



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 10:12 PM UTC

PDB ID : 8Q0A / pdb_00008q0a
EMDB ID : EMD-18051
Title : Inward-facing, closed proteoliposome complex I at 3.1 Å. Initially purified in DDM.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-07-28
Resolution : 3.10 Å(reported)
Based on initial model : 7QSK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

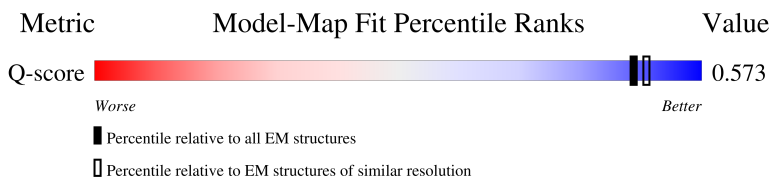
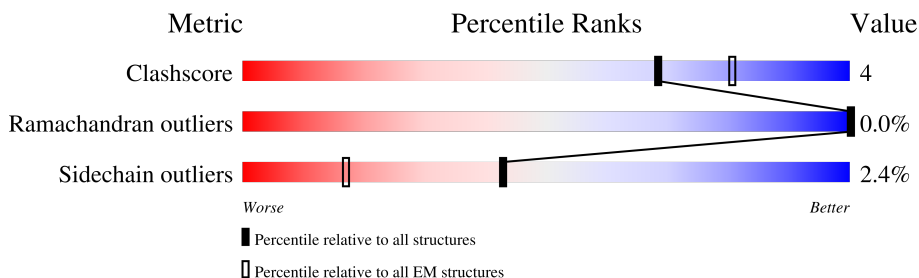
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



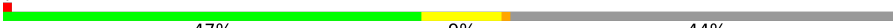
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	115	 88% 10% .
2	B	216	 66% 6% 28%
3	C	266	 73% 6% 21%
4	D	463	 86% 7% 7%

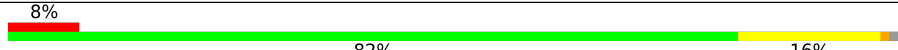
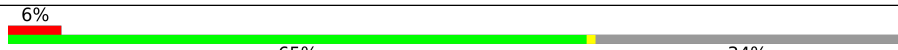
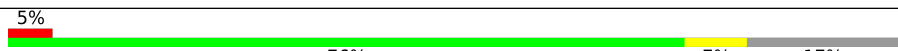
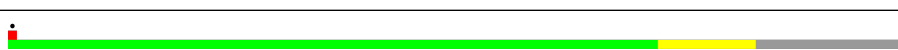
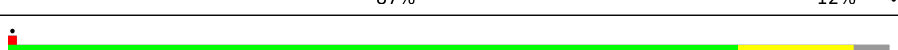
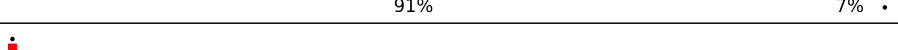
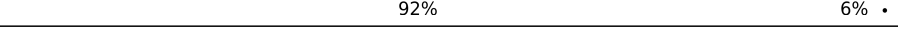
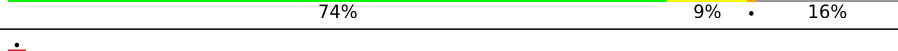
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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26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

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

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 69719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	155	Total	C	N	O	S	0	0
			1241	792	224	211	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1738	1120	298	317	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	430	Total	C	N	O	S	0	0
			3459	2209	596	629	25		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5279	3307	920	1013	39		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	342	Total	C	N	O	S	0	0
			2754	1781	487	481	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	115	Total	C	N	O	S	0	0
			928	600	157	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			976	625	181	166	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	141	Total	C	N	O	S	0	0
			1152	740	201	202	9		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

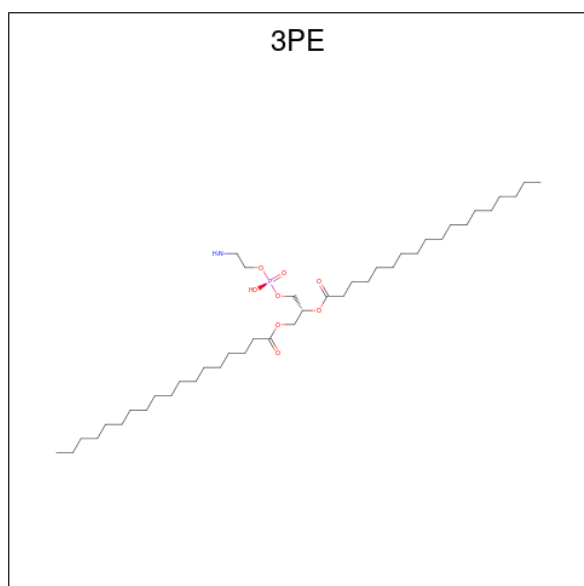
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	45	Total	C	N	O	S	0	0
			380	238	67	74	1		

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



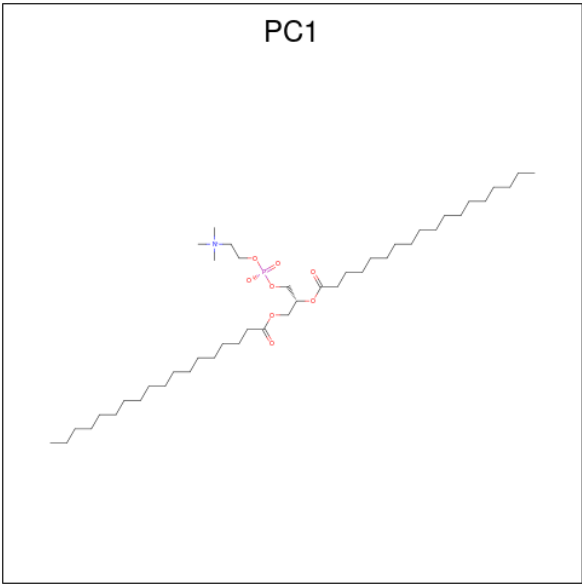
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	J	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	L	1	Total	C	N	O	P	0
			45	35	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
45	L	1	Total 40	C 30	N 1	O 8	P 1	0
45	L	1	Total 23	C 13	N 1	O 8	P 1	0
45	L	1	Total 51	C 41	N 1	O 8	P 1	0
45	L	1	Total 51	C 41	N 1	O 8	P 1	0
45	L	1	Total 39	C 29	N 1	O 8	P 1	0
45	M	1	Total 40	C 30	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 35	C 25	N 1	O 8	P 1	0
45	P	1	Total 32	C 22	N 1	O 8	P 1	0
45	Y	1	Total 51	C 41	N 1	O 8	P 1	0
45	Y	1	Total 47	C 37	N 1	O 8	P 1	0
45	Z	1	Total 42	C 32	N 1	O 8	P 1	0
45	b	1	Total 41	C 31	N 1	O 8	P 1	0
45	b	1	Total 47	C 37	N 1	O 8	P 1	0
45	b	1	Total 51	C 41	N 1	O 8	P 1	0
45	e	1	Total 49	C 39	N 1	O 8	P 1	0
45	m	1	Total 50	C 40	N 1	O 8	P 1	0
45	m	1	Total 41	C 31	N 1	O 8	P 1	0
45	m	1	Total 42	C 32	N 1	O 8	P 1	0
45	q	1	Total 21	C 11	N 1	O 8	P 1	0

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



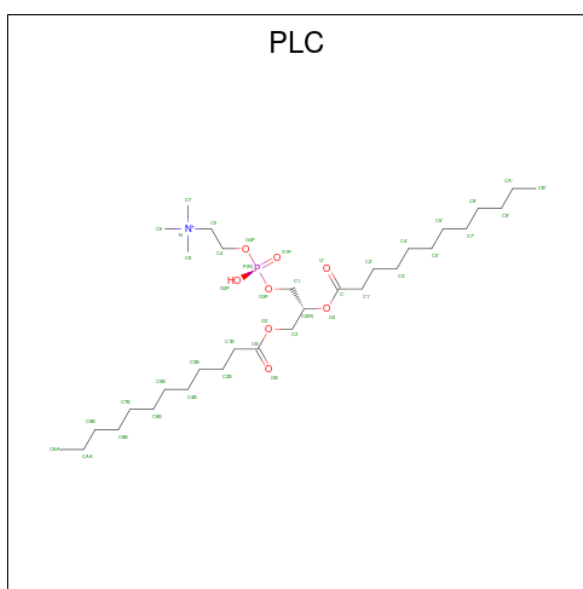
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	H	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
46	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	Y	1	Total	C	N	O	P	0
			45	35	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
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
			47	37	1	8	1	
46	q	1	Total	C	N	O	P	0
			38	28	1	8	1	

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



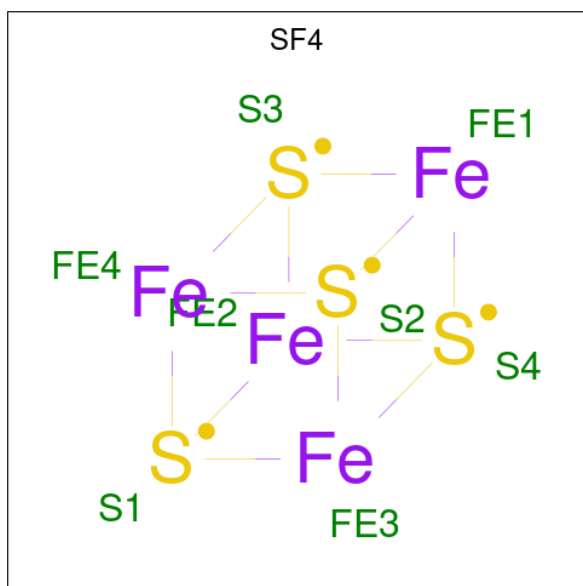
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
47	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
47	J	1	Total	C	N	O	P	0
			38	28	1	8	1	
47	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
47	O	1	Total	C	N	O	P	0
			32	22	1	8	1	
47	P	1	Total	C	N	O	P	0
			27	17	1	8	1	
47	d	1	Total	C	N	O	P	0
			36	26	1	8	1	

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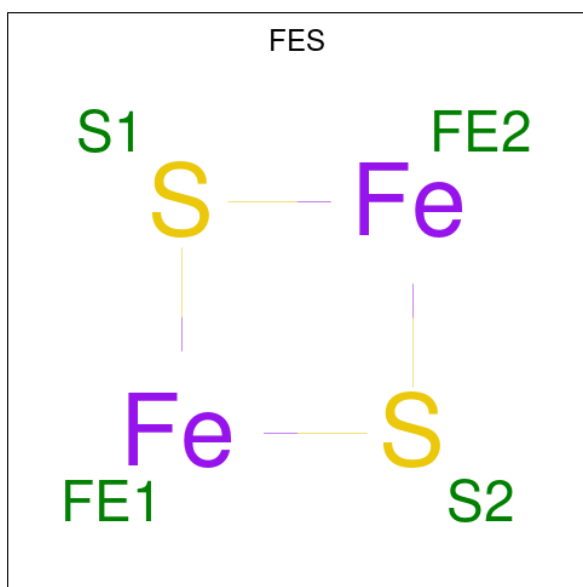
Mol	Chain	Residues	Atoms					AltConf
47	g	1	Total	C	N	O	P	0
			32	22	1	8	1	

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



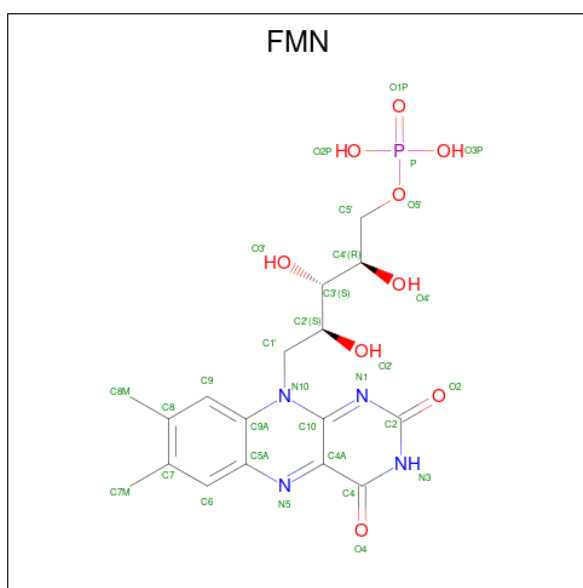
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

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



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

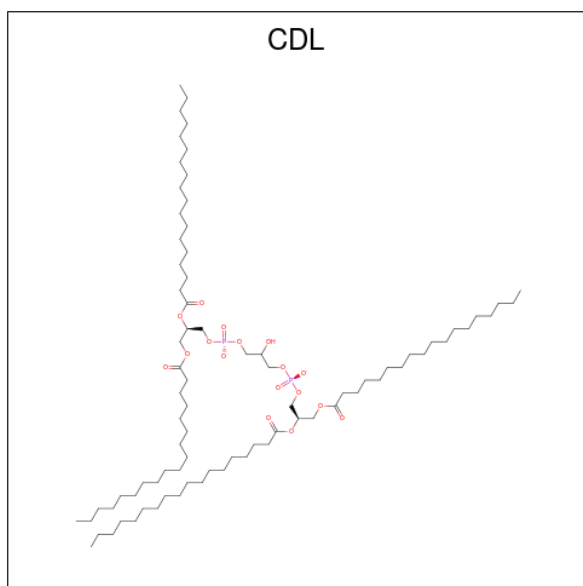


Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

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

- Molecule 52 is 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
			83	64	17	2	
52	J	1	Total	C	O	P	0
			70	51	17	2	
52	L	1	Total	C	O	P	0
			76	57	17	2	
52	M	1	Total	C	O	P	0
			100	81	17	2	
52	N	1	Total	C	O	P	0
			80	61	17	2	
52	X	1	Total	C	O	P	0
			100	81	17	2	
52	d	1	Total	C	O	P	0
			65	46	17	2	
52	i	1	Total	C	O	P	0
			80	61	17	2	
52	r	1	Total	C	O	P	0
			61	42	17	2	

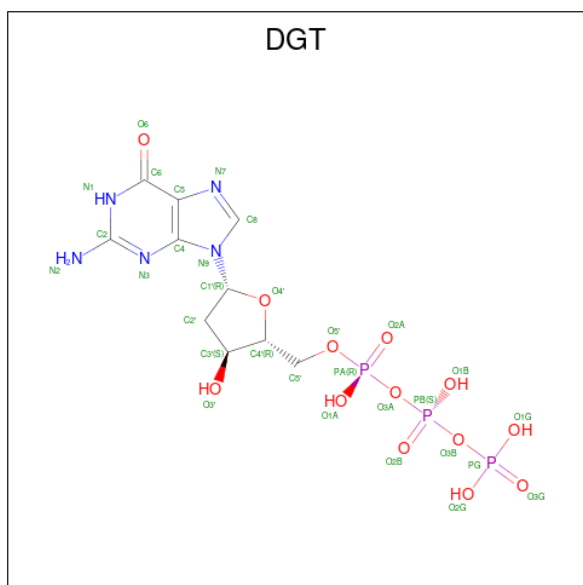
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



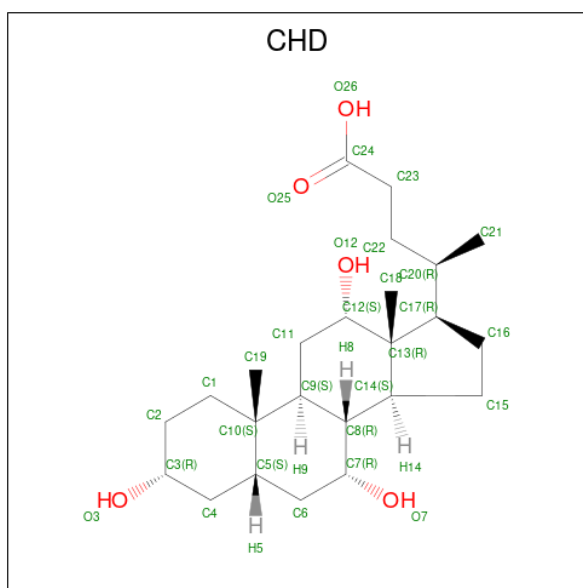
Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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



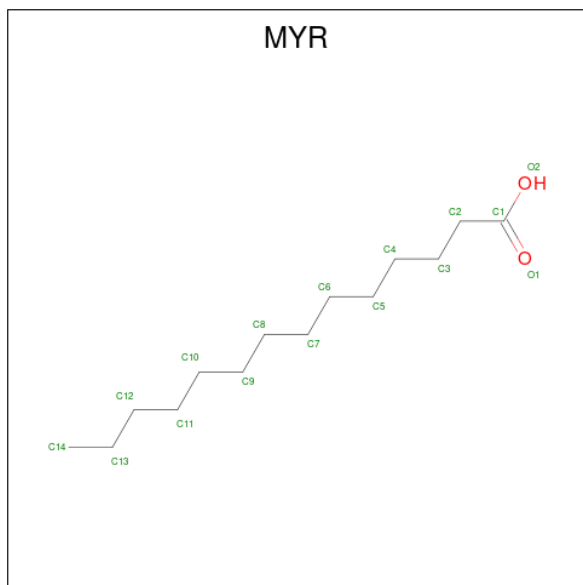
Mol	Chain	Residues	Atoms						AltConf
57	T	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
57	U	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

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



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

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



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

3 Residue-property plots [i](#)

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

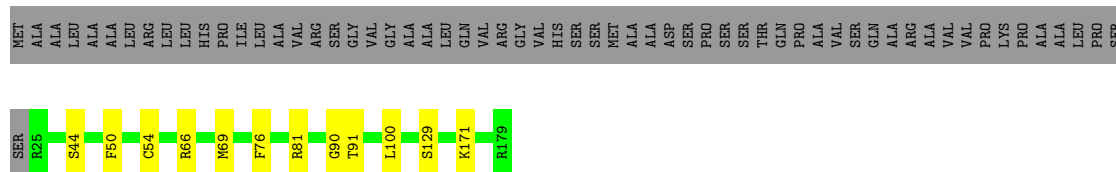
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



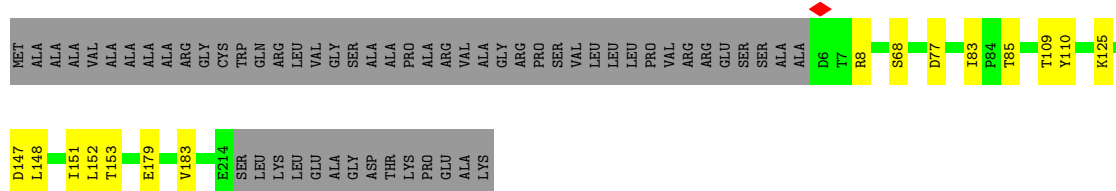
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B: 



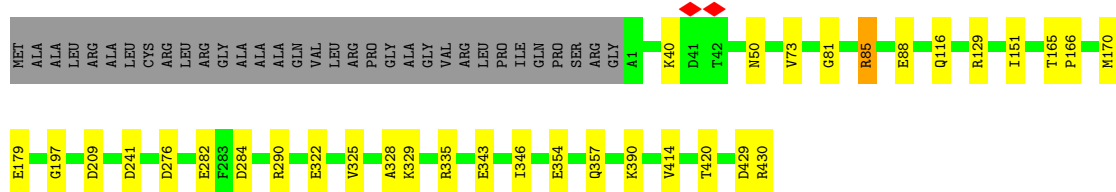
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 



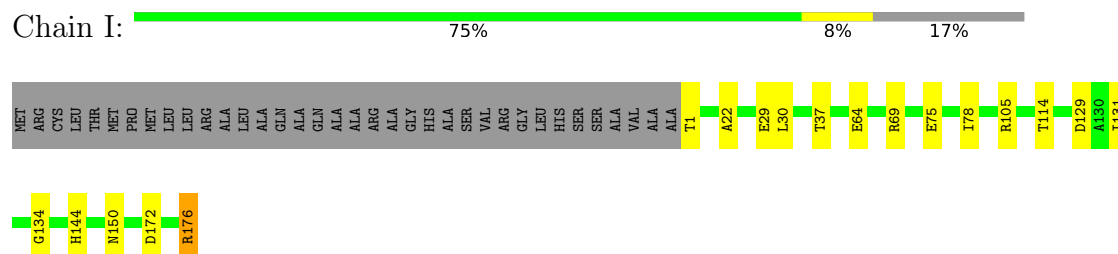
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D: 

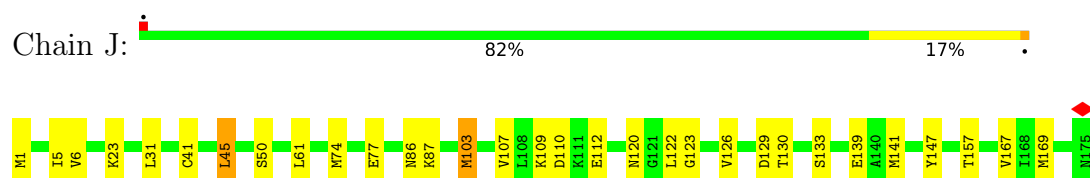


- | | |
|------|------|
| R195 | M1 |
| F198 | F2 |
| L207 | I6 |
| V208 | I11 |
| S209 | P12 |
| E214 | I13 |
| I231 | L14 |
| N235 | A18 |
| I236 | T21 |
| T245 | E24 |
| S246 | L28 |
| P249 | I49 |
| F259 | A50 |
| L271 | D51 |
| A275 | T65 |
| S276 | M70 |
| Y277 | F71 |
| R281 | I76 |
| Q284 | I87 |
| L285 | P88 |
| T318 | Y93 |
| | N99 |
| | V102 |
| | Y114 |
| | M124 |
| | Y127 |
| | Q138 |
| | F160 |
| | E170 |
| | Q171 |
| | M172 |
| | P177 |
| | A178 |
| | W179 |
| | P180 |
| | A191 |

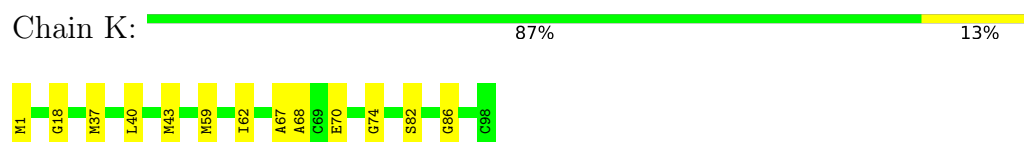
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



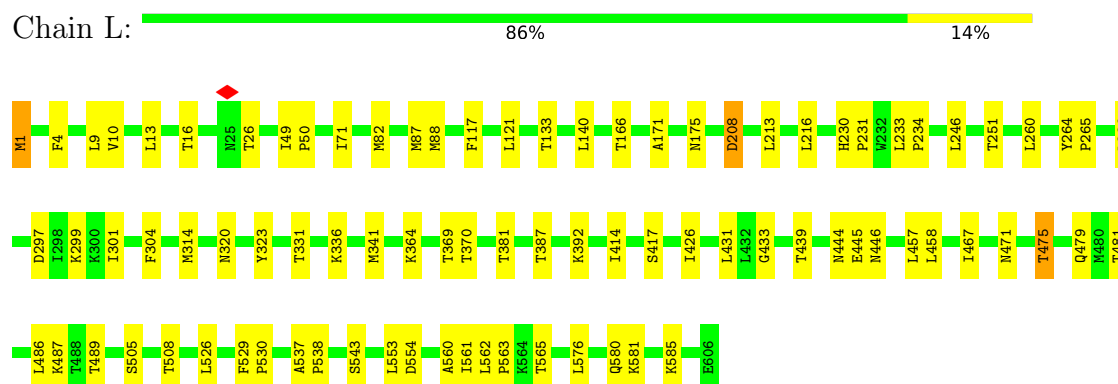
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



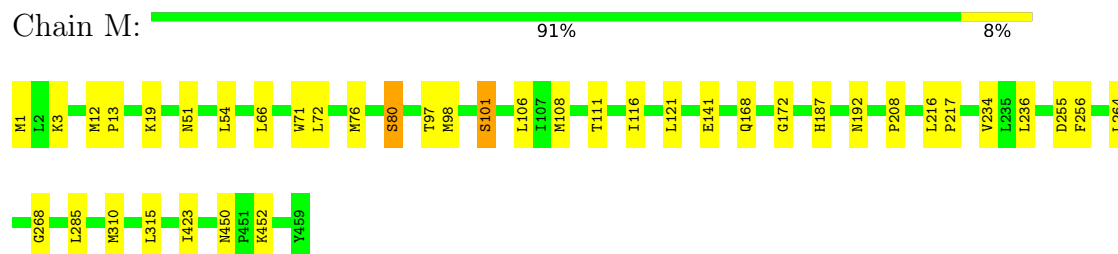
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

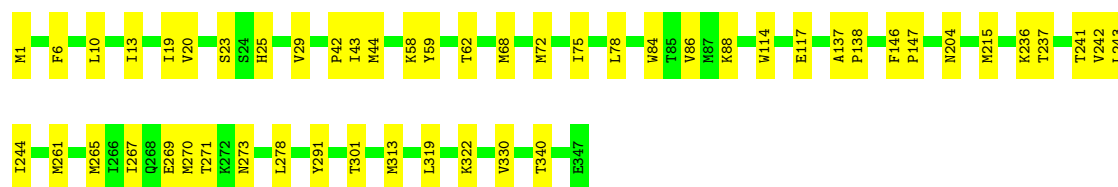


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



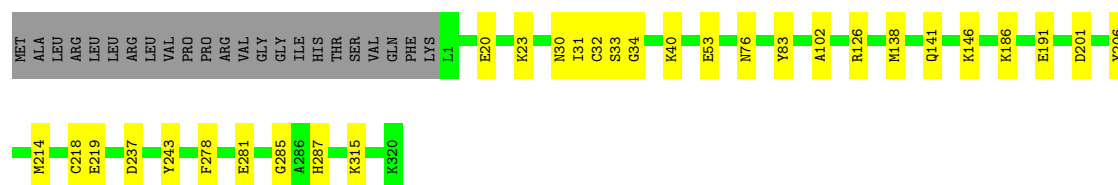
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  85% 15%



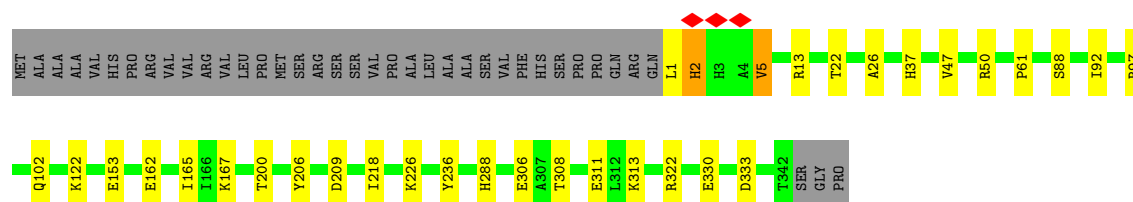
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  85% 9% 7%



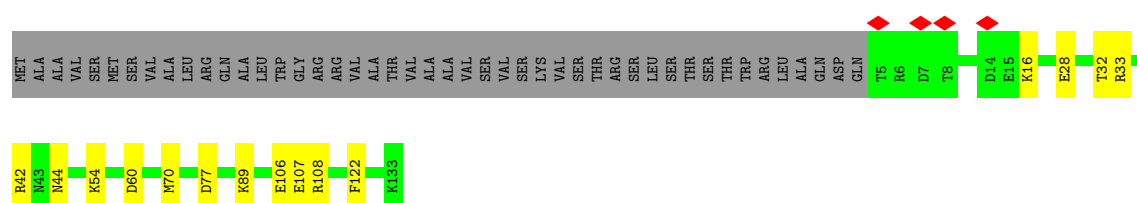
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  81% 8% 10%



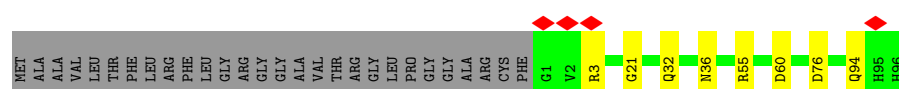
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  65% 9% 26%



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

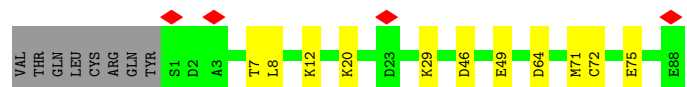
Chain R:  71% 6% 23%



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



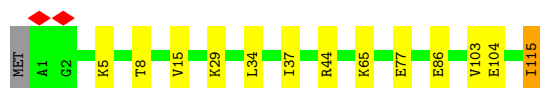
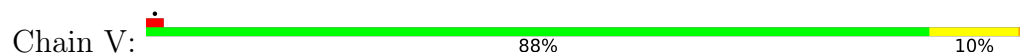
- Molecule 20: Acyl carrier protein, mitochondrial



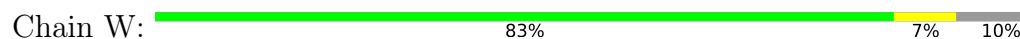
- Molecule 20: Acyl carrier protein, mitochondrial



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



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

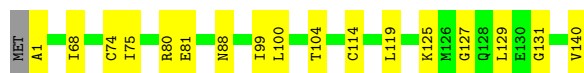


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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

Chain Y:  87% 12%



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

Chain Z:  90% 8%

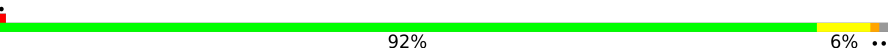


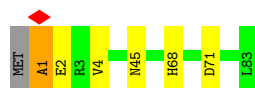
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  91% 9%



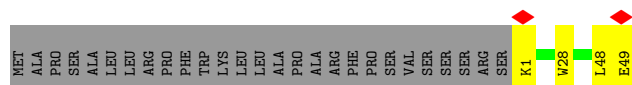
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  92% 6%



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

Chain c:  59% 5% 36%



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

Chain d:  90% 10%

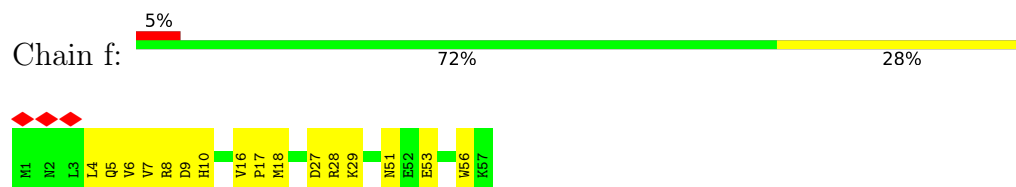


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

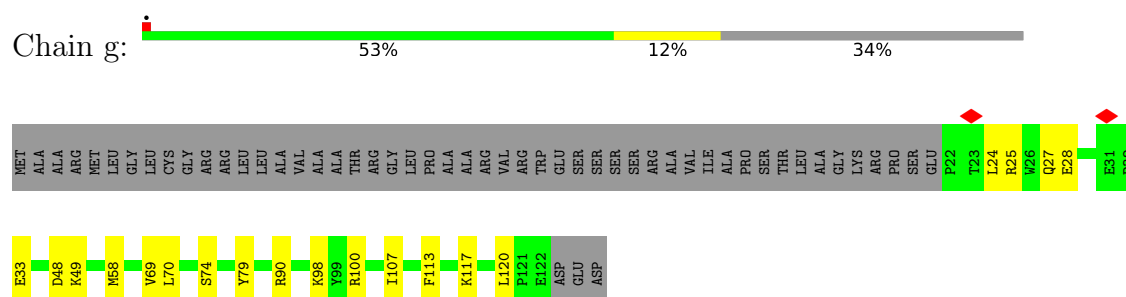
Chain e:  86% 8% 7%



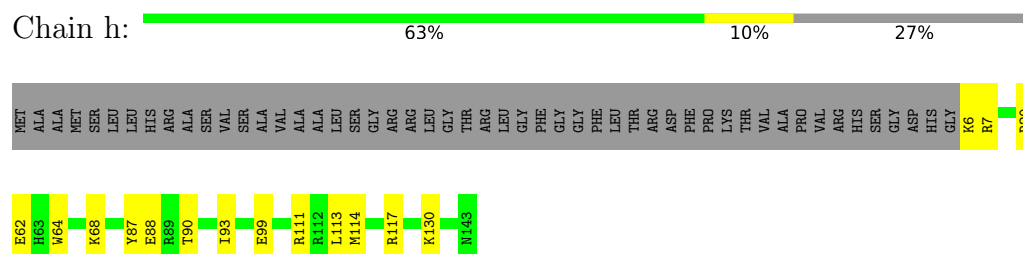
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



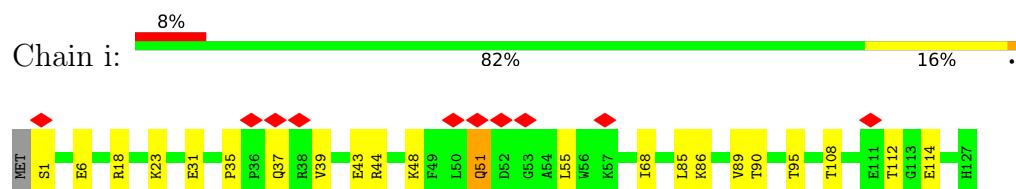
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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



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

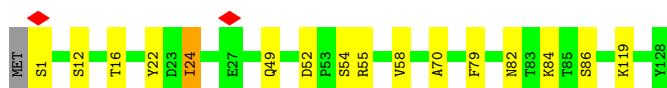
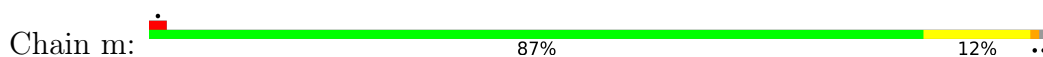




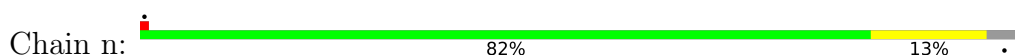
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



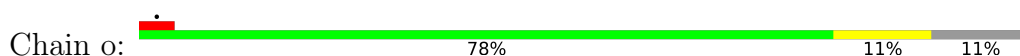
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



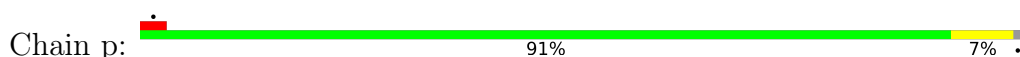
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



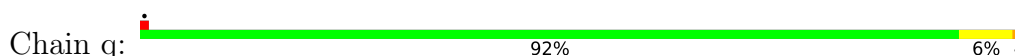
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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

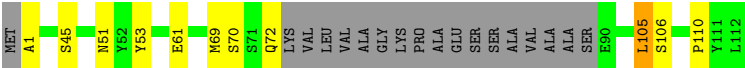


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

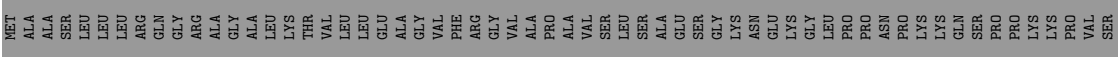




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- 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	68095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/936	0.26	0/1281
2	B	0.27	0/1272	0.27	0/1720
3	C	0.26	0/1789	0.28	0/2436
4	D	0.26	0/3537	0.27	0/4794
5	E	0.18	0/1699	0.27	0/2312
6	F	0.19	0/3401	0.25	0/4595
7	G	0.21	0/5367	0.27	0/7274
8	H	0.25	0/2571	0.29	0/3513
9	I	0.28	0/1445	0.29	0/1956
10	J	0.21	0/1370	0.26	0/1859
11	K	0.22	0/745	0.27	0/1008
12	L	0.19	0/4920	0.26	0/6694
13	M	0.23	0/3738	0.26	0/5097
14	N	0.24	0/2792	0.27	0/3800
15	O	0.19	0/2651	0.24	0/3587
16	P	0.21	0/2831	0.25	0/3841
17	Q	0.22	0/1072	0.26	0/1449
18	R	0.22	0/753	0.23	0/1014
19	S	0.15	0/711	0.24	0/956
20	T	0.15	0/719	0.23	0/971
20	U	0.15	0/719	0.24	0/971
21	V	0.19	0/948	0.23	0/1284
22	W	0.20	0/1000	0.26	0/1344
23	X	0.20	0/1439	0.25	0/1942
24	Y	0.17	0/1042	0.22	0/1414
25	Z	0.21	0/1181	0.23	0/1592
26	a	0.21	0/584	0.25	0/786
27	b	0.18	0/667	0.23	0/916
28	c	0.20	0/427	0.23	0/579
29	d	0.21	0/1018	0.27	0/1375
30	e	0.20	0/850	0.24	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.17	0/505	0.27	0/681
32	g	0.18	0/873	0.26	0/1186
33	h	0.20	0/1188	0.23	0/1607
34	i	0.15	0/1127	0.24	0/1534
35	j	0.16	0/624	0.22	0/855
36	k	0.13	0/672	0.24	0/906
37	l	0.17	0/1369	0.26	0/1873
38	m	0.18	0/1088	0.23	0/1472
39	n	0.16	0/1540	0.23	0/2085
40	o	0.15	0/1073	0.23	0/1437
41	p	0.18	0/1491	0.23	0/2011
42	q	0.21	0/1242	0.26	0/1688
43	r	0.21	0/789	0.26	0/1068
44	s	0.14	0/392	0.24	0/531
All	All	0.21	0/68167	0.26	0/92430

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	12	0
2	B	1241	0	1251	9	0
3	C	1738	0	1685	12	0
4	D	3459	0	3404	23	0
5	E	1659	0	1664	16	0
6	F	3326	0	3282	37	0
7	G	5279	0	5301	53	0
8	H	2509	0	2621	36	0
9	I	1414	0	1370	11	0
10	J	1345	0	1352	16	0
11	K	745	0	785	10	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4802	0	4960	52	0
13	M	3654	0	3852	26	0
14	N	2733	0	2912	32	0
15	O	2589	0	2565	21	0
16	P	2754	0	2773	17	0
17	Q	1049	0	1045	5	0
18	R	740	0	714	4	0
19	S	700	0	719	8	0
20	T	707	0	700	3	0
20	U	707	0	700	10	0
21	V	928	0	972	9	0
22	W	976	0	991	7	0
23	X	1402	0	1379	7	0
24	Y	1030	0	1039	9	0
25	Z	1152	0	1151	5	0
26	a	569	0	568	4	0
27	b	654	0	663	3	0
28	c	414	0	415	3	0
29	d	999	0	988	10	0
30	e	829	0	829	3	0
31	f	492	0	501	10	0
32	g	846	0	798	15	0
33	h	1154	0	1168	14	0
34	i	1097	0	1108	15	0
35	j	597	0	536	0	0
36	k	653	0	639	4	0
37	l	1314	0	1210	11	0
38	m	1070	0	1068	8	0
39	n	1487	0	1433	15	0
40	o	1048	0	1016	6	0
41	p	1458	0	1430	9	0
42	q	1212	0	1183	4	0
43	r	776	0	782	8	0
44	s	380	0	349	9	0
45	A	82	0	118	0	0
45	I	38	0	53	0	0
45	J	75	0	98	1	0
45	L	284	0	407	1	0
45	M	85	0	121	0	0
45	N	49	0	75	1	0
45	P	67	0	82	0	0
45	Y	98	0	153	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Z	42	0	61	0	0
45	b	139	0	212	0	0
45	e	49	0	75	0	0
45	m	133	0	197	1	0
45	q	21	0	16	0	0
46	A	103	0	128	1	0
46	B	94	0	136	0	0
46	H	87	0	128	2	0
46	I	54	0	88	1	0
46	L	45	0	67	2	0
46	M	79	0	109	2	0
46	Y	45	0	67	1	0
46	Z	44	0	62	1	0
46	d	39	0	52	0	0
46	h	47	0	71	0	0
46	q	38	0	53	0	0
47	A	38	0	53	0	0
47	B	37	0	51	0	0
47	J	38	0	53	0	0
47	L	31	0	36	0	0
47	O	32	0	41	0	0
47	P	27	0	28	0	0
47	d	36	0	49	0	0
47	g	32	0	41	1	0
48	B	8	0	0	1	0
48	F	8	0	0	0	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	E	4	0	0	0	0
49	G	4	0	0	0	0
50	F	31	0	19	1	0
51	G	1	0	0	0	0
52	H	83	0	116	1	0
52	J	70	0	84	0	0
52	L	76	0	99	1	0
52	M	100	0	156	4	0
52	N	80	0	107	0	0
52	X	100	0	156	1	0
52	d	65	0	77	1	0
52	i	80	0	104	4	0
52	r	61	0	66	0	0
53	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	R	1	0	0	0	0
54	O	1	0	0	0	0
55	O	31	0	12	6	0
56	P	48	0	24	1	0
57	T	37	0	0	1	0
57	U	37	0	0	0	0
58	i	29	0	38	7	0
59	o	15	0	27	0	0
All	All	69719	0	70889	520	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 (520) 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)
6:F:131:ALA:O	6:F:171:TYR:OH	1.91	0.88
13:M:51:ASN:OD1	33:h:90:THR:OG1	1.91	0.86
33:h:49:GLU:OE1	33:h:68:LYS:NZ	2.09	0.86
34:i:35:PRO:O	34:i:37:GLN:NE2	2.10	0.85
7:G:45:ARG:NH1	7:G:260:GLU:OE1	2.10	0.84
22:W:39:TYR:O	22:W:59:ARG:NH1	2.11	0.84
42:q:78:ASP:OD1	42:q:80:SER:OG	1.94	0.84
7:G:140:LYS:O	7:G:148:THR:OG1	1.96	0.82
33:h:87:TYR:OH	41:p:86:GLU:OE1	1.98	0.81
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.63	0.80
15:O:20:GLU:O	15:O:23:LYS:NZ	2.14	0.80
1:A:71:LEU:O	10:J:147:TYR:OH	2.01	0.79
34:i:48:LYS:O	34:i:51:GLN:NE2	2.15	0.79
10:J:77:GLU:N	10:J:77:GLU:OE1	2.15	0.79
7:G:40:PHE:O	7:G:158:ARG:NH1	2.15	0.78
6:F:15:LEU:O	6:F:20:ARG:NH1	2.17	0.78
15:O:281:GLU:N	15:O:281:GLU:OE1	2.17	0.78
7:G:47:SER:OG	7:G:165:GLU:OE2	2.02	0.77
5:E:63:ILE:O	5:E:67:ASN:ND2	2.17	0.77
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.18	0.77
8:H:114:TYR:OH	10:J:61:LEU:O	2.02	0.77
34:i:89:VAL:O	34:i:95:THR:HG21	1.85	0.77
31:f:5:GLN:OE1	31:f:8:ARG:NH1	2.18	0.77
10:J:23:LYS:NZ	11:K:18:GLY:O	2.18	0.76
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:237:ASP:OD1	21:V:29:LYS:NZ	2.19	0.75
20:T:49:GLU:OE2	22:W:63:ARG:NH2	2.18	0.75
12:L:561:ILE:O	12:L:565:THR:OG1	2.04	0.75
14:N:291:TYR:OH	45:N:402:3PE:O14	2.05	0.74
40:o:43:GLN:NE2	40:o:47:ASP:OD1	2.20	0.74
5:E:112:ASN:OD1	5:E:115:SER:OG	2.01	0.74
13:M:187:HIS:O	13:M:192:ASN:ND2	2.20	0.73
8:H:249:PRO:O	26:a:28:ARG:NH2	2.21	0.73
7:G:260:GLU:OE2	7:G:397:LYS:NZ	2.21	0.73
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.21	0.72
6:F:248:GLU:OE1	6:F:249:ARG:NE	2.23	0.72
6:F:370:ASP:OD2	6:F:374:LYS:NZ	2.23	0.72
37:l:141:GLU:N	37:l:141:GLU:OE1	2.23	0.72
1:A:1:FME:O1	1:A:2:ASN:N	2.22	0.72
4:D:282:GLU:N	4:D:282:GLU:OE1	2.22	0.72
58:i:201:CHD:H212	58:i:201:CHD:H12	1.72	0.71
2:B:44:SER:OG	8:H:51:ASP:OD1	2.07	0.71
32:g:58:MET:HE1	47:g:201:PLC:H82	1.72	0.70
7:G:577:GLU:OE2	7:G:579:ARG:NH2	2.24	0.70
14:N:19:ILE:O	14:N:23:SER:OG	2.08	0.69
32:g:33:GLU:N	32:g:33:GLU:OE1	2.25	0.69
23:X:138:GLU:N	23:X:138:GLU:OE1	2.26	0.69
8:H:231:ILE:O	8:H:235:ASN:ND2	2.25	0.69
14:N:269:GLU:O	14:N:273:ASN:ND2	2.25	0.69
13:M:3:LYS:NZ	31:f:27:ASP:OD2	2.22	0.69
7:G:35:MET:HE2	7:G:81:THR:HB	1.75	0.68
40:o:102:GLU:OE2	40:o:105:ARG:NH1	2.26	0.68
6:F:154:ARG:HA	44:s:58:LEU:HD21	1.76	0.68
10:J:167:VAL:HG13	14:N:42:PRO:HG3	1.76	0.68
16:P:306:GLU:N	16:P:306:GLU:OE1	2.27	0.68
10:J:129:ASP:OD1	10:J:130:THR:N	2.27	0.68
32:g:100:ARG:NH2	32:g:107:ILE:O	2.27	0.67
29:d:60:ARG:NH1	52:d:201:CDL:OA3	2.28	0.66
45:J:203:3PE:O14	12:L:585:LYS:NZ	2.27	0.66
15:O:33:SER:N	55:O:402:DGT:O3G	2.28	0.66
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.28	0.66
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.09	0.65
16:P:13:ARG:NH2	16:P:61:PRO:O	2.29	0.65
13:M:255:ASP:OD1	13:M:256:PHE:N	2.29	0.65
8:H:138:GLN:NE2	8:H:191:ALA:O	2.29	0.65
3:C:77:ASP:OD1	4:D:390:LYS:NZ	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:198:PHE:CD1	8:H:285:LEU:HD13	2.32	0.64
19:S:30:GLN:OE1	19:S:33:ARG:NH2	2.29	0.64
3:C:148:LEU:O	22:W:87:MET:HE2	1.96	0.64
25:Z:55:GLU:OE1	25:Z:58:ARG:NH2	2.31	0.64
10:J:109:LYS:NZ	10:J:110:ASP:OD1	2.30	0.64
12:L:467:ILE:O	12:L:471:ASN:ND2	2.30	0.64
15:O:30:ASN:OD1	15:O:31:ILE:N	2.30	0.64
37:l:157:GLU:O	40:o:33:ARG:NE	2.31	0.63
12:L:140:LEU:O	12:L:140:LEU:HD23	1.99	0.63
7:G:366:THR:HB	7:G:450:MET:HE3	1.79	0.63
12:L:171:ALA:O	12:L:175:ASN:ND2	2.32	0.63
25:Z:89:ASN:ND2	25:Z:122:GLU:O	2.31	0.63
39:n:169:ILE:O	39:n:172:ARG:NH1	2.31	0.62
12:L:246:LEU:O	12:L:251:THR:OG1	2.17	0.62
4:D:284:ASP:OD1	9:I:1:THR:OG1	2.17	0.62
46:M:605:PC1:H142	52:i:202:CDL:OA3	1.99	0.62
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.32	0.62
40:o:28:TYR:OH	40:o:110:ARG:NH1	2.31	0.62
7:G:326:GLU:N	7:G:326:GLU:OE1	2.32	0.62
13:M:76:MET:O	13:M:80:SER:OG	2.18	0.62
20:U:56:ASP:OD1	39:n:24:ARG:NH2	2.32	0.62
15:O:83:TYR:HH	55:O:402:DGT:HO3'	1.47	0.61
17:Q:33:ARG:NH1	17:Q:77:ASP:OD1	2.34	0.61
12:L:414:ILE:O	12:L:417:SER:OG	2.17	0.61
5:E:121:GLN:O	5:E:125:GLY:N	2.33	0.61
18:R:55:ARG:NE	18:R:76:ASP:OD1	2.32	0.61
12:L:341:MET:HE2	12:L:457:LEU:HD12	1.82	0.61
37:l:20:ARG:NH2	37:l:35:GLU:OE1	2.34	0.61
28:c:48:LEU:HD12	28:c:49:GLU:N	2.16	0.61
40:o:82:GLU:N	40:o:82:GLU:OE1	2.33	0.61
38:m:16:THR:O	38:m:22:TYR:OH	2.10	0.60
37:l:47:TYR:OH	37:l:77:MET:O	2.10	0.60
27:b:68:HIS:N	27:b:71:ASP:OD2	2.34	0.60
7:G:194:GLU:OE1	7:G:385:ARG:NE	2.34	0.60
43:r:69:MET:SD	43:r:70:SER:N	2.75	0.60
6:F:224:ASN:ND2	50:F:501:FMN:O2	2.35	0.60
34:i:18:ARG:NH1	39:n:170:VAL:O	2.34	0.60
11:K:43:MET:SD	14:N:72:MET:HE1	2.42	0.60
13:M:97:THR:O	13:M:101:SER:OG	2.20	0.60
16:P:92:ILE:HD11	16:P:218:ILE:HD11	1.84	0.60
11:K:37:MET:SD	14:N:68:MET:HE1	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:GLY:N	55:O:402:DGT:O3G	2.34	0.59
52:M:602:CDL:H473	52:X:201:CDL:H461	1.85	0.59
6:F:380:VAL:O	6:F:429:ARG:NH1	2.34	0.59
12:L:560:ALA:O	12:L:565:THR:HG23	2.02	0.59
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.34	0.59
31:f:53:GLU:N	31:f:53:GLU:OE1	2.36	0.59
44:s:72:SER:OG	44:s:75:HIS:ND1	2.29	0.59
6:F:250:ASN:ND2	6:F:318:ASP:OD2	2.35	0.58
7:G:415:LEU:O	7:G:416:THR:OG1	2.20	0.58
23:X:109:CYS:SG	23:X:110:VAL:N	2.76	0.58
7:G:433:ALA:O	7:G:476:LYS:NZ	2.18	0.58
15:O:138:MET:CE	55:O:402:DGT:HN2	2.16	0.58
15:O:53:GLU:OE2	15:O:126:ARG:NH1	2.37	0.58
1:A:35:SER:O	2:B:81:ARG:NH2	2.36	0.58
6:F:120:GLU:OE2	6:F:236:ARG:NH1	2.34	0.58
6:F:175:VAL:O	44:s:62:ARG:NH1	2.34	0.58
7:G:375:ASP:OD1	7:G:375:ASP:N	2.35	0.58
7:G:615:THR:OG1	7:G:617:ASP:OD1	2.13	0.58
8:H:18:ALA:O	8:H:21:THR:OG1	2.17	0.58
58:i:201:CHD:H212	58:i:201:CHD:H183	1.85	0.58
12:L:508:THR:O	39:n:35:LYS:NZ	2.18	0.58
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.37	0.58
3:C:85:THR:HG21	21:V:115:ILE:HG13	1.85	0.58
7:G:371:VAL:HG22	7:G:450:MET:HE1	1.86	0.58
36:k:17:ASP:OD1	36:k:18:TYR:N	2.36	0.58
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.12	0.57
38:m:52:ASP:OD2	38:m:54:SER:OG	2.15	0.57
4:D:88:GLU:OE2	4:D:430:ARG:NH1	2.36	0.57
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.85	0.57
13:M:450:ASN:OD1	13:M:452:LYS:NZ	2.37	0.57
15:O:285:GLY:N	32:g:27:GLN:O	2.33	0.57
5:E:105:THR:HG22	5:E:106:THR:H	1.69	0.57
6:F:263:ASN:ND2	6:F:285:GLY:O	2.36	0.57
14:N:243:LEU:HD22	14:N:330:VAL:HG11	1.86	0.57
15:O:287:HIS:ND1	32:g:28:GLU:OE2	2.33	0.57
39:n:56:MET:HA	39:n:56:MET:HE2	1.86	0.57
45:m:202:3PE:O22	45:m:202:3PE:N	2.38	0.57
5:E:55:GLN:O	5:E:59:GLY:N	2.35	0.56
5:E:123:LYS:NZ	5:E:174:ASP:OD1	2.34	0.56
5:E:96:GLY:N	5:E:138:THR:OG1	2.35	0.56
7:G:201:ASP:OD2	7:G:268:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:332:LYS:NZ	7:G:505:LEU:O	2.32	0.56
2:B:69:MET:HE1	2:B:76:PHE:CD2	2.40	0.56
7:G:339:ASP:OD1	19:S:16:ARG:NH1	2.38	0.56
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.37	0.56
57:T:101:EHZ:O1	57:T:101:EHZ:O2	2.19	0.56
3:C:151:ILE:HG23	3:C:152:LEU:HG	1.87	0.56
12:L:341:MET:CE	12:L:457:LEU:HD12	2.35	0.56
13:M:208:PRO:HD3	13:M:236:LEU:HD22	1.88	0.56
4:D:81:GLY:N	4:D:429:ASP:OD1	2.39	0.56
7:G:156:CYS:O	7:G:157:THR:OG1	2.16	0.56
9:I:64:GLU:O	9:I:134:GLY:N	2.39	0.56
7:G:475:GLN:OE1	7:G:479:THR:HG21	2.06	0.56
6:F:94:VAL:HG11	6:F:192:LEU:HD21	1.88	0.56
13:M:141:GLU:N	13:M:141:GLU:OE1	2.39	0.56
58:i:201:CHD:H232	58:i:201:CHD:H161	1.87	0.55
6:F:356:HIS:O	7:G:177:ARG:NH1	2.39	0.55
14:N:215:MET:HE1	14:N:244:ILE:HG23	1.88	0.55
15:O:32:CYS:SG	15:O:186:LYS:NZ	2.78	0.55
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.35	0.55
44:s:48:THR:HG23	44:s:49:TYR:CD2	2.42	0.55
7:G:285:ARG:NH2	7:G:555:PRO:O	2.40	0.55
11:K:82:SER:O	11:K:86:GLY:N	2.37	0.55
29:d:100:ASP:OD2	33:h:117:ARG:NH2	2.39	0.55
1:A:114:THR:OG1	1:A:115:GLU:N	2.38	0.55
8:H:207:LEU:O	8:H:209:SER:N	2.40	0.55
6:F:314:THR:HG22	6:F:314:THR:O	2.07	0.55
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.15	0.55
32:g:48:ASP:OD1	32:g:49:LYS:N	2.40	0.55
5:E:217:LEU:HD11	6:F:48:ILE:HG12	1.89	0.54
32:g:25:ARG:O	32:g:25:ARG:NE	2.31	0.54
34:i:39:VAL:O	34:i:44:ARG:NH1	2.39	0.54
8:H:99:ASN:N	46:H:402:PC1:O12	2.38	0.54
6:F:188:GLU:OE1	6:F:190:THR:N	2.38	0.54
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.42	0.54
26:a:52:ARG:NH1	26:a:58:ASN:OD1	2.41	0.54
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.43	0.54
24:Y:68:ILE:HG21	24:Y:99:ILE:HD12	1.90	0.54
24:Y:81:GLU:OE1	24:Y:81:GLU:N	2.41	0.54
3:C:85:THR:HG21	21:V:115:ILE:CG1	2.38	0.53
31:f:56:TRP:NE1	33:h:88:GLU:OE1	2.38	0.53
34:i:86:LYS:O	34:i:90:THR:OG1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:MET:O	6:F:91:LYS:NZ	2.32	0.53
7:G:276:ARG:NH1	7:G:680:ALA:O	2.39	0.53
21:V:8:THR:HG23	21:V:15:VAL:HG22	1.90	0.53
15:O:20:GLU:N	15:O:20:GLU:OE1	2.37	0.53
37:l:82:ASP:N	37:l:82:ASP:OD1	2.41	0.53
34:i:108:THR:O	41:p:18:ALA:N	2.40	0.53
10:J:103:MET:HA	10:J:103:MET:HE2	1.92	0.52
58:i:201:CHD:O3	58:i:201:CHD:H9	2.09	0.52
17:Q:107:GLU:OE1	17:Q:108:ARG:N	2.41	0.52
7:G:475:GLN:O	7:G:479:THR:OG1	2.25	0.52
39:n:30:CYS:O	39:n:32:HIS:N	2.39	0.52
8:H:102:VAL:HG23	8:H:160:PHE:O	2.09	0.52
12:L:562:LEU:HB2	12:L:563:PRO:HD3	1.92	0.52
44:s:72:SER:HG	44:s:75:HIS:HD1	1.37	0.52
3:C:8:ARG:NH1	43:r:61:GLU:OE2	2.34	0.52
5:E:18:GLU:N	5:E:18:GLU:OE1	2.43	0.52
16:P:153:GLU:HG3	16:P:165:ILE:HD13	1.91	0.52
9:I:172:ASP:OD2	9:I:176:ARG:NH1	2.41	0.52
15:O:278:PHE:O	32:g:25:ARG:NH2	2.42	0.52
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.43	0.52
16:P:200:THR:HG21	16:P:288:HIS:HA	1.92	0.52
58:i:201:CHD:H232	58:i:201:CHD:C16	2.39	0.52
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.25	0.51
3:C:83:ILE:HG22	3:C:85:THR:HG22	1.93	0.51
12:L:208:ASP:N	12:L:208:ASP:OD1	2.42	0.51
30:e:58:GLU:N	30:e:58:GLU:OE1	2.40	0.51
6:F:407:LEU:HD23	6:F:407:LEU:O	2.11	0.51
14:N:236:LYS:HG3	14:N:237:THR:HG23	1.93	0.51
24:Y:127:GLY:O	24:Y:131:GLY:N	2.43	0.51
34:i:6:GLU:OE2	39:n:157:ARG:NH1	2.43	0.51
20:U:88:GLU:OE1	34:i:23:LYS:NZ	2.40	0.51
1:A:18:VAL:HG21	8:H:76:ILE:CG1	2.41	0.51
7:G:615:THR:O	7:G:619:VAL:HG23	2.11	0.51
8:H:65:THR:O	8:H:124:ASN:ND2	2.41	0.51
13:M:216:LEU:HD23	13:M:216:LEU:C	2.36	0.51
11:K:70:GLU:O	11:K:74:GLY:N	2.36	0.51
32:g:79:TYR:OH	52:i:202:CDL:OA4	2.29	0.51
6:F:96:ASN:ND2	6:F:187:GLY:O	2.43	0.50
3:C:8:ARG:O	4:D:129:ARG:NH2	2.45	0.50
6:F:301:GLY:O	6:F:335:ILE:HD12	2.11	0.50
11:K:43:MET:CE	14:N:72:MET:HE1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:57:GLU:OE2	38:m:12:SER:OG	2.18	0.50
9:I:22:ALA:HB1	25:Z:34:MET:HE3	1.93	0.50
7:G:355:GLY:O	7:G:361:ASN:ND2	2.45	0.50
7:G:455:SER:O	7:G:459:GLN:NE2	2.43	0.50
12:L:297:ASP:OD1	12:L:299:LYS:N	2.44	0.49
33:h:7:ARG:NH1	34:i:31:GLU:O	2.43	0.49
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.94	0.49
14:N:44:MET:HE1	14:N:59:TYR:CG	2.46	0.49
41:p:48:ARG:NH1	41:p:52:GLU:OE2	2.45	0.49
14:N:270:MET:HE1	14:N:278:LEU:HD23	1.94	0.49
6:F:17:ASP:OD1	6:F:20:ARG:NH1	2.45	0.49
8:H:198:PHE:CE1	8:H:285:LEU:HD13	2.46	0.49
46:I:204:PC1:O13	46:I:204:PC1:H132	2.12	0.49
20:U:39:ASP:OD1	20:U:39:ASP:N	2.45	0.49
1:A:18:VAL:HG21	8:H:76:ILE:HG12	1.95	0.49
44:s:42:GLN:OE1	44:s:42:GLN:N	2.41	0.49
46:H:402:PC1:O13	46:H:402:PC1:H133	2.13	0.49
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.48	0.49
43:r:105:LEU:HD22	43:r:110:PRO:HB3	1.95	0.49
12:L:264:TYR:N	12:L:265:PRO:CD	2.76	0.48
17:Q:89:LYS:NZ	17:Q:107:GLU:OE2	2.25	0.48
1:A:115:GLU:N	1:A:115:GLU:OE1	2.46	0.48
10:J:31:LEU:C	10:J:31:LEU:HD23	2.39	0.48
52:M:602:CDL:H872	52:M:602:CDL:H232	1.95	0.48
4:D:322:GLU:OE1	4:D:322:GLU:N	2.39	0.48
12:L:230:HIS:N	12:L:231:PRO:CD	2.76	0.48
15:O:214:MET:O	15:O:218:CYS:N	2.45	0.48
14:N:146:PHE:N	14:N:147:PRO:CD	2.76	0.48
7:G:190:MET:HE1	7:G:690:ALA:HB1	1.95	0.48
16:P:153:GLU:OE1	16:P:167:LYS:NZ	2.47	0.48
43:r:45:SER:O	43:r:51:ASN:ND2	2.47	0.48
9:I:75:GLU:O	9:I:105:ARG:NH1	2.46	0.48
3:C:183:VAL:O	22:W:100:THR:OG1	2.32	0.48
14:N:265:MET:HA	14:N:265:MET:HE2	1.95	0.48
15:O:186:LYS:NZ	15:O:191:GLU:OE1	2.39	0.48
58:i:201:CHD:H12	58:i:201:CHD:C21	2.43	0.48
4:D:165:THR:HG21	8:H:275:ALA:O	2.14	0.47
12:L:369:THR:O	12:L:369:THR:HG22	2.14	0.47
13:M:12:MET:HB2	13:M:13:PRO:HD3	1.95	0.47
19:S:17:GLU:OE1	19:S:67:ARG:NH2	2.45	0.47
7:G:272:ASP:OD1	7:G:681:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:71:TRP:CZ3	32:g:69:VAL:HG11	2.49	0.47
18:R:60:ASP:N	18:R:60:ASP:OD1	2.46	0.47
5:E:105:THR:HG22	5:E:106:THR:N	2.30	0.47
40:o:112:LYS:O	40:o:115:GLU:N	2.47	0.47
7:G:601:ARG:NH2	7:G:614:ASP:OD2	2.47	0.47
7:G:632:ARG:NH2	19:S:58:SER:O	2.46	0.47
12:L:133:THR:HG22	12:L:133:THR:O	2.14	0.47
13:M:285:LEU:HD23	13:M:285:LEU:O	2.14	0.47
46:Y:203:PC1:H142	46:Y:203:PC1:O13	2.14	0.47
29:d:93:TYR:CD1	33:h:114:MET:HE2	2.50	0.47
3:C:109:THR:OG1	3:C:110:TYR:N	2.43	0.47
31:f:51:ASN:O	31:f:51:ASN:ND2	2.48	0.47
37:l:15:LYS:N	37:l:19:GLU:OE1	2.41	0.47
6:F:258:ILE:N	6:F:258:ILE:HD12	2.29	0.47
7:G:617:ASP:OD1	7:G:617:ASP:N	2.48	0.47
8:H:179:TRP:N	8:H:180:PRO:CD	2.77	0.47
14:N:261:MET:HG3	14:N:340:THR:HG23	1.95	0.47
36:k:60:VAL:HG12	36:k:61:SER:N	2.30	0.47
4:D:328:ALA:HB3	7:G:126:ASP:HB2	1.97	0.47
41:p:117:GLY:O	41:p:120:HIS:ND1	2.42	0.47
6:F:127:ARG:O	6:F:127:ARG:NE	2.39	0.47
12:L:13:LEU:O	12:L:16:THR:OG1	2.32	0.47
13:M:423:ILE:CD1	38:m:58:VAL:HG13	2.45	0.47
29:d:112:VAL:O	41:p:159:LYS:NZ	2.47	0.47
6:F:109:GLU:OE1	6:F:112:ARG:NH2	2.48	0.47
6:F:381:ARG:NH2	6:F:383:ASP:OD2	2.48	0.47
14:N:68:MET:HE2	14:N:68:MET:HA	1.96	0.47
15:O:219:GLU:OE2	15:O:243:TYR:N	2.39	0.47
29:d:3:THR:HG23	29:d:4:GLY:N	2.29	0.47
12:L:71:ILE:CG2	13:M:310:MET:HE1	2.45	0.46
52:L:701:CDL:H671	52:i:202:CDL:C44	2.45	0.46
19:S:40:TYR:CD1	19:S:54:ILE:HD11	2.50	0.46
37:l:66:HIS:O	37:l:70:ARG:N	2.43	0.46
4:D:343:GLU:OE1	4:D:343:GLU:N	2.46	0.46
12:L:439:THR:OG1	20:U:57:GLU:OE1	2.28	0.46
14:N:270:MET:CE	14:N:278:LEU:HD23	2.45	0.46
16:P:50:ARG:NE	56:P:501:NDP:O2X	2.44	0.46
6:F:306:LEU:C	6:F:306:LEU:HD12	2.40	0.46
12:L:301:ILE:CG2	12:L:426:ILE:HD11	2.45	0.46
6:F:188:GLU:OE1	6:F:189:GLU:N	2.49	0.46
7:G:227:SER:OG	7:G:228:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:37:MET:HE2	11:K:67:ALA:HB2	1.96	0.46
13:M:264:LEU:O	13:M:268:GLY:N	2.49	0.46
24:Y:100:LEU:O	24:Y:104:THR:HG22	2.15	0.46
12:L:433:GLY:O	36:k:59:ASN:ND2	2.43	0.46
3:C:68:SER:N	21:V:86:GLU:OE1	2.46	0.46
3:C:179:GLU:OE1	16:P:37:HIS:NE2	2.45	0.46
8:H:245:THR:HG22	8:H:246:SER:N	2.31	0.46
12:L:1:FME:O	12:L:4:PHE:N	2.48	0.46
41:p:127:GLU:OE1	41:p:127:GLU:N	2.46	0.46
42:q:5:GLN:N	42:q:5:GLN:OE1	2.49	0.46
16:P:162:GLU:OE1	16:P:162:GLU:N	2.43	0.46
12:L:286:LEU:C	12:L:286:LEU:HD13	2.41	0.46
12:L:323:TYR:CZ	12:L:475:THR:HG21	2.52	0.46
32:g:98:LYS:NZ	41:p:5:ASP:OD2	2.43	0.46
12:L:9:LEU:HD12	34:i:85:LEU:HD11	1.97	0.45
27:b:1:AYA:OT	27:b:4:VAL:N	2.39	0.45
44:s:58:LEU:O	44:s:62:ARG:NE	2.49	0.45
19:S:92:ASN:O	19:S:96:SER:OG	2.33	0.45
20:T:64:ASP:OD2	22:W:32:ARG:NH2	2.44	0.45
20:U:17:TYR:HH	36:k:21:TRP:HE1	1.64	0.45
6:F:318:ASP:OD1	6:F:321:ALA:HB3	2.16	0.45
12:L:381:THR:O	12:L:392:LYS:NZ	2.42	0.45
4:D:50:ASN:O	8:H:127:TYR:OH	2.26	0.45
12:L:82:MET:HB3	12:L:87:MET:HE3	1.98	0.45
32:g:70:LEU:O	32:g:74:SER:OG	2.21	0.45
32:g:79:TYR:OH	52:i:202:CDL:OA7	2.27	0.45
34:i:112:THR:HG23	34:i:114:GLU:HG2	1.98	0.45
6:F:28:ARG:NH1	44:s:35:ASN:O	2.46	0.45
8:H:87:ILE:N	8:H:88:PRO:CD	2.80	0.45
24:Y:80:ARG:NH1	24:Y:88:ASN:OD1	2.50	0.45
13:M:168:GLN:O	13:M:172:GLY:N	2.40	0.45
23:X:122:GLY:N	25:Z:65:GLU:OE2	2.47	0.45
14:N:13:ILE:CD1	14:N:43:ILE:HD12	2.47	0.45
14:N:13:ILE:HD11	14:N:43:ILE:HD12	1.98	0.45
5:E:44:ALA:O	5:E:47:VAL:HG23	2.17	0.45
8:H:277:TYR:OH	9:I:30:LEU:O	2.26	0.45
10:J:103:MET:O	10:J:107:VAL:HG12	2.17	0.45
52:M:602:CDL:H541	14:N:242:VAL:HG11	1.99	0.45
43:r:105:LEU:HD22	43:r:110:PRO:CB	2.47	0.45
2:B:50:PHE:CE2	2:B:100:LEU:HD12	2.51	0.45
5:E:164:LEU:HD13	5:E:169:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.98	0.45
10:J:157:THR:HG21	11:K:62:ILE:HD12	1.98	0.45
13:M:285:LEU:HD23	13:M:285:LEU:C	2.41	0.45
21:V:5:LYS:NZ	21:V:77:GLU:OE1	2.50	0.45
9:I:69:ARG:NH2	18:R:36:ASN:OD1	2.50	0.44
31:f:9:ASP:OD1	31:f:10:HIS:N	2.50	0.44
58:i:201:CHD:H112	58:i:201:CHD:H12A	1.73	0.44
8:H:28:LEU:HD22	8:H:275:ALA:HB2	2.00	0.44
10:J:45:LEU:HD12	10:J:50:SER:HA	1.98	0.44
12:L:576:LEU:HD22	45:L:707:3PE:O22	2.18	0.44
29:d:93:TYR:CG	33:h:114:MET:HE2	2.52	0.44
7:G:243:ARG:O	7:G:244:THR:OG1	2.27	0.44
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.99	0.44
29:d:3:THR:HG23	29:d:4:GLY:H	1.83	0.44
2:B:81:ARG:NE	8:H:214:GLU:OE1	2.43	0.44
6:F:41:ASP:OD1	6:F:117:LYS:NZ	2.49	0.44
8:H:49:ILE:N	8:H:49:ILE:HD12	2.32	0.44
12:L:166:THR:HG21	46:L:709:PC1:H153	1.99	0.44
38:m:49:GLN:O	38:m:55:ARG:NE	2.51	0.44
4:D:151:ILE:HG23	4:D:170:MET:HB3	2.00	0.44
5:E:26:GLU:OE1	5:E:26:GLU:N	2.46	0.44
12:L:331:THR:HB	12:L:387:THR:HG22	1.98	0.44
7:G:366:THR:HG22	7:G:366:THR:O	2.18	0.44
12:L:71:ILE:HG23	13:M:310:MET:HE1	1.99	0.44
37:l:53:ARG:NE	37:l:57:GLU:OE1	2.50	0.44
1:A:27:LEU:HD12	46:A:203:PC1:H133	2.00	0.44
13:M:54:LEU:HD23	33:h:93:ILE:HG23	1.99	0.44
16:P:2:HIS:NE2	18:R:21:GLY:O	2.51	0.44
19:S:22:LEU:HD23	19:S:22:LEU:N	2.33	0.44
7:G:41:CYS:O	7:G:161:ARG:NH2	2.36	0.44
7:G:347:GLU:O	7:G:510:GLY:N	2.51	0.44
8:H:72:ILE:HD12	52:H:401:CDL:OA9	2.18	0.44
6:F:362:CYS:HB3	6:F:404:ILE:HD12	2.00	0.43
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.00	0.43
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.99	0.43
20:U:85:ASP:OD2	39:n:175:GLU:N	2.40	0.43
34:i:31:GLU:OE2	39:n:116:ASP:N	2.51	0.43
38:m:22:TYR:C	38:m:24:ILE:HD13	2.43	0.43
13:M:108:MET:HB3	13:M:121:LEU:HD13	2.00	0.43
4:D:73:VAL:HG21	4:D:414:VAL:HG21	2.01	0.43
29:d:100:ASP:HB3	33:h:113:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:105:LEU:HD23	43:r:106:SER:H	1.84	0.43
4:D:335:ARG:NH2	9:I:129:ASP:OD1	2.47	0.43
31:f:4:LEU:O	31:f:5:GLN:HB3	2.18	0.43
7:G:58:GLU:OE1	7:G:83:SER:OG	2.15	0.43
7:G:294:THR:OG1	7:G:295:THR:N	2.49	0.43
10:J:5:ILE:HG23	10:J:6:VAL:N	2.34	0.43
10:J:123:GLY:O	10:J:126:VAL:HG22	2.18	0.43
14:N:241:THR:O	14:N:301:THR:OG1	2.34	0.43
22:W:95:VAL:HG12	22:W:95:VAL:O	2.19	0.43
24:Y:140:VAL:O	33:h:111:ARG:NH2	2.52	0.43
39:n:134:ARG:NE	39:n:161:ASP:OD2	2.46	0.43
12:L:369:THR:OG1	12:L:445:GLU:OE1	2.31	0.43
12:L:87:MET:HA	12:L:87:MET:HE2	2.00	0.43
46:L:709:PC1:H142	46:L:709:PC1:O13	2.17	0.43
20:U:49:GLU:OE2	39:n:19:TYR:OH	2.34	0.43
32:g:113:PHE:CE1	41:p:73:ILE:HG22	2.53	0.43
4:D:346:ILE:HG23	7:G:117:GLN:HG2	2.01	0.43
14:N:20:VAL:HG13	14:N:29:VAL:HG13	2.00	0.43
26:a:27:HIS:O	26:a:31:ASN:ND2	2.50	0.43
1:A:54:LYS:O	1:A:114:THR:HG22	2.19	0.43
8:H:195:ARG:O	8:H:198:PHE:N	2.44	0.43
34:i:6:GLU:OE2	39:n:157:ARG:NH2	2.49	0.43
12:L:458:LEU:HD23	12:L:458:LEU:C	2.44	0.42
13:M:66:LEU:HD11	13:M:111:THR:CG2	2.49	0.42
24:Y:74:CYS:SG	24:Y:75:ILE:N	2.91	0.42
24:Y:125:LYS:NZ	24:Y:129:LEU:HD21	2.34	0.42
2:B:66:ARG:NH2	4:D:179:GLU:OE2	2.47	0.42
12:L:444:ASN:OD1	12:L:446:ASN:ND2	2.52	0.42
38:m:82:ASN:OD1	38:m:84:LYS:N	2.43	0.42
7:G:262:TRP:HB2	7:G:390:LEU:HD11	2.01	0.42
10:J:120:ASN:OD1	10:J:122:LEU:HD13	2.19	0.42
7:G:273:GLY:O	7:G:549:HIS:NE2	2.49	0.42
11:K:40:LEU:HD22	14:N:75:ILE:HD12	2.01	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.00	0.42
16:P:330:GLU:N	16:P:333:ASP:OD2	2.46	0.42
19:S:42:GLU:N	19:S:42:GLU:OE1	2.52	0.42
6:F:224:ASN:HB3	6:F:227:THR:HG22	2.00	0.42
23:X:143:SER:OG	30:e:38:GLU:OE1	2.33	0.42
31:f:7:VAL:HG12	31:f:7:VAL:O	2.18	0.42
20:U:68:GLU:OE2	39:n:13:GLN:NE2	2.49	0.42
8:H:285:LEU:HD12	8:H:285:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.55	0.42
13:M:98:MET:HE1	52:M:602:CDL:C87	2.50	0.42
20:U:32:VAL:HG23	20:U:33:ASN:N	2.35	0.42
33:h:52:LEU:C	33:h:52:LEU:HD13	2.45	0.42
44:s:31:GLU:N	44:s:32:PRO:CD	2.81	0.42
6:F:99:GLU:O	6:F:139:ARG:NE	2.53	0.42
7:G:569:LYS:O	7:G:583:THR:OG1	2.37	0.42
8:H:87:ILE:CG1	8:H:88:PRO:HD3	2.50	0.42
15:O:138:MET:HE2	55:O:402:DGT:HN2	1.83	0.42
16:P:209:ASP:OD2	16:P:308:THR:N	2.50	0.42
4:D:165:THR:N	4:D:166:PRO:CD	2.83	0.42
7:G:156:CYS:C	7:G:157:THR:HG1	2.15	0.42
14:N:267:ILE:O	14:N:271:THR:HG23	2.20	0.42
16:P:26:ALA:HB3	16:P:47:VAL:HG13	2.00	0.42
23:X:79:GLU:HB3	23:X:80:PRO:HD3	2.00	0.42
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.45	0.41
14:N:313:MET:HE1	15:O:102:ALA:HB3	2.02	0.41
16:P:1:LEU:HD12	16:P:5:VAL:CG1	2.50	0.41
21:V:34:LEU:O	21:V:44:ARG:NH1	2.53	0.41
37:l:68:ASP:OD1	37:l:69:LEU:N	2.51	0.41
2:B:50:PHE:CZ	2:B:100:LEU:HD12	2.55	0.41
6:F:165:ASN:OD1	6:F:168:GLY:HA2	2.20	0.41
9:I:131:ILE:HG23	9:I:131:ILE:O	2.20	0.41
12:L:537:ALA:HB3	12:L:538:PRO:HD3	2.01	0.41
12:L:561:ILE:HG13	12:L:562:LEU:N	2.35	0.41
31:f:4:LEU:C	31:f:6:VAL:H	2.27	0.41
2:B:129:SER:OG	4:D:85:2MR:O	2.32	0.41
8:H:172:MET:HE3	8:H:177:PRO:HD3	2.02	0.41
12:L:260:LEU:HD12	12:L:314:MET:HE2	2.00	0.41
46:Z:202:PC1:H142	46:Z:202:PC1:O13	2.20	0.41
32:g:120:LEU:HD21	41:p:162:MET:HE3	2.02	0.41
7:G:143:GLY:HA2	7:G:190:MET:HE2	2.03	0.41
12:L:304:PHE:CZ	12:L:526:LEU:HD22	2.55	0.41
46:M:606:PC1:C38	24:Y:119:LEU:HD11	2.50	0.41
16:P:22:THR:OG1	16:P:88:SER:OG	2.21	0.41
33:h:62:GLU:OE1	33:h:64:TRP:NE1	2.53	0.41
43:r:72:GLN:OE1	43:r:72:GLN:N	2.54	0.41
4:D:197:GLY:O	4:D:325:VAL:N	2.52	0.41
4:D:329:LYS:HD2	43:r:53:TYR:CZ	2.56	0.41
25:Z:12:VAL:HG13	25:Z:13:GLY:N	2.34	0.41
34:i:55:LEU:HD13	34:i:55:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:323:VAL:HG12	7:G:324:ASP:N	2.35	0.41
12:L:213:LEU:HD23	12:L:216:LEU:HD12	2.03	0.41
7:G:534:ARG:NH2	7:G:556:ILE:O	2.52	0.41
8:H:281:ARG:O	8:H:284:GLN:N	2.53	0.41
13:M:108:MET:CB	13:M:121:LEU:HD13	2.51	0.41
6:F:94:VAL:HG11	6:F:192:LEU:CD2	2.50	0.41
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.51	0.41
42:q:138:VAL:HG23	42:q:138:VAL:O	2.21	0.41
2:B:90:GLY:HA2	48:B:201:SF4:S2	2.61	0.41
12:L:486:LEU:HA	12:L:489:THR:HG23	2.02	0.41
28:c:48:LEU:HD12	28:c:48:LEU:C	2.45	0.41
37:l:10:PRO:HG2	38:m:70:ALA:HB2	2.02	0.41
39:n:177:PRO:O	39:n:178:MET:C	2.64	0.41
9:I:114:THR:HG21	9:I:144:HIS:CE1	2.56	0.41
8:H:11:ILE:HB	8:H:12:PRO:HD3	2.03	0.40
12:L:260:LEU:CD1	12:L:314:MET:HE2	2.51	0.40
14:N:25:HIS:N	14:N:86:VAL:HG23	2.36	0.40
14:N:322:LYS:O	29:d:49:ARG:NH2	2.55	0.40
16:P:206:TYR:CZ	16:P:313:LYS:HG2	2.55	0.40
17:Q:60:ASP:N	17:Q:60:ASP:OD1	2.54	0.40
1:A:81:THR:O	27:b:45:ASN:ND2	2.53	0.40
7:G:316:ALA:HB3	7:G:519:PRO:HG3	2.02	0.40
7:G:688:VAL:O	7:G:692:THR:HG23	2.21	0.40
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.56	0.40
12:L:505:SER:O	12:L:508:THR:OG1	2.32	0.40
21:V:103:VAL:HG23	21:V:104:GLU:N	2.35	0.40
5:E:132:THR:OG1	5:E:134:ASP:OD1	2.37	0.40
5:E:190:ARG:NE	5:E:192:SER:O	2.54	0.40
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.02	0.40
12:L:458:LEU:HD23	12:L:458:LEU:O	2.22	0.40
15:O:83:TYR:OH	55:O:402:DGT:O3'	2.20	0.40
42:q:1:AME:HA	42:q:1:AME:HE1	2.02	0.40
1:A:108:GLN:HB2	10:J:169:MET:HE1	2.03	0.40
6:F:103:GLY:O	6:F:333:ALA:HB1	2.22	0.40
6:F:193:ILE:HG23	6:F:215:VAL:HA	2.03	0.40
9:I:150:ASN:OD1	9:I:150:ASN:C	2.63	0.40
12:L:562:LEU:CB	12:L:563:PRO:HD3	2.51	0.40
14:N:6:PHE:CE2	14:N:10:LEU:HD11	2.56	0.40
21:V:37:ILE:O	21:V:44:ARG:NH1	2.55	0.40
30:e:50:ARG:NE	30:e:54:GLU:OE2	2.47	0.40
31:f:16:VAL:HB	31:f:17:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.04	0.40
20:U:31:SER:OG	20:U:34:SER:OG	2.23	0.40
39:n:139:LEU:O	39:n:143:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
2	B	153/216 (71%)	150 (98%)	3 (2%)	0	100	100
3	C	207/266 (78%)	200 (97%)	7 (3%)	0	100	100
4	D	427/463 (92%)	411 (96%)	16 (4%)	0	100	100
5	E	212/249 (85%)	198 (93%)	13 (6%)	1 (0%)	24	57
6	F	430/464 (93%)	413 (96%)	17 (4%)	0	100	100
7	G	686/727 (94%)	664 (97%)	22 (3%)	0	100	100
8	H	316/318 (99%)	303 (96%)	12 (4%)	1 (0%)	36	67
9	I	174/212 (82%)	167 (96%)	7 (4%)	0	100	100
10	J	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
12	L	604/606 (100%)	572 (95%)	32 (5%)	0	100	100
13	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
14	N	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
15	O	318/343 (93%)	311 (98%)	7 (2%)	0	100	100
16	P	340/380 (90%)	330 (97%)	10 (3%)	0	100	100
17	Q	127/175 (73%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	94/124 (76%)	92 (98%)	2 (2%)	0	100	100
19	S	85/99 (86%)	82 (96%)	3 (4%)	0	100	100
20	T	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
22	W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
25	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	97/106 (92%)	94 (97%)	3 (3%)	0	100	100
31	f	55/57 (96%)	50 (91%)	5 (9%)	0	100	100
32	g	99/154 (64%)	91 (92%)	8 (8%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
35	j	69/108 (64%)	67 (97%)	2 (3%)	0	100	100
36	k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
37	l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	m	126/129 (98%)	118 (94%)	8 (6%)	0	100	100
39	n	169/179 (94%)	165 (98%)	4 (2%)	0	100	100
40	o	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
41	p	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
43	r	91/113 (80%)	88 (97%)	3 (3%)	0	100	100
44	s	43/109 (39%)	40 (93%)	3 (7%)	0	100	100
All	All	8193/9213 (89%)	7886 (96%)	305 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	157	ASN
8	H	208	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	97 (97%)	3 (3%)	36	65
2	B	131/175 (75%)	128 (98%)	3 (2%)	44	70
3	C	190/228 (83%)	187 (98%)	3 (2%)	55	75
4	D	370/392 (94%)	367 (99%)	3 (1%)	73	81
5	E	183/205 (89%)	177 (97%)	6 (3%)	33	63
6	F	346/368 (94%)	338 (98%)	8 (2%)	44	70
7	G	578/608 (95%)	571 (99%)	7 (1%)	63	78
8	H	274/274 (100%)	272 (99%)	2 (1%)	76	82
9	I	151/175 (86%)	147 (97%)	4 (3%)	40	68
10	J	141/141 (100%)	131 (93%)	10 (7%)	13	41
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	78
12	L	533/533 (100%)	517 (97%)	16 (3%)	36	65
13	M	412/412 (100%)	406 (98%)	6 (2%)	57	75
14	N	315/315 (100%)	312 (99%)	3 (1%)	68	79
15	O	283/303 (93%)	278 (98%)	5 (2%)	51	73
16	P	296/327 (90%)	289 (98%)	7 (2%)	43	69
17	Q	116/153 (76%)	109 (94%)	7 (6%)	17	47
18	R	79/97 (81%)	76 (96%)	3 (4%)	29	60
19	S	77/82 (94%)	75 (97%)	2 (3%)	40	68
20	T	81/135 (60%)	73 (90%)	8 (10%)	7	29
20	U	81/135 (60%)	77 (95%)	4 (5%)	22	53
21	V	101/102 (99%)	99 (98%)	2 (2%)	48	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	W	107/114 (94%)	105 (98%)	2 (2%)	50	73
23	X	154/155 (99%)	151 (98%)	3 (2%)	50	73
24	Y	101/102 (99%)	100 (99%)	1 (1%)	68	79
25	Z	120/121 (99%)	116 (97%)	4 (3%)	33	63
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	70 (99%)	1 (1%)	59	76
28	c	45/68 (66%)	44 (98%)	1 (2%)	45	71
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	66
30	e	89/96 (93%)	85 (96%)	4 (4%)	24	56
31	f	54/54 (100%)	51 (94%)	3 (6%)	19	49
32	g	92/131 (70%)	89 (97%)	3 (3%)	33	63
33	h	121/158 (77%)	118 (98%)	3 (2%)	42	69
34	i	120/121 (99%)	117 (98%)	3 (2%)	42	69
35	j	61/84 (73%)	60 (98%)	1 (2%)	55	75
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	75
37	l	140/159 (88%)	136 (97%)	4 (3%)	37	66
38	m	113/114 (99%)	109 (96%)	4 (4%)	32	62
39	n	156/161 (97%)	151 (97%)	5 (3%)	34	64
40	o	110/120 (92%)	105 (96%)	5 (4%)	24	56
41	p	155/157 (99%)	153 (99%)	2 (1%)	61	77
42	q	130/130 (100%)	123 (95%)	7 (5%)	20	50
43	r	85/97 (88%)	84 (99%)	1 (1%)	63	78
44	s	44/92 (48%)	44 (100%)	0	100	100
All	All	7218/7891 (92%)	7044 (98%)	174 (2%)	43	69

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	109	LYS
1	A	114	THR
2	B	54	CYS
2	B	91	THR
2	B	171	LYS

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Mol	Chain	Res	Type
3	C	125	LYS
3	C	147	ASP
3	C	153	THR
4	D	40	LYS
4	D	209	ASP
4	D	420	THR
5	E	68	LYS
5	E	72	ILE
5	E	88	THR
5	E	165	THR
5	E	183	LYS
5	E	190	ARG
6	F	8	LYS
6	F	34	LYS
6	F	46	LYS
6	F	84	LYS
6	F	127	ARG
6	F	132	ARG
6	F	359	CYS
6	F	365	CYS
7	G	122	MET
7	G	229	ASP
7	G	249	ARG
7	G	287	GLU
7	G	375	ASP
7	G	516	LYS
7	G	669	LYS
8	H	14	LEU
8	H	70	MET
9	I	29	GLU
9	I	37	THR
9	I	78	ILE
9	I	176	ARG
10	J	41	CYS
10	J	45	LEU
10	J	74	MET
10	J	86	ASN
10	J	87	LYS
10	J	103	MET
10	J	112	GLU
10	J	133	SER
10	J	139	GLU

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Mol	Chain	Res	Type
10	J	141	MET
11	K	59	MET
12	L	10	VAL
12	L	26	THR
12	L	88	MET
12	L	208	ASP
12	L	320	ASN
12	L	336	LYS
12	L	364	LYS
12	L	475	THR
12	L	479	GLN
12	L	481	THR
12	L	487	LYS
12	L	543	SER
12	L	553	LEU
12	L	554	ASP
12	L	580	GLN
12	L	581	LYS
13	M	19	LYS
13	M	72	LEU
13	M	80	SER
13	M	101	SER
13	M	116	ILE
13	M	315	LEU
14	N	88	LYS
14	N	204	ASN
14	N	319	LEU
15	O	40	LYS
15	O	76	ASN
15	O	146	LYS
15	O	206	TYR
15	O	315	LYS
16	P	2	HIS
16	P	5	VAL
16	P	97	ARG
16	P	102	GLN
16	P	122	LYS
16	P	226	LYS
16	P	322	ARG
17	Q	16	LYS
17	Q	42	ARG
17	Q	44	ASN

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Mol	Chain	Res	Type
17	Q	54	LYS
17	Q	70	MET
17	Q	106	GLU
17	Q	122	PHE
18	R	3	ARG
18	R	32	GLN
18	R	94	GLN
19	S	61	GLN
19	S	74	LYS
20	T	7	THR
20	T	8	LEU
20	T	12	LYS
20	T	20	LYS
20	T	29	LYS
20	T	71	MET
20	T	72	CYS
20	T	75	GLU
20	U	12	LYS
20	U	39	ASP
20	U	71	MET
20	U	83	LYS
21	V	65	LYS
21	V	115	ILE
22	W	86	LYS
22	W	115	LYS
23	X	15	GLN
23	X	64	GLN
23	X	132	THR
24	Y	114	CYS
25	Z	4	LYS
25	Z	50	MET
25	Z	51	LYS
25	Z	98	LYS
27	b	2	GLU
28	c	1	LYS
29	d	25	LYS
29	d	111	GLU
29	d	120	ARG
30	e	7	LYS
30	e	18	THR
30	e	80	ARG
30	e	97	HIS

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Mol	Chain	Res	Type
31	f	18	MET
31	f	28	ARG
31	f	29	LYS
32	g	24	LEU
32	g	90	ARG
32	g	117	LYS
33	h	6	LYS
33	h	20	ARG
33	h	130	LYS
34	i	43	GLU
34	i	51	GLN
34	i	68	ILE
35	j	39	ARG
36	k	91	LYS
37	l	4	ILE
37	l	6	LYS
37	l	25	LYS
37	l	126	GLN
38	m	24	ILE
38	m	79	PHE
38	m	86	SER
38	m	119	LYS
39	n	14	LYS
39	n	46	ARG
39	n	111	LYS
39	n	135	GLU
39	n	137	LYS
40	o	7	ARG
40	o	15	GLU
40	o	21	MET
40	o	34	LYS
40	o	83	ARG
41	p	69	ARG
41	p	126	LYS
42	q	5	GLN
42	q	59	HIS
42	q	95	ASP
42	q	107	LYS
42	q	122	GLN
42	q	136	GLU
42	q	144	TYR
43	r	105	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	94	ASN
4	D	79	HIS
4	D	217	ASN
5	E	27	ASN
5	E	121	GLN
6	F	421	HIS
8	H	248	ASN
12	L	194	ASN
12	L	541	ASN
13	M	220	HIS
13	M	304	GLN
13	M	331	ASN
14	N	49	ASN
15	O	114	HIS
16	P	49	HIS
16	P	87	HIS
16	P	93	ASN
16	P	131	HIS
17	Q	29	HIS
18	R	94	GLN
21	V	95	GLN
22	W	125	HIS
23	X	63	ASN
23	X	105	GLN
25	Z	75	GLN
29	d	79	GLN
30	e	6	GLN
30	e	20	GLN
30	e	26	HIS
30	e	76	HIS
32	g	119	GLN
34	i	127	HIS
37	l	66	HIS
39	n	32	HIS
40	o	43	GLN
40	o	53	GLN
42	q	31	ASN
42	q	91	HIS
43	r	12	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	H	1	8	8,9,10	1.50	1 (12%)	8,9,11	1.56	3 (37%)
1	FME	A	1	1	8,9,10	1.47	1 (12%)	8,9,11	1.32	1 (12%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.50	2 (25%)
24	AYA	Y	1	24	6,7,8	1.88	2 (33%)	6,8,10	1.48	1 (16%)
13	FME	M	1	13	8,9,10	1.48	1 (12%)	8,9,11	1.52	3 (37%)
29	AME	d	1	29	9,10,11	1.52	1 (11%)	9,11,13	1.20	1 (11%)
34	SAC	i	1	34	7,8,9	1.75	1 (14%)	7,9,11	1.62	1 (14%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.49	3 (37%)
27	AYA	b	1	27	6,7,8	1.90	1 (16%)	6,8,10	1.31	1 (16%)
42	AME	q	1	42	9,10,11	1.55	1 (11%)	9,11,13	1.33	2 (22%)
11	FME	K	1	11	8,9,10	1.52	1 (12%)	8,9,11	1.27	0
43	AYA	r	1	43	6,7,8	1.86	2 (33%)	6,8,10	1.33	1 (16%)
38	SAC	m	1	38	7,8,9	1.77	1 (14%)	7,9,11	1.30	1 (14%)
10	FME	J	1	10	8,9,10	1.53	1 (12%)	8,9,11	1.39	2 (25%)
4	2MR	D	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.43	1 (20%)

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
8	FME	H	1	8	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	2/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
24	AYA	Y	1	24	-	1/5/6/8	-
13	FME	M	1	13	-	2/7/9/11	-
29	AME	d	1	29	-	0/9/10/12	-
34	SAC	i	1	34	-	4/7/8/10	-
14	FME	N	1	14	-	2/7/9/11	-
27	AYA	b	1	27	-	0/5/6/8	-
42	AME	q	1	42	-	5/9/10/12	-
11	FME	K	1	11	-	5/7/9/11	-
43	AYA	r	1	43	-	1/5/6/8	-
38	SAC	m	1	38	-	3/7/8/10	-
10	FME	J	1	10	-	4/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.46	1.44	1.33
4	D	85	2MR	CZ-NE	5.10	1.45	1.34
11	K	1	FME	CN-N	3.81	1.45	1.33
10	J	1	FME	CN-N	3.78	1.45	1.33
14	N	1	FME	CN-N	3.76	1.45	1.33
12	L	1	FME	CN-N	3.69	1.45	1.33
38	m	1	SAC	C1A-N	3.68	1.46	1.34
8	H	1	FME	CN-N	3.66	1.45	1.33
13	M	1	FME	CN-N	3.66	1.45	1.33
1	A	1	FME	CN-N	3.65	1.45	1.33
34	i	1	SAC	C1A-N	3.57	1.45	1.34
42	q	1	AME	CT1-N	3.57	1.45	1.34
27	b	1	AYA	CT-N	3.53	1.45	1.34
29	d	1	AME	CT1-N	3.48	1.45	1.34
24	Y	1	AYA	CT-N	3.46	1.45	1.34
43	r	1	AYA	CT-N	3.37	1.45	1.34
43	r	1	AYA	OT-CT	-2.10	1.18	1.23
24	Y	1	AYA	OT-CT	-2.04	1.18	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C2A-C1A-N	3.17	121.38	116.12
42	q	1	AME	CE-SD-CG	2.61	113.83	100.32
4	D	85	2MR	CD-NE-CZ	-2.60	118.48	123.36
24	Y	1	AYA	CM-CT-N	2.56	120.37	116.12
27	b	1	AYA	CM-CT-N	2.37	120.05	116.12
43	r	1	AYA	CM-CT-N	2.35	120.02	116.12
38	m	1	SAC	C2A-C1A-N	2.25	119.86	116.12
12	L	1	FME	CA-N-CN	-2.25	119.36	122.82
8	H	1	FME	O1-CN-N	-2.24	119.54	125.32
8	H	1	FME	CA-N-CN	-2.18	119.47	122.82
13	M	1	FME	CA-N-CN	-2.17	119.48	122.82
12	L	1	FME	O1-CN-N	-2.15	119.77	125.32
14	N	1	FME	CA-N-CN	-2.14	119.53	122.82
8	H	1	FME	CE-SD-CG	2.12	111.30	100.32
1	A	1	FME	O1-CN-N	-2.11	119.87	125.32
13	M	1	FME	O-C-CA	-2.07	119.44	124.77
42	q	1	AME	CT2-CT1-N	2.07	119.55	116.12
10	J	1	FME	O1-CN-N	-2.05	120.01	125.32
13	M	1	FME	O1-CN-N	-2.05	120.03	125.32
29	d	1	AME	CT2-CT1-N	2.04	119.50	116.12
14	N	1	FME	CE-SD-CG	2.03	110.85	100.32
14	N	1	FME	O1-CN-N	-2.02	120.09	125.32
10	J	1	FME	CA-N-CN	-2.02	119.71	122.82

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-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
24	Y	1	AYA	O-C-CA-CB
34	i	1	SAC	N-CA-CB-OG
34	i	1	SAC	C-CA-CB-OG
38	m	1	SAC	O-C-CA-CB
38	m	1	SAC	C-CA-CB-OG
42	q	1	AME	C-CA-CB-CG
43	r	1	AYA	O-C-CA-CB
8	H	1	FME	CB-CG-SD-CE
14	N	1	FME	CB-CG-SD-CE
34	i	1	SAC	C2A-C1A-N-CA

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

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
12	L	1	FME	1	0
27	b	1	AYA	1	0
42	q	1	AME	1	0
4	D	85	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 80 ligands modelled in this entry, 4 are monoatomic - leaving 76 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	J	203	-	43,43,50	0.95	4 (9%)	46,48,55	1.15	2 (4%)
45	3PE	e	201	-	48,48,50	0.90	4 (8%)	51,53,55	1.09	2 (3%)
45	3PE	L	708	-	38,38,50	0.99	4 (10%)	41,43,55	1.15	2 (4%)
47	PLC	g	201	-	31,31,41	0.57	0	37,39,49	0.56	0
45	3PE	b	103	-	50,50,50	0.88	4 (8%)	53,55,55	1.06	2 (3%)
47	PLC	O	403	-	31,31,41	0.58	0	37,39,49	0.59	0
45	3PE	b	102	-	46,46,50	0.89	3 (6%)	49,51,55	1.10	2 (4%)
46	PC1	B	203	-	47,47,53	1.01	4 (8%)	53,55,61	1.05	2 (3%)
45	3PE	A	201	-	30,30,50	1.12	4 (13%)	33,35,55	1.12	2 (6%)
48	SF4	B	201	2	0,12,12	-	-	-	-	-
45	3PE	q	201	-	20,20,50	1.33	4 (20%)	23,25,55	1.05	2 (8%)
46	PC1	h	201	-	46,46,53	1.02	4 (8%)	52,54,61	1.06	2 (3%)
45	3PE	L	706	-	50,50,50	0.87	4 (8%)	53,55,55	1.07	2 (3%)
47	PLC	d	203	-	35,35,41	0.55	0	41,43,49	0.54	0
47	PLC	B	204	-	36,36,41	0.55	0	42,44,49	0.52	0
52	CDL	H	401	-	82,82,99	0.97	8 (9%)	88,94,111	1.10	4 (4%)
47	PLC	P	504	-	26,26,41	0.63	0	32,34,49	0.62	0
57	EHZ	U	101	20	31,36,37	1.56	5 (16%)	36,44,47	1.73	7 (19%)
57	EHZ	T	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.80	8 (22%)
48	SF4	F	502	6	0,12,12	-	-	-	-	-
48	SF4	G	801	7	0,12,12	-	-	-	-	-
47	PLC	A	206	-	37,37,41	0.55	0	43,45,49	0.60	0
52	CDL	i	202	-	79,79,99	0.98	8 (10%)	85,91,111	1.15	4 (4%)
45	3PE	I	203	-	37,37,50	1.00	4 (10%)	40,42,55	1.12	2 (5%)
45	3PE	m	203	-	41,41,50	0.95	4 (9%)	44,46,55	1.15	2 (4%)
48	SF4	I	202	9	0,12,12	-	-	-	-	-
52	CDL	M	602	-	99,99,99	0.89	8 (8%)	105,111,111	1.12	4 (3%)
46	PC1	M	605	-	43,43,53	1.05	4 (9%)	49,51,61	1.03	2 (4%)
45	3PE	P	503	-	31,31,50	1.06	4 (12%)	34,36,55	1.14	2 (5%)
50	FMN	F	501	-	33,33,33	2.73	10 (30%)	48,50,50	1.74	13 (27%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
58	CHD	i	201	-	32,32,32	3.25	11 (34%)	51,51,51	2.33	18 (35%)
46	PC1	H	402	-	47,47,53	1.04	4 (8%)	53,55,61	1.03	2 (3%)
47	PLC	J	204	-	37,37,41	0.54	0	43,45,49	0.54	0
45	3PE	Y	201	-	50,50,50	0.88	4 (8%)	53,55,55	1.11	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	A	203	-	34,34,53	1.18	4 (11%)	40,42,61	1.01	2 (5%)
55	DGT	O	402	54	32,33,33	3.29	14 (43%)	48,52,52	1.92	14 (29%)
45	3PE	Y	202	-	46,46,50	0.90	4 (8%)	49,51,55	1.09	2 (4%)
46	PC1	M	606	-	34,34,53	1.17	4 (11%)	40,42,61	1.11	2 (5%)
45	3PE	N	402	-	48,48,50	0.88	4 (8%)	51,53,55	1.01	2 (3%)
45	3PE	L	702	-	34,34,50	0.98	3 (8%)	37,39,55	1.07	1 (2%)
46	PC1	A	205	-	32,32,53	1.23	4 (12%)	38,40,61	1.10	2 (5%)
46	PC1	Y	203	-	44,44,53	1.06	4 (9%)	50,52,61	1.03	2 (4%)
46	PC1	q	202	-	37,37,53	1.07	3 (8%)	43,45,61	0.91	1 (2%)
59	MYR	o	201	40	13,14,15	0.40	0	12,13,15	0.86	0
45	3PE	Z	201	-	41,41,50	0.97	4 (9%)	44,46,55	1.10	2 (4%)
47	PLC	L	710	-	30,30,41	0.59	0	36,38,49	0.59	0
45	3PE	L	707	-	50,50,50	0.88	4 (8%)	53,55,55	1.09	2 (3%)
52	CDL	L	701	-	75,75,99	1.01	8 (10%)	81,87,111	1.10	4 (4%)
46	PC1	Z	202	-	43,43,53	1.07	4 (9%)	49,51,61	1.02	2 (4%)
52	CDL	r	201	-	60,60,99	1.11	8 (13%)	66,72,111	1.22	4 (6%)
45	3PE	m	201	-	49,49,50	0.87	4 (8%)	52,54,55	1.07	2 (3%)
45	3PE	M	603	-	39,39,50	0.99	4 (10%)	42,44,55	1.09	2 (4%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	L	704	-	39,39,50	0.98	4 (10%)	42,44,55	1.10	2 (4%)
45	3PE	M	604	-	44,44,50	0.91	4 (9%)	47,49,55	1.07	2 (4%)
46	PC1	d	202	-	38,38,53	1.12	4 (10%)	44,46,61	1.09	2 (4%)
46	PC1	H	403	-	38,38,53	1.13	4 (10%)	44,46,61	0.96	2 (4%)
48	SF4	I	201	9	0,12,12	-	-	-	-	-
52	CDL	N	401	-	79,79,99	0.98	8 (10%)	85,91,111	1.14	4 (4%)
45	3PE	J	202	-	30,30,50	1.10	4 (13%)	33,35,55	1.25	3 (9%)
56	NDP	P	501	-	51,52,52	3.99	27 (52%)	71,80,80	1.96	14 (19%)
45	3PE	m	202	-	40,40,50	0.97	4 (10%)	43,45,55	1.06	2 (4%)
45	3PE	A	202	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	2 (3%)
52	CDL	d	201	-	64,64,99	1.08	8 (12%)	70,76,111	1.12	4 (5%)
46	PC1	I	204	-	53,53,53	0.95	4 (7%)	59,61,61	0.99	2 (3%)
48	SF4	G	802	7	0,12,12	-	-	-	-	-
46	PC1	A	204	-	34,34,53	1.16	4 (11%)	40,42,61	1.06	2 (5%)
46	PC1	B	202	-	45,45,53	1.03	3 (6%)	51,53,61	1.07	3 (5%)
52	CDL	J	201	-	69,69,99	1.06	8 (11%)	75,81,111	1.19	4 (5%)
46	PC1	L	709	-	44,44,53	1.04	4 (9%)	50,52,61	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	CDL	X	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.08	4 (3%)
45	3PE	L	703	-	44,44,50	0.91	4 (9%)	47,49,55	1.11	2 (4%)
45	3PE	L	705	-	22,22,50	1.28	4 (18%)	25,27,55	1.31	2 (8%)
45	3PE	b	101	-	40,40,50	0.96	3 (7%)	43,45,55	1.09	2 (4%)
45	3PE	P	502	-	34,34,50	1.05	4 (11%)	37,39,55	1.15	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	J	203	-	-	23/47/47/54	-
45	3PE	e	201	-	-	23/52/52/54	-
45	3PE	L	708	-	-	12/42/42/54	-
47	PLC	g	201	-	-	7/34/34/45	-
45	3PE	b	103	-	-	26/54/54/54	-
47	PLC	O	403	-	-	9/34/34/45	-
45	3PE	b	102	-	-	21/50/50/54	-
46	PC1	B	203	-	-	17/51/51/57	-
45	3PE	A	201	-	-	17/34/34/54	-
48	SF4	B	201	2	-	-	0/6/5/5
45	3PE	q	201	-	-	13/24/24/54	-
46	PC1	h	201	-	-	28/50/50/57	-
45	3PE	L	706	-	-	21/54/54/54	-
47	PLC	d	203	-	-	20/39/39/45	-
47	PLC	B	204	-	-	12/40/40/45	-
52	CDL	H	401	-	-	41/93/93/110	-
47	PLC	P	504	-	-	4/29/29/45	-
57	EHZ	U	101	20	-	10/42/44/45	-
57	EHZ	T	101	20	-	4/42/44/45	-
48	SF4	F	502	6	-	-	0/6/5/5
48	SF4	G	801	7	-	-	0/6/5/5
47	PLC	A	206	-	-	18/41/41/45	-
52	CDL	i	202	-	-	27/90/90/110	-
45	3PE	I	203	-	-	20/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	m	203	-	-	14/45/45/54	-
52	CDL	M	602	-	-	52/110/110/110	-
48	SF4	I	202	9	-	-	0/6/5/5
46	PC1	M	605	-	-	19/47/47/57	-
45	3PE	P	503	-	-	15/35/35/54	-
50	FMN	F	501	-	-	9/18/18/18	0/3/3/3
49	FES	G	803	7	-	-	0/1/1/1
58	CHD	i	201	-	-	4/9/74/74	0/4/4/4
46	PC1	H	402	-	-	16/51/51/57	-
47	PLC	J	204	-	-	18/41/41/45	-
45	3PE	Y	201	-	-	27/54/54/54	-
46	PC1	A	203	-	-	25/38/38/57	-
55	DGT	O	402	54	-	7/22/34/34	0/3/3/3
45	3PE	Y	202	-	-	18/50/50/54	-
46	PC1	M	606	-	-	15/38/38/57	-
45	3PE	N	402	-	-	25/52/52/54	-
45	3PE	L	702	-	-	11/37/37/54	-
46	PC1	A	205	-	-	17/36/36/57	-
46	PC1	Y	203	-	-	23/48/48/57	-
46	PC1	q	202	-	-	18/40/40/57	-
59	MYR	o	201	40	-	6/12/12/13	-
45	3PE	Z	201	-	-	18/45/45/54	-
47	PLC	L	710	-	-	16/34/34/45	-
45	3PE	L	707	-	-	18/54/54/54	-
52	CDL	L	701	-	-	31/86/86/110	-
46	PC1	Z	202	-	-	18/47/47/57	-
52	CDL	r	201	-	-	31/71/71/110	-
45	3PE	m	201	-	-	24/53/53/54	-
45	3PE	M	603	-	-	24/43/43/54	-
49	FES	E	301	5	-	-	0/1/1/1
45	3PE	L	704	-	-	17/43/43/54	-
45	3PE	M	604	-	-	23/48/48/54	-
46	PC1	d	202	-	-	12/42/42/57	-
46	PC1	H	403	-	-	16/42/42/57	-
52	CDL	N	401	-	-	40/90/90/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	I	201	9	-	-	0/6/5/5
45	3PE	J	202	-	-	14/34/34/54	-
56	NDP	P	501	-	-	10/34/77/77	0/5/5/5
45	3PE	m	202	-	-	22/44/44/54	-
45	3PE	A	202	-	-	25/54/54/54	-
52	CDL	d	201	-	-	42/75/75/110	-
46	PC1	I	204	-	-	12/57/57/57	-
52	CDL	J	201	-	-	35/80/80/110	-
46	PC1	A	204	-	-	17/38/38/57	-
46	PC1	B	202	-	-	28/49/49/57	-
48	SF4	G	802	7	-	-	0/6/5/5
46	PC1	L	709	-	-	25/48/48/57	-
52	CDL	X	201	-	-	40/110/110/110	-
45	3PE	L	703	-	-	18/48/48/54	-
45	3PE	L	705	-	-	11/26/26/54	-
45	3PE	b	101	-	-	19/44/44/54	-
45	3PE	P	502	-	-	18/38/38/54	-

All (315) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	PA-O3	10.14	1.70	1.59
56	P	501	NDP	C2B-C1B	-9.13	1.30	1.53
55	O	402	DGT	O6-C6	8.76	1.40	1.23
58	i	201	CHD	C11-C12	8.72	1.67	1.53
56	P	501	NDP	O4B-C1B	8.35	1.61	1.42
56	P	501	NDP	O4D-C1D	8.30	1.61	1.42
56	P	501	NDP	C7N-N7N	7.60	1.55	1.33
56	P	501	NDP	C2D-C1D	-7.47	1.30	1.53
56	P	501	NDP	C6N-C5N	7.12	1.55	1.33
58	i	201	CHD	C16-C15	7.09	1.73	1.54
55	O	402	DGT	C5-N7	6.74	1.52	1.39
56	P	501	NDP	O4D-C4D	-6.59	1.30	1.45
50	F	501	FMN	C10-N1	6.54	1.46	1.33
50	F	501	FMN	C4A-N5	6.44	1.44	1.30
58	i	201	CHD	C20-C17	-5.95	1.44	1.54
56	P	501	NDP	P2B-O2B	5.56	1.69	1.59
58	i	201	CHD	C13-C17	5.53	1.64	1.55
58	i	201	CHD	O12-C12	-5.45	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	O4B-C4B	-5.41	1.33	1.45
50	F	501	FMN	C5A-N5	5.39	1.49	1.39
58	i	201	CHD	C8-C9	5.39	1.64	1.53
56	P	501	NDP	C6A-N6A	5.26	1.47	1.34
55	O	402	DGT	PB-O3B	5.16	1.65	1.59
57	T	101	EHZ	C12-N1	5.14	1.45	1.33
55	O	402	DGT	PB-O3A	5.04	1.64	1.59
57	U	101	EHZ	C12-N1	4.96	1.45	1.33
55	O	402	DGT	PA-O3A	4.95	1.64	1.59
50	F	501	FMN	C2-N1	4.94	1.47	1.36
50	F	501	FMN	C9A-N10	4.94	1.49	1.41
57	U	101	EHZ	C15-N2	4.88	1.45	1.33
57	T	101	EHZ	C15-N2	4.79	1.44	1.33
55	O	402	DGT	C2-N2	4.76	1.45	1.34
58	i	201	CHD	C6-C5	4.72	1.61	1.53
55	O	402	DGT	C2-N1	4.71	1.49	1.37
56	P	501	NDP	C2N-C3N	4.55	1.47	1.35
50	F	501	FMN	C2-N3	4.49	1.48	1.39
56	P	501	NDP	C5A-C4A	-4.46	1.31	1.39
55	O	402	DGT	C2-N3	4.26	1.43	1.33
56	P	501	NDP	PN-O3	4.25	1.64	1.59
55	O	402	DGT	C8-N9	-4.23	1.28	1.37
56	P	501	NDP	O7N-C7N	-4.16	1.14	1.24
55	O	402	DGT	C4-N9	-4.05	1.27	1.38
56	P	501	NDP	C8A-N9A	-4.00	1.30	1.37
58	i	201	CHD	C15-C14	3.98	1.62	1.54
56	P	501	NDP	O2D-C2D	3.73	1.52	1.43
50	F	501	FMN	C10-N10	3.66	1.45	1.37
58	i	201	CHD	C6-C7	3.60	1.59	1.52
50	F	501	FMN	C4-N3	3.59	1.45	1.38
56	P	501	NDP	C4N-C3N	3.17	1.56	1.50
46	B	202	PC1	O21-C2	-2.99	1.39	1.46
50	F	501	FMN	O2-C2	-2.94	1.18	1.24
52	M	602	CDL	OB6-CB4	-2.93	1.39	1.46
52	r	201	CDL	OA6-CA4	-2.90	1.39	1.46
45	J	203	3PE	O21-C2	-2.86	1.39	1.46
52	M	602	CDL	OA6-CA4	-2.86	1.39	1.46
52	L	701	CDL	OA6-CA4	-2.86	1.39	1.46
52	H	401	CDL	OA6-CA4	-2.84	1.39	1.46
46	Z	202	PC1	O21-C2	-2.81	1.40	1.46
45	b	101	3PE	O21-C2	-2.81	1.40	1.46
52	r	201	CDL	OB6-CB4	-2.80	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	X	201	CDL	OB6-CB4	-2.80	1.40	1.46
50	F	501	FMN	O4-C4	-2.80	1.18	1.23
46	L	709	PC1	O21-C2	-2.78	1.40	1.46
46	A	203	PC1	O21-C2	-2.78	1.40	1.46
52	d	201	CDL	OA6-CA4	-2.77	1.40	1.46
52	i	202	CDL	OA6-CA4	-2.76	1.40	1.46
46	d	202	PC1	O21-C2	-2.76	1.40	1.46
52	L	701	CDL	OB6-CB4	-2.76	1.40	1.46
56	P	501	NDP	C5A-N7A	-2.75	1.34	1.39
52	i	202	CDL	OB6-CB4	-2.75	1.40	1.46
46	I	204	PC1	O21-C2	-2.74	1.40	1.46
45	b	102	3PE	O21-C2	-2.74	1.40	1.46
45	L	702	3PE	O21-C2	-2.74	1.40	1.46
45	P	502	3PE	O21-C2	-2.74	1.40	1.46
46	A	205	PC1	O21-C2	-2.73	1.40	1.46
46	B	203	PC1	O21-C2	-2.72	1.40	1.46
45	e	201	3PE	O21-C2	-2.72	1.40	1.46
45	L	705	3PE	O21-C2	-2.71	1.40	1.46
52	N	401	CDL	OA6-CA4	-2.71	1.40	1.46
45	L	708	3PE	O21-C2	-2.71	1.40	1.46
46	H	402	PC1	O21-C2	-2.71	1.40	1.46
52	H	401	CDL	OB6-CB4	-2.70	1.40	1.46
46	M	606	PC1	O21-C2	-2.70	1.40	1.46
45	m	201	3PE	O21-C2	-2.69	1.40	1.46
46	H	403	PC1	O21-C2	-2.68	1.40	1.46
52	d	201	CDL	OB6-CB4	-2.68	1.40	1.46
52	N	401	CDL	OB6-CB4	-2.67	1.40	1.46
52	J	201	CDL	OA6-CA4	-2.67	1.40	1.46
45	Y	201	3PE	O21-C2	-2.67	1.40	1.46
55	O	402	DGT	C1'-N9	-2.66	1.41	1.48
45	A	201	3PE	O21-C2	-2.65	1.40	1.46
45	Z	201	3PE	O21-C2	-2.65	1.40	1.46
45	q	201	3PE	O21-C2	-2.65	1.40	1.46
45	m	202	3PE	O21-C2	-2.64	1.40	1.46
56	P	501	NDP	C4N-C5N	2.64	1.55	1.49
52	J	201	CDL	OB6-CB4	-2.63	1.40	1.46
45	J	202	3PE	O21-C2	-2.63	1.40	1.46
45	A	202	3PE	O21-C2	-2.62	1.40	1.46
46	A	204	PC1	O21-C2	-2.62	1.40	1.46
46	M	605	PC1	O21-C2	-2.61	1.40	1.46
58	i	201	CHD	C13-C12	-2.60	1.50	1.54
45	I	203	3PE	O21-C2	-2.59	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	L	706	3PE	O21-C2	-2.59	1.40	1.46
45	Y	202	3PE	O21-C2	-2.58	1.40	1.46
57	T	101	EHZ	O4-C15	-2.56	1.18	1.23
46	h	201	PC1	O21-C2	-2.56	1.40	1.46
56	P	501	NDP	O3D-C3D	-2.56	1.36	1.43
45	L	704	3PE	O31-C31	2.56	1.40	1.33
45	b	103	3PE	O21-C2	-2.56	1.40	1.46
45	m	203	3PE	O21-C2	-2.56	1.40	1.46
46	Y	203	PC1	O31-C31	2.54	1.40	1.33
45	M	603	3PE	O21-C2	-2.53	1.40	1.46
52	X	201	CDL	OA8-CA7	2.52	1.40	1.33
52	r	201	CDL	OB8-CB7	2.52	1.40	1.33
52	X	201	CDL	OA6-CA4	-2.51	1.40	1.46
45	N	402	3PE	O21-C2	-2.51	1.40	1.46
52	J	201	CDL	OB8-CB7	2.50	1.40	1.33
56	P	501	NDP	O3B-C3B	-2.49	1.36	1.43
46	Y	203	PC1	O21-C2	-2.49	1.40	1.46
52	L	701	CDL	OB8-CB7	2.49	1.40	1.33
46	M	605	PC1	O31-C31	2.48	1.40	1.33
57	U	101	EHZ	O3-C12	-2.47	1.18	1.23
45	L	707	3PE	O31-C3	-2.47	1.39	1.45
45	m	202	3PE	O31-C31	2.47	1.40	1.33
45	L	703	3PE	O21-C2	-2.47	1.40	1.46
46	q	202	PC1	O21-C2	-2.47	1.40	1.46
45	L	707	3PE	O21-C2	-2.46	1.40	1.46
52	N	401	CDL	OA8-CA7	2.46	1.40	1.33
46	A	204	PC1	O31-C31	2.46	1.40	1.33
52	X	201	CDL	OB8-CB6	-2.46	1.39	1.45
45	I	203	3PE	O31-C31	2.45	1.40	1.33
45	L	703	3PE	O31-C31	2.44	1.40	1.33
45	Y	201	3PE	O31-C3	-2.43	1.39	1.45
46	Z	202	PC1	O31-C31	2.43	1.40	1.33
45	M	604	3PE	O21-C2	-2.43	1.40	1.46
57	T	101	EHZ	O3-C12	-2.42	1.18	1.23
52	i	202	CDL	OB8-CB7	2.42	1.40	1.33
57	U	101	EHZ	O4-C15	-2.41	1.18	1.23
45	P	503	3PE	O21-C2	-2.41	1.40	1.46
45	e	201	3PE	O31-C31	2.41	1.40	1.33
52	H	401	CDL	OA8-CA6	-2.40	1.39	1.45
45	Z	201	3PE	O31-C31	2.40	1.40	1.33
57	T	101	EHZ	C9-S1	2.40	1.81	1.76
52	i	202	CDL	OA8-CA7	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	402	PC1	O31-C31	2.39	1.40	1.33
45	m	203	3PE	O31-C31	2.39	1.40	1.33
46	M	606	PC1	O31-C31	2.39	1.40	1.33
52	r	201	CDL	OA8-CA6	-2.38	1.39	1.45
46	I	204	PC1	O31-C31	2.38	1.40	1.33
45	L	704	3PE	O21-C2	-2.38	1.41	1.46
52	d	201	CDL	OB8-CB7	2.37	1.40	1.33
52	J	201	CDL	OA8-CA7	2.37	1.40	1.33
52	M	602	CDL	OA8-CA7	2.37	1.40	1.33
46	A	205	PC1	O31-C31	2.37	1.40	1.33
52	H	401	CDL	OB8-CB7	2.37	1.40	1.33
45	b	101	3PE	O31-C31	2.37	1.40	1.33
56	P	501	NDP	C6N-N1N	2.36	1.43	1.37
45	A	201	3PE	O31-C31	2.36	1.40	1.33
45	J	203	3PE	O31-C3	-2.36	1.39	1.45
45	b	102	3PE	O31-C3	-2.36	1.39	1.45
46	h	201	PC1	O31-C31	2.35	1.40	1.33
45	A	201	3PE	O31-C3	-2.35	1.39	1.45
52	M	602	CDL	OB8-CB7	2.35	1.40	1.33
45	M	603	3PE	O31-C31	2.35	1.40	1.33
46	d	202	PC1	O31-C3	-2.34	1.39	1.45
45	q	201	3PE	O31-C31	2.34	1.40	1.33
46	Y	203	PC1	O21-C21	2.34	1.40	1.34
45	P	502	3PE	O31-C3	-2.34	1.39	1.45
45	P	503	3PE	O31-C31	2.33	1.40	1.33
45	A	202	3PE	O31-C3	-2.33	1.40	1.45
46	d	202	PC1	O31-C31	2.33	1.40	1.33
45	L	708	3PE	O31-C31	2.33	1.40	1.33
45	M	604	3PE	O31-C31	2.33	1.40	1.33
52	d	201	CDL	OA8-CA7	2.33	1.40	1.33
46	H	403	PC1	O31-C3	-2.33	1.40	1.45
46	H	403	PC1	O31-C31	2.32	1.40	1.33
46	B	203	PC1	O31-C31	2.31	1.40	1.33
46	L	709	PC1	O31-C31	2.31	1.40	1.33
52	M	602	CDL	OB8-CB6	-2.30	1.40	1.45
45	Y	202	3PE	O31-C3	-2.30	1.40	1.45
46	Z	202	PC1	O31-C3	-2.30	1.40	1.45
52	L	701	CDL	OA8-CA7	2.30	1.40	1.33
45	J	202	3PE	O31-C31	2.29	1.40	1.33
45	b	103	3PE	O31-C3	-2.29	1.40	1.45
45	M	603	3PE	O31-C3	-2.29	1.40	1.45
52	H	401	CDL	OB8-CB6	-2.29	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	b	103	3PE	O31-C31	2.29	1.40	1.33
56	P	501	NDP	C7N-C3N	2.29	1.53	1.48
45	M	603	3PE	O21-C21	2.29	1.40	1.34
45	L	705	3PE	O31-C31	2.28	1.40	1.33
45	N	402	3PE	O31-C3	-2.28	1.40	1.45
46	B	202	PC1	O31-C31	2.28	1.40	1.33
46	H	402	PC1	O31-C3	-2.28	1.40	1.45
55	O	402	DGT	PG-O2G	-2.28	1.46	1.54
57	U	101	EHZ	C9-S1	2.27	1.81	1.76
46	A	203	PC1	O31-C31	2.27	1.40	1.33
52	N	401	CDL	OB8-CB7	2.27	1.40	1.33
45	J	203	3PE	O31-C31	2.26	1.40	1.33
52	N	401	CDL	OB8-CB6	-2.26	1.40	1.45
45	m	201	3PE	O31-C31	2.26	1.39	1.33
45	Z	201	3PE	O31-C3	-2.26	1.40	1.45
45	e	201	3PE	O31-C3	-2.26	1.40	1.45
45	m	201	3PE	O31-C3	-2.26	1.40	1.45
45	q	201	3PE	O31-C3	-2.26	1.40	1.45
56	P	501	NDP	P2B-O1X	2.26	1.57	1.50
45	L	706	3PE	O31-C31	2.26	1.39	1.33
46	h	201	PC1	O31-C3	-2.26	1.40	1.45
46	L	709	PC1	O31-C3	-2.25	1.40	1.45
52	d	201	CDL	OA8-CA6	-2.25	1.40	1.45
45	N	402	3PE	O31-C31	2.25	1.39	1.33
45	L	705	3PE	O31-C3	-2.25	1.40	1.45
52	X	201	CDL	OA6-CA5	2.24	1.40	1.34
45	A	202	3PE	O31-C31	2.24	1.39	1.33
46	A	203	PC1	O31-C3	-2.24	1.40	1.45
45	Y	201	3PE	O31-C31	2.23	1.39	1.33
45	Y	202	3PE	O31-C31	2.23	1.39	1.33
45	L	707	3PE	O21-C21	2.23	1.40	1.34
45	m	202	3PE	O21-C21	2.23	1.40	1.34
45	P	502	3PE	O31-C31	2.23	1.39	1.33
52	r	201	CDL	OA8-CA7	2.22	1.39	1.33
55	O	402	DGT	PG-O1G	-2.22	1.46	1.54
46	q	202	PC1	O21-C21	2.22	1.40	1.34
52	J	201	CDL	OA8-CA6	-2.22	1.40	1.45
46	B	202	PC1	O31-C3	-2.22	1.40	1.45
45	L	704	3PE	O21-C21	2.21	1.40	1.34
45	L	706	3PE	O31-C3	-2.21	1.40	1.45
45	b	101	3PE	O31-C3	-2.21	1.40	1.45
46	H	403	PC1	O21-C21	2.21	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Z	201	3PE	O21-C21	2.21	1.40	1.34
45	L	708	3PE	O31-C3	-2.20	1.40	1.45
45	L	707	3PE	O31-C31	2.20	1.39	1.33
52	J	201	CDL	OA6-CA5	2.20	1.40	1.34
46	h	201	PC1	O21-C21	2.20	1.40	1.34
45	b	102	3PE	O31-C31	2.20	1.39	1.33
52	d	201	CDL	OB8-CB6	-2.20	1.40	1.45
45	b	103	3PE	O21-C21	2.20	1.40	1.34
46	B	203	PC1	O21-C21	2.20	1.40	1.34
52	H	401	CDL	OA8-CA7	2.20	1.39	1.33
56	P	501	NDP	PA-O5B	2.19	1.68	1.59
45	J	202	3PE	O31-C3	-2.19	1.40	1.45
45	M	604	3PE	O21-C21	2.19	1.40	1.34
52	i	202	CDL	OB8-CB6	-2.19	1.40	1.45
52	L	701	CDL	OB8-CB6	-2.18	1.40	1.45
52	d	201	CDL	OB6-CB5	2.18	1.40	1.34
46	M	605	PC1	O31-C3	-2.18	1.40	1.45
45	m	201	3PE	O21-C21	2.18	1.40	1.34
52	J	201	CDL	OB6-CB5	2.18	1.40	1.34
52	M	602	CDL	OA8-CA6	-2.17	1.40	1.45
46	A	205	PC1	O31-C3	-2.17	1.40	1.45
45	N	402	3PE	O21-C21	2.16	1.40	1.34
46	H	402	PC1	O21-C21	2.16	1.40	1.34
45	m	203	3PE	O31-C3	-2.16	1.40	1.45
46	A	204	PC1	O21-C21	2.15	1.40	1.34
46	I	204	PC1	O31-C3	-2.15	1.40	1.45
45	L	704	3PE	O31-C3	-2.15	1.40	1.45
45	I	203	3PE	O21-C21	2.15	1.40	1.34
45	m	202	3PE	O31-C3	-2.15	1.40	1.45
45	P	503	3PE	O21-C21	2.14	1.40	1.34
52	r	201	CDL	OB8-CB6	-2.14	1.40	1.45
45	L	703	3PE	O31-C3	-2.13	1.40	1.45
45	m	203	3PE	O21-C21	2.13	1.40	1.34
52	J	201	CDL	OB8-CB6	-2.13	1.40	1.45
45	I	203	3PE	O31-C3	-2.13	1.40	1.45
46	A	205	PC1	O21-C21	2.13	1.40	1.34
46	I	204	PC1	O21-C21	2.13	1.40	1.34
45	q	201	3PE	O21-C21	2.12	1.40	1.34
45	A	201	3PE	O21-C21	2.12	1.40	1.34
46	L	709	PC1	O21-C21	2.12	1.40	1.34
52	N	401	CDL	OB6-CB5	2.12	1.40	1.34
46	Z	202	PC1	O21-C21	2.12	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	q	202	PC1	O31-C3	-2.11	1.40	1.45
45	Y	202	3PE	O21-C21	2.11	1.40	1.34
45	L	702	3PE	O21-C21	2.11	1.40	1.34
46	M	606	PC1	O21-C21	2.11	1.40	1.34
52	H	401	CDL	OB6-CB5	2.11	1.40	1.34
45	L	703	3PE	O21-C21	2.11	1.40	1.34
46	M	606	PC1	O31-C3	-2.10	1.40	1.45
45	J	202	3PE	O21-C21	2.10	1.40	1.34
52	L	701	CDL	OA8-CA6	-2.10	1.40	1.45
46	M	605	PC1	O21-C21	2.10	1.40	1.34
45	L	706	3PE	O21-C21	2.09	1.40	1.34
52	N	401	CDL	OA8-CA6	-2.08	1.40	1.45
45	M	604	3PE	O31-C3	-2.08	1.40	1.45
58	i	201	CHD	C11-C9	-2.08	1.50	1.53
52	r	201	CDL	OB6-CB5	2.07	1.40	1.34
45	P	503	3PE	O31-C3	-2.07	1.40	1.45
46	A	204	PC1	O31-C3	-2.07	1.40	1.45
52	i	202	CDL	OA8-CA6	-2.07	1.40	1.45
52	N	401	CDL	OA6-CA5	2.07	1.40	1.34
45	L	708	3PE	O21-C21	2.06	1.40	1.34
45	L	702	3PE	O31-C3	-2.06	1.40	1.45
45	Y	201	3PE	O21-C21	2.06	1.40	1.34
52	i	202	CDL	OB6-CB5	2.05	1.40	1.34
46	B	203	PC1	O31-C3	-2.05	1.40	1.45
45	A	202	3PE	O21-C21	2.05	1.40	1.34
45	L	705	3PE	O21-C21	2.05	1.40	1.34
52	X	201	CDL	OA8-CA6	-2.04	1.40	1.45
45	J	203	3PE	O21-C21	2.04	1.40	1.34
46	A	203	PC1	O21-C21	2.04	1.40	1.34
45	P	502	3PE	O21-C21	2.03	1.40	1.34
52	M	602	CDL	OB6-CB5	2.03	1.40	1.34
52	H	401	CDL	OA6-CA5	2.03	1.40	1.34
52	d	201	CDL	OA6-CA5	2.03	1.40	1.34
52	X	201	CDL	OB6-CB5	2.03	1.40	1.34
56	P	501	NDP	P2B-O3X	-2.03	1.47	1.54
52	i	202	CDL	OA6-CA5	2.02	1.40	1.34
46	d	202	PC1	O21-C21	2.02	1.40	1.34
52	L	701	CDL	OA6-CA5	2.02	1.40	1.34
45	e	201	3PE	O21-C21	2.02	1.40	1.34
46	Y	203	PC1	O31-C3	-2.02	1.40	1.45
52	L	701	CDL	OB6-CB5	2.02	1.40	1.34
52	r	201	CDL	OA6-CA5	2.02	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	X	201	CDL	OB8-CB7	2.02	1.39	1.33
52	M	602	CDL	OA6-CA5	2.01	1.40	1.34
55	O	402	DGT	C4-N3	2.00	1.38	1.34

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	O	402	DGT	C8-N9-C4	7.49	120.06	106.03
57	T	101	EHZ	C8-C9-S1	6.46	121.71	113.56
58	i	201	CHD	C17-C13-C14	6.13	106.27	100.11
56	P	501	NDP	N3A-C2A-N1A	-5.79	119.81	128.58
57	U	101	EHZ	C8-C9-S1	5.72	120.78	113.56
56	P	501	NDP	C4A-N9A-C1B	-5.70	113.31	126.63
56	P	501	NDP	N6A-C6A-N1A	-5.65	105.79	118.38
58	i	201	CHD	C13-C17-C20	-5.44	112.89	119.48
58	i	201	CHD	C17-C13-C12	5.27	122.41	117.67
56	P	501	NDP	C1B-N9A-C8A	5.04	138.27	127.09
56	P	501	NDP	C5A-C4A-N3A	-4.79	120.12	126.72
50	F	501	FMN	C7M-C7-C6	4.76	127.95	119.57
52	J	201	CDL	OA6-CA5-C11	4.61	121.46	111.48
45	M	603	3PE	O21-C21-C22	4.57	121.37	111.48
58	i	201	CHD	C18-C13-C12	-4.49	104.56	109.06
50	F	501	FMN	C9-C8-C7	4.48	126.26	119.69
45	m	203	3PE	O21-C21-C22	4.44	121.09	111.48
52	J	201	CDL	OB6-CB5-C51	4.40	121.00	111.48
58	i	201	CHD	C14-C13-C12	4.36	111.40	107.42
45	L	707	3PE	O21-C21-C22	4.35	120.90	111.48
52	N	401	CDL	OB6-CB5-C51	4.30	120.78	111.48
56	P	501	NDP	N9A-C8A-N7A	-4.27	107.87	113.94
46	A	205	PC1	O21-C21-C22	4.27	120.71	111.48
52	i	202	CDL	OA6-CA5-C11	4.25	120.69	111.48
52	M	602	CDL	OB6-CB5-C51	4.25	120.68	111.48
45	L	705	3PE	O21-C21-C22	4.21	120.59	111.48
52	d	201	CDL	OA6-CA5-C11	4.20	120.56	111.48
45	L	703	3PE	O21-C21-C22	4.19	120.55	111.48
45	e	201	3PE	O21-C21-C22	4.19	120.55	111.48
45	I	203	3PE	O21-C21-C22	4.18	120.53	111.48
52	M	602	CDL	OA6-CA5-C11	4.18	120.53	111.48
45	J	202	3PE	O21-C21-C22	4.16	120.49	111.48
45	b	103	3PE	O21-C21-C22	4.15	120.47	111.48
46	Y	203	PC1	O21-C21-C22	4.14	120.44	111.48
45	Y	201	3PE	O21-C21-C22	4.14	120.44	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	402	PC1	O21-C21-C22	4.14	120.44	111.48
45	P	502	3PE	O21-C21-C22	4.10	120.36	111.48
56	P	501	NDP	C5A-C6A-N6A	4.09	133.41	123.29
46	A	204	PC1	O21-C21-C22	4.09	120.33	111.48
52	N	401	CDL	OA6-CA5-C11	4.07	120.29	111.48
52	r	201	CDL	OA6-CA5-C11	4.06	120.27	111.48
52	X	201	CDL	OB6-CB5-C51	4.06	120.27	111.48
46	h	201	PC1	O21-C21-C22	4.05	120.23	111.48
46	M	606	PC1	O21-C21-C22	4.03	120.20	111.48
52	r	201	CDL	OB6-CB5-C51	4.02	120.18	111.48
45	Y	202	3PE	O21-C21-C22	4.02	120.17	111.48
45	L	708	3PE	O21-C21-C22	4.01	120.17	111.48
45	L	704	3PE	O21-C21-C22	4.00	120.14	111.48
45	Z	201	3PE	O21-C21-C22	4.00	120.13	111.48
58	i	201	CHD	C1-C10-C5	4.00	113.48	107.75
45	P	503	3PE	O21-C21-C22	3.98	120.09	111.48
52	L	701	CDL	OA6-CA5-C11	3.97	120.08	111.48
45	L	706	3PE	O21-C21-C22	3.93	119.99	111.48
46	I	204	PC1	O21-C21-C22	3.93	119.98	111.48
45	A	202	3PE	O21-C21-C22	3.92	119.96	111.48
46	B	203	PC1	O21-C21-C22	3.91	119.95	111.48
52	H	401	CDL	OB6-CB5-C51	3.91	119.93	111.48
46	d	202	PC1	O21-C21-C22	3.90	119.92	111.48
52	H	401	CDL	OA6-CA5-C11	3.89	119.89	111.48
52	X	201	CDL	OA6-CA5-C11	3.88	119.88	111.48
45	M	604	3PE	O21-C21-C22	3.87	119.86	111.48
52	i	202	CDL	OB6-CB5-C51	3.87	119.86	111.48
46	L	709	PC1	O21-C21-C22	3.87	119.85	111.48
45	A	201	3PE	O21-C21-C22	3.84	119.80	111.48
58	i	201	CHD	C18-C13-C14	-3.83	105.19	111.20
52	L	701	CDL	OB6-CB5-C51	3.83	119.77	111.48
46	A	203	PC1	O21-C21-C22	3.81	119.73	111.48
45	J	203	3PE	O21-C21-C22	3.79	119.69	111.48
46	Z	202	PC1	O21-C21-C22	3.78	119.66	111.48
45	L	702	3PE	O21-C21-C22	3.78	119.65	111.48
46	B	202	PC1	O21-C21-C22	3.76	119.61	111.48
46	M	605	PC1	O21-C21-C22	3.75	119.59	111.48
45	b	102	3PE	O21-C21-C22	3.74	119.57	111.48
45	m	202	3PE	O21-C21-C22	3.72	119.53	111.48
45	b	101	3PE	O21-C21-C22	3.71	119.50	111.48
45	N	402	3PE	O21-C21-C22	3.69	119.47	111.48
45	m	201	3PE	O21-C21-C22	3.63	119.34	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	i	201	CHD	C18-C13-C17	-3.55	105.64	111.20
50	F	501	FMN	C4-N3-C2	-3.53	119.36	125.64
56	P	501	NDP	C2A-N3A-C4A	3.50	120.38	111.83
55	O	402	DGT	C1'-N9-C8	-3.46	120.15	127.91
50	F	501	FMN	C8M-C8-C7	-3.32	113.99	120.76
57	U	101	EHZ	C14-C13-C12	-3.24	106.99	112.39
46	q	202	PC1	O21-C21-C22	3.22	118.45	111.48
58	i	201	CHD	C9-C11-C12	-3.20	110.11	114.29
55	O	402	DGT	C2-N1-C6	-3.19	119.33	125.11
52	i	202	CDL	OA8-CA7-C31	3.18	121.52	111.83
56	P	501	NDP	C2B-C1B-N9A	-3.13	108.60	113.75
58	i	201	CHD	C6-C5-C4	-3.09	107.69	111.23
52	J	201	CDL	OB8-CB7-C71	3.08	121.23	111.83
45	J	203	3PE	O31-C31-C32	3.07	121.19	111.83
57	T	101	EHZ	O2-C9-C8	-3.03	118.97	123.74
52	d	201	CDL	OB8-CB7-C71	3.01	121.02	111.83
56	P	501	NDP	N3A-C4A-N9A	2.96	132.21	127.17
46	M	605	PC1	O31-C31-C32	2.94	120.80	111.83
52	r	201	CDL	OB8-CB7-C71	2.92	120.75	111.83
46	Y	203	PC1	O31-C31-C32	2.90	120.69	111.83
45	M	604	3PE	O31-C31-C32	2.89	120.66	111.83
46	Z	202	PC1	O31-C31-C32	2.89	120.64	111.83
52	L	701	CDL	OA8-CA7-C31	2.86	120.54	111.83
46	d	202	PC1	O31-C31-C32	2.85	120.53	111.83
52	M	602	CDL	OA8-CA7-C31	2.85	120.53	111.83
45	L	704	3PE	O31-C31-C32	2.85	120.52	111.83
57	T	101	EHZ	C13-C14-N2	-2.84	105.96	112.00
57	U	101	EHZ	O2-C9-S1	-2.84	119.07	122.68
45	Y	201	3PE	O31-C31-C32	2.83	120.48	111.83
56	P	501	NDP	C5A-N7A-C8A	2.83	107.90	103.45
45	L	703	3PE	O31-C31-C32	2.83	120.47	111.83
46	H	403	PC1	O31-C31-C32	2.82	120.42	111.83
45	L	708	3PE	O31-C31-C32	2.81	120.42	111.83
58	i	201	CHD	C11-C9-C10	-2.81	110.85	113.70
45	m	203	3PE	O31-C31-C32	2.80	120.38	111.83
52	X	201	CDL	OA8-CA7-C31	2.80	120.37	111.83
45	m	201	3PE	O31-C31-C32	2.80	120.36	111.83
46	B	202	PC1	O31-C31-C32	2.80	120.36	111.83
52	H	401	CDL	OA8-CA7-C31	2.80	120.36	111.83
46	M	606	PC1	O31-C31-C32	2.79	120.35	111.83
55	O	402	DGT	O2G-PG-O3B	2.79	113.98	104.64
52	H	401	CDL	OB8-CB7-C71	2.78	120.32	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	h	201	PC1	O31-C31-C32	2.78	120.31	111.83
46	B	203	PC1	O31-C31-C32	2.78	120.31	111.83
52	i	202	CDL	OB8-CB7-C71	2.77	120.30	111.83
55	O	402	DGT	C2'-C3'-C4'	2.75	108.38	102.80
45	L	705	3PE	O31-C31-C32	2.75	120.21	111.83
52	M	602	CDL	OB8-CB7-C71	2.74	120.20	111.83
52	X	201	CDL	OB8-CB7-C71	2.74	120.20	111.83
45	L	706	3PE	O31-C31-C32	2.74	120.19	111.83
58	i	201	CHD	C19-C10-C9	-2.73	107.51	111.18
55	O	402	DGT	O1G-PG-O3B	2.72	113.76	104.64
45	J	202	3PE	O31-C31-C32	2.72	120.12	111.83
45	P	503	3PE	O31-C31-C32	2.70	120.06	111.83
45	Z	201	3PE	O31-C31-C32	2.68	120.00	111.83
45	m	202	3PE	O31-C31-C32	2.68	120.00	111.83
52	N	401	CDL	OB8-CB7-C71	2.68	119.99	111.83
52	J	201	CDL	OA8-CA7-C31	2.68	119.99	111.83
58	i	201	CHD	C23-C22-C20	-2.67	109.47	114.46
45	A	201	3PE	O31-C31-C32	2.66	119.95	111.83
46	A	204	PC1	O31-C31-C32	2.66	119.94	111.83
50	F	501	FMN	C4A-C10-N10	2.66	120.28	116.48
46	L	709	PC1	O31-C31-C32	2.65	119.93	111.83
45	q	201	3PE	O21-C21-C22	2.65	120.67	110.93
45	N	402	3PE	O31-C31-C32	2.65	119.92	111.83
57	T	101	EHZ	O2-C9-S1	-2.64	119.33	122.68
52	d	201	CDL	OA8-CA7-C31	2.63	119.87	111.83
45	Y	202	3PE	O31-C31-C32	2.63	119.85	111.83
45	P	502	3PE	O31-C31-C32	2.63	119.84	111.83
52	N	401	CDL	OA8-CA7-C31	2.62	119.84	111.83
50	F	501	FMN	C4A-C4-N3	2.62	119.93	113.25
57	T	101	EHZ	C13-C12-N1	2.62	121.12	116.34
52	r	201	CDL	OA8-CA7-C31	2.62	119.83	111.83
45	I	203	3PE	O31-C31-C32	2.62	119.81	111.83
45	b	102	3PE	O31-C31-C32	2.61	119.79	111.83
45	A	202	3PE	O31-C31-C32	2.61	119.78	111.83
45	L	707	3PE	O31-C31-C32	2.60	119.77	111.83
57	T	101	EHZ	C14-C13-C12	-2.60	108.06	112.39
45	b	103	3PE	O31-C31-C32	2.59	119.74	111.83
50	F	501	FMN	O4-C4-C4A	-2.58	119.71	126.53
45	M	603	3PE	O31-C31-C32	2.57	119.67	111.83
52	L	701	CDL	OB8-CB7-C71	2.56	119.66	111.83
56	P	501	NDP	C4A-N9A-C8A	2.55	108.42	105.74
50	F	501	FMN	C6-C7-C8	-2.55	115.94	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	402	PC1	O31-C31-C32	2.53	119.56	111.83
50	F	501	FMN	C5A-C9A-N10	2.53	120.26	117.97
46	A	203	PC1	O31-C31-C32	2.51	119.50	111.83
46	A	205	PC1	O31-C31-C32	2.49	119.44	111.83
45	e	201	3PE	O31-C31-C32	2.49	119.42	111.83
45	q	201	3PE	O31-C31-C32	2.49	118.69	111.15
45	b	101	3PE	O31-C31-C32	2.48	119.40	111.83
57	T	101	EHZ	C19-C17-C16	2.48	112.99	108.77
52	d	201	CDL	OB6-CB5-C51	2.47	120.00	110.93
55	O	402	DGT	C5-C6-N1	2.44	119.47	113.25
46	H	403	PC1	O21-C21-C22	2.42	119.81	110.93
55	O	402	DGT	O6-C6-C5	-2.40	120.19	126.53
46	I	204	PC1	O31-C31-C32	2.39	119.12	111.83
58	i	201	CHD	C15-C14-C8	2.39	121.64	118.36
58	i	201	CHD	C16-C17-C13	2.36	105.83	103.54
50	F	501	FMN	C9A-C5A-N5	-2.34	119.97	122.45
55	O	402	DGT	O1B-PB-O2B	-2.34	101.54	112.44
57	U	101	EHZ	C13-C12-N1	2.33	120.60	116.34
55	O	402	DGT	O1A-PA-O2A	-2.33	101.60	112.44
57	U	101	EHZ	O2-C9-C8	-2.28	120.15	123.74
50	F	501	FMN	C7M-C7-C8	-2.28	116.10	120.76
50	F	501	FMN	C6-C5A-C9A	2.19	122.06	119.05
55	O	402	DGT	C5-C4-N9	-2.18	101.75	105.66
58	i	201	CHD	C16-C17-C20	-2.18	108.88	112.18
50	F	501	FMN	C10-C4A-N5	-2.15	120.42	124.81
56	P	501	NDP	C4A-C5A-N7A	-2.14	108.14	110.58
57	T	101	EHZ	C7-C8-C9	-2.13	109.09	113.86
55	O	402	DGT	C1'-N9-C4	-2.12	119.78	125.50
57	U	101	EHZ	C11-N1-C12	-2.12	118.88	122.82
58	i	201	CHD	C1-C2-C3	2.09	113.25	110.48
55	O	402	DGT	N9-C8-N7	-2.09	109.53	113.40
57	U	101	EHZ	C7-C8-C9	-2.07	109.23	113.86
45	J	202	3PE	C2-O21-C21	-2.07	112.84	117.80
58	i	201	CHD	C9-C10-C5	2.04	111.35	108.51
46	B	202	PC1	C2-O21-C21	-2.04	112.92	117.80
56	P	501	NDP	C3N-C2N-N1N	-2.01	120.25	123.20
55	O	402	DGT	C8-N7-C5	-2.01	100.68	104.26

There are no chirality outliers.

All (1336) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O12
45	A	201	3PE	C11-O13-P-O14
45	A	201	3PE	O13-C11-C12-N
45	A	202	3PE	O22-C21-O21-C2
45	A	202	3PE	C22-C21-O21-C2
45	I	203	3PE	C1-O11-P-O12
45	I	203	3PE	C1-O11-P-O13
45	I	203	3PE	C1-O11-P-O14
45	I	203	3PE	C11-O13-P-O11
45	I	203	3PE	C11-O13-P-O14
45	J	202	3PE	C11-O13-P-O11
45	J	202	3PE	C11-O13-P-O12
45	J	202	3PE	C12-C11-O13-P
45	J	203	3PE	C1-O11-P-O13
45	J	203	3PE	C11-O13-P-O12
45	J	203	3PE	O13-C11-C12-N
45	J	203	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
45	L	704	3PE	C22-C21-O21-C2
45	L	705	3PE	C11-O13-P-O14
45	L	705	3PE	O13-C11-C12-N
45	L	705	3PE	C22-C21-O21-C2
45	L	706	3PE	C22-C21-O21-C2
45	L	707	3PE	C1-O11-P-O12
45	L	707	3PE	C1-O11-P-O13
45	L	707	3PE	C1-O11-P-O14
45	L	708	3PE	O11-C1-C2-O21
45	L	708	3PE	O22-C21-O21-C2
45	L	708	3PE	C22-C21-O21-C2
45	M	603	3PE	C1-O11-P-O13
45	M	603	3PE	C1-O11-P-O14
45	M	603	3PE	O13-C11-C12-N
45	M	603	3PE	O21-C2-C3-O31
45	M	603	3PE	O22-C21-O21-C2
45	M	603	3PE	C22-C21-O21-C2
45	M	604	3PE	C11-O13-P-O11
45	M	604	3PE	C11-O13-P-O12
45	M	604	3PE	C22-C21-O21-C2
45	N	402	3PE	O13-C11-C12-N
45	P	502	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
45	P	502	3PE	C1-O11-P-O13
45	P	503	3PE	O13-C11-C12-N
45	P	503	3PE	C22-C21-O21-C2
45	Y	202	3PE	C12-C11-O13-P
45	Z	201	3PE	C11-O13-P-O14
45	Z	201	3PE	C12-C11-O13-P
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	103	3PE	C1-O11-P-O12
45	b	103	3PE	C1-O11-P-O13
45	b	103	3PE	O13-C11-C12-N
45	b	103	3PE	C22-C21-O21-C2
45	e	201	3PE	C1-O11-P-O12
45	e	201	3PE	C1-O11-P-O13
45	e	201	3PE	C1-O11-P-O14
45	m	201	3PE	C1-O11-P-O12
45	m	201	3PE	C1-O11-P-O13
45	m	201	3PE	C1-O11-P-O14
45	m	201	3PE	O11-C1-C2-O21
45	m	202	3PE	C1-O11-P-O12
45	m	202	3PE	C1-O11-P-O13
45	m	202	3PE	C1-O11-P-O14
45	m	202	3PE	C12-C11-O13-P
45	m	202	3PE	O13-C11-C12-N
45	m	202	3PE	O32-C31-O31-C3
45	m	203	3PE	C11-O13-P-O14
45	m	203	3PE	O22-C21-O21-C2
45	q	201	3PE	C1-O11-P-O14
45	q	201	3PE	C11-O13-P-O11
45	q	201	3PE	C22-C21-O21-C2
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	C22-C21-O21-C2
46	A	205	PC1	C11-O13-P-O12
46	A	205	PC1	C11-O13-P-O11
46	A	205	PC1	O22-C21-O21-C2
46	A	205	PC1	C22-C21-O21-C2
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	C1-O11-P-O13
46	B	202	PC1	O11-C1-C2-O21
46	B	202	PC1	C22-C21-O21-C2
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	C22-C21-O21-C2
46	H	402	PC1	C1-O11-P-O12
46	H	402	PC1	C1-O11-P-O14
46	H	402	PC1	C1-O11-P-O13
46	I	204	PC1	C11-O13-P-O12
46	I	204	PC1	C11-O13-P-O14
46	I	204	PC1	C11-O13-P-O11
46	L	709	PC1	C11-O13-P-O12
46	L	709	PC1	C11-O13-P-O11
46	L	709	PC1	O13-C11-C12-N
46	M	606	PC1	C1-O11-P-O12
46	M	606	PC1	C1-O11-P-O14
46	M	606	PC1	C1-O11-P-O13
46	M	606	PC1	C22-C21-O21-C2
46	Y	203	PC1	C11-O13-P-O11
46	Y	203	PC1	C1-O11-P-O12
46	Y	203	PC1	C1-O11-P-O14
46	Y	203	PC1	C1-O11-P-O13
46	Y	203	PC1	O21-C2-C3-O31
46	Y	203	PC1	C22-C21-O21-C2
46	Z	202	PC1	O11-C1-C2-O21
46	h	201	PC1	C11-O13-P-O14
46	q	202	PC1	C11-O13-P-O12
46	q	202	PC1	C11-O13-P-O11
46	q	202	PC1	O13-C11-C12-N
46	q	202	PC1	C2-C1-O11-P
47	A	206	PLC	C1-O3P-P-O2P
47	A	206	PLC	C1-O3P-P-O4P
47	A	206	PLC	C4-O4P-P-O3P
47	B	204	PLC	C1'-C'-O2-C2
47	J	204	PLC	C1'-C'-O2-C2
47	J	204	PLC	C4-O4P-P-O1P
47	J	204	PLC	C4-O4P-P-O2P
47	J	204	PLC	C4-O4P-P-O3P
47	L	710	PLC	C2-C1-O3P-P
47	L	710	PLC	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
47	L	710	PLC	C1-O3P-P-O2P
47	L	710	PLC	C1-O3P-P-O4P
47	L	710	PLC	C4-O4P-P-O2P
47	L	710	PLC	C4-O4P-P-O3P
47	P	504	PLC	C1-O3P-P-O2P
47	d	203	PLC	O4P-C4-C5-N
47	d	203	PLC	C1-O3P-P-O2P
47	d	203	PLC	C1-O3P-P-O4P
50	F	501	FMN	C5'-O5'-P-O1P
50	F	501	FMN	C5'-O5'-P-O2P
52	H	401	CDL	C11-CA5-OA6-CA4
52	H	401	CDL	CB2-OB2-PB2-OB3
52	H	401	CDL	CB2-OB2-PB2-OB5
52	J	201	CDL	OA7-CA5-OA6-CA4
52	J	201	CDL	C11-CA5-OA6-CA4
52	J	201	CDL	C1-CB2-OB2-PB2
52	J	201	CDL	CB3-OB5-PB2-OB2
52	J	201	CDL	CB3-OB5-PB2-OB4
52	J	201	CDL	OB7-CB5-OB6-CB4
52	L	701	CDL	O1-C1-CA2-OA2
52	L	701	CDL	CA2-OA2-PA1-OA3
52	L	701	CDL	CA3-OA5-PA1-OA2
52	L	701	CDL	CA3-OA5-PA1-OA3
52	L	701	CDL	CB2-OB2-PB2-OB4
52	L	701	CDL	CB2-OB2-PB2-OB5
52	L	701	CDL	CB3-OB5-PB2-OB4
52	M	602	CDL	C1-CA2-OA2-PA1
52	M	602	CDL	C11-CA5-OA6-CA4
52	M	602	CDL	CB2-OB2-PB2-OB4
52	M	602	CDL	OB5-CB3-CB4-OB6
52	M	602	CDL	OB7-CB5-OB6-CB4
52	M	602	CDL	C51-CB5-OB6-CB4
52	N	401	CDL	CA3-OA5-PA1-OA4
52	N	401	CDL	OA7-CA5-OA6-CA4
52	N	401	CDL	C11-CA5-OA6-CA4
52	N	401	CDL	CB2-OB2-PB2-OB3
52	N	401	CDL	CB2-OB2-PB2-OB5
52	N	401	CDL	OB6-CB4-CB6-OB8
52	N	401	CDL	C51-CB5-OB6-CB4
52	X	201	CDL	O1-C1-CB2-OB2
52	X	201	CDL	C11-CA5-OA6-CA4
52	X	201	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
52	d	201	CDL	O1-C1-CA2-OA2
52	d	201	CDL	CA2-OA2-PA1-OA3
52	d	201	CDL	CA2-OA2-PA1-OA4
52	d	201	CDL	CA2-OA2-PA1-OA5
52	d	201	CDL	CA3-OA5-PA1-OA2
52	d	201	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	CB3-OB5-PB2-OB2
52	d	201	CDL	CB3-OB5-PB2-OB3
52	d	201	CDL	CB3-OB5-PB2-OB4
52	i	202	CDL	C11-CA5-OA6-CA4
52	i	202	CDL	CB3-OB5-PB2-OB2
52	i	202	CDL	OB7-CB5-OB6-CB4
52	r	201	CDL	CA3-OA5-PA1-OA3
52	r	201	CDL	C11-CA5-OA6-CA4
52	r	201	CDL	CB2-OB2-PB2-OB3
52	r	201	CDL	CB2-OB2-PB2-OB5
52	r	201	CDL	CB3-OB5-PB2-OB2
52	r	201	CDL	CB3-OB5-PB2-OB3
52	r	201	CDL	CB3-OB5-PB2-OB4
55	O	402	DGT	PB-O3B-PG-O1G
56	P	501	NDP	O4D-C4D-C5D-O5D
57	T	101	EHZ	C6-C7-C8-C9
57	U	101	EHZ	O1-C7-C8-C9
57	U	101	EHZ	C6-C7-C8-C9
57	U	101	EHZ	C11-C10-S1-C9
58	i	201	CHD	C17-C20-C22-C23
45	P	502	3PE	O32-C31-O31-C3
46	H	403	PC1	O32-C31-O31-C3
52	J	201	CDL	OB9-CB7-OB8-CB6
52	d	201	CDL	OB9-CB7-OB8-CB6
45	L	704	3PE	C32-C31-O31-C3
45	P	502	3PE	C32-C31-O31-C3
46	H	403	PC1	C32-C31-O31-C3
52	J	201	CDL	C71-CB7-OB8-CB6
52	d	201	CDL	C71-CB7-OB8-CB6
45	A	201	3PE	O32-C31-O31-C3
45	A	202	3PE	O32-C31-O31-C3
45	J	202	3PE	O32-C31-O31-C3
45	L	704	3PE	O32-C31-O31-C3
45	L	708	3PE	O32-C31-O31-C3
45	Y	201	3PE	O32-C31-O31-C3
45	Y	202	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	m	203	3PE	O32-C31-O31-C3
46	M	605	PC1	O32-C31-O31-C3
46	Z	202	PC1	O32-C31-O31-C3
46	d	202	PC1	O32-C31-O31-C3
46	h	201	PC1	O32-C31-O31-C3
52	J	201	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OA9-CA7-OA8-CA6
52	M	602	CDL	OB9-CB7-OB8-CB6
52	i	202	CDL	OB9-CB7-OB8-CB6
47	g	201	PLC	C1B-CB-O3-C3
45	J	202	3PE	O22-C21-O21-C2
45	L	704	3PE	O22-C21-O21-C2
45	L	705	3PE	O22-C21-O21-C2
45	M	604	3PE	O22-C21-O21-C2
45	b	101	3PE	O22-C21-O21-C2
45	b	103	3PE	O22-C21-O21-C2
45	q	201	3PE	O22-C21-O21-C2
46	B	202	PC1	O22-C21-O21-C2
46	B	203	PC1	O22-C21-O21-C2
46	Y	203	PC1	O22-C21-O21-C2
47	B	204	PLC	O'-C'-O2-C2
47	J	204	PLC	O'-C'-O2-C2
52	H	401	CDL	OA7-CA5-OA6-CA4
52	M	602	CDL	OA7-CA5-OA6-CA4
52	N	401	CDL	OB7-CB5-OB6-CB4
52	X	201	CDL	OA7-CA5-OA6-CA4
52	X	201	CDL	OB7-CB5-OB6-CB4
52	i	202	CDL	OA7-CA5-OA6-CA4
52	r	201	CDL	OA7-CA5-OA6-CA4
45	A	201	3PE	C32-C31-O31-C3
45	A	202	3PE	C32-C31-O31-C3
45	Y	201	3PE	C32-C31-O31-C3
45	e	201	3PE	C32-C31-O31-C3
45	m	202	3PE	C32-C31-O31-C3
45	m	203	3PE	C32-C31-O31-C3
46	Z	202	PC1	C32-C31-O31-C3
46	d	202	PC1	C32-C31-O31-C3
46	h	201	PC1	C32-C31-O31-C3
52	J	201	CDL	C31-CA7-OA8-CA6
52	M	602	CDL	C31-CA7-OA8-CA6
45	J	202	3PE	C22-C21-O21-C2
45	m	203	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
52	J	201	CDL	C51-CB5-OB6-CB4
52	i	202	CDL	C51-CB5-OB6-CB4
52	N	401	CDL	OA9-CA7-OA8-CA6
45	J	202	3PE	C32-C31-O31-C3
45	L	707	3PE	C32-C31-O31-C3
45	L	708	3PE	C32-C31-O31-C3
45	M	603	3PE	C32-C31-O31-C3
45	Y	202	3PE	C32-C31-O31-C3
46	M	605	PC1	C32-C31-O31-C3
52	M	602	CDL	C71-CB7-OB8-CB6
52	N	401	CDL	C71-CB7-OB8-CB6
52	i	202	CDL	C71-CB7-OB8-CB6
45	M	603	3PE	O32-C31-O31-C3
45	e	201	3PE	O32-C31-O31-C3
46	Y	203	PC1	O32-C31-O31-C3
52	N	401	CDL	OB9-CB7-OB8-CB6
45	L	703	3PE	O22-C21-O21-C2
45	L	706	3PE	O22-C21-O21-C2
45	P	503	3PE	O22-C21-O21-C2
46	A	204	PC1	O22-C21-O21-C2
46	M	606	PC1	O22-C21-O21-C2
52	J	201	CDL	O1-C1-CB2-OB2
52	N	401	CDL	C31-CA7-OA8-CA6
45	P	502	3PE	C22-C21-O21-C2
46	Z	202	PC1	C22-C21-O21-C2
46	h	201	PC1	C22-C21-O21-C2
47	A	206	PLC	C1'-C'-O2-C2
45	L	707	3PE	O32-C31-O31-C3
47	g	201	PLC	OB-CB-O3-C3
46	Y	203	PC1	C32-C31-O31-C3
46	Z	202	PC1	O22-C21-O21-C2
52	J	201	CDL	CA2-C1-CB2-OB2
52	L	701	CDL	CB2-C1-CA2-OA2
52	d	201	CDL	CB2-C1-CA2-OA2
47	A	206	PLC	C1B-CB-O3-C3
52	H	401	CDL	O1-C1-CA2-OA2
45	M	604	3PE	C31-C32-C33-C34
52	M	602	CDL	CA5-C11-C12-C13
45	P	502	3PE	O22-C21-O21-C2
45	I	203	3PE	C22-C21-O21-C2
47	P	504	PLC	C1'-C'-O2-C2
45	P	502	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	M	606	PC1	O21-C2-C3-O31
52	H	401	CDL	C31-CA7-OA8-CA6
45	I	203	3PE	C21-C22-C23-C24
47	A	206	PLC	OB-CB-O3-C3
47	B	204	PLC	C'-C1'-C2'-C3'
50	F	501	FMN	O3'-C3'-C4'-C5'
50	F	501	FMN	C2'-C3'-C4'-C5'
46	H	402	PC1	C11-C12-N-C13
46	H	402	PC1	C11-C12-N-C15
45	P	503	3PE	C21-C22-C23-C24
46	B	203	PC1	C21-C22-C23-C24
47	d	203	PLC	C'-C1'-C2'-C3'
52	H	401	CDL	CB7-C71-C72-C73
52	J	201	CDL	CA5-C11-C12-C13
52	J	201	CDL	CB7-C71-C72-C73
52	N	401	CDL	CA7-C31-C32-C33
45	J	203	3PE	C31-C32-C33-C34
45	e	201	3PE	C31-C32-C33-C34
46	B	202	PC1	C31-C32-C33-C34
46	q	202	PC1	C21-C22-C23-C24
47	A	206	PLC	C'-C1'-C2'-C3'
47	g	201	PLC	C'-C1'-C2'-C3'
52	H	401	CDL	CB5-C51-C52-C53
52	L	701	CDL	CA5-C11-C12-C13
52	X	201	CDL	CA7-C31-C32-C33
52	M	602	CDL	CB5-C51-C52-C53
46	h	201	PC1	O22-C21-O21-C2
47	A	206	PLC	O'-C'-O2-C2
52	H	401	CDL	OA9-CA7-OA8-CA6
46	A	205	PC1	C21-C22-C23-C24
46	H	402	PC1	C31-C32-C33-C34
46	L	709	PC1	C21-C22-C23-C24
47	d	203	PLC	C1B-CB-O3-C3
45	Z	201	3PE	C22-C21-O21-C2
45	L	706	3PE	C31-C32-C33-C34
45	I	203	3PE	O22-C21-O21-C2
45	Z	201	3PE	O22-C21-O21-C2
47	P	504	PLC	O'-C'-O2-C2
52	X	201	CDL	CA2-C1-CB2-OB2
45	J	203	3PE	C32-C31-O31-C3
47	L	710	PLC	C1B-CB-O3-C3
52	r	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
46	q	202	PC1	C32-C31-O31-C3
52	d	201	CDL	CB7-C71-C72-C73
56	P	501	NDP	C3D-C4D-C5D-O5D
45	b	102	3PE	C22-C21-O21-C2
46	L	709	PC1	C22-C21-O21-C2
45	b	102	3PE	O22-C21-O21-C2
46	L	709	PC1	O22-C21-O21-C2
52	i	202	CDL	O1-C1-CA2-OA2
46	q	202	PC1	O11-C1-C2-O21
45	L	707	3PE	C22-C21-O21-C2
47	O	403	PLC	O2-C2-C3-O3
45	J	203	3PE	O32-C31-O31-C3
45	b	102	3PE	C2D-C2E-C2F-C2G
46	B	202	PC1	C3C-C3D-C3E-C3F
46	h	201	PC1	C27-C28-C29-C2A
46	h	201	PC1	C37-C38-C39-C3A
45	J	202	3PE	C33-C34-C35-C36
45	J	203	3PE	C32-C33-C34-C35
45	J	203	3PE	C25-C26-C27-C28
45	J	203	3PE	C26-C27-C28-C29
45	L	702	3PE	C29-C2A-C2B-C2C
45	L	703	3PE	C38-C39-C3A-C3B
45	L	703	3PE	C23-C24-C25-C26
45	L	708	3PE	C29-C2A-C2B-C2C
45	M	603	3PE	C38-C39-C3A-C3B
45	N	402	3PE	C24-C25-C26-C27
45	Y	201	3PE	C27-C28-C29-C2A
45	m	203	3PE	C24-C25-C26-C27
46	L	709	PC1	C23-C24-C25-C26
52	N	401	CDL	C55-C56-C57-C58
45	L	703	3PE	C32-C33-C34-C35
52	d	201	CDL	C72-C73-C74-C75
47	d	203	PLC	OB-CB-O3-C3
46	A	205	PC1	C32-C31-O31-C3
45	Y	201	3PE	C23-C24-C25-C26
45	m	202	3PE	C32-C33-C34-C35
47	J	204	PLC	C5B-C6B-C7B-C8B
52	H	401	CDL	C78-C79-C80-C81
52	X	201	CDL	C82-C83-C84-C85
45	M	603	3PE	C21-C22-C23-C24
45	A	202	3PE	C36-C37-C38-C39
45	b	103	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
52	M	602	CDL	C83-C84-C85-C86
45	L	702	3PE	C22-C21-O21-C2
45	Y	201	3PE	C22-C21-O21-C2
47	d	203	PLC	C1'-C'-O2-C2
45	A	202	3PE	C38-C39-C3A-C3B
45	Y	201	3PE	C22-C23-C24-C25
45	L	702	3PE	C2E-C2F-C2G-C2H
45	b	103	3PE	C35-C36-C37-C38
46	A	204	PC1	C23-C24-C25-C26
52	X	201	CDL	C16-C17-C18-C19
52	M	602	CDL	CB7-C71-C72-C73
45	e	201	3PE	C24-C25-C26-C27
47	O	403	PLC	C2'-C3'-C4'-C5'
52	H	401	CDL	C72-C73-C74-C75
52	J	201	CDL	C31-C32-C33-C34
52	M	602	CDL	C12-C13-C14-C15
52	M	602	CDL	C34-C35-C36-C37
52	X	201	CDL	C58-C59-C60-C61
47	L	710	PLC	OB-CB-O3-C3
52	r	201	CDL	OA9-CA7-OA8-CA6
46	B	202	PC1	C25-C26-C27-C28
46	L	709	PC1	C35-C36-C37-C38
46	q	202	PC1	C28-C29-C2A-C2B
47	B	204	PLC	C5B-C6B-C7B-C8B
45	L	706	3PE	C27-C28-C29-C2A
45	Y	202	3PE	C28-C29-C2A-C2B
52	H	401	CDL	C59-C60-C61-C62
52	X	201	CDL	C35-C36-C37-C38
46	B	203	PC1	C31-C32-C33-C34
46	Y	203	PC1	C31-C32-C33-C34
46	Z	202	PC1	C37-C38-C39-C3A
52	d	201	CDL	C42-C43-C44-C45
45	L	707	3PE	O22-C21-O21-C2
45	L	703	3PE	C25-C26-C27-C28
45	L	708	3PE	C25-C26-C27-C28
45	e	201	3PE	C2A-C2B-C2C-C2D
46	Y	203	PC1	C24-C25-C26-C27
52	M	602	CDL	C16-C17-C18-C19
52	M	602	CDL	C39-C40-C41-C42
52	i	202	CDL	CB2-C1-CA2-OA2
50	F	501	FMN	O3'-C3'-C4'-O4'
45	e	201	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
47	d	203	PLC	CB-C1B-C2B-C3B
52	r	201	CDL	CB7-C71-C72-C73
45	A	201	3PE	C24-C25-C26-C27
45	L	702	3PE	C23-C24-C25-C26
45	M	603	3PE	C39-C3A-C3B-C3C
45	P	502	3PE	C34-C35-C36-C37
45	Y	202	3PE	C3A-C3B-C3C-C3D
45	m	201	3PE	C32-C33-C34-C35
46	I	204	PC1	C3E-C3F-C3G-C3H
47	B	204	PLC	C4B-C5B-C6B-C7B
52	M	602	CDL	C56-C57-C58-C59
52	r	201	CDL	C71-C72-C73-C74
45	b	103	3PE	C2B-C2C-C2D-C2E
52	i	202	CDL	C57-C58-C59-C60
46	H	402	PC1	C11-C12-N-C14
45	Z	201	3PE	C28-C29-C2A-C2B
45	b	101	3PE	C2A-C2B-C2C-C2D
45	e	201	3PE	C26-C27-C28-C29
46	B	203	PC1	C3A-C3B-C3C-C3D
46	Z	202	PC1	C35-C36-C37-C38
46	h	201	PC1	C22-C23-C24-C25
52	d	201	CDL	C35-C36-C37-C38
45	N	402	3PE	C21-C22-C23-C24
46	A	204	PC1	C21-C22-C23-C24
45	m	201	3PE	C39-C3A-C3B-C3C
46	L	709	PC1	C36-C37-C38-C39
52	L	701	CDL	C52-C53-C54-C55
52	d	201	CDL	C11-CA5-OA6-CA4
50	F	501	FMN	C2'-C3'-C4'-O4'
45	Y	202	3PE	C33-C34-C35-C36
46	B	203	PC1	C36-C37-C38-C39
46	M	606	PC1	C23-C24-C25-C26
46	H	402	PC1	C28-C29-C2A-C2B
52	X	201	CDL	C22-C23-C24-C25
46	A	205	PC1	O32-C31-O31-C3
45	e	201	3PE	C34-C35-C36-C37
45	L	702	3PE	O22-C21-O21-C2
45	Y	201	3PE	O22-C21-O21-C2
47	d	203	PLC	O'-C'-O2-C2
45	A	202	3PE	C2E-C2F-C2G-C2H
45	L	706	3PE	C25-C26-C27-C28
46	B	202	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
46	M	606	PC1	C32-C33-C34-C35
52	H	401	CDL	C11-C12-C13-C14
45	Y	202	3PE	C36-C37-C38-C39
46	A	203	PC1	C32-C33-C34-C35
47	J	204	PLC	C1B-CB-O3-C3
45	A	202	3PE	C25-C26-C27-C28
45	J	203	3PE	C39-C3A-C3B-C3C
46	h	201	PC1	C28-C29-C2A-C2B
45	b	101	3PE	C26-C27-C28-C29
46	L	709	PC1	C39-C3A-C3B-C3C
52	i	202	CDL	C74-C75-C76-C77
46	L	709	PC1	C3E-C3F-C3G-C3H
52	H	401	CDL	C14-C15-C16-C17
52	J	201	CDL	C53-C54-C55-C56
46	Z	202	PC1	C22-C23-C24-C25
46	M	605	PC1	C22-C21-O21-C2
52	H	401	CDL	C51-CB5-OB6-CB4
52	L	701	CDL	C11-CA5-OA6-CA4
45	N	402	3PE	C35-C36-C37-C38
46	q	202	PC1	C2D-C2E-C2F-C2G
52	H	401	CDL	OB7-CB5-OB6-CB4
45	m	201	3PE	C22-C23-C24-C25
45	Y	201	3PE	C21-C22-C23-C24
46	A	205	PC1	C31-C32-C33-C34
58	i	201	CHD	C21-C20-C22-C23
52	J	201	CDL	C38-C39-C40-C41
52	L	701	CDL	C36-C37-C38-C39
45	A	202	3PE	C2B-C2C-C2D-C2E
47	d	203	PLC	C5B-C6B-C7B-C8B
52	H	401	CDL	C60-C61-C62-C63
52	M	602	CDL	C18-C19-C20-C21
46	q	202	PC1	O32-C31-O31-C3
45	M	603	3PE	C35-C36-C37-C38
52	L	701	CDL	C39-C40-C41-C42
52	i	202	CDL	CA5-C11-C12-C13
52	M	602	CDL	C37-C38-C39-C40
45	N	402	3PE	O11-C1-C2-O21
46	A	205	PC1	O11-C1-C2-O21
52	M	602	CDL	OA5-CA3-CA4-OA6
52	X	201	CDL	C39-C40-C41-C42
52	r	201	CDL	C51-CB5-OB6-CB4
46	h	201	PC1	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
52	d	201	CDL	C40-C41-C42-C43
52	N	401	CDL	C32-C33-C34-C35
45	L	703	3PE	C21-C22-C23-C24
45	Y	202	3PE	C2D-C2E-C2F-C2G
46	A	205	PC1	C23-C24-C25-C26
45	Z	201	3PE	O21-C2-C3-O31
45	L	706	3PE	C34-C35-C36-C37
52	X	201	CDL	C52-C53-C54-C55
45	P	503	3PE	C32-C31-O31-C3
46	M	606	PC1	C32-C31-O31-C3
45	L	707	3PE	C33-C34-C35-C36
46	H	402	PC1	C27-C28-C29-C2A
47	d	203	PLC	C7B-C8B-C9B-CAA
45	b	103	3PE	C2E-C2F-C2G-C2H
46	A	204	PC1	C33-C34-C35-C36
46	I	204	PC1	C2A-C2B-C2C-C2D
52	L	701	CDL	OA7-CA5-OA6-CA4
45	L	706	3PE	C22-C23-C24-C25
52	H	401	CDL	C54-C55-C56-C57
52	i	202	CDL	CB5-C51-C52-C53
45	m	201	3PE	C22-C21-O21-C2
45	b	101	3PE	C2D-C2E-C2F-C2G
46	M	605	PC1	C34-C35-C36-C37
47	J	204	PLC	OB-CB-O3-C3
45	L	707	3PE	C25-C26-C27-C28
45	M	603	3PE	C3A-C3B-C3C-C3D
45	Y	201	3PE	C2E-C2F-C2G-C2H
45	Y	202	3PE	C2B-C2C-C2D-C2E
47	J	204	PLC	C1'-C2'-C3'-C4'
52	M	602	CDL	C14-C15-C16-C17
45	b	102	3PE	C26-C27-C28-C29
45	Y	202	3PE	C2E-C2F-C2G-C2H
46	H	402	PC1	C37-C38-C39-C3A
45	L	703	3PE	O11-C1-C2-C3
45	L	708	3PE	O11-C1-C2-C3
45	N	402	3PE	O11-C1-C2-C3
45	m	202	3PE	O11-C1-C2-C3
46	B	202	PC1	O11-C1-C2-C3
46	Z	202	PC1	O11-C1-C2-C3
52	M	602	CDL	OA5-CA3-CA4-CA6
52	M	602	CDL	OB5-CB3-CB4-CB6
52	d	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
46	M	605	PC1	O22-C21-O21-C2
52	d	201	CDL	OA7-CA5-OA6-CA4
45	L	706	3PE	C3A-C3B-C3C-C3D
46	B	203	PC1	C26-C27-C28-C29
55	O	402	DGT	O4'-C4'-C5'-O5'
45	L	702	3PE	C27-C28-C29-C2A
46	H	402	PC1	C32-C33-C34-C35
56	P	501	NDP	C2B-O2B-P2B-O1X
52	H	401	CDL	C74-C75-C76-C77
45	I	203	3PE	C29-C2A-C2B-C2C
46	Z	202	PC1	C32-C33-C34-C35
52	N	401	CDL	C16-C17-C18-C19
52	N	401	CDL	C22-C23-C24-C25
45	A	202	3PE	C32-C33-C34-C35
45	b	103	3PE	C32-C33-C34-C35
52	H	401	CDL	C31-C32-C33-C34
45	L	702	3PE	C1-C2-C3-O31
45	M	604	3PE	C1-C2-C3-O31
45	P	502	3PE	C1-C2-C3-O31
45	b	101	3PE	C1-C2-C3-O31
46	M	606	PC1	C1-C2-C3-O31
47	A	206	PLC	C1-C2-C3-O3
47	J	204	PLC	C1-C2-C3-O3
52	d	201	CDL	CA3-CA4-CA6-OA8
45	N	402	3PE	C33-C34-C35-C36
46	q	202	PC1	C29-C2A-C2B-C2C
45	Z	201	3PE	C32-C31-O31-C3
46	L	709	PC1	C32-C31-O31-C3
45	m	203	3PE	C22-C23-C24-C25
47	B	204	PLC	C2B-C3B-C4B-C5B
47	A	206	PLC	C3'-C4'-C5'-C6'
45	m	201	3PE	C28-C29-C2A-C2B
45	P	503	3PE	O32-C31-O31-C3
45	Y	202	3PE	C2-C1-O11-P
52	r	201	CDL	C12-C13-C14-C15
46	M	606	PC1	O32-C31-O31-C3
45	Y	201	3PE	C28-C29-C2A-C2B
45	m	201	3PE	C3C-C3D-C3E-C3F
59	o	201	MYR	C5-C6-C7-C8
46	L	709	PC1	O32-C31-O31-C3
45	q	201	3PE	C32-C31-O31-C3
52	d	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
45	M	604	3PE	C1-C2-O21-C21
52	M	602	CDL	C81-C82-C83-C84
45	N	402	3PE	C2C-C2D-C2E-C2F
52	i	202	CDL	C31-C32-C33-C34
45	L	702	3PE	C25-C26-C27-C28
45	e	201	3PE	C22-C23-C24-C25
45	L	708	3PE	C33-C34-C35-C36
46	L	709	PC1	O11-C1-C2-O21
46	h	201	PC1	O11-C1-C2-O21
45	m	203	3PE	C3D-C3E-C3F-C3G
52	N	401	CDL	C71-C72-C73-C74
59	o	201	MYR	C9-C10-C11-C12
45	I	203	3PE	C32-C31-O31-C3
46	A	203	PC1	C25-C26-C27-C28
56	P	501	NDP	O4D-C1D-N1N-C6N
46	H	402	PC1	C23-C24-C25-C26
52	H	401	CDL	C13-C14-C15-C16
52	J	201	CDL	C56-C57-C58-C59
45	b	101	3PE	C24-C25-C26-C27
52	X	201	CDL	C63-C64-C65-C66
46	B	203	PC1	C3D-C3E-C3F-C3G
52	i	202	CDL	C71-C72-C73-C74
47	J	204	PLC	C8B-C9B-CAA-CBA
46	I	204	PC1	C31-C32-C33-C34
46	B	202	PC1	C33-C34-C35-C36
46	M	605	PC1	C2D-C2E-C2F-C2G
47	A	206	PLC	C6'-C7'-C8'-C9'
52	X	201	CDL	C44-C45-C46-C47
45	A	202	3PE	C3B-C3C-C3D-C3E
45	m	201	3PE	C3F-C3G-C3H-C3I
52	M	602	CDL	C64-C65-C66-C67
55	O	402	DGT	PB-O3A-PA-O2A
52	X	201	CDL	C71-CB7-OB8-CB6
45	J	202	3PE	C36-C37-C38-C39
46	M	605	PC1	C23-C24-C25-C26
46	M	605	PC1	C27-C28-C29-C2A
46	A	203	PC1	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
46	B	202	PC1	C28-C29-C2A-C2B
52	L	701	CDL	CA7-C31-C32-C33
46	d	202	PC1	C23-C24-C25-C26
45	N	402	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
52	X	201	CDL	C77-C78-C79-C80
46	A	203	PC1	C22-C23-C24-C25
45	m	201	3PE	C2-C1-O11-P
52	d	201	CDL	CA4-CA3-OA5-PA1
45	Z	201	3PE	O32-C31-O31-C3
52	H	401	CDL	C57-C58-C59-C60
45	e	201	3PE	C39-C3A-C3B-C3C
45	L	703	3PE	C31-C32-C33-C34
45	b	103	3PE	C3F-C3G-C3H-C3I
45	L	707	3PE	O11-C1-C2-C3
45	q	201	3PE	O11-C1-C2-C3
46	A	205	PC1	O11-C1-C2-C3
46	L	709	PC1	O11-C1-C2-C3
46	Y	203	PC1	O11-C1-C2-C3
46	q	202	PC1	O11-C1-C2-C3
47	L	710	PLC	O3P-C1-C2-C3
52	X	201	CDL	OA5-CA3-CA4-CA6
52	d	201	CDL	OA5-CA3-CA4-CA6
52	i	202	CDL	OB5-CB3-CB4-CB6
45	N	402	3PE	C37-C38-C39-C3A
45	P	503	3PE	C27-C28-C29-C2A
52	r	201	CDL	O1-C1-CB2-OB2
46	A	204	PC1	C31-C32-C33-C34
52	r	201	CDL	OB7-CB5-OB6-CB4
45	Y	202	3PE	C25-C26-C27-C28
45	Z	201	3PE	C27-C28-C29-C2A
52	i	202	CDL	C13-C14-C15-C16
52	r	201	CDL	C16-C17-C18-C19
45	A	201	3PE	C32-C33-C34-C35
45	L	706	3PE	C35-C36-C37-C38
47	g	201	PLC	C1'-C2'-C3'-C4'
45	q	201	3PE	O32-C31-O31-C3
46	I	204	PC1	C33-C34-C35-C36
52	i	202	CDL	C76-C77-C78-C79
52	d	201	CDL	OA9-CA7-OA8-CA6
52	d	201	CDL	C41-C42-C43-C44
52	i	202	CDL	C54-C55-C56-C57
52	L	701	CDL	C51-CB5-OB6-CB4
45	A	202	3PE	C1-C2-C3-O31
45	J	203	3PE	C1-C2-C3-O31
45	M	603	3PE	C1-C2-C3-O31
45	Z	201	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	A	203	PC1	C1-C2-C3-O31
52	N	401	CDL	CB3-CB4-CB6-OB8
52	i	202	CDL	CA3-CA4-CA6-OA8
52	d	201	CDL	C11-C12-C13-C14
45	m	202	3PE	C2A-C2B-C2C-C2D
52	d	201	CDL	C44-C45-C46-C47
52	J	201	CDL	C51-C52-C53-C54
52	N	401	CDL	C76-C77-C78-C79
45	A	202	3PE	C31-C32-C33-C34
45	A	201	3PE	O11-C1-C2-O21
45	L	706	3PE	O11-C1-C2-O21
45	P	503	3PE	O11-C1-C2-O21
45	b	101	3PE	O11-C1-C2-O21
45	b	102	3PE	O11-C1-C2-O21
46	A	203	PC1	O11-C1-C2-O21
46	M	606	PC1	O11-C1-C2-O21
52	H	401	CDL	OB5-CB3-CB4-OB6
52	r	201	CDL	OB5-CB3-CB4-OB6
52	M	602	CDL	C24-C25-C26-C27
52	H	401	CDL	C73-C74-C75-C76
45	I	203	3PE	C26-C27-C28-C29
52	X	201	CDL	C32-C33-C34-C35
57	T	101	EHZ	O1-C7-C8-C9
57	U	101	EHZ	O2-C9-S1-C10
45	Y	202	3PE	O21-C2-C3-O31
46	A	203	PC1	O21-C2-C3-O31
52	d	201	CDL	OA6-CA4-CA6-OA8
52	i	202	CDL	OA6-CA4-CA6-OA8
45	Z	201	3PE	C25-C26-C27-C28
45	m	203	3PE	C38-C39-C3A-C3B
55	O	402	DGT	C3'-C4'-C5'-O5'
45	m	201	3PE	O22-C21-O21-C2
45	I	203	3PE	O32-C31-O31-C3
52	d	201	CDL	C36-C37-C38-C39
52	M	602	CDL	CA7-C31-C32-C33
52	N	401	CDL	C78-C79-C80-C81
46	M	605	PC1	C32-C33-C34-C35
45	J	203	3PE	C23-C24-C25-C26
45	b	101	3PE	C23-C24-C25-C26
45	m	202	3PE	C33-C34-C35-C36
45	b	102	3PE	C28-C29-C2A-C2B
59	o	201	MYR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
47	A	206	PLC	C4'-C5'-C6'-C7'
52	L	701	CDL	C55-C56-C57-C58
57	U	101	EHZ	C8-C9-S1-C10
46	Y	203	PC1	C36-C37-C38-C39
52	H	401	CDL	CB2-C1-CA2-OA2
45	M	604	3PE	C36-C37-C38-C39
45	b	102	3PE	C22-C23-C24-C25
46	h	201	PC1	C29-C2A-C2B-C2C
46	Y	203	PC1	C21-C22-C23-C24
45	L	707	3PE	C36-C37-C38-C39
45	L	704	3PE	C35-C36-C37-C38
46	Z	202	PC1	C38-C39-C3A-C3B
45	A	202	3PE	O11-C1-C2-C3
45	M	603	3PE	O11-C1-C2-C3
45	m	201	3PE	O11-C1-C2-C3
46	A	204	PC1	O11-C1-C2-C3
46	h	201	PC1	O11-C1-C2-C3
47	B	204	PLC	O3P-C1-C2-C3
52	N	401	CDL	OB5-CB3-CB4-CB6
45	M	603	3PE	C33-C34-C35-C36
45	I	203	3PE	C2E-C2F-C2G-C2H
52	M	602	CDL	C59-C60-C61-C62
52	N	401	CDL	C18-C19-C20-C21
47	L	710	PLC	C1'-C'-O2-C2
46	H	402	PC1	O21-C21-C22-C23
46	A	203	PC1	O32-C31-O31-C3
52	X	201	CDL	OB9-CB7-OB8-CB6
52	M	602	CDL	C79-C80-C81-C82
45	P	502	3PE	C32-C33-C34-C35
45	e	201	3PE	C2C-C2D-C2E-C2F
45	L	707	3PE	C3-C2-O21-C21
45	P	503	3PE	C3-C2-O21-C21
52	N	401	CDL	CA6-CA4-OA6-CA5
52	X	201	CDL	CA6-CA4-OA6-CA5
55	O	402	DGT	PB-O3B-PG-O2G
57	U	101	EHZ	O3-C12-C13-C14
45	M	604	3PE	C32-C33-C34-C35
45	m	201	3PE	C36-C37-C38-C39
52	M	602	CDL	C62-C63-C64-C65
46	Z	202	PC1	C25-C26-C27-C28
46	B	202	PC1	O32-C31-O31-C3
45	A	202	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
45	I	203	3PE	O11-C1-C2-O21
45	L	703	3PE	O11-C1-C2-O21
45	L	707	3PE	O11-C1-C2-O21
45	M	603	3PE	O11-C1-C2-O21
45	e	201	3PE	O11-C1-C2-O21
46	A	204	PC1	O11-C1-C2-O21
46	Y	203	PC1	O11-C1-C2-O21
47	L	710	PLC	O3P-C1-C2-O2
52	i	202	CDL	OB5-CB3-CB4-OB6
47	g	201	PLC	C7'-C8'-C9'-CA'
45	J	203	3PE	C3D-C3E-C3F-C3G
45	L	705	3PE	C1-C2-C3-O31
46	B	202	PC1	C1-C2-C3-O31
46	Y	203	PC1	C1-C2-C3-O31
47	L	710	PLC	C1-C2-C3-O3
47	O	403	PLC	C1-C2-C3-O3
47	d	203	PLC	C1-C2-C3-O3
52	M	602	CDL	CB3-CB4-CB6-OB8
45	b	103	3PE	C38-C39-C3A-C3B
52	d	201	CDL	C38-C39-C40-C41
45	A	202	3PE	C34-C35-C36-C37
45	I	203	3PE	C12-C11-O13-P
45	L	702	3PE	C12-C11-O13-P
45	M	603	3PE	C12-C11-O13-P
45	M	604	3PE	C12-C11-O13-P
45	N	402	3PE	C12-C11-O13-P
45	Y	201	3PE	C12-C11-O13-P
45	b	103	3PE	C12-C11-O13-P
45	e	201	3PE	C12-C11-O13-P
45	m	201	3PE	C12-C11-O13-P
45	m	203	3PE	C12-C11-O13-P
45	q	201	3PE	C12-C11-O13-P
47	J	204	PLC	C5-C4-O4P-P
47	d	203	PLC	C5-C4-O4P-P
47	J	204	PLC	C1B-C2B-C3B-C4B
57	T	101	EHZ	C4-C5-C6-C7
45	M	604	3PE	O21-C2-C3-O31
45	b	101	3PE	O21-C2-C3-O31
46	H	403	PC1	O21-C2-C3-O31
52	J	201	CDL	OB6-CB4-CB6-OB8
52	M	602	CDL	OB6-CB4-CB6-OB8
46	M	605	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
52	X	201	CDL	C31-CA7-OA8-CA6
46	I	204	PC1	C2C-C2D-C2E-C2F
45	M	604	3PE	C38-C39-C3A-C3B
52	r	201	CDL	C72-C73-C74-C75
52	d	201	CDL	C31-C32-C33-C34
45	Z	201	3PE	C21-C22-C23-C24
45	q	201	3PE	O21-C21-C22-C23
46	h	201	PC1	C36-C37-C38-C39
46	A	204	PC1	O13-C11-C12-N
47	A	206	PLC	O4P-C4-C5-N
47	B	204	PLC	O4P-C4-C5-N
45	e	201	3PE	C36-C37-C38-C39
45	A	202	3PE	C24-C25-C26-C27
46	h	201	PC1	C23-C24-C25-C26
52	H	401	CDL	C62-C63-C64-C65
52	r	201	CDL	C18-C19-C20-C21
45	Z	201	3PE	C32-C33-C34-C35
52	H	401	CDL	C56-C57-C58-C59
52	X	201	CDL	C71-C72-C73-C74
52	i	202	CDL	C37-C38-C39-C40
45	L	703	3PE	C39-C3A-C3B-C3C
52	H	401	CDL	C12-C13-C14-C15
45	A	201	3PE	O11-C1-C2-C3
45	b	101	3PE	O11-C1-C2-C3
45	b	103	3PE	O11-C1-C2-C3
45	e	201	3PE	O11-C1-C2-C3
46	H	403	PC1	C22-C21-O21-C2
52	L	701	CDL	OB7-CB5-OB6-CB4
52	X	201	CDL	C80-C81-C82-C83
45	M	604	3PE	C22-C23-C24-C25
45	Y	201	3PE	C2C-C2D-C2E-C2F
52	H	401	CDL	C71-CB7-OB8-CB6
52	X	201	CDL	C54-C55-C56-C57
45	M	603	3PE	C3F-C3G-C3H-C3I
57	U	101	EHZ	N1-C12-C13-C14
52	X	201	CDL	OA9-CA7-OA8-CA6
45	N	402	3PE	C2-C1-O11-P
50	F	501	FMN	C4'-C5'-O5'-P
45	b	103	3PE	C23-C24-C25-C26
46	M	605	PC1	C26-C27-C28-C29
47	L	710	PLC	O'-C'-O2-C2
45	A	202	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	O11-C1-C2-O21
45	m	202	3PE	O11-C1-C2-O21
45	q	201	3PE	O11-C1-C2-O21
47	B	204	PLC	O3P-C1-C2-O2
52	N	401	CDL	OB5-CB3-CB4-OB6
52	X	201	CDL	OA5-CA3-CA4-OA6
52	d	201	CDL	OA5-CA3-CA4-OA6
52	d	201	CDL	OB5-CB3-CB4-OB6
46	H	403	PC1	C11-C12-N-C13
46	H	403	PC1	C11-C12-N-C14
46	H	403	PC1	C11-C12-N-C15
45	I	203	3PE	C2F-C2G-C2H-C2I
45	Y	201	3PE	C38-C39-C3A-C3B
52	X	201	CDL	C13-C14-C15-C16
45	b	101	3PE	C2F-C2G-C2H-C2I
46	I	204	PC1	C29-C2A-C2B-C2C
45	A	202	3PE	O21-C2-C3-O31
45	Y	201	3PE	O21-C2-C3-O31
45	b	103	3PE	O21-C2-C3-O31
46	B	202	PC1	O21-C2-C3-O31
46	d	202	PC1	O21-C2-C3-O31
47	A	206	PLC	O2-C2-C3-O3
47	J	204	PLC	O2-C2-C3-O3
47	d	203	PLC	O2-C2-C3-O3
52	X	201	CDL	OA6-CA4-CA6-OA8
52	r	201	CDL	OA6-CA4-CA6-OA8
45	Y	201	3PE	C1-C2-C3-O31
45	Y	202	3PE	C1-C2-C3-O31
45	b	103	3PE	C1-C2-C3-O31
46	A	204	PC1	C1-C2-C3-O31
46	d	202	PC1	C1-C2-C3-O31
52	H	401	CDL	CB3-CB4-CB6-OB8
52	J	201	CDL	CB3-CB4-CB6-OB8
45	b	103	3PE	C3B-C3C-C3D-C3E
52	X	201	CDL	C37-C38-C39-C40
45	A	202	3PE	C3D-C3E-C3F-C3G
46	Y	203	PC1	C37-C38-C39-C3A
46	h	201	PC1	C32-C33-C34-C35
45	b	102	3PE	C2C-C2D-C2E-C2F
45	J	202	3PE	C11-O13-P-O14
45	J	203	3PE	C1-O11-P-O14
45	J	203	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	L	704	3PE	C1-O11-P-O14
45	L	705	3PE	C1-O11-P-O14
45	M	603	3PE	C11-O13-P-O11
45	M	603	3PE	C11-O13-P-O14
45	M	604	3PE	C11-O13-P-O14
45	N	402	3PE	C11-O13-P-O11
45	N	402	3PE	C11-O13-P-O12
45	N	402	3PE	C11-O13-P-O14
45	P	502	3PE	C1-O11-P-O14
45	P	502	3PE	C11-O13-P-O11
45	P	502	3PE	C11-O13-P-O12
45	P	502	3PE	C11-O13-P-O14
45	P	503	3PE	C11-O13-P-O14
45	Y	202	3PE	O13-C11-C12-N
45	Z	201	3PE	C1-O11-P-O13
45	Z	201	3PE	C1-O11-P-O14
45	b	102	3PE	C11-O13-P-O11
45	b	102	3PE	C11-O13-P-O12
45	b	102	3PE	C11-O13-P-O14
45	b	102	3PE	O13-C11-C12-N
45	b	103	3PE	C1-O11-P-O14
45	e	201	3PE	O13-C11-C12-N
45	m	201	3PE	C11-O13-P-O11
45	m	201	3PE	C11-O13-P-O12
45	m	201	3PE	C11-O13-P-O14
45	m	202	3PE	C11-O13-P-O11
45	m	202	3PE	C11-O13-P-O12
45	m	202	3PE	C11-O13-P-O14
45	m	203	3PE	C11-O13-P-O11
45	q	201	3PE	C1-O11-P-O12
45	q	201	3PE	C1-O11-P-O13
46	A	203	PC1	C11-O13-P-O12
46	A	203	PC1	C11-O13-P-O14
46	A	203	PC1	C11-O13-P-O11
46	A	203	PC1	C1-O11-P-O12
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	B	203	PC1	C11-O13-P-O11
46	L	709	PC1	C11-O13-P-O14
46	L	709	PC1	C1-O11-P-O12
46	L	709	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	L	709	PC1	C1-O11-P-O13
46	M	605	PC1	C1-O11-P-O14
46	M	605	PC1	C1-O11-P-O13
46	Y	203	PC1	C11-O13-P-O12
46	Z	202	PC1	C11-O13-P-O12
46	Z	202	PC1	C11-O13-P-O14
46	Z	202	PC1	C11-O13-P-O11
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	q	202	PC1	C11-O13-P-O14
47	A	206	PLC	C4-O4P-P-O1P
47	O	403	PLC	C1-O3P-P-O1P
47	d	203	PLC	C4-O4P-P-O1P
52	H	401	CDL	CA2-OA2-PA1-OA3
52	H	401	CDL	CA2-OA2-PA1-OA5
52	J	201	CDL	CB3-OB5-PB2-OB3
52	L	701	CDL	CA3-OA5-PA1-OA4
52	L	701	CDL	CB3-OB5-PB2-OB2
52	L	701	CDL	CB3-OB5-PB2-OB3
52	M	602	CDL	CB2-OB2-PB2-OB3
52	M	602	CDL	CB2-OB2-PB2-OB5
52	N	401	CDL	CA2-OA2-PA1-OA4
52	N	401	CDL	CA3-OA5-PA1-OA2
52	N	401	CDL	CA3-OA5-PA1-OA3
52	d	201	CDL	CB2-OB2-PB2-OB3
52	i	202	CDL	CB3-OB5-PB2-OB3
56	P	501	NDP	C5D-O5D-PN-O3
56	P	501	NDP	C5D-O5D-PN-O1N
56	P	501	NDP	C5D-O5D-PN-O2N
52	L	701	CDL	C31-C32-C33-C34
45	L	704	3PE	C2-C1-O11-P
45	b	103	3PE	C2-C1-O11-P
46	h	201	PC1	C2-C1-O11-P
47	A	206	PLC	C2-C1-O3P-P
52	d	201	CDL	C1-CA2-OA2-PA1
46	L	709	PC1	C33-C34-C35-C36
46	H	403	PC1	O22-C21-O21-C2
46	B	203	PC1	C3B-C3C-C3D-C3E
45	I	203	3PE	C27-C28-C29-C2A
45	L	706	3PE	C2E-C2F-C2G-C2H
46	H	403	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C3D-C3E-C3F-C3G
57	T	101	EHZ	C3-C4-C5-C6
45	Y	201	3PE	C2A-C2B-C2C-C2D
52	i	202	CDL	C52-C53-C54-C55
45	Y	202	3PE	C31-C32-C33-C34
52	H	401	CDL	OB9-CB7-OB8-CB6
47	O	403	PLC	C8'-C9'-CA'-CB'
45	L	703	3PE	C3-C2-O21-C21
45	L	704	3PE	C1-C2-O21-C21
45	L	705	3PE	C3-C2-O21-C21
46	q	202	PC1	C1-C2-O21-C21
47	J	204	PLC	C1-C2-O2-C'
45	M	604	3PE	C28-C29-C2A-C2B
52	L	701	CDL	C62-C63-C64-C65
45	L	703	3PE	C3C-C3D-C3E-C3F
45	J	203	3PE	C38-C39-C3A-C3B
45	L	706	3PE	O11-C1-C2-C3
45	Y	201	3PE	O11-C1-C2-C3
45	b	102	3PE	O11-C1-C2-C3
46	A	203	PC1	O11-C1-C2-C3
52	M	602	CDL	C33-C34-C35-C36
47	O	403	PLC	C1B-CB-O3-C3
52	r	201	CDL	C31-C32-C33-C34
45	b	103	3PE	O11-C1-C2-O21
45	b	103	3PE	C3E-C3F-C3G-C3H
46	h	201	PC1	C2A-C2B-C2C-C2D
45	b	103	3PE	C2A-C2B-C2C-C2D
45	L	704	3PE	C33-C34-C35-C36
45	Y	201	3PE	C36-C37-C38-C39
46	L	709	PC1	C3A-C3B-C3C-C3D
45	L	703	3PE	O32-C31-O31-C3
45	L	706	3PE	C24-C25-C26-C27
46	H	403	PC1	C36-C37-C38-C39
45	N	402	3PE	C2A-C2B-C2C-C2D
45	Y	201	3PE	C34-C35-C36-C37
52	X	201	CDL	C31-C32-C33-C34
45	L	702	3PE	O21-C2-C3-O31
45	L	705	3PE	O21-C2-C3-O31
46	M	605	PC1	O21-C2-C3-O31
46	h	201	PC1	C11-C12-N-C13
45	M	604	3PE	O32-C31-O31-C3
45	L	703	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	A	204	PC1	O32-C31-O31-C3
52	M	602	CDL	C40-C41-C42-C43
45	J	203	3PE	O21-C21-C22-C23
46	H	403	PC1	C1-C2-C3-O31
46	M	605	PC1	C1-C2-C3-O31
55	O	402	DGT	PA-O3A-PB-O1B
56	P	501	NDP	PN-O3-PA-O2A
47	A	206	PLC	C2-C3-O3-CB
46	Y	203	PC1	C3C-C3D-C3E-C3F
45	L	706	3PE	C3F-C3G-C3H-C3I
45	M	604	3PE	C2E-C2F-C2G-C2H
45	b	101	3PE	C31-C32-C33-C34
45	m	201	3PE	C21-C22-C23-C24
45	e	201	3PE	C2E-C2F-C2G-C2H
52	J	201	CDL	C35-C36-C37-C38
46	Y	203	PC1	C38-C39-C3A-C3B
46	d	202	PC1	C34-C35-C36-C37
45	L	707	3PE	C2C-C2D-C2E-C2F
45	L	703	3PE	O21-C21-C22-C23
45	M	604	3PE	C32-C31-O31-C3
46	A	204	PC1	C32-C31-O31-C3
46	B	203	PC1	C2-C1-O11-P
57	U	101	EHZ	S1-C10-C11-N1
52	X	201	CDL	C20-C21-C22-C23
46	H	403	PC1	C3B-C3C-C3D-C3E
52	J	201	CDL	C76-C77-C78-C79
45	M	603	3PE	C3D-C3E-C3F-C3G
46	Z	202	PC1	C36-C37-C38-C39
46	Z	202	PC1	C39-C3A-C3B-C3C
52	X	201	CDL	C72-C73-C74-C75
46	H	402	PC1	C36-C37-C38-C39
52	r	201	CDL	OB5-CB3-CB4-CB6
52	H	401	CDL	C79-C80-C81-C82
46	I	204	PC1	C22-C23-C24-C25
46	L	709	PC1	C32-C33-C34-C35
46	A	205	PC1	C32-C33-C34-C35
52	N	401	CDL	C74-C75-C76-C77
45	m	201	3PE	C26-C27-C28-C29
57	U	101	EHZ	N2-C15-C16-C17
45	m	203	3PE	C35-C36-C37-C38
45	N	402	3PE	C29-C2A-C2B-C2C
52	L	701	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
45	N	402	3PE	C34-C35-C36-C37
52	M	602	CDL	C31-C32-C33-C34
45	q	201	3PE	O22-C21-C22-C23
45	P	503	3PE	C25-C26-C27-C28
45	P	502	3PE	C21-C22-C23-C24
52	L	701	CDL	C33-C34-C35-C36
45	P	503	3PE	C2-C1-O11-P
52	i	202	CDL	C1-CA2-OA2-PA1
46	I	204	PC1	C34-C35-C36-C37
52	N	401	CDL	C34-C35-C36-C37
45	M	604	3PE	C33-C34-C35-C36
45	J	203	3PE	C33-C34-C35-C36
45	L	707	3PE	C2A-C2B-C2C-C2D
45	b	102	3PE	C33-C34-C35-C36
52	N	401	CDL	CB2-C1-CA2-OA2
46	H	403	PC1	C35-C36-C37-C38
45	m	202	3PE	C35-C36-C37-C38
45	L	708	3PE	C26-C27-C28-C29
45	m	201	3PE	C2A-C2B-C2C-C2D
45	b	102	3PE	C34-C35-C36-C37
45	b	103	3PE	C3D-C3E-C3F-C3G
45	L	706	3PE	C3-C2-O21-C21
47	J	204	PLC	C3-C2-O2-C'
45	A	202	3PE	C28-C29-C2A-C2B
52	L	701	CDL	C14-C15-C16-C17
45	M	604	3PE	C24-C25-C26-C27
46	A	203	PC1	C23-C24-C25-C26
58	i	201	CHD	C22-C23-C24-O25
45	Y	201	3PE	C2B-C2C-C2D-C2E
46	M	605	PC1	C33-C34-C35-C36
46	h	201	PC1	C11-C12-N-C14
45	L	704	3PE	C23-C24-C25-C26
47	d	203	PLC	O3P-C1-C2-O2
45	b	102	3PE	C32-C33-C34-C35
45	e	201	3PE	C37-C38-C39-C3A
45	P	502	3PE	C2-C1-O11-P
45	P	503	3PE	O11-C1-C2-C3
52	M	602	CDL	C51-C52-C53-C54
58	i	201	CHD	C22-C23-C24-O26
45	A	201	3PE	O21-C2-C3-O31
45	N	402	3PE	O21-C2-C3-O31
45	L	702	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C33-C34-C35-C36
52	M	602	CDL	C13-C14-C15-C16
52	J	201	CDL	C73-C74-C75-C76
45	Z	201	3PE	C23-C24-C25-C26
45	e	201	3PE	O22-C21-O21-C2
52	X	201	CDL	C62-C63-C64-C65
45	L	704	3PE	C27-C28-C29-C2A
46	q	202	PC1	C2B-C2C-C2D-C2E
52	X	201	CDL	C19-C20-C21-C22
52	i	202	CDL	C61-C62-C63-C64
45	m	202	3PE	C23-C24-C25-C26
46	h	201	PC1	C35-C36-C37-C38
45	L	706	3PE	C39-C3A-C3B-C3C
46	A	205	PC1	C2-C1-O11-P
46	M	605	PC1	C2-C1-O11-P
52	H	401	CDL	CA4-CA3-OA5-PA1
52	H	401	CDL	C1-CB2-OB2-PB2
45	L	706	3PE	C36-C37-C38-C39
45	b	102	3PE	C2A-C2B-C2C-C2D
45	P	503	3PE	C24-C25-C26-C27
45	Z	201	3PE	C2C-C2D-C2E-C2F
45	b	102	3PE	C29-C2A-C2B-C2C
52	J	201	CDL	C33-C34-C35-C36
52	X	201	CDL	C34-C35-C36-C37
47	B	204	PLC	C1-C2-C3-O3
52	r	201	CDL	CA3-CA4-CA6-OA8
52	M	602	CDL	C17-C18-C19-C20
52	X	201	CDL	C72-C71-CB7-OB8
52	r	201	CDL	O1-C1-CA2-OA2
59	o	201	MYR	C6-C7-C8-C9
45	M	604	3PE	C37-C38-C39-C3A
46	M	605	PC1	C2C-C2D-C2E-C2F
52	r	201	CDL	C14-C15-C16-C17
52	r	201	CDL	C52-C51-CB5-OB6
45	Y	201	3PE	C39-C3A-C3B-C3C
46	A	203	PC1	O22-C21-O21-C2
52	d	201	CDL	CA2-C1-CB2-OB2
52	J	201	CDL	C74-C75-C76-C77
52	M	602	CDL	C74-C75-C76-C77
46	h	201	PC1	C11-C12-N-C15
45	m	202	3PE	O21-C21-C22-C23
59	o	201	MYR	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
45	Y	201	3PE	C3B-C3C-C3D-C3E
45	I	203	3PE	O11-C1-C2-C3
46	M	606	PC1	O11-C1-C2-C3
52	H	401	CDL	OB5-CB3-CB4-CB6
52	L	701	CDL	C32-C31-CA7-OA8
52	X	201	CDL	C78-C79-C80-C81
45	L	707	3PE	C3A-C3B-C3C-C3D
46	B	202	PC1	C38-C39-C3A-C3B
46	Y	203	PC1	C35-C36-C37-C38
46	I	204	PC1	C2D-C2E-C2F-C2G
46	h	201	PC1	C33-C34-C35-C36
52	J	201	CDL	C36-C37-C38-C39
52	d	201	CDL	O1-C1-CB2-OB2
45	m	203	3PE	C3C-C3D-C3E-C3F
45	J	202	3PE	C35-C36-C37-C38
50	F	501	FMN	C5'-O5'-P-O3P
46	A	204	PC1	O31-C31-C32-C33
46	q	202	PC1	C2F-C2G-C2H-C2I
52	N	401	CDL	C24-C25-C26-C27
55	O	402	DGT	PB-O3B-PG-O3G
46	A	203	PC1	C34-C35-C36-C37
46	H	403	PC1	C3E-C3F-C3G-C3H
46	q	202	PC1	C26-C27-C28-C29
45	b	103	3PE	C3C-C3D-C3E-C3F
47	A	206	PLC	C4B-C5B-C6B-C7B
45	L	708	3PE	C27-C28-C29-C2A
46	B	202	PC1	C34-C35-C36-C37
45	L	707	3PE	C27-C28-C29-C2A
45	m	202	3PE	C2B-C2C-C2D-C2E
52	L	701	CDL	C64-C65-C66-C67
46	M	605	PC1	C35-C36-C37-C38
46	H	402	PC1	C2B-C2C-C2D-C2E
45	N	402	3PE	C38-C39-C3A-C3B
45	J	202	3PE	O11-C1-C2-O21
46	H	403	PC1	O11-C1-C2-O21
45	Y	201	3PE	C29-C2A-C2B-C2C
52	X	201	CDL	CA3-CA4-CA6-OA8
45	L	706	3PE	O31-C31-C32-C33
45	I	203	3PE	C25-C26-C27-C28
45	L	708	3PE	C2B-C2C-C2D-C2E
45	m	201	3PE	C3B-C3C-C3D-C3E
45	b	101	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	L	703	3PE	C3B-C3C-C3D-C3E
45	m	203	3PE	C3F-C3G-C3H-C3I
45	b	102	3PE	O21-C21-C22-C23
45	P	503	3PE	C12-C11-O13-P
47	L	710	PLC	C1'-C2'-C3'-C4'
47	g	201	PLC	C4'-C5'-C6'-C7'
52	r	201	CDL	C15-C16-C17-C18
46	B	203	PC1	C32-C33-C34-C35
46	Y	203	PC1	C3A-C3B-C3C-C3D
45	Y	202	3PE	O31-C31-C32-C33
46	B	203	PC1	O21-C21-C22-C23
52	N	401	CDL	C11-C12-C13-C14
45	L	704	3PE	C24-C25-C26-C27
52	d	201	CDL	C34-C35-C36-C37
45	b	101	3PE	O31-C31-C32-C33
46	A	205	PC1	O21-C21-C22-C23
45	J	202	3PE	O11-C1-C2-C3
46	d	202	PC1	C11-C12-N-C14
45	J	203	3PE	C3A-C3B-C3C-C3D
45	A	201	3PE	O31-C31-C32-C33
45	N	402	3PE	C2E-C2F-C2G-C2H
52	L	701	CDL	C13-C14-C15-C16
46	B	202	PC1	C21-C22-C23-C24
52	d	201	CDL	C52-C51-CB5-OB6
45	J	203	3PE	C37-C38-C39-C3A
46	d	202	PC1	C37-C38-C39-C3A
46	q	202	PC1	C25-C26-C27-C28
45	L	706	3PE	C2F-C2G-C2H-C2I
46	B	202	PC1	O31-C31-C32-C33
47	B	204	PLC	C2B-C1B-CB-O3
46	H	403	PC1	C3F-C3G-C3H-C3I
52	M	602	CDL	C55-C56-C57-C58
46	B	202	PC1	O13-C11-C12-N
46	h	201	PC1	O13-C11-C12-N
45	N	402	3PE	C36-C37-C38-C39
52	N	401	CDL	C20-C21-C22-C23
45	L	707	3PE	C34-C35-C36-C37
45	N	402	3PE	C27-C28-C29-C2A
45	e	201	3PE	C22-C21-O21-C2
45	Z	201	3PE	C2E-C2F-C2G-C2H
45	A	201	3PE	O21-C21-C22-C23
52	N	401	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
46	L	709	PC1	C11-C12-N-C14
46	L	709	PC1	C11-C12-N-C15
46	d	202	PC1	C11-C12-N-C15
45	A	202	3PE	C27-C28-C29-C2A
45	P	502	3PE	O31-C31-C32-C33
45	b	102	3PE	O31-C31-C32-C33
47	d	203	PLC	C2B-C1B-CB-O3
57	U	101	EHZ	O4-C15-C16-C17
59	o	201	MYR	C1-C2-C3-C4
46	M	606	PC1	C25-C26-C27-C28
45	J	202	3PE	C38-C39-C3A-C3B
46	A	203	PC1	C22-C21-O21-C2
52	J	201	CDL	C75-C76-C77-C78
52	r	201	CDL	C53-C54-C55-C56
52	N	401	CDL	C57-C58-C59-C60
56	P	501	NDP	C2B-O2B-P2B-O2X
45	m	202	3PE	C2-C1-O11-P
52	J	201	CDL	CA7-C31-C32-C33
45	L	705	3PE	O31-C31-C32-C33
45	N	402	3PE	O31-C31-C32-C33
52	L	701	CDL	C52-C51-CB5-OB6
52	M	602	CDL	C80-C81-C82-C83
46	h	201	PC1	C26-C27-C28-C29
47	O	403	PLC	C4'-C5'-C6'-C7'
46	B	202	PC1	C11-C12-N-C14
46	B	202	PC1	C11-C12-N-C15
45	b	103	3PE	C34-C35-C36-C37
45	L	704	3PE	O21-C21-C22-C23
46	A	205	PC1	O31-C31-C32-C33
47	J	204	PLC	C2B-C1B-CB-O3
45	m	202	3PE	C2E-C2F-C2G-C2H
45	Y	201	3PE	O31-C31-C32-C33
47	L	710	PLC	O2-C'-C1'-C2'
52	J	201	CDL	C12-C11-CA5-OA6
52	J	201	CDL	C72-C71-CB7-OB8
45	I	203	3PE	C22-C23-C24-C25
45	J	203	3PE	C36-C37-C38-C39
52	d	201	CDL	C37-C38-C39-C40
50	F	501	FMN	N10-C1'-C2'-O2'
46	H	402	PC1	O22-C21-C22-C23
46	B	203	PC1	C37-C38-C39-C3A
45	L	705	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
45	L	706	3PE	C1-C2-O21-C21
45	M	603	3PE	C1-C2-O21-C21
47	P	504	PLC	C3-C2-O2-C'
46	A	203	PC1	C11-C12-N-C14
46	A	203	PC1	O21-C21-C22-C23
52	H	401	CDL	C81-C82-C83-C84
45	b	101	3PE	O32-C31-C32-C33
45	A	202	3PE	C33-C34-C35-C36
45	L	706	3PE	C23-C24-C25-C26
45	A	201	3PE	C2-C1-O11-P
46	A	205	PC1	O22-C21-C22-C23
46	B	203	PC1	O22-C21-C22-C23
47	B	204	PLC	C2B-C1B-CB-OB
47	d	203	PLC	O2-C'-C1'-C2'
52	d	201	CDL	C76-C77-C78-C79
46	Z	202	PC1	C34-C35-C36-C37
46	M	606	PC1	C26-C27-C28-C29
45	M	603	3PE	C3B-C3C-C3D-C3E
45	A	201	3PE	O22-C21-C22-C23
45	P	502	3PE	O32-C31-C32-C33
46	B	202	PC1	O32-C31-C32-C33
47	d	203	PLC	C2B-C1B-CB-OB
45	M	604	3PE	C21-C22-C23-C24
46	A	203	PC1	C11-C12-N-C15
46	L	709	PC1	C11-C12-N-C13
46	d	202	PC1	C11-C12-N-C13
45	M	604	3PE	C23-C24-C25-C26
45	b	102	3PE	O32-C31-C32-C33
52	M	602	CDL	C72-C73-C74-C75
52	N	401	CDL	C51-C52-C53-C54
46	d	202	PC1	C35-C36-C37-C38
52	r	201	CDL	C13-C14-C15-C16
47	O	403	PLC	C7'-C8'-C9'-CA'
45	A	201	3PE	O32-C31-C32-C33
45	L	705	3PE	O32-C31-C32-C33
52	M	602	CDL	C15-C16-C17-C18
46	A	204	PC1	O21-C2-C3-O31
45	N	402	3PE	O32-C31-C32-C33
45	Y	202	3PE	O32-C31-C32-C33
52	N	401	CDL	C52-C51-CB5-OB7
45	L	704	3PE	C25-C26-C27-C28
45	A	201	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
47	O	403	PLC	OB-CB-O3-C3
46	d	202	PC1	C22-C23-C24-C25
45	Y	201	3PE	O32-C31-C32-C33
46	A	205	PC1	O32-C31-C32-C33
52	J	201	CDL	C72-C71-CB7-OB9
46	B	203	PC1	C2B-C2C-C2D-C2E
45	A	202	3PE	C2-C1-O11-P
45	m	201	3PE	O21-C21-C22-C23
52	H	401	CDL	C72-C71-CB7-OB8
52	N	401	CDL	C72-C71-CB7-OB8
52	M	602	CDL	C77-C78-C79-C80
52	N	401	CDL	C56-C57-C58-C59
46	A	203	PC1	C11-C12-N-C13
46	B	202	PC1	C11-C12-N-C13
46	Y	203	PC1	C39-C3A-C3B-C3C
52	r	201	CDL	CA7-C31-C32-C33
47	d	203	PLC	O3P-C1-C2-C3
47	g	201	PLC	O3P-C1-C2-C3
47	J	204	PLC	C2B-C1B-CB-OB
45	A	202	3PE	O21-C21-C22-C23
52	L	701	CDL	C52-C51-CB5-OB7
52	M	602	CDL	C12-C11-CA5-OA6
52	M	602	CDL	C72-C71-CB7-OB8
52	H	401	CDL	C34-C35-C36-C37
52	H	401	CDL	C52-C53-C54-C55
56	P	501	NDP	PN-O3-PA-O1A
45	m	202	3PE	C31-C32-C33-C34
45	J	203	3PE	C34-C35-C36-C37
45	L	704	3PE	O22-C21-C22-C23
46	A	203	PC1	O22-C21-C22-C23
47	L	710	PLC	O'-C'-C1'-C2'
52	J	201	CDL	C12-C11-CA5-OA7
52	M	602	CDL	C32-C33-C34-C35

There are no ring outliers.

25 monomers are involved in 41 short contacts:

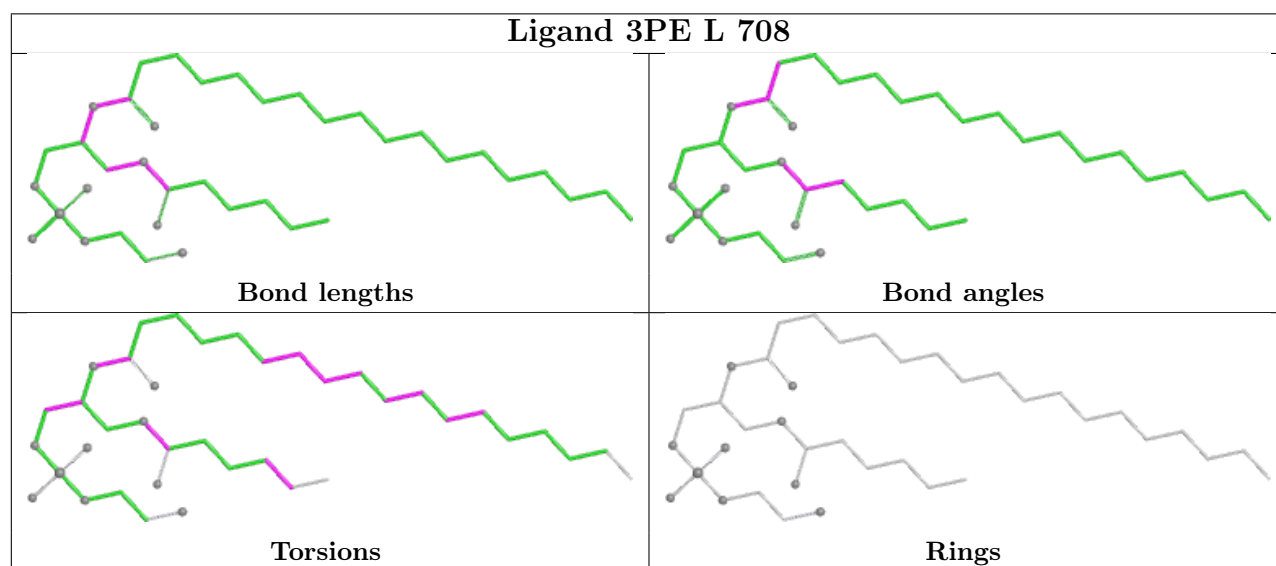
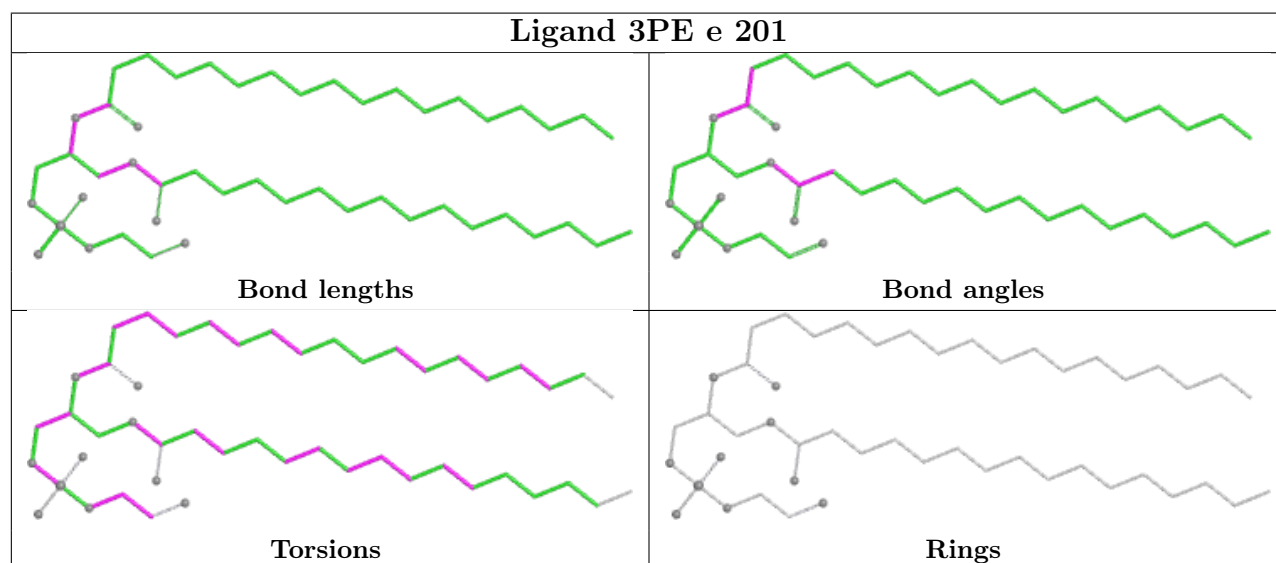
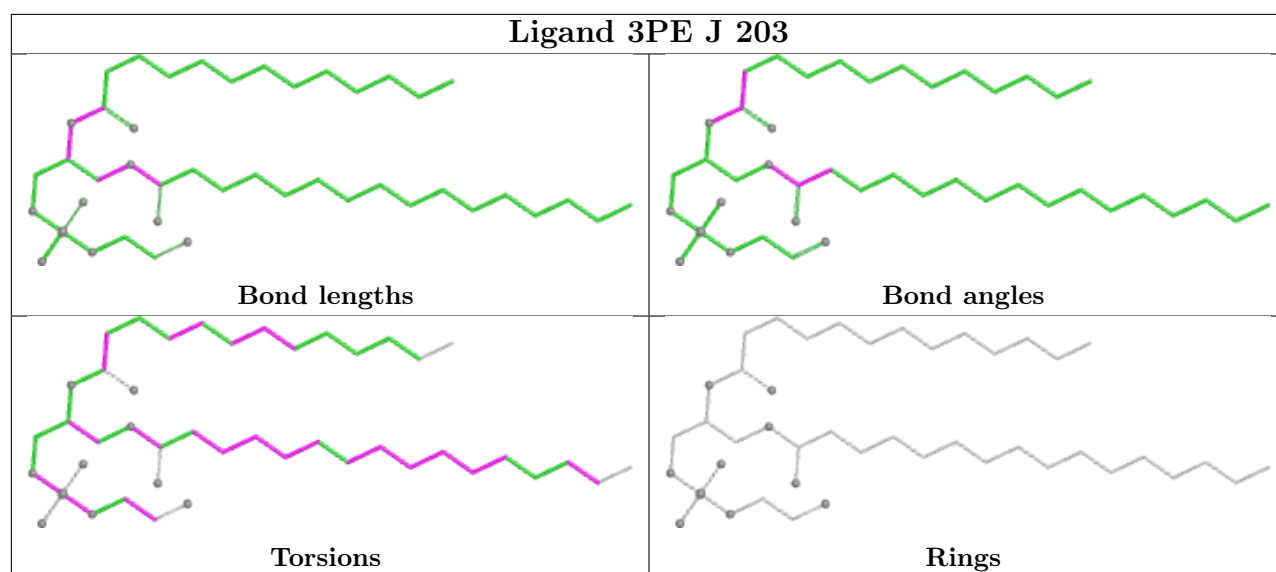
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	J	203	3PE	1	0
47	g	201	PLC	1	0
48	B	201	SF4	1	0
52	H	401	CDL	1	0

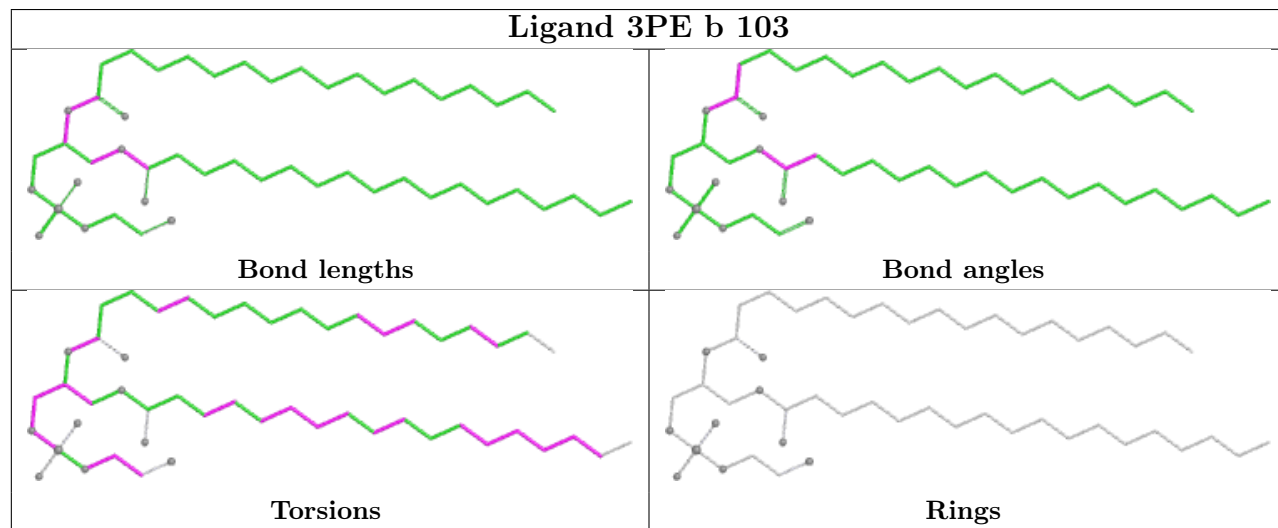
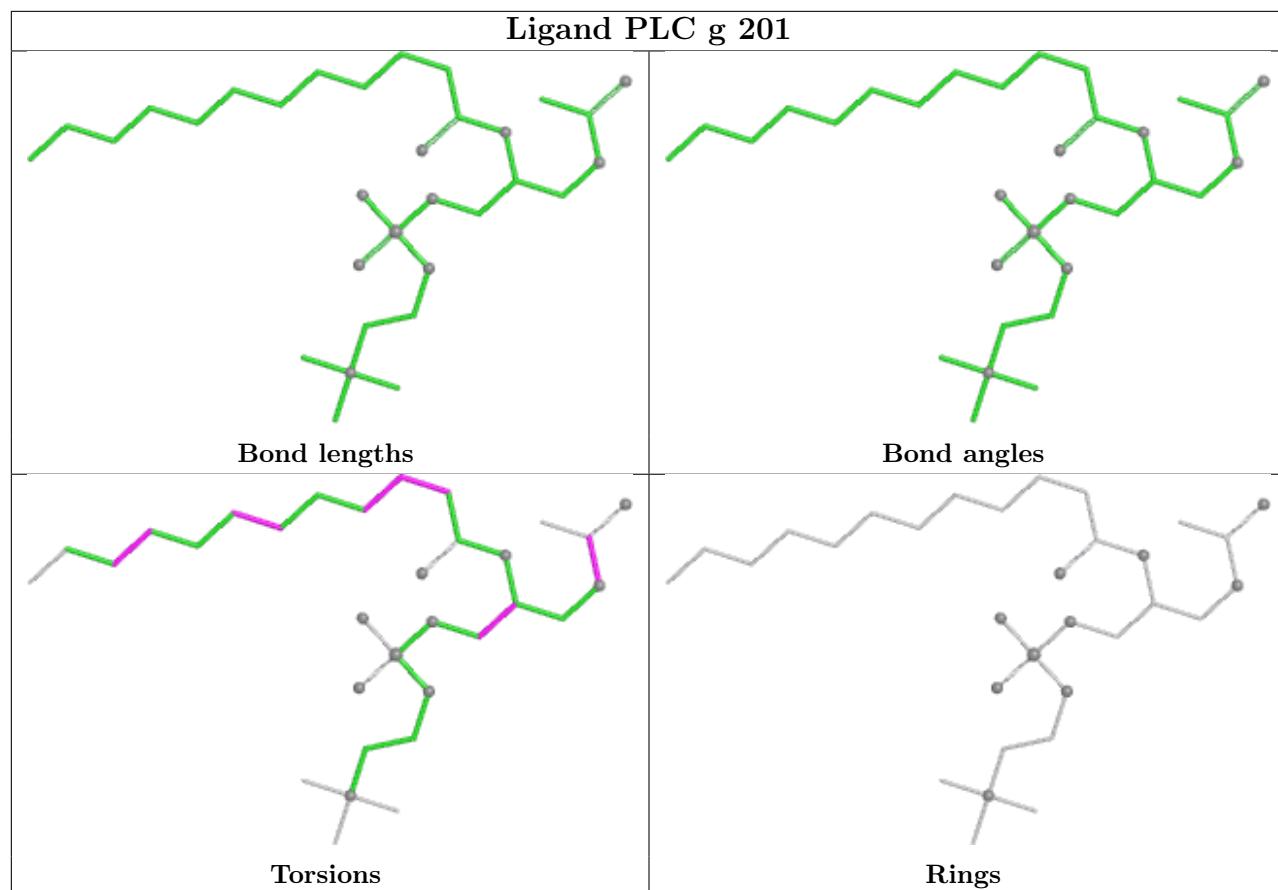
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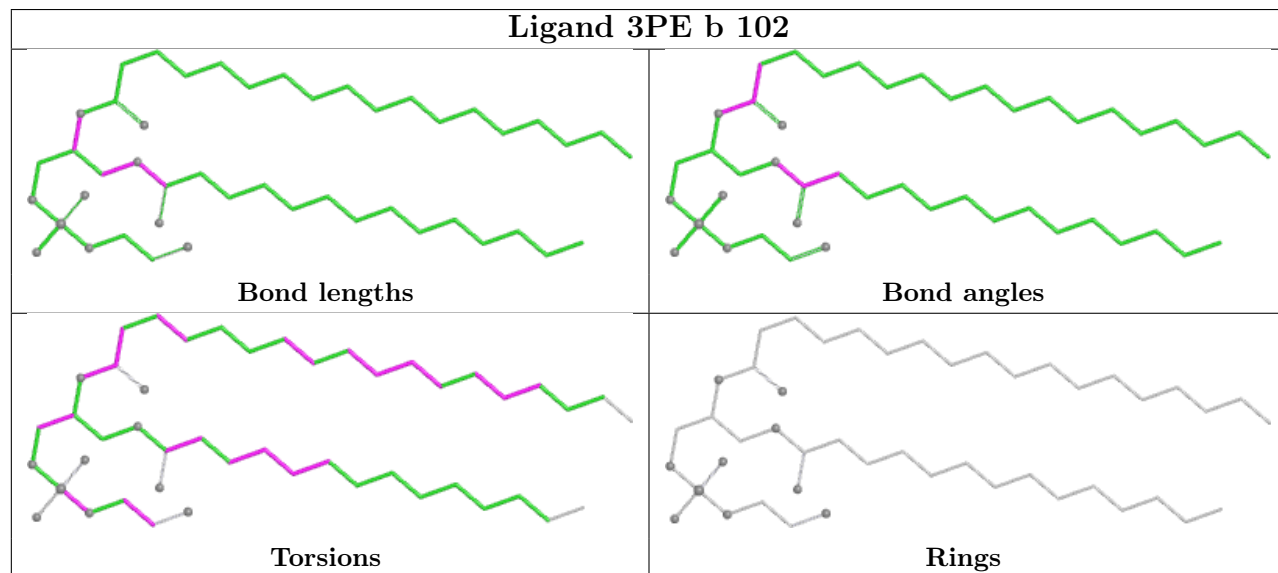
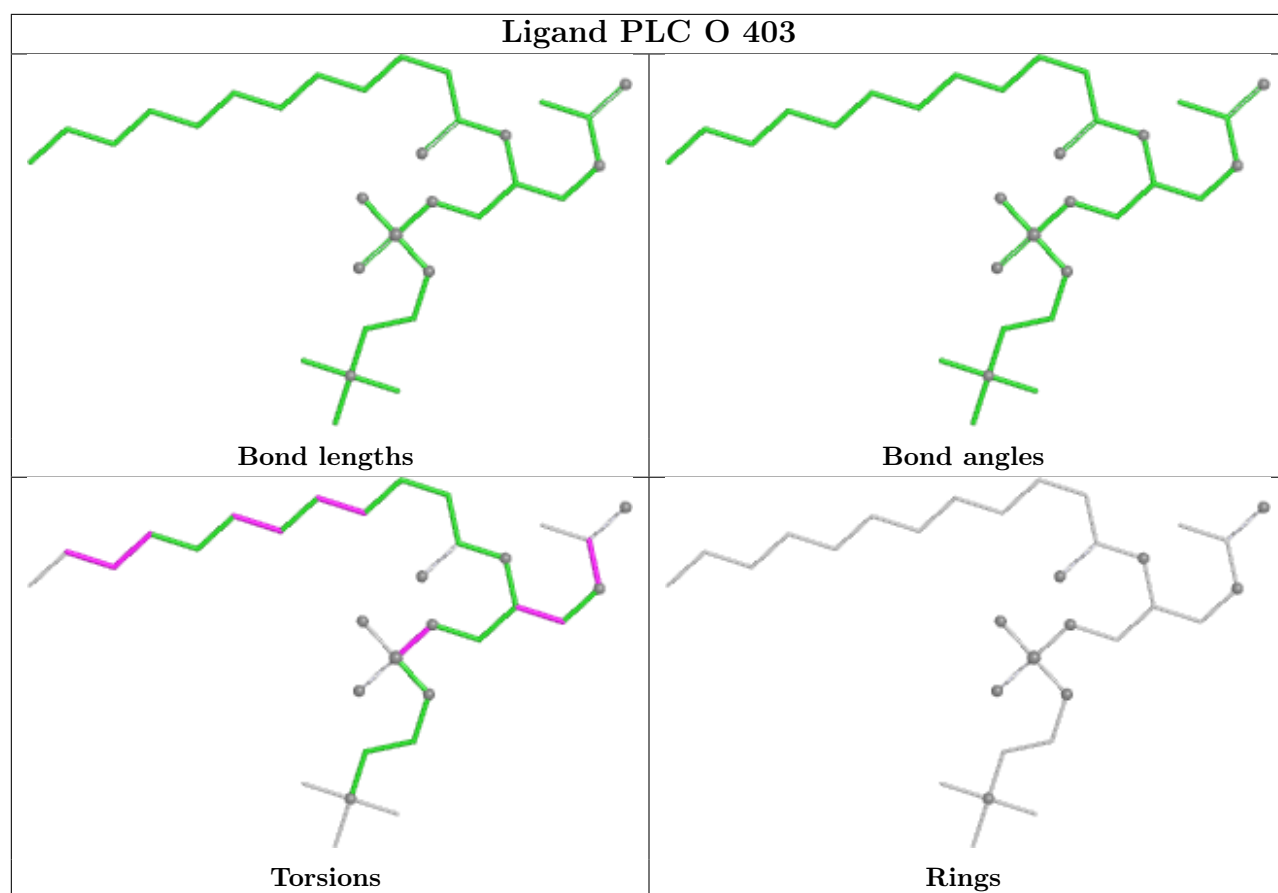
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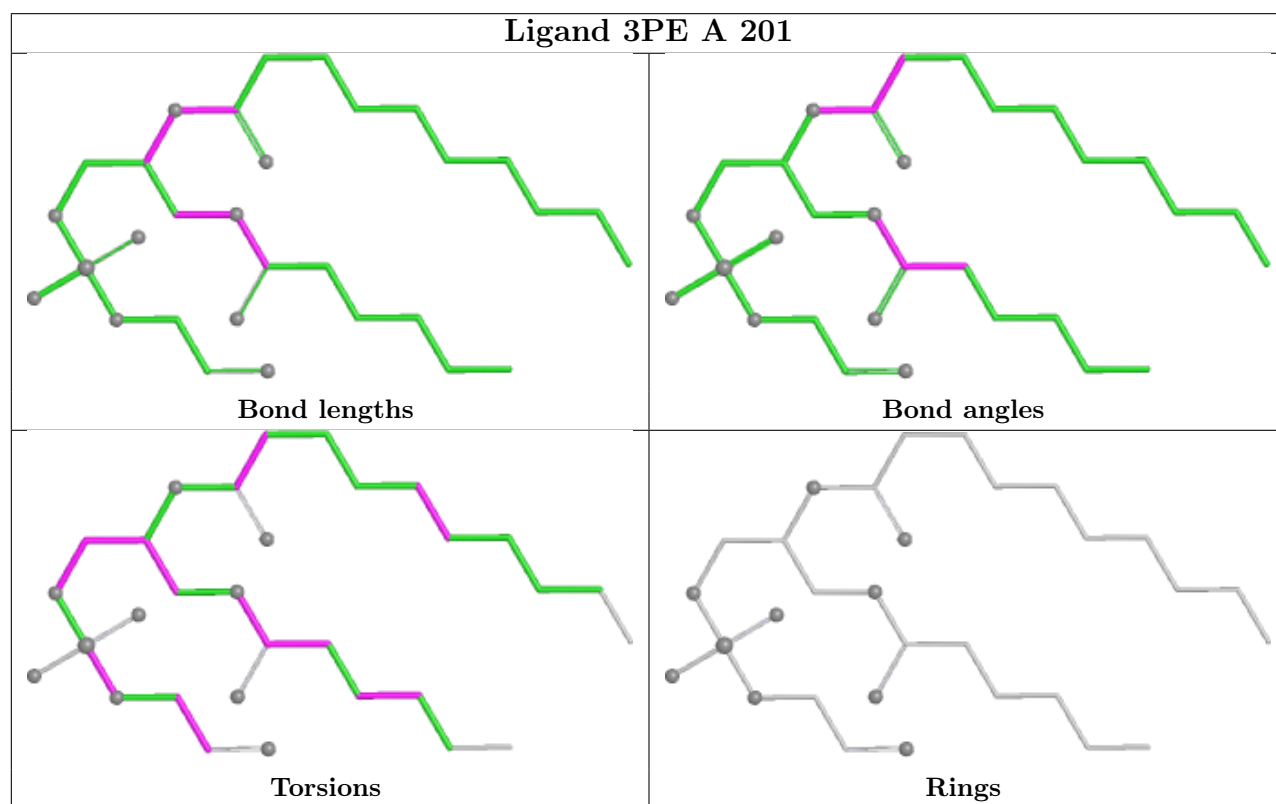
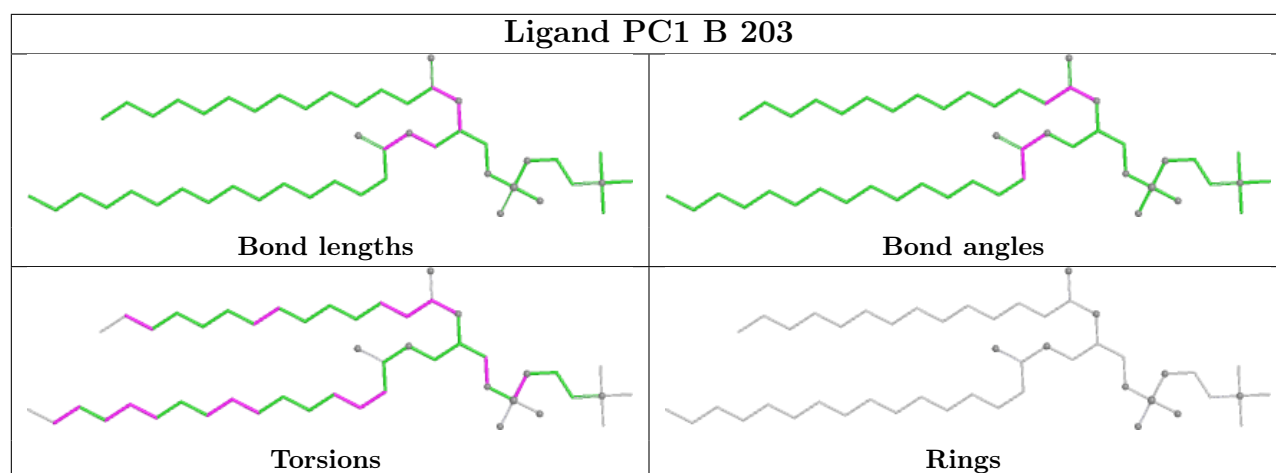
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	T	101	EHZ	1	0
52	i	202	CDL	4	0
52	M	602	CDL	4	0
46	M	605	PC1	1	0
50	F	501	FMN	1	0
58	i	201	CHD	7	0
46	H	402	PC1	2	0
46	A	203	PC1	1	0
55	O	402	DGT	6	0
46	M	606	PC1	1	0
45	N	402	3PE	1	0
46	Y	203	PC1	1	0
45	L	707	3PE	1	0
52	L	701	CDL	1	0
46	Z	202	PC1	1	0
56	P	501	NDP	1	0
45	m	202	3PE	1	0
52	d	201	CDL	1	0
46	I	204	PC1	1	0
46	L	709	PC1	2	0
52	X	201	CDL	1	0

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

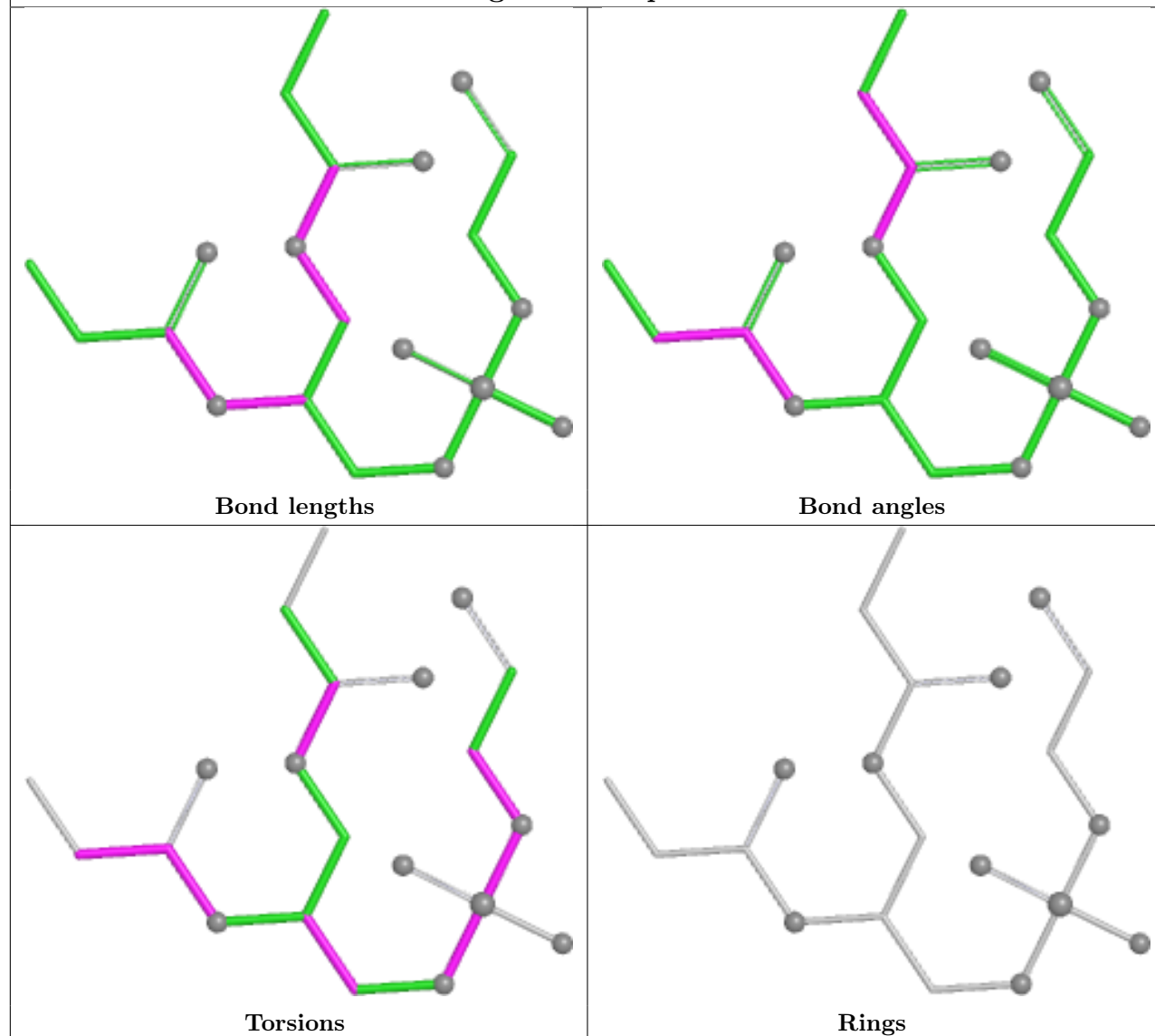




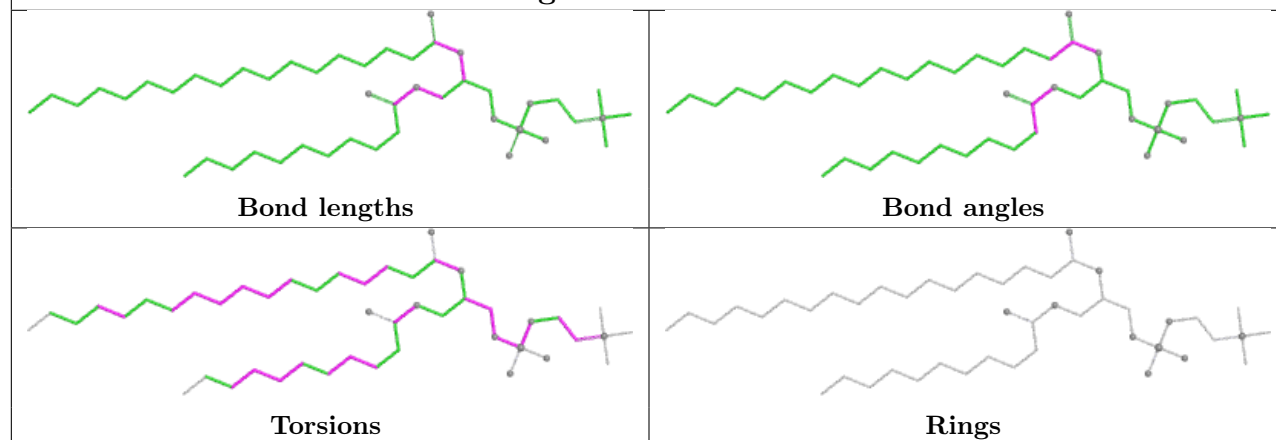


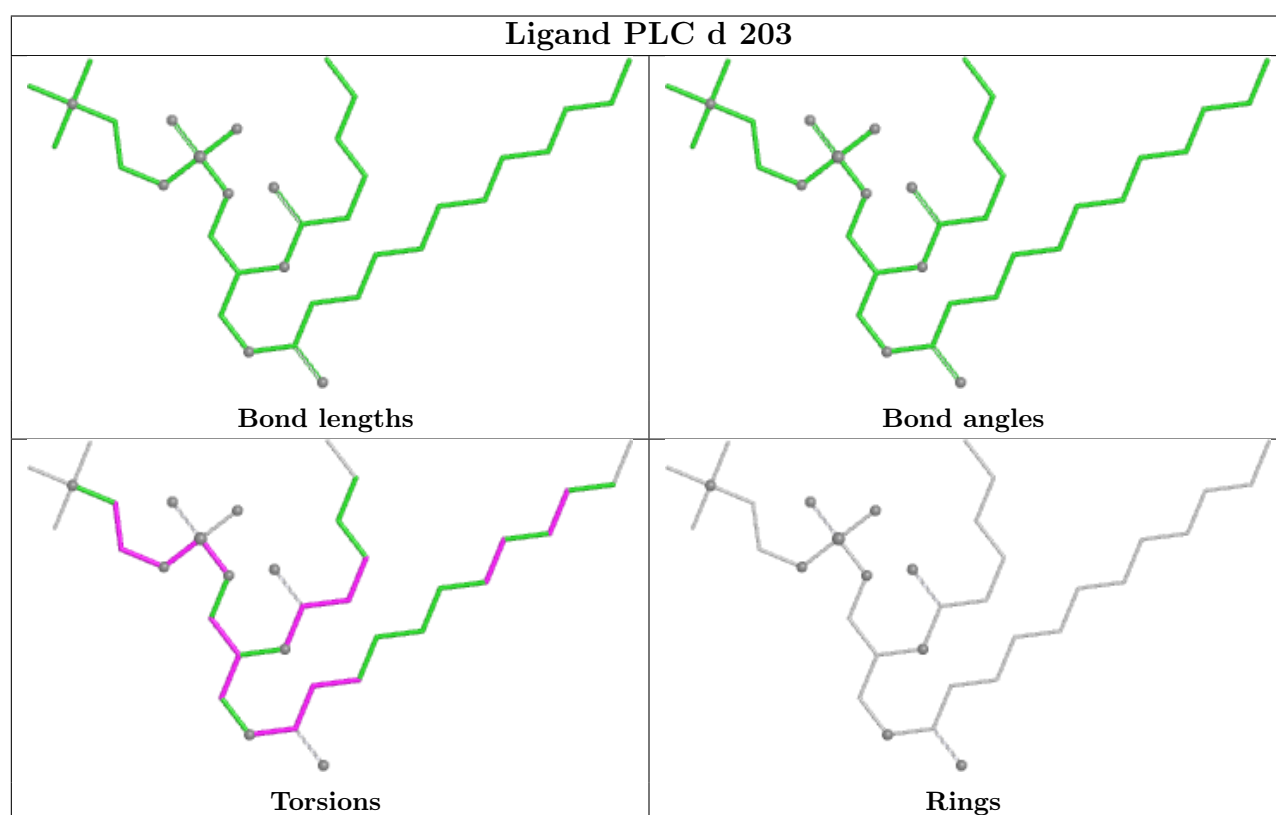
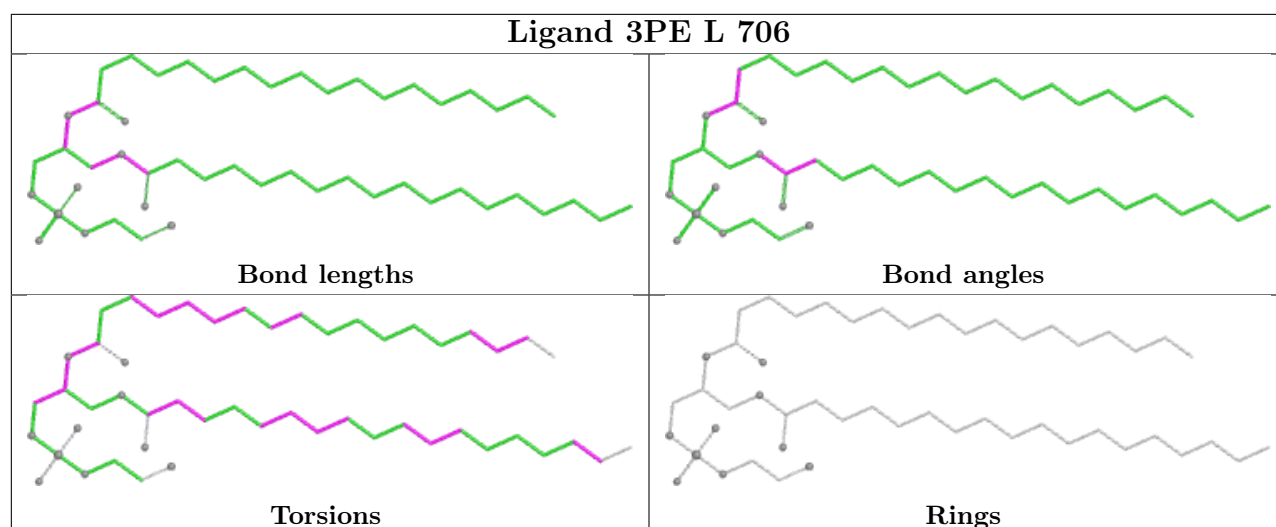


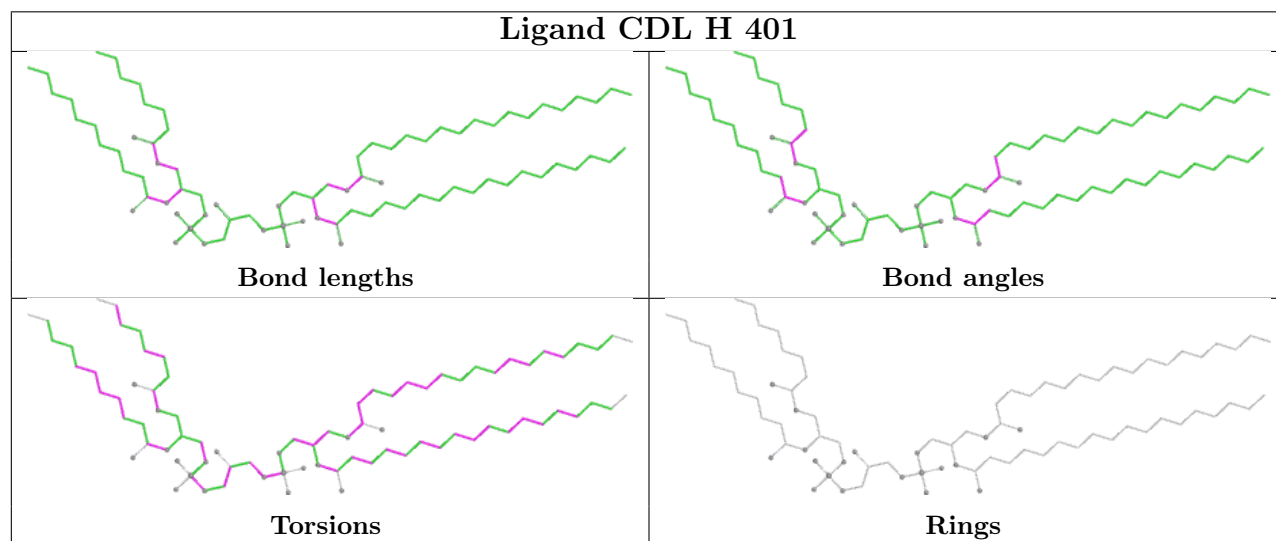
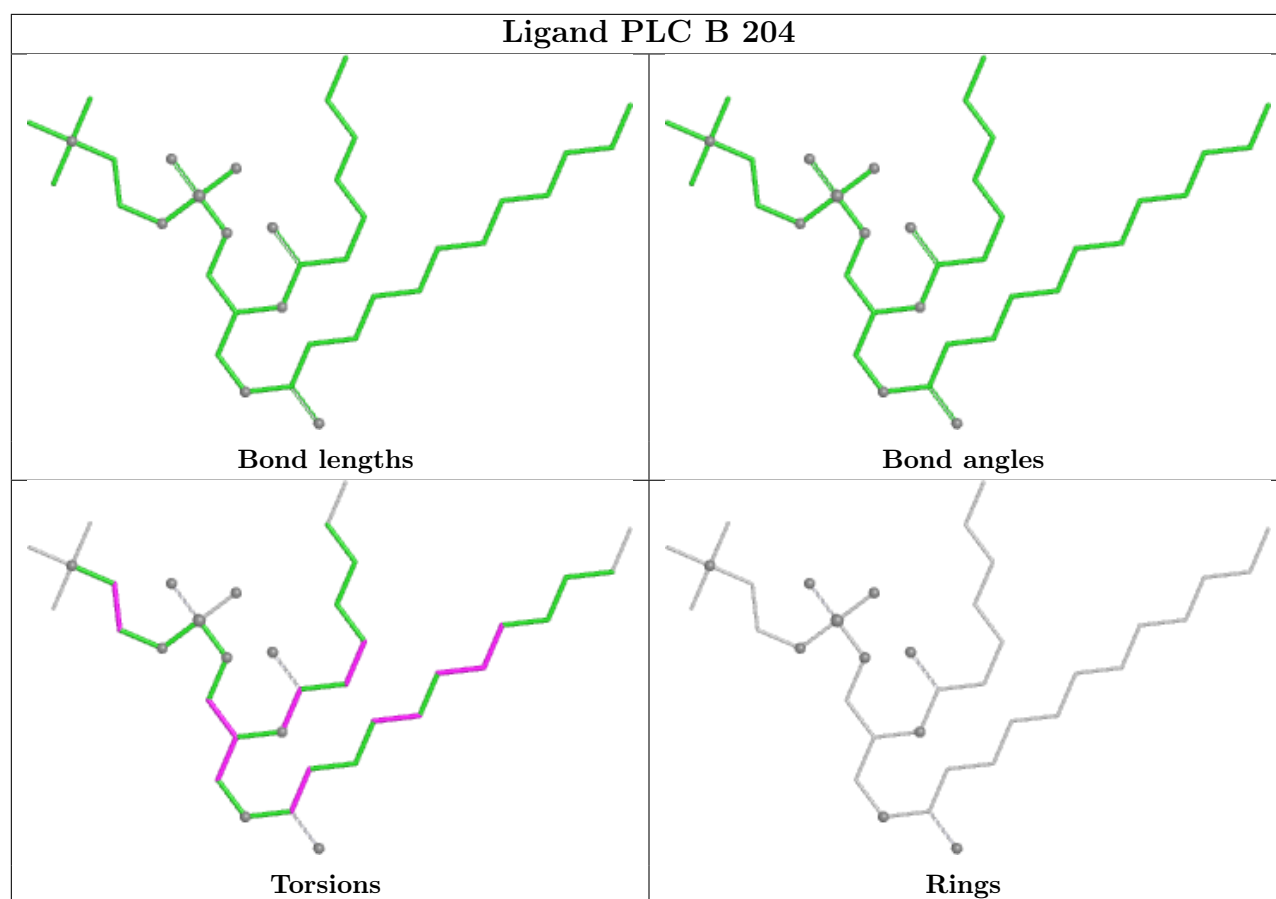
Ligand 3PE q 201



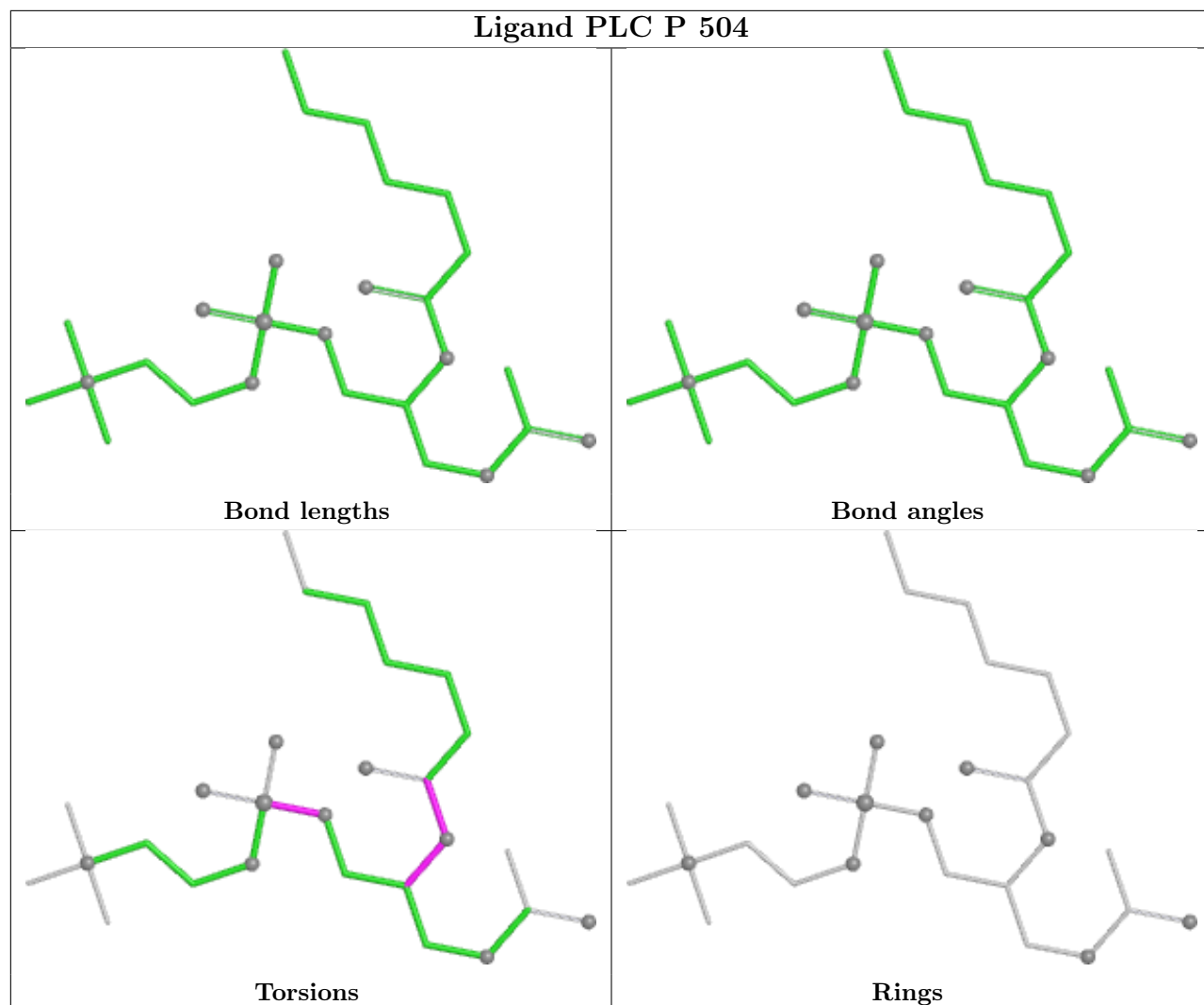
Ligand PC1 h 201

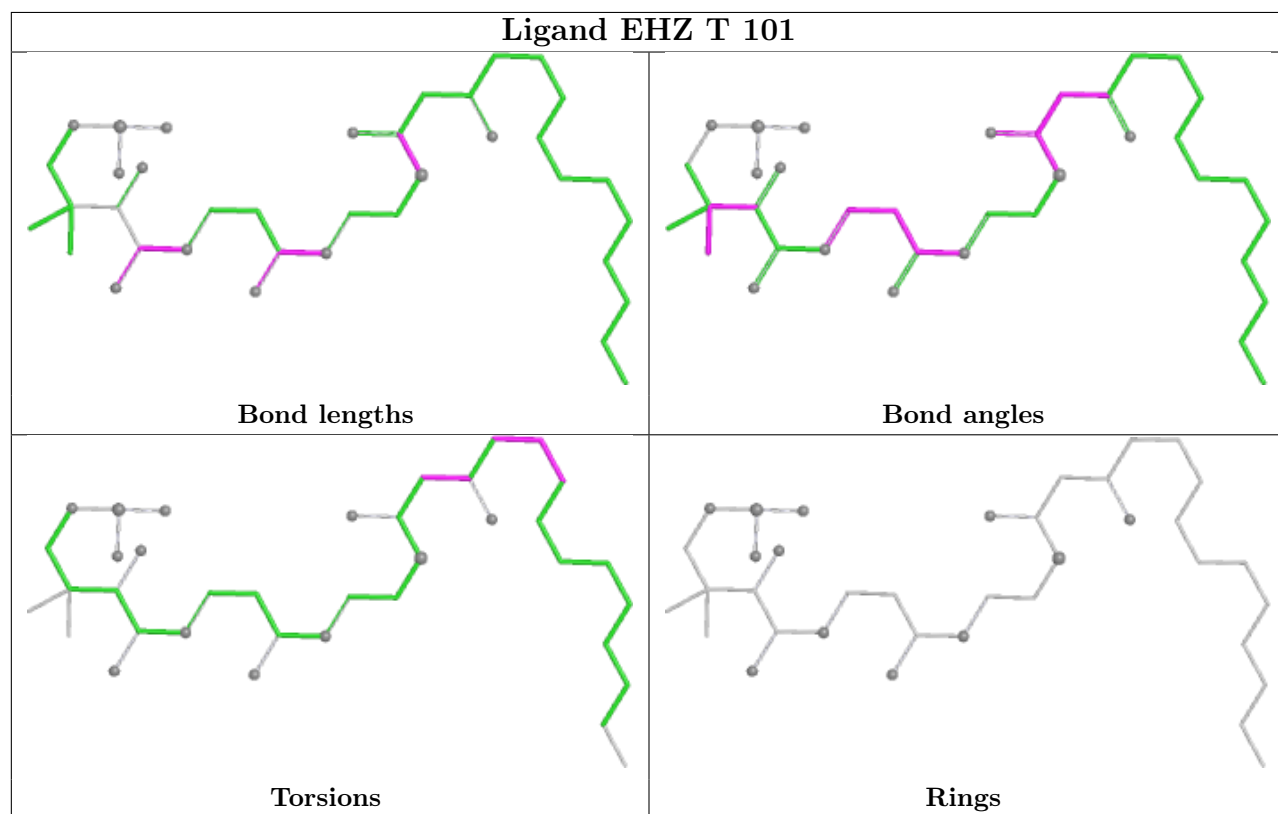
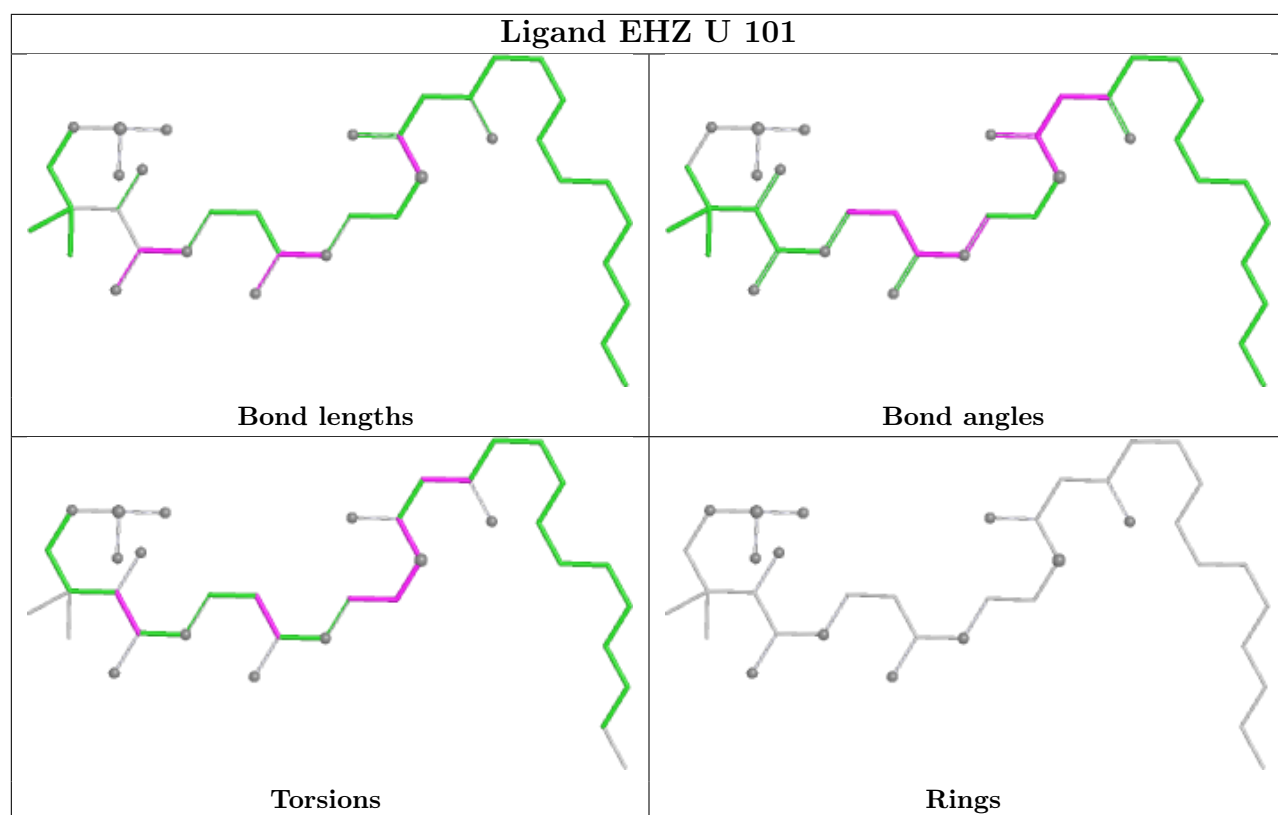


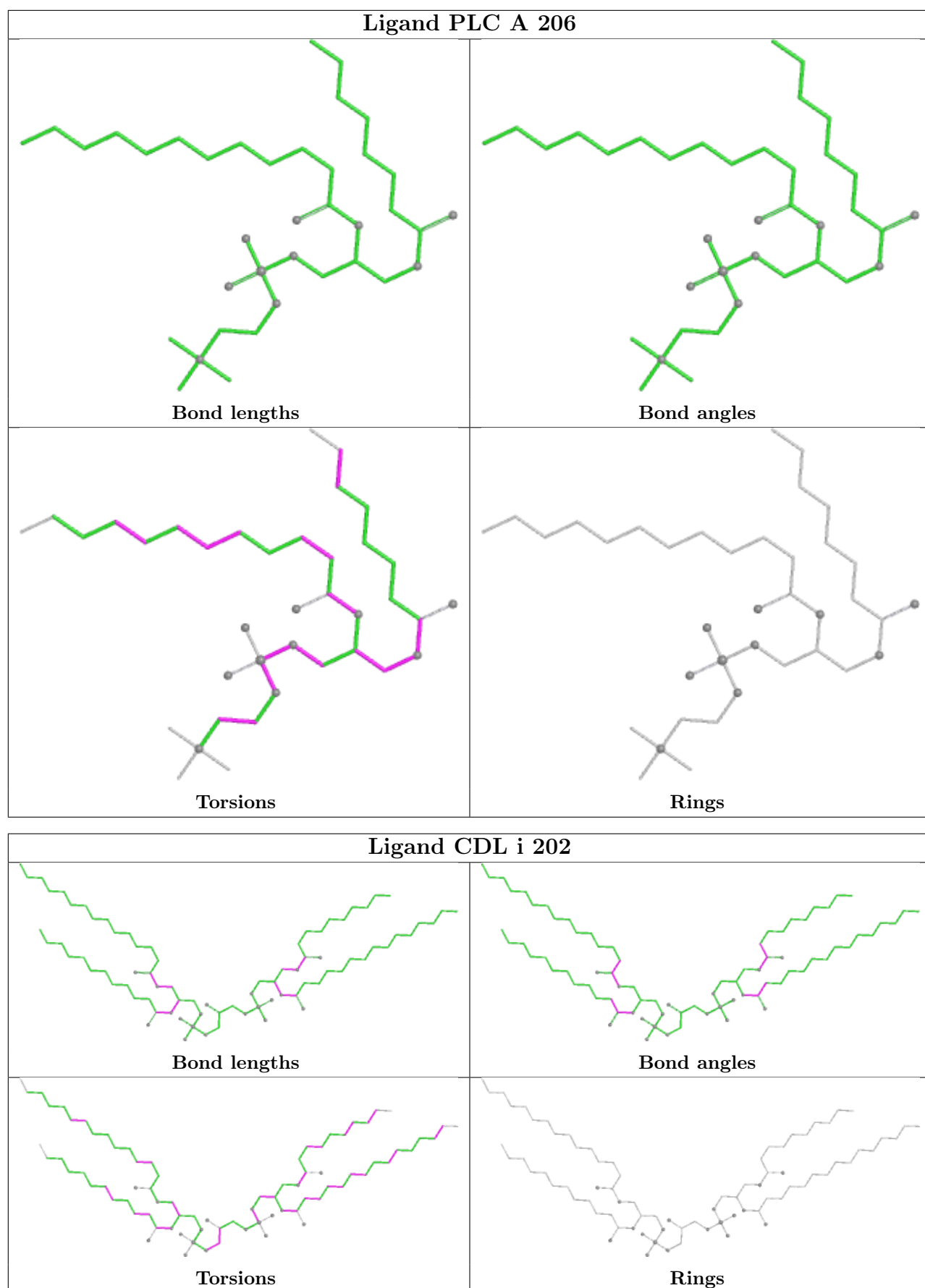


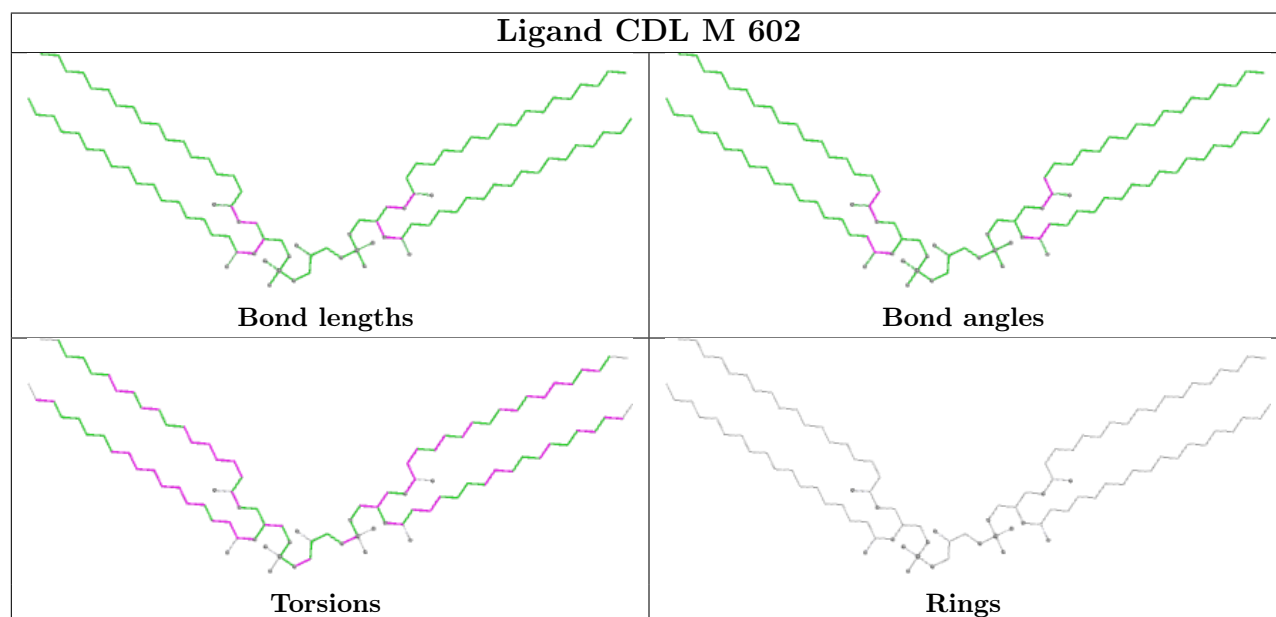
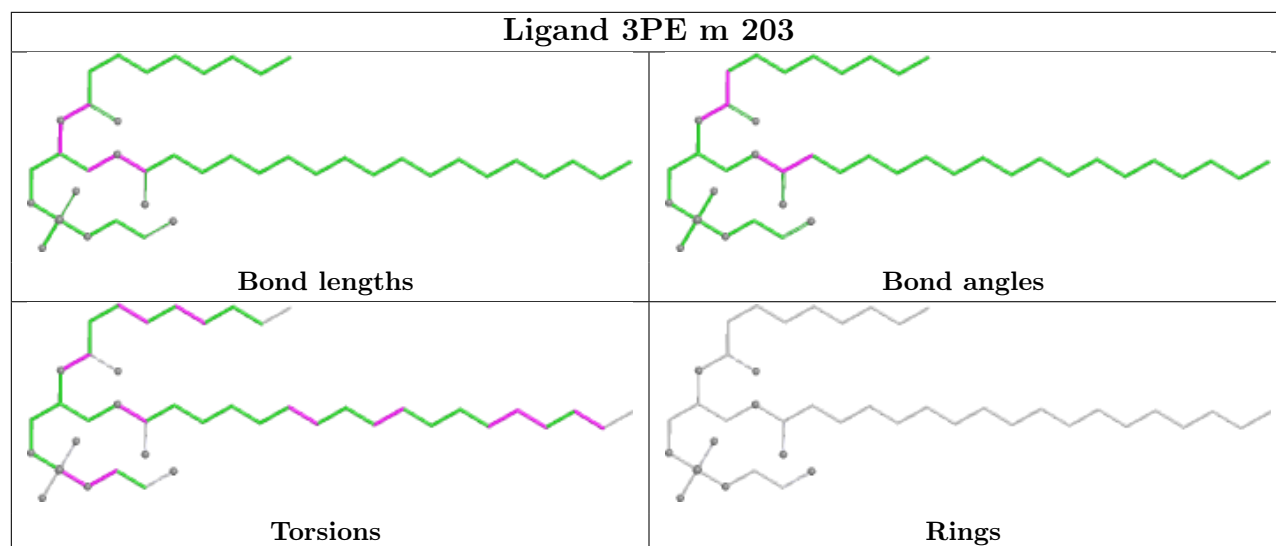
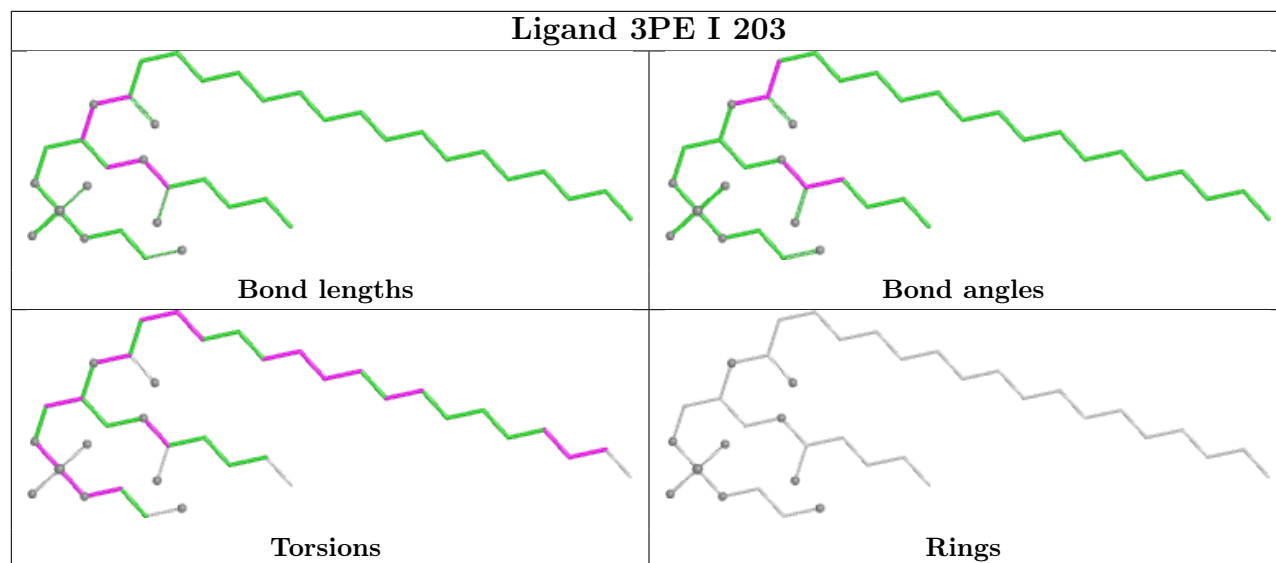


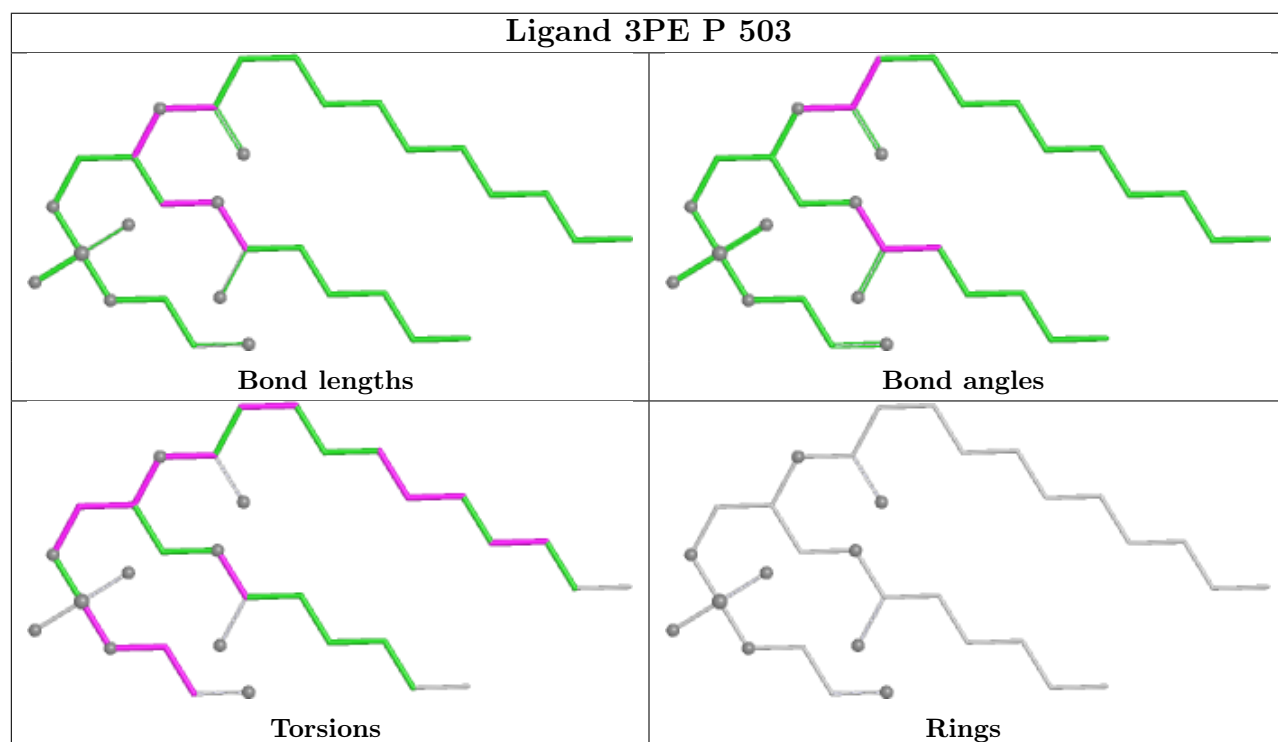
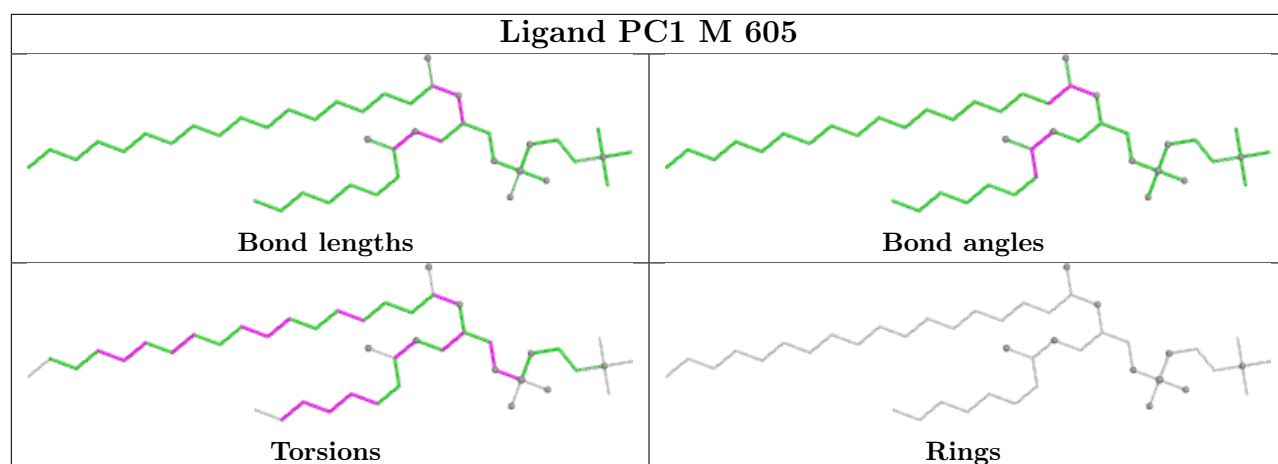
Ligand PLC P 504

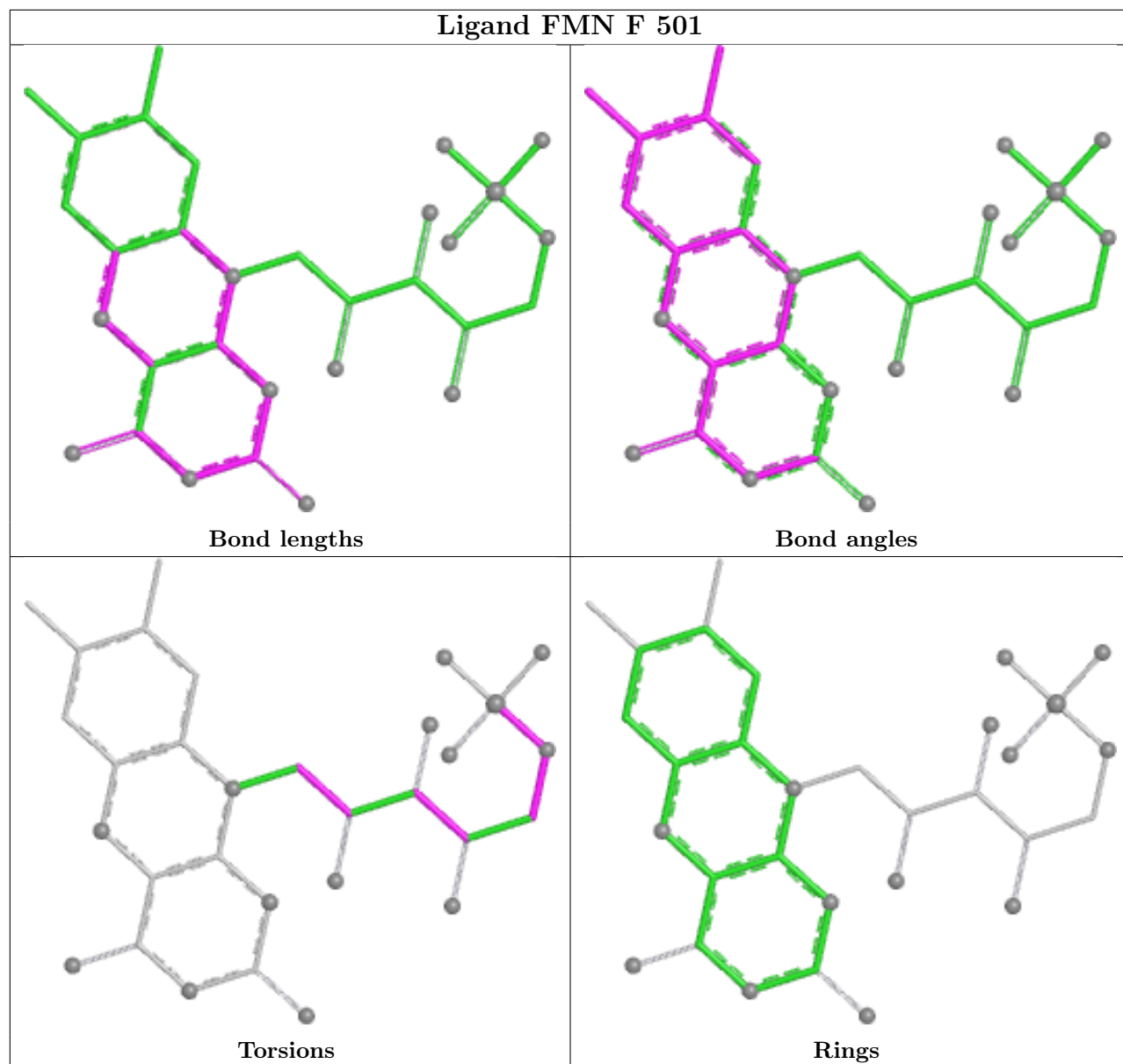


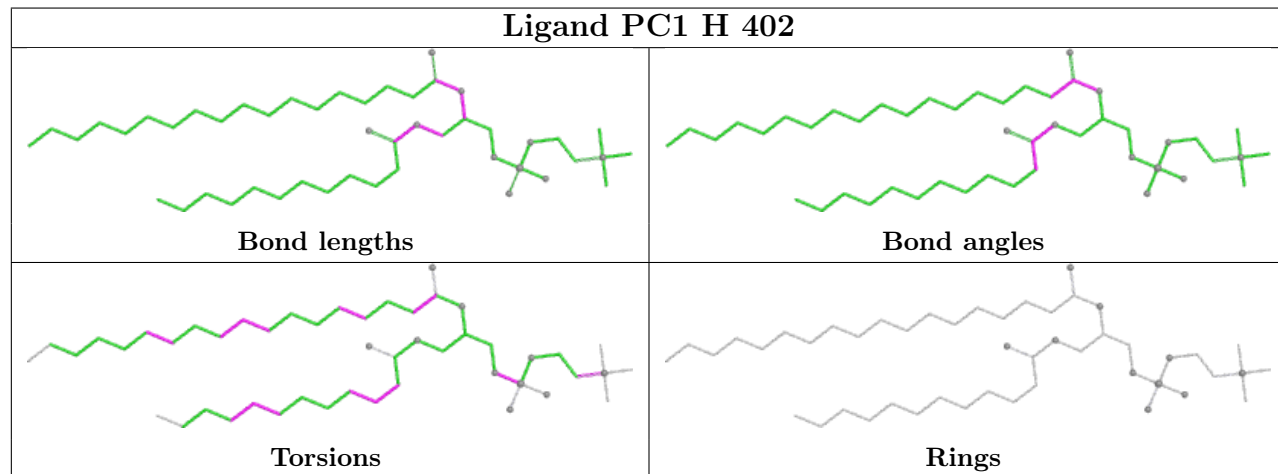
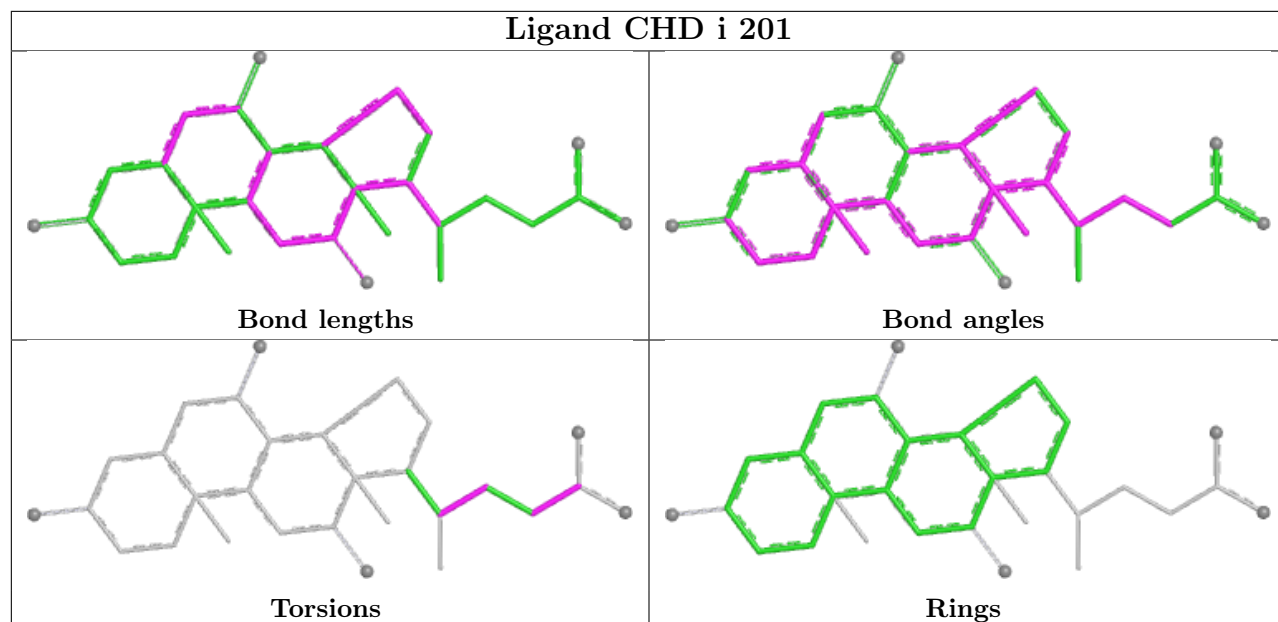


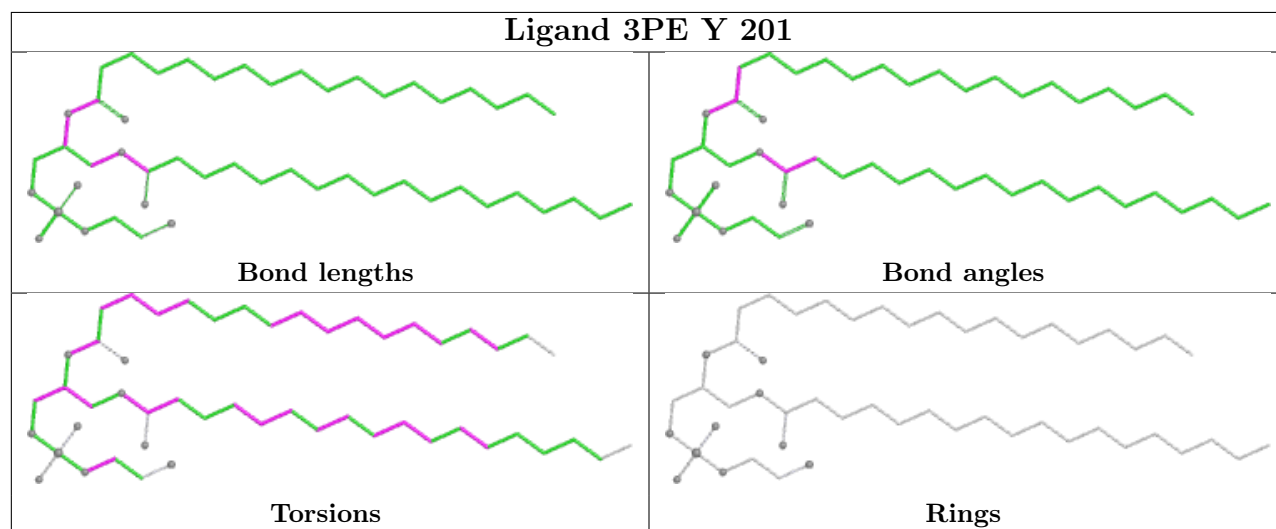
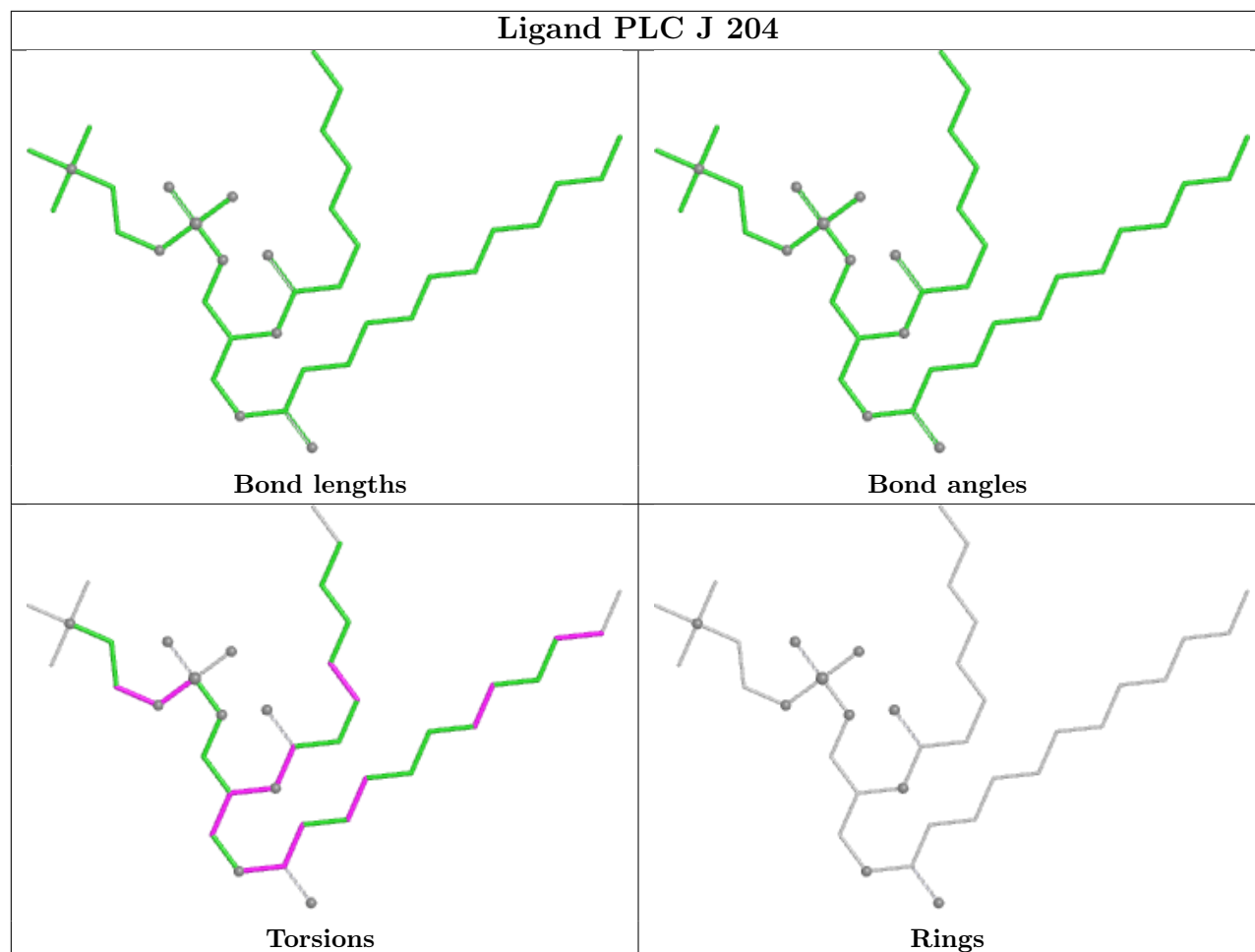




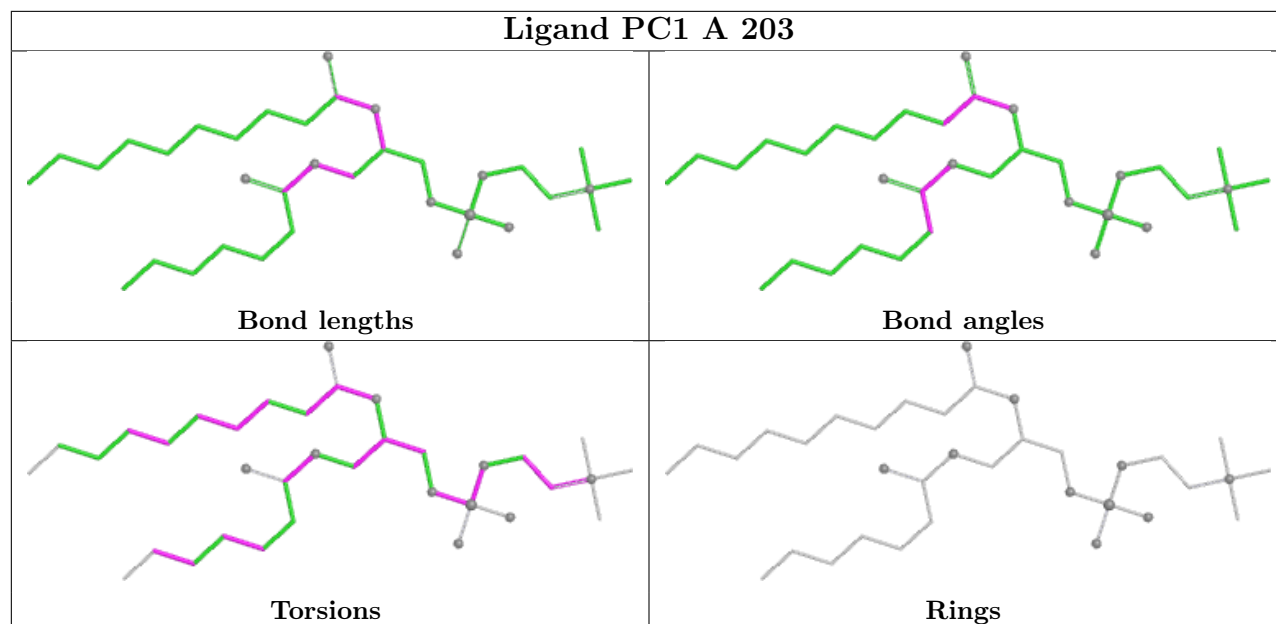




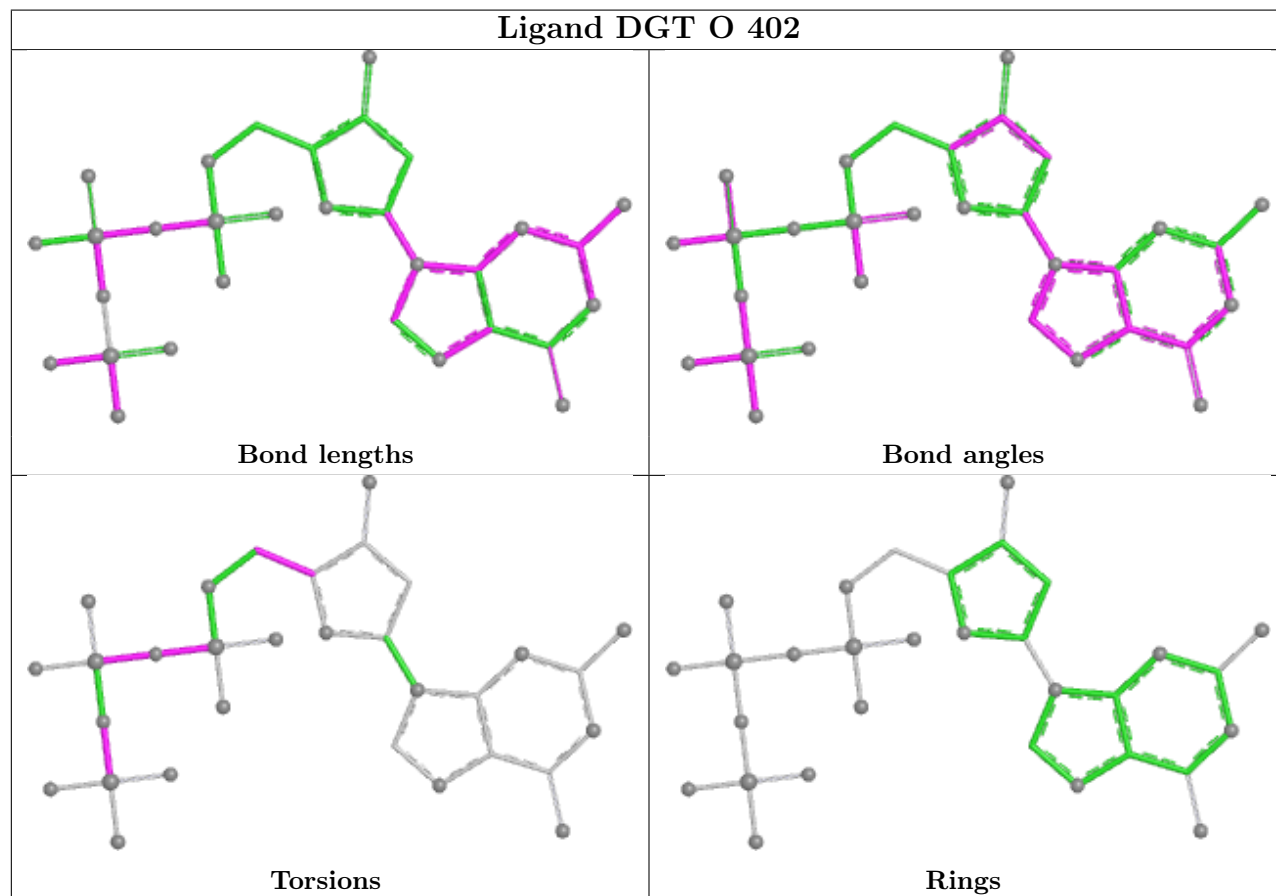


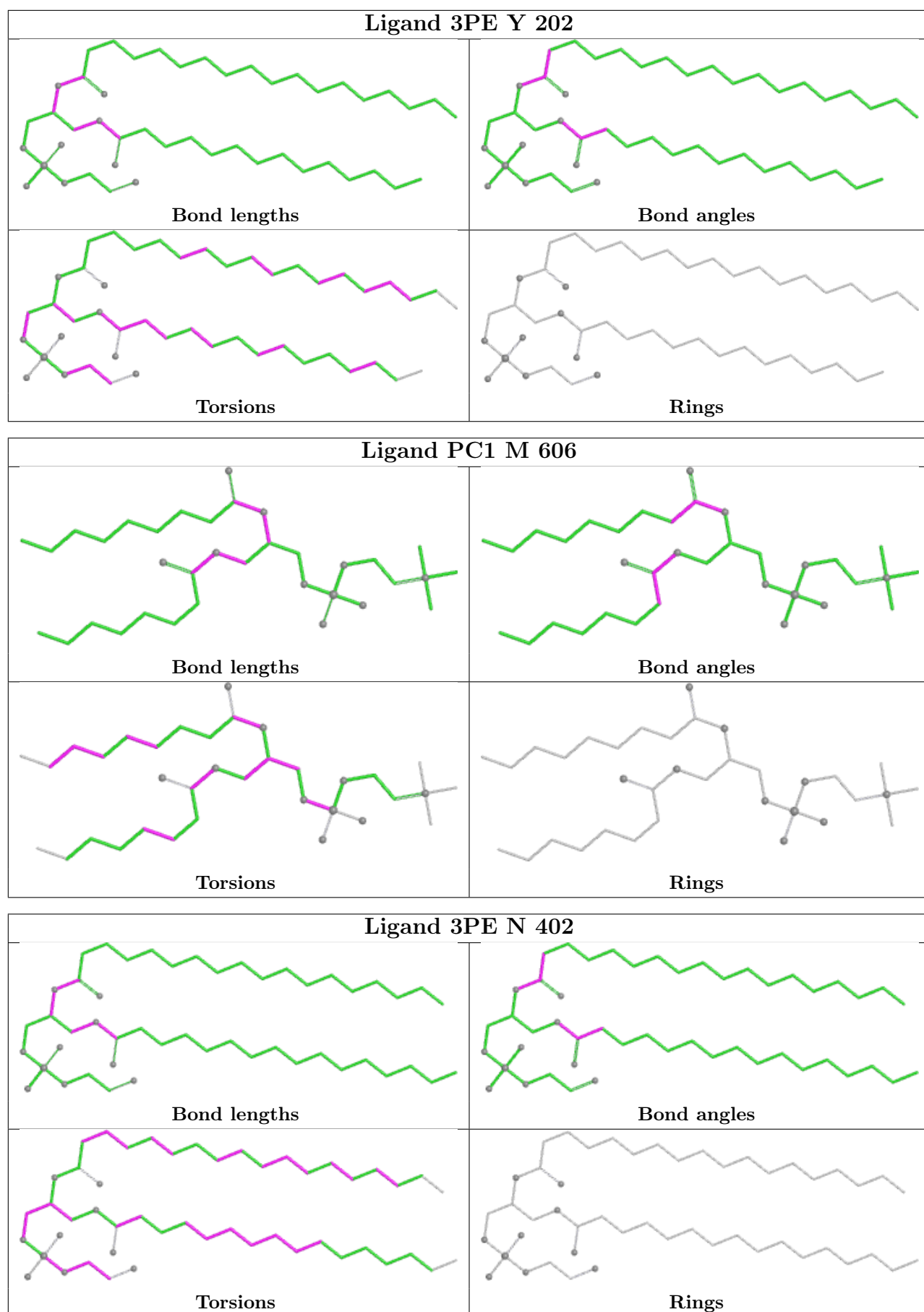


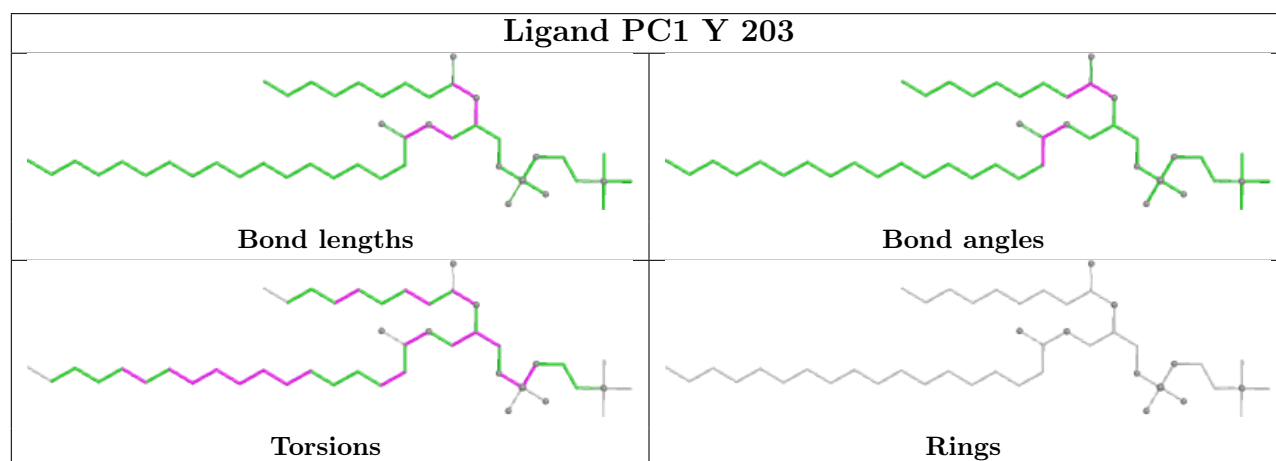
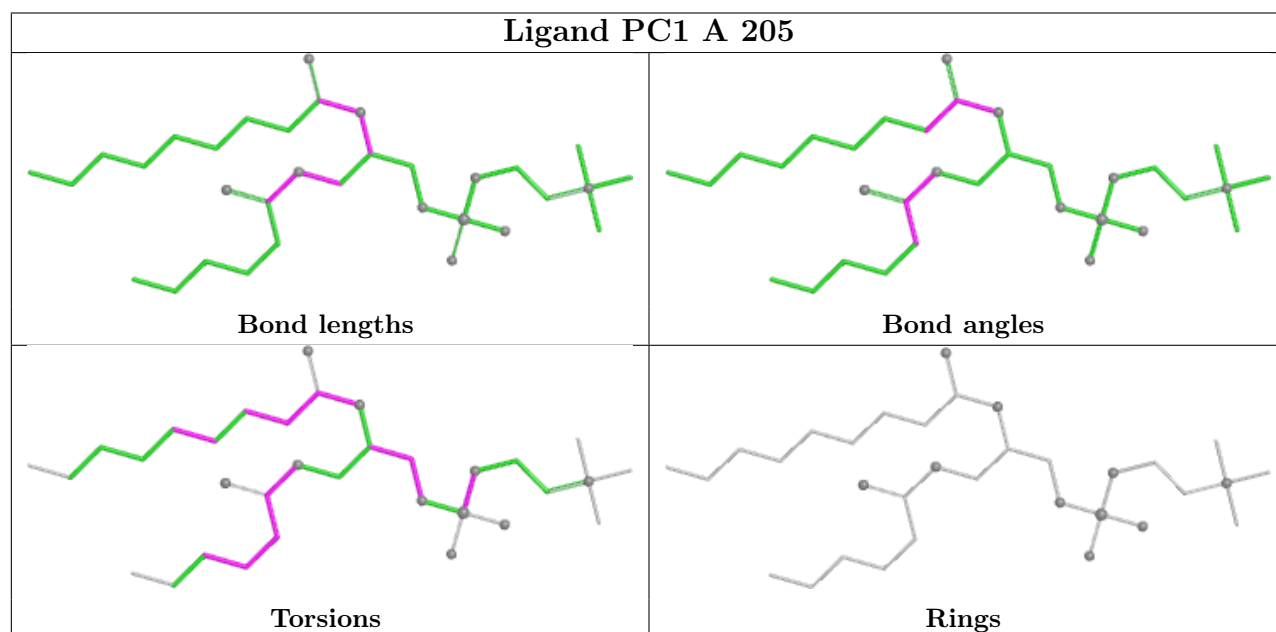
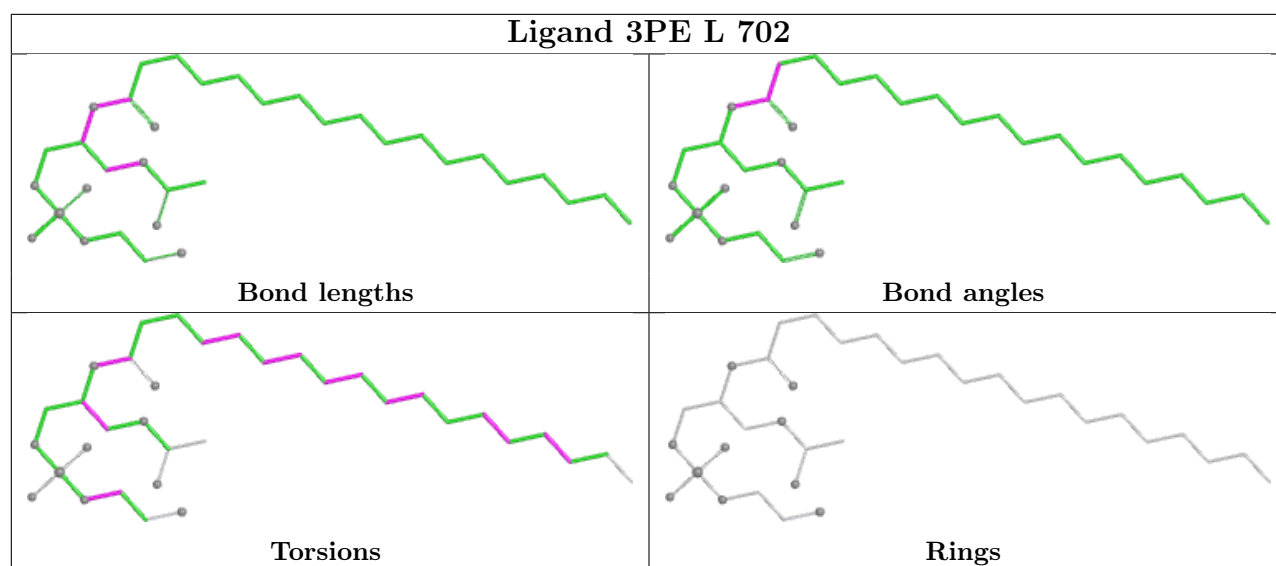
Ligand PC1 A 203

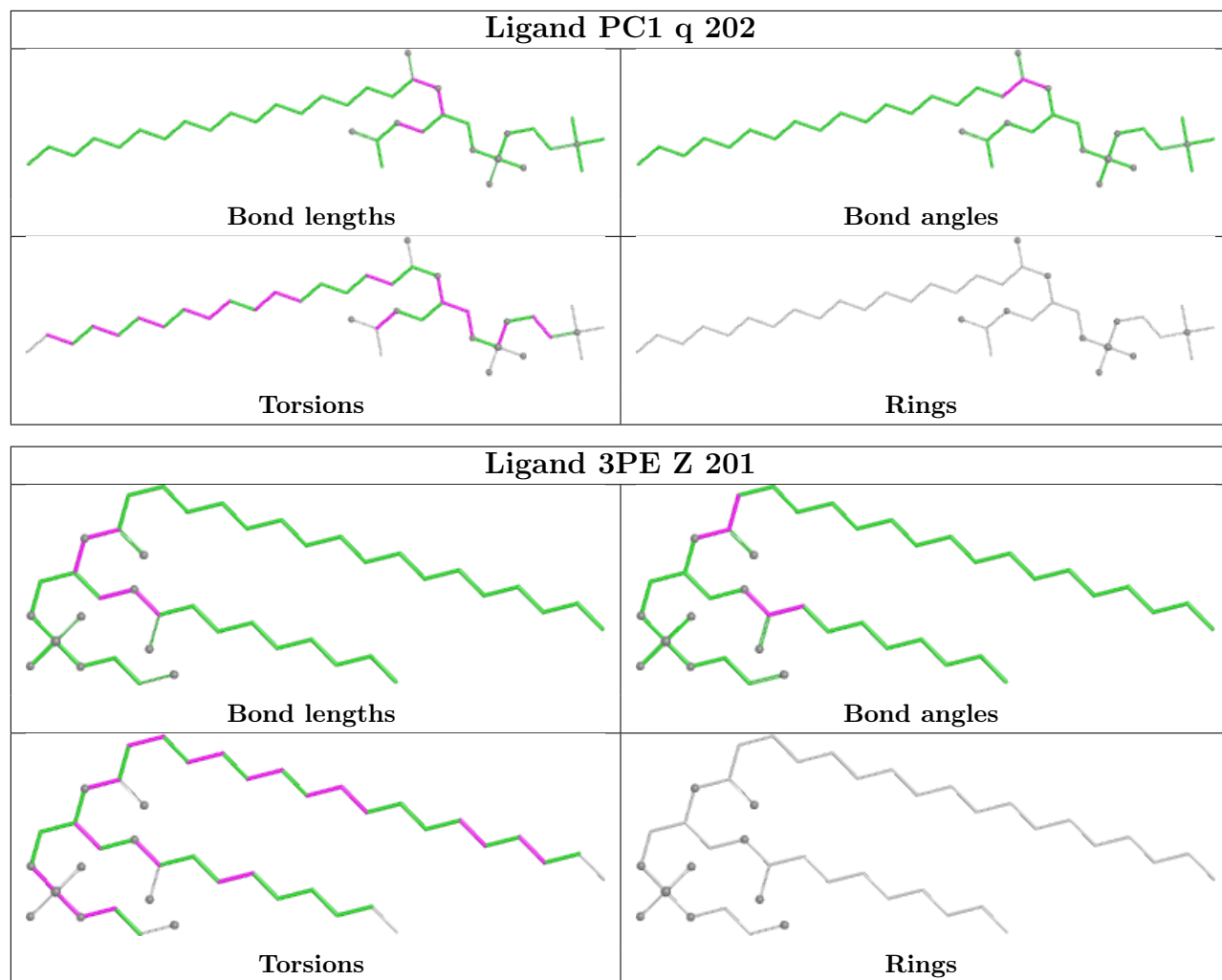


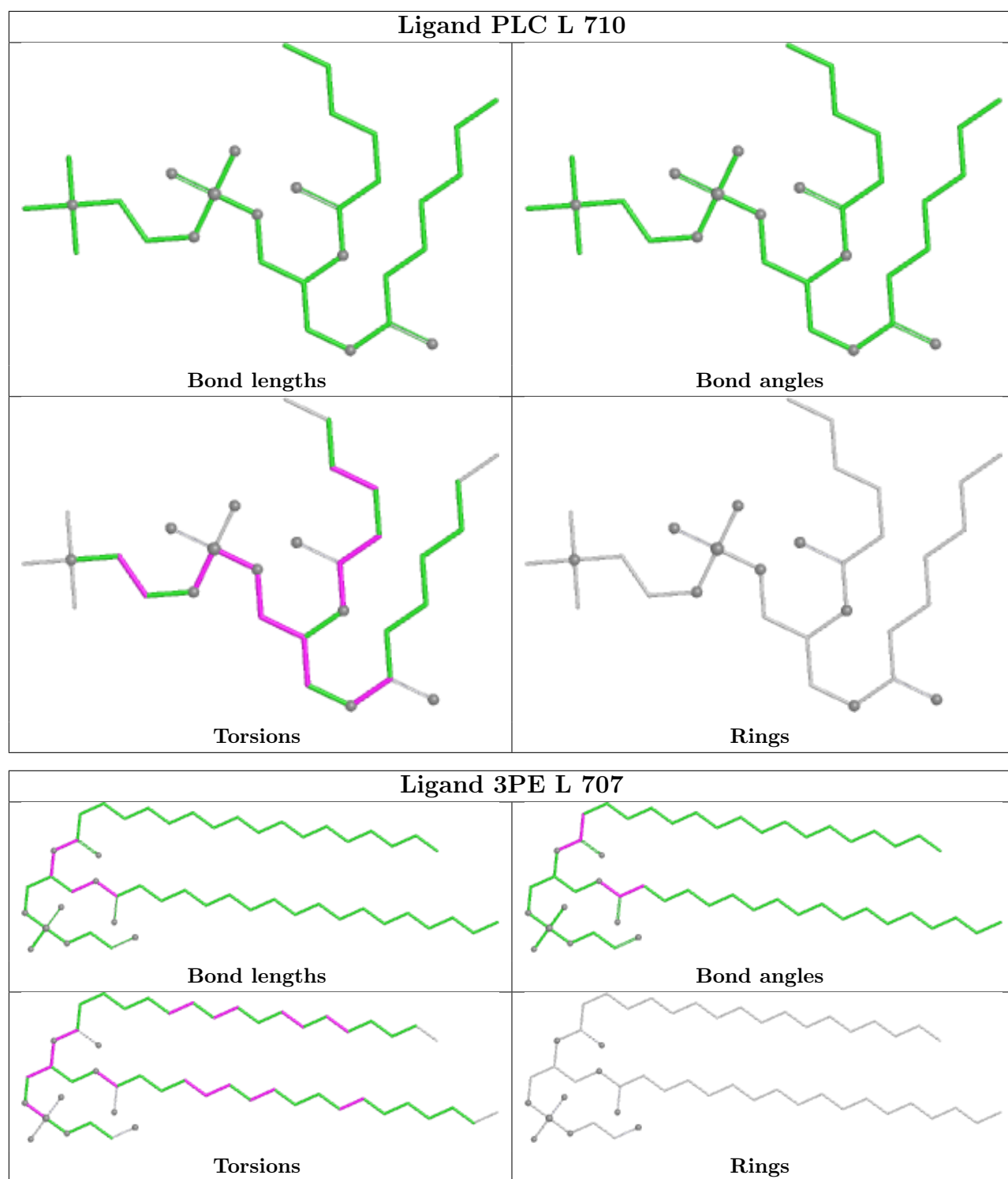
Ligand DGT O 402

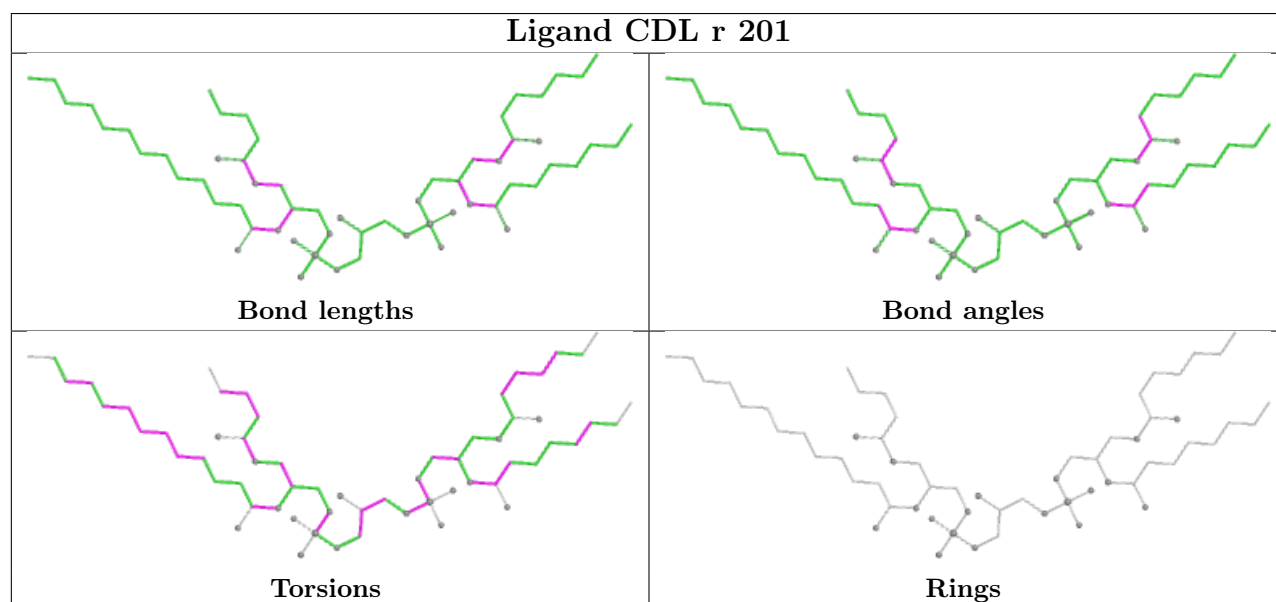
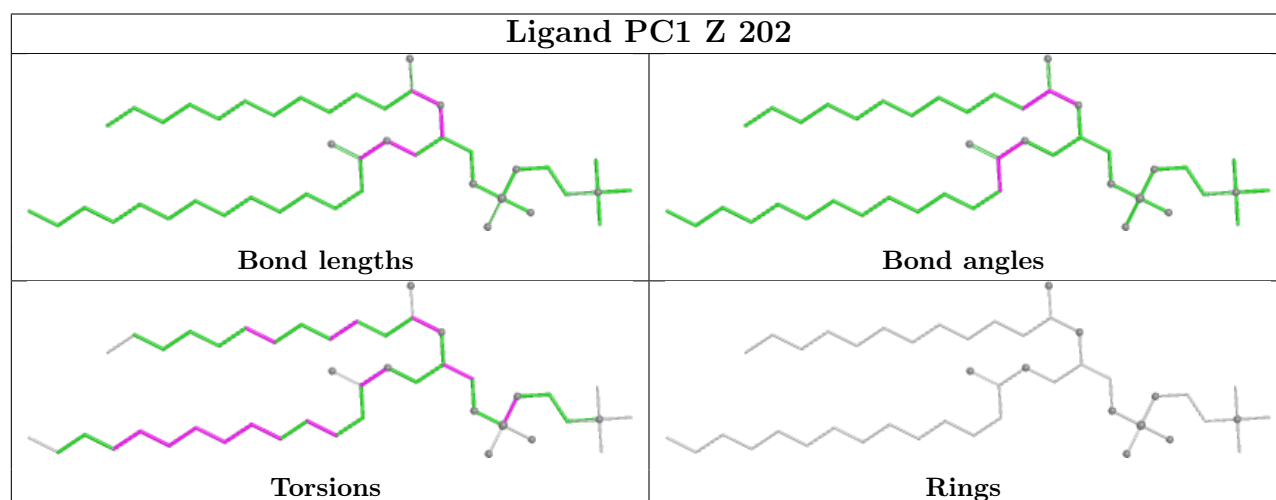
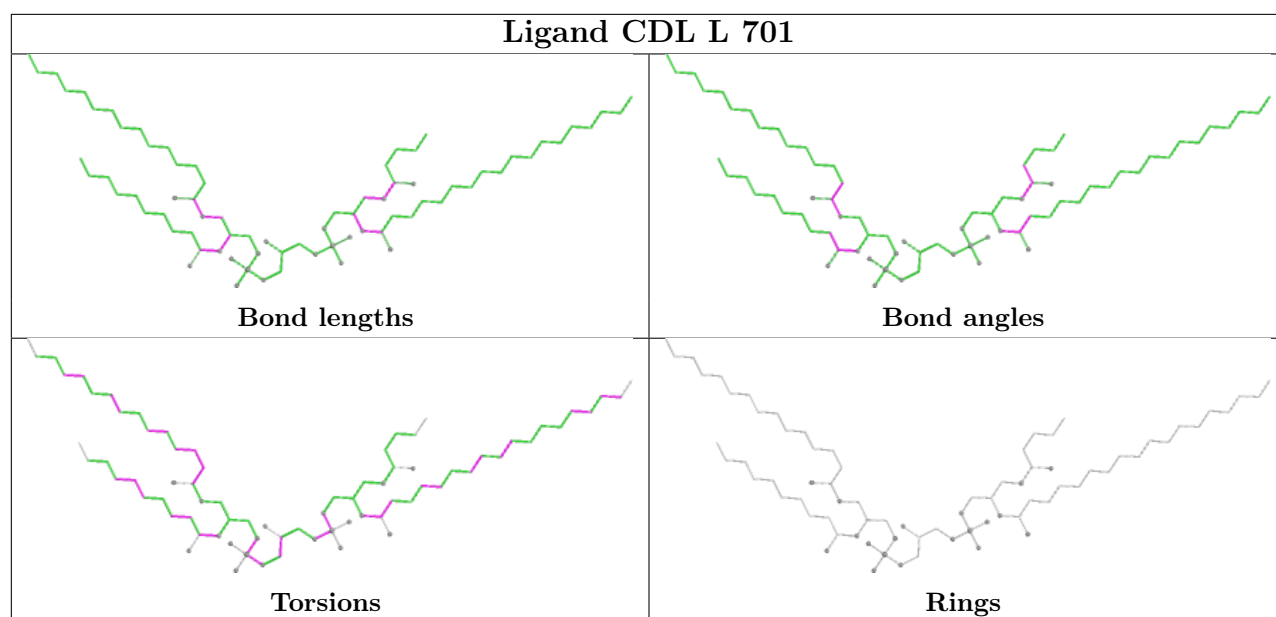


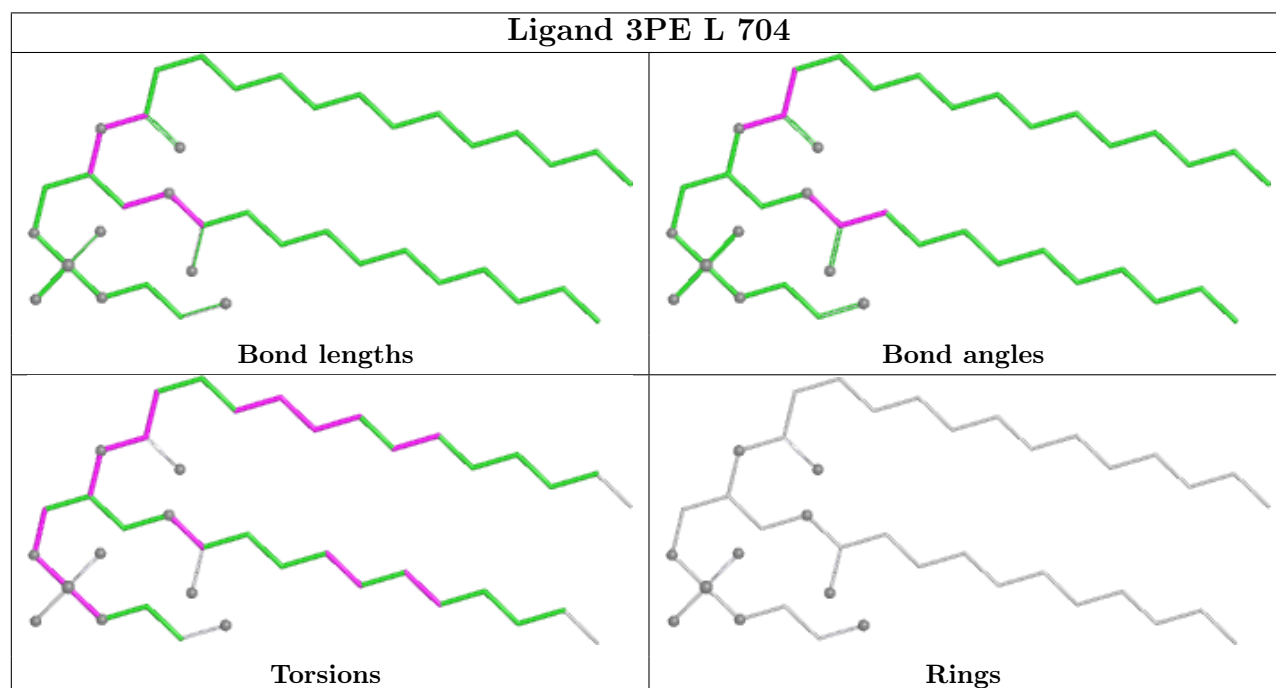
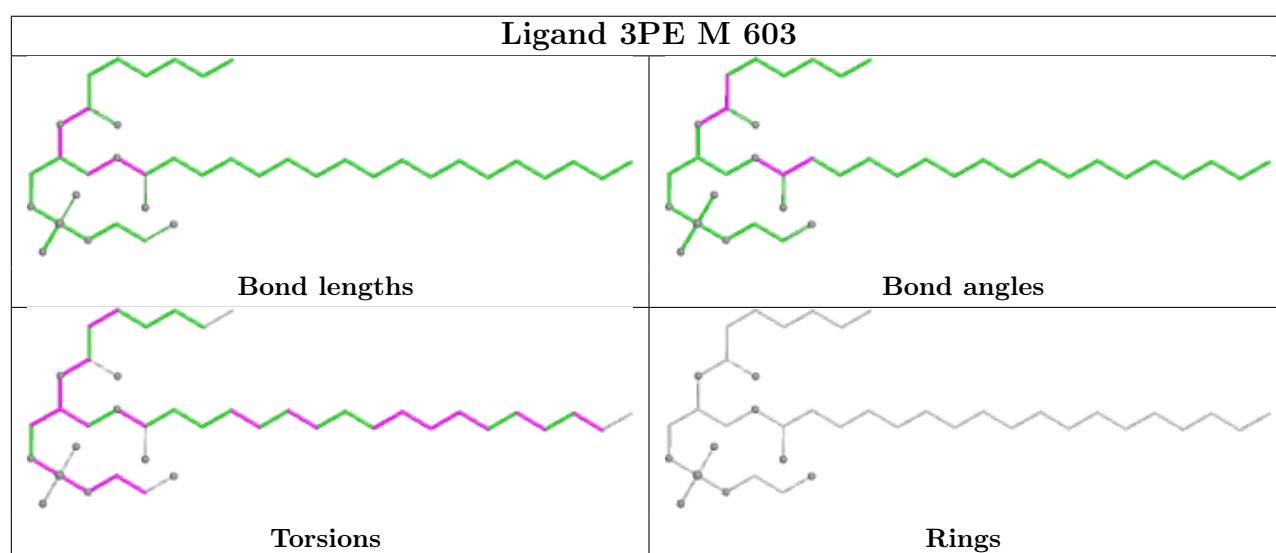
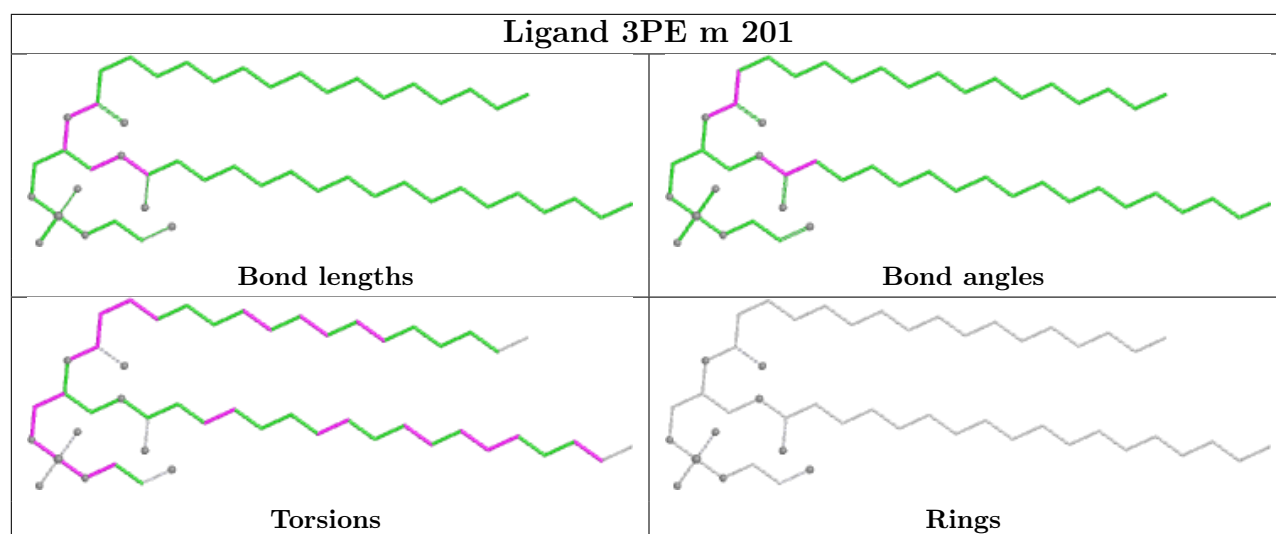


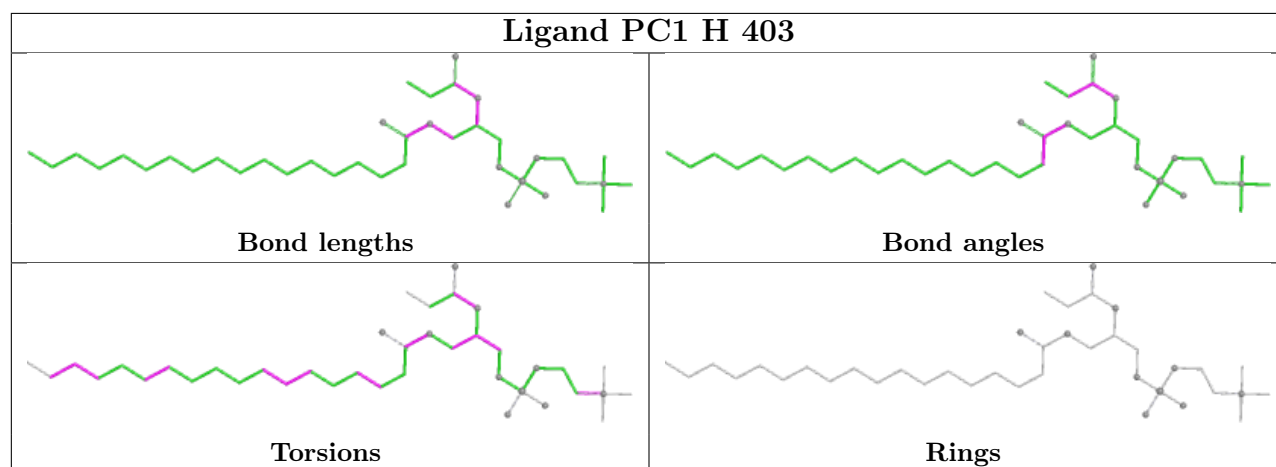
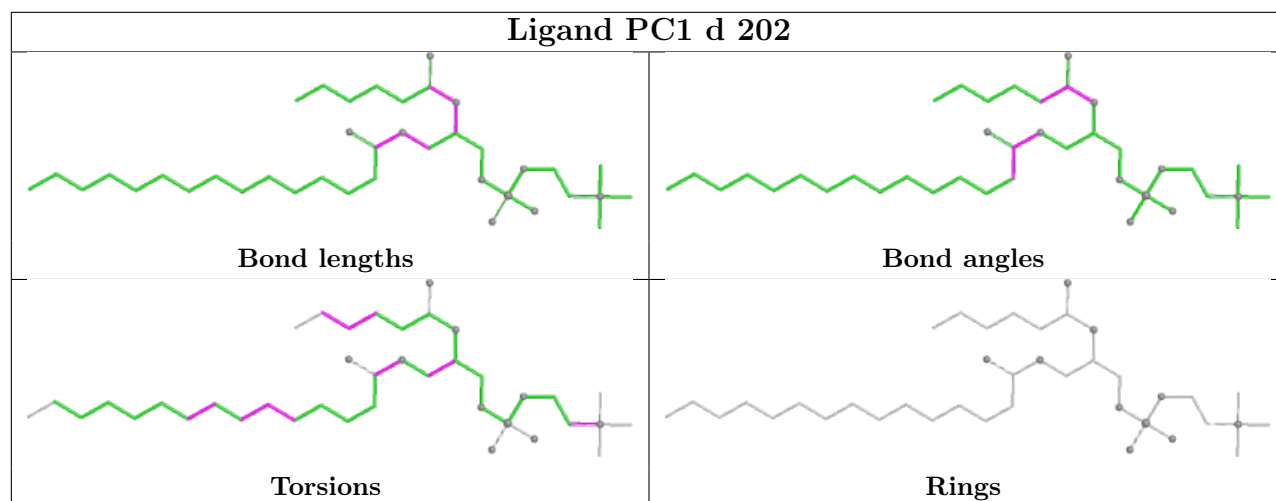
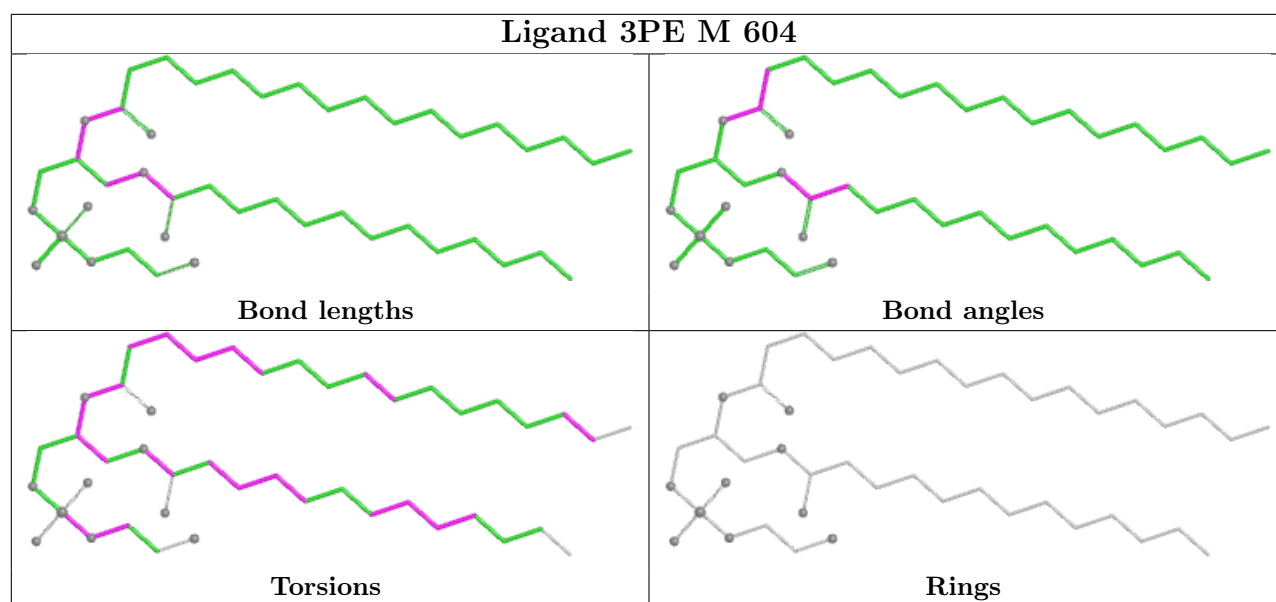


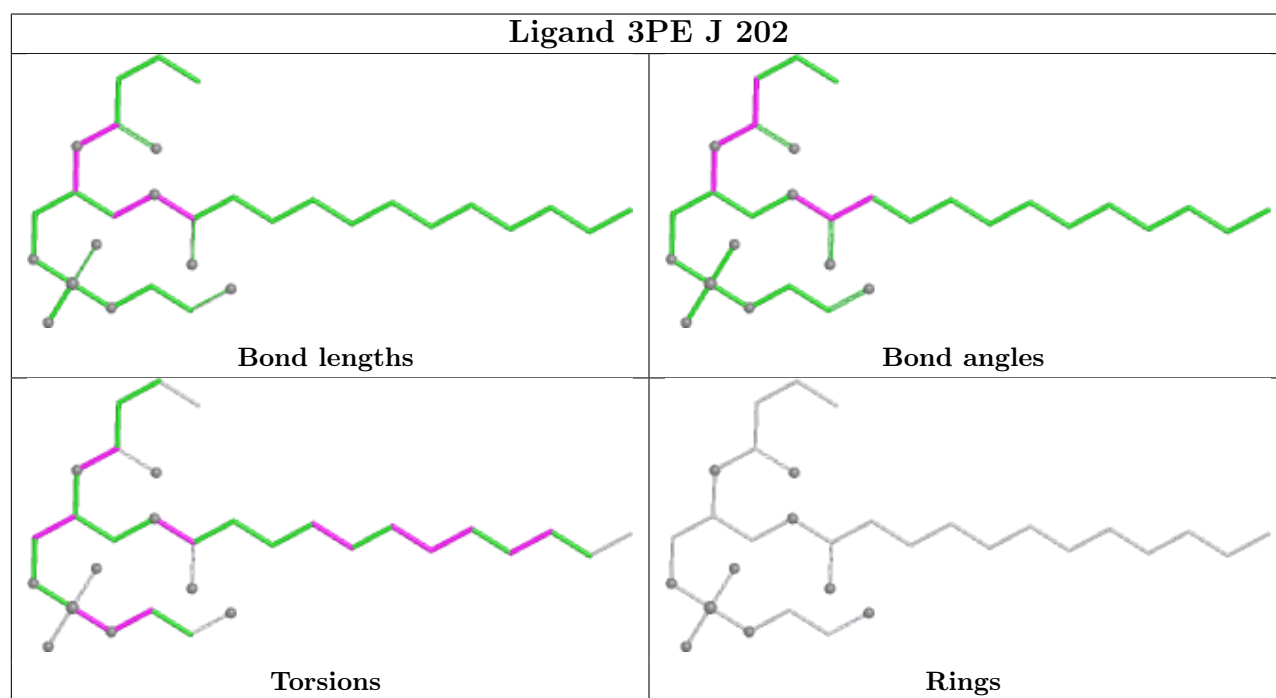
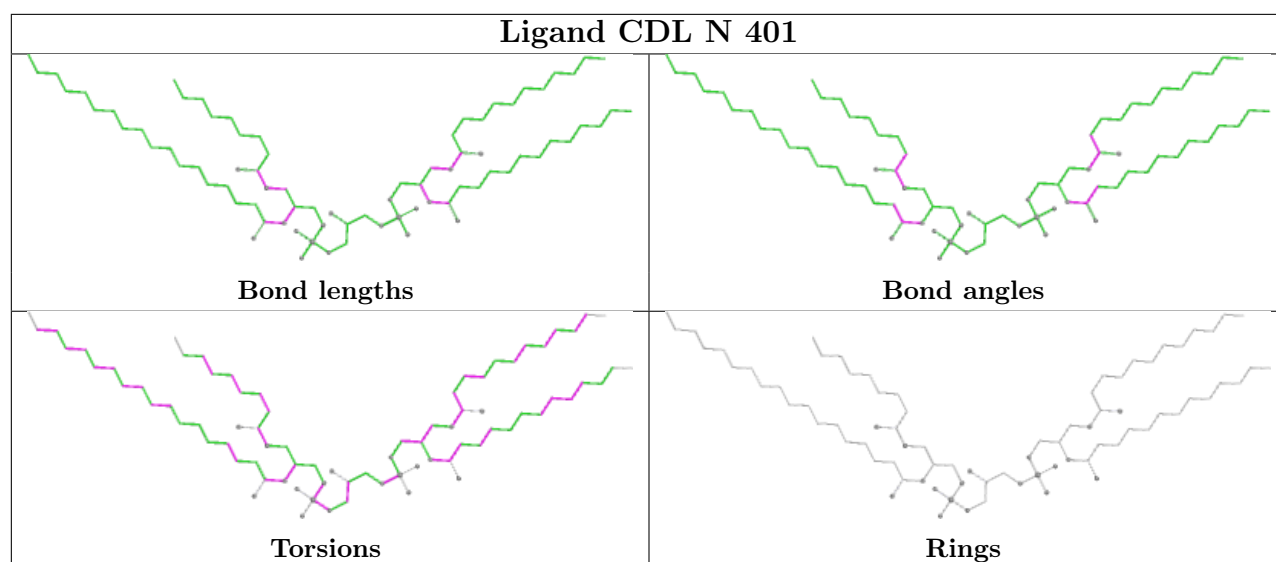


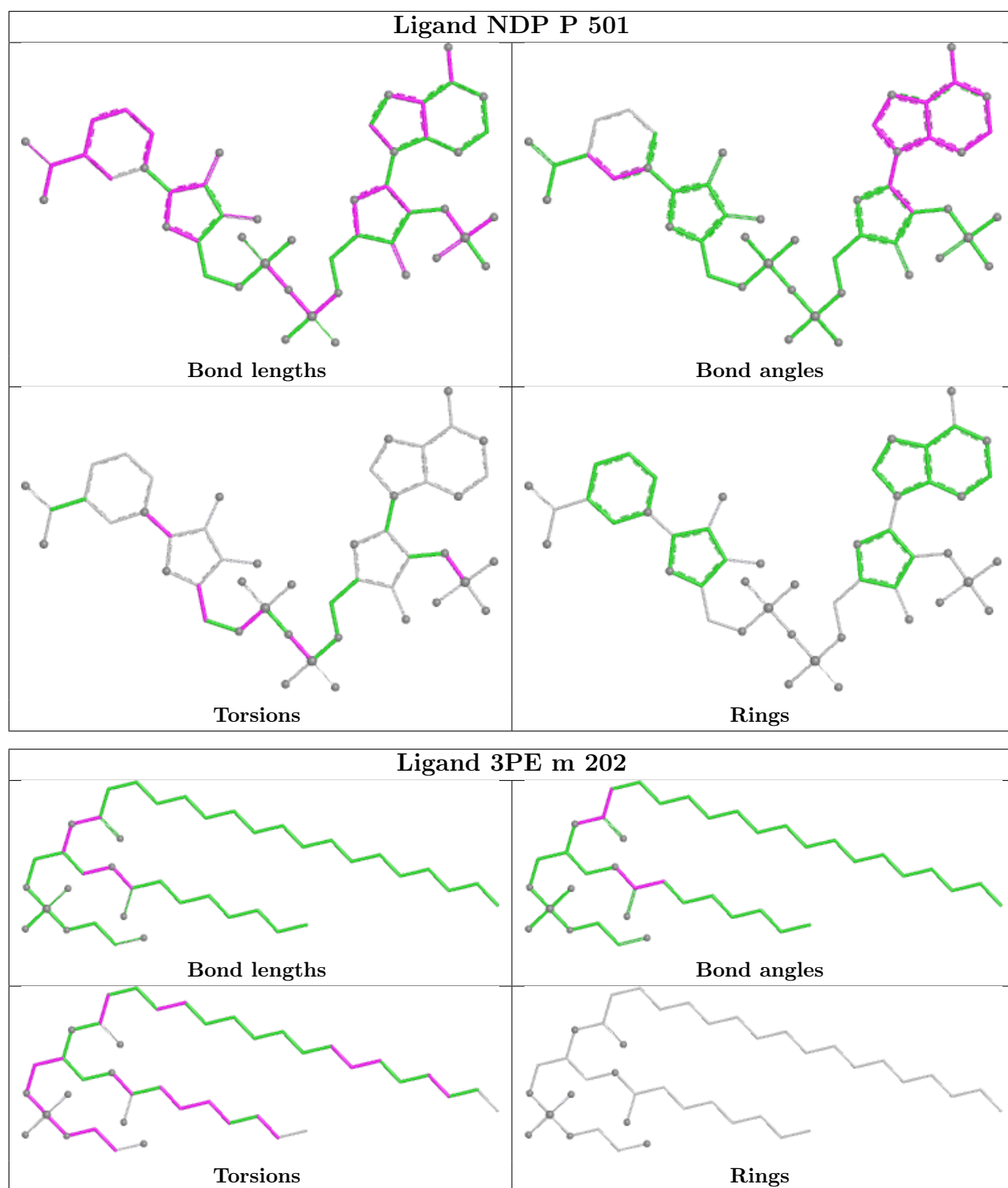


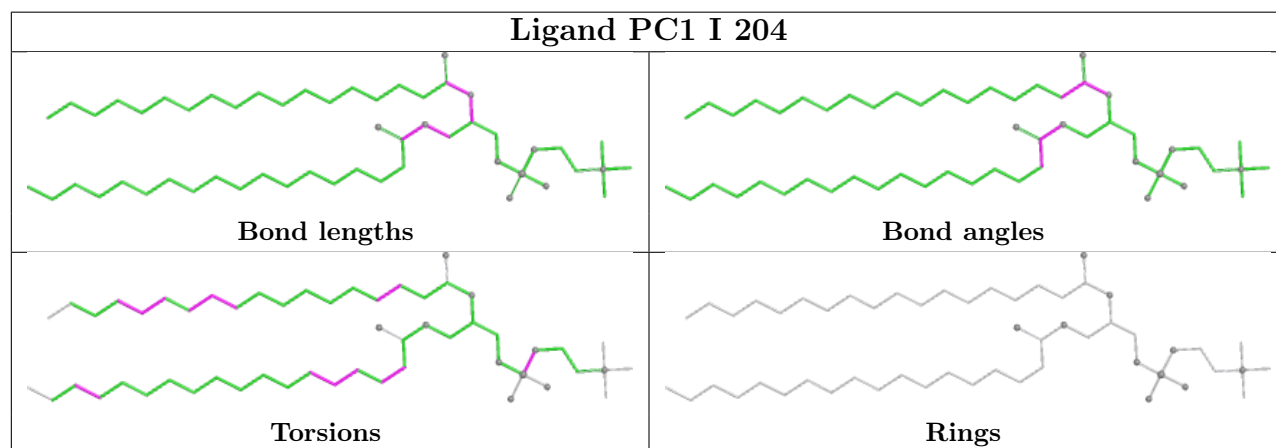
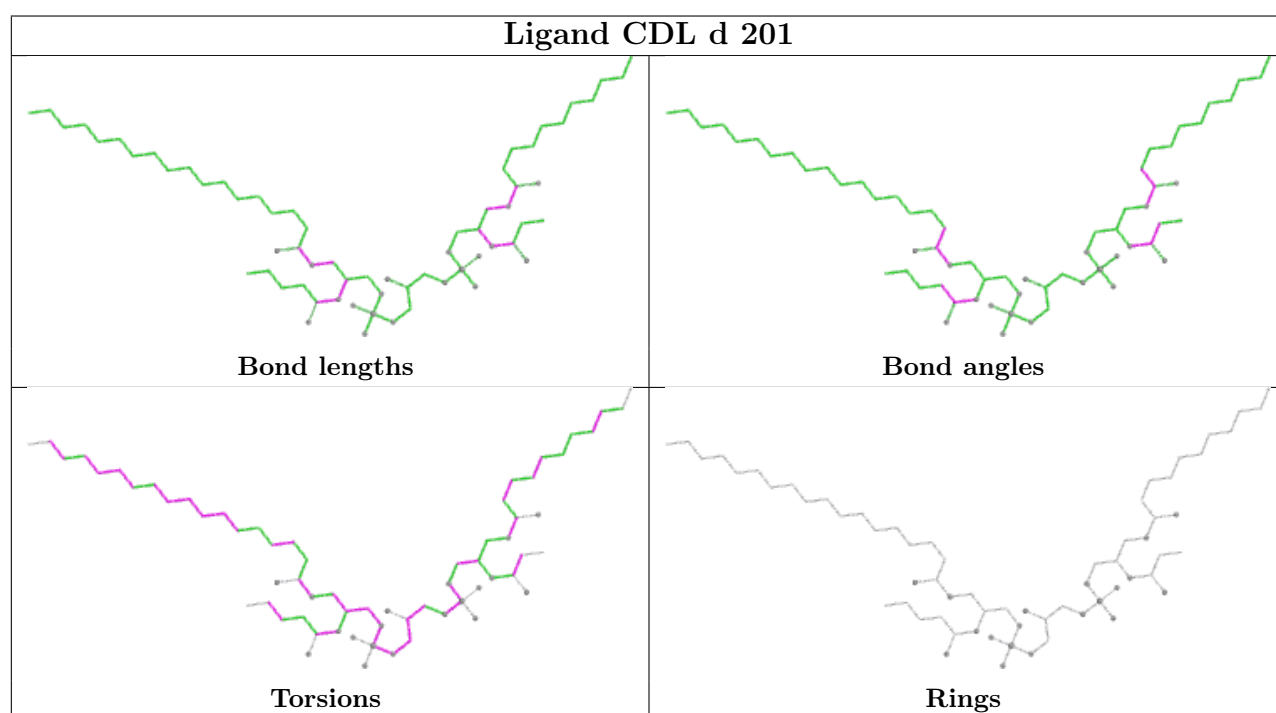
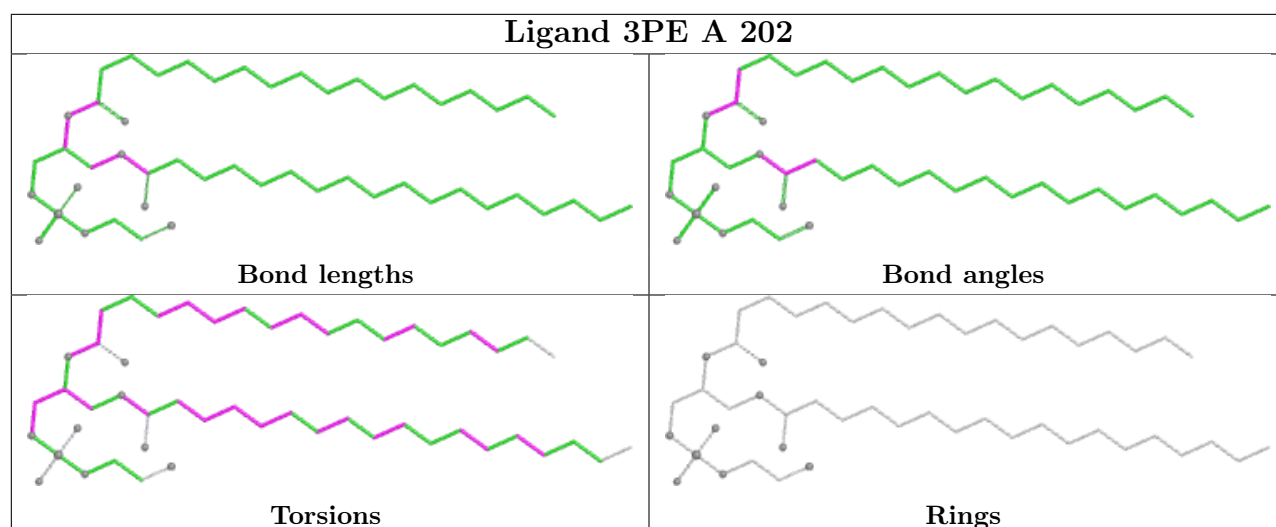


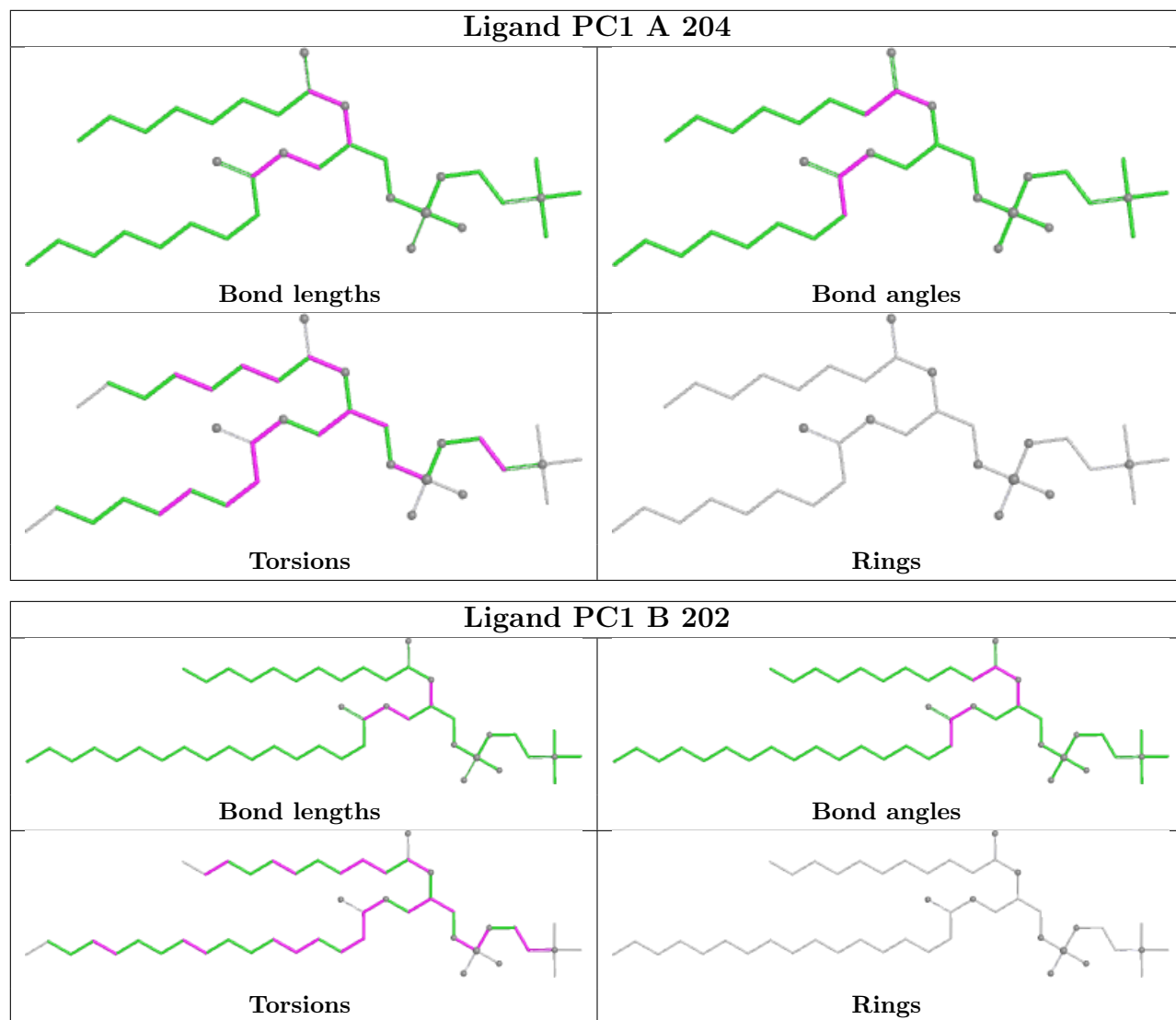


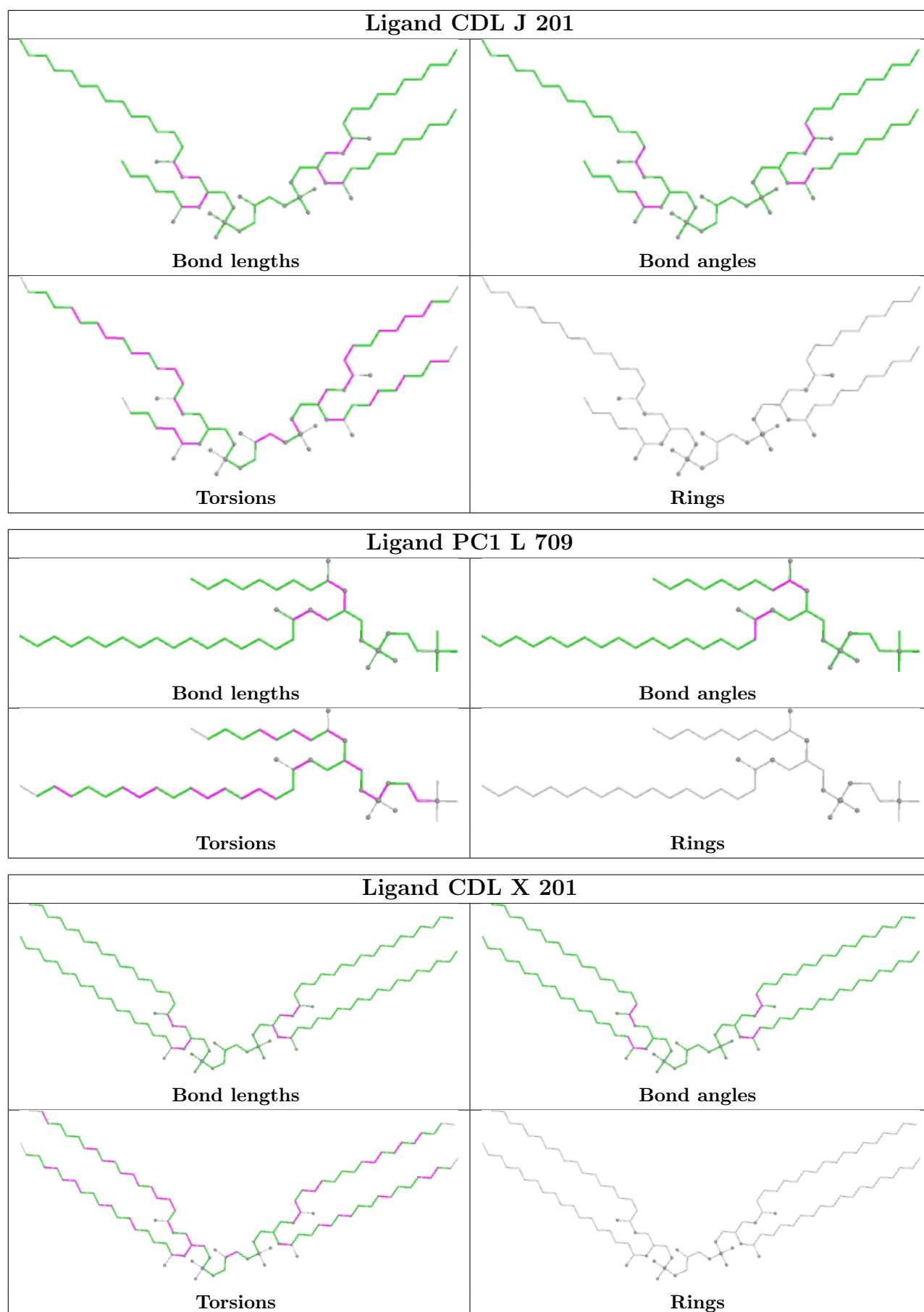


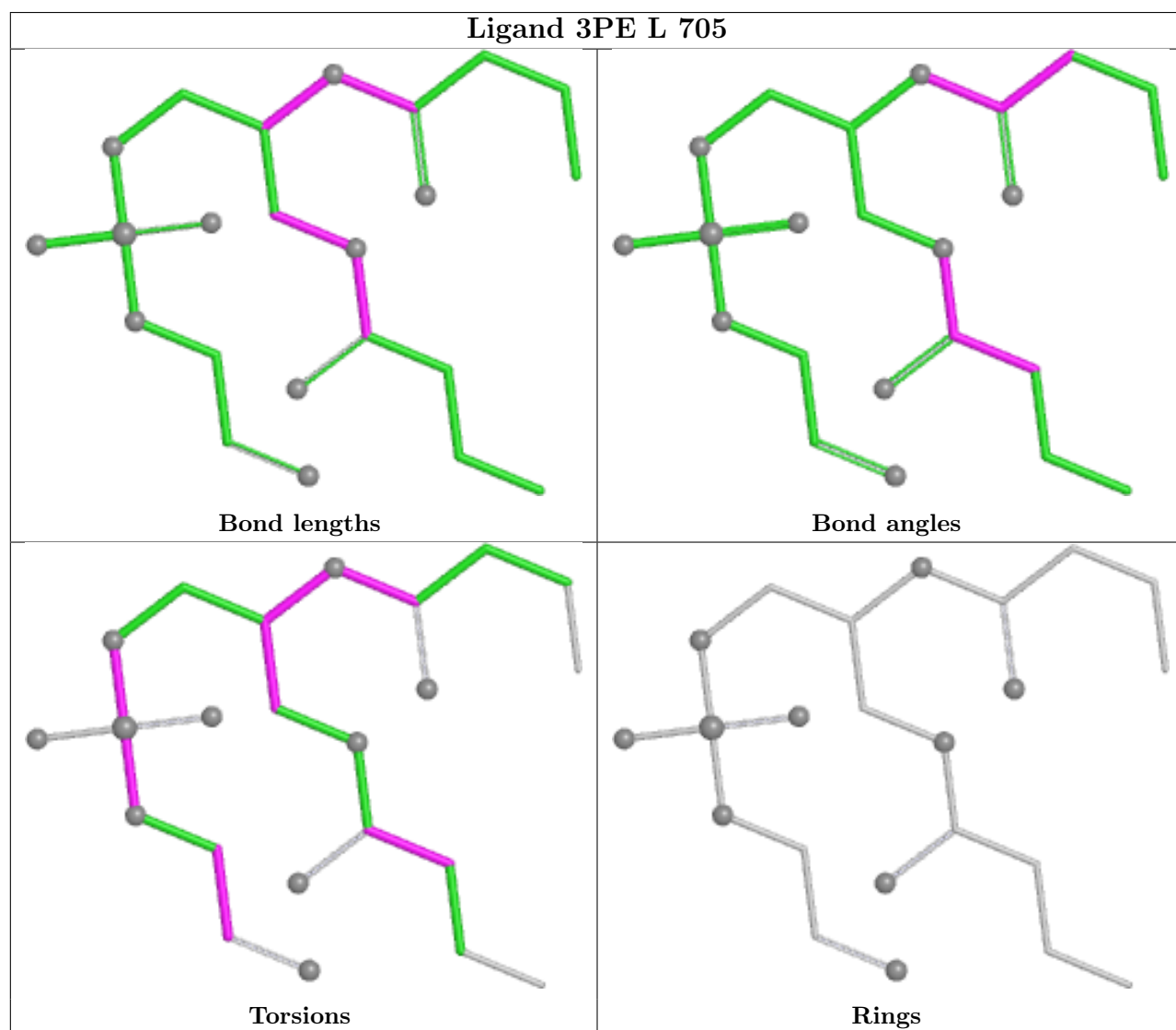
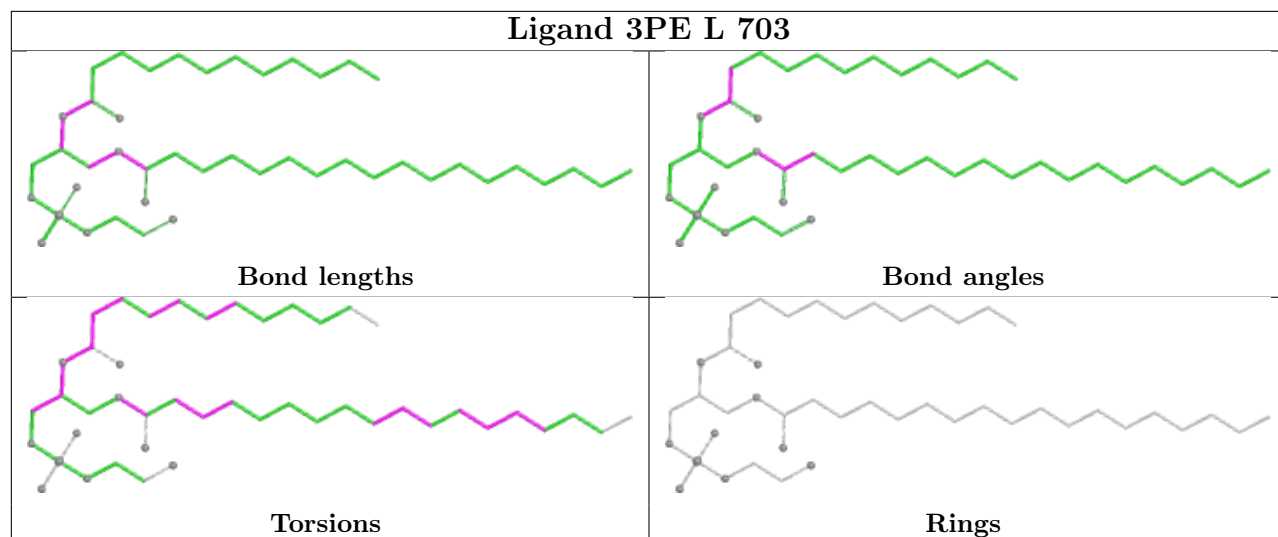


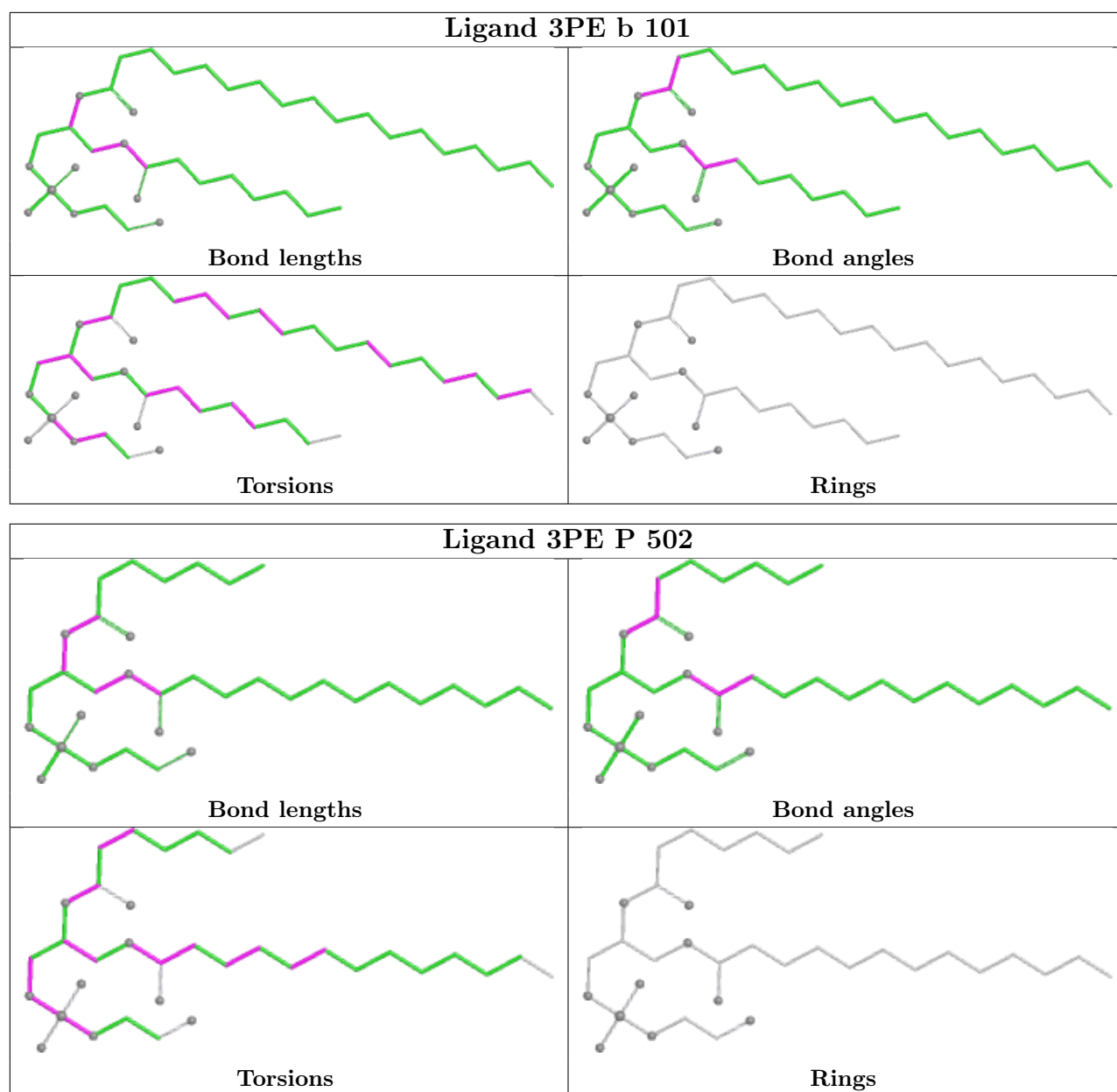












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

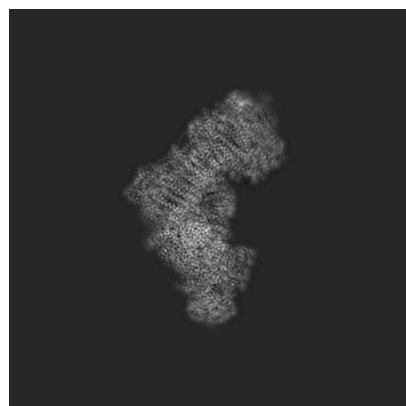
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18051. These allow visual inspection of the internal detail of the map and identification of artifacts.

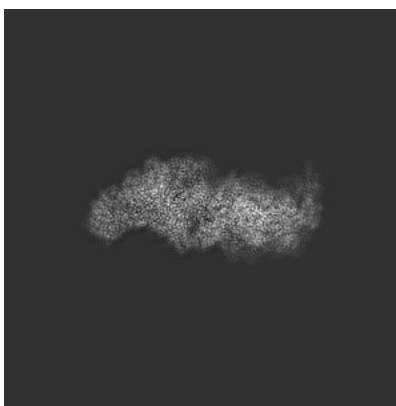
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

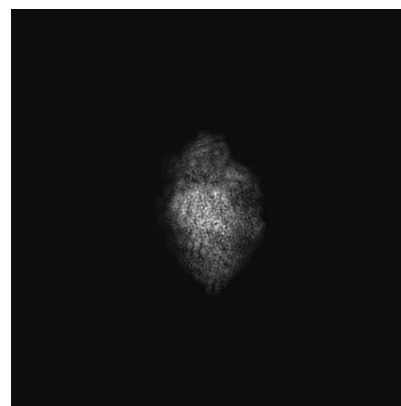
6.1.1 Primary map



X

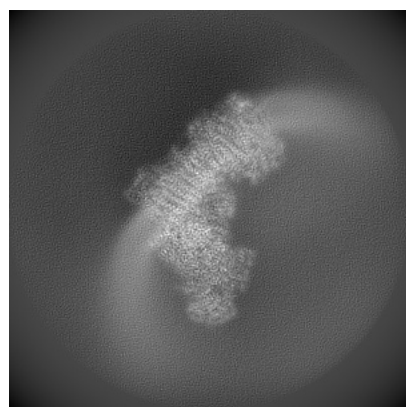


Y

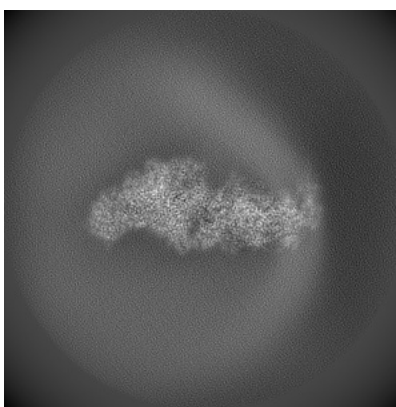


Z

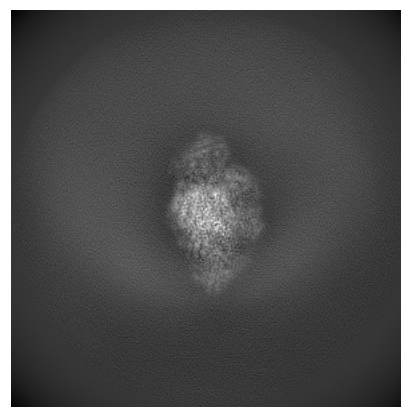
6.1.2 Raw map



X



Y



Z

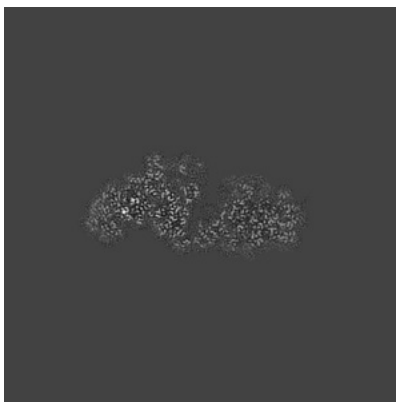
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

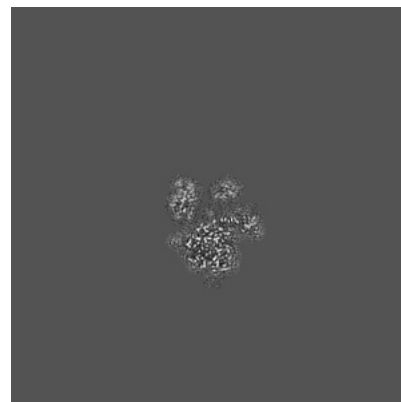
6.2.1 Primary map



X Index: 180

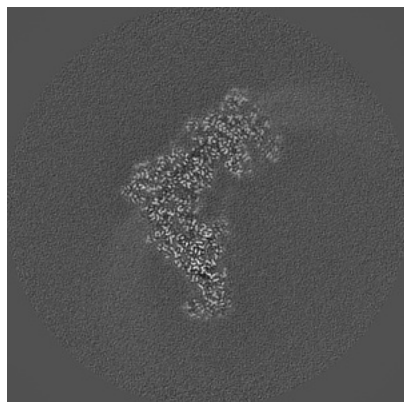


Y Index: 180

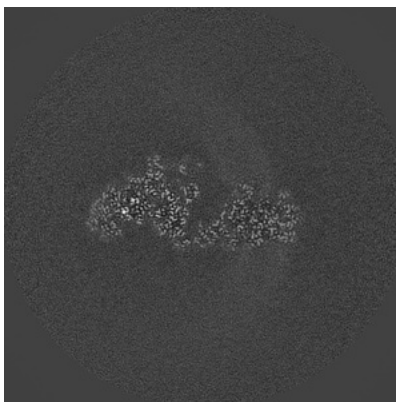


Z Index: 180

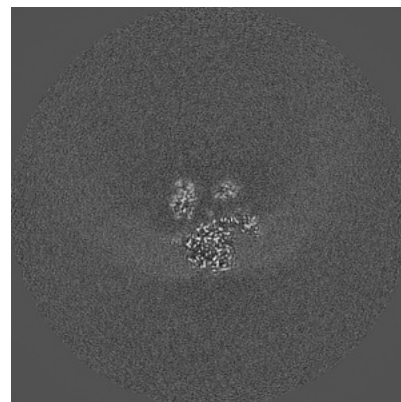
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

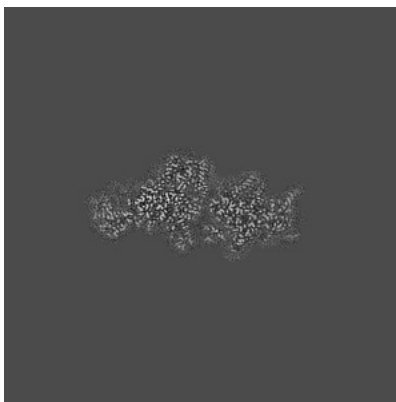
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 176

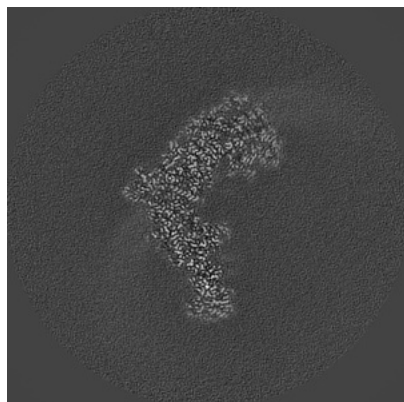


Y Index: 169

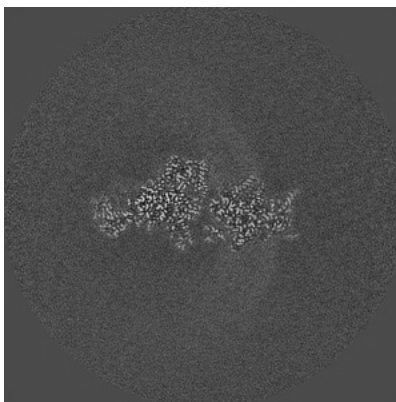


Z Index: 148

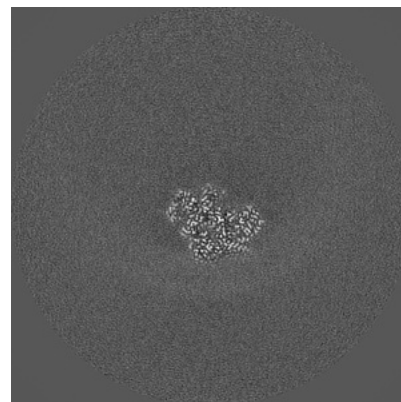
6.3.2 Raw map



X Index: 176



Y Index: 169

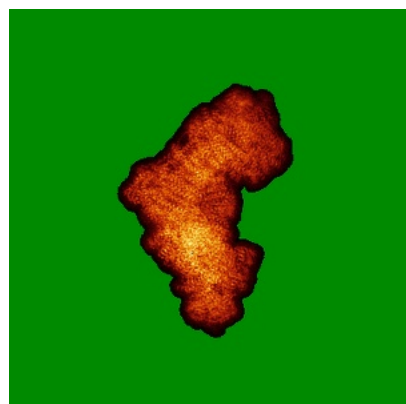


Z Index: 158

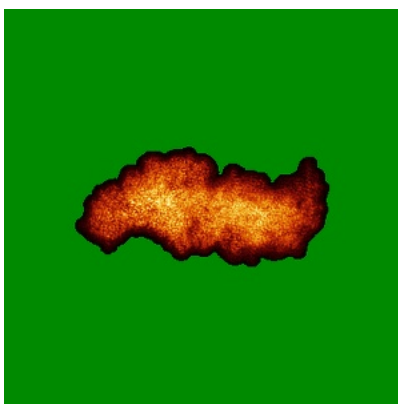
The images above show the largest variance slices of the map in three orthogonal directions.

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

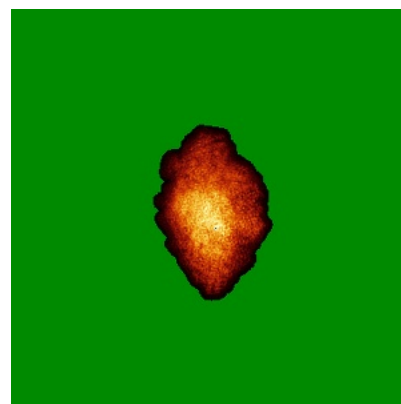
6.4.1 Primary map



X

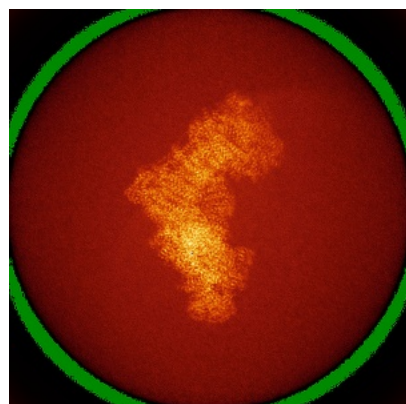


Y

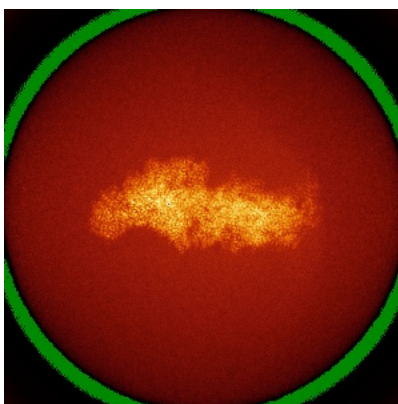


Z

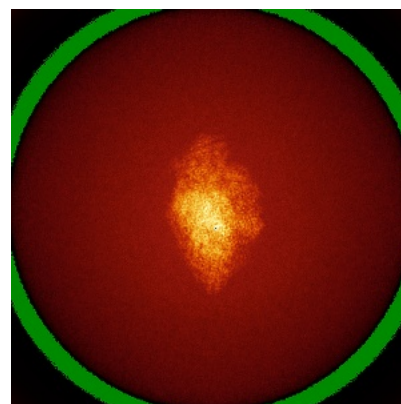
6.4.2 Raw map



X



Y



Z

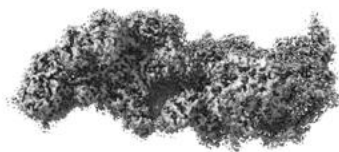
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

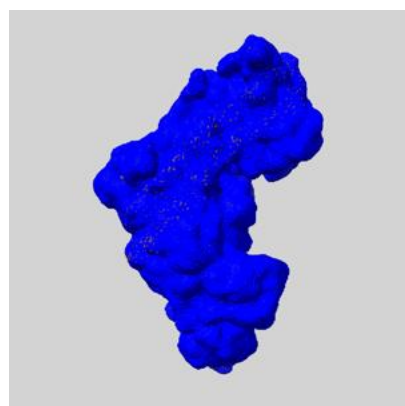
6.6 Mask visualisation [i](#)

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

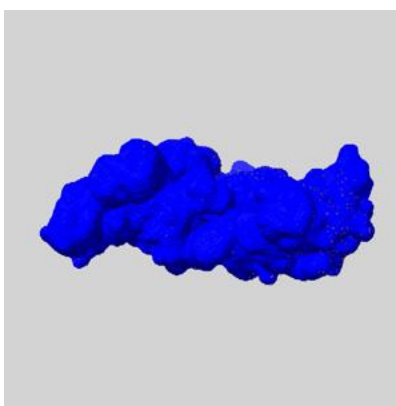
A mask typically either:

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

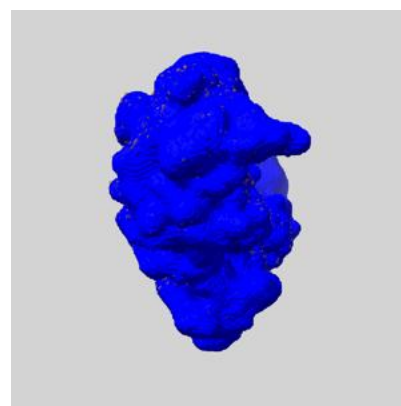
6.6.1 emd_18051_msk_1.map [i](#)



X



Y

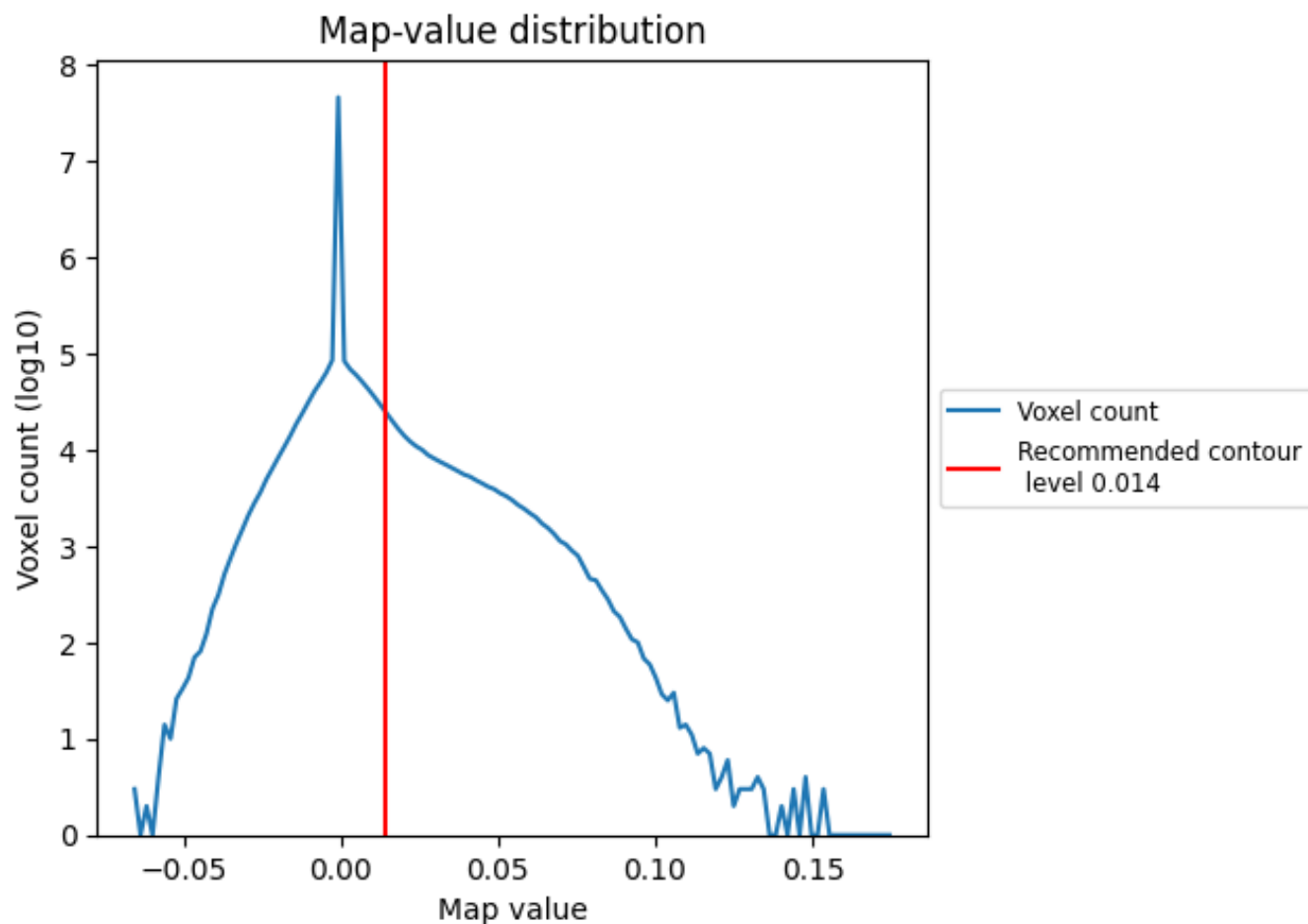


Z

7 Map analysis [i](#)

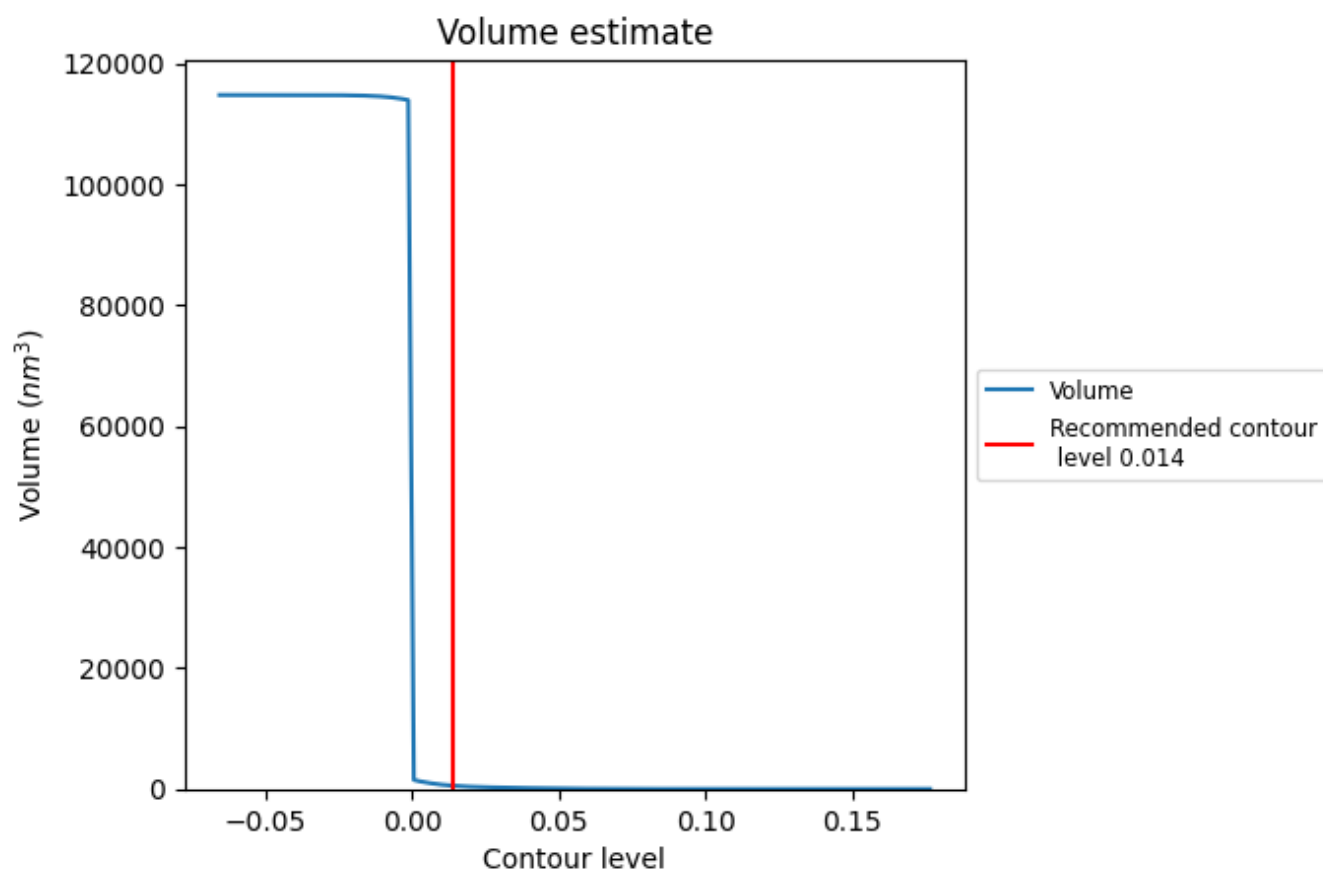
This section contains the results of statistical analysis of the map.

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.

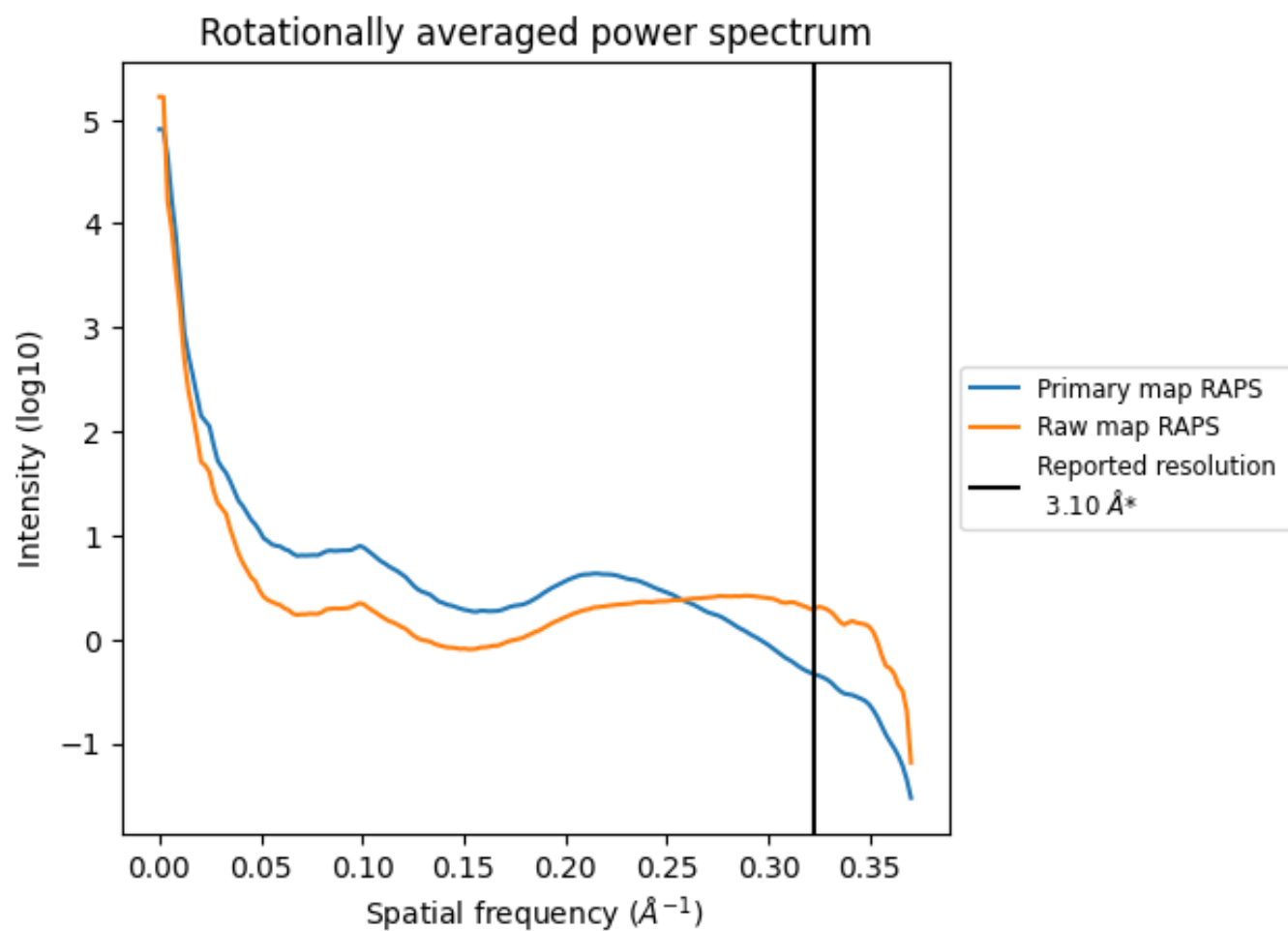
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm^3 ; this corresponds to an approximate mass of 483 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

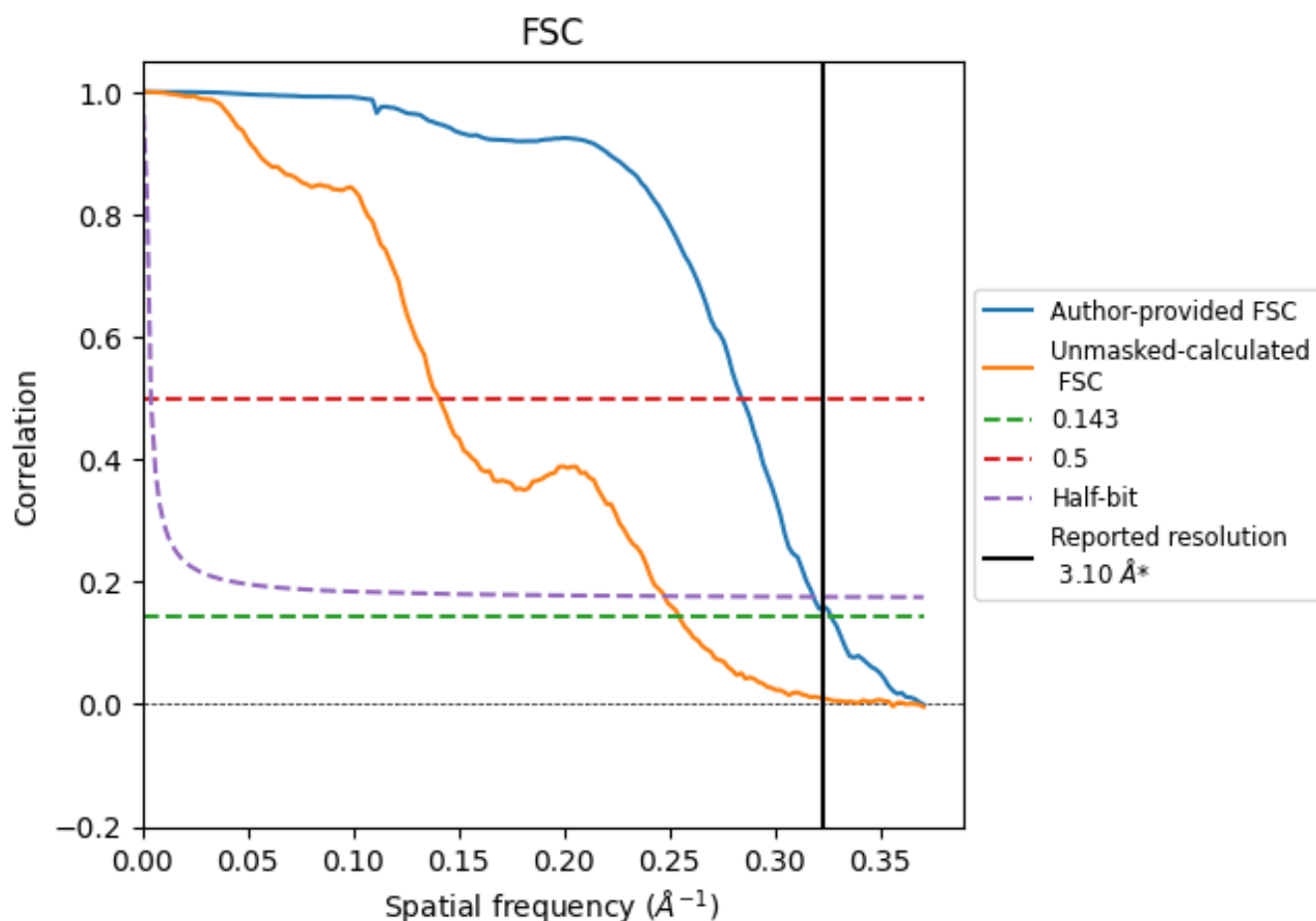


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.52	3.14
Unmasked-calculated*	3.93	7.11	4.04

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

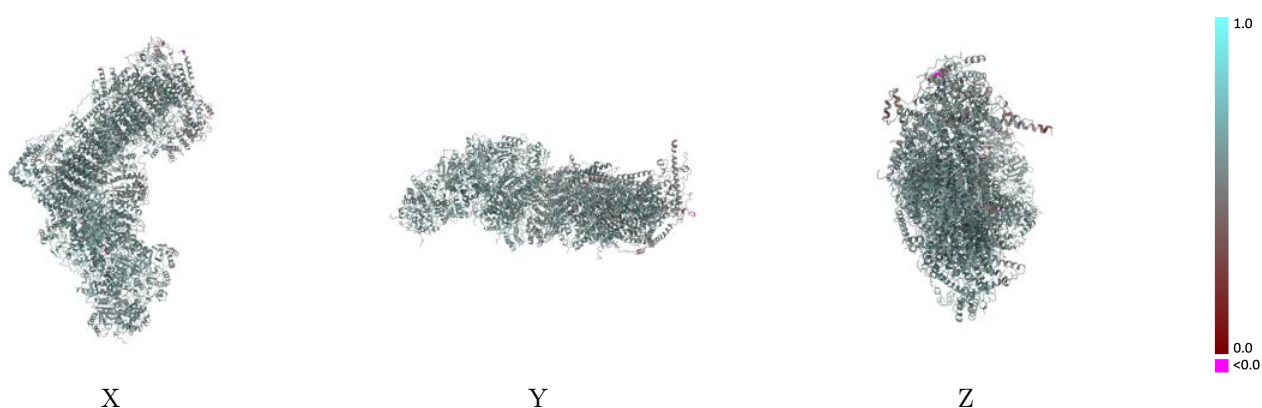
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18051 and PDB model 8Q0A. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)

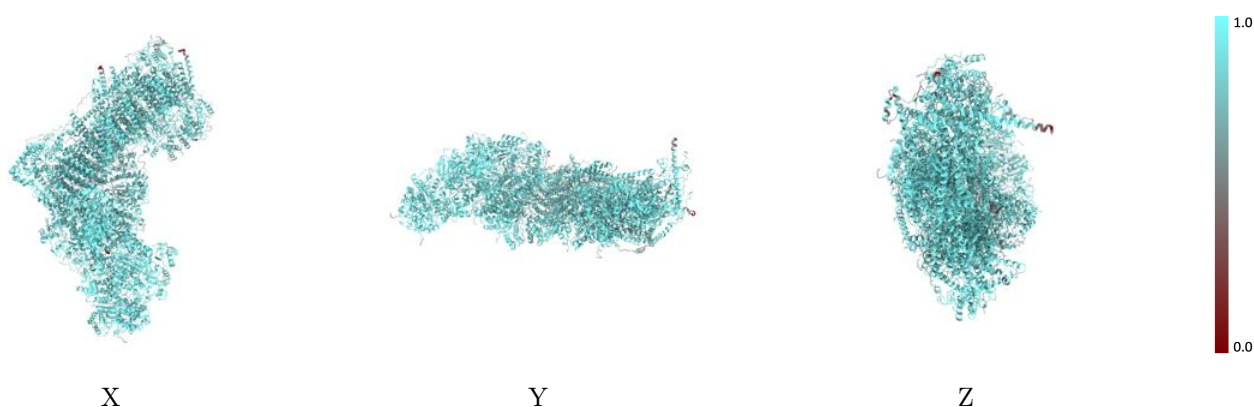
This section was not generated.

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



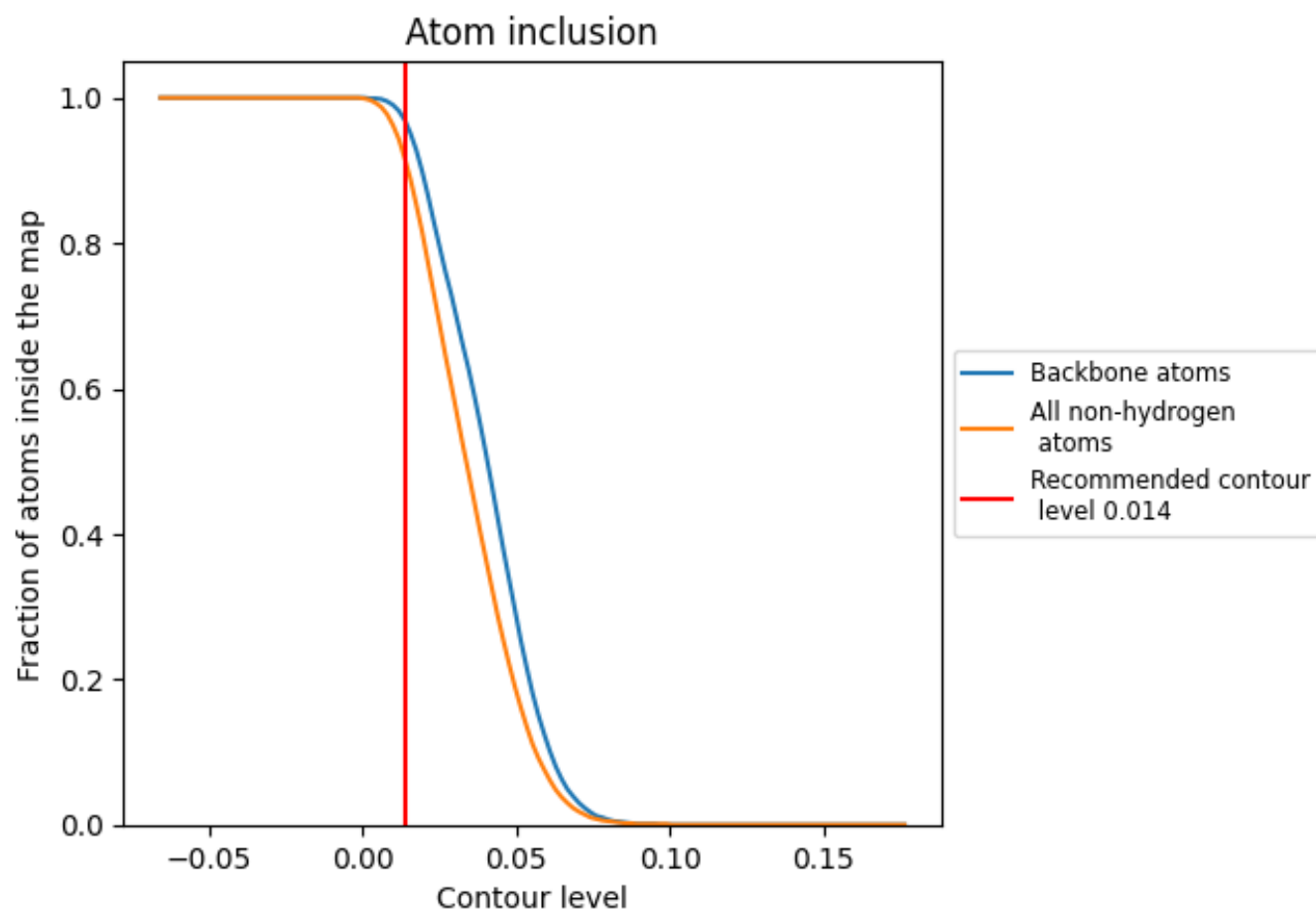
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.5730
A	 0.9030	 0.5920
B	 0.9540	 0.6110
C	 0.9640	 0.6130
D	 0.9600	 0.6110
E	 0.9180	 0.5560
F	 0.9370	 0.5700
G	 0.9380	 0.5840
H	 0.9620	 0.6050
I	 0.9620	 0.6150
J	 0.8940	 0.5810
K	 0.9530	 0.5990
L	 0.8970	 0.5650
M	 0.9500	 0.5990
N	 0.9670	 0.6070
O	 0.9090	 0.5600
P	 0.9260	 0.5860
Q	 0.9150	 0.5880
R	 0.8960	 0.5750
S	 0.8850	 0.5270
T	 0.8330	 0.4950
U	 0.8280	 0.4940
V	 0.9220	 0.5820
W	 0.9230	 0.5870
X	 0.8910	 0.5660
Y	 0.8840	 0.5600
Z	 0.9190	 0.5710
a	 0.9560	 0.6030
b	 0.8470	 0.5610
c	 0.8590	 0.5500
d	 0.9000	 0.5780
e	 0.9000	 0.5650
f	 0.8310	 0.5300
g	 0.8770	 0.5560
h	 0.9260	 0.5850



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7890	 0.4870
j	 0.7970	 0.4890
k	 0.7930	 0.4770
l	 0.8980	 0.5480
m	 0.8590	 0.5510
n	 0.8780	 0.5350
o	 0.8390	 0.4970
p	 0.8880	 0.5430
q	 0.9180	 0.5860
r	 0.9330	 0.5840
s	 0.8460	 0.5190