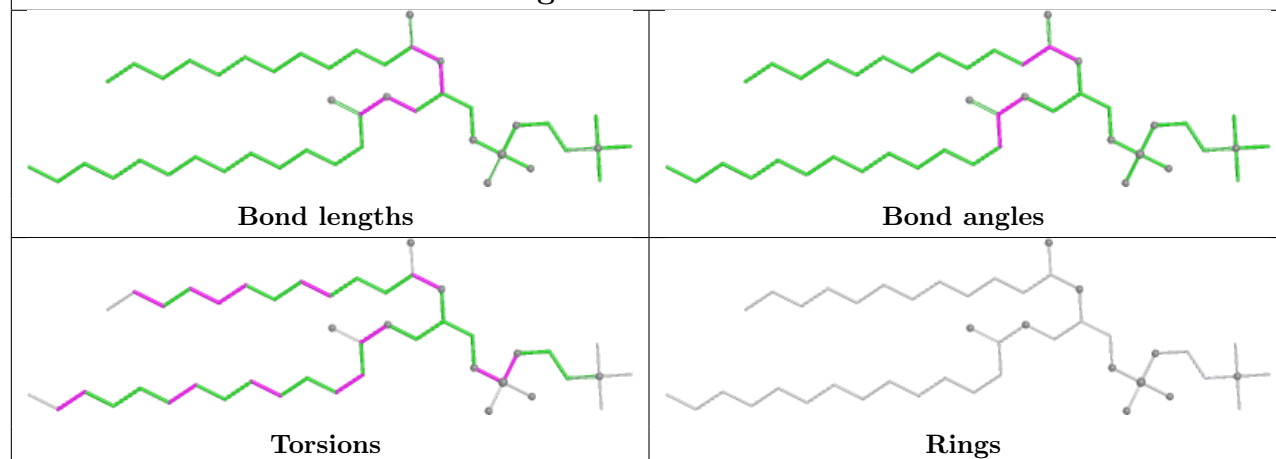
Ligand 3PE J 201

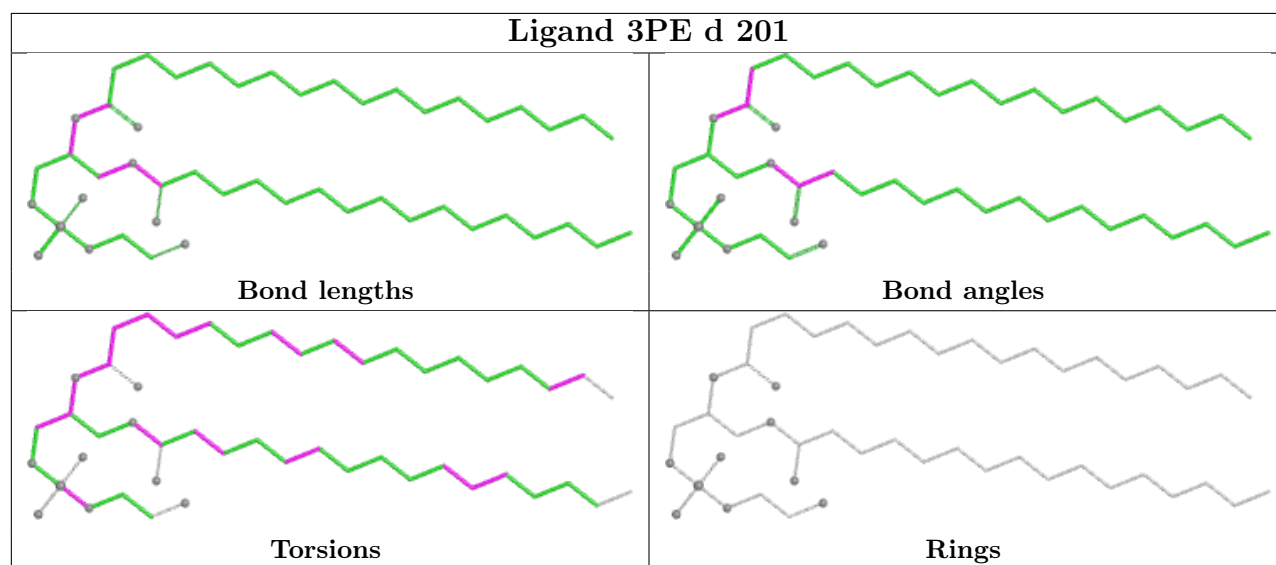
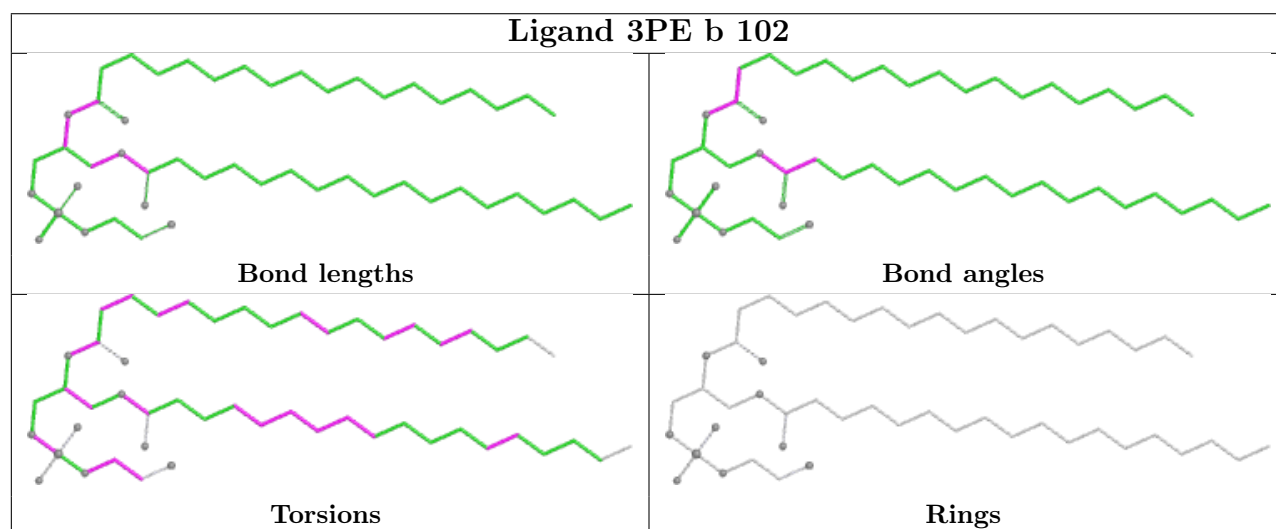
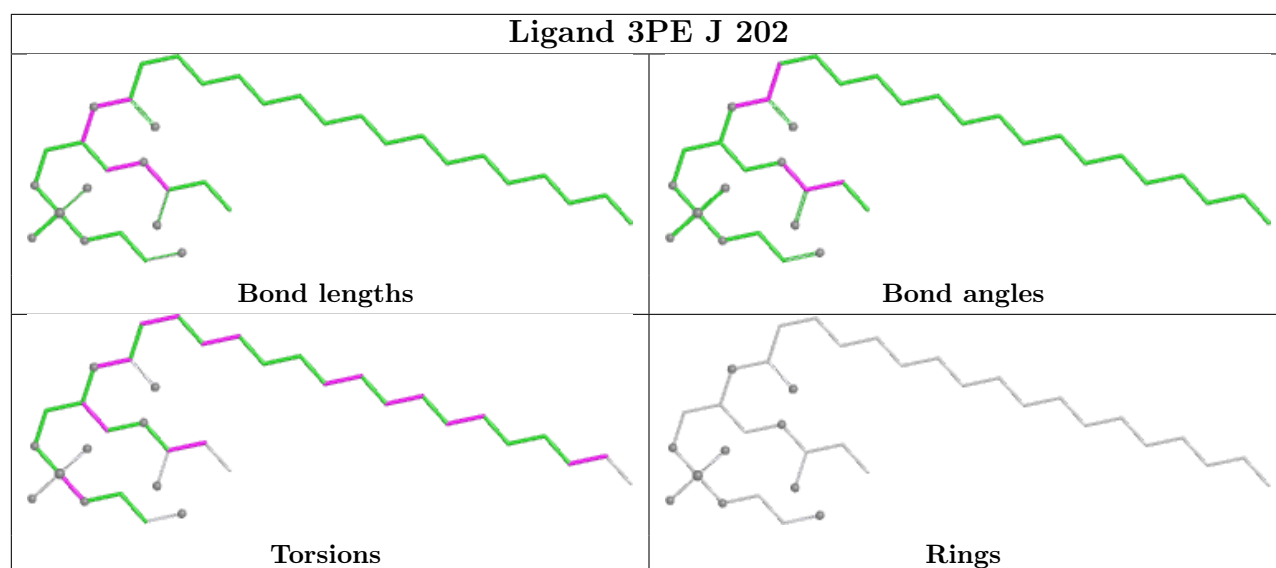


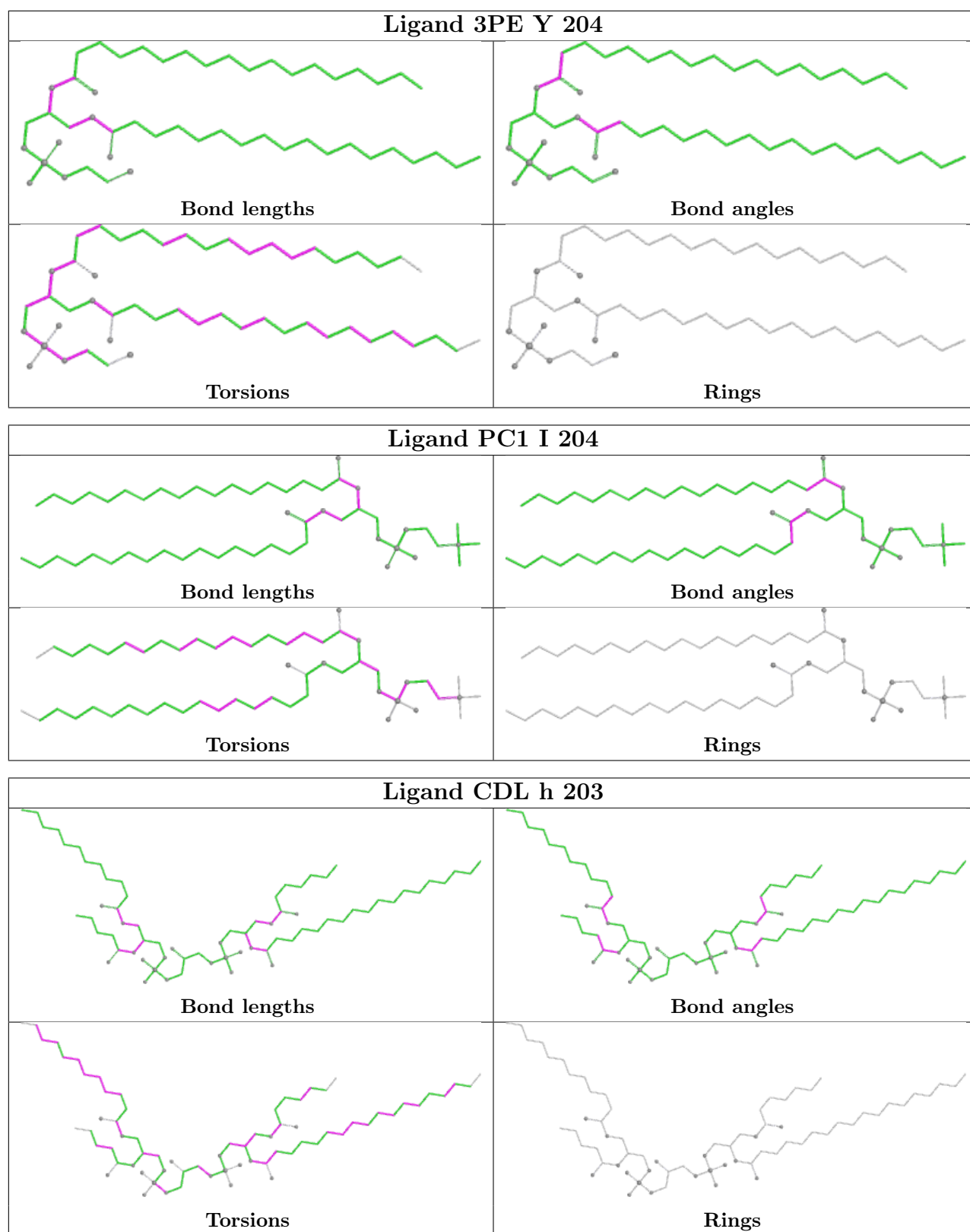
Ligand PLC Y 208

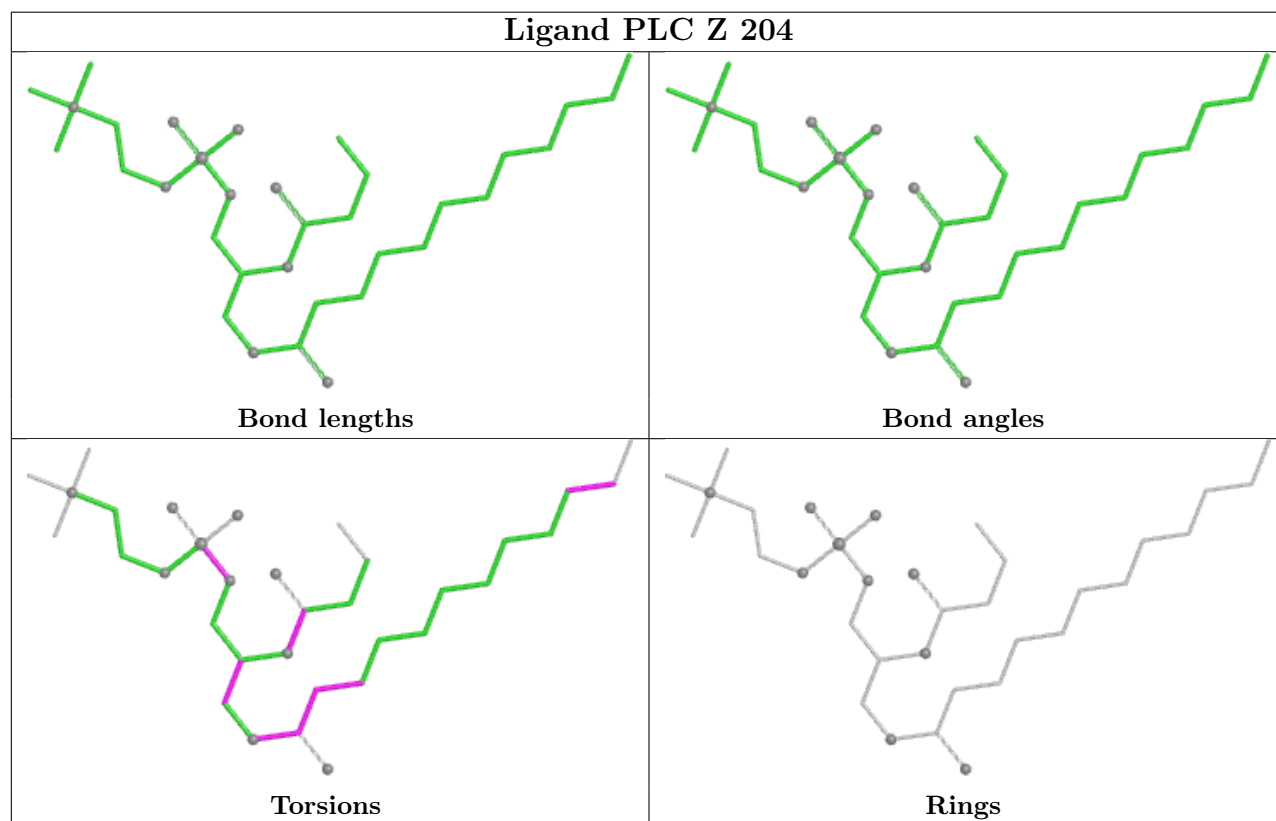
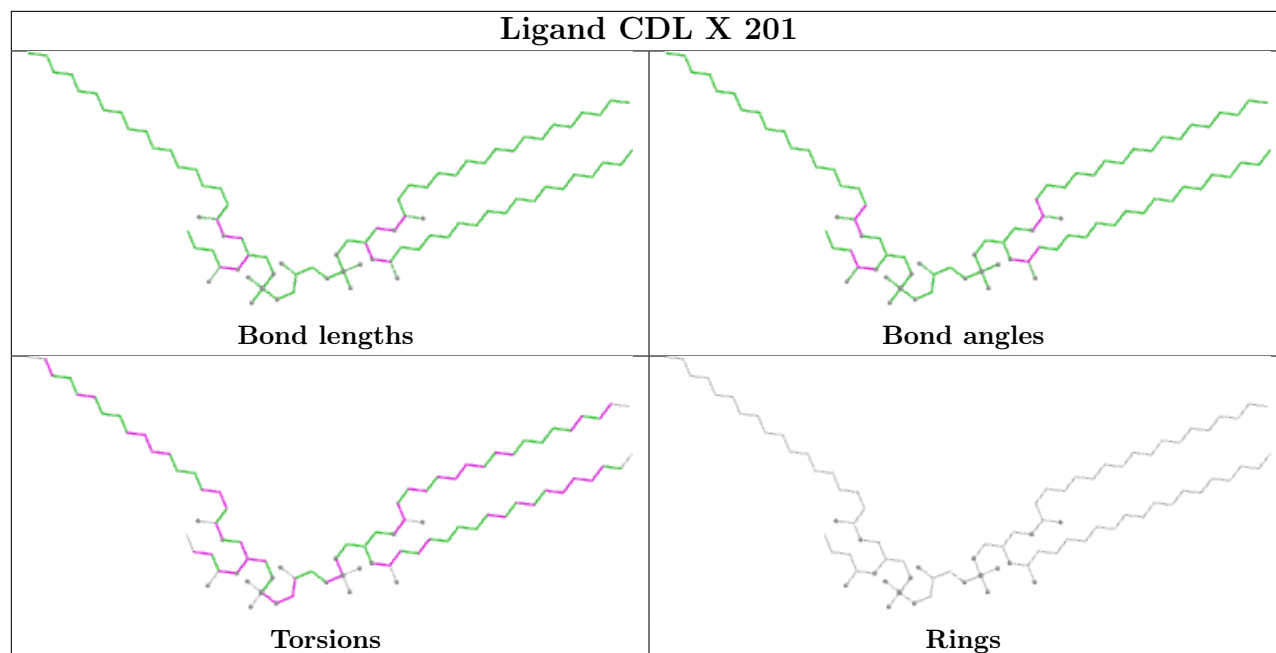


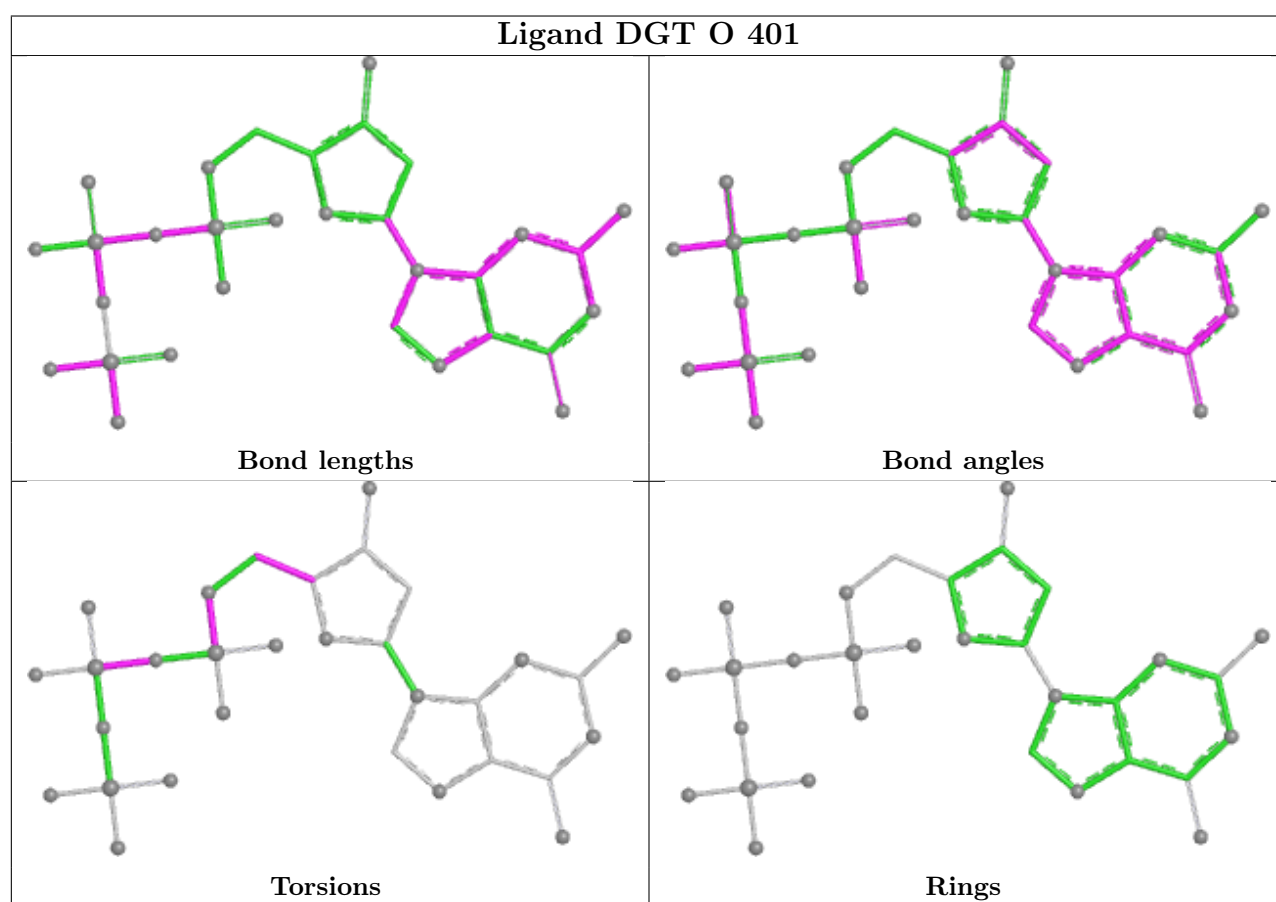
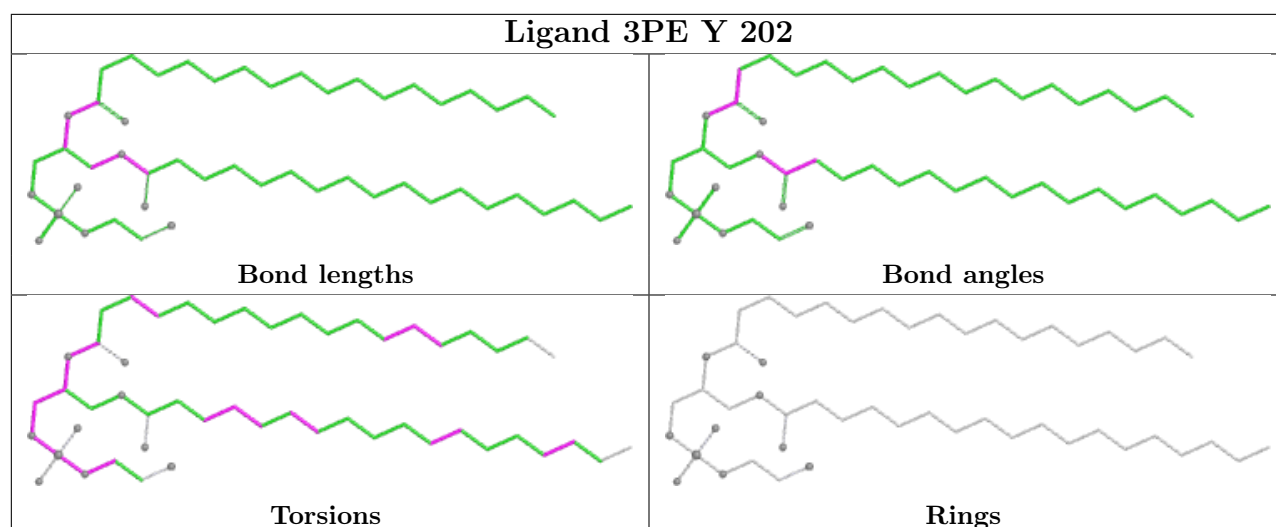
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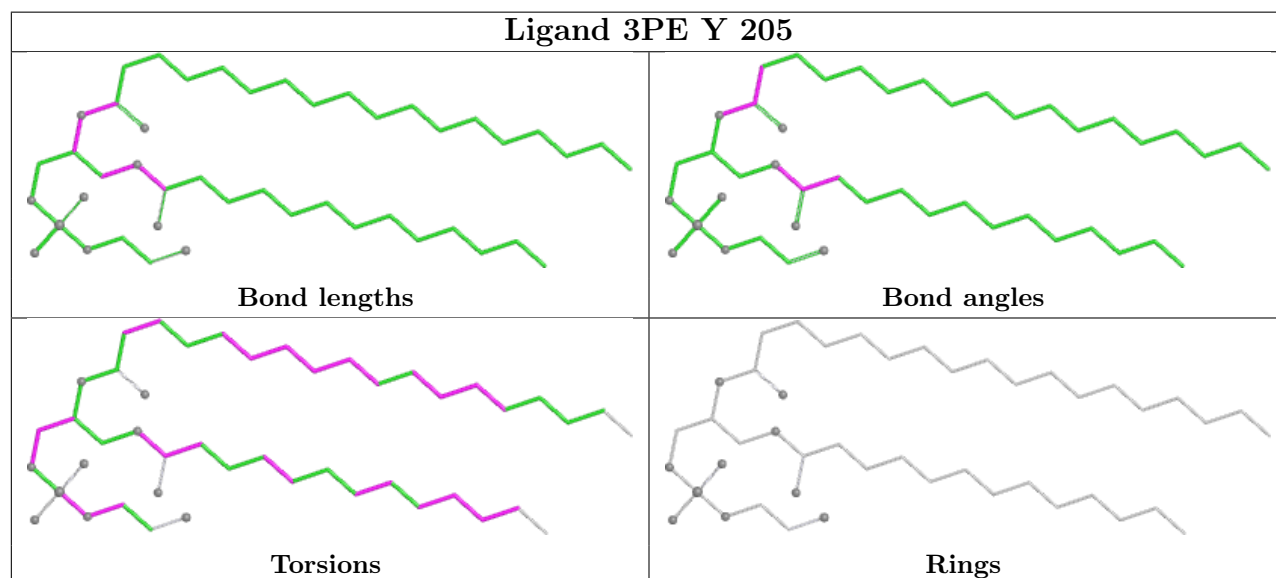
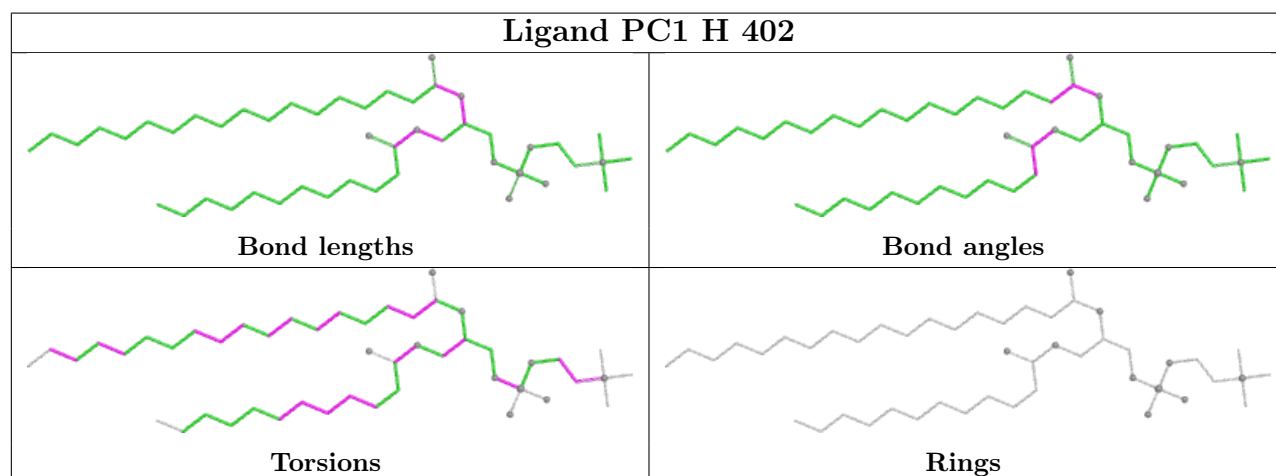
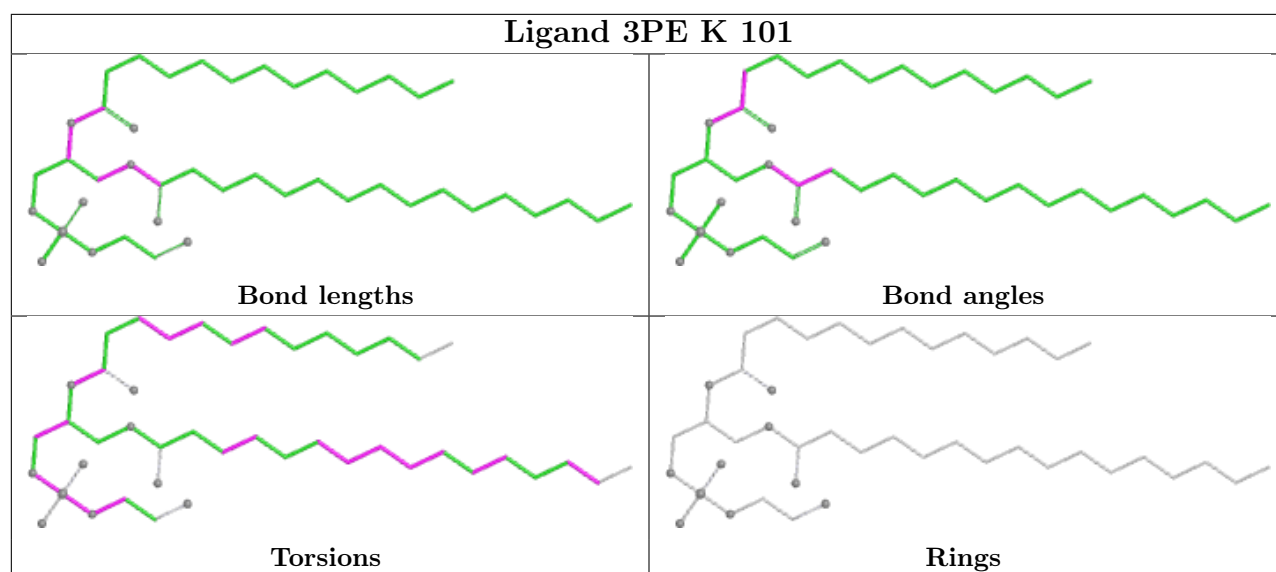


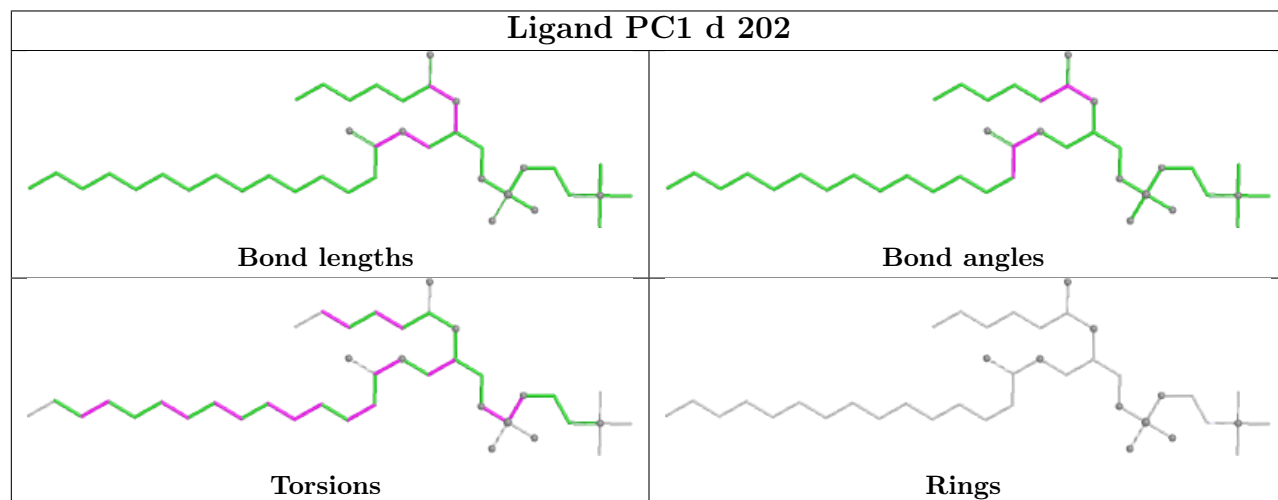
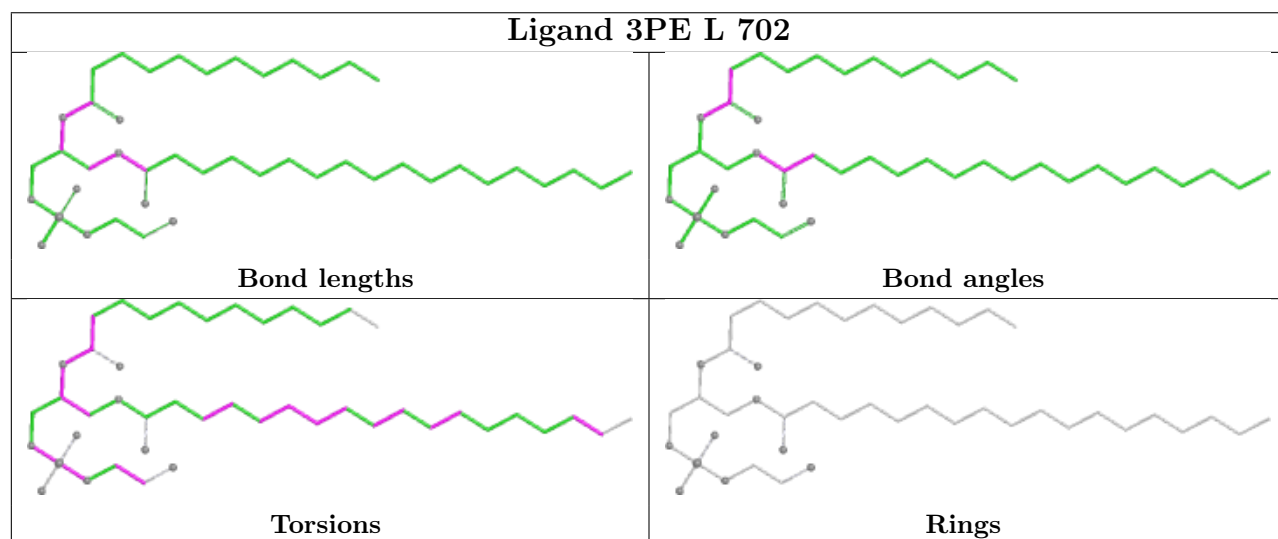
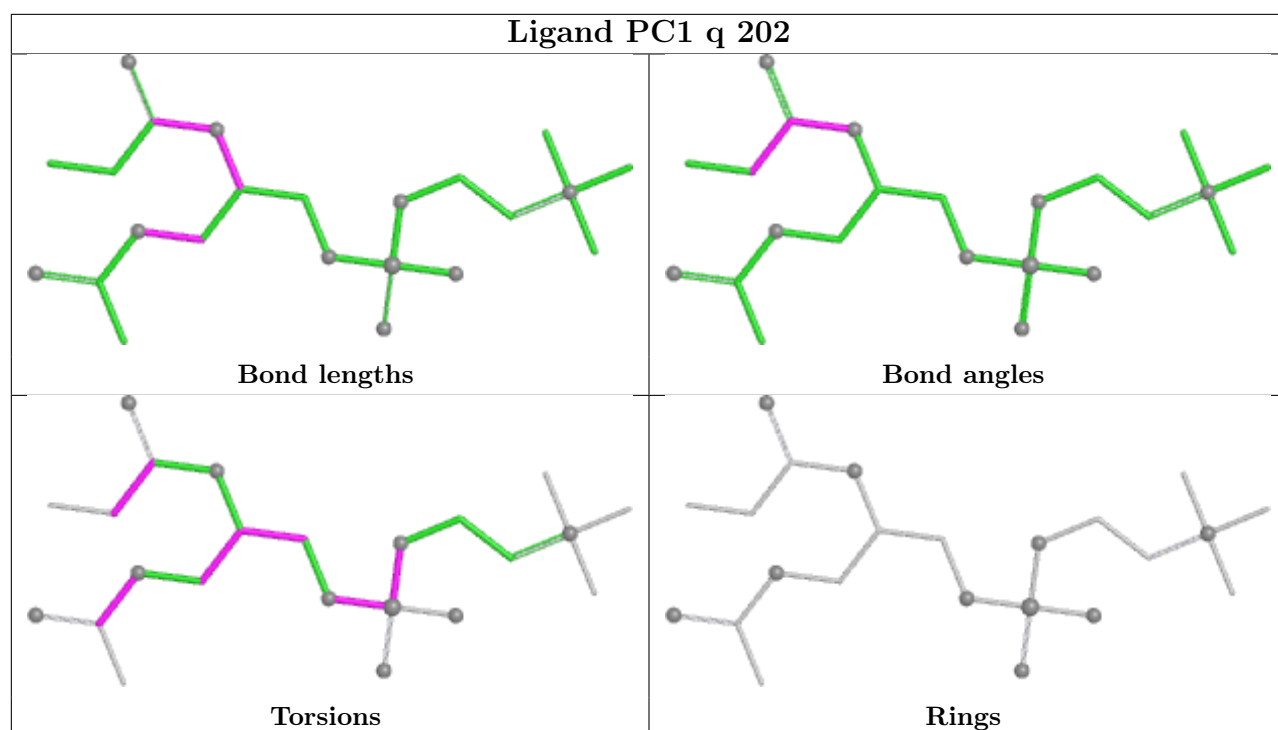


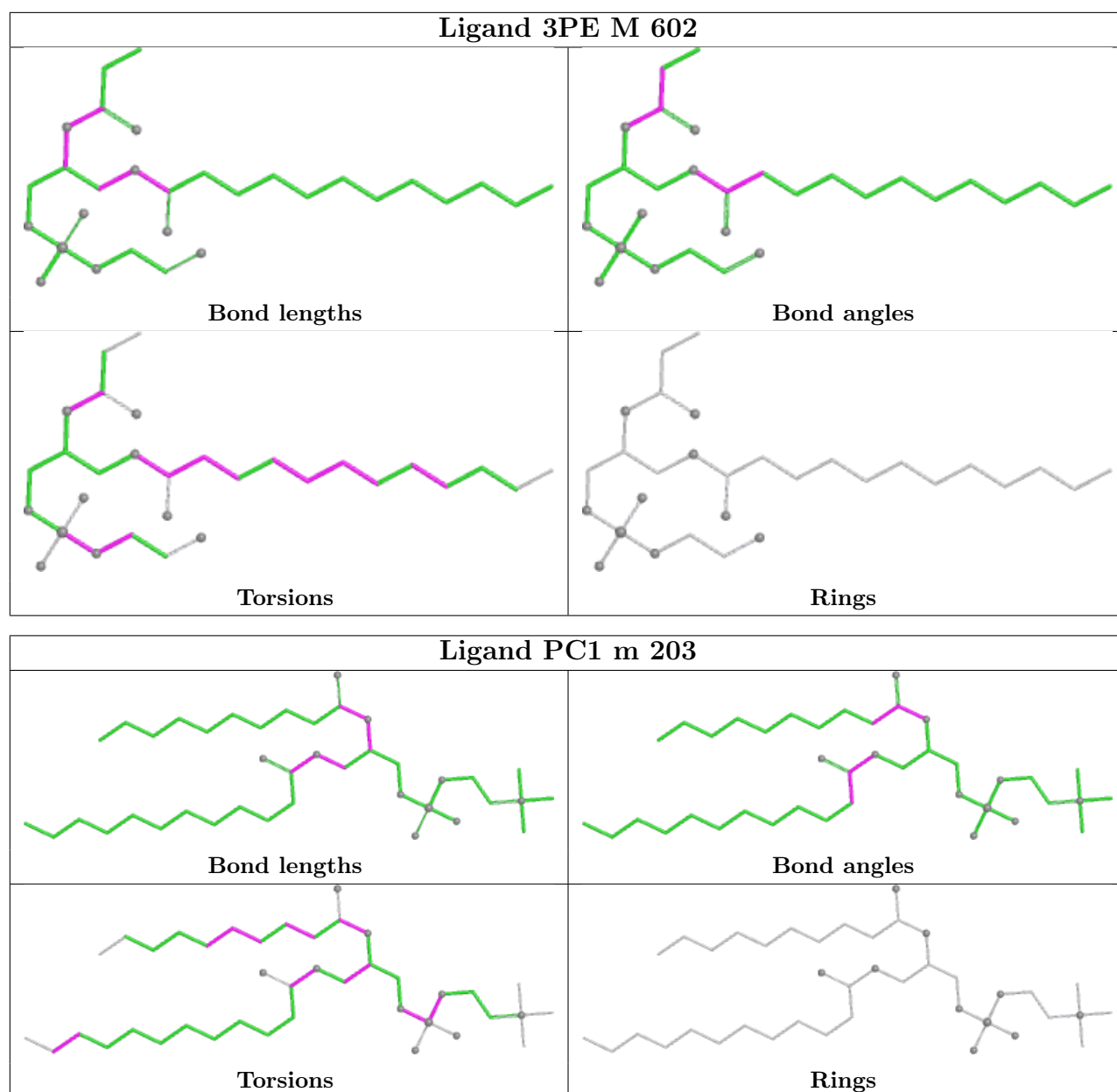


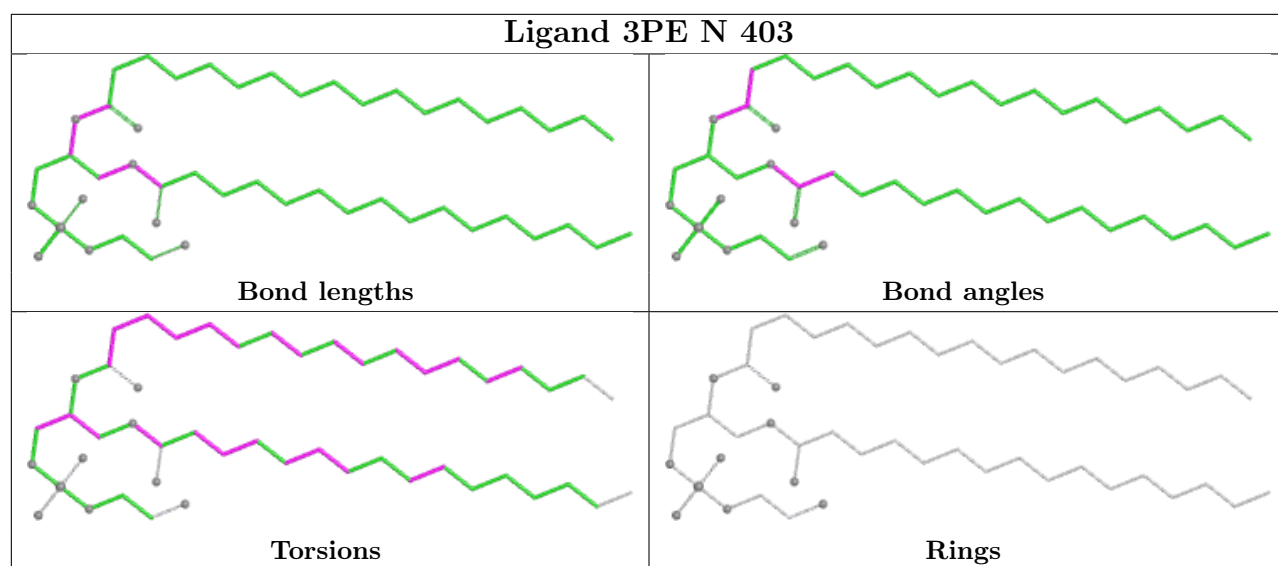


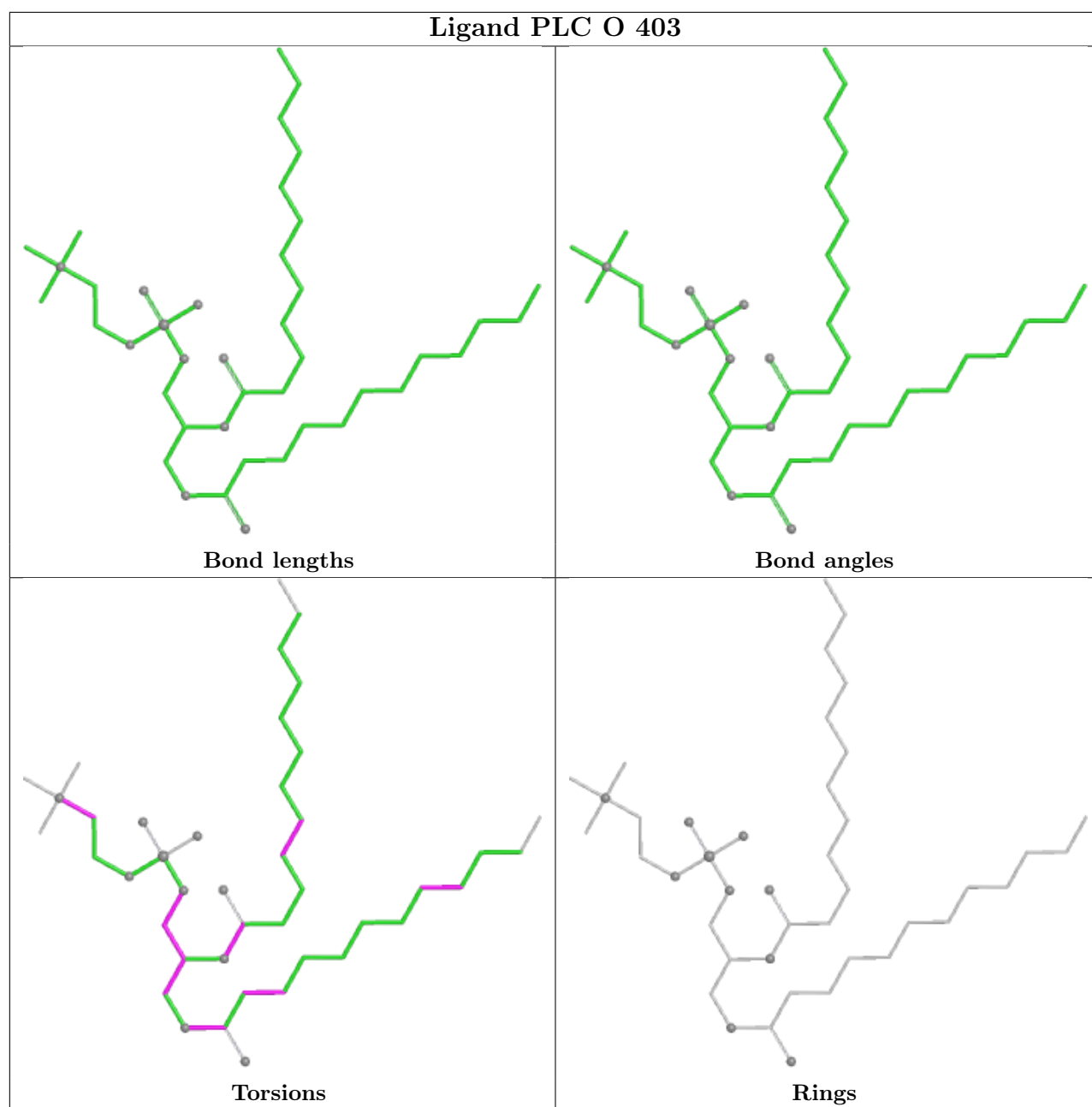


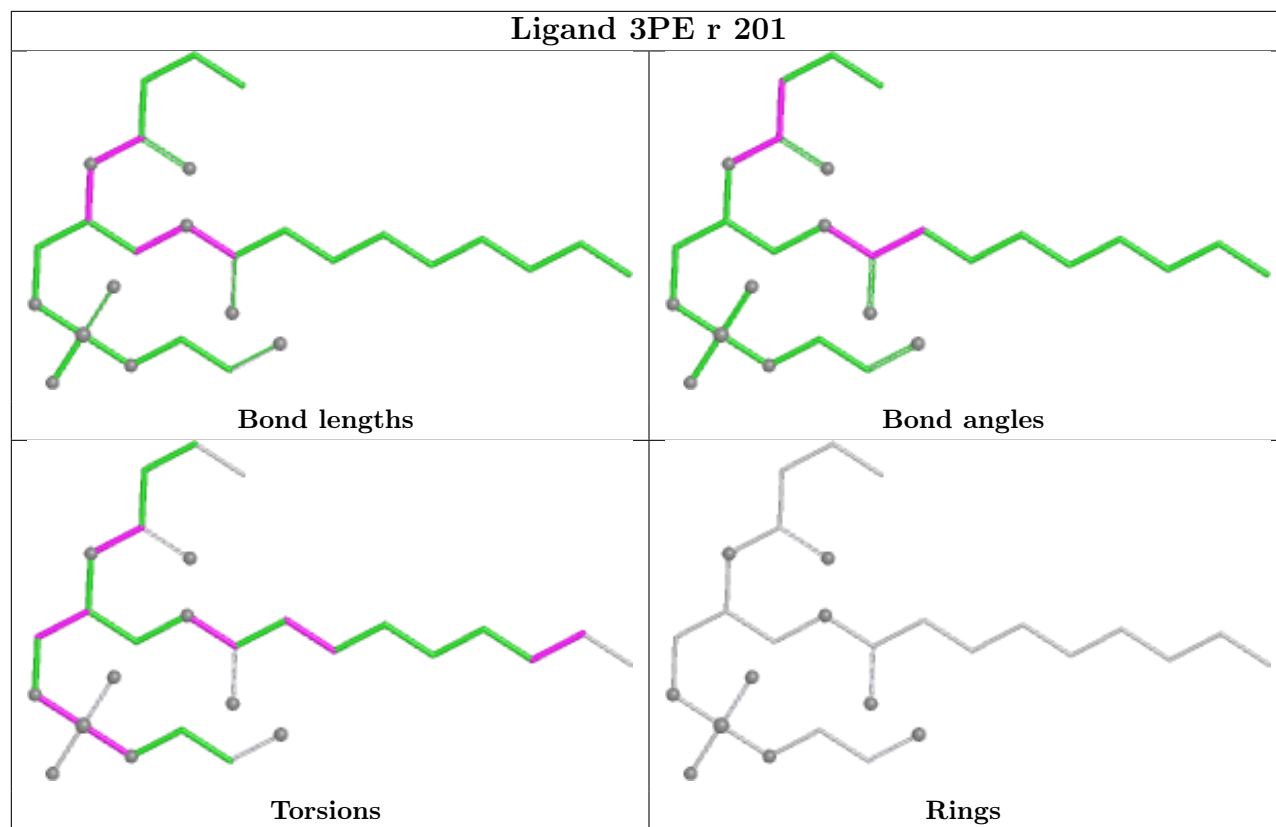


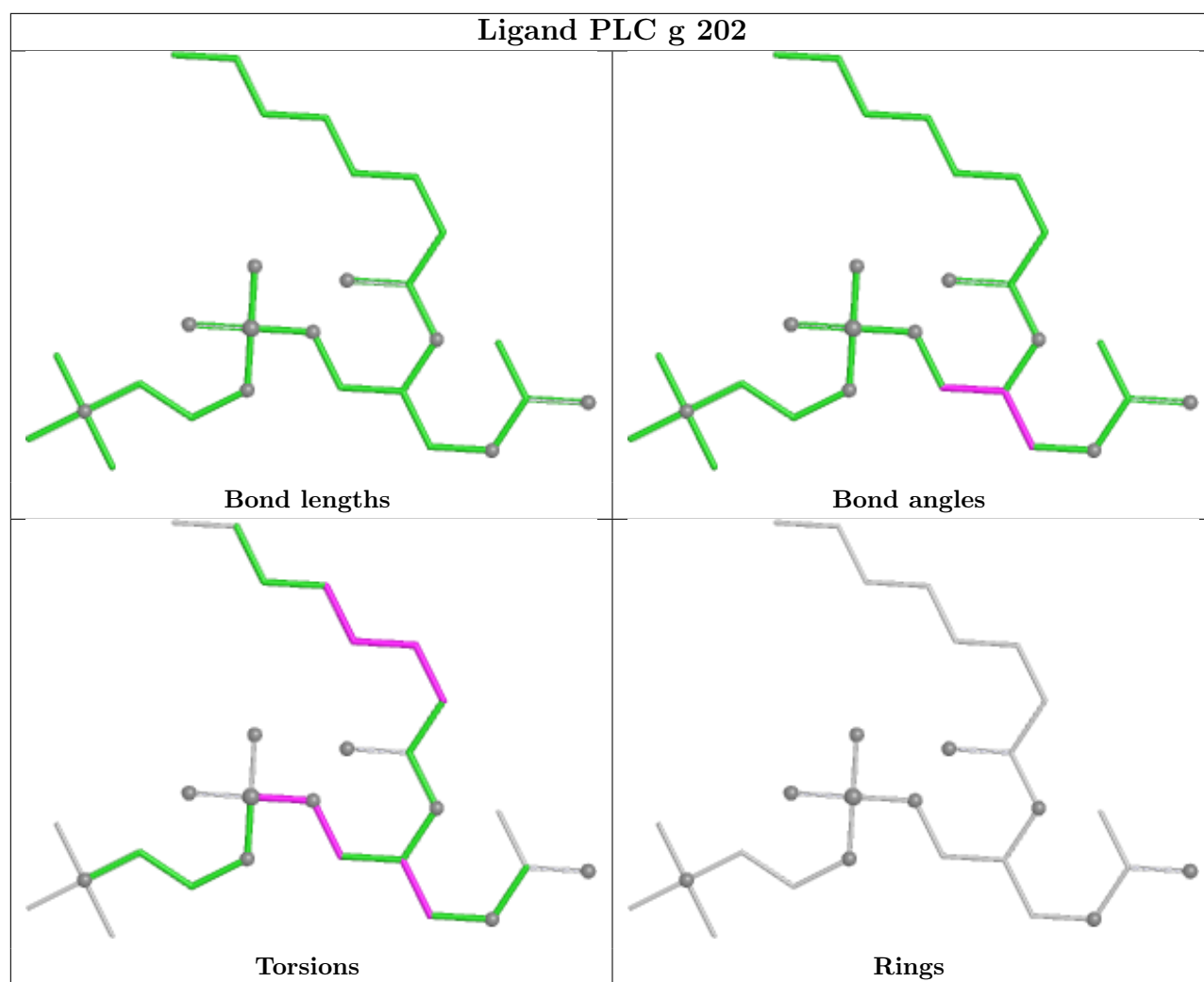












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

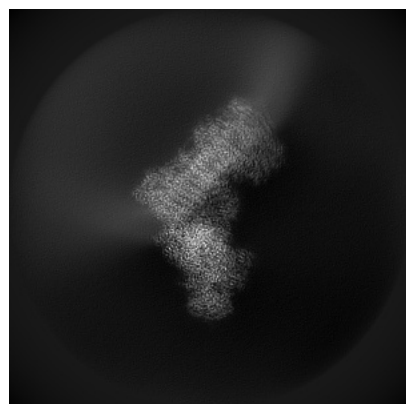
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18068. These allow visual inspection of the internal detail of the map and identification of artifacts.

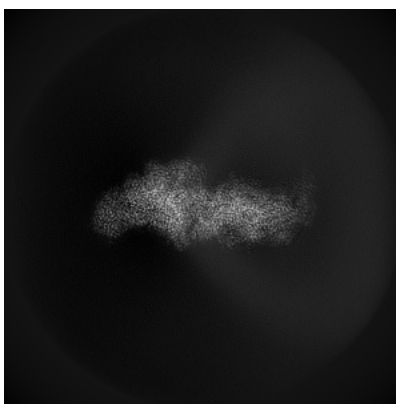
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

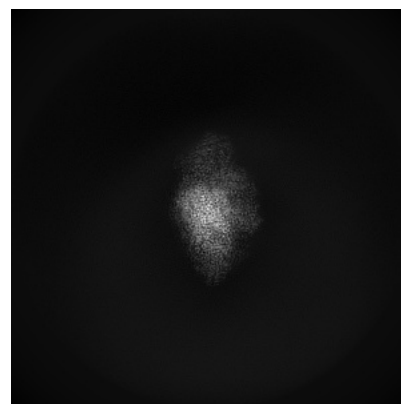
6.1.1 Primary map



X

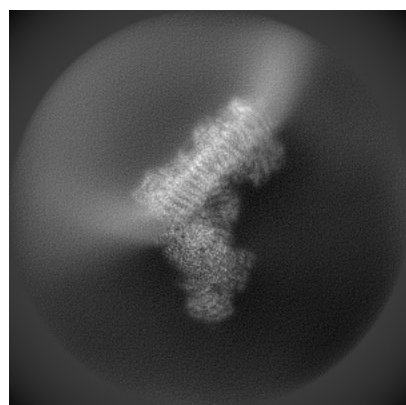


Y

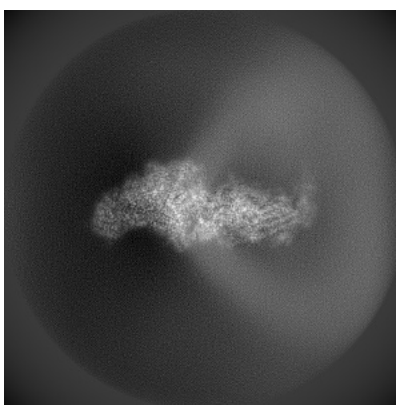


Z

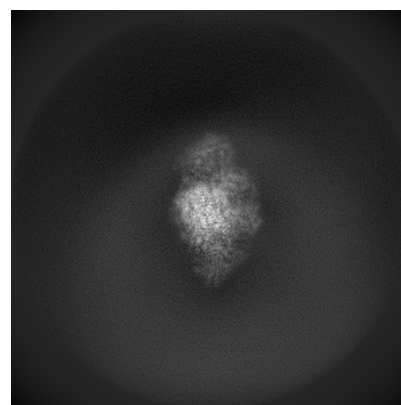
6.1.2 Raw map



X



Y



Z

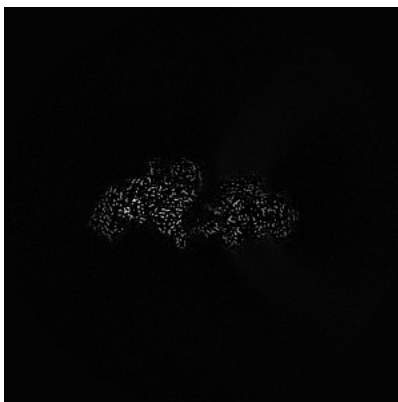
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240

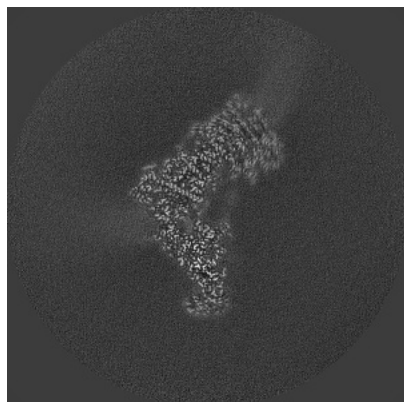


Y Index: 240

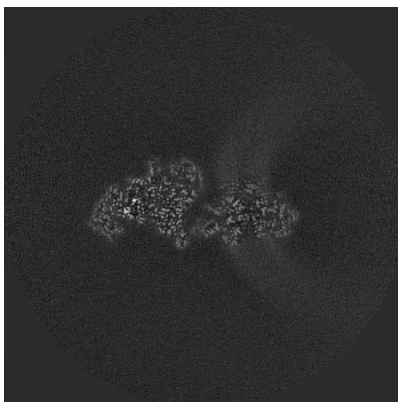


Z Index: 240

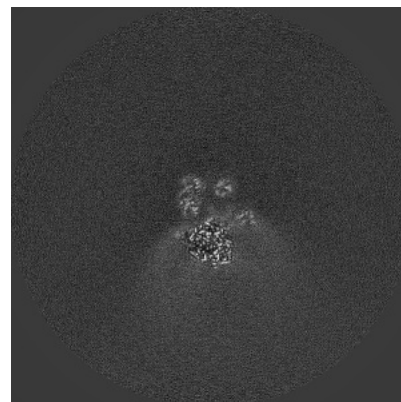
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

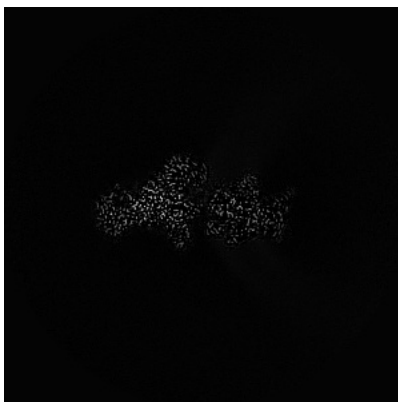
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 236

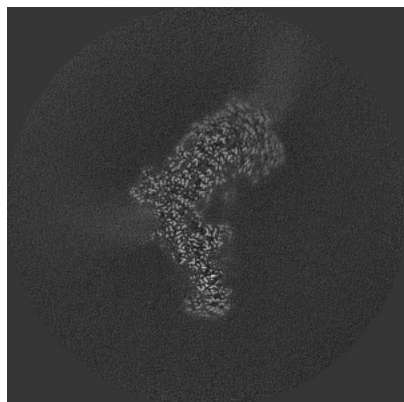


Y Index: 228

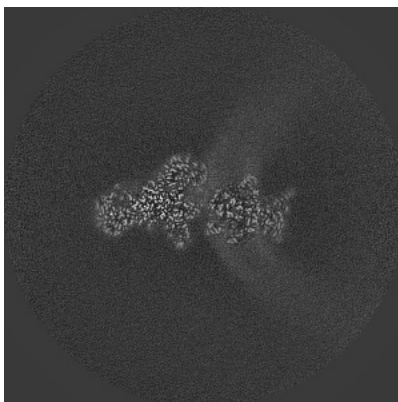


Z Index: 198

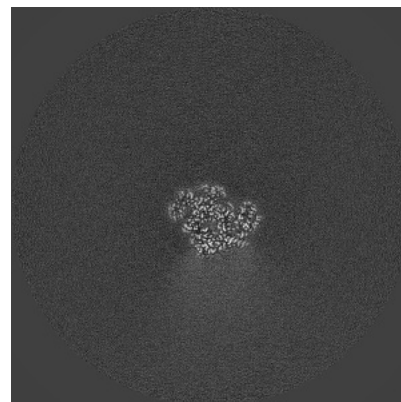
6.3.2 Raw map



X Index: 236



Y Index: 228

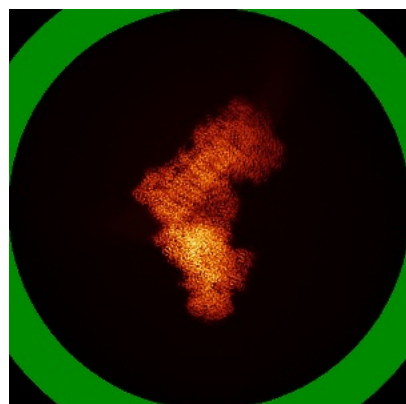


Z Index: 211

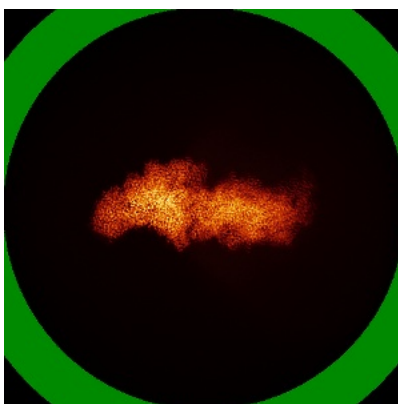
The images above show the largest variance slices of the map in three orthogonal directions.

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

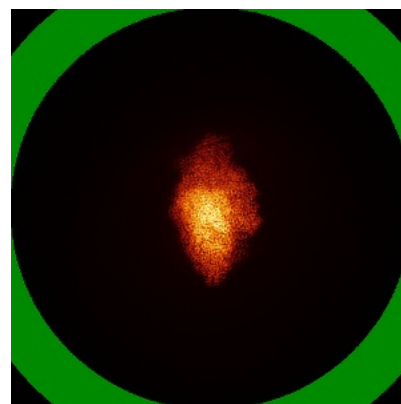
6.4.1 Primary map



X

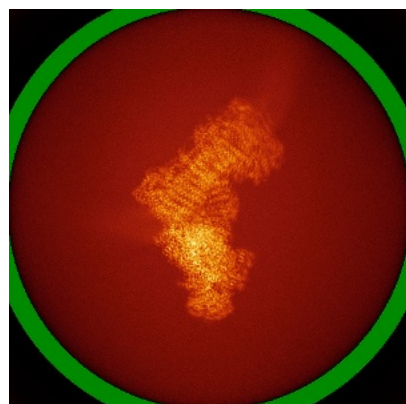


Y

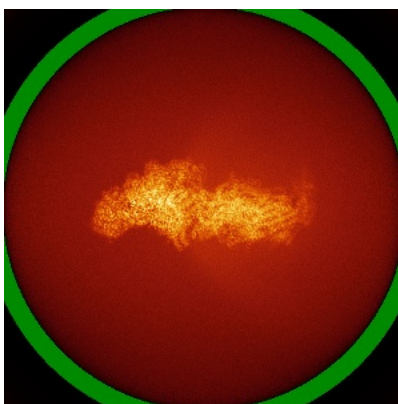


Z

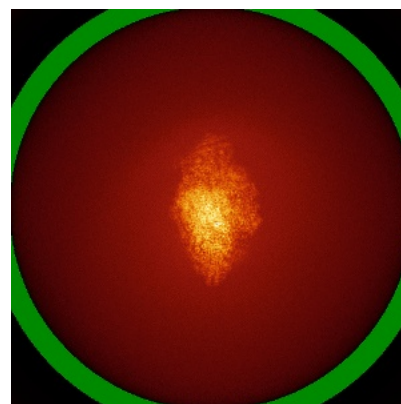
6.4.2 Raw map



X



Y

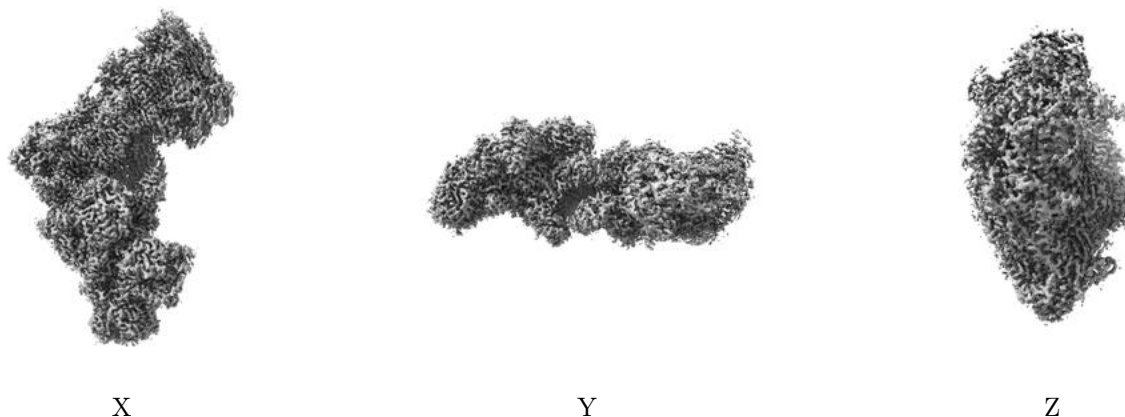


Z

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

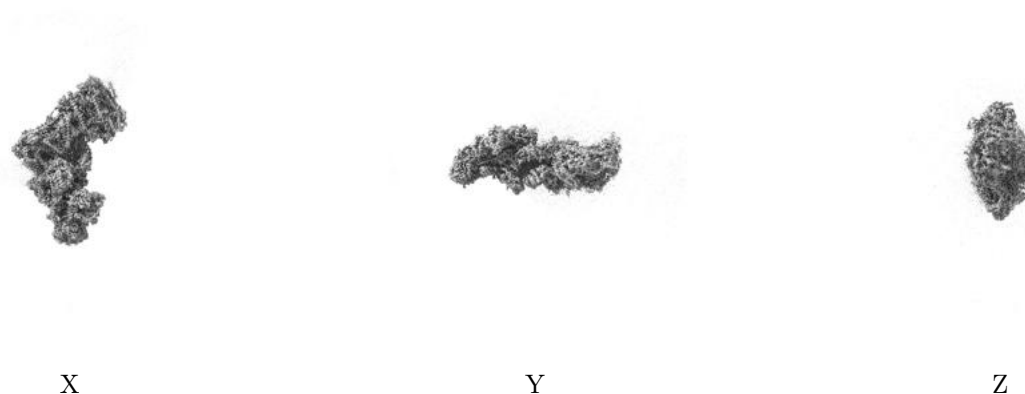
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

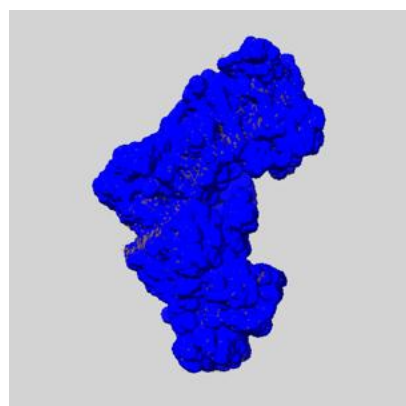
6.6 Mask visualisation [i](#)

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

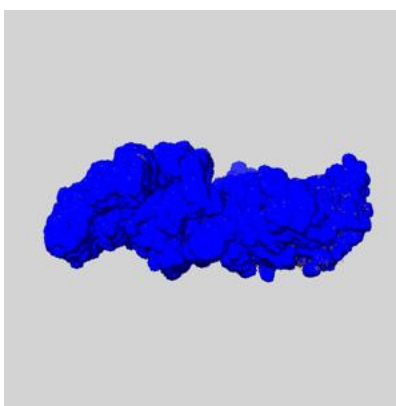
A mask typically either:

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

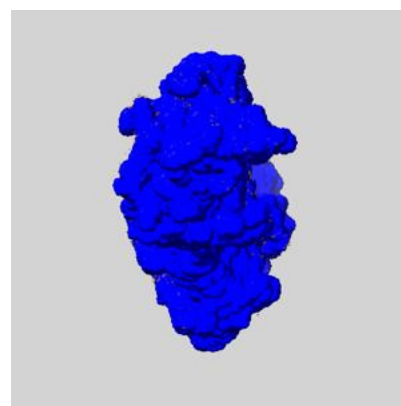
6.6.1 emd_18068_msk_1.map [i](#)



X



Y

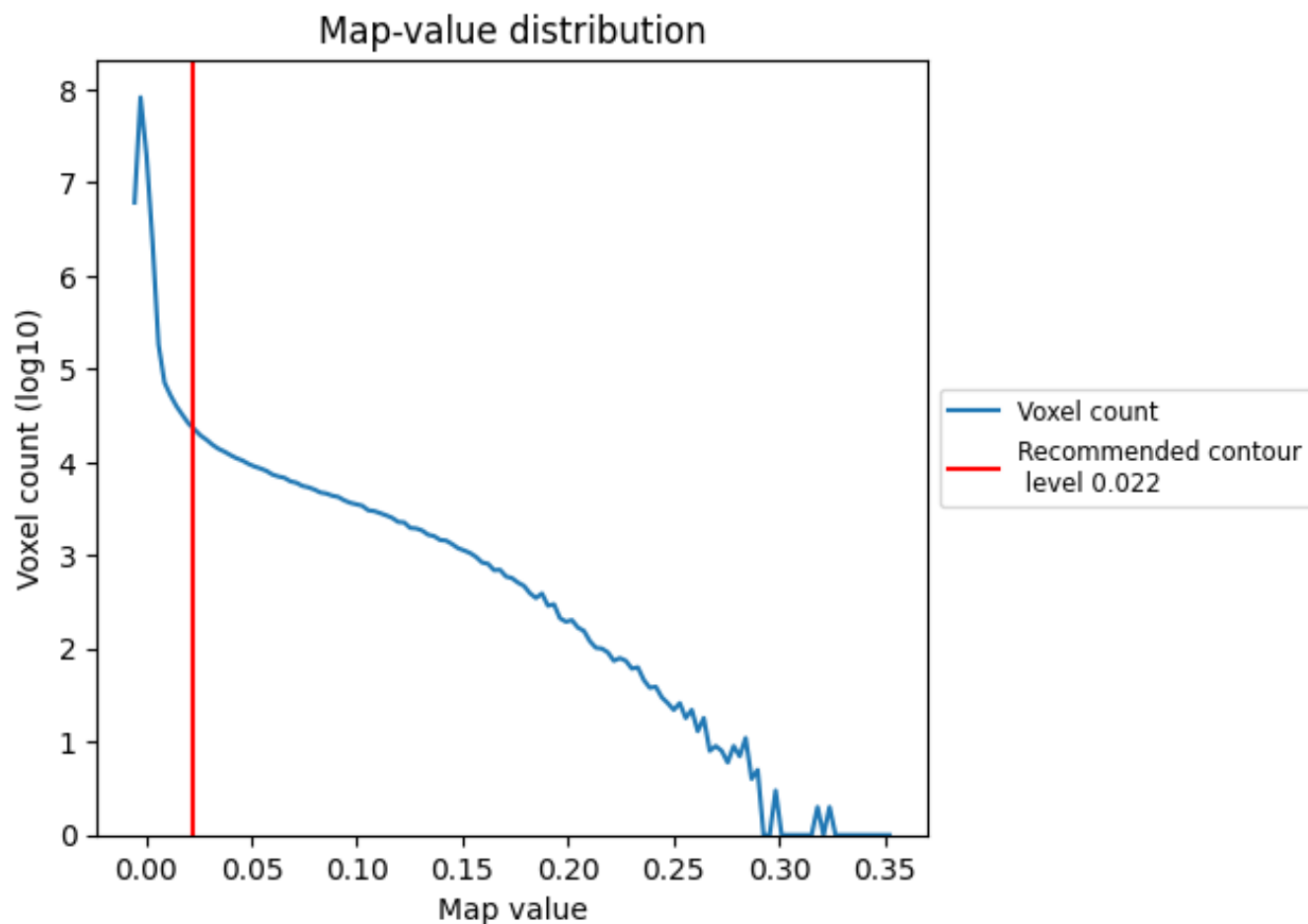


Z

7 Map analysis [i](#)

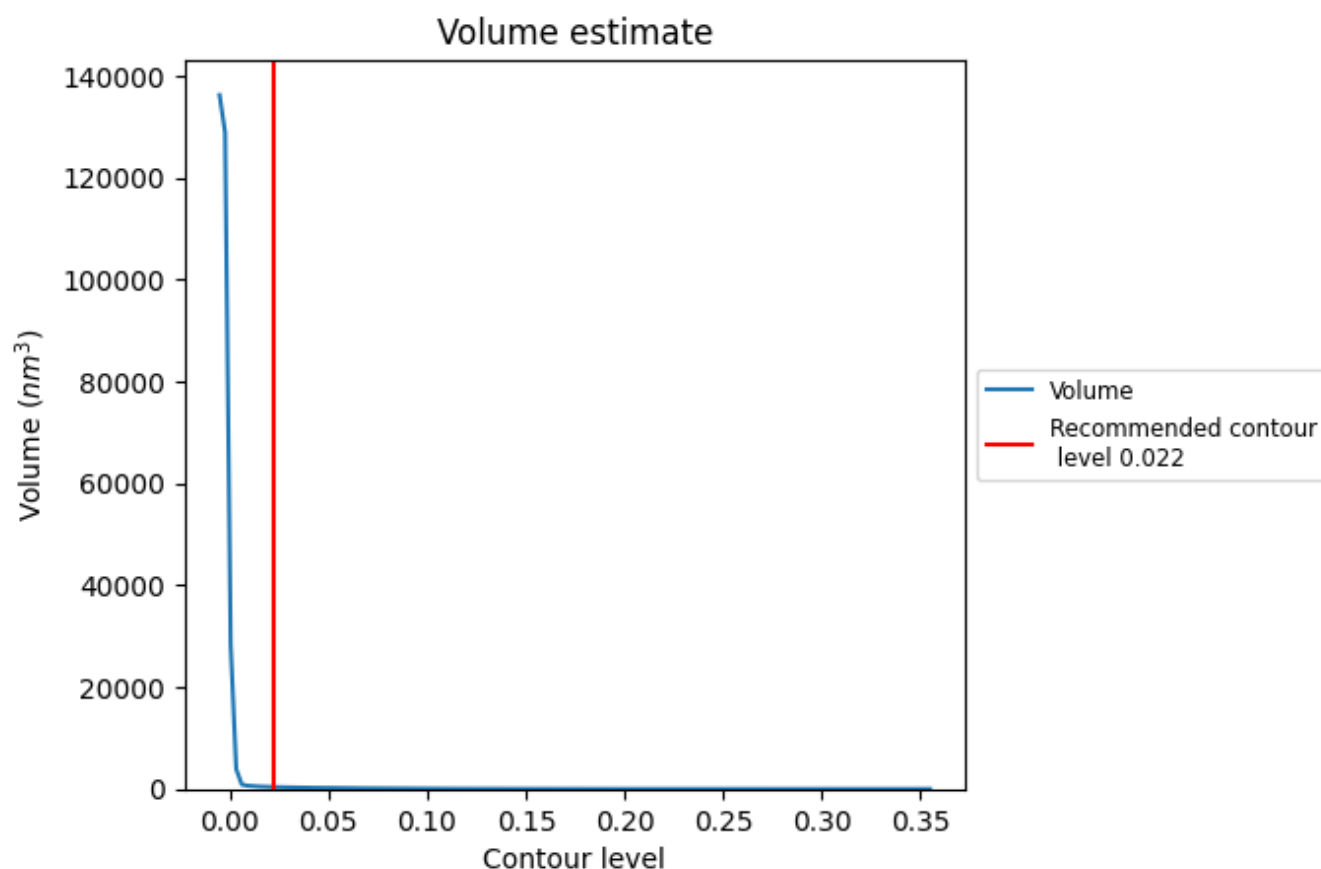
This section contains the results of statistical analysis of the map.

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.

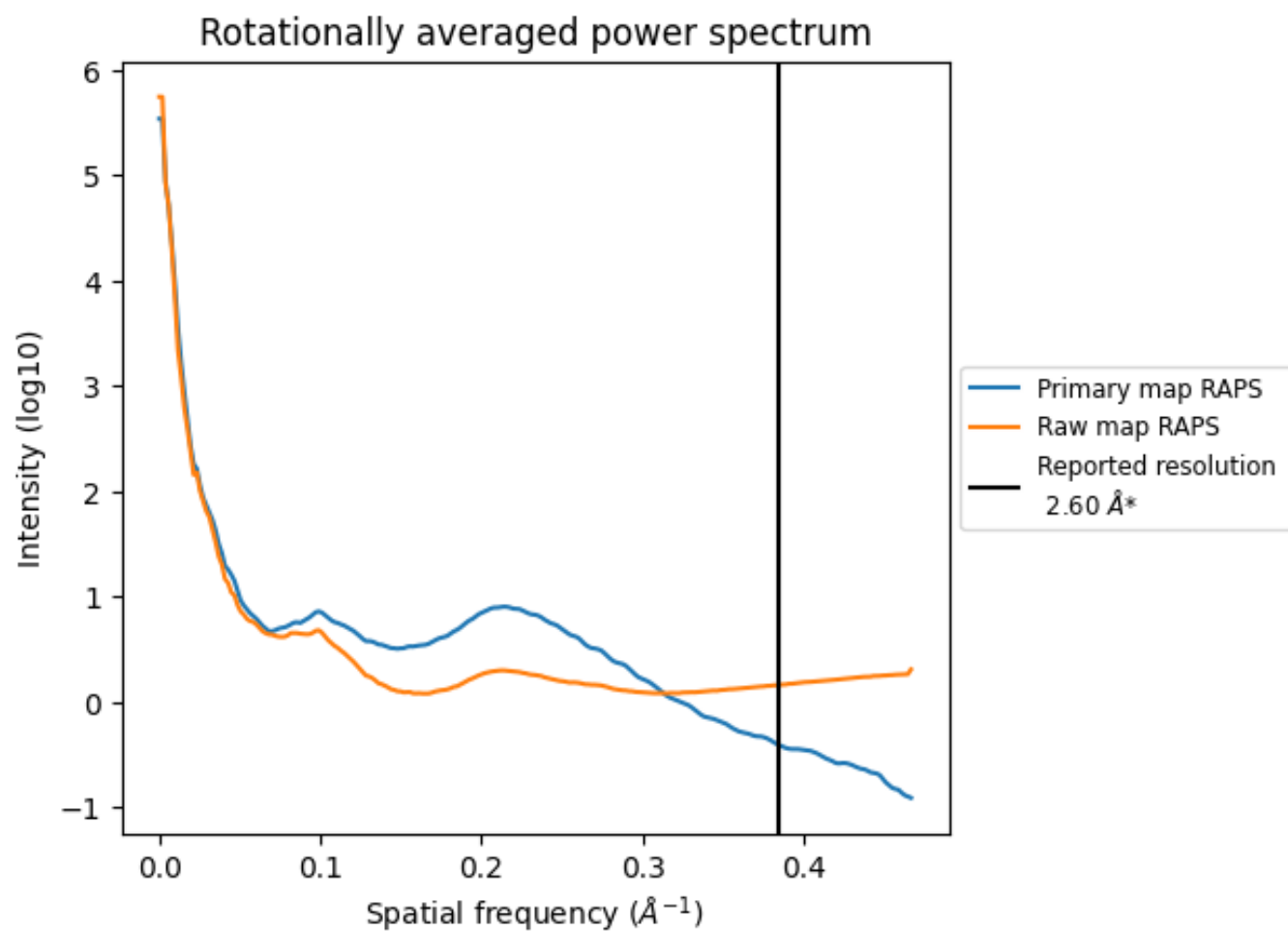
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm^3 ; this corresponds to an approximate mass of 341 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

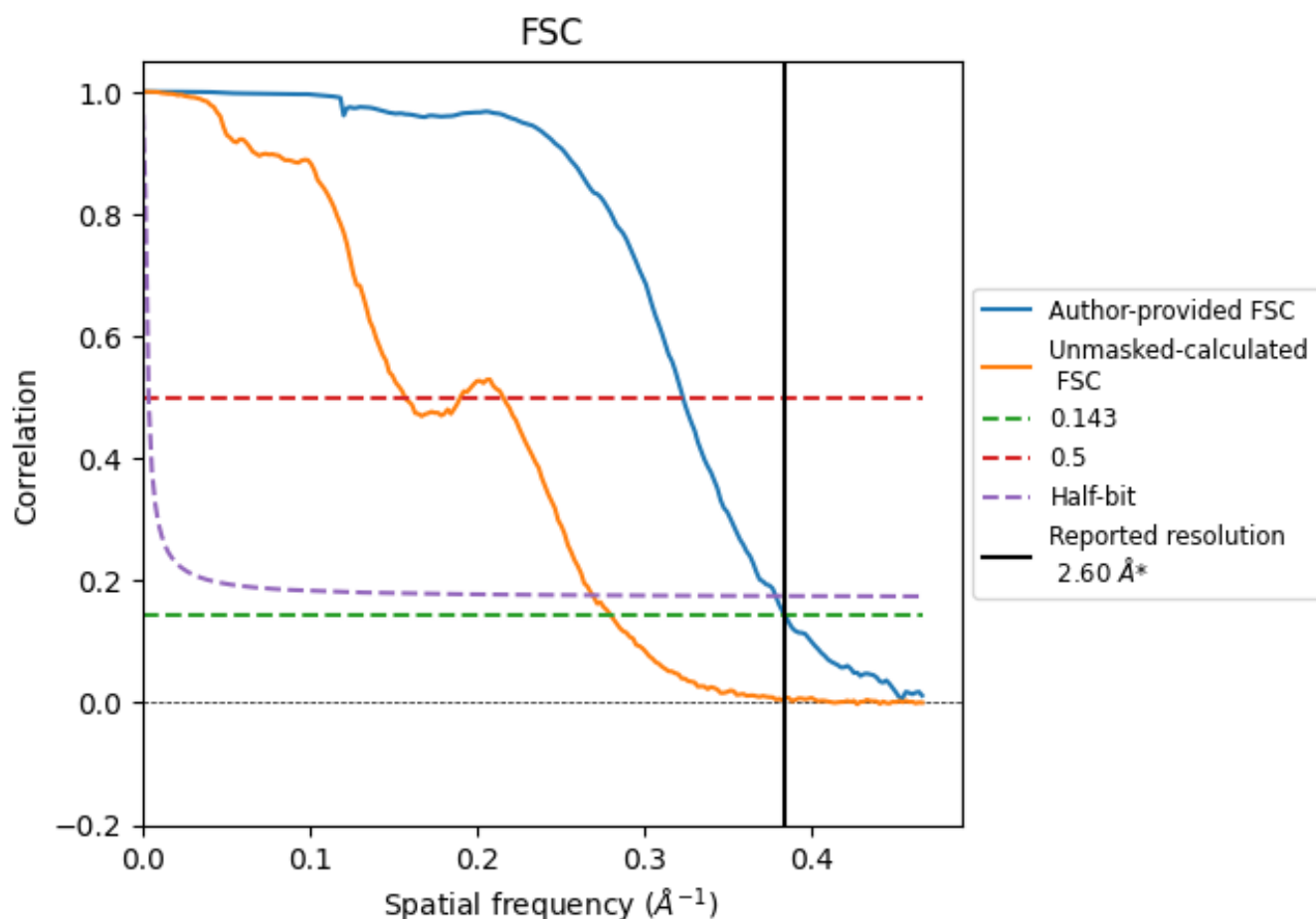


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

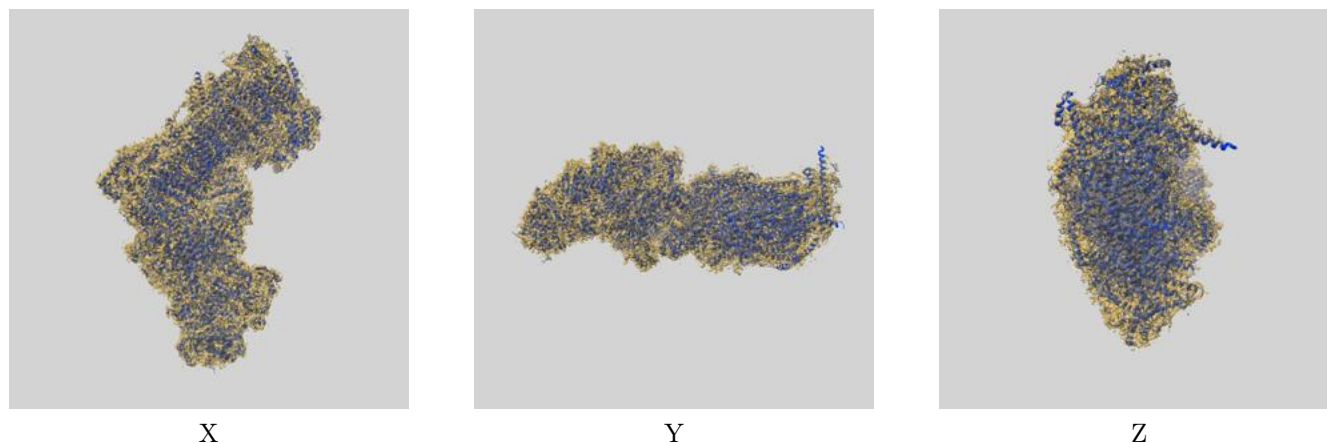
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.60	3.09	2.64
Unmasked-calculated*	3.57	6.37	3.71

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

9 Map-model fit [i](#)

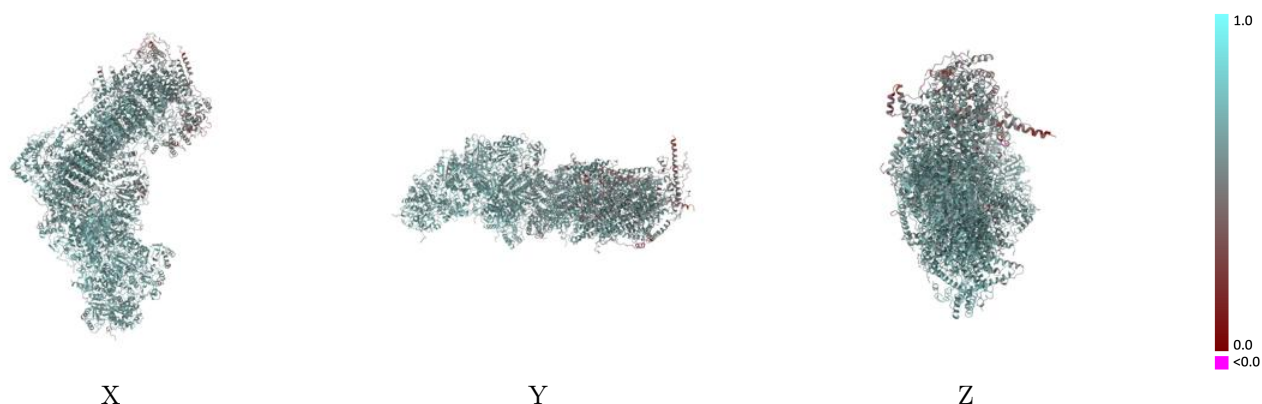
This section contains information regarding the fit between EMDB map EMD-18068 and PDB model 8Q1Y. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



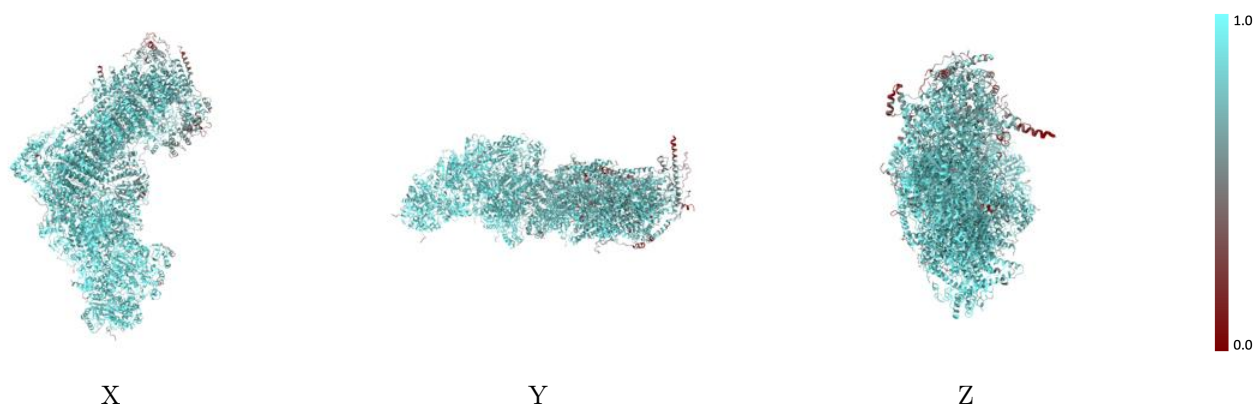
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



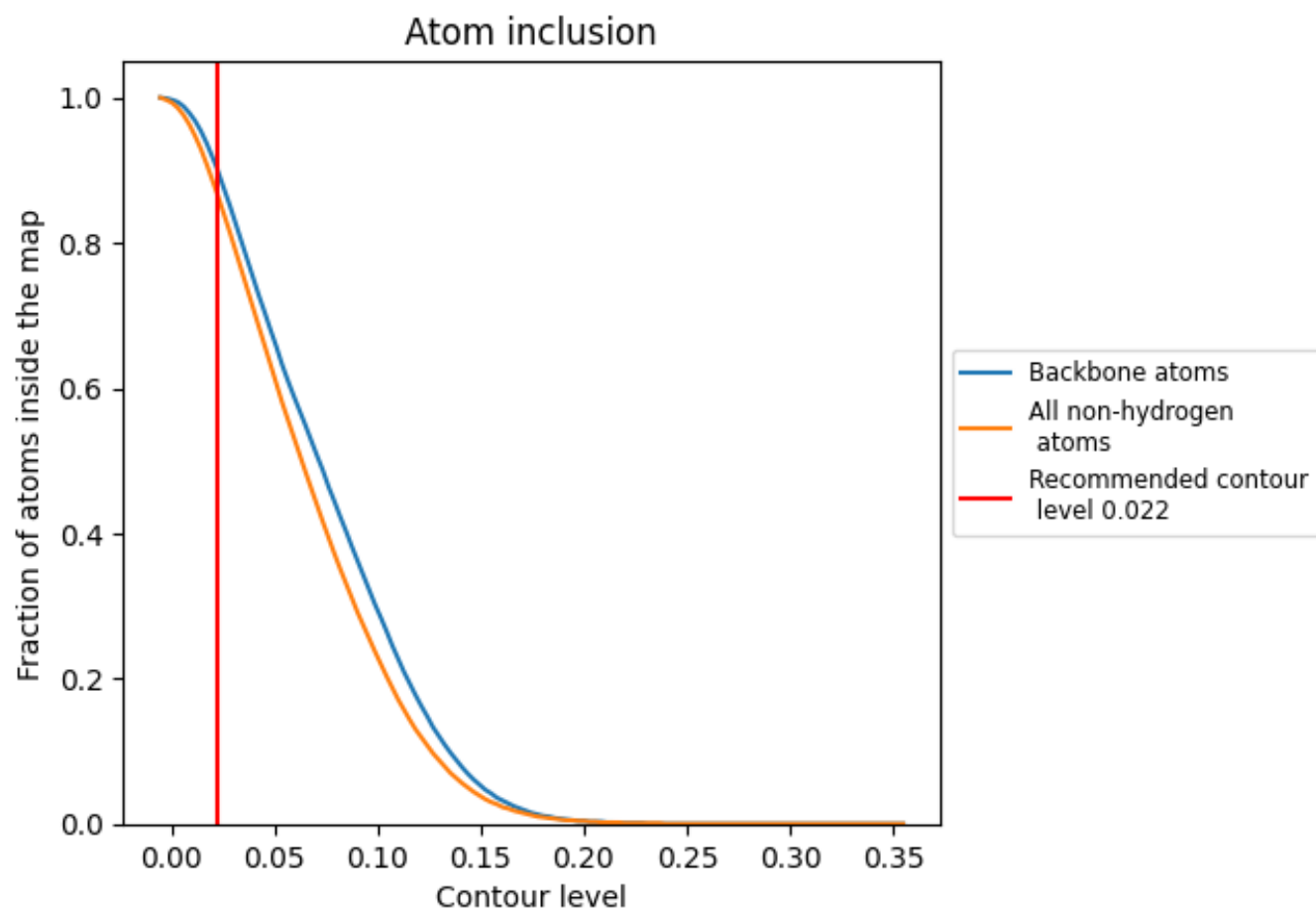
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.6140
A	 0.8780	 0.6130
B	 0.9480	 0.6720
C	 0.9660	 0.6810
D	 0.9650	 0.6770
E	 0.8900	 0.6190
F	 0.9150	 0.6310
G	 0.9230	 0.6480
H	 0.9340	 0.6480
I	 0.9730	 0.6840
J	 0.8890	 0.6210
K	 0.9590	 0.6620
L	 0.8520	 0.5900
M	 0.9430	 0.6520
N	 0.9630	 0.6670
O	 0.8380	 0.5960
P	 0.8750	 0.6160
Q	 0.9230	 0.6570
R	 0.9160	 0.6460
S	 0.7960	 0.5780
T	 0.6970	 0.5290
U	 0.5960	 0.4500
V	 0.9050	 0.6380
W	 0.9080	 0.6390
X	 0.8930	 0.6270
Y	 0.8240	 0.5950
Z	 0.8960	 0.6340
a	 0.9490	 0.6540
b	 0.8680	 0.6220
c	 0.8350	 0.5970
d	 0.8810	 0.6220
e	 0.8690	 0.6230
f	 0.6930	 0.5300
g	 0.8010	 0.5790
h	 0.8950	 0.6270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6170	 0.4760
j	 0.5810	 0.4600
k	 0.4870	 0.4200
l	 0.7730	 0.5390
m	 0.7820	 0.5620
n	 0.7260	 0.5070
o	 0.5070	 0.4100
p	 0.7670	 0.5590
q	 0.9280	 0.6530
r	 0.9330	 0.6520
s	 0.7960	 0.5740