



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:45 PM UTC

PDB ID : 8Q25 / pdb_00008q25
EMDB ID : EMD-18069
Title : Outward-facing, open1 proteoliposome complex I at 2.8 Å, after deactivation treatment. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-01
Resolution : 2.80 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:

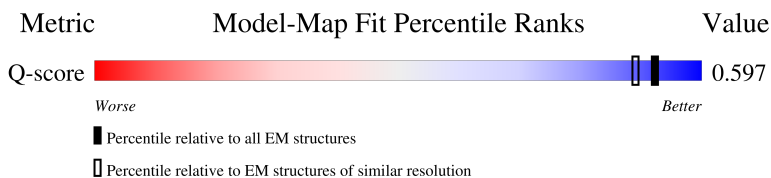
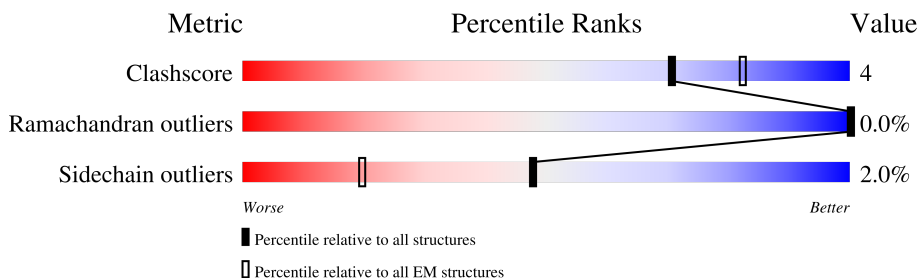
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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	11806 (2.30 - 3.30)

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	

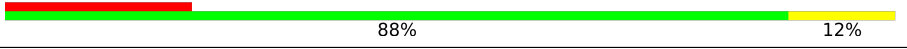
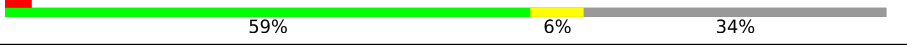
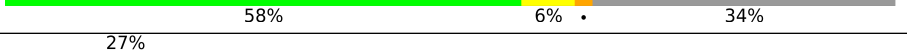
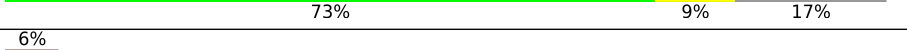
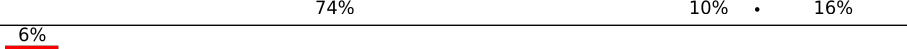
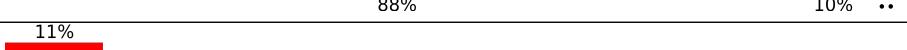
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	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 60 unique types of molecules in this entry. The entry contains 69693 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	419	Total	C	N	O	S	0	0
			3377	2159	580	613	25		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2728	1765	484	474	5		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

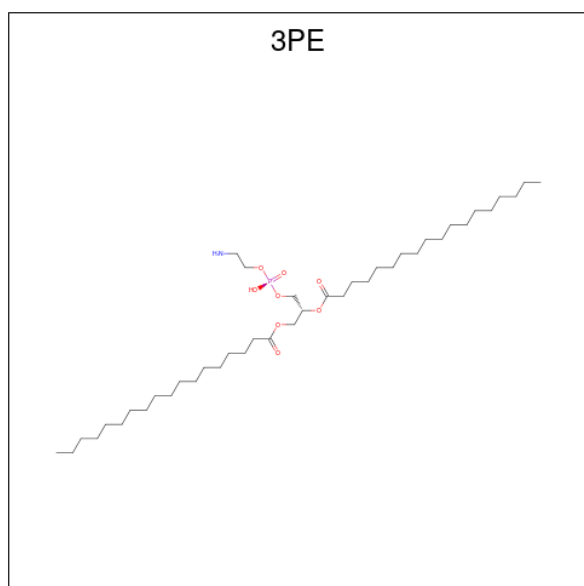
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

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



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	A	1	Total	C	N	O	P	0
			42	32	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
			37	27	1	8	1	
45	J	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	
45	L	1	Total	C	N	O	P	0
			34	24	1	8	1	

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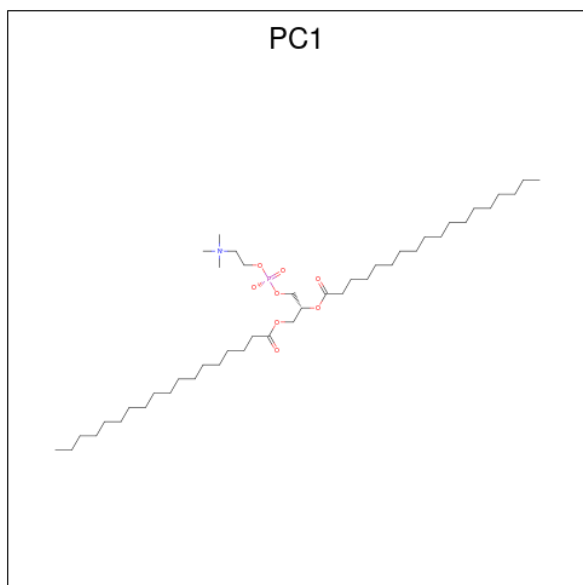
Mol	Chain	Residues	Atoms					AltConf
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45	M	1	Total 50	C 40	N 1	O 8	P 1	0
45	M	1	Total 45	C 35	N 1	O 8	P 1	0
45	N	1	Total 49	C 39	N 1	O 8	P 1	0
45	P	1	Total 38	C 28	N 1	O 8	P 1	0
45	Y	1	Total 41	C 31	N 1	O 8	P 1	0
45	Y	1	Total 27	C 17	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 45	C 35	N 1	O 8	P 1	0
45	Y	1	Total 36	C 26	N 1	O 8	P 1	0
45	Z	1	Total 42	C 32	N 1	O 8	P 1	0
45	a	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 36	C 26	N 1	O 8	P 1	0
45	b	1	Total 47	C 37	N 1	O 8	P 1	0
45	d	1	Total 49	C 39	N 1	O 8	P 1	0
45	f	1	Total 24	C 14	N 1	O 8	P 1	0
45	g	1	Total 29	C 19	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0
45	q	1	Total 51	C 41	N 1	O 8	P 1	0

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

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



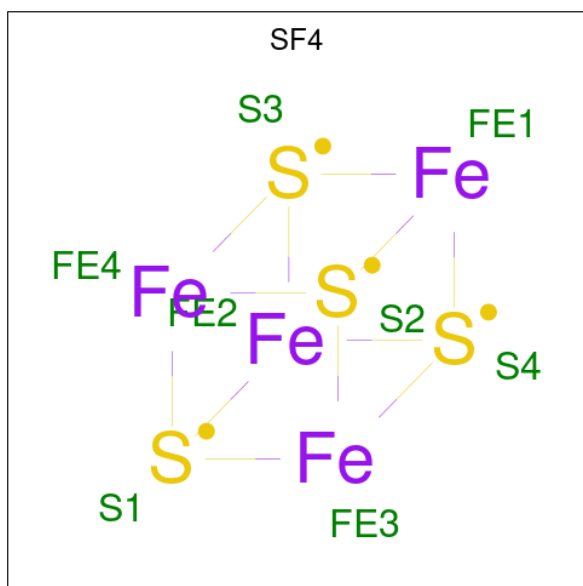
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	M	1	Total	C	N	O	P	0
			44	34	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	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	l	1	Total	C	N	O	P	0
			47	37	1	8	1	
46	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	q	1	Total	C	N	O	P	0
			49	39	1	8	1	

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



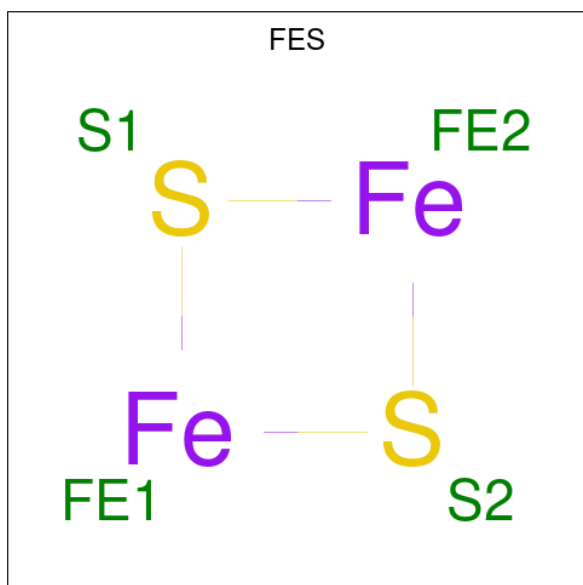
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	

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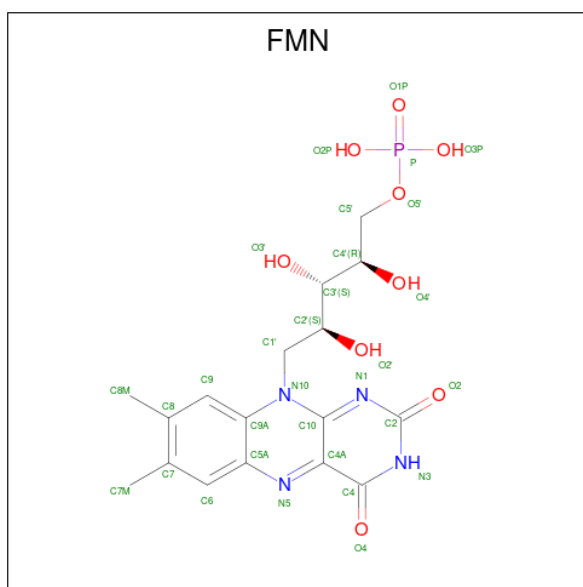
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

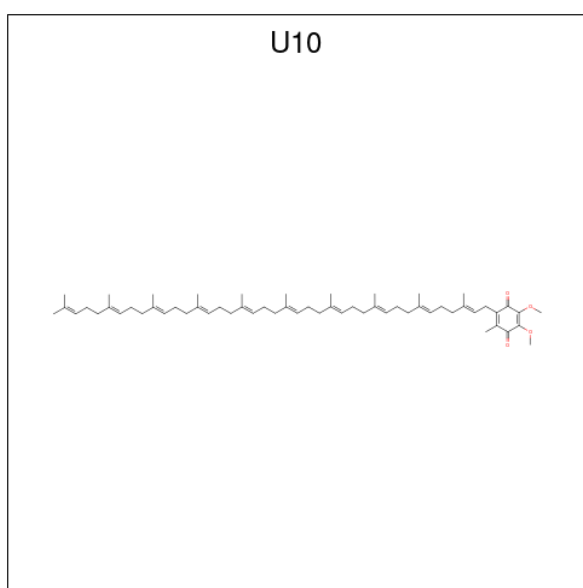


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

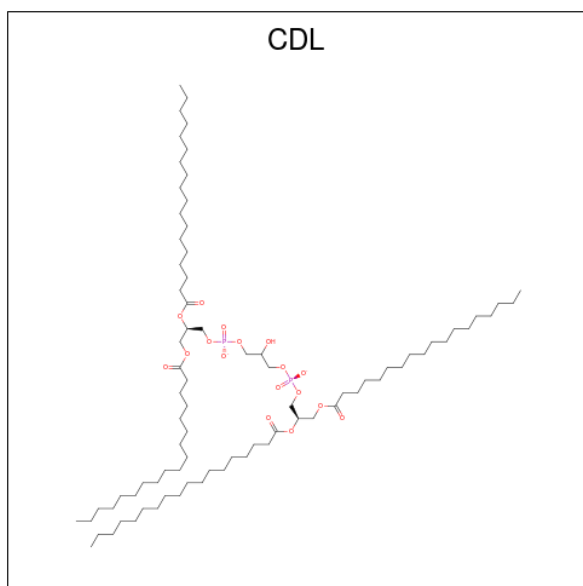
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



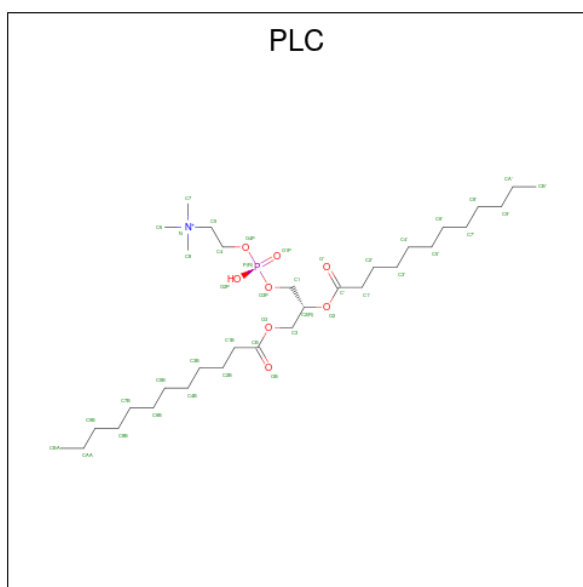
Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			34	30	4	

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



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

- Molecule 53 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
53	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	M	1	Total	C	N	O	P	0
			34	24	1	8	1	
53	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
53	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
53	Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
53	Z	1	Total	C	N	O	P	0
			36	26	1	8	1	
53	b	1	Total	C	N	O	P	0
			38	28	1	8	1	
53	g	1	Total	C	N	O	P	0
			42	32	1	8	1	

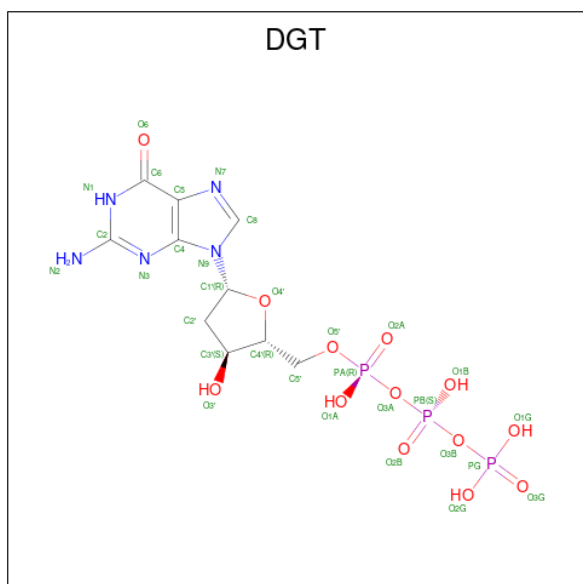
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

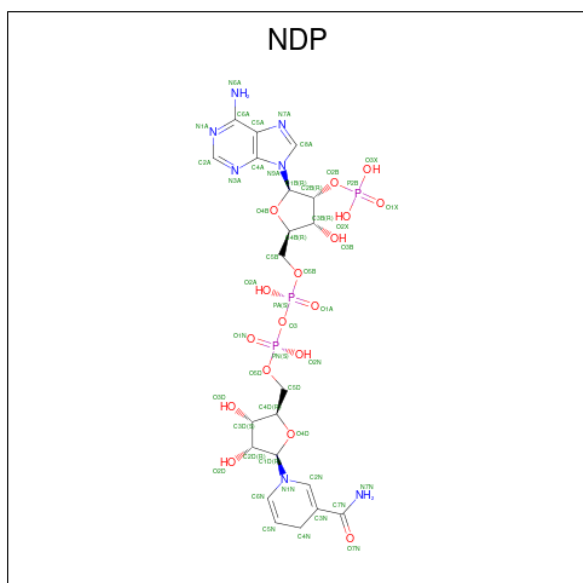
Mol	Chain	Residues	Atoms		AltConf
55	O	1	Total 1	Mg 1	0

- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



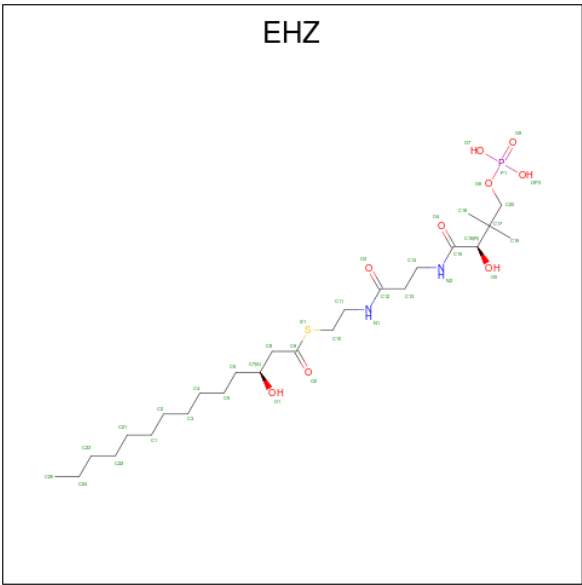
Mol	Chain	Residues	Atoms					AltConf
56	O	1	Total 31	C 10	N 5	O 13	P 3	0

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



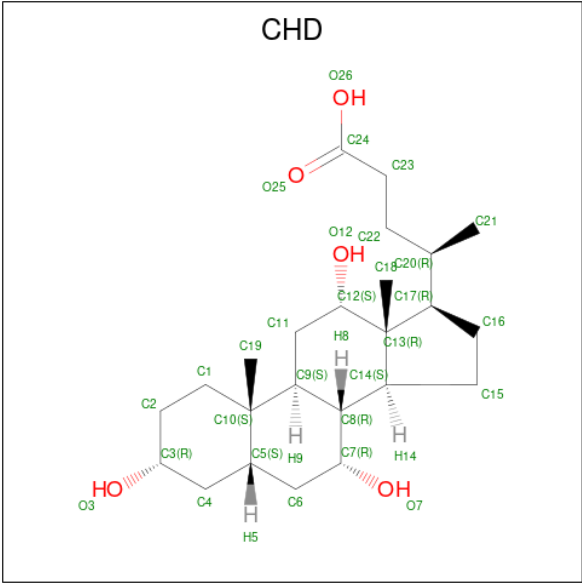
Mol	Chain	Residues	Atoms					AltConf
57	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 58 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



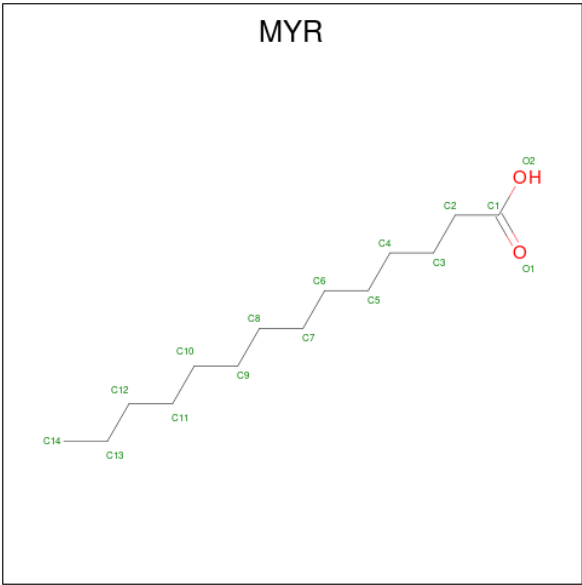
Mol	Chain	Residues	Atoms						AltConf
58	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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



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

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



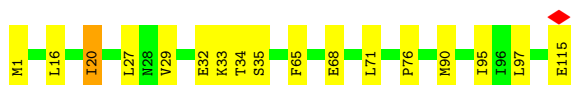
Mol	Chain	Residues	Atoms			AltConf
60	o	1	Total	C	O	0
			15	14	1	

3 Residue-property plots [i](#)

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

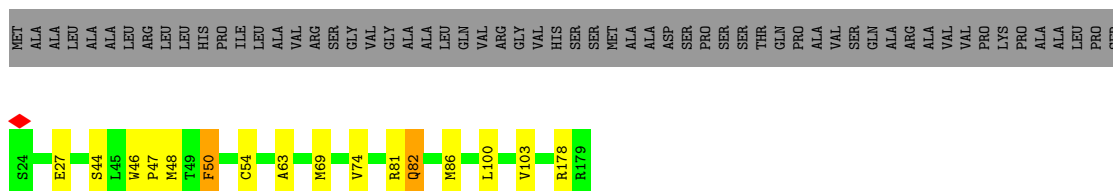
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



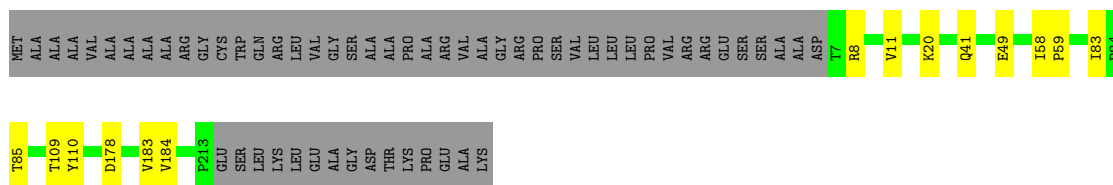
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



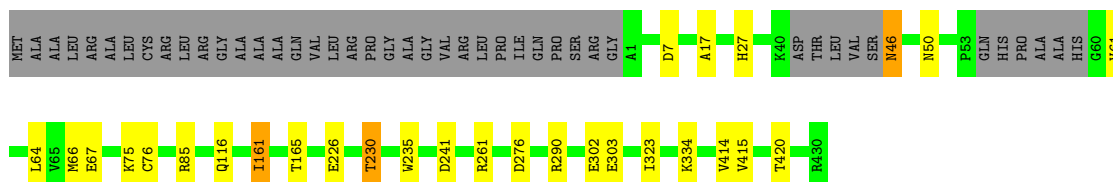
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



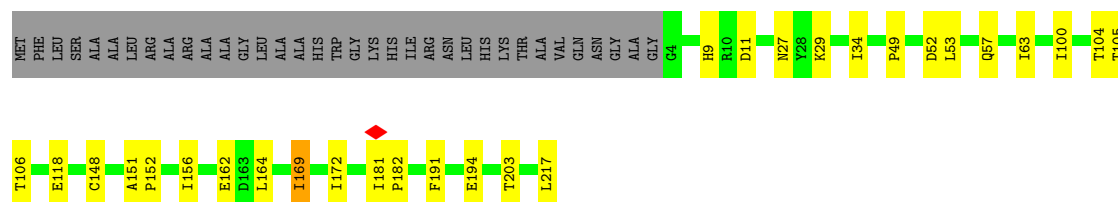
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 



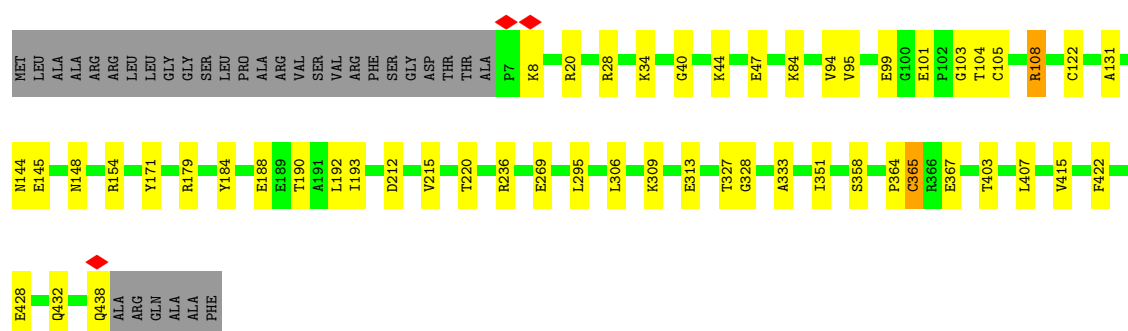
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  74% 11% 14%



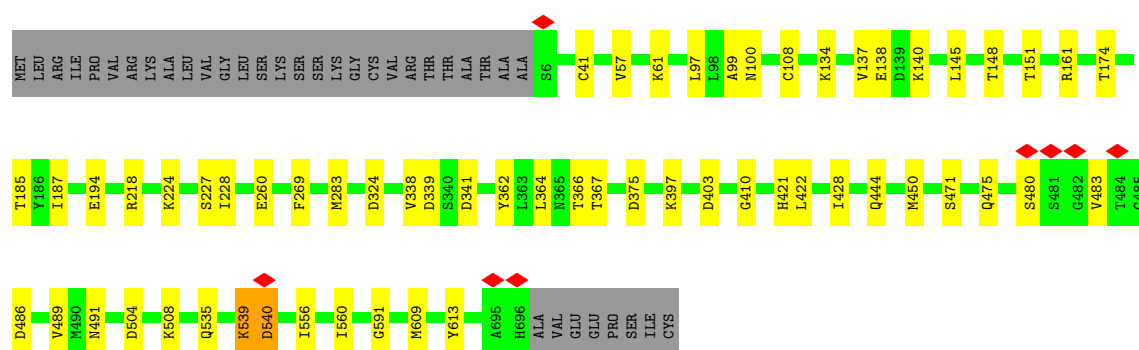
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  82% 11% 7%



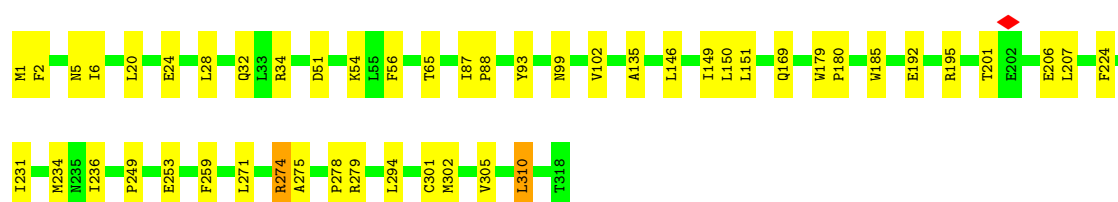
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  87% 8% 5%



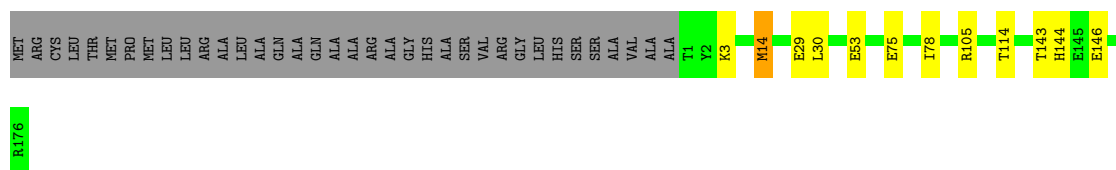
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  85% 15%



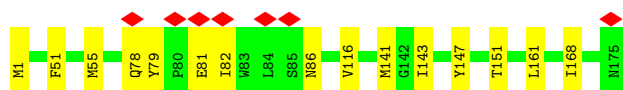
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  77% 5% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  91% 9%



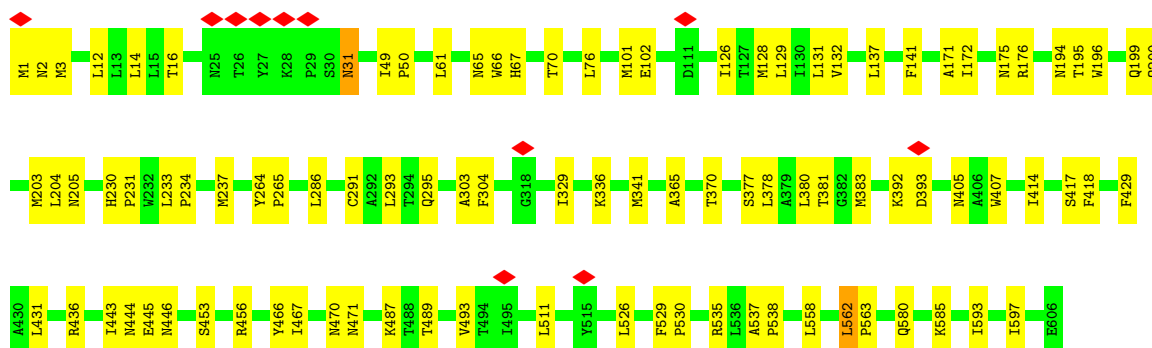
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  93% 7%

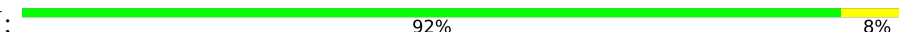


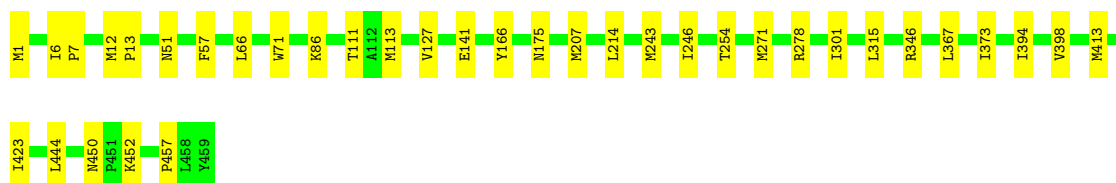
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  84% 16%



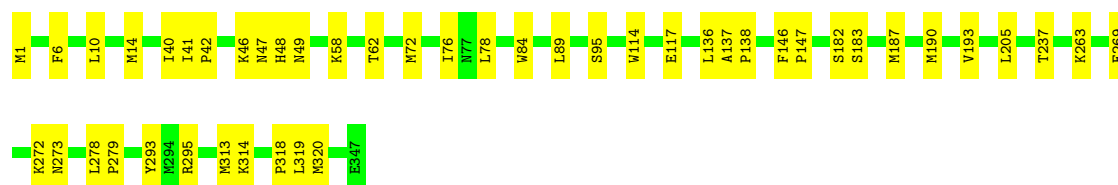
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  92% 8%



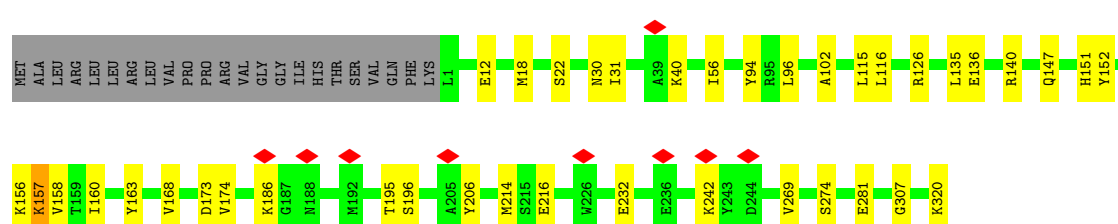
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  87% 13%



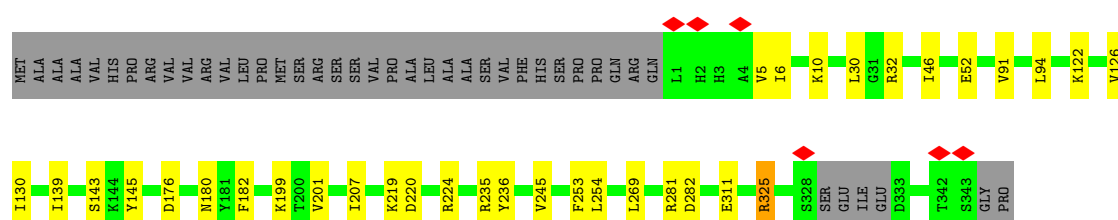
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  82% 11% 7%



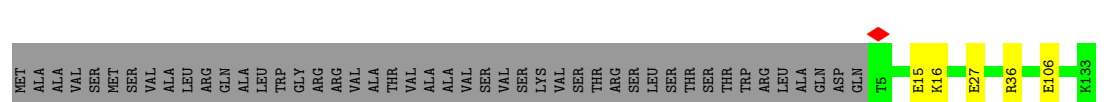
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  80% 9% 11%



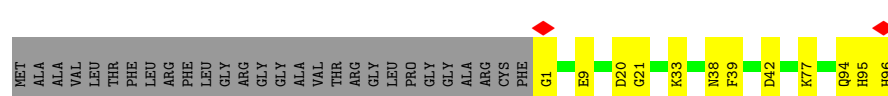
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  71% 26%

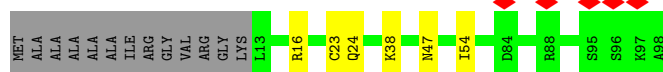
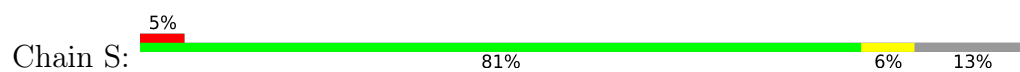


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

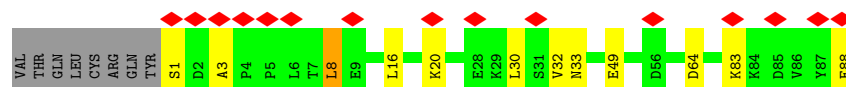
Chain R:  68% 10% 23%



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



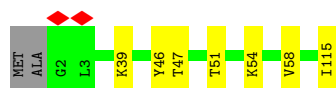
- Molecule 20: Acyl carrier protein, mitochondrial



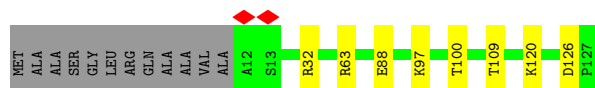
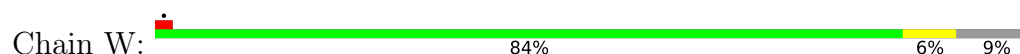
- Molecule 20: Acyl carrier protein, mitochondrial



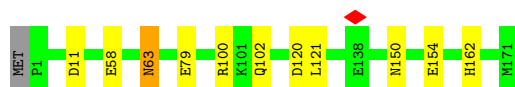
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- 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:  89% 11%



- 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:  89% 11%



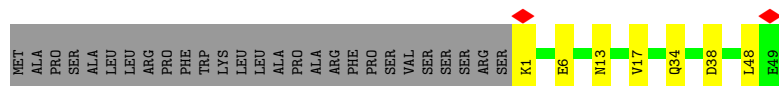
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  93% 6%



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

Chain c:  55% 9% 36%



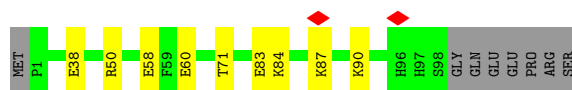
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  92% 7%

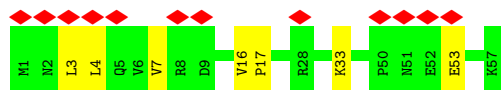
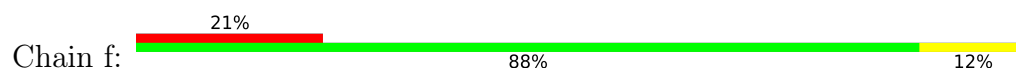


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

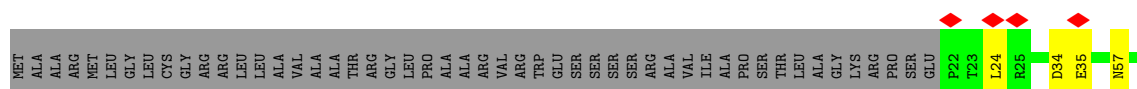
Chain e:  84% 8% 8%



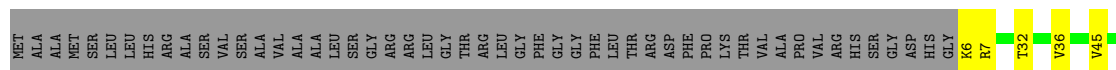
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



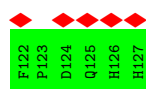
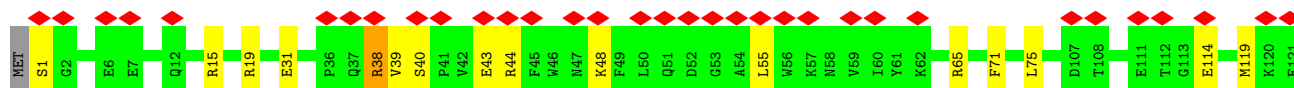
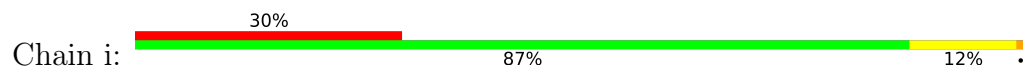
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

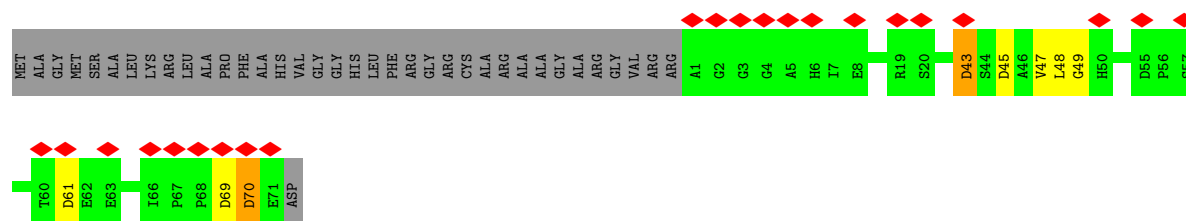


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

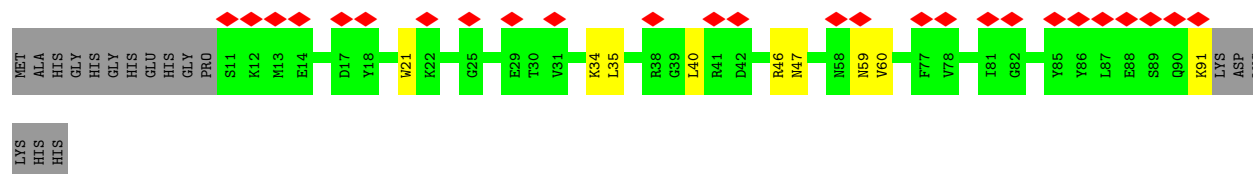
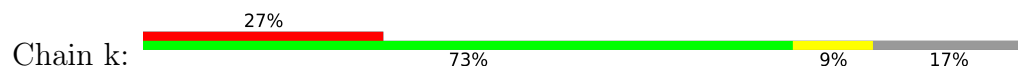


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

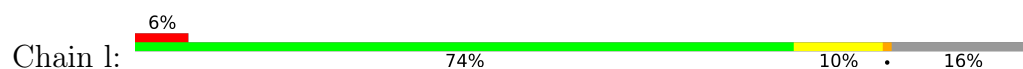




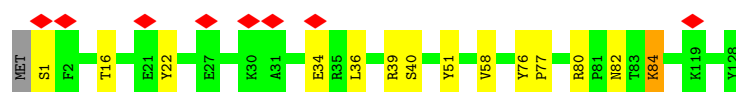
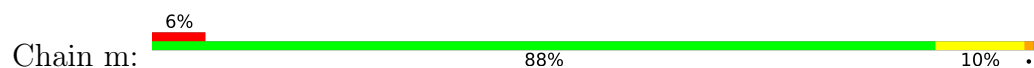
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



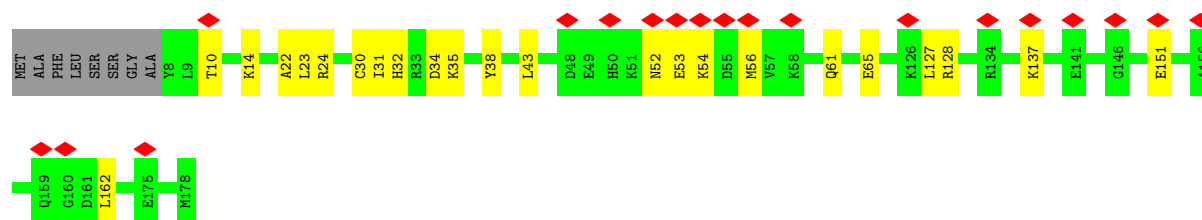
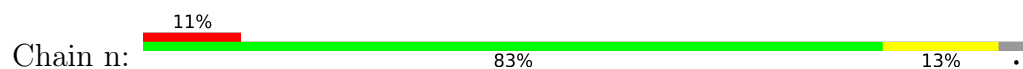
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



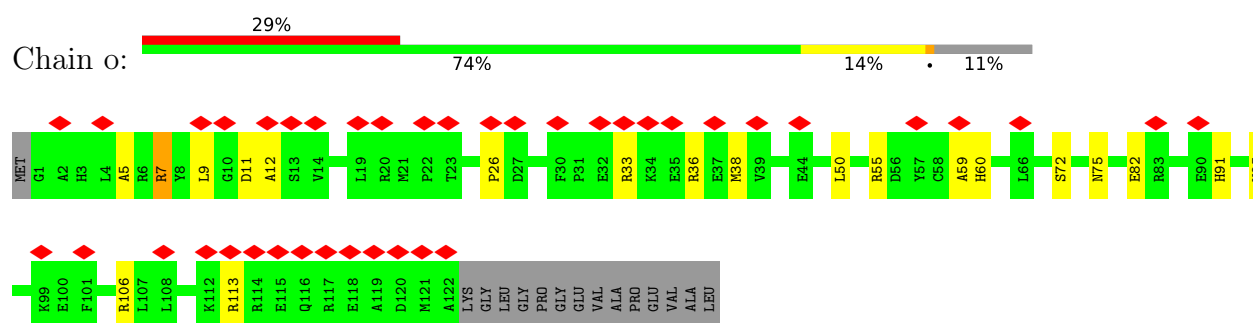
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



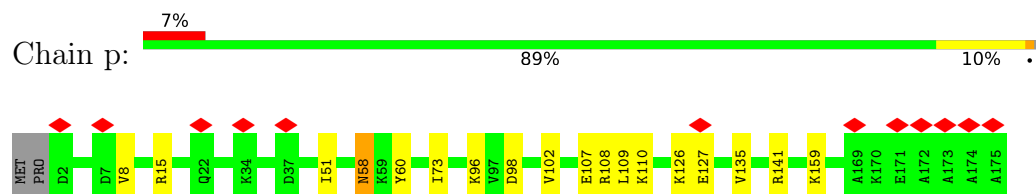
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



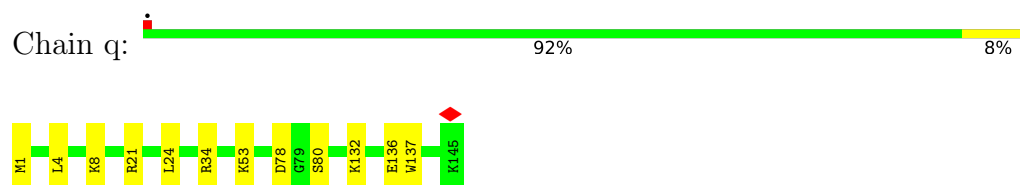
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



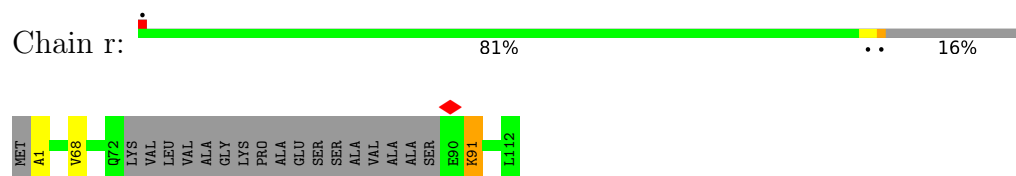
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



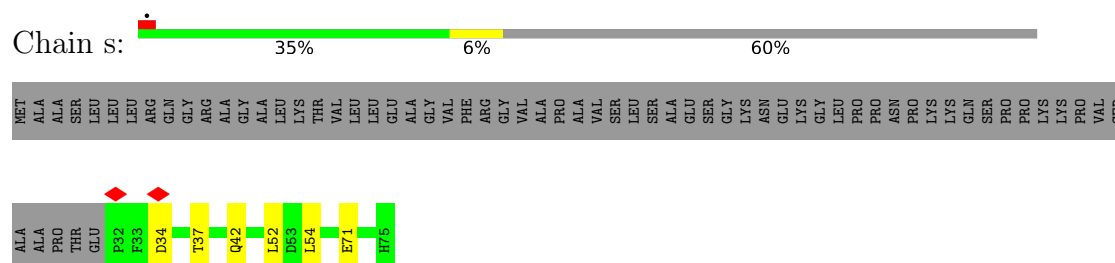
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45912	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	0.382	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	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: AYA, FES, K, U10, PLC, MYR, ZN, CHD, SF4, NDP, FME, PC1, FMN, CDL, 3PE, MG, EHZ, 2MR, SAC, DGT, AME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/936	0.23	0/1281
2	B	0.19	0/1278	0.27	0/1728
3	C	0.17	0/1772	0.27	0/2413
4	D	0.18	0/3450	0.25	0/4670
5	E	0.12	0/1699	0.29	0/2312
6	F	0.13	0/3401	0.25	0/4595
7	G	0.15	0/5387	0.26	0/7301
8	H	0.16	0/2571	0.28	0/3513
9	I	0.19	0/1445	0.28	0/1956
10	J	0.14	0/1370	0.24	0/1859
11	K	0.14	0/745	0.24	0/1008
12	L	0.11	0/4920	0.24	0/6694
13	M	0.14	0/3738	0.23	0/5097
14	N	0.15	0/2792	0.26	0/3800
15	O	0.11	0/2651	0.22	0/3587
16	P	0.14	0/2804	0.25	0/3803
17	Q	0.15	0/1072	0.24	0/1449
18	R	0.16	0/753	0.23	0/1014
19	S	0.09	0/702	0.23	0/945
20	T	0.11	0/719	0.22	0/971
20	U	0.10	0/719	0.21	0/971
21	V	0.12	0/943	0.22	0/1277
22	W	0.13	0/1006	0.24	0/1352
23	X	0.12	0/1439	0.22	0/1942
24	Y	0.11	0/1042	0.20	0/1414
25	Z	0.13	0/1186	0.22	0/1599
26	a	0.16	0/584	0.24	0/786
27	b	0.11	0/667	0.22	0/916
28	c	0.13	0/427	0.18	0/579
29	d	0.13	0/1018	0.22	0/1375
30	e	0.13	0/846	0.24	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.12	0/505	0.22	0/681
32	g	0.11	0/873	0.25	0/1186
33	h	0.12	0/1188	0.23	0/1607
34	i	0.09	0/1127	0.24	0/1534
35	j	0.11	0/624	0.20	0/855
36	k	0.07	0/672	0.19	0/906
37	l	0.10	0/1369	0.24	0/1873
38	m	0.10	0/1088	0.22	0/1472
39	n	0.09	0/1540	0.22	0/2085
40	o	0.12	0/1073	0.22	0/1437
41	p	0.09	0/1491	0.20	0/2011
42	q	0.14	0/1242	0.24	0/1688
43	r	0.15	0/789	0.28	0/1068
44	s	0.10	0/383	0.21	0/518
All	All	0.14	0/68046	0.24	0/92259

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	921	0	952	14	0
2	B	1247	0	1256	10	0
3	C	1721	0	1675	8	0
4	D	3377	0	3327	18	0
5	E	1659	0	1664	19	0
6	F	3326	0	3282	35	0
7	G	5298	0	5316	34	0
8	H	2509	0	2621	36	0
9	I	1414	0	1370	9	0
10	J	1345	0	1352	12	0
11	K	745	0	785	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	59	0
13	M	3654	0	3852	22	0
14	N	2733	0	2912	25	0
15	O	2589	0	2566	21	0
16	P	2728	0	2749	19	0
17	Q	1049	0	1045	3	0
18	R	740	0	714	6	0
19	S	691	0	706	3	0
20	T	707	0	700	7	0
20	U	707	0	700	10	0
21	V	923	0	964	3	0
22	W	982	0	999	6	0
23	X	1402	0	1383	10	0
24	Y	1030	0	1039	10	0
25	Z	1157	0	1156	12	0
26	a	569	0	568	6	0
27	b	654	0	663	1	0
28	c	414	0	415	3	0
29	d	999	0	988	8	0
30	e	825	0	826	5	0
31	f	492	0	501	5	0
32	g	846	0	798	8	0
33	h	1154	0	1168	11	0
34	i	1097	0	1108	10	0
35	j	597	0	536	6	0
36	k	653	0	639	7	0
37	l	1314	0	1210	14	0
38	m	1070	0	1068	9	0
39	n	1487	0	1433	17	0
40	o	1048	0	1016	12	0
41	p	1458	0	1430	15	0
42	q	1212	0	1183	7	0
43	r	776	0	782	1	0
44	s	371	0	344	6	0
45	A	82	0	115	0	0
45	I	37	0	51	2	0
45	J	81	0	113	2	0
45	L	120	0	168	0	0
45	M	95	0	141	1	0
45	N	49	0	75	0	0
45	P	38	0	50	0	0
45	Y	302	0	449	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	42	0	58	0	0
45	a	36	0	49	0	0
45	b	83	0	117	0	0
45	d	49	0	75	0	0
45	f	24	0	22	0	0
45	g	29	0	32	0	0
45	m	41	0	59	0	0
45	q	51	0	82	1	0
45	r	30	0	34	0	0
46	A	68	0	84	1	0
46	B	94	0	136	1	0
46	H	136	0	203	3	0
46	I	54	0	88	2	0
46	J	35	0	44	0	0
46	M	79	0	109	2	0
46	Z	44	0	62	0	0
46	d	39	0	52	2	0
46	h	38	0	53	0	0
46	l	47	0	71	0	0
46	m	41	0	56	0	0
46	q	49	0	75	2	0
47	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	0	0
48	E	4	0	0	0	0
48	G	4	0	0	0	0
49	F	31	0	19	0	0
50	G	1	0	0	0	0
51	H	34	0	41	14	0
52	H	58	0	63	1	0
52	L	100	0	156	0	0
52	M	100	0	156	1	0
52	N	94	0	141	1	0
52	d	152	0	204	2	0
52	i	76	0	96	0	0
52	r	61	0	66	0	0
53	J	35	0	47	0	0
53	L	36	0	49	0	0
53	M	34	0	45	0	0
53	O	62	0	77	0	0
53	Y	42	0	64	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	Z	36	0	49	0	0
53	b	38	0	53	0	0
53	g	42	0	64	0	0
54	M	1	0	0	0	0
54	R	1	0	0	0	0
55	O	1	0	0	0	0
56	O	31	0	12	0	0
57	P	48	0	26	2	0
58	T	37	0	0	1	0
58	U	37	0	0	1	0
59	i	29	0	38	6	0
60	o	15	0	27	0	0
All	All	69693	0	70937	493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (493) 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)
51:H:401:U10:H101	51:H:401:U10:H13	1.54	0.89
13:M:457:PRO:O	32:g:84:ARG:NH2	2.05	0.89
5:E:194:GLU:OE1	6:F:28:ARG:NH1	2.08	0.86
40:o:59:ALA:O	40:o:60:HIS:ND1	2.09	0.85
8:H:224:PHE:CE1	51:H:401:U10:H72	2.14	0.82
7:G:366:THR:O	7:G:367:THR:OG1	1.98	0.81
38:m:36:LEU:O	38:m:40:SER:OG	1.99	0.80
37:l:62:TYR:OH	39:n:151:GLU:OE2	1.99	0.79
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.63	0.78
20:T:88:GLU:OE1	20:T:88:GLU:N	2.18	0.77
20:U:22:TYR:OH	20:U:49:GLU:OE2	2.03	0.77
39:n:10:THR:O	39:n:14:LYS:NZ	2.18	0.77
7:G:260:GLU:OE2	7:G:397:LYS:NZ	2.18	0.77
23:X:154:GLU:N	23:X:154:GLU:OE1	2.17	0.77
4:D:66:MET:HE1	4:D:414:VAL:HG21	1.67	0.77
33:h:48:GLY:O	41:p:60:TYR:OH	2.03	0.77
34:i:39:VAL:O	34:i:44:ARG:NH2	2.17	0.76
33:h:7:ARG:NH2	34:i:31:GLU:O	2.18	0.76
1:A:71:LEU:O	10:J:147:TYR:OH	2.05	0.75
16:P:143:SER:OG	16:P:282:ASP:OD1	2.04	0.75
35:j:61:ASP:OD1	40:o:106:ARG:NH1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:i:201:CHD:H212	59:i:201:CHD:H12	1.67	0.74
12:L:31:ASN:OD1	12:L:31:ASN:N	2.20	0.74
7:G:341:ASP:O	7:G:508:LYS:NZ	2.20	0.74
14:N:182:SER:OG	14:N:293:TYR:OH	2.05	0.74
15:O:307:GLY:O	15:O:320:LYS:NZ	2.20	0.74
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.20	0.73
12:L:414:ILE:O	12:L:417:SER:OG	2.07	0.73
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.23	0.72
24:Y:81:GLU:OE1	24:Y:81:GLU:N	2.21	0.72
42:q:21:ARG:NH2	46:q:202:PC1:O14	2.22	0.72
2:B:48:MET:HE1	2:B:86:MET:HE2	1.70	0.72
44:s:34:ASP:OD2	44:s:37:THR:OG1	2.06	0.72
37:l:141:GLU:N	37:l:141:GLU:OE1	2.22	0.72
25:Z:130:GLU:N	25:Z:130:GLU:OE1	2.23	0.71
4:D:226:GLU:O	4:D:230:THR:OG1	2.07	0.71
25:Z:87:ARG:NH1	25:Z:91:GLU:OE2	2.24	0.70
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.25	0.69
16:P:10:LYS:NZ	22:W:126:ASP:OD2	2.21	0.69
6:F:358:SER:OG	6:F:365:CYS:SG	2.49	0.69
20:T:49:GLU:OE2	22:W:63:ARG:NH2	2.25	0.69
23:X:58:GLU:N	23:X:58:GLU:OE1	2.26	0.69
5:E:34:ILE:HG21	5:E:49:PRO:HB2	1.74	0.68
59:i:201:CHD:O7	59:i:201:CHD:O3	2.08	0.68
12:L:67:HIS:HE2	12:L:70:THR:HG1	1.41	0.68
23:X:63:ASN:OD1	25:Z:80:ARG:NH2	2.27	0.68
12:L:444:ASN:OD1	12:L:446:ASN:ND2	2.27	0.68
13:M:141:GLU:N	13:M:141:GLU:OE1	2.27	0.68
41:p:127:GLU:N	41:p:127:GLU:OE1	2.27	0.68
40:o:26:PRO:O	40:o:33:ARG:NH1	2.26	0.67
7:G:444:GLN:OE1	7:G:480:SER:OG	2.09	0.67
6:F:99:GLU:OE2	6:F:104:THR:HG22	1.95	0.67
12:L:429:PHE:O	12:L:436:ARG:NH2	2.28	0.67
13:M:51:ASN:OD1	33:h:90:THR:OG1	2.12	0.66
5:E:162:GLU:OE2	6:F:108:ARG:NH2	2.28	0.66
12:L:467:ILE:O	12:L:471:ASN:ND2	2.27	0.66
42:q:78:ASP:OD2	42:q:80:SER:OG	2.13	0.66
15:O:281:GLU:N	15:O:281:GLU:OE1	2.28	0.66
13:M:166:TYR:OH	45:M:604:3PE:O12	2.06	0.65
16:P:145:TYR:HH	57:P:501:NDP:HO2N	1.43	0.65
7:G:339:ASP:OD1	19:S:16:ARG:NH1	2.29	0.65
18:R:1:GLY:N	18:R:42:ASP:OD2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:125:TYR:OH	40:o:7:ARG:NH1	2.30	0.65
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.78	0.65
51:H:401:U10:H101	51:H:401:U10:C13	2.26	0.65
15:O:147:GLN:N	15:O:147:GLN:OE1	2.29	0.65
13:M:278:ARG:NE	37:l:82:ASP:OD1	2.30	0.65
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.13	0.65
23:X:150:ASN:OD1	30:e:50:ARG:NH1	2.30	0.64
6:F:101:GLU:OE1	6:F:184:TYR:OH	2.11	0.64
15:O:232:GLU:OE1	15:O:232:GLU:N	2.30	0.64
2:B:46:TRP:CH2	51:H:401:U10:H1M2	2.32	0.64
12:L:237:MET:HE3	12:L:303:ALA:HB2	1.79	0.64
6:F:364:PRO:HG2	6:F:403:THR:HG22	1.79	0.63
7:G:535:GLN:N	7:G:535:GLN:OE1	2.32	0.63
51:H:401:U10:C8	51:H:401:U10:H1M1	2.28	0.63
25:Z:142:TYR:CE2	26:a:48:MET:HE1	2.34	0.63
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.31	0.63
17:Q:27:GLU:N	17:Q:27:GLU:OE1	2.30	0.63
20:U:28:GLU:N	20:U:28:GLU:OE1	2.31	0.63
2:B:44:SER:O	8:H:54:LYS:NZ	2.32	0.63
29:d:5:ARG:NH1	29:d:89:ASP:OD1	2.32	0.63
26:a:49:GLU:OE1	26:a:52:ARG:NH2	2.32	0.62
10:J:78:GLN:OE1	10:J:78:GLN:N	2.32	0.62
44:s:71:GLU:OE1	44:s:71:GLU:N	2.33	0.62
22:W:88:GLU:OE2	22:W:97:LYS:NZ	2.29	0.62
6:F:438:GLN:N	6:F:438:GLN:OE1	2.32	0.62
2:B:27:GLU:OE2	2:B:178:ARG:NH2	2.32	0.62
5:E:172:ILE:HG23	5:E:182:PRO:HG2	1.81	0.62
9:I:75:GLU:O	9:I:105:ARG:NH1	2.34	0.61
15:O:30:ASN:OD1	15:O:31:ILE:N	2.33	0.61
4:D:241:ASP:OD1	4:D:290:ARG:NH1	2.32	0.61
34:i:114:GLU:OE1	41:p:15:ARG:NH2	2.34	0.61
35:j:43:ASP:OD1	35:j:43:ASP:N	2.33	0.61
8:H:65:THR:HG21	16:P:325:ARG:HG2	1.82	0.60
51:H:401:U10:H201	51:H:401:U10:H23	1.81	0.60
9:I:30:LEU:HD13	46:I:204:PC1:H262	1.84	0.60
5:E:9:HIS:NE2	5:E:11:ASP:OD1	2.35	0.60
7:G:591:GLY:HA2	16:P:6:ILE:HG21	1.84	0.60
6:F:40:GLY:O	6:F:236:ARG:NH2	2.35	0.60
21:V:46:TYR:OH	43:r:91:LYS:NZ	2.34	0.60
6:F:407:LEU:HD23	6:F:407:LEU:O	2.01	0.59
4:D:66:MET:HE3	4:D:76:CYS:SG	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:40:ASP:OD2	38:m:84:LYS:NZ	2.34	0.59
5:E:151:ALA:HB1	5:E:152:PRO:HD2	1.85	0.59
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.37	0.59
12:L:293:LEU:HD11	12:L:418:PHE:CD2	2.38	0.59
6:F:108:ARG:NH1	6:F:145:GLU:OE2	2.34	0.59
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.85	0.59
5:E:151:ALA:HB1	5:E:152:PRO:CD	2.33	0.59
29:d:112:VAL:O	41:p:159:LYS:NZ	2.35	0.59
40:o:50:LEU:O	40:o:55:ARG:NH1	2.35	0.59
8:H:301:CYS:O	8:H:305:VAL:HG23	2.02	0.58
37:l:132:GLN:OE1	40:o:36:ARG:NH1	2.34	0.58
2:B:46:TRP:CZ2	51:H:401:U10:H1M2	2.38	0.58
11:K:43:MET:HE1	14:N:72:MET:HE1	1.84	0.58
33:h:140:THR:O	33:h:143:ASN:ND2	2.36	0.58
20:U:52:MET:HE3	39:n:24:ARG:CD	2.32	0.58
34:i:55:LEU:HD13	34:i:55:LEU:O	2.03	0.58
4:D:46:ASN:ND2	4:D:67:GLU:OE2	2.36	0.58
7:G:138:GLU:OE2	18:R:77:LYS:NZ	2.23	0.58
12:L:511:LEU:HD21	39:n:38:TYR:CD1	2.39	0.58
34:i:43:GLU:N	34:i:43:GLU:OE1	2.36	0.58
40:o:82:GLU:N	40:o:82:GLU:OE1	2.35	0.58
8:H:249:PRO:O	26:a:28:ARG:NH2	2.37	0.57
14:N:314:LYS:NZ	15:O:274:SER:OG	2.36	0.57
59:i:201:CHD:O3	59:i:201:CHD:H9	2.04	0.57
5:E:105:THR:HG22	5:E:106:THR:H	1.70	0.57
7:G:422:LEU:O	7:G:428:ILE:HD13	2.04	0.57
21:V:54:LYS:O	21:V:58:VAL:HG23	2.04	0.57
39:n:61:GLN:NE2	39:n:65:GLU:OE2	2.35	0.57
20:U:23:ASP:OD1	36:k:46:ARG:NH2	2.37	0.57
24:Y:12:PRO:O	24:Y:15:THR:OG1	2.22	0.57
1:A:115:GLU:N	1:A:115:GLU:OE1	2.37	0.57
15:O:136:GLU:OE1	15:O:140:ARG:NH1	2.38	0.57
5:E:104:THR:HG22	5:E:104:THR:O	2.04	0.56
16:P:253:PHE:C	16:P:254:LEU:HD22	2.30	0.56
20:U:21:LEU:HD13	36:k:47:ASN:HA	1.87	0.56
31:f:4:LEU:HD13	31:f:4:LEU:O	2.05	0.56
34:i:15:ARG:HD2	34:i:19:ARG:HH21	1.69	0.56
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.35	0.56
1:A:90:MET:SD	10:J:151:THR:HG23	2.45	0.56
15:O:216:GLU:N	15:O:216:GLU:OE1	2.38	0.56
29:d:1:AME:HT22	29:d:3:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:40:SER:OG	34:i:43:GLU:OE1	2.24	0.56
14:N:47:ASN:O	14:N:49:ASN:ND2	2.38	0.56
15:O:94:TYR:OH	15:O:151:HIS:ND1	2.36	0.56
40:o:5:ALA:O	40:o:9:LEU:N	2.38	0.56
19:S:23:CYS:SG	19:S:24:GLN:N	2.79	0.56
38:m:16:THR:O	38:m:22:TYR:OH	2.15	0.56
14:N:313:MET:HE1	15:O:102:ALA:HB3	1.87	0.55
20:U:17:TYR:OH	36:k:21:TRP:NE1	2.39	0.55
39:n:56:MET:HA	39:n:56:MET:HE2	1.88	0.55
4:D:302:GLU:OE2	9:I:3:LYS:NZ	2.38	0.55
6:F:20:ARG:NH1	6:F:269:GLU:O	2.39	0.55
15:O:156:LYS:O	15:O:160:ILE:HG22	2.07	0.55
12:L:489:THR:O	12:L:493:VAL:HG22	2.07	0.55
4:D:64:LEU:HD22	4:D:76:CYS:SG	2.47	0.55
10:J:51:PHE:CD1	10:J:143:ILE:HD13	2.42	0.54
7:G:556:ILE:HD12	7:G:556:ILE:O	2.08	0.54
20:T:32:VAL:HG13	20:T:33:ASN:OD1	2.07	0.54
7:G:375:ASP:OD1	7:G:375:ASP:N	2.40	0.54
13:M:271:MET:HE2	13:M:271:MET:HA	1.90	0.54
18:R:20:ASP:OD1	18:R:21:GLY:N	2.41	0.54
29:d:63:LEU:HD23	52:d:201:CDL:OA9	2.07	0.54
8:H:146:LEU:HD11	8:H:192:GLU:HG3	1.89	0.54
12:L:2:ASN:OD1	12:L:3:MET:N	2.41	0.54
25:Z:49:MET:HE3	25:Z:49:MET:HA	1.89	0.54
41:p:98:ASP:OD2	41:p:141:ARG:NH2	2.41	0.54
10:J:51:PHE:CE1	10:J:55:MET:HE3	2.43	0.53
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.39	0.53
37:l:8:MET:HE2	37:l:8:MET:HA	1.91	0.53
29:d:1:AME:HT22	29:d:3:THR:CG2	2.39	0.53
6:F:84:LYS:NZ	6:F:212:ASP:OD1	2.41	0.53
12:L:535:ARG:NH1	37:l:90:ASP:O	2.40	0.53
12:L:76:LEU:HD21	12:L:196:TRP:HE3	1.73	0.53
33:h:52:LEU:HD13	33:h:53:ALA:N	2.24	0.53
35:j:47:VAL:HG22	35:j:47:VAL:O	2.07	0.53
12:L:102:GLU:OE1	12:L:456:ARG:NH1	2.39	0.53
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.91	0.53
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.39	0.53
5:E:191:PHE:N	5:E:194:GLU:OE2	2.37	0.53
12:L:293:LEU:HD11	12:L:418:PHE:CE2	2.43	0.52
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.42	0.52
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:H:401:U10:O4	51:H:401:U10:H3M3	2.10	0.52
51:H:401:U10:H222	45:q:201:3PE:H3I2	1.92	0.52
8:H:169:GLN:O	46:H:404:PC1:H141	2.09	0.52
1:A:33:LYS:O	1:A:34:THR:OG1	2.22	0.52
44:s:42:GLN:OE1	44:s:42:GLN:N	2.41	0.51
10:J:141:MET:HA	10:J:141:MET:HE2	1.92	0.51
6:F:145:GLU:OE1	6:F:145:GLU:N	2.38	0.51
25:Z:128:ALA:O	25:Z:132:VAL:HG23	2.10	0.51
14:N:193:VAL:O	14:N:193:VAL:HG22	2.11	0.51
37:l:126:GLN:OE1	37:l:126:GLN:N	2.44	0.51
38:m:34:GLU:N	38:m:34:GLU:OE1	2.43	0.51
41:p:8:VAL:O	41:p:108:ARG:NH1	2.43	0.51
12:L:264:TYR:N	12:L:265:PRO:CD	2.74	0.51
5:E:148:CYS:N	6:F:105:CYS:SG	2.83	0.50
13:M:71:TRP:HZ3	32:g:69:VAL:HG11	1.76	0.50
12:L:194:ASN:O	12:L:194:ASN:ND2	2.45	0.50
59:i:201:CHD:H212	59:i:201:CHD:H183	1.93	0.50
35:j:69:ASP:OD2	40:o:113:ARG:NE	2.43	0.50
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.94	0.50
51:H:401:U10:H201	51:H:401:U10:C23	2.41	0.50
7:G:471:SER:O	7:G:475:GLN:NE2	2.42	0.50
16:P:30:LEU:HD23	16:P:94:LEU:HD22	1.93	0.50
42:q:24:LEU:HD13	46:q:202:PC1:H221	1.94	0.50
28:c:13:ASN:O	28:c:17:VAL:HG23	2.12	0.50
34:i:38:ARG:NE	34:i:38:ARG:O	2.45	0.50
7:G:283:MET:HE3	7:G:560:ILE:HD12	1.94	0.50
13:M:394:ILE:O	13:M:398:VAL:HG23	2.11	0.50
1:A:68:GLU:HG2	10:J:161:LEU:HD13	1.93	0.50
6:F:428:GLU:OE2	6:F:432:GLN:NE2	2.44	0.50
9:I:143:THR:OG1	9:I:146:GLU:OE2	2.25	0.49
4:D:161:ILE:HD12	8:H:278:PRO:HB2	1.93	0.49
14:N:72:MET:HE3	14:N:76:ILE:HD11	1.94	0.49
16:P:5:VAL:HG12	16:P:5:VAL:O	2.12	0.49
46:B:202:PC1:H142	46:B:202:PC1:O13	2.12	0.49
8:H:99:ASN:N	46:H:403:PC1:O12	2.45	0.49
23:X:79:GLU:N	23:X:79:GLU:OE1	2.46	0.49
24:Y:16:GLU:OE1	24:Y:19:ARG:NE	2.45	0.49
16:P:91:VAL:HG23	16:P:126:VAL:HG11	1.94	0.49
20:U:52:MET:HE1	39:n:23:LEU:HB3	1.94	0.49
45:J:202:3PE:O14	12:L:585:LYS:NZ	2.32	0.49
12:L:365:ALA:HB1	12:L:443:ILE:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:405:ASN:OD1	12:L:407:TRP:N	2.45	0.49
14:N:183:SER:O	14:N:187:MET:HE2	2.12	0.49
6:F:94:VAL:HG11	6:F:192:LEU:HD22	1.94	0.49
6:F:154:ARG:NH2	44:s:54:LEU:HD23	2.28	0.49
12:L:466:TYR:O	12:L:470:ASN:ND2	2.41	0.49
1:A:35:SER:O	2:B:81:ARG:NH2	2.46	0.49
46:A:203:PC1:O13	46:A:203:PC1:H132	2.13	0.49
9:I:14:MET:HE3	45:I:203:3PE:C27	2.42	0.49
12:L:131:LEU:HD23	12:L:131:LEU:C	2.38	0.49
3:C:41:GLN:NE2	3:C:49:GLU:OE1	2.45	0.48
6:F:47:GLU:OE1	6:F:47:GLU:N	2.42	0.48
7:G:283:MET:HE1	42:q:137:TRP:CZ3	2.48	0.48
7:G:410:GLY:O	7:G:421:HIS:NE2	2.39	0.48
8:H:135:ALA:HB2	8:H:201:THR:HG21	1.95	0.48
12:L:176:ARG:NH2	13:M:367:LEU:HD13	2.28	0.48
25:Z:142:TYR:CZ	26:a:48:MET:HE1	2.47	0.48
15:O:126:ARG:NE	15:O:206:TYR:OH	2.46	0.48
1:A:95:ILE:HG21	8:H:302:MET:HG3	1.94	0.48
10:J:81:GLU:OE1	10:J:86:ASN:ND2	2.44	0.48
6:F:95:VAL:HG21	6:F:122:CYS:SG	2.53	0.48
6:F:309:LYS:NZ	6:F:313:GLU:OE2	2.46	0.48
14:N:136:LEU:HD22	46:d:204:PC1:H391	1.94	0.48
40:o:11:ASP:OD1	40:o:12:ALA:N	2.47	0.48
7:G:99:ALA:O	7:G:134:LYS:NZ	2.47	0.48
13:M:113:MET:SD	13:M:175:ASN:ND2	2.84	0.48
39:n:30:CYS:O	39:n:32:HIS:N	2.47	0.48
7:G:366:THR:HB	7:G:450:MET:HE3	1.95	0.48
2:B:82:GLN:HG3	51:H:401:U10:H3M2	1.95	0.48
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.48	0.47
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.30	0.47
12:L:199:GLN:NE2	41:p:110:LYS:O	2.46	0.47
8:H:224:PHE:CZ	51:H:401:U10:H72	2.48	0.47
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.78	0.47
58:T:101:EHZ:O2	58:T:101:EHZ:O1	2.32	0.47
12:L:378:LEU:HD13	12:L:383:MET:SD	2.55	0.47
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.49	0.47
12:L:76:LEU:HD21	12:L:196:TRP:CE3	2.49	0.47
8:H:179:TRP:N	8:H:180:PRO:CD	2.78	0.47
6:F:188:GLU:OE1	6:F:190:THR:N	2.48	0.47
7:G:227:SER:OG	7:G:228:ILE:N	2.48	0.47
13:M:450:ASN:OD1	13:M:452:LYS:NZ	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:146:PHE:N	14:N:147:PRO:CD	2.77	0.47
31:f:3:LEU:O	31:f:7:VAL:HG12	2.15	0.47
6:F:327:THR:OG1	6:F:328:GLY:N	2.48	0.47
51:H:401:U10:C8	51:H:401:U10:C1M	2.92	0.47
12:L:203:MET:HG2	41:p:109:LEU:HD11	1.96	0.47
15:O:173:ASP:OD1	15:O:174:VAL:N	2.48	0.47
15:O:186:LYS:HZ3	15:O:186:LYS:HB3	1.80	0.47
18:R:9:GLU:OE2	18:R:33:LYS:NZ	2.42	0.47
29:d:63:LEU:HD23	52:d:201:CDL:HA62	1.97	0.47
39:n:127:LEU:HD21	39:n:162:LEU:HD11	1.97	0.46
58:U:101:EHZ:O2	58:U:101:EHZ:O1	2.32	0.46
25:Z:124:TYR:HB3	25:Z:132:VAL:HG22	1.98	0.46
36:k:35:LEU:HD12	36:k:40:LEU:HB2	1.96	0.46
4:D:415:VAL:HG22	8:H:207:LEU:HD13	1.98	0.46
8:H:51:ASP:HB2	51:H:401:U10:H152	1.97	0.46
14:N:237:THR:HG21	14:N:319:LEU:HD11	1.97	0.46
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.50	0.46
2:B:63:ALA:HB2	2:B:69:MET:HE2	1.98	0.46
4:D:17:ALA:HB1	11:K:98:CYS:SG	2.56	0.46
39:n:34:ASP:OD1	39:n:35:LYS:N	2.49	0.46
1:A:32:GLU:OE1	1:A:32:GLU:N	2.47	0.46
12:L:230:HIS:N	12:L:231:PRO:CD	2.79	0.46
15:O:22:SER:HB3	15:O:115:LEU:HD11	1.98	0.46
6:F:192:LEU:HD23	6:F:192:LEU:O	2.16	0.45
46:I:204:PC1:O13	46:I:204:PC1:H132	2.16	0.45
15:O:18:MET:HE3	15:O:116:LEU:HD23	1.98	0.45
8:H:20:LEU:HD13	26:a:12:MET:HE1	1.99	0.45
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.34	0.45
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.50	0.45
19:S:54:ILE:N	19:S:54:ILE:HD12	2.32	0.45
32:g:64:PHE:O	32:g:69:VAL:HG23	2.16	0.45
7:G:145:LEU:HD22	7:G:269:PHE:CD2	2.52	0.45
14:N:318:PRO:HG2	14:N:320:MET:HE2	1.98	0.45
41:p:102:VAL:O	41:p:102:VAL:HG12	2.16	0.45
36:k:59:ASN:OD1	36:k:60:VAL:N	2.50	0.45
6:F:131:ALA:O	6:F:171:TYR:OH	2.17	0.45
8:H:149:ILE:HG21	8:H:185:TRP:HB2	1.98	0.45
14:N:14:MET:HE1	52:N:401:CDL:H371	1.99	0.45
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.98	0.45
4:D:161:ILE:HD11	4:D:235:TRP:CE3	2.51	0.45
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:407:LEU:HD23	6:F:407:LEU:C	2.41	0.45
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.99	0.45
16:P:145:TYR:OH	57:P:501:NDP:O2D	2.21	0.45
4:D:165:THR:OG1	8:H:275:ALA:O	2.30	0.45
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.99	0.45
46:M:606:PC1:C35	24:Y:90:LEU:HD12	2.47	0.45
20:U:17:TYR:HH	36:k:21:TRP:CD1	2.35	0.45
27:b:58:ASP:HA	27:b:62:MET:HE2	1.99	0.45
28:c:34:GLN:NE2	28:c:38:ASP:OD2	2.46	0.45
39:n:22:ALA:HB3	39:n:43:LEU:HD21	1.99	0.45
24:Y:90:LEU:HD23	24:Y:90:LEU:C	2.42	0.45
6:F:306:LEU:C	6:F:306:LEU:HD12	2.42	0.44
14:N:47:ASN:O	14:N:48:HIS:C	2.59	0.44
16:P:201:VAL:HG11	16:P:235:ARG:HE	1.82	0.44
7:G:140:LYS:O	7:G:148:THR:OG1	2.35	0.44
10:J:116:VAL:N	45:J:201:3PE:O14	2.44	0.44
25:Z:92:GLU:N	25:Z:92:GLU:OE1	2.50	0.44
52:H:402:CDL:H111	10:J:82:ILE:HG22	1.99	0.44
12:L:380:LEU:O	12:L:392:LYS:NZ	2.38	0.44
14:N:6:PHE:CE2	14:N:10:LEU:HD11	2.52	0.44
33:h:32:THR:O	33:h:36:VAL:HG23	2.17	0.44
8:H:24:GLU:OE2	8:H:274:ARG:NH2	2.50	0.44
12:L:128:MET:O	12:L:132:VAL:HG23	2.17	0.44
37:l:127:PRO:O	37:l:128:VAL:HG13	2.17	0.44
1:A:76:PRO:HD3	8:H:151:LEU:HD11	1.99	0.44
33:h:45:VAL:HG13	41:p:51:ILE:HG12	2.00	0.44
7:G:41:CYS:O	7:G:161:ARG:NH2	2.41	0.44
7:G:338:VAL:HG13	7:G:609:MET:HE1	1.99	0.44
7:G:539:LYS:O	7:G:540:ASP:OD1	2.36	0.44
8:H:253:GLU:N	8:H:253:GLU:OE1	2.49	0.44
17:Q:36:ARG:NE	17:Q:106:GLU:OE2	2.44	0.44
25:Z:111:HIS:NE2	30:e:60:GLU:OE1	2.50	0.44
1:A:20:ILE:HD11	8:H:56:PHE:CD1	2.52	0.44
3:C:8:ARG:HB2	3:C:11:VAL:HG22	1.99	0.44
5:E:52:ASP:OD2	6:F:179:ARG:NH1	2.45	0.44
12:L:61:LEU:HD12	12:L:61:LEU:O	2.18	0.44
12:L:65:ASN:OD1	12:L:66:TRP:N	2.50	0.44
12:L:171:ALA:O	12:L:175:ASN:ND2	2.40	0.44
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.53	0.44
37:l:39:ASP:O	38:m:80:ARG:NH2	2.50	0.44
40:o:72:SER:O	40:o:75:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:VAL:O	22:W:100:THR:OG1	2.31	0.43
7:G:194:GLU:OE1	7:G:194:GLU:N	2.39	0.43
46:H:403:PC1:H133	46:H:403:PC1:O13	2.17	0.43
12:L:511:LEU:HD21	39:n:38:TYR:CE1	2.52	0.43
12:L:593:ILE:HG22	12:L:597:ILE:HD12	2.00	0.43
13:M:12:MET:HB2	13:M:13:PRO:HD3	2.00	0.43
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.53	0.43
29:d:109:TYR:HA	29:d:112:VAL:HG22	2.00	0.43
34:i:71:PHE:HD1	34:i:75:LEU:HD23	1.83	0.43
9:I:14:MET:HE3	45:I:203:3PE:H272	1.99	0.43
12:L:341:MET:HE1	12:L:453:SER:C	2.43	0.43
20:T:64:ASP:OD2	22:W:32:ARG:NH1	2.51	0.43
23:X:120:ASP:OD1	23:X:121:LEU:N	2.48	0.43
35:j:70:ASP:OD1	35:j:70:ASP:N	2.51	0.43
8:H:310:LEU:HD12	8:H:310:LEU:O	2.19	0.43
12:L:137:LEU:O	12:L:141:PHE:N	2.47	0.43
12:L:237:MET:HE3	12:L:303:ALA:CB	2.47	0.43
13:M:346:ARG:NE	37:l:68:ASP:OD2	2.51	0.43
16:P:30:LEU:HD12	16:P:207:ILE:HD11	1.99	0.43
23:X:11:ASP:OD1	23:X:11:ASP:N	2.51	0.43
36:k:35:LEU:HD12	36:k:40:LEU:CB	2.49	0.43
7:G:489:VAL:O	7:G:489:VAL:HG12	2.18	0.43
8:H:87:ILE:N	8:H:88:PRO:CD	2.81	0.43
15:O:56:ILE:HD11	15:O:96:LEU:CD1	2.49	0.43
31:f:53:GLU:OE1	31:f:53:GLU:N	2.42	0.43
33:h:114:MET:HE2	33:h:121:PRO:HD2	2.00	0.43
5:E:217:LEU:HD13	5:E:217:LEU:C	2.43	0.43
59:i:201:CHD:H12	59:i:201:CHD:C21	2.42	0.43
1:A:16:LEU:O	1:A:20:ILE:HG23	2.18	0.43
5:E:151:ALA:O	5:E:152:PRO:C	2.60	0.43
18:R:38:ASN:O	18:R:39:PHE:C	2.61	0.43
23:X:100:ARG:NH2	25:Z:62:GLU:OE1	2.52	0.43
32:g:84:ARG:O	41:p:96:LYS:NZ	2.52	0.43
41:p:58:ASN:OD1	41:p:58:ASN:N	2.51	0.43
3:C:109:THR:OG1	3:C:110:TYR:N	2.52	0.43
10:J:79:TYR:O	10:J:81:GLU:N	2.52	0.43
13:M:423:ILE:CD1	38:m:58:VAL:HG13	2.48	0.43
15:O:135:LEU:HD22	15:O:152:TYR:CG	2.54	0.43
6:F:215:VAL:HG12	6:F:220:THR:OG1	2.19	0.42
12:L:14:LEU:HD23	12:L:14:LEU:O	2.19	0.42
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:15:GLU:OE1	17:Q:15:GLU:N	2.52	0.42
30:e:58:GLU:OE1	30:e:58:GLU:N	2.50	0.42
39:n:22:ALA:CB	39:n:43:LEU:HD21	2.49	0.42
31:f:4:LEU:HD13	31:f:4:LEU:C	2.44	0.42
14:N:41:ILE:N	14:N:42:PRO:HD2	2.34	0.42
39:n:52:ASN:OD1	39:n:53:GLU:N	2.53	0.42
4:D:161:ILE:HD11	4:D:235:TRP:HE3	1.84	0.42
12:L:562:LEU:HB2	12:L:563:PRO:CD	2.50	0.42
13:M:127:VAL:HG11	52:M:602:CDL:H842	2.00	0.42
21:V:47:THR:O	21:V:51:THR:OG1	2.27	0.42
3:C:184:VAL:HG11	22:W:109:THR:HG21	2.01	0.42
4:D:27:HIS:NE2	20:T:1:SER:O	2.52	0.42
6:F:295:LEU:HD11	6:F:422:PHE:HE2	1.84	0.42
7:G:324:ASP:OD1	7:G:324:ASP:N	2.51	0.42
12:L:49:ILE:HD12	12:L:49:ILE:H	1.85	0.42
12:L:203:MET:CG	41:p:109:LEU:HD11	2.49	0.42
35:j:45:ASP:O	35:j:49:GLY:N	2.52	0.42
42:q:4:LEU:HD11	42:q:8:LYS:HE3	2.00	0.42
37:l:30:ARG:NH2	37:l:32:GLU:OE1	2.52	0.42
6:F:306:LEU:HD12	6:F:306:LEU:O	2.20	0.42
13:M:6:ILE:HB	13:M:7:PRO:HD3	2.02	0.42
24:Y:90:LEU:HD23	24:Y:90:LEU:O	2.20	0.42
38:m:51:TYR:O	39:n:128:ARG:NH2	2.51	0.42
6:F:103:GLY:O	6:F:333:ALA:HB1	2.20	0.42
30:e:83:GLU:OE2	30:e:87:LYS:NZ	2.53	0.42
7:G:137:VAL:HG12	7:G:151:THR:HA	2.02	0.42
12:L:291:CYS:O	12:L:295:GLN:HG2	2.20	0.42
6:F:144:ASN:O	6:F:148:ASN:ND2	2.50	0.41
42:q:4:LEU:C	42:q:4:LEU:HD13	2.45	0.41
6:F:351:ILE:HD11	6:F:415:VAL:HG23	2.02	0.41
8:H:32:GLN:OE1	8:H:34:ARG:NH2	2.53	0.41
8:H:87:ILE:HG12	8:H:88:PRO:HD3	2.02	0.41
3:C:178:ASP:OD2	16:P:32:ARG:NH1	2.51	0.41
12:L:429:PHE:HE1	39:n:31:ILE:HD13	1.85	0.41
14:N:278:LEU:HB3	14:N:279:PRO:HD3	2.02	0.41
20:T:8:LEU:HD13	20:T:8:LEU:O	2.20	0.41
28:c:48:LEU:C	28:c:48:LEU:HD12	2.45	0.41
38:m:82:ASN:OD1	38:m:84:LYS:N	2.53	0.41
7:G:137:VAL:HG22	7:G:138:GLU:N	2.34	0.41
13:M:373:ILE:HD11	13:M:444:LEU:CD1	2.50	0.41
16:P:46:ILE:N	16:P:46:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:130:ILE:N	16:P:130:ILE:HD12	2.35	0.41
18:R:94:GLN:O	18:R:95:HIS:ND1	2.53	0.41
20:U:25:ILE:HG22	20:U:26:ASP:N	2.35	0.41
20:U:52:MET:HE1	39:n:23:LEU:CB	2.50	0.41
24:Y:62:ALA:HB2	45:Y:204:3PE:H341	2.02	0.41
46:d:204:PC1:O13	46:d:204:PC1:H142	2.20	0.41
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.55	0.41
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.02	0.41
4:D:261:ARG:NH2	4:D:303:GLU:OE2	2.48	0.41
9:I:29:GLU:N	9:I:29:GLU:OE1	2.53	0.41
12:L:12:LEU:CD2	12:L:129:LEU:HD23	2.51	0.41
12:L:195:THR:HG21	12:L:200:GLN:HB3	2.01	0.41
37:l:68:ASP:OD1	37:l:68:ASP:N	2.54	0.41
5:E:53:LEU:HD13	44:s:52:LEU:HD13	2.02	0.41
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.49	0.41
7:G:364:LEU:HD12	7:G:491:ASN:HB3	2.03	0.41
12:L:16:THR:HG22	12:L:126:ILE:HD13	2.01	0.41
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.02	0.41
15:O:195:THR:OG1	15:O:196:SER:N	2.54	0.41
7:G:540:ASP:O	7:G:540:ASP:CG	2.63	0.41
12:L:562:LEU:CB	12:L:563:PRO:CD	2.98	0.41
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.03	0.41
32:g:90:ARG:NH2	41:p:107:GLU:OE1	2.54	0.41
8:H:87:ILE:CG1	8:H:88:PRO:HD3	2.51	0.41
12:L:49:ILE:HD12	12:L:49:ILE:N	2.35	0.41
12:L:377:SER:O	12:L:381:THR:HG23	2.21	0.41
15:O:157:LYS:HG3	15:O:158:VAL:HG13	2.03	0.41
16:P:220:ASP:O	16:P:224:ARG:NH2	2.54	0.41
23:X:102:GLN:OE1	23:X:102:GLN:N	2.50	0.41
34:i:65:ARG:HB3	59:i:201:CHD:H232	2.03	0.41
38:m:76:TYR:N	38:m:77:PRO:HD2	2.36	0.41
1:A:29:VAL:HG13	1:A:34:THR:HG21	2.03	0.41
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.41
12:L:537:ALA:HB3	12:L:538:PRO:HD3	2.01	0.41
12:L:558:LEU:C	13:M:214:LEU:HD11	2.46	0.41
14:N:89:LEU:HD12	14:N:95:SER:HA	2.03	0.41
29:d:94:ILE:HD13	33:h:106:LYS:HD3	2.03	0.41
32:g:34:ASP:OD1	32:g:35:GLU:N	2.54	0.41
1:A:68:GLU:CG	10:J:161:LEU:HD13	2.51	0.40
4:D:7:ASP:OD1	4:D:7:ASP:N	2.54	0.40
7:G:185:THR:O	7:G:187:ILE:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:272:LYS:HB3	24:Y:140:VAL:HG21	2.02	0.40
40:o:91:HIS:O	40:o:95:VAL:HG23	2.20	0.40
11:K:63:LEU:HD23	11:K:63:LEU:C	2.45	0.40
12:L:204:LEU:O	12:L:205:ASN:C	2.64	0.40
20:T:1:SER:O	20:T:3:ALA:N	2.55	0.40
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.54	0.40
25:Z:119:MET:HE2	30:e:71:THR:CG2	2.51	0.40
2:B:50:PHE:HE2	2:B:103:VAL:HG11	1.86	0.40
8:H:206:GLU:OE2	8:H:279:ARG:NH1	2.39	0.40
13:M:254:THR:O	13:M:254:THR:HG22	2.21	0.40
14:N:269:GLU:O	14:N:273:ASN:ND2	2.51	0.40
16:P:182:PHE:O	16:P:245:VAL:HG11	2.22	0.40
5:E:164:LEU:HD13	5:E:169:ILE:HG12	2.03	0.40
12:L:131:LEU:HD23	12:L:131:LEU:O	2.22	0.40
14:N:190:MET:HE2	14:N:205:LEU:HA	2.03	0.40
2:B:47:PRO:HD3	2:B:74:VAL:HG13	2.03	0.40
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.03	0.40
4:D:323:ILE:HD12	4:D:323:ILE:C	2.47	0.40
7:G:108:CYS:O	7:G:218:ARG:NH1	2.54	0.40
46:M:606:PC1:H351	24:Y:90:LEU:HD12	2.04	0.40
24:Y:127:GLY:O	24:Y:131:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	154/216 (71%)	148 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	200 (98%)	5 (2%)	0	100	100
4	D	412/463 (89%)	399 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
6	F	430/464 (93%)	412 (96%)	18 (4%)	0	100	100
7	G	689/727 (95%)	668 (97%)	21 (3%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
10	J	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
11	K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	38
12	L	604/606 (100%)	577 (96%)	26 (4%)	1 (0%)	43	72
13	M	457/459 (100%)	452 (99%)	5 (1%)	0	100	100
14	N	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
15	O	318/343 (93%)	315 (99%)	3 (1%)	0	100	100
16	P	335/380 (88%)	327 (98%)	8 (2%)	0	100	100
17	Q	127/175 (73%)	127 (100%)	0	0	100	100
18	R	94/124 (76%)	89 (95%)	5 (5%)	0	100	100
19	S	84/99 (85%)	84 (100%)	0	0	100	100
20	T	86/156 (55%)	79 (92%)	7 (8%)	0	100	100
20	U	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
21	V	112/116 (97%)	108 (96%)	4 (4%)	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%)	137 (99%)	1 (1%)	0	100	100
25	Z	140/144 (97%)	137 (98%)	3 (2%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
28	c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
32	g	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	i	125/128 (98%)	119 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	j	69/108 (64%)	66 (96%)	3 (4%)	0	100	100
36	k	79/98 (81%)	78 (99%)	1 (1%)	0	100	100
37	l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	m	126/129 (98%)	123 (98%)	3 (2%)	0	100	100
39	n	169/179 (94%)	161 (95%)	8 (5%)	0	100	100
40	o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	p	172/176 (98%)	167 (97%)	5 (3%)	0	100	100
42	q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	42 (100%)	0	0	100	100
All	All	8173/9213 (89%)	7927 (97%)	244 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	97 (97%)	3 (3%)	36	72
2	B	132/175 (75%)	128 (97%)	4 (3%)	36	72
3	C	188/228 (82%)	187 (100%)	1 (0%)	81	93
4	D	361/392 (92%)	353 (98%)	8 (2%)	45	78
5	E	183/205 (89%)	177 (97%)	6 (3%)	33	69
6	F	346/368 (94%)	341 (99%)	5 (1%)	59	85
7	G	579/608 (95%)	568 (98%)	11 (2%)	50	81
8	H	274/274 (100%)	269 (98%)	5 (2%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	151/175 (86%)	149 (99%)	2 (1%)	61	86
10	J	141/141 (100%)	140 (99%)	1 (1%)	76	91
11	K	85/85 (100%)	83 (98%)	2 (2%)	43	77
12	L	533/533 (100%)	523 (98%)	10 (2%)	50	81
13	M	412/412 (100%)	406 (98%)	6 (2%)	57	84
14	N	315/315 (100%)	311 (99%)	4 (1%)	61	86
15	O	283/303 (93%)	277 (98%)	6 (2%)	47	79
16	P	293/327 (90%)	285 (97%)	8 (3%)	39	74
17	Q	116/153 (76%)	115 (99%)	1 (1%)	70	89
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	86
19	S	76/82 (93%)	74 (97%)	2 (3%)	40	75
20	T	81/135 (60%)	76 (94%)	5 (6%)	16	45
20	U	81/135 (60%)	80 (99%)	1 (1%)	63	87
21	V	101/102 (99%)	99 (98%)	2 (2%)	48	80
22	W	108/114 (95%)	107 (99%)	1 (1%)	70	89
23	X	154/155 (99%)	153 (99%)	1 (1%)	78	92
24	Y	101/102 (99%)	97 (96%)	4 (4%)	28	63
25	Z	120/121 (99%)	119 (99%)	1 (1%)	73	90
26	a	59/59 (100%)	57 (97%)	2 (3%)	32	68
27	b	71/72 (99%)	69 (97%)	2 (3%)	38	73
28	c	45/68 (66%)	43 (96%)	2 (4%)	25	59
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	73
30	e	89/96 (93%)	86 (97%)	3 (3%)	32	68
31	f	54/54 (100%)	53 (98%)	1 (2%)	50	81
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	69
33	h	121/158 (77%)	119 (98%)	2 (2%)	53	83
34	i	120/121 (99%)	117 (98%)	3 (2%)	42	76
35	j	61/84 (73%)	58 (95%)	3 (5%)	22	55
36	k	63/76 (83%)	61 (97%)	2 (3%)	34	70
37	l	140/159 (88%)	135 (96%)	5 (4%)	31	66
38	m	113/114 (99%)	111 (98%)	2 (2%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	n	156/161 (97%)	154 (99%)	2 (1%)	61	86
40	o	110/120 (92%)	108 (98%)	2 (2%)	51	82
41	p	155/157 (99%)	152 (98%)	3 (2%)	50	81
42	q	130/130 (100%)	127 (98%)	3 (2%)	44	78
43	r	85/97 (88%)	83 (98%)	2 (2%)	43	77
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7205/7891 (91%)	7059 (98%)	146 (2%)	48	80

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	27	LEU
1	A	97	LEU
2	B	50	PHE
2	B	54	CYS
2	B	82	GLN
2	B	100	LEU
3	C	20	LYS
4	D	46	ASN
4	D	50	ASN
4	D	61	VAL
4	D	75	LYS
4	D	161	ILE
4	D	230	THR
4	D	334	LYS
4	D	420	THR
5	E	29	LYS
5	E	63	ILE
5	E	118	GLU
5	E	169	ILE
5	E	181	ILE
5	E	203	THR
6	F	8	LYS
6	F	34	LYS
6	F	44	LYS
6	F	108	ARG
6	F	365	CYS
7	G	57	VAL
7	G	61	LYS

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Mol	Chain	Res	Type
7	G	97	LEU
7	G	174	THR
7	G	224	LYS
7	G	403	ASP
7	G	483	VAL
7	G	486	ASP
7	G	539	LYS
7	G	540	ASP
7	G	613	TYR
8	H	5	ASN
8	H	28	LEU
8	H	234	MET
8	H	274	ARG
8	H	310	LEU
9	I	14	MET
9	I	78	ILE
10	J	168	ILE
11	K	34	GLU
11	K	37	MET
12	L	31	ASN
12	L	101	MET
12	L	172	ILE
12	L	286	LEU
12	L	329	ILE
12	L	336	LYS
12	L	393	ASP
12	L	445	GLU
12	L	487	LYS
12	L	580	GLN
13	M	57	PHE
13	M	86	LYS
13	M	207	MET
13	M	246	ILE
13	M	315	LEU
13	M	413	MET
14	N	40	ILE
14	N	46	LYS
14	N	263	LYS
14	N	295	ARG
15	O	12	GLU
15	O	40	LYS
15	O	157	LYS

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Mol	Chain	Res	Type
15	O	168	VAL
15	O	214	MET
15	O	242	LYS
16	P	52	GLU
16	P	122	LYS
16	P	139	ILE
16	P	199	LYS
16	P	219	LYS
16	P	269	LEU
16	P	281	ARG
16	P	325	ARG
17	Q	16	LYS
18	R	96	HIS
19	S	38	LYS
19	S	47	ASN
20	T	8	LEU
20	T	16	LEU
20	T	20	LYS
20	T	30	LEU
20	T	83	LYS
20	U	50	ILE
21	V	39	LYS
21	V	115	ILE
22	W	120	LYS
23	X	63	ASN
24	Y	2	LYS
24	Y	50	GLU
24	Y	85	ASP
24	Y	114	CYS
25	Z	133	LEU
26	a	1	MET
26	a	69	ILE
27	b	3	ARG
27	b	9	LYS
28	c	1	LYS
28	c	6	GLU
29	d	5	ARG
29	d	8	ARG
29	d	104	LYS
30	e	38	GLU
30	e	84	LYS
30	e	90	LYS

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Mol	Chain	Res	Type
31	f	33	LYS
32	g	24	LEU
32	g	57	ASN
32	g	117	LYS
33	h	6	LYS
33	h	113	LEU
34	i	38	ARG
34	i	48	LYS
34	i	119	MET
35	j	43	ASP
35	j	48	LEU
35	j	70	ASP
36	k	34	LYS
36	k	91	LYS
37	l	6	LYS
37	l	89	VAL
37	l	126	GLN
37	l	148	LYS
37	l	157	GLU
38	m	39	ARG
38	m	84	LYS
39	n	54	LYS
39	n	137	LYS
40	o	7	ARG
40	o	38	MET
41	p	58	ASN
41	p	126	LYS
41	p	135	VAL
42	q	53	LYS
42	q	132	LYS
42	q	136	GLU
43	r	68	VAL
43	r	91	LYS

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

Mol	Chain	Res	Type
1	A	83	ASN
3	C	95	ASN
3	C	160	HIS
3	C	192	GLN
4	D	190	HIS

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Mol	Chain	Res	Type
4	D	217	ASN
5	E	58	ASN
5	E	121	GLN
5	E	214	GLN
6	F	402	HIS
6	F	421	HIS
7	G	179	ASN
7	G	402	ASN
7	G	696	HIS
8	H	5	ASN
8	H	47	GLN
8	H	250	HIS
12	L	348	HIS
13	M	43	ASN
13	M	220	HIS
13	M	293	HIS
13	M	304	GLN
13	M	331	ASN
15	O	190	HIS
15	O	271	ASN
16	P	93	ASN
16	P	131	HIS
19	S	47	ASN
21	V	82	GLN
22	W	50	GLN
29	d	79	GLN
29	d	97	HIS
30	e	76	HIS
33	h	124	HIS
34	i	82	HIS
36	k	20	GLN
36	k	90	GLN
37	l	28	ASN
37	l	78	HIS
39	n	11	HIS
40	o	91	HIS
42	q	17	HIS
42	q	91	HIS
43	r	72	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
4	2MR	D	85	4	10,12,13	2.44	2 (20%)	5,13,15	1.33	1 (20%)
11	FME	K	1	11	8,9,10	1.51	1 (12%)	8,9,11	1.41	2 (25%)
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.24	1 (11%)
27	AYA	b	1	27	6,7,8	1.88	1 (16%)	6,8,10	1.32	1 (16%)
34	SAC	i	1	34	7,8,9	1.73	1 (14%)	7,9,11	1.51	1 (14%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	8,9,11	1.39	1 (12%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	8,9,11	1.44	1 (12%)
42	AME	q	1	42	9,10,11	1.50	1 (11%)	9,11,13	1.33	1 (11%)
8	FME	H	1	8	8,9,10	1.49	1 (12%)	8,9,11	1.48	2 (25%)
1	FME	A	1	1	8,9,10	1.51	1 (12%)	8,9,11	1.38	1 (12%)
38	SAC	m	1	38	7,8,9	1.74	1 (14%)	7,9,11	1.29	1 (14%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	8,9,11	1.38	1 (12%)
43	AYA	r	1	43	6,7,8	1.87	2 (33%)	6,8,10	1.23	1 (16%)
24	AYA	Y	1	24	6,7,8	1.87	2 (33%)	6,8,10	1.42	1 (16%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	8,9,11	1.40	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	0/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	K	1	11	-	4/7/9/11	-
29	AME	d	1	29	-	5/9/10/12	-
27	AYA	b	1	27	-	0/5/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
12	FME	L	1	12	-	2/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
42	AME	q	1	42	-	4/9/10/12	-
8	FME	H	1	8	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
38	SAC	m	1	38	-	1/7/8/10	-
14	FME	N	1	14	-	3/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
24	AYA	Y	1	24	-	0/5/6/8	-
13	FME	M	1	13	-	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	5.42	1.44	1.33
4	D	85	2MR	CZ-NE	5.10	1.45	1.34
10	J	1	FME	CN-N	3.74	1.45	1.33
12	L	1	FME	CN-N	3.73	1.45	1.33
13	M	1	FME	CN-N	3.72	1.45	1.33
1	A	1	FME	CN-N	3.72	1.45	1.33
11	K	1	FME	CN-N	3.70	1.45	1.33
14	N	1	FME	CN-N	3.70	1.45	1.33
8	H	1	FME	CN-N	3.63	1.45	1.33
27	b	1	AYA	CT-N	3.54	1.45	1.34
34	i	1	SAC	C1A-N	3.53	1.45	1.34
38	m	1	SAC	C1A-N	3.51	1.45	1.34
29	d	1	AME	CT1-N	3.46	1.45	1.34
24	Y	1	AYA	CT-N	3.44	1.45	1.34
43	r	1	AYA	CT-N	3.39	1.45	1.34
42	q	1	AME	CT1-N	3.39	1.45	1.34
43	r	1	AYA	OT-CT	-2.09	1.18	1.23
24	Y	1	AYA	OT-CT	-2.03	1.18	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	2.87	120.88	116.12
24	Y	1	AYA	CM-CT-N	2.50	120.27	116.12
42	q	1	AME	CT2-CT1-N	2.40	120.10	116.12
38	m	1	SAC	C2A-C1A-N	2.36	120.04	116.12
27	b	1	AYA	CM-CT-N	2.33	119.98	116.12
4	D	85	2MR	CD-NE-CZ	-2.22	119.19	123.36
8	H	1	FME	CA-N-CN	-2.18	119.47	122.82
12	L	1	FME	O1-CN-N	-2.18	119.70	125.32
43	r	1	AYA	CM-CT-N	2.16	119.71	116.12
8	H	1	FME	O1-CN-N	-2.15	119.76	125.32
29	d	1	AME	CT2-CT1-N	2.14	119.67	116.12
10	J	1	FME	O1-CN-N	-2.14	119.79	125.32
11	K	1	FME	O1-CN-N	-2.12	119.85	125.32
14	N	1	FME	O1-CN-N	-2.12	119.85	125.32
1	A	1	FME	O1-CN-N	-2.04	120.04	125.32
13	M	1	FME	O1-CN-N	-2.03	120.08	125.32
11	K	1	FME	CA-N-CN	-2.00	119.75	122.82

There are no chirality outliers.

All (26) 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
29	d	1	AME	C-CA-CB-CG
42	q	1	AME	C-CA-CB-CG
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
10	J	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
29	d	1	AME	N-CA-CB-CG
42	q	1	AME	N-CA-CB-CG
12	L	1	FME	CA-CB-CG-SD
29	d	1	AME	CB-CG-SD-CE
42	q	1	AME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE
14	N	1	FME	N-CA-CB-CG
42	q	1	AME	CA-CB-CG-SD
38	m	1	SAC	C-CA-CB-OG
29	d	1	AME	CB-CA-N-CT1
12	L	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
13	M	1	FME	N-CA-CB-CG
14	N	1	FME	CB-CG-SD-CE
29	d	1	AME	C-CA-N-CT1
11	K	1	FME	CB-CA-N-CN
11	K	1	FME	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	1	AME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 83 ligands modelled in this entry, 4 are monoatomic - leaving 79 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	3PE	L	704	-	40,40,50	0.97	4 (10%)	43,45,55	1.14	2 (4%)
53	PLC	O	403	-	30,30,41	0.55	0	34,37,49	0.59	0
60	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.84	0
45	3PE	Y	206	-	44,44,50	0.93	4 (9%)	47,49,55	1.09	2 (4%)
52	CDL	r	201	-	60,60,99	1.12	8 (13%)	66,72,111	1.13	4 (6%)
58	EHZ	U	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.60	6 (16%)
53	PLC	Z	203	-	35,35,41	0.54	0	41,43,49	0.64	1 (2%)
46	PC1	B	203	-	47,47,53	1.01	4 (8%)	53,55,61	1.08	2 (3%)
57	NDP	P	501	-	51,52,52	4.01	28 (54%)	71,80,80	1.89	14 (19%)
52	CDL	L	701	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	b	102	-	46,46,50	0.91	4 (8%)	49,51,55	1.05	2 (4%)
46	PC1	I	204	-	53,53,53	0.94	4 (7%)	59,61,61	1.03	2 (3%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
52	CDL	M	602	-	99,99,99	0.88	8 (8%)	105,111,111	1.11	4 (3%)
52	CDL	i	202	-	75,75,99	1.01	8 (10%)	81,87,111	1.13	4 (4%)
47	SF4	I	201	9	0,12,12	-	-	-	-	-
45	3PE	q	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.05	2 (3%)
45	3PE	d	203	-	48,48,50	0.89	4 (8%)	51,53,55	1.03	2 (3%)
46	PC1	H	404	-	40,40,53	1.09	4 (10%)	46,48,61	1.01	2 (4%)
53	PLC	L	705	-	35,35,41	0.54	0	41,43,49	0.54	0
46	PC1	B	202	-	45,45,53	1.03	4 (8%)	51,53,61	1.03	2 (3%)
46	PC1	h	201	-	37,37,53	1.07	3 (8%)	43,45,61	0.96	1 (2%)
59	CHD	i	201	-	32,32,32	3.26	11 (34%)	51,51,51	2.39	17 (33%)
45	3PE	Y	204	-	50,50,50	0.87	4 (8%)	53,55,55	1.07	2 (3%)
52	CDL	N	401	-	93,93,99	0.90	8 (8%)	99,105,111	1.09	4 (4%)
53	PLC	J	204	-	34,34,41	0.55	0	40,42,49	0.56	0
47	SF4	I	202	9	0,12,12	-	-	-	-	-
47	SF4	G	802	7	0,12,12	-	-	-	-	-
45	3PE	b	101	-	35,35,50	1.03	4 (11%)	38,40,55	1.13	2 (5%)
52	CDL	d	202	-	86,86,99	0.94	8 (9%)	92,98,111	1.12	4 (4%)
52	CDL	H	402	-	57,57,99	1.11	7 (12%)	63,69,111	1.17	3 (4%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
46	PC1	Z	202	-	43,43,53	1.05	4 (9%)	49,51,61	1.01	2 (4%)
45	3PE	I	203	-	36,36,50	1.02	4 (11%)	39,41,55	1.09	2 (5%)
49	FMN	F	502	-	33,33,33	2.73	10 (30%)	48,50,50	1.76	13 (27%)
45	3PE	Y	207	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
45	3PE	P	502	-	37,37,50	1.00	4 (10%)	40,42,55	1.12	2 (5%)
53	PLC	Y	208	-	41,41,41	0.51	0	47,49,49	0.51	0
45	3PE	J	202	-	43,43,50	0.93	3 (6%)	46,48,55	1.12	2 (4%)
51	U10	H	401	-	34,34,63	1.99	17 (50%)	42,44,79	1.70	10 (23%)
46	PC1	A	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.06	2 (5%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
52	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.12	4 (5%)
46	PC1	A	204	-	32,32,53	1.22	4 (12%)	38,40,61	1.05	2 (5%)
46	PC1	d	204	-	38,38,53	1.12	3 (7%)	44,46,61	1.05	2 (4%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
53	PLC	O	404	-	30,30,41	0.59	0	36,38,49	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
45	3PE	A	202	-	41,41,50	0.95	4 (9%)	44,46,55	1.10	2 (4%)
45	3PE	f	101	-	23,23,50	1.25	4 (17%)	26,28,55	1.39	2 (7%)
53	PLC	g	202	-	41,41,41	0.51	0	47,49,49	0.49	0
46	PC1	M	606	-	34,34,53	1.17	4 (11%)	40,42,61	1.09	2 (5%)
45	3PE	Y	205	-	50,50,50	0.87	4 (8%)	53,55,55	1.04	2 (3%)
45	3PE	m	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.15	2 (4%)
45	3PE	g	201	-	28,28,50	1.15	4 (14%)	31,33,55	1.35	3 (9%)
46	PC1	l	701	-	46,46,53	1.02	4 (8%)	52,54,61	0.97	2 (3%)
46	PC1	H	405	-	46,46,53	1.02	4 (8%)	52,54,61	1.05	2 (3%)
45	3PE	Y	202	-	26,26,50	1.19	4 (15%)	29,31,55	1.16	2 (6%)
46	PC1	J	203	-	34,34,53	1.17	4 (11%)	40,42,61	1.08	2 (5%)
46	PC1	q	202	-	48,48,53	1.01	4 (8%)	54,56,61	1.02	2 (3%)
53	PLC	b	103	-	37,37,41	0.55	0	43,45,49	0.52	0
45	3PE	L	702	-	44,44,50	0.92	4 (9%)	47,49,55	1.05	2 (4%)
46	PC1	m	202	-	40,40,53	1.08	4 (10%)	46,48,61	1.01	2 (4%)
56	DGT	O	402	55	32,33,33	3.32	14 (43%)	48,52,52	1.95	13 (27%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	L	703	-	33,33,50	1.06	4 (12%)	36,38,55	1.16	2 (5%)
45	3PE	J	201	-	36,36,50	1.02	4 (11%)	39,41,55	1.19	2 (5%)
46	PC1	H	403	-	47,47,53	1.02	4 (8%)	53,55,61	1.06	2 (3%)
45	3PE	a	101	-	35,35,50	1.02	4 (11%)	38,40,55	1.01	2 (5%)
45	3PE	Y	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.12	2 (4%)
45	3PE	Z	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.05	2 (4%)
45	3PE	M	603	-	49,49,50	0.88	4 (8%)	52,54,55	1.09	2 (3%)
53	PLC	M	607	-	33,33,41	0.57	0	39,41,49	0.52	0
45	3PE	A	201	-	39,39,50	0.98	4 (10%)	42,44,55	1.04	2 (4%)
45	3PE	r	202	-	29,29,50	1.13	4 (13%)	32,34,55	1.21	2 (6%)
45	3PE	M	604	-	44,44,50	0.93	4 (9%)	47,49,55	1.10	2 (4%)
45	3PE	N	402	-	48,48,50	0.88	4 (8%)	51,53,55	1.07	2 (3%)
46	PC1	M	605	-	43,43,53	1.05	4 (9%)	49,51,61	1.00	2 (4%)
58	EHZ	T	101	20	31,36,37	1.57	5 (16%)	36,44,47	1.72	8 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	L	704	-	-	20/44/44/54	-
53	PLC	O	403	-	-	10/33/33/45	-
60	MYR	o	201	40	-	2/12/12/13	-
45	3PE	Y	206	-	-	18/48/48/54	-
52	CDL	r	201	-	-	28/71/71/110	-
58	EHZ	U	101	20	-	10/42/44/45	-
53	PLC	Z	203	-	-	14/39/39/45	-
46	PC1	B	203	-	-	19/51/51/57	-
57	NDP	P	501	-	-	9/34/77/77	0/5/5/5
52	CDL	L	701	-	-	40/110/110/110	-
45	3PE	b	102	-	-	21/50/50/54	-
46	PC1	I	204	-	-	16/57/57/57	-
47	SF4	F	501	6	-	-	0/6/5/5
52	CDL	M	602	-	-	49/110/110/110	-
52	CDL	i	202	-	-	38/86/86/110	-
47	SF4	I	201	9	-	-	0/6/5/5
45	3PE	q	201	-	-	24/54/54/54	-
45	3PE	d	203	-	-	25/52/52/54	-
46	PC1	H	404	-	-	14/44/44/57	-
53	PLC	L	705	-	-	13/39/39/45	-
46	PC1	B	202	-	-	20/49/49/57	-
46	PC1	h	201	-	-	10/40/40/57	-
59	CHD	i	201	-	-	3/9/74/74	0/4/4/4
45	3PE	Y	204	-	-	25/54/54/54	-
52	CDL	N	401	-	-	40/104/104/110	-
53	PLC	J	204	-	-	12/38/38/45	-
47	SF4	I	202	9	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
45	3PE	b	101	-	-	20/39/39/54	-
52	CDL	d	202	-	-	48/97/97/110	-
52	CDL	H	402	-	-	32/67/67/110	-
47	SF4	B	201	2	-	-	0/6/5/5
46	PC1	Z	202	-	-	18/47/47/57	-
45	3PE	I	203	-	-	13/40/40/54	-
49	FMN	F	502	-	-	3/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Y	207	-	-	15/39/39/54	-
45	3PE	P	502	-	-	17/41/41/54	-
53	PLC	Y	208	-	-	16/45/45/45	-
45	3PE	J	202	-	-	13/47/47/54	-
51	U10	H	401	-	-	10/29/53/87	0/1/1/1
46	PC1	A	203	-	-	17/38/38/57	-
48	FES	E	301	5	-	-	0/1/1/1
52	CDL	d	201	-	-	33/75/75/110	-
46	PC1	A	204	-	-	18/36/36/57	-
46	PC1	d	204	-	-	16/42/42/57	-
48	FES	G	803	7	-	-	0/1/1/1
53	PLC	O	404	-	-	9/34/34/45	-
45	3PE	Y	203	-	-	20/54/54/54	-
45	3PE	A	202	-	-	23/45/45/54	-
45	3PE	f	101	-	-	14/26/26/54	-
53	PLC	g	202	-	-	13/45/45/45	-
46	PC1	M	606	-	-	14/38/38/57	-
45	3PE	Y	205	-	-	22/54/54/54	-
45	3PE	m	201	-	-	15/44/44/54	-
45	3PE	g	201	-	-	16/31/31/54	-
46	PC1	l	701	-	-	17/50/50/57	-
46	PC1	H	405	-	-	24/50/50/57	-
45	3PE	Y	202	-	-	15/30/30/54	-
46	PC1	J	203	-	-	13/38/38/57	-
46	PC1	q	202	-	-	15/52/52/57	-
53	PLC	b	103	-	-	18/41/41/45	-
45	3PE	L	702	-	-	22/48/48/54	-
46	PC1	m	202	-	-	14/44/44/57	-
56	DGT	O	402	55	-	5/22/34/34	0/3/3/3
47	SF4	G	801	7	-	-	0/6/5/5
45	3PE	L	703	-	-	17/37/37/54	-
45	3PE	J	201	-	-	11/40/40/54	-
46	PC1	H	403	-	-	25/51/51/57	-
45	3PE	a	101	-	-	15/39/39/54	-
45	3PE	Y	201	-	-	17/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	Z	201	-	-	13/45/45/54	-
45	3PE	M	603	-	-	20/53/53/54	-
53	PLC	M	607	-	-	14/37/37/45	-
45	3PE	A	201	-	-	21/43/43/54	-
45	3PE	r	202	-	-	13/33/33/54	-
45	3PE	M	604	-	-	23/48/48/54	-
45	3PE	N	402	-	-	32/52/52/54	-
46	PC1	M	605	-	-	17/47/47/57	-
58	EHZ	T	101	20	-	8/42/44/45	-

All (334) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	PA-O3	10.42	1.70	1.59
57	P	501	NDP	C2B-C1B	-9.01	1.30	1.53
59	i	201	CHD	C11-C12	8.89	1.67	1.53
56	O	402	DGT	O6-C6	8.78	1.40	1.23
57	P	501	NDP	O4B-C1B	8.67	1.62	1.42
57	P	501	NDP	O4D-C1D	8.38	1.61	1.42
57	P	501	NDP	C7N-N7N	7.66	1.55	1.33
57	P	501	NDP	C2D-C1D	-7.22	1.30	1.53
59	i	201	CHD	C16-C15	7.17	1.73	1.54
57	P	501	NDP	C6N-C5N	7.09	1.54	1.33
56	O	402	DGT	C5-N7	6.74	1.52	1.39
49	F	502	FMN	C10-N1	6.55	1.46	1.33
57	P	501	NDP	O4D-C4D	-6.47	1.30	1.45
49	F	502	FMN	C4A-N5	6.42	1.44	1.30
59	i	201	CHD	C20-C17	-5.97	1.44	1.54
57	P	501	NDP	P2B-O2B	5.61	1.69	1.59
59	i	201	CHD	C13-C17	5.57	1.64	1.55
49	F	502	FMN	C5A-N5	5.43	1.49	1.39
57	P	501	NDP	C6A-N6A	5.43	1.48	1.34
59	i	201	CHD	C8-C9	5.33	1.64	1.53
59	i	201	CHD	O12-C12	-5.26	1.35	1.43
56	O	402	DGT	PB-O3B	5.26	1.65	1.59
56	O	402	DGT	PB-O3A	5.18	1.65	1.59
56	O	402	DGT	PA-O3A	5.10	1.65	1.59
57	P	501	NDP	O4B-C4B	-5.08	1.33	1.45
58	T	101	EHZ	C12-N1	5.08	1.45	1.33
58	U	101	EHZ	C12-N1	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	U	101	EHZ	C15-N2	4.99	1.45	1.33
49	F	502	FMN	C2-N1	4.99	1.47	1.36
59	i	201	CHD	C6-C5	4.98	1.61	1.53
49	F	502	FMN	C9A-N10	4.97	1.49	1.41
58	T	101	EHZ	C15-N2	4.94	1.45	1.33
56	O	402	DGT	C2-N1	4.81	1.49	1.37
56	O	402	DGT	C2-N2	4.80	1.45	1.34
57	P	501	NDP	C2N-C3N	4.67	1.48	1.35
57	P	501	NDP	PN-O3	4.57	1.64	1.59
56	O	402	DGT	C2-N3	4.40	1.43	1.33
49	F	502	FMN	C2-N3	4.35	1.48	1.39
57	P	501	NDP	C5A-C4A	-4.25	1.31	1.39
56	O	402	DGT	C8-N9	-4.22	1.28	1.37
59	i	201	CHD	C15-C14	4.16	1.62	1.54
57	P	501	NDP	O7N-C7N	-4.11	1.14	1.24
56	O	402	DGT	C4-N9	-3.89	1.28	1.38
57	P	501	NDP	C8A-N9A	-3.81	1.31	1.37
57	P	501	NDP	O2D-C2D	3.80	1.52	1.43
49	F	502	FMN	C10-N10	3.73	1.45	1.37
49	F	502	FMN	C4-N3	3.61	1.45	1.38
51	H	401	U10	C4-C5	-3.29	1.39	1.48
57	P	501	NDP	C4N-C3N	3.25	1.56	1.50
59	i	201	CHD	C6-C7	3.24	1.58	1.52
51	H	401	U10	C3-C2	-3.07	1.40	1.48
51	H	401	U10	C20-C19	2.96	1.57	1.50
49	F	502	FMN	O2-C2	-2.94	1.18	1.24
46	l	701	PC1	O21-C2	-2.87	1.39	1.46
51	H	401	U10	C6-C1	2.84	1.40	1.35
46	d	204	PC1	O21-C2	-2.83	1.39	1.46
57	P	501	NDP	C5A-N7A	-2.80	1.34	1.39
45	J	202	3PE	O21-C2	-2.79	1.40	1.46
52	M	602	CDL	OB6-CB4	-2.78	1.40	1.46
52	d	202	CDL	OB6-CB4	-2.78	1.40	1.46
52	H	402	CDL	OB6-CB4	-2.77	1.40	1.46
51	H	401	U10	C7-C8	2.77	1.54	1.50
52	r	201	CDL	OB6-CB4	-2.75	1.40	1.46
52	d	201	CDL	OA6-CA4	-2.75	1.40	1.46
46	A	203	PC1	O21-C2	-2.75	1.40	1.46
51	H	401	U10	C11-C9	2.74	1.56	1.51
52	r	201	CDL	OA6-CA4	-2.73	1.40	1.46
45	M	603	3PE	O21-C2	-2.73	1.40	1.46
52	N	401	CDL	OB6-CB4	-2.73	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	i	202	CDL	OB6-CB4	-2.72	1.40	1.46
57	P	501	NDP	C4N-C5N	2.72	1.56	1.49
46	I	204	PC1	O21-C2	-2.71	1.40	1.46
46	H	404	PC1	O21-C2	-2.71	1.40	1.46
46	q	202	PC1	O21-C2	-2.71	1.40	1.46
46	J	203	PC1	O21-C2	-2.71	1.40	1.46
46	B	202	PC1	O21-C2	-2.71	1.40	1.46
46	M	606	PC1	O21-C2	-2.71	1.40	1.46
52	H	402	CDL	OA6-CA4	-2.70	1.40	1.46
52	M	602	CDL	OA6-CA4	-2.70	1.40	1.46
49	F	502	FMN	O4-C4	-2.70	1.18	1.23
46	H	403	PC1	O21-C2	-2.70	1.40	1.46
52	L	701	CDL	OB6-CB4	-2.69	1.40	1.46
45	Y	202	3PE	O21-C2	-2.69	1.40	1.46
52	L	701	CDL	OA6-CA4	-2.69	1.40	1.46
45	a	101	3PE	O21-C2	-2.68	1.40	1.46
46	A	204	PC1	O21-C2	-2.68	1.40	1.46
45	M	604	3PE	O21-C2	-2.67	1.40	1.46
46	H	405	PC1	O21-C2	-2.67	1.40	1.46
52	i	202	CDL	OA6-CA4	-2.67	1.40	1.46
45	I	203	3PE	O21-C2	-2.67	1.40	1.46
45	L	703	3PE	O21-C2	-2.67	1.40	1.46
46	M	605	PC1	O21-C2	-2.66	1.40	1.46
45	N	402	3PE	O21-C2	-2.66	1.40	1.46
52	d	201	CDL	OB6-CB4	-2.66	1.40	1.46
45	g	201	3PE	O21-C2	-2.66	1.40	1.46
45	r	202	3PE	O21-C2	-2.66	1.40	1.46
45	b	102	3PE	O21-C2	-2.65	1.40	1.46
46	Z	202	PC1	O21-C2	-2.65	1.40	1.46
46	h	201	PC1	O21-C2	-2.65	1.40	1.46
45	d	203	3PE	O21-C2	-2.64	1.40	1.46
46	B	203	PC1	O21-C2	-2.64	1.40	1.46
45	Y	204	3PE	O21-C2	-2.64	1.40	1.46
45	P	502	3PE	O21-C2	-2.63	1.40	1.46
45	f	101	3PE	O21-C2	-2.62	1.40	1.46
46	m	202	PC1	O21-C2	-2.61	1.40	1.46
59	i	201	CHD	C13-C12	-2.61	1.50	1.54
56	O	402	DGT	C1'-N9	-2.59	1.41	1.48
45	Y	207	3PE	O21-C2	-2.59	1.40	1.46
45	A	202	3PE	O21-C2	-2.59	1.40	1.46
45	A	201	3PE	O21-C2	-2.59	1.40	1.46
45	L	704	3PE	O21-C2	-2.58	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	m	201	3PE	O21-C2	-2.58	1.40	1.46
45	Y	206	3PE	O21-C2	-2.57	1.40	1.46
45	J	201	3PE	O21-C2	-2.56	1.40	1.46
45	b	101	3PE	O21-C2	-2.55	1.40	1.46
45	Y	201	3PE	O21-C2	-2.53	1.40	1.46
45	q	201	3PE	O21-C2	-2.53	1.40	1.46
51	H	401	U10	C15-C14	2.53	1.56	1.50
52	d	202	CDL	OA6-CA4	-2.51	1.40	1.46
45	L	702	3PE	O21-C2	-2.50	1.40	1.46
52	r	201	CDL	OB8-CB7	2.49	1.40	1.33
45	A	201	3PE	O31-C31	2.49	1.40	1.33
52	L	701	CDL	OB8-CB7	2.47	1.40	1.33
57	P	501	NDP	O3D-C3D	-2.47	1.36	1.43
45	Z	201	3PE	O21-C2	-2.46	1.40	1.46
57	P	501	NDP	C6N-N1N	2.46	1.43	1.37
57	P	501	NDP	O3B-C3B	-2.46	1.36	1.43
46	A	203	PC1	O31-C31	2.45	1.40	1.33
52	d	201	CDL	OB8-CB7	2.45	1.40	1.33
52	N	401	CDL	OA6-CA4	-2.45	1.40	1.46
52	i	202	CDL	OB8-CB7	2.44	1.40	1.33
45	Y	203	3PE	O21-C2	-2.44	1.40	1.46
46	H	405	PC1	O31-C31	2.44	1.40	1.33
45	L	704	3PE	O31-C31	2.44	1.40	1.33
45	J	201	3PE	O31-C31	2.43	1.40	1.33
52	d	202	CDL	OA8-CA7	2.43	1.40	1.33
45	Y	203	3PE	O31-C31	2.43	1.40	1.33
45	L	703	3PE	O31-C31	2.43	1.40	1.33
46	m	202	PC1	O31-C31	2.43	1.40	1.33
46	q	202	PC1	O31-C31	2.43	1.40	1.33
45	b	102	3PE	O31-C31	2.43	1.40	1.33
52	i	202	CDL	OA8-CA7	2.42	1.40	1.33
45	d	203	3PE	O31-C31	2.42	1.40	1.33
52	H	402	CDL	OA8-CA7	2.42	1.40	1.33
46	Z	202	PC1	O31-C31	2.41	1.40	1.33
45	Z	201	3PE	O31-C31	2.41	1.40	1.33
52	N	401	CDL	OA8-CA7	2.41	1.40	1.33
46	M	606	PC1	O31-C31	2.41	1.40	1.33
58	T	101	EHZ	O4-C15	-2.41	1.18	1.23
46	A	204	PC1	O31-C31	2.39	1.40	1.33
46	d	204	PC1	O31-C31	2.39	1.40	1.33
52	r	201	CDL	OA8-CA7	2.39	1.40	1.33
46	H	404	PC1	O31-C31	2.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	M	605	PC1	O31-C31	2.38	1.40	1.33
45	Y	201	3PE	O31-C31	2.38	1.40	1.33
45	Y	202	3PE	O31-C31	2.38	1.40	1.33
45	q	201	3PE	O31-C31	2.38	1.40	1.33
46	H	403	PC1	O31-C31	2.38	1.40	1.33
52	L	701	CDL	OA8-CA7	2.38	1.40	1.33
46	l	701	PC1	O31-C31	2.38	1.40	1.33
45	m	201	3PE	O31-C31	2.38	1.40	1.33
52	M	602	CDL	OA8-CA7	2.38	1.40	1.33
45	b	101	3PE	O31-C31	2.37	1.40	1.33
46	B	202	PC1	O31-C31	2.37	1.40	1.33
52	d	201	CDL	OA8-CA6	-2.37	1.39	1.45
46	I	204	PC1	O31-C31	2.37	1.40	1.33
58	T	101	EHZ	C9-S1	2.37	1.81	1.76
45	Y	207	3PE	O31-C31	2.37	1.40	1.33
52	M	602	CDL	OB8-CB7	2.36	1.40	1.33
45	J	202	3PE	O31-C3	-2.36	1.39	1.45
45	I	203	3PE	O31-C31	2.36	1.40	1.33
45	Y	205	3PE	O21-C2	-2.36	1.41	1.46
51	H	401	U10	C7-C6	2.36	1.55	1.51
45	f	101	3PE	O31-C31	2.35	1.40	1.33
58	U	101	EHZ	O4-C15	-2.35	1.18	1.23
45	L	702	3PE	O31-C31	2.34	1.40	1.33
45	Y	204	3PE	O31-C31	2.34	1.40	1.33
45	r	202	3PE	O31-C3	-2.34	1.39	1.45
45	Y	206	3PE	O31-C3	-2.33	1.39	1.45
45	M	604	3PE	O31-C31	2.33	1.40	1.33
45	M	603	3PE	O31-C31	2.33	1.40	1.33
52	d	202	CDL	OB8-CB6	-2.33	1.40	1.45
58	U	101	EHZ	C9-S1	2.33	1.81	1.76
51	H	401	U10	C16-C14	2.33	1.56	1.51
45	g	201	3PE	O31-C31	2.33	1.40	1.33
46	B	203	PC1	O31-C3	-2.32	1.40	1.45
45	A	202	3PE	O31-C31	2.32	1.40	1.33
45	a	101	3PE	O31-C31	2.32	1.40	1.33
45	Y	206	3PE	O31-C31	2.32	1.40	1.33
46	J	203	PC1	O31-C31	2.31	1.40	1.33
46	B	203	PC1	O31-C31	2.31	1.40	1.33
58	T	101	EHZ	O3-C12	-2.31	1.18	1.23
57	P	501	NDP	C7N-C3N	2.31	1.53	1.48
45	g	201	3PE	O21-C21	2.31	1.40	1.35
52	N	401	CDL	OB8-CB6	-2.30	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	f	101	3PE	O21-C21	2.30	1.40	1.35
52	N	401	CDL	OB8-CB7	2.30	1.40	1.33
45	Y	205	3PE	O31-C31	2.29	1.40	1.33
45	N	402	3PE	O31-C31	2.29	1.40	1.33
45	r	202	3PE	O31-C31	2.28	1.40	1.33
46	J	203	PC1	O31-C3	-2.28	1.40	1.45
51	H	401	U10	C1M-C1	2.28	1.55	1.50
45	P	502	3PE	O31-C3	-2.26	1.40	1.45
45	q	201	3PE	O31-C3	-2.26	1.40	1.45
45	P	502	3PE	O31-C31	2.26	1.39	1.33
46	l	701	PC1	O31-C3	-2.26	1.40	1.45
57	P	501	NDP	PA-O5B	2.26	1.68	1.59
58	U	101	EHZ	O3-C12	-2.25	1.18	1.23
46	I	204	PC1	O31-C3	-2.24	1.40	1.45
45	g	201	3PE	O31-C3	-2.24	1.40	1.45
45	N	402	3PE	O31-C3	-2.24	1.40	1.45
56	O	402	DGT	PG-O2G	-2.23	1.46	1.54
57	P	501	NDP	P2B-O1X	2.23	1.57	1.50
46	B	202	PC1	O31-C3	-2.23	1.40	1.45
45	J	201	3PE	O31-C3	-2.23	1.40	1.45
45	b	101	3PE	O31-C3	-2.22	1.40	1.45
45	Y	202	3PE	O31-C3	-2.22	1.40	1.45
52	M	602	CDL	OA8-CA6	-2.22	1.40	1.45
45	b	102	3PE	O31-C3	-2.22	1.40	1.45
56	O	402	DGT	PG-O1G	-2.22	1.46	1.54
45	a	101	3PE	O31-C3	-2.22	1.40	1.45
45	A	202	3PE	O31-C3	-2.22	1.40	1.45
46	Z	202	PC1	O21-C21	2.21	1.40	1.34
45	Z	201	3PE	O21-C21	2.21	1.40	1.34
46	h	201	PC1	O21-C21	2.21	1.40	1.34
45	Y	204	3PE	O31-C3	-2.21	1.40	1.45
45	Y	205	3PE	O21-C21	2.21	1.40	1.34
52	d	201	CDL	OA8-CA7	2.21	1.39	1.33
45	L	702	3PE	O31-C3	-2.21	1.40	1.45
46	H	404	PC1	O31-C3	-2.21	1.40	1.45
45	Y	203	3PE	O31-C3	-2.21	1.40	1.45
45	Y	205	3PE	O31-C3	-2.21	1.40	1.45
46	H	405	PC1	O21-C21	2.20	1.40	1.34
45	Y	201	3PE	O31-C3	-2.20	1.40	1.45
46	M	605	PC1	O31-C3	-2.20	1.40	1.45
45	Y	203	3PE	O21-C21	2.20	1.40	1.34
45	M	603	3PE	O31-C3	-2.20	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	i	202	CDL	OB8-CB6	-2.19	1.40	1.45
52	N	401	CDL	OA6-CA5	2.19	1.40	1.34
51	H	401	U10	O3-C3	2.19	1.42	1.36
45	Z	201	3PE	O31-C3	-2.19	1.40	1.45
46	m	202	PC1	O21-C21	2.19	1.40	1.34
45	Y	207	3PE	O21-C21	2.19	1.40	1.34
52	d	201	CDL	OB6-CB5	2.19	1.40	1.34
45	Y	201	3PE	O21-C21	2.19	1.40	1.34
45	m	201	3PE	O31-C3	-2.18	1.40	1.45
52	r	201	CDL	OA8-CA6	-2.18	1.40	1.45
52	L	701	CDL	OB6-CB5	2.18	1.40	1.34
46	d	204	PC1	O31-C3	-2.18	1.40	1.45
52	M	602	CDL	OB8-CB6	-2.18	1.40	1.45
45	f	101	3PE	O31-C3	-2.18	1.40	1.45
56	O	402	DGT	C4-N3	2.18	1.39	1.34
45	d	203	3PE	O21-C21	2.18	1.40	1.34
45	J	202	3PE	O31-C31	2.17	1.39	1.33
52	N	401	CDL	OA8-CA6	-2.17	1.40	1.45
51	H	401	U10	O4-C4	2.17	1.42	1.36
46	A	204	PC1	O31-C3	-2.17	1.40	1.45
46	A	204	PC1	O21-C21	2.17	1.40	1.34
45	A	202	3PE	O21-C21	2.17	1.40	1.34
46	M	605	PC1	O21-C21	2.17	1.40	1.34
52	r	201	CDL	OA6-CA5	2.17	1.40	1.34
45	L	702	3PE	O21-C21	2.16	1.40	1.34
45	Y	207	3PE	O31-C3	-2.16	1.40	1.45
45	m	201	3PE	O21-C21	2.16	1.40	1.34
45	M	604	3PE	O31-C3	-2.16	1.40	1.45
45	I	203	3PE	O31-C3	-2.16	1.40	1.45
45	b	102	3PE	O21-C21	2.16	1.40	1.34
46	B	203	PC1	O21-C21	2.16	1.40	1.34
46	h	201	PC1	O31-C3	-2.16	1.40	1.45
46	q	202	PC1	O21-C21	2.16	1.40	1.34
45	d	203	3PE	O31-C3	-2.15	1.40	1.45
45	b	101	3PE	O21-C21	2.15	1.40	1.34
52	i	202	CDL	OA8-CA6	-2.15	1.40	1.45
51	H	401	U10	C6-C5	-2.15	1.40	1.46
45	L	704	3PE	O21-C21	2.15	1.40	1.34
45	L	704	3PE	O31-C3	-2.15	1.40	1.45
45	Y	206	3PE	O21-C21	2.14	1.40	1.34
46	J	203	PC1	O21-C21	2.14	1.40	1.34
51	H	401	U10	C1-C2	-2.14	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A	201	3PE	O21-C21	2.14	1.40	1.34
52	L	701	CDL	OB8-CB6	-2.14	1.40	1.45
46	I	204	PC1	O21-C21	2.14	1.40	1.34
52	d	202	CDL	OA6-CA5	2.14	1.40	1.34
45	J	201	3PE	O21-C21	2.14	1.40	1.34
52	L	701	CDL	OA6-CA5	2.14	1.40	1.34
52	d	201	CDL	OB8-CB6	-2.14	1.40	1.45
46	Z	202	PC1	O31-C3	-2.13	1.40	1.45
46	M	606	PC1	O21-C21	2.13	1.40	1.34
45	r	202	3PE	O21-C21	2.13	1.40	1.34
52	d	201	CDL	OA6-CA5	2.13	1.40	1.34
46	B	202	PC1	O21-C21	2.13	1.40	1.34
52	H	402	CDL	OB8-CB6	-2.13	1.40	1.45
52	r	201	CDL	OB8-CB6	-2.13	1.40	1.45
52	H	402	CDL	OA8-CA6	-2.13	1.40	1.45
46	q	202	PC1	O31-C3	-2.12	1.40	1.45
45	I	203	3PE	O21-C21	2.12	1.40	1.34
46	H	403	PC1	O21-C21	2.12	1.40	1.34
45	q	201	3PE	O21-C21	2.12	1.40	1.34
52	d	202	CDL	OB8-CB7	2.11	1.39	1.33
51	H	401	U10	C25-C24	2.11	1.55	1.50
45	Y	204	3PE	O21-C21	2.11	1.40	1.34
52	N	401	CDL	OB6-CB5	2.11	1.40	1.34
45	L	703	3PE	O31-C3	-2.11	1.40	1.45
46	M	606	PC1	O31-C3	-2.11	1.40	1.45
46	H	404	PC1	O21-C21	2.11	1.40	1.34
46	m	202	PC1	O31-C3	-2.10	1.40	1.45
45	N	402	3PE	O21-C21	2.10	1.40	1.34
46	H	405	PC1	O31-C3	-2.10	1.40	1.45
52	M	602	CDL	OA6-CA5	2.10	1.40	1.34
52	L	701	CDL	OA8-CA6	-2.10	1.40	1.45
45	a	101	3PE	O21-C21	2.09	1.40	1.34
45	A	201	3PE	O31-C3	-2.09	1.40	1.45
45	L	703	3PE	O21-C21	2.08	1.40	1.34
52	i	202	CDL	OB6-CB5	2.08	1.40	1.34
52	d	202	CDL	OB6-CB5	2.08	1.40	1.34
46	A	203	PC1	O31-C3	-2.08	1.40	1.45
45	M	603	3PE	O21-C21	2.08	1.40	1.34
45	P	502	3PE	O21-C21	2.08	1.40	1.34
46	H	403	PC1	O31-C3	-2.07	1.40	1.45
45	Y	202	3PE	O21-C21	2.07	1.40	1.34
51	H	401	U10	C22-C23	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	NDP	C5D-C4D	2.07	1.57	1.51
52	H	402	CDL	OA6-CA5	2.07	1.40	1.34
46	l	701	PC1	O21-C21	2.06	1.40	1.34
52	i	202	CDL	OA6-CA5	2.06	1.40	1.34
57	P	501	NDP	C5B-C4B	2.06	1.57	1.51
52	d	202	CDL	OA8-CA6	-2.06	1.40	1.45
51	H	401	U10	C10-C9	2.05	1.55	1.50
45	M	604	3PE	O21-C21	2.04	1.40	1.34
52	H	402	CDL	OB6-CB5	2.04	1.40	1.34
52	r	201	CDL	OB6-CB5	2.04	1.40	1.34
46	A	203	PC1	O21-C21	2.02	1.40	1.34
59	i	201	CHD	O7-C7	-2.02	1.39	1.43
52	M	602	CDL	OB6-CB5	2.00	1.39	1.34

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	O	402	DGT	C8-N9-C4	7.41	119.91	106.03
59	i	201	CHD	C17-C13-C14	6.54	106.68	100.11
59	i	201	CHD	C13-C17-C20	-6.20	111.98	119.48
58	T	101	EHZ	C8-C9-S1	6.00	121.13	113.56
57	P	501	NDP	N6A-C6A-N1A	-5.63	105.84	118.38
58	U	101	EHZ	C8-C9-S1	5.37	120.34	113.56
57	P	501	NDP	N3A-C2A-N1A	-5.28	120.58	128.58
57	P	501	NDP	C5A-C4A-N3A	-5.27	119.46	126.72
57	P	501	NDP	C4A-N9A-C1B	-5.17	114.55	126.63
45	f	101	3PE	O21-C21-C22	5.15	120.27	111.09
51	H	401	U10	C10-C9-C11	5.04	123.98	115.23
45	g	201	3PE	O21-C21-C22	4.97	119.95	111.09
57	P	501	NDP	C1B-N9A-C8A	4.75	137.64	127.09
59	i	201	CHD	C9-C10-C5	4.73	115.09	108.51
59	i	201	CHD	C17-C13-C12	4.72	121.91	117.67
49	F	502	FMN	C7M-C7-C6	4.63	127.72	119.57
49	F	502	FMN	C9-C8-C7	4.49	126.28	119.69
45	L	704	3PE	O21-C21-C22	4.44	121.08	111.48
45	m	201	3PE	O21-C21-C22	4.36	120.91	111.48
45	M	604	3PE	O21-C21-C22	4.31	120.81	111.48
45	Y	207	3PE	O21-C21-C22	4.31	120.80	111.48
46	H	403	PC1	O21-C21-C22	4.28	120.75	111.48
46	H	405	PC1	O21-C21-C22	4.26	120.70	111.48
46	M	606	PC1	O21-C21-C22	4.26	120.69	111.48
45	r	202	3PE	O21-C21-C22	4.22	120.60	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	I	204	PC1	O21-C21-C22	4.18	120.53	111.48
45	Y	201	3PE	O21-C21-C22	4.18	120.52	111.48
51	H	401	U10	C7-C8-C9	4.16	134.00	126.83
57	P	501	NDP	C5A-C6A-N6A	4.14	133.53	123.29
52	r	201	CDL	OA6-CA5-C11	4.13	120.41	111.48
52	d	201	CDL	OA6-CA5-C11	4.12	120.39	111.48
52	i	202	CDL	OA6-CA5-C11	4.11	120.37	111.48
46	B	203	PC1	O21-C21-C22	4.09	120.33	111.48
45	J	201	3PE	O21-C21-C22	4.08	120.31	111.48
45	b	101	3PE	O21-C21-C22	4.06	120.27	111.48
46	A	204	PC1	O21-C21-C22	4.06	120.27	111.48
45	J	202	3PE	O21-C21-C22	4.05	120.24	111.48
45	A	202	3PE	O21-C21-C22	4.05	120.23	111.48
52	H	402	CDL	OB6-CB5-C51	4.04	120.22	111.48
52	d	202	CDL	OB6-CB5-C51	4.01	120.17	111.48
52	M	602	CDL	OB6-CB5-C51	4.01	120.15	111.48
52	M	602	CDL	OA6-CA5-C11	4.01	120.15	111.48
46	A	203	PC1	O21-C21-C22	4.00	120.14	111.48
59	i	201	CHD	C14-C13-C12	4.00	111.07	107.42
45	Y	206	3PE	O21-C21-C22	4.00	120.13	111.48
45	Y	203	3PE	O21-C21-C22	3.99	120.12	111.48
46	q	202	PC1	O21-C21-C22	3.98	120.10	111.48
52	N	401	CDL	OB6-CB5-C51	3.98	120.09	111.48
51	H	401	U10	C8-C7-C6	3.98	121.88	112.08
45	Y	205	3PE	O21-C21-C22	3.98	120.08	111.48
45	L	703	3PE	O21-C21-C22	3.97	120.08	111.48
52	r	201	CDL	OB6-CB5-C51	3.97	120.06	111.48
45	P	502	3PE	O21-C21-C22	3.96	120.05	111.48
52	i	202	CDL	OB6-CB5-C51	3.95	120.03	111.48
59	i	201	CHD	C18-C13-C12	-3.95	105.10	109.06
45	A	201	3PE	O21-C21-C22	3.95	120.02	111.48
52	d	202	CDL	OA6-CA5-C11	3.94	120.01	111.48
45	Y	204	3PE	O21-C21-C22	3.94	120.00	111.48
45	q	201	3PE	O21-C21-C22	3.94	120.00	111.48
45	b	102	3PE	O21-C21-C22	3.93	119.98	111.48
52	L	701	CDL	OA6-CA5-C11	3.91	119.93	111.48
57	P	501	NDP	N9A-C8A-N7A	-3.90	108.40	113.94
45	N	402	3PE	O21-C21-C22	3.90	119.91	111.48
45	Y	202	3PE	O21-C21-C22	3.90	119.91	111.48
46	J	203	PC1	O21-C21-C22	3.88	119.87	111.48
52	H	402	CDL	OA6-CA5-C11	3.88	119.87	111.48
45	M	603	3PE	O21-C21-C22	3.86	119.82	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B	202	PC1	O21-C21-C22	3.85	119.82	111.48
45	Z	201	3PE	O21-C21-C22	3.85	119.80	111.48
59	i	201	CHD	C18-C13-C14	-3.84	105.18	111.20
46	H	404	PC1	O21-C21-C22	3.82	119.74	111.48
45	d	203	3PE	O21-C21-C22	3.80	119.71	111.48
46	Z	202	PC1	O21-C21-C22	3.80	119.70	111.48
46	m	202	PC1	O21-C21-C22	3.78	119.65	111.48
45	L	702	3PE	O21-C21-C22	3.75	119.59	111.48
46	M	605	PC1	O21-C21-C22	3.74	119.57	111.48
45	I	203	3PE	O21-C21-C22	3.73	119.55	111.48
46	d	204	PC1	O21-C21-C22	3.68	119.44	111.48
46	h	201	PC1	O21-C21-C22	3.68	119.44	111.48
52	L	701	CDL	OB6-CB5-C51	3.64	119.36	111.48
59	i	201	CHD	C18-C13-C17	-3.59	105.58	111.20
52	N	401	CDL	OA6-CA5-C11	3.52	119.09	111.48
56	O	402	DGT	C1'-N9-C8	-3.51	120.05	127.91
49	F	502	FMN	C4-N3-C2	-3.48	119.46	125.64
57	P	501	NDP	C2A-N3A-C4A	3.45	120.25	111.83
46	l	701	PC1	O21-C21-C22	3.35	118.73	111.48
58	T	101	EHZ	C13-C12-N1	3.34	122.43	116.34
49	F	502	FMN	C8M-C8-C7	-3.29	114.04	120.76
57	P	501	NDP	N3A-C4A-N9A	3.23	132.65	127.17
56	O	402	DGT	C2-N1-C6	-3.20	119.31	125.11
59	i	201	CHD	C23-C22-C20	-3.16	108.56	114.46
52	d	202	CDL	OA8-CA7-C31	3.08	121.22	111.83
46	l	701	PC1	O31-C31-C32	3.03	121.08	111.83
56	O	402	DGT	C2'-C3'-C4'	3.02	108.93	102.80
45	J	201	3PE	O31-C31-C32	3.01	121.03	111.83
56	O	402	DGT	O2G-PG-O3B	3.01	114.72	104.64
45	M	603	3PE	O31-C31-C32	3.00	120.99	111.83
46	B	203	PC1	O31-C31-C32	3.00	120.98	111.83
52	L	701	CDL	OA8-CA7-C31	2.96	120.85	111.83
52	H	402	CDL	OA8-CA7-C31	2.95	120.09	111.15
52	M	602	CDL	OB8-CB7-C71	2.95	120.81	111.83
59	i	201	CHD	C11-C9-C10	-2.94	110.72	113.70
52	d	202	CDL	OB8-CB7-C71	2.92	120.74	111.83
45	g	201	3PE	O31-C31-C32	2.89	120.66	111.83
45	Y	203	3PE	O31-C31-C32	2.84	120.50	111.83
46	H	403	PC1	O31-C31-C32	2.84	120.49	111.83
49	F	502	FMN	C4A-C10-N10	2.84	120.55	116.48
52	i	202	CDL	OB8-CB7-C71	2.83	120.46	111.83
46	B	202	PC1	O31-C31-C32	2.83	120.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	H	401	U10	C10-C9-C8	-2.82	116.38	123.63
45	L	704	3PE	O31-C31-C32	2.80	120.38	111.83
56	O	402	DGT	O1G-PG-O3B	2.79	113.99	104.64
45	Y	207	3PE	O31-C31-C32	2.79	119.61	111.15
45	N	402	3PE	O31-C31-C32	2.77	120.27	111.83
46	d	204	PC1	O31-C31-C32	2.76	120.26	111.83
52	d	201	CDL	OB8-CB7-C71	2.75	120.23	111.83
45	M	604	3PE	O31-C31-C32	2.74	120.19	111.83
45	f	101	3PE	O31-C31-C32	2.74	120.19	111.83
45	m	201	3PE	O31-C31-C32	2.73	120.17	111.83
46	J	203	PC1	O31-C31-C32	2.73	120.15	111.83
58	T	101	EHZ	O2-C9-C8	-2.72	119.46	123.74
45	Z	201	3PE	O31-C31-C32	2.71	120.11	111.83
52	r	201	CDL	OB8-CB7-C71	2.70	120.08	111.83
59	i	201	CHD	C15-C14-C8	2.70	122.06	118.36
52	N	401	CDL	OB8-CB7-C71	2.70	120.05	111.83
46	q	202	PC1	O31-C31-C32	2.69	120.05	111.83
46	H	405	PC1	O31-C31-C32	2.69	120.03	111.83
57	P	501	NDP	C5A-N7A-C8A	2.69	107.67	103.45
45	r	202	3PE	O31-C31-C32	2.68	120.02	111.83
49	F	502	FMN	C6-C7-C8	-2.68	115.75	119.69
45	L	703	3PE	O31-C31-C32	2.67	119.99	111.83
45	Y	201	3PE	O31-C31-C32	2.67	119.99	111.83
45	Y	205	3PE	O31-C31-C32	2.67	119.99	111.83
45	Y	206	3PE	O31-C31-C32	2.67	119.99	111.83
52	N	401	CDL	OA8-CA7-C31	2.67	119.98	111.83
46	H	404	PC1	O31-C31-C32	2.67	119.98	111.83
45	q	201	3PE	O31-C31-C32	2.67	119.97	111.83
45	I	203	3PE	O31-C31-C32	2.67	119.97	111.83
45	A	202	3PE	O31-C31-C32	2.66	119.95	111.83
52	M	602	CDL	OA8-CA7-C31	2.66	119.95	111.83
46	A	203	PC1	O31-C31-C32	2.65	119.91	111.83
46	M	606	PC1	O31-C31-C32	2.63	119.85	111.83
58	T	101	EHZ	C10-S1-C9	2.63	109.60	101.84
45	Y	202	3PE	O31-C31-C32	2.63	119.84	111.83
46	Z	202	PC1	O31-C31-C32	2.62	119.83	111.83
45	J	202	3PE	O31-C31-C32	2.62	119.83	111.83
45	b	102	3PE	O31-C31-C32	2.62	119.82	111.83
45	L	702	3PE	O31-C31-C32	2.61	119.78	111.83
45	a	101	3PE	O31-C31-C32	2.60	119.76	111.83
51	H	401	U10	C20-C19-C21	2.59	119.73	115.23
46	A	204	PC1	O31-C31-C32	2.59	119.73	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	i	201	CHD	C19-C10-C9	-2.59	107.70	111.18
59	i	201	CHD	C16-C17-C13	2.58	106.05	103.54
52	d	201	CDL	OB6-CB5-C51	2.58	120.40	110.93
59	i	201	CHD	C1-C10-C9	-2.57	107.34	111.34
58	T	101	EHZ	O2-C9-S1	-2.57	119.41	122.68
49	F	502	FMN	C4A-C4-N3	2.57	119.79	113.25
45	Y	204	3PE	O31-C31-C32	2.56	119.66	111.83
45	P	502	3PE	O31-C31-C32	2.56	119.65	111.83
45	A	201	3PE	O31-C31-C32	2.56	119.64	111.83
51	H	401	U10	C12-C11-C9	2.55	121.64	113.19
45	b	101	3PE	O31-C31-C32	2.53	119.56	111.83
46	M	605	PC1	O31-C31-C32	2.53	119.54	111.83
46	I	204	PC1	O31-C31-C32	2.52	119.53	111.83
45	a	101	3PE	O21-C21-C22	2.52	120.20	110.93
52	L	701	CDL	OB8-CB7-C71	2.52	119.53	111.83
51	H	401	U10	C7-C6-C5	-2.52	115.59	118.52
52	i	202	CDL	OA8-CA7-C31	2.51	119.48	111.83
52	d	201	CDL	OA8-CA7-C31	2.50	119.47	111.83
45	d	203	3PE	O31-C31-C32	2.50	119.46	111.83
56	O	402	DGT	C5-C6-N1	2.49	119.59	113.25
46	m	202	PC1	O31-C31-C32	2.49	119.41	111.83
49	F	502	FMN	O4-C4-C4A	-2.48	119.98	126.53
49	F	502	FMN	C9A-C5A-N5	-2.47	119.83	122.45
49	F	502	FMN	C5A-C9A-N10	2.47	120.20	117.97
58	T	101	EHZ	C11-N1-C12	-2.47	118.23	122.82
52	r	201	CDL	OA8-CA7-C31	2.47	119.36	111.83
56	O	402	DGT	O1B-PB-O2B	-2.46	101.00	112.44
58	U	101	EHZ	O2-C9-C8	-2.43	119.91	123.74
56	O	402	DGT	O6-C6-C5	-2.41	120.16	126.53
56	O	402	DGT	O1A-PA-O2A	-2.41	101.23	112.44
59	i	201	CHD	C4-C3-C2	2.38	113.52	110.62
57	P	501	NDP	C2B-C1B-N9A	-2.34	109.90	113.75
59	i	201	CHD	C9-C11-C12	-2.34	111.24	114.29
58	U	101	EHZ	O2-C9-S1	-2.31	119.74	122.68
57	P	501	NDP	P2B-O2B-C2B	-2.30	117.29	123.43
51	H	401	U10	C15-C14-C16	2.29	119.21	115.23
49	F	502	FMN	C10-C4A-N5	-2.28	120.16	124.81
49	F	502	FMN	C6-C5A-C9A	2.25	122.14	119.05
51	H	401	U10	C22-C23-C24	-2.24	122.50	127.62
58	T	101	EHZ	O3-C12-N1	-2.23	118.65	123.03
56	O	402	DGT	C5-C4-N9	-2.20	101.71	105.66
58	U	101	EHZ	C7-C8-C9	-2.20	108.95	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	O	402	DGT	N9-C4-N3	2.16	130.27	125.95
58	U	101	EHZ	C13-C12-N1	2.16	120.27	116.34
45	g	201	3PE	C2-O21-C21	-2.14	114.07	117.85
53	Z	203	PLC	C3-C2-C1	2.13	116.76	111.78
58	U	101	EHZ	C14-C13-C12	-2.12	108.86	112.39
49	F	502	FMN	C7M-C7-C8	-2.08	116.52	120.76
57	P	501	NDP	C4A-C5A-N7A	-2.07	108.22	110.58
57	P	501	NDP	C6A-C5A-C4A	2.05	119.98	117.18
58	T	101	EHZ	C14-N2-C15	-2.05	118.87	122.55
51	H	401	U10	C25-C24-C26	2.05	118.54	116.13
56	O	402	DGT	C1'-N9-C4	-2.02	120.04	125.50
59	i	201	CHD	C6-C5-C4	-2.02	108.92	111.23

There are no chirality outliers.

All (1304) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C22-C21-O21-C2
45	A	202	3PE	C1-O11-P-O13
45	A	202	3PE	C1-O11-P-O14
45	A	202	3PE	C11-O13-P-O11
45	A	202	3PE	C11-O13-P-O12
45	A	202	3PE	C11-O13-P-O14
45	A	202	3PE	O22-C21-O21-C2
45	I	203	3PE	O11-C1-C2-O21
45	J	201	3PE	O32-C31-O31-C3
45	L	702	3PE	C1-O11-P-O12
45	L	702	3PE	C1-O11-P-O13
45	L	702	3PE	C1-O11-P-O14
45	L	702	3PE	C22-C21-O21-C2
45	L	703	3PE	C11-O13-P-O11
45	L	703	3PE	C11-O13-P-O12
45	L	703	3PE	C11-O13-P-O14
45	L	703	3PE	O21-C2-C3-O31
45	L	703	3PE	C22-C21-O21-C2
45	L	704	3PE	C11-O13-P-O11
45	L	704	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
45	L	704	3PE	O22-C21-O21-C2
45	M	603	3PE	C11-O13-P-O11
45	M	603	3PE	C11-O13-P-O12
45	M	604	3PE	C1-O11-P-O12
45	M	604	3PE	C1-O11-P-O13
45	M	604	3PE	C1-O11-P-O14
45	M	604	3PE	C11-O13-P-O11
45	M	604	3PE	C11-O13-P-O12
45	M	604	3PE	C11-O13-P-O14
45	N	402	3PE	C1-O11-P-O12
45	N	402	3PE	C1-O11-P-O13
45	N	402	3PE	C1-O11-P-O14
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C12-C11-O13-P
45	N	402	3PE	O13-C11-C12-N
45	P	502	3PE	C1-O11-P-O12
45	P	502	3PE	C1-O11-P-O13
45	P	502	3PE	C1-O11-P-O14
45	P	502	3PE	C11-O13-P-O14
45	P	502	3PE	C2-C1-O11-P
45	P	502	3PE	C22-C21-O21-C2
45	Y	201	3PE	C11-O13-P-O14
45	Y	201	3PE	O32-C31-O31-C3
45	Y	202	3PE	C1-O11-P-O12
45	Y	202	3PE	C11-O13-P-O14
45	Y	203	3PE	C1-O11-P-O13
45	Y	203	3PE	C1-O11-P-O14
45	Y	203	3PE	C22-C21-O21-C2
45	Y	205	3PE	C1-O11-P-O12
45	Y	205	3PE	C1-O11-P-O13
45	Y	205	3PE	C11-O13-P-O11
45	Y	205	3PE	C12-C11-O13-P
45	Y	205	3PE	C22-C21-O21-C2
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	207	3PE	C11-O13-P-O11
45	Y	207	3PE	C11-O13-P-O12
45	Y	207	3PE	C11-O13-P-O14
45	Y	207	3PE	O22-C21-O21-C2
45	Z	201	3PE	C11-O13-P-O11
45	Z	201	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
45	Z	201	3PE	C11-O13-P-O14
45	a	101	3PE	C11-O13-P-O11
45	a	101	3PE	C11-O13-P-O12
45	a	101	3PE	O22-C21-O21-C2
45	b	101	3PE	C1-O11-P-O12
45	b	101	3PE	C1-O11-P-O14
45	b	101	3PE	C11-O13-P-O11
45	b	101	3PE	C11-O13-P-O14
45	b	101	3PE	C12-C11-O13-P
45	b	101	3PE	C22-C21-O21-C2
45	b	102	3PE	C11-O13-P-O11
45	b	102	3PE	C11-O13-P-O12
45	b	102	3PE	C11-O13-P-O14
45	b	102	3PE	O21-C2-C3-O31
45	d	203	3PE	C1-O11-P-O12
45	d	203	3PE	C1-O11-P-O13
45	d	203	3PE	C1-O11-P-O14
45	d	203	3PE	C11-O13-P-O11
45	d	203	3PE	C11-O13-P-O12
45	d	203	3PE	O21-C2-C3-O31
45	f	101	3PE	C1-O11-P-O14
45	f	101	3PE	C11-O13-P-O11
45	f	101	3PE	C11-O13-P-O12
45	f	101	3PE	C11-O13-P-O14
45	f	101	3PE	O13-C11-C12-N
45	f	101	3PE	O22-C21-O21-C2
45	f	101	3PE	C22-C21-O21-C2
45	m	201	3PE	C11-O13-P-O14
45	m	201	3PE	O22-C21-O21-C2
45	q	201	3PE	C11-O13-P-O11
45	r	202	3PE	O22-C21-O21-C2
45	r	202	3PE	C22-C21-O21-C2
46	A	203	PC1	C1-O11-P-O12
46	A	203	PC1	C1-O11-P-O14
46	A	203	PC1	C1-O11-P-O13
46	A	203	PC1	O13-C11-C12-N
46	A	204	PC1	C11-O13-P-O12
46	A	204	PC1	C11-O13-P-O11
46	A	204	PC1	C1-O11-P-O12
46	A	204	PC1	C1-O11-P-O14
46	A	204	PC1	C1-O11-P-O13
46	A	204	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	203	PC1	C11-O13-P-O12
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C11-O13-P-O11
46	B	203	PC1	C1-O11-P-O12
46	B	203	PC1	C1-O11-P-O13
46	B	203	PC1	C22-C21-O21-C2
46	H	403	PC1	C1-O11-P-O12
46	H	403	PC1	C1-O11-P-O14
46	H	403	PC1	C1-O11-P-O13
46	H	403	PC1	O13-C11-C12-N
46	H	405	PC1	C11-O13-P-O12
46	H	405	PC1	C11-O13-P-O11
46	H	405	PC1	C1-O11-P-O12
46	H	405	PC1	C1-O11-P-O14
46	H	405	PC1	C1-O11-P-O13
46	H	405	PC1	C22-C21-O21-C2
46	I	204	PC1	O13-C11-C12-N
46	J	203	PC1	C1-O11-P-O12
46	J	203	PC1	C1-O11-P-O14
46	J	203	PC1	C1-O11-P-O13
46	J	203	PC1	C22-C21-O21-C2
46	M	605	PC1	C1-O11-P-O12
46	M	605	PC1	C1-O11-P-O13
46	M	606	PC1	C11-O13-P-O12
46	M	606	PC1	C11-O13-P-O14
46	M	606	PC1	C11-O13-P-O11
46	M	606	PC1	C1-O11-P-O12
46	Z	202	PC1	C1-O11-P-O12
46	Z	202	PC1	C1-O11-P-O13
46	h	201	PC1	C1-O11-P-O12
46	h	201	PC1	C1-O11-P-O14
46	h	201	PC1	C1-O11-P-O13
46	l	701	PC1	C11-O13-P-O12
46	l	701	PC1	C11-O13-P-O14
46	m	202	PC1	C1-O11-P-O12
46	m	202	PC1	C1-O11-P-O14
46	m	202	PC1	C1-O11-P-O13
46	q	202	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
46	q	202	PC1	C11-O13-P-O11
46	q	202	PC1	C22-C21-O21-C2
51	H	401	U10	C1-C6-C7-C8
51	H	401	U10	C5-C6-C7-C8
51	H	401	U10	C12-C11-C9-C8
52	H	402	CDL	C1-CA2-OA2-PA1
52	H	402	CDL	CA2-OA2-PA1-OA4
52	H	402	CDL	CA2-OA2-PA1-OA5
52	H	402	CDL	C11-CA5-OA6-CA4
52	H	402	CDL	CB3-OB5-PB2-OB2
52	H	402	CDL	CB3-OB5-PB2-OB3
52	H	402	CDL	C51-CB5-OB6-CB4
52	L	701	CDL	CA3-OA5-PA1-OA2
52	L	701	CDL	CA3-OA5-PA1-OA3
52	M	602	CDL	O1-C1-CA2-OA2
52	M	602	CDL	CA3-OA5-PA1-OA2
52	M	602	CDL	CA3-OA5-PA1-OA3
52	M	602	CDL	CA3-OA5-PA1-OA4
52	M	602	CDL	C51-CB5-OB6-CB4
52	N	401	CDL	CA2-OA2-PA1-OA3
52	N	401	CDL	OB7-CB5-OB6-CB4
52	d	201	CDL	O1-C1-CA2-OA2
52	d	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	C11-CA5-OA6-CA4
52	d	201	CDL	CB2-OB2-PB2-OB3
52	d	201	CDL	CB2-OB2-PB2-OB5
52	d	201	CDL	OB5-CB3-CB4-OB6
52	d	201	CDL	OB7-CB5-OB6-CB4
52	d	201	CDL	C51-CB5-OB6-CB4
52	d	202	CDL	O1-C1-CA2-OA2
52	d	202	CDL	CA2-OA2-PA1-OA4
52	d	202	CDL	CA2-OA2-PA1-OA5
52	d	202	CDL	CA3-OA5-PA1-OA2
52	d	202	CDL	CA3-OA5-PA1-OA4
52	d	202	CDL	OB7-CB5-OB6-CB4
52	d	202	CDL	C51-CB5-OB6-CB4
52	i	202	CDL	O1-C1-CB2-OB2
52	i	202	CDL	CA3-OA5-PA1-OA2
52	i	202	CDL	CA3-OA5-PA1-OA3
52	i	202	CDL	CA3-OA5-PA1-OA4
52	i	202	CDL	C51-CB5-OB6-CB4
52	r	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CB2-OB2-PB2-OB3
52	r	201	CDL	CB2-OB2-PB2-OB4
53	J	204	PLC	O4P-C4-C5-N
53	J	204	PLC	C1-O3P-P-O1P
53	J	204	PLC	C4-O4P-P-O2P
53	J	204	PLC	C4-O4P-P-O3P
53	L	705	PLC	O4P-C4-C5-N
53	L	705	PLC	C1-O3P-P-O1P
53	L	705	PLC	C4-O4P-P-O1P
53	L	705	PLC	C4-O4P-P-O3P
53	M	607	PLC	C4-O4P-P-O3P
53	O	403	PLC	O2-C2-C3-O3
53	O	403	PLC	O4P-C4-C5-N
53	O	403	PLC	OB-CB-O3-C3
53	O	404	PLC	C1'-C'-O2-C2
53	O	404	PLC	C4-O4P-P-O3P
53	Y	208	PLC	O4P-C4-C5-N
53	Y	208	PLC	C1-O3P-P-O2P
53	Y	208	PLC	C1-O3P-P-O4P
53	Y	208	PLC	C4-O4P-P-O1P
53	Z	203	PLC	C1'-C'-O2-C2
53	Z	203	PLC	O'-C'-O2-C2
53	Z	203	PLC	C1-O3P-P-O2P
53	Z	203	PLC	C1-O3P-P-O4P
53	Z	203	PLC	C4-O4P-P-O2P
53	Z	203	PLC	C4-O4P-P-O3P
53	b	103	PLC	O3P-C1-C2-O2
53	b	103	PLC	C1-O3P-P-O1P
53	b	103	PLC	C1-O3P-P-O2P
53	b	103	PLC	C1-O3P-P-O4P
53	b	103	PLC	C4-O4P-P-O1P
53	b	103	PLC	C4-O4P-P-O2P
53	b	103	PLC	C4-O4P-P-O3P
53	g	202	PLC	C1-O3P-P-O2P
53	g	202	PLC	C1-O3P-P-O4P
56	O	402	DGT	C5'-O5'-PA-O1A
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	C12-C13-C14-N2
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	O2-C9-S1-C10

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Mol	Chain	Res	Type	Atoms
58	U	101	EHZ	C8-C9-S1-C10
45	I	203	3PE	O32-C31-O31-C3
45	Y	205	3PE	O32-C31-O31-C3
46	A	204	PC1	O32-C31-O31-C3
46	d	204	PC1	O32-C31-O31-C3
52	L	701	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OB9-CB7-OB8-CB6
45	Y	205	3PE	C32-C31-O31-C3
46	d	204	PC1	C32-C31-O31-C3
52	M	602	CDL	C71-CB7-OB8-CB6
45	A	202	3PE	O32-C31-O31-C3
45	Z	201	3PE	O32-C31-O31-C3
45	a	101	3PE	O32-C31-O31-C3
45	m	201	3PE	O32-C31-O31-C3
45	r	202	3PE	O32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
46	B	203	PC1	O32-C31-O31-C3
46	H	405	PC1	O32-C31-O31-C3
46	l	701	PC1	O32-C31-O31-C3
52	d	201	CDL	OB9-CB7-OB8-CB6
52	d	202	CDL	OA9-CA7-OA8-CA6
52	r	201	CDL	OB9-CB7-OB8-CB6
52	H	402	CDL	OB9-CB7-OB8-CB6
52	H	402	CDL	C71-CB7-OB8-CB6
45	g	201	3PE	O32-C31-O31-C3
45	A	201	3PE	O22-C21-O21-C2
45	L	702	3PE	O22-C21-O21-C2
45	Y	203	3PE	O22-C21-O21-C2
45	Y	205	3PE	O22-C21-O21-C2
45	b	101	3PE	O22-C21-O21-C2
46	B	203	PC1	O22-C21-O21-C2
46	H	405	PC1	O22-C21-O21-C2
46	J	203	PC1	O22-C21-O21-C2
46	m	202	PC1	O22-C21-O21-C2
52	H	402	CDL	OA7-CA5-OA6-CA4
52	H	402	CDL	OB7-CB5-OB6-CB4
52	d	201	CDL	OA7-CA5-OA6-CA4
52	i	202	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	OA7-CA5-OA6-CA4
53	O	404	PLC	O'-C'-O2-C2
45	I	203	3PE	C32-C31-O31-C3
45	J	201	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C32-C31-O31-C3
45	Z	201	3PE	C32-C31-O31-C3
45	a	101	3PE	C32-C31-O31-C3
45	r	202	3PE	C32-C31-O31-C3
46	A	204	PC1	C32-C31-O31-C3
46	B	203	PC1	C32-C31-O31-C3
46	H	405	PC1	C32-C31-O31-C3
46	l	701	PC1	C32-C31-O31-C3
52	L	701	CDL	C31-CA7-OA8-CA6
52	d	201	CDL	C71-CB7-OB8-CB6
52	r	201	CDL	C71-CB7-OB8-CB6
45	g	201	3PE	C22-C21-O21-C2
46	h	201	PC1	O32-C31-O31-C3
45	A	202	3PE	C22-C21-O21-C2
45	L	704	3PE	C22-C21-O21-C2
45	Y	207	3PE	C22-C21-O21-C2
45	a	101	3PE	C22-C21-O21-C2
45	m	201	3PE	C22-C21-O21-C2
46	A	204	PC1	C22-C21-O21-C2
46	m	202	PC1	C22-C21-O21-C2
52	N	401	CDL	C51-CB5-OB6-CB4
45	A	202	3PE	C32-C31-O31-C3
45	g	201	3PE	C32-C31-O31-C3
45	m	201	3PE	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
52	d	202	CDL	C31-CA7-OA8-CA6
46	h	201	PC1	C32-C31-O31-C3
45	N	402	3PE	O32-C31-O31-C3
45	Y	206	3PE	O32-C31-O31-C3
45	f	101	3PE	O32-C31-O31-C3
45	L	703	3PE	O22-C21-O21-C2
45	P	502	3PE	O22-C21-O21-C2
46	q	202	PC1	O22-C21-O21-C2
52	M	602	CDL	OB7-CB5-OB6-CB4
45	L	704	3PE	C32-C31-O31-C3
45	f	101	3PE	C32-C31-O31-C3
46	J	203	PC1	C32-C31-O31-C3
52	H	402	CDL	C31-CA7-OA8-CA6
52	d	202	CDL	C11-CA5-OA6-CA4
57	P	501	NDP	C3B-C4B-C5B-O5B
57	P	501	NDP	O4D-C4D-C5D-O5D
57	P	501	NDP	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	C32-C31-O31-C3
45	Y	206	3PE	C32-C31-O31-C3
51	H	401	U10	C12-C11-C9-C10
51	H	401	U10	C20-C19-C21-C22
46	J	203	PC1	O32-C31-O31-C3
51	H	401	U10	C14-C16-C17-C18
46	B	203	PC1	C2-C1-O11-P
45	L	704	3PE	O32-C31-O31-C3
52	H	402	CDL	OA9-CA7-OA8-CA6
52	N	401	CDL	C11-CA5-OA6-CA4
52	d	202	CDL	OA7-CA5-OA6-CA4
52	M	602	CDL	CB2-C1-CA2-OA2
52	d	201	CDL	CB2-C1-CA2-OA2
52	d	202	CDL	CB2-C1-CA2-OA2
45	P	502	3PE	C32-C31-O31-C3
46	q	202	PC1	C32-C31-O31-C3
52	N	401	CDL	C31-CA7-OA8-CA6
52	N	401	CDL	C71-CB7-OB8-CB6
52	i	202	CDL	C71-CB7-OB8-CB6
53	M	607	PLC	C1B-CB-O3-C3
53	Z	203	PLC	C1B-CB-O3-C3
53	Z	203	PLC	OB-CB-O3-C3
51	H	401	U10	C18-C19-C21-C22
52	i	202	CDL	OB9-CB7-OB8-CB6
52	N	401	CDL	OB9-CB7-OB8-CB6
45	q	201	3PE	C22-C21-O21-C2
52	i	202	CDL	OB6-CB4-CB6-OB8
45	Y	202	3PE	C32-C31-O31-C3
52	M	602	CDL	CB5-C51-C52-C53
52	d	202	CDL	CA7-C31-C32-C33
45	Z	201	3PE	C31-C32-C33-C34
57	P	501	NDP	O4B-C4B-C5B-O5B
52	M	602	CDL	C31-CA7-OA8-CA6
45	b	102	3PE	C31-C32-C33-C34
46	H	404	PC1	C21-C22-C23-C24
45	I	203	3PE	C21-C22-C23-C24
45	L	704	3PE	C21-C22-C23-C24
45	Y	204	3PE	C31-C32-C33-C34
46	H	403	PC1	C31-C32-C33-C34
46	J	203	PC1	C21-C22-C23-C24
53	Y	208	PLC	CB-C1B-C2B-C3B
52	r	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
45	Y	206	3PE	C31-C32-C33-C34
46	I	204	PC1	C21-C22-C23-C24
46	q	202	PC1	O32-C31-O31-C3
52	N	401	CDL	OA9-CA7-OA8-CA6
53	M	607	PLC	OB-CB-O3-C3
45	g	201	3PE	O22-C21-O21-C2
45	P	502	3PE	O32-C31-O31-C3
52	r	201	CDL	CB7-C71-C72-C73
52	N	401	CDL	OA7-CA5-OA6-CA4
45	Y	202	3PE	O32-C31-O31-C3
45	q	201	3PE	C32-C31-O31-C3
53	g	202	PLC	C1B-CB-O3-C3
45	J	202	3PE	C22-C21-O21-C2
46	I	204	PC1	C22-C21-O21-C2
53	g	202	PLC	C1'-C'-O2-C2
45	J	202	3PE	O22-C21-O21-C2
45	q	201	3PE	O22-C21-O21-C2
46	I	204	PC1	O22-C21-O21-C2
52	r	201	CDL	OB7-CB5-OB6-CB4
53	g	202	PLC	O'-C'-O2-C2
52	i	202	CDL	CA2-C1-CB2-OB2
46	Z	202	PC1	C32-C31-O31-C3
46	M	606	PC1	C21-C22-C23-C24
45	M	604	3PE	C22-C21-O21-C2
52	M	602	CDL	OA9-CA7-OA8-CA6
45	M	604	3PE	O22-C21-O21-C2
45	q	201	3PE	O32-C31-O31-C3
45	Y	205	3PE	C3-C2-O21-C21
52	N	401	CDL	CA6-CA4-OA6-CA5
58	U	101	EHZ	C5-C6-C7-O1
46	H	404	PC1	O21-C2-C3-O31
45	L	702	3PE	C24-C25-C26-C27
45	m	201	3PE	C35-C36-C37-C38
52	i	202	CDL	C31-C32-C33-C34
52	i	202	CDL	C35-C36-C37-C38
46	M	605	PC1	C2E-C2F-C2G-C2H
52	M	602	CDL	C32-C33-C34-C35
45	Y	201	3PE	C31-C32-C33-C34
45	N	402	3PE	C2A-C2B-C2C-C2D
45	Y	205	3PE	C26-C27-C28-C29
45	Y	206	3PE	C28-C29-C2A-C2B
45	d	203	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
45	m	201	3PE	C33-C34-C35-C36
46	Z	202	PC1	C32-C33-C34-C35
52	H	402	CDL	C11-C12-C13-C14
52	d	202	CDL	C40-C41-C42-C43
53	g	202	PLC	OB-CB-O3-C3
45	I	203	3PE	C23-C24-C25-C26
45	M	603	3PE	C3C-C3D-C3E-C3F
45	M	604	3PE	C33-C34-C35-C36
45	Y	203	3PE	C2A-C2B-C2C-C2D
45	b	102	3PE	C33-C34-C35-C36
46	B	202	PC1	C25-C26-C27-C28
46	H	404	PC1	C2B-C2C-C2D-C2E
58	U	101	EHZ	S1-C10-C11-N1
45	L	704	3PE	C27-C28-C29-C2A
45	Y	202	3PE	C23-C24-C25-C26
46	m	202	PC1	C25-C26-C27-C28
45	Y	204	3PE	C26-C27-C28-C29
53	M	607	PLC	O3P-C1-C2-C3
46	H	404	PC1	C22-C21-O21-C2
52	i	202	CDL	C11-CA5-OA6-CA4
45	P	502	3PE	C35-C36-C37-C38
45	a	101	3PE	C36-C37-C38-C39
45	f	101	3PE	C32-C33-C34-C35
46	H	403	PC1	C22-C23-C24-C25
52	H	402	CDL	C60-C61-C62-C63
45	L	702	3PE	C31-C32-C33-C34
45	Y	203	3PE	C21-C22-C23-C24
46	M	605	PC1	C32-C31-O31-C3
45	Y	205	3PE	C36-C37-C38-C39
46	B	203	PC1	C39-C3A-C3B-C3C
52	M	602	CDL	C62-C63-C64-C65
45	Y	201	3PE	C28-C29-C2A-C2B
46	I	204	PC1	C23-C24-C25-C26
52	M	602	CDL	C83-C84-C85-C86
52	N	401	CDL	C16-C17-C18-C19
45	Y	204	3PE	C33-C34-C35-C36
46	Z	202	PC1	O32-C31-O31-C3
46	H	405	PC1	C26-C27-C28-C29
52	L	701	CDL	C17-C18-C19-C20
45	J	201	3PE	C29-C2A-C2B-C2C
45	J	202	3PE	C32-C33-C34-C35
45	M	603	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	C35-C36-C37-C38
45	Y	203	3PE	C35-C36-C37-C38
45	q	201	3PE	C2D-C2E-C2F-C2G
52	i	202	CDL	C37-C38-C39-C40
51	H	401	U10	C9-C11-C12-C13
46	H	404	PC1	C26-C27-C28-C29
52	d	202	CDL	C58-C59-C60-C61
52	d	202	CDL	C76-C77-C78-C79
45	d	203	3PE	C31-C32-C33-C34
45	A	201	3PE	C35-C36-C37-C38
45	Y	206	3PE	C2A-C2B-C2C-C2D
45	Y	207	3PE	C29-C2A-C2B-C2C
45	f	101	3PE	C33-C34-C35-C36
46	A	204	PC1	C22-C23-C24-C25
46	M	605	PC1	C26-C27-C28-C29
46	h	201	PC1	C22-C23-C24-C25
52	H	402	CDL	C57-C58-C59-C60
53	J	204	PLC	C4B-C5B-C6B-C7B
45	Y	203	3PE	C33-C34-C35-C36
45	Y	205	3PE	C34-C35-C36-C37
45	Y	206	3PE	C33-C34-C35-C36
45	Z	201	3PE	C39-C3A-C3B-C3C
52	r	201	CDL	C16-C17-C18-C19
45	d	203	3PE	C21-C22-C23-C24
45	A	201	3PE	C23-C24-C25-C26
45	J	202	3PE	C3C-C3D-C3E-C3F
45	L	703	3PE	C33-C34-C35-C36
53	O	404	PLC	C1B-C2B-C3B-C4B
45	Y	201	3PE	C25-C26-C27-C28
46	H	403	PC1	C37-C38-C39-C3A
52	N	401	CDL	C35-C36-C37-C38
58	T	101	EHZ	C2-C3-C4-C5
45	A	202	3PE	C21-C22-C23-C24
53	M	607	PLC	C6B-C7B-C8B-C9B
53	M	607	PLC	C7B-C8B-C9B-CAA
52	r	201	CDL	C13-C14-C15-C16
46	H	404	PC1	O22-C21-O21-C2
46	B	203	PC1	C36-C37-C38-C39
52	L	701	CDL	C74-C75-C76-C77
53	b	103	PLC	C2'-C3'-C4'-C5'
45	M	604	3PE	C38-C39-C3A-C3B
45	N	402	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	q	201	3PE	C37-C38-C39-C3A
46	I	204	PC1	C32-C33-C34-C35
45	M	604	3PE	C34-C35-C36-C37
46	I	204	PC1	C36-C37-C38-C39
52	M	602	CDL	C18-C19-C20-C21
53	Y	208	PLC	C2B-C3B-C4B-C5B
45	N	402	3PE	C28-C29-C2A-C2B
46	l	701	PC1	C39-C3A-C3B-C3C
52	d	201	CDL	C72-C73-C74-C75
45	g	201	3PE	C33-C34-C35-C36
60	o	201	MYR	C3-C4-C5-C6
45	N	402	3PE	C2C-C2D-C2E-C2F
52	L	701	CDL	O1-C1-CA2-OA2
52	N	401	CDL	C22-C23-C24-C25
52	d	201	CDL	C34-C35-C36-C37
45	M	603	3PE	C22-C21-O21-C2
45	Y	201	3PE	C22-C21-O21-C2
45	Y	202	3PE	C22-C21-O21-C2
45	L	702	3PE	C21-C22-C23-C24
45	Y	201	3PE	O22-C21-O21-C2
52	i	202	CDL	OA7-CA5-OA6-CA4
45	M	604	3PE	C28-C29-C2A-C2B
46	Z	202	PC1	C35-C36-C37-C38
46	l	701	PC1	C23-C24-C25-C26
46	M	605	PC1	O32-C31-O31-C3
52	i	202	CDL	C74-C75-C76-C77
52	r	201	CDL	C11-C12-C13-C14
46	d	204	PC1	C33-C34-C35-C36
52	d	202	CDL	C81-C82-C83-C84
45	N	402	3PE	C37-C38-C39-C3A
52	L	701	CDL	C20-C21-C22-C23
52	M	602	CDL	C40-C41-C42-C43
52	N	401	CDL	C38-C39-C40-C41
46	m	202	PC1	C24-C25-C26-C27
52	N	401	CDL	C19-C20-C21-C22
52	d	202	CDL	C52-C53-C54-C55
45	M	603	3PE	O22-C21-O21-C2
45	L	704	3PE	O11-C1-C2-O21
46	A	203	PC1	O11-C1-C2-O21
52	L	701	CDL	OA5-CA3-CA4-OA6
45	Y	201	3PE	C33-C34-C35-C36
52	M	602	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
46	A	203	PC1	C22-C21-O21-C2
46	H	403	PC1	C22-C21-O21-C2
45	L	702	3PE	C28-C29-C2A-C2B
45	A	202	3PE	C34-C35-C36-C37
53	L	705	PLC	C1B-C2B-C3B-C4B
45	Y	206	3PE	C21-C22-C23-C24
45	Z	201	3PE	C23-C24-C25-C26
46	M	605	PC1	C2C-C2D-C2E-C2F
45	g	201	3PE	O21-C2-C3-O31
46	l	701	PC1	O21-C2-C3-O31
45	d	203	3PE	C32-C31-O31-C3
46	H	403	PC1	C34-C35-C36-C37
46	H	404	PC1	C22-C23-C24-C25
46	l	701	PC1	C32-C33-C34-C35
45	Y	203	3PE	C27-C28-C29-C2A
46	M	606	PC1	C23-C24-C25-C26
46	h	201	PC1	C2-C1-O11-P
45	q	201	3PE	C3A-C3B-C3C-C3D
45	a	101	3PE	C33-C34-C35-C36
45	g	201	3PE	C36-C37-C38-C39
46	A	203	PC1	C25-C26-C27-C28
45	M	603	3PE	C38-C39-C3A-C3B
46	d	204	PC1	C3B-C3C-C3D-C3E
52	i	202	CDL	C13-C14-C15-C16
45	J	202	3PE	C37-C38-C39-C3A
52	H	402	CDL	CA5-C11-C12-C13
45	J	202	3PE	C35-C36-C37-C38
52	L	701	CDL	C15-C16-C17-C18
46	q	202	PC1	C26-C27-C28-C29
52	d	202	CDL	C71-C72-C73-C74
46	q	202	PC1	C29-C2A-C2B-C2C
52	i	202	CDL	C51-C52-C53-C54
45	q	201	3PE	C3C-C3D-C3E-C3F
46	m	202	PC1	C38-C39-C3A-C3B
52	M	602	CDL	C43-C44-C45-C46
45	A	202	3PE	O11-C1-C2-C3
45	I	203	3PE	O11-C1-C2-C3
46	A	203	PC1	O11-C1-C2-C3
46	l	701	PC1	O11-C1-C2-C3
46	m	202	PC1	O11-C1-C2-C3
52	M	602	CDL	OA5-CA3-CA4-CA6
52	N	401	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
52	d	201	CDL	OA5-CA3-CA4-CA6
53	Y	208	PLC	O3P-C1-C2-C3
53	Z	203	PLC	O3P-C1-C2-C3
45	b	102	3PE	C28-C29-C2A-C2B
46	H	405	PC1	C24-C25-C26-C27
46	M	606	PC1	C33-C34-C35-C36
45	Y	206	3PE	C36-C37-C38-C39
46	I	204	PC1	C2B-C2C-C2D-C2E
46	Z	202	PC1	C31-C32-C33-C34
46	q	202	PC1	C25-C26-C27-C28
45	L	702	3PE	C34-C35-C36-C37
46	H	403	PC1	C33-C34-C35-C36
52	M	602	CDL	C73-C74-C75-C76
45	A	201	3PE	C21-C22-C23-C24
52	M	602	CDL	CA5-C11-C12-C13
45	g	201	3PE	C35-C36-C37-C38
52	d	201	CDL	C41-C42-C43-C44
46	Z	202	PC1	C25-C26-C27-C28
45	r	202	3PE	C33-C34-C35-C36
46	Z	202	PC1	C22-C23-C24-C25
46	H	403	PC1	C21-C22-C23-C24
45	J	202	3PE	C1-C2-C3-O31
45	Y	202	3PE	C1-C2-C3-O31
45	Y	204	3PE	C1-C2-C3-O31
45	d	203	3PE	C1-C2-C3-O31
46	A	203	PC1	C1-C2-C3-O31
46	H	404	PC1	C1-C2-C3-O31
46	J	203	PC1	C1-C2-C3-O31
46	d	204	PC1	C1-C2-C3-O31
52	i	202	CDL	CB3-CB4-CB6-OB8
46	H	403	PC1	C2B-C2C-C2D-C2E
52	N	401	CDL	C21-C22-C23-C24
52	M	602	CDL	C36-C37-C38-C39
45	r	202	3PE	C35-C36-C37-C38
46	I	204	PC1	C3E-C3F-C3G-C3H
45	M	604	3PE	C37-C38-C39-C3A
45	a	101	3PE	C32-C33-C34-C35
52	i	202	CDL	C15-C16-C17-C18
52	i	202	CDL	C33-C34-C35-C36
52	i	202	CDL	C54-C55-C56-C57
52	N	401	CDL	CA5-C11-C12-C13
45	d	203	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C22-C23-C24-C25
45	q	201	3PE	C2-C1-O11-P
46	B	203	PC1	C25-C26-C27-C28
52	L	701	CDL	C12-C13-C14-C15
52	d	202	CDL	C54-C55-C56-C57
45	Y	203	3PE	C32-C33-C34-C35
52	d	202	CDL	C61-C62-C63-C64
52	i	202	CDL	CB5-C51-C52-C53
52	L	701	CDL	C53-C54-C55-C56
45	b	101	3PE	C3-C2-O21-C21
45	q	201	3PE	C3-C2-O21-C21
45	Y	206	3PE	C38-C39-C3A-C3B
52	M	602	CDL	CB7-C71-C72-C73
45	Y	205	3PE	C3A-C3B-C3C-C3D
45	A	201	3PE	O11-C1-C2-O21
45	M	604	3PE	O11-C1-C2-O21
45	Y	204	3PE	C35-C36-C37-C38
45	A	202	3PE	C33-C34-C35-C36
45	Y	203	3PE	C2E-C2F-C2G-C2H
45	L	704	3PE	C2F-C2G-C2H-C2I
45	d	203	3PE	C34-C35-C36-C37
46	H	405	PC1	C3E-C3F-C3G-C3H
52	L	701	CDL	C71-C72-C73-C74
52	M	602	CDL	C16-C17-C18-C19
52	d	202	CDL	C37-C38-C39-C40
45	I	203	3PE	C25-C26-C27-C28
45	M	604	3PE	C26-C27-C28-C29
45	Y	205	3PE	C33-C34-C35-C36
52	M	602	CDL	C38-C39-C40-C41
45	J	201	3PE	C22-C23-C24-C25
45	a	101	3PE	C3E-C3F-C3G-C3H
46	d	204	PC1	C38-C39-C3A-C3B
52	L	701	CDL	C40-C41-C42-C43
45	N	402	3PE	O21-C2-C3-O31
45	Y	204	3PE	O21-C2-C3-O31
45	Y	206	3PE	O21-C2-C3-O31
45	Y	204	3PE	C2C-C2D-C2E-C2F
45	M	604	3PE	O21-C21-C22-C23
53	J	204	PLC	C2B-C1B-CB-O3
45	Y	203	3PE	C38-C39-C3A-C3B
52	d	201	CDL	C77-C78-C79-C80
45	M	603	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
56	O	402	DGT	PA-O3A-PB-O2B
57	P	501	NDP	PN-O3-PA-O1A
46	Z	202	PC1	C23-C24-C25-C26
45	P	502	3PE	C26-C27-C28-C29
53	L	705	PLC	C2'-C3'-C4'-C5'
52	H	402	CDL	C13-C14-C15-C16
52	i	202	CDL	C31-CA7-OA8-CA6
53	g	202	PLC	C'-C1'-C2'-C3'
46	q	202	PC1	C28-C29-C2A-C2B
52	d	201	CDL	C31-C32-C33-C34
53	L	705	PLC	C1'-C2'-C3'-C4'
46	H	403	PC1	O22-C21-O21-C2
53	L	705	PLC	C2-C1-O3P-P
45	b	102	3PE	C27-C28-C29-C2A
45	J	201	3PE	C2E-C2F-C2G-C2H
53	g	202	PLC	C7'-C8'-C9'-CA'
45	Y	204	3PE	C32-C31-O31-C3
52	d	202	CDL	C44-C45-C46-C47
52	M	602	CDL	C58-C59-C60-C61
52	N	401	CDL	C56-C57-C58-C59
45	b	102	3PE	C25-C26-C27-C28
46	H	405	PC1	C37-C38-C39-C3A
53	O	403	PLC	C2'-C3'-C4'-C5'
45	L	704	3PE	O11-C1-C2-C3
45	Y	201	3PE	O11-C1-C2-C3
45	Y	204	3PE	O11-C1-C2-C3
46	M	606	PC1	O11-C1-C2-C3
52	L	701	CDL	OA5-CA3-CA4-CA6
52	d	201	CDL	OB5-CB3-CB4-CB6
46	H	403	PC1	C25-C26-C27-C28
52	d	202	CDL	C80-C81-C82-C83
52	L	701	CDL	C64-C65-C66-C67
53	b	103	PLC	C8'-C9'-CA'-CB'
45	J	201	3PE	C27-C28-C29-C2A
52	L	701	CDL	C63-C64-C65-C66
46	A	203	PC1	C31-C32-C33-C34
52	N	401	CDL	C24-C25-C26-C27
46	A	203	PC1	C22-C23-C24-C25
52	L	701	CDL	C36-C37-C38-C39
45	d	203	3PE	C2F-C2G-C2H-C2I
45	q	201	3PE	C36-C37-C38-C39
53	b	103	PLC	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
46	B	203	PC1	C22-C23-C24-C25
46	B	202	PC1	C22-C21-O21-C2
52	d	201	CDL	C31-CA7-OA8-CA6
52	N	401	CDL	C76-C77-C78-C79
45	L	702	3PE	C1-C2-C3-O31
45	L	704	3PE	C1-C2-C3-O31
45	g	201	3PE	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31
46	h	201	PC1	C1-C2-C3-O31
52	d	202	CDL	CB3-CB4-CB6-OB8
52	r	201	CDL	CA3-CA4-CA6-OA8
53	J	204	PLC	C1-C2-C3-O3
53	O	403	PLC	C1-C2-C3-O3
52	d	202	CDL	C35-C36-C37-C38
52	d	202	CDL	C32-C33-C34-C35
45	Y	202	3PE	O22-C21-O21-C2
46	A	203	PC1	O22-C21-O21-C2
45	A	202	3PE	O11-C1-C2-O21
45	N	402	3PE	O11-C1-C2-O21
45	Y	202	3PE	O11-C1-C2-O21
45	Y	204	3PE	O11-C1-C2-O21
45	b	101	3PE	O11-C1-C2-O21
46	B	202	PC1	O11-C1-C2-O21
46	d	204	PC1	O11-C1-C2-O21
46	l	701	PC1	O11-C1-C2-O21
52	N	401	CDL	OB5-CB3-CB4-OB6
53	L	705	PLC	O3P-C1-C2-O2
53	b	103	PLC	C4B-C5B-C6B-C7B
45	Y	207	3PE	C2A-C2B-C2C-C2D
45	b	102	3PE	O21-C21-C22-C23
46	B	202	PC1	C26-C27-C28-C29
58	T	101	EHZ	O1-C7-C8-C9
45	Y	201	3PE	C2B-C2C-C2D-C2E
46	B	202	PC1	C39-C3A-C3B-C3C
52	d	202	CDL	C34-C35-C36-C37
45	L	702	3PE	O21-C2-C3-O31
45	L	704	3PE	O21-C2-C3-O31
45	Y	202	3PE	O21-C2-C3-O31
46	A	203	PC1	O21-C2-C3-O31
53	J	204	PLC	O2-C2-C3-O3
53	O	404	PLC	O2-C2-C3-O3
45	q	201	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
46	H	405	PC1	C33-C34-C35-C36
52	M	602	CDL	C11-C12-C13-C14
53	b	103	PLC	C2B-C3B-C4B-C5B
46	A	204	PC1	C25-C26-C27-C28
46	H	405	PC1	C34-C35-C36-C37
52	M	602	CDL	C34-C35-C36-C37
45	L	704	3PE	C33-C34-C35-C36
57	P	501	NDP	PN-O3-PA-O5B
52	d	201	CDL	C11-C12-C13-C14
52	r	201	CDL	C18-C19-C20-C21
52	d	202	CDL	C77-C78-C79-C80
52	d	202	CDL	C42-C43-C44-C45
45	b	102	3PE	C39-C3A-C3B-C3C
46	M	605	PC1	C2A-C2B-C2C-C2D
46	A	204	PC1	C23-C24-C25-C26
52	d	201	CDL	C44-C45-C46-C47
52	r	201	CDL	C31-C32-C33-C34
46	m	202	PC1	C32-C31-O31-C3
46	H	405	PC1	C28-C29-C2A-C2B
52	L	701	CDL	C59-C60-C61-C62
52	i	202	CDL	OA9-CA7-OA8-CA6
46	M	606	PC1	C34-C35-C36-C37
45	M	604	3PE	O11-C1-C2-C3
52	d	202	CDL	OA5-CA3-CA4-CA6
45	J	202	3PE	C26-C27-C28-C29
45	d	203	3PE	C39-C3A-C3B-C3C
45	g	201	3PE	C34-C35-C36-C37
53	M	607	PLC	C2B-C3B-C4B-C5B
46	M	605	PC1	C29-C2A-C2B-C2C
46	l	701	PC1	C3C-C3D-C3E-C3F
52	d	201	CDL	C36-C37-C38-C39
46	B	202	PC1	O22-C21-O21-C2
45	a	101	3PE	C38-C39-C3A-C3B
46	B	202	PC1	C34-C35-C36-C37
52	d	202	CDL	CA6-CA4-OA6-CA5
58	T	101	EHZ	O3-C12-C13-C14
45	P	502	3PE	C25-C26-C27-C28
45	b	101	3PE	C34-C35-C36-C37
45	m	201	3PE	C25-C26-C27-C28
45	Y	204	3PE	O32-C31-O31-C3
45	P	502	3PE	C32-C33-C34-C35
45	q	201	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	O11-C1-C2-O21
52	d	201	CDL	OA5-CA3-CA4-OA6
53	M	607	PLC	O3P-C1-C2-O2
53	Z	203	PLC	O3P-C1-C2-O2
45	L	703	3PE	C1-C2-C3-O31
45	P	502	3PE	C1-C2-C3-O31
45	Y	207	3PE	C1-C2-C3-O31
45	b	102	3PE	C1-C2-C3-O31
58	T	101	EHZ	N1-C12-C13-C14
52	d	202	CDL	CB7-C71-C72-C73
45	d	203	3PE	C3A-C3B-C3C-C3D
45	q	201	3PE	C2A-C2B-C2C-C2D
46	d	204	PC1	C3C-C3D-C3E-C3F
45	I	203	3PE	C28-C29-C2A-C2B
45	A	202	3PE	C12-C11-O13-P
45	L	702	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	M	604	3PE	C12-C11-O13-P
45	Y	201	3PE	C12-C11-O13-P
45	Y	206	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P
45	a	101	3PE	C12-C11-O13-P
45	b	102	3PE	C12-C11-O13-P
45	g	201	3PE	C12-C11-O13-P
53	L	705	PLC	C5-C4-O4P-P
53	M	607	PLC	C5-C4-O4P-P
53	Y	208	PLC	C5-C4-O4P-P
53	g	202	PLC	C5-C4-O4P-P
52	r	201	CDL	CA5-C11-C12-C13
52	d	201	CDL	OA9-CA7-OA8-CA6
52	i	202	CDL	C39-C40-C41-C42
53	g	202	PLC	C6B-C7B-C8B-C9B
45	J	202	3PE	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
46	J	203	PC1	O21-C2-C3-O31
46	h	201	PC1	O21-C2-C3-O31
52	r	201	CDL	OA6-CA4-CA6-OA8
45	d	203	3PE	C33-C34-C35-C36
52	i	202	CDL	C72-C73-C74-C75
45	a	101	3PE	C3C-C3D-C3E-C3F
53	g	202	PLC	C7B-C8B-C9B-CAA

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Mol	Chain	Res	Type	Atoms
45	A	202	3PE	C24-C25-C26-C27
46	m	202	PC1	O32-C31-O31-C3
46	d	204	PC1	C35-C36-C37-C38
53	Y	208	PLC	C3B-C4B-C5B-C6B
46	H	405	PC1	C38-C39-C3A-C3B
52	d	202	CDL	C63-C64-C65-C66
53	M	607	PLC	O4P-C4-C5-N
53	b	103	PLC	O4P-C4-C5-N
45	b	101	3PE	C24-C25-C26-C27
45	L	704	3PE	C35-C36-C37-C38
46	B	203	PC1	C21-C22-C23-C24
46	B	202	PC1	C3C-C3D-C3E-C3F
52	M	602	CDL	C33-C34-C35-C36
45	L	702	3PE	C3A-C3B-C3C-C3D
45	A	201	3PE	O11-C1-C2-C3
45	N	402	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
53	L	705	PLC	O3P-C1-C2-C3
53	b	103	PLC	O3P-C1-C2-C3
58	U	101	EHZ	C19-C17-C20-O6
46	d	204	PC1	C31-C32-C33-C34
46	l	701	PC1	C37-C38-C39-C3A
52	L	701	CDL	C81-C82-C83-C84
46	B	203	PC1	C3C-C3D-C3E-C3F
46	H	403	PC1	C28-C29-C2A-C2B
45	m	201	3PE	C37-C38-C39-C3A
46	M	605	PC1	C2-C1-O11-P
49	F	502	FMN	C4'-C5'-O5'-P
58	T	101	EHZ	C11-C10-S1-C9
45	m	201	3PE	C3F-C3G-C3H-C3I
46	B	203	PC1	C29-C2A-C2B-C2C
45	g	201	3PE	O11-C1-C2-O21
46	A	204	PC1	O11-C1-C2-O21
46	M	606	PC1	O11-C1-C2-O21
46	m	202	PC1	O11-C1-C2-O21
52	M	602	CDL	OA5-CA3-CA4-OA6
52	d	202	CDL	OA5-CA3-CA4-OA6
53	Y	208	PLC	O3P-C1-C2-O2
45	Y	207	3PE	C21-C22-C23-C24
46	Z	202	PC1	C22-C21-O21-C2
46	H	403	PC1	C11-C12-N-C13
45	L	704	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	M	605	PC1	C25-C26-C27-C28
45	d	203	3PE	C25-C26-C27-C28
45	J	201	3PE	O21-C2-C3-O31
45	P	502	3PE	O21-C2-C3-O31
45	Y	207	3PE	O21-C2-C3-O31
46	A	204	PC1	O21-C2-C3-O31
46	d	204	PC1	O21-C2-C3-O31
52	d	202	CDL	OB6-CB4-CB6-OB8
45	J	201	3PE	C1-C2-C3-O31
45	N	402	3PE	C1-C2-C3-O31
45	b	101	3PE	C1-C2-C3-O31
46	l	701	PC1	C1-C2-C3-O31
52	r	201	CDL	CB3-CB4-CB6-OB8
53	O	404	PLC	C1-C2-C3-O3
46	Z	202	PC1	C21-C22-C23-C24
53	g	202	PLC	C8'-C9'-CA'-CB'
45	M	604	3PE	C2A-C2B-C2C-C2D
45	A	201	3PE	C11-O13-P-O14
45	I	203	3PE	C11-O13-P-O11
45	I	203	3PE	C11-O13-P-O12
45	L	703	3PE	O13-C11-C12-N
45	L	704	3PE	C11-O13-P-O12
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	O13-C11-C12-N
45	M	604	3PE	O13-C11-C12-N
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O14
45	Y	201	3PE	C11-O13-P-O11
45	Y	201	3PE	C11-O13-P-O12
45	Y	202	3PE	C1-O11-P-O13
45	Y	202	3PE	C1-O11-P-O14
45	Y	204	3PE	C1-O11-P-O14
45	Y	204	3PE	C11-O13-P-O11
45	Y	204	3PE	C11-O13-P-O12
45	Y	205	3PE	C1-O11-P-O14
45	Y	205	3PE	C11-O13-P-O14
45	Z	201	3PE	C1-O11-P-O14
45	b	101	3PE	C1-O11-P-O13
45	b	101	3PE	O13-C11-C12-N
45	m	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O12
45	q	201	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
45	q	201	3PE	C1-O11-P-O13
45	q	201	3PE	C1-O11-P-O14
45	r	202	3PE	C11-O13-P-O11
45	r	202	3PE	C11-O13-P-O12
45	r	202	3PE	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O11
46	B	202	PC1	C11-O13-P-O12
46	B	203	PC1	C1-O11-P-O14
46	H	403	PC1	C11-C12-N-C14
46	M	605	PC1	C1-O11-P-O14
46	M	606	PC1	C1-O11-P-O14
46	M	606	PC1	C1-O11-P-O13
46	d	204	PC1	C1-O11-P-O14
46	h	201	PC1	C11-O13-P-O14
46	l	701	PC1	C11-O13-P-O11
46	m	202	PC1	C11-O13-P-O11
52	H	402	CDL	CB3-OB5-PB2-OB4
52	L	701	CDL	CA2-OA2-PA1-OA3
52	N	401	CDL	CB2-OB2-PB2-OB3
52	d	202	CDL	CA3-OA5-PA1-OA3
52	d	202	CDL	CB3-OB5-PB2-OB2
52	d	202	CDL	CB3-OB5-PB2-OB3
52	d	202	CDL	CB3-OB5-PB2-OB4
52	r	201	CDL	CA3-OA5-PA1-OA3
52	r	201	CDL	CB2-OB2-PB2-OB5
53	L	705	PLC	C1-O3P-P-O4P
53	L	705	PLC	C4-O4P-P-O2P
53	M	607	PLC	C4-O4P-P-O1P
53	O	404	PLC	C4-O4P-P-O1P
56	O	402	DGT	C5'-O5'-PA-O3A
57	P	501	NDP	C5D-O5D-PN-O1N
45	Y	206	3PE	C2C-C2D-C2E-C2F
45	q	201	3PE	C39-C3A-C3B-C3C
52	H	402	CDL	C64-C65-C66-C67
45	J	202	3PE	C36-C37-C38-C39
46	I	204	PC1	C28-C29-C2A-C2B
45	L	703	3PE	C2-C1-O11-P
52	M	602	CDL	C1-CA2-OA2-PA1
45	q	201	3PE	C32-C33-C34-C35
45	J	202	3PE	O21-C21-C22-C23
52	N	401	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
52	L	701	CDL	C84-C85-C86-C87
45	M	604	3PE	C23-C24-C25-C26
45	N	402	3PE	C39-C3A-C3B-C3C
52	L	701	CDL	C32-C33-C34-C35
45	r	202	3PE	C23-C24-C25-C26
52	N	401	CDL	C62-C63-C64-C65
46	H	405	PC1	C3B-C3C-C3D-C3E
52	H	402	CDL	CA6-CA4-OA6-CA5
53	Y	208	PLC	C1-C2-O2-C'
52	M	602	CDL	C13-C14-C15-C16
45	Y	204	3PE	C23-C24-C25-C26
45	Y	207	3PE	C2B-C2C-C2D-C2E
46	B	202	PC1	C3B-C3C-C3D-C3E
53	O	403	PLC	C4-C5-N-C8
46	q	202	PC1	O11-C1-C2-C3
52	H	402	CDL	C55-C56-C57-C58
53	b	103	PLC	C3B-C4B-C5B-C6B
45	Y	203	3PE	C32-C31-O31-C3
45	N	402	3PE	C2F-C2G-C2H-C2I
45	Y	207	3PE	C24-C25-C26-C27
45	Y	205	3PE	C32-C33-C34-C35
45	Y	202	3PE	C25-C26-C27-C28
45	N	402	3PE	C24-C25-C26-C27
45	P	502	3PE	C22-C23-C24-C25
45	J	201	3PE	C2D-C2E-C2F-C2G
46	H	403	PC1	C35-C36-C37-C38
45	Y	205	3PE	C35-C36-C37-C38
46	H	405	PC1	C3C-C3D-C3E-C3F
52	N	401	CDL	C44-C45-C46-C47
46	H	404	PC1	C31-C32-C33-C34
52	L	701	CDL	CA5-C11-C12-C13
52	L	701	CDL	OB7-CB5-OB6-CB4
45	N	402	3PE	C2-C1-O11-P
45	r	202	3PE	C22-C23-C24-C25
52	d	201	CDL	C39-C40-C41-C42
46	q	202	PC1	O21-C2-C3-O31
52	N	401	CDL	OB6-CB4-CB6-OB8
45	J	201	3PE	C23-C24-C25-C26
52	N	401	CDL	C33-C34-C35-C36
52	L	701	CDL	C51-CB5-OB6-CB4
45	Y	203	3PE	O32-C31-O31-C3
52	L	701	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
46	Z	202	PC1	O22-C21-O21-C2
52	L	701	CDL	C32-C31-CA7-OA8
45	Y	206	3PE	C1-C2-C3-O31
46	A	204	PC1	C1-C2-C3-O31
52	d	202	CDL	C78-C79-C80-C81
52	r	201	CDL	C52-C53-C54-C55
46	H	405	PC1	C22-C23-C24-C25
52	L	701	CDL	C58-C59-C60-C61
45	M	603	3PE	C3A-C3B-C3C-C3D
46	A	203	PC1	C32-C33-C34-C35
46	A	203	PC1	C21-C22-C23-C24
45	N	402	3PE	C25-C26-C27-C28
53	O	403	PLC	C4-C5-N-C7
45	N	402	3PE	C22-C23-C24-C25
46	d	204	PC1	C34-C35-C36-C37
46	m	202	PC1	C32-C33-C34-C35
52	N	401	CDL	C58-C59-C60-C61
58	U	101	EHZ	C21-C22-C23-C24
45	Y	206	3PE	C26-C27-C28-C29
46	H	405	PC1	C36-C37-C38-C39
52	M	602	CDL	C22-C23-C24-C25
52	H	402	CDL	C61-C62-C63-C64
45	A	202	3PE	C3C-C3D-C3E-C3F
45	b	102	3PE	C35-C36-C37-C38
45	Y	204	3PE	C32-C33-C34-C35
46	l	701	PC1	C38-C39-C3A-C3B
46	H	405	PC1	C25-C26-C27-C28
45	d	203	3PE	C28-C29-C2A-C2B
52	M	602	CDL	C51-C52-C53-C54
46	H	403	PC1	C11-C12-N-C15
45	J	202	3PE	C24-C25-C26-C27
45	Y	203	3PE	C3A-C3B-C3C-C3D
52	L	701	CDL	C41-C42-C43-C44
53	Y	208	PLC	C1B-CB-O3-C3
46	M	606	PC1	O21-C21-C22-C23
52	N	401	CDL	C55-C56-C57-C58
53	J	204	PLC	C2B-C1B-CB-OB
46	Z	202	PC1	O21-C2-C3-O31
45	M	603	3PE	C24-C25-C26-C27
45	L	702	3PE	C35-C36-C37-C38
53	Z	203	PLC	C'-C1'-C2'-C3'
45	Y	205	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
45	Y	207	3PE	C22-C23-C24-C25
46	M	605	PC1	C22-C23-C24-C25
57	P	501	NDP	O4D-C1D-N1N-C6N
45	I	203	3PE	C29-C2A-C2B-C2C
52	M	602	CDL	C31-C32-C33-C34
52	d	201	CDL	C1-CB2-OB2-PB2
52	N	401	CDL	C23-C24-C25-C26
52	L	701	CDL	C82-C83-C84-C85
52	M	602	CDL	C72-C73-C74-C75
52	i	202	CDL	C11-C12-C13-C14
45	L	703	3PE	C23-C24-C25-C26
59	i	201	CHD	C22-C23-C24-O25
52	M	602	CDL	C41-C42-C43-C44
51	H	401	U10	C2-C3-O3-C3M
46	Z	202	PC1	C26-C27-C28-C29
45	M	604	3PE	O22-C21-C22-C23
59	i	201	CHD	C17-C20-C22-C23
45	b	101	3PE	C33-C34-C35-C36
52	H	402	CDL	C53-C54-C55-C56
52	L	701	CDL	C42-C43-C44-C45
53	Y	208	PLC	C6'-C7'-C8'-C9'
58	T	101	EHZ	C1-C21-C22-C23
45	Y	204	3PE	C3D-C3E-C3F-C3G
45	L	702	3PE	C33-C34-C35-C36
45	q	201	3PE	C28-C29-C2A-C2B
45	M	603	3PE	C29-C2A-C2B-C2C
45	L	702	3PE	C1-C2-O21-C21
45	Y	203	3PE	C1-C2-O21-C21
45	Y	203	3PE	C3-C2-O21-C21
52	d	202	CDL	CA5-C11-C12-C13
52	i	202	CDL	CA5-C11-C12-C13
45	b	102	3PE	C32-C31-O31-C3
53	Y	208	PLC	OB-CB-O3-C3
52	H	402	CDL	C52-C53-C54-C55
45	g	201	3PE	C31-C32-C33-C34
46	M	606	PC1	C31-C32-C33-C34
45	L	703	3PE	O11-C1-C2-O21
52	H	402	CDL	OB5-CB3-CB4-OB6
53	J	204	PLC	O3P-C1-C2-O2
45	L	703	3PE	C26-C27-C28-C29
45	M	604	3PE	C2-C1-O11-P
45	Z	201	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
45	Y	205	3PE	C38-C39-C3A-C3B
59	i	201	CHD	C22-C23-C24-O26
45	N	402	3PE	C26-C27-C28-C29
46	H	404	PC1	C24-C25-C26-C27
52	i	202	CDL	C52-C53-C54-C55
45	A	201	3PE	C27-C28-C29-C2A
46	d	204	PC1	C39-C3A-C3B-C3C
45	b	101	3PE	O21-C2-C3-O31
52	M	602	CDL	OA6-CA4-CA6-OA8
52	d	202	CDL	OA6-CA4-CA6-OA8
52	L	701	CDL	C16-C17-C18-C19
53	Z	203	PLC	C1'-C2'-C3'-C4'
45	d	203	3PE	C3B-C3C-C3D-C3E
52	M	602	CDL	C52-C53-C54-C55
46	H	403	PC1	O21-C21-C22-C23
53	O	403	PLC	C4-C5-N-C6
52	H	402	CDL	CB2-C1-CA2-OA2
52	L	701	CDL	C35-C36-C37-C38
52	r	201	CDL	C71-C72-C73-C74
52	L	701	CDL	C31-C32-C33-C34
45	M	603	3PE	C28-C29-C2A-C2B
53	O	404	PLC	C2-C1-O3P-P
46	H	403	PC1	C39-C3A-C3B-C3C
45	b	102	3PE	O32-C31-O31-C3
53	M	607	PLC	O'-C'-O2-C2
45	Z	201	3PE	C29-C2A-C2B-C2C
52	N	401	CDL	CB3-CB4-CB6-OB8
52	i	202	CDL	CA3-CA4-CA6-OA8
52	L	701	CDL	C56-C57-C58-C59
53	g	202	PLC	CB-C1B-C2B-C3B
45	A	201	3PE	O31-C31-C32-C33
52	d	201	CDL	C42-C43-C44-C45
46	d	204	PC1	C32-C33-C34-C35
45	d	203	3PE	C27-C28-C29-C2A
46	q	202	PC1	O11-C1-C2-O21
45	a	101	3PE	C34-C35-C36-C37
53	Z	203	PLC	C7B-C8B-C9B-CAA
45	N	402	3PE	C23-C24-C25-C26
53	Y	208	PLC	O2-C'-C1'-C2'
45	Y	206	3PE	C29-C2A-C2B-C2C
45	M	603	3PE	C39-C3A-C3B-C3C
52	i	202	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
45	Y	202	3PE	O11-C1-C2-C3
45	g	201	3PE	O11-C1-C2-C3
46	A	204	PC1	O11-C1-C2-C3
46	B	202	PC1	O11-C1-C2-C3
46	d	204	PC1	O11-C1-C2-C3
52	d	201	CDL	C52-C51-CB5-OB6
53	b	103	PLC	C2-C1-O3P-P
45	A	201	3PE	C22-C23-C24-C25
46	l	701	PC1	C3B-C3C-C3D-C3E
45	d	203	3PE	C2B-C2C-C2D-C2E
46	H	403	PC1	C32-C31-O31-C3
45	b	102	3PE	O22-C21-C22-C23
45	d	203	3PE	C29-C2A-C2B-C2C
52	N	401	CDL	C11-C12-C13-C14
46	H	404	PC1	C2F-C2G-C2H-C2I
52	M	602	CDL	CA7-C31-C32-C33
52	N	401	CDL	C63-C64-C65-C66
45	A	201	3PE	C38-C39-C3A-C3B
46	I	204	PC1	C26-C27-C28-C29
45	A	201	3PE	C1-C2-O21-C21
45	A	201	3PE	C3-C2-O21-C21
46	B	202	PC1	C23-C24-C25-C26
46	Z	202	PC1	C3A-C3B-C3C-C3D
52	L	701	CDL	C61-C62-C63-C64
45	L	704	3PE	C31-C32-C33-C34
52	r	201	CDL	O1-C1-CB2-OB2
46	J	203	PC1	C22-C23-C24-C25
52	M	602	CDL	C59-C60-C61-C62
46	A	204	PC1	C26-C27-C28-C29
45	Y	207	3PE	C2E-C2F-C2G-C2H
45	Y	202	3PE	C24-C25-C26-C27
57	P	501	NDP	C2D-C1D-N1N-C6N
45	g	201	3PE	C2-C1-O11-P
45	q	201	3PE	C33-C34-C35-C36
45	f	101	3PE	O11-C1-C2-O21
46	l	701	PC1	C3F-C3G-C3H-C3I
52	L	701	CDL	C78-C79-C80-C81
46	q	202	PC1	C1-C2-C3-O31
60	o	201	MYR	C11-C10-C9-C8
52	M	602	CDL	C12-C11-CA5-OA6
45	L	703	3PE	C22-C23-C24-C25
45	g	201	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	Z	202	PC1	C27-C28-C29-C2A
52	i	202	CDL	C36-C37-C38-C39
52	i	202	CDL	C71-C72-C73-C74
45	A	201	3PE	C12-C11-O13-P
45	Y	204	3PE	C12-C11-O13-P
46	H	403	PC1	O32-C31-O31-C3
45	b	102	3PE	C2B-C2C-C2D-C2E
45	N	402	3PE	O31-C31-C32-C33
45	Y	204	3PE	C3F-C3G-C3H-C3I
52	N	401	CDL	C14-C15-C16-C17
52	d	202	CDL	C64-C65-C66-C67
45	q	201	3PE	C3B-C3C-C3D-C3E
52	H	402	CDL	OA5-CA3-CA4-CA6
52	H	402	CDL	OB5-CB3-CB4-CB6
46	I	204	PC1	C38-C39-C3A-C3B
52	N	401	CDL	C73-C74-C75-C76
45	L	703	3PE	O21-C21-C22-C23
52	d	202	CDL	C31-C32-C33-C34
45	L	702	3PE	C3F-C3G-C3H-C3I
53	M	607	PLC	C1'-C'-O2-C2
52	r	201	CDL	CA4-CA3-OA5-PA1
53	Y	208	PLC	C8'-C9'-CA'-CB'
45	Y	205	3PE	C28-C29-C2A-C2B
45	A	201	3PE	C33-C34-C35-C36
46	A	204	PC1	O13-C11-C12-N
56	O	402	DGT	PB-O3A-PA-O1A
45	b	101	3PE	C32-C31-O31-C3
45	r	202	3PE	C34-C35-C36-C37
52	d	201	CDL	CB7-C71-C72-C73
45	Y	204	3PE	O21-C21-C22-C23
46	I	204	PC1	O31-C31-C32-C33
52	M	602	CDL	C78-C79-C80-C81
52	d	202	CDL	C36-C37-C38-C39
45	M	603	3PE	O31-C31-C32-C33
58	U	101	EHZ	C3-C4-C5-C6
45	b	102	3PE	O31-C31-C32-C33
52	L	701	CDL	OB5-CB3-CB4-OB6
52	N	401	CDL	OA5-CA3-CA4-OA6
51	H	401	U10	C15-C14-C16-C17
53	M	607	PLC	CB-C1B-C2B-C3B
46	B	203	PC1	C23-C24-C25-C26
45	M	603	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
46	H	404	PC1	O31-C31-C32-C33
52	d	201	CDL	C72-C71-CB7-OB8
53	J	204	PLC	O2-C'-C1'-C2'
52	N	401	CDL	C17-C18-C19-C20
45	N	402	3PE	C3A-C3B-C3C-C3D
46	Z	202	PC1	C38-C39-C3A-C3B
45	Y	204	3PE	O31-C31-C32-C33
52	M	602	CDL	C52-C51-CB5-OB6
45	J	201	3PE	C2C-C2D-C2E-C2F
53	b	103	PLC	C'-C1'-C2'-C3'
46	J	203	PC1	O21-C21-C22-C23
46	H	404	PC1	C27-C28-C29-C2A
45	b	101	3PE	O32-C31-O31-C3
45	f	101	3PE	C1-C2-C3-O31
53	O	404	PLC	C2'-C3'-C4'-C5'
45	I	203	3PE	O21-C21-C22-C23
45	L	702	3PE	O21-C21-C22-C23
45	A	202	3PE	O21-C2-C3-O31
45	Y	203	3PE	O21-C2-C3-O31
45	Y	207	3PE	C25-C26-C27-C28
45	L	702	3PE	C37-C38-C39-C3A
45	A	202	3PE	O31-C31-C32-C33
45	r	202	3PE	O31-C31-C32-C33
45	M	603	3PE	C32-C33-C34-C35
45	Y	203	3PE	O31-C31-C32-C33
45	Y	204	3PE	C24-C25-C26-C27
49	F	502	FMN	N10-C1'-C2'-O2'
58	U	101	EHZ	C18-C17-C20-O6
45	L	702	3PE	C27-C28-C29-C2A
46	H	405	PC1	O31-C31-C32-C33
52	i	202	CDL	C12-C11-CA5-OA6
45	b	102	3PE	C2C-C2D-C2E-C2F
52	r	201	CDL	C53-C54-C55-C56
45	L	704	3PE	C3-C2-O21-C21
53	O	403	PLC	C1-C2-O2-C'
46	M	605	PC1	C11-C12-N-C14
53	b	103	PLC	O2-C'-C1'-C2'
45	Y	205	3PE	C39-C3A-C3B-C3C
52	M	602	CDL	OA7-CA5-OA6-CA4
45	A	202	3PE	C36-C37-C38-C39
45	N	402	3PE	C34-C35-C36-C37
45	L	704	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	A	202	3PE	C2-C1-O11-P
45	a	101	3PE	C2-C1-O11-P
53	Z	203	PLC	C2-C1-O3P-P
45	J	202	3PE	C23-C24-C25-C26
52	L	701	CDL	CA4-CA6-OA8-CA7
45	Y	204	3PE	C22-C23-C24-C25
46	q	202	PC1	C36-C37-C38-C39
53	O	403	PLC	C3'-C4'-C5'-C6'
52	H	402	CDL	OA5-CA3-CA4-OA6
45	L	703	3PE	O22-C21-C22-C23
45	Y	204	3PE	O22-C21-C22-C23
45	b	102	3PE	O32-C31-C32-C33
52	H	402	CDL	C51-C52-C53-C54
46	I	204	PC1	C27-C28-C29-C2A
52	N	401	CDL	C77-C78-C79-C80
52	M	602	CDL	C56-C57-C58-C59
52	r	201	CDL	C12-C13-C14-C15
52	d	201	CDL	C33-C34-C35-C36
45	I	203	3PE	O22-C21-C22-C23
45	L	702	3PE	O22-C21-C22-C23
45	N	402	3PE	O32-C31-C32-C33
52	d	202	CDL	C41-C42-C43-C44
45	f	101	3PE	O21-C2-C3-O31
52	r	201	CDL	OB6-CB4-CB6-OB8
49	F	502	FMN	O3'-C3'-C4'-C5'
46	H	404	PC1	O32-C31-C32-C33
46	J	203	PC1	O22-C21-C22-C23
52	M	602	CDL	C52-C51-CB5-OB7
52	d	202	CDL	C72-C71-CB7-OB8
45	d	203	3PE	C2D-C2E-C2F-C2G
46	H	403	PC1	C2E-C2F-C2G-C2H
46	M	605	PC1	C27-C28-C29-C2A
45	A	202	3PE	C3E-C3F-C3G-C3H
45	m	201	3PE	C1-C2-C3-O31
52	d	201	CDL	C72-C71-CB7-OB9
53	J	204	PLC	O'-C'-C1'-C2'
52	H	402	CDL	C52-C51-CB5-OB6
52	i	202	CDL	C76-C77-C78-C79
46	M	605	PC1	C11-C12-N-C13
46	M	605	PC1	C11-C12-N-C15
45	Y	204	3PE	O32-C31-C32-C33
46	H	405	PC1	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
52	i	202	CDL	C12-C11-CA5-OA7
45	Y	201	3PE	O21-C21-C22-C23
45	d	203	3PE	C36-C37-C38-C39
46	I	204	PC1	O32-C31-C32-C33
45	Y	203	3PE	C39-C3A-C3B-C3C
45	m	201	3PE	O11-C1-C2-C3
45	M	603	3PE	O22-C21-C22-C23
45	m	201	3PE	C3C-C3D-C3E-C3F
52	M	602	CDL	C37-C38-C39-C40
45	P	502	3PE	O21-C21-C22-C23
45	Z	201	3PE	O21-C21-C22-C23
46	H	403	PC1	O31-C31-C32-C33
56	O	402	DGT	PB-O3A-PA-O2A
45	A	202	3PE	O32-C31-C32-C33
46	I	204	PC1	C25-C26-C27-C28
45	q	201	3PE	O31-C31-C32-C33
52	N	401	CDL	C72-C71-CB7-OB8
52	i	202	CDL	C32-C31-CA7-OA8
45	b	101	3PE	C21-C22-C23-C24

There are no ring outliers.

23 monomers are involved in 48 short contacts:

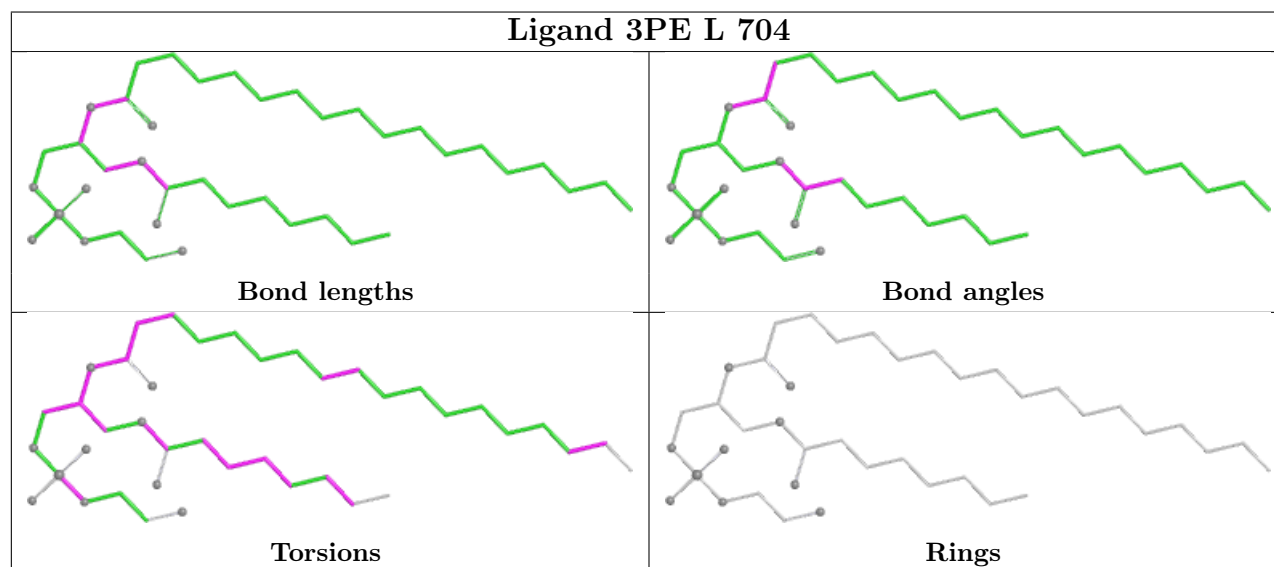
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	U	101	EHZ	1	0
57	P	501	NDP	2	0
46	I	204	PC1	2	0
52	M	602	CDL	1	0
45	q	201	3PE	1	0
46	H	404	PC1	1	0
46	B	202	PC1	1	0
59	i	201	CHD	6	0
45	Y	204	3PE	1	0
52	N	401	CDL	1	0
52	H	402	CDL	1	0
45	I	203	3PE	2	0
45	J	202	3PE	1	0
51	H	401	U10	14	0
46	A	203	PC1	1	0
52	d	201	CDL	2	0
46	d	204	PC1	2	0
46	M	606	PC1	2	0

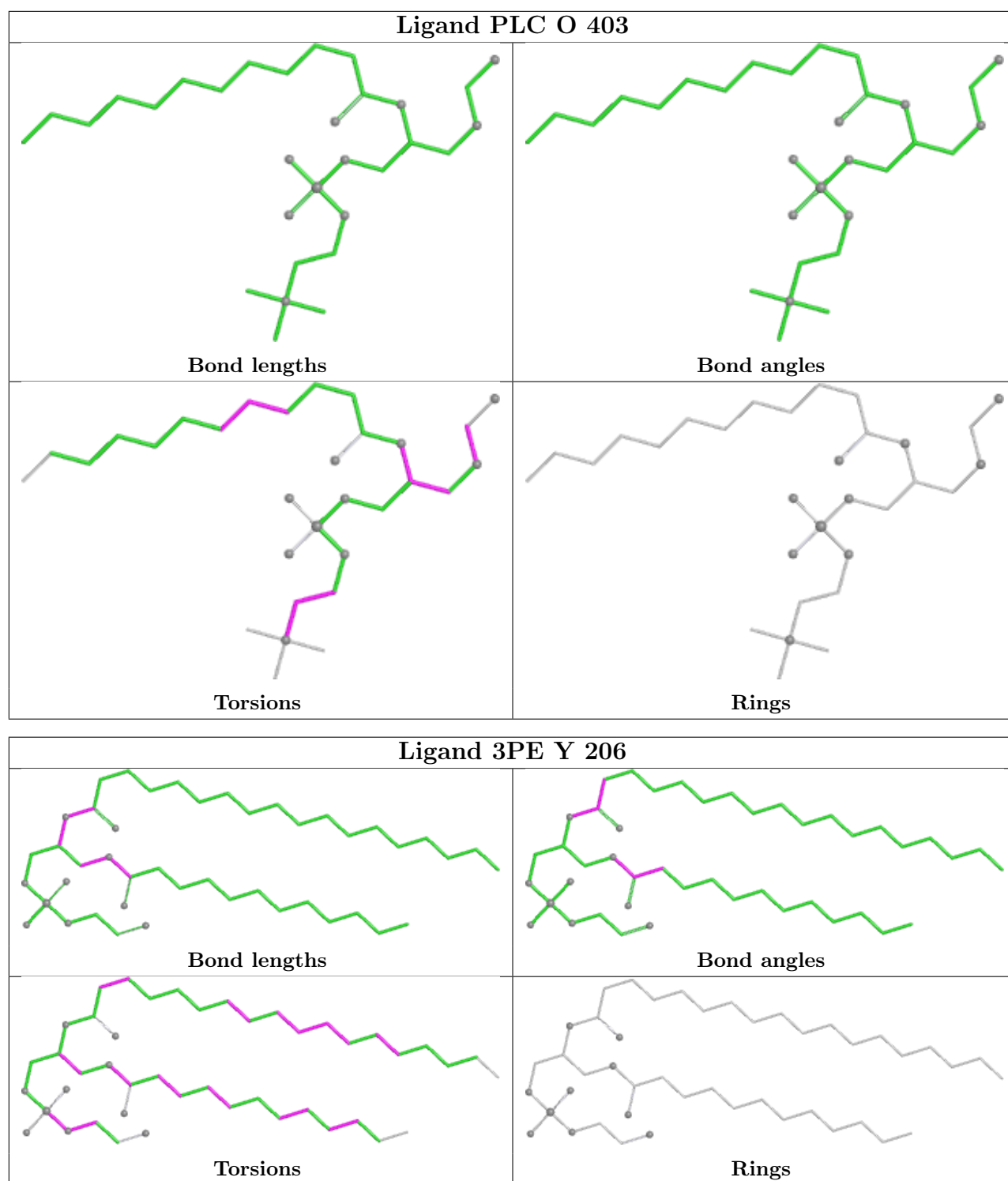
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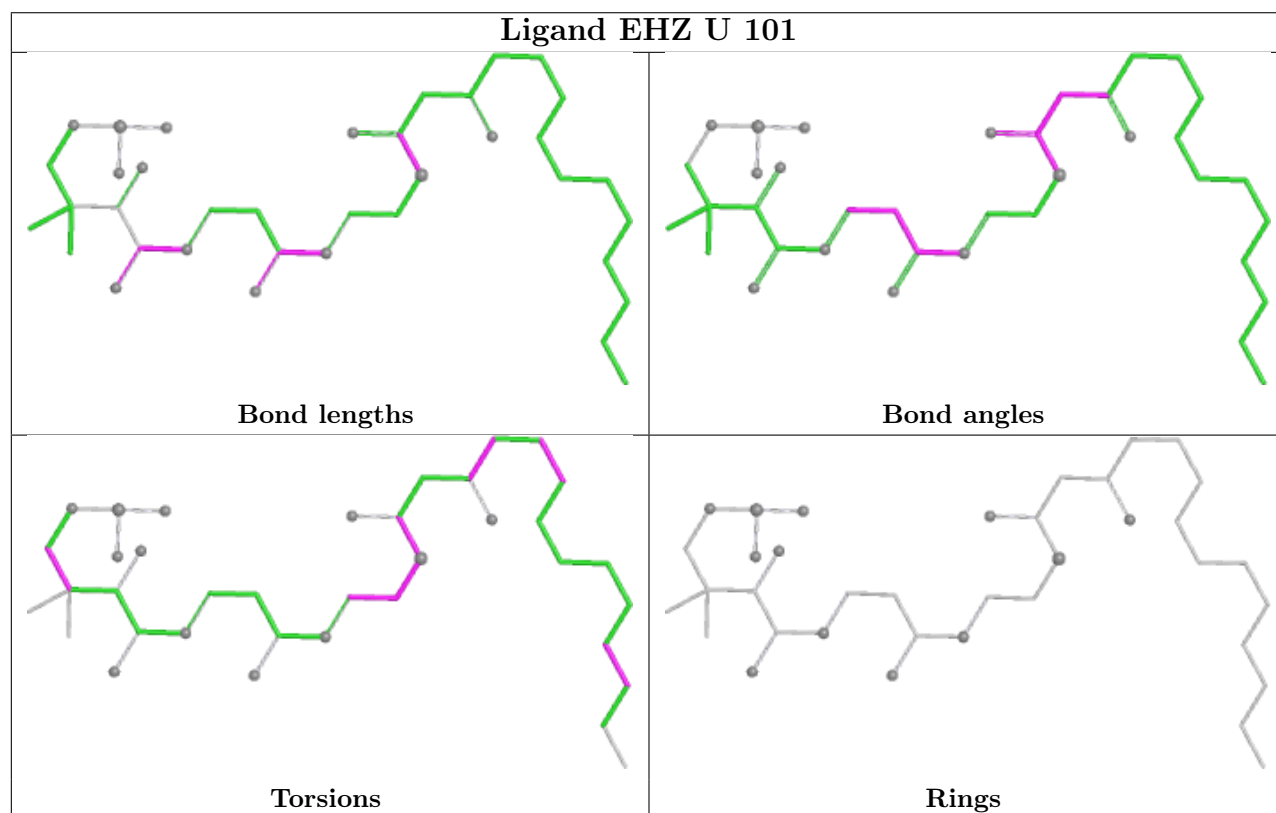
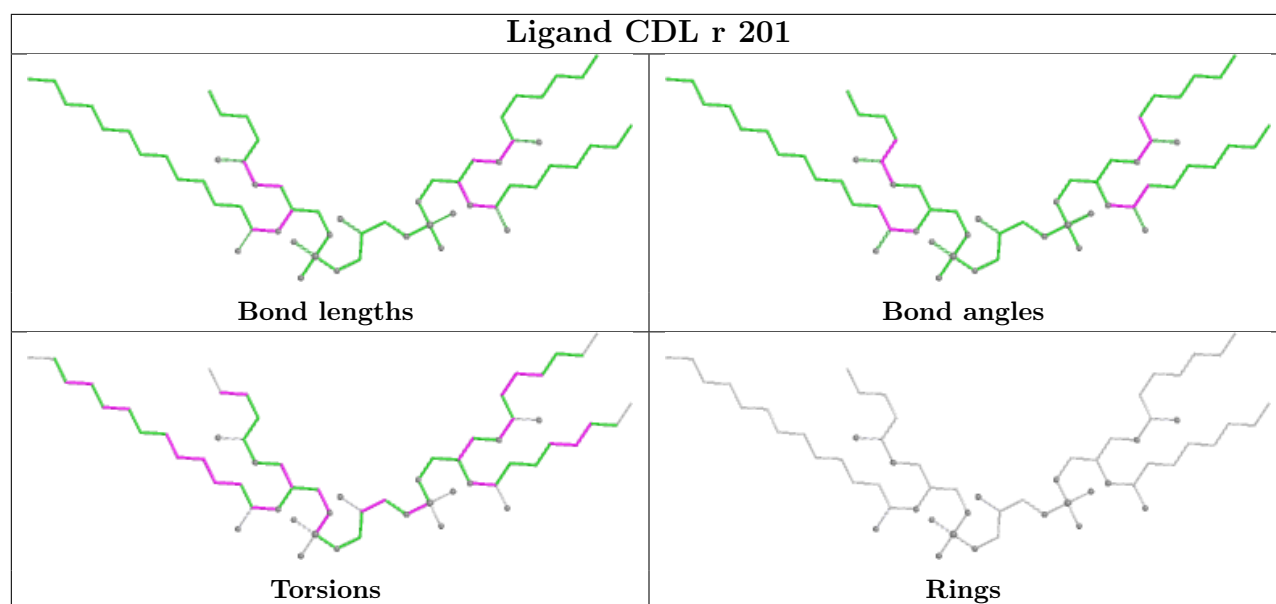
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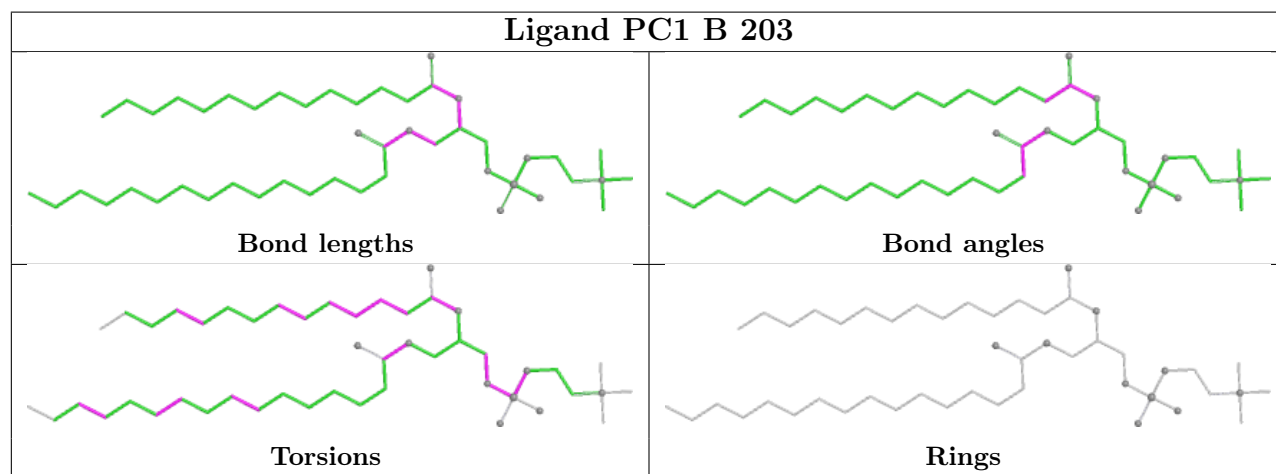
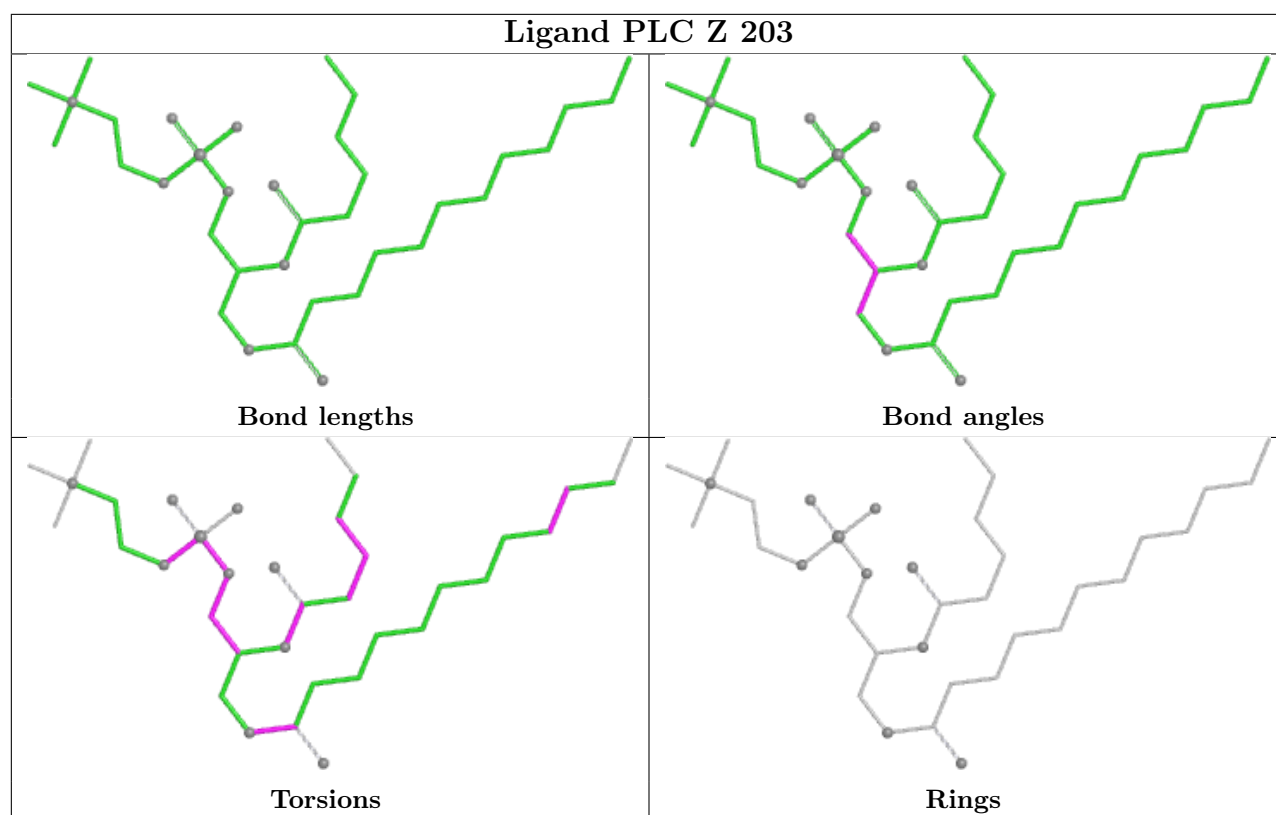
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	q	202	PC1	2	0
45	J	201	3PE	1	0
46	H	403	PC1	2	0
45	M	604	3PE	1	0
58	T	101	EHZ	1	0

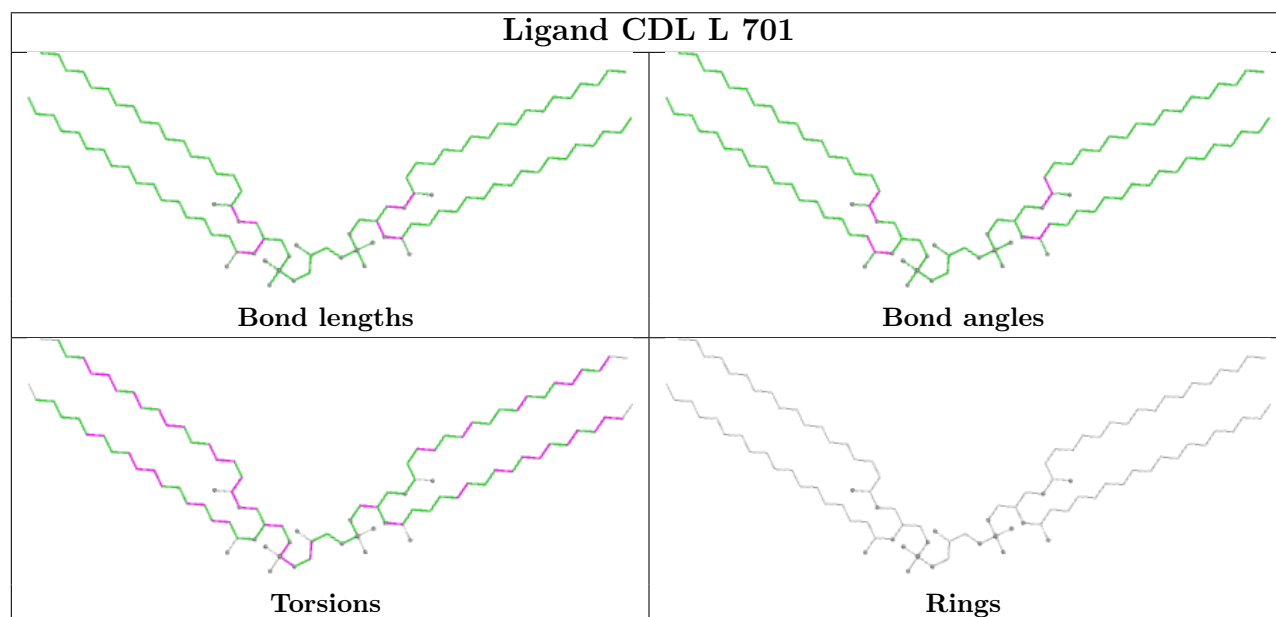
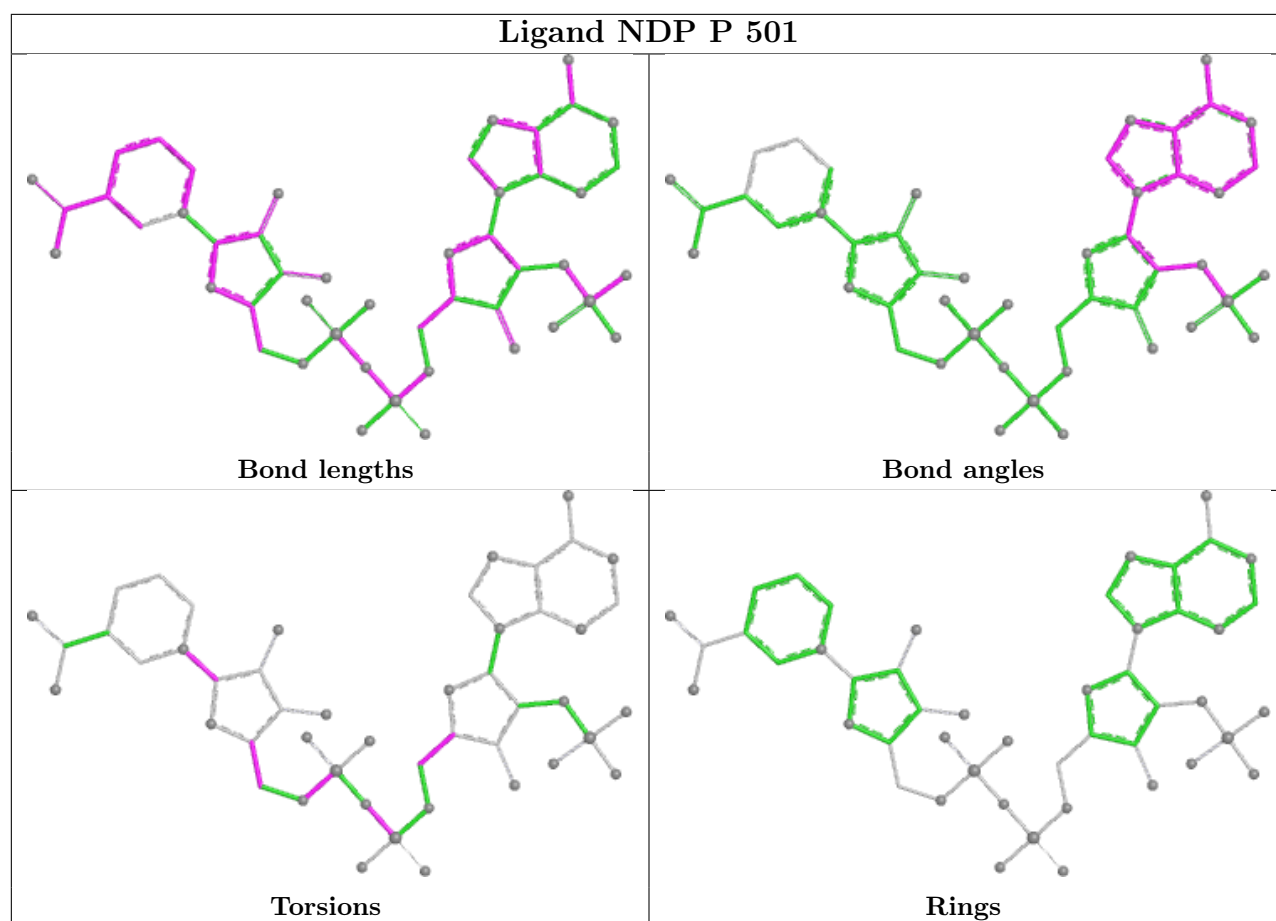
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

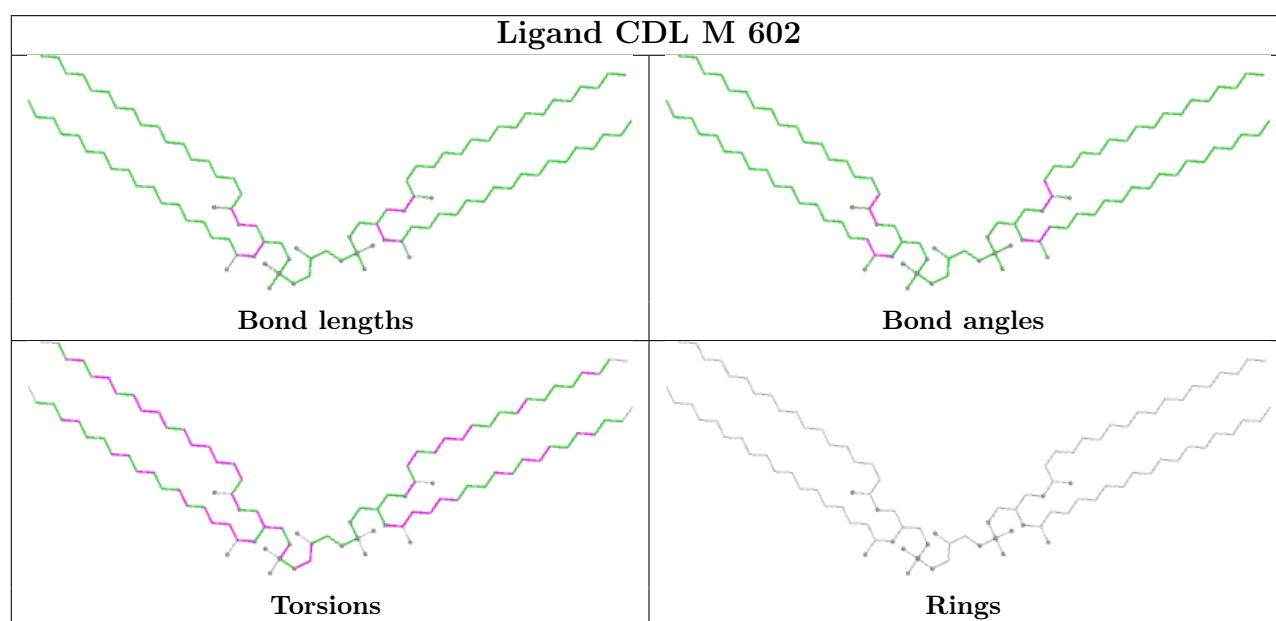
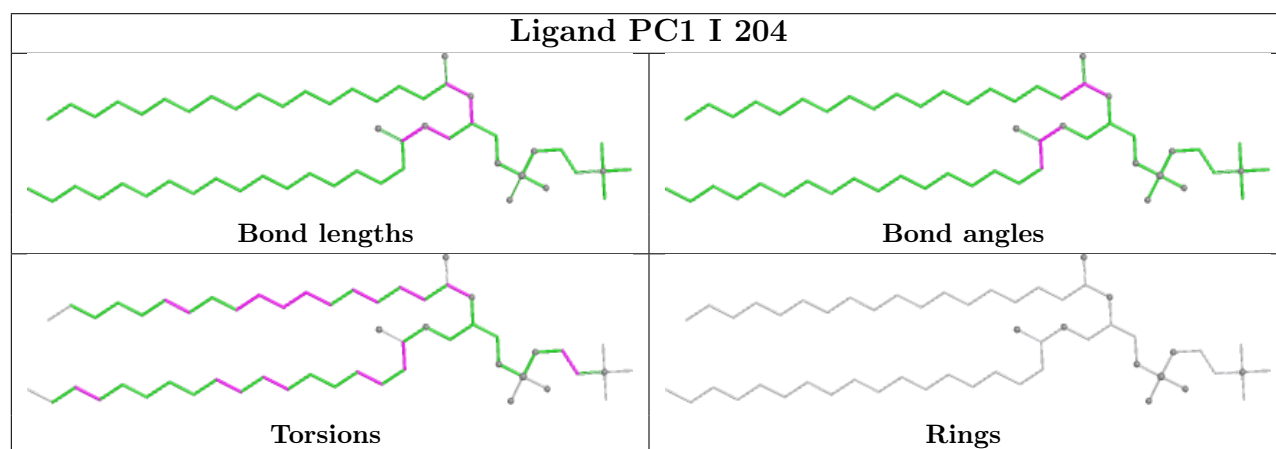
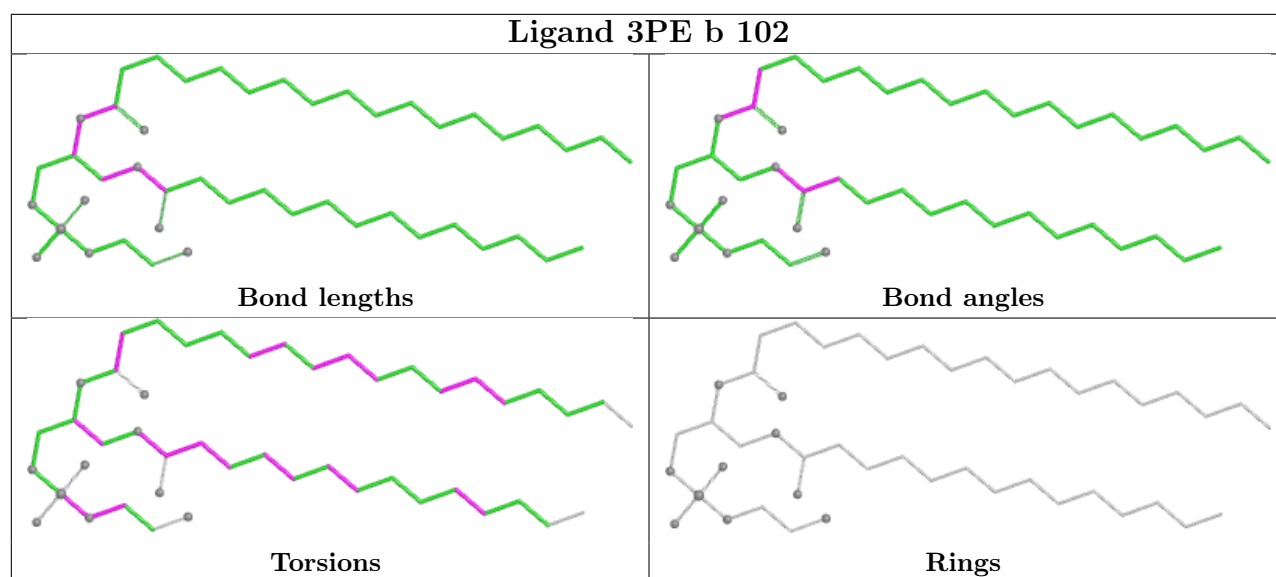


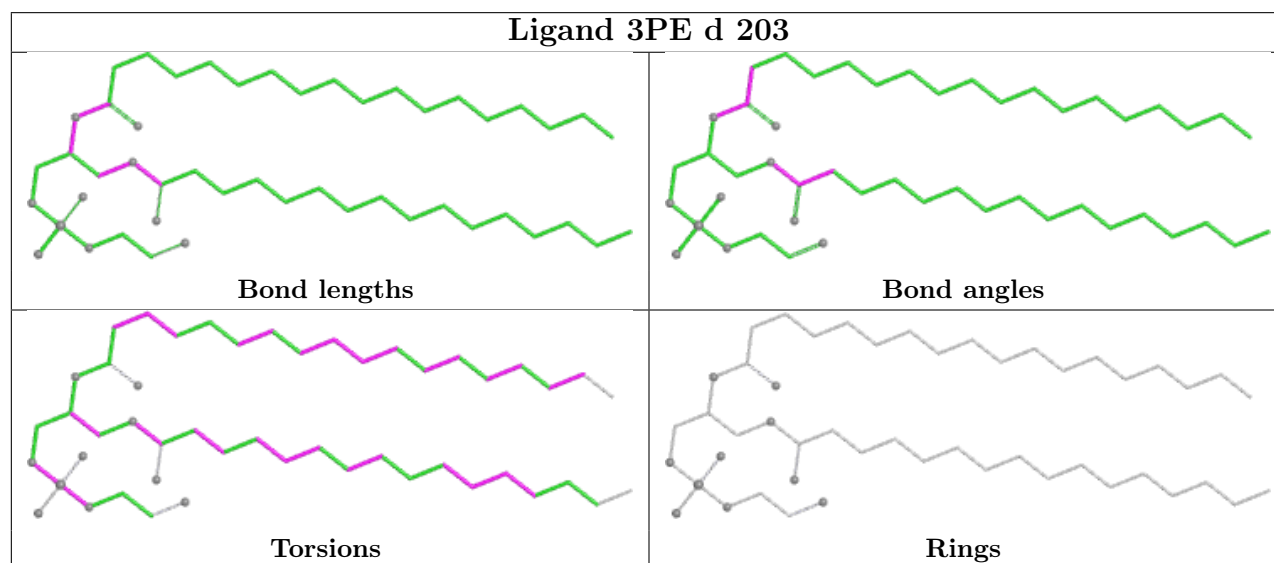
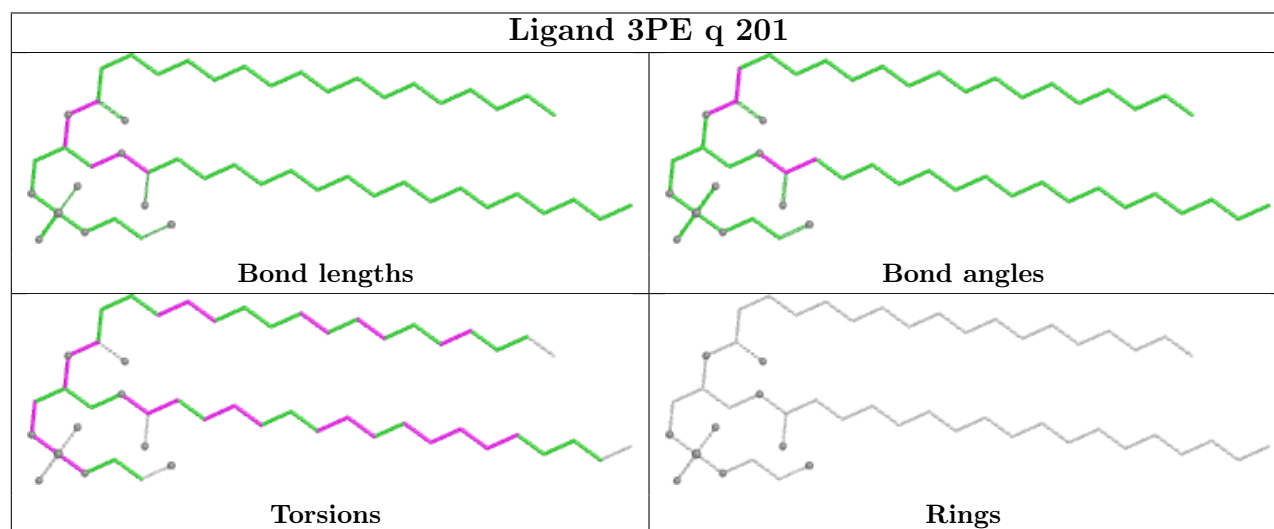
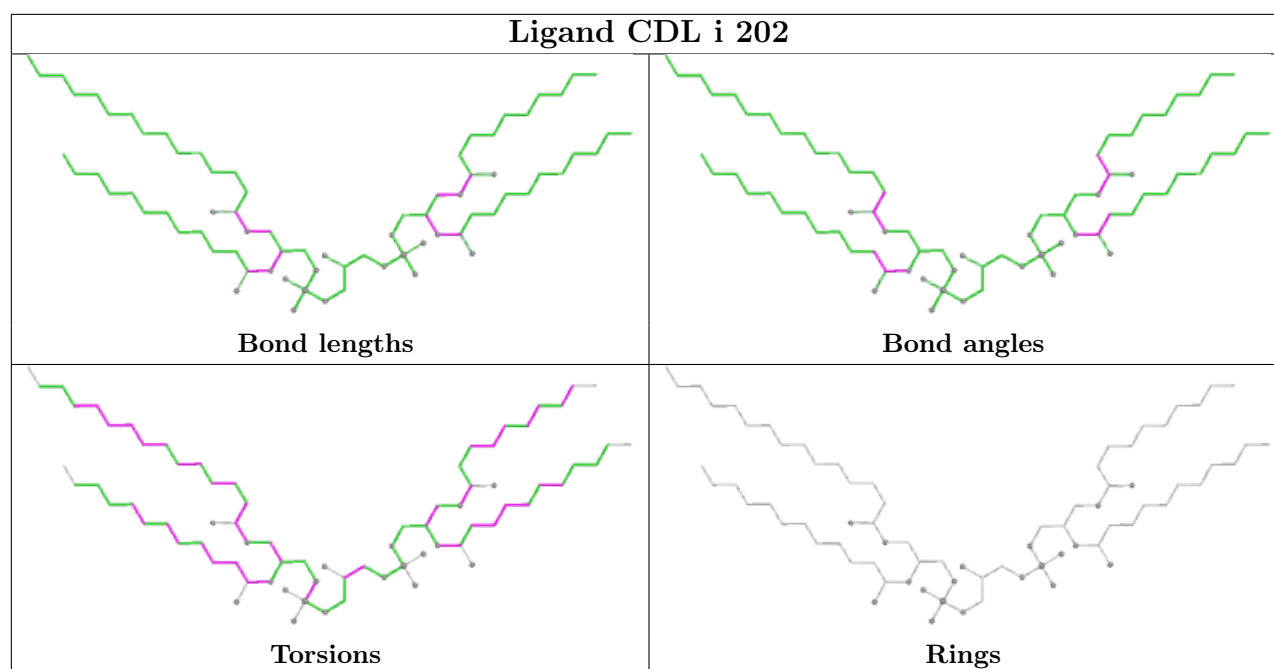


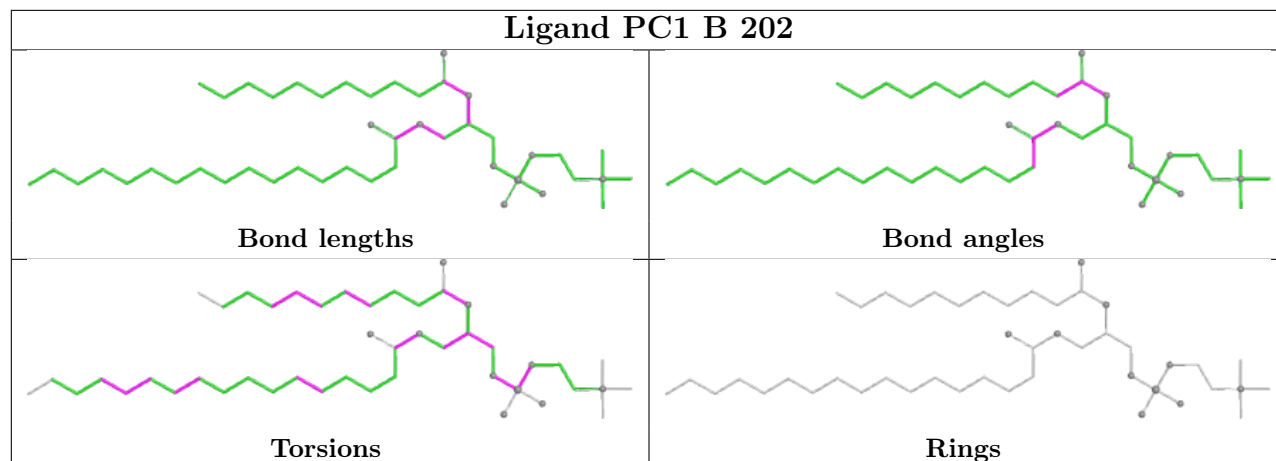
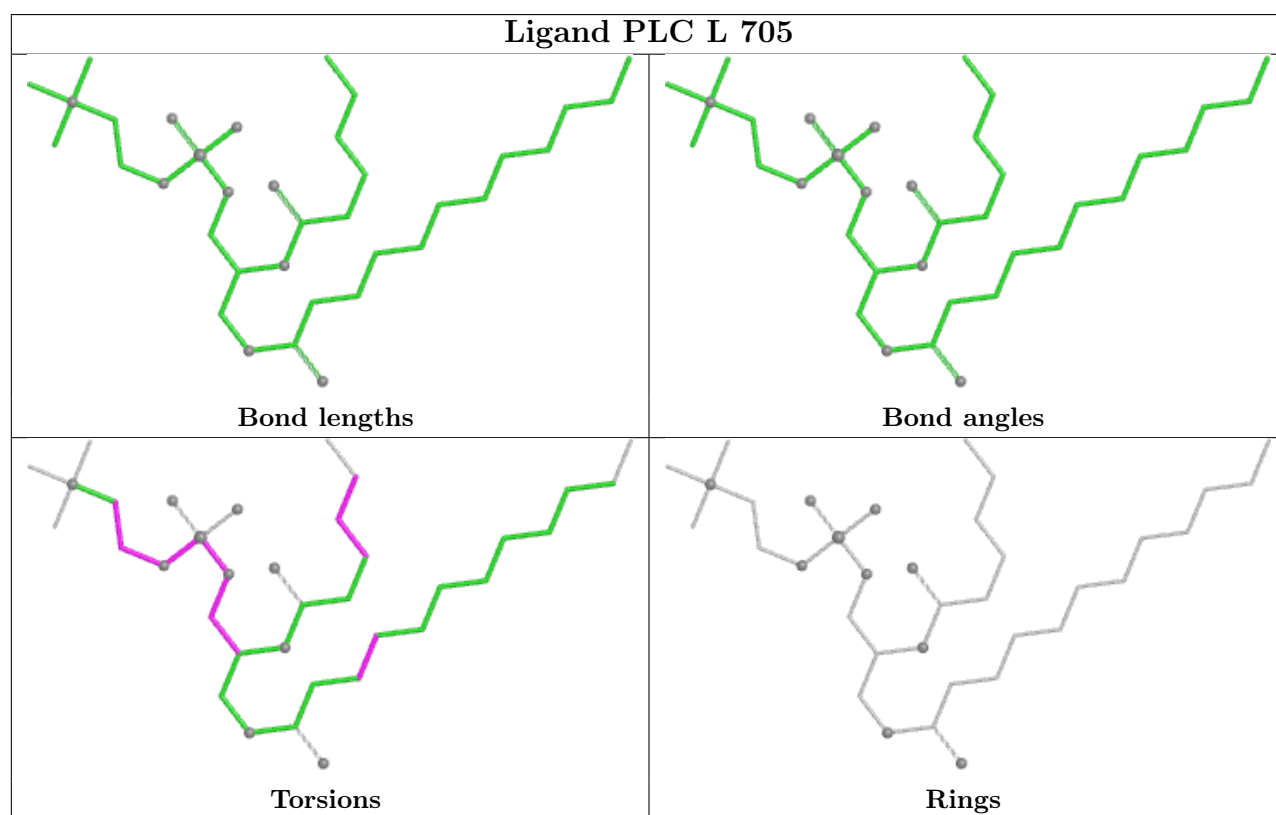
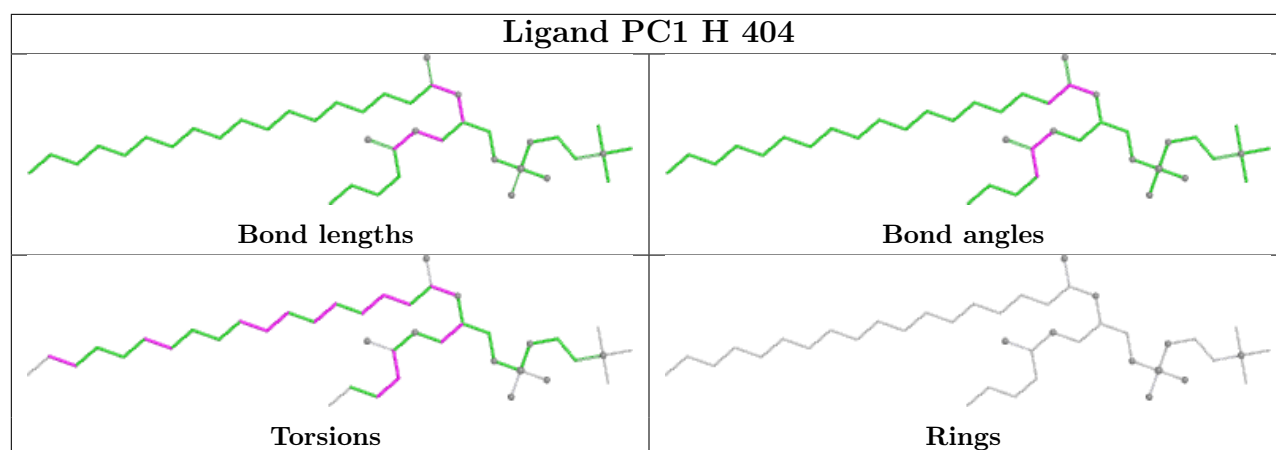




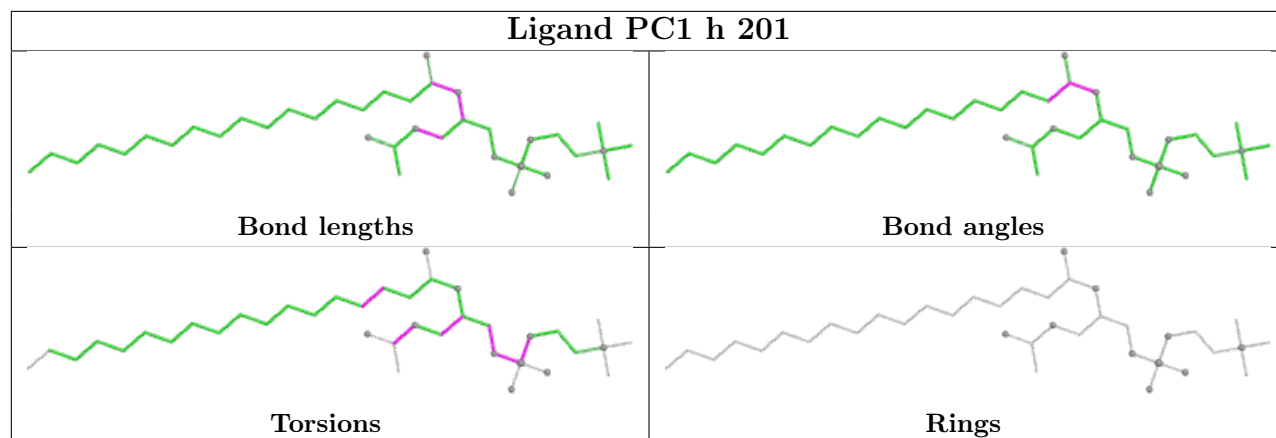




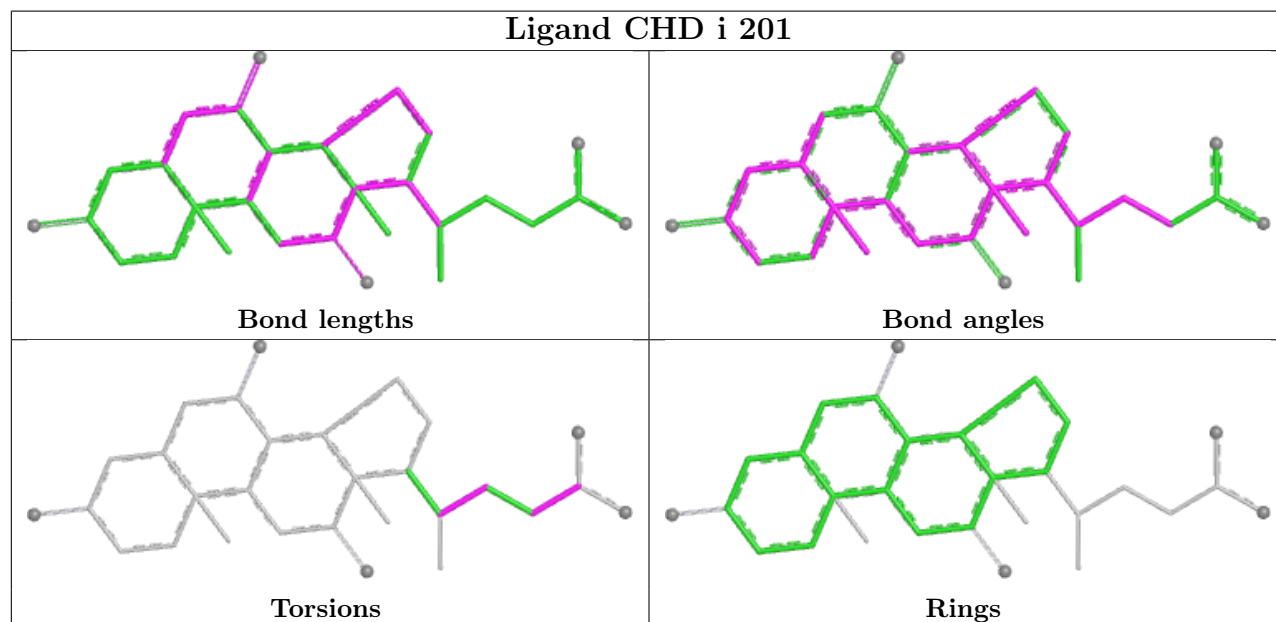




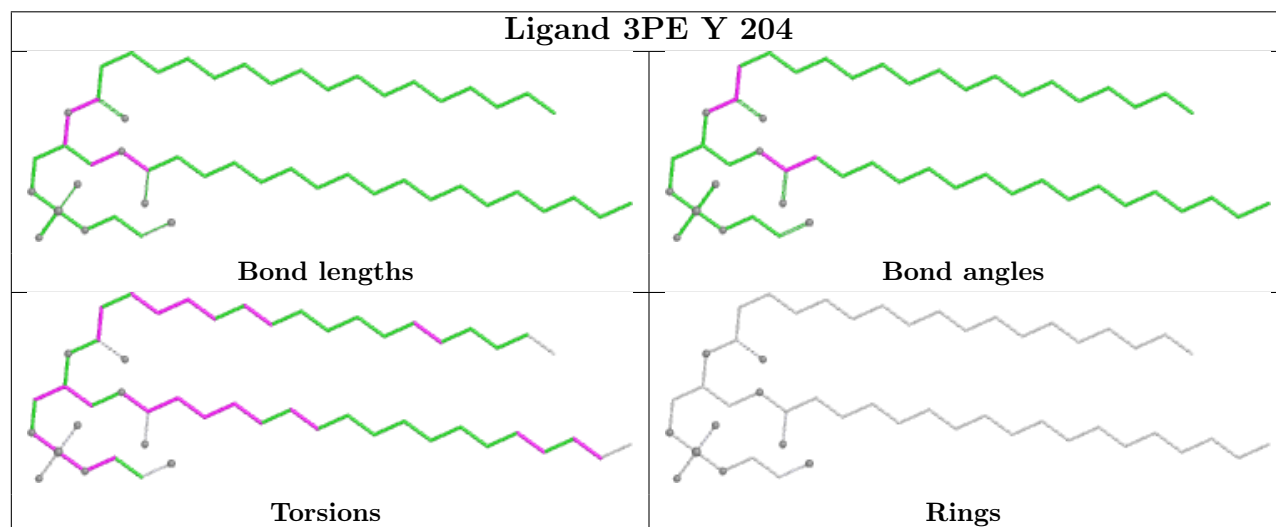
Ligand PC1 h 201

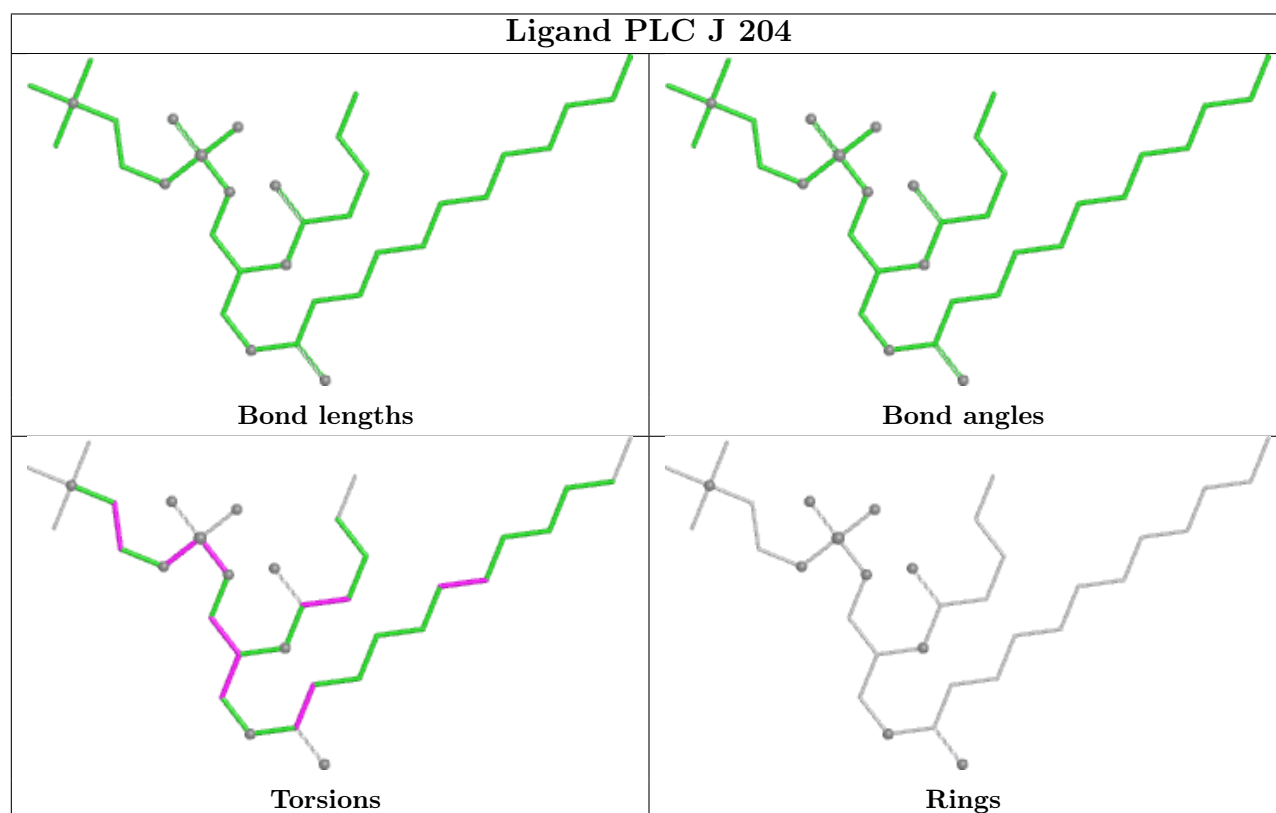
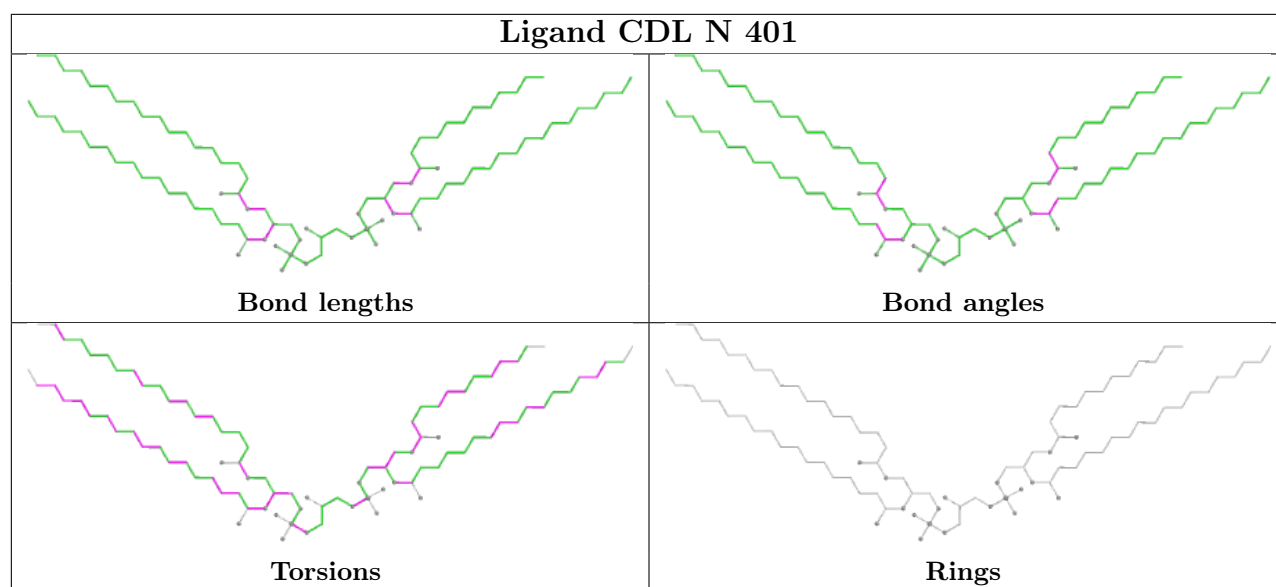


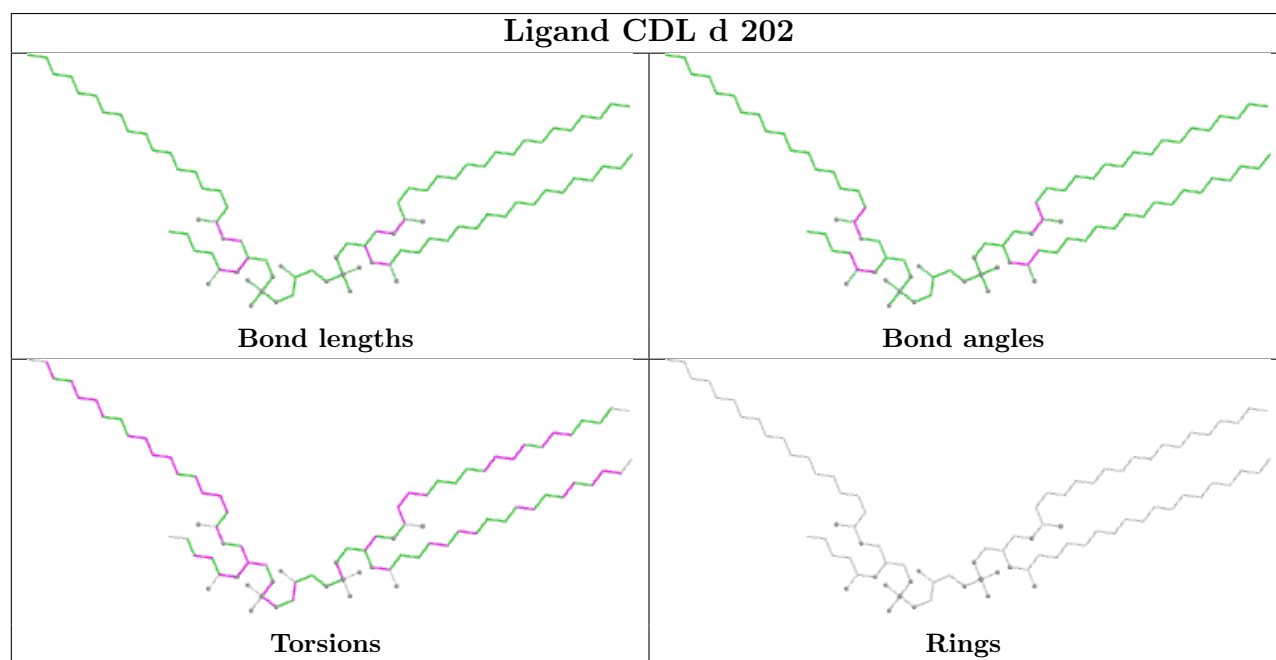
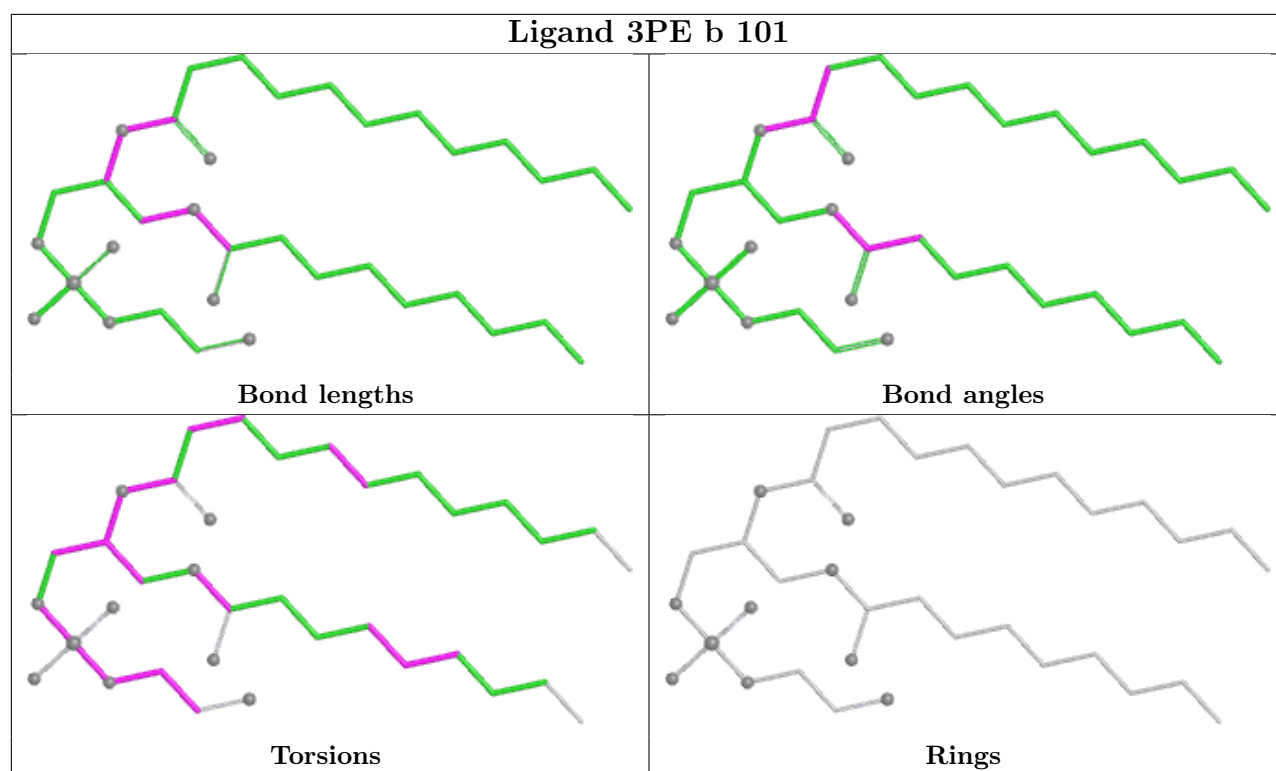
Ligand CHD i 201

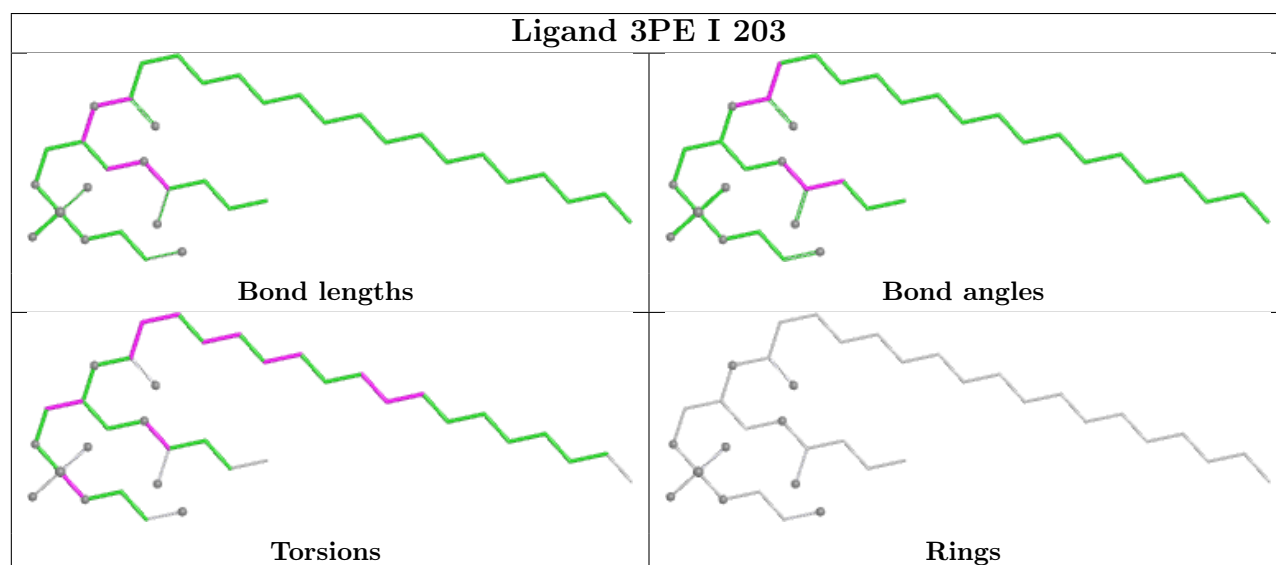
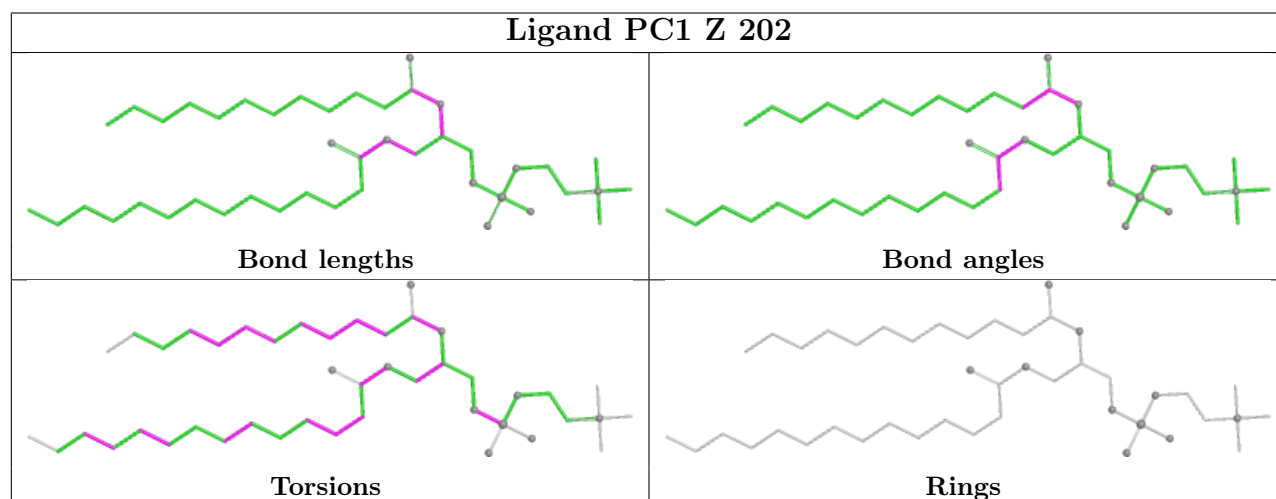
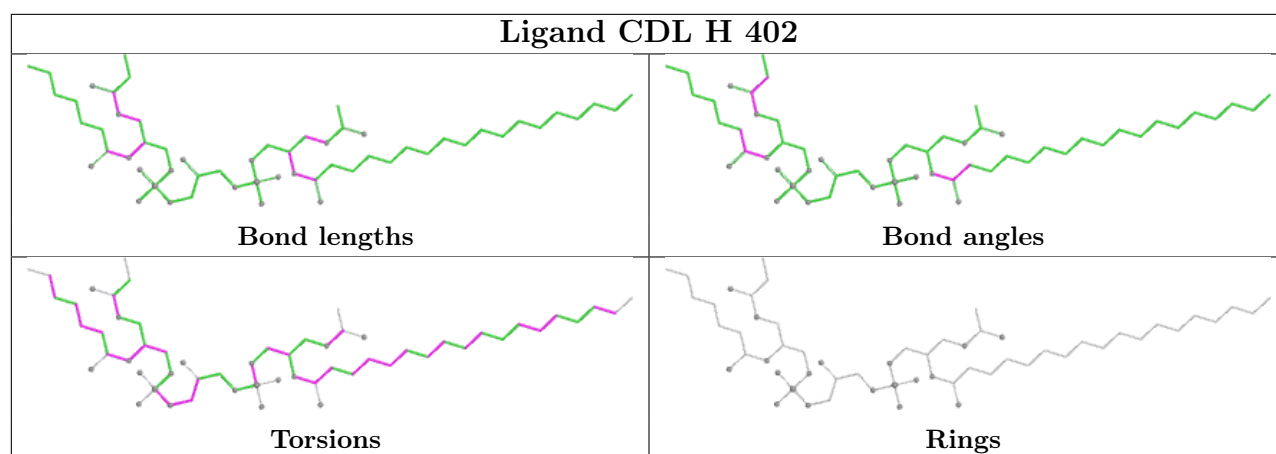


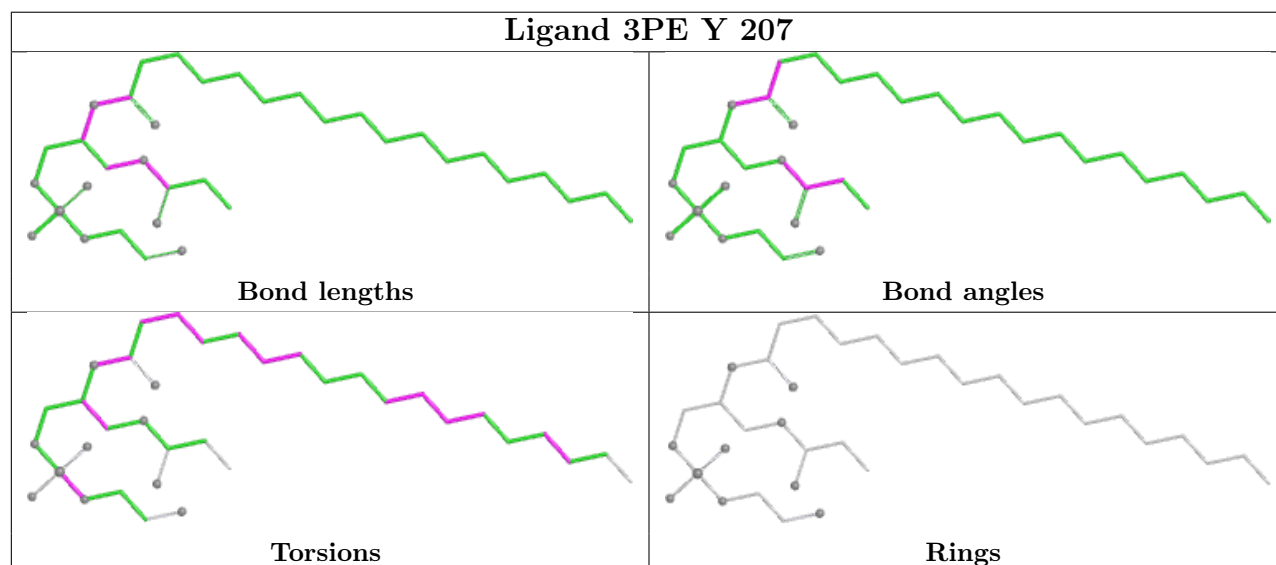
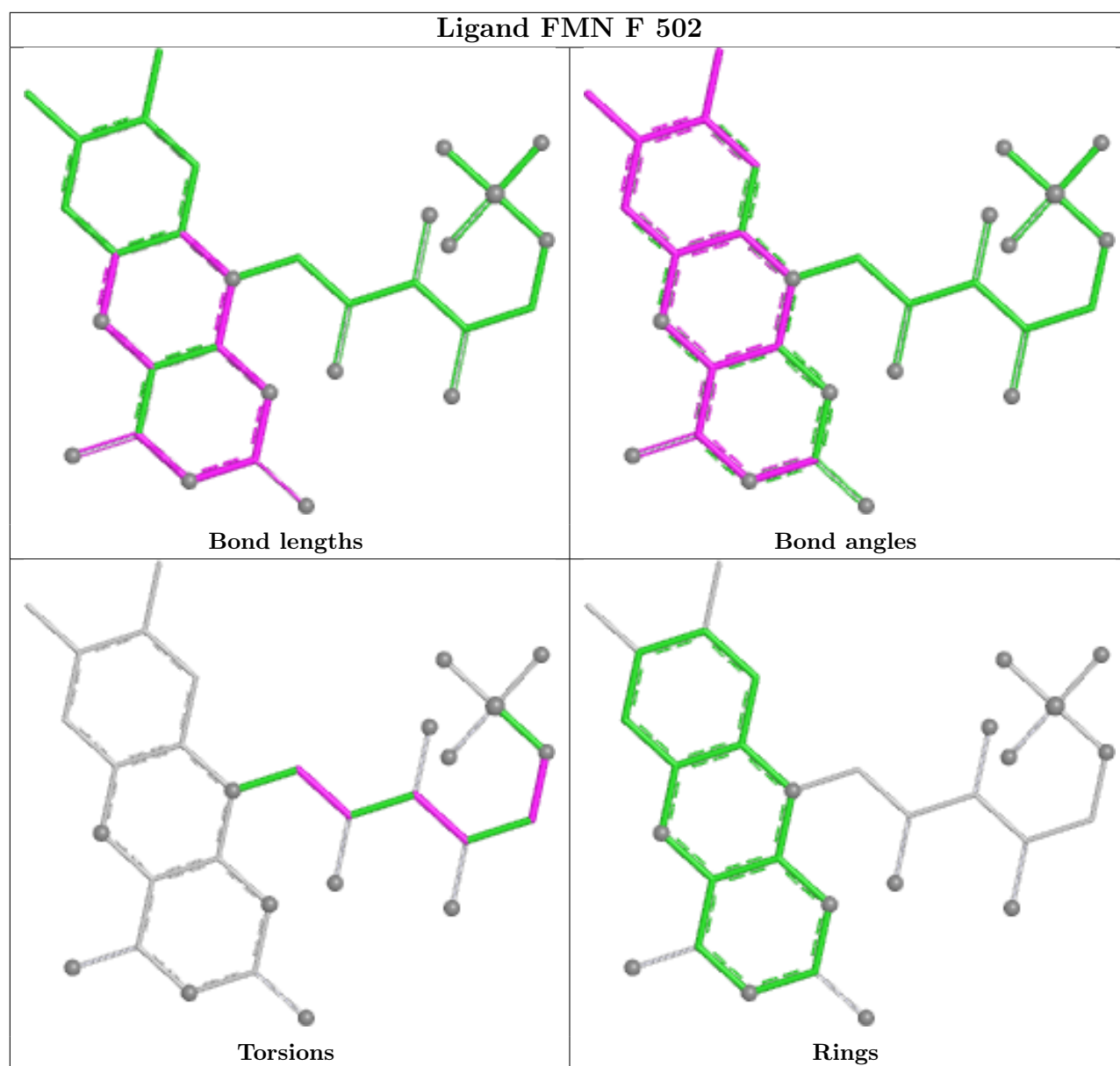
Ligand 3PE Y 204

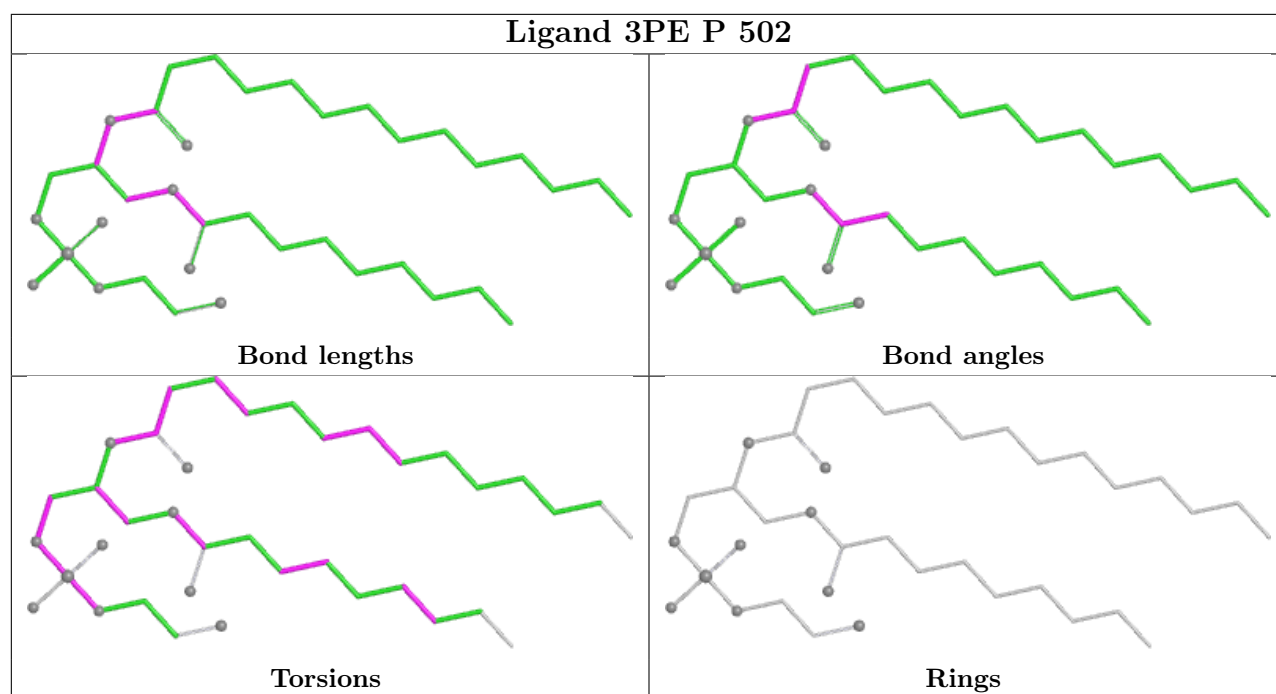


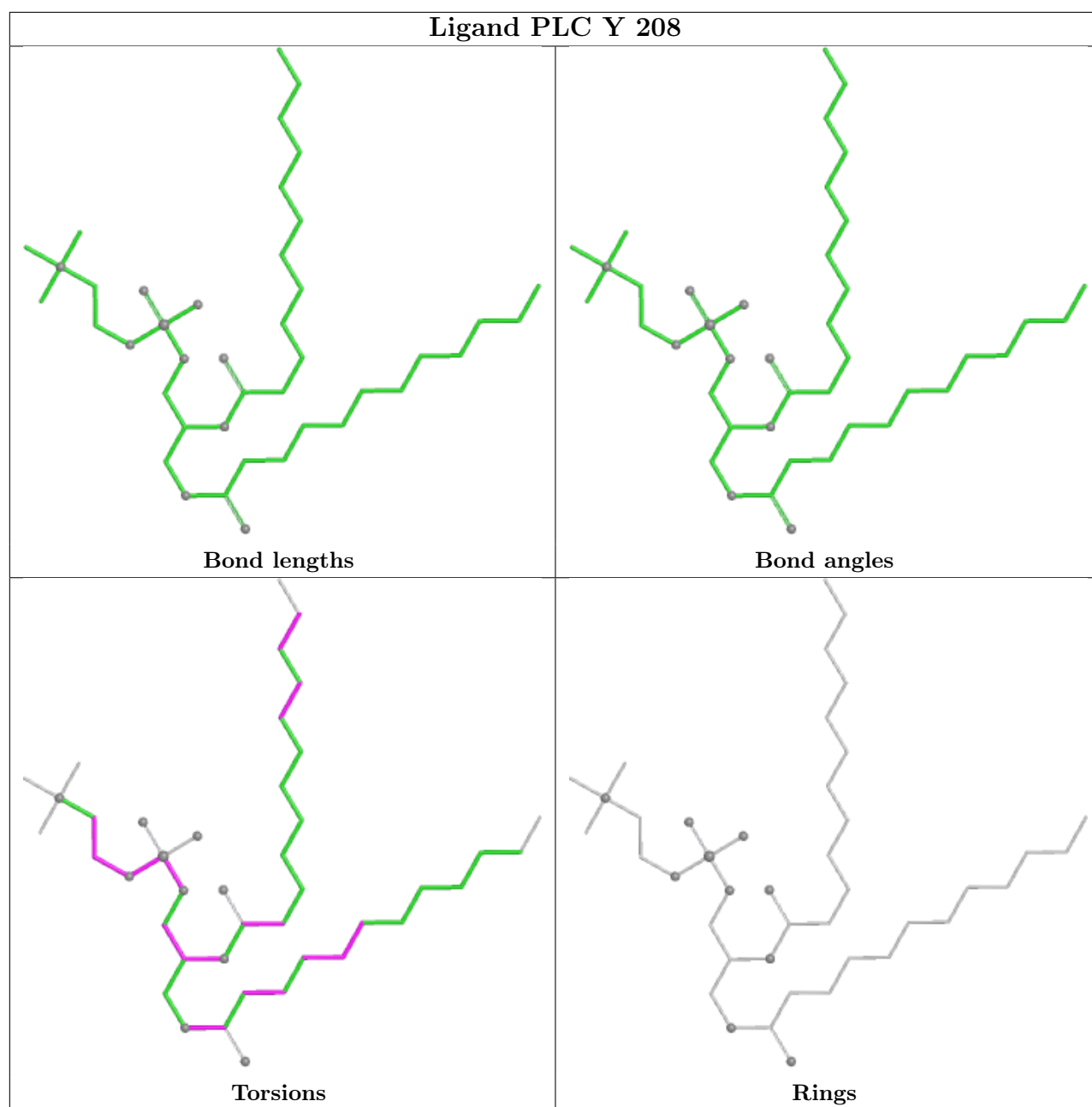


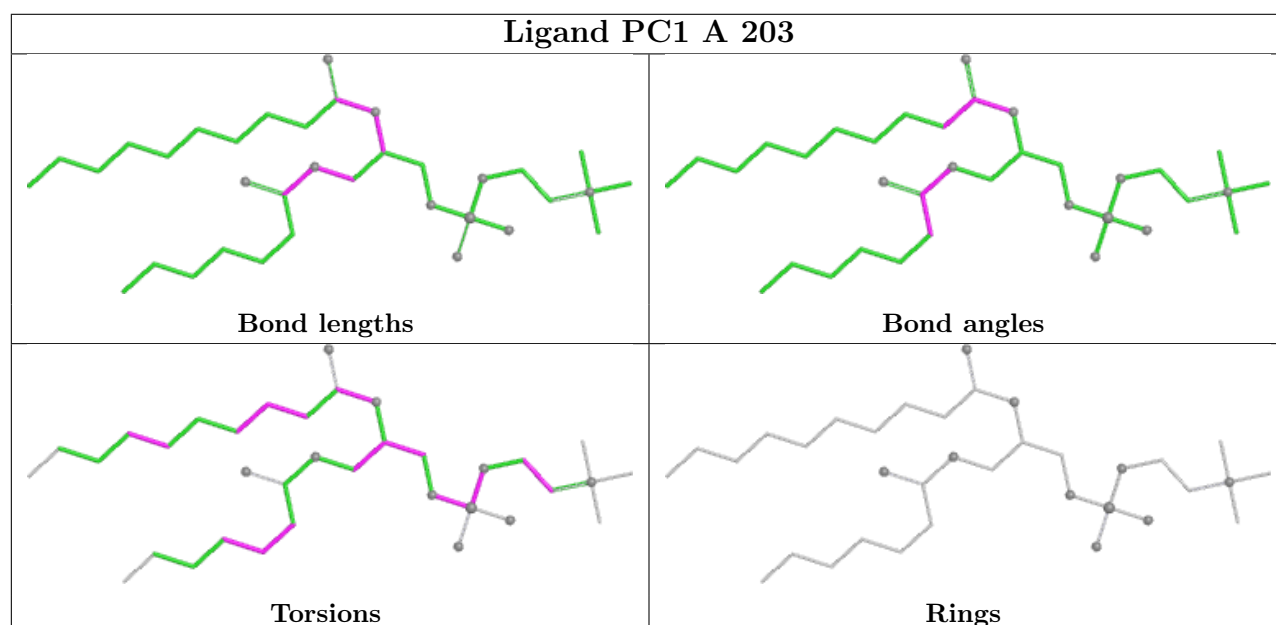
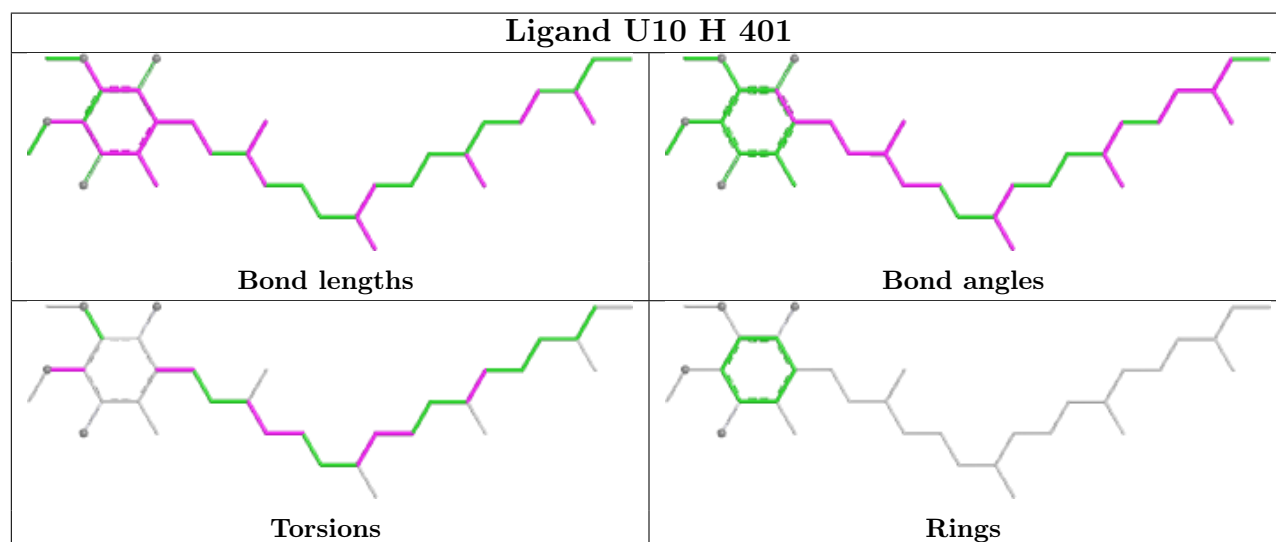
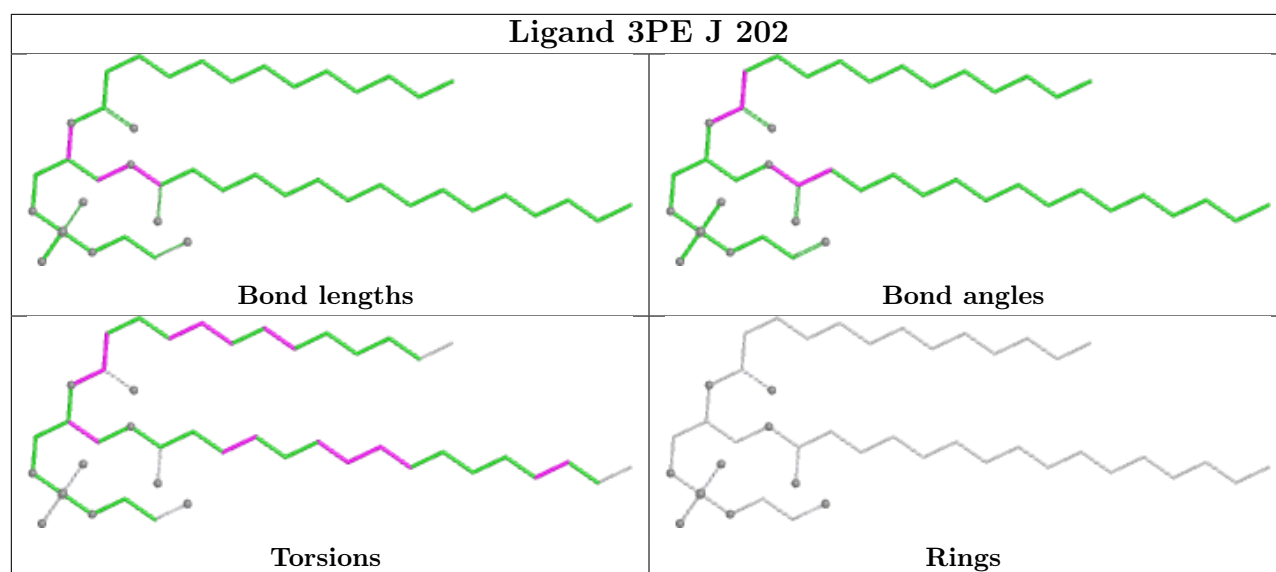


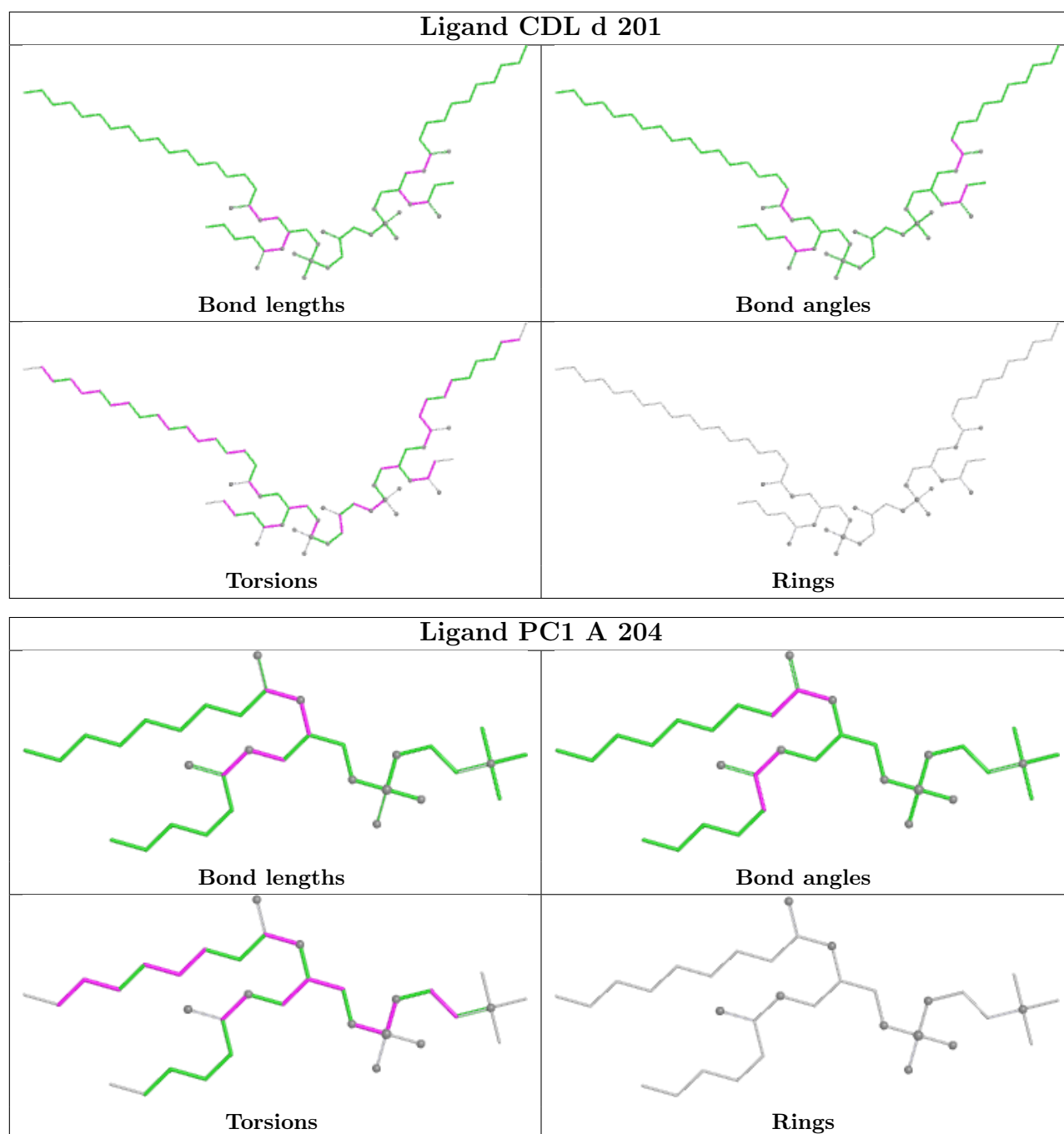


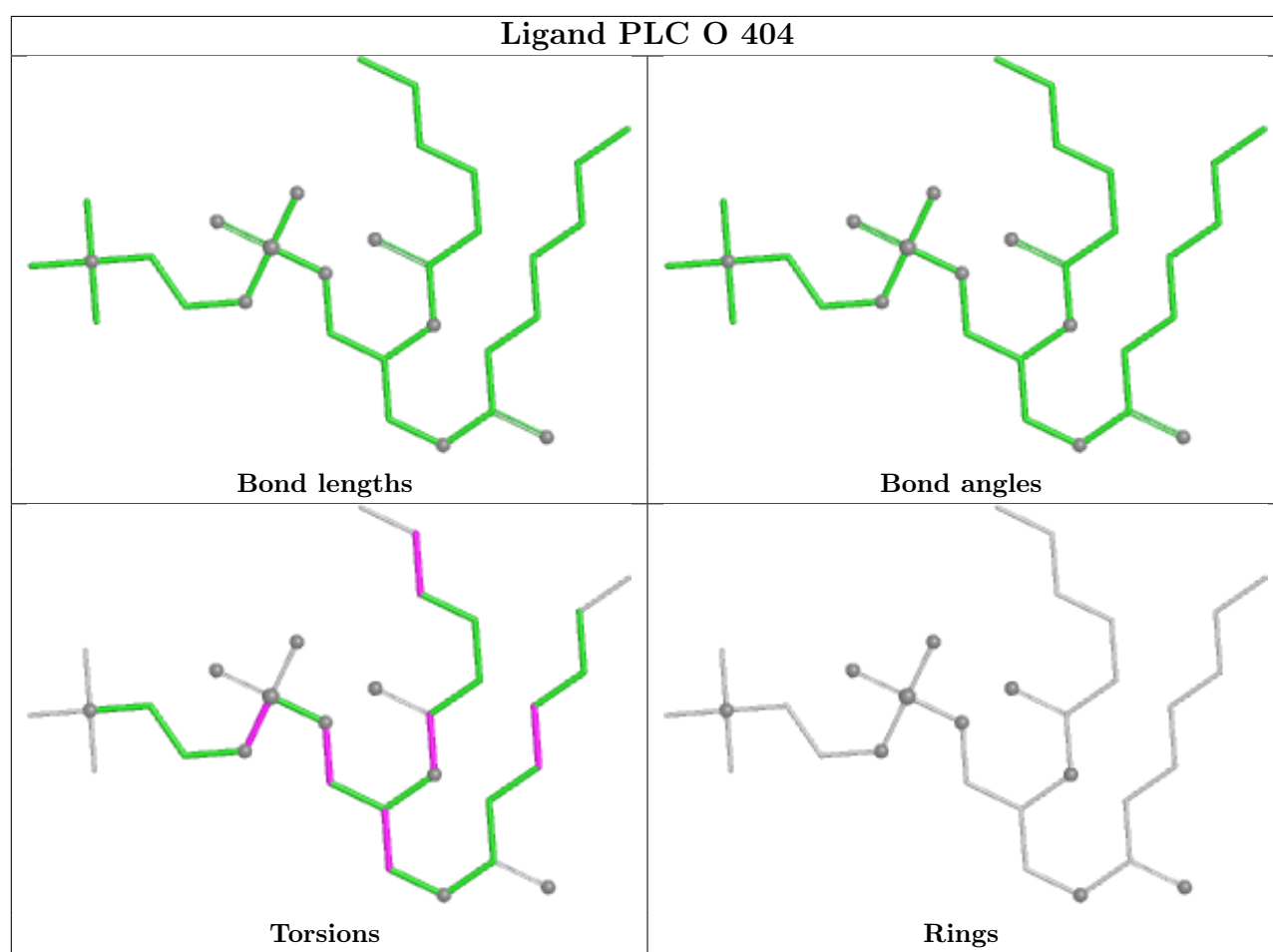
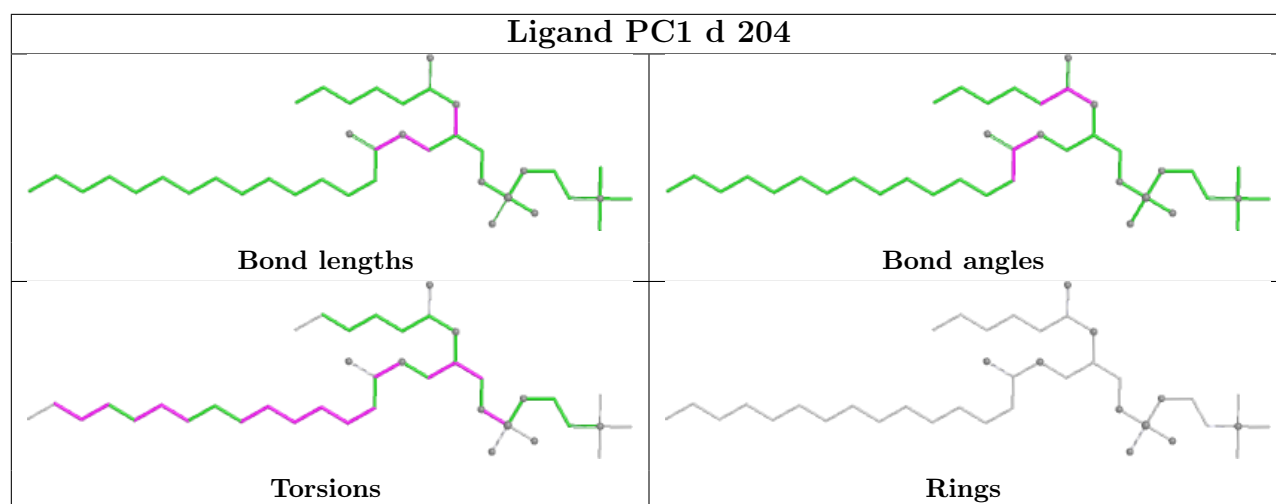


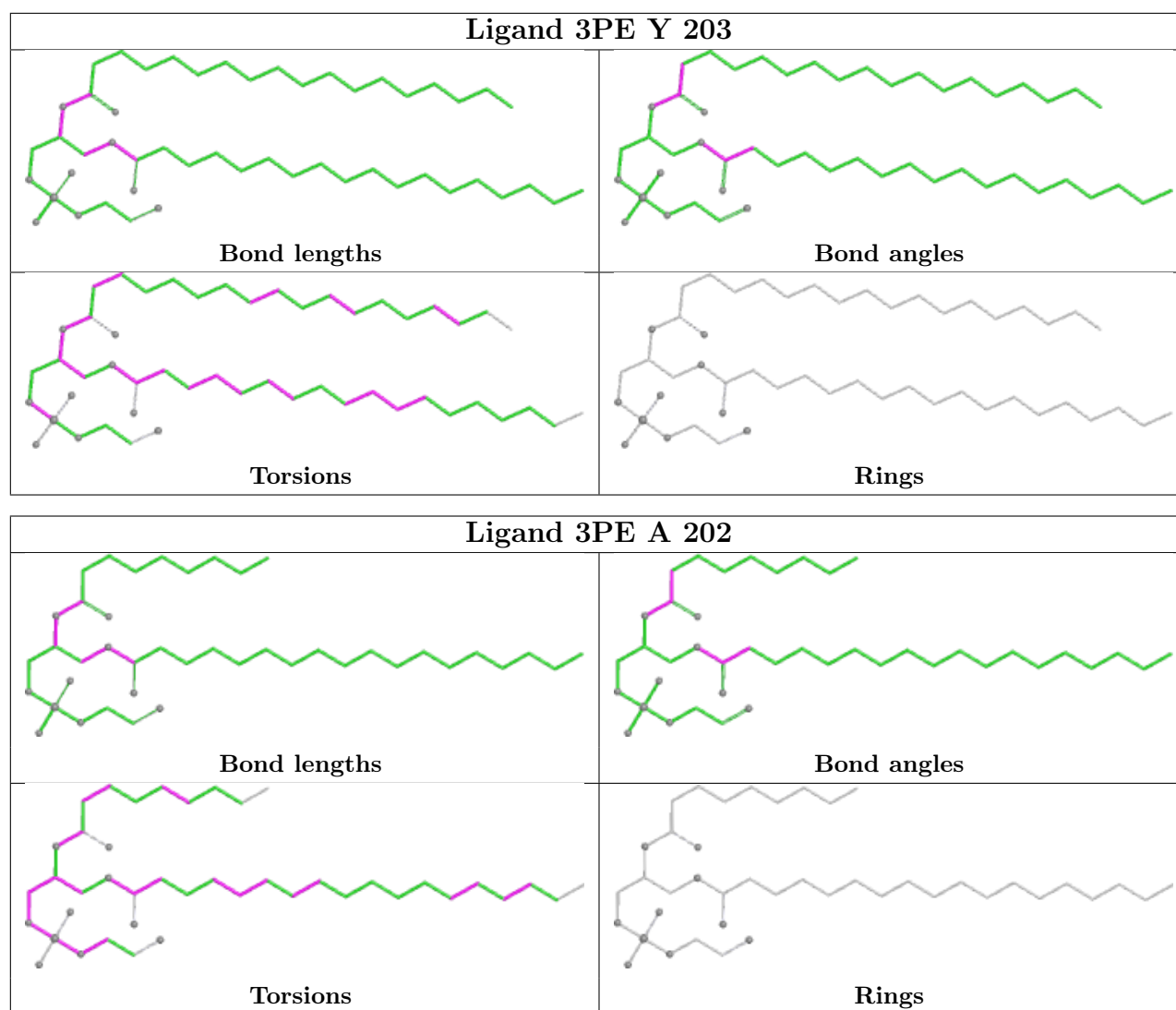


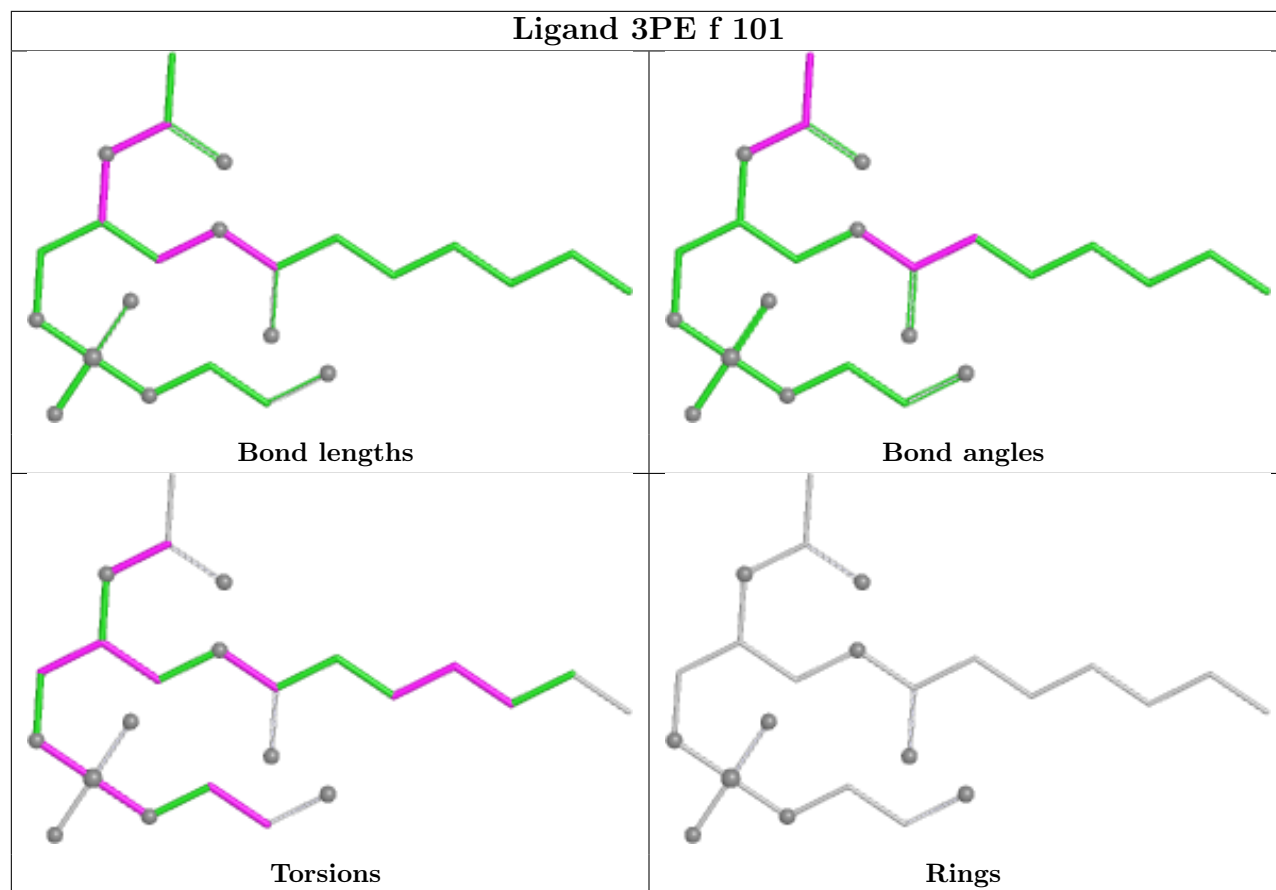


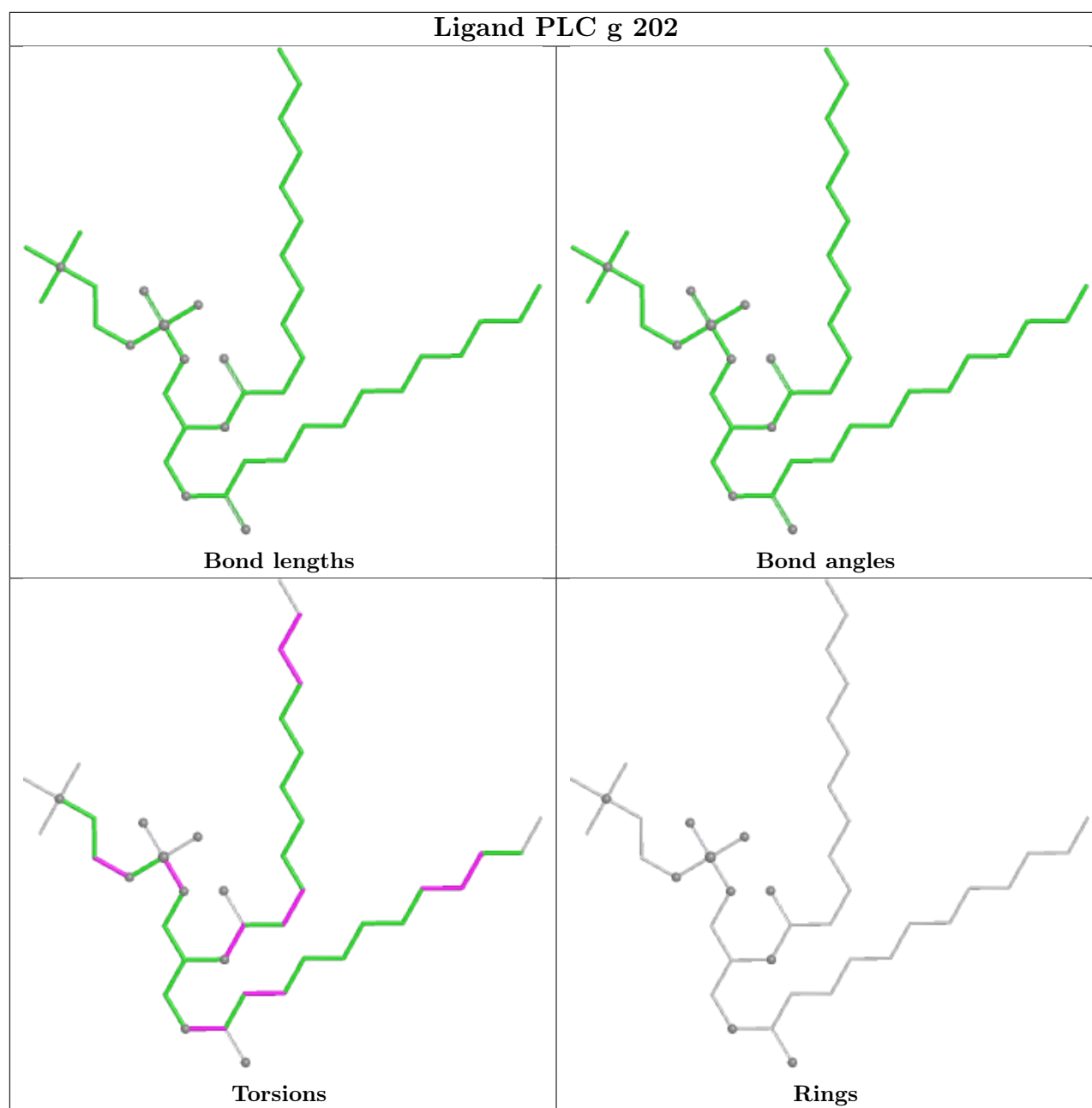


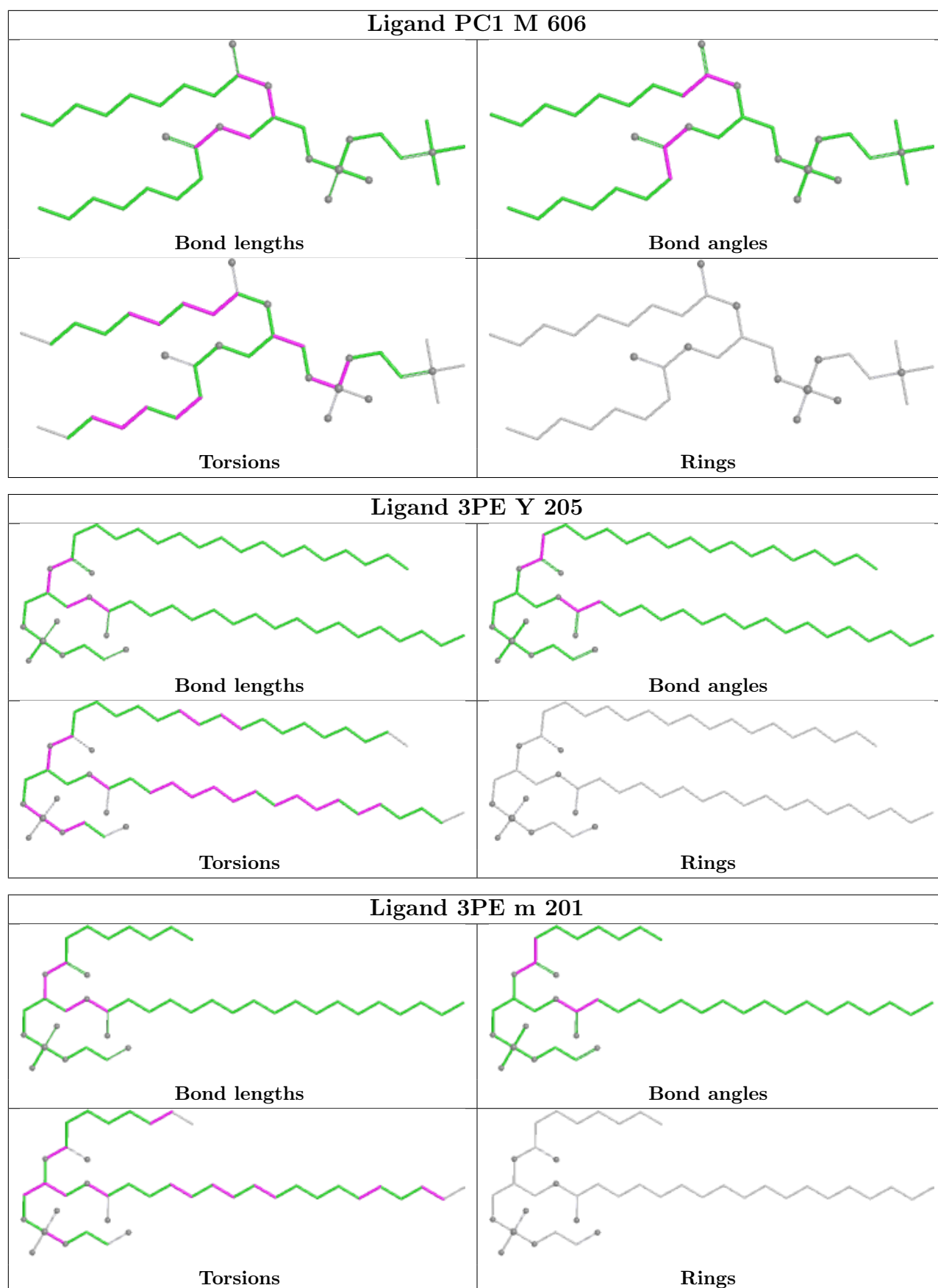


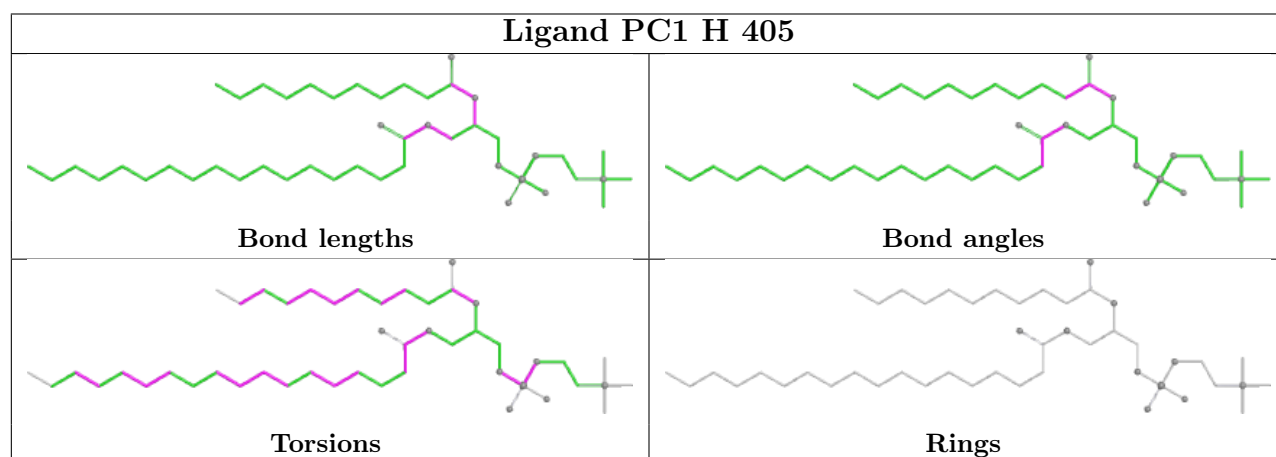
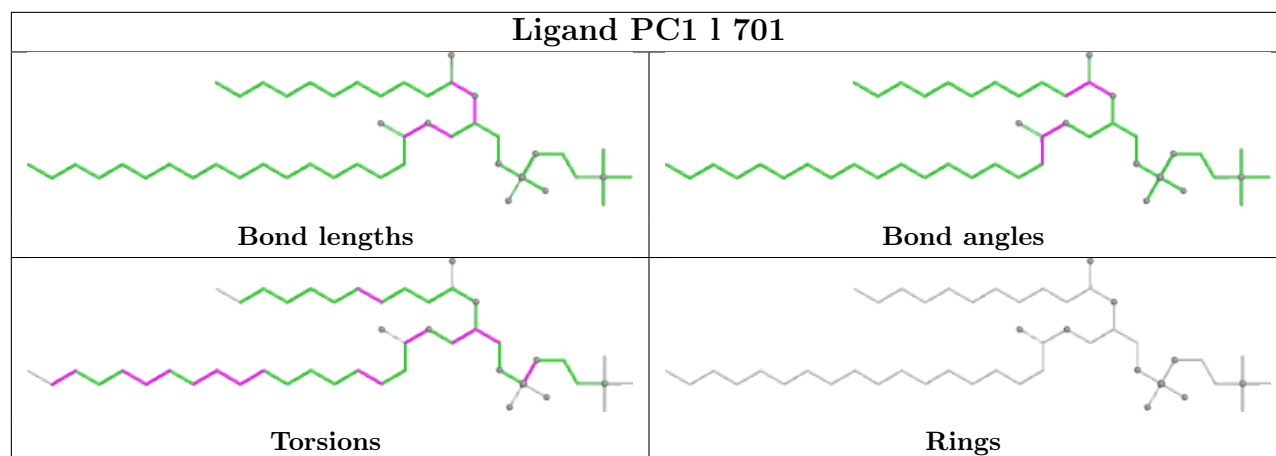
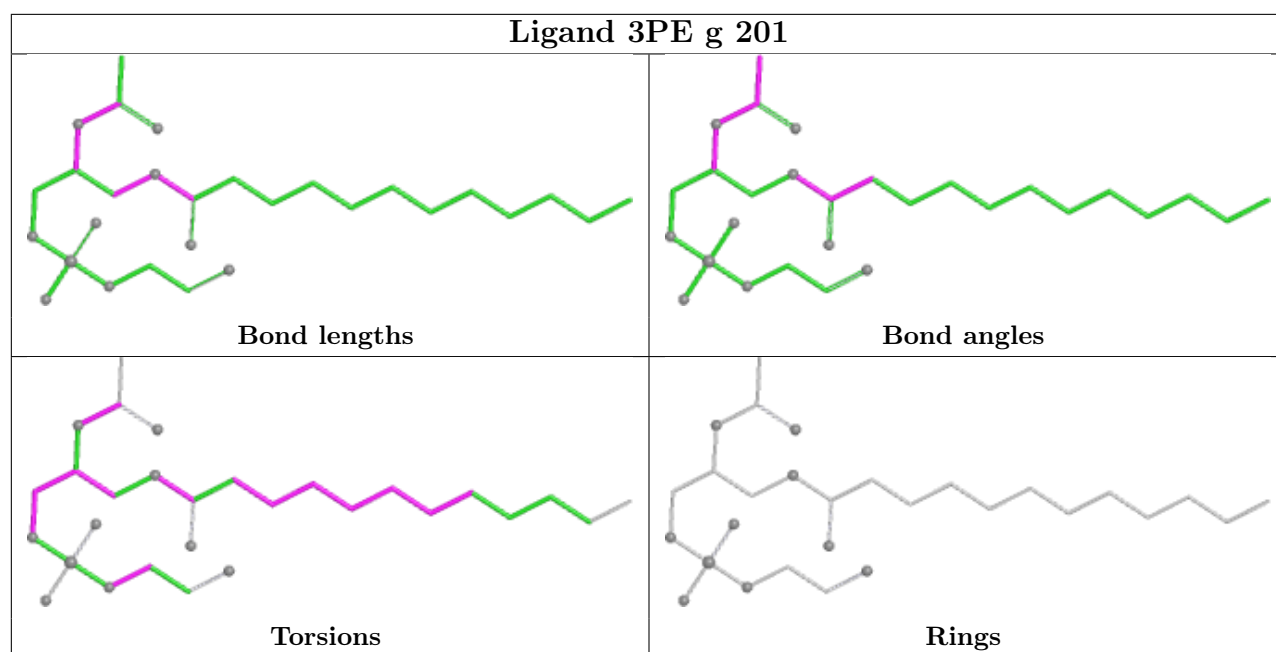




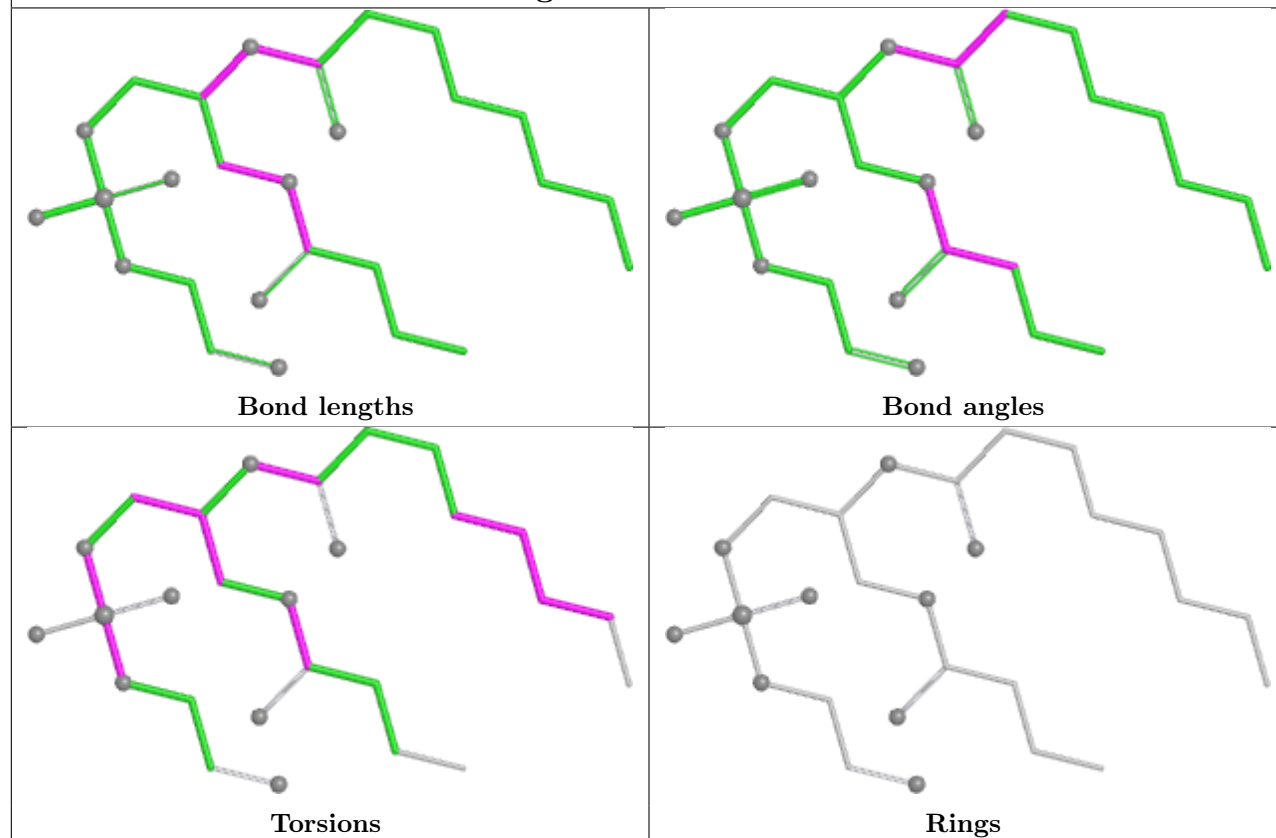




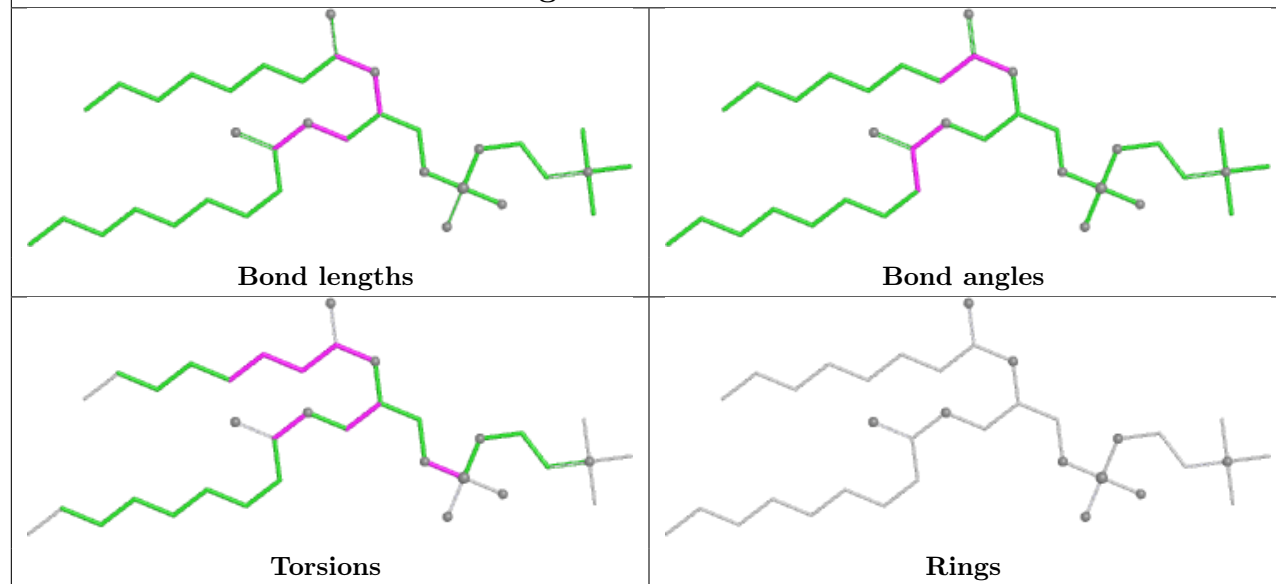


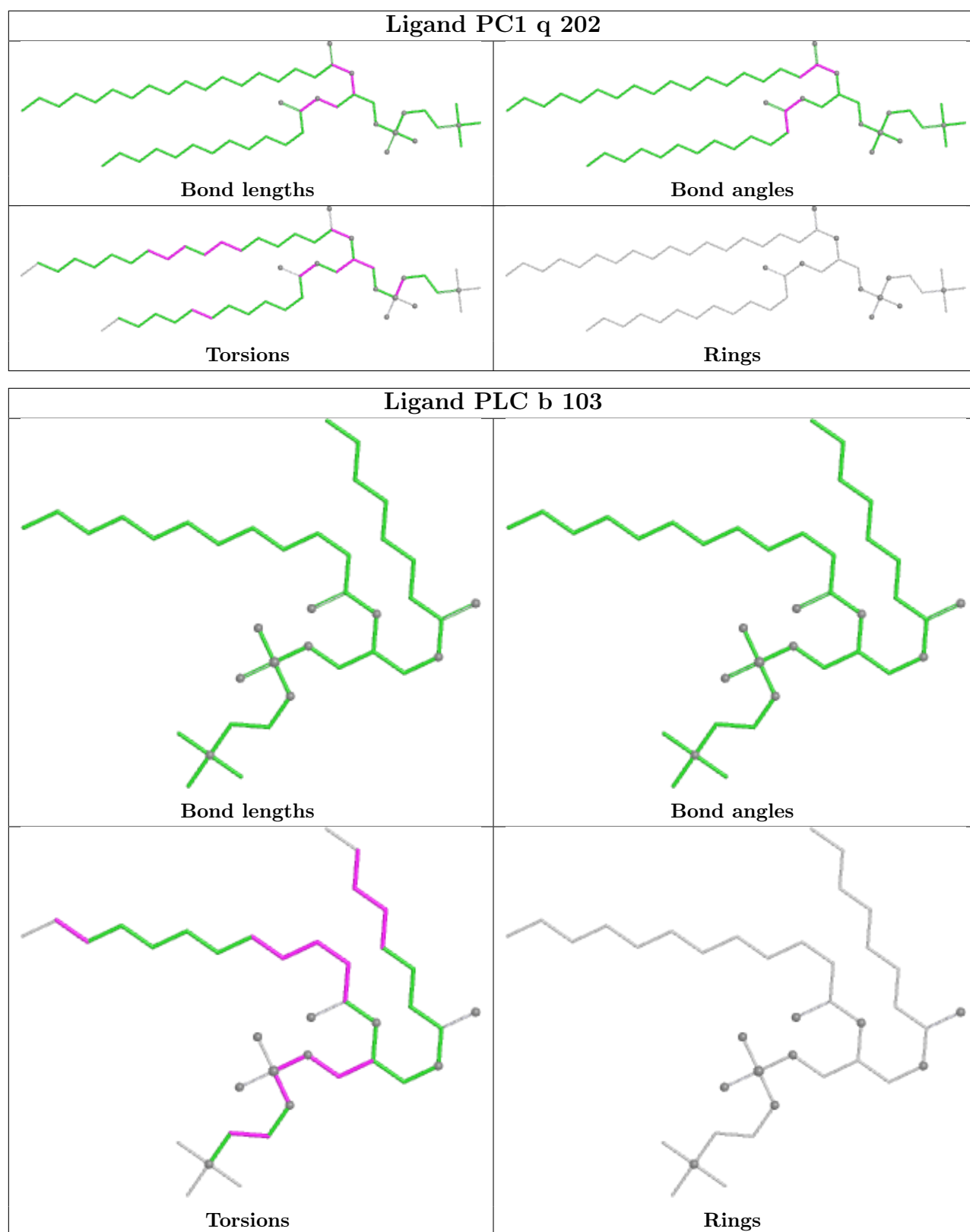


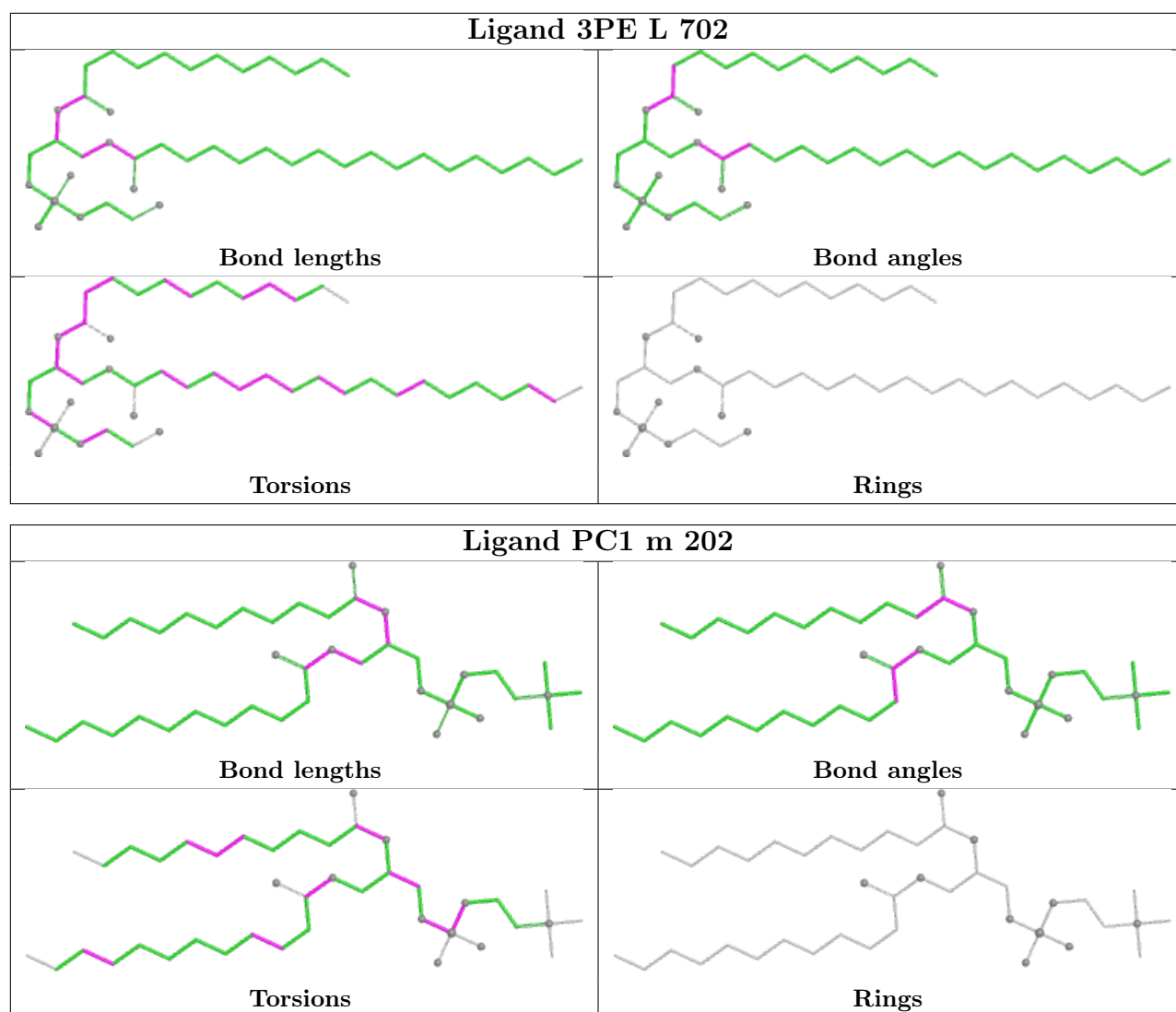
Ligand 3PE Y 202

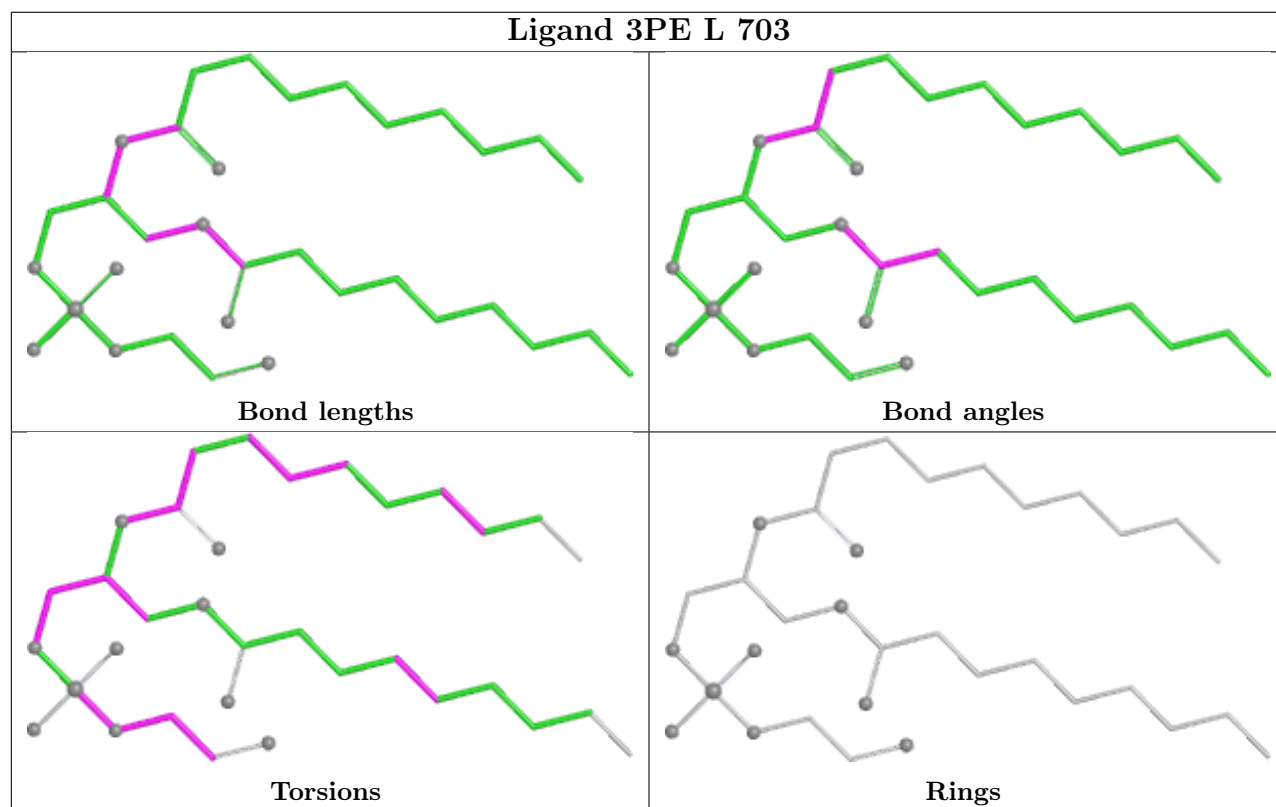
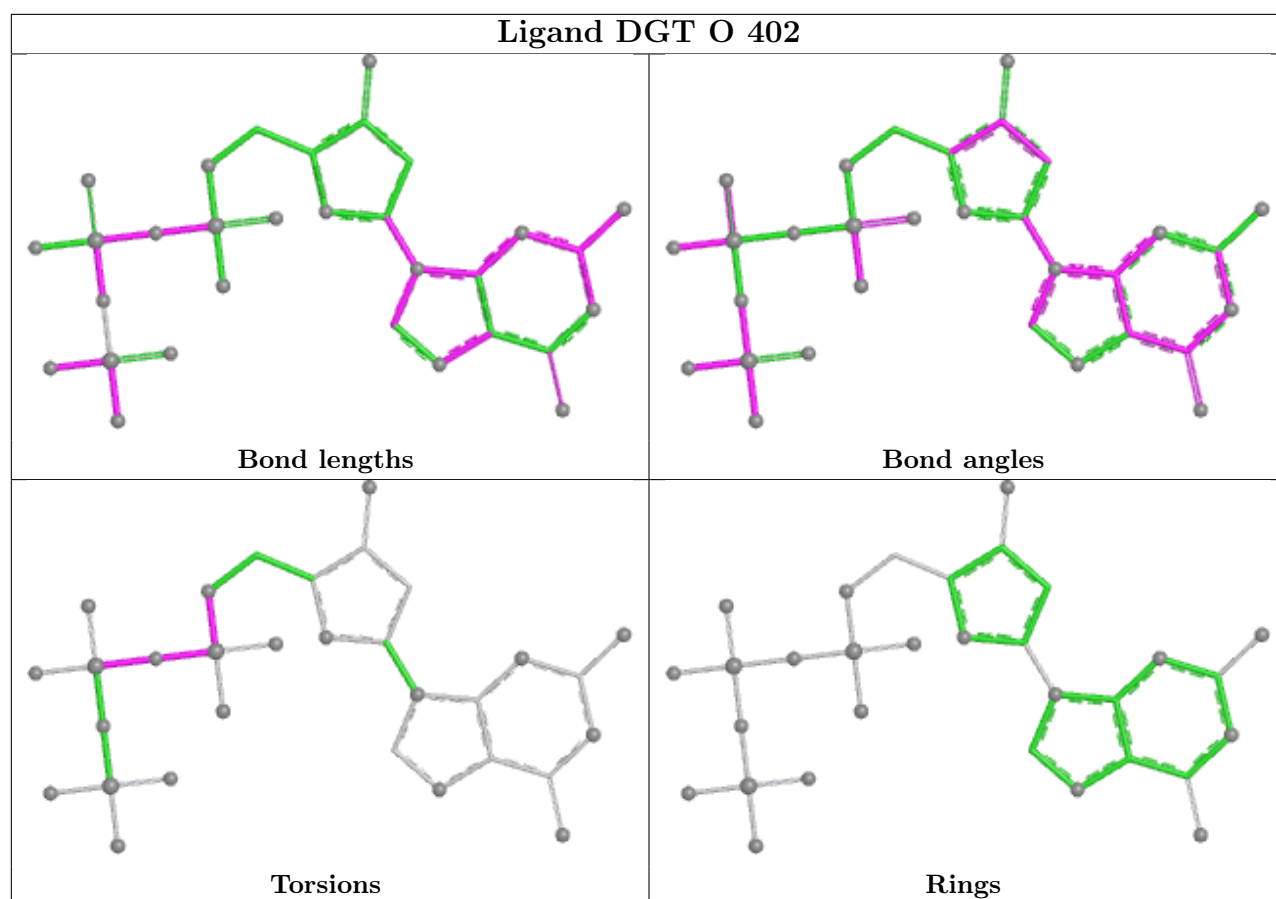


Ligand PC1 J 203

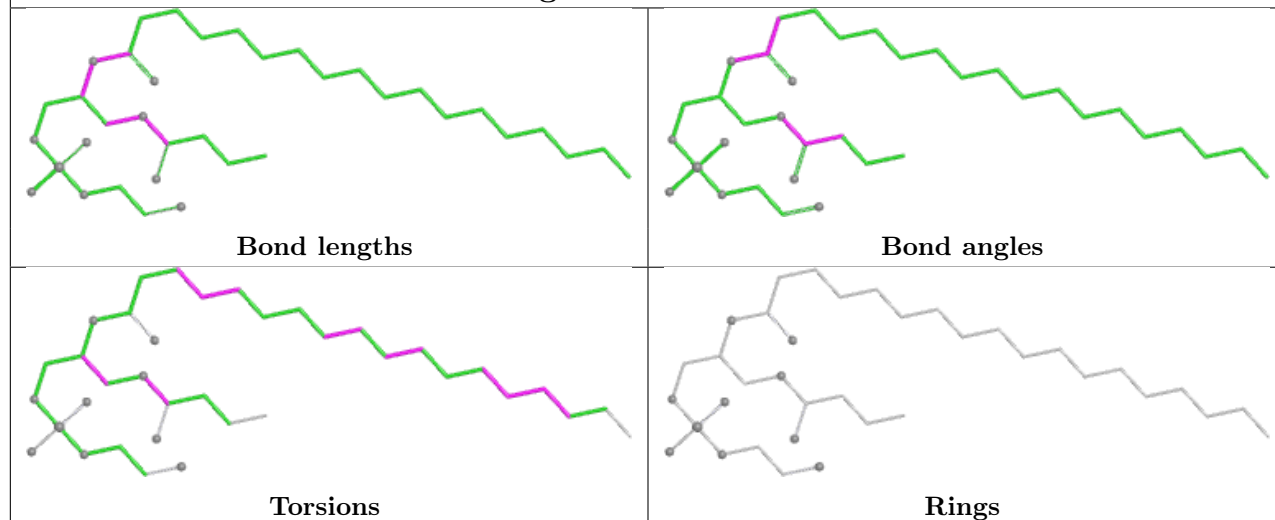




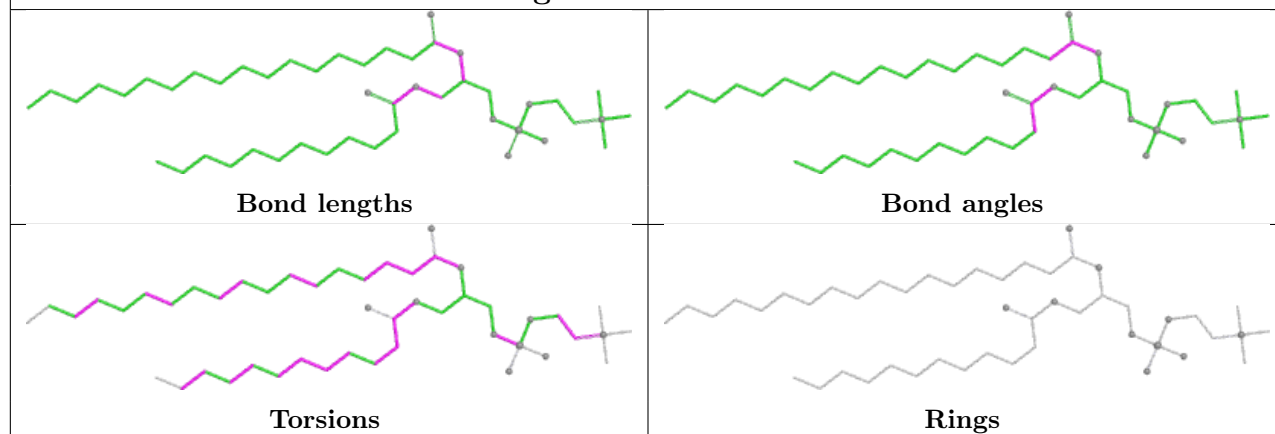




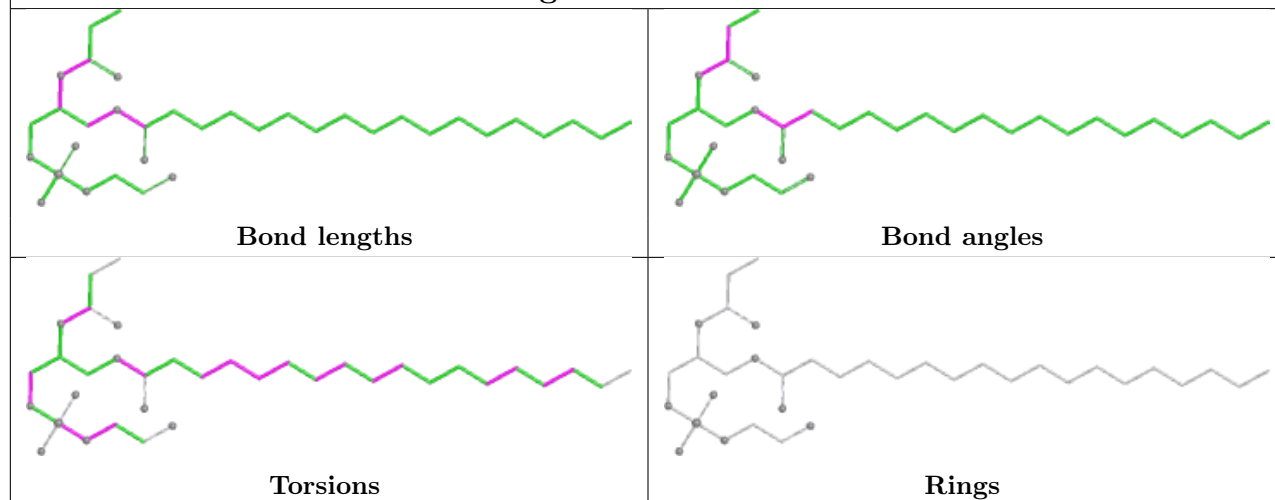
Ligand 3PE J 201

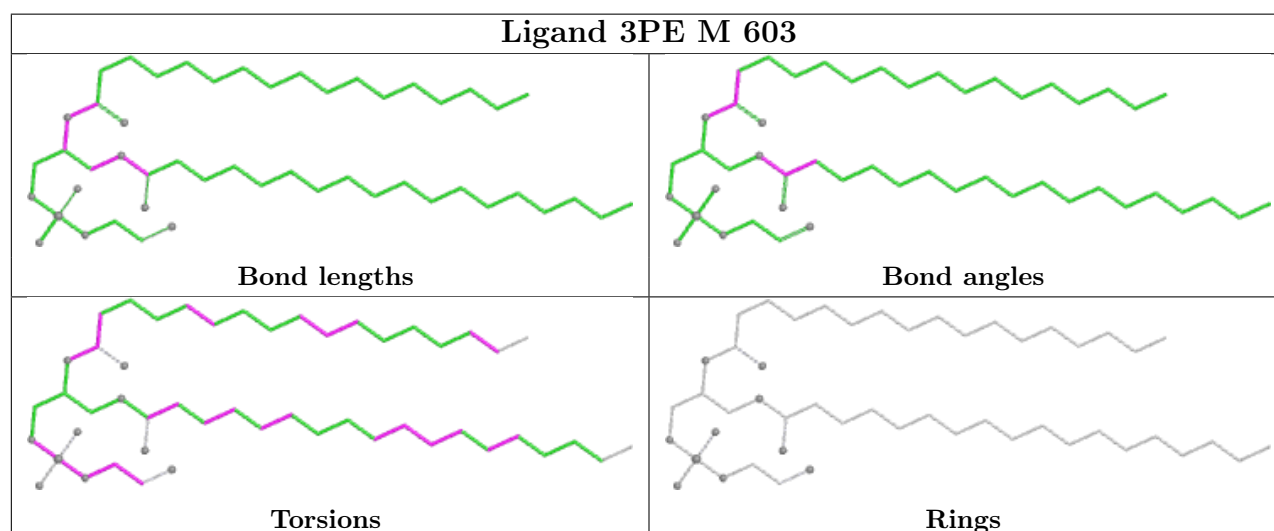
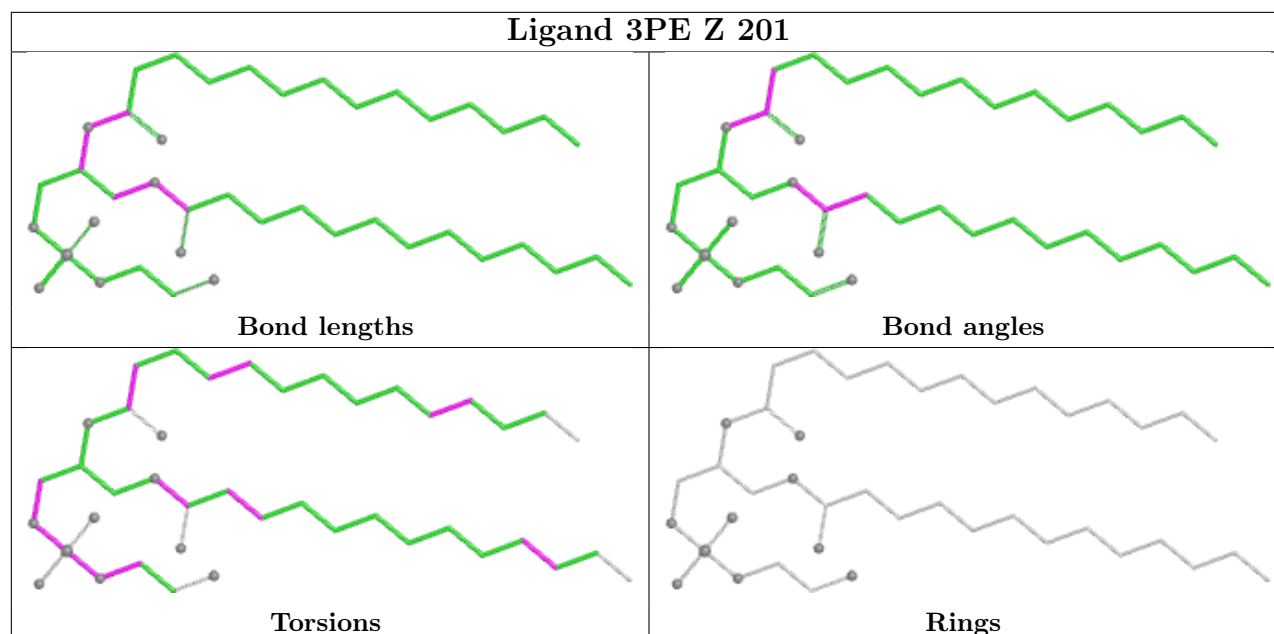
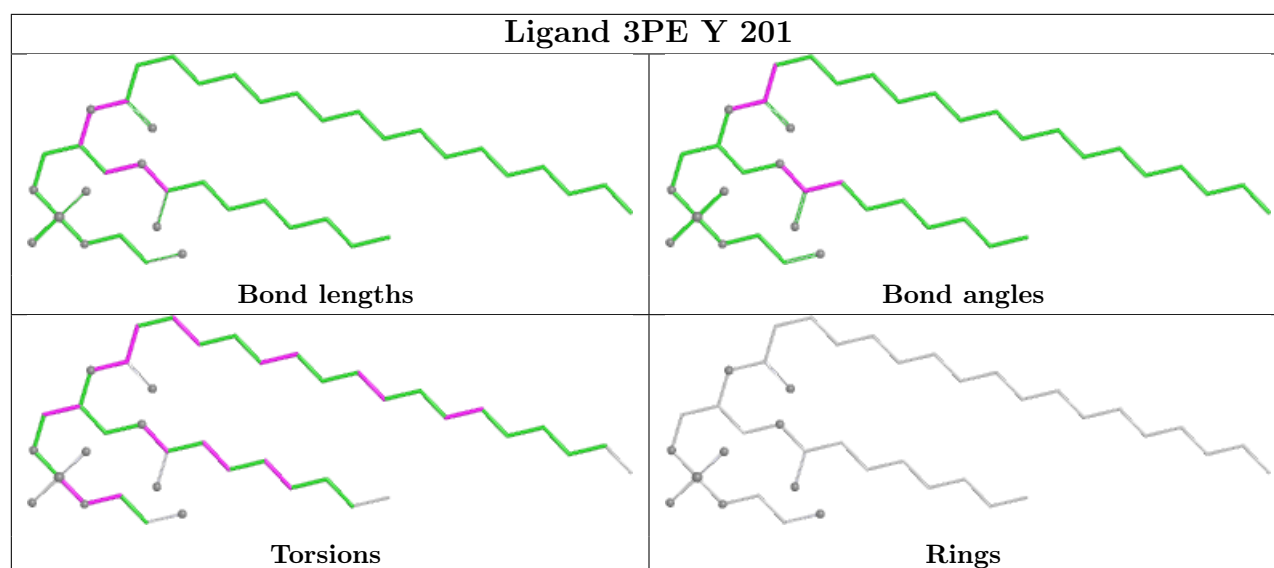


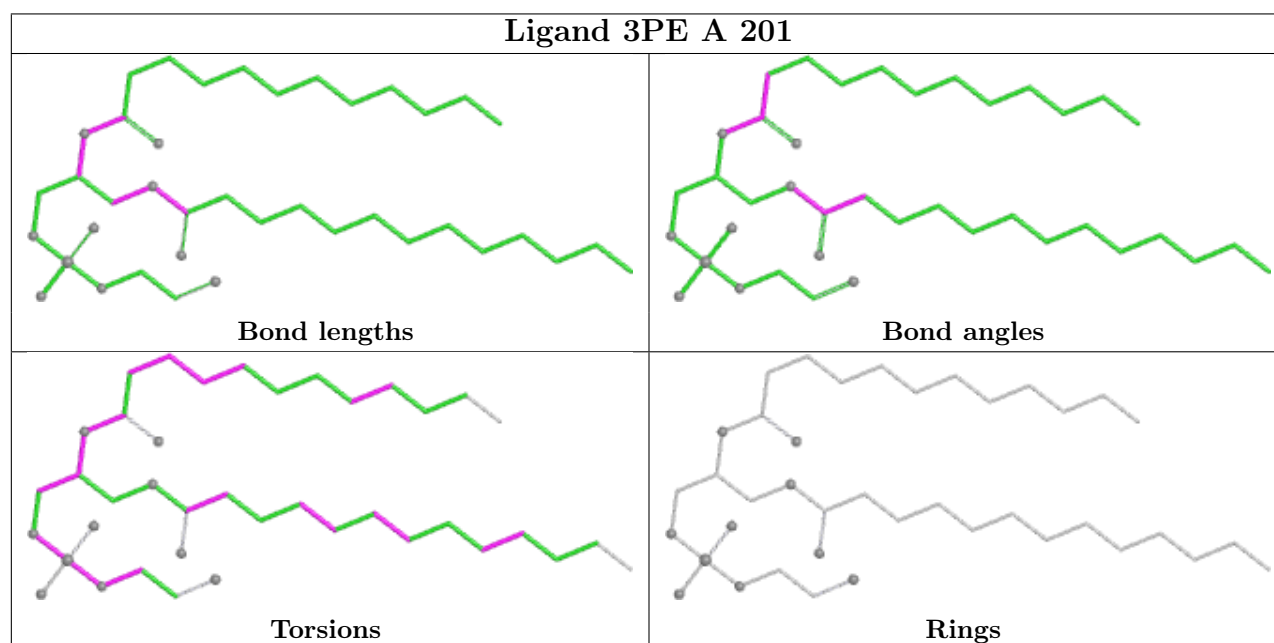
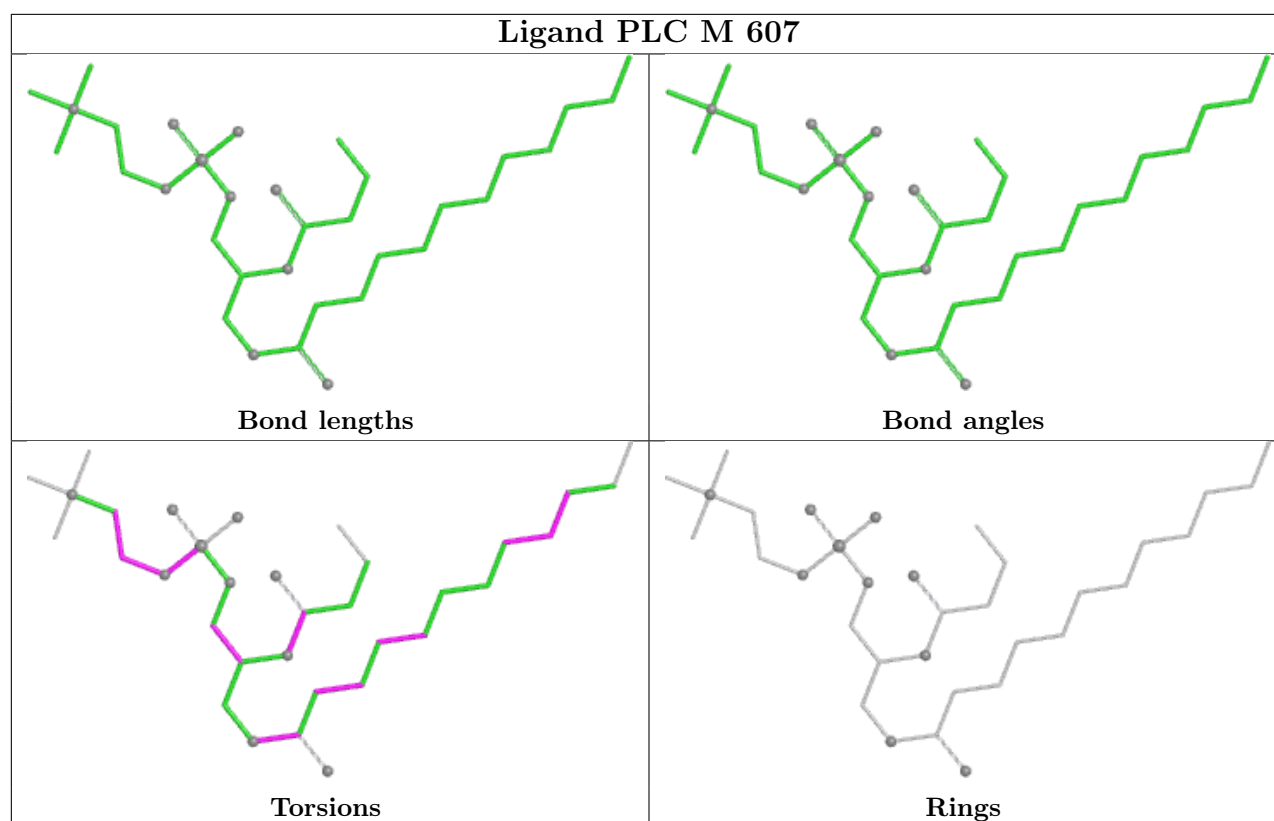
Ligand PC1 H 403

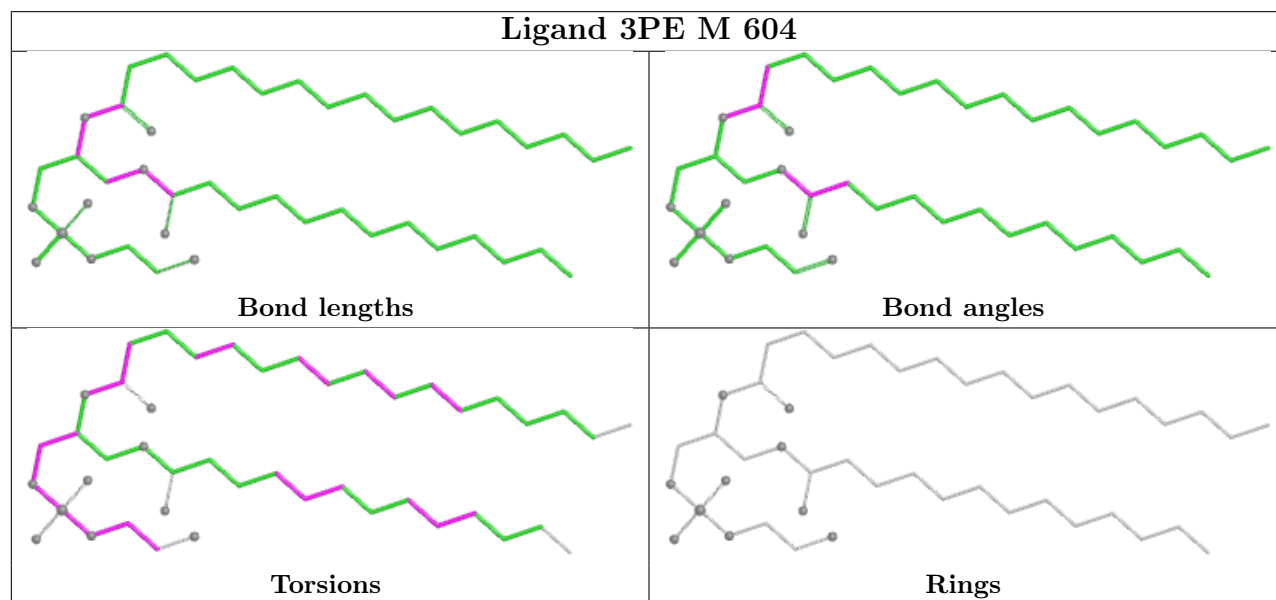
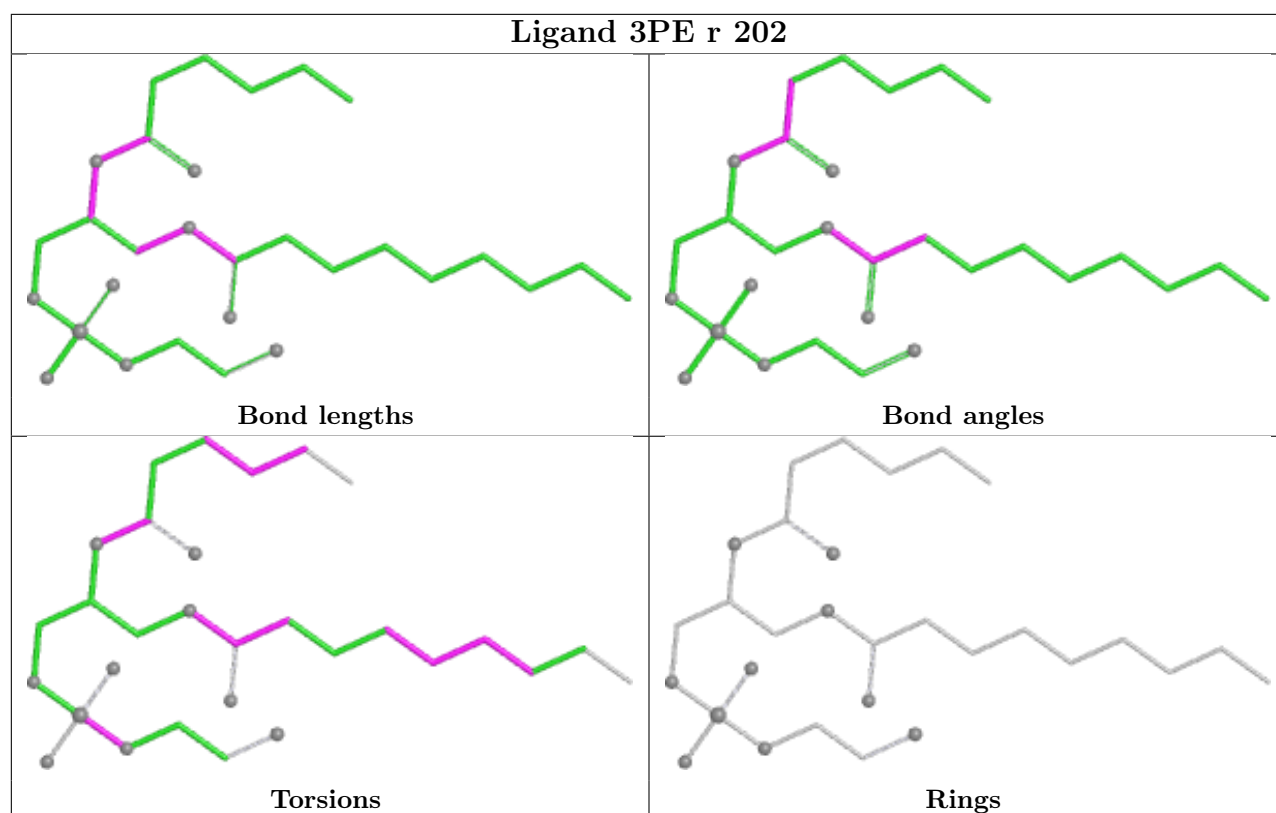


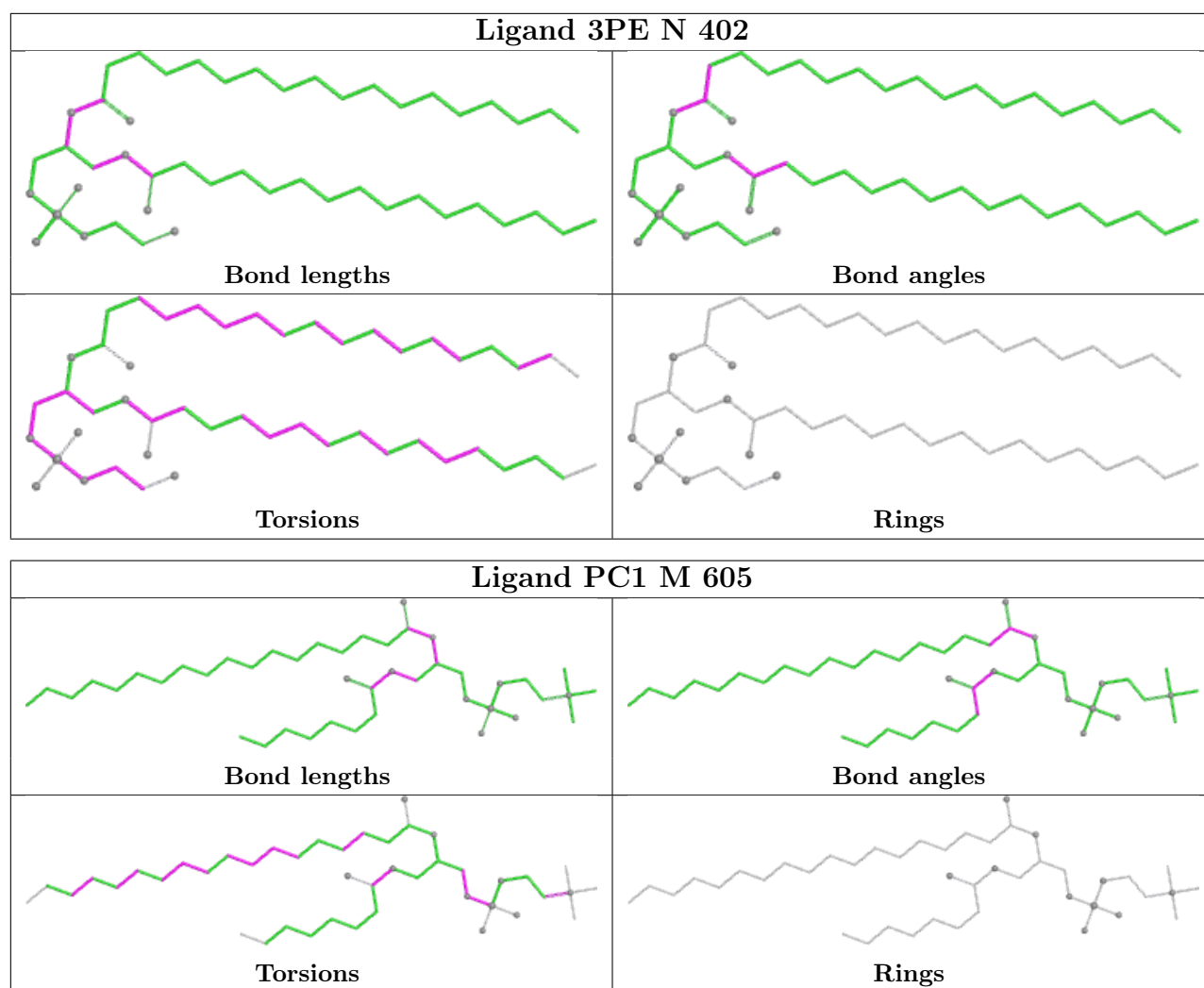
Ligand 3PE a 101

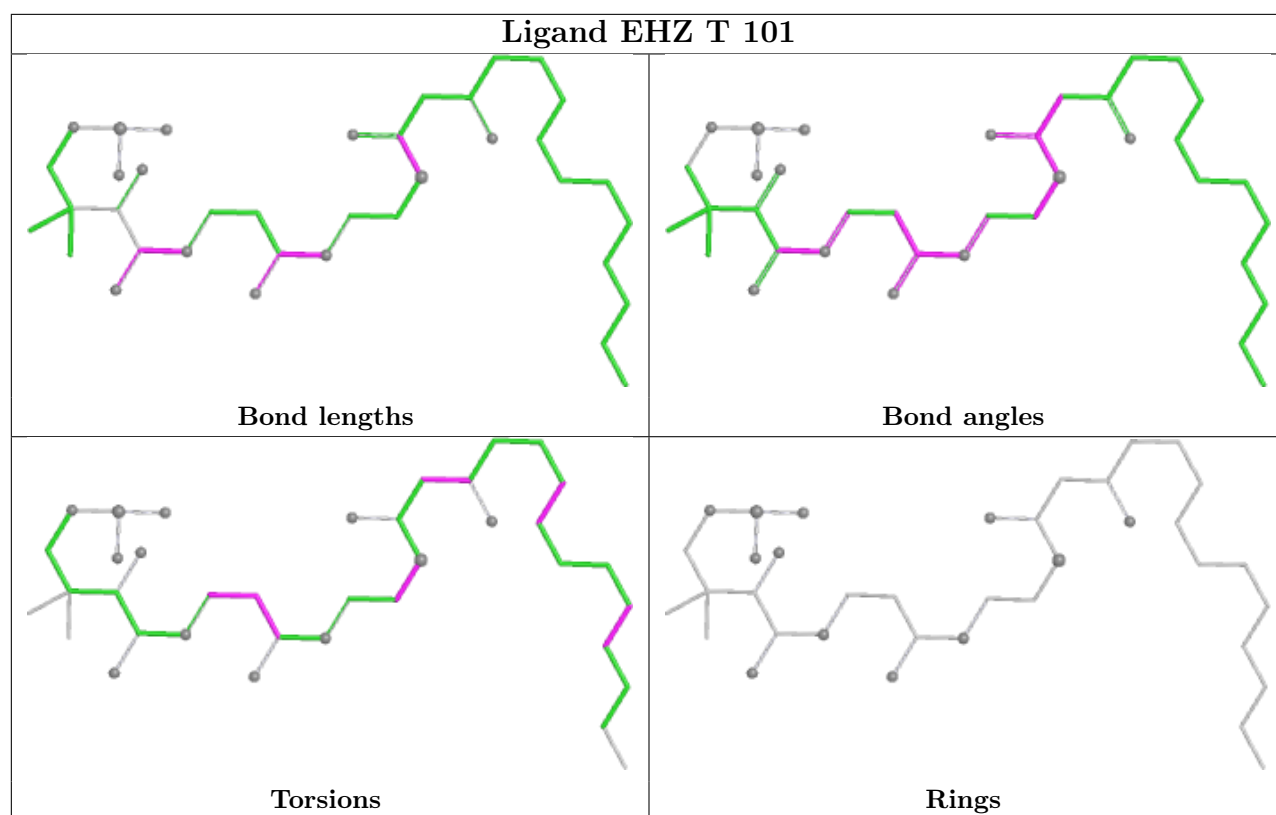












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

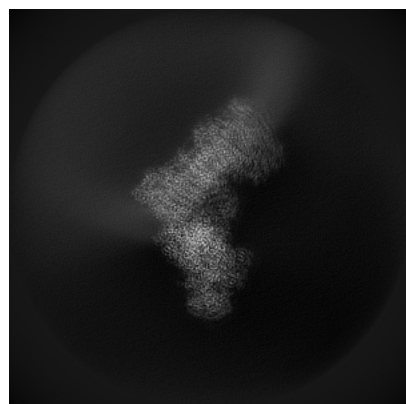
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18069. These allow visual inspection of the internal detail of the map and identification of artifacts.

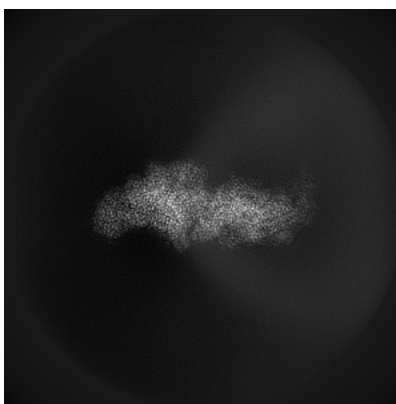
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

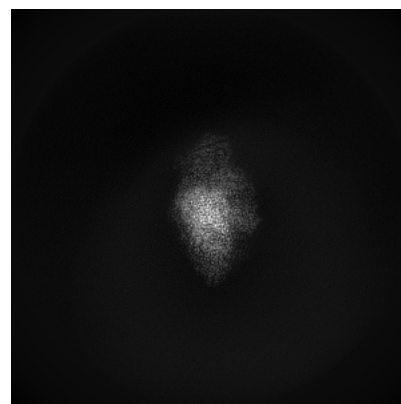
6.1.1 Primary map



X

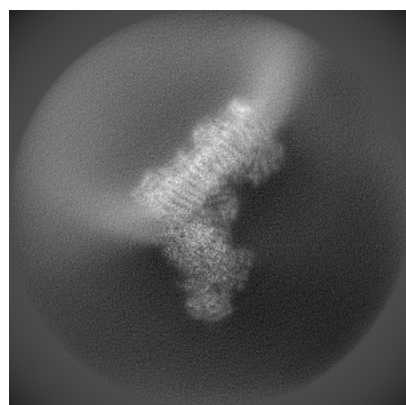


Y

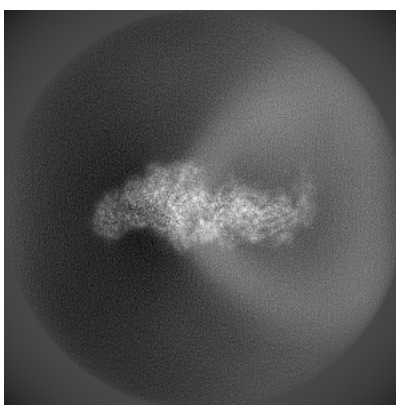


Z

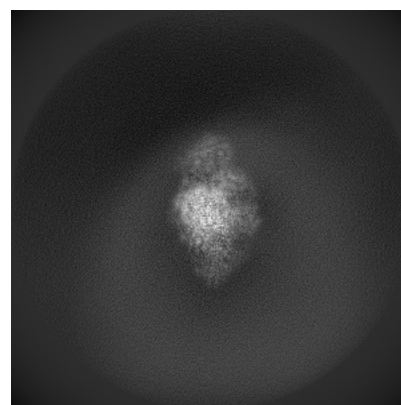
6.1.2 Raw map



X



Y



Z

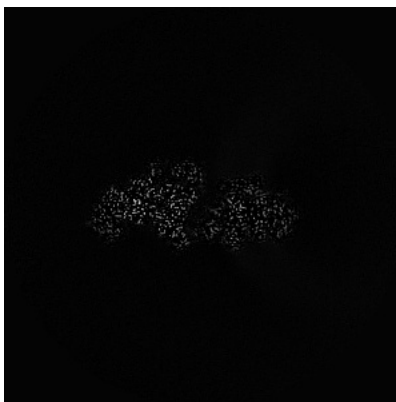
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

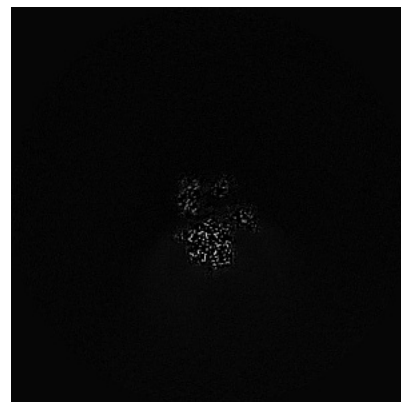
6.2.1 Primary map



X Index: 240

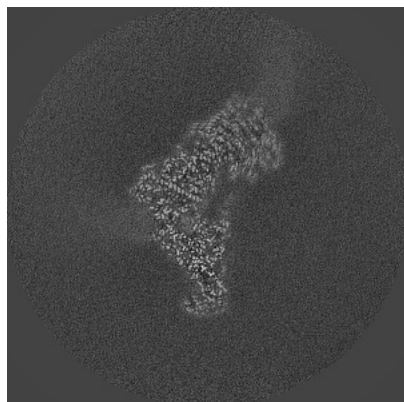


Y Index: 240

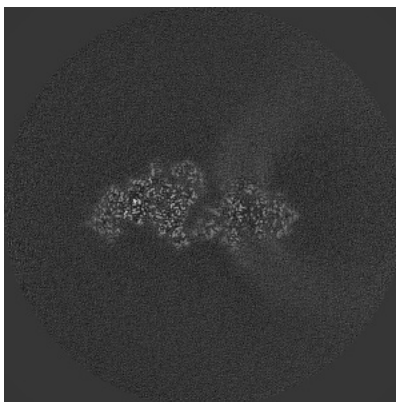


Z Index: 240

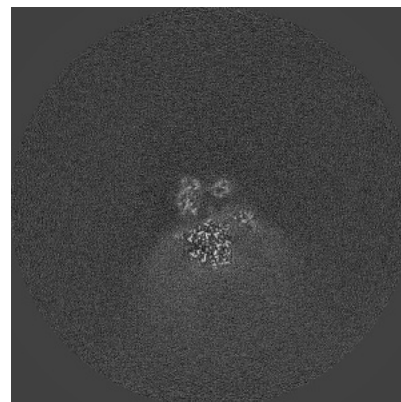
6.2.2 Raw map



X Index: 240



Y Index: 240

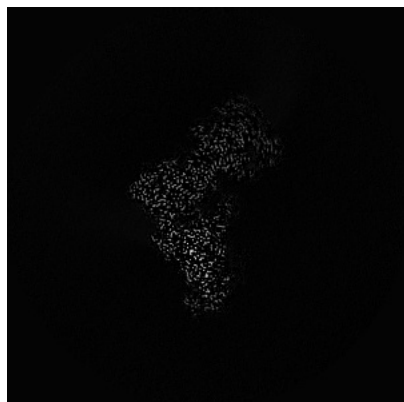


Z Index: 240

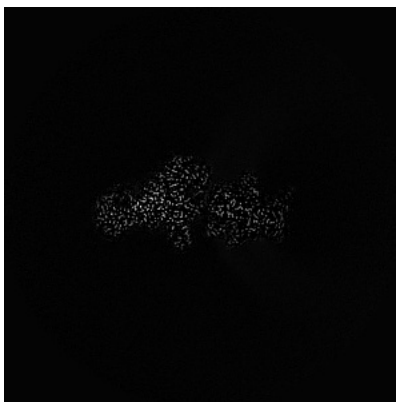
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 247

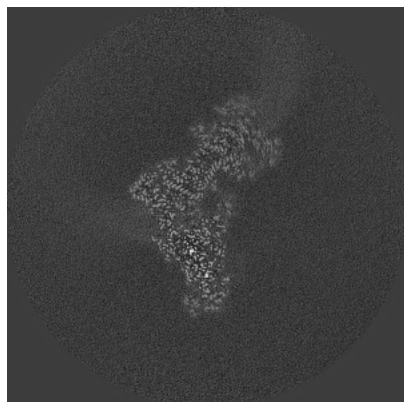


Y Index: 227

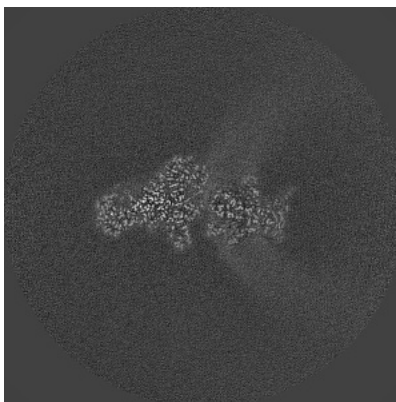


Z Index: 198

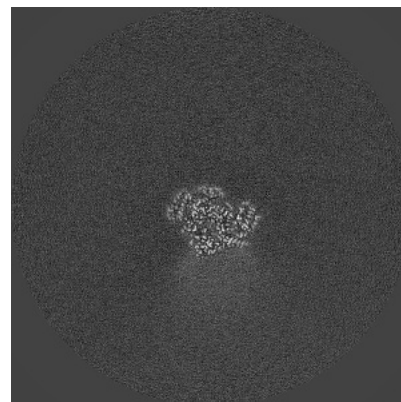
6.3.2 Raw map



X Index: 247



Y Index: 227

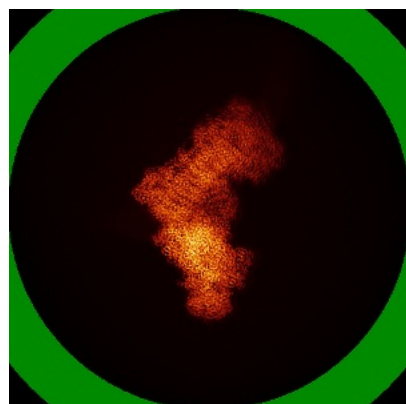


Z Index: 212

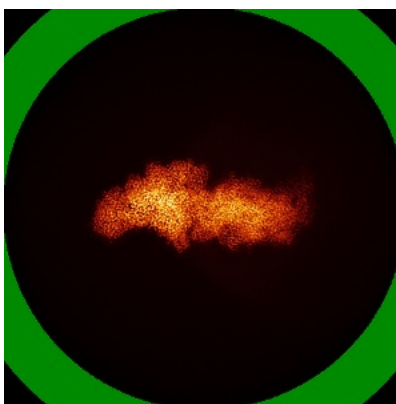
The images above show the largest variance slices of the map in three orthogonal directions.

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

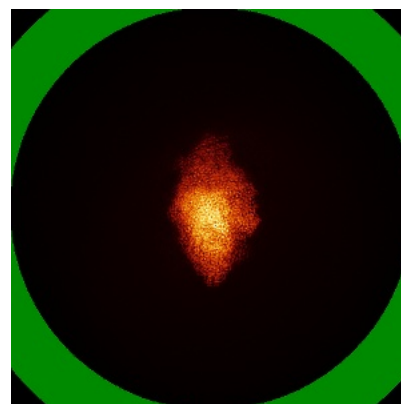
6.4.1 Primary map



X

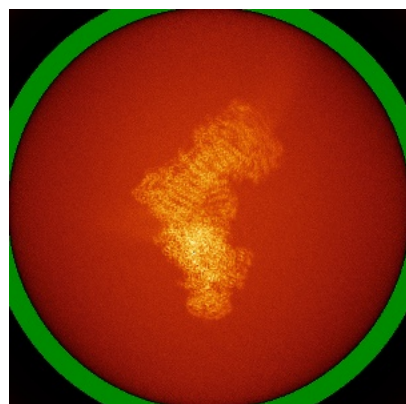


Y

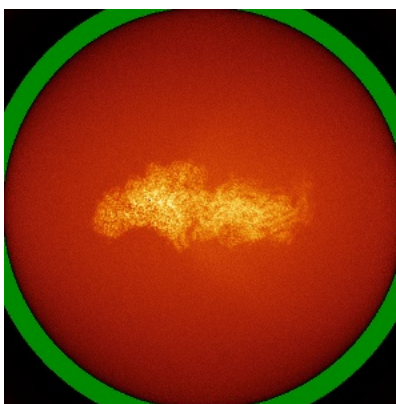


Z

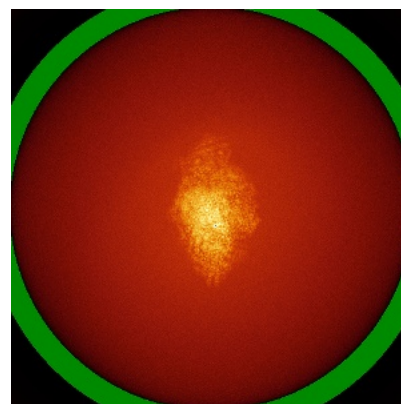
6.4.2 Raw map



X



Y

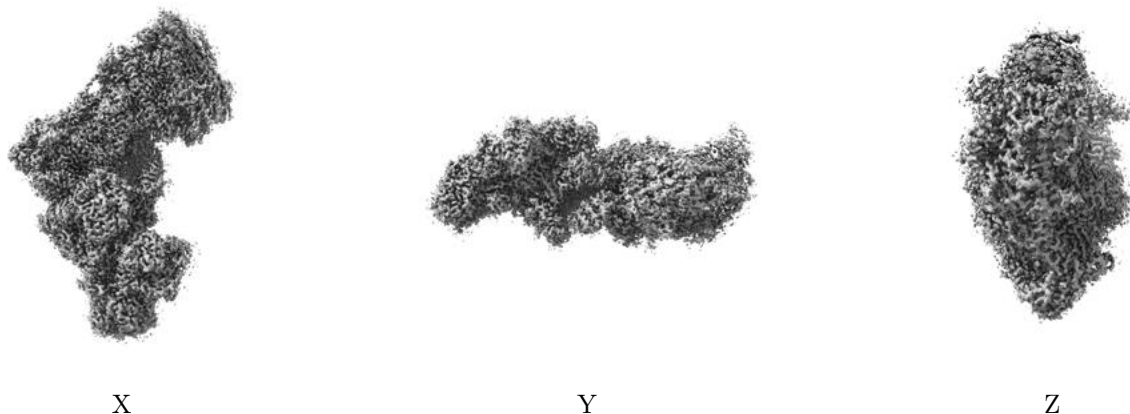


Z

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.

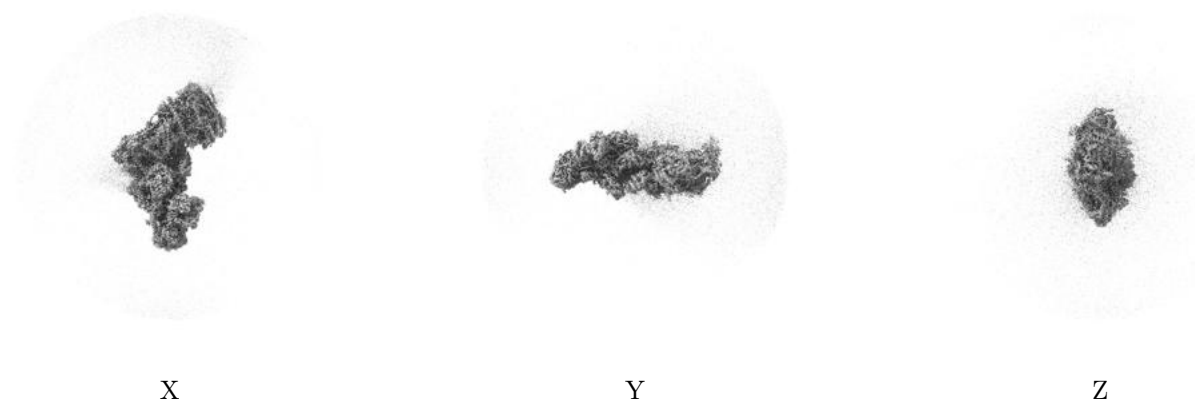
6.5 Orthogonal surface views [i](#)

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.

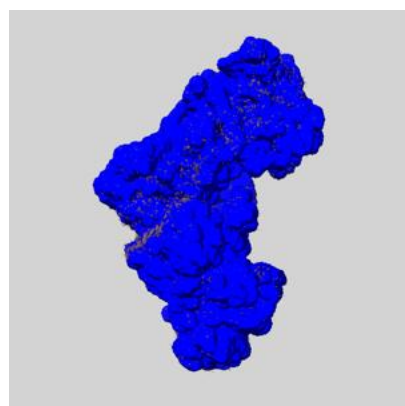
6.6 Mask visualisation [i](#)

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

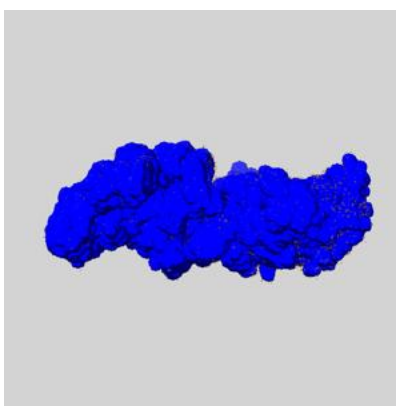
A mask typically either:

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

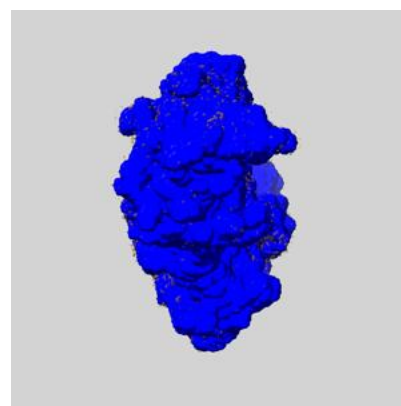
6.6.1 emd_18069_msk_1.map [i](#)



X



Y

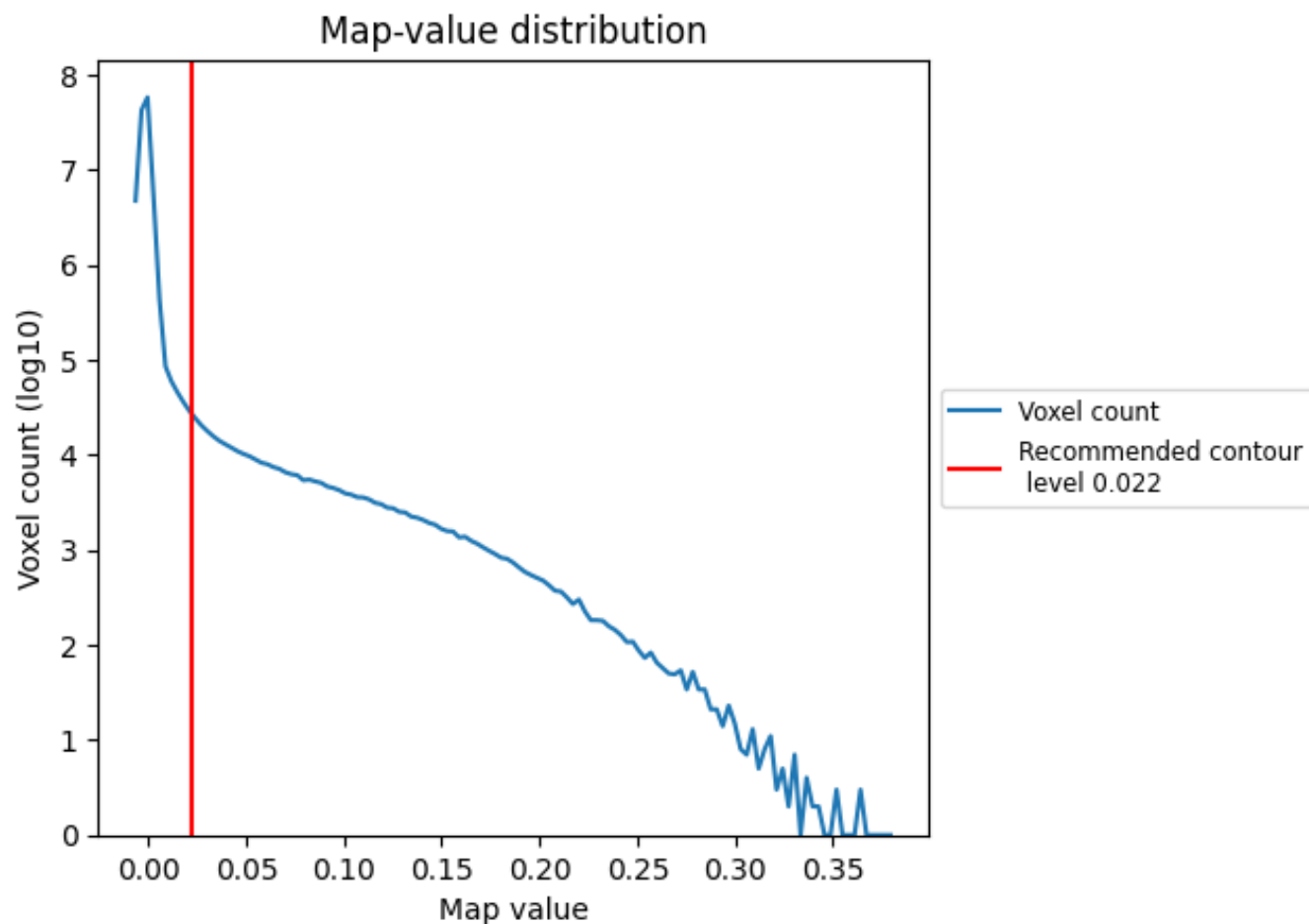


Z

7 Map analysis [i](#)

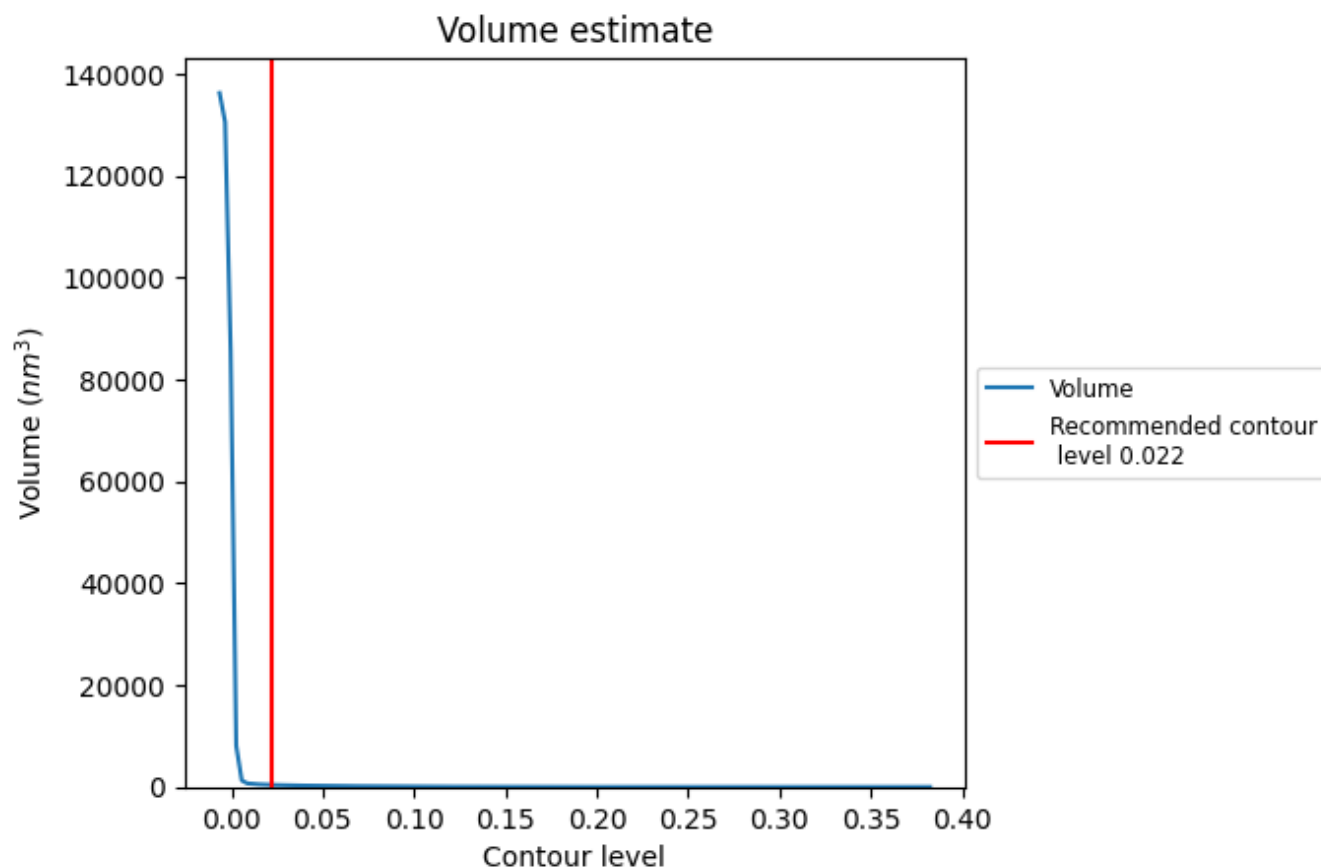
This section contains the results of statistical analysis of the map.

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.

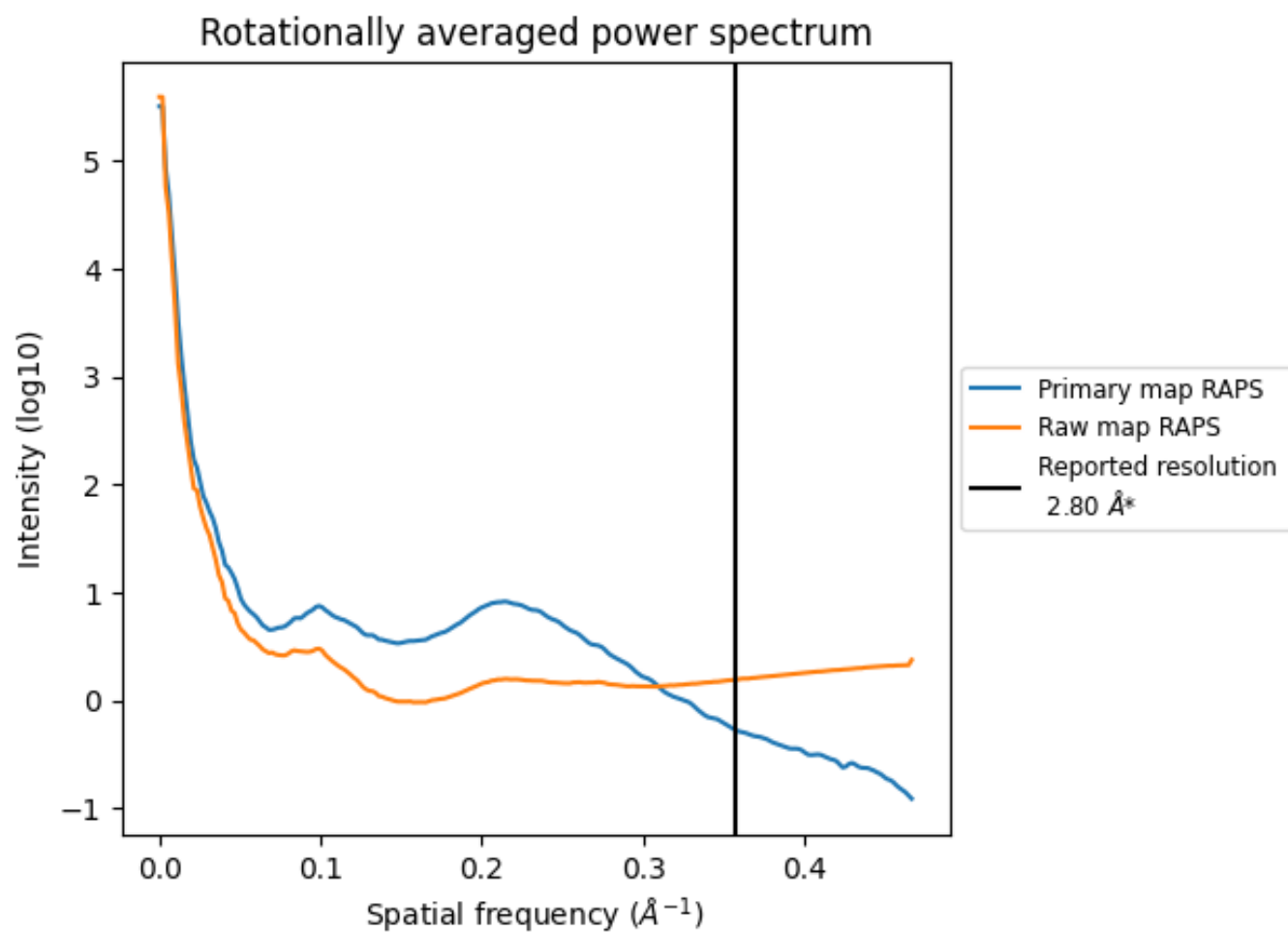
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm^3 ; this corresponds to an approximate mass of 365 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 ⓘ

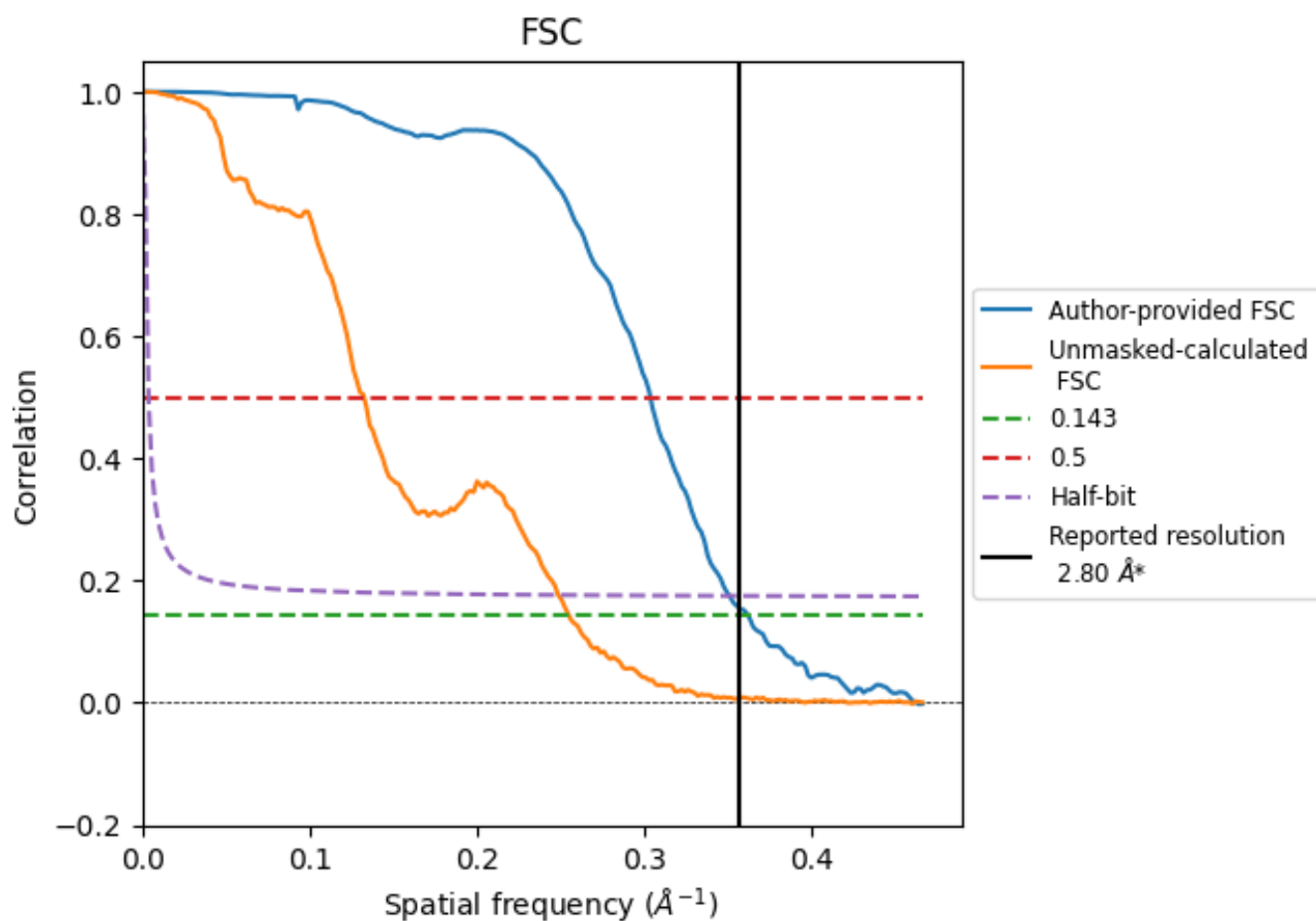


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

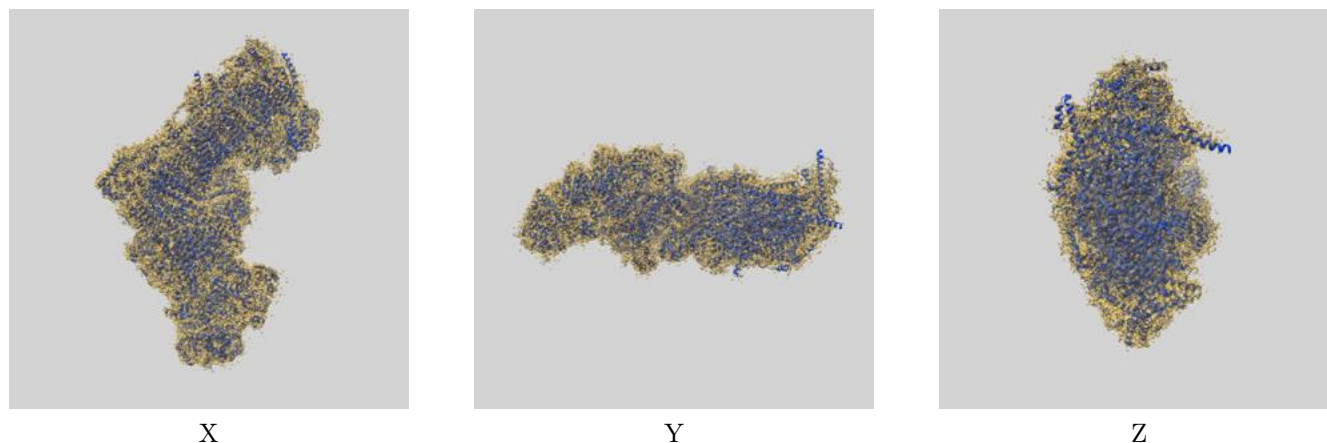
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.29	2.85
Unmasked-calculated*	3.92	7.55	4.02

*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 3.92 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

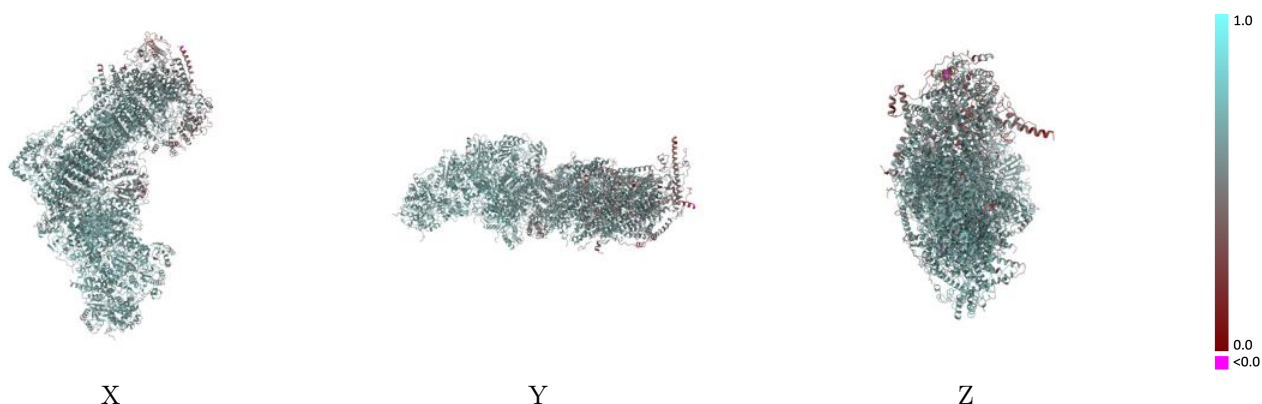
This section contains information regarding the fit between EMDB map EMD-18069 and PDB model 8Q25. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.022 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](#)

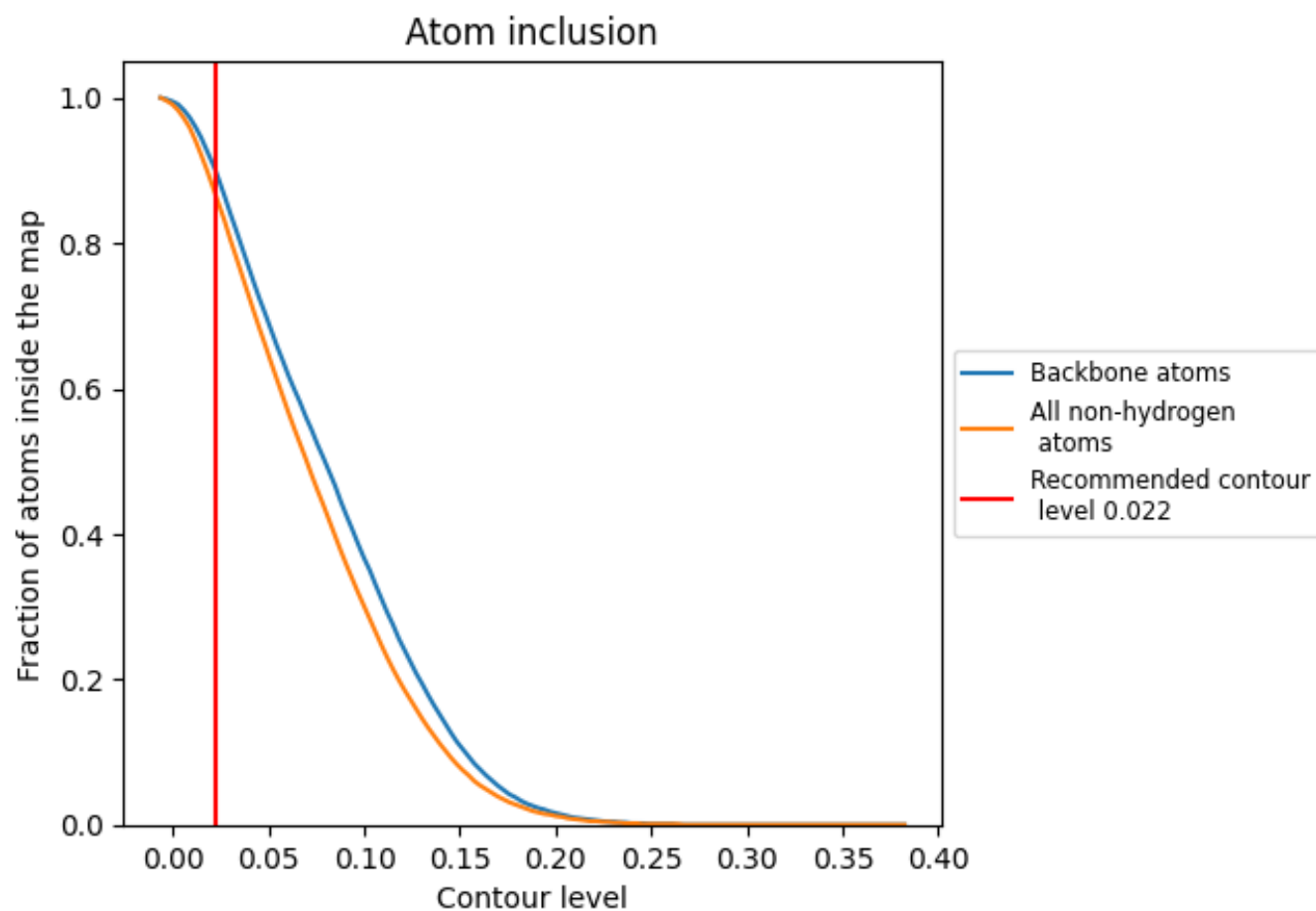


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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	 0.8690	 0.5970
A	 0.8980	 0.6190
B	 0.9580	 0.6580
C	 0.9680	 0.6650
D	 0.9580	 0.6630
E	 0.8860	 0.5980
F	 0.9120	 0.6170
G	 0.9280	 0.6370
H	 0.9400	 0.6390
I	 0.9590	 0.6690
J	 0.8900	 0.6010
K	 0.9590	 0.6480
L	 0.8370	 0.5630
M	 0.9350	 0.6330
N	 0.9570	 0.6540
O	 0.8160	 0.5560
P	 0.9020	 0.6180
Q	 0.9270	 0.6500
R	 0.9110	 0.6340
S	 0.7930	 0.5560
T	 0.6820	 0.4770
U	 0.6190	 0.4390
V	 0.8890	 0.6050
W	 0.9140	 0.6360
X	 0.9020	 0.6190
Y	 0.8460	 0.5860
Z	 0.8900	 0.6140
a	 0.9330	 0.6310
b	 0.8680	 0.5980
c	 0.8350	 0.5750
d	 0.9000	 0.6120
e	 0.8730	 0.6090
f	 0.7060	 0.5350
g	 0.8010	 0.5550
h	 0.8840	 0.6010



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Chain	Atom inclusion	Q-score
i	 0.5930	 0.4400
j	 0.5620	 0.4110
k	 0.4960	 0.3830
l	 0.7760	 0.5140
m	 0.7880	 0.5470
n	 0.7330	 0.4970
o	 0.5330	 0.3980
p	 0.7700	 0.5260
q	 0.8980	 0.6300
r	 0.9160	 0.6420
s	 0.8090	 0.5600