



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 06:20 pm BST

PDB ID : 6YJ4 / pdb\_00006yj4  
EMDB ID : EMD-10815  
Title : Structure of Yarrowia lipolytica complex I at 2.7 Å  
Authors : Hirst, J.; Grba, D.  
Deposited on : 2020-04-02  
Resolution : 2.70 Å(reported)  
Based on initial model : 6G2J

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

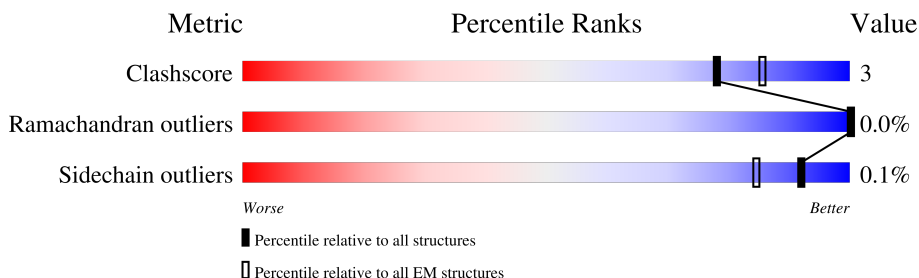
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.


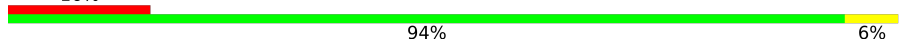
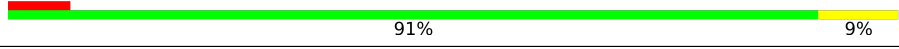
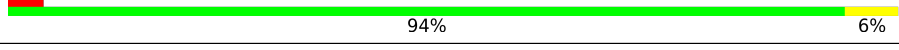
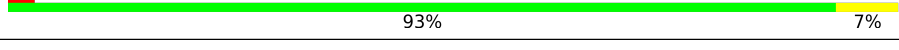
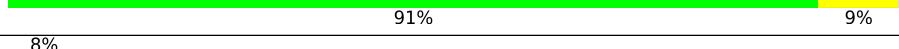
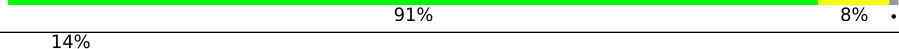
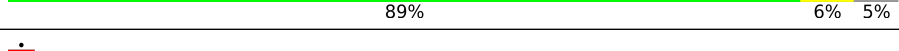
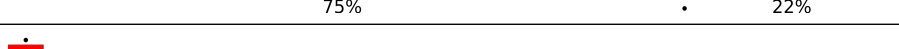
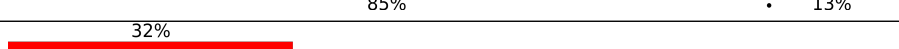


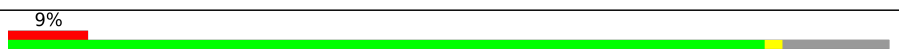
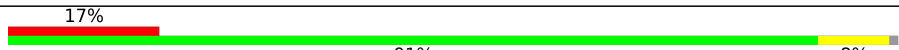
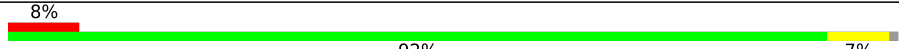

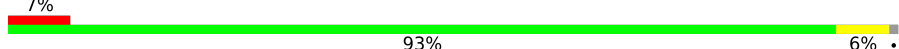
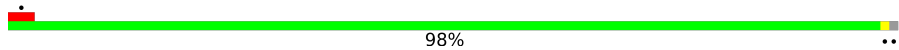
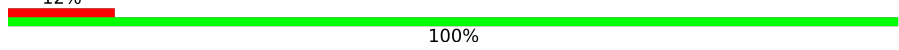
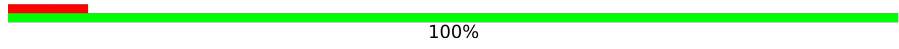
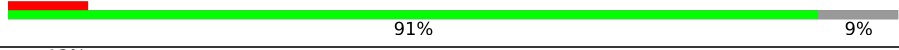
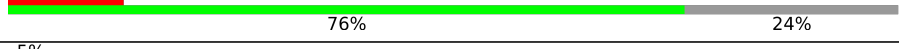
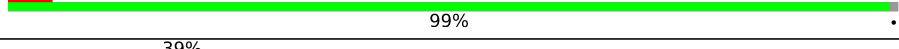




The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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	128	<div> <div>40%</div> <div> <div>92%</div> <div>8%</div> </div> </div>
2	B	210	<div> <div>79%</div> <div>5%</div> <div>16%</div> </div>
3	C	293	<div> <div>78%</div> <div>5%</div> <div>17%</div> </div>
4	D	466	<div> <div>6%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
5	E	243	<div> <div>22%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
6	F	488	<div> <div>14%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
7	G	728	<div> <div>7%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
8	H	341	<div> <div>13%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	229	
10	J	185	
11	K	89	
12	L	655	
13	M	486	
14	N	469	
15	O	169	
16	P	375	
17	Q	161	
18	R	136	
19	S	87	
20	T	109	
21	U	132	
22	V	144	
23	W	124	
24	X	172	
25	Y	198	
26	Z	123	
27	a	87	
28	b	78	
29	c	182	
30	d	74	
31	e	89	
32	f	138	
33	g	249	

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Mol	Chain	Length	Quality of chain
34	h	139	
35	i	90	
36	j	91	
37	k	60	
38	l	149	
39	m	93	
40	n	109	
41	o	99	
42	p	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	3PE	A	501	X	-	-	-
43	3PE	H	602	X	-	-	-
43	3PE	M	502	X	-	-	-
43	3PE	Y	4203	X	-	-	-
43	3PE	Z	202	X	-	-	-
43	3PE	d	4603	X	-	-	-
45	LMT	B	302	X	-	-	-
45	LMT	M	503	X	-	-	-
45	LMT	Y	4201	X	-	-	-
45	LMT	Y	4202	X	-	-	-
45	LMT	Y	4204	X	-	-	-
48	FMN	F	501	X	-	-	-
52	EHZ	T	201	X	-	-	-
52	EHZ	U	201	X	-	-	-

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 66311 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	128	Total	C	N	O	S	0	0
			1006	684	150	169	3		

- Molecule 2 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	177	Total	C	N	O	S	0	0
			1395	885	246	249	15		

- Molecule 3 is a protein called NUGM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total	C	N	O	S	0	0
			1999	1285	339	371	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	282	ALA	-	expression tag	UNP Q9UUU0
C	283	ALA	-	expression tag	UNP Q9UUU0
C	284	ALA	-	expression tag	UNP Q9UUU0
C	285	ALA	-	expression tag	UNP Q9UUU0
C	286	ALA	-	expression tag	UNP Q9UUU0
C	287	ALA	-	expression tag	UNP Q9UUU0
C	288	HIS	-	expression tag	UNP Q9UUU0
C	289	HIS	-	expression tag	UNP Q9UUU0
C	290	HIS	-	expression tag	UNP Q9UUU0
C	291	HIS	-	expression tag	UNP Q9UUU0
C	292	HIS	-	expression tag	UNP Q9UUU0
C	293	HIS	-	expression tag	UNP Q9UUU0

- Molecule 4 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	437	Total	C	N	O	S	0	0
			3465	2202	594	647	22		

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1688	1060	284	326	18		

- Molecule 6 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	460	Total	C	N	O	S	0	0
			3559	2248	629	658	24		

- Molecule 7 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	694	Total	C	N	O	S	0	0
			5274	3275	928	1042	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2709	1843	394	465	7		

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	191	Total	C	N	O	S	0	0
			1526	972	255	289	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	185	Total	C	N	O	S	0	0
			1462	990	209	254	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	89	Total	C	N	O	S	0	0
			693	465	109	116	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	655	Total	C	N	O	S	0	0
			5207	3485	786	907	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	486	Total	C	N	O	S	0	0
			3857	2601	586	655	15		

- Molecule 14 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	469	Total	C	N	O	S	0	0
			3776	2558	550	656	12		

- Molecule 15 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	168	Total	C	N	O	S	0	0
			1305	845	223	233	4		

- Molecule 16 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	355	Total	C	N	O	S	0	0
			2812	1785	493	524	10		

- Molecule 17 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1037	659	190	186	2		

- Molecule 18 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	118	Total	C	N	O	S	0	0
			922	574	166	177	5		

- Molecule 19 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	86	Total	C	N	O	S	0	0
			667	418	126	122	1		

- Molecule 20 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	81	Total	C	N	O	S	0	0
			620	391	98	131			

- Molecule 21 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	88	Total	C	N	O	S	0	0
			667	416	106	143	2		

- Molecule 22 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	126	Total	C	N	O	S	0	0
			1028	653	173	200	2		

- Molecule 23 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).



Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	123	Total	C	N	O	S	0	0
			1036	667	182	185	2		

- Molecule 24 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 25 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	179	Total	C	N	O	S	0	0
			1327	842	240	240	5		

- Molecule 26 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	122	Total	C	N	O	S	0	0
			983	629	180	169	5		

- Molecule 27 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 28 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	78	Total	C	N	O	S	0	0
			639	418	115	105	1		

- Molecule 29 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	182	Total	C	N	O	S	0	0
			1397	898	241	256	2		

- Molecule 30 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	67	Total	C	N	O	S	0	0
			510	339	86	85			

- Molecule 31 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	68	Total	C	N	O	S	0	0
			546	336	102	102	6		

- Molecule 32 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	137	Total	C	N	O	S	0	0
			1136	730	194	210	2		

- Molecule 33 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	198	Total	C	N	O	S	0	0
			1585	1019	273	291	2		

- Molecule 34 is a protein called subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	113	Total	C	N	O	S	0	0
			909	585	153	170	1		

- Molecule 35 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	86	Total	C	N	O	S	0	0
			659	420	120	118	1		

- Molecule 36 is a protein called subunit NIGM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	53	Total	C	N	O	S	0	0
			445	299	77	66	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-23	MET	-	initiating methionine	UNP A0A1D8NFX6
j	-22	HIS	-	expression tag	UNP A0A1D8NFX6
j	-21	ASN	-	expression tag	UNP A0A1D8NFX6
j	-20	SER	-	expression tag	UNP A0A1D8NFX6
j	-19	SER	-	expression tag	UNP A0A1D8NFX6
j	-18	SER	-	expression tag	UNP A0A1D8NFX6
j	-17	VAL	-	expression tag	UNP A0A1D8NFX6
j	-16	HIS	-	expression tag	UNP A0A1D8NFX6
j	-15	HIS	-	expression tag	UNP A0A1D8NFX6
j	-14	HIS	-	expression tag	UNP A0A1D8NFX6
j	-13	TYR	-	expression tag	UNP A0A1D8NFX6
j	-12	ILE	-	expression tag	UNP A0A1D8NFX6
j	-11	SER	-	expression tag	UNP A0A1D8NFX6
j	-10	LYS	-	expression tag	UNP A0A1D8NFX6
j	-9	THR	-	expression tag	UNP A0A1D8NFX6
j	-8	THR	-	expression tag	UNP A0A1D8NFX6
j	-7	GLY	-	expression tag	UNP A0A1D8NFX6
j	-6	PHE	-	expression tag	UNP A0A1D8NFX6
j	-5	PHE	-	expression tag	UNP A0A1D8NFX6
j	-4	ARG	-	expression tag	UNP A0A1D8NFX6
j	-3	PHE	-	expression tag	UNP A0A1D8NFX6
j	-2	ARG	-	expression tag	UNP A0A1D8NFX6
j	-1	TYR	-	expression tag	UNP A0A1D8NFX6
j	0	LYS	-	expression tag	UNP A0A1D8NFX6

- Molecule 37 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	47	Total	C	N	O	0	0
			373	242	70	61		

- Molecule 38 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	125	Total	C	N	O	S	0	0
			1039	674	166	197	2		

- Molecule 39 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	92	Total	C	N	O	0	0
			735	472	134	129		

- Molecule 40 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	108	Total	C	N	O	S	0	0
			900	571	172	154	3		

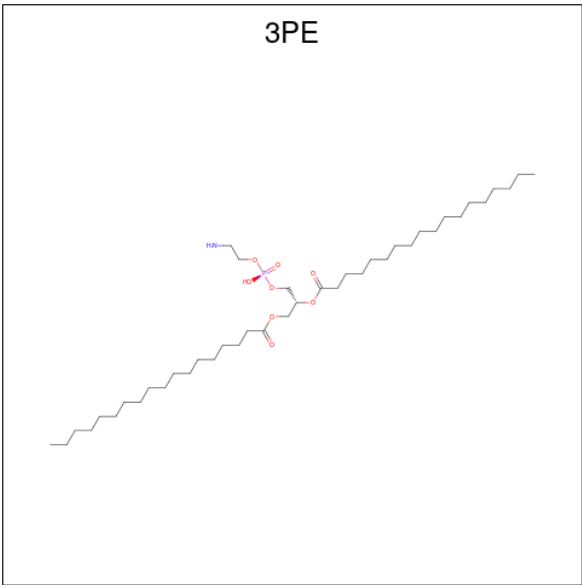
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	83	Total	C	N	O	S	0	0
			681	431	123	119	8		

- Molecule 42 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	91	Total	C	N	O	S	0	0
			766	475	138	150	3		

- Molecule 43 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



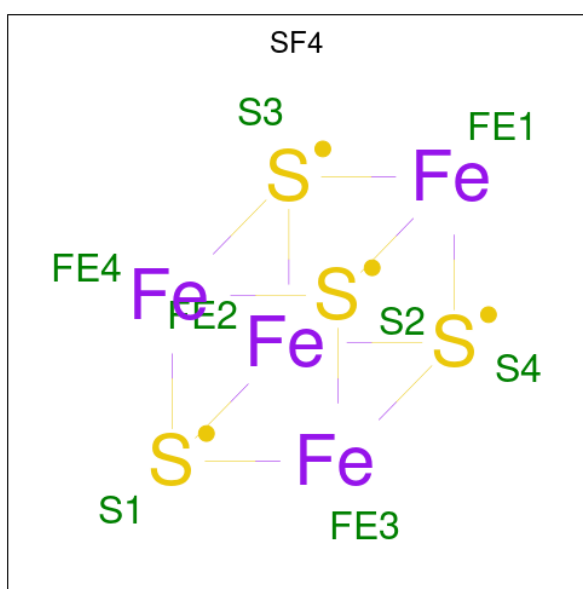
Mol	Chain	Residues	Atoms					AltConf
43	A	1	Total	C	N	O	P	0
			27	17	1	8	1	
43	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	H	1	Total	C	N	O	P	0
			22	12	1	8	1	
43	I	1	Total	C	N	O	P	0
			46	36	1	8	1	
43	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	L	1	Total	C	N	O	P	0
			33	23	1	8	1	
43	M	1	Total	C	N	O	P	0
			30	20	1	8	1	
43	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
43	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
43	Y	1	Total	C	N	O	P	0
			24	14	1	8	1	
43	Z	1	Total	C	N	O	P	0
			32	22	1	8	1	
43	Z	1	Total	C	N	O	P	0
			43	33	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
43	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
43	b	1	Total	C	N	O	P	0
			26	16	1	8	1	
43	d	1	Total	C	N	O	P	0
			24	14	1	8	1	
43	d	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 45 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $\text{C}_{24}\text{H}_{46}\text{O}_{11}$ ).



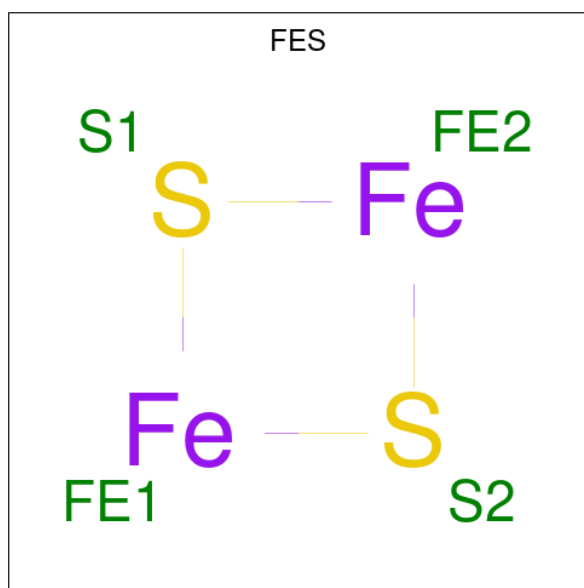
Mol	Chain	Residues	Atoms			AltCon
45	B	1	Total 35	C 24	O 11	0
45	M	1	Total 35	C 24	O 11	0
45	Y	1	Total 35	C 24	O 11	0
45	Y	1	Total 35	C 24	O 11	0
45	Y	1	Total 35	C 24	O 11	0

- Molecule 46 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $C_{32}H_{65}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
46	D	1	Total	C	N	O	P	0
			27	17	1	8	1	
46	H	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	L	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	L	1	Total	C	N	O	P	0
			29	19	1	8	1	
46	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	P	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	d	1	Total	C	N	O	P	0
			27	17	1	8	1	

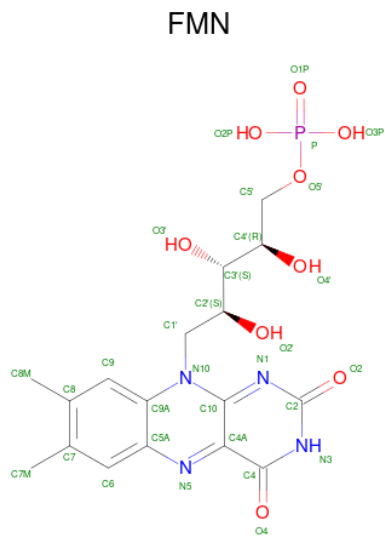
- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



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

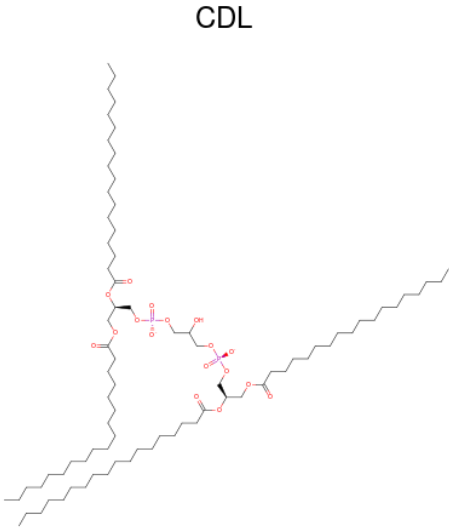
- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).





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

- Molecule 49 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ).



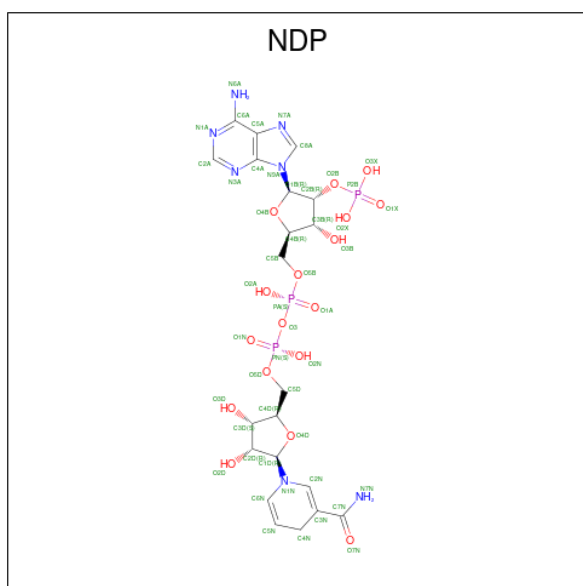
Mol	Chain	Residues	Atoms				AltConf
49	M	1	Total 83	C 64	O 17	P 2	0
49	O	1	Total 63	C 44	O 17	P 2	0
49	P	1	Total 48	C 29	O 17	P 2	0

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Mol	Chain	Residues	Atoms				AltConf
49	Z	1	Total	C	O	P	0
			57	38	17	2	
49	a	1	Total	C	O	P	0
			52	33	17	2	
49	b	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

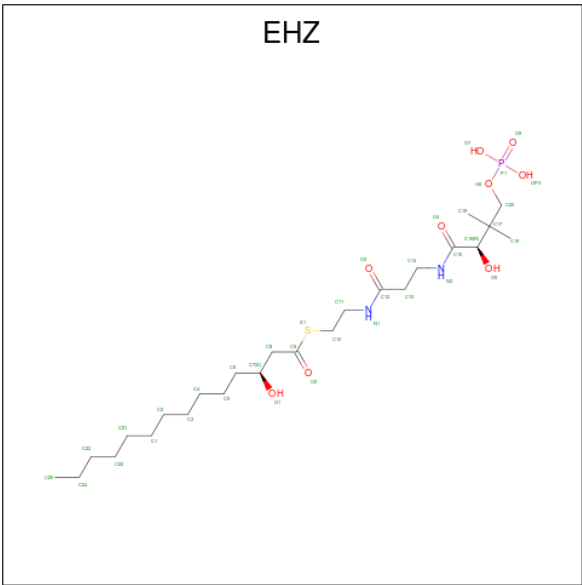


Mol	Chain	Residues	Atoms					AltConf
50	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
51	R	1	Total	Zn	0
			1	1	

- Molecule 52 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula:  $C_{25}H_{49}N_2O_9PS$ ).



Mol	Chain	Residues	Atoms						AltConf
52	T	1	Total	C	N	O	P	S	0
			34	22	2	8	1	1	
52	U	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 53 is water.

Mol	Chain	Residues	Atoms		AltConf
53	A	2	Total	O	0
			2	2	
53	B	15	Total	O	0
			15	15	
53	C	15	Total	O	0
			15	15	
53	D	20	Total	O	0
			20	20	
53	E	2	Total	O	0
			2	2	
53	F	7	Total	O	0
			7	7	
53	G	25	Total	O	0
			25	25	
53	H	10	Total	O	0
			10	10	
53	I	18	Total	O	0
			18	18	
53	J	4	Total	O	0
			4	4	

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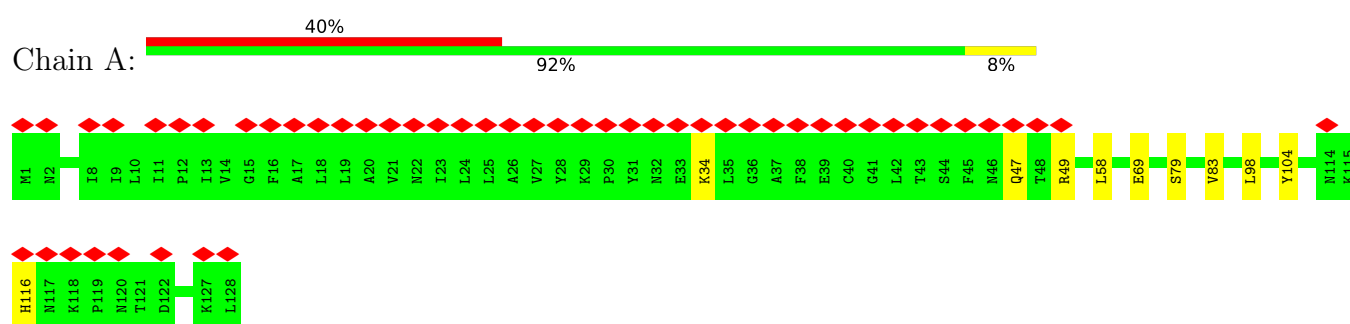
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Mol	Chain	Residues	Atoms		AltConf
53	K	3	Total 3	O 3	0
53	L	27	Total 27	O 27	0
53	M	25	Total 25	O 25	0
53	N	37	Total 37	O 37	0
53	O	4	Total 4	O 4	0
53	P	14	Total 14	O 14	0
53	Q	7	Total 7	O 7	0
53	R	3	Total 3	O 3	0
53	W	4	Total 4	O 4	0
53	X	1	Total 1	O 1	0
53	Z	3	Total 3	O 3	0
53	a	3	Total 3	O 3	0
53	c	3	Total 3	O 3	0
53	f	4	Total 4	O 4	0
53	h	1	Total 1	O 1	0
53	i	2	Total 2	O 2	0
53	l	4	Total 4	O 4	0
53	m	4	Total 4	O 4	0
53	n	2	Total 2	O 2	0
53	o	1	Total 1	O 1	0
53	p	5	Total 5	O 5	0

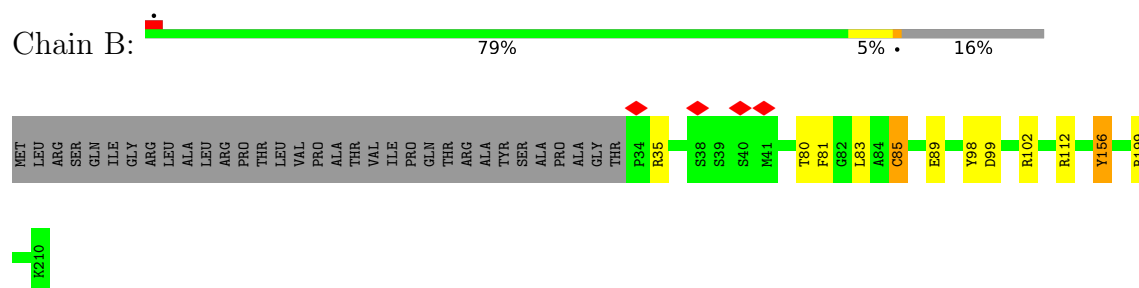
### 3 Residue-property plots [i](#)

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

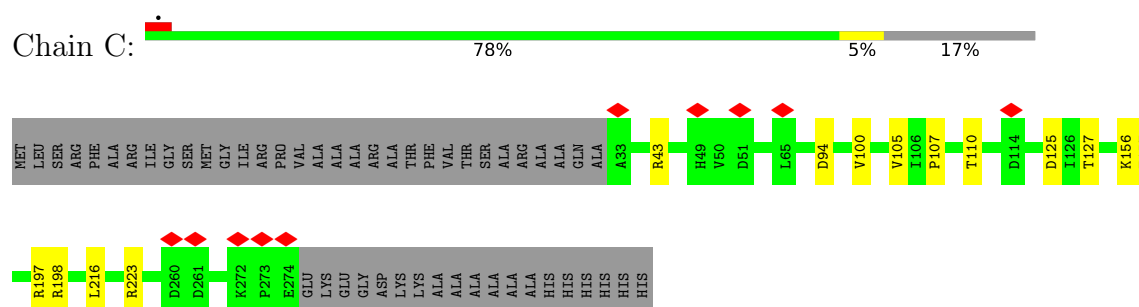
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



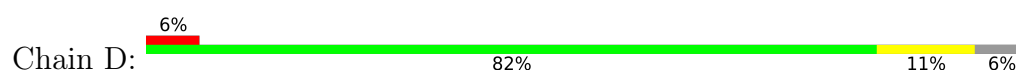
- Molecule 2: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

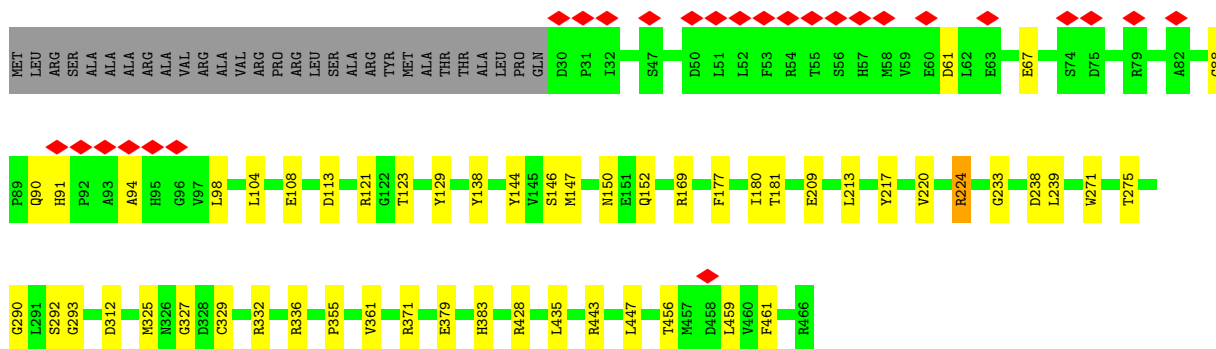


- Molecule 3: NUGM protein

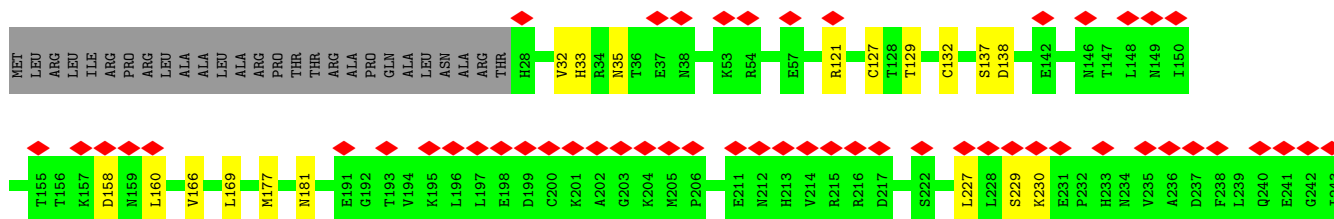
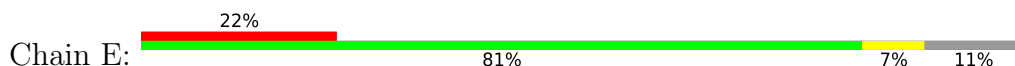


- Molecule 4: NUCM protein

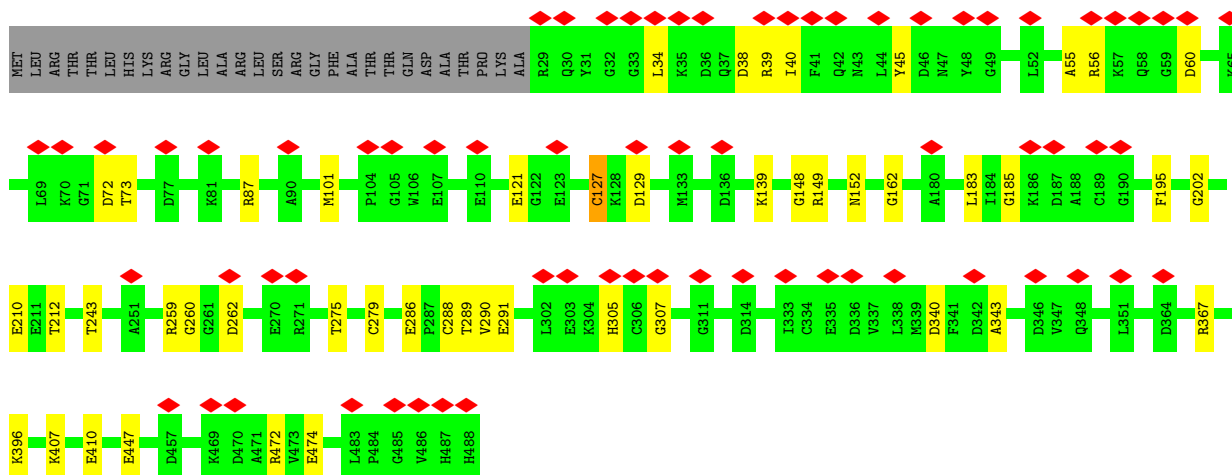
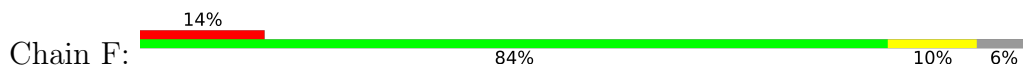




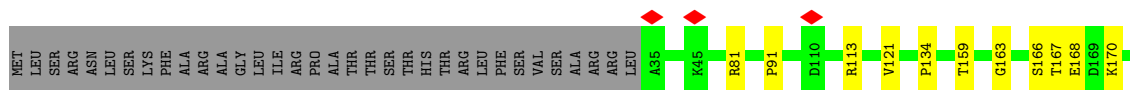
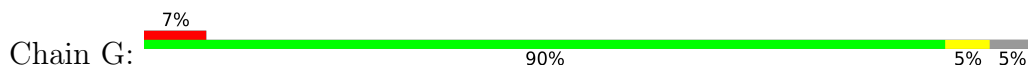
• Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

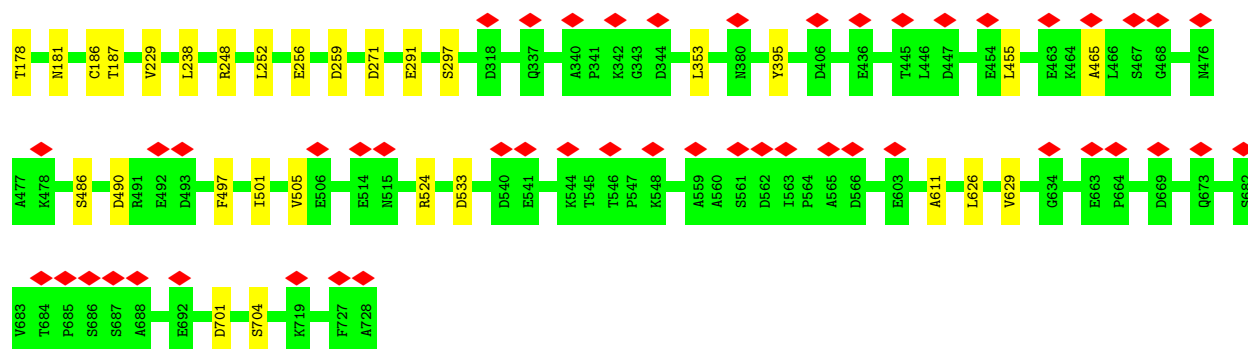


• Molecule 6: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)

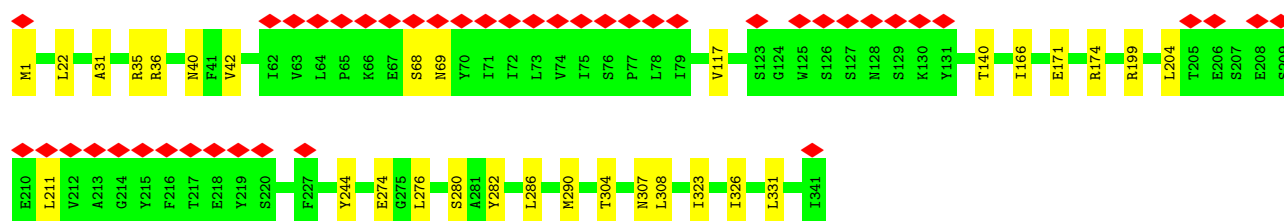


• Molecule 7: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

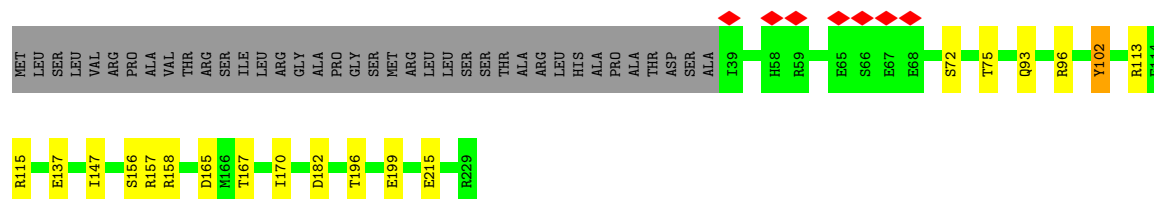




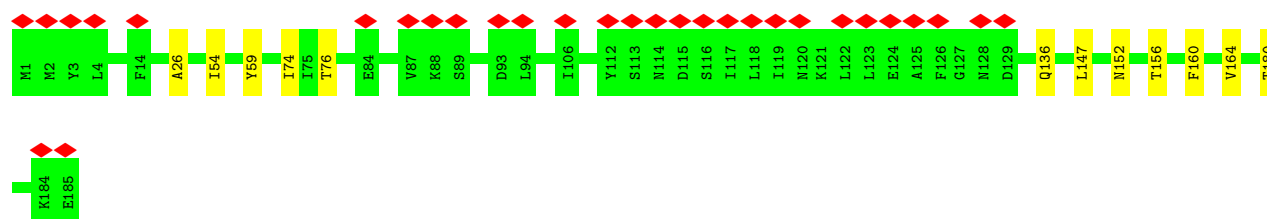
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



• Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

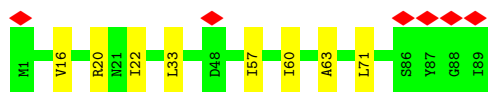


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



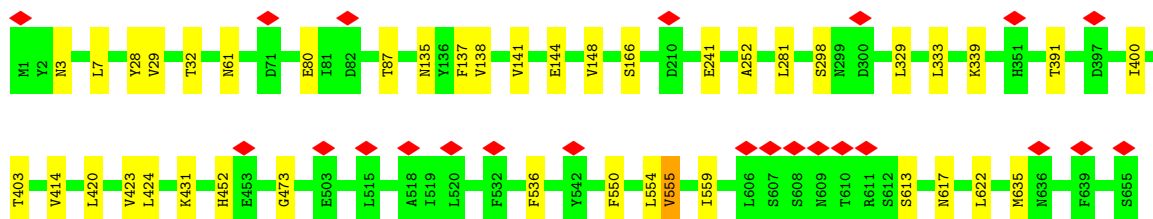
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L





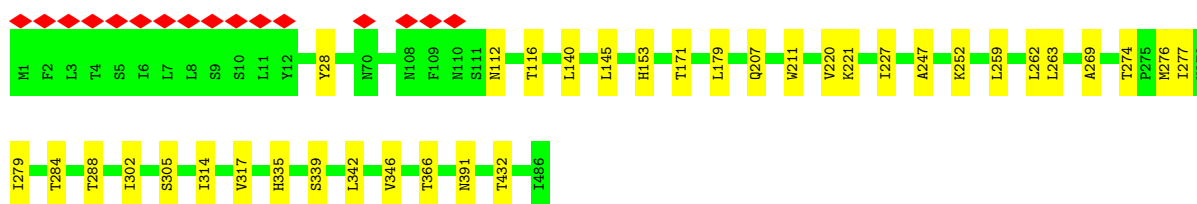
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 94% 6%



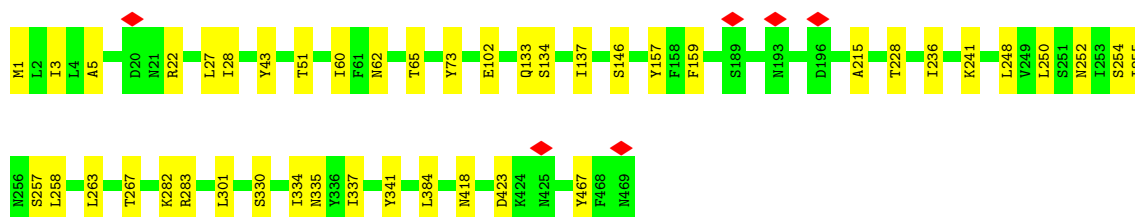
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 93% 7%



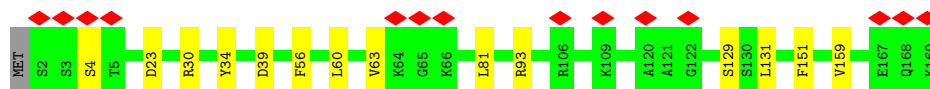
- Molecule 14: NADH dehydrogenase subunit 2

Chain N: 91% 9%



- Molecule 15: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

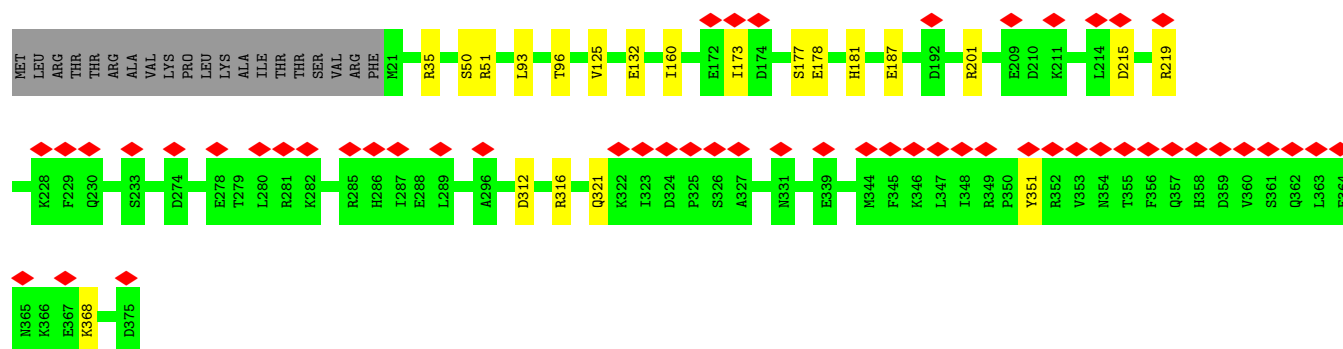
Chain O: 8% 91% 8%



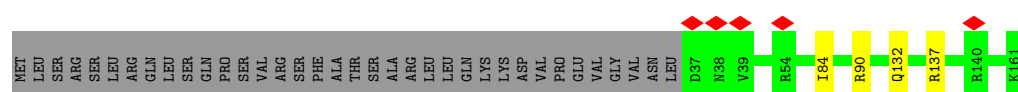
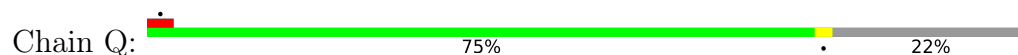
- Molecule 16: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain P: 14% 89% 6% 5%

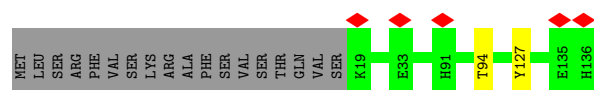
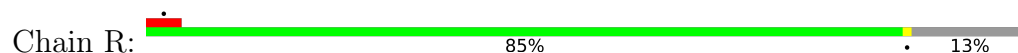




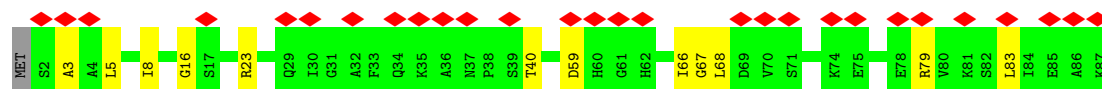
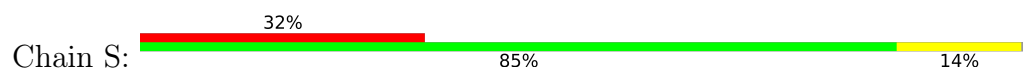
- Molecule 17: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



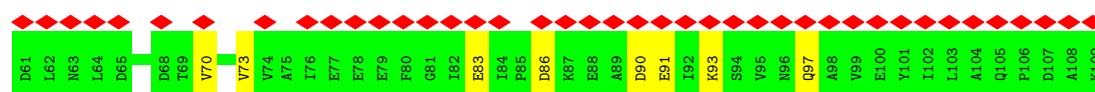
- Molecule 18: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



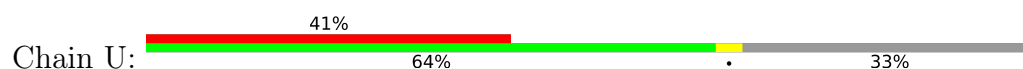
- Molecule 19: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

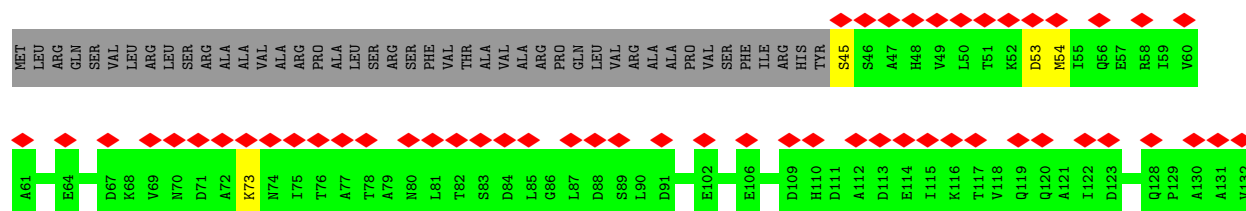


- Molecule 20: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

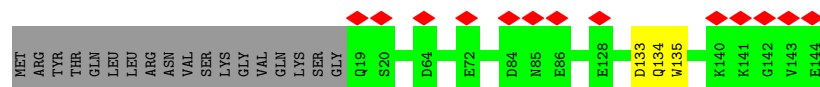
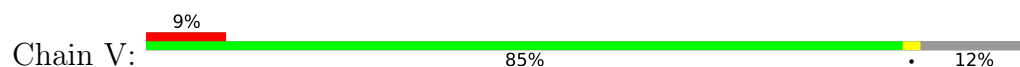


- Molecule 21: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

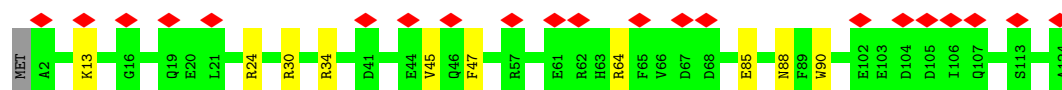




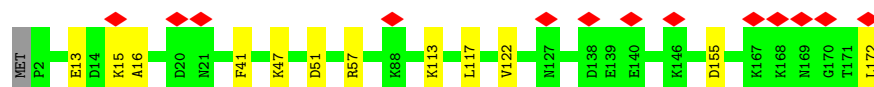
- Molecule 22: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



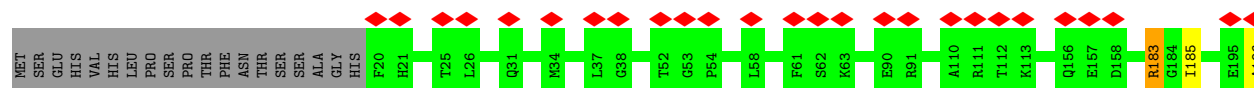
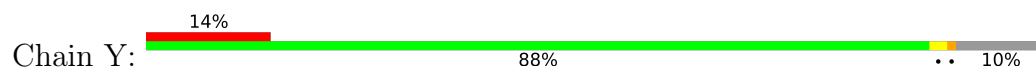
- Molecule 23: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



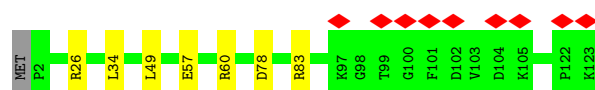
- Molecule 24: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 25: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

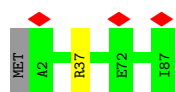


- Molecule 26: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)



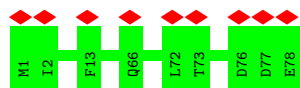
- Molecule 27: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain a:  98%



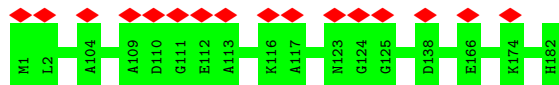
- Molecule 28: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain b:  12% 100%



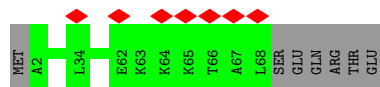
- Molecule 29: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain c:  9% 100%




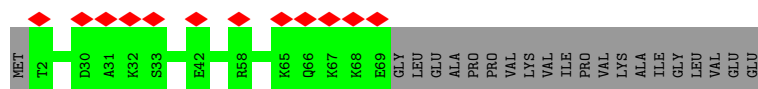
- Molecule 30: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain d:  9% 91% 9%



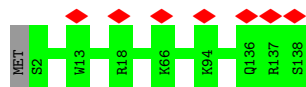
- Molecule 31: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain e:  13% 76% 24%




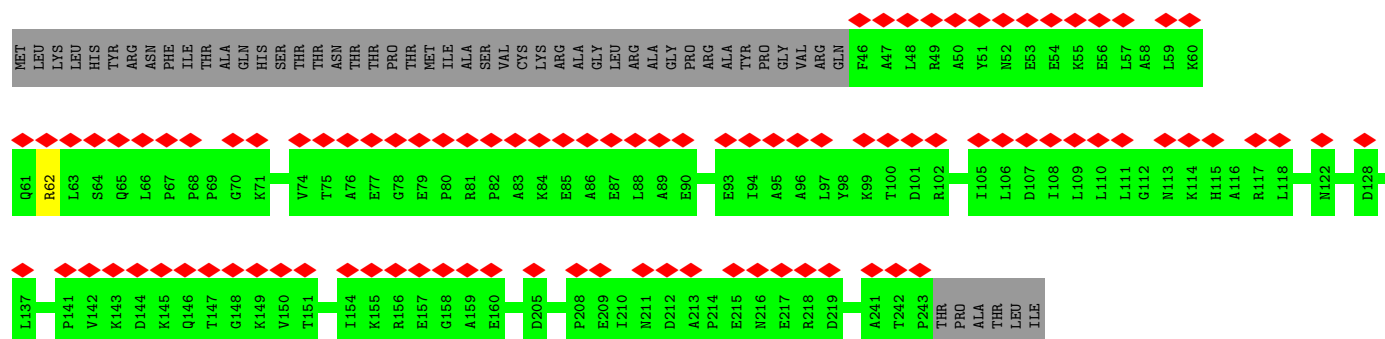
- Molecule 32: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain f:  5% 99%

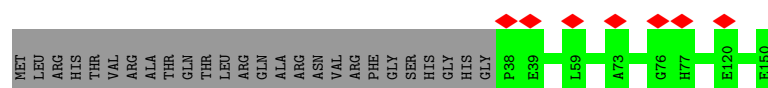
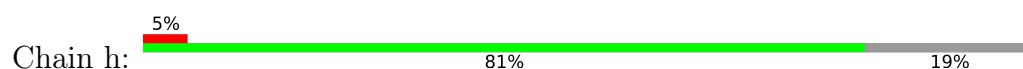


- Molecule 33: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

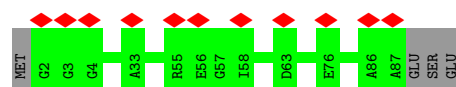
Chain g:  39% 79% 20%



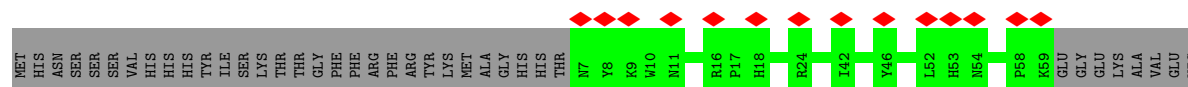
- Molecule 34: subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



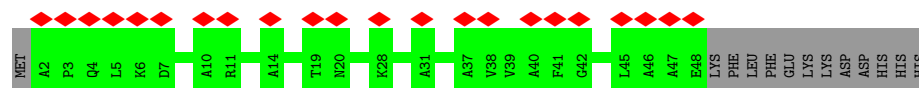
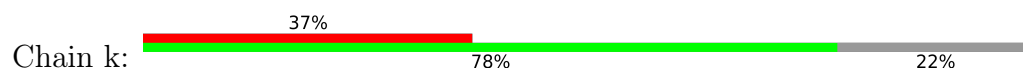
- Molecule 35: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



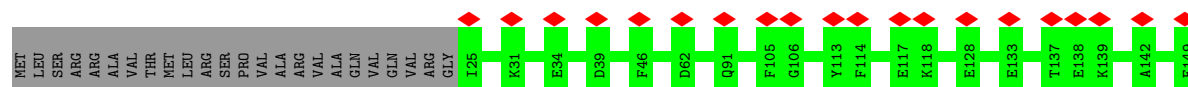
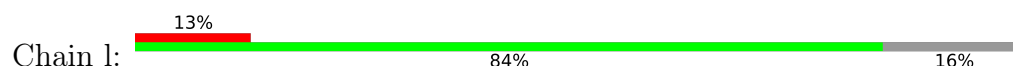
- Molecule 36: subunit NIGM of protein NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 37: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

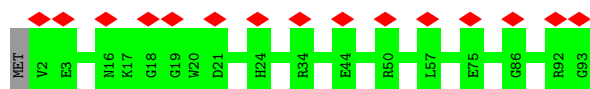


- Molecule 38: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



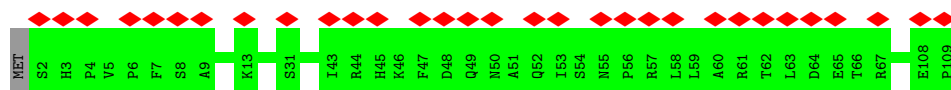
- Molecule 39: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain m:  16% 99%




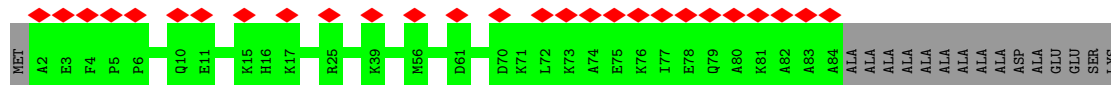
- Molecule 40: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain n:  28% 99%



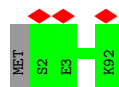
- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain o:  27% 84% 16%



- Molecule 42: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain p:  99%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49669	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	474.74997, 474.74997, 474.74997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, FMN, NDP, CDL, PLC, LMT, FES, SF4, FME, ZN, EHZ, 3PE

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	0.43	0/1018	0.56	0/1390
2	B	0.65	3/1434 (0.2%)	0.68	1/1950 (0.1%)
3	C	0.55	0/2062	0.62	2/2813 (0.1%)
4	D	0.54	0/3533	0.61	2/4788 (0.0%)
5	E	0.44	0/1725	0.62	0/2343
6	F	0.45	1/3638 (0.0%)	0.62	0/4910
7	G	0.47	0/5368	0.59	0/7285
8	H	0.51	0/2772	0.64	3/3786 (0.1%)
9	I	0.66	1/1564 (0.1%)	0.67	2/2121 (0.1%)
10	J	0.41	0/1477	0.53	0/2015
11	K	0.45	0/692	0.61	0/937
12	L	0.46	0/5327	0.56	0/7273
13	M	0.50	0/3941	0.58	0/5382
14	N	0.55	0/3846	0.56	0/5242
15	O	0.46	0/1344	0.56	0/1822
16	P	0.41	0/2873	0.60	0/3894
17	Q	0.49	0/1067	0.58	1/1442 (0.1%)
18	R	0.48	0/946	0.56	0/1283
19	S	0.36	0/677	0.63	0/907
20	T	0.48	1/628 (0.2%)	0.72	1/854 (0.1%)
21	U	0.32	0/673	0.54	0/916
22	V	0.44	0/1049	0.57	0/1420
23	W	0.45	0/1061	0.57	0/1427
24	X	0.43	0/1374	0.59	0/1856
25	Y	0.40	0/1359	0.58	0/1851
26	Z	0.48	0/1007	0.69	0/1357
27	a	0.44	0/697	0.60	1/940 (0.1%)
28	b	0.47	0/665	0.57	0/909
29	c	0.48	0/1438	0.58	0/1965
30	d	0.44	0/523	0.50	0/707
31	e	0.40	0/555	0.53	0/740
32	f	0.53	0/1174	0.56	0/1597

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g	0.39	0/1614	0.58	0/2182
34	h	0.44	0/937	0.52	0/1270
35	i	0.37	0/679	0.59	0/924
36	j	0.36	0/465	0.53	0/630
37	k	0.37	0/385	0.62	0/522
38	l	0.41	0/1073	0.54	0/1451
39	m	0.44	0/756	0.59	0/1021
40	n	0.38	0/926	0.57	0/1253
41	o	0.38	0/695	0.54	0/930
42	p	0.47	0/782	0.61	0/1051
All	All	0.48	6/65819 (0.0%)	0.59	13/89356 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	102	TYR	CD1-CE1	-8.28	1.26	1.39
2	B	156	TYR	CD2-CE2	-7.00	1.28	1.39
6	F	279	CYS	CB-SG	6.17	1.92	1.82
2	B	156	TYR	CD1-CE1	-5.16	1.31	1.39
20	T	33	GLU	CG-CD	-5.09	1.44	1.51
2	B	85	CYS	CB-SG	-5.02	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	94	ASP	CB-CG-OD1	7.05	124.65	118.30
8	H	211	LEU	CB-CG-CD1	6.04	121.27	111.00
20	T	31	ASP	CB-CG-OD2	5.75	123.47	118.30
8	H	199	ARG	NE-CZ-NH2	5.54	123.07	120.30
9	I	115	ARG	NE-CZ-NH1	5.48	123.04	120.30
8	H	199	ARG	NE-CZ-NH1	-5.47	117.57	120.30
3	C	43	ARG	NE-CZ-NH1	5.29	122.94	120.30
9	I	157	ARG	NE-CZ-NH1	5.18	122.89	120.30
17	Q	90	ARG	NE-CZ-NH1	5.17	122.88	120.30
27	a	37	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	B	199	ARG	NE-CZ-NH2	5.04	122.82	120.30
4	D	224	ARG	NE-CZ-NH1	5.04	122.82	120.30
4	D	443	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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	1006	0	1056	10	0
2	B	1395	0	1375	11	0
3	C	1999	0	1925	10	0
4	D	3465	0	3397	37	0
5	E	1688	0	1660	13	0
6	F	3559	0	3513	30	0
7	G	5274	0	5173	25	0
8	H	2709	0	2805	17	0
9	I	1526	0	1471	12	0
10	J	1462	0	1582	11	0
11	K	693	0	753	9	0
12	L	5207	0	5364	27	0
13	M	3857	0	4053	26	0
14	N	3776	0	4004	34	0
15	O	1305	0	1281	10	0
16	P	2812	0	2763	13	0
17	Q	1037	0	994	3	0
18	R	922	0	876	2	0
19	S	667	0	684	8	0
20	T	620	0	614	6	0
21	U	667	0	655	2	0
22	V	1028	0	1021	2	0
23	W	1036	0	1018	7	0
24	X	1345	0	1333	7	0
25	Y	1327	0	1310	2	0
26	Z	983	0	1000	6	0
27	a	681	0	671	0	0
28	b	639	0	620	0	0
29	c	1397	0	1407	0	0
30	d	510	0	532	0	0
31	e	546	0	536	0	0
32	f	1136	0	1089	0	0
33	g	1585	0	1603	0	0
34	h	909	0	877	0	0
35	i	659	0	641	0	0
36	j	445	0	439	0	0
37	k	373	0	361	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	l	1039	0	973	0	0
39	m	735	0	718	0	0
40	n	900	0	904	0	0
41	o	681	0	685	0	0
42	p	766	0	726	0	0
43	A	78	0	110	0	0
43	H	22	0	18	0	0
43	I	46	0	69	1	0
43	L	186	0	286	1	0
43	M	70	0	91	1	0
43	N	51	0	82	1	0
43	Y	24	0	22	0	0
43	Z	75	0	98	0	0
43	b	69	0	89	0	0
43	d	54	0	56	0	0
44	B	8	0	0	0	0
44	F	8	0	0	0	0
44	G	16	0	0	0	0
44	I	16	0	0	0	0
45	B	35	0	46	0	0
45	M	35	0	46	0	0
45	Y	105	0	138	0	0
46	D	27	0	28	0	0
46	H	28	0	30	0	0
46	L	105	0	138	3	0
46	N	42	0	64	0	0
46	P	35	0	47	0	0
46	d	27	0	28	0	0
47	E	4	0	0	1	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	M	83	0	113	1	0
49	O	63	0	73	2	0
49	P	48	0	40	0	0
49	Z	57	0	58	1	0
49	a	52	0	48	0	0
49	b	48	0	40	0	0
50	P	48	0	26	0	0
51	R	1	0	0	0	0
52	T	34	0	0	2	0
52	U	35	0	0	2	0
53	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B	15	0	0	3	0
53	C	15	0	0	2	0
53	D	20	0	0	2	0
53	E	2	0	0	0	0
53	F	7	0	0	0	0
53	G	25	0	0	0	0
53	H	10	0	0	2	0
53	I	18	0	0	1	0
53	J	4	0	0	1	0
53	K	3	0	0	0	0
53	L	27	0	0	1	0
53	M	25	0	0	1	0
53	N	37	0	0	5	0
53	O	4	0	0	0	0
53	P	14	0	0	2	0
53	Q	7	0	0	0	0
53	R	3	0	0	0	0
53	W	4	0	0	1	0
53	X	1	0	0	0	0
53	Z	3	0	0	0	0
53	a	3	0	0	0	0
53	c	3	0	0	0	0
53	f	4	0	0	0	0
53	h	1	0	0	0	0
53	i	2	0	0	0	0
53	l	4	0	0	0	0
53	m	4	0	0	0	0
53	n	2	0	0	0	0
53	o	1	0	0	0	0
53	p	5	0	0	0	0
All	All	66311	0	66365	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:T:201:EHZ:O9	23:W:64:ARG:NH2	1.66	1.25
14:N:137:ILE:HD11	14:N:236:ILE:HG22	1.46	0.93
2:B:102:ARG:NH2	53:B:403:HOH:O	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:THR:OG1	47:E:301:FES:S2	2.46	0.74
2:B:80:THR:O	4:D:90:GLN:NE2	2.20	0.74
4:D:61:ASP:OD1	14:N:283:ARG:NE	2.21	0.73
1:A:47:GLN:NE2	1:A:49:ARG:O	2.22	0.72
2:B:99:ASP:OD2	53:B:401:HOH:O	2.07	0.71
13:M:247:ALA:O	13:M:252:LYS:NZ	2.23	0.71
4:D:209:GLU:OE2	53:D:601:HOH:O	2.09	0.71
8:H:274:GLU:OE2	53:H:701:HOH:O	2.07	0.71
3:C:125:ASP:OD2	3:C:127:THR:OG1	2.07	0.71
4:D:336:ARG:NH1	53:D:602:HOH:O	2.22	0.71
8:H:35:ARG:NH2	53:H:702:HOH:O	2.24	0.70
12:L:281:LEU:HD21	12:L:414:VAL:HG21	1.73	0.70
3:C:198:ARG:O	53:C:301:HOH:O	2.10	0.69
14:N:133:GLN:OE1	53:N:2501:HOH:O	2.10	0.69
12:L:400:ILE:O	12:L:403:THR:OG1	2.11	0.69
6:F:340:ASP:OD1	6:F:343:ALA:N	2.26	0.69
16:P:132:GLU:OE1	16:P:316:ARG:NH1	2.27	0.68
13:M:220:VAL:HG22	13:M:227:ILE:HG21	1.75	0.68
2:B:80:THR:OG1	4:D:90:GLN:NE2	2.26	0.68
5:E:127:CYS:SG	5:E:129:THR:OG1	2.52	0.68
24:X:47:LYS:NZ	24:X:51:ASP:OD2	2.26	0.68
15:O:129:SER:OG	49:O:401:CDL:OB3	2.08	0.68
20:T:86:ASP:OD1	23:W:30:ARG:NH1	2.28	0.67
10:J:74:ILE:HD13	11:K:71:LEU:HD22	1.75	0.67
20:T:83:GLU:OE1	23:W:34:ARG:NH1	2.28	0.67
4:D:371:ARG:NH2	9:I:182:ASP:OD1	2.28	0.67
14:N:423:ASP:OD2	53:N:2502:HOH:O	2.11	0.67
24:X:113:LYS:NZ	24:X:155:ASP:OD2	2.28	0.67
16:P:215:ASP:OD2	16:P:219:ARG:NH1	2.29	0.66
9:I:215:GLU:OE1	53:I:6401:HOH:O	2.13	0.66
23:W:13:LYS:O	23:W:24:ARG:NH2	2.29	0.65
46:L:1007:PLC:H81	13:M:366:THR:HG22	1.79	0.65
8:H:276:LEU:O	8:H:280:SER:OG	2.07	0.65
13:M:171:THR:HG23	13:M:221:LYS:HD3	1.78	0.65
52:T:201:EHZ:O2	52:T:201:EHZ:O1	2.11	0.65
14:N:137:ILE:HG23	14:N:157:TYR:HE2	1.62	0.65
14:N:248:LEU:O	53:N:2503:HOH:O	2.15	0.65
13:M:366:THR:OG1	13:M:432:THR:O	2.10	0.64
3:C:197:ARG:NH2	4:D:113:ASP:OD1	2.31	0.64
12:L:252:ALA:HB1	12:L:339:LYS:HG3	1.77	0.64
5:E:121:ARG:O	5:E:181:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:215:ASP:OD1	16:P:351:TYR:OH	2.11	0.63
15:O:23:ASP:OD2	15:O:30:ARG:NH1	2.31	0.63
12:L:87:THR:HG21	12:L:329:LEU:CD2	2.29	0.63
14:N:254:SER:O	14:N:301:LEU:HD23	1.99	0.63
12:L:298:SER:O	12:L:431:LYS:NZ	2.32	0.62
12:L:452:HIS:NE2	21:U:45:SER:OG	2.29	0.62
12:L:536:PHE:O	46:L:1001:PLC:H62	1.98	0.62
15:O:39:ASP:OD1	15:O:93:ARG:NH1	2.32	0.62
2:B:98:TYR:OH	53:B:402:HOH:O	2.15	0.62
4:D:181:THR:OG1	4:D:217:TYR:OH	2.09	0.60
20:T:54:PRO:O	20:T:55:THR:OG1	2.12	0.60
6:F:149:ARG:NH2	6:F:152:ASN:OD1	2.35	0.60
10:J:54:ILE:HD11	10:J:147:LEU:HD22	1.83	0.60
6:F:39:ARG:NH1	6:F:291:GLU:O	2.35	0.60
43:I:6301:3PE:H2I2	26:Z:34:LEU:HD13	1.83	0.59
6:F:72:ASP:OD1	6:F:73:THR:N	2.35	0.59
8:H:40:ASN:HD21	9:I:102:TYR:HE1	1.50	0.59
1:A:49:ARG:NH2	10:J:76:THR:O	2.35	0.59
10:J:136:GLN:NE2	53:J:201:HOH:O	2.33	0.59
12:L:61:ASN:ND2	12:L:80:GLU:OE1	2.34	0.59
4:D:123:THR:HG23	4:D:138:TYR:CD2	2.38	0.58
12:L:87:THR:HG21	12:L:329:LEU:HD21	1.86	0.58
13:M:342:LEU:O	13:M:346:VAL:HG22	2.04	0.58
7:G:701:ASP:OD1	7:G:704:SER:OG	2.10	0.58
13:M:112:ASN:O	13:M:116:THR:HG23	2.04	0.58
4:D:325:MET:SD	4:D:325:MET:N	2.77	0.57
7:G:259:ASP:OD2	7:G:297:SER:OG	2.22	0.57
13:M:153:HIS:NE2	14:N:418:ASN:OD1	2.37	0.57
12:L:3:ASN:O	12:L:7:LEU:HD23	2.04	0.57
14:N:137:ILE:CD1	14:N:236:ILE:HG22	2.28	0.57
3:C:105:VAL:HG22	3:C:157:THR:HG21	1.85	0.57
4:D:98:LEU:HD13	4:D:461:PHE:CE1	2.40	0.57
14:N:263:LEU:O	14:N:267:THR:HG23	2.04	0.57
24:X:57:ARG:NH1	26:Z:78:ASP:OD2	2.37	0.57
7:G:395:TYR:OH	7:G:533:ASP:OD1	2.17	0.56
13:M:284:THR:O	13:M:288:THR:OG1	2.10	0.56
6:F:38:ASP:OD1	6:F:259:ARG:NH2	2.38	0.56
11:K:33:LEU:HD13	11:K:63:ALA:HB2	1.85	0.56
13:M:28:TYR:OH	13:M:116:THR:HG22	2.06	0.56
13:M:211:TRP:HZ2	13:M:277:ILE:HD11	1.70	0.56
14:N:27:LEU:HD21	15:O:81:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:335:ASN:ND2	53:N:2504:HOH:O	2.34	0.56
4:D:220:VAL:O	9:I:113:ARG:NH2	2.35	0.56
14:N:257:SER:OG	43:N:2402:3PE:O12	2.10	0.56
9:I:93:GLN:OE1	9:I:96:ARG:NH1	2.39	0.56
4:D:88:GLY:O	4:D:91:HIS:ND1	2.38	0.55
3:C:105:VAL:CG2	3:C:157:THR:HG21	2.35	0.55
16:P:173:ILE:O	16:P:181:HIS:ND1	2.33	0.55
4:D:67:GLU:OE2	16:P:368:LYS:NZ	2.39	0.55
12:L:166:SER:OG	43:L:1003:3PE:N	2.40	0.55
14:N:252:ASN:HB3	14:N:255:ILE:HD11	1.89	0.55
4:D:152:GLN:NE2	4:D:312:ASP:OD2	2.40	0.54
14:N:73:TYR:OH	15:O:151:PHE:O	2.26	0.54
16:P:187:GLU:OE2	16:P:201:ARG:NH1	2.41	0.54
8:H:323:ILE:HA	8:H:326:ILE:HG22	1.90	0.54
13:M:211:TRP:HE1	13:M:262:LEU:HD21	1.73	0.54
12:L:635:MET:SD	14:N:258:LEU:HD23	2.48	0.54
14:N:228:THR:O	14:N:282:LYS:NZ	2.41	0.53
2:B:156:TYR:CD1	9:I:170:ILE:HG21	2.42	0.53
10:J:152:ASN:O	10:J:156:THR:OG1	2.21	0.53
5:E:138:ASP:OD2	6:F:367:ARG:NH2	2.42	0.53
12:L:391:THR:HG22	12:L:473:GLY:H	1.74	0.53
14:N:134:SER:HA	14:N:137:ILE:HG22	1.90	0.53
19:S:67:GLY:O	19:S:79:ARG:NH1	2.41	0.53
16:P:93:LEU:O	16:P:96:THR:OG1	2.19	0.53
14:N:3:ILE:HD13	49:O:401:CDL:H652	1.91	0.53
15:O:131:LEU:HD12	15:O:159:VAL:HG13	1.90	0.53
7:G:256:GLU:OE1	17:Q:132:GLN:NE2	2.43	0.52
8:H:171:GLU:OE2	8:H:174:ARG:NH1	2.42	0.52
12:L:550:PHE:CE1	12:L:554:LEU:HD21	2.45	0.52
21:U:53:ASP:OD1	21:U:54:MET:N	2.42	0.52
20:T:93:LYS:N	20:T:97:GLN:OE1	2.39	0.52
6:F:56:ARG:HH12	6:F:183:LEU:HD21	1.74	0.52
9:I:72:SER:O	9:I:75:THR:OG1	2.23	0.52
13:M:276:MET:HA	13:M:279:ILE:HD12	1.92	0.52
14:N:62:ASN:HD21	14:N:250:LEU:HD11	1.73	0.52
14:N:215:ALA:H	14:N:267:THR:HG22	1.74	0.52
10:J:74:ILE:CD1	11:K:71:LEU:HD22	2.40	0.52
13:M:211:TRP:NE1	13:M:262:LEU:HD21	2.25	0.52
7:G:186:CYS:O	7:G:187:THR:OG1	2.19	0.52
19:S:3:ALA:HB3	19:S:59:ASP:OD2	2.10	0.52
4:D:180:ILE:HG23	4:D:213:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:MET:SD	6:F:243:THR:OG1	2.52	0.51
4:D:147:MET:SD	4:D:147:MET:N	2.84	0.51
13:M:274:THR:HA	13:M:277:ILE:HD12	1.92	0.51
5:E:166:VAL:HG21	5:E:169:LEU:HD11	1.93	0.51
12:L:28:TYR:O	12:L:32:THR:HG23	2.11	0.51
7:G:252:LEU:HD13	7:G:271:ASP:HB3	1.92	0.50
13:M:145:LEU:HD21	13:M:171:THR:HG21	1.94	0.50
4:D:98:LEU:HD13	4:D:461:PHE:CZ	2.46	0.50
13:M:179:LEU:HD11	14:N:384:LEU:HD13	1.93	0.50
12:L:137:PHE:O	12:L:141:VAL:HG23	2.11	0.50
6:F:56:ARG:NH1	6:F:183:LEU:HD11	2.27	0.50
7:G:167:THR:N	7:G:181:ASN:OD1	2.45	0.50
26:Z:26:ARG:NH1	49:Z:201:CDL:OA3	2.44	0.50
13:M:140:LEU:HD21	43:M:504:3PE:H2I3	1.94	0.50
1:A:83:VAL:HG23	1:A:83:VAL:O	2.12	0.49
6:F:40:ILE:O	6:F:139:LYS:NZ	2.44	0.49
4:D:146:SER:O	4:D:150:ASN:ND2	2.45	0.49
19:S:16:GLY:O	19:S:23:ARG:NH2	2.46	0.49
19:S:66:ILE:HG12	19:S:83:LEU:HD22	1.95	0.49
4:D:329:CYS:HB3	4:D:456:THR:HG21	1.93	0.49
12:L:613:SER:O	12:L:617:ASN:ND2	2.43	0.49
6:F:447:GLU:OE1	6:F:447:GLU:N	2.45	0.49
7:G:353:LEU:HD11	7:G:701:ASP:OD2	2.13	0.48
11:K:16:VAL:HG11	12:L:622:LEU:HD22	1.95	0.48
11:K:22:ILE:HD11	14:N:159:PHE:CE2	2.48	0.48
5:E:169:LEU:HB2	5:E:177:MET:HE3	1.94	0.48
12:L:87:THR:HG21	12:L:329:LEU:HD23	1.95	0.48
3:C:107:PRO:O	3:C:110:THR:OG1	2.29	0.48
15:O:56:PHE:CE2	15:O:60:LEU:HD11	2.49	0.48
10:J:59:TYR:HE1	11:K:60:ILE:HD11	1.79	0.48
4:D:104:LEU:HD21	4:D:447:LEU:HD21	1.95	0.48
5:E:227:LEU:HD12	6:F:45:TYR:HD2	1.79	0.48
3:C:223:ARG:NE	53:C:304:HOH:O	2.47	0.48
11:K:57:ILE:HA	11:K:60:ILE:HD12	1.96	0.48
7:G:170:LYS:O	7:G:178:THR:OG1	2.22	0.47
6:F:121:GLU:OE2	6:F:129:ASP:N	2.44	0.47
7:G:134:PRO:O	7:G:248:ARG:NH1	2.47	0.47
13:M:207:GLN:HB3	13:M:269:ALA:HB2	1.95	0.47
19:S:5:LEU:HD23	19:S:40:THR:HG21	1.97	0.47
14:N:43:TYR:HE2	14:N:467:TYR:HH	1.60	0.47
4:D:177:PHE:CZ	4:D:220:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:162:GLY:N	6:F:202:GLY:O	2.47	0.47
7:G:455:LEU:HD13	7:G:465:ALA:HB2	1.95	0.47
15:O:30:ARG:NH2	15:O:34:TYR:OH	2.48	0.47
7:G:497:PHE:O	7:G:501:ILE:HD12	2.15	0.47
12:L:420:LEU:HA	12:L:423:VAL:HG22	1.97	0.47
23:W:88:ASN:O	23:W:90:TRP:N	2.48	0.47
24:X:41:PHE:CE1	24:X:122:VAL:HG21	2.50	0.47
4:D:336:ARG:NH2	4:D:456:THR:O	2.48	0.47
5:E:132:CYS:O	5:E:137:SER:N	2.46	0.46
6:F:288:CYS:SG	6:F:290:VAL:HG13	2.55	0.46
10:J:160:PHE:O	10:J:164:VAL:HG23	2.14	0.46
6:F:34:LEU:O	6:F:39:ARG:NH2	2.48	0.46
7:G:611:ALA:O	17:Q:84:ILE:HD12	2.16	0.46
14:N:62:ASN:OD1	14:N:65:THR:HG23	2.16	0.46
14:N:146:SER:OG	14:N:341:TYR:OH	2.16	0.46
22:V:133:ASP:OD1	22:V:134:GLN:N	2.49	0.46
8:H:304:THR:OG1	8:H:307:ASN:OD1	2.27	0.46
4:D:379:GLU:O	4:D:383:HIS:ND1	2.48	0.46
5:E:158:ASP:OD1	5:E:160:LEU:HD22	2.15	0.46
1:A:58:LEU:HD21	10:J:180:THR:OG1	2.16	0.46
6:F:290:VAL:HG11	6:F:305:HIS:HB3	1.96	0.46
10:J:26:ALA:O	11:K:20:ARG:NH2	2.45	0.46
6:F:396:LYS:NZ	7:G:163:GLY:O	2.48	0.46
24:X:16:ALA:O	26:Z:83:ARG:NH1	2.46	0.45
1:A:104:TYR:OH	14:N:102:GLU:OE1	2.35	0.45
6:F:286:GLU:OE1	6:F:307:GLY:HA3	2.16	0.45
24:X:13:GLU:OE1	24:X:15:LYS:NZ	2.40	0.45
2:B:81:PHE:CE2	2:B:83:LEU:HD11	2.51	0.45
6:F:148:GLY:O	6:F:152:ASN:N	2.50	0.45
12:L:241:GLU:O	53:L:1101:HOH:O	2.21	0.45
16:P:177:SER:OG	16:P:312:ASP:OD1	2.23	0.45
3:C:216:LEU:HD13	4:D:129:TYR:CD2	2.52	0.44
4:D:233:GLY:O	4:D:361:VAL:HG23	2.16	0.44
6:F:185:GLY:N	6:F:195:PHE:O	2.45	0.44
12:L:144:GLU:O	12:L:148:VAL:HG23	2.17	0.44
1:A:69:GLU:OE1	1:A:98:LEU:HD22	2.17	0.44
12:L:555:VAL:O	12:L:559:ILE:HG12	2.17	0.44
2:B:35:ARG:NE	16:P:178:GLU:OE1	2.51	0.44
2:B:89:GLU:OE1	4:D:224:ARG:NH1	2.50	0.44
24:X:117:LEU:HD23	24:X:172:LEU:HD11	1.99	0.44
13:M:259:LEU:HD23	13:M:263:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:196:ALA:O	25:Y:198:ASN:N	2.50	0.44
4:D:271:TRP:O	4:D:275:THR:OG1	2.33	0.44
5:E:227:LEU:HD12	6:F:45:TYR:CD2	2.52	0.44
9:I:156:SER:OG	9:I:158:ARG:NH1	2.51	0.44
26:Z:57:GLU:OE2	26:Z:60:ARG:NH1	2.50	0.44
13:M:302:ILE:O	13:M:305:SER:OG	2.21	0.44
14:N:241:LYS:NZ	53:N:2507:HOH:O	2.49	0.44
6:F:260:GLY:O	6:F:262:ASP:N	2.50	0.44
8:H:31:ALA:HB1	8:H:36:ARG:HG3	1.99	0.44
14:N:137:ILE:HG23	14:N:157:TYR:CE2	2.49	0.44
6:F:472:ARG:NH2	6:F:474:GLU:OE1	2.44	0.44
52:U:201:EHZ:O3	52:U:201:EHZ:N2	2.51	0.44
52:U:201:EHZ:O5	52:U:201:EHZ:O6	2.36	0.44
9:I:165:ASP:OD1	9:I:167:THR:OG1	2.28	0.43
19:S:68:LEU:HD23	19:S:79:ARG:HD2	1.99	0.43
20:T:90:ASP:OD1	20:T:91:GLU:N	2.51	0.43
7:G:291:GLU:OE2	17:Q:137:ARG:NH2	2.51	0.43
12:L:29:VAL:O	12:L:32:THR:OG1	2.31	0.43
12:L:135:ASN:OD1	12:L:138:VAL:HG23	2.19	0.43
19:S:5:LEU:HD11	19:S:8:ILE:HD11	2.00	0.43
6:F:55:ALA:HB1	6:F:60:ASP:HB2	2.00	0.43
2:B:85:CYS:HB3	4:D:144:TYR:CG	2.53	0.43
13:M:391:ASN:ND2	53:M:604:HOH:O	2.45	0.43
1:A:69:GLU:HG2	1:A:98:LEU:HD13	2.01	0.43
7:G:626:LEU:HA	7:G:629:VAL:HG12	2.00	0.43
16:P:50:SER:O	16:P:51:ARG:NH1	2.48	0.43
23:W:85:GLU:OE2	53:W:201:HOH:O	2.21	0.43
1:A:79:SER:O	1:A:83:VAL:HG22	2.19	0.42
8:H:331:LEU:HD23	26:Z:49:LEU:CD2	2.49	0.42
49:M:501:CDL:OA3	49:M:501:CDL:O1	2.36	0.42
14:N:51:THR:CG2	14:N:60:ILE:HD11	2.49	0.42
9:I:137:GLU:HB2	9:I:147:ILE:HD12	2.00	0.42
8:H:22:LEU:HD13	8:H:290:MET:SD	2.59	0.42
8:H:22:LEU:HD22	8:H:290:MET:SD	2.58	0.42
14:N:330:SER:O	14:N:334:ILE:HG23	2.18	0.42
16:P:125:VAL:HG23	16:P:160:ILE:HG21	2.01	0.42
19:S:5:LEU:HD21	19:S:8:ILE:HD11	2.02	0.42
1:A:34:LYS:O	2:B:112:ARG:NH1	2.52	0.42
14:N:22:ARG:HD2	15:O:63:VAL:HG13	2.02	0.42
14:N:334:ILE:HD11	14:N:337:ILE:HD13	2.01	0.42
4:D:91:HIS:CE1	4:D:94:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:229:VAL:CG1	7:G:238:LEU:HD13	2.50	0.42
1:A:116:HIS:N	4:D:108:GLU:OE2	2.52	0.42
4:D:290:GLY:O	4:D:428:ARG:NH2	2.50	0.42
6:F:87:ARG:NH2	6:F:275:THR:O	2.52	0.42
14:N:5:ALA:HB1	14:N:28:ILE:HD11	2.01	0.42
4:D:292:SER:OG	4:D:293:GLY:N	2.52	0.42
9:I:196:THR:OG1	9:I:199:GLU:OE2	2.34	0.42
4:D:169:ARG:NH2	4:D:355:PRO:O	2.46	0.42
8:H:204:LEU:HD23	8:H:308:LEU:HD13	2.01	0.41
16:P:35:ARG:NH1	53:P:506:HOH:O	2.53	0.41
23:W:45:VAL:HG12	23:W:47:PHE:H	1.85	0.41
7:G:166:SER:HB2	18:R:94:THR:HG22	2.03	0.41
12:L:420:LEU:O	12:L:424:LEU:HD13	2.20	0.41
3:C:156:LYS:HB2	22:V:135:TRP:HH2	1.85	0.41
5:E:229:SER:OG	5:E:230:LYS:N	2.53	0.41
6:F:407:LYS:N	6:F:410:GLU:OE1	2.46	0.41
5:E:32:VAL:HG21	7:G:168:GLU:OE2	2.19	0.41
6:F:127:CYS:SG	6:F:289:THR:OG1	2.78	0.41
3:C:100:VAL:HG23	3:C:157:THR:HG22	2.02	0.41
4:D:238:ASP:OD1	4:D:239:LEU:N	2.49	0.41
4:D:435:LEU:HD13	4:D:459:LEU:CD1	2.50	0.41
46:L:1007:PLC:H61	13:M:366:THR:O	2.21	0.41
7:G:501:ILE:O	7:G:505:VAL:HG23	2.21	0.41
8:H:42:VAL:O	8:H:42:VAL:HG12	2.21	0.41
10:J:59:TYR:CE1	11:K:60:ILE:HD11	2.55	0.41
13:M:335:HIS:O	13:M:339:SER:OG	2.31	0.41
5:E:33:HIS:NE2	5:E:35:ASN:OD1	2.49	0.41
13:M:227:ILE:O	13:M:227:ILE:HG22	2.21	0.41
15:O:4:SER:O	15:O:4:SER:OG	2.31	0.41
4:D:327:GLY:O	4:D:332:ARG:NH2	2.53	0.41
9:I:158:ARG:NH2	18:R:127:TYR:O	2.54	0.41
7:G:81:ARG:O	7:G:121:VAL:HG21	2.21	0.41
8:H:68:SER:OG	8:H:69:ASN:N	2.53	0.41
8:H:166:ILE:HG23	8:H:244:TYR:CD2	2.56	0.41
12:L:87:THR:HG23	12:L:333:LEU:HD22	2.03	0.41
25:Y:183:ARG:NH1	25:Y:185:ILE:HD13	2.36	0.41
6:F:288:CYS:SG	6:F:289:THR:N	2.94	0.41
7:G:91:PRO:O	7:G:113:ARG:NH1	2.52	0.41
7:G:159:THR:HG22	7:G:159:THR:O	2.21	0.41
6:F:210:GLU:OE1	6:F:212:THR:OG1	2.38	0.40
7:G:490:ASP:OD1	7:G:524:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:117:VAL:CG1	8:H:140:THR:HG23	2.51	0.40
13:M:314:ILE:HA	13:M:317:VAL:HG12	2.03	0.40
8:H:282:TYR:CE2	8:H:286:LEU:HD11	2.56	0.40
7:G:486:SER:OG	7:G:524:ARG:NH1	2.48	0.40
20:T:70:VAL:HA	20:T:73:VAL:HG12	2.02	0.40
16:P:321:GLN:NE2	53:P:501:HOH:O	2.54	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	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
2	B	175/210 (83%)	169 (97%)	6 (3%)	0	100	100
3	C	240/293 (82%)	234 (98%)	6 (2%)	0	100	100
4	D	434/466 (93%)	417 (96%)	17 (4%)	0	100	100
5	E	214/243 (88%)	204 (95%)	10 (5%)	0	100	100
6	F	458/488 (94%)	433 (94%)	25 (6%)	0	100	100
7	G	692/728 (95%)	657 (95%)	35 (5%)	0	100	100
8	H	339/341 (99%)	324 (96%)	15 (4%)	0	100	100
9	I	189/229 (82%)	179 (95%)	10 (5%)	0	100	100
10	J	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
11	K	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
12	L	653/655 (100%)	624 (96%)	28 (4%)	1 (0%)	44	68
13	M	484/486 (100%)	469 (97%)	15 (3%)	0	100	100
14	N	467/469 (100%)	460 (98%)	7 (2%)	0	100	100
15	O	166/169 (98%)	158 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	353/375 (94%)	340 (96%)	13 (4%)	0	100	100
17	Q	123/161 (76%)	119 (97%)	4 (3%)	0	100	100
18	R	116/136 (85%)	111 (96%)	5 (4%)	0	100	100
19	S	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
20	T	79/109 (72%)	71 (90%)	8 (10%)	0	100	100
21	U	86/132 (65%)	83 (96%)	3 (4%)	0	100	100
22	V	124/144 (86%)	116 (94%)	8 (6%)	0	100	100
23	W	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
24	X	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
25	Y	177/198 (89%)	171 (97%)	6 (3%)	0	100	100
26	Z	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
27	a	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
28	b	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
29	c	180/182 (99%)	168 (93%)	12 (7%)	0	100	100
30	d	65/74 (88%)	65 (100%)	0	0	100	100
31	e	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
32	f	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
33	g	196/249 (79%)	190 (97%)	6 (3%)	0	100	100
34	h	111/139 (80%)	107 (96%)	4 (4%)	0	100	100
35	i	84/90 (93%)	82 (98%)	2 (2%)	0	100	100
36	j	51/91 (56%)	50 (98%)	1 (2%)	0	100	100
37	k	45/60 (75%)	40 (89%)	5 (11%)	0	100	100
38	l	123/149 (83%)	113 (92%)	10 (8%)	0	100	100
39	m	90/93 (97%)	86 (96%)	4 (4%)	0	100	100
40	n	106/109 (97%)	101 (95%)	5 (5%)	0	100	100
41	o	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
42	p	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
All	All	8041/8759 (92%)	7707 (96%)	333 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	555	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	107/113 (95%)	107 (100%)	0	100	100
2	B	154/180 (86%)	154 (100%)	0	100	100
3	C	218/251 (87%)	218 (100%)	0	100	100
4	D	372/393 (95%)	372 (100%)	0	100	100
5	E	191/212 (90%)	191 (100%)	0	100	100
6	F	367/389 (94%)	366 (100%)	1 (0%)	91	97
7	G	566/595 (95%)	566 (100%)	0	100	100
8	H	298/301 (99%)	298 (100%)	0	100	100
9	I	157/187 (84%)	157 (100%)	0	100	100
10	J	166/166 (100%)	166 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	579/579 (100%)	579 (100%)	0	100	100
13	M	433/433 (100%)	433 (100%)	0	100	100
14	N	432/432 (100%)	432 (100%)	0	100	100
15	O	132/133 (99%)	132 (100%)	0	100	100
16	P	299/329 (91%)	299 (100%)	0	100	100
17	Q	107/140 (76%)	107 (100%)	0	100	100
18	R	98/115 (85%)	98 (100%)	0	100	100
19	S	72/73 (99%)	72 (100%)	0	100	100
20	T	68/91 (75%)	68 (100%)	0	100	100
21	U	75/111 (68%)	74 (99%)	1 (1%)	65	85
22	V	113/129 (88%)	113 (100%)	0	100	100
23	W	109/110 (99%)	109 (100%)	0	100	100
24	X	147/148 (99%)	147 (100%)	0	100	100
25	Y	130/147 (88%)	129 (99%)	1 (1%)	79	91
26	Z	101/102 (99%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	68/69 (99%)	68 (100%)	0	100	100
28	b	65/65 (100%)	65 (100%)	0	100	100
29	c	148/148 (100%)	148 (100%)	0	100	100
30	d	52/59 (88%)	52 (100%)	0	100	100
31	e	59/76 (78%)	59 (100%)	0	100	100
32	f	122/123 (99%)	122 (100%)	0	100	100
33	g	161/211 (76%)	160 (99%)	1 (1%)	84	94
34	h	98/119 (82%)	98 (100%)	0	100	100
35	i	64/68 (94%)	64 (100%)	0	100	100
36	j	45/78 (58%)	45 (100%)	0	100	100
37	k	32/45 (71%)	32 (100%)	0	100	100
38	l	109/129 (84%)	109 (100%)	0	100	100
39	m	72/73 (99%)	72 (100%)	0	100	100
40	n	99/100 (99%)	99 (100%)	0	100	100
41	o	70/76 (92%)	70 (100%)	0	100	100
42	p	84/85 (99%)	84 (100%)	0	100	100
All	All	6915/7459 (93%)	6911 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	127	CYS
21	U	73	LYS
25	Y	183	ARG
33	g	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	86	ASN
4	D	90	GLN
4	D	193	HIS
4	D	434	HIS
5	E	174	ASN
12	L	636	ASN

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Mol	Chain	Res	Type
14	N	180	ASN
16	P	237	HIS
23	W	22	GLN
33	g	207	HIS
40	n	11	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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$
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	1.10	0
1	FME	A	1	1	8,9,10	0.99	0	7,9,11	0.84	0
8	FME	H	1	8	8,9,10	0.98	0	7,9,11	1.35	1 (14%)
11	FME	K	1	11	8,9,10	0.96	0	7,9,11	1.00	0
12	FME	L	1	12	8,9,10	0.98	0	7,9,11	0.95	0
4	2MR	D	121	4	10,12,13	2.41	3 (30%)	5,13,15	2.15	1 (20%)
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	0.90	0
14	FME	N	1	14	8,9,10	1.10	1 (12%)	7,9,11	1.22	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FME	J	1	10	-	3/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	H	1	8	-	3/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
4	2MR	D	121	4	-	3/10/13/15	-
13	FME	M	1	13	-	0/7/9/11	-
14	FME	N	1	14	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	121	2MR	CZ-NE	5.01	1.45	1.34
4	D	121	2MR	CZ-NH2	4.72	1.43	1.33
4	D	121	2MR	CQ1-NH1	-2.54	1.41	1.46
14	N	1	FME	CA-N	-2.46	1.42	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	121	2MR	CD-NE-CZ	4.46	131.76	123.41
8	H	1	FME	C-CA-N	2.90	114.96	109.73
14	N	1	FME	C-CA-N	2.73	114.66	109.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
4	D	121	2MR	O-C-CA-CB
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	O-C-CA-CB
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	O-C-CA-CB
11	K	1	FME	N-CA-CB-CG
4	D	121	2MR	NE-CD-CG-CB
14	N	1	FME	CB-CG-SD-CE
12	L	1	FME	N-CA-CB-CG
4	D	121	2MR	CA-CB-CG-CD
10	J	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 1 is monoatomic - leaving 49 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
43	3PE	A	501	-	26,26,50	1.26	3 (11%)	29,31,55	1.31	3 (10%)
44	SF4	G	802	7	0,12,12	-	-	-	-	-
49	CDL	Z	201	-	56,56,99	1.22	8 (14%)	62,68,111	1.12	6 (9%)
49	CDL	b	401	-	47,47,99	1.33	9 (19%)	53,59,111	1.36	6 (11%)
52	EHZ	U	201	21	27,34,37	1.74	6 (22%)	33,42,47	1.37	7 (21%)
46	PLC	L	1007	-	41,41,41	1.28	6 (14%)	47,49,49	1.11	3 (6%)
49	CDL	P	403	-	47,47,99	1.31	8 (17%)	53,59,111	1.23	6 (11%)
49	CDL	O	401	-	62,62,99	1.14	8 (12%)	68,74,111	1.16	6 (8%)
52	EHZ	T	201	20	26,33,37	1.71	5 (19%)	32,41,47	1.60	6 (18%)
44	SF4	I	6302	9	0,12,12	-	-	-	-	-
46	PLC	d	4602	-	26,26,41	1.38	2 (7%)	32,34,49	1.24	3 (9%)
43	3PE	M	504	-	39,39,50	1.03	4 (10%)	42,44,55	1.12	3 (7%)
43	3PE	L	1005	-	50,50,50	0.91	3 (6%)	53,55,55	1.29	3 (5%)
43	3PE	b	403	-	25,25,50	1.27	4 (16%)	28,30,55	1.25	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	LMT	Y	4201	-	36,36,36	0.85	0	47,47,47	1.07	5 (10%)
43	3PE	H	602	-	21,21,50	1.31	2 (9%)	24,26,55	1.21	2 (8%)
49	CDL	M	501	-	82,82,99	1.32	7 (8%)	88,94,111	1.05	6 (6%)
43	3PE	Z	203	-	42,42,50	0.97	4 (9%)	45,47,55	1.08	3 (6%)
44	SF4	G	801	7	0,12,12	-	-	-	-	-
46	PLC	L	1001	-	33,33,41	1.38	3 (9%)	39,41,49	1.09	3 (7%)
46	PLC	H	601	-	27,27,41	1.44	3 (11%)	33,35,49	3.95	8 (24%)
46	PLC	P	401	-	34,34,41	1.34	4 (11%)	40,42,49	1.15	3 (7%)
45	LMT	Y	4204	-	36,36,36	0.88	2 (5%)	47,47,47	1.65	10 (21%)
50	NDP	P	402	-	45,52,52	2.22	5 (11%)	53,80,80	1.66	9 (16%)
46	PLC	N	2401	-	41,41,41	1.11	4 (9%)	47,49,49	1.10	3 (6%)
47	FES	E	301	5	0,4,4	-	-	-	-	-
43	3PE	d	4603	-	29,29,50	1.18	4 (13%)	32,34,55	1.15	3 (9%)
46	PLC	L	1002	-	28,28,41	1.30	4 (14%)	34,36,49	1.12	3 (8%)
44	SF4	I	6303	9	0,12,12	-	-	-	-	-
43	3PE	M	502	-	29,29,50	1.18	4 (13%)	32,34,55	1.22	3 (9%)
43	3PE	Y	4203	-	23,23,50	1.32	4 (17%)	26,28,55	1.53	4 (15%)
45	LMT	B	302	-	36,36,36	0.83	1 (2%)	47,47,47	0.80	1 (2%)
46	PLC	D	501	-	26,26,41	1.39	4 (15%)	32,34,49	1.15	3 (9%)
49	CDL	a	101	-	51,51,99	1.26	8 (15%)	57,63,111	1.25	6 (10%)
43	3PE	A	502	-	50,50,50	0.90	4 (8%)	53,55,55	1.12	5 (9%)
43	3PE	L	1003	-	50,50,50	0.88	4 (8%)	53,55,55	0.93	2 (3%)
47	FES	G	803	7	0,4,4	-	-	-	-	-
43	3PE	L	1004	-	50,50,50	0.88	3 (6%)	53,55,55	1.03	2 (3%)
43	3PE	d	4601	-	23,23,50	1.29	4 (17%)	26,28,55	1.31	3 (11%)
48	FMN	F	501	6	33,33,33	2.89	10 (30%)	48,50,50	1.99	16 (33%)
45	LMT	M	503	-	36,36,36	0.77	0	47,47,47	0.85	2 (4%)
43	3PE	N	2402	-	50,50,50	0.89	3 (6%)	53,55,55	0.97	2 (3%)
45	LMT	Y	4202	-	36,36,36	0.79	0	47,47,47	1.25	7 (14%)
43	3PE	I	6301	-	45,45,50	1.21	3 (6%)	48,50,55	1.01	3 (6%)
43	3PE	Z	202	-	31,31,50	1.15	4 (12%)	34,36,55	1.31	3 (8%)
44	SF4	B	301	2	0,12,12	-	-	-	-	-
44	SF4	F	502	6	0,12,12	-	-	-	-	-
43	3PE	L	1006	-	32,32,50	1.13	4 (12%)	35,37,55	1.17	3 (8%)
43	3PE	b	402	-	42,42,50	1.21	4 (9%)	45,47,55	1.02	3 (6%)

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
43	3PE	A	501	-	1/1/4/4	16/30/30/54	-
44	SF4	G	802	7	-	-	0/6/5/5
52	EHZ	U	201	21	1/1/7/9	11/40/42/45	-
49	CDL	Z	201	-	-	33/67/67/110	-
49	CDL	b	401	-	-	19/58/58/110	-
46	PLC	L	1007	-	-	21/45/45/45	-
49	CDL	P	403	-	-	26/58/58/110	-
49	CDL	O	401	-	-	26/73/73/110	-
52	EHZ	T	201	20	1/1/7/9	7/39/41/45	-
44	SF4	I	6302	9	-	-	0/6/5/5
46	PLC	d	4602	-	-	9/30/30/45	-
43	3PE	M	504	-	-	17/43/43/54	-
43	3PE	L	1005	-	-	25/54/54/54	-
43	3PE	b	403	-	-	9/29/29/54	-
45	LMT	Y	4201	-	4/4/10/10	4/21/61/61	0/2/2/2
43	3PE	H	602	-	1/1/4/4	11/24/24/54	-
49	CDL	M	501	-	-	41/93/93/110	-
43	3PE	Z	203	-	-	14/46/46/54	-
44	SF4	G	801	7	-	-	0/6/5/5
46	PLC	L	1001	-	-	18/37/37/45	-
46	PLC	H	601	-	-	12/31/31/45	-
46	PLC	P	401	-	-	9/38/38/45	-
45	LMT	Y	4204	-	4/4/10/10	13/21/61/61	0/2/2/2
50	NDP	P	402	-	-	9/30/77/77	0/5/5/5
46	PLC	N	2401	-	-	18/45/45/45	-
47	FES	E	301	5	-	-	0/1/1/1
43	3PE	d	4603	-	1/1/4/4	16/33/33/54	-
46	PLC	L	1002	-	-	10/32/32/45	-
44	SF4	I	6303	9	-	-	0/6/5/5
43	3PE	M	502	-	1/1/4/4	18/33/33/54	-
43	3PE	Y	4203	-	1/1/4/4	13/26/26/54	-
45	LMT	B	302	-	4/4/10/10	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PLC	D	501	-	-	12/30/30/45	-
49	CDL	a	101	-	-	25/62/62/110	-
43	3PE	A	502	-	-	20/54/54/54	-
43	3PE	L	1003	-	-	20/54/54/54	-
47	FES	G	803	7	-	-	0/1/1/1
43	3PE	L	1004	-	-	27/54/54/54	-
48	FMN	F	501	6	2/2/4/4	8/18/18/18	0/3/3/3
43	3PE	d	4601	-	-	8/27/27/54	-
45	LMT	M	503	-	4/4/10/10	13/21/61/61	0/2/2/2
45	LMT	Y	4202	-	4/4/10/10	13/21/61/61	0/2/2/2
43	3PE	N	2402	-	-	27/54/54/54	-
43	3PE	I	6301	-	-	17/49/49/54	-
43	3PE	Z	202	-	1/1/4/4	18/35/35/54	-
44	SF4	B	301	2	-	-	0/6/5/5
44	SF4	F	502	6	-	-	0/6/5/5
43	3PE	L	1006	-	-	11/36/36/54	-
43	3PE	b	402	-	-	12/46/46/54	-

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	P	402	NDP	P2B-O2B	11.90	1.81	1.59
48	F	501	FMN	O2-C2	8.75	1.40	1.24
48	F	501	FMN	O4-C4	8.61	1.40	1.23
48	F	501	FMN	C2-N1	5.84	1.50	1.36
52	U	201	EHZ	C15-N2	5.19	1.44	1.33
52	T	201	EHZ	C12-N1	4.97	1.44	1.33
52	U	201	EHZ	C12-N1	4.96	1.44	1.33
52	T	201	EHZ	C15-N2	4.80	1.44	1.33
50	P	402	NDP	PN-O5D	4.75	1.78	1.59
48	F	501	FMN	C10-N1	4.38	1.42	1.33
43	I	6301	3PE	O31-C31	3.62	1.43	1.33
49	M	501	CDL	OA6-CA5	3.51	1.44	1.34
48	F	501	FMN	C6-C7	-3.40	1.34	1.39
46	L	1001	PLC	O3-CB	3.39	1.43	1.33
43	I	6301	3PE	O21-C21	3.30	1.43	1.34
48	F	501	FMN	C4A-N5	3.23	1.37	1.30
49	M	501	CDL	OB8-CB7	3.23	1.42	1.33
48	F	501	FMN	C6-C5A	-3.21	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	L	1001	PLC	O2-C'	3.19	1.43	1.34
43	b	402	3PE	O31-C31	3.18	1.42	1.33
46	L	1007	PLC	O3-CB	3.15	1.42	1.33
50	P	402	NDP	O2B-C2B	-3.06	1.33	1.44
43	b	402	3PE	O21-C21	3.02	1.42	1.34
49	M	501	CDL	OA8-CA7	3.00	1.42	1.33
43	b	402	3PE	O21-C2	-2.91	1.39	1.46
49	O	401	CDL	OB6-CB4	-2.90	1.39	1.46
49	M	501	CDL	OB6-CB5	2.90	1.42	1.34
43	L	1004	3PE	O21-C2	-2.86	1.39	1.46
46	H	601	PLC	O3-CB	2.84	1.41	1.33
46	P	401	PLC	O3-CB	2.84	1.41	1.33
49	Z	201	CDL	OA6-CA4	-2.78	1.39	1.46
46	L	1007	PLC	O2-C'	2.77	1.42	1.34
49	M	501	CDL	OB6-CB4	-2.76	1.39	1.46
43	Z	202	3PE	O21-C2	-2.75	1.39	1.46
46	H	601	PLC	O2-C'	2.74	1.42	1.34
49	b	401	CDL	OA6-CA4	-2.72	1.39	1.46
43	I	6301	3PE	O21-C2	-2.72	1.39	1.46
43	L	1005	3PE	O21-C21	2.68	1.41	1.34
52	U	201	EHZ	O3-C12	-2.67	1.17	1.23
46	H	601	PLC	O2-C2	-2.66	1.39	1.46
46	d	4602	PLC	O2-C2	-2.65	1.40	1.46
43	Z	202	3PE	O31-C3	-2.60	1.39	1.45
49	b	401	CDL	OB6-CB4	-2.58	1.40	1.46
43	M	502	3PE	O21-C2	-2.56	1.40	1.46
43	Y	4203	3PE	O21-C2	-2.56	1.40	1.46
45	Y	4204	LMT	O2'-C2'	-2.56	1.37	1.43
43	A	501	3PE	O31-C31	2.54	1.40	1.33
46	P	401	PLC	O2-C'	2.53	1.41	1.34
49	O	401	CDL	OB8-CB6	-2.52	1.39	1.45
49	P	403	CDL	OA8-CA7	2.50	1.40	1.33
49	a	101	CDL	OB6-CB4	-2.50	1.40	1.46
43	N	2402	3PE	O21-C21	2.50	1.41	1.34
49	a	101	CDL	OA8-CA7	2.49	1.40	1.33
43	A	501	3PE	O21-C2	-2.48	1.40	1.46
43	A	502	3PE	O31-C31	2.48	1.40	1.33
43	A	502	3PE	O21-C2	-2.48	1.40	1.46
49	P	403	CDL	OB6-CB4	-2.48	1.40	1.46
43	b	403	3PE	O21-C2	-2.47	1.40	1.46
46	L	1002	PLC	O2-C2	-2.47	1.40	1.46
43	H	602	3PE	O21-C2	-2.47	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	4601	3PE	O31-C31	2.46	1.40	1.33
43	L	1003	3PE	O21-C21	2.45	1.41	1.34
49	P	403	CDL	OB8-CB7	2.45	1.40	1.33
43	M	504	3PE	O21-C2	-2.45	1.40	1.46
49	a	101	CDL	OB8-CB6	-2.44	1.39	1.45
49	Z	201	CDL	OA8-CA7	2.44	1.40	1.33
43	L	1005	3PE	O31-C31	2.43	1.40	1.33
45	Y	4204	LMT	O5B-C5B	-2.42	1.38	1.44
52	T	201	EHZ	O4-C15	-2.41	1.18	1.23
49	O	401	CDL	OA6-CA4	-2.41	1.40	1.46
46	N	2401	PLC	O2-C2	-2.41	1.40	1.46
43	d	4603	3PE	O21-C2	-2.40	1.40	1.46
46	d	4602	PLC	O3-CB	2.40	1.40	1.33
49	b	401	CDL	OA8-CA7	2.40	1.40	1.33
46	P	401	PLC	O2-C2	-2.40	1.40	1.46
49	Z	201	CDL	OB6-CB4	-2.39	1.40	1.46
48	F	501	FMN	P-O3P	-2.39	1.45	1.54
43	b	403	3PE	O31-C31	2.38	1.40	1.33
43	Z	203	3PE	O31-C31	2.38	1.40	1.33
43	L	1006	3PE	O31-C31	2.37	1.40	1.33
43	N	2402	3PE	O31-C31	2.37	1.40	1.33
46	N	2401	PLC	O2-C'	2.37	1.41	1.34
43	Y	4203	3PE	O31-C31	2.36	1.40	1.33
49	P	403	CDL	OA6-CA5	2.36	1.41	1.34
52	U	201	EHZ	O4-C15	-2.36	1.18	1.23
43	L	1004	3PE	O31-C31	2.36	1.40	1.33
49	Z	201	CDL	OB6-CB5	2.36	1.41	1.34
43	d	4603	3PE	O31-C31	2.36	1.40	1.33
43	L	1006	3PE	O21-C2	-2.35	1.40	1.46
49	Z	201	CDL	OB8-CB7	2.35	1.40	1.33
49	a	101	CDL	OA6-CA4	-2.35	1.40	1.46
52	T	201	EHZ	O3-C12	-2.34	1.18	1.23
43	L	1006	3PE	O21-C21	2.34	1.40	1.34
45	B	302	LMT	O1'-C1'	-2.34	1.36	1.40
43	L	1003	3PE	O31-C31	2.32	1.40	1.33
46	N	2401	PLC	O3-CB	2.32	1.40	1.33
43	M	504	3PE	O31-C31	2.32	1.40	1.33
46	D	501	PLC	O2-C2	-2.31	1.40	1.46
46	L	1007	PLC	O2-C2	-2.31	1.40	1.46
49	P	403	CDL	OA6-CA4	-2.31	1.40	1.46
49	b	401	CDL	OB8-CB7	2.30	1.40	1.33
43	M	502	3PE	O31-C3	-2.30	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	b	401	CDL	OB8-CB6	-2.30	1.39	1.45
43	Z	203	3PE	O21-C2	-2.29	1.40	1.46
46	L	1002	PLC	O3-C3	-2.29	1.39	1.45
43	M	504	3PE	O21-C21	2.28	1.40	1.34
43	L	1004	3PE	O31-C3	-2.28	1.40	1.45
46	D	501	PLC	O2-C'	2.28	1.40	1.34
43	Y	4203	3PE	O31-C3	-2.27	1.40	1.45
46	L	1002	PLC	O3-CB	2.27	1.40	1.33
49	O	401	CDL	OA8-CA7	2.27	1.40	1.33
46	D	501	PLC	O3-CB	2.26	1.39	1.33
43	A	502	3PE	O21-C21	2.26	1.40	1.34
49	b	401	CDL	OA8-CA6	-2.26	1.40	1.45
43	N	2402	3PE	O31-C3	-2.25	1.40	1.45
48	F	501	FMN	P-O2P	-2.25	1.46	1.54
52	U	201	EHZ	O6-C20	-2.24	1.39	1.44
52	U	201	EHZ	C9-S1	2.24	1.81	1.76
43	M	502	3PE	O31-C31	2.24	1.39	1.33
43	L	1003	3PE	O31-C3	-2.23	1.40	1.45
43	M	504	3PE	O31-C3	-2.23	1.40	1.45
49	Z	201	CDL	OA8-CA6	-2.23	1.40	1.45
52	T	201	EHZ	C9-S1	2.22	1.81	1.76
43	Z	203	3PE	O31-C3	-2.21	1.40	1.45
49	O	401	CDL	OA8-CA6	-2.21	1.40	1.45
43	H	602	3PE	O21-C21	2.20	1.40	1.34
43	b	403	3PE	O31-C3	-2.20	1.40	1.45
43	A	501	3PE	O21-C21	2.20	1.40	1.34
49	P	403	CDL	OB6-CB5	2.20	1.40	1.34
49	a	101	CDL	OA6-CA5	2.19	1.40	1.34
49	a	101	CDL	OB6-CB5	2.19	1.40	1.34
43	L	1006	3PE	O31-C3	-2.19	1.40	1.45
46	L	1002	PLC	O2-C'	2.18	1.40	1.34
43	d	4601	3PE	O21-C21	2.17	1.40	1.34
43	L	1003	3PE	O21-C2	-2.16	1.41	1.46
43	d	4603	3PE	O31-C3	-2.16	1.40	1.45
49	O	401	CDL	OB8-CB7	2.14	1.39	1.33
46	D	501	PLC	O3-C3	-2.14	1.40	1.45
43	b	402	3PE	P-O11	2.13	1.67	1.59
49	a	101	CDL	OA8-CA6	-2.13	1.40	1.45
46	L	1007	PLC	P-O2P	-2.12	1.45	1.55
43	b	403	3PE	O21-C21	2.12	1.40	1.34
49	a	101	CDL	OB8-CB7	2.11	1.39	1.33
43	M	502	3PE	O21-C21	2.11	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	Y	4203	3PE	O21-C21	2.11	1.39	1.35
49	b	401	CDL	OB6-CB5	2.10	1.40	1.34
46	L	1001	PLC	P-O3P	2.10	1.67	1.59
46	P	401	PLC	C8-N	-2.10	1.43	1.50
49	M	501	CDL	PB2-OB4	-2.09	1.45	1.55
49	Z	201	CDL	OB8-CB6	-2.09	1.40	1.45
43	d	4601	3PE	O31-C3	-2.08	1.40	1.45
43	Z	202	3PE	O31-C31	2.07	1.39	1.33
49	M	501	CDL	PA1-OA4	-2.07	1.45	1.55
46	N	2401	PLC	O3-C3	-2.07	1.40	1.45
46	L	1007	PLC	P-O3P	2.07	1.67	1.59
49	b	401	CDL	OA6-CA5	2.06	1.40	1.34
49	b	401	CDL	PB2-OB4	-2.05	1.45	1.55
43	d	4603	3PE	O21-C21	2.05	1.40	1.34
43	Z	203	3PE	O21-C21	2.05	1.40	1.34
43	d	4601	3PE	O21-C2	-2.05	1.41	1.46
46	L	1007	PLC	C8-N	-2.05	1.44	1.50
50	P	402	NDP	C7N-N7N	2.05	1.38	1.33
49	P	403	CDL	OA8-CA6	-2.04	1.40	1.45
43	Z	202	3PE	P-O12	-2.03	1.45	1.55
43	A	502	3PE	O31-C3	-2.03	1.40	1.45
43	L	1005	3PE	O21-C2	-2.03	1.41	1.46
49	O	401	CDL	PB2-OB4	-2.03	1.45	1.55
48	F	501	FMN	C4-N3	-2.02	1.35	1.38
50	P	402	NDP	O5B-C5B	-2.01	1.37	1.44
49	Z	201	CDL	OA6-CA5	2.00	1.40	1.34
49	O	401	CDL	OA6-CA5	2.00	1.40	1.34
49	P	403	CDL	OB8-CB6	-2.00	1.40	1.45

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	601	PLC	C8-N-C7	14.48	146.20	108.97
46	H	601	PLC	C6-N-C5	10.05	151.06	109.92
46	H	601	PLC	C7-N-C6	-8.86	86.19	108.97
46	H	601	PLC	C8-N-C6	-8.00	88.39	108.97
43	L	1005	3PE	O21-C21-C22	6.46	125.43	111.50
50	P	402	NDP	PN-O3-PA	-6.32	111.15	132.83
52	T	201	EHZ	C8-C9-S1	5.66	120.63	113.63
48	F	501	FMN	C4-C4A-C10	4.84	124.93	116.79
45	Y	4204	LMT	O5B-C5B-C4B	-4.81	100.96	109.69
46	N	2401	PLC	O2-C'-C1'	4.79	121.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	Y	4203	3PE	O21-C21-C22	4.74	119.80	111.09
43	A	501	3PE	O21-C21-C22	4.72	121.67	111.50
48	F	501	FMN	C4A-C10-N1	-4.45	114.40	124.73
49	b	401	CDL	OA6-CA5-C11	4.43	121.04	111.50
46	L	1007	PLC	O2-C'-C1'	4.36	120.90	111.50
49	a	101	CDL	OA6-CA5-C11	4.33	120.83	111.50
43	Z	202	3PE	O21-C21-C22	4.32	120.81	111.50
46	D	501	PLC	O2-C'-C1'	4.16	120.48	111.50
49	O	401	CDL	OA6-CA5-C11	4.16	120.47	111.50
46	d	4602	PLC	O2-C'-C1'	4.15	120.44	111.50
49	a	101	CDL	OB6-CB5-C51	4.13	120.40	111.50
48	F	501	FMN	C6-C5A-C9A	4.07	124.69	118.94
43	L	1006	3PE	O21-C21-C22	4.04	120.22	111.50
43	b	403	3PE	O21-C21-C22	4.02	120.17	111.50
43	N	2402	3PE	O21-C21-C22	4.01	120.15	111.50
46	H	601	PLC	O2-C'-C1'	4.00	120.12	111.50
46	P	401	PLC	O2-C'-C1'	3.99	120.10	111.50
43	d	4601	3PE	O21-C21-C22	3.98	120.08	111.50
49	b	401	CDL	OB6-CB5-C51	3.95	120.02	111.50
43	d	4603	3PE	O21-C21-C22	3.91	119.92	111.50
48	F	501	FMN	C4-C4A-N5	-3.90	112.68	118.23
43	H	602	3PE	O21-C21-C22	3.77	119.64	111.50
49	P	403	CDL	OA6-CA5-C11	3.75	119.58	111.50
43	M	502	3PE	O21-C21-C22	3.72	119.51	111.50
49	Z	201	CDL	OA6-CA5-C11	3.68	119.43	111.50
43	A	502	3PE	O31-C31-C32	3.67	123.41	111.91
43	M	504	3PE	O21-C21-C22	3.66	119.38	111.50
49	M	501	CDL	OA6-CA5-C11	3.59	119.24	111.50
43	Z	203	3PE	O21-C21-C22	3.58	119.21	111.50
49	P	403	CDL	OB6-CB5-C51	3.58	119.21	111.50
49	P	403	CDL	OB8-CB7-C71	3.52	120.62	111.38
45	Y	4204	LMT	C1-O1'-C1'	3.51	119.65	113.84
45	Y	4202	LMT	C1-O1'-C1'	3.49	119.63	113.84
46	L	1002	PLC	O2-C'-C1'	3.49	120.54	110.80
43	L	1003	3PE	O21-C21-C22	3.49	119.02	111.50
43	L	1004	3PE	C3-C2-C1	-3.47	103.58	111.79
43	A	502	3PE	C3-C2-C1	-3.37	103.82	111.79
45	Y	4202	LMT	O1B-C4'-C3'	3.30	116.05	107.28
49	b	401	CDL	OA8-CA7-C31	3.26	119.93	111.38
49	M	501	CDL	OB6-CB5-C51	3.26	118.52	111.50
43	b	402	3PE	O21-C21-C22	3.24	118.49	111.50
49	Z	201	CDL	OB6-CB5-C51	3.24	118.49	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	F	501	FMN	C4-N3-C2	-3.22	119.69	125.64
50	P	402	NDP	O2B-P2B-O1X	-3.19	97.09	109.39
45	Y	4201	LMT	C1B-O1B-C4'	-3.18	110.10	117.96
46	L	1001	PLC	O2-C'-C1'	3.18	118.35	111.50
43	L	1004	3PE	O21-C21-C22	3.16	118.32	111.50
45	Y	4204	LMT	C1B-O5B-C5B	3.16	119.90	113.69
52	U	201	EHZ	C13-C12-N1	3.15	121.73	116.42
50	P	402	NDP	PA-O5B-C5B	-3.15	103.20	121.68
43	L	1005	3PE	O31-C31-C32	3.12	121.71	111.91
46	H	601	PLC	C7-N-C5	-3.10	97.22	109.92
46	H	601	PLC	O3-CB-C1B	3.10	119.50	111.38
48	F	501	FMN	O2P-P-O5'	3.04	114.83	106.73
45	Y	4204	LMT	O1B-C4'-C5'	3.04	117.77	109.45
43	Y	4203	3PE	O31-C31-C32	3.03	121.42	111.91
52	T	201	EHZ	C13-C12-N1	3.02	121.51	116.42
45	B	302	LMT	C1B-O5B-C5B	3.01	119.59	113.69
43	I	6301	3PE	O21-C21-C22	2.98	117.93	111.50
50	P	402	NDP	PN-O5D-C5D	-2.97	104.29	121.68
45	Y	4204	LMT	O1B-C1B-O5B	-2.91	102.55	110.67
48	F	501	FMN	C6-C5A-N5	-2.89	113.46	118.51
43	N	2402	3PE	O31-C31-C32	2.84	120.81	111.91
49	O	401	CDL	OB6-CB5-C51	2.83	117.60	111.50
48	F	501	FMN	C5A-C9A-N10	2.82	120.86	117.95
52	T	201	EHZ	C11-N1-C12	-2.81	117.61	122.84
43	A	502	3PE	O21-C21-C22	2.80	117.54	111.50
46	d	4602	PLC	O3-CB-C1B	2.80	120.68	111.91
45	Y	4204	LMT	C1'-C2'-C3'	2.78	115.78	110.00
43	M	504	3PE	O31-C31-C32	2.76	120.58	111.91
48	F	501	FMN	C4A-C10-N10	2.76	120.51	116.48
45	Y	4201	LMT	C1-O1'-C1'	2.74	118.39	113.84
46	D	501	PLC	O3-CB-C1B	2.73	118.53	111.38
48	F	501	FMN	C9-C9A-C5A	-2.72	114.97	120.11
46	L	1001	PLC	O3-CB-C1B	2.71	120.41	111.91
52	U	201	EHZ	C8-C9-S1	2.70	116.97	113.63
43	M	502	3PE	O31-C31-C32	2.65	120.23	111.91
43	L	1003	3PE	O31-C31-C32	2.65	120.22	111.91
49	Z	201	CDL	OB8-CB7-C71	2.62	120.14	111.91
50	P	402	NDP	O7N-C7N-N7N	-2.56	116.88	122.88
48	F	501	FMN	O3P-P-O5'	2.56	113.55	106.73
43	L	1005	3PE	O21-C21-O22	-2.56	117.51	123.70
43	A	502	3PE	O31-C31-O32	-2.56	117.13	123.59
50	P	402	NDP	O3X-P2B-O2X	2.56	117.42	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	P	402	NDP	C2A-N1A-C6A	-2.55	114.39	118.75
48	F	501	FMN	O4-C4-C4A	-2.53	119.88	126.60
43	b	403	3PE	O31-C31-C32	2.51	119.78	111.91
46	P	401	PLC	O3-CB-C1B	2.50	119.77	111.91
48	F	501	FMN	C4A-C4-N3	2.49	119.52	113.19
49	O	401	CDL	OA8-CA7-C31	2.49	119.72	111.91
52	U	201	EHZ	C19-C17-C16	2.49	113.13	108.82
49	M	501	CDL	OA8-CA7-C31	2.49	119.71	111.91
45	Y	4202	LMT	O5'-C1'-O1'	-2.49	104.09	109.97
45	Y	4202	LMT	O5'-C5'-C4'	2.47	114.97	109.75
46	P	401	PLC	O2P-P-O1P	-2.46	100.08	112.24
46	H	601	PLC	O2P-P-O1P	-2.45	100.13	112.24
43	b	402	3PE	O31-C31-C32	2.44	119.58	111.91
43	H	602	3PE	O12-P-O14	-2.44	100.16	112.24
49	Z	201	CDL	OB4-PB2-OB3	-2.44	100.18	112.24
43	Z	202	3PE	O31-C31-C32	2.43	119.54	111.91
50	P	402	NDP	O4B-C4B-C3B	2.42	109.90	105.11
49	b	401	CDL	OB8-CB7-C71	2.42	119.49	111.91
48	F	501	FMN	C9A-N10-C10	-2.41	117.01	120.77
45	Y	4204	LMT	O1B-C4'-C3'	-2.41	100.87	107.28
49	Z	201	CDL	OA8-CA7-C31	2.40	119.45	111.91
52	U	201	EHZ	C11-N1-C12	-2.40	118.39	122.84
49	a	101	CDL	OA8-CA7-C31	2.40	119.43	111.91
46	L	1007	PLC	O3-CB-C1B	2.39	119.41	111.91
46	N	2401	PLC	O2P-P-O1P	-2.39	100.43	112.24
45	M	503	LMT	O1B-C4'-C3'	2.39	113.63	107.28
43	Y	4203	3PE	O12-P-O14	-2.37	100.55	112.24
48	F	501	FMN	O5'-P-O1P	2.36	113.10	106.47
45	Y	4201	LMT	C1'-C2'-C3'	2.36	114.91	110.00
45	Y	4201	LMT	C6'-C5'-C4'	-2.36	106.46	113.33
43	d	4601	3PE	O12-P-O14	-2.35	100.61	112.24
45	Y	4202	LMT	C1'-O5'-C5'	2.35	118.30	113.69
48	F	501	FMN	N10-C10-N1	2.35	125.09	118.35
49	a	101	CDL	OA4-PA1-OA3	-2.34	100.66	112.24
43	Y	4203	3PE	C2-O21-C21	-2.34	113.54	117.90
46	N	2401	PLC	O3-CB-C1B	2.33	119.23	111.91
43	L	1006	3PE	O12-P-O14	-2.33	100.72	112.24
43	d	4603	3PE	O31-C31-C32	2.33	119.22	111.91
49	P	403	CDL	OB4-PB2-OB3	-2.32	100.78	112.24
43	Z	203	3PE	O31-C31-C32	2.32	119.18	111.91
49	M	501	CDL	OA4-PA1-OA3	-2.31	100.81	112.24
43	b	403	3PE	O12-P-O14	-2.31	100.81	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	O	401	CDL	OB8-CB7-C71	2.31	119.15	111.91
43	I	6301	3PE	O12-P-O14	-2.31	100.84	112.24
43	L	1006	3PE	O31-C31-C32	2.31	119.15	111.91
43	I	6301	3PE	O31-C31-C32	2.30	119.12	111.91
43	A	501	3PE	O31-C31-C32	2.29	119.10	111.91
46	d	4602	PLC	O2P-P-O1P	-2.29	100.91	112.24
43	d	4603	3PE	O12-P-O14	-2.29	100.91	112.24
46	L	1001	PLC	O2P-P-O1P	-2.28	100.97	112.24
43	M	504	3PE	O12-P-O14	-2.28	100.98	112.24
49	b	401	CDL	OB4-PB2-OB3	-2.27	101.01	112.24
43	Z	203	3PE	O12-P-O14	-2.27	101.02	112.24
49	O	401	CDL	OB4-PB2-OB3	-2.27	101.02	112.24
49	P	403	CDL	OA8-CA7-C31	2.27	119.02	111.91
46	D	501	PLC	O2P-P-O1P	-2.27	101.04	112.24
49	b	401	CDL	OA4-PA1-OA3	-2.26	101.04	112.24
43	M	502	3PE	O12-P-O14	-2.26	101.06	112.24
52	T	201	EHZ	O3-C12-N1	-2.26	118.76	123.01
43	A	501	3PE	O12-P-O14	-2.25	101.10	112.24
49	P	403	CDL	OA4-PA1-OA3	-2.24	101.16	112.24
49	M	501	CDL	OB8-CB7-C71	2.24	118.93	111.91
46	L	1002	PLC	O3-CB-C1B	2.23	118.92	111.91
45	Y	4204	LMT	C3B-C4B-C5B	-2.22	106.27	110.24
46	L	1002	PLC	O2P-P-O1P	-2.21	101.30	112.24
43	Z	202	3PE	O12-P-O14	-2.21	101.31	112.24
52	U	201	EHZ	C10-S1-C9	2.21	108.75	101.87
43	d	4601	3PE	O31-C31-C32	2.19	118.77	111.91
45	Y	4204	LMT	O5'-C5'-C6'	-2.16	101.07	106.44
49	a	101	CDL	OB4-PB2-OB3	-2.15	101.61	112.24
45	Y	4204	LMT	C1B-C2B-C3B	2.14	114.46	110.00
49	O	401	CDL	OA4-PA1-OA3	-2.14	101.66	112.24
49	a	101	CDL	OB8-CB7-C71	2.14	118.62	111.91
43	b	402	3PE	O12-P-O14	-2.14	101.67	112.24
52	T	201	EHZ	C14-N2-C15	-2.13	118.80	122.59
45	Y	4202	LMT	O5'-C1'-C2'	2.12	114.84	110.35
45	Y	4201	LMT	C2'-C3'-C4'	2.12	114.52	109.68
49	Z	201	CDL	OA4-PA1-OA3	-2.09	101.88	112.24
46	L	1007	PLC	O2P-P-O1P	-2.09	101.90	112.24
50	P	402	NDP	C5B-C4B-C3B	-2.09	107.37	115.18
52	U	201	EHZ	C13-C14-N2	-2.05	107.75	111.90
45	Y	4202	LMT	C1B-O5B-C5B	2.05	117.72	113.69
45	M	503	LMT	C1B-O5B-C5B	2.05	117.71	113.69
49	M	501	CDL	OB4-PB2-OB3	-2.03	102.21	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	T	201	EHZ	O2-C9-S1	-2.03	119.98	122.61
52	U	201	EHZ	O3-C12-N1	-2.02	119.19	123.01
43	A	502	3PE	P-O11-C1	-2.01	109.88	121.68

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	A	501	3PE	C2
43	H	602	3PE	C2
43	M	502	3PE	C2
43	Y	4203	3PE	C2
43	Z	202	3PE	C2
43	d	4603	3PE	C2
45	B	302	LMT	C5B
45	B	302	LMT	C2B
45	B	302	LMT	C4B
45	B	302	LMT	C1'
45	M	503	LMT	C5B
45	M	503	LMT	C2B
45	M	503	LMT	C4B
45	M	503	LMT	C1'
45	Y	4201	LMT	C5B
45	Y	4201	LMT	C2B
45	Y	4201	LMT	C4B
45	Y	4201	LMT	C1'
45	Y	4202	LMT	C5B
45	Y	4202	LMT	C2B
45	Y	4202	LMT	C4B
45	Y	4202	LMT	C1'
45	Y	4204	LMT	C5B
45	Y	4204	LMT	C2B
45	Y	4204	LMT	C4B
45	Y	4204	LMT	C1'
48	F	501	FMN	C3'
48	F	501	FMN	C2'
52	T	201	EHZ	C16
52	U	201	EHZ	C16

All (665) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	501	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
43	A	501	3PE	C11-O13-P-O14
43	A	501	3PE	O13-C11-C12-N
43	A	501	3PE	C22-C21-O21-C2
43	A	502	3PE	C1-O11-P-O14
43	H	602	3PE	C1-O11-P-O12
43	H	602	3PE	C1-O11-P-O14
43	H	602	3PE	C11-O13-P-O11
43	H	602	3PE	C11-O13-P-O12
43	H	602	3PE	C11-O13-P-O14
43	H	602	3PE	C22-C21-O21-C2
43	I	6301	3PE	C11-O13-P-O12
43	I	6301	3PE	C11-O13-P-O14
43	L	1003	3PE	C11-O13-P-O12
43	L	1003	3PE	C11-O13-P-O14
43	L	1003	3PE	O13-C11-C12-N
43	L	1004	3PE	C11-O13-P-O12
43	L	1004	3PE	C11-O13-P-O14
43	L	1005	3PE	O13-C11-C12-N
43	L	1005	3PE	O22-C21-O21-C2
43	L	1005	3PE	C22-C21-O21-C2
43	L	1006	3PE	O13-C11-C12-N
43	M	502	3PE	C1-O11-P-O12
43	M	502	3PE	C1-O11-P-O14
43	M	502	3PE	C12-C11-O13-P
43	M	502	3PE	O13-C11-C12-N
43	M	502	3PE	C22-C21-O21-C2
43	M	504	3PE	C1-O11-P-O14
43	M	504	3PE	O13-C11-C12-N
43	N	2402	3PE	C11-O13-P-O14
43	N	2402	3PE	C22-C21-O21-C2
43	Y	4203	3PE	C1-O11-P-O12
43	Y	4203	3PE	C1-O11-P-O14
43	Y	4203	3PE	O13-C11-C12-N
43	Y	4203	3PE	O32-C31-O31-C3
43	Y	4203	3PE	C22-C21-O21-C2
43	Z	202	3PE	C1-O11-P-O12
43	Z	202	3PE	C11-O13-P-O11
43	Z	202	3PE	C11-O13-P-O12
43	Z	202	3PE	C11-O13-P-O14
43	d	4601	3PE	C1-O11-P-O14
43	d	4601	3PE	C11-O13-P-O11
43	d	4601	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
43	d	4603	3PE	C1-O11-P-O14
43	d	4603	3PE	O13-C11-C12-N
45	M	503	LMT	C2'-C1'-O1'-C1
45	M	503	LMT	O5'-C1'-O1'-C1
45	Y	4202	LMT	O5'-C1'-O1'-C1
45	Y	4202	LMT	C2-C1-O1'-C1'
45	Y	4204	LMT	O5'-C1'-O1'-C1
46	D	501	PLC	O4P-C4-C5-N
46	D	501	PLC	C1-O3P-P-O1P
46	D	501	PLC	C1-O3P-P-O2P
46	D	501	PLC	C1-O3P-P-O4P
46	H	601	PLC	O3P-C1-C2-O2
46	H	601	PLC	O4P-C4-C5-N
46	H	601	PLC	C4-O4P-P-O1P
46	H	601	PLC	C4-O4P-P-O2P
46	L	1001	PLC	O4P-C4-C5-N
46	L	1001	PLC	C1-O3P-P-O1P
46	L	1001	PLC	C4-O4P-P-O1P
46	L	1001	PLC	C4-O4P-P-O2P
46	L	1001	PLC	C4-O4P-P-O3P
46	L	1007	PLC	O4P-C4-C5-N
46	L	1007	PLC	C1'-C'-O2-C2
46	L	1007	PLC	C1-O3P-P-O1P
46	L	1007	PLC	C1-O3P-P-O2P
46	N	2401	PLC	O4P-C4-C5-N
46	N	2401	PLC	C1'-C'-O2-C2
46	N	2401	PLC	O'-C'-O2-C2
46	P	401	PLC	O3P-C1-C2-O2
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	O3'-C3'-C4'-C5'
49	M	501	CDL	OA6-CA4-CA6-OA8
49	M	501	CDL	CB2-OB2-PB2-OB3
49	M	501	CDL	CB2-OB2-PB2-OB4
49	M	501	CDL	CB2-OB2-PB2-OB5
49	M	501	CDL	CB3-OB5-PB2-OB2
49	M	501	CDL	CB3-OB5-PB2-OB3
49	M	501	CDL	CB3-OB5-PB2-OB4
49	M	501	CDL	OB6-CB4-CB6-OB8
49	O	401	CDL	CA3-OA5-PA1-OA2
49	O	401	CDL	CA3-OA5-PA1-OA3
49	O	401	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
49	O	401	CDL	CB3-OB5-PB2-OB2
49	O	401	CDL	CB3-OB5-PB2-OB3
49	P	403	CDL	CA2-C1-CB2-OB2
49	Z	201	CDL	CA2-OA2-PA1-OA3
49	Z	201	CDL	CA2-OA2-PA1-OA4
49	Z	201	CDL	C11-CA5-OA6-CA4
49	Z	201	CDL	CB3-OB5-PB2-OB4
49	a	101	CDL	CA2-OA2-PA1-OA4
49	a	101	CDL	CA3-OA5-PA1-OA2
49	a	101	CDL	C11-CA5-OA6-CA4
49	a	101	CDL	CB2-OB2-PB2-OB3
49	b	401	CDL	OA7-CA5-OA6-CA4
49	b	401	CDL	C11-CA5-OA6-CA4
49	b	401	CDL	CB2-OB2-PB2-OB3
49	b	401	CDL	CB2-OB2-PB2-OB4
50	P	402	NDP	C5D-O5D-PN-O3
52	T	201	EHZ	C6-C7-C8-C9
52	T	201	EHZ	C12-C13-C14-N2
52	U	201	EHZ	O2-C9-S1-C10
52	U	201	EHZ	C8-C9-S1-C10
43	Y	4203	3PE	O22-C21-O21-C2
45	Y	4202	LMT	C3'-C4'-O1B-C1B
43	A	502	3PE	O32-C31-O31-C3
46	L	1002	PLC	OB-CB-O3-C3
43	A	502	3PE	C32-C31-O31-C3
43	Y	4203	3PE	C32-C31-O31-C3
46	H	601	PLC	OB-CB-O3-C3
46	N	2401	PLC	OB-CB-O3-C3
46	d	4602	PLC	OB-CB-O3-C3
49	P	403	CDL	OB9-CB7-OB8-CB6
43	A	501	3PE	O22-C21-O21-C2
43	H	602	3PE	O22-C21-O21-C2
43	N	2402	3PE	O22-C21-O21-C2
46	L	1001	PLC	O'-C'-O2-C2
46	L	1007	PLC	O'-C'-O2-C2
49	Z	201	CDL	OA7-CA5-OA6-CA4
43	Z	202	3PE	C32-C31-O31-C3
46	H	601	PLC	C1B-CB-O3-C3
46	L	1002	PLC	C1B-CB-O3-C3
46	N	2401	PLC	C1B-CB-O3-C3
46	d	4602	PLC	C1B-CB-O3-C3
49	P	403	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
46	L	1001	PLC	C1'-C'-O2-C2
43	M	502	3PE	O22-C21-O21-C2
49	a	101	CDL	OA7-CA5-OA6-CA4
49	M	501	CDL	O1-C1-CB2-OB2
49	P	403	CDL	O1-C1-CB2-OB2
43	L	1004	3PE	C32-C31-O31-C3
49	Z	201	CDL	C71-CB7-OB8-CB6
43	Z	202	3PE	O32-C31-O31-C3
43	d	4603	3PE	C22-C21-O21-C2
45	B	302	LMT	O5B-C5B-C6B-O6B
45	Y	4204	LMT	O5'-C5'-C6'-O6'
45	B	302	LMT	C4B-C5B-C6B-O6B
50	P	402	NDP	O4B-C4B-C5B-O5B
50	P	402	NDP	O4D-C4D-C5D-O5D
45	B	302	LMT	O5'-C5'-C6'-O6'
45	M	503	LMT	C4'-C5'-C6'-O6'
48	F	501	FMN	C2'-C3'-C4'-O4'
43	L	1004	3PE	O32-C31-O31-C3
49	Z	201	CDL	OB9-CB7-OB8-CB6
43	M	502	3PE	C32-C31-O31-C3
43	N	2402	3PE	C32-C31-O31-C3
45	M	503	LMT	O5B-C5B-C6B-O6B
48	F	501	FMN	C2'-C3'-C4'-C5'
46	L	1002	PLC	C1'-C'-O2-C2
49	O	401	CDL	C51-CB5-OB6-CB4
49	M	501	CDL	CA2-C1-CB2-OB2
49	a	101	CDL	CB2-C1-CA2-OA2
43	d	4603	3PE	O22-C21-O21-C2
45	Y	4204	LMT	C4'-C5'-C6'-O6'
43	N	2402	3PE	O32-C31-O31-C3
43	L	1003	3PE	C32-C31-O31-C3
43	b	402	3PE	C32-C31-O31-C3
43	d	4603	3PE	C32-C31-O31-C3
46	L	1007	PLC	C1B-CB-O3-C3
46	P	401	PLC	C1B-CB-O3-C3
49	O	401	CDL	C71-CB7-OB8-CB6
49	b	401	CDL	C71-CB7-OB8-CB6
45	M	503	LMT	C3'-C4'-O1B-C1B
49	a	101	CDL	O1-C1-CA2-OA2
45	Y	4202	LMT	C2'-C1'-O1'-C1
45	Y	4204	LMT	C2'-C1'-O1'-C1
43	M	502	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
49	O	401	CDL	OB9-CB7-OB8-CB6
45	M	503	LMT	O5'-C5'-C6'-O6'
43	I	6301	3PE	C22-C21-O21-C2
46	D	501	PLC	C'-C1'-C2'-C3'
43	L	1003	3PE	O32-C31-O31-C3
43	Z	202	3PE	C31-C32-C33-C34
43	N	2402	3PE	C21-C22-C23-C24
43	Z	202	3PE	C21-C22-C23-C24
46	P	401	PLC	C'-C1'-C2'-C3'
49	O	401	CDL	CB7-C71-C72-C73
50	P	402	NDP	C3B-C4B-C5B-O5B
49	M	501	CDL	C1-CB2-OB2-PB2
43	I	6301	3PE	C31-C32-C33-C34
43	b	402	3PE	O32-C31-O31-C3
46	L	1007	PLC	OB-CB-O3-C3
46	P	401	PLC	OB-CB-O3-C3
49	a	101	CDL	CB7-C71-C72-C73
43	d	4603	3PE	O32-C31-O31-C3
46	L	1002	PLC	O'-C'-O2-C2
49	O	401	CDL	OB7-CB5-OB6-CB4
49	Z	201	CDL	C31-CA7-OA8-CA6
49	b	401	CDL	OB9-CB7-OB8-CB6
46	L	1001	PLC	CB-C1B-C2B-C3B
45	Y	4204	LMT	O1'-C1-C2-C3
43	A	501	3PE	C1-O11-P-O13
43	A	502	3PE	C1-O11-P-O13
43	H	602	3PE	C1-O11-P-O13
43	I	6301	3PE	C11-O13-P-O11
43	L	1003	3PE	C1-O11-P-O13
43	L	1003	3PE	C11-O13-P-O11
43	L	1004	3PE	C11-O13-P-O11
43	L	1005	3PE	C1-O11-P-O13
43	L	1006	3PE	C1-O11-P-O13
43	M	502	3PE	C1-O11-P-O13
43	M	504	3PE	C1-O11-P-O13
43	N	2402	3PE	C11-O13-P-O11
43	Y	4203	3PE	C1-O11-P-O13
43	Z	202	3PE	C1-O11-P-O13
43	d	4603	3PE	C1-O11-P-O13
46	H	601	PLC	C4-O4P-P-O3P
46	L	1001	PLC	C1-O3P-P-O4P
46	L	1007	PLC	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
49	Z	201	CDL	CA2-OA2-PA1-OA5
49	Z	201	CDL	CA3-OA5-PA1-OA2
49	Z	201	CDL	CB3-OB5-PB2-OB2
49	a	101	CDL	CA2-OA2-PA1-OA5
49	b	401	CDL	CB2-OB2-PB2-OB5
43	I	6301	3PE	O22-C21-O21-C2
48	F	501	FMN	O3'-C3'-C4'-O4'
43	N	2402	3PE	C22-C23-C24-C25
46	d	4602	PLC	C1'-C'-O2-C2
43	A	502	3PE	C24-C25-C26-C27
43	I	6301	3PE	C35-C36-C37-C38
43	L	1004	3PE	C38-C39-C3A-C3B
43	L	1005	3PE	C2C-C2D-C2E-C2F
43	N	2402	3PE	C3A-C3B-C3C-C3D
43	b	402	3PE	C24-C25-C26-C27
49	M	501	CDL	C71-C72-C73-C74
46	N	2401	PLC	C4B-C5B-C6B-C7B
46	d	4602	PLC	O'-C'-O2-C2
45	Y	4201	LMT	C7-C8-C9-C10
45	Y	4204	LMT	C2-C3-C4-C5
43	Z	203	3PE	C29-C2A-C2B-C2C
45	B	302	LMT	C7-C8-C9-C10
45	Y	4202	LMT	C11-C10-C9-C8
46	N	2401	PLC	C3'-C4'-C5'-C6'
49	M	501	CDL	C14-C15-C16-C17
49	O	401	CDL	C60-C61-C62-C63
45	Y	4202	LMT	C7-C8-C9-C10
49	M	501	CDL	C54-C55-C56-C57
45	B	302	LMT	C4-C5-C6-C7
46	L	1001	PLC	C3B-C4B-C5B-C6B
46	P	401	PLC	C4'-C5'-C6'-C7'
43	L	1003	3PE	C2A-C2B-C2C-C2D
43	M	504	3PE	C2C-C2D-C2E-C2F
49	M	501	CDL	C17-C18-C19-C20
49	O	401	CDL	C55-C56-C57-C58
52	U	201	EHZ	C2-C1-C21-C22
43	A	502	3PE	C32-C33-C34-C35
43	I	6301	3PE	C23-C24-C25-C26
43	L	1004	3PE	C32-C33-C34-C35
43	L	1004	3PE	C37-C38-C39-C3A
49	Z	201	CDL	OA9-CA7-OA8-CA6
43	I	6301	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
43	L	1005	3PE	C2B-C2C-C2D-C2E
46	L	1007	PLC	C6'-C7'-C8'-C9'
43	b	402	3PE	C36-C37-C38-C39
49	M	501	CDL	C20-C21-C22-C23
43	L	1004	3PE	O13-C11-C12-N
43	Z	202	3PE	O13-C11-C12-N
43	L	1003	3PE	C3C-C3D-C3E-C3F
43	L	1004	3PE	C35-C36-C37-C38
43	N	2402	3PE	C25-C26-C27-C28
43	Z	203	3PE	C3A-C3B-C3C-C3D
43	b	402	3PE	C2D-C2E-C2F-C2G
46	H	601	PLC	C2'-C3'-C4'-C5'
49	M	501	CDL	C37-C38-C39-C40
46	L	1007	PLC	C'-C1'-C2'-C3'
49	Z	201	CDL	CA7-C31-C32-C33
43	A	502	3PE	C2A-C2B-C2C-C2D
43	I	6301	3PE	C32-C33-C34-C35
46	N	2401	PLC	C1'-C2'-C3'-C4'
46	N	2401	PLC	C1B-C2B-C3B-C4B
46	N	2401	PLC	C5B-C6B-C7B-C8B
43	N	2402	3PE	C36-C37-C38-C39
43	N	2402	3PE	C1-C2-C3-O31
43	L	1005	3PE	C3D-C3E-C3F-C3G
46	L	1007	PLC	C4'-C5'-C6'-C7'
49	M	501	CDL	C79-C80-C81-C82
43	A	502	3PE	C29-C2A-C2B-C2C
43	L	1004	3PE	C3B-C3C-C3D-C3E
49	P	403	CDL	C51-C52-C53-C54
49	M	501	CDL	C53-C54-C55-C56
49	M	501	CDL	C18-C19-C20-C21
43	N	2402	3PE	C34-C35-C36-C37
43	b	402	3PE	C33-C34-C35-C36
43	M	502	3PE	C35-C36-C37-C38
43	b	402	3PE	C29-C2A-C2B-C2C
46	D	501	PLC	C1B-CB-O3-C3
46	L	1001	PLC	C1B-CB-O3-C3
49	M	501	CDL	C71-CB7-OB8-CB6
45	M	503	LMT	C4B-C5B-C6B-O6B
43	A	502	3PE	C22-C21-O21-C2
43	L	1004	3PE	C22-C21-O21-C2
43	M	504	3PE	C22-C21-O21-C2
43	b	403	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
49	M	501	CDL	C22-C23-C24-C25
49	a	101	CDL	C32-C33-C34-C35
46	N	2401	PLC	C6'-C7'-C8'-C9'
43	L	1005	3PE	C28-C29-C2A-C2B
45	Y	4204	LMT	C4-C5-C6-C7
49	M	501	CDL	OB9-CB7-OB8-CB6
49	a	101	CDL	C71-CB7-OB8-CB6
46	N	2401	PLC	C7B-C8B-C9B-CAA
43	Z	202	3PE	C33-C34-C35-C36
45	Y	4202	LMT	C5-C6-C7-C8
45	Y	4201	LMT	C3-C4-C5-C6
43	Z	202	3PE	C22-C21-O21-C2
43	d	4601	3PE	C22-C21-O21-C2
49	a	101	CDL	C51-CB5-OB6-CB4
49	b	401	CDL	C51-CB5-OB6-CB4
43	A	502	3PE	O22-C21-O21-C2
43	M	504	3PE	O22-C21-O21-C2
43	Z	202	3PE	O22-C21-O21-C2
43	b	403	3PE	O22-C21-O21-C2
45	Y	4202	LMT	C3-C4-C5-C6
49	O	401	CDL	C62-C63-C64-C65
46	D	501	PLC	OB-CB-O3-C3
46	L	1001	PLC	OB-CB-O3-C3
43	d	4601	3PE	O22-C21-O21-C2
49	b	401	CDL	OB7-CB5-OB6-CB4
43	A	501	3PE	C11-O13-P-O11
46	D	501	PLC	C4-O4P-P-O3P
46	N	2401	PLC	C1-O3P-P-O4P
49	P	403	CDL	CA3-OA5-PA1-OA2
43	Z	203	3PE	O11-C1-C2-C3
46	H	601	PLC	O3P-C1-C2-C3
46	P	401	PLC	O3P-C1-C2-C3
49	P	403	CDL	OB5-CB3-CB4-CB6
49	Z	201	CDL	OB5-CB3-CB4-CB6
49	a	101	CDL	OB5-CB3-CB4-CB6
49	M	501	CDL	C35-C36-C37-C38
45	B	302	LMT	C4'-C5'-C6'-O6'
49	Z	201	CDL	CB2-C1-CA2-OA2
43	L	1004	3PE	O22-C21-O21-C2
43	L	1003	3PE	C38-C39-C3A-C3B
43	N	2402	3PE	C26-C27-C28-C29
43	N	2402	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
49	Z	201	CDL	C52-C53-C54-C55
43	d	4601	3PE	C21-C22-C23-C24
43	H	602	3PE	C1-C2-C3-O31
43	L	1005	3PE	C1-C2-C3-O31
43	L	1006	3PE	C1-C2-C3-O31
43	M	504	3PE	C1-C2-C3-O31
46	L	1001	PLC	C1-C2-C3-O3
46	L	1002	PLC	C1-C2-C3-O3
49	M	501	CDL	CB3-CB4-CB6-OB8
49	O	401	CDL	CA3-CA4-CA6-OA8
49	b	401	CDL	CB3-CB4-CB6-OB8
45	M	503	LMT	C9-C10-C11-C12
43	A	502	3PE	C37-C38-C39-C3A
43	A	501	3PE	C34-C35-C36-C37
45	M	503	LMT	C5'-C4'-O1B-C1B
43	A	502	3PE	C34-C35-C36-C37
43	L	1005	3PE	C29-C2A-C2B-C2C
43	N	2402	3PE	C23-C24-C25-C26
52	T	201	EHZ	C3-C4-C5-C6
50	P	402	NDP	C3D-C4D-C5D-O5D
45	B	302	LMT	C9-C10-C11-C12
43	b	403	3PE	C32-C31-O31-C3
43	M	502	3PE	C38-C39-C3A-C3B
43	b	403	3PE	C33-C34-C35-C36
49	a	101	CDL	OB9-CB7-OB8-CB6
43	I	6301	3PE	C27-C28-C29-C2A
43	N	2402	3PE	C3F-C3G-C3H-C3I
49	M	501	CDL	C74-C75-C76-C77
49	O	401	CDL	OB5-CB3-CB4-OB6
49	M	501	CDL	CB7-C71-C72-C73
46	H	601	PLC	C'-C1'-C2'-C3'
43	Z	203	3PE	C37-C38-C39-C3A
49	b	401	CDL	C11-C12-C13-C14
49	a	101	CDL	OB7-CB5-OB6-CB4
43	A	501	3PE	C32-C33-C34-C35
43	N	2402	3PE	C2B-C2C-C2D-C2E
43	N	2402	3PE	C3E-C3F-C3G-C3H
52	U	201	EHZ	C5-C6-C7-C8
43	N	2402	3PE	C2F-C2G-C2H-C2I
45	Y	4204	LMT	C11-C10-C9-C8
43	b	403	3PE	C21-C22-C23-C24
49	O	401	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
45	M	503	LMT	C6-C7-C8-C9
43	Y	4203	3PE	O11-C1-C2-C3
46	L	1007	PLC	O3P-C1-C2-C3
46	d	4602	PLC	O3P-C1-C2-C3
49	P	403	CDL	OA5-CA3-CA4-CA6
45	Y	4201	LMT	C2-C3-C4-C5
52	U	201	EHZ	C2-C3-C4-C5
43	b	403	3PE	O32-C31-O31-C3
43	M	504	3PE	C29-C2A-C2B-C2C
48	F	501	FMN	O2'-C2'-C3'-C4'
45	Y	4204	LMT	C3'-C4'-O1B-C1B
49	O	401	CDL	C56-C57-C58-C59
43	L	1003	3PE	C37-C38-C39-C3A
49	M	501	CDL	C1-CA2-OA2-PA1
49	P	403	CDL	CB4-CB3-OB5-PB2
45	B	302	LMT	C2-C1-O1'-C1'
46	L	1001	PLC	C1'-C2'-C3'-C4'
43	M	502	3PE	C1-C2-C3-O31
49	M	501	CDL	CA3-CA4-CA6-OA8
49	P	403	CDL	CB3-CB4-CB6-OB8
45	B	302	LMT	C2-C3-C4-C5
49	M	501	CDL	C51-C52-C53-C54
49	M	501	CDL	C11-C12-C13-C14
49	O	401	CDL	C64-C65-C66-C67
49	Z	201	CDL	CB2-OB2-PB2-OB5
43	L	1005	3PE	C27-C28-C29-C2A
43	N	2402	3PE	C38-C39-C3A-C3B
49	P	403	CDL	OA5-CA3-CA4-OA6
49	P	403	CDL	OB5-CB3-CB4-OB6
49	b	401	CDL	OA5-CA3-CA4-OA6
49	a	101	CDL	CA5-C11-C12-C13
49	Z	201	CDL	O1-C1-CA2-OA2
43	L	1003	3PE	C33-C34-C35-C36
43	M	504	3PE	C22-C23-C24-C25
46	L	1002	PLC	C4B-C5B-C6B-C7B
52	U	201	EHZ	C5-C6-C7-O1
43	A	501	3PE	O21-C2-C3-O31
43	H	602	3PE	O21-C2-C3-O31
43	M	504	3PE	O21-C2-C3-O31
46	L	1002	PLC	O2-C2-C3-O3
46	H	601	PLC	C1'-C'-O2-C2
45	M	503	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
43	b	402	3PE	C2B-C2C-C2D-C2E
43	d	4603	3PE	C22-C23-C24-C25
46	H	601	PLC	O'-C'-O2-C2
49	M	501	CDL	CA4-CA3-OA5-PA1
43	N	2402	3PE	C33-C34-C35-C36
46	D	501	PLC	C1'-C'-O2-C2
43	b	402	3PE	C31-C32-C33-C34
43	b	403	3PE	C31-C32-C33-C34
43	d	4603	3PE	C21-C22-C23-C24
50	P	402	NDP	PA-O3-PN-O5D
46	L	1007	PLC	C1'-C2'-C3'-C4'
46	N	2401	PLC	O3P-C1-C2-C3
49	b	401	CDL	OA5-CA3-CA4-CA6
49	P	403	CDL	C33-C34-C35-C36
49	M	501	CDL	C12-C13-C14-C15
46	D	501	PLC	O'-C'-O2-C2
43	L	1006	3PE	C26-C27-C28-C29
46	P	401	PLC	C6'-C7'-C8'-C9'
43	L	1004	3PE	C2E-C2F-C2G-C2H
45	M	503	LMT	C2-C3-C4-C5
49	b	401	CDL	C72-C73-C74-C75
43	L	1005	3PE	C32-C33-C34-C35
46	L	1002	PLC	C1B-C2B-C3B-C4B
43	Z	203	3PE	C3-C2-O21-C21
43	M	502	3PE	C32-C33-C34-C35
43	A	501	3PE	C1-C2-C3-O31
49	a	101	CDL	CA4-CA3-OA5-PA1
43	A	501	3PE	O11-C1-C2-O21
43	L	1005	3PE	O11-C1-C2-O21
43	Y	4203	3PE	O11-C1-C2-O21
43	Z	203	3PE	O11-C1-C2-O21
43	d	4603	3PE	O11-C1-C2-O21
46	L	1007	PLC	O3P-C1-C2-O2
46	N	2401	PLC	O3P-C1-C2-O2
46	d	4602	PLC	O3P-C1-C2-O2
43	A	501	3PE	O21-C21-C22-C23
43	L	1004	3PE	C3E-C3F-C3G-C3H
43	L	1005	3PE	O21-C2-C3-O31
43	L	1006	3PE	O21-C2-C3-O31
43	N	2402	3PE	O21-C2-C3-O31
49	O	401	CDL	OA6-CA4-CA6-OA8
49	P	403	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
49	b	401	CDL	OB6-CB4-CB6-OB8
46	L	1007	PLC	C3B-C4B-C5B-C6B
45	Y	4204	LMT	C5'-C4'-O1B-C1B
43	I	6301	3PE	C1-O11-P-O13
43	L	1006	3PE	C11-O13-P-O11
49	M	501	CDL	CA2-OA2-PA1-OA5
49	P	403	CDL	CA2-OA2-PA1-OA5
43	A	501	3PE	C1-O11-P-O12
43	A	502	3PE	C11-O13-P-O14
43	L	1003	3PE	C1-O11-P-O12
43	L	1003	3PE	C1-O11-P-O14
43	L	1005	3PE	C1-O11-P-O12
43	L	1006	3PE	C1-O11-P-O12
43	L	1006	3PE	C1-O11-P-O14
43	L	1006	3PE	C11-O13-P-O12
43	M	502	3PE	C11-O13-P-O14
43	M	504	3PE	C1-O11-P-O12
43	N	2402	3PE	C11-O13-P-O12
43	Z	202	3PE	C1-O11-P-O14
43	d	4603	3PE	C1-O11-P-O12
43	d	4603	3PE	C11-O13-P-O12
46	L	1002	PLC	C4-O4P-P-O1P
49	M	501	CDL	CA3-OA5-PA1-OA3
49	O	401	CDL	CA2-OA2-PA1-OA3
49	P	403	CDL	CA3-OA5-PA1-OA3
49	Z	201	CDL	CA3-OA5-PA1-OA3
49	Z	201	CDL	CB3-OB5-PB2-OB3
49	a	101	CDL	CA2-OA2-PA1-OA3
49	a	101	CDL	CB3-OB5-PB2-OB3
50	P	402	NDP	C5D-O5D-PN-O2N
43	d	4603	3PE	O11-C1-C2-C3
46	L	1007	PLC	C7B-C8B-C9B-CAA
49	a	101	CDL	C34-C35-C36-C37
43	L	1003	3PE	C27-C28-C29-C2A
43	I	6301	3PE	C2B-C2C-C2D-C2E
43	L	1005	3PE	O31-C31-C32-C33
49	Z	201	CDL	OB5-CB3-CB4-OB6
49	a	101	CDL	OB5-CB3-CB4-OB6
43	M	504	3PE	C32-C33-C34-C35
46	d	4602	PLC	O4P-C4-C5-N
43	M	502	3PE	O21-C2-C3-O31
52	U	201	EHZ	C21-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
43	I	6301	3PE	C33-C34-C35-C36
46	L	1007	PLC	C7'-C8'-C9'-CA'
49	a	101	CDL	CA7-C31-C32-C33
43	M	504	3PE	C2B-C2C-C2D-C2E
43	Z	202	3PE	C24-C25-C26-C27
45	Y	4201	LMT	C1-C2-C3-C4
43	N	2402	3PE	C1-C2-O21-C21
43	d	4601	3PE	C3-C2-O21-C21
43	A	501	3PE	O11-C1-C2-C3
49	O	401	CDL	OB5-CB3-CB4-CB6
43	L	1004	3PE	C23-C24-C25-C26
43	d	4603	3PE	C23-C24-C25-C26
43	Z	202	3PE	C22-C23-C24-C25
43	b	403	3PE	C1-O11-P-O13
46	P	401	PLC	C4-O4P-P-O3P
46	d	4602	PLC	C4-O4P-P-O3P
49	P	403	CDL	CB3-OB5-PB2-OB2
43	L	1005	3PE	C2E-C2F-C2G-C2H
43	Z	203	3PE	C31-C32-C33-C34
49	O	401	CDL	C12-C13-C14-C15
49	b	401	CDL	C1-CA2-OA2-PA1
43	Z	203	3PE	C33-C34-C35-C36
49	Z	201	CDL	C33-C34-C35-C36
52	U	201	EHZ	C1-C2-C3-C4
52	T	201	EHZ	O4-C15-C16-C17
43	L	1003	3PE	C32-C33-C34-C35
43	L	1004	3PE	C3D-C3E-C3F-C3G
49	P	403	CDL	C31-CA7-OA8-CA6
43	L	1006	3PE	C22-C23-C24-C25
52	U	201	EHZ	S1-C10-C11-N1
43	Z	203	3PE	O22-C21-O21-C2
46	d	4602	PLC	O2-C'-C1'-C2'
43	L	1004	3PE	C33-C34-C35-C36
43	Y	4203	3PE	C32-C33-C34-C35
49	M	501	CDL	C75-C76-C77-C78
50	P	402	NDP	O4D-C1D-N1N-C6N
46	L	1007	PLC	C2'-C3'-C4'-C5'
43	L	1003	3PE	C2C-C2D-C2E-C2F
46	P	401	PLC	C1'-C2'-C3'-C4'
43	H	602	3PE	C22-C23-C24-C25
43	L	1005	3PE	C3B-C3C-C3D-C3E
52	T	201	EHZ	N2-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
43	L	1004	3PE	C1-C2-O21-C21
43	L	1005	3PE	C3-C2-O21-C21
46	L	1001	PLC	C1-C2-O2-C'
49	a	101	CDL	CA3-CA4-OA6-CA5
49	P	403	CDL	OA9-CA7-OA8-CA6
46	D	501	PLC	C2'-C3'-C4'-C5'
49	Z	201	CDL	C11-C12-C13-C14
45	Y	4202	LMT	C4B-C5B-C6B-O6B
43	L	1004	3PE	C28-C29-C2A-C2B
45	Y	4204	LMT	C5-C6-C7-C8
43	M	504	3PE	C27-C28-C29-C2A
49	P	403	CDL	CA5-C11-C12-C13
43	Z	203	3PE	C26-C27-C28-C29
49	Z	201	CDL	C14-C15-C16-C17
52	T	201	EHZ	C11-C10-S1-C9
52	U	201	EHZ	C11-C10-S1-C9
49	O	401	CDL	CB2-C1-CA2-OA2
43	I	6301	3PE	C37-C38-C39-C3A
43	N	2402	3PE	C2-C1-O11-P
46	N	2401	PLC	C2-C1-O3P-P
48	F	501	FMN	O2'-C2'-C3'-O3'
45	M	503	LMT	O1'-C1-C2-C3
49	M	501	CDL	C55-C56-C57-C58
49	Z	201	CDL	C12-C13-C14-C15
43	A	502	3PE	C2E-C2F-C2G-C2H
46	L	1001	PLC	C5B-C6B-C7B-C8B
43	L	1004	3PE	C2A-C2B-C2C-C2D
49	P	403	CDL	C72-C71-CB7-OB8
45	Y	4202	LMT	O1'-C1-C2-C3
46	L	1001	PLC	O2-C2-C3-O3
43	b	402	3PE	O31-C31-C32-C33
43	A	502	3PE	C33-C34-C35-C36
45	Y	4202	LMT	C4-C5-C6-C7
43	L	1005	3PE	C11-O13-P-O11
43	M	502	3PE	C11-O13-P-O11
49	b	401	CDL	CA2-OA2-PA1-OA5
43	L	1004	3PE	C36-C37-C38-C39
43	L	1005	3PE	C34-C35-C36-C37
50	P	402	NDP	C2D-C1D-N1N-C6N
49	P	403	CDL	C72-C71-CB7-OB9
49	Z	201	CDL	C13-C14-C15-C16
43	A	502	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
43	M	502	3PE	O31-C31-C32-C33
49	Z	201	CDL	C32-C31-CA7-OA8
45	Y	4204	LMT	C9-C10-C11-C12
43	L	1004	3PE	C3F-C3G-C3H-C3I
43	A	502	3PE	C2C-C2D-C2E-C2F
43	L	1003	3PE	C22-C23-C24-C25
49	Z	201	CDL	C12-C11-CA5-OA6
43	d	4603	3PE	C25-C26-C27-C28
43	L	1005	3PE	C33-C34-C35-C36
46	N	2401	PLC	C7'-C8'-C9'-CA'
43	M	504	3PE	O32-C31-O31-C3
43	A	502	3PE	O31-C31-C32-C33
43	Z	203	3PE	O31-C31-C32-C33
43	M	504	3PE	C24-C25-C26-C27
52	T	201	EHZ	O1-C7-C8-C9
52	U	201	EHZ	O1-C7-C8-C9
43	L	1004	3PE	O31-C31-C32-C33
43	I	6301	3PE	C34-C35-C36-C37
43	L	1005	3PE	O11-C1-C2-C3
49	a	101	CDL	C72-C71-CB7-OB8
43	I	6301	3PE	C28-C29-C2A-C2B
49	O	401	CDL	C52-C53-C54-C55
49	P	403	CDL	OB7-CB5-OB6-CB4
43	L	1006	3PE	C21-C22-C23-C24
43	L	1003	3PE	O31-C31-C32-C33
49	M	501	CDL	C52-C51-CB5-OB6
43	Z	203	3PE	C22-C21-O21-C2
43	Z	202	3PE	C25-C26-C27-C28
49	O	401	CDL	OA9-CA7-OA8-CA6
49	P	403	CDL	C12-C11-CA5-OA6
49	Z	201	CDL	C72-C71-CB7-OB8
45	Y	4204	LMT	C3-C4-C5-C6
49	M	501	CDL	CB5-C51-C52-C53
49	O	401	CDL	C31-CA7-OA8-CA6
46	L	1007	PLC	C2B-C3B-C4B-C5B
43	A	501	3PE	C21-C22-C23-C24
43	M	504	3PE	C32-C31-O31-C3
43	Z	203	3PE	C24-C25-C26-C27
43	L	1004	3PE	C31-C32-C33-C34
43	A	502	3PE	C11-O13-P-O11
43	A	502	3PE	O32-C31-C32-C33
49	M	501	CDL	C52-C51-CB5-OB7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
49	Z	201	CDL	C12-C11-CA5-OA7
49	Z	201	CDL	C32-C31-CA7-OA9
46	N	2401	PLC	C1-O3P-P-O1P
49	M	501	CDL	CA2-OA2-PA1-OA3
49	P	403	CDL	CA2-OA2-PA1-OA3
49	b	401	CDL	CA2-OA2-PA1-OA4
49	b	401	CDL	CA3-OA5-PA1-OA3
43	L	1004	3PE	O32-C31-C32-C33
43	M	502	3PE	O32-C31-C32-C33
43	Z	203	3PE	O32-C31-C32-C33
43	b	402	3PE	O32-C31-C32-C33
49	P	403	CDL	C12-C11-CA5-OA7
43	b	403	3PE	O11-C1-C2-C3
43	N	2402	3PE	C32-C33-C34-C35
43	b	402	3PE	C25-C26-C27-C28
43	L	1004	3PE	C12-C11-O13-P
43	Z	202	3PE	C12-C11-O13-P
43	d	4601	3PE	C12-C11-O13-P
46	L	1001	PLC	C5-C4-O4P-P
43	L	1005	3PE	C31-C32-C33-C34
43	L	1005	3PE	C35-C36-C37-C38
46	L	1007	PLC	O2-C'-C1'-C2'
43	Y	4203	3PE	C2-C1-O11-P
45	Y	4202	LMT	O5B-C1B-O1B-C4'
46	L	1002	PLC	O2-C'-C1'-C2'
46	L	1007	PLC	O'-C'-C1'-C2'
49	Z	201	CDL	C72-C71-CB7-OB9
49	a	101	CDL	C72-C71-CB7-OB9
49	Z	201	CDL	C15-C16-C17-C18
46	D	501	PLC	O2-C'-C1'-C2'
43	d	4603	3PE	C24-C25-C26-C27
43	Y	4203	3PE	O31-C31-C32-C33
45	Y	4202	LMT	C2B-C1B-O1B-C4'
43	L	1003	3PE	O32-C31-C32-C33

There are no ring outliers.

12 monomers are involved in 16 short contacts:

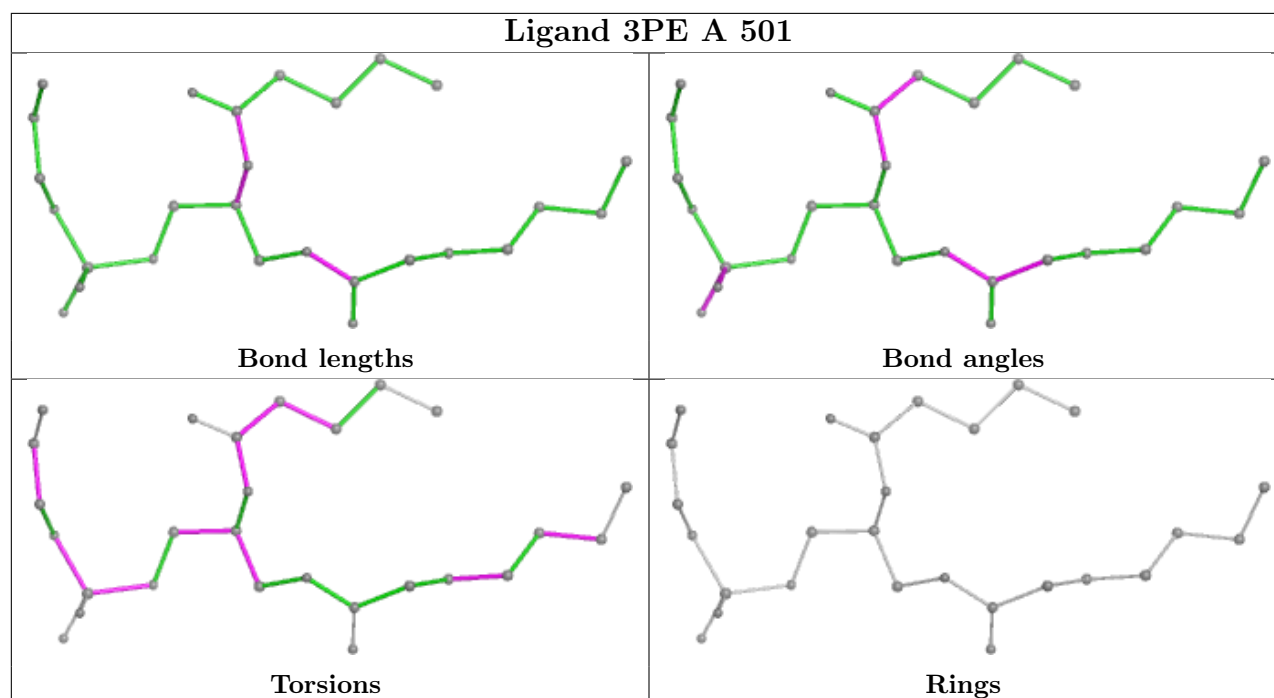
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	Z	201	CDL	1	0
52	U	201	EHZ	2	0
46	L	1007	PLC	2	0

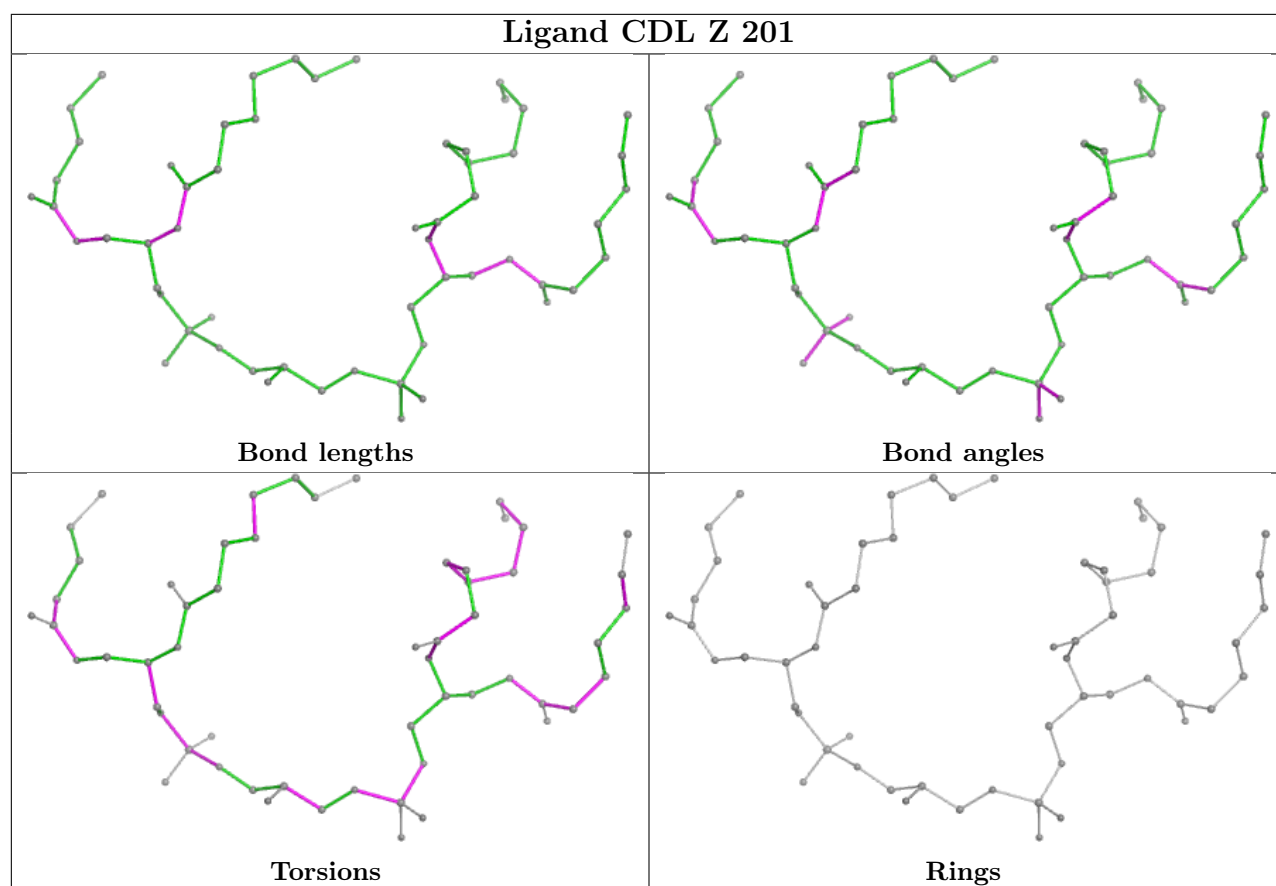
*Continued on next page...*

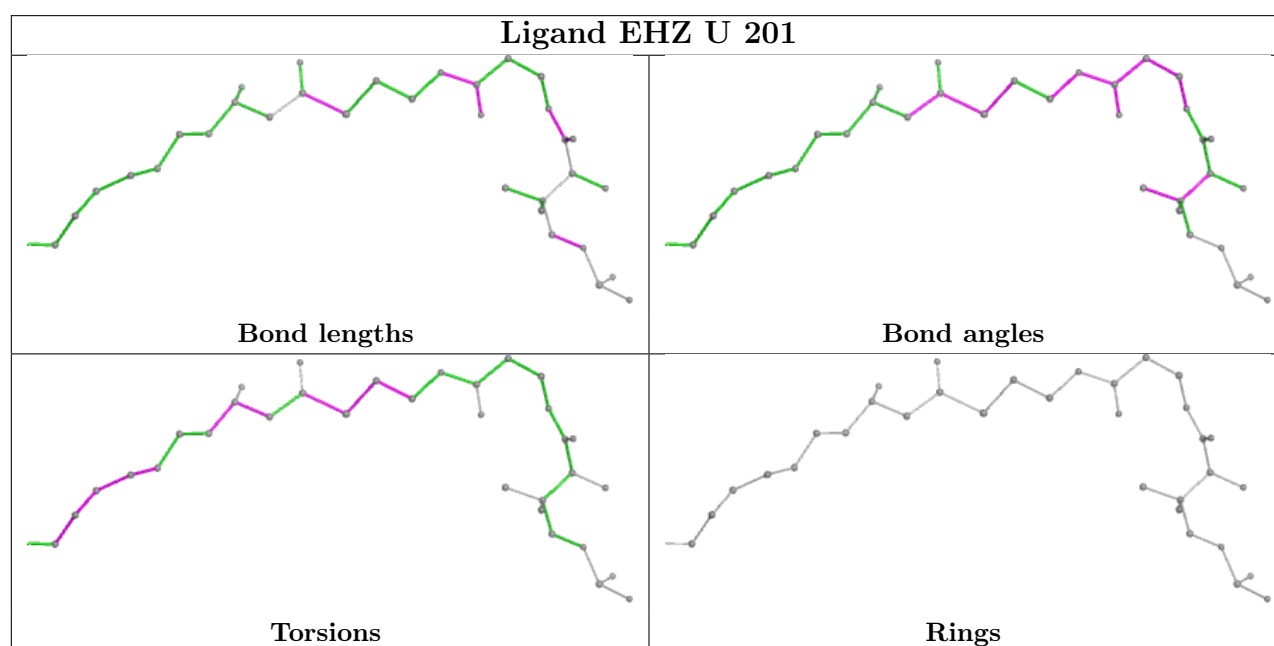
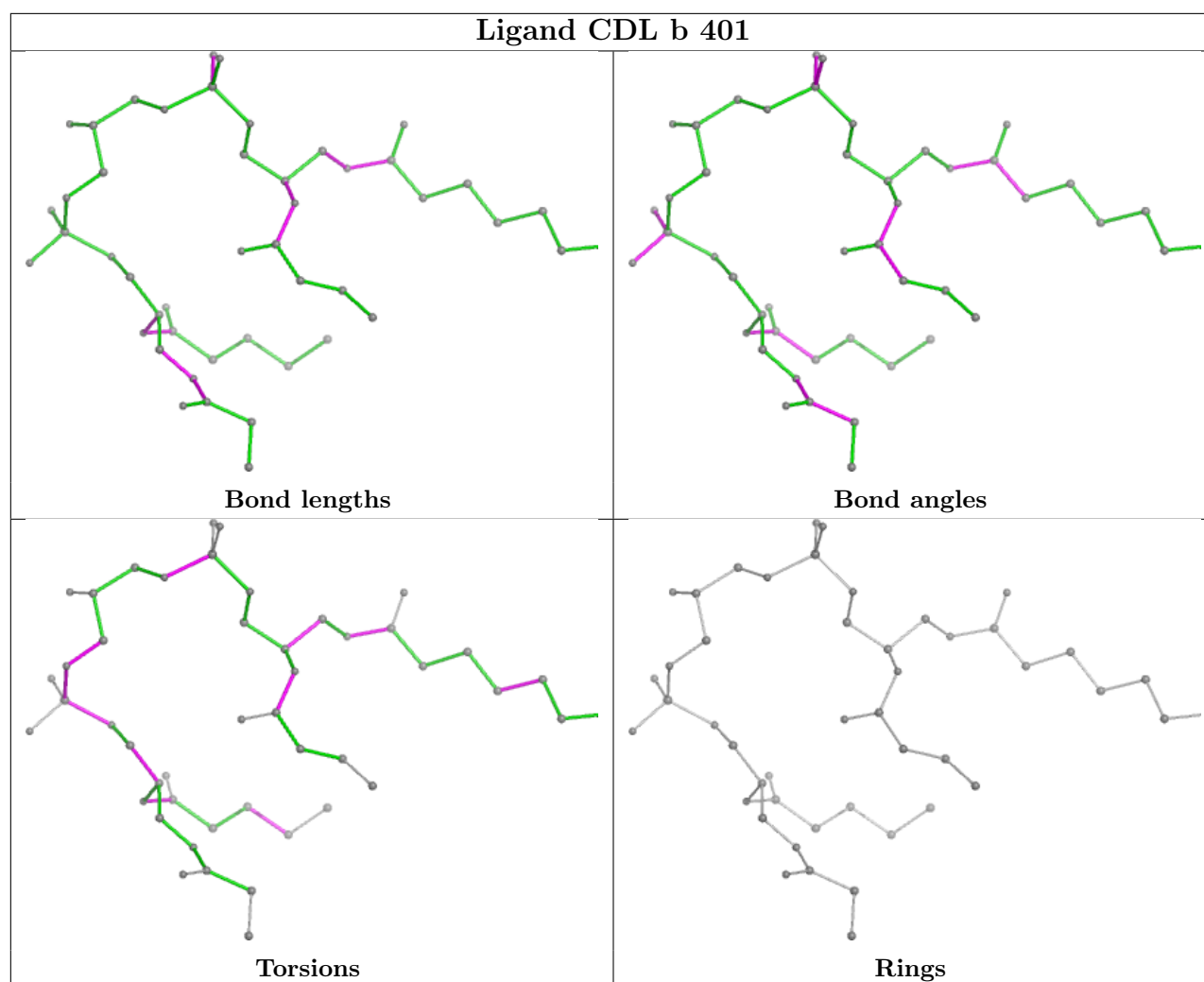
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	O	401	CDL	2	0
52	T	201	EHZ	2	0
43	M	504	3PE	1	0
49	M	501	CDL	1	0
46	L	1001	PLC	1	0
47	E	301	FES	1	0
43	L	1003	3PE	1	0
43	N	2402	3PE	1	0
43	I	6301	3PE	1	0

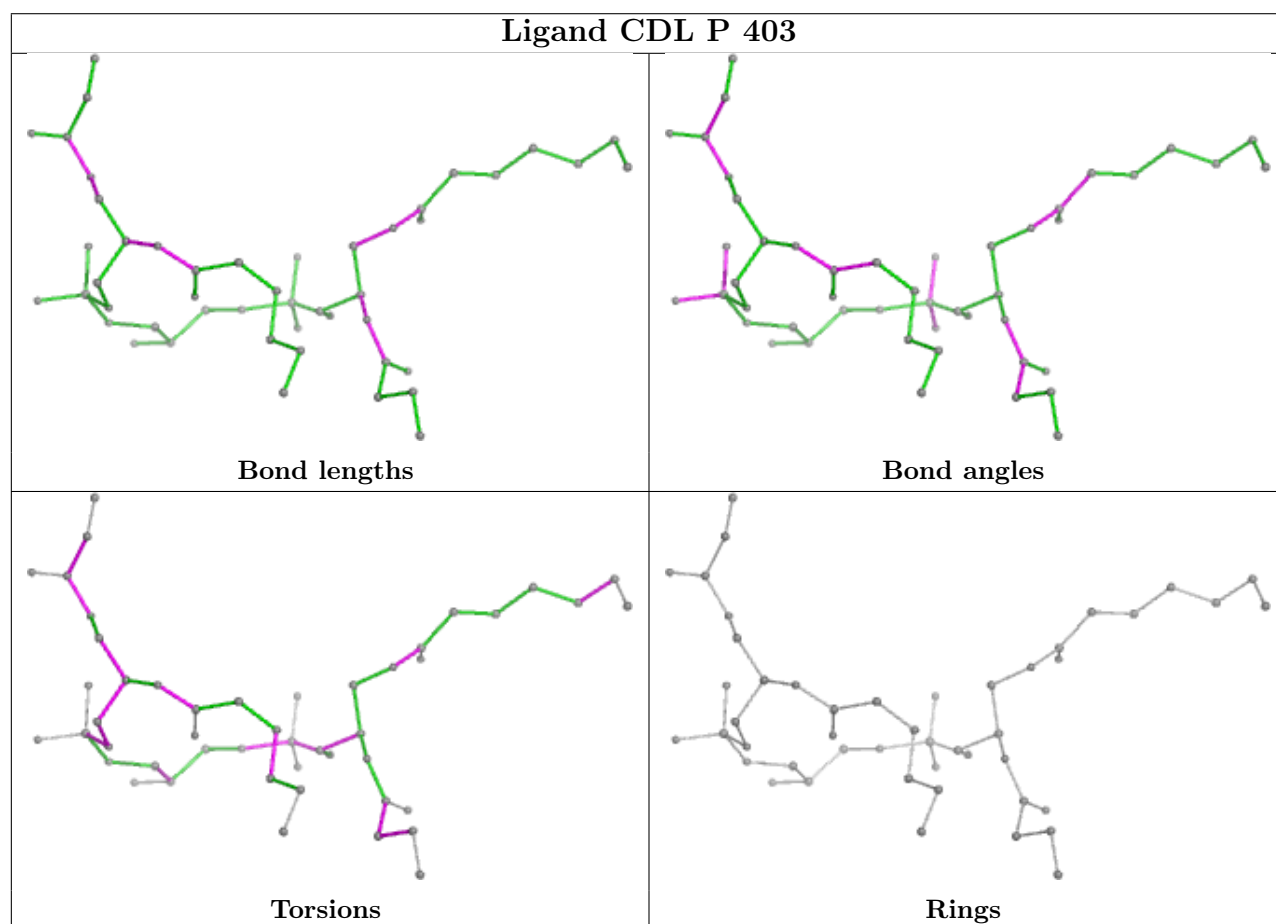
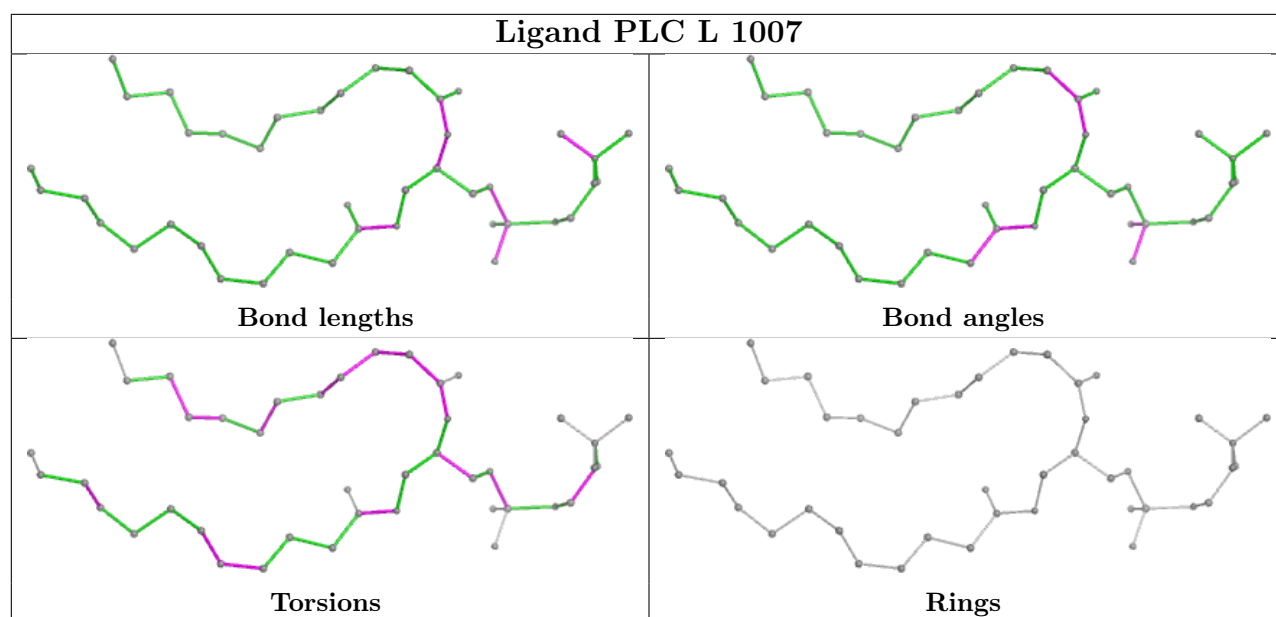
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

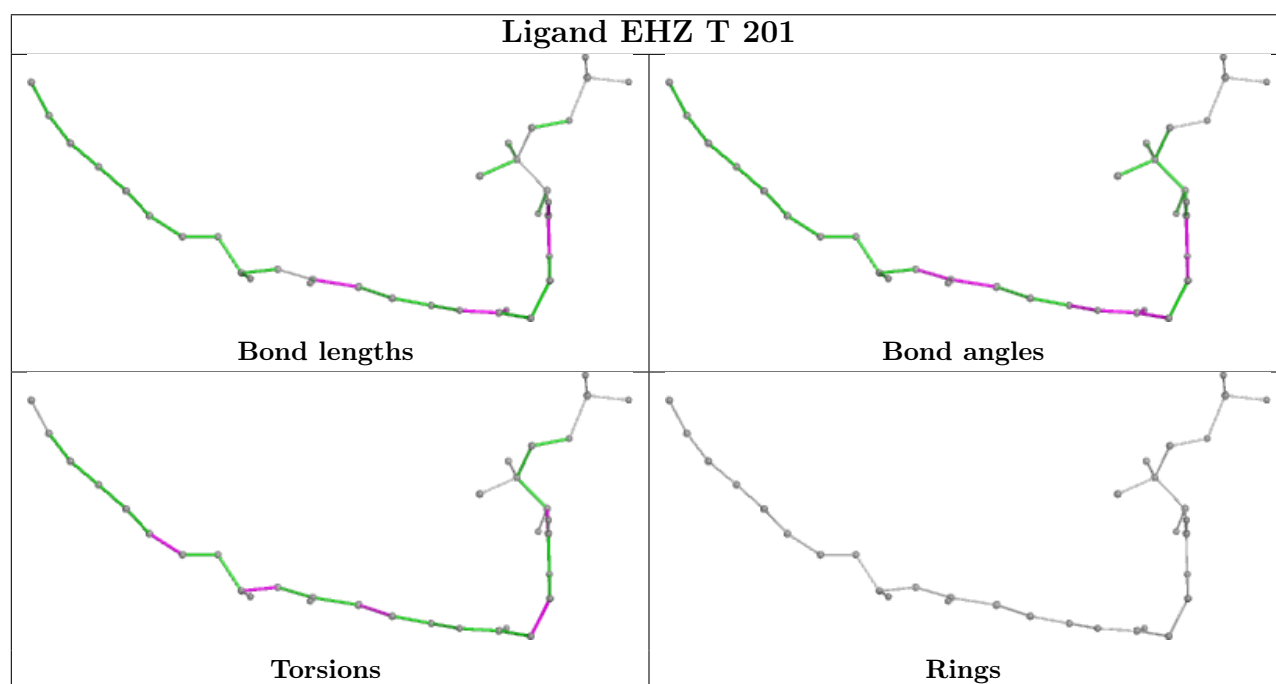
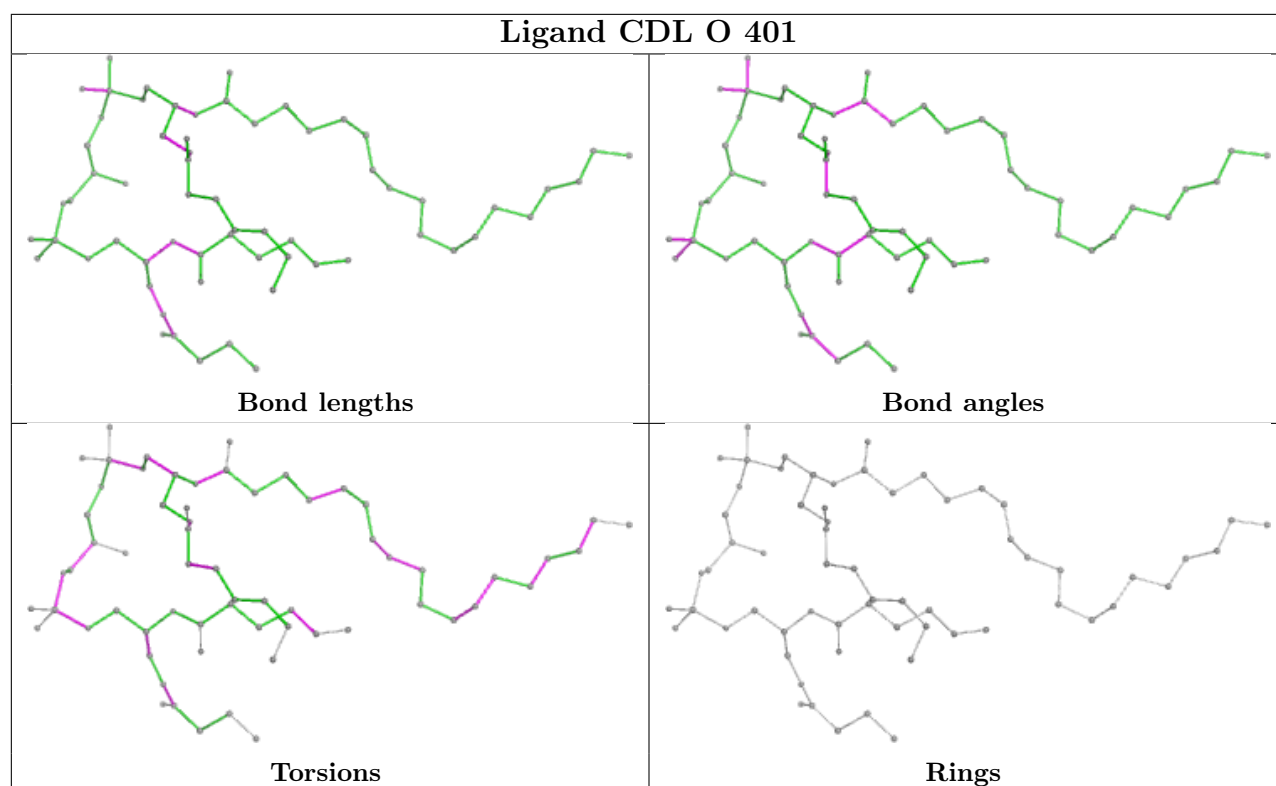


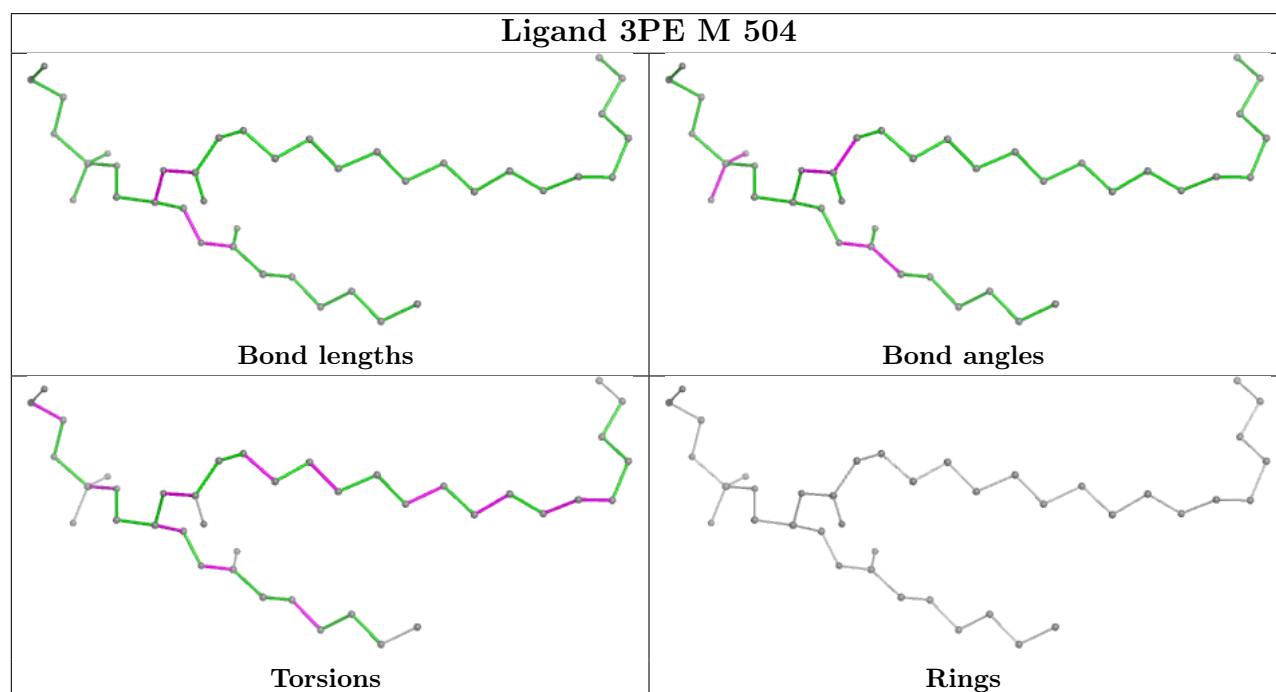
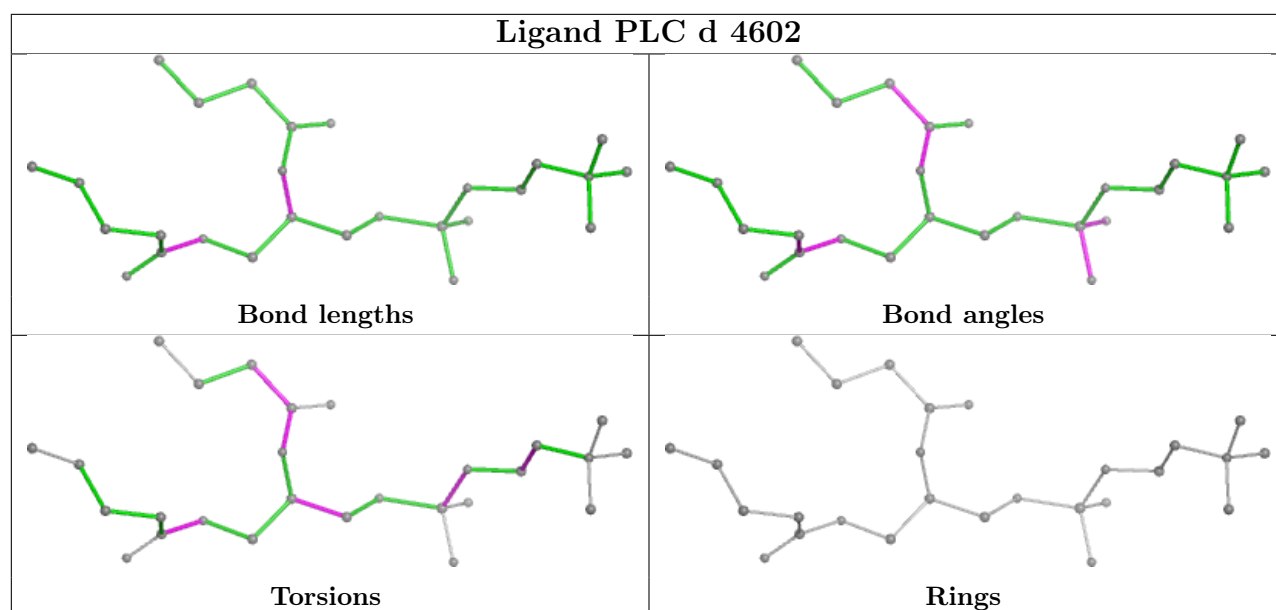


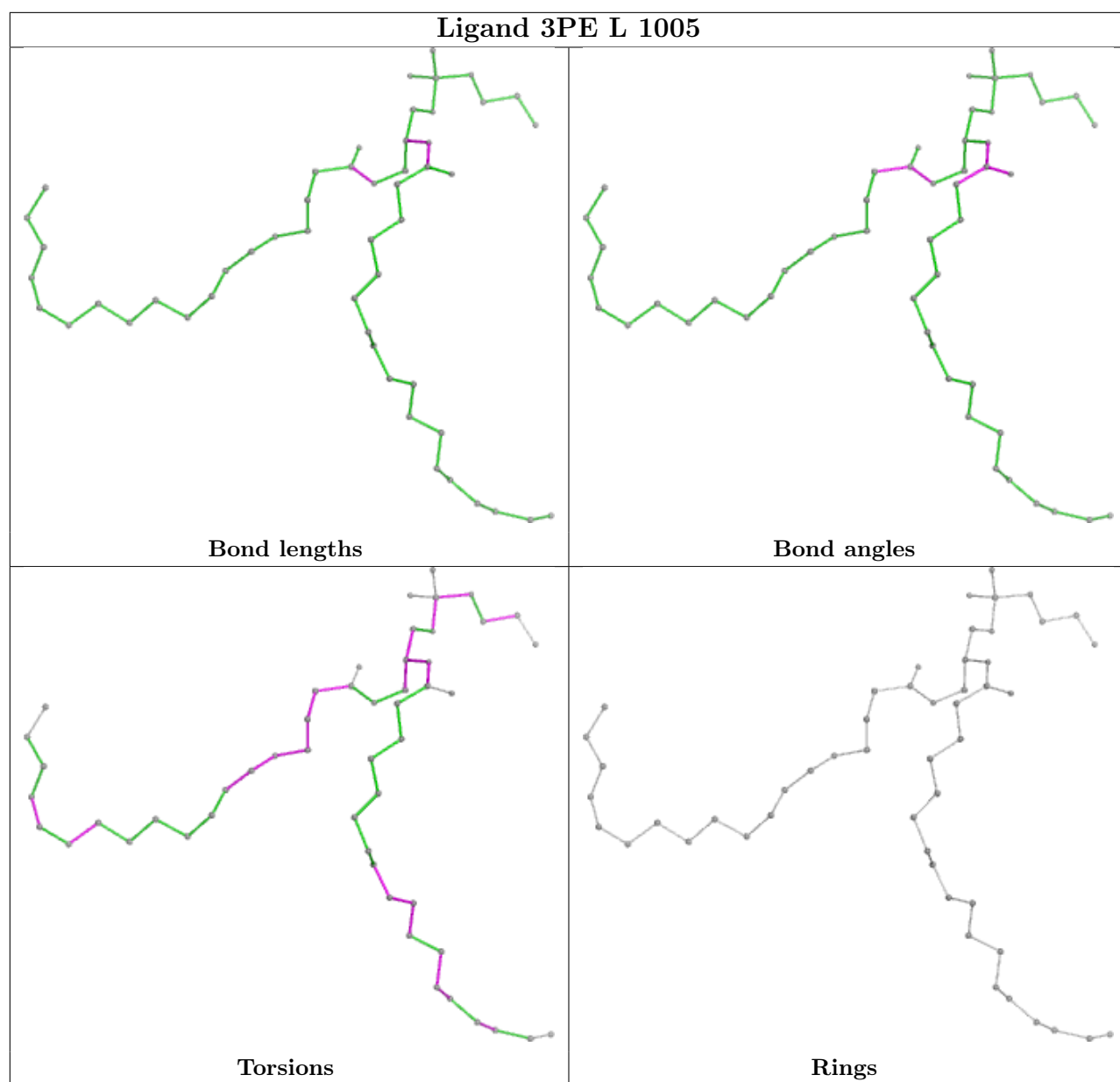


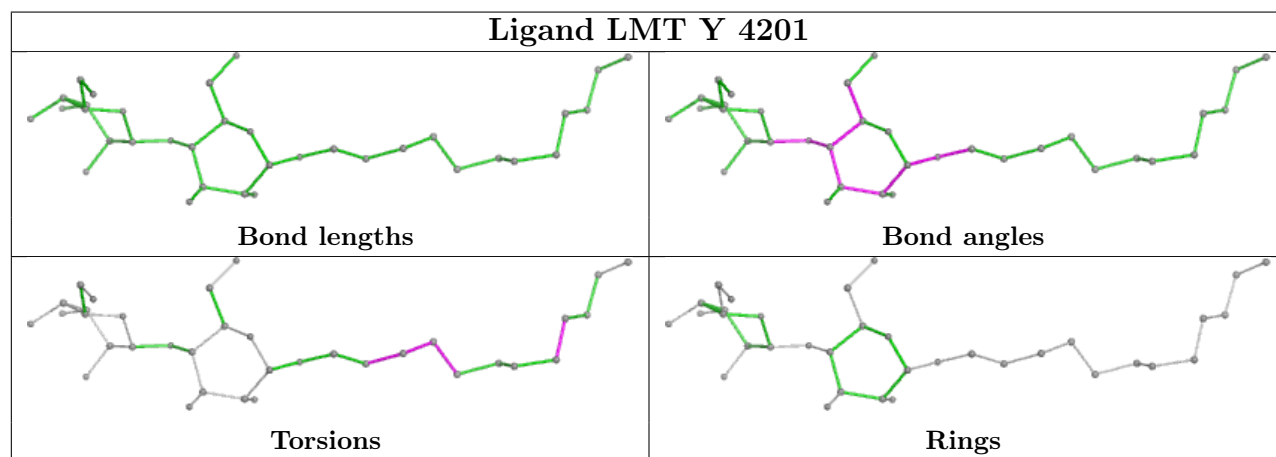
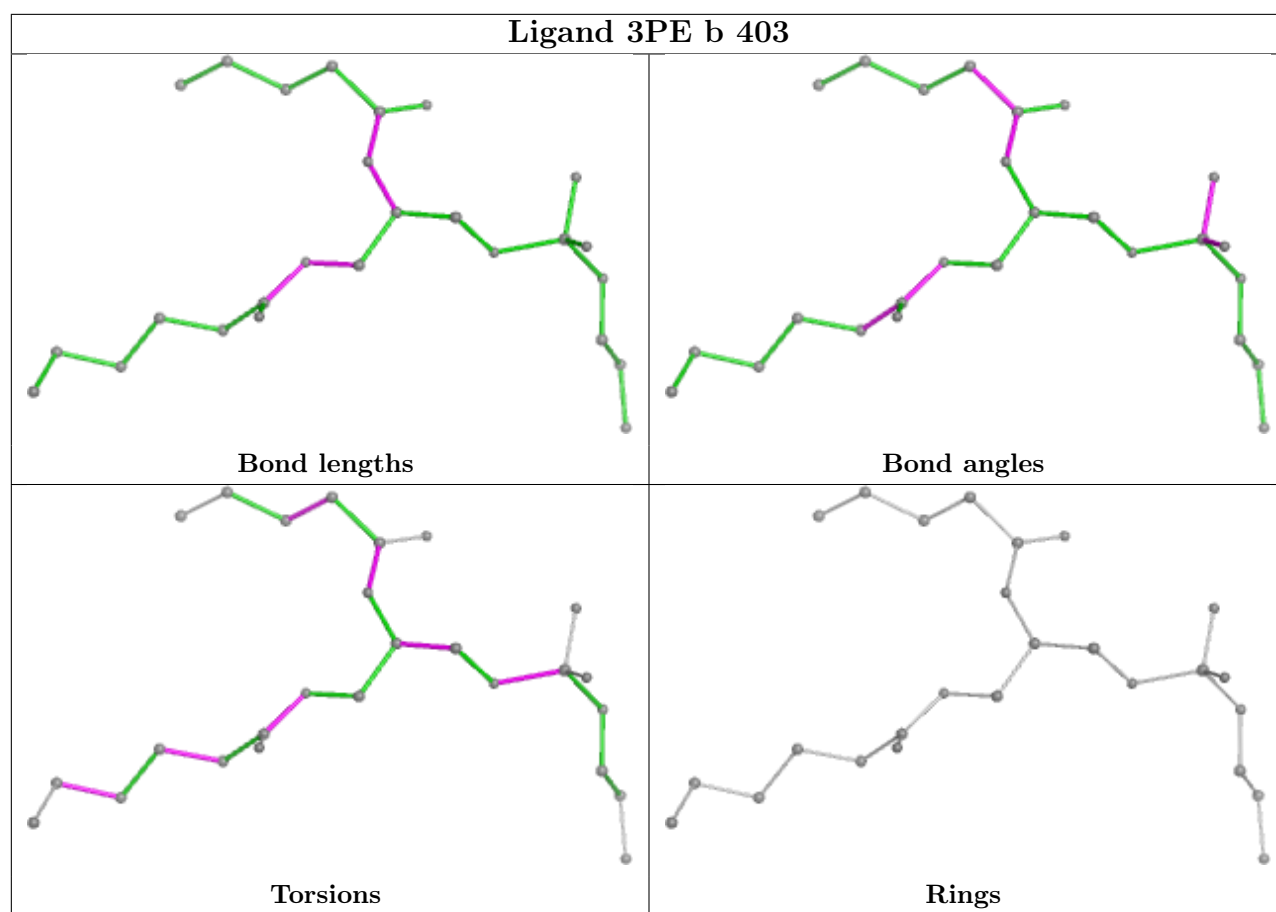


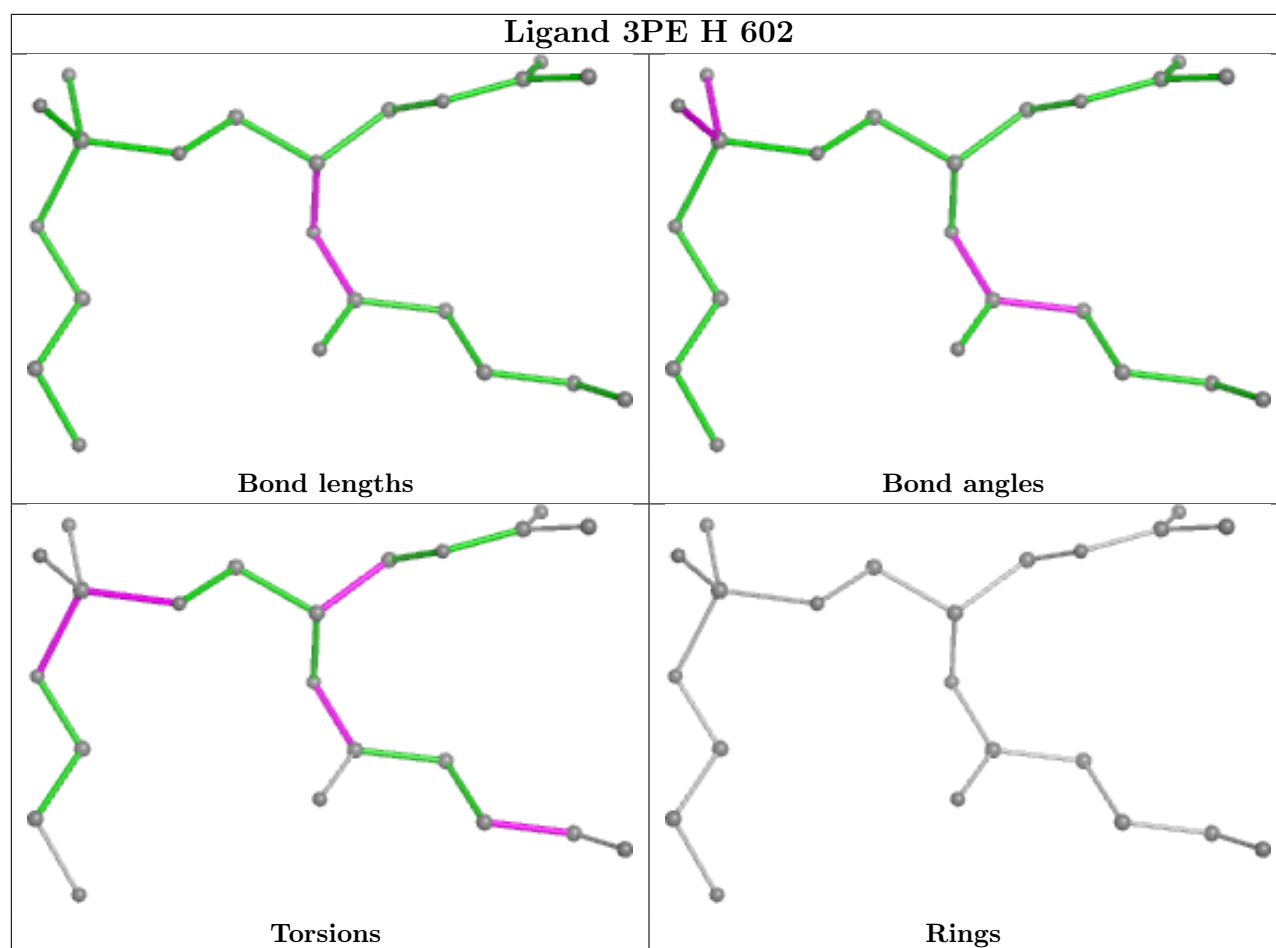


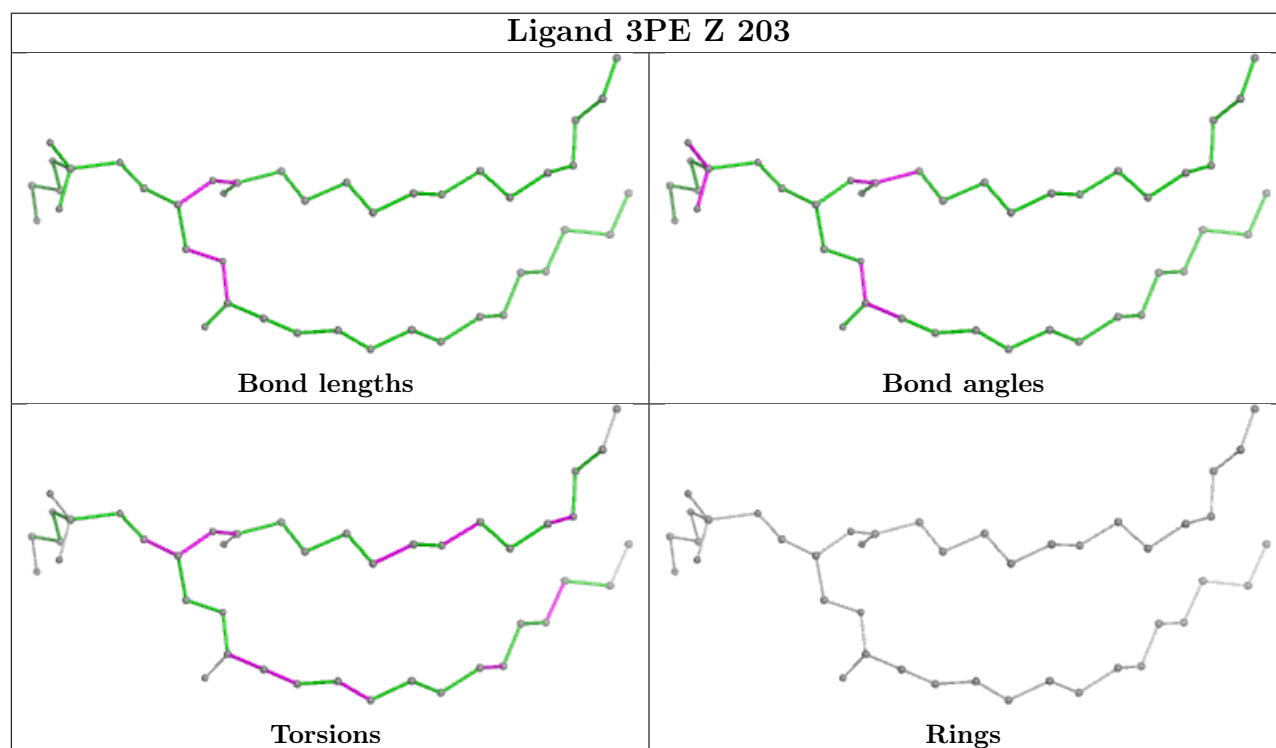
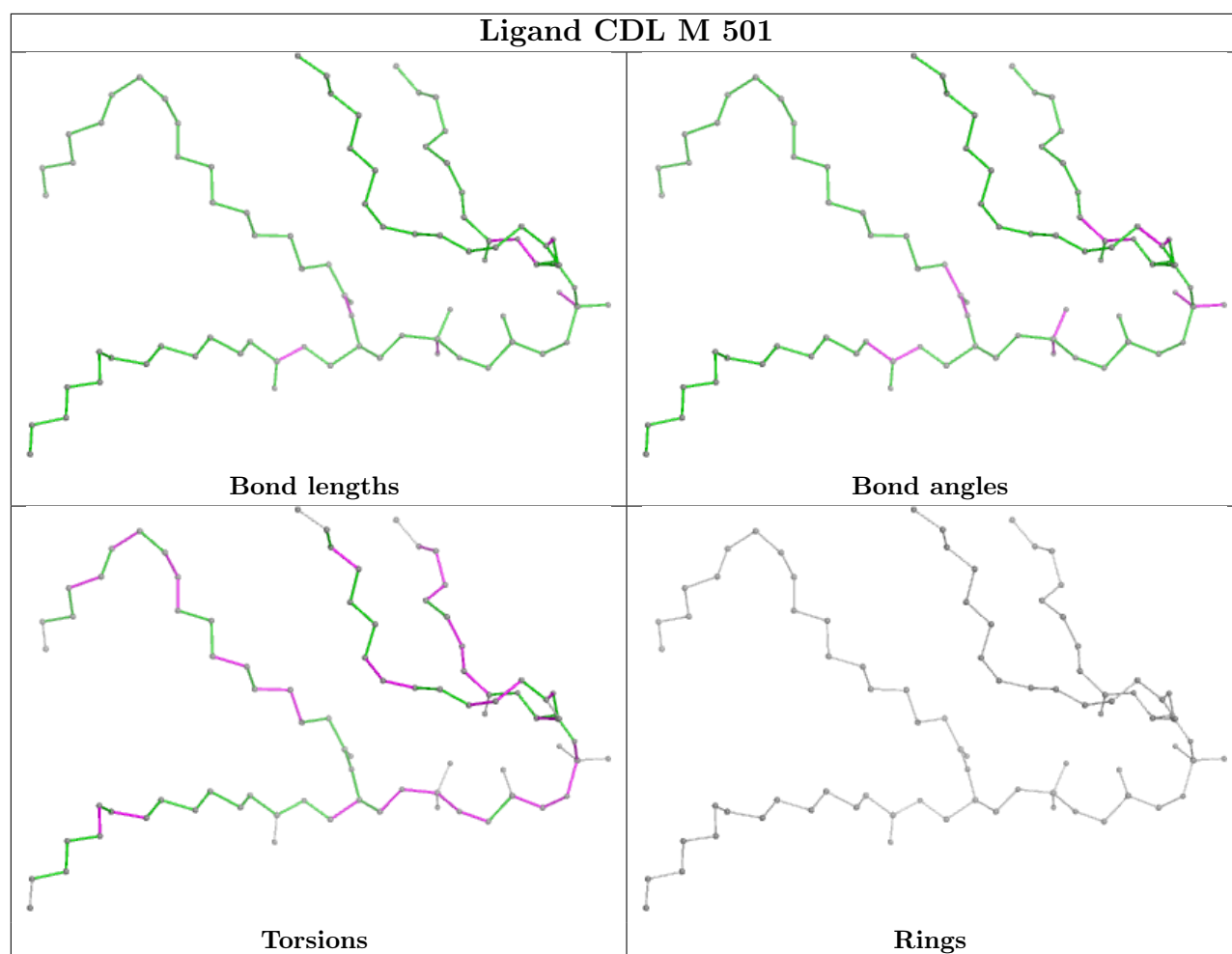


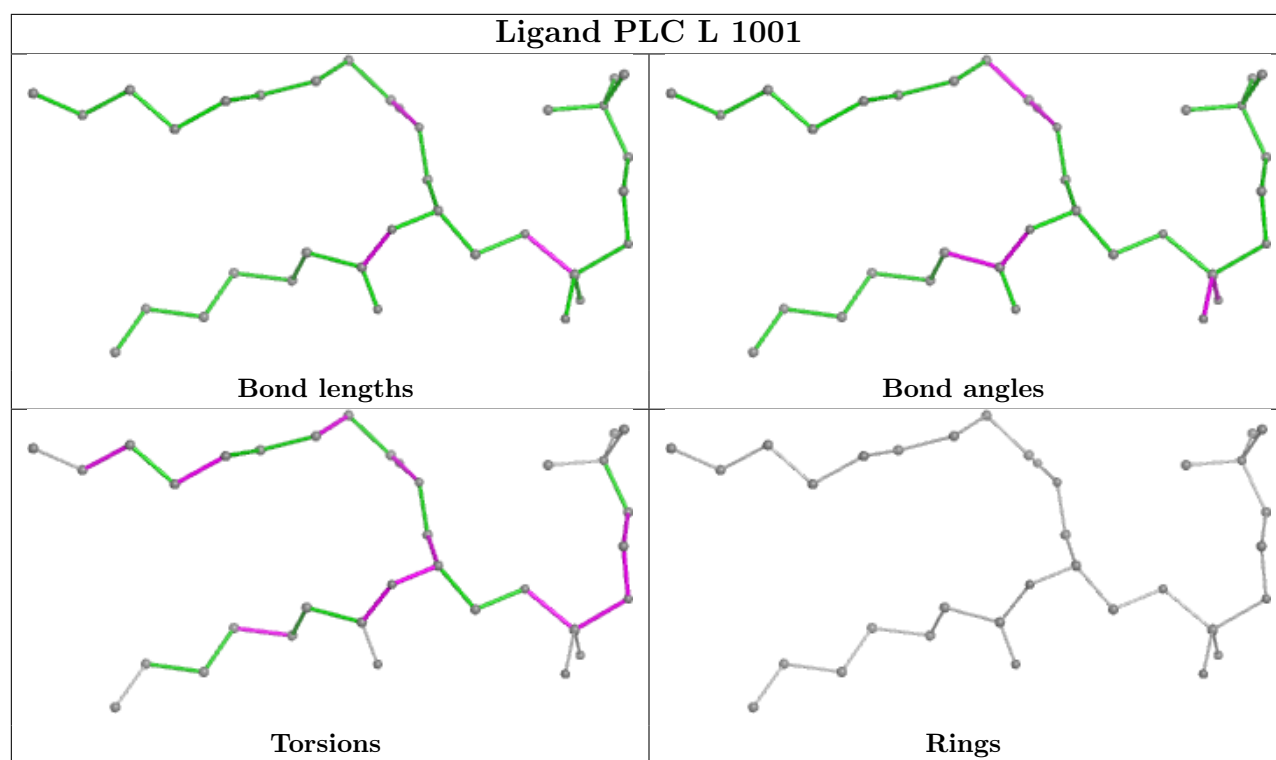




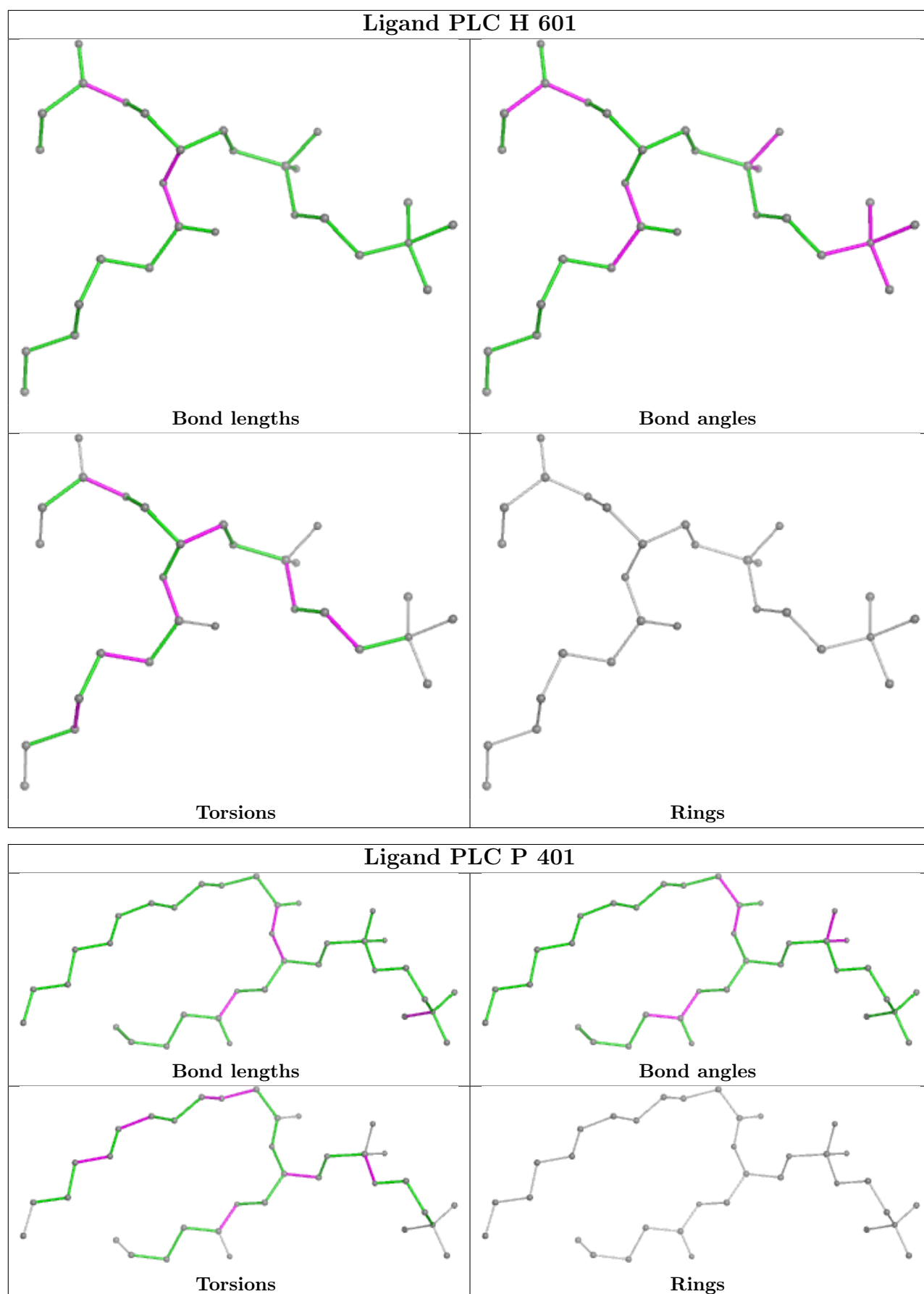


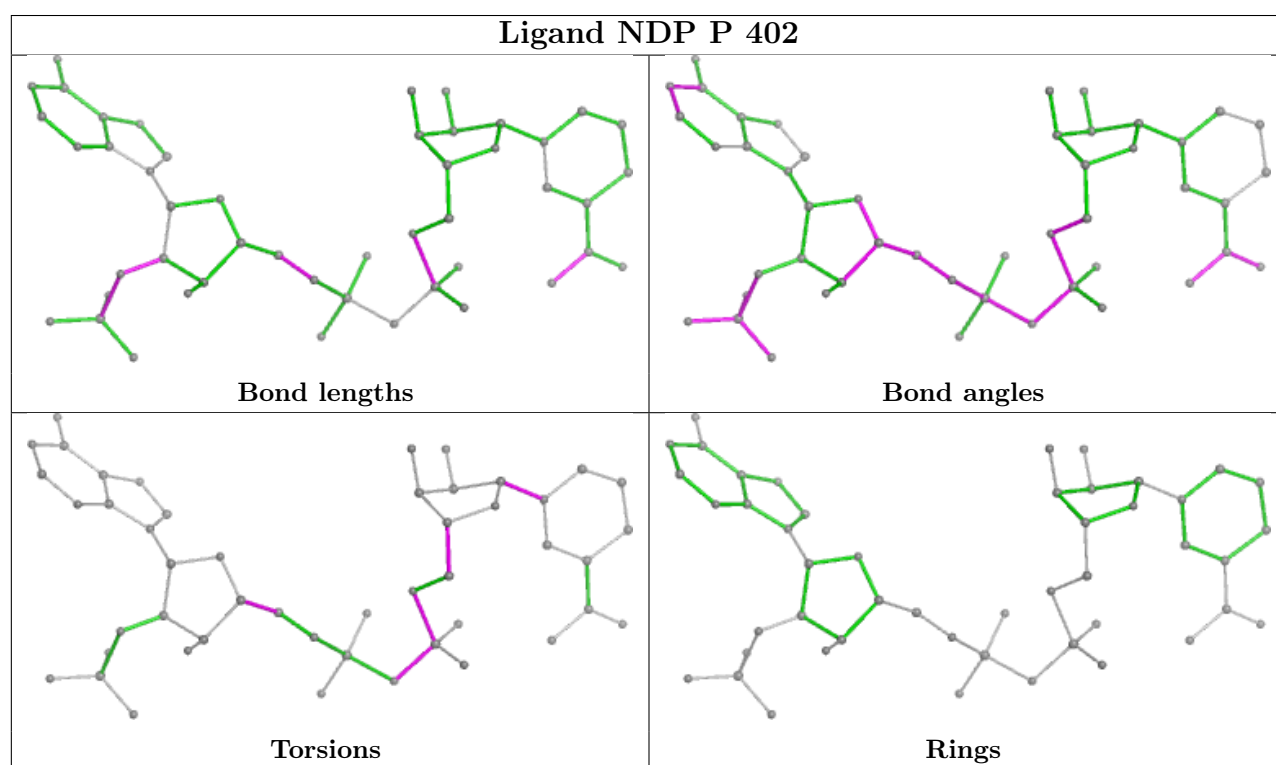
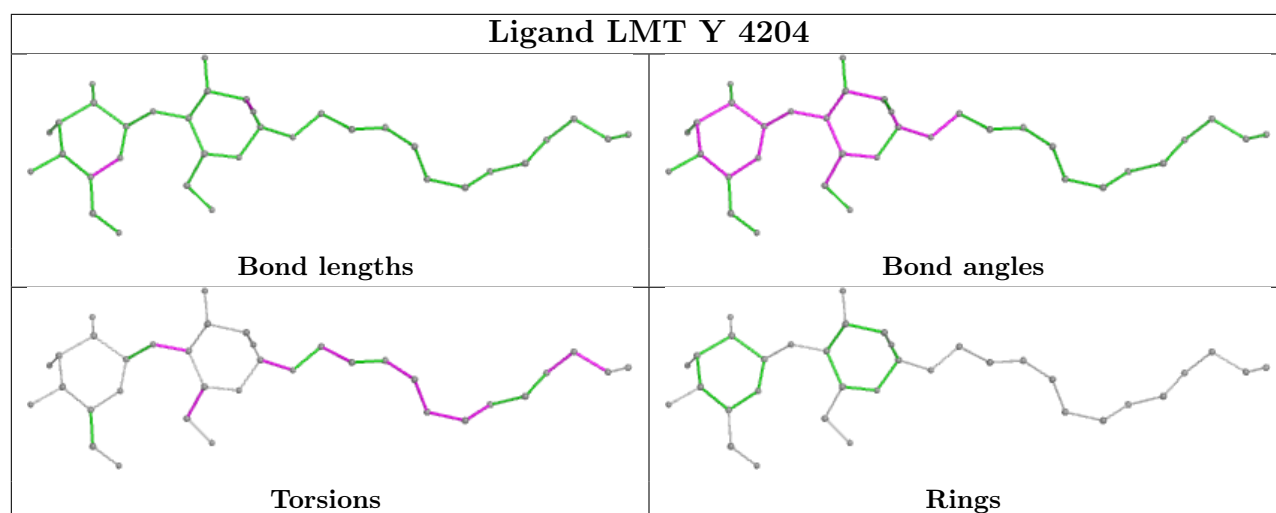


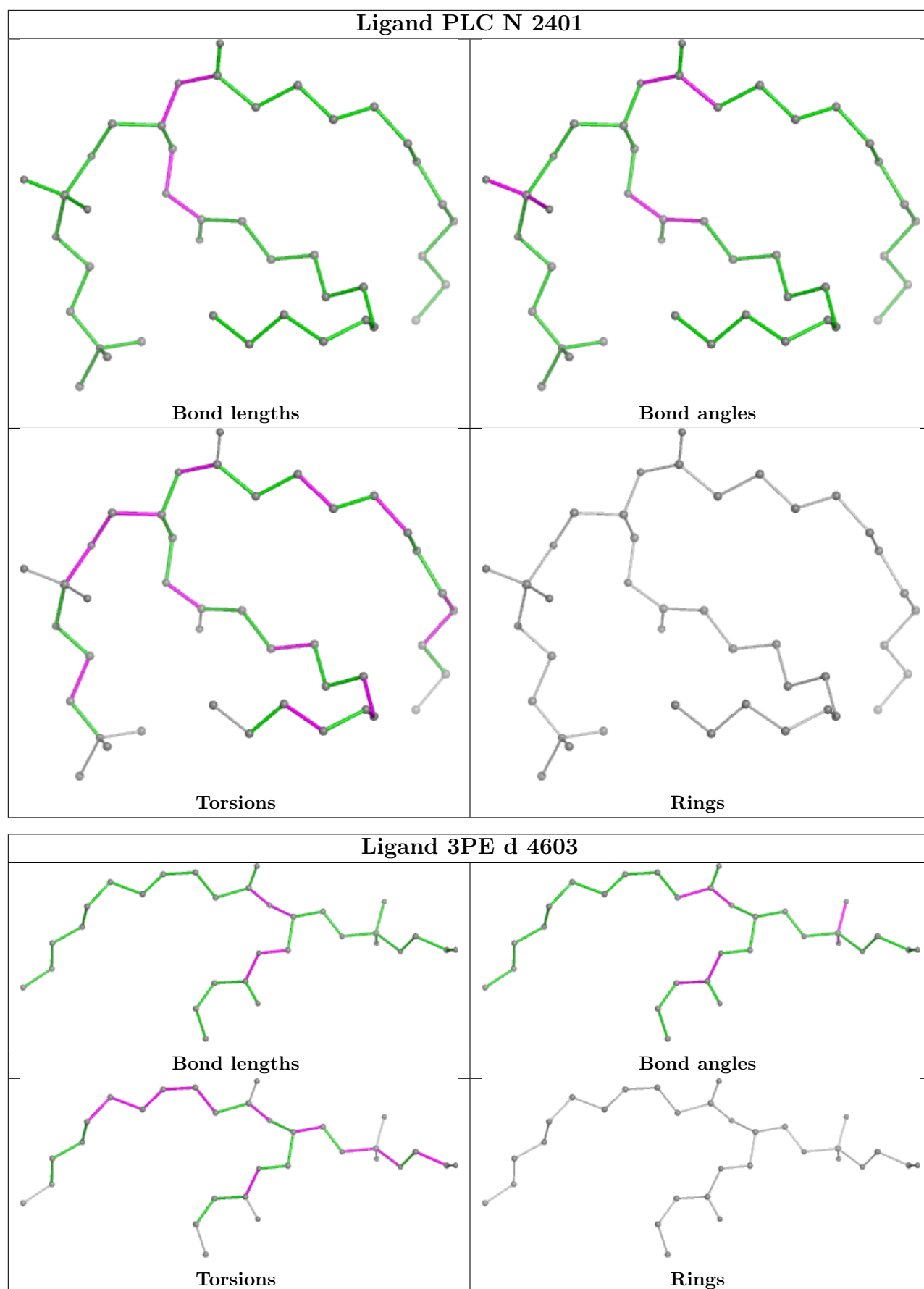


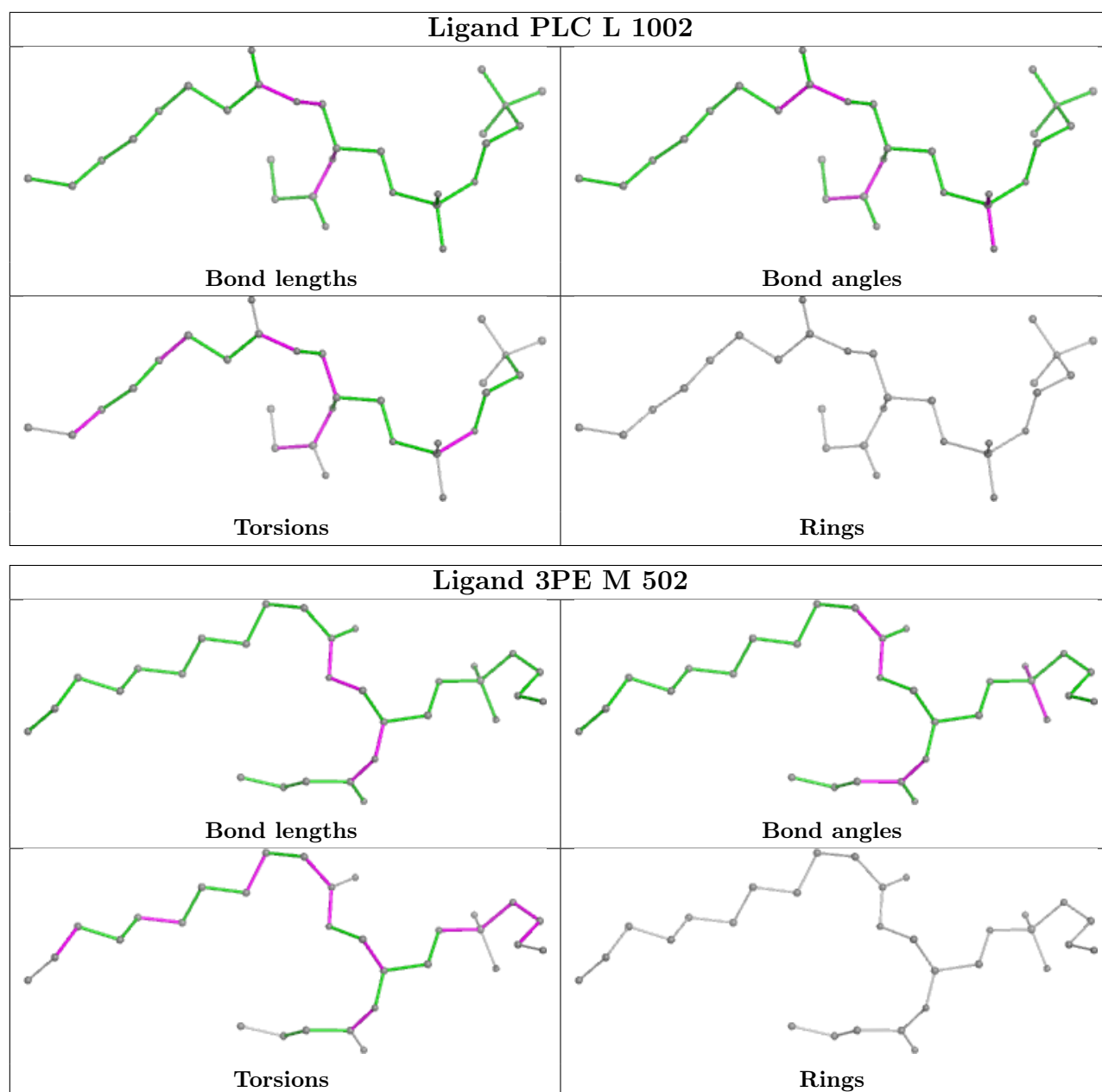


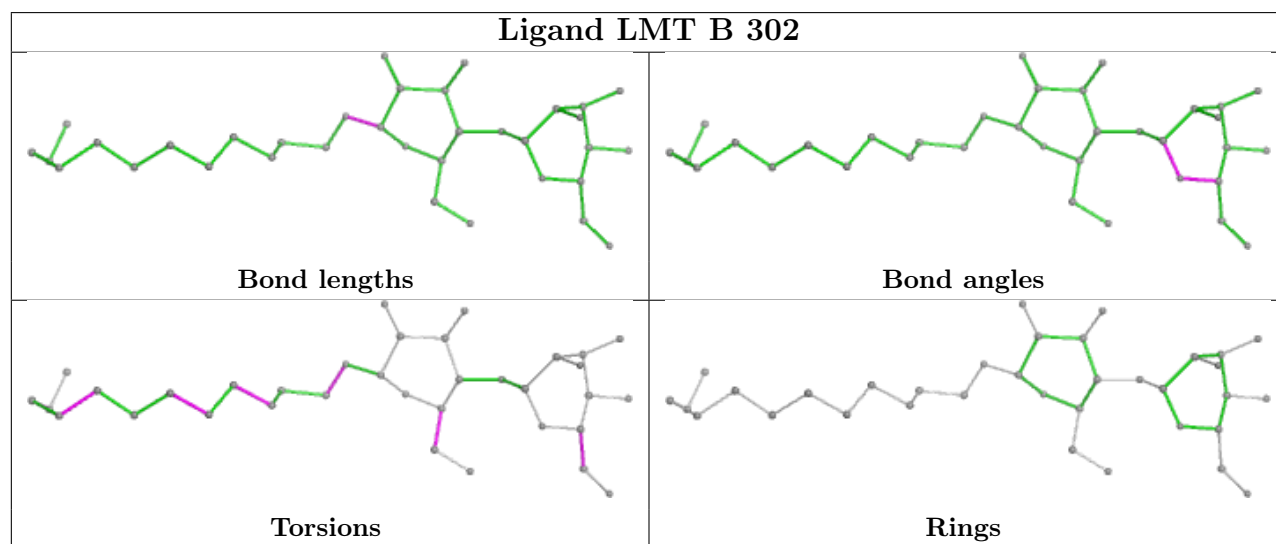
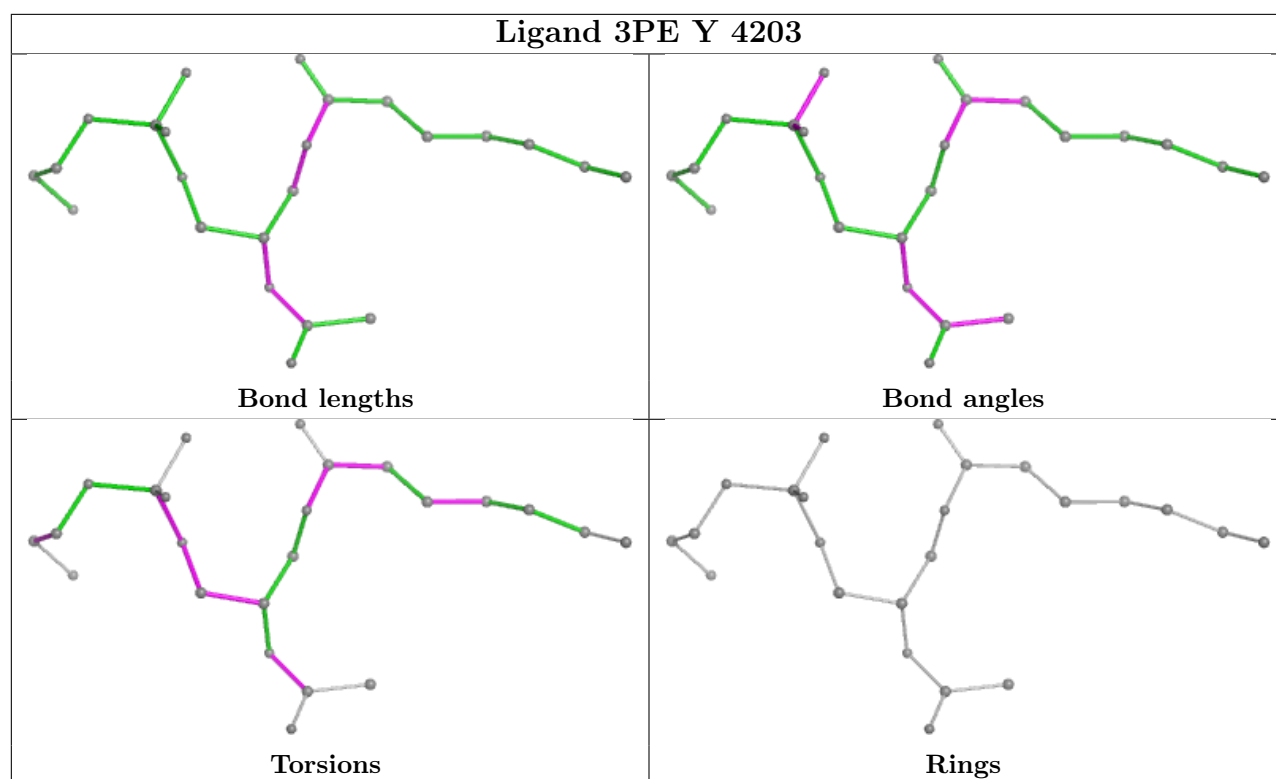


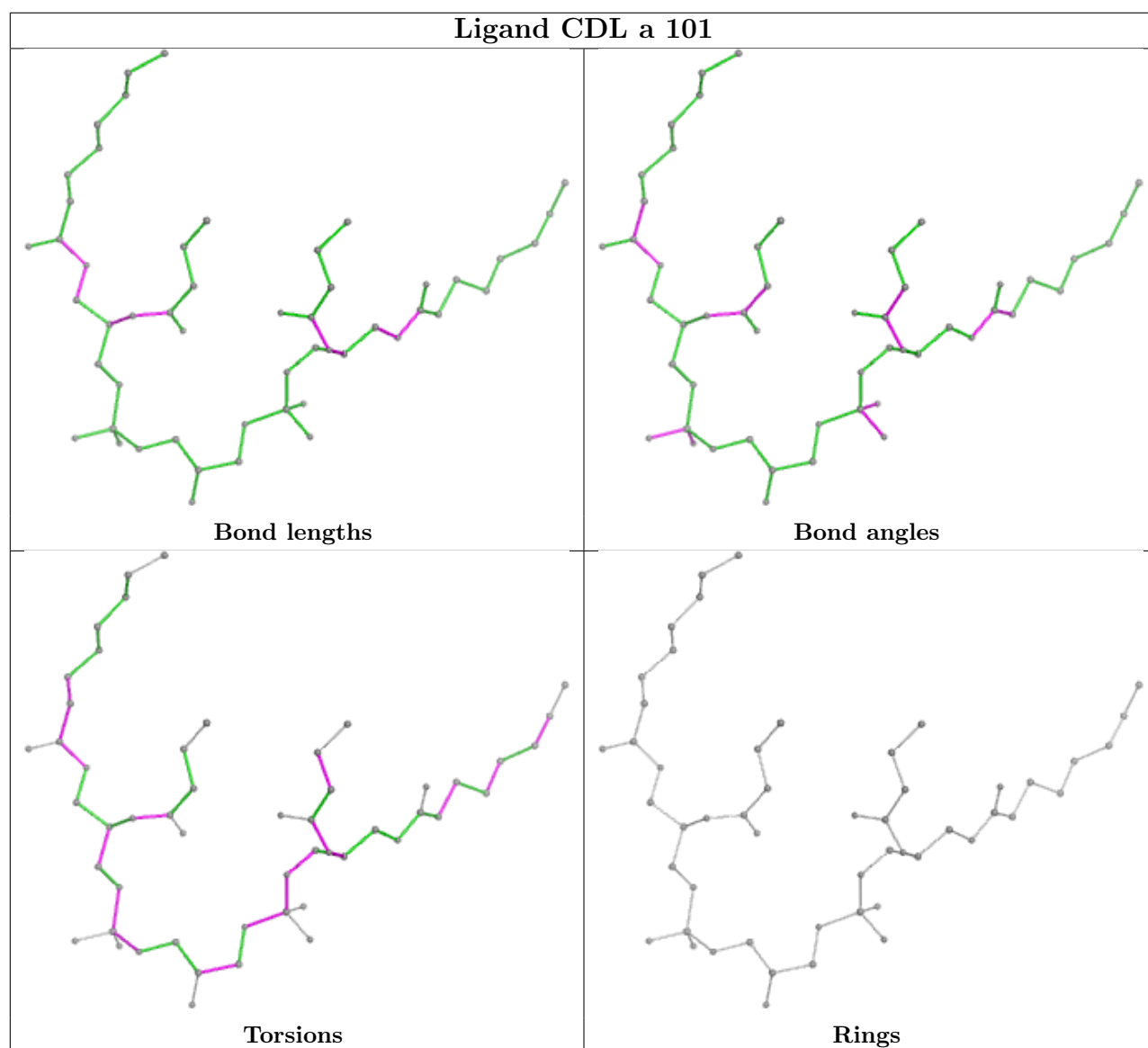
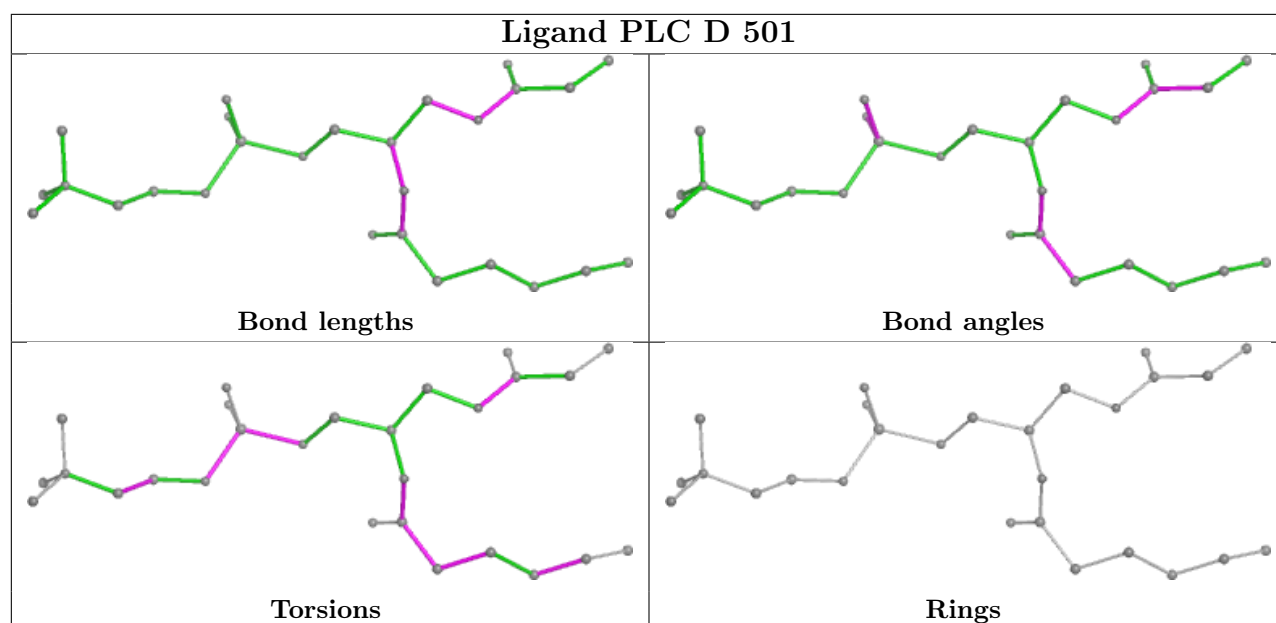


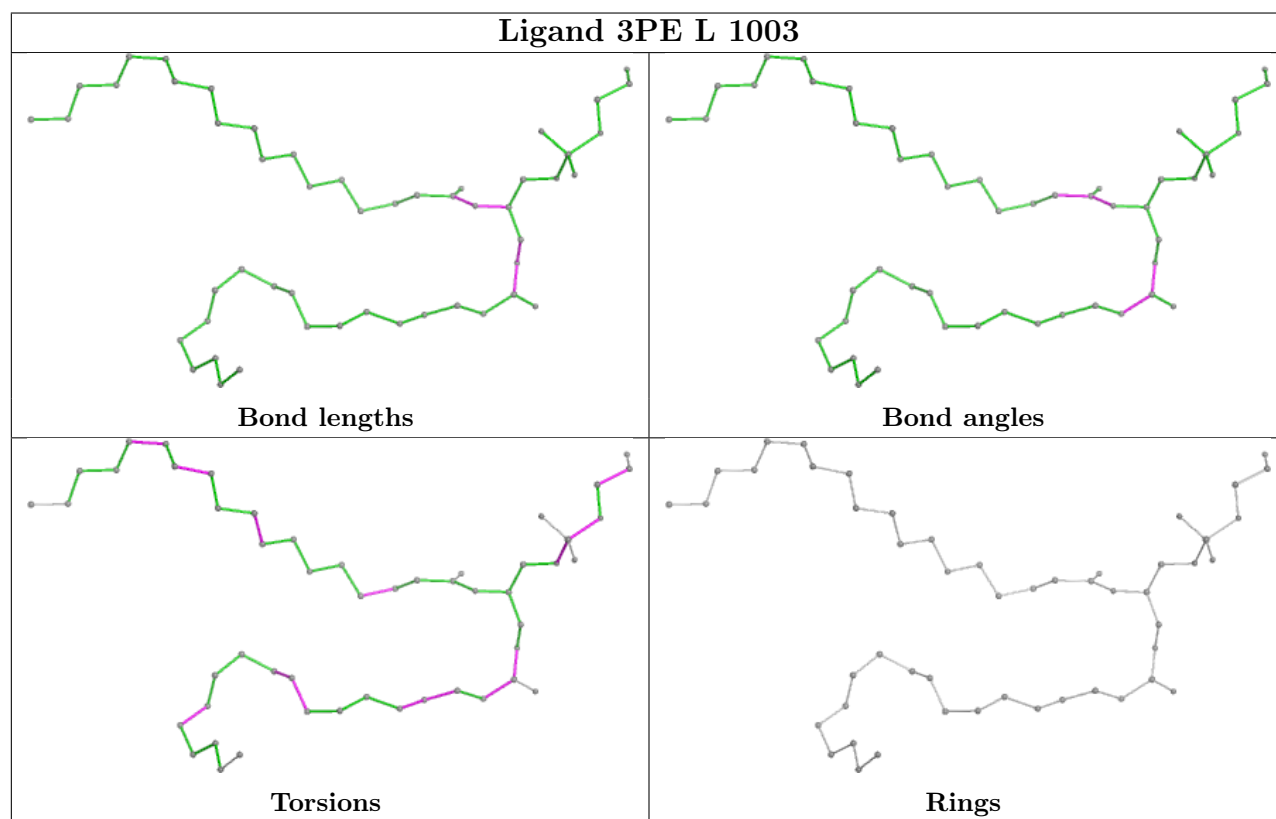
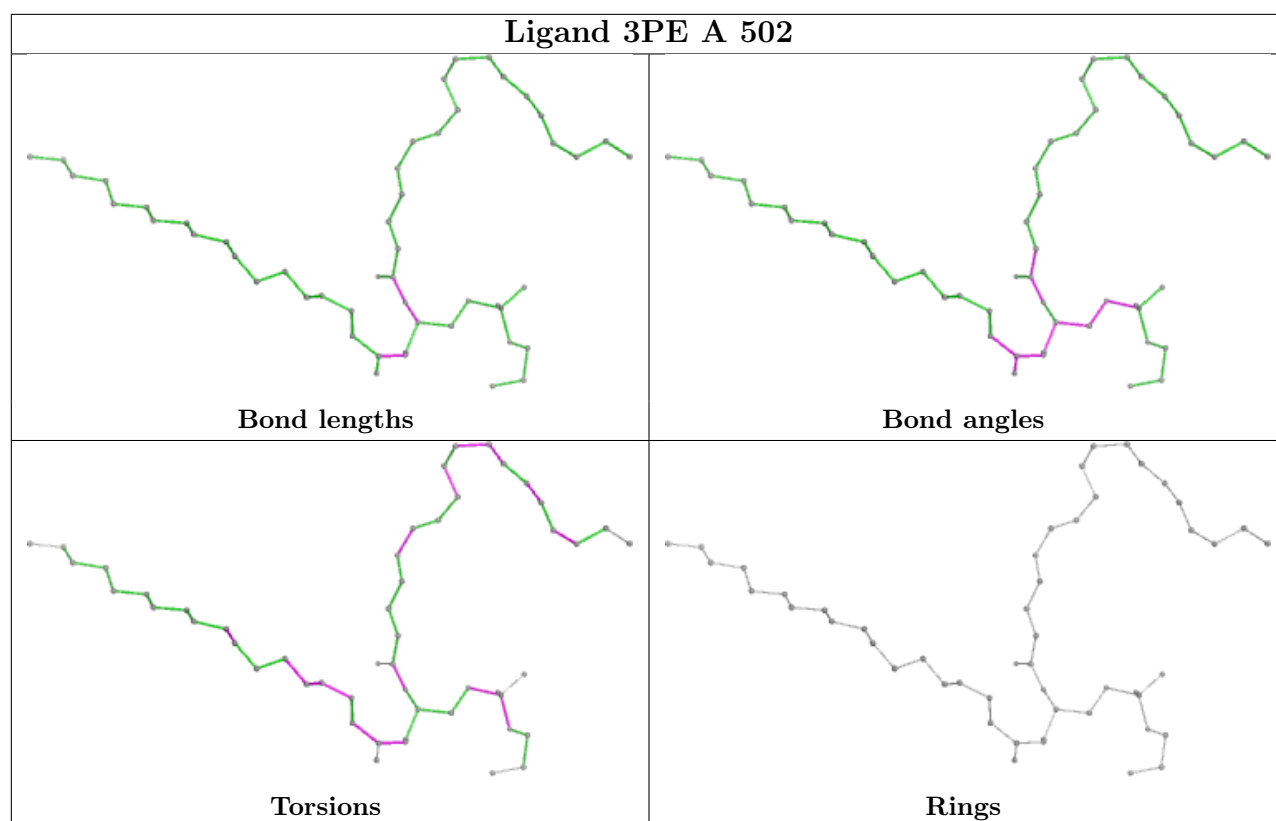


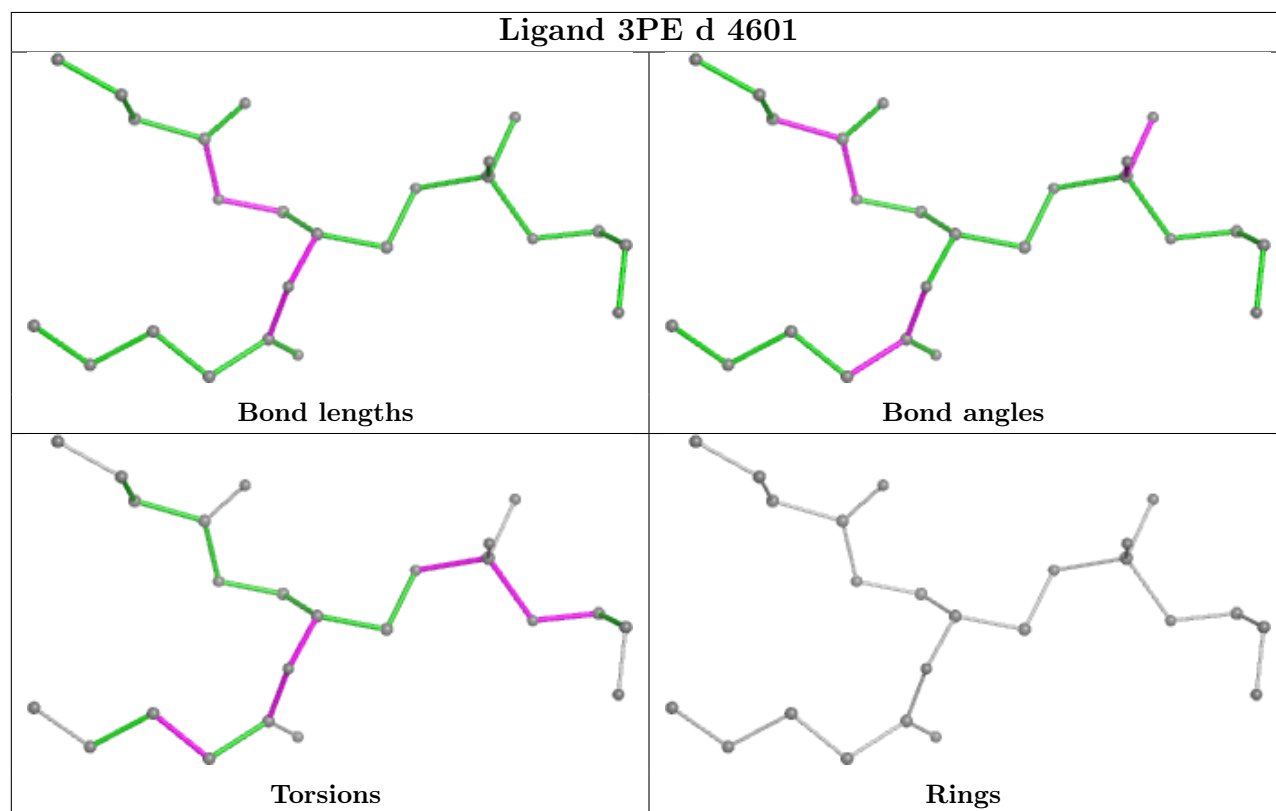
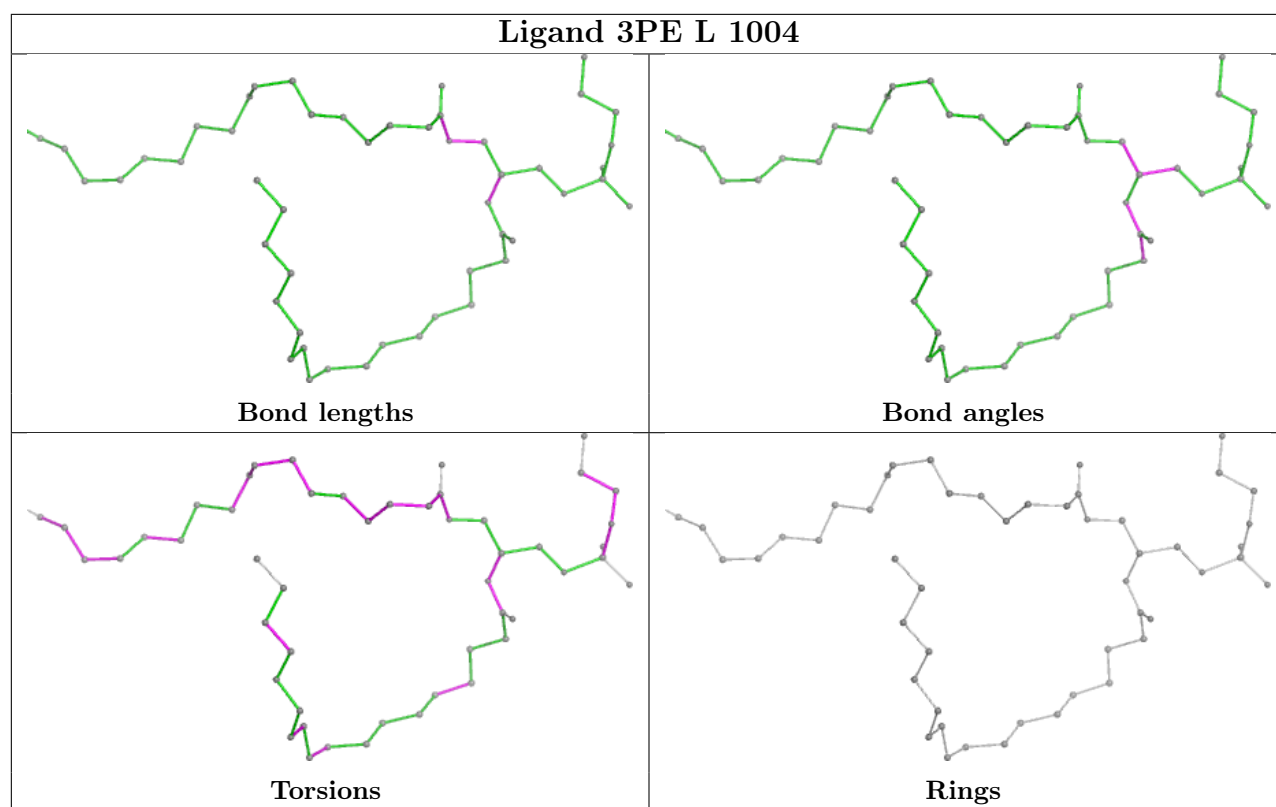




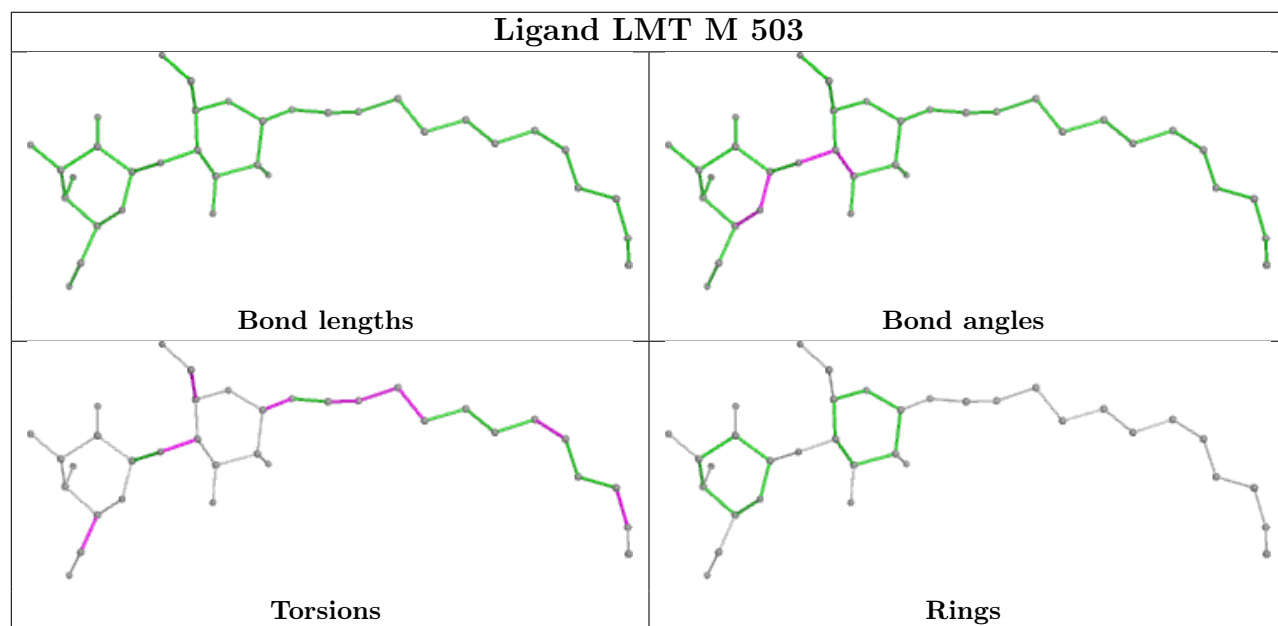
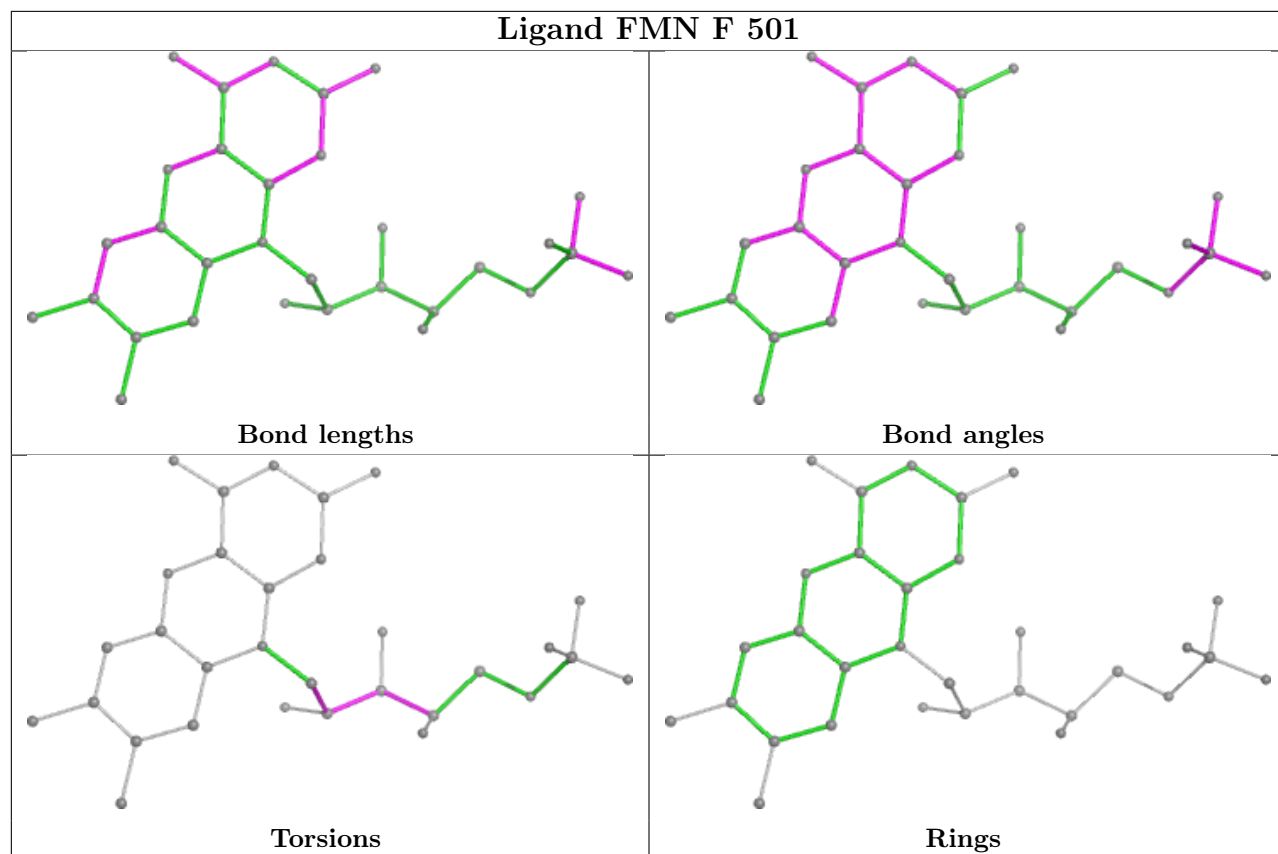


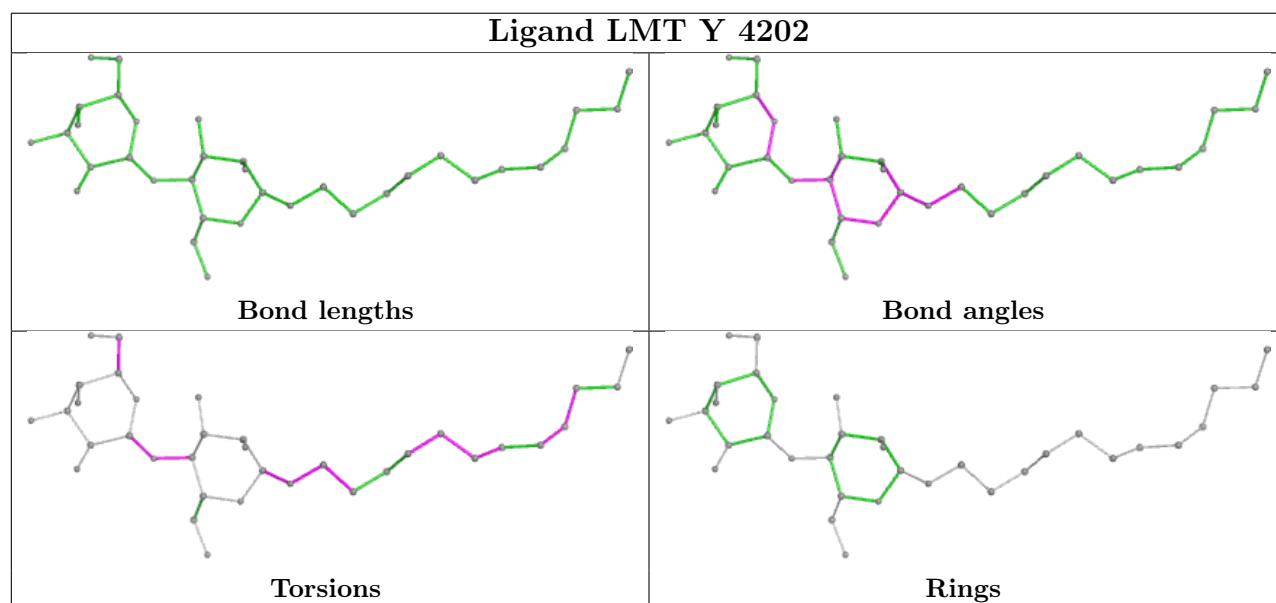
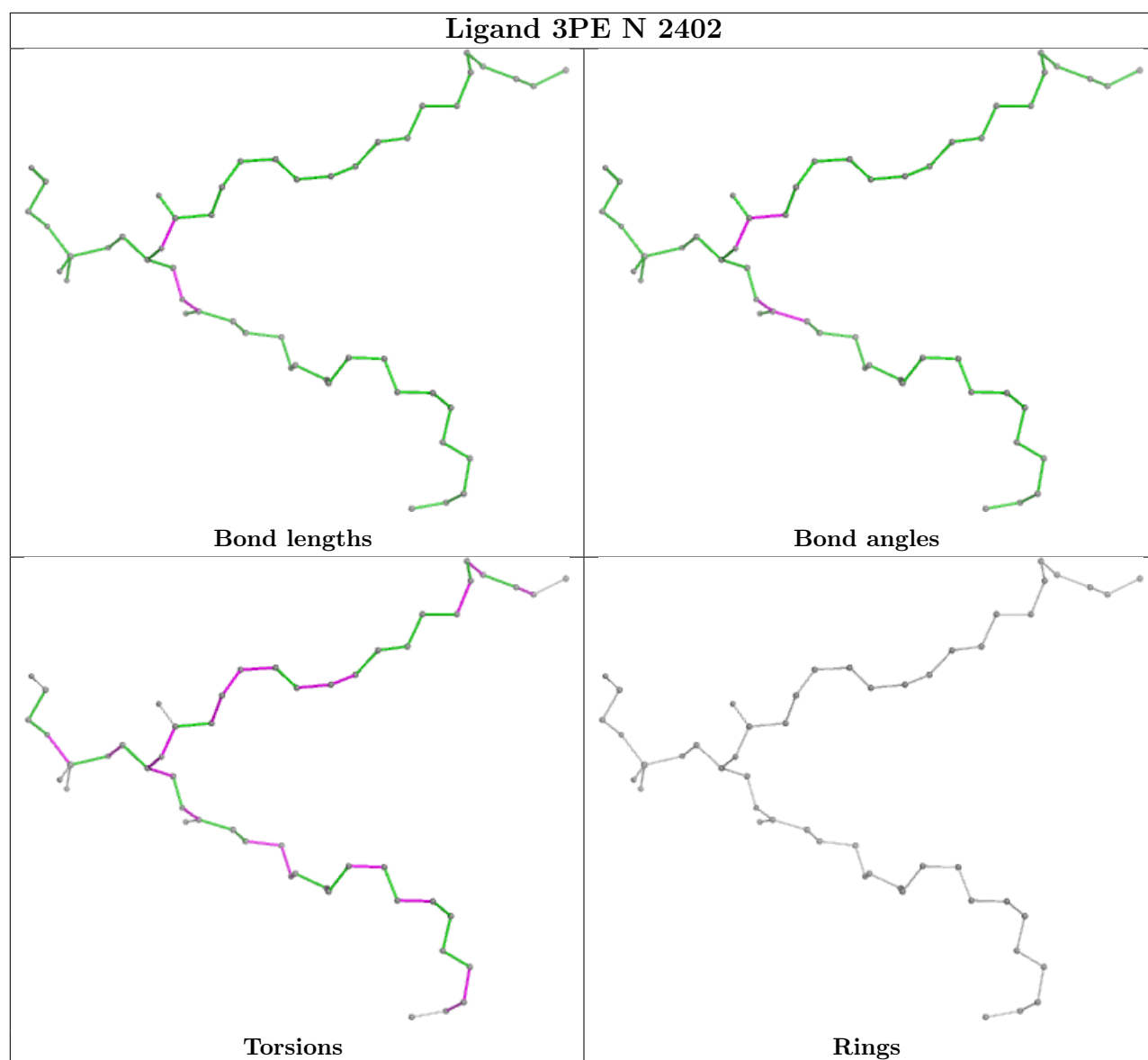


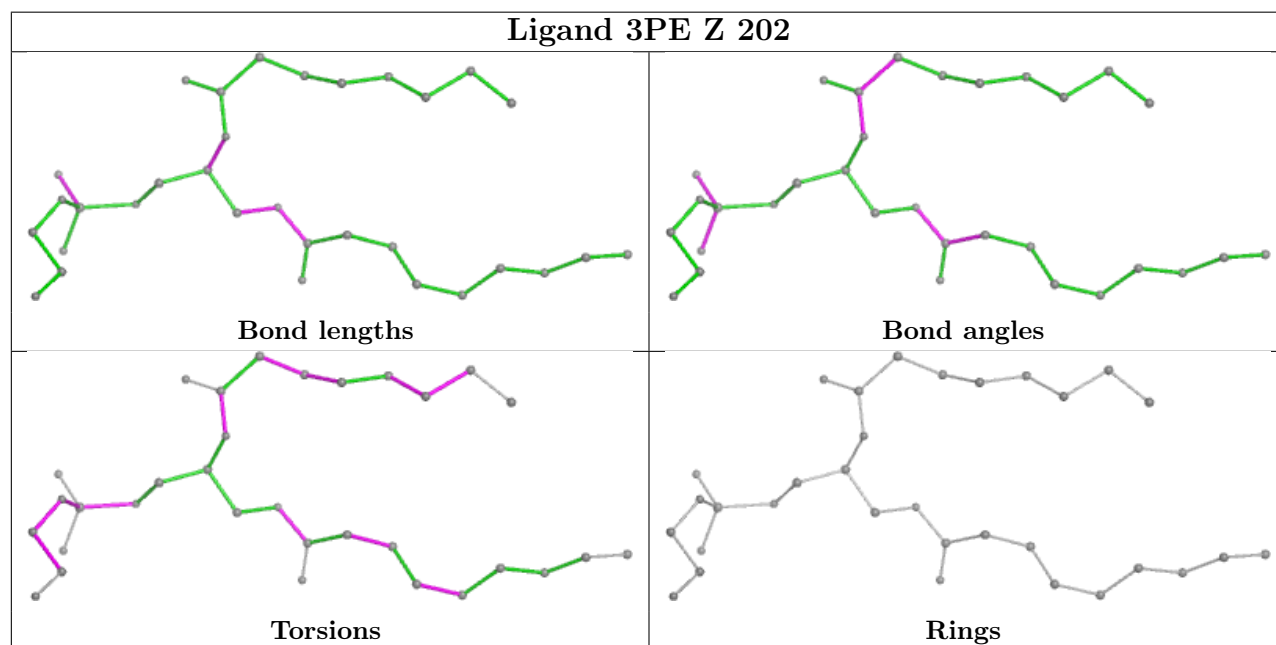
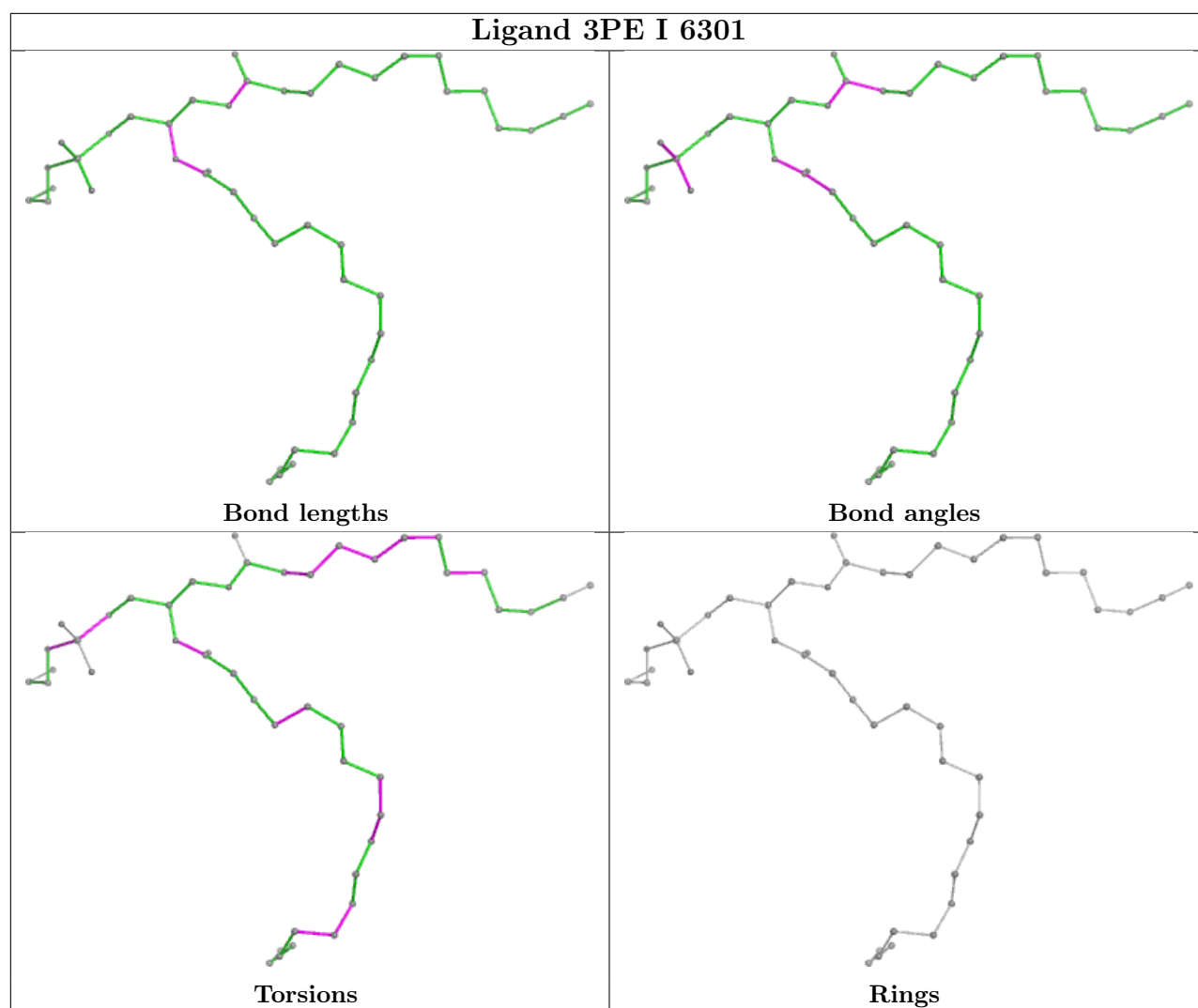


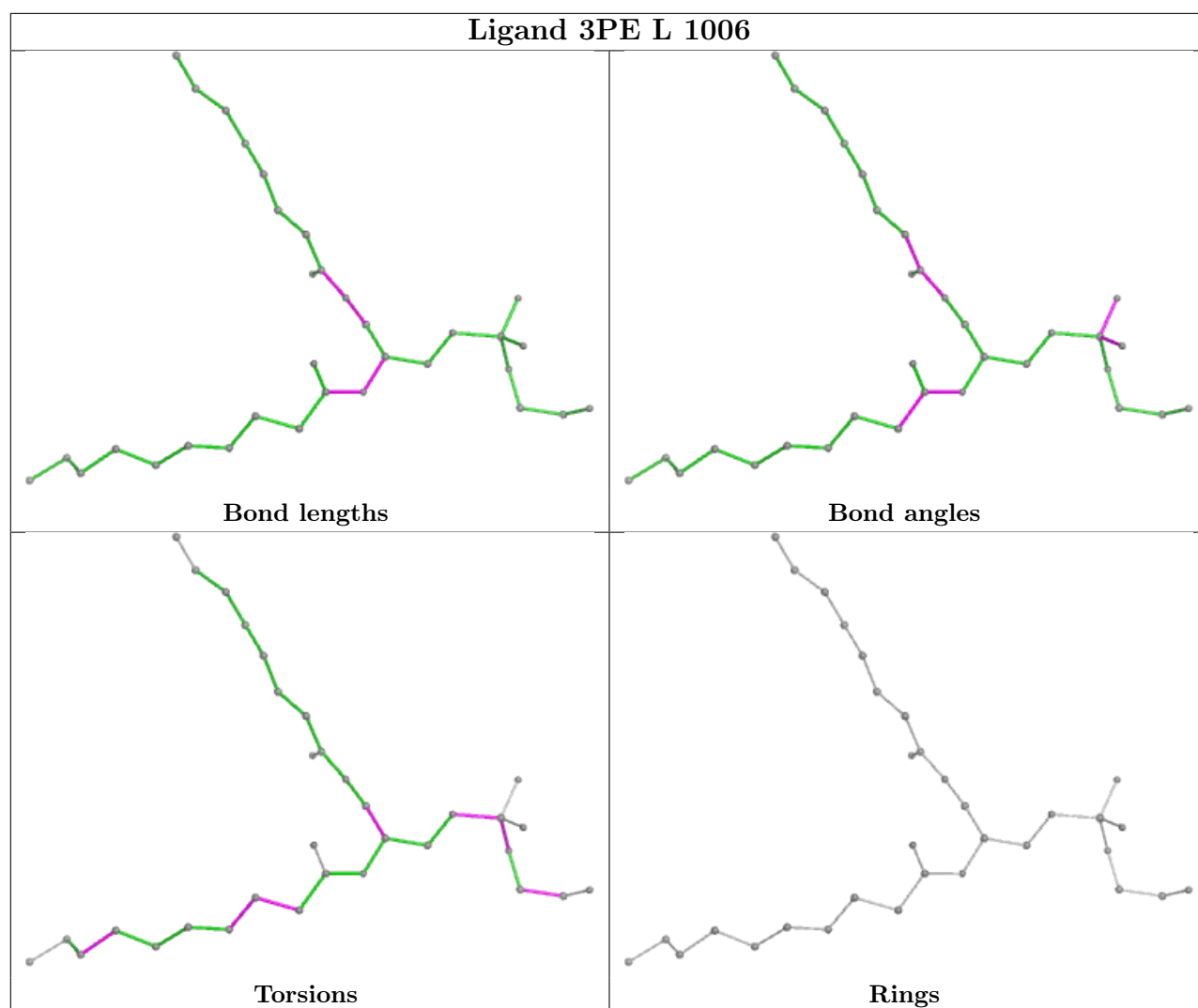


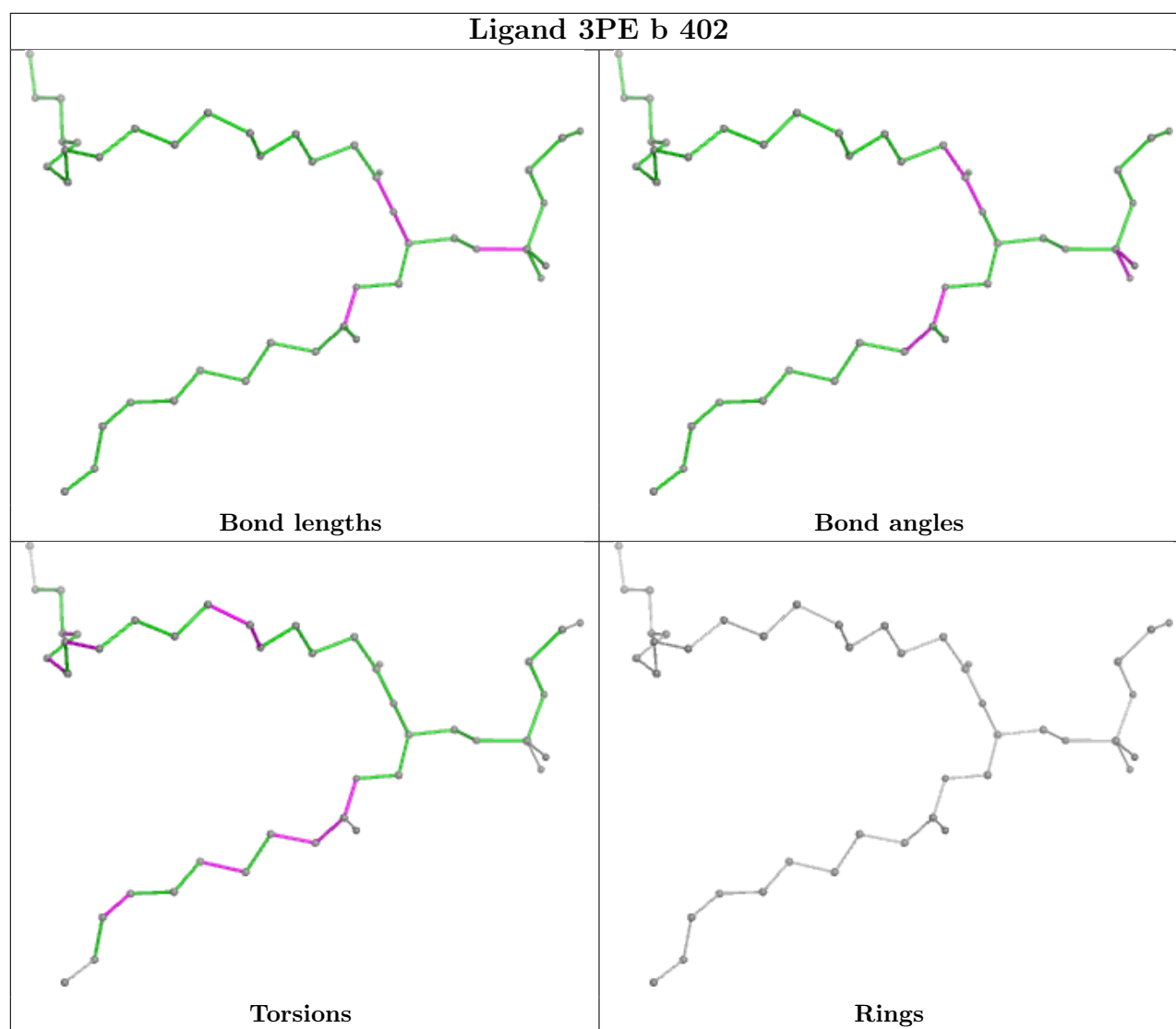












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

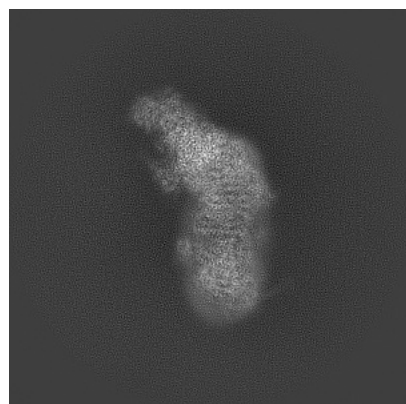
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10815. These allow visual inspection of the internal detail of the map and identification of artifacts.

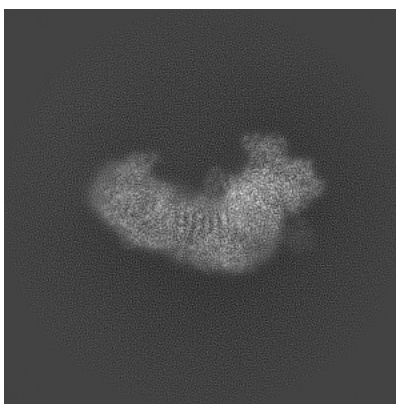
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

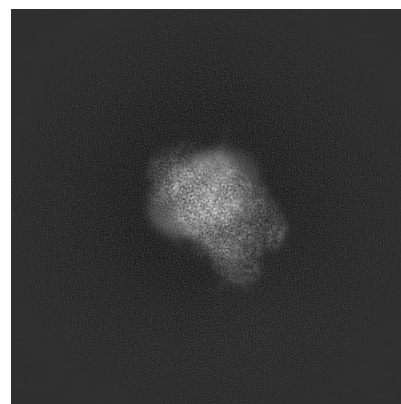
#### 6.1.1 Primary map



X

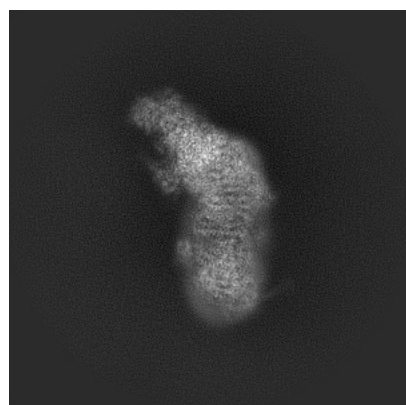


Y

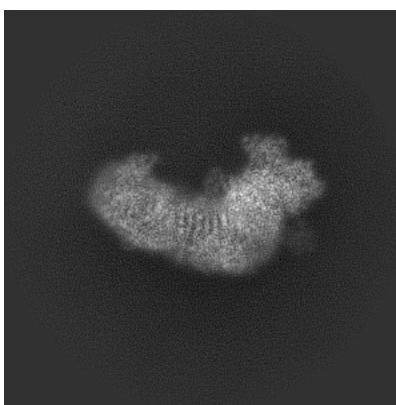


Z

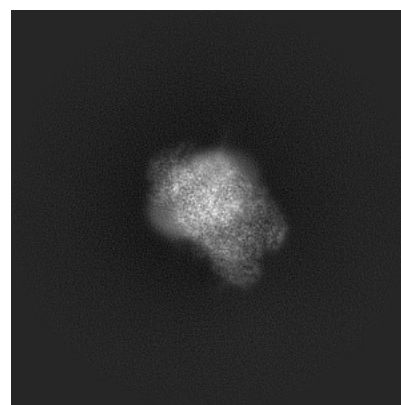
#### 6.1.2 Raw map



X



Y

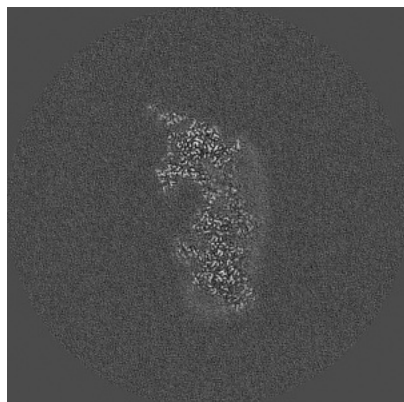


Z

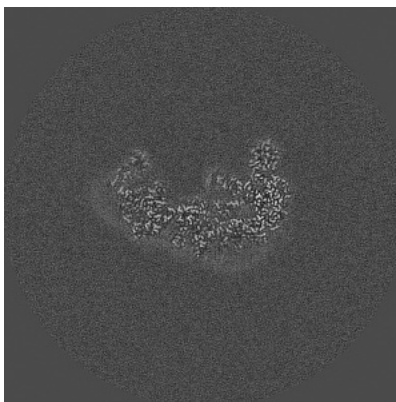
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

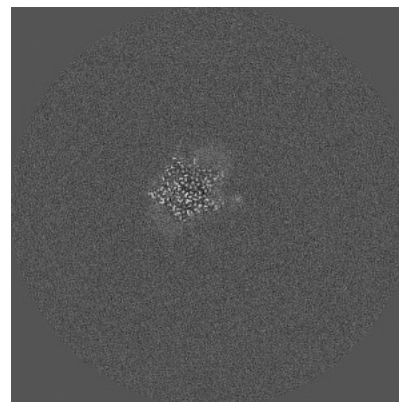
### 6.2.1 Primary map



X Index: 225

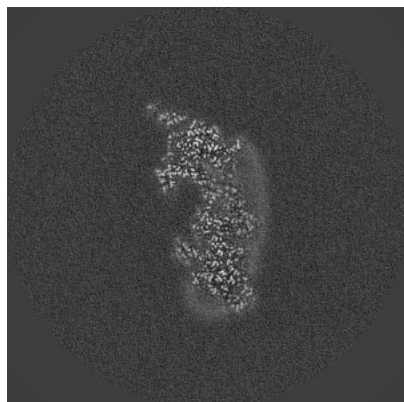


Y Index: 225

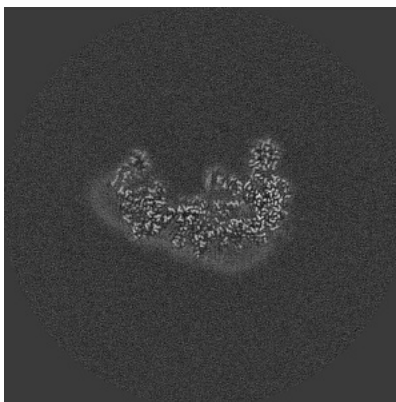


Z Index: 225

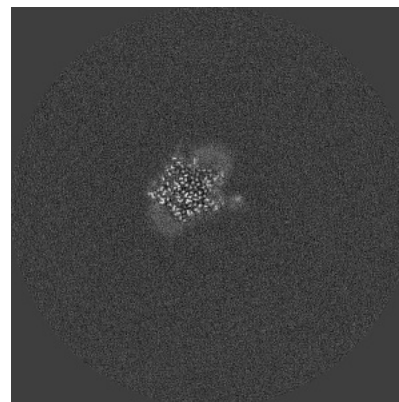
### 6.2.2 Raw map



X Index: 225



Y Index: 225



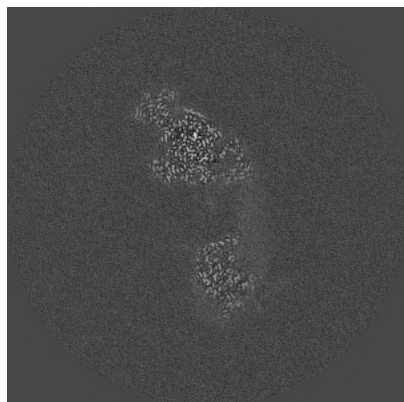
Z Index: 225

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

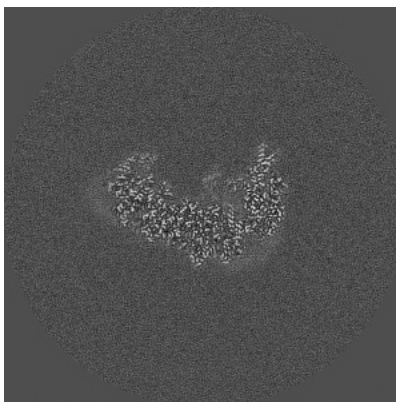


## 6.3 Largest variance slices [i](#)

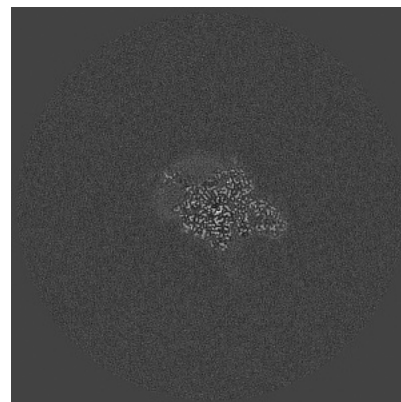
### 6.3.1 Primary map



X Index: 242

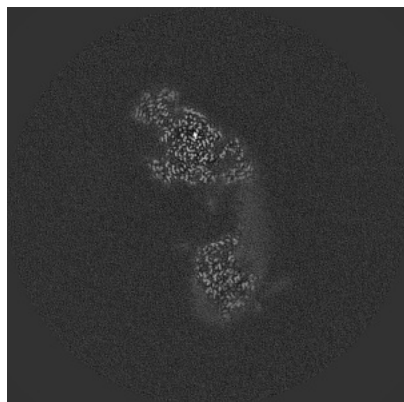


Y Index: 234

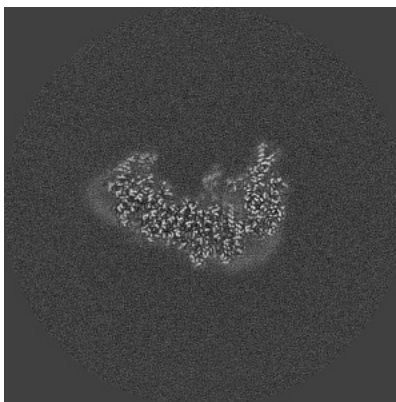


Z Index: 284

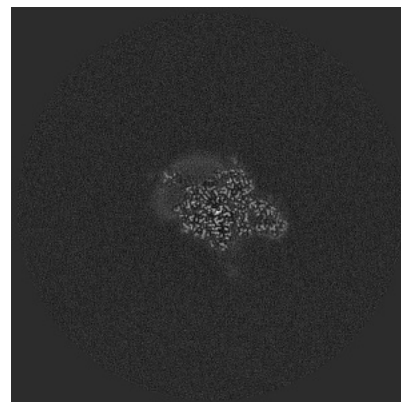
### 6.3.2 Raw map



X Index: 242



Y Index: 234



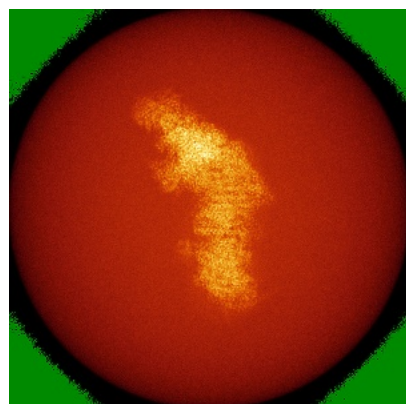
Z Index: 284

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

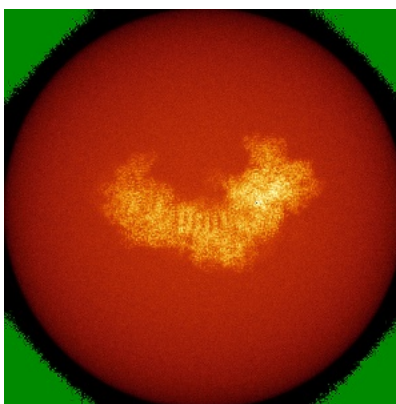


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

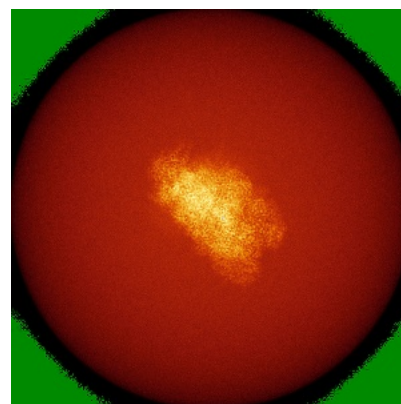
### 6.4.1 Primary map



X

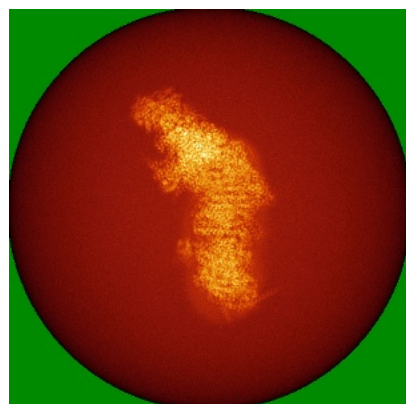


Y

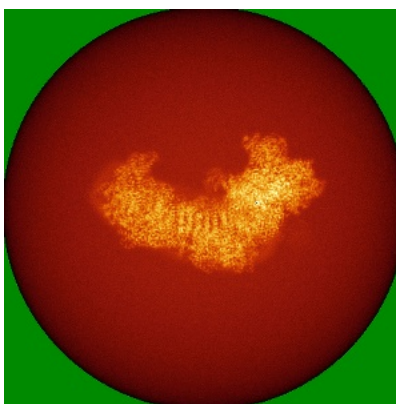


Z

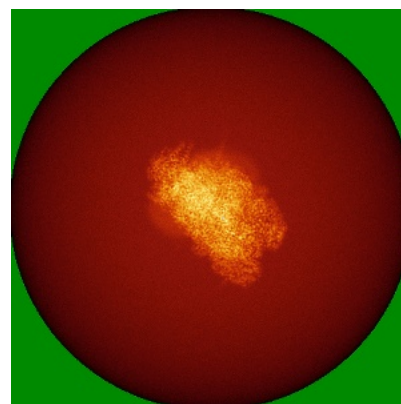
### 6.4.2 Raw map



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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

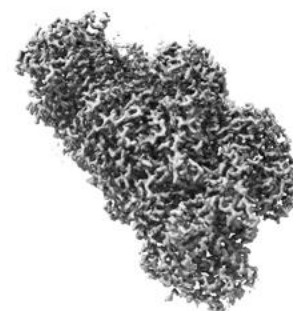
### 6.5.2 Raw map



X



Y



Z

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

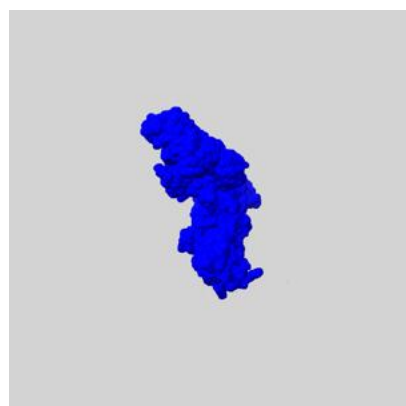
## 6.6 Mask visualisation [i](#)

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

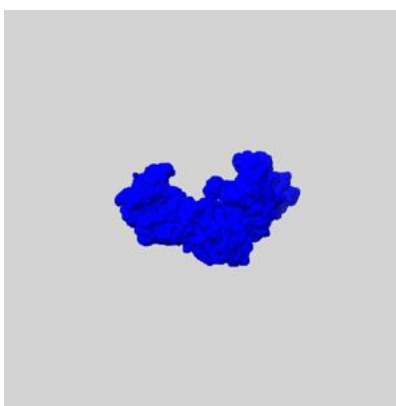
A mask typically either:

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

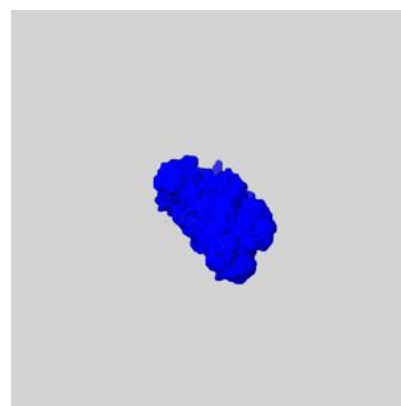
### 6.6.1 emd\_10815\_msk\_1.map [i](#)



X



Y

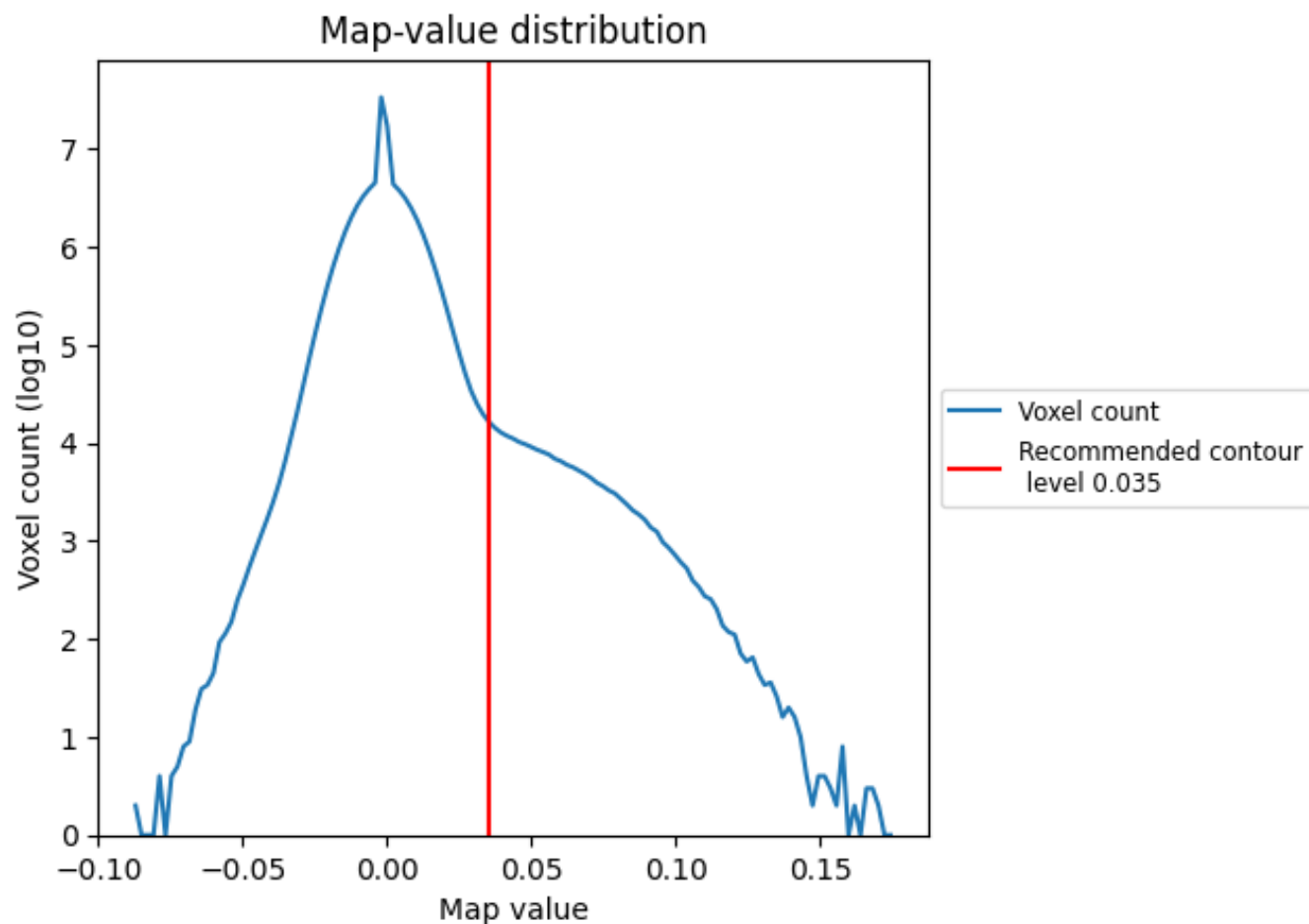


Z

## 7 Map analysis [i](#)

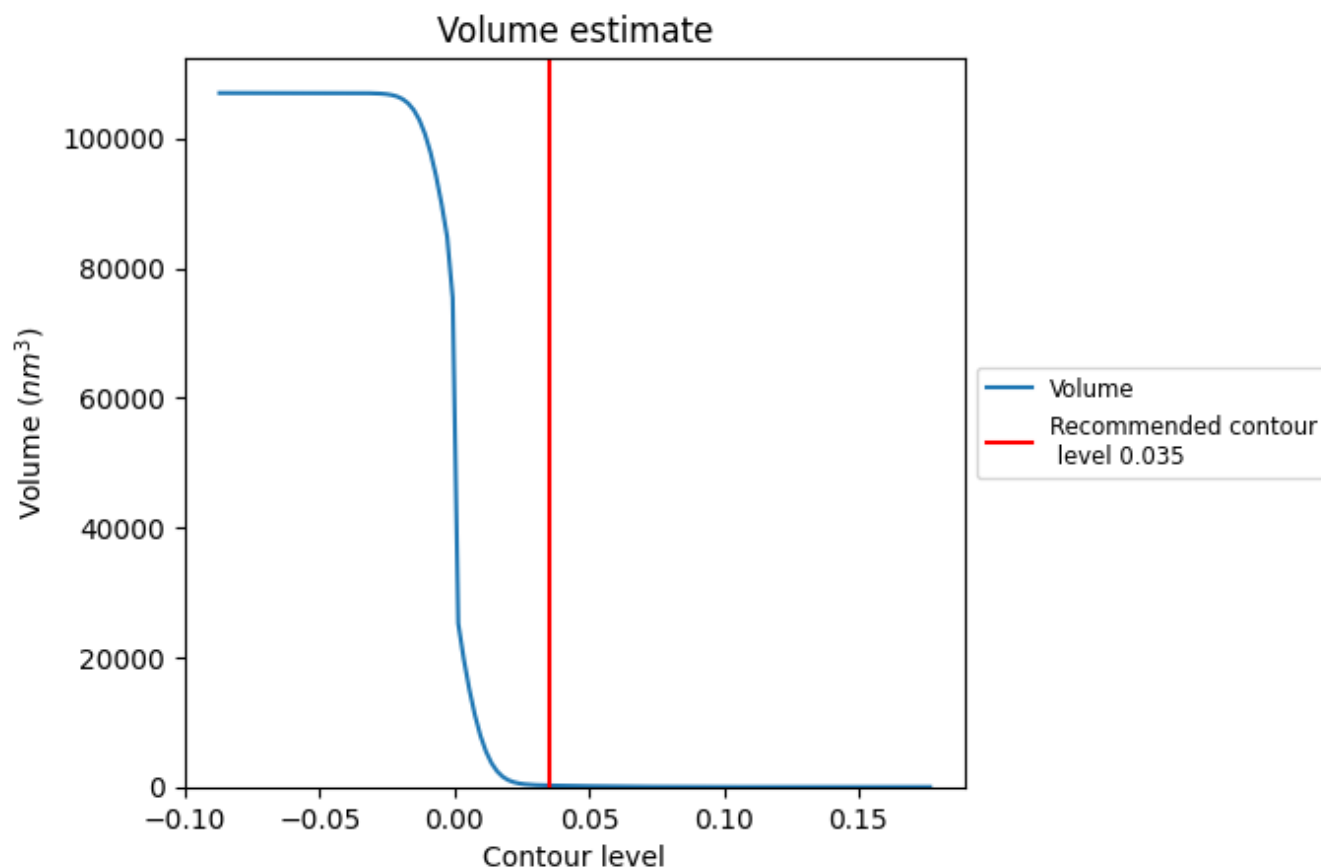
This section contains the results of statistical analysis of the map.

### 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.

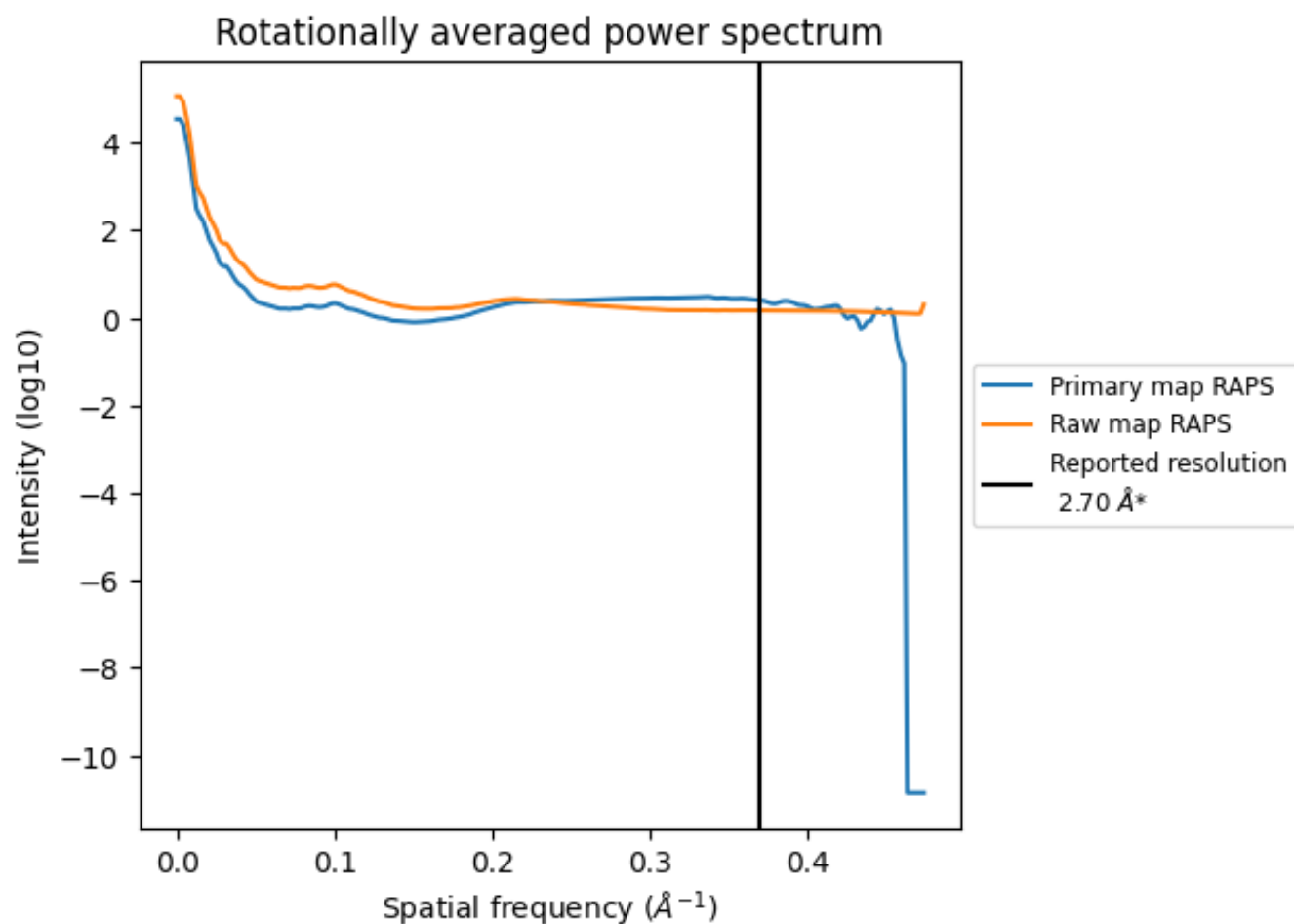
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $230 \text{ nm}^3$ ; this corresponds to an approximate mass of 208 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 ⓘ

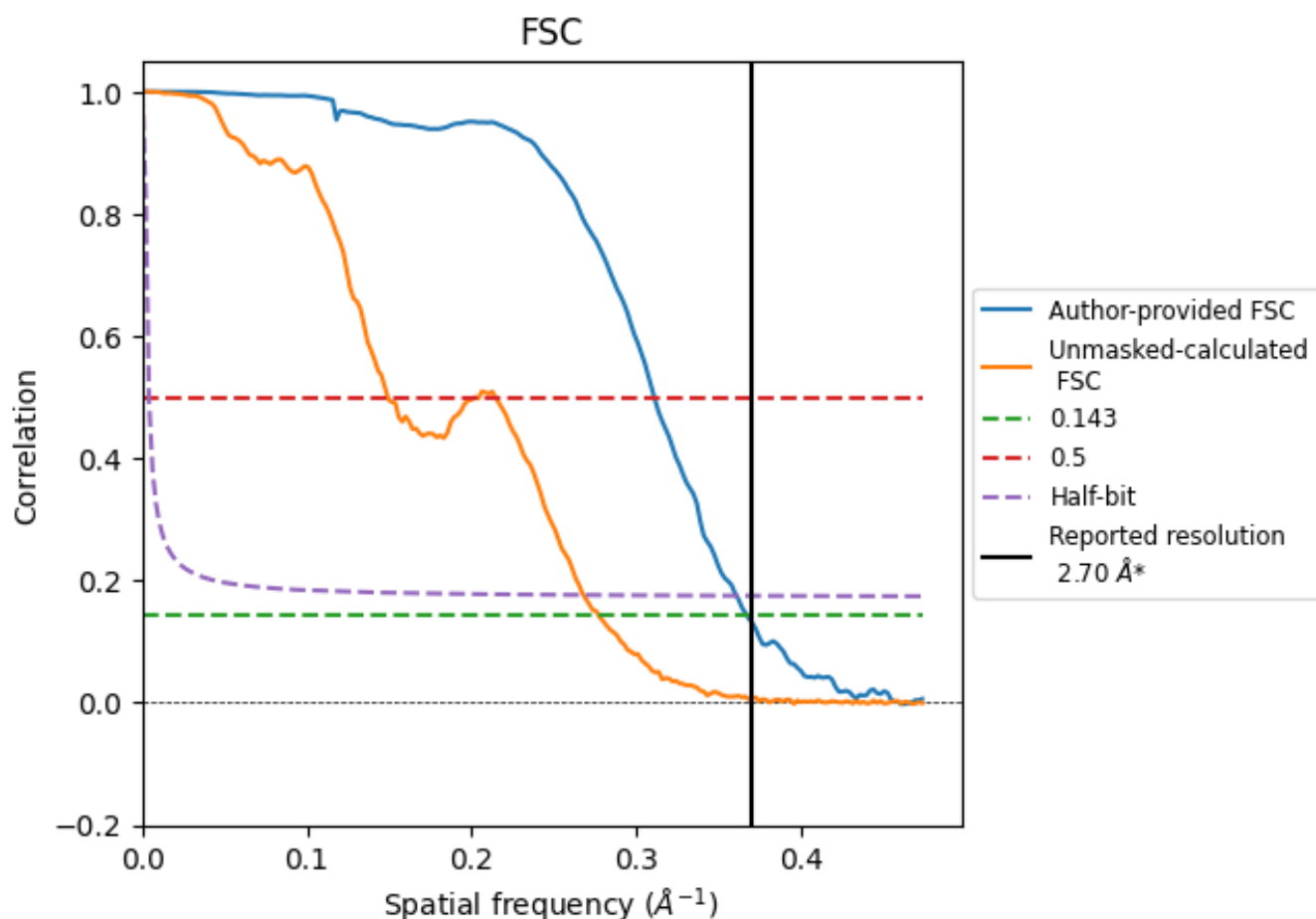


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 0.370  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.21	2.77
Unmasked-calculated*	3.60	6.70	3.73

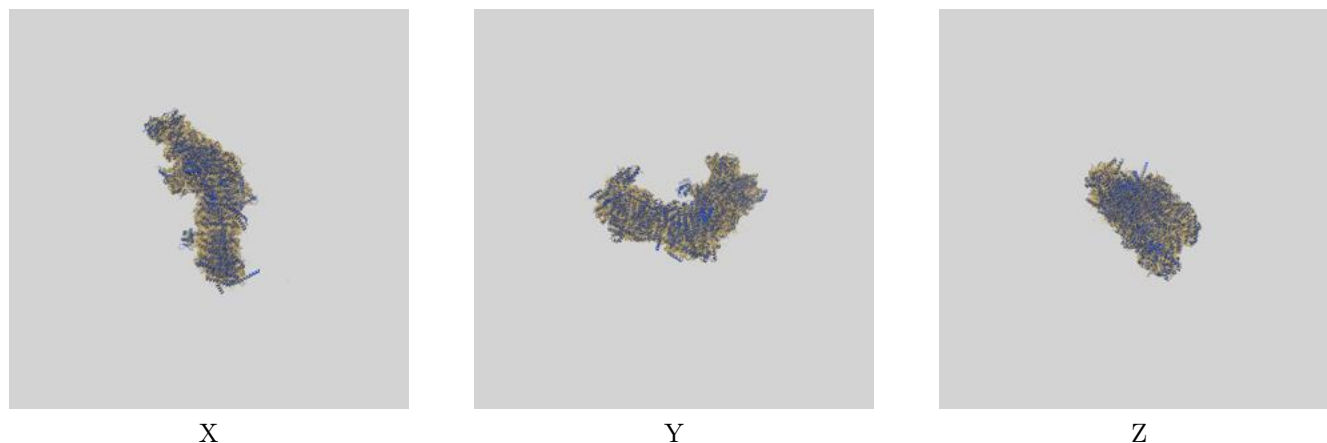
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 2.7 by more than 10 %



## 9 Map-model fit [i](#)

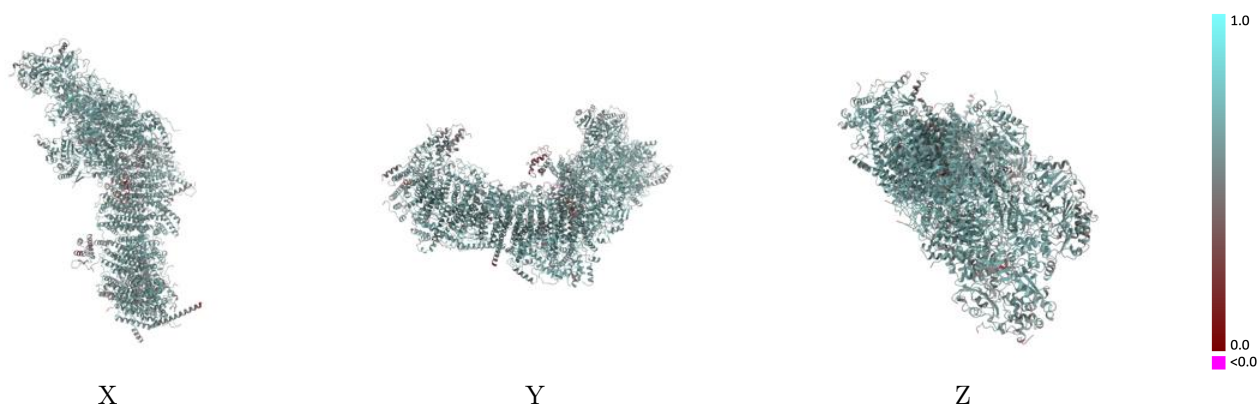
This section contains information regarding the fit between EMDB map EMD-10815 and PDB model 6YJ4. Per-residue inclusion information can be found in section [3](#) on page [21](#).

### 9.1 Map-model overlay [i](#)



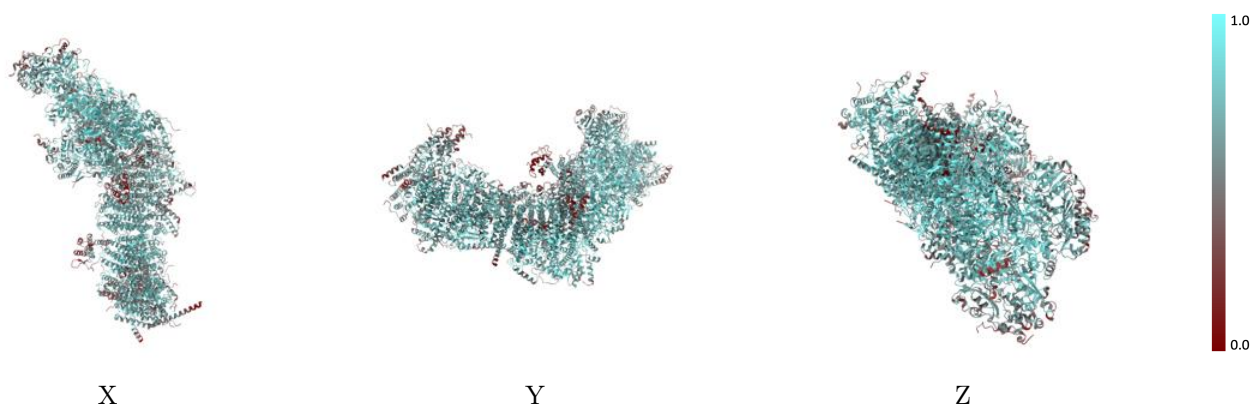
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



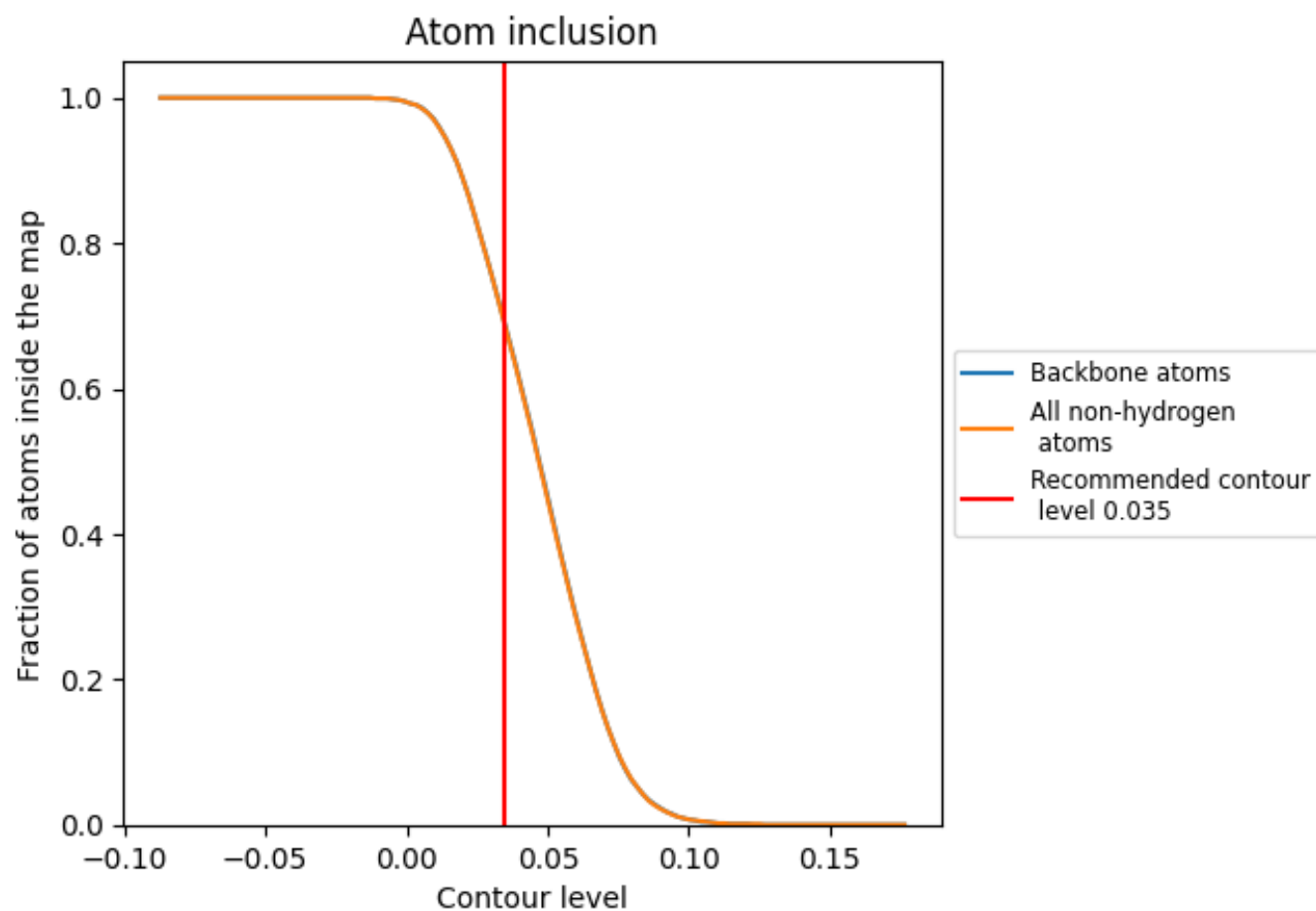
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.6020
A	 0.4610	 0.5350
B	 0.8240	 0.6470
C	 0.8190	 0.6420
D	 0.7970	 0.6390
E	 0.5920	 0.5690
F	 0.6420	 0.5810
G	 0.7410	 0.6130
H	 0.6950	 0.6100
I	 0.8330	 0.6520
J	 0.6420	 0.6030
K	 0.7370	 0.6340
L	 0.7050	 0.6110
M	 0.7730	 0.6360
N	 0.8170	 0.6520
O	 0.7280	 0.6170
P	 0.6590	 0.5860
Q	 0.7760	 0.6310
R	 0.7860	 0.6210
S	 0.5240	 0.5430
T	 0.1930	 0.3900
U	 0.3660	 0.4980
V	 0.6410	 0.5800
W	 0.6870	 0.5970
X	 0.6850	 0.6030
Y	 0.5840	 0.5790
Z	 0.6840	 0.6050
a	 0.7460	 0.6120
b	 0.6580	 0.5910
c	 0.7280	 0.6100
d	 0.6630	 0.5910
e	 0.6650	 0.5800
f	 0.7710	 0.6210
g	 0.4430	 0.4960
h	 0.6740	 0.6030



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Chain	Atom inclusion	Q-score
i	 0.6460	 0.5860
j	 0.5070	 0.5320
k	 0.4650	 0.5150
l	 0.6210	 0.5830
m	 0.6740	 0.5990
n	 0.5490	 0.5260
o	 0.5120	 0.5380
p	 0.7520	 0.6180