



Full wwPDB EM Validation Report ⓘ

May 19, 2022 – 03:34 pm BST

PDB ID : 7QSD
EMDB ID : EMD-14127
Title : Bovine complex I in the active state at 3.1 Å
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-01-13
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

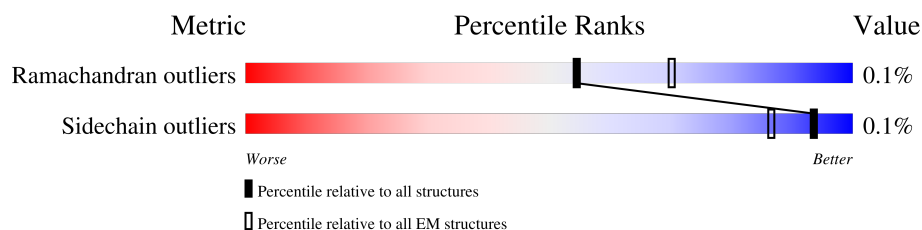
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	115	<div> <div>8%</div> <div>99%</div> <div>.</div> </div>
2	B	216	<div> <div>71%</div> <div>28%</div> </div>
3	C	266	<div> <div>78%</div> <div>22%</div> </div>
4	D	463	<div> <div>93%</div> <div>7%</div> </div>
5	E	249	<div> <div>6%</div> <div>86%</div> <div>14%</div> </div>
6	F	464	<div> <div>93%</div> <div>7%</div> </div>
7	G	727	<div> <div>95%</div> <div>5%</div> </div>
8	H	318	<div> <div>100%</div> </div>
9	I	212	<div> <div>83%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	154	
33	h	189	

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Mol	Chain	Length	Quality of chain
34	i	127	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 67258 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1655	1057	277	311	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	431	Total	C	N	O	S	0	0
			3319	2091	593	615	20		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1337	902	189	234	12		

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	341	Total	C	N	O	S	0	0
			2747	1777	486	479	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	95	Total	C	N	O	S	0	0
			730	448	137	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			677	425	126	124	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	76	Total	C	N	O	S	0	0
			612	393	90	124	5		
20	U	86	Total	C	N	O	S	0	0
			692	447	102	138	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	113	Total	C	N	O	S	0	0
			919	595	155	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			971	622	180	165	4		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	425	109	115	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	48	Total	C	N	O	0	0
			405	268	69	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			993	647	169	172	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			819	518	156	139	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	50	Total	C	N	O	S	0	0
			437	286	77	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	98	Total	C	N	O	S	0	0
			824	529	137	154	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	107	Total	C	N	O	S	0	0
			920	605	158	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	64	Total	C	N	O	S	0	0
			556	367	90	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	80	Total	C	N	O	S	0	0
			644	421	108	113	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	844	213	239	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	127	Total	C	N	O	S	0	0
			1061	681	187	193			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	172	Total	C	N	O	S	0	0
			1492	955	273	257	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	171	Total	C	N	O	S	0	0
			1443	904	266	265	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	144	Total	C	N	O	S	0	0
			1201	773	215	209	4		

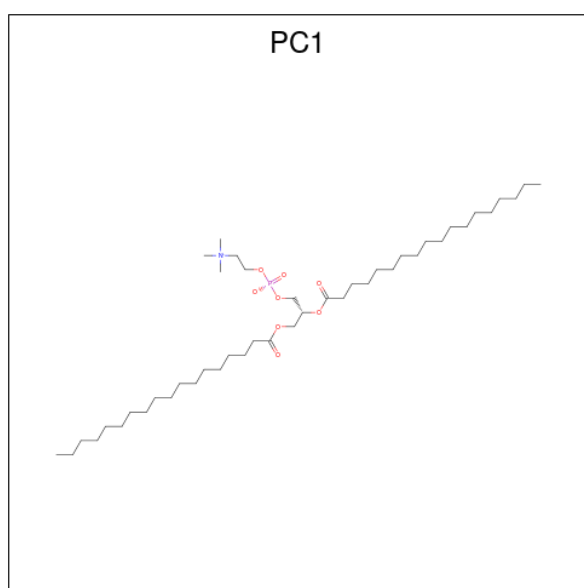
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	94	Total	C	N	O	S	0	0
			767	485	143	136	3		

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

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

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			21	11	1	8	1	
45	B	1	Total	C	N	O	P	0
			78	58	2	16	2	
45	B	1	Total	C	N	O	P	0
			78	58	2	16	2	
45	d	1	Total	C	N	O	P	0
			26	16	1	8	1	
45	g	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	I	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	J	1	Total	C	N	O	P	0
			28	18	1	8	1	
46	K	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	L	1	Total	C	N	O	P	0
			118	88	3	24	3	
46	L	1	Total	C	N	O	P	0
			118	88	3	24	3	
46	L	1	Total	C	N	O	P	0
			118	88	3	24	3	
46	M	1	Total	C	N	O	P	0
			86	66	2	16	2	
46	M	1	Total	C	N	O	P	0
			86	66	2	16	2	
46	N	1	Total	C	N	O	P	0
			85	65	2	16	2	
46	N	1	Total	C	N	O	P	0
			85	65	2	16	2	
46	X	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	c	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



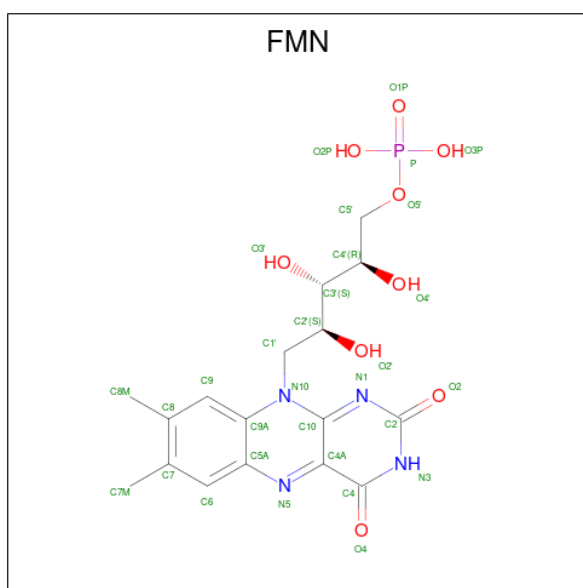
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			16	8	8	
47	G	1	Total	Fe	S	0
			16	8	8	
47	I	1	Total	Fe	S	0
			16	8	8	
47	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



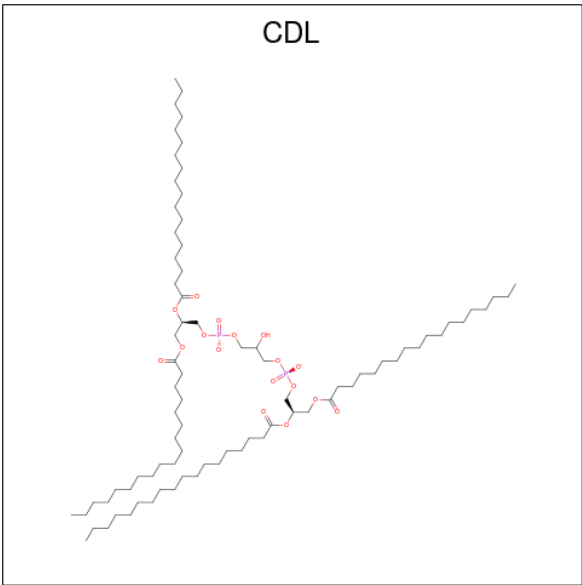
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



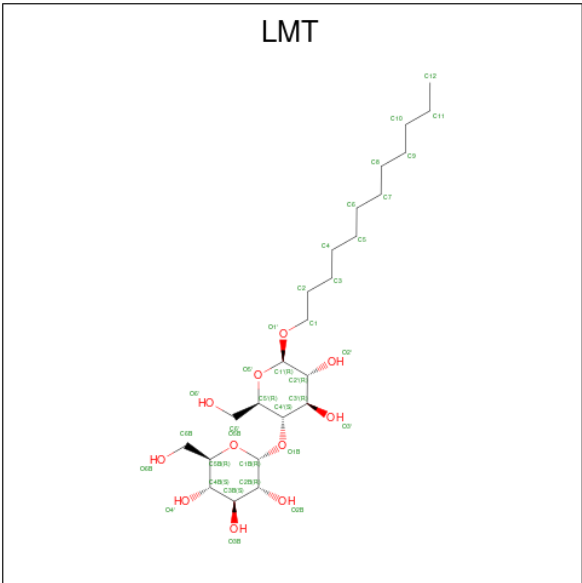
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



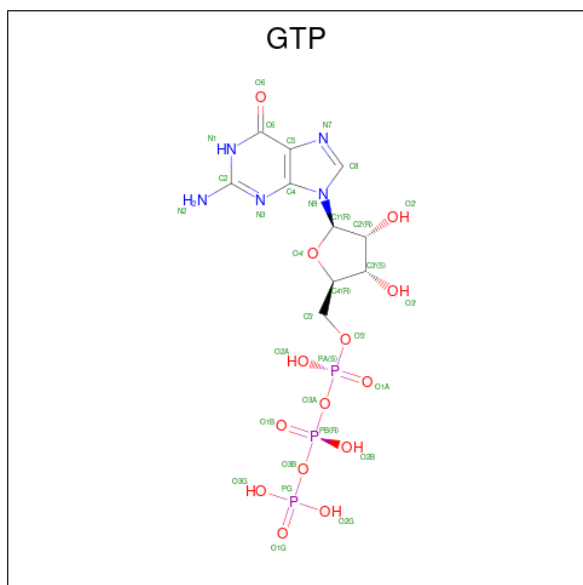
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O	P	0
			62	43	17	2	
50	Y	1	Total	C	O	P	0
			50	31	17	2	
50	h	1	Total	C	O	P	0
			64	45	17	2	
50	q	1	Total	C	O	P	0
			69	50	17	2	

- Molecule 51 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
51	M	1	Total	C	O	0
			35	24	11	
51	N	1	Total	C	O	0
			35	24	11	
51	b	1	Total	C	O	0
			35	24	11	

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
52	O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

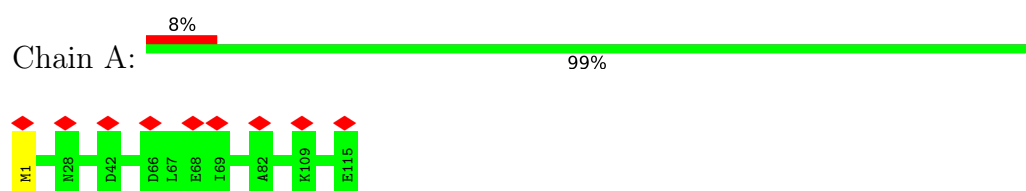


Mol	Chain	Residues	Atoms						AltConf
56	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

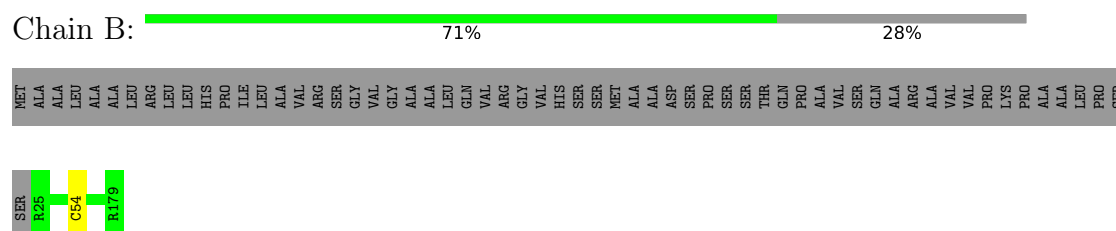
3 Residue-property plots [i](#)

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

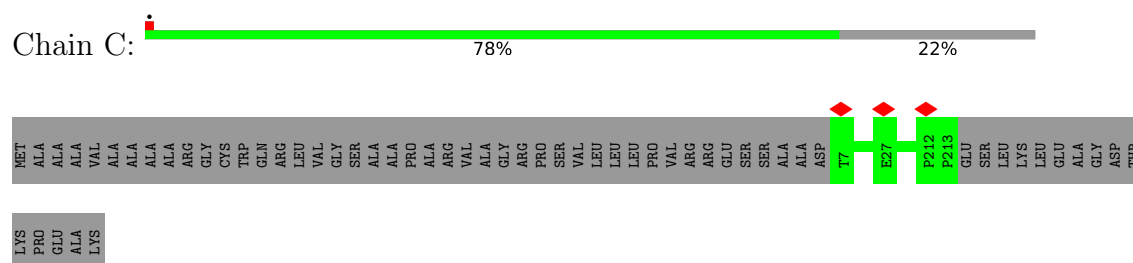
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



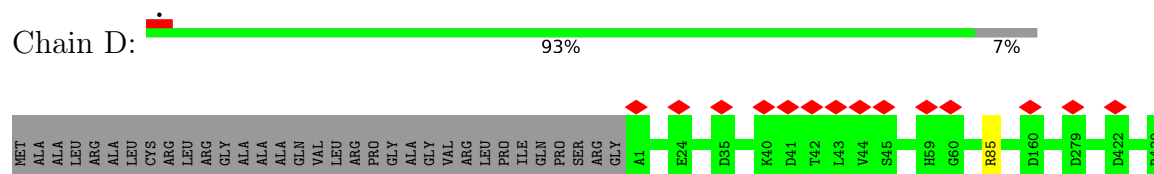
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



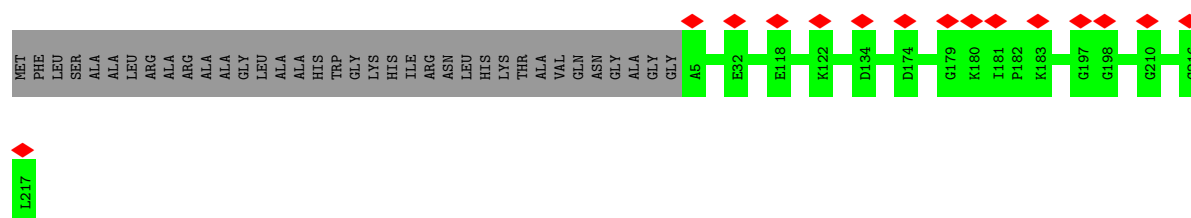
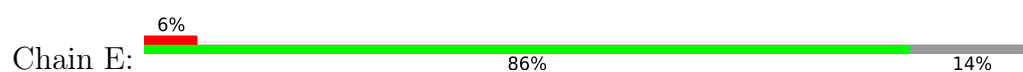
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



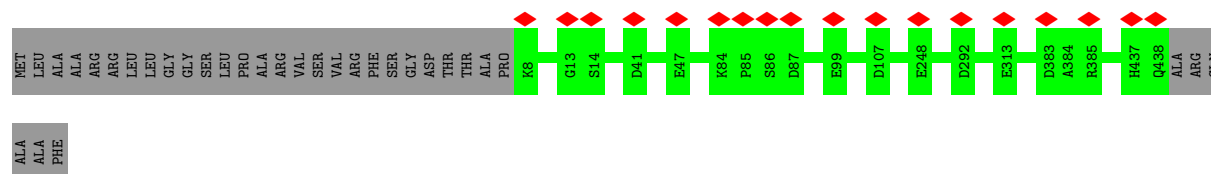
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



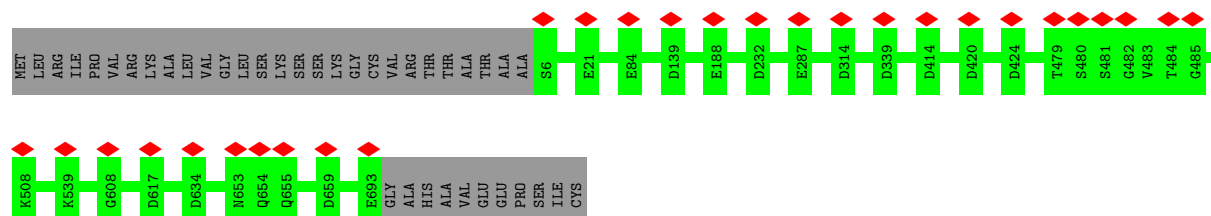
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



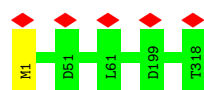
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



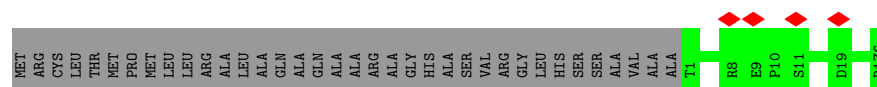
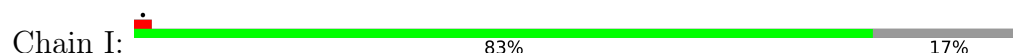
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

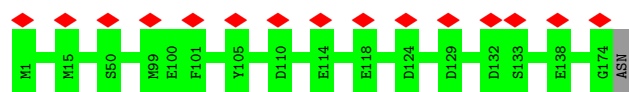


- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6





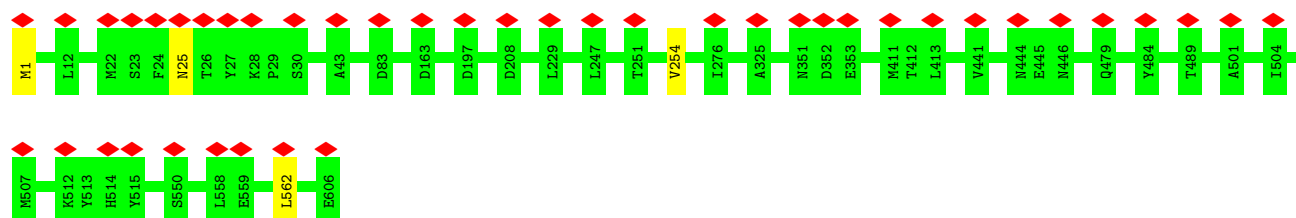
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 100%



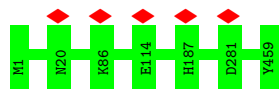
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 99% 7%



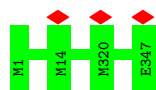
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 100%



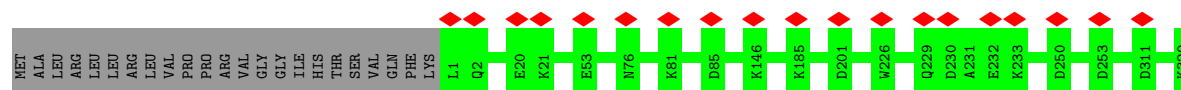
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 100%



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

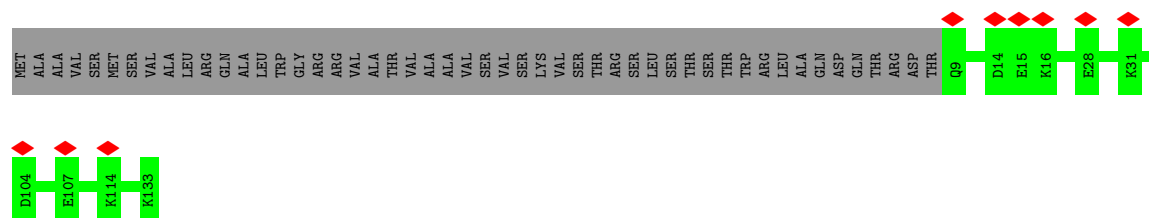
Chain O: 93% 6% 7%



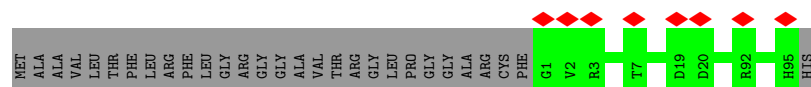
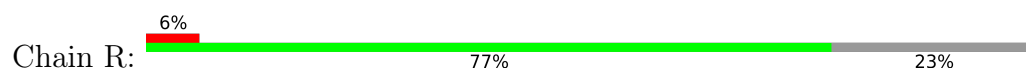
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 90% 10%

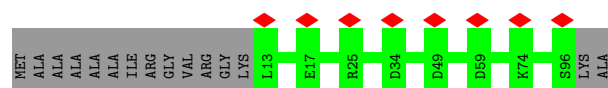
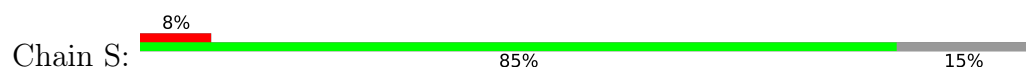
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



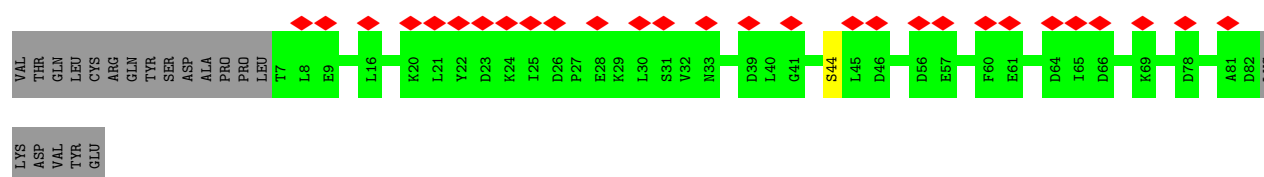
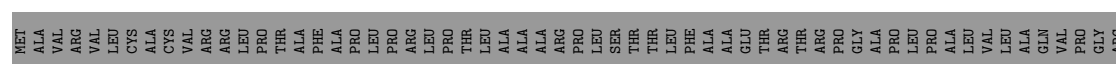
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



- Molecule 20: Acyl carrier protein, mitochondrial



- Molecule 20: Acyl carrier protein, mitochondrial



MET ALA VAL ARG LEU CYS ALA CYS ARG VAL ARG LEU PRO THR ALA PHE ALA PRO LEU PRO ARG LEU PRO THR LEU ALA ALA ARG PRO LEU SER THR THR PHE ALA ALA GLU THR ARG THR ARG PRO GLY ALA PRO PRO PRO ALA VAL VAL VAL GLN VAL VAL PRO GLY ARG

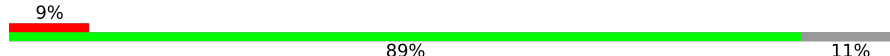
VAL THR GLN LEU CYS ARG GLN TYR SER ASP A3 K29 D39 D43 S44 D56 G59 D64 D78 E88

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

Chain V:  9% 97%

MET ALA GLY L3 L4 K5 K6 E17 E21 D32 E51 K65 K66 E78 I115

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

Chain W:  9% 89% 11%

MET ALA ALA SER GLY LEU ARG GLN ALA VAL ALA ALA SER T15 S16 D24 M25 N26 D53 K57 T74 E111 R114 D117 P128

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

Chain X:  6% 99%

MET P1 E10 R75 E79 C99 D133 E152 V153 E154 G155 D156 M171

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

Chain Y:  11% 99%

MET A1 K2 Q7 D10 E13 T46 L49 E50 E81 D84 G83 R103 T104 R105 A111 A112 Y116 L119 V140

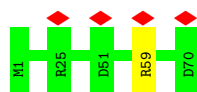
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  6% 98%

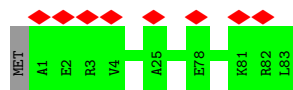
MET ALA ALA S4 G14 L25 L30 D64 D100 G103 T144

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

Chain a:  6% 99%



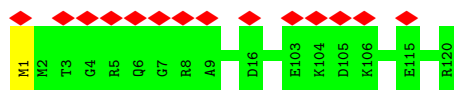
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



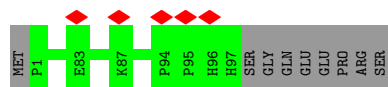
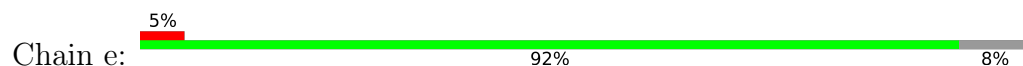
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



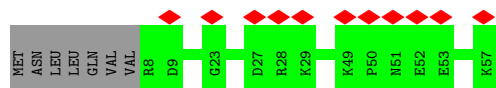
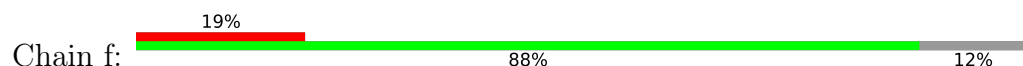
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

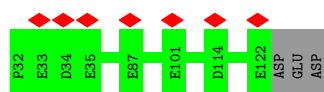


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

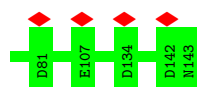
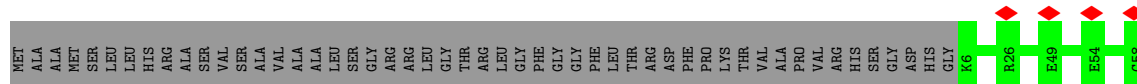


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

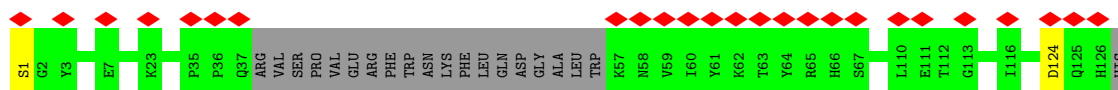
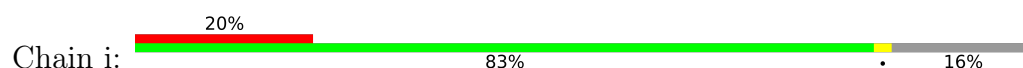




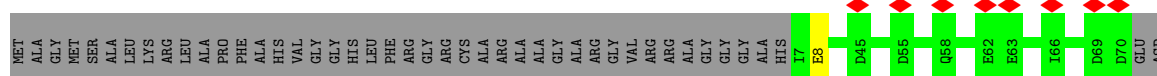
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



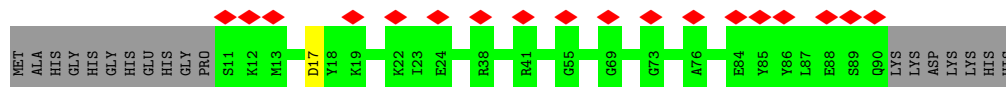
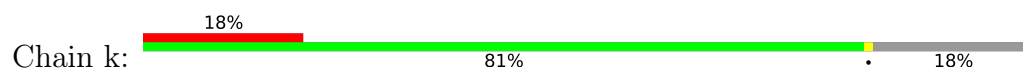
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



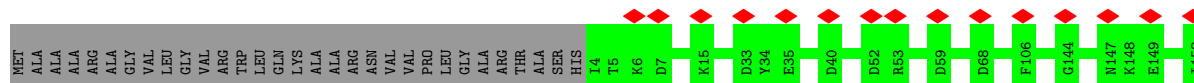
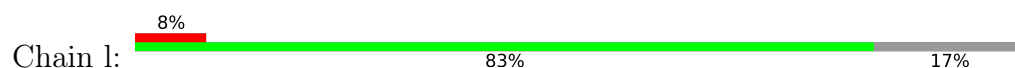
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



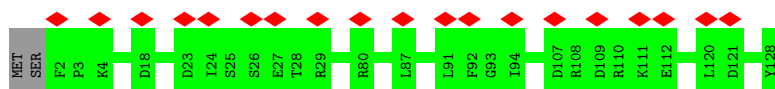
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



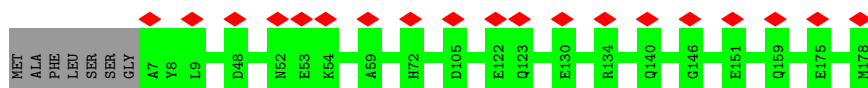
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



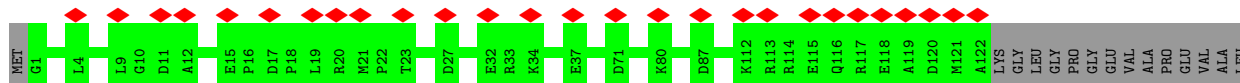
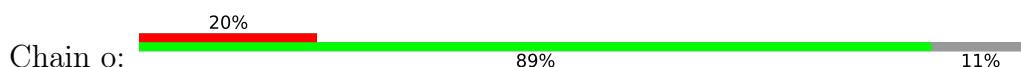
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



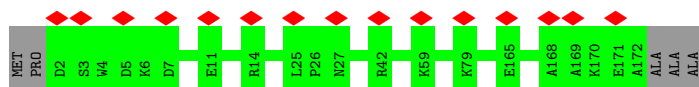
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



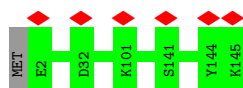
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



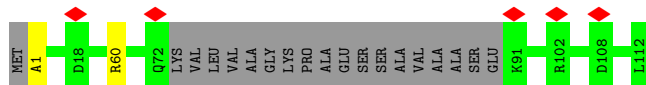
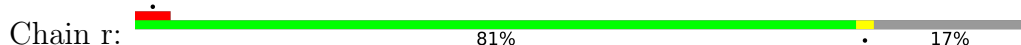
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

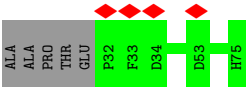


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18231	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	27.341	Depositor
Minimum map value	-13.287	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.973	Depositor
Recommended contour level	5.08	Depositor
Map size (Å)	475.2, 475.2, 475.2	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, GTP, ZN, SF4, FES, LMT, SAC, AYA, 3PE, 2MR, FME, MG, FMN, PC1, AME, CDL, EH2

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	0.34	0/936	0.43	0/1281
2	B	0.45	1/1272 (0.1%)	0.48	0/1720
3	C	0.43	0/1772	0.46	0/2413
4	D	0.41	0/3537	0.44	0/4794
5	E	0.37	0/1695	0.44	0/2307
6	F	0.36	0/3393	0.47	0/4584
7	G	0.37	0/5367	0.46	0/7274
8	H	0.38	0/2571	0.44	0/3513
9	I	0.44	0/1445	0.47	0/1956
10	J	0.39	0/1362	0.43	0/1848
11	K	0.36	0/745	0.43	0/1008
12	L	0.34	0/4920	0.43	0/6694
13	M	0.36	0/3738	0.44	0/5097
14	N	0.35	0/2792	0.44	0/3800
15	O	0.37	0/2651	0.42	0/3587
16	P	0.37	0/2824	0.45	0/3831
17	Q	0.37	0/1039	0.45	0/1404
18	R	0.41	0/742	0.46	0/999
19	S	0.33	0/688	0.45	0/927
20	T	0.30	0/621	0.40	0/837
20	U	0.35	0/704	0.42	0/950
21	V	0.33	0/939	0.40	0/1272
22	W	0.37	0/995	0.42	0/1337
23	X	0.37	0/1439	0.44	0/1942
24	Y	0.31	0/1042	0.43	0/1414
25	Z	0.37	0/1181	0.42	0/1592
26	a	0.36	0/584	0.42	0/786
27	b	0.34	0/672	0.42	0/923
28	c	0.34	0/418	0.37	0/567
29	d	0.42	0/1012	0.42	0/1368
30	e	0.34	0/840	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.34	0/450	0.42	0/606
32	g	0.37	0/850	0.42	0/1154
33	h	0.36	0/1188	0.41	0/1607
34	i	0.34	0/941	0.41	0/1279
35	j	0.36	0/582	0.38	0/799
36	k	0.31	0/663	0.40	0/895
37	l	0.38	0/1358	0.42	0/1858
38	m	0.36	0/1088	0.42	0/1472
39	n	0.36	0/1545	0.39	0/2092
40	o	0.32	0/1073	0.39	0/1437
41	p	0.37	0/1476	0.41	0/1990
42	q	0.40	0/1242	0.45	0/1688
43	r	0.37	0/780	0.42	0/1056
44	s	0.34	0/383	0.43	0/518
All	All	0.37	1/67555 (0.0%)	0.44	0/91599

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	CYS	CB-SG	-5.31	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	B	153/216 (71%)	145 (95%)	8 (5%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100
4	D	427/463 (92%)	397 (93%)	30 (7%)	0	100	100
5	E	211/249 (85%)	192 (91%)	19 (9%)	0	100	100
6	F	429/464 (92%)	410 (96%)	19 (4%)	0	100	100
7	G	686/727 (94%)	642 (94%)	44 (6%)	0	100	100
8	H	316/318 (99%)	293 (93%)	23 (7%)	0	100	100
9	I	174/212 (82%)	165 (95%)	9 (5%)	0	100	100
10	J	172/175 (98%)	160 (93%)	12 (7%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	557 (92%)	44 (7%)	3 (0%)	29	64
13	M	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	O	318/343 (93%)	300 (94%)	18 (6%)	0	100	100
16	P	339/380 (89%)	318 (94%)	21 (6%)	0	100	100
17	Q	123/175 (70%)	117 (95%)	6 (5%)	0	100	100
18	R	93/124 (75%)	88 (95%)	5 (5%)	0	100	100
19	S	82/99 (83%)	76 (93%)	6 (7%)	0	100	100
20	T	74/156 (47%)	71 (96%)	3 (4%)	0	100	100
20	U	84/156 (54%)	82 (98%)	1 (1%)	1 (1%)	13	44
21	V	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
22	W	112/128 (88%)	106 (95%)	6 (5%)	0	100	100
23	X	169/172 (98%)	154 (91%)	14 (8%)	1 (1%)	25	59
24	Y	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
25	Z	139/144 (96%)	129 (93%)	10 (7%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
30	e	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
31	f	48/57 (84%)	44 (92%)	4 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	96/154 (62%)	89 (93%)	7 (7%)	0	100	100
33	h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	i	103/127 (81%)	92 (89%)	10 (10%)	1 (1%)	15	49
35	j	62/108 (57%)	59 (95%)	2 (3%)	1 (2%)	9	37
36	k	78/98 (80%)	72 (92%)	5 (6%)	1 (1%)	12	42
37	l	153/186 (82%)	142 (93%)	11 (7%)	0	100	100
38	m	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
39	n	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
40	o	120/137 (88%)	107 (89%)	13 (11%)	0	100	100
41	p	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	82 (91%)	8 (9%)	0	100	100
44	s	42/109 (38%)	38 (90%)	4 (10%)	0	100	100
All	All	8112/9212 (88%)	7640 (94%)	464 (6%)	8 (0%)	54	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	99	CYS
12	L	562	LEU
20	U	43	ASP
35	j	8	GLU
12	L	25	ASN
34	i	124	ASP
36	k	17	ASP
12	L	254	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	533/533 (100%)	533 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	295/327 (90%)	295 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	78/97 (80%)	78 (100%)	0	100	100
19	S	75/82 (92%)	75 (100%)	0	100	100
20	T	70/135 (52%)	69 (99%)	1 (1%)	67	86
20	U	79/135 (58%)	78 (99%)	1 (1%)	69	87
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	120/121 (99%)	120 (100%)	0	100	100
26	a	59/59 (100%)	58 (98%)	1 (2%)	60	83
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	104/105 (99%)	104 (100%)	0	100	100
30	e	88/96 (92%)	88 (100%)	0	100	100
31	f	47/54 (87%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	89/131 (68%)	89 (100%)	0	100	100
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	102/120 (85%)	102 (100%)	0	100	100
35	j	59/84 (70%)	59 (100%)	0	100	100
36	k	62/76 (82%)	62 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	113/115 (98%)	113 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	110/120 (92%)	110 (100%)	0	100	100
41	p	155/157 (99%)	155 (100%)	0	100	100
42	q	130/131 (99%)	130 (100%)	0	100	100
43	r	84/97 (87%)	83 (99%)	1 (1%)	71	88
44	s	43/92 (47%)	43 (100%)	0	100	100
All	All	7156/7892 (91%)	7152 (100%)	4 (0%)	93	98

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

Mol	Chain	Res	Type
20	T	44	SER
20	U	44	SER
26	a	59	ARG
43	r	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
7	G	401	HIS
12	L	248	HIS
12	L	514	HIS
22	W	48	HIS
22	W	108	HIS
44	s	43	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	FME	H	1	8	8,9,10	0.90	0	7,9,11	1.08	1 (14%)
34	SAC	i	1	34	7,8,9	0.91	0	8,9,11	1.02	1 (12%)
1	FME	A	1	1	8,9,10	1.03	1 (12%)	7,9,11	0.61	0
29	AME	d	1	29	9,10,11	1.48	1 (11%)	9,11,13	1.54	2 (22%)
10	FME	J	1	10	8,9,10	0.91	0	7,9,11	0.89	0
4	2MR	D	85	4	10,12,13	2.40	2 (20%)	5,13,15	1.30	0
13	FME	M	1	13	8,9,10	0.94	0	7,9,11	0.96	0
43	AYA	r	1	43	6,7,8	1.41	1 (16%)	5,8,10	0.98	0
12	FME	L	1	12	8,9,10	1.00	1 (12%)	7,9,11	0.75	0
24	AYA	Y	1	24	6,7,8	1.29	1 (16%)	5,8,10	1.54	1 (20%)
14	FME	N	1	14	8,9,10	0.96	0	7,9,11	0.94	0
11	FME	K	1	11	8,9,10	0.97	0	7,9,11	0.72	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	H	1	8	-	3/7/9/11	-
34	SAC	i	1	34	-	2/7/8/10	-
1	FME	A	1	1	-	0/7/9/11	-
29	AME	d	1	29	-	6/9/10/12	-
10	FME	J	1	10	-	3/7/9/11	-
4	2MR	D	85	4	-	1/10/13/15	-
13	FME	M	1	13	-	0/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
12	FME	L	1	12	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AYA	Y	1	24	-	0/4/6/8	-
14	FME	N	1	14	-	3/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.30	1.45	1.33
4	D	85	2MR	CZ-NE	4.89	1.44	1.34
29	d	1	AME	CT1-N	3.38	1.46	1.34
43	r	1	AYA	CA-N	-2.99	1.43	1.46
24	Y	1	AYA	CA-N	-2.67	1.43	1.46
1	A	1	FME	CA-N	-2.22	1.43	1.46
12	L	1	FME	CA-N	-2.08	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	1	AYA	CB-CA-N	3.29	113.27	109.61
29	d	1	AME	CE-SD-CG	2.60	109.32	100.40
29	d	1	AME	CT2-CT1-N	2.36	120.10	116.10
34	i	1	SAC	OG-CB-CA	-2.23	105.27	110.97
8	H	1	FME	C-CA-N	2.08	113.48	109.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
12	L	1	FME	O1-CN-N-CA
12	L	1	FME	CA-CB-CG-SD
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	CB-CA-N-CN
29	d	1	AME	O-C-CA-CB
29	d	1	AME	CB-CA-N-CT1
34	i	1	SAC	C-CA-N-C1A
34	i	1	SAC	CB-CA-N-C1A
29	d	1	AME	CA-CB-CG-SD
10	J	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
14	N	1	FME	N-CA-CB-CG
29	d	1	AME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
29	d	1	AME	CB-CG-SD-CE
11	K	1	FME	CA-CB-CG-SD
29	d	1	AME	C-CA-N-CT1
8	H	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	$\# Z > 2$
46	3PE	K	101	-	38,38,50	1.00	4 (10%)	41,43,55	1.11	2 (4%)
46	3PE	c	301	-	37,37,50	0.99	3 (8%)	40,42,55	0.99	2 (5%)
46	3PE	A	702	-	38,38,50	0.98	4 (10%)	41,43,55	1.11	2 (4%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
50	CDL	Y	701	-	49,49,99	1.21	8 (16%)	55,61,111	1.31	4 (7%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
46	3PE	N	902	-	43,43,50	0.92	3 (6%)	46,48,55	1.04	2 (4%)
50	CDL	L	702	-	61,61,99	1.12	8 (13%)	67,73,111	1.14	4 (5%)
51	LMT	N	901	-	36,36,36	1.13	2 (5%)	47,47,47	1.17	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	PC1	g	1501	-	48,48,53	1.00	3 (6%)	54,56,61	1.08	2 (3%)
50	CDL	q	201	-	68,68,99	1.03	8 (11%)	74,80,111	1.11	4 (5%)
45	PC1	d	501	-	25,25,53	1.37	4 (16%)	31,33,61	1.03	2 (6%)
51	LMT	M	602	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	1 (2%)
46	3PE	L	701	-	37,37,50	1.01	4 (10%)	40,42,55	1.13	2 (5%)
46	3PE	M	601	-	45,45,50	0.91	4 (8%)	48,50,55	1.22	2 (4%)
46	3PE	J	401	-	27,27,50	1.08	3 (11%)	30,32,55	1.10	1 (3%)
47	SF4	G	801	7	0,12,12	-	-	-		
47	SF4	F	502	6	0,12,12	-	-	-		
47	SF4	I	202	9	0,12,12	-	-	-		
49	FMN	F	501	-	31,33,33	1.33	6 (19%)	40,50,50	1.81	6 (15%)
56	EHZ	U	101	20	29,36,37	1.64	5 (17%)	35,44,47	1.35	3 (8%)
45	PC1	B	202	-	42,42,53	1.05	4 (9%)	48,50,61	1.04	2 (4%)
45	PC1	A	701	-	20,20,53	1.89	3 (15%)	24,27,61	1.13	1 (4%)
45	PC1	B	203	-	34,34,53	1.19	4 (11%)	40,42,61	1.09	2 (5%)
46	3PE	L	703	-	44,44,50	0.90	4 (9%)	47,49,55	1.14	3 (6%)
46	3PE	M	603	-	39,39,50	0.96	4 (10%)	42,44,55	1.07	2 (4%)
46	3PE	N	903	-	40,40,50	0.95	4 (10%)	43,45,55	1.20	2 (4%)
47	SF4	B	201	2	0,12,12	-	-	-		
51	LMT	b	301	-	36,36,36	1.19	3 (8%)	47,47,47	1.34	5 (10%)
50	CDL	h	1001	-	63,63,99	1.10	8 (12%)	69,75,111	1.22	5 (7%)
48	FES	G	803	7	0,4,4	-	-	-		
56	EHZ	T	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.73	7 (20%)
54	NDP	P	501	-	45,52,52	2.09	8 (17%)	53,80,80	1.75	10 (18%)
52	GTP	O	401	53	26,34,34	2.95	10 (38%)	33,54,54	2.02	14 (42%)
47	SF4	G	802	7	0,12,12	-	-	-		
46	3PE	X	401	-	30,30,50	1.09	3 (10%)	33,35,55	1.24	2 (6%)
46	3PE	L	704	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
46	3PE	I	201	-	41,41,50	0.93	3 (7%)	44,46,55	1.18	2 (4%)

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
46	3PE	K	101	-	-	19/42/42/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	c	301	-	-	22/41/41/54	-
46	3PE	A	702	-	-	16/42/42/54	-
48	FES	E	301	5	-	-	0/1/1/1
50	CDL	Y	701	-	-	23/59/59/110	-
50	CDL	L	702	-	-	34/72/72/110	-
46	3PE	N	902	-	-	24/47/47/54	-
51	LMT	N	901	-	-	5/21/61/61	0/2/2/2
47	SF4	I	203	9	-	-	0/6/5/5
45	PC1	g	1501	-	-	23/52/52/57	-
50	CDL	q	201	-	-	35/79/79/110	-
45	PC1	d	501	-	-	11/29/29/57	-
51	LMT	M	602	-	-	6/21/61/61	0/2/2/2
46	3PE	L	701	-	-	19/41/41/54	-
46	3PE	M	601	-	-	20/49/49/54	-
46	3PE	J	401	-	-	12/30/30/54	-
56	EHZ	U	101	20	-	7/42/44/45	-
47	SF4	F	502	6	-	-	0/6/5/5
47	SF4	G	801	7	-	-	0/6/5/5
49	FMN	F	501	-	-	3/18/18/18	0/3/3/3
47	SF4	I	202	9	-	-	0/6/5/5
45	PC1	B	202	-	-	22/46/46/57	-
45	PC1	A	701	-	-	13/22/22/57	-
45	PC1	B	203	-	-	12/38/38/57	-
46	3PE	L	703	-	-	23/48/48/54	-
46	3PE	M	603	-	-	20/43/43/54	-
46	3PE	N	903	-	-	19/44/44/54	-
47	SF4	B	201	2	-	-	0/6/5/5
51	LMT	b	301	-	-	8/21/61/61	0/2/2/2
50	CDL	h	1001	-	-	28/74/74/110	-
48	FES	G	803	7	-	-	0/1/1/1
56	EHZ	T	101	20	-	11/42/44/45	-
54	NDP	P	501	-	-	9/30/77/77	0/5/5/5
52	GTP	O	401	53	-	0/18/38/38	0/3/3/3
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	X	401	-	-	16/34/34/54	-
46	3PE	L	704	-	-	20/38/38/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	I	201	-	-	18/45/45/54	-

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	P2B-O2B	10.95	1.80	1.59
52	O	401	GTP	C2-N1	8.08	1.49	1.35
52	O	401	GTP	O6-C6	6.17	1.40	1.24
45	A	701	PC1	O21-C2	-5.79	1.40	1.46
52	O	401	GTP	C2-N2	5.54	1.45	1.33
56	T	101	EHZ	C12-N1	5.29	1.45	1.33
52	O	401	GTP	O4'-C1'	5.28	1.48	1.41
56	U	101	EHZ	C15-N2	5.15	1.44	1.33
56	U	101	EHZ	C12-N1	4.99	1.44	1.33
56	T	101	EHZ	C15-N2	4.93	1.44	1.33
54	P	501	NDP	PN-O5D	3.51	1.73	1.59
51	b	301	LMT	O5B-C1B	3.45	1.50	1.41
52	O	401	GTP	C2'-C1'	-3.30	1.48	1.53
51	M	602	LMT	O5B-C1B	3.30	1.50	1.41
54	P	501	NDP	O2B-C2B	-3.29	1.32	1.44
51	N	901	LMT	O5B-C1B	3.22	1.50	1.41
49	F	501	FMN	C10-N1	3.20	1.37	1.33
51	b	301	LMT	O5'-C1'	3.14	1.49	1.41
45	A	701	PC1	O21-C21	3.09	1.40	1.33
54	P	501	NDP	C7N-C3N	-2.83	1.42	1.48
49	F	501	FMN	C1'-N10	2.82	1.51	1.48
51	M	602	LMT	O5'-C1'	2.80	1.49	1.41
51	N	901	LMT	O5'-C1'	2.78	1.48	1.41
50	h	1001	CDL	OA6-CA4	-2.78	1.39	1.46
46	L	701	3PE	O21-C2	-2.77	1.39	1.46
50	L	702	CDL	OA6-CA4	-2.76	1.39	1.46
52	O	401	GTP	C6-N1	2.73	1.37	1.33
50	L	702	CDL	OB6-CB4	-2.73	1.39	1.46
45	B	203	PC1	O21-C2	-2.72	1.39	1.46
50	q	201	CDL	OA6-CA4	-2.72	1.39	1.46
46	X	401	3PE	O21-C2	-2.71	1.39	1.46
46	L	704	3PE	O21-C2	-2.70	1.39	1.46
45	g	1501	PC1	O21-C2	-2.69	1.39	1.46
49	F	501	FMN	C4-N3	2.67	1.37	1.33
46	I	201	3PE	O21-C2	-2.67	1.39	1.46
56	T	101	EHZ	O3-C12	-2.64	1.17	1.23
46	K	101	3PE	O31-C31	2.63	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B	202	PC1	O21-C2	-2.63	1.40	1.46
46	A	702	3PE	O21-C2	-2.61	1.40	1.46
50	h	1001	CDL	OB6-CB4	-2.59	1.40	1.46
46	L	703	3PE	O21-C2	-2.59	1.40	1.46
46	N	902	3PE	O21-C2	-2.59	1.40	1.46
45	d	501	PC1	O21-C2	-2.57	1.40	1.46
50	L	702	CDL	OB8-CB7	2.56	1.40	1.33
46	c	301	3PE	O21-C2	-2.55	1.40	1.46
46	J	401	3PE	O21-C2	-2.52	1.40	1.46
50	q	201	CDL	OB6-CB4	-2.51	1.40	1.46
46	L	701	3PE	O31-C3	-2.51	1.39	1.45
56	T	101	EHZ	O4-C15	-2.50	1.18	1.23
50	h	1001	CDL	OB8-CB7	2.50	1.40	1.33
50	L	702	CDL	OA8-CA7	2.49	1.40	1.33
46	M	603	3PE	O21-C2	-2.48	1.40	1.46
46	M	601	3PE	O21-C2	-2.48	1.40	1.46
46	c	301	3PE	O31-C31	2.47	1.40	1.33
45	d	501	PC1	O31-C31	2.46	1.40	1.33
50	h	1001	CDL	OA8-CA7	2.46	1.40	1.33
56	U	101	EHZ	O4-C15	-2.46	1.18	1.23
46	L	704	3PE	O31-C31	2.45	1.40	1.33
46	K	101	3PE	O21-C2	-2.45	1.40	1.46
52	O	401	GTP	C2'-C3'	-2.45	1.46	1.53
50	Y	701	CDL	OA6-CA4	-2.44	1.40	1.46
46	M	603	3PE	O31-C31	2.44	1.40	1.33
54	P	501	NDP	O5D-C5D	-2.42	1.35	1.44
50	q	201	CDL	OA8-CA7	2.42	1.40	1.33
46	N	903	3PE	O21-C2	-2.40	1.40	1.46
50	Y	701	CDL	OA8-CA7	2.40	1.40	1.33
46	I	201	3PE	O31-C3	-2.38	1.39	1.45
56	T	101	EHZ	C9-S1	2.38	1.81	1.76
50	Y	701	CDL	OB6-CB4	-2.37	1.40	1.46
45	B	203	PC1	O31-C31	2.37	1.40	1.33
46	L	703	3PE	O31-C3	-2.37	1.39	1.45
50	Y	701	CDL	OB8-CB7	2.36	1.40	1.33
45	g	1501	PC1	O31-C3	-2.32	1.39	1.45
50	q	201	CDL	OB8-CB7	2.31	1.40	1.33
56	U	101	EHZ	O3-C12	-2.31	1.18	1.23
49	F	501	FMN	C4A-N5	2.30	1.36	1.33
45	B	202	PC1	O31-C31	2.30	1.40	1.33
50	h	1001	CDL	OB6-CB5	2.30	1.40	1.34
50	Y	701	CDL	OB6-CB5	2.30	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	N	902	3PE	O31-C31	2.30	1.40	1.33
46	M	601	3PE	O31-C3	-2.29	1.39	1.45
46	A	702	3PE	O31-C31	2.28	1.40	1.33
46	X	401	3PE	O31-C31	2.27	1.40	1.33
46	J	401	3PE	O31-C3	-2.25	1.40	1.45
46	N	903	3PE	O31-C31	2.25	1.39	1.33
52	O	401	GTP	PG-O2G	-2.25	1.46	1.54
45	g	1501	PC1	O31-C31	2.24	1.39	1.33
46	N	903	3PE	O31-C3	-2.23	1.40	1.45
46	c	301	3PE	O31-C3	-2.21	1.40	1.45
46	M	601	3PE	O31-C31	2.21	1.39	1.33
52	O	401	GTP	PG-O3G	-2.20	1.46	1.54
46	L	701	3PE	O31-C31	2.20	1.39	1.33
45	d	501	PC1	O31-C3	-2.19	1.40	1.45
56	U	101	EHZ	C9-S1	2.19	1.81	1.76
46	K	101	3PE	O21-C21	2.19	1.40	1.34
46	A	702	3PE	O21-C21	2.19	1.40	1.34
49	F	501	FMN	C6-C5A	-2.18	1.38	1.41
46	N	902	3PE	O31-C3	-2.18	1.40	1.45
46	N	903	3PE	O21-C21	2.17	1.40	1.34
46	M	601	3PE	O21-C21	2.17	1.40	1.34
46	A	702	3PE	O31-C3	-2.17	1.40	1.45
50	h	1001	CDL	OB8-CB6	-2.16	1.40	1.45
46	L	703	3PE	O31-C31	2.16	1.39	1.33
50	L	702	CDL	OA8-CA6	-2.15	1.40	1.45
46	I	201	3PE	O31-C31	2.15	1.39	1.33
46	J	401	3PE	O21-C21	2.15	1.40	1.34
50	q	201	CDL	OB6-CB5	2.15	1.40	1.34
50	q	201	CDL	OB8-CB6	-2.14	1.40	1.45
46	M	603	3PE	O21-C21	2.13	1.40	1.34
51	b	301	LMT	O5B-C5B	2.13	1.49	1.44
45	B	202	PC1	O31-C3	-2.12	1.40	1.45
46	X	401	3PE	O31-C3	-2.12	1.40	1.45
50	q	201	CDL	OA8-CA6	-2.12	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.12	1.40	1.45
50	Y	701	CDL	OB8-CB6	-2.11	1.40	1.45
45	A	701	PC1	O31-C3	-2.11	1.40	1.45
54	P	501	NDP	O3B-C3B	-2.11	1.38	1.43
50	q	201	CDL	OA6-CA5	2.10	1.40	1.34
50	L	702	CDL	OB6-CB5	2.09	1.40	1.34
49	F	501	FMN	C4A-C4	-2.09	1.37	1.41
45	B	203	PC1	O31-C3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	h	1001	CDL	OA8-CA6	-2.08	1.40	1.45
54	P	501	NDP	O2D-C2D	-2.08	1.38	1.43
45	d	501	PC1	O21-C21	2.08	1.40	1.34
46	M	603	3PE	O31-C3	-2.07	1.40	1.45
50	Y	701	CDL	OA8-CA6	-2.07	1.40	1.45
54	P	501	NDP	O3D-C3D	-2.06	1.38	1.43
45	B	203	PC1	O21-C21	2.06	1.40	1.34
50	h	1001	CDL	OA6-CA5	2.05	1.40	1.34
45	B	202	PC1	O21-C21	2.05	1.40	1.34
46	L	703	3PE	O21-C21	2.04	1.40	1.34
46	L	704	3PE	O31-C3	-2.03	1.40	1.45
46	K	101	3PE	O31-C3	-2.03	1.40	1.45
50	L	702	CDL	OA6-CA5	2.01	1.40	1.34
46	L	704	3PE	O21-C21	2.01	1.40	1.34
46	L	701	3PE	O21-C21	2.01	1.40	1.34
52	O	401	GTP	C2-N3	2.00	1.44	1.34
50	Y	701	CDL	OA6-CA5	2.00	1.40	1.34

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	F	501	FMN	C1'-N10-C9A	7.50	124.20	118.29
54	P	501	NDP	PN-O3-PA	-7.29	107.80	132.83
56	T	101	EHZ	C8-C9-S1	6.21	121.31	113.63
50	Y	701	CDL	OB6-CB5-C51	5.54	121.29	111.09
56	U	101	EHZ	C8-C9-S1	5.06	119.89	113.63
49	F	501	FMN	C2-N3-C4	5.03	119.39	115.14
50	h	1001	CDL	OB6-CB5-C51	5.01	122.30	111.50
46	M	601	3PE	O21-C21-C22	4.75	121.74	111.50
46	N	903	3PE	O21-C21-C22	4.54	121.28	111.50
45	A	701	PC1	O21-C21-O22	-4.33	120.05	125.57
46	I	201	3PE	O21-C21-C22	4.31	120.78	111.50
52	O	401	GTP	C2-N3-C4	-4.21	110.55	115.36
46	L	703	3PE	O21-C21-C22	4.16	120.46	111.50
46	X	401	3PE	O21-C21-C22	4.13	120.40	111.50
46	A	702	3PE	O21-C21-C22	4.09	120.31	111.50
46	L	704	3PE	O21-C21-C22	4.08	120.29	111.50
45	g	1501	PC1	O21-C21-C22	4.07	120.27	111.50
50	L	702	CDL	OA6-CA5-C11	4.07	120.27	111.50
50	q	201	CDL	OB6-CB5-C51	4.05	120.24	111.50
46	L	701	3PE	O21-C21-C22	4.00	120.13	111.50
45	B	203	PC1	O21-C21-C22	3.92	119.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	K	101	3PE	O21-C21-C22	3.90	119.90	111.50
45	B	202	PC1	O21-C21-C22	3.89	119.89	111.50
46	J	401	3PE	O21-C21-C22	3.87	119.84	111.50
50	h	1001	CDL	OA6-CA5-C11	3.82	119.72	111.50
46	M	603	3PE	O21-C21-C22	3.80	119.70	111.50
50	L	702	CDL	OB6-CB5-C51	3.80	119.69	111.50
50	Y	701	CDL	OA6-CA5-C11	3.79	119.66	111.50
52	O	401	GTP	C1'-N9-C4	-3.77	120.02	126.64
50	q	201	CDL	OA6-CA5-C11	3.68	119.42	111.50
54	P	501	NDP	O2B-P2B-O1X	-3.54	95.72	109.39
51	b	301	LMT	C1'-C2'-C3'	3.46	117.21	110.00
56	T	101	EHZ	C10-S1-C9	3.40	112.47	101.87
56	T	101	EHZ	C13-C12-N1	3.30	121.98	116.42
46	K	101	3PE	O31-C31-C32	3.30	122.27	111.91
52	O	401	GTP	N3-C2-N1	-3.17	123.00	127.22
46	N	902	3PE	O21-C21-C22	3.15	118.29	111.50
52	O	401	GTP	PB-O3B-PG	-3.14	122.06	132.83
52	O	401	GTP	C5-C6-N1	-3.12	119.17	123.43
46	c	301	3PE	O21-C21-C22	3.08	118.15	111.50
52	O	401	GTP	C3'-C2'-C1'	3.05	105.57	100.98
46	X	401	3PE	O31-C31-C32	3.03	121.43	111.91
50	h	1001	CDL	OB8-CB7-C71	3.00	121.31	111.91
45	d	501	PC1	O21-C21-C22	2.94	119.00	110.80
46	N	903	3PE	O31-C31-C32	2.94	121.13	111.91
46	N	902	3PE	O31-C31-C32	2.91	121.03	111.91
45	B	203	PC1	O31-C31-C32	2.91	121.03	111.91
54	P	501	NDP	PA-O5B-C5B	-2.89	104.73	121.68
52	O	401	GTP	PA-O3A-PB	-2.88	122.93	132.83
45	d	501	PC1	O31-C31-C32	2.83	120.78	111.91
52	O	401	GTP	O2G-PG-O3B	2.83	114.12	104.64
49	F	501	FMN	C5A-C9A-N10	2.82	119.76	117.72
50	h	1001	CDL	OA8-CA7-C31	2.78	120.65	111.91
45	g	1501	PC1	O31-C31-C32	2.78	120.64	111.91
46	L	704	3PE	O31-C31-C32	2.78	120.62	111.91
45	B	202	PC1	O31-C31-C32	2.77	120.59	111.91
52	O	401	GTP	O3G-PG-O3B	2.75	113.85	104.64
51	b	301	LMT	C3B-C4B-C5B	2.72	115.09	110.24
52	O	401	GTP	C4-C5-C6	-2.71	118.21	120.80
54	P	501	NDP	PN-O5D-C5D	-2.71	105.82	121.68
51	N	901	LMT	C1B-O1B-C4'	-2.69	111.31	117.96
46	A	702	3PE	O31-C31-C32	2.68	120.31	111.91
50	Y	701	CDL	OB8-CB7-C71	2.66	120.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	F	501	FMN	C4A-C4-N3	-2.64	119.82	123.43
49	F	501	FMN	C9A-N10-C10	-2.60	118.50	121.91
50	q	201	CDL	OA8-CA7-C31	2.60	120.07	111.91
54	P	501	NDP	O3X-P2B-O2X	2.58	117.49	107.64
51	b	301	LMT	O5'-C1'-C2'	2.57	115.79	110.35
46	M	601	3PE	O31-C31-C32	2.56	119.95	111.91
46	L	703	3PE	O31-C31-C32	2.56	119.94	111.91
46	M	603	3PE	O31-C31-C32	2.55	119.91	111.91
46	I	201	3PE	O31-C31-C32	2.53	119.86	111.91
50	q	201	CDL	OB8-CB7-C71	2.53	119.83	111.91
50	L	702	CDL	OB8-CB7-C71	2.53	119.83	111.91
56	T	101	EHZ	C13-C14-N2	-2.50	106.85	111.90
50	L	702	CDL	OA8-CA7-C31	2.48	119.69	111.91
46	c	301	3PE	O31-C31-C32	2.47	119.66	111.91
54	P	501	NDP	C2A-N1A-C6A	-2.45	114.57	118.75
50	Y	701	CDL	OA8-CA7-C31	2.43	119.53	111.91
46	L	701	3PE	O31-C31-C32	2.40	119.43	111.91
51	N	901	LMT	C1B-C2B-C3B	2.38	114.96	110.00
54	P	501	NDP	O4B-C4B-C3B	2.38	109.83	105.11
51	b	301	LMT	C1B-C2B-C3B	2.32	114.83	110.00
56	T	101	EHZ	C14-N2-C15	-2.32	118.46	122.59
56	T	101	EHZ	C19-C17-C20	2.31	112.00	108.23
54	P	501	NDP	O2N-PN-O1N	2.30	123.63	112.24
49	F	501	FMN	C4A-N5-C5A	2.29	119.06	116.77
56	U	101	EHZ	C10-S1-C9	2.27	108.95	101.87
52	O	401	GTP	C2-N1-C6	2.26	119.52	115.93
54	P	501	NDP	C5B-C4B-C3B	-2.26	106.72	115.18
52	O	401	GTP	O2B-PB-O1B	-2.26	101.09	112.24
51	M	602	LMT	C3B-C4B-C5B	2.21	114.17	110.24
56	U	101	EHZ	O2-C9-S1	-2.12	119.86	122.61
52	O	401	GTP	C2'-C3'-C4'	2.11	106.74	102.64
51	N	901	LMT	C4B-C3B-C2B	2.11	114.50	110.82
50	h	1001	CDL	OB6-CB5-OB7	-2.09	118.64	123.70
51	b	301	LMT	O5B-C1B-C2B	2.08	114.75	110.35
54	P	501	NDP	O5D-PN-O1N	-2.08	100.95	109.07
52	O	401	GTP	O2A-PA-O1A	-2.06	102.03	112.24
46	L	703	3PE	C2-O21-C21	-2.01	112.85	117.79
56	T	101	EHZ	O2-C9-S1	-2.00	120.01	122.61

There are no chirality outliers.

All (498) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	701	PC1	C1-O11-P-O14
45	A	701	PC1	O13-C11-C12-N
45	A	701	PC1	C1-C2-O21-C21
45	A	701	PC1	O22-C21-O21-C2
45	B	202	PC1	C11-O13-P-O14
45	B	202	PC1	C11-O13-P-O11
45	B	202	PC1	C1-O11-P-O14
45	B	202	PC1	O13-C11-C12-N
45	d	501	PC1	C11-O13-P-O12
45	d	501	PC1	C11-O13-P-O14
45	d	501	PC1	C11-O13-P-O11
45	d	501	PC1	O13-C11-C12-N
45	g	1501	PC1	C1-O11-P-O14
45	g	1501	PC1	C1-O11-P-O13
45	g	1501	PC1	O13-C11-C12-N
46	A	702	3PE	O13-C11-C12-N
46	A	702	3PE	C22-C21-O21-C2
46	I	201	3PE	C1-O11-P-O12
46	J	401	3PE	C11-O13-P-O11
46	J	401	3PE	C11-O13-P-O12
46	J	401	3PE	C11-O13-P-O14
46	J	401	3PE	O21-C2-C3-O31
46	K	101	3PE	O13-C11-C12-N
46	L	701	3PE	C11-O13-P-O12
46	L	701	3PE	C11-O13-P-O14
46	L	701	3PE	O13-C11-C12-N
46	L	701	3PE	C22-C21-O21-C2
46	L	703	3PE	O13-C11-C12-N
46	L	704	3PE	O22-C21-O21-C2
46	L	704	3PE	C22-C21-O21-C2
46	M	601	3PE	C12-C11-O13-P
46	M	601	3PE	O13-C11-C12-N
46	M	601	3PE	C22-C21-O21-C2
46	M	603	3PE	C1-O11-P-O12
46	M	603	3PE	C1-O11-P-O14
46	M	603	3PE	C11-O13-P-O12
46	M	603	3PE	C11-O13-P-O14
46	N	902	3PE	C1-O11-P-O12
46	N	902	3PE	C1-O11-P-O14
46	N	902	3PE	C11-O13-P-O14
46	N	903	3PE	C1-O11-P-O12
46	N	903	3PE	C1-O11-P-O13
46	N	903	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
46	N	903	3PE	O22-C21-O21-C2
46	N	903	3PE	C22-C21-O21-C2
46	X	401	3PE	C11-O13-P-O11
46	X	401	3PE	C11-O13-P-O12
46	X	401	3PE	C11-O13-P-O14
46	X	401	3PE	C12-C11-O13-P
46	X	401	3PE	O13-C11-C12-N
46	X	401	3PE	O22-C21-O21-C2
46	c	301	3PE	C1-O11-P-O12
46	c	301	3PE	C11-O13-P-O11
46	c	301	3PE	C11-O13-P-O14
46	c	301	3PE	C22-C21-O21-C2
49	F	501	FMN	C5'-O5'-P-O1P
49	F	501	FMN	C5'-O5'-P-O2P
50	L	702	CDL	CA2-OA2-PA1-OA3
50	L	702	CDL	CA3-OA5-PA1-OA3
50	L	702	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	OA9-CA7-OA8-CA6
50	L	702	CDL	CB2-OB2-PB2-OB3
50	L	702	CDL	CB2-OB2-PB2-OB5
50	Y	701	CDL	CA2-OA2-PA1-OA3
50	Y	701	CDL	CB2-OB2-PB2-OB3
50	Y	701	CDL	C51-CB5-OB6-CB4
50	h	1001	CDL	CB3-OB5-PB2-OB3
50	h	1001	CDL	CB3-OB5-PB2-OB4
50	h	1001	CDL	OB7-CB5-OB6-CB4
50	h	1001	CDL	C51-CB5-OB6-CB4
50	q	201	CDL	CA2-C1-CB2-OB2
50	q	201	CDL	CA3-OA5-PA1-OA2
50	q	201	CDL	CA3-OA5-PA1-OA4
51	N	901	LMT	C2-C1-O1'-C1'
54	P	501	NDP	C5B-O5B-PA-O1A
54	P	501	NDP	C5B-O5B-PA-O2A
54	P	501	NDP	O4B-C4B-C5B-O5B
54	P	501	NDP	C3B-C4B-C5B-O5B
54	P	501	NDP	C2B-O2B-P2B-O2X
56	T	101	EHZ	C16-C17-C20-O6
56	T	101	EHZ	C18-C17-C20-O6
56	T	101	EHZ	O2-C9-S1-C10
56	T	101	EHZ	C8-C9-S1-C10
56	U	101	EHZ	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
56	U	101	EHZ	O2-C9-S1-C10
56	U	101	EHZ	C8-C9-S1-C10
50	Y	701	CDL	OB7-CB5-OB6-CB4
45	g	1501	PC1	O32-C31-O31-C3
46	K	101	3PE	O32-C31-O31-C3
46	L	703	3PE	O32-C31-O31-C3
46	N	903	3PE	O32-C31-O31-C3
46	K	101	3PE	C32-C31-O31-C3
46	N	903	3PE	C32-C31-O31-C3
50	L	702	CDL	C31-CA7-OA8-CA6
46	J	401	3PE	C32-C31-O31-C3
45	d	501	PC1	O32-C31-O31-C3
46	L	704	3PE	O32-C31-O31-C3
50	h	1001	CDL	OB9-CB7-OB8-CB6
46	L	701	3PE	O22-C21-O21-C2
46	M	601	3PE	O22-C21-O21-C2
46	c	301	3PE	O22-C21-O21-C2
45	d	501	PC1	C32-C31-O31-C3
45	g	1501	PC1	C32-C31-O31-C3
46	L	703	3PE	C32-C31-O31-C3
46	L	704	3PE	C32-C31-O31-C3
46	N	902	3PE	C32-C31-O31-C3
46	X	401	3PE	C22-C21-O21-C2
45	A	701	PC1	O32-C31-O31-C3
46	M	603	3PE	C32-C31-O31-C3
50	h	1001	CDL	C71-CB7-OB8-CB6
46	J	401	3PE	O32-C31-O31-C3
45	A	701	PC1	C32-C31-O31-C3
46	A	702	3PE	O22-C21-O21-C2
46	N	902	3PE	O32-C31-O31-C3
51	M	602	LMT	O5'-C5'-C6'-O6'
51	b	301	LMT	O5'-C5'-C6'-O6'
50	L	702	CDL	O1-C1-CA2-OA2
50	L	702	CDL	O1-C1-CB2-OB2
46	M	603	3PE	C22-C21-O21-C2
46	M	603	3PE	O32-C31-O31-C3
51	N	901	LMT	O5B-C5B-C6B-O6B
51	b	301	LMT	C4'-C5'-C6'-O6'
54	P	501	NDP	O4D-C4D-C5D-O5D
51	M	602	LMT	C4'-C5'-C6'-O6'
50	Y	701	CDL	C1-CB2-OB2-PB2
50	Y	701	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
50	Y	701	CDL	C71-CB7-OB8-CB6
45	B	203	PC1	C32-C31-O31-C3
46	L	701	3PE	C32-C31-O31-C3
51	N	901	LMT	C4B-C5B-C6B-O6B
45	B	203	PC1	O32-C31-O31-C3
50	Y	701	CDL	OA5-CA3-CA4-OA6
50	q	201	CDL	O1-C1-CB2-OB2
51	M	602	LMT	C2'-C1'-O1'-C1
50	Y	701	CDL	C11-CA5-OA6-CA4
46	L	701	3PE	O32-C31-O31-C3
50	h	1001	CDL	C31-CA7-OA8-CA6
45	g	1501	PC1	C21-C22-C23-C24
50	L	702	CDL	CB5-C51-C52-C53
51	b	301	LMT	C5'-C4'-O1B-C1B
46	M	601	3PE	C21-C22-C23-C24
46	N	902	3PE	C21-C22-C23-C24
50	L	702	CDL	CA5-C11-C12-C13
50	q	201	CDL	CA7-C31-C32-C33
46	M	603	3PE	O22-C21-O21-C2
50	q	201	CDL	CA5-C11-C12-C13
45	B	203	PC1	C22-C21-O21-C2
50	q	201	CDL	O1-C1-CA2-OA2
46	I	201	3PE	C22-C21-O21-C2
45	A	701	PC1	C11-O13-P-O11
45	A	701	PC1	C1-O11-P-O13
45	B	203	PC1	C11-O13-P-O11
46	A	702	3PE	C1-O11-P-O13
46	L	701	3PE	C11-O13-P-O11
46	L	703	3PE	C11-O13-P-O11
46	M	601	3PE	C1-O11-P-O13
46	M	603	3PE	C1-O11-P-O13
46	M	603	3PE	C11-O13-P-O11
46	N	902	3PE	C1-O11-P-O13
46	c	301	3PE	C1-O11-P-O13
50	Y	701	CDL	CA2-OA2-PA1-OA5
50	Y	701	CDL	CB2-OB2-PB2-OB5
50	h	1001	CDL	CB3-OB5-PB2-OB2
50	q	201	CDL	CB2-OB2-PB2-OB5
50	q	201	CDL	CB3-OB5-PB2-OB2
50	q	201	CDL	CB2-C1-CA2-OA2
45	B	203	PC1	O22-C21-O21-C2
46	I	201	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
50	Y	701	CDL	OA7-CA5-OA6-CA4
50	L	702	CDL	C71-CB7-OB8-CB6
50	q	201	CDL	C31-CA7-OA8-CA6
45	B	202	PC1	C25-C26-C27-C28
46	N	902	3PE	C22-C21-O21-C2
46	N	902	3PE	C37-C38-C39-C3A
50	L	702	CDL	C53-C54-C55-C56
56	T	101	EHZ	C19-C17-C20-O6
46	K	101	3PE	C35-C36-C37-C38
50	q	201	CDL	C52-C53-C54-C55
46	L	704	3PE	C31-C32-C33-C34
50	h	1001	CDL	C22-C23-C24-C25
50	h	1001	CDL	OA9-CA7-OA8-CA6
46	L	704	3PE	C35-C36-C37-C38
46	M	601	3PE	C2E-C2F-C2G-C2H
46	N	902	3PE	C28-C29-C2A-C2B
46	K	101	3PE	C32-C33-C34-C35
46	M	601	3PE	C34-C35-C36-C37
50	L	702	CDL	C59-C60-C61-C62
51	N	901	LMT	O1'-C1-C2-C3
46	N	902	3PE	C2D-C2E-C2F-C2G
46	c	301	3PE	C3E-C3F-C3G-C3H
50	Y	701	CDL	C31-C32-C33-C34
50	h	1001	CDL	CB7-C71-C72-C73
45	g	1501	PC1	C34-C35-C36-C37
46	J	401	3PE	C22-C23-C24-C25
46	I	201	3PE	C33-C34-C35-C36
46	K	101	3PE	O22-C21-O21-C2
46	K	101	3PE	C22-C21-O21-C2
46	L	701	3PE	C35-C36-C37-C38
46	M	603	3PE	C35-C36-C37-C38
46	L	701	3PE	C33-C34-C35-C36
46	N	903	3PE	C33-C34-C35-C36
50	L	702	CDL	C54-C55-C56-C57
45	B	202	PC1	C3A-C3B-C3C-C3D
50	q	201	CDL	C37-C38-C39-C40
46	N	902	3PE	C31-C32-C33-C34
50	L	702	CDL	OB9-CB7-OB8-CB6
46	M	603	3PE	C33-C34-C35-C36
56	T	101	EHZ	C2-C1-C21-C22
45	g	1501	PC1	C29-C2A-C2B-C2C
46	N	902	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	g	1501	PC1	C23-C24-C25-C26
46	L	703	3PE	C34-C35-C36-C37
45	g	1501	PC1	C38-C39-C3A-C3B
46	L	704	3PE	C32-C33-C34-C35
50	h	1001	CDL	C11-CA5-OA6-CA4
45	g	1501	PC1	C27-C28-C29-C2A
50	q	201	CDL	OA9-CA7-OA8-CA6
50	L	702	CDL	C52-C53-C54-C55
50	h	1001	CDL	C16-C17-C18-C19
51	M	602	LMT	C5-C6-C7-C8
54	P	501	NDP	C3D-C4D-C5D-O5D
46	A	702	3PE	C27-C28-C29-C2A
46	N	902	3PE	C2A-C2B-C2C-C2D
56	U	101	EHZ	C5-C6-C7-O1
46	L	701	3PE	C22-C23-C24-C25
50	L	702	CDL	CA2-C1-CB2-OB2
50	h	1001	CDL	OA7-CA5-OA6-CA4
45	g	1501	PC1	C26-C27-C28-C29
51	N	901	LMT	C4-C5-C6-C7
46	M	603	3PE	C22-C23-C24-C25
46	N	903	3PE	C38-C39-C3A-C3B
45	g	1501	PC1	C32-C33-C34-C35
46	M	603	3PE	C32-C33-C34-C35
51	b	301	LMT	C3'-C4'-O1B-C1B
50	h	1001	CDL	CA5-C11-C12-C13
50	q	201	CDL	C71-C72-C73-C74
46	L	704	3PE	C34-C35-C36-C37
50	Y	701	CDL	C12-C13-C14-C15
46	L	704	3PE	C21-C22-C23-C24
50	L	702	CDL	C34-C35-C36-C37
46	M	601	3PE	C26-C27-C28-C29
45	d	501	PC1	C22-C21-O21-C2
46	L	703	3PE	C22-C21-O21-C2
56	U	101	EHZ	C3-C4-C5-C6
46	L	703	3PE	O22-C21-O21-C2
46	I	201	3PE	C37-C38-C39-C3A
46	M	601	3PE	C38-C39-C3A-C3B
45	B	202	PC1	C22-C21-O21-C2
46	I	201	3PE	C1-O11-P-O13
46	N	902	3PE	C11-O13-P-O11
50	L	702	CDL	CA2-OA2-PA1-OA5
46	N	902	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
46	c	301	3PE	C33-C34-C35-C36
45	B	202	PC1	C36-C37-C38-C39
45	B	202	PC1	O11-C1-C2-C3
46	K	101	3PE	O11-C1-C2-C3
46	L	704	3PE	O11-C1-C2-C3
46	N	902	3PE	O11-C1-C2-C3
50	Y	701	CDL	OA5-CA3-CA4-CA6
46	L	703	3PE	C33-C34-C35-C36
46	A	702	3PE	C32-C33-C34-C35
46	I	201	3PE	C26-C27-C28-C29
46	J	401	3PE	C24-C25-C26-C27
46	K	101	3PE	C29-C2A-C2B-C2C
45	g	1501	PC1	C22-C21-O21-C2
45	B	203	PC1	C1-C2-C3-O31
46	J	401	3PE	C1-C2-C3-O31
46	K	101	3PE	C1-C2-C3-O31
46	L	704	3PE	C1-C2-C3-O31
45	g	1501	PC1	C2F-C2G-C2H-C2I
46	L	704	3PE	C3B-C3C-C3D-C3E
46	X	401	3PE	C36-C37-C38-C39
46	L	701	3PE	C37-C38-C39-C3A
46	X	401	3PE	C22-C23-C24-C25
51	b	301	LMT	O5B-C5B-C6B-O6B
50	Y	701	CDL	CA6-CA4-OA6-CA5
46	M	601	3PE	C28-C29-C2A-C2B
46	N	903	3PE	C2A-C2B-C2C-C2D
50	h	1001	CDL	C72-C73-C74-C75
56	T	101	EHZ	C21-C22-C23-C24
46	L	701	3PE	C32-C33-C34-C35
46	L	703	3PE	C31-C32-C33-C34
46	M	603	3PE	C28-C29-C2A-C2B
45	d	501	PC1	O21-C2-C3-O31
45	d	501	PC1	O22-C21-O21-C2
54	P	501	NDP	O4D-C1D-N1N-C6N
46	N	903	3PE	C36-C37-C38-C39
50	L	702	CDL	CB2-C1-CA2-OA2
46	N	902	3PE	C25-C26-C27-C28
46	A	702	3PE	O11-C1-C2-C3
46	K	101	3PE	C28-C29-C2A-C2B
46	M	601	3PE	C31-C32-C33-C34
45	B	202	PC1	O22-C21-O21-C2
46	c	301	3PE	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
45	g	1501	PC1	C24-C25-C26-C27
46	N	902	3PE	C32-C33-C34-C35
45	B	202	PC1	C37-C38-C39-C3A
50	L	702	CDL	CB3-CB4-CB6-OB8
50	L	702	CDL	C35-C36-C37-C38
46	c	301	3PE	C39-C3A-C3B-C3C
56	U	101	EHZ	C2-C1-C21-C22
50	L	702	CDL	CA3-OA5-PA1-OA2
46	c	301	3PE	C22-C23-C24-C25
46	N	902	3PE	O11-C1-C2-O21
46	c	301	3PE	O11-C1-C2-O21
45	B	203	PC1	O21-C2-C3-O31
46	K	101	3PE	O21-C2-C3-O31
46	L	704	3PE	O21-C2-C3-O31
46	N	903	3PE	O21-C2-C3-O31
50	L	702	CDL	OB6-CB4-CB6-OB8
50	Y	701	CDL	OB6-CB4-CB6-OB8
50	q	201	CDL	OA6-CA4-CA6-OA8
46	I	201	3PE	C32-C31-O31-C3
45	g	1501	PC1	O22-C21-O21-C2
45	g	1501	PC1	C2-C1-O11-P
50	q	201	CDL	CB4-CB3-OB5-PB2
46	L	703	3PE	C37-C38-C39-C3A
50	L	702	CDL	C60-C61-C62-C63
46	c	301	3PE	C32-C33-C34-C35
45	A	701	PC1	O11-C1-C2-C3
46	N	903	3PE	O11-C1-C2-C3
46	X	401	3PE	O11-C1-C2-C3
46	X	401	3PE	C34-C35-C36-C37
50	q	201	CDL	OA7-CA5-OA6-CA4
45	g	1501	PC1	C2A-C2B-C2C-C2D
46	L	703	3PE	C39-C3A-C3B-C3C
50	q	201	CDL	C11-CA5-OA6-CA4
49	F	501	FMN	C5'-O5'-P-O3P
50	h	1001	CDL	CA6-CA4-OA6-CA5
50	Y	701	CDL	C13-C14-C15-C16
46	M	601	3PE	C32-C31-O31-C3
46	M	601	3PE	C2-C1-O11-P
50	Y	701	CDL	CB3-CB4-CB6-OB8
50	h	1001	CDL	CB4-CB3-OB5-PB2
50	q	201	CDL	CA3-CA4-CA6-OA8
46	I	201	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	A	702	3PE	O11-C1-C2-O21
46	L	704	3PE	O11-C1-C2-O21
46	N	903	3PE	O11-C1-C2-O21
46	X	401	3PE	O11-C1-C2-O21
46	I	201	3PE	C39-C3A-C3B-C3C
56	T	101	EHZ	C5-C6-C7-O1
45	B	202	PC1	C1-O11-P-O13
46	A	702	3PE	C11-O13-P-O11
46	L	703	3PE	C1-O11-P-O13
46	L	704	3PE	C11-O13-P-O11
46	X	401	3PE	C1-O11-P-O13
46	L	703	3PE	C32-C33-C34-C35
50	h	1001	CDL	O1-C1-CB2-OB2
46	L	704	3PE	C2-C1-O11-P
46	M	603	3PE	C2-C1-O11-P
45	A	701	PC1	C11-O13-P-O12
45	A	701	PC1	C1-O11-P-O12
45	B	202	PC1	C11-O13-P-O12
45	B	203	PC1	C11-O13-P-O12
46	A	702	3PE	C1-O11-P-O12
46	A	702	3PE	C11-O13-P-O12
46	A	702	3PE	C11-O13-P-O14
46	I	201	3PE	C1-O11-P-O14
46	L	703	3PE	C11-O13-P-O12
46	L	703	3PE	C11-O13-P-O14
46	L	704	3PE	C11-O13-P-O12
46	M	601	3PE	C1-O11-P-O14
46	N	903	3PE	C1-O11-P-O14
46	c	301	3PE	C1-O11-P-O14
50	L	702	CDL	CA2-OA2-PA1-OA4
50	Y	701	CDL	CB2-OB2-PB2-OB4
50	q	201	CDL	CA3-OA5-PA1-OA3
50	q	201	CDL	CB2-OB2-PB2-OB3
50	q	201	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	CB3-OB5-PB2-OB4
51	M	602	LMT	O5'-C1'-O1'-C1
51	b	301	LMT	O5'-C1'-O1'-C1
46	L	701	3PE	O11-C1-C2-C3
46	c	301	3PE	O11-C1-C2-C3
45	B	203	PC1	C23-C24-C25-C26
50	L	702	CDL	C57-C58-C59-C60
46	N	902	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
45	B	202	PC1	C12-C11-O13-P
46	A	702	3PE	C12-C11-O13-P
46	L	703	3PE	C12-C11-O13-P
46	M	601	3PE	O32-C31-O31-C3
46	L	701	3PE	C24-C25-C26-C27
45	B	202	PC1	O11-C1-C2-O21
46	K	101	3PE	O11-C1-C2-O21
46	L	701	3PE	O11-C1-C2-O21
46	K	101	3PE	C26-C27-C28-C29
46	c	301	3PE	C31-C32-C33-C34
45	B	203	PC1	O13-C11-C12-N
45	g	1501	PC1	C1-C2-C3-O31
45	g	1501	PC1	O21-C2-C3-O31
50	q	201	CDL	CA4-CA3-OA5-PA1
50	q	201	CDL	C51-C52-C53-C54
46	K	101	3PE	C37-C38-C39-C3A
46	M	603	3PE	C23-C24-C25-C26
46	X	401	3PE	C31-C32-C33-C34
45	A	701	PC1	O11-C1-C2-O21
46	L	703	3PE	C28-C29-C2A-C2B
50	h	1001	CDL	OA6-CA4-CA6-OA8
45	d	501	PC1	C1-O11-P-O13
46	J	401	3PE	C1-O11-P-O13
46	L	704	3PE	C1-O11-P-O13
46	N	903	3PE	C11-O13-P-O11
50	h	1001	CDL	CA2-OA2-PA1-OA5
50	h	1001	CDL	CA3-OA5-PA1-OA2
50	q	201	CDL	CA2-OA2-PA1-OA5
46	L	701	3PE	C23-C24-C25-C26
45	d	501	PC1	C1-C2-C3-O31
45	B	203	PC1	C22-C23-C24-C25
50	h	1001	CDL	C31-C32-C33-C34
50	q	201	CDL	C73-C74-C75-C76
46	K	101	3PE	C27-C28-C29-C2A
46	X	401	3PE	C32-C33-C34-C35
45	B	202	PC1	C2-C1-O11-P
46	N	902	3PE	C2-C1-O11-P
50	h	1001	CDL	CA4-CA3-OA5-PA1
46	M	601	3PE	C32-C33-C34-C35
46	A	702	3PE	C37-C38-C39-C3A
46	M	603	3PE	C31-C32-C33-C34
45	B	202	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
50	q	201	CDL	C15-C16-C17-C18
46	L	703	3PE	O31-C31-C32-C33
56	T	101	EHZ	S1-C10-C11-N1
46	A	702	3PE	C29-C2A-C2B-C2C
46	I	201	3PE	C23-C24-C25-C26
46	I	201	3PE	C22-C23-C24-C25
46	M	601	3PE	C2A-C2B-C2C-C2D
46	L	703	3PE	C1-C2-O21-C21
46	L	703	3PE	C3-C2-O21-C21
50	Y	701	CDL	CB6-CB4-OB6-CB5
46	I	201	3PE	C24-C25-C26-C27
46	L	704	3PE	C33-C34-C35-C36
46	X	401	3PE	C2-C1-O11-P
50	q	201	CDL	C38-C39-C40-C41
51	M	602	LMT	O1'-C1-C2-C3
46	L	703	3PE	C36-C37-C38-C39
46	L	703	3PE	C21-C22-C23-C24
56	T	101	EHZ	C11-C10-S1-C9
46	J	401	3PE	C21-C22-C23-C24
46	N	902	3PE	C34-C35-C36-C37
46	N	903	3PE	C3A-C3B-C3C-C3D
46	I	201	3PE	C38-C39-C3A-C3B
46	L	704	3PE	C38-C39-C3A-C3B
46	M	603	3PE	C37-C38-C39-C3A
45	B	202	PC1	C33-C34-C35-C36
51	b	301	LMT	O1'-C1-C2-C3
46	L	701	3PE	C34-C35-C36-C37
50	q	201	CDL	OB5-CB3-CB4-OB6
50	h	1001	CDL	C12-C13-C14-C15
56	U	101	EHZ	C21-C22-C23-C24
46	M	601	3PE	O21-C2-C3-O31
50	L	702	CDL	OA6-CA4-CA6-OA8
46	N	903	3PE	C32-C33-C34-C35
46	L	701	3PE	C38-C39-C3A-C3B
46	M	603	3PE	C34-C35-C36-C37
50	L	702	CDL	OB7-CB5-OB6-CB4
50	h	1001	CDL	C52-C53-C54-C55
46	c	301	3PE	C3-C2-O21-C21
46	K	101	3PE	C2A-C2B-C2C-C2D
50	q	201	CDL	C36-C37-C38-C39
46	N	903	3PE	C1-C2-C3-O31
45	B	202	PC1	O31-C31-C32-C33

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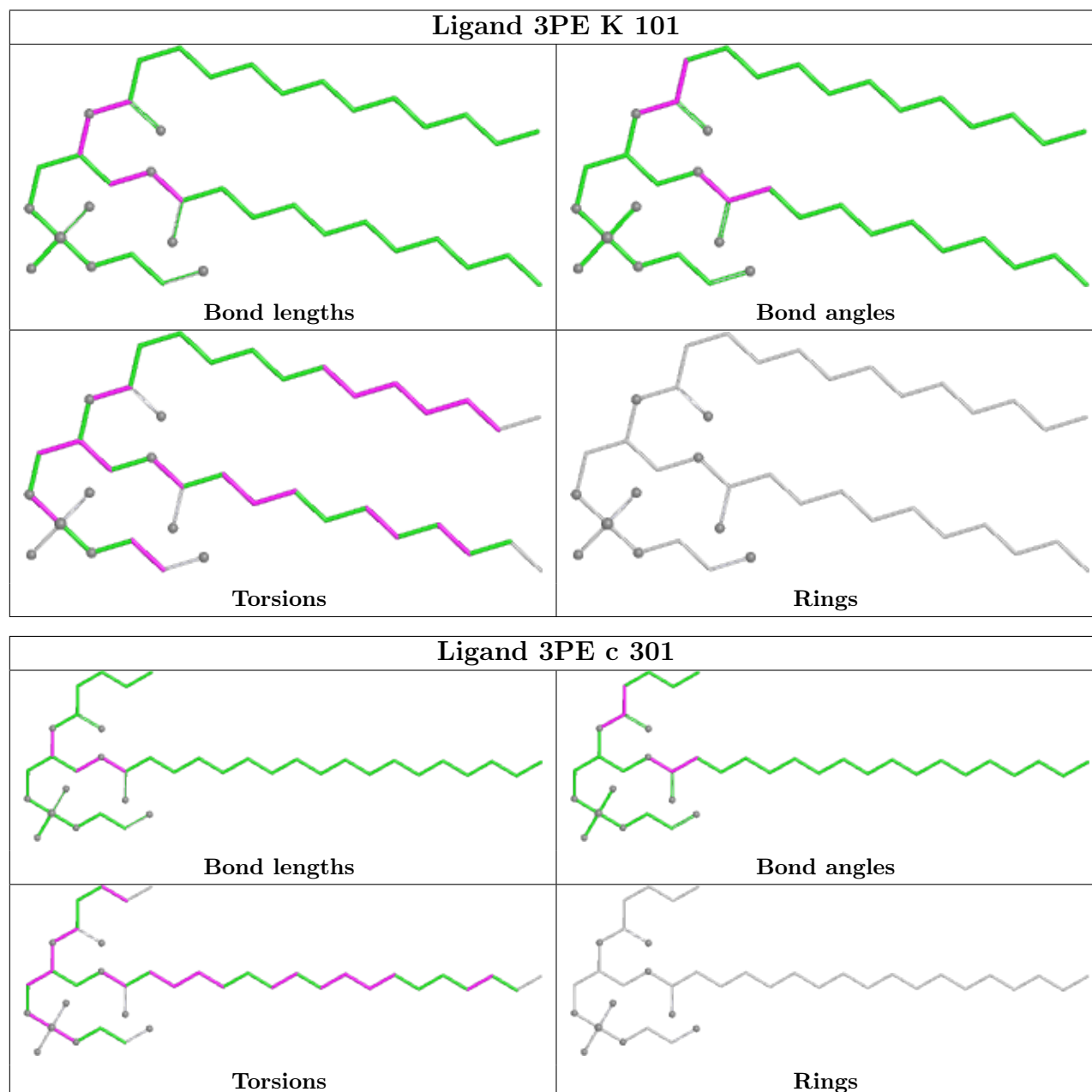
Mol	Chain	Res	Type	Atoms
45	g	1501	PC1	O31-C31-C32-C33
50	q	201	CDL	C72-C71-CB7-OB8
50	h	1001	CDL	C15-C16-C17-C18
46	N	902	3PE	C36-C37-C38-C39
46	I	201	3PE	C2B-C2C-C2D-C2E
51	b	301	LMT	C4-C5-C6-C7
45	B	202	PC1	O21-C21-C22-C23
46	K	101	3PE	C31-C32-C33-C34
46	I	201	3PE	C34-C35-C36-C37
46	c	301	3PE	C36-C37-C38-C39
54	P	501	NDP	C5B-O5B-PA-O3
46	c	301	3PE	C32-C31-O31-C3
50	L	702	CDL	C51-CB5-OB6-CB4
45	g	1501	PC1	O32-C31-C32-C33
50	q	201	CDL	C72-C71-CB7-OB9
50	h	1001	CDL	CA3-CA4-CA6-OA8
46	c	301	3PE	C38-C39-C3A-C3B
45	A	701	PC1	C11-O13-P-O14
46	I	201	3PE	C11-O13-P-O12
46	K	101	3PE	C1-O11-P-O14
46	L	703	3PE	C1-O11-P-O14
46	M	601	3PE	C1-O11-P-O12
56	T	101	EHZ	C6-C7-C8-C9
45	B	202	PC1	O32-C31-C32-C33
50	q	201	CDL	C32-C31-CA7-OA8
46	c	301	3PE	O32-C31-O31-C3
50	L	702	CDL	CB4-CB6-OB8-CB7
46	J	401	3PE	C28-C29-C2A-C2B
46	c	301	3PE	C1-C2-O21-C21
45	B	203	PC1	C35-C36-C37-C38
46	A	702	3PE	C2A-C2B-C2C-C2D
50	L	702	CDL	OA5-CA3-CA4-OA6
45	B	202	PC1	O22-C21-C22-C23
50	Y	701	CDL	C15-C16-C17-C18
50	Y	701	CDL	CA7-C31-C32-C33

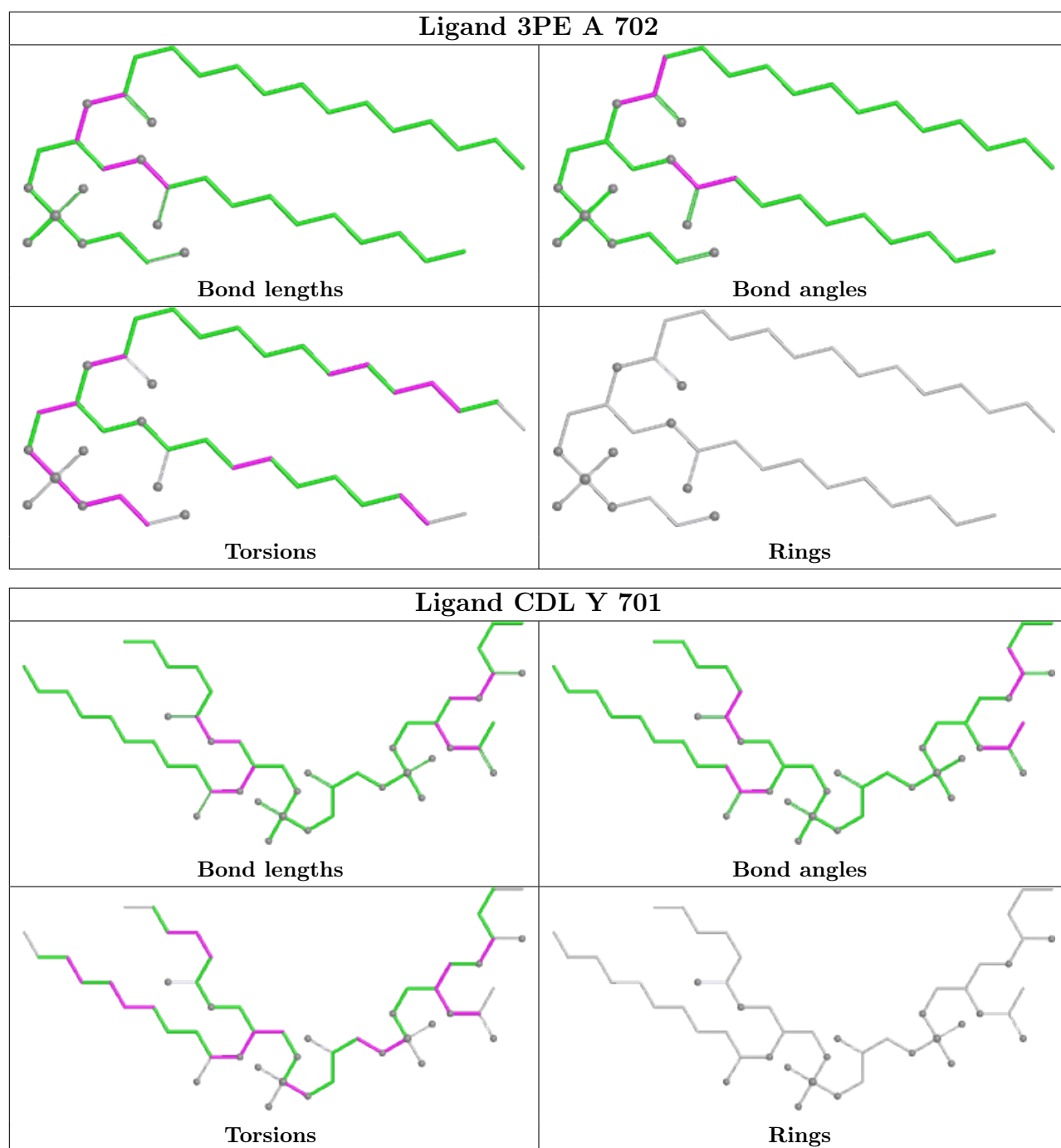
There are no ring outliers.

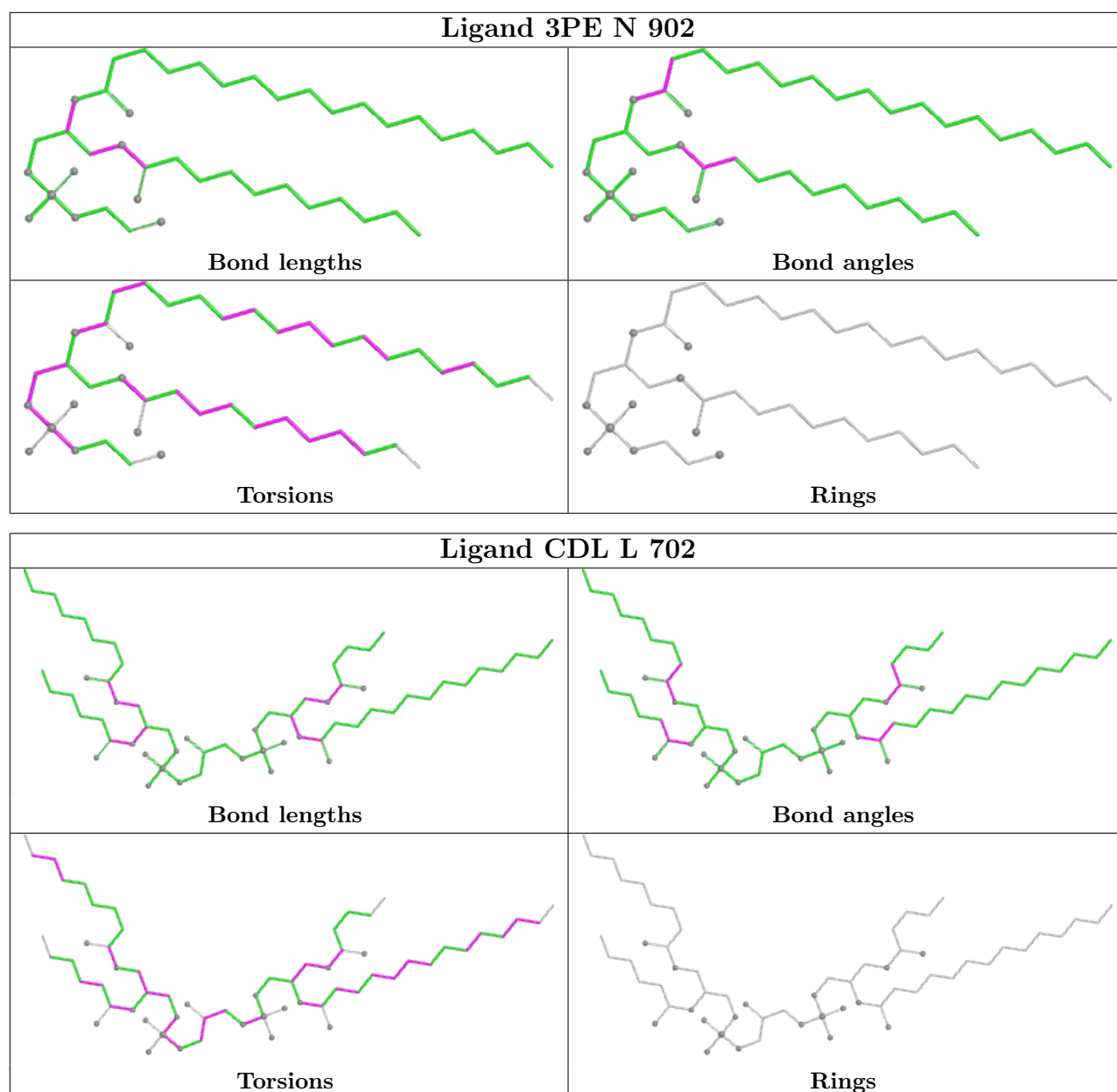
No monomer is involved in short contacts.

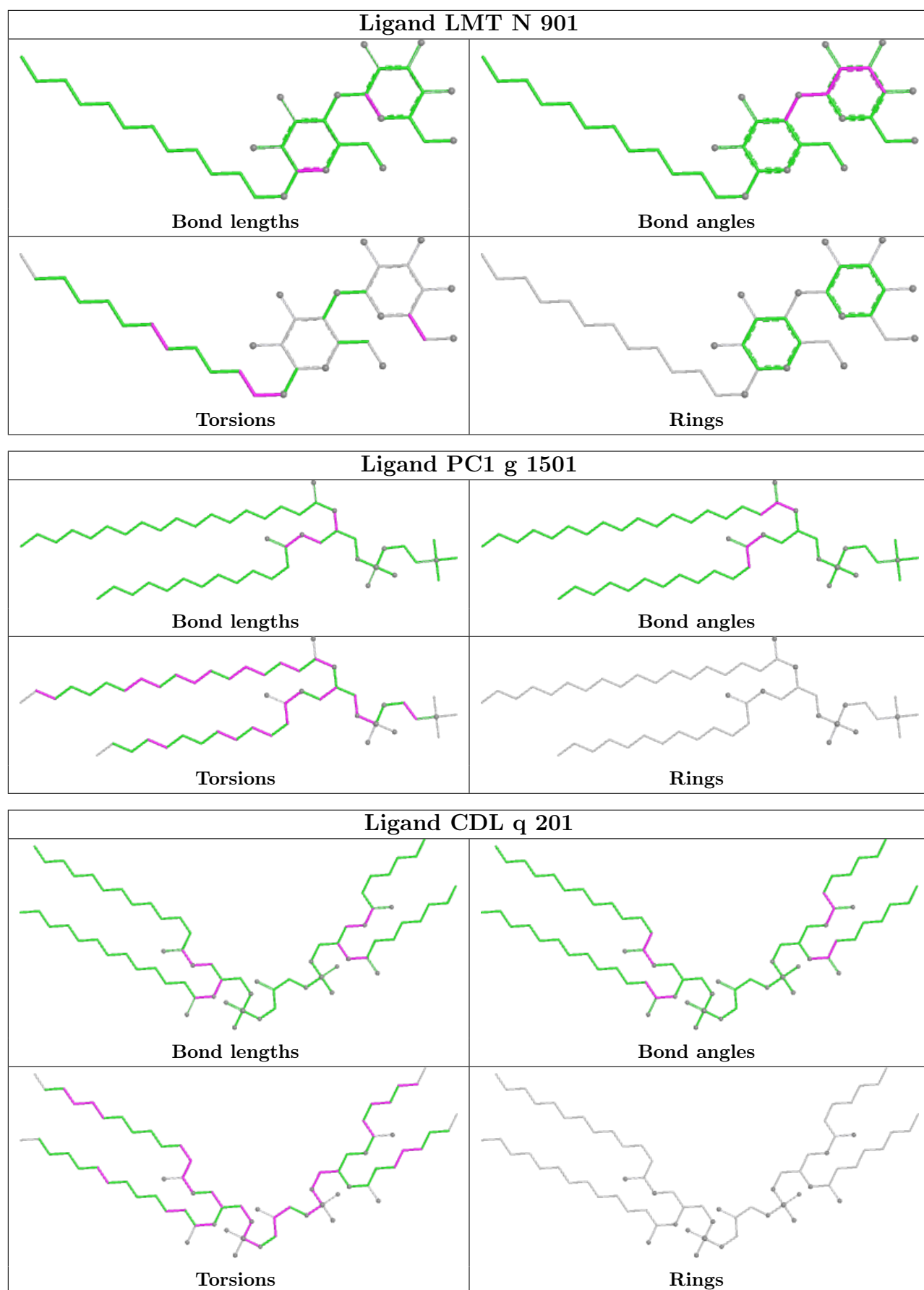
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

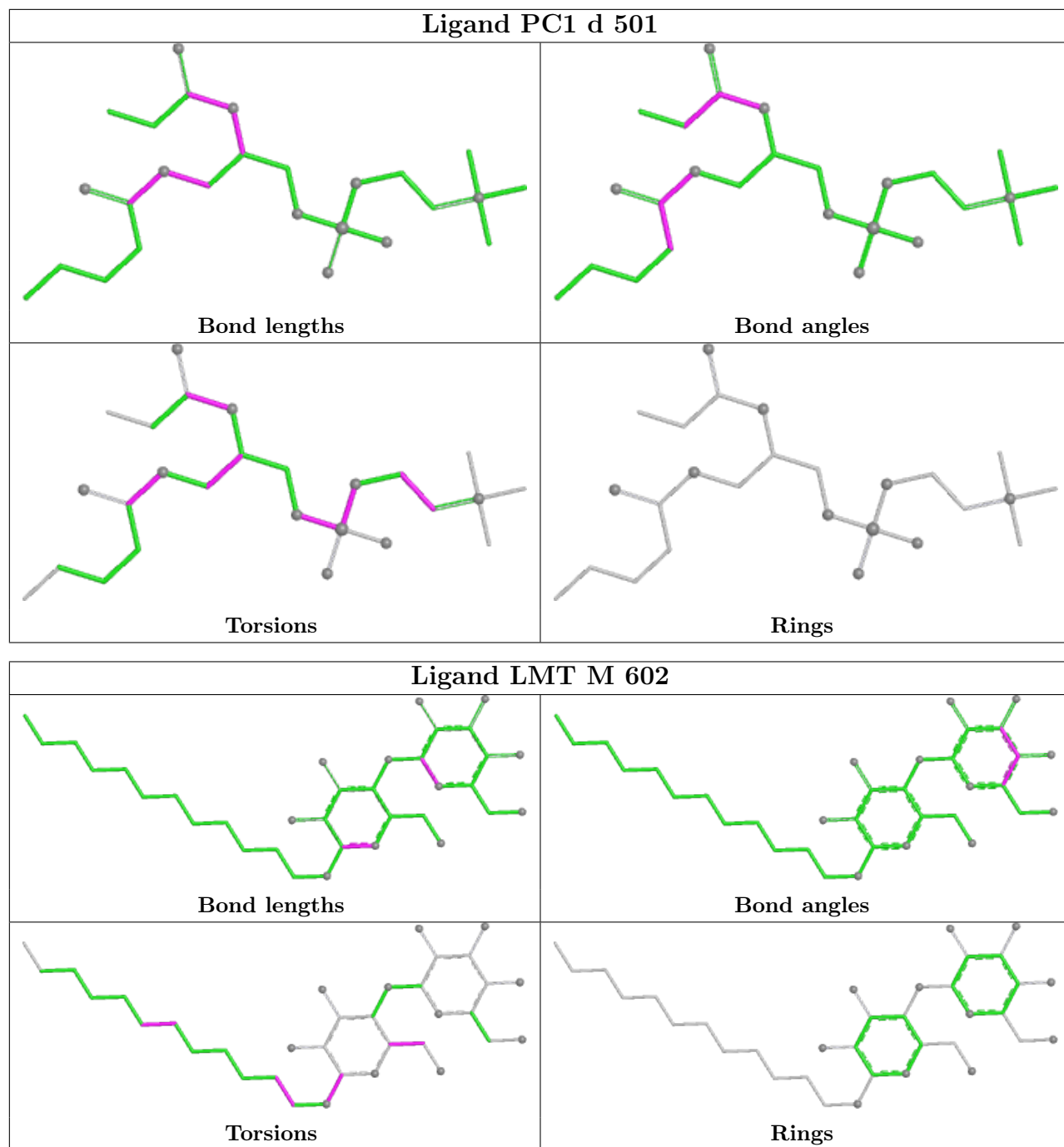
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

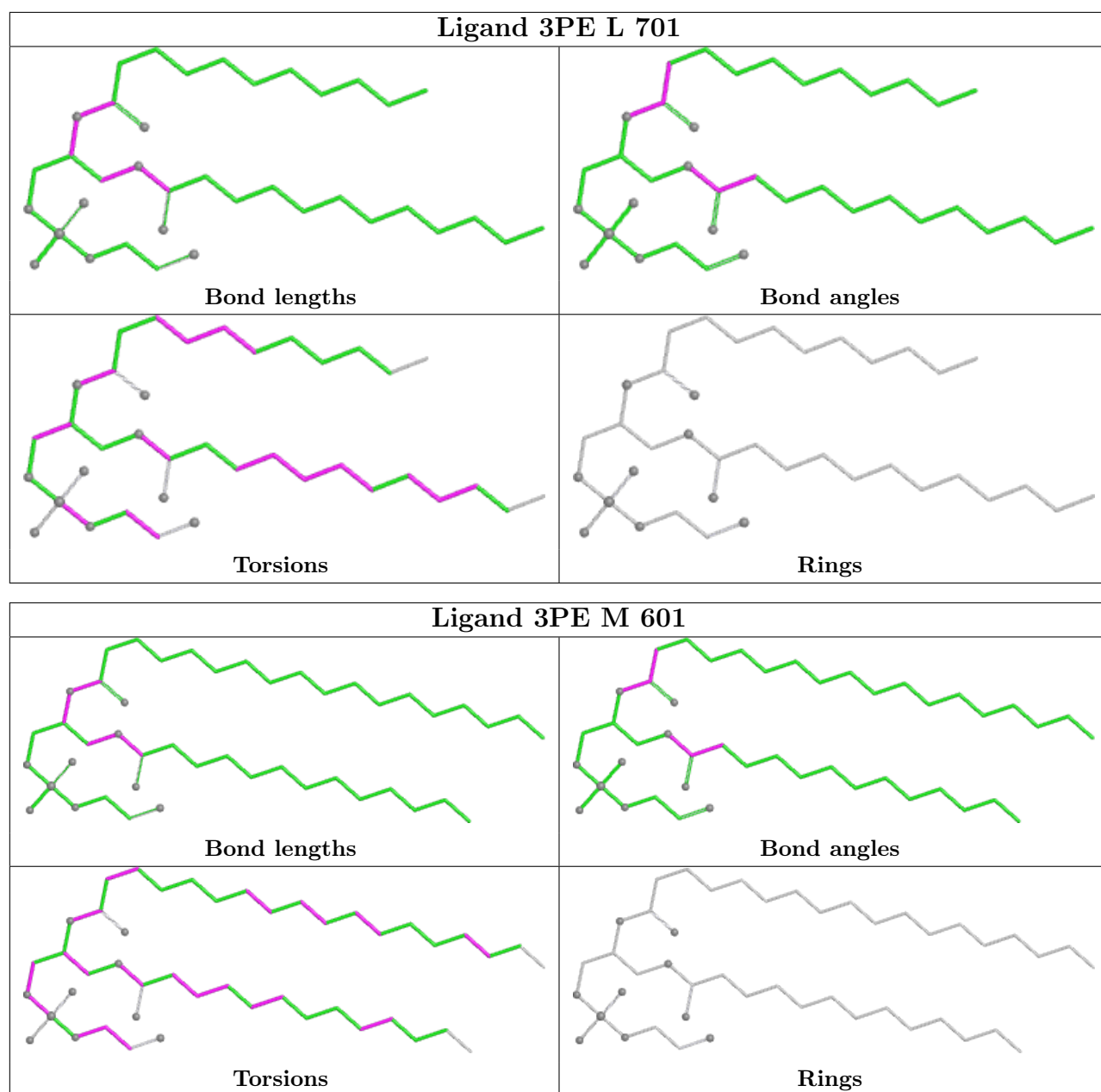


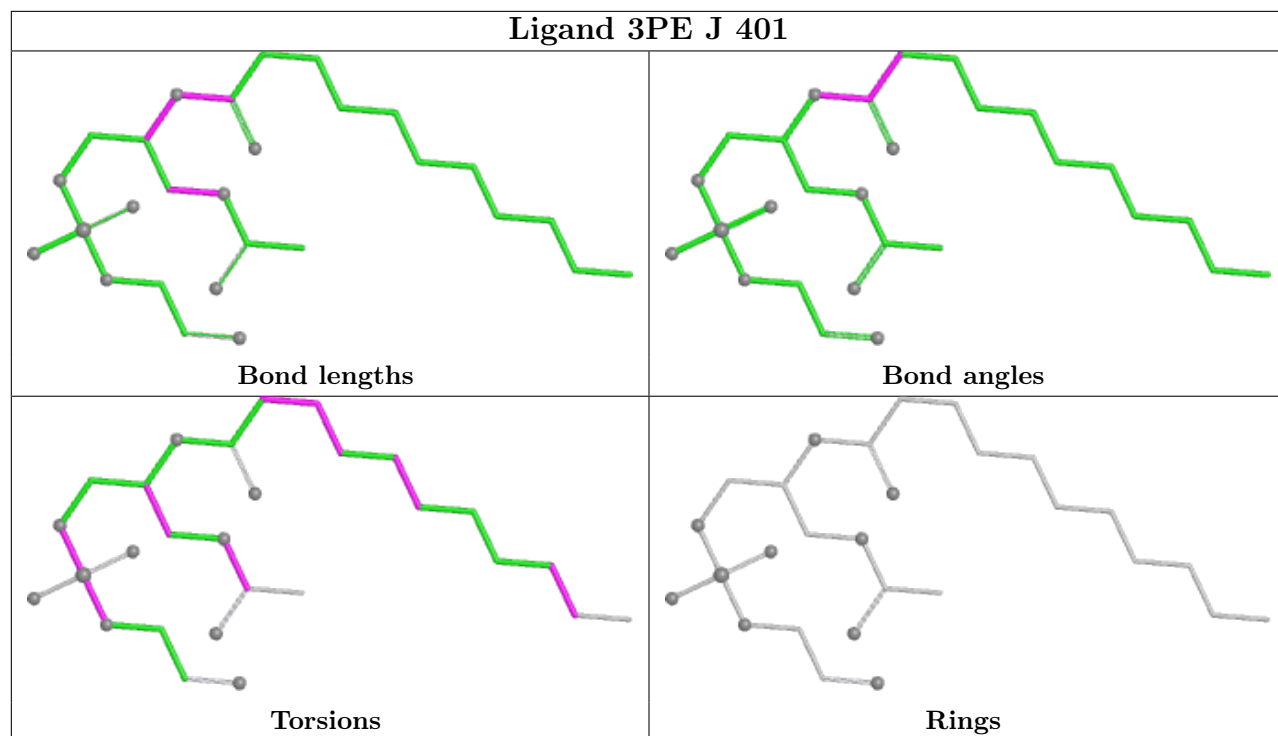


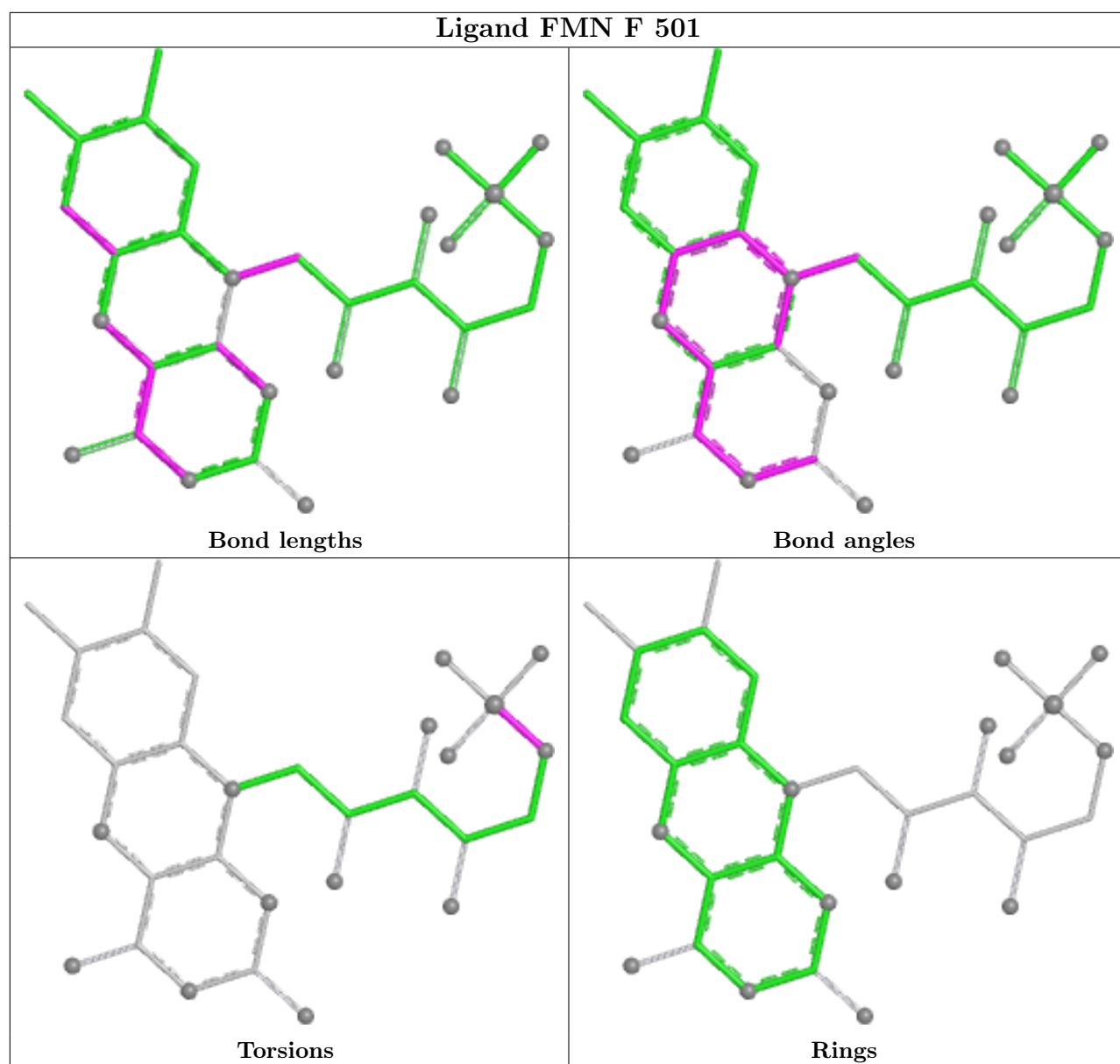


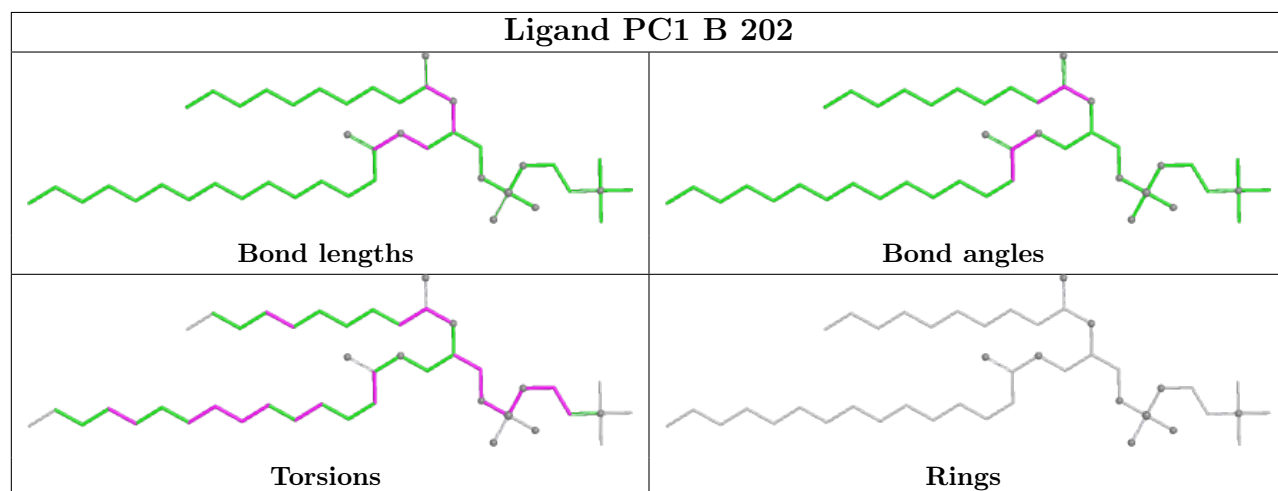
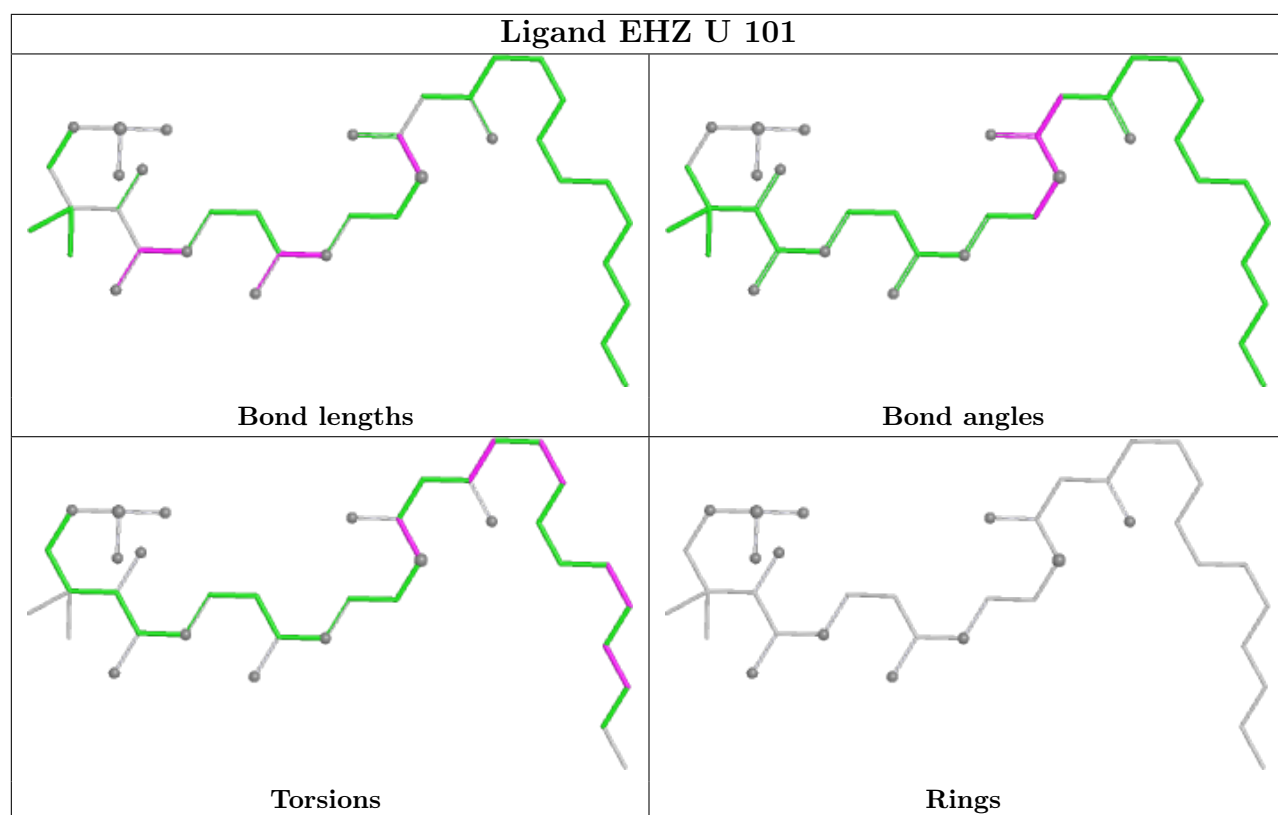


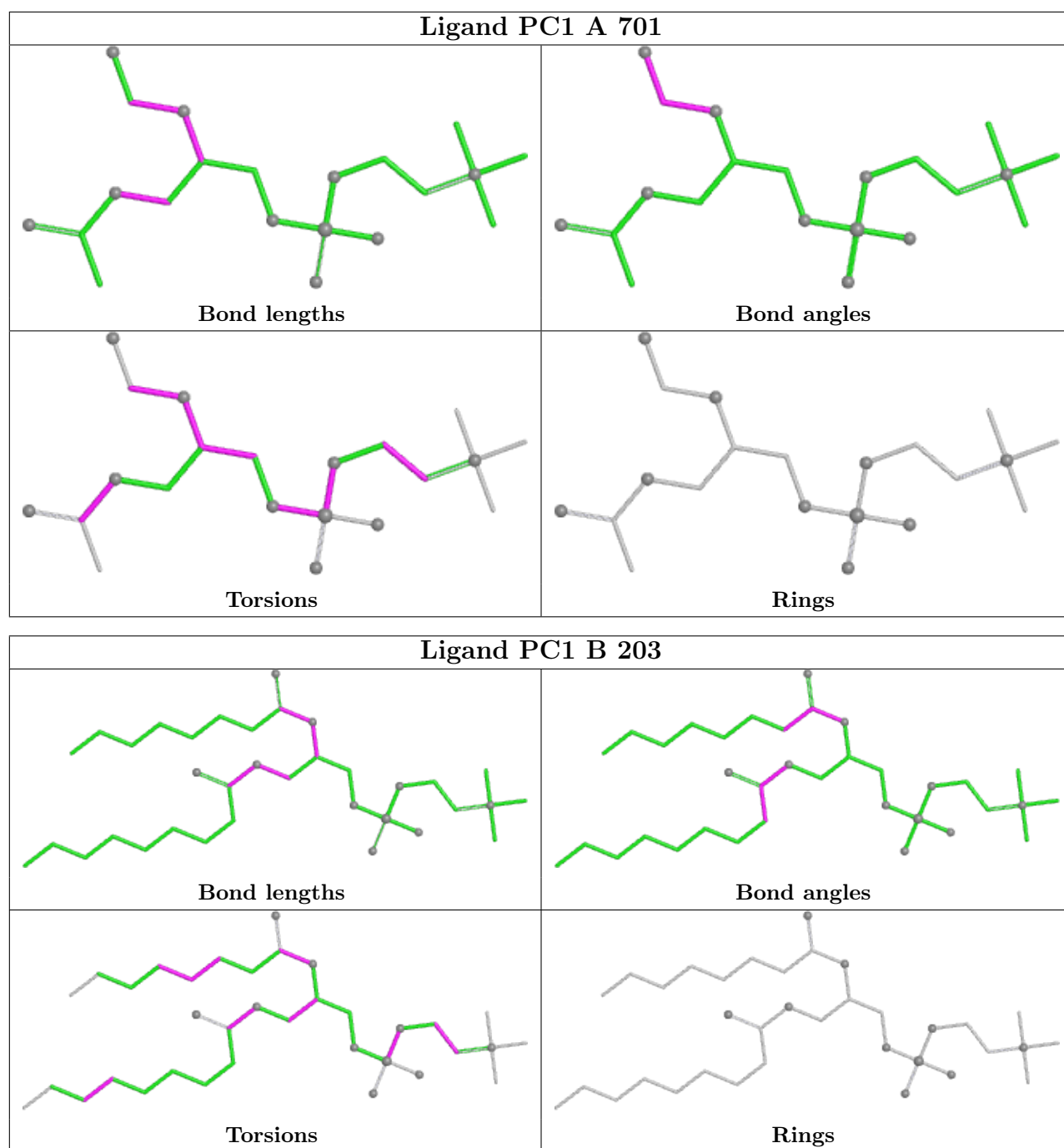


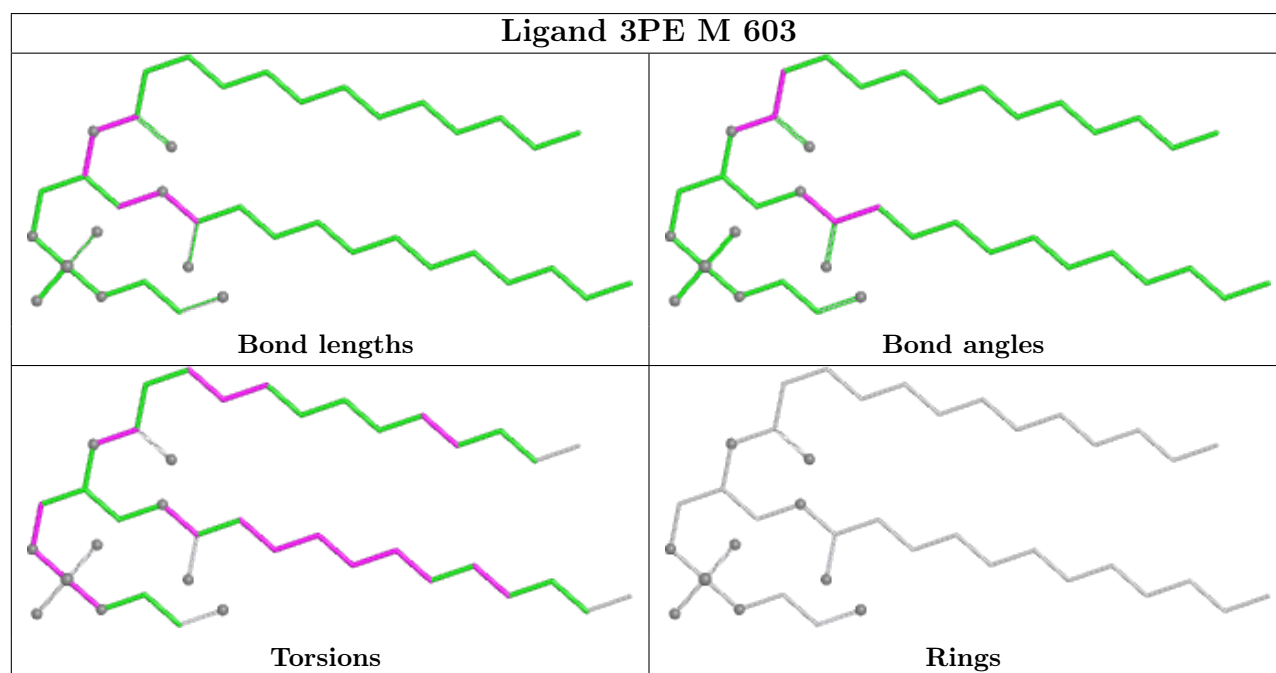
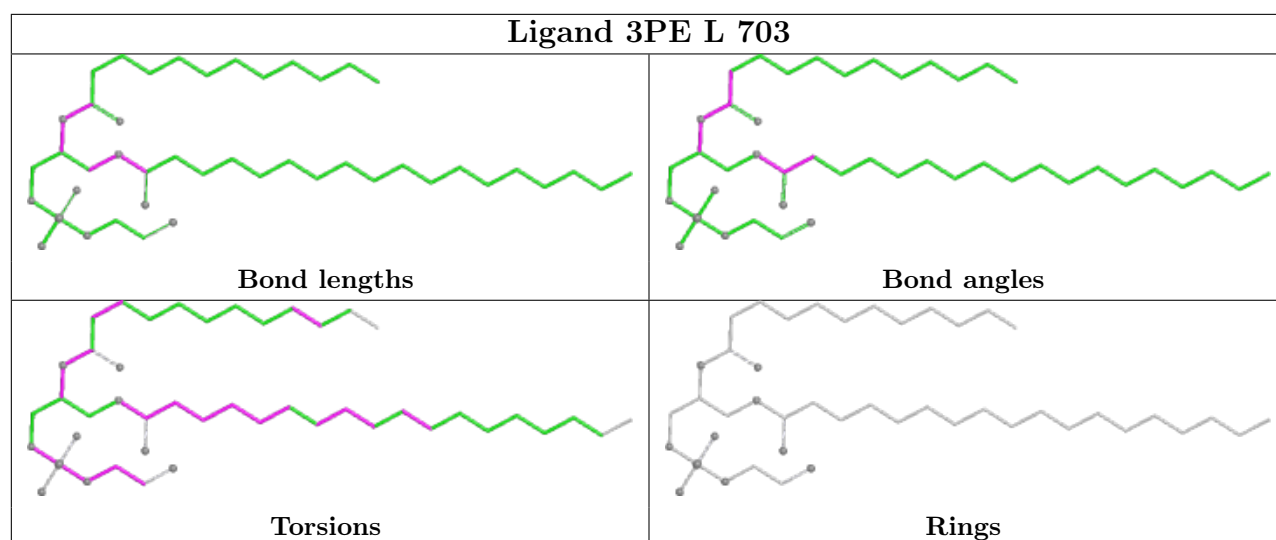


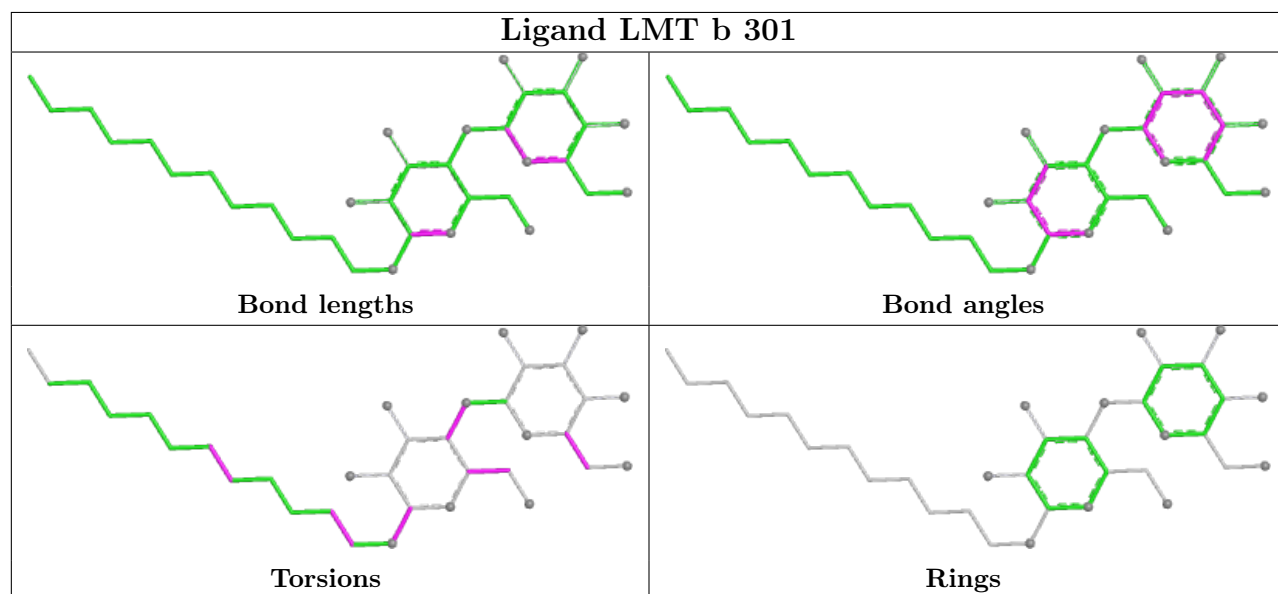
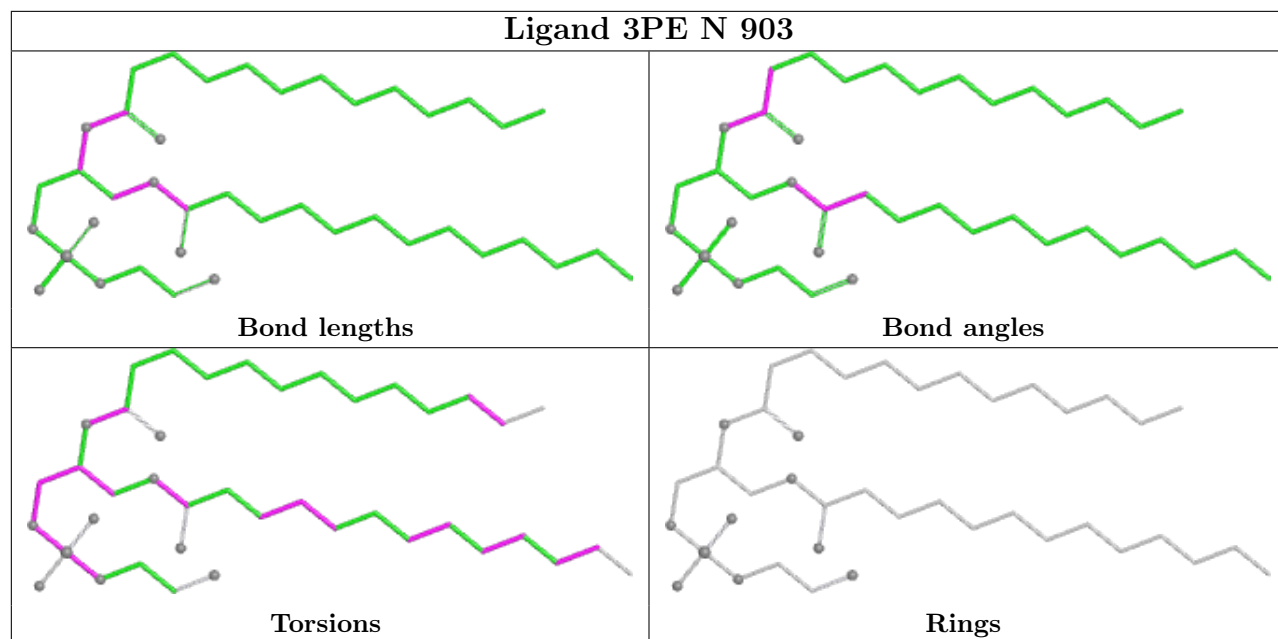


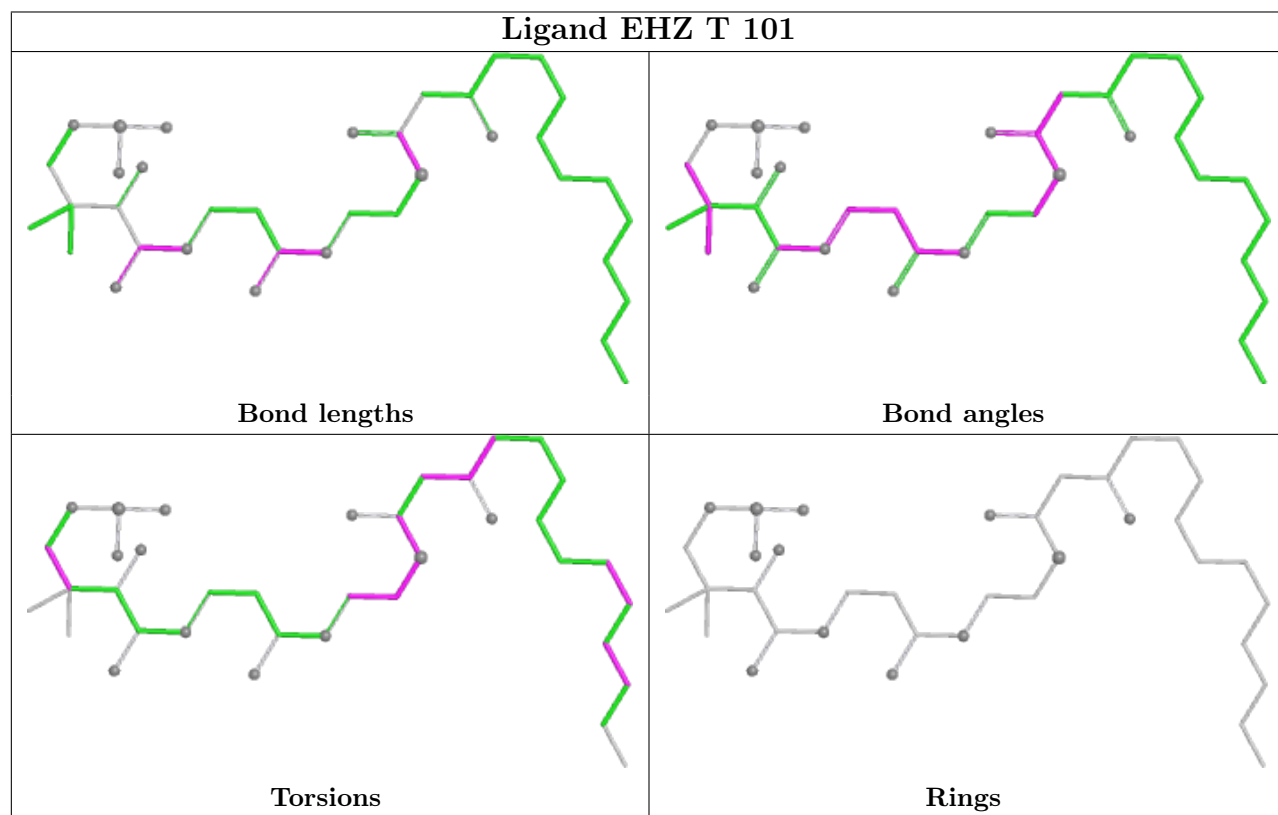
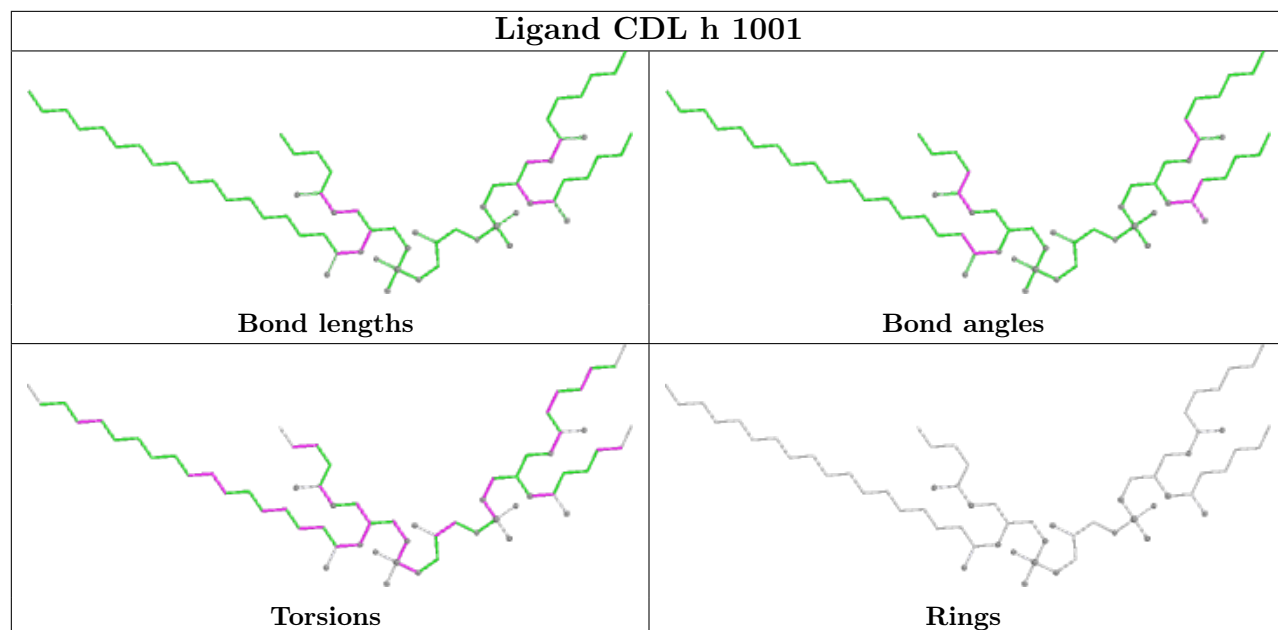


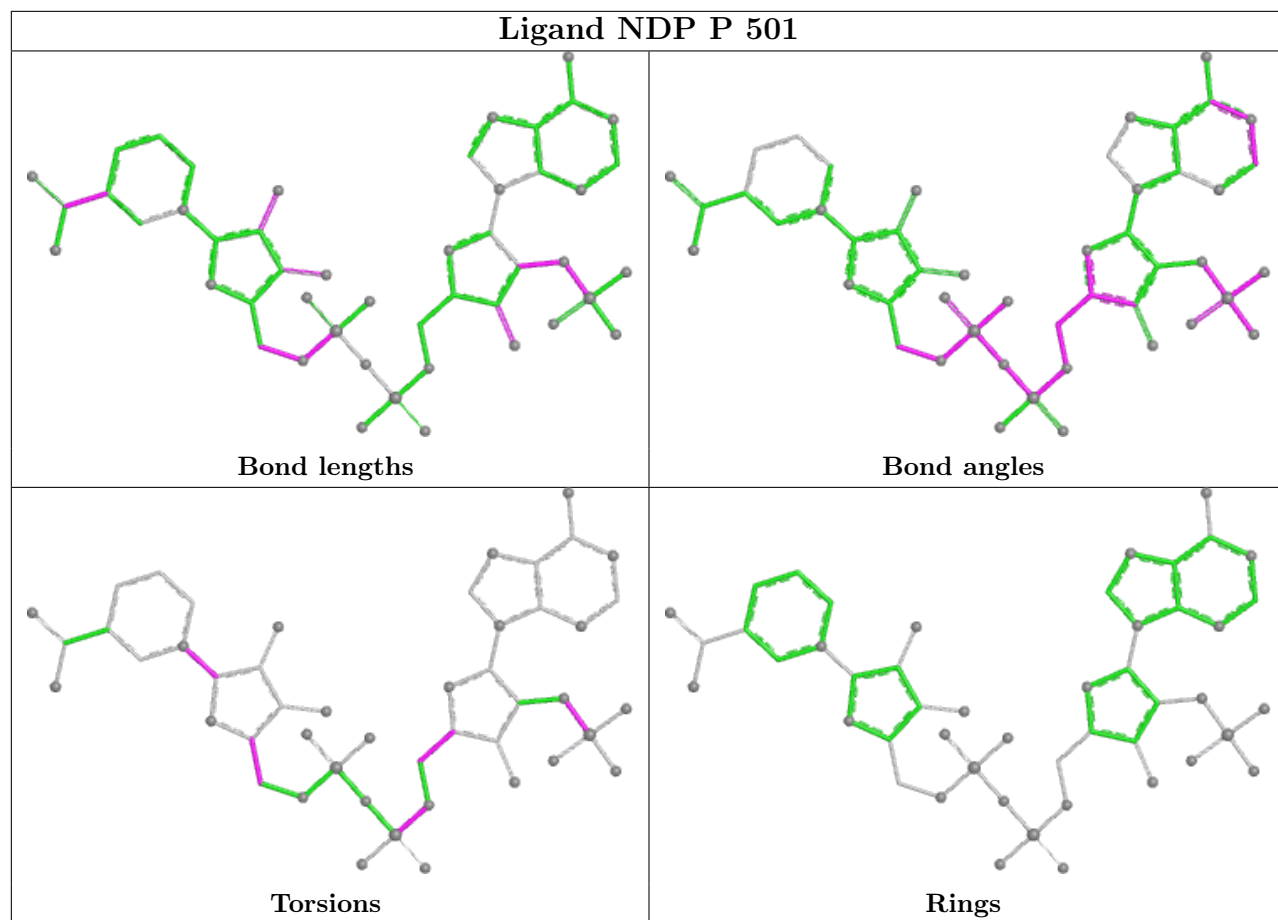


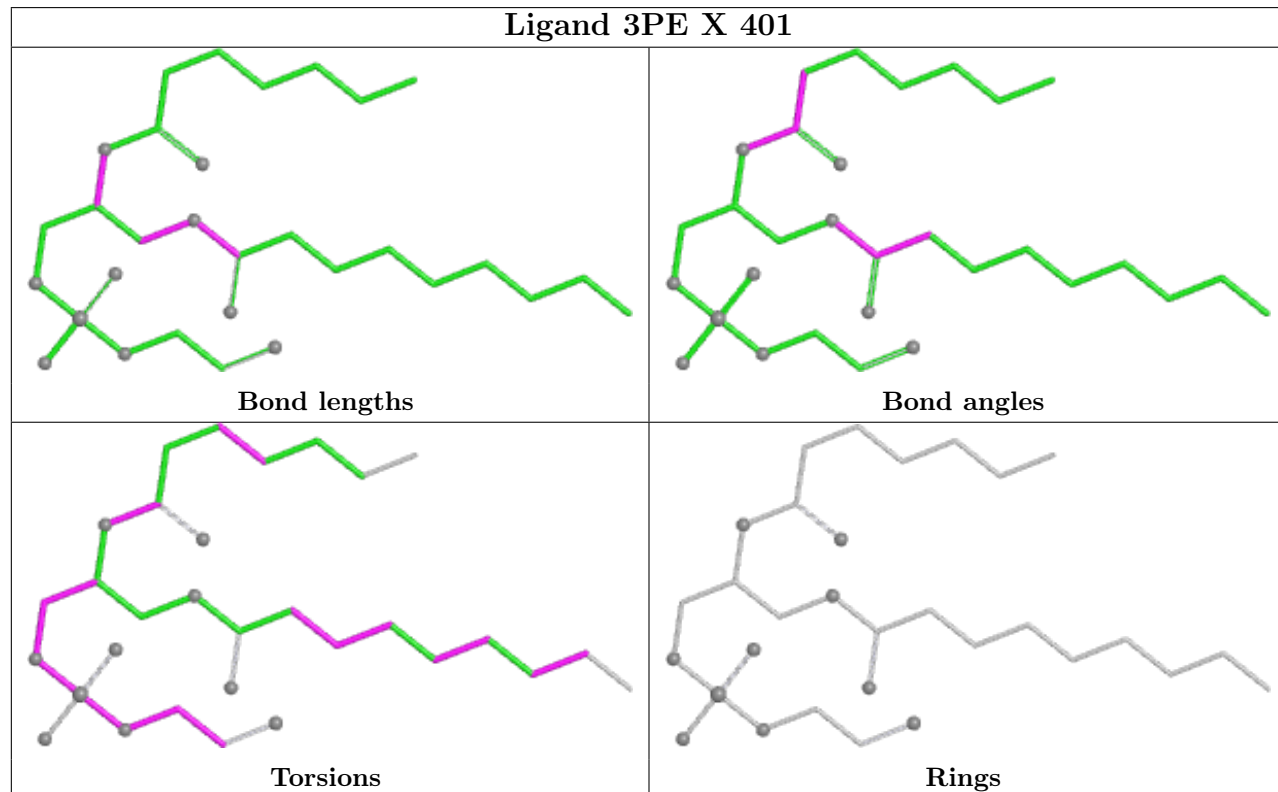
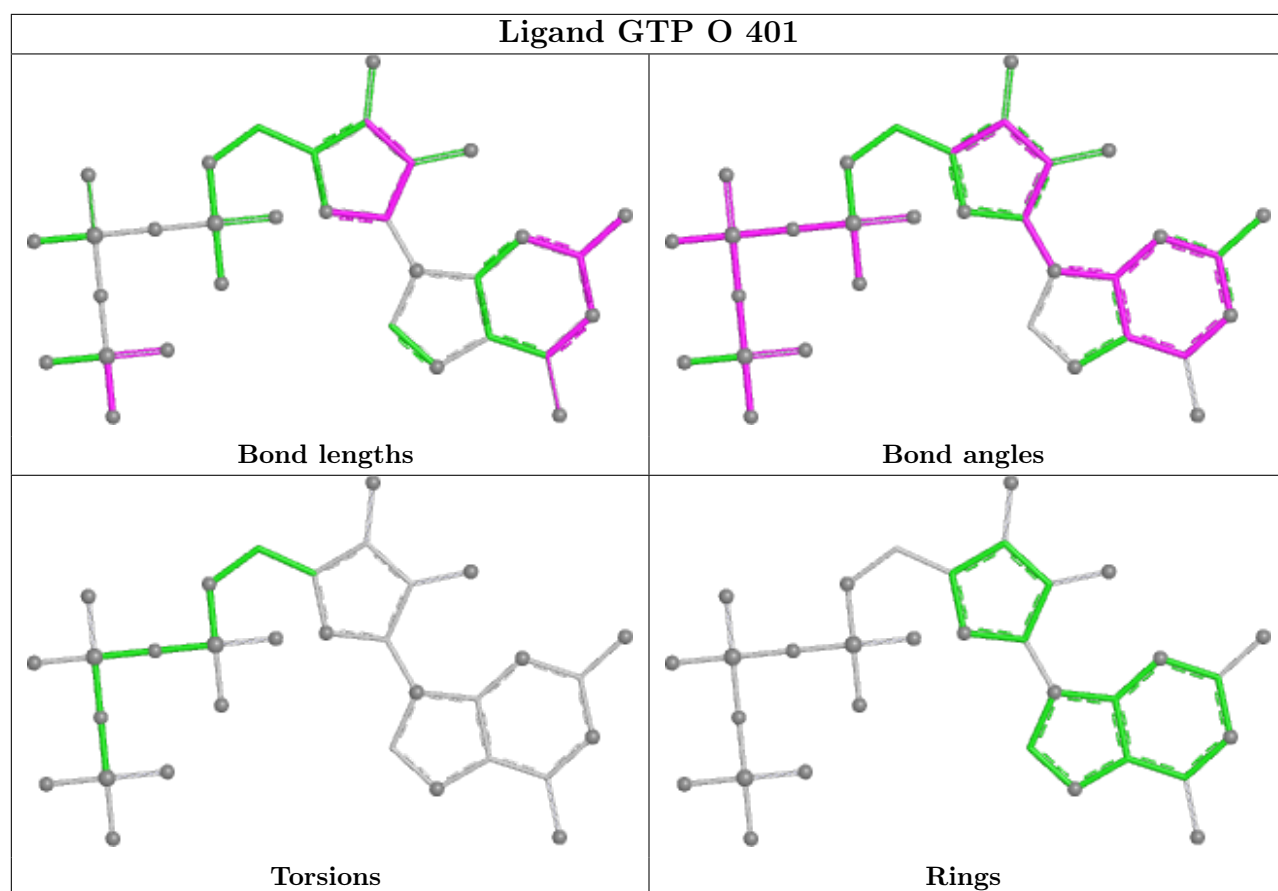


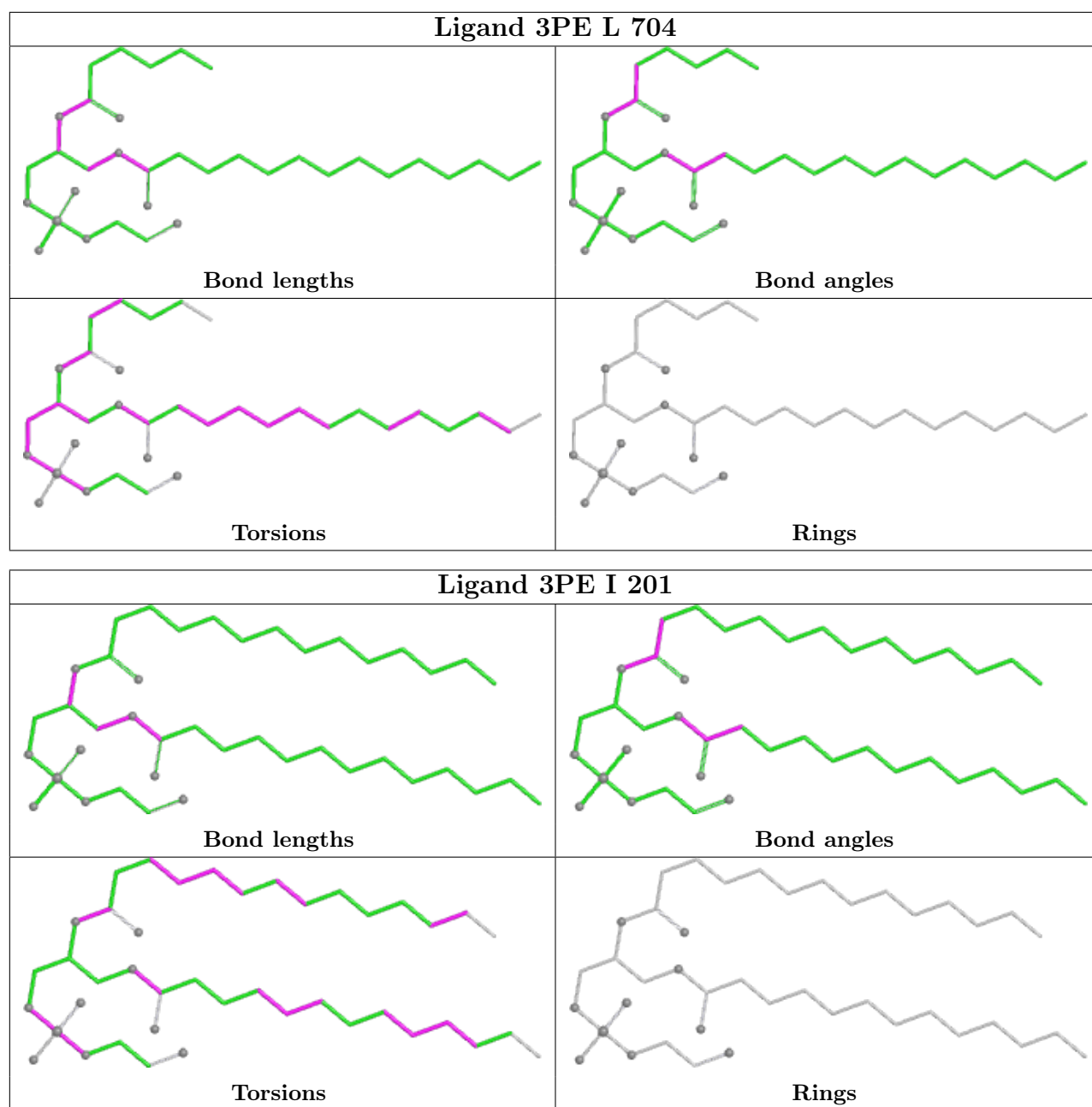












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

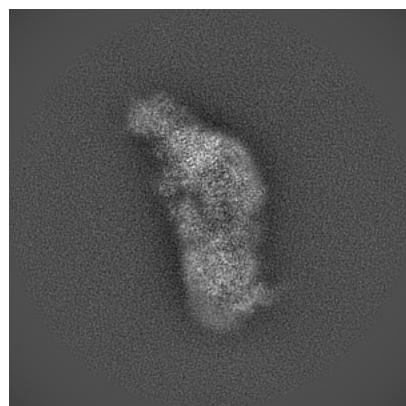
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14127. These allow visual inspection of the internal detail of the map and identification of artifacts.

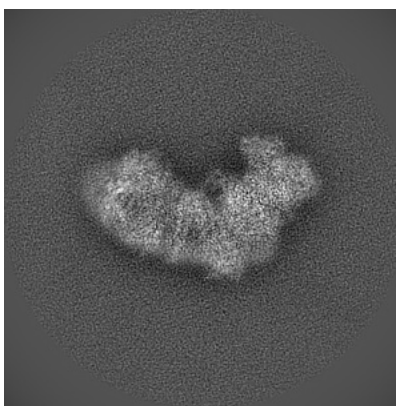
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

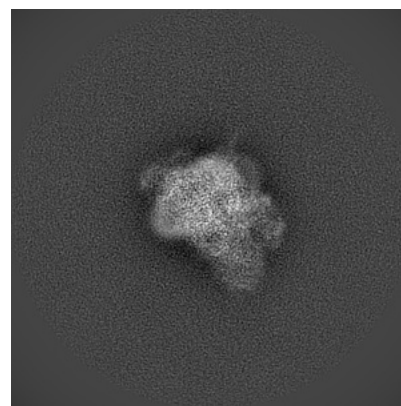
6.1.1 Primary map



X

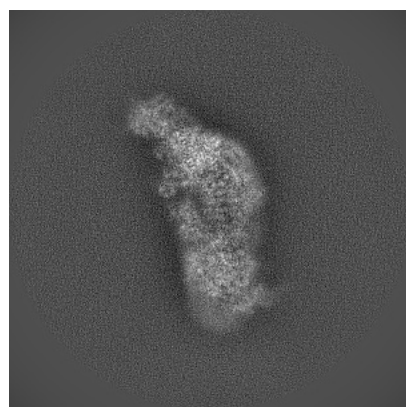


Y

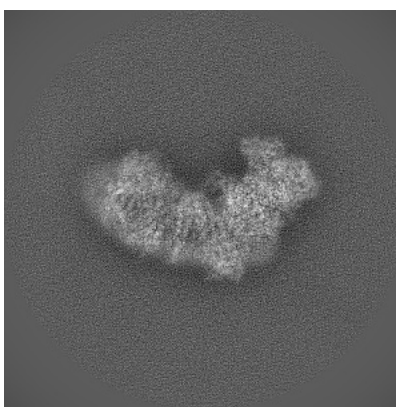


Z

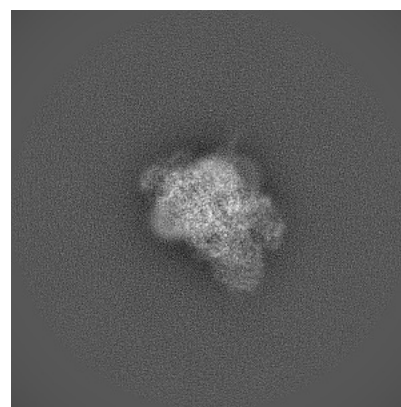
6.1.2 Raw map



X



Y

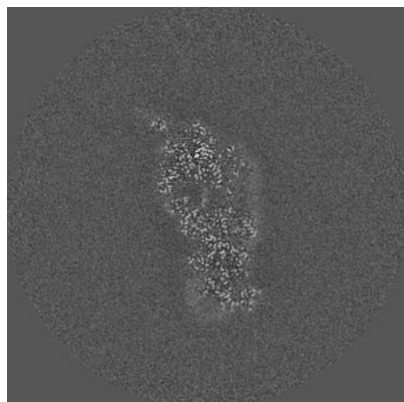


Z

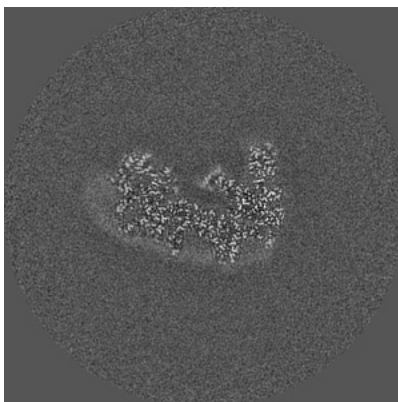
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

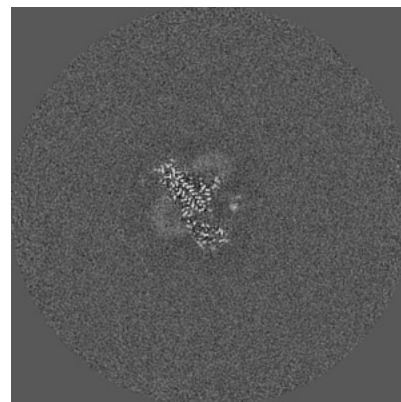
6.2.1 Primary map



X Index: 225

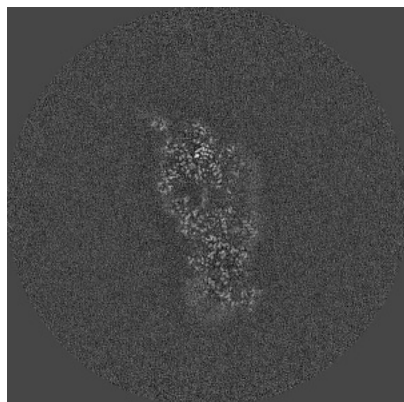


Y Index: 225

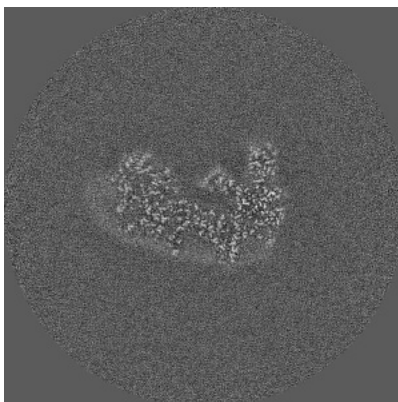


Z Index: 225

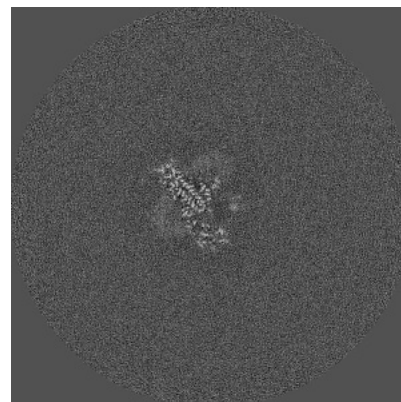
6.2.2 Raw map



X Index: 225



Y Index: 225

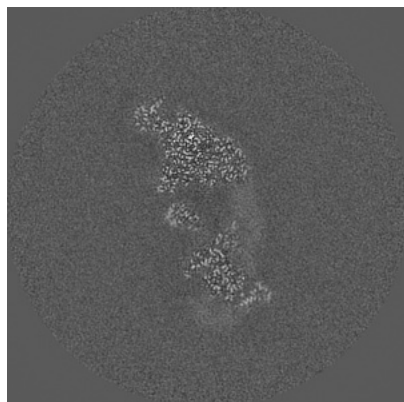


Z Index: 225

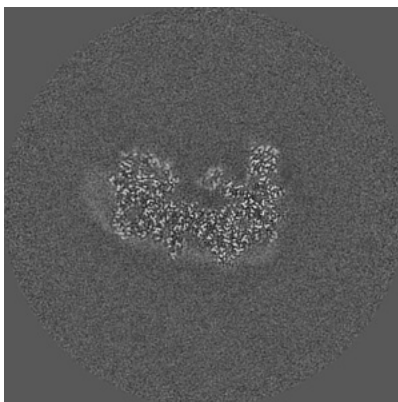
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

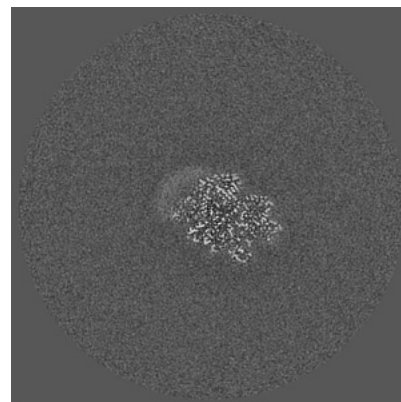
6.3.1 Primary map



X Index: 238

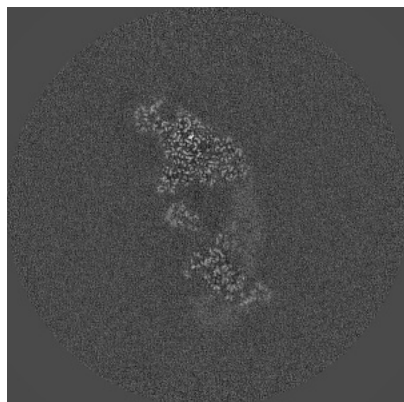


Y Index: 229

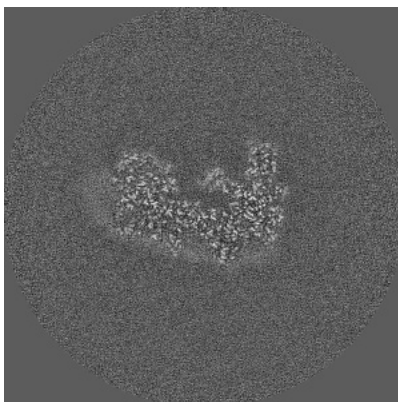


Z Index: 290

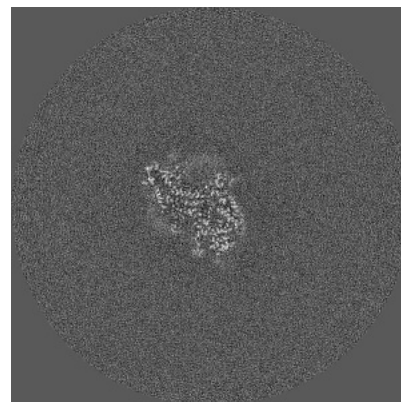
6.3.2 Raw map



X Index: 238



Y Index: 227

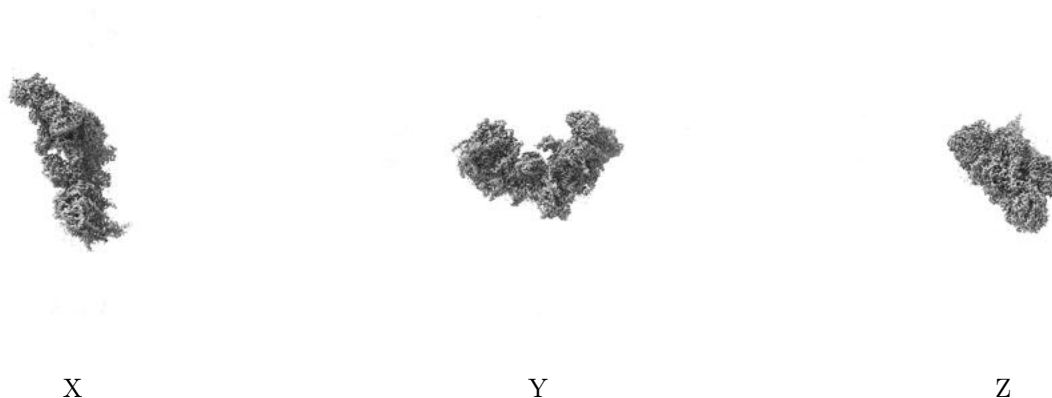


Z Index: 254

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

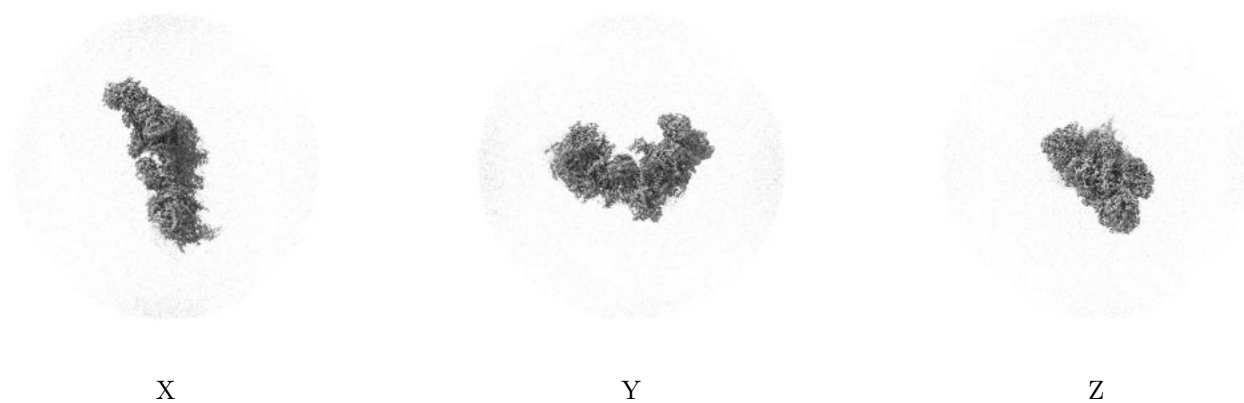
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

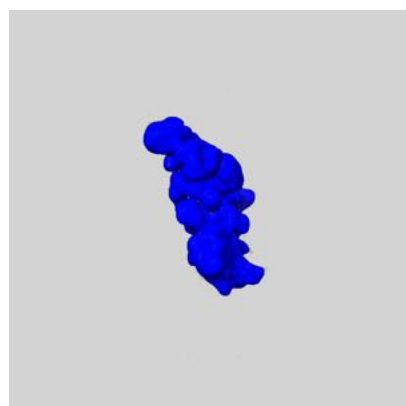
6.5 Mask visualisation [i](#)

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

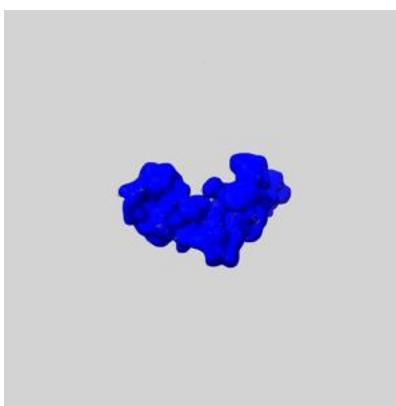
A mask typically either:

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

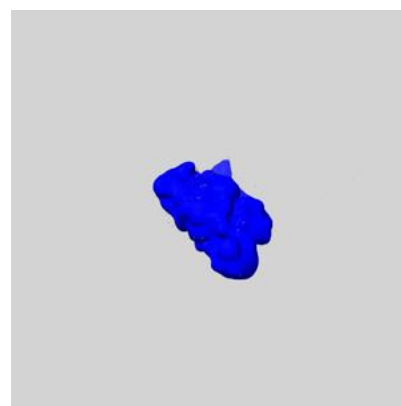
6.5.1 emd_14127_msk_1.map [i](#)



X



Y

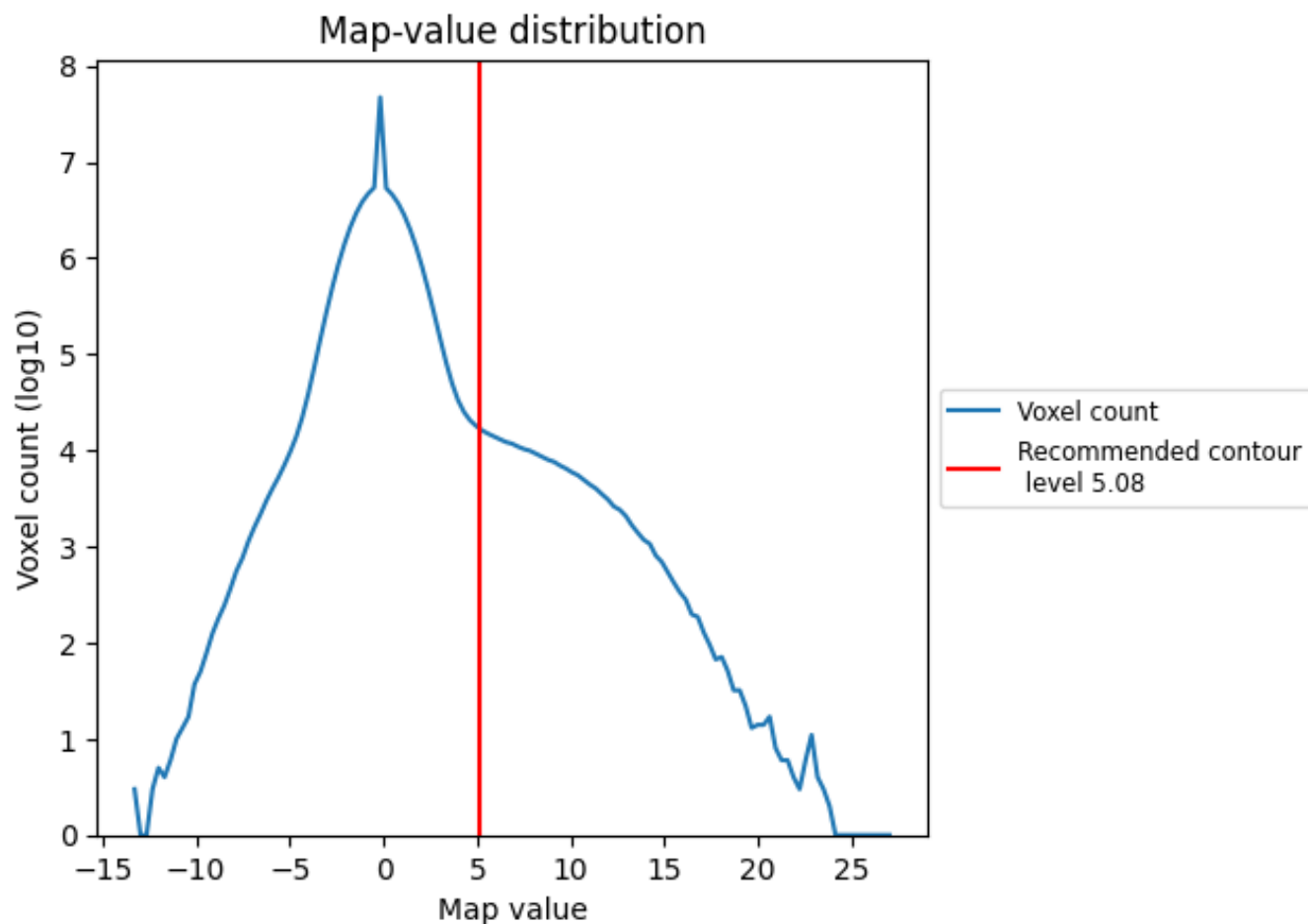


Z

7 Map analysis [i](#)

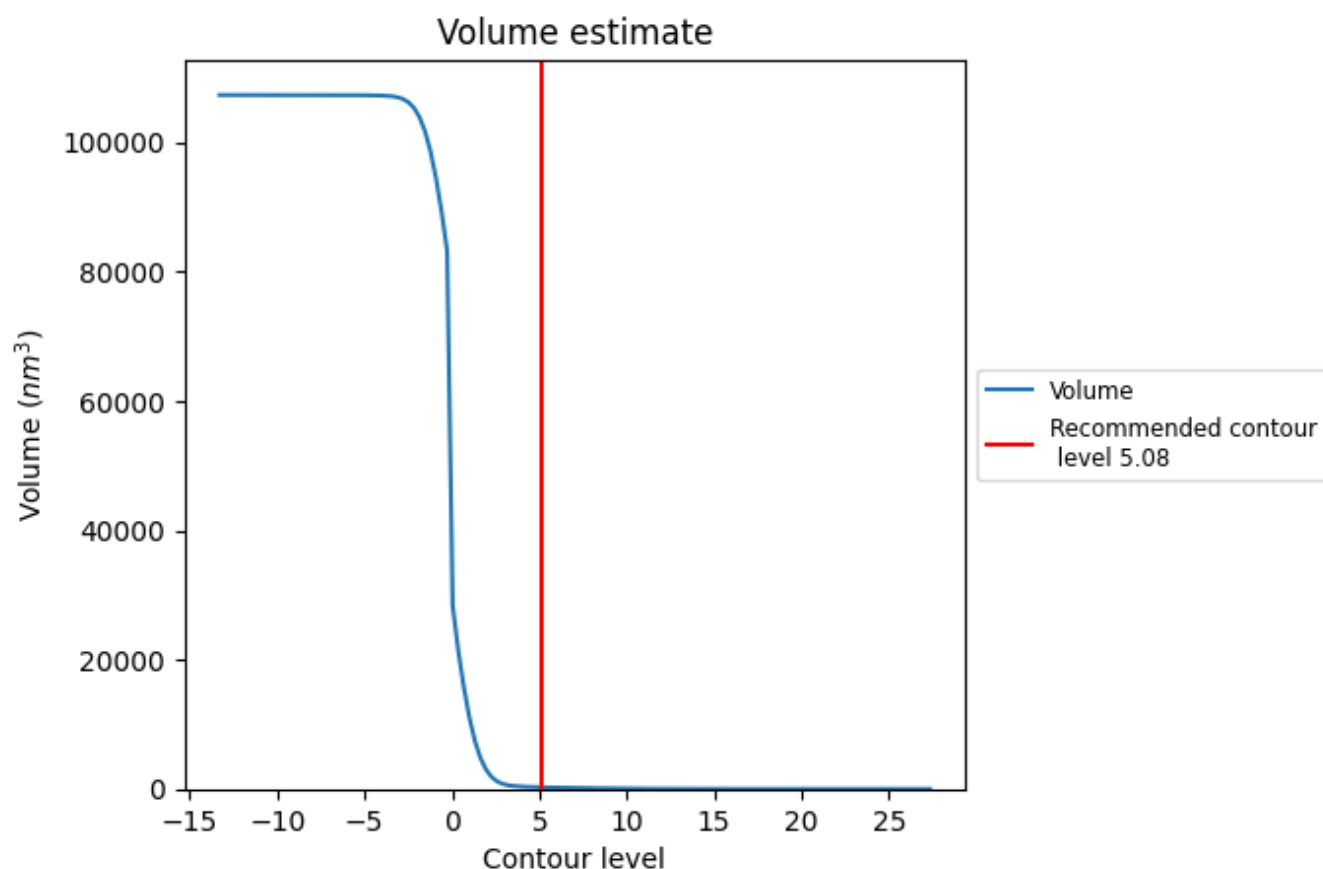
This section contains the results of statistical analysis of the map.

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.

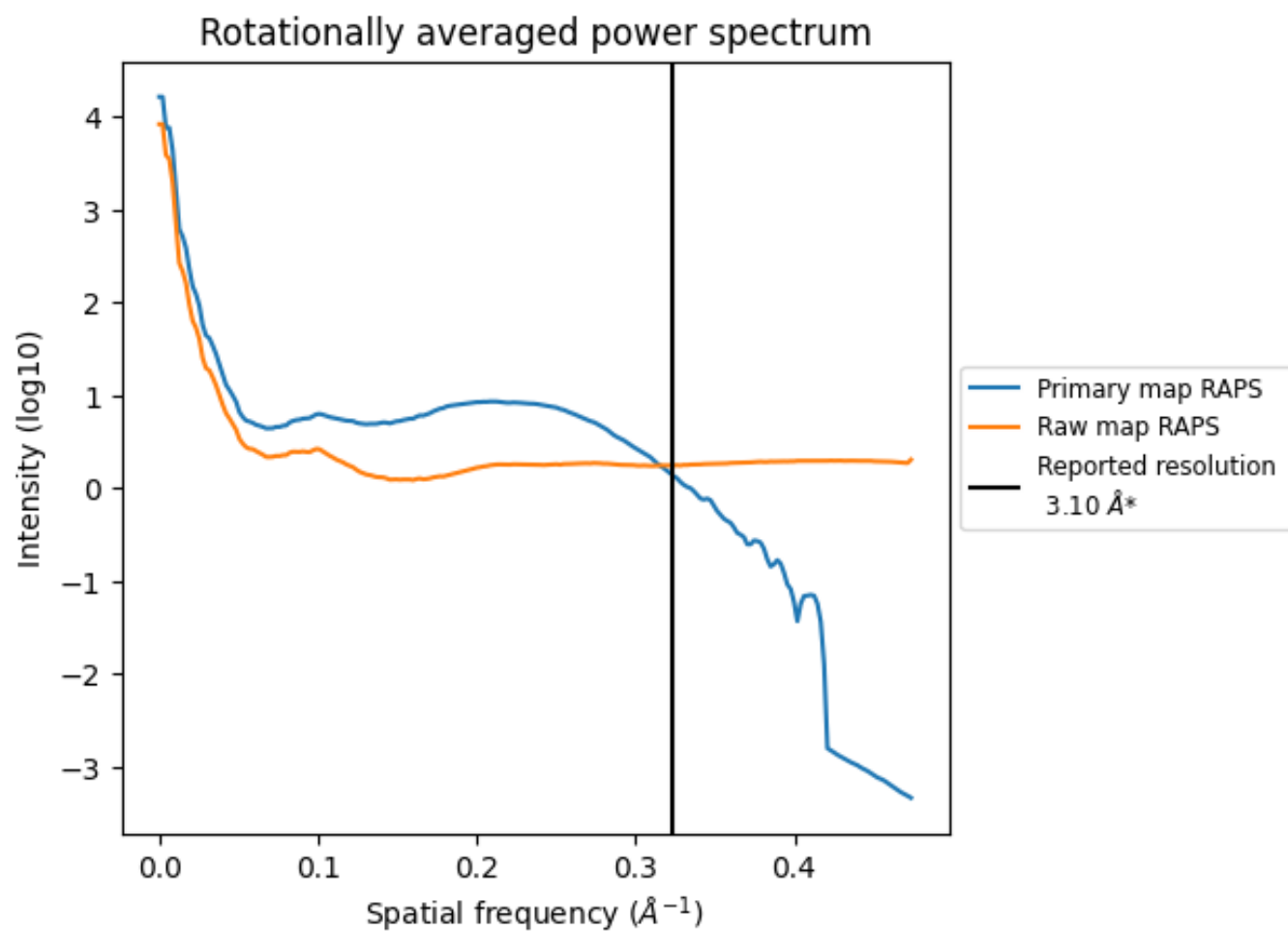
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm^3 ; this corresponds to an approximate mass of 232 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

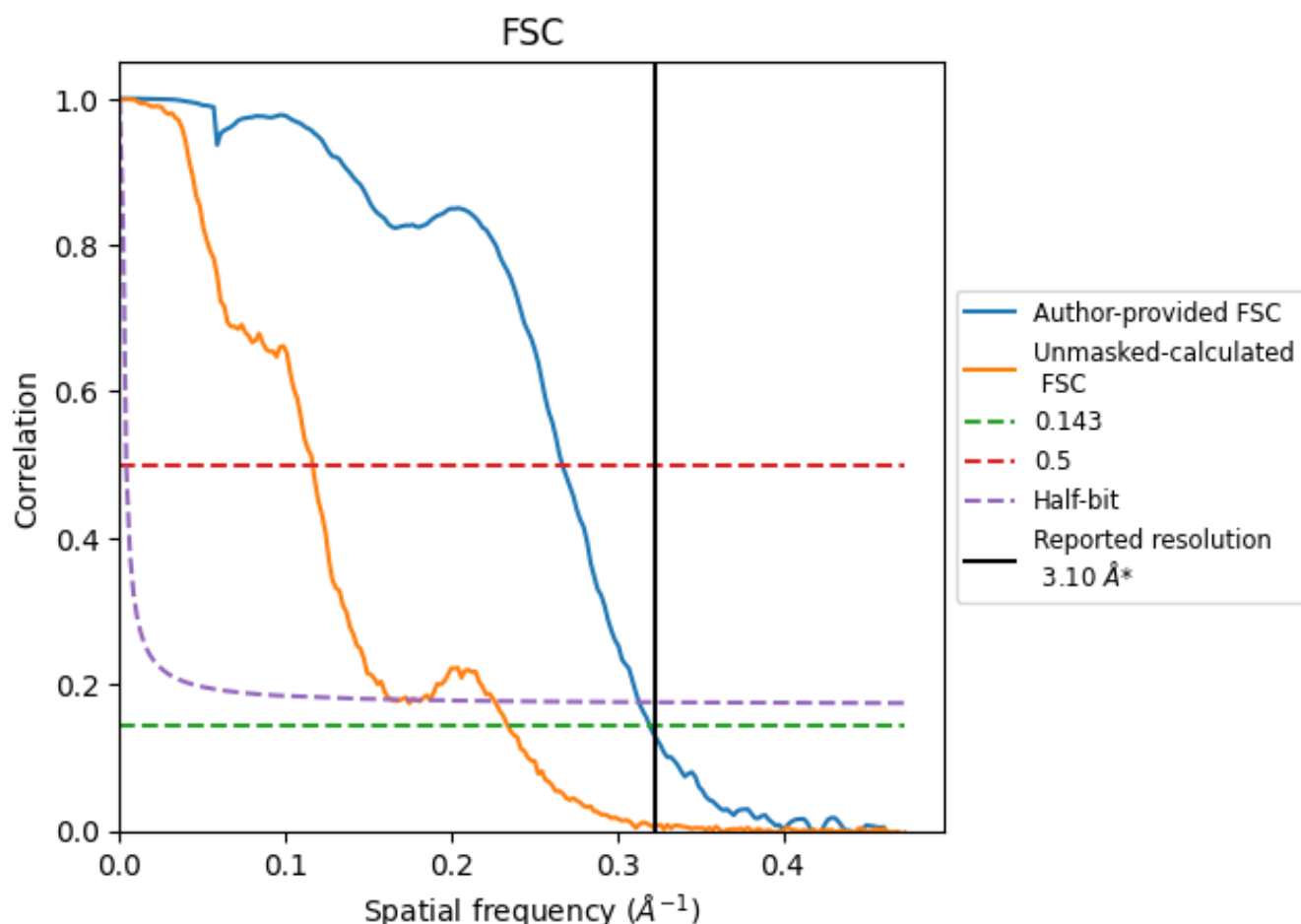


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

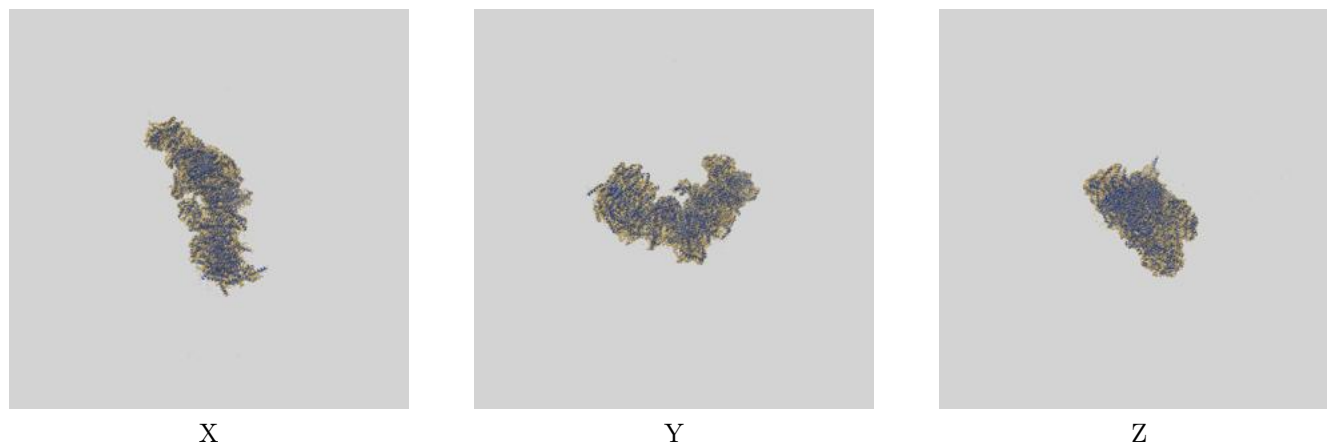
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.75	3.19
Unmasked-calculated*	4.27	8.58	6.11

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

9 Map-model fit [i](#)

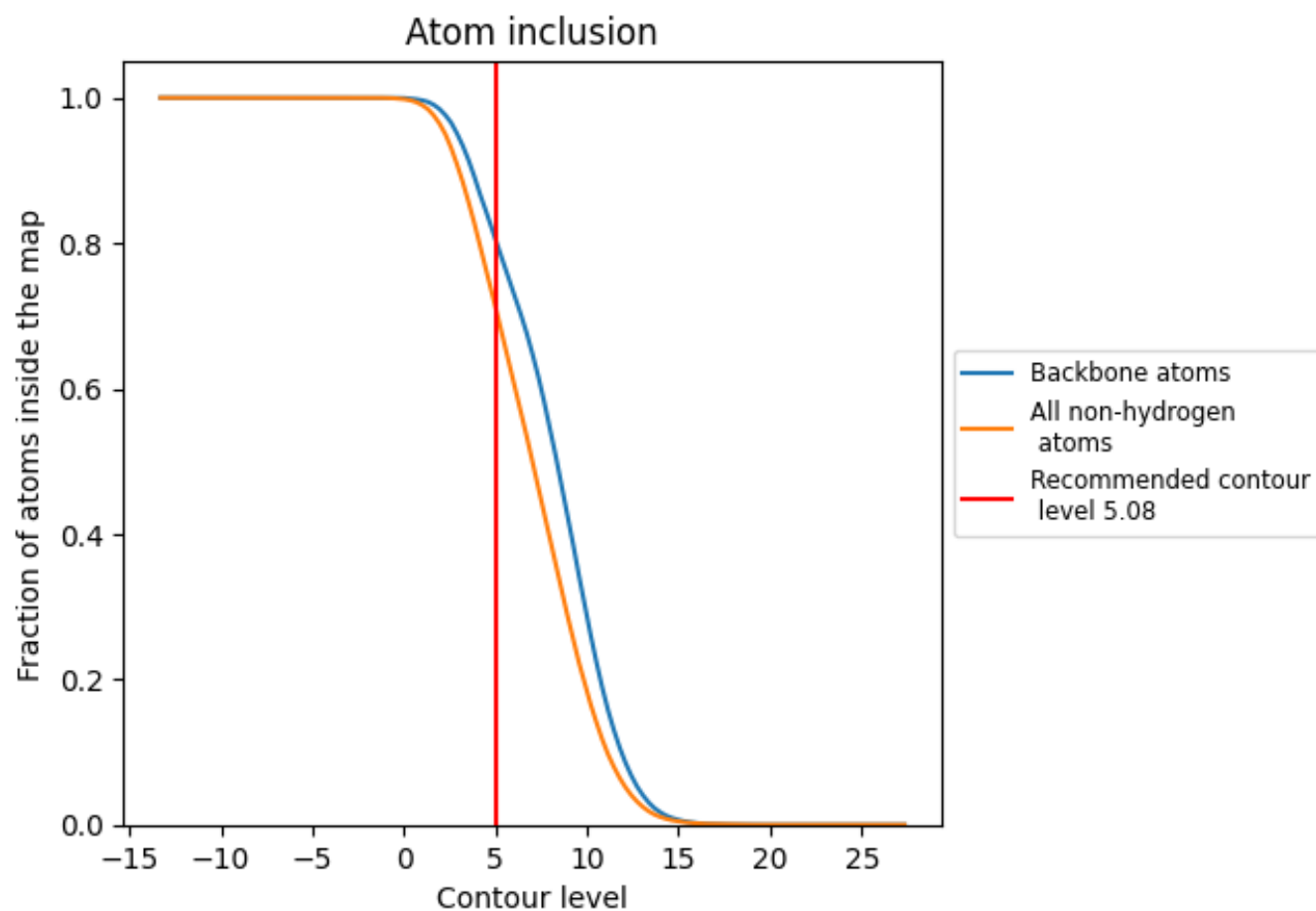
This section contains information regarding the fit between EMDB map EMD-14127 and PDB model 7QSD. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.08 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 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.