



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 02:59 pm BST

PDB ID : 7ZMH
EMDB ID : EMD-14798
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (state 1) - membrane arm
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.47 Å (reported)
Based on initial models : 6RFQ, 6RFR

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

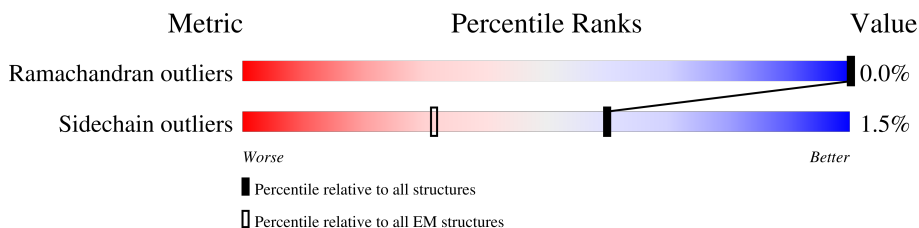
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.47 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.



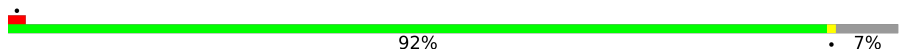
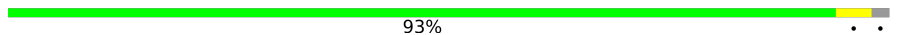
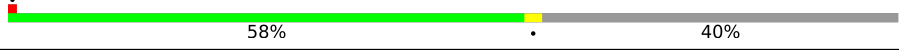
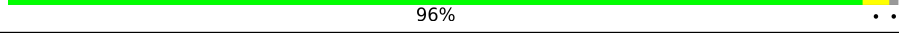



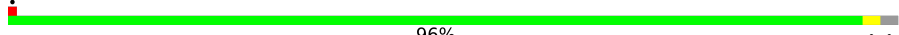



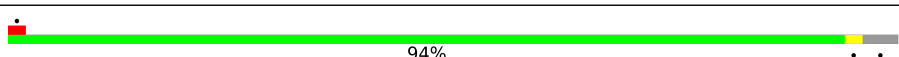

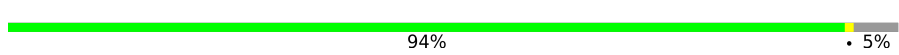

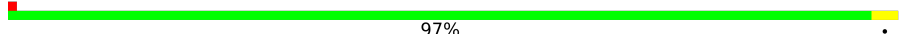

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	378	88% 12%
2	2	571	96% ..
3	3	146	69% 31%
4	4	542	89% . 9%
5	5	679	97% ..
6	6	224	82% . 15%
7	8	86	91% 9%
8	9	785	13% 87%
9	D	86	99% .

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Mol	Chain	Length	Quality of chain
10	J	199	 92% 7%
11	L	89	 93%
12	Q	141	 58% 40%
13	R	99	 96%
14	S	143	 51% 48%
15	U	186	 90% 10%
16	W	121	 81% 18%
17	X	191	 96%
18	a	815	 17% 82%
19	b	94	 86% 14%
20	c	93	 66% 34%
21	d	105	 94%
22	e	46	 83% 17%
23	g	82	 94% 5%
24	i	93	 85% 13%
25	j	75	 97%
26	n	184	 73% 27%

2 Entry composition i

There are 32 unique types of molecules in this entry. The entry contains 37605 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	334	2566	1722	388	445	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	558	4459	2994	672	782	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	101	788	541	113	132	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	494	3904	2650	572	670	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	670	5273	3551	792	905	25	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	445	ARG	-	insertion	UNP G1DJA3
5	446	LEU	-	insertion	UNP G1DJA3
5	447	ALA	-	insertion	UNP G1DJA3

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Chain	Residue	Modelled	Actual	Comment	Reference
5	448	ILE	-	insertion	UNP G1DJA3
5	449	ASP	-	insertion	UNP G1DJA3
5	450	ASN	-	insertion	UNP G1DJA3
5	451	PHE	-	insertion	UNP G1DJA3
5	452	PHE	-	insertion	UNP G1DJA3
5	453	SER	-	insertion	UNP G1DJA3
5	454	ALA	-	insertion	UNP G1DJA3
5	455	GLN	-	insertion	UNP G1DJA3
5	456	ALA	-	insertion	UNP G1DJA3
5	457	ILE	-	insertion	UNP G1DJA3
5	458	LYS	-	insertion	UNP G1DJA3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	190	1468	988	221	253	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	78	663	411	127	119	6	0	0

- Molecule 8 is a protein called Subunit NDUFS5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	9	103	807	500	147	154	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	100	VAL	-	insertion	UNP G0SG48

- Molecule 9 is a protein called Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	85	Total	C	N	O	S	0	0
			678	432	127	115	4		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	186	Total	C	N	O	S	0	0
			1388	877	259	250	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	87	Total	C	N	O	S	0	0
			673	453	102	115	3		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	85	Total	C	N	O	S	0	0
			673	422	109	141	1		

- Molecule 13 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	98	Total	C	N	O	S	0	0
			807	520	149	137	1		

- Molecule 14 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	74	Total	C	N	O	0	0
			612	402	98	112		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	167	Total	C	N	O	S	0	0
			1357	854	253	241	9		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	99	816	521	154	139	2	0	0

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	X	187	1484	943	268	265	8	0	0

- Molecule 18 is a protein called NADH dehydrogenase (Ubiquinone)-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	a	144	1172	753	196	218	5	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	166	VAL	ALA	conflict	UNP G0RXU4
a	168	ALA	MET	conflict	UNP G0RXU4
a	?	-	GLU	deletion	UNP G0RXU4
a	?	-	GLY	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4
a	?	-	ASP	deletion	UNP G0RXU4
a	?	-	PRO	deletion	UNP G0RXU4

- Molecule 19 is a protein called Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	b	81	683	445	125	110	3	0	0

- Molecule 20 is a protein called Subunit NDUFB3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	c	61	505	329	91	83	2	0	0

- Molecule 21 is a protein called Subunit NDUFB10 of NADH-ubiquinone oxidoreductase

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	d	101	843	535	149	155	4	0	0

- Molecule 22 is a protein called Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	e	38	317	215	55	46	1	0	0

- Molecule 23 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	g	78	610	399	105	105	1	0	0

- Molecule 24 is a protein called Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	i	81	682	450	118	112	2	0	0

- Molecule 25 is a protein called Subunit NDUF4 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	j	75	616	399	110	103	4	0	0

- Molecule 26 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	n	135	1061	680	186	194	1	0	0

There are 52 discrepancies between the modelled and reference sequences:

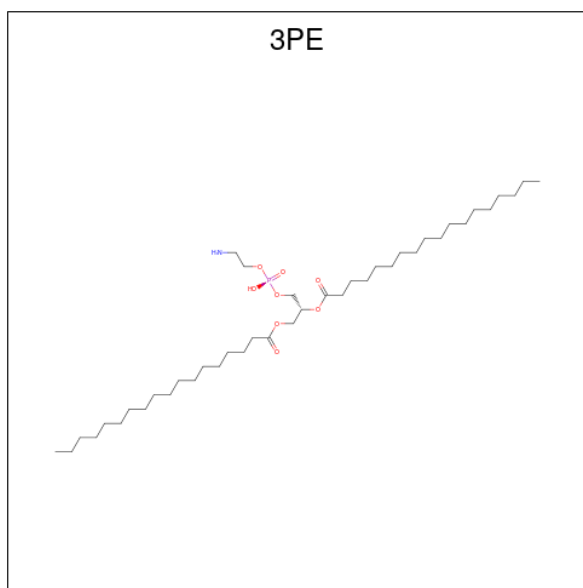
Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP G0S086
n	9	ALA	-	insertion	UNP G0S086
n	10	LEU	-	insertion	UNP G0S086
n	11	LEU	-	insertion	UNP G0S086
n	12	ALA	-	insertion	UNP G0S086
n	13	ARG	-	insertion	UNP G0S086
n	14	ARG	-	insertion	UNP G0S086
n	15	VAL	-	insertion	UNP G0S086
n	16	ARG	-	insertion	UNP G0S086
n	17	PRO	-	insertion	UNP G0S086
n	18	THR	-	insertion	UNP G0S086
n	19	VAL	-	insertion	UNP G0S086
n	20	VAL	-	insertion	UNP G0S086
n	21	VAL	-	insertion	UNP G0S086
n	22	PRO	-	insertion	UNP G0S086
n	23	ARG	-	insertion	UNP G0S086
n	24	ASN	-	insertion	UNP G0S086
n	25	ALA	-	insertion	UNP G0S086
n	26	ARG	-	insertion	UNP G0S086
n	27	THR	-	insertion	UNP G0S086
n	28	TYR	-	insertion	UNP G0S086
n	29	ALA	-	insertion	UNP G0S086
n	30	SER	-	insertion	UNP G0S086
n	31	SER	-	insertion	UNP G0S086
n	32	HIS	-	insertion	UNP G0S086
n	33	ASP	-	insertion	UNP G0S086
n	34	HIS	-	insertion	UNP G0S086
n	35	ASP	-	insertion	UNP G0S086
n	36	HIS	-	insertion	UNP G0S086
n	37	HIS	-	insertion	UNP G0S086
n	38	ASP	-	insertion	UNP G0S086
n	39	HIS	-	insertion	UNP G0S086
n	40	HIS	-	insertion	UNP G0S086
n	41	HIS	-	insertion	UNP G0S086
n	42	ASP	-	insertion	UNP G0S086
n	43	HIS	-	insertion	UNP G0S086

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Chain	Residue	Modelled	Actual	Comment	Reference
n	44	GLY	-	insertion	UNP G0S086
n	45	HIS	-	insertion	UNP G0S086
n	46	ASN	-	insertion	UNP G0S086
n	47	VAL	-	insertion	UNP G0S086
n	48	GLU	-	insertion	UNP G0S086
n	49	GLU	-	insertion	UNP G0S086
n	50	PRO	-	insertion	UNP G0S086
n	51	LEU	-	insertion	UNP G0S086
n	52	GLY	-	insertion	UNP G0S086

- Molecule 27 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



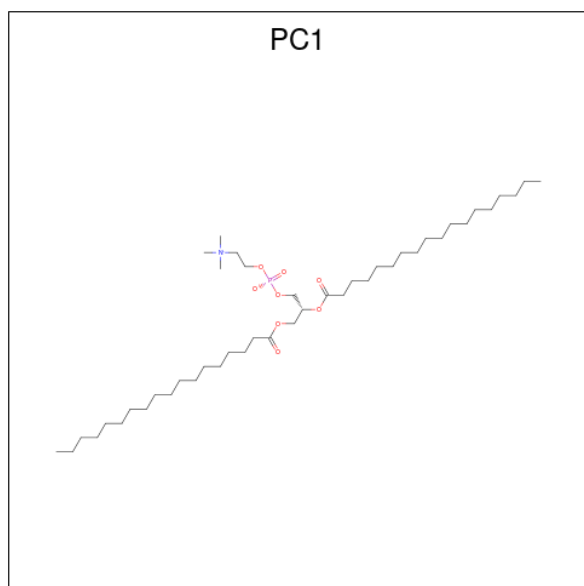
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	1	1	Total	C	N	O	P	0
			45	35	1	8	1	
27	4	1	Total	C	N	O	P	0
			45	35	1	8	1	
27	4	1	Total	C	N	O	P	0
			34	24	1	8	1	
27	5	1	Total	C	N	O	P	0
			35	25	1	8	1	
27	5	1	Total	C	N	O	P	0
			33	23	1	8	1	
27	5	1	Total	C	N	O	P	0
			35	25	1	8	1	

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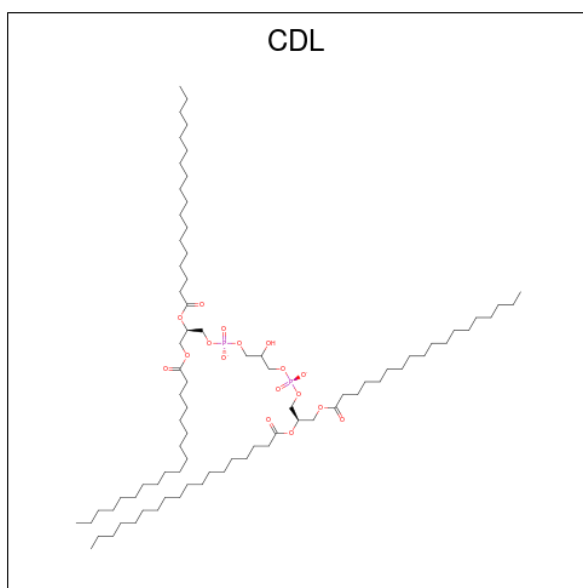
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	5	1	Total 43	C 33	N 1	O 8	P 1	0
27	5	1	Total 33	C 23	N 1	O 8	P 1	0
27	6	1	Total 36	C 26	N 1	O 8	P 1	0
27	J	1	Total 30	C 20	N 1	O 8	P 1	0
27	W	1	Total 38	C 28	N 1	O 8	P 1	0
27	W	1	Total 39	C 29	N 1	O 8	P 1	0
27	g	1	Total 36	C 26	N 1	O 8	P 1	0
27	g	1	Total 44	C 34	N 1	O 8	P 1	0
27	i	1	Total 41	C 31	N 1	O 8	P 1	0
27	n	1	Total 51	C 41	N 1	O 8	P 1	0
27	n	1	Total 39	C 29	N 1	O 8	P 1	0

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			42	32	1	8	1	
28	3	1	Total	C	N	O	P	0
			43	33	1	8	1	
28	4	1	Total	C	N	O	P	0
			50	40	1	8	1	
28	5	1	Total	C	N	O	P	0
			54	44	1	8	1	
28	5	1	Total	C	N	O	P	0
			43	33	1	8	1	
28	S	1	Total	C	N	O	P	0
			52	42	1	8	1	
28	X	1	Total	C	N	O	P	0
			39	29	1	8	1	
28	X	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 29 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



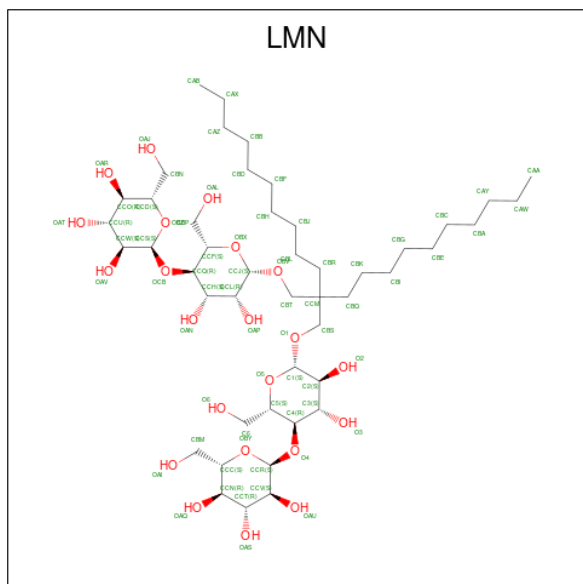
Mol	Chain	Residues	Atoms				AltConf
29	2	1	Total	C	O	P	0
			74	55	17	2	
29	D	1	Total	C	O	P	0
			65	46	17	2	
29	S	1	Total	C	O	P	0
			79	60	17	2	
29	X	1	Total	C	O	P	0
			70	51	17	2	

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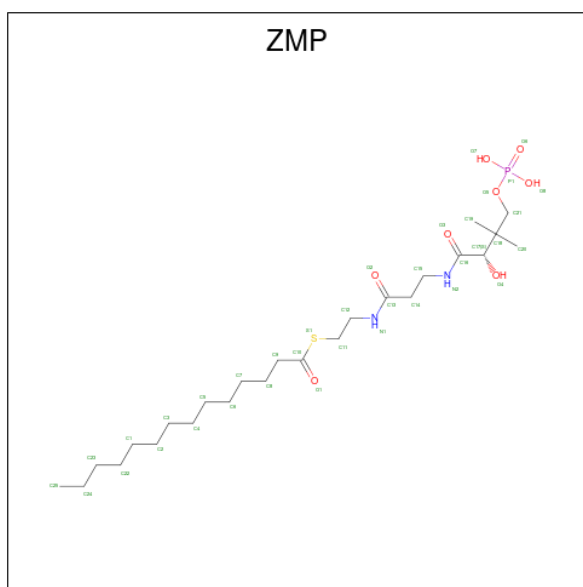
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
29	X	1	79	60	17	2	0

- Molecule 30 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	2	1	58	41	17	0
30	4	1	47	35	12	0
30	j	1	69	47	22	0

- Molecule 31 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
31	Q	1	36	25	2	7	1	1	0

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	1	110	Total	O	0
			110	110	
32	2	224	Total	O	0
			224	224	
32	3	25	Total	O	0
			25	25	
32	4	181	Total	O	0
			181	181	
32	5	100	Total	O	0
			100	100	
32	6	52	Total	O	0
			52	52	
32	9	23	Total	O	0
			23	23	
32	D	36	Total	O	0
			36	36	
32	J	1	Total	O	0
			1	1	
32	L	23	Total	O	0
			23	23	
32	Q	1	Total	O	0
			1	1	

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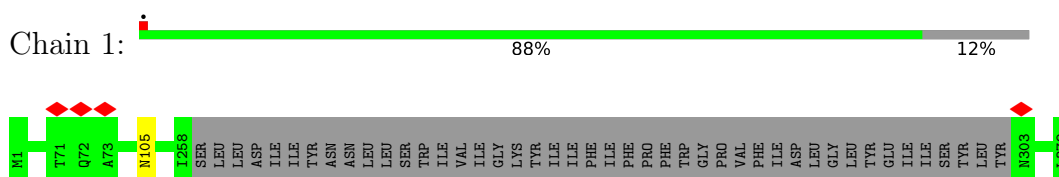
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Mol	Chain	Residues	Atoms		AltConf
32	R	15	Total 15	O 15	0
32	S	6	Total 6	O 6	0
32	U	60	Total 60	O 60	0
32	W	43	Total 43	O 43	0
32	X	71	Total 71	O 71	0
32	a	23	Total 23	O 23	0
32	b	13	Total 13	O 13	0
32	d	18	Total 18	O 18	0
32	g	15	Total 15	O 15	0
32	i	11	Total 11	O 11	0
32	j	18	Total 18	O 18	0
32	n	42	Total 42	O 42	0

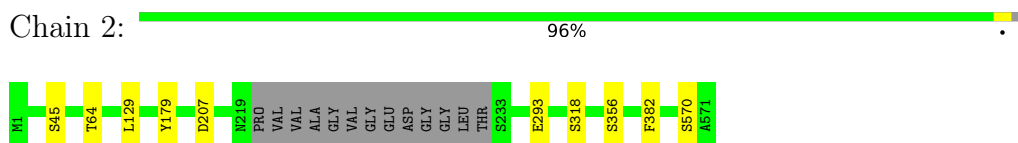
3 Residue-property plots [i](#)

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

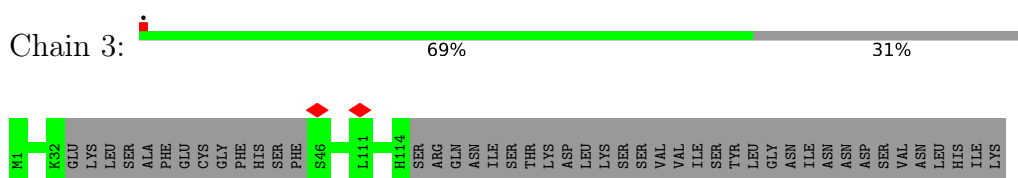
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



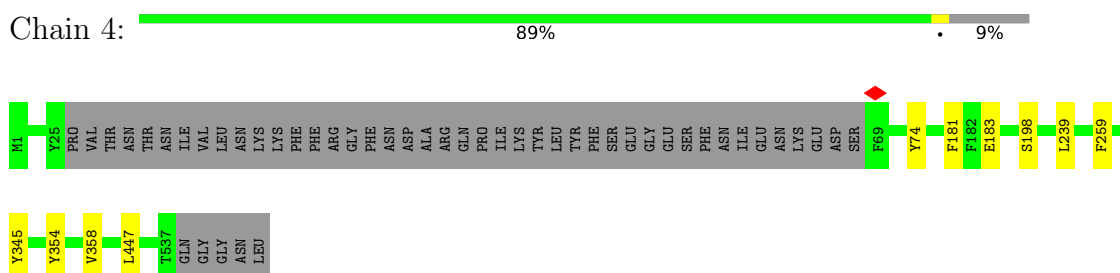
- Molecule 2: NADH dehydrogenase subunit 2



- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



- Molecule 4: NADH-ubiquinone oxidoreductase chain 4

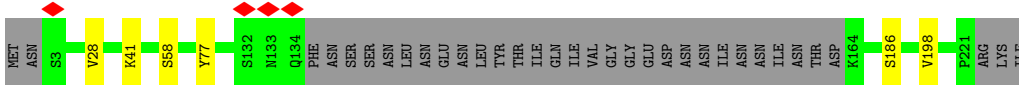
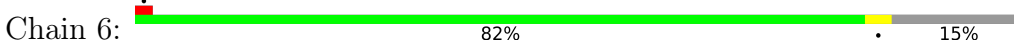


- Molecule 5: NADH-ubiquinone oxidoreductase chain 5

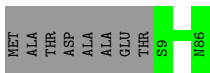
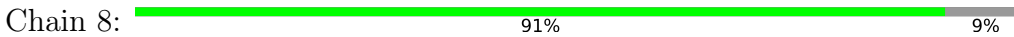




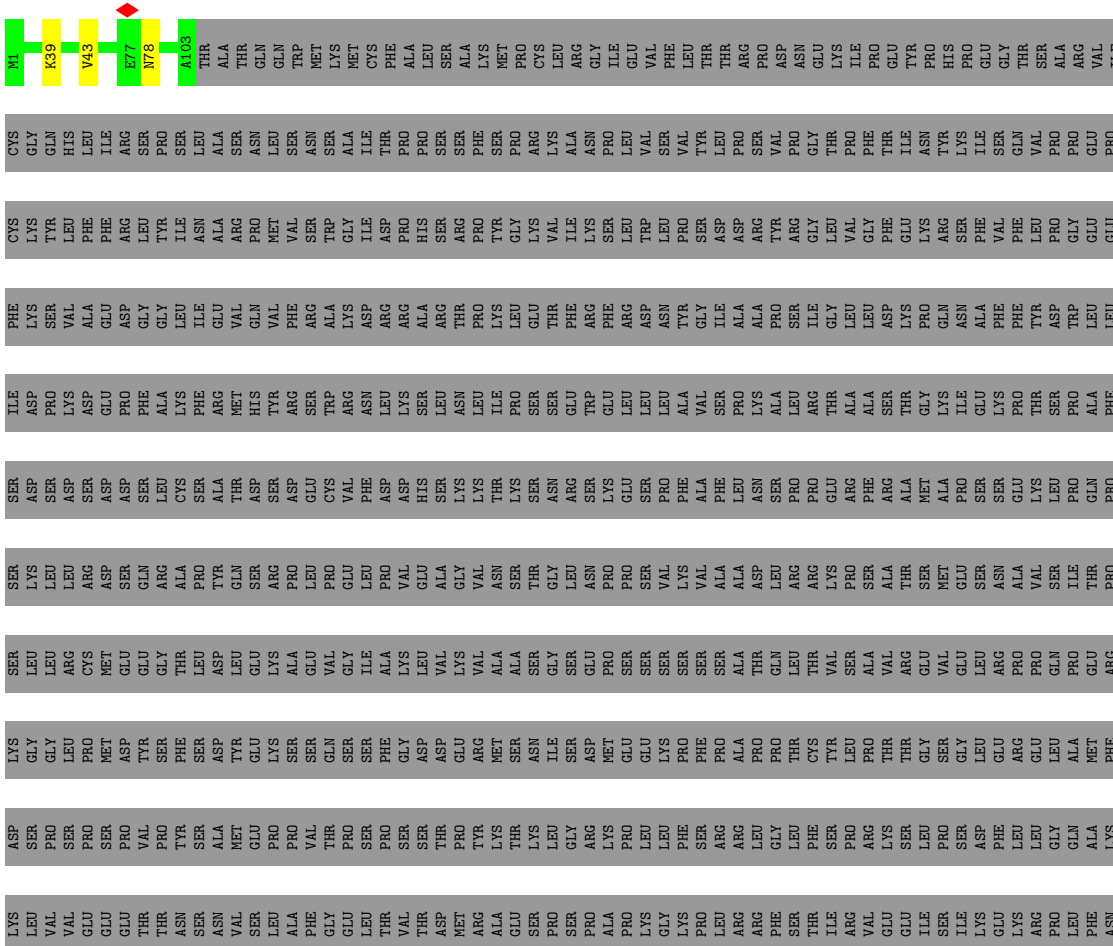
● Molecule 6: NADH-ubiquinone oxidoreductase chain 6



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



● Molecule 8: Subunit NDUF55 of NADH-ubiquinone oxidoreductase (Complex I)




SER
LEU
ARG
ARG
ILE
ALA
SER
SER
ALA
SER
PRO
ARG
ARG
LYS
LEU
ALA
GLY
ARG
VAL
LEU
SER
SER
MET
ASP
LEU
GLY
LYS
LYS
GLY
GLY
GLU
LYS
GLU
GLY

- Molecule 9: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

Chain D:  99%

MET
P2
X86

- Molecule 10: NADH-ubiquinone oxidoreductase-like protein

Chain J:  92% 7%

MET
ALA
PRO
ILE
GLU
GLU
HIS
GLU
HIS
TYR
HIS
P13
F112
G132
V133
R136
E157
G198
ALA

- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain L:  93%

MET
P2
S35
F38
I51
E66
Y88
LYS

- Molecule 12: Acyl carrier protein

Chain Q:  58% 40%

MET
PHE
ARG
SER
ALA
VAL
LEU
ARG
SER
ALA
ALA
ALA
THR
ARG
THR
THR
ILE
ILE
ARG
SER
ILE
PRO
PRO
ALA
ALA
ALA
LYS
LYS
PHE
ALA
ALA
VAL
VAL
ALA
PRO
VAL
VAL
SER
ARG
VAL
THR
SER
PHE
ILE
PRO
LYS
THR
ALA
SER
TRP
GLN
VAL
ILE
ARG
CYS
TYR
ALA
SER
ASN
E57
S98

E111
Q137
H141

- Molecule 13: Complex I-B22

Chain R:  96%

MET
S2
L61
L91
E92
F99


- Molecule 14: Complex I-ESSS

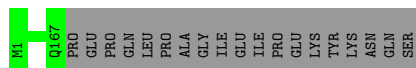
Chain S: 51% 48%

MET
ASP
GLY
GLY
PRO
PRO
THR
PHE
ALA
PHE
ARG
PRO
THR
ALA
ALA
GLN
GLN
ALA
PRO
GLY
LYS
LEU
SER
SER
ALA
PRO
VAL
THR
THR
ARG
ARG
LEU
ALA
ALA
ALA
LEU
LEU
SER
SER
ARG
ALA
SER
SER
VAL
SER
SER
LYS
ALA
LEU
THR
PRO
ALA
ALA
ARG
PHE
ARG
PHE
PHE
SER
THR
THR
GLN
ARG
ARG




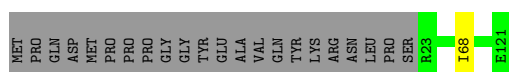
- Molecule 15: NADH-ubiquinone oxidoreductase

Chain U:  90% 10%



- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  81% 18%



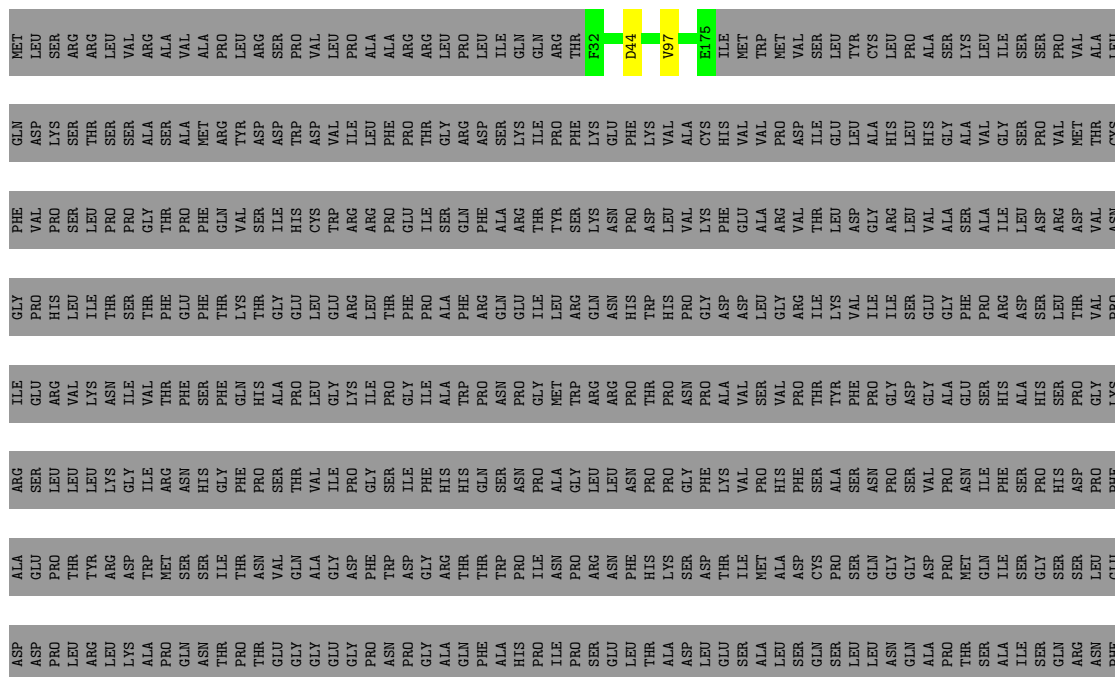
- Molecule 17: NADH-ubiquinone oxidoreductase-like protein

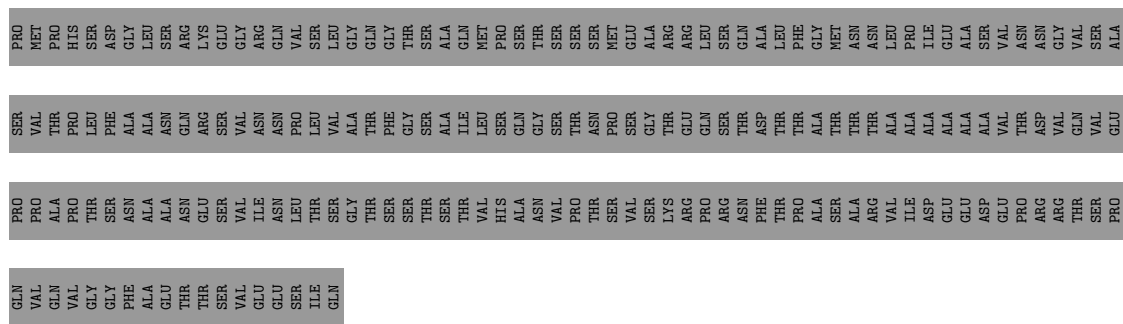
Chain X:  96% ..



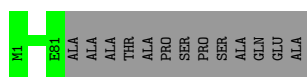
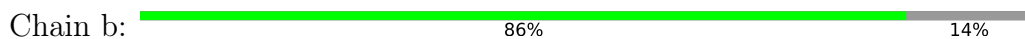
- Molecule 18: NADH dehydrogenase (Ubiquinone)-like protein

Chain a:  17% 82%

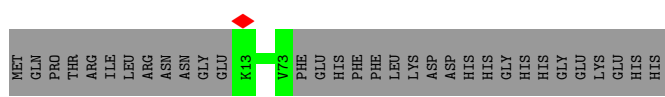




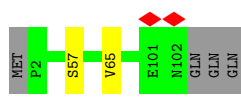
- Molecule 19: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)



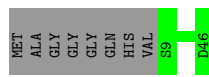
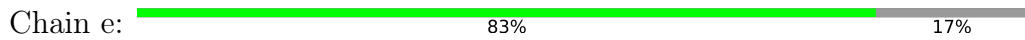
- Molecule 20: Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I)



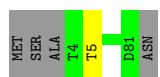
- Molecule 21: Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I)



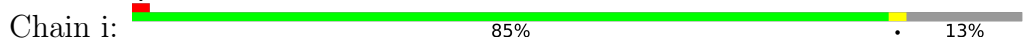
- Molecule 22: Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I)

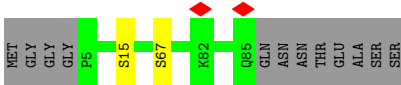


- Molecule 23: Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I)

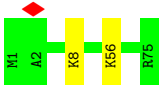


- Molecule 24: Subunit NDUF6 of NADH-ubiquinone oxidoreductase (Complex I)

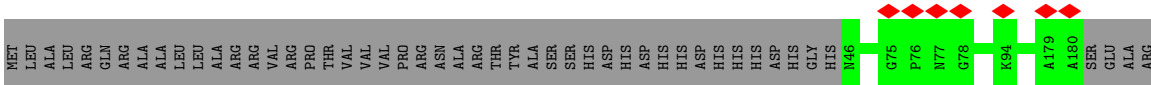




- Molecule 25: Subunit NDUFB4 of NADH-ubiquinone oxidoreductase (Complex I)



- Molecule 26: Subunit NDUFB5 of NADH-ubiquinone oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153568	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.221	Depositor
Minimum map value	-2.124	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.168	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	143.964, 218.457, 227.664	wwPDB
Map dimensions	272, 261, 172	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.837, 0.837, 0.837	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: CDL, ZMP, 3PE, LMN, PC1

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	1	0.42	0/2625	0.53	0/3582
2	2	0.42	0/4565	0.55	0/6209
3	3	0.42	0/809	0.56	0/1102
4	4	0.44	0/4002	0.60	3/5454 (0.1%)
5	5	0.41	0/5415	0.55	2/7372 (0.0%)
6	6	0.39	0/1495	0.52	0/2038
7	8	0.45	0/676	0.48	0/903
8	9	0.38	0/824	0.52	0/1112
9	D	0.38	0/674	0.53	0/911
10	J	0.36	0/1413	0.50	0/1908
11	L	0.36	0/680	0.56	0/921
12	Q	0.47	0/683	0.60	0/926
13	R	0.37	0/832	0.47	0/1133
14	S	0.45	0/637	0.54	0/872
15	U	0.36	0/1394	0.52	0/1890
16	W	0.39	0/834	0.58	0/1125
17	X	0.41	0/1523	0.55	1/2058 (0.0%)
18	a	0.38	0/1209	0.52	0/1639
19	b	0.36	0/701	0.42	0/939
20	c	0.31	0/524	0.50	0/710
21	d	0.53	1/861 (0.1%)	0.54	2/1157 (0.2%)
22	e	0.28	0/332	0.36	0/451
23	g	0.37	0/631	0.47	0/868
24	i	0.36	0/711	0.45	0/967
25	j	0.42	0/630	0.55	0/847
26	n	0.32	0/1092	0.40	0/1481
All	All	0.41	1/35772 (0.0%)	0.53	8/48575 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	d	65	VAL	C-N	10.83	1.58	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	144	ARG	CG-CD-NE	7.30	127.13	111.80
21	d	65	VAL	O-C-N	7.02	133.93	122.70
5	5	278	LEU	CA-CB-CG	5.63	128.24	115.30
21	d	65	VAL	CA-C-N	-5.62	104.83	117.20
4	4	259	PHE	CB-CA-C	5.33	121.07	110.40

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	1	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	545 (98%)	8 (1%)	1 (0%)	44	62
3	3	97/146 (66%)	93 (96%)	4 (4%)	0	100	100
4	4	490/542 (90%)	479 (98%)	11 (2%)	0	100	100
5	5	668/679 (98%)	636 (95%)	31 (5%)	1 (0%)	48	67
6	6	186/224 (83%)	183 (98%)	3 (2%)	0	100	100
7	8	76/86 (88%)	71 (93%)	5 (7%)	0	100	100
8	9	101/785 (13%)	101 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
10	J	184/199 (92%)	178 (97%)	6 (3%)	0	100	100
11	L	85/89 (96%)	85 (100%)	0	0	100	100
12	Q	83/141 (59%)	82 (99%)	1 (1%)	0	100	100
13	R	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
14	S	72/143 (50%)	72 (100%)	0	0	100	100
15	U	165/186 (89%)	163 (99%)	2 (1%)	0	100	100
16	W	97/121 (80%)	97 (100%)	0	0	100	100
17	X	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
18	a	142/815 (17%)	136 (96%)	6 (4%)	0	100	100
19	b	79/94 (84%)	77 (98%)	2 (2%)	0	100	100
20	c	59/93 (63%)	55 (93%)	4 (7%)	0	100	100
21	d	99/105 (94%)	97 (98%)	2 (2%)	0	100	100
22	e	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
23	g	76/82 (93%)	73 (96%)	3 (4%)	0	100	100
24	i	79/93 (85%)	76 (96%)	3 (4%)	0	100	100
25	j	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
26	n	133/184 (72%)	129 (97%)	4 (3%)	0	100	100
All	All	4324/6253 (69%)	4206 (97%)	116 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	5	68	GLU
2	2	570	SER

5.3.2 Protein sidechains [i](#)

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	1	283/326 (87%)	282 (100%)	1 (0%)	89	95
2	2	510/518 (98%)	501 (98%)	9 (2%)	54	76
3	3	82/128 (64%)	82 (100%)	0	100	100
4	4	431/477 (90%)	424 (98%)	7 (2%)	58	79
5	5	580/596 (97%)	574 (99%)	6 (1%)	73	87
6	6	168/203 (83%)	162 (96%)	6 (4%)	30	53
7	8	69/75 (92%)	69 (100%)	0	100	100
8	9	84/687 (12%)	81 (96%)	3 (4%)	30	53
9	D	68/69 (99%)	68 (100%)	0	100	100
10	J	129/146 (88%)	127 (98%)	2 (2%)	58	79
11	L	74/76 (97%)	70 (95%)	4 (5%)	18	35
12	Q	75/119 (63%)	72 (96%)	3 (4%)	27	48
13	R	87/89 (98%)	84 (97%)	3 (3%)	32	55
14	S	60/111 (54%)	59 (98%)	1 (2%)	56	77
15	U	149/167 (89%)	149 (100%)	0	100	100
16	W	83/102 (81%)	82 (99%)	1 (1%)	67	84
17	X	146/152 (96%)	144 (99%)	2 (1%)	62	81
18	a	123/697 (18%)	121 (98%)	2 (2%)	58	79
19	b	67/74 (90%)	67 (100%)	0	100	100
20	c	49/80 (61%)	49 (100%)	0	100	100
21	d	90/94 (96%)	89 (99%)	1 (1%)	70	86
22	e	30/35 (86%)	30 (100%)	0	100	100
23	g	65/69 (94%)	64 (98%)	1 (2%)	60	80
24	i	68/78 (87%)	66 (97%)	2 (3%)	37	61
25	j	64/64 (100%)	62 (97%)	2 (3%)	35	59
26	n	106/150 (71%)	106 (100%)	0	100	100
All	All	3740/5382 (70%)	3684 (98%)	56 (2%)	60	80

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	198	VAL
25	j	56	LYS
11	L	38	PHE

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Mol	Chain	Res	Type
25	j	8	LYS
18	a	97	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
13	R	42	ASN
18	a	101	HIS
13	R	51	GLN
26	n	161	GLN
16	W	66	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 ligands 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	$\# Z > 2$
27	3PE	W	202	-	38,38,50	0.97	4 (10%)	41,43,55	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	3PE	J	201	-	29,29,50	1.11	4 (13%)	32,34,55	1.16	2 (6%)
28	PC1	5	701	-	53,53,53	0.98	5 (9%)	59,61,61	1.25	4 (6%)
28	PC1	3	201	-	42,42,53	1.05	4 (9%)	48,50,61	1.10	2 (4%)
28	PC1	1	402	-	41,41,53	1.07	4 (9%)	47,49,61	1.07	2 (4%)
27	3PE	g	102	-	43,43,50	0.92	4 (9%)	46,48,55	1.09	2 (4%)
27	3PE	5	702	-	34,34,50	1.03	4 (11%)	37,39,55	1.13	2 (5%)
29	CDL	D	101	-	64,64,99	1.08	8 (12%)	70,76,111	1.14	4 (5%)
27	3PE	5	703	-	32,32,50	1.06	4 (12%)	35,37,55	1.12	2 (5%)
28	PC1	S	202	-	51,51,53	0.96	4 (7%)	57,59,61	1.08	2 (3%)
30	LMN	4	602	-	48,48,72	1.85	13 (27%)	60,62,98	1.01	1 (1%)
29	CDL	X	202	-	78,78,99	0.97	7 (8%)	84,90,111	1.18	5 (5%)
29	CDL	2	601	-	73,73,99	0.34	0	79,85,111	0.50	0
27	3PE	i	101	-	40,40,50	0.96	4 (10%)	43,45,55	1.15	2 (4%)
27	3PE	4	604	-	33,33,50	1.04	4 (12%)	36,38,55	1.15	2 (5%)
30	LMN	2	602	-	60,60,72	1.72	10 (16%)	78,80,98	1.08	3 (3%)
30	LMN	j	101	-	72,72,72	1.63	14 (19%)	96,98,98	1.04	6 (6%)
27	3PE	W	201	-	37,37,50	0.99	4 (10%)	40,42,55	1.12	2 (5%)
27	3PE	n	201	-	50,50,50	0.86	4 (8%)	53,55,55	1.12	2 (3%)
27	3PE	5	705	-	42,42,50	0.94	4 (9%)	45,47,55	1.14	2 (4%)
28	PC1	X	203	-	38,38,53	1.10	4 (10%)	44,46,61	1.07	2 (4%)
27	3PE	5	704	-	34,34,50	1.04	4 (11%)	37,39,55	1.20	2 (5%)
27	3PE	n	202	-	38,38,50	1.00	4 (10%)	41,43,55	1.13	2 (4%)
28	PC1	4	603	-	49,49,53	0.98	4 (8%)	55,57,61	1.15	2 (3%)
27	3PE	5	707	-	32,32,50	1.06	4 (12%)	35,37,55	1.17	2 (5%)
27	3PE	g	101	-	35,35,50	1.00	4 (11%)	38,40,55	1.17	2 (5%)
27	3PE	1	401	-	44,44,50	0.92	4 (9%)	47,49,55	1.20	4 (8%)
31	ZMP	Q	201	12	29,35,36	0.21	0	34,42,45	0.43	0
27	3PE	6	301	-	35,35,50	1.03	4 (11%)	38,40,55	1.20	2 (5%)
28	PC1	X	204	-	31,31,53	1.21	4 (12%)	37,39,61	1.10	2 (5%)
28	PC1	5	706	-	42,42,53	1.08	4 (9%)	48,50,61	1.15	2 (4%)
29	CDL	X	201	-	69,69,99	1.03	7 (10%)	75,81,111	1.17	5 (6%)
27	3PE	4	601	-	44,44,50	0.90	4 (9%)	47,49,55	1.10	2 (4%)
29	CDL	S	201	-	78,78,99	0.97	8 (10%)	84,90,111	1.14	4 (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
27	3PE	W	202	-	-	15/42/42/54	-
27	3PE	J	201	-	-	16/33/33/54	-
28	PC1	5	701	-	-	26/57/57/57	-
28	PC1	3	201	-	-	14/46/46/57	-
28	PC1	1	402	-	-	23/45/45/57	-
27	3PE	g	102	-	-	20/47/47/54	-
27	3PE	5	702	-	-	15/38/38/54	-
29	CDL	D	101	-	-	27/75/75/110	-
27	3PE	5	703	-	-	17/36/36/54	-
28	PC1	S	202	-	-	18/55/55/57	-
30	LMN	4	602	-	-	24/38/78/130	0/2/2/4
29	CDL	X	202	-	-	44/89/89/110	-
29	CDL	2	601	-	-	26/84/84/110	-
27	3PE	i	101	-	-	18/44/44/54	-
27	3PE	4	604	-	-	14/37/37/54	-
30	LMN	2	602	-	-	25/44/104/130	0/3/3/4
30	LMN	j	101	-	-	23/50/130/130	0/4/4/4
27	3PE	W	201	-	-	15/41/41/54	-
27	3PE	n	201	-	-	21/54/54/54	-
27	3PE	5	705	-	-	17/46/46/54	-
28	PC1	X	203	-	-	19/42/42/57	-
27	3PE	5	704	-	-	12/38/38/54	-
27	3PE	n	202	-	-	22/42/42/54	-
28	PC1	4	603	-	-	27/53/53/57	-
27	3PE	5	707	-	-	11/36/36/54	-
27	3PE	g	101	-	-	15/39/39/54	-
27	3PE	1	401	-	-	21/48/48/54	-
31	ZMP	Q	201	12	-	10/40/42/43	-
27	3PE	6	301	-	-	20/39/39/54	-
28	PC1	X	204	-	-	15/35/35/57	-
28	PC1	5	706	-	-	23/46/46/57	-
29	CDL	X	201	-	-	27/80/80/110	-
27	3PE	4	601	-	-	14/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	S	201	-	-	36/89/89/110	-

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	j	101	LMN	O5-C1	4.70	1.53	1.41
30	4	602	LMN	O5-C1	4.70	1.53	1.41
30	2	602	LMN	O5-C1	4.66	1.53	1.41
30	j	101	LMN	CBS-CCM	4.24	1.63	1.53
30	4	602	LMN	CBS-CCM	4.20	1.63	1.53

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	603	PC1	O21-C21-C22	4.95	122.17	111.50
28	5	701	PC1	O21-C21-C22	4.93	122.12	111.50
28	5	706	PC1	O21-C21-C22	4.64	121.50	111.50
27	1	401	3PE	O21-C21-C22	4.55	121.30	111.50
27	5	704	3PE	O21-C21-C22	4.39	120.96	111.50

There are no chirality outliers.

5 of 690 torsion outliers are listed below:

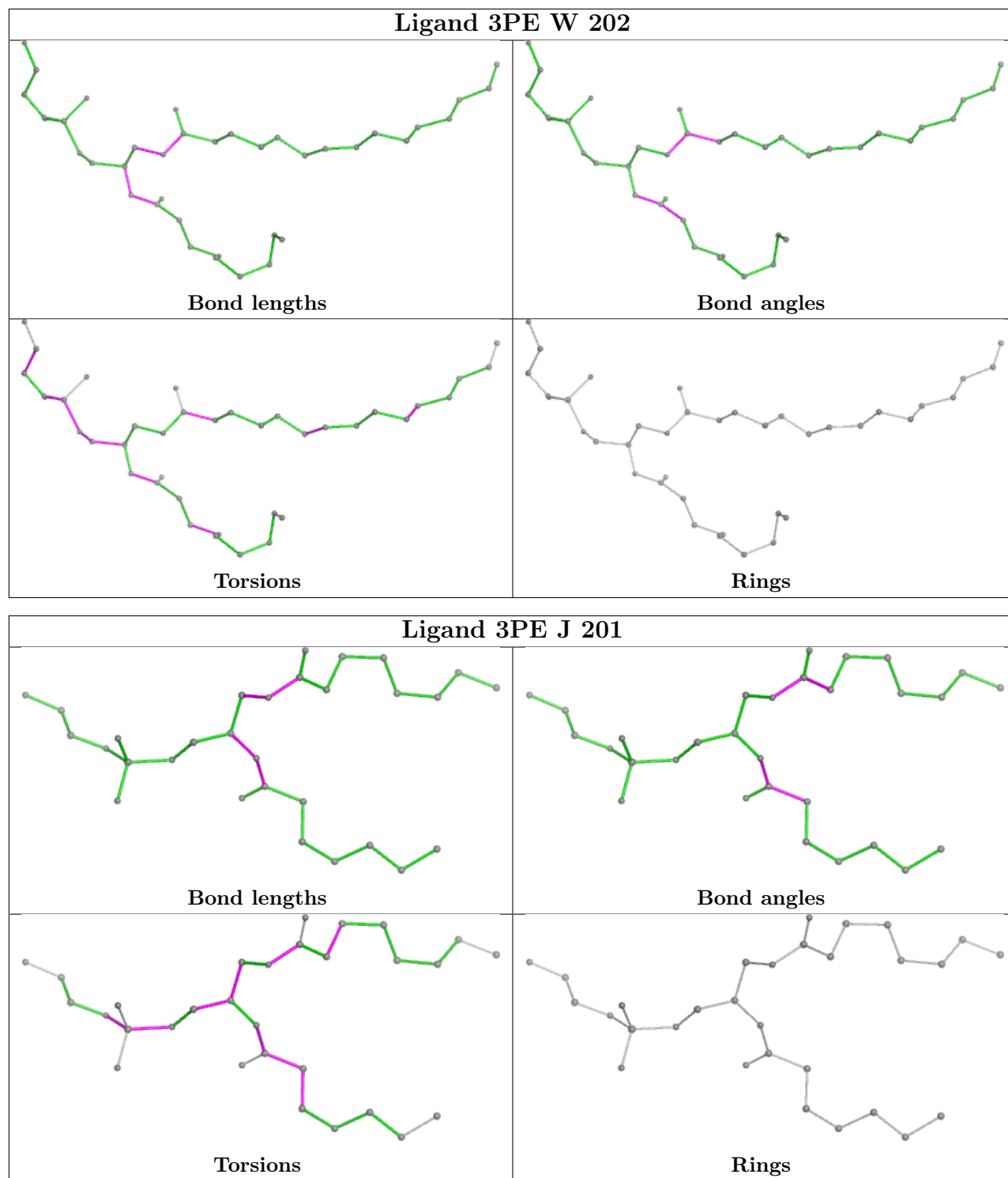
Mol	Chain	Res	Type	Atoms
27	1	401	3PE	C1-O11-P-O12
27	1	401	3PE	C1-O11-P-O14
27	4	604	3PE	O22-C21-O21-C2
27	5	702	3PE	C1-O11-P-O12
27	5	702	3PE	C1-O11-P-O13

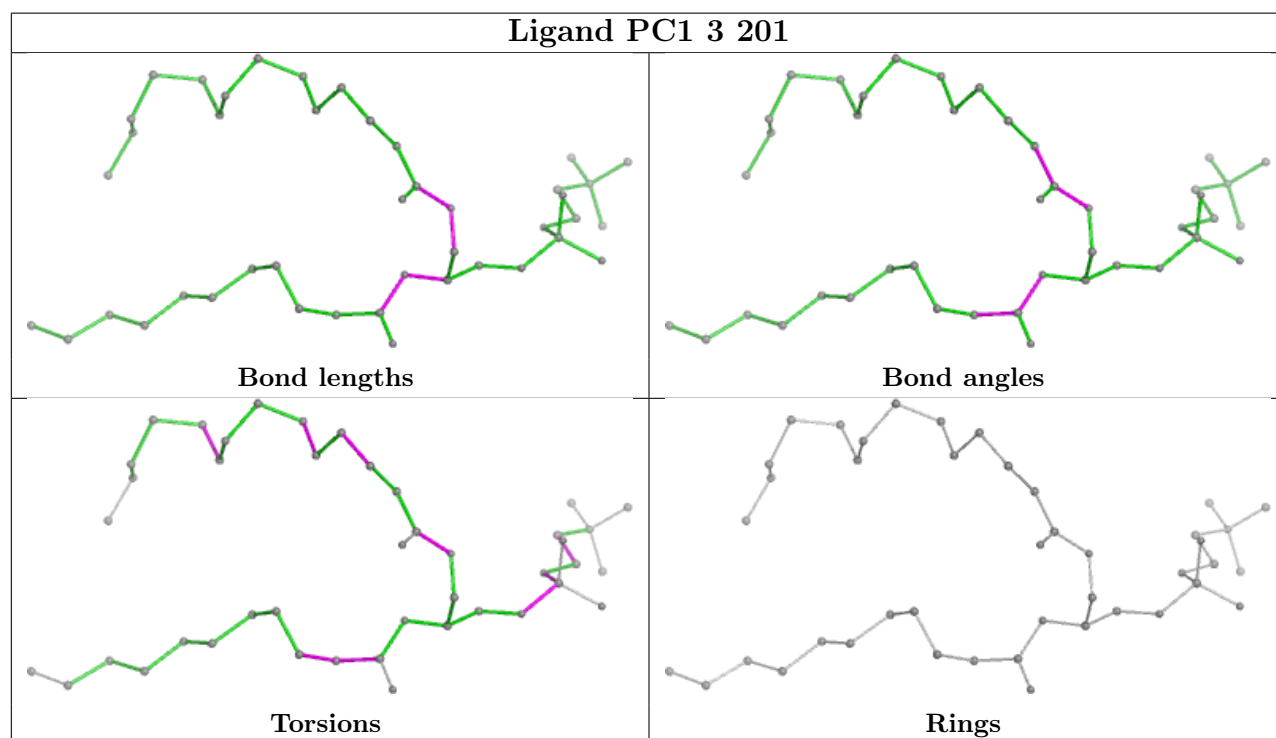
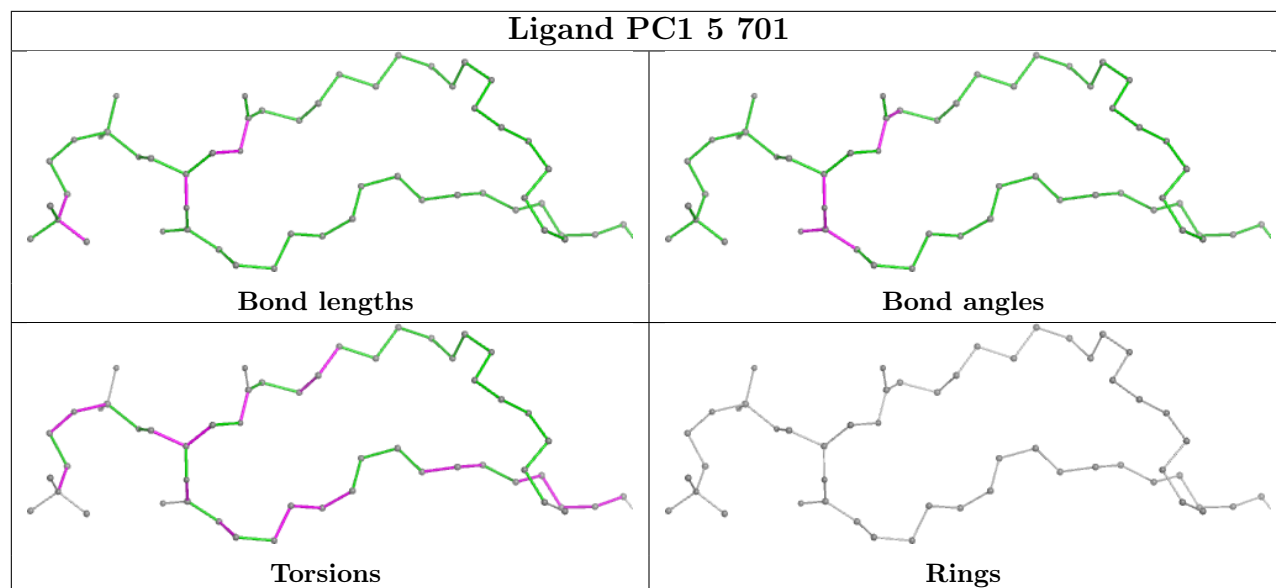
There are no ring outliers.

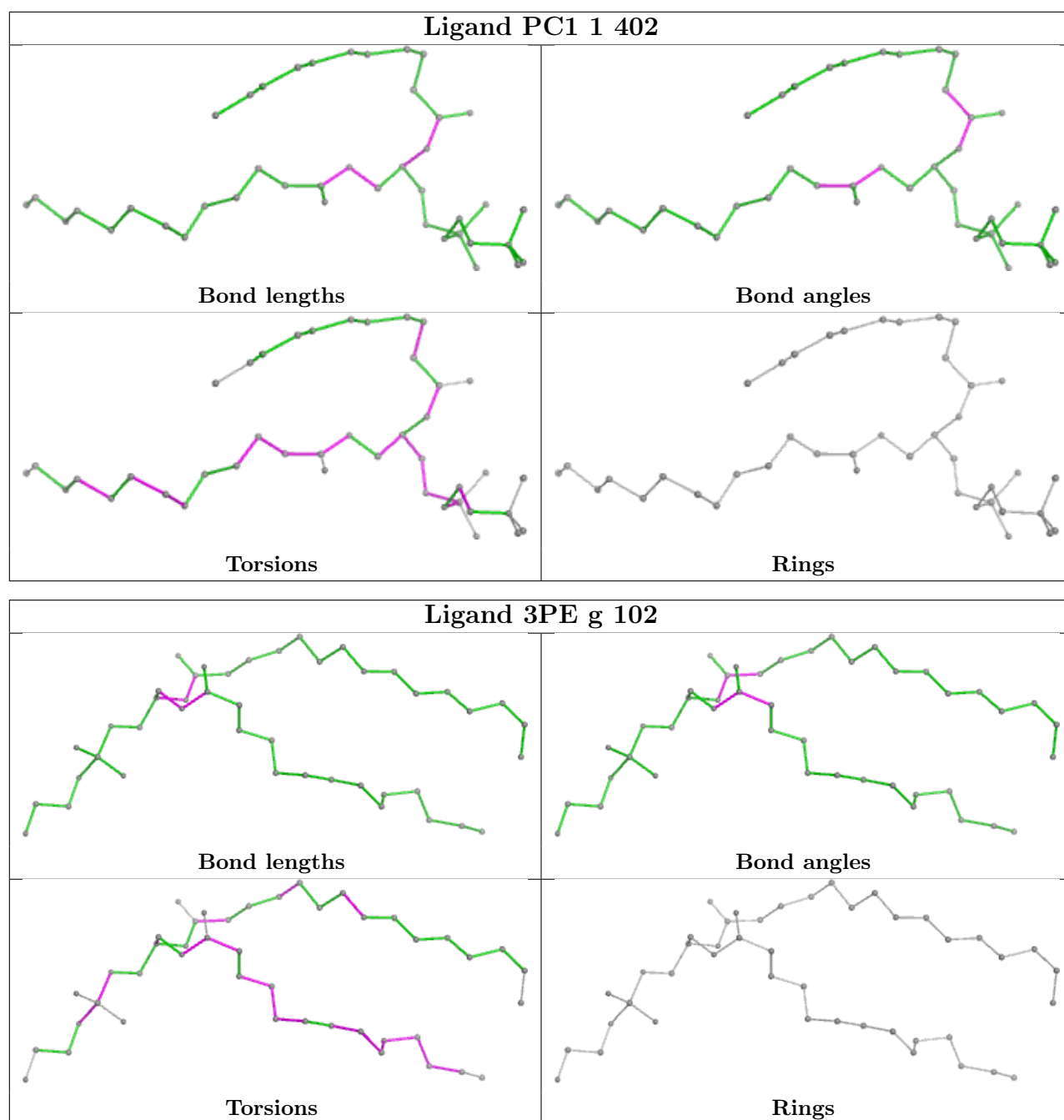
No monomer is involved in short contacts.

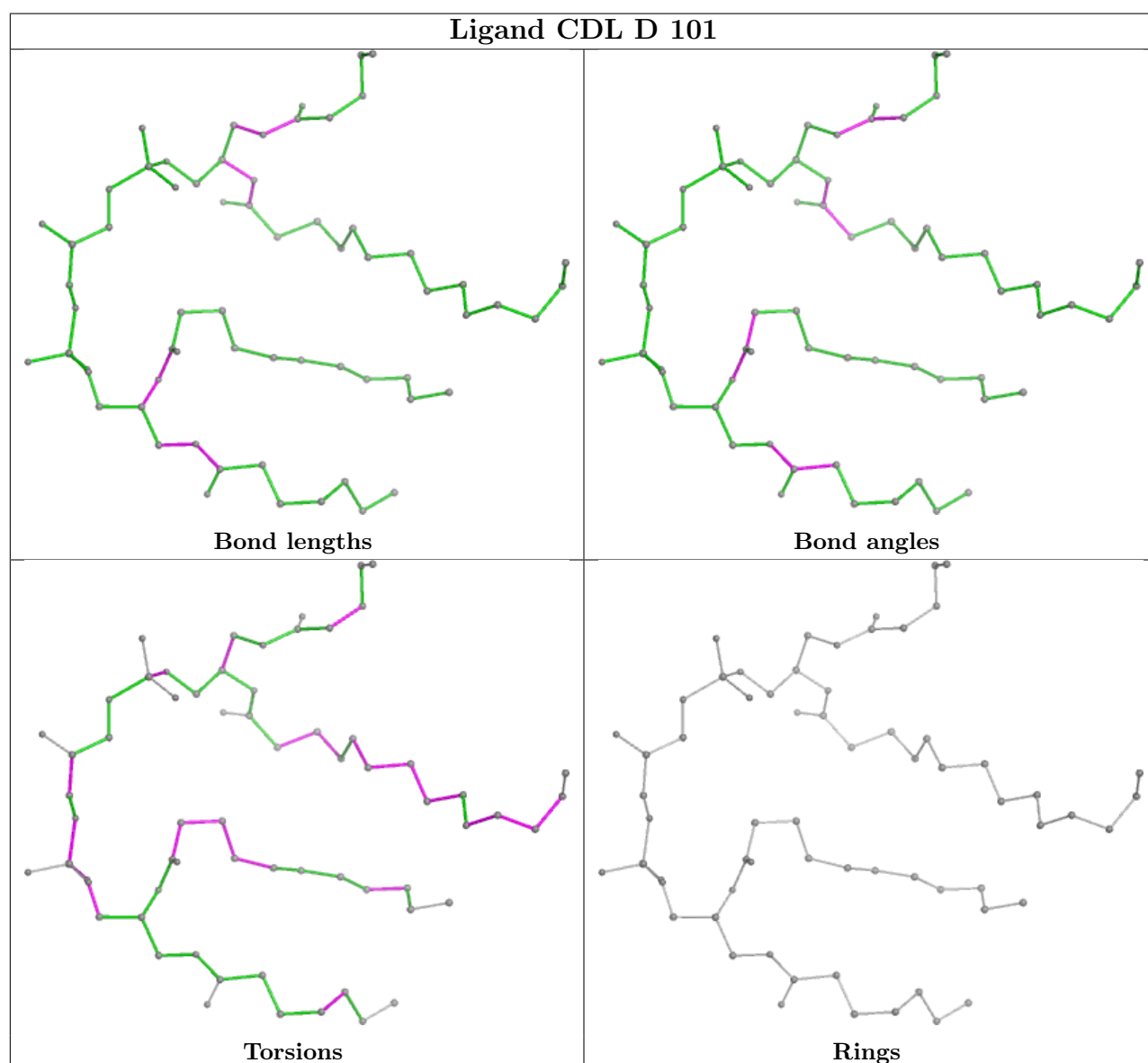
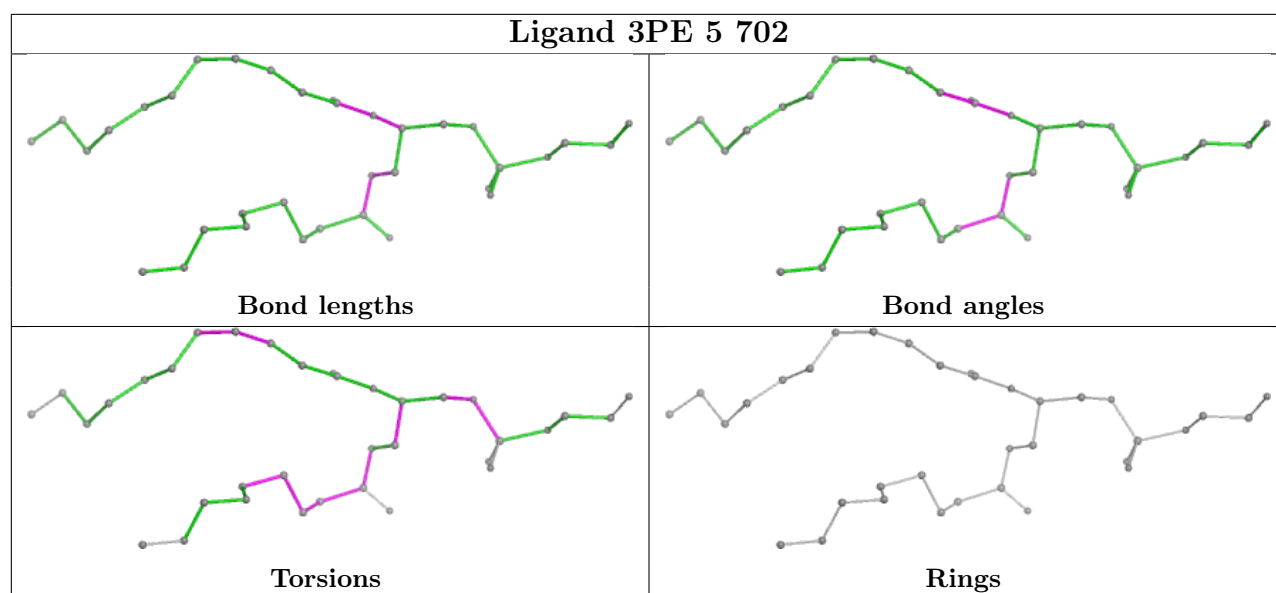
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

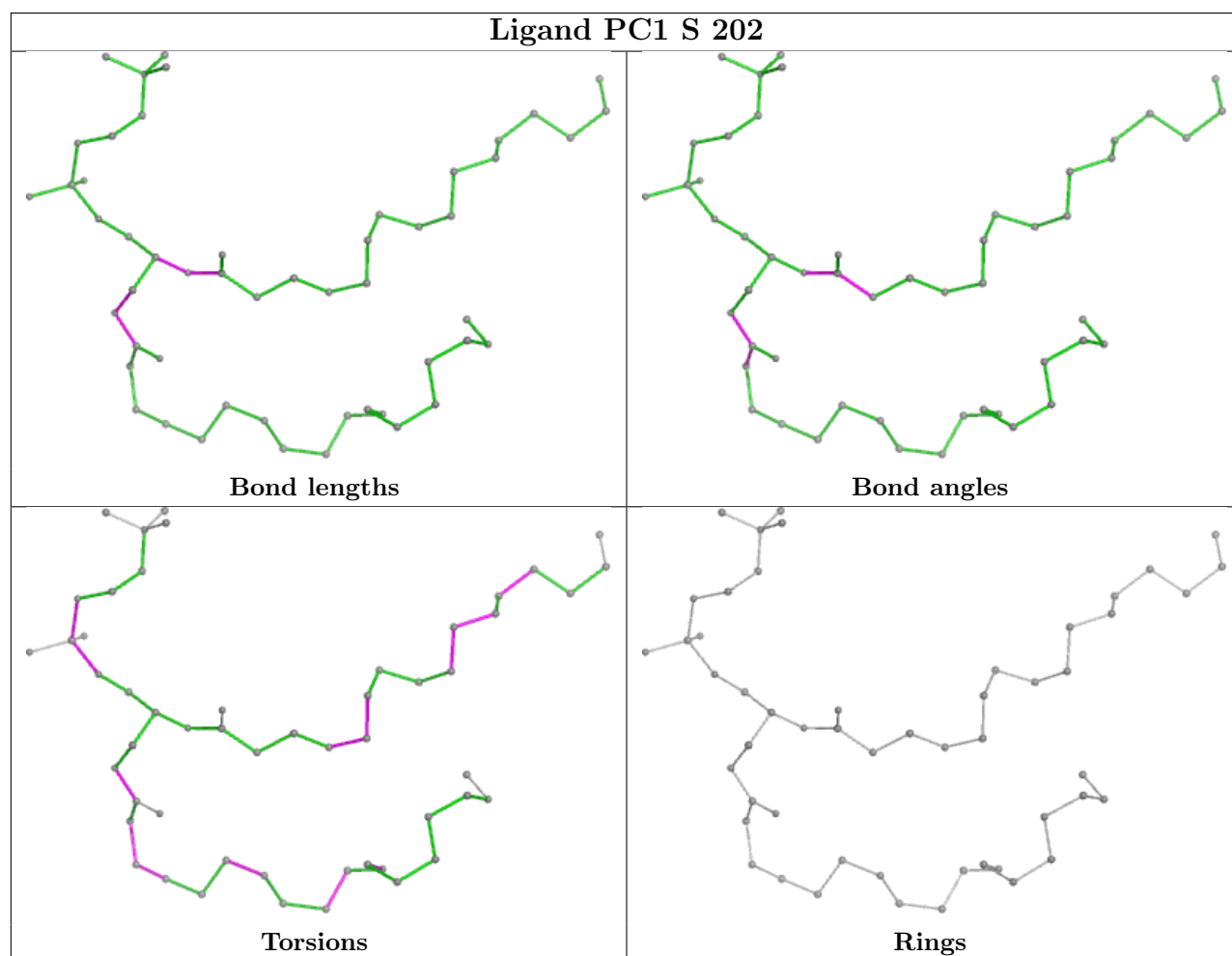
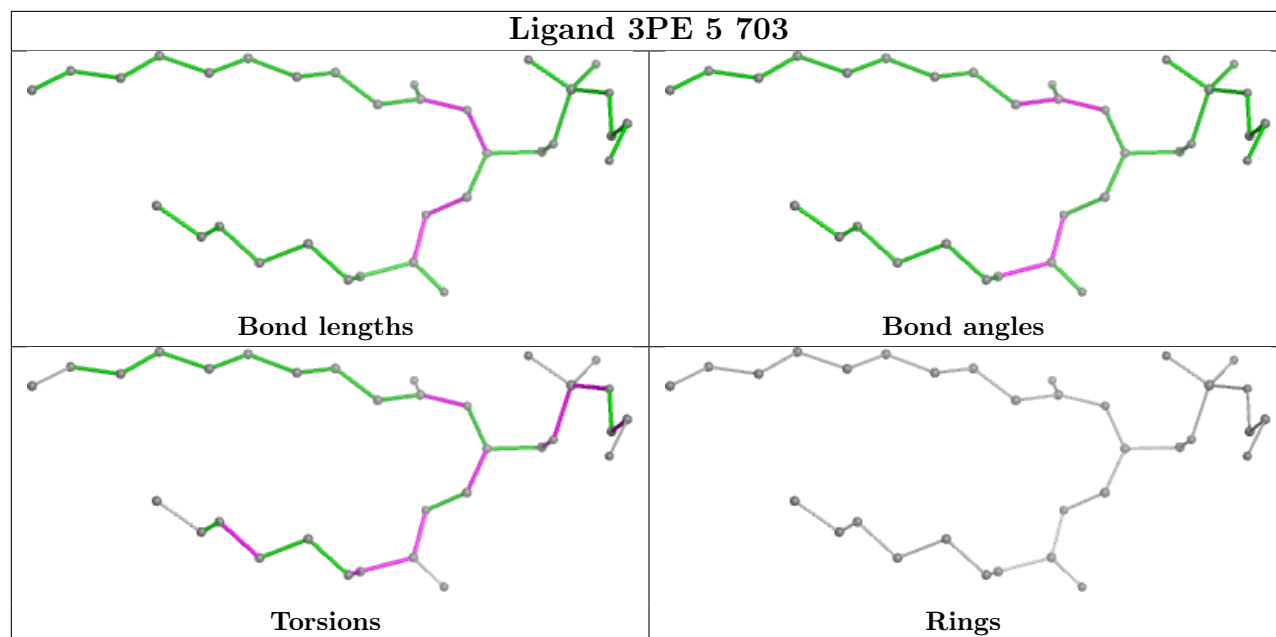
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

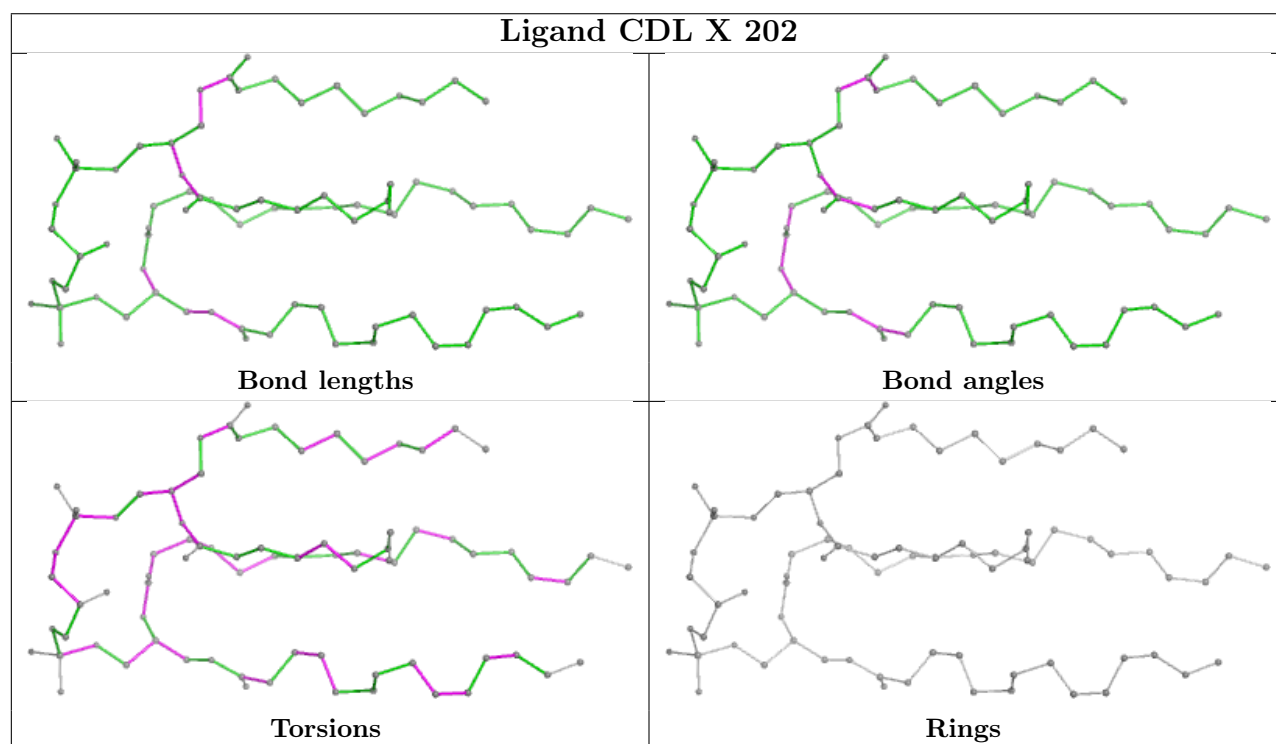
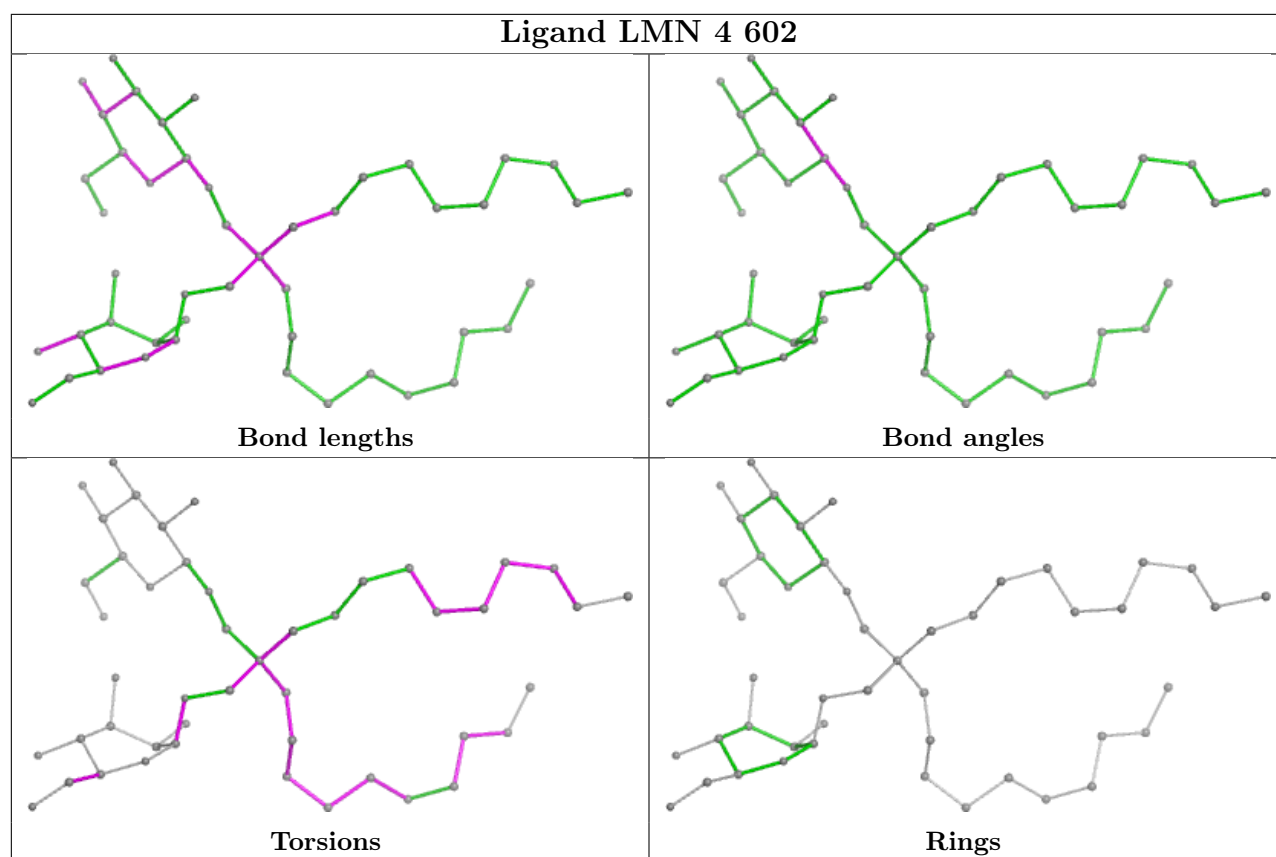


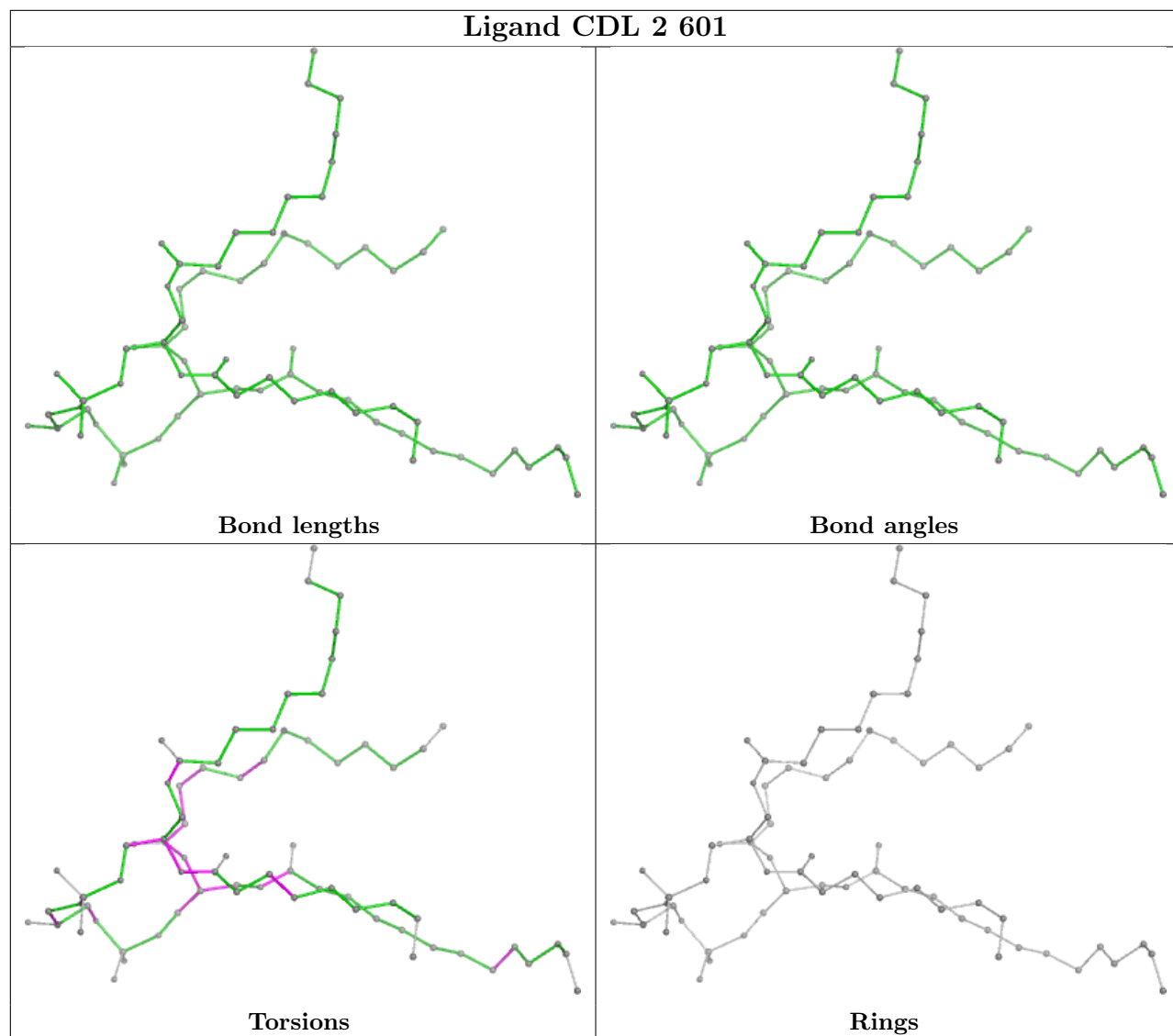


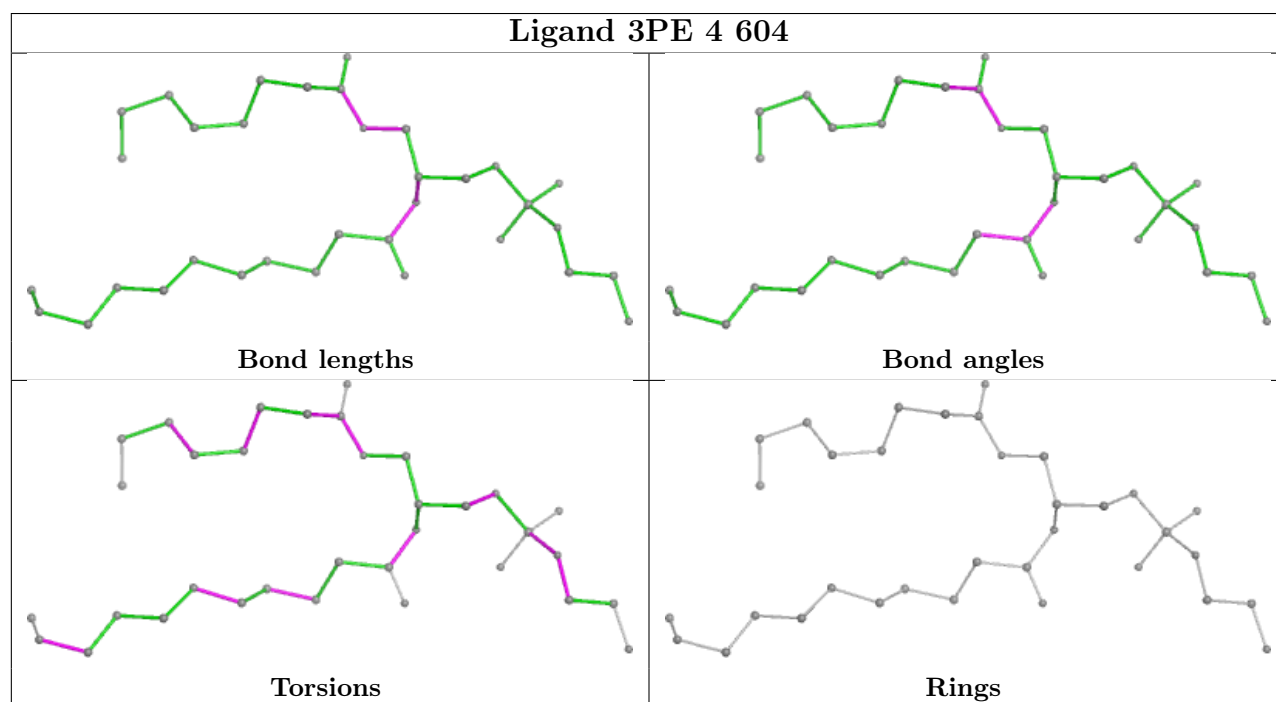
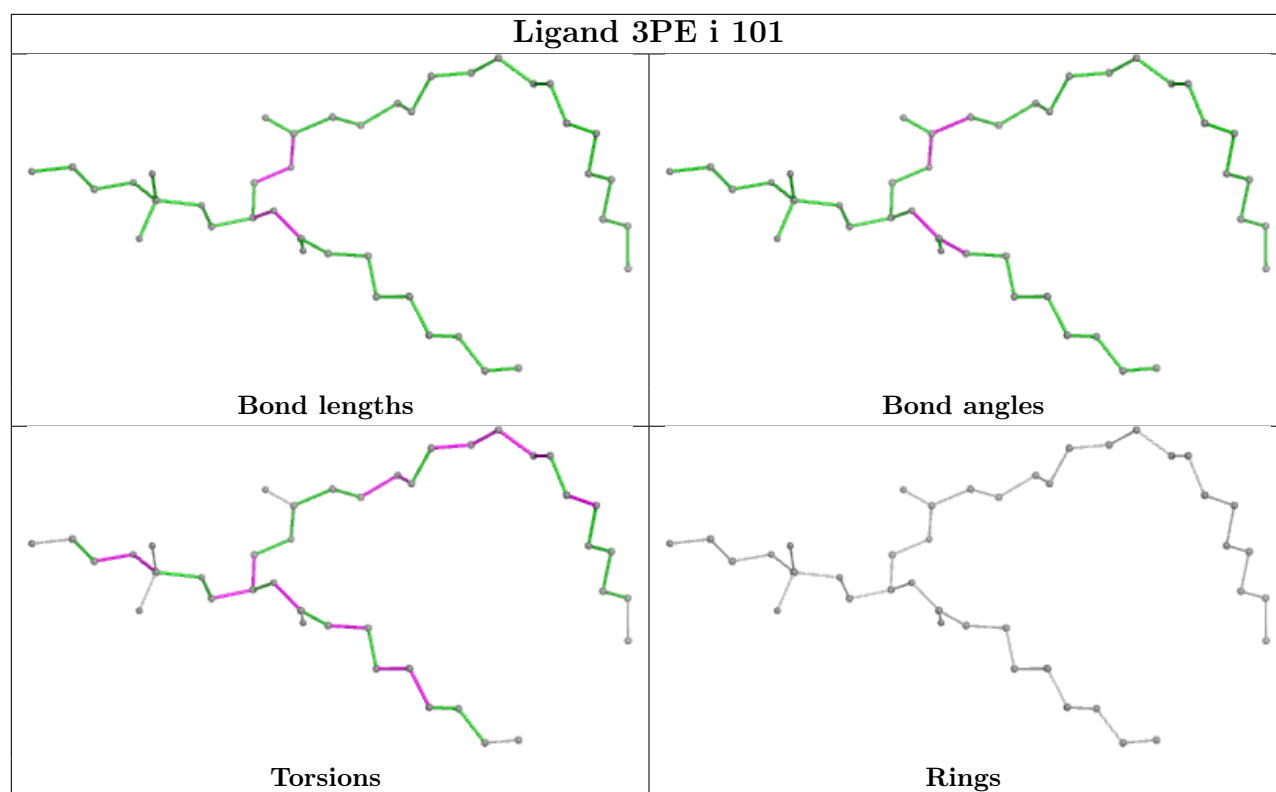


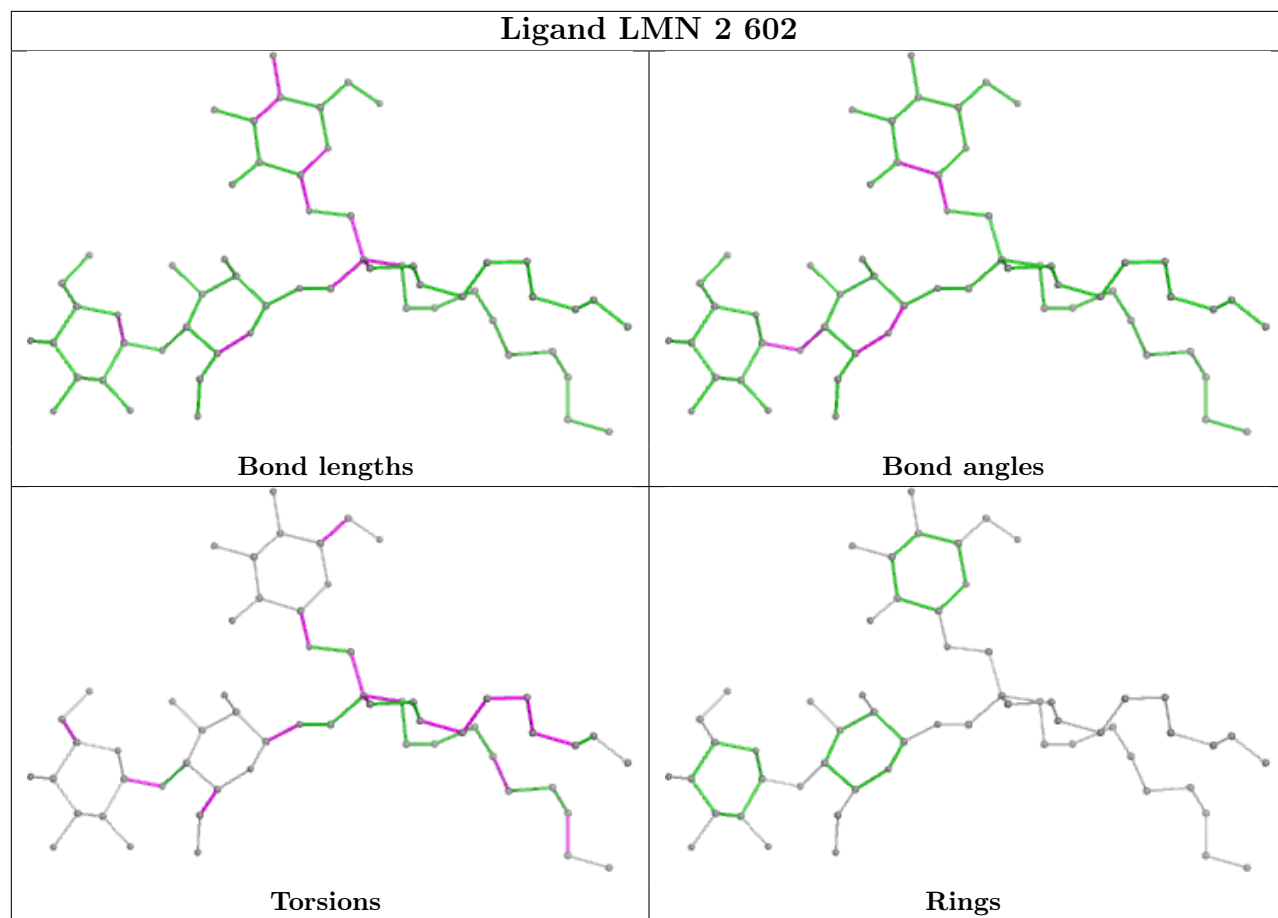


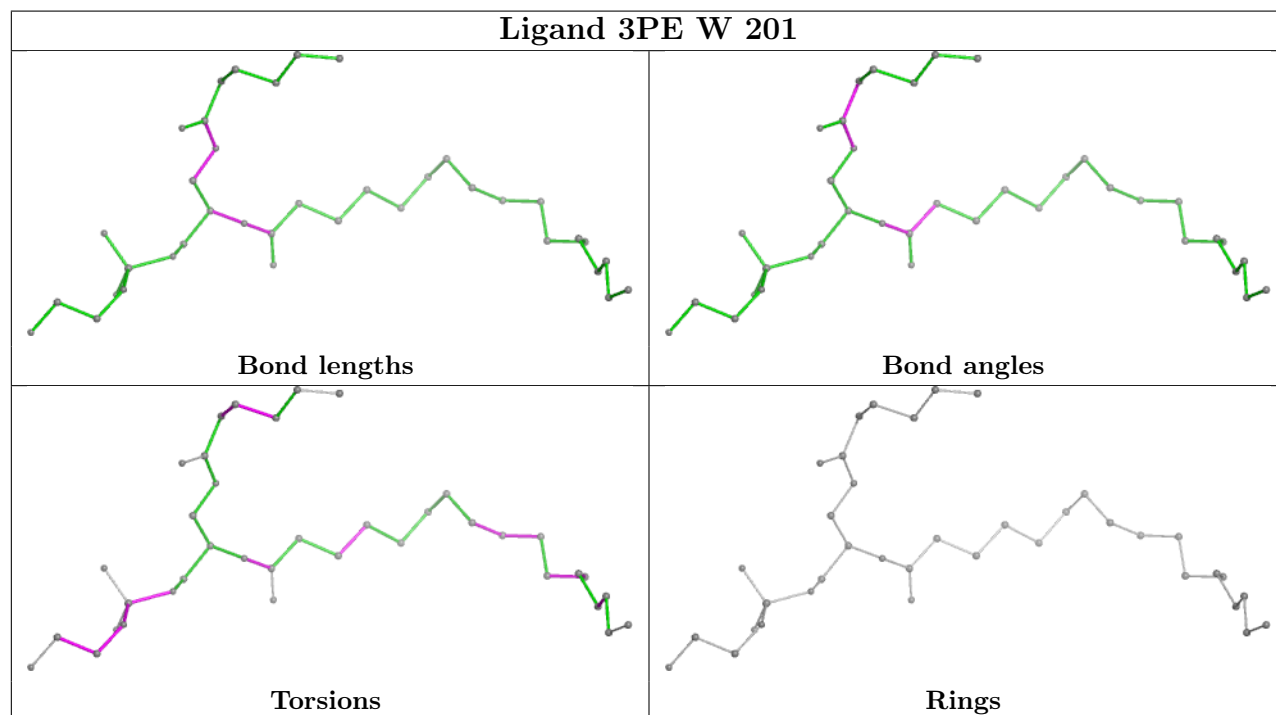
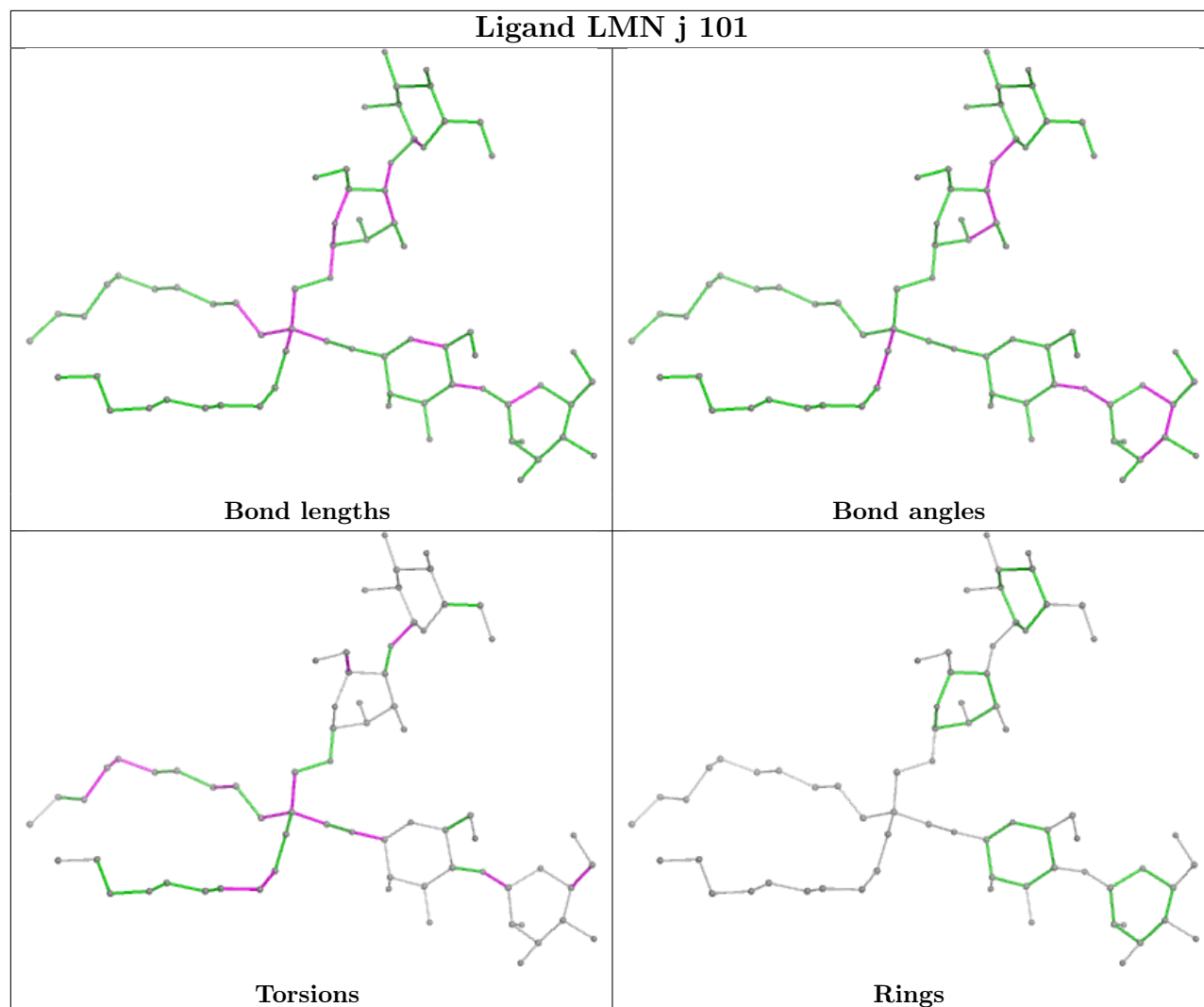


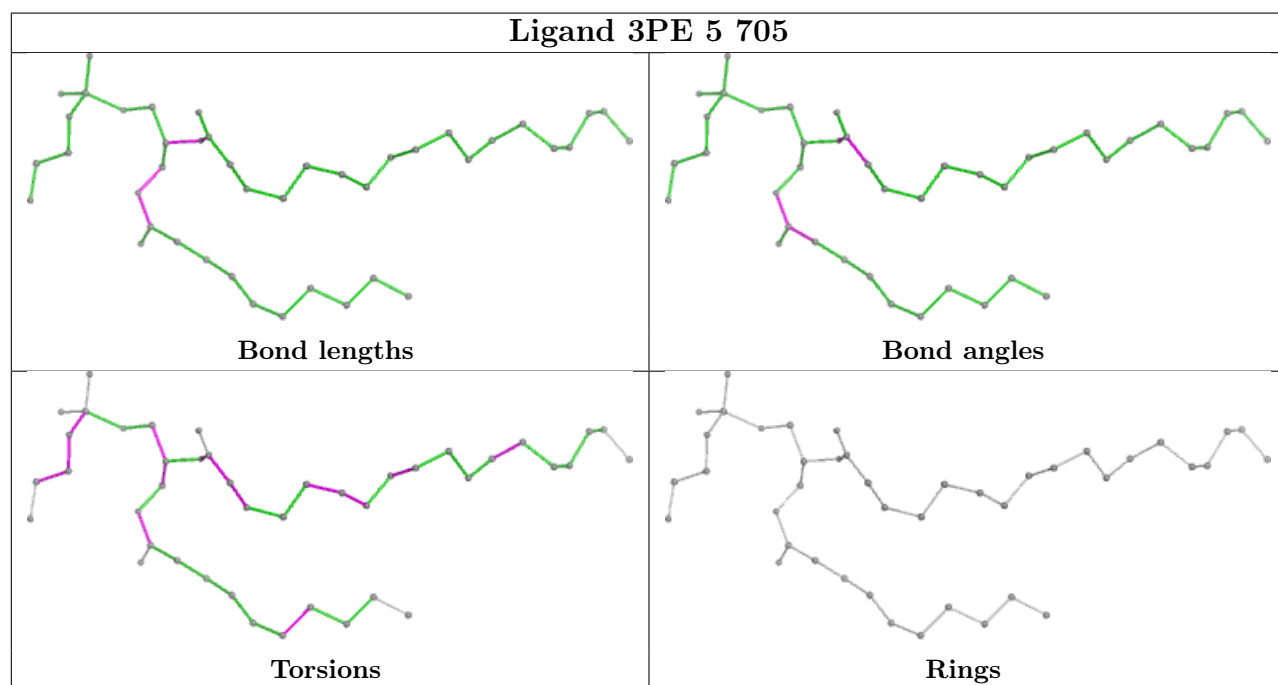
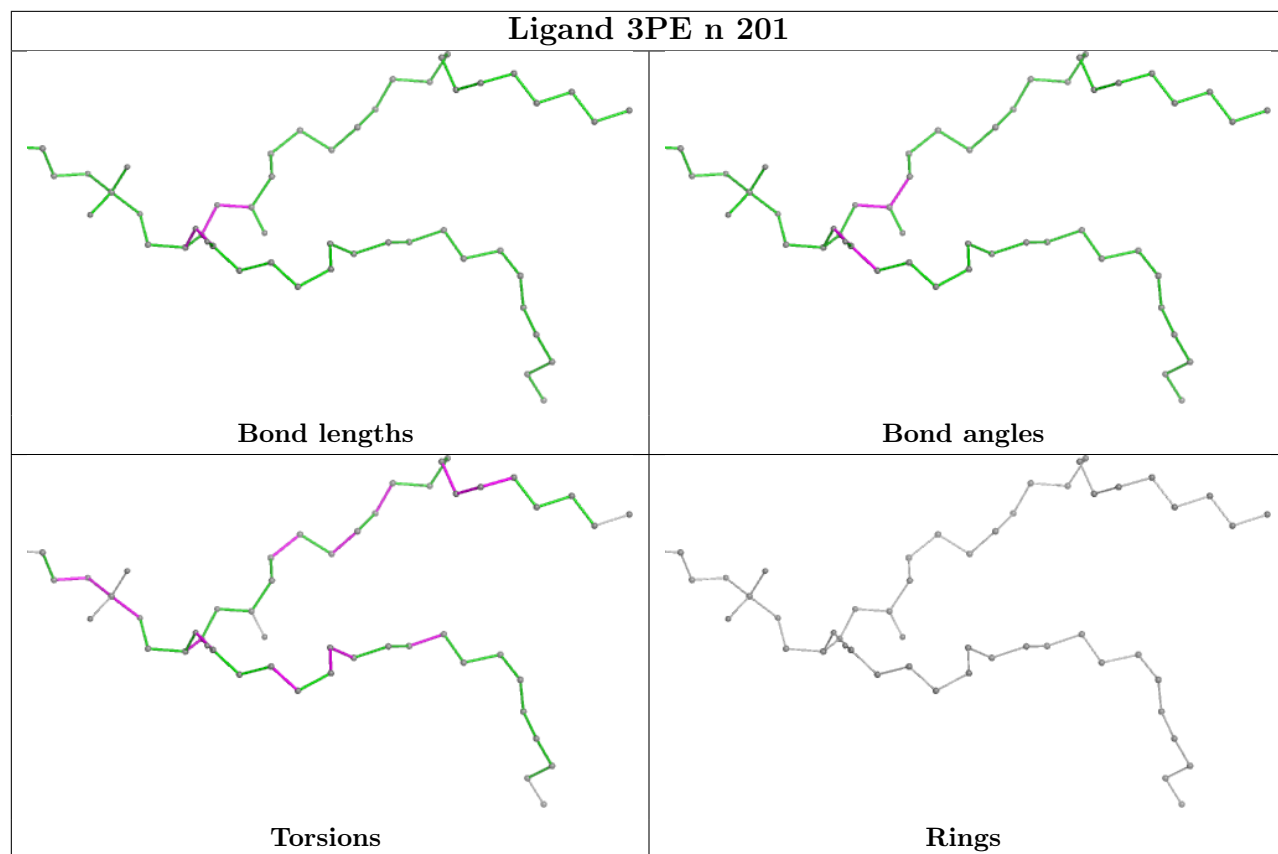


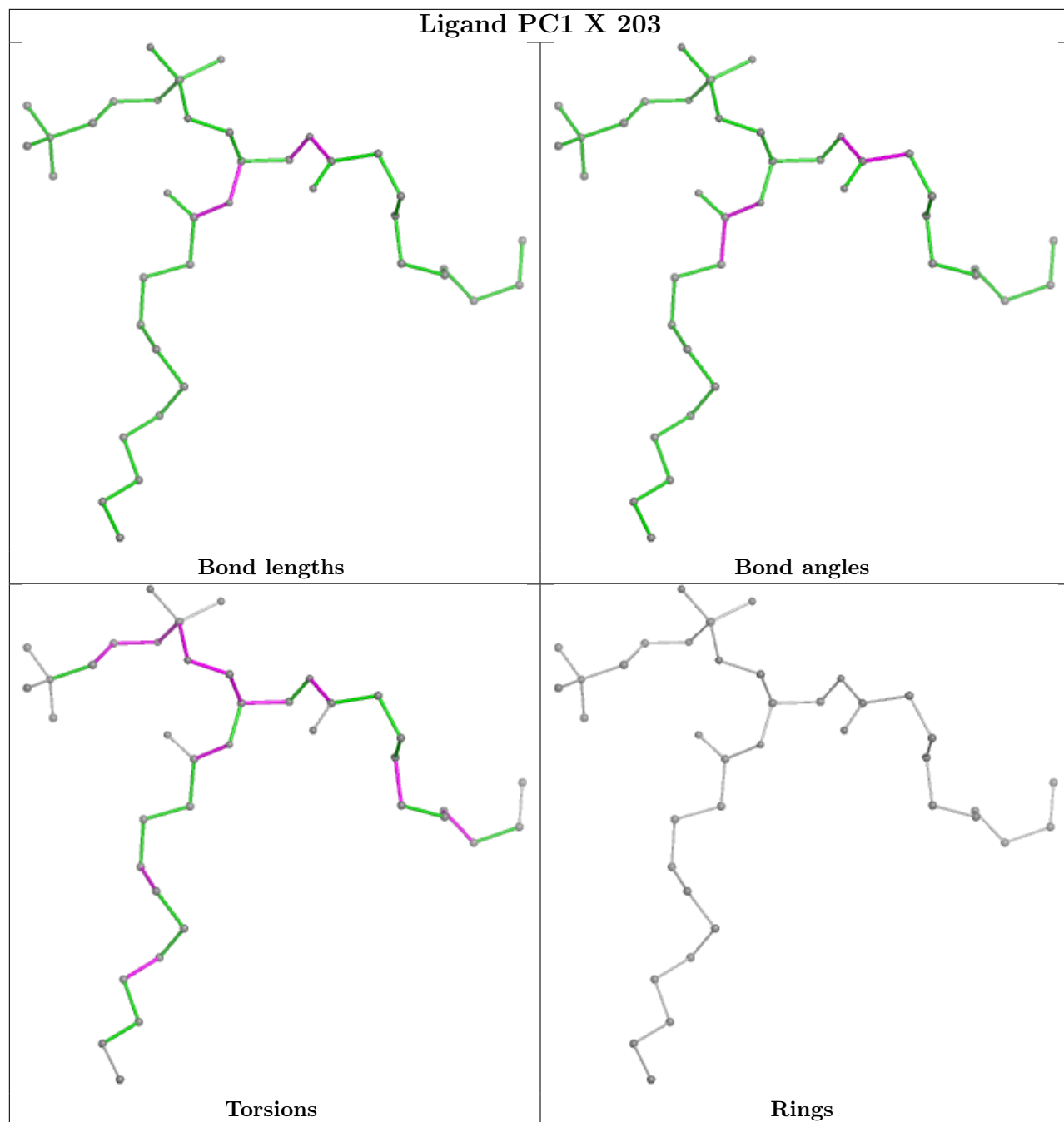


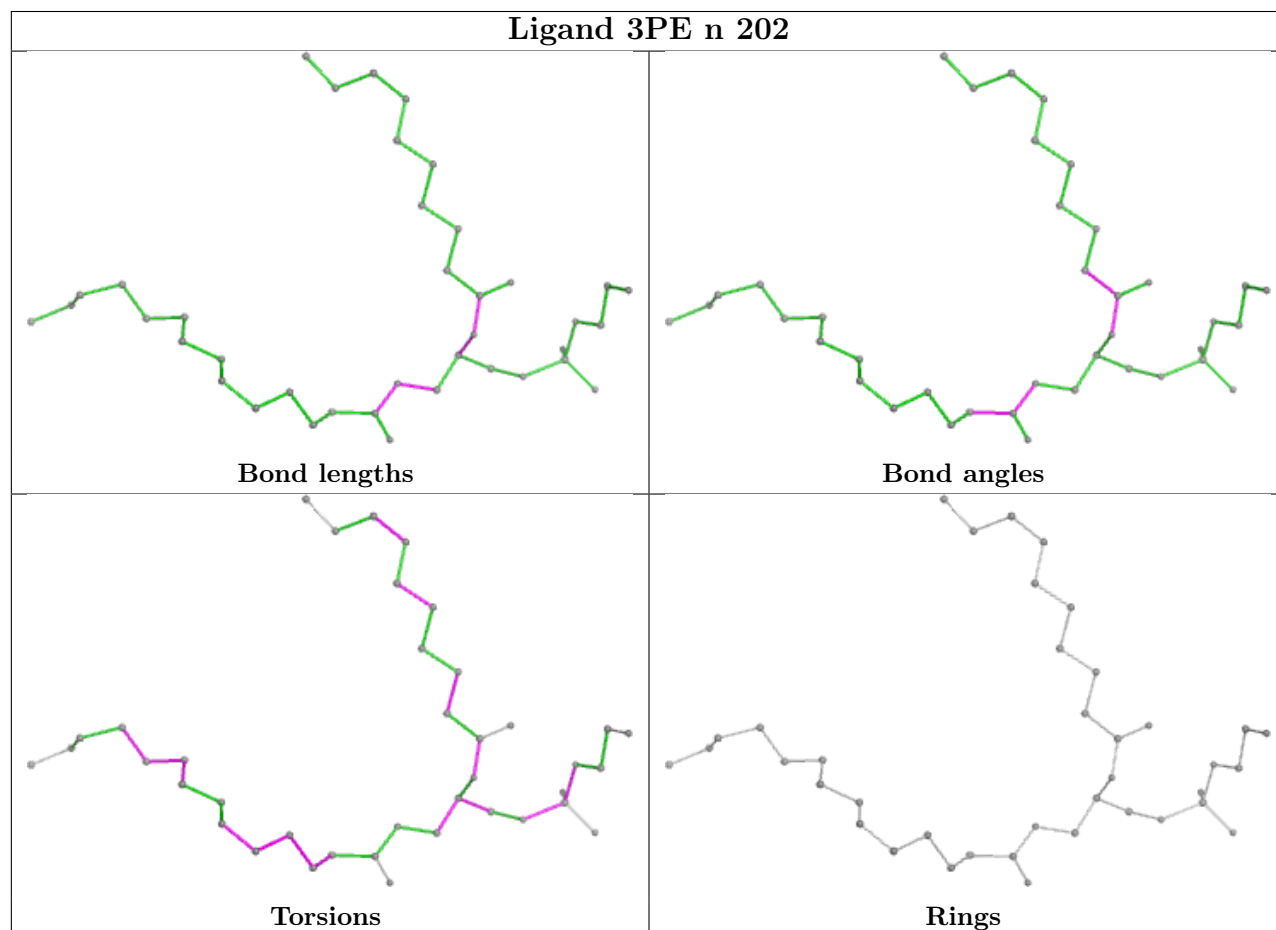
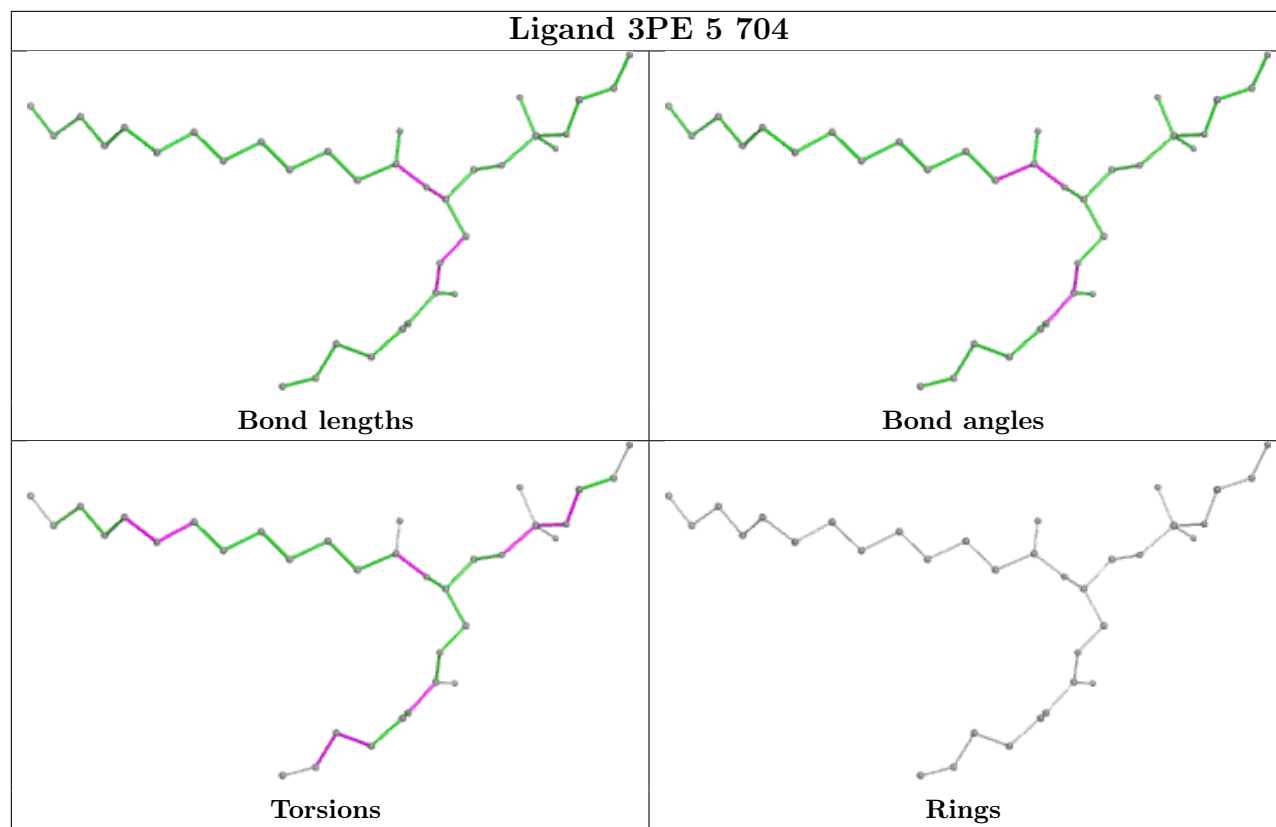


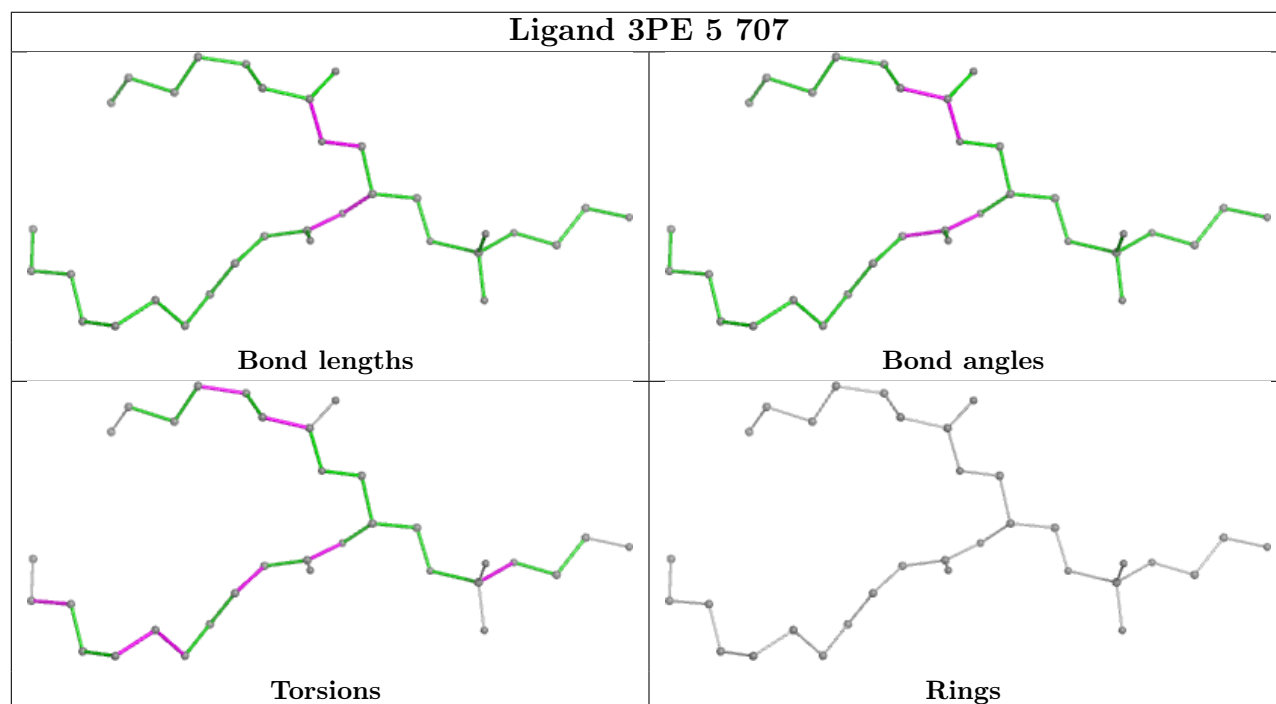
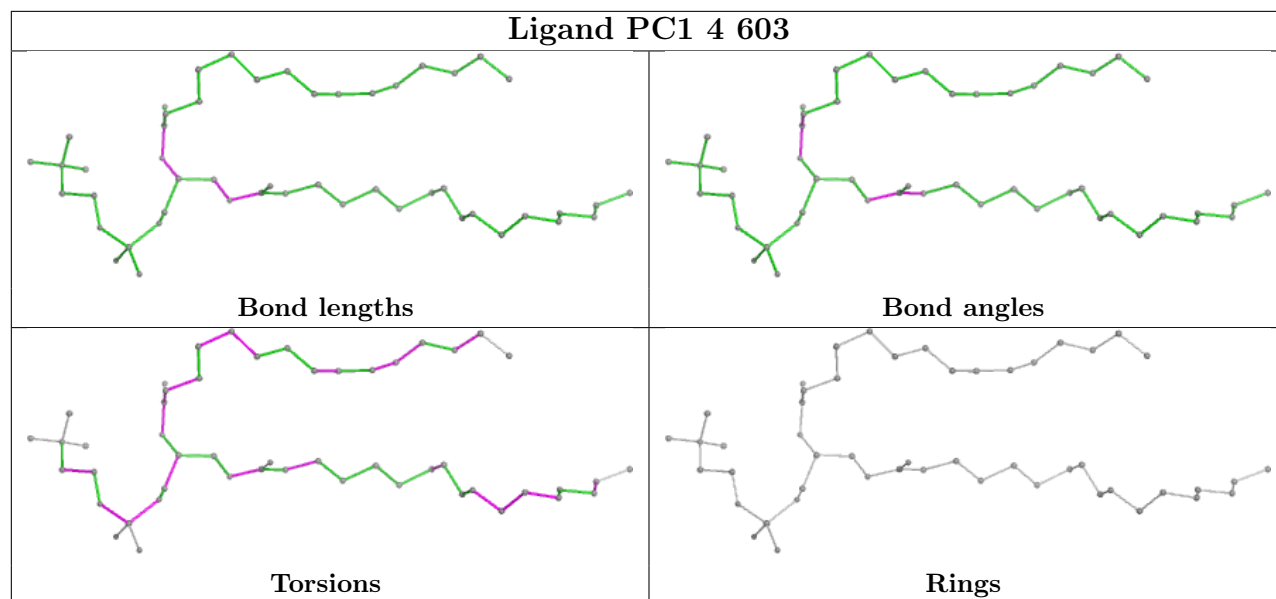


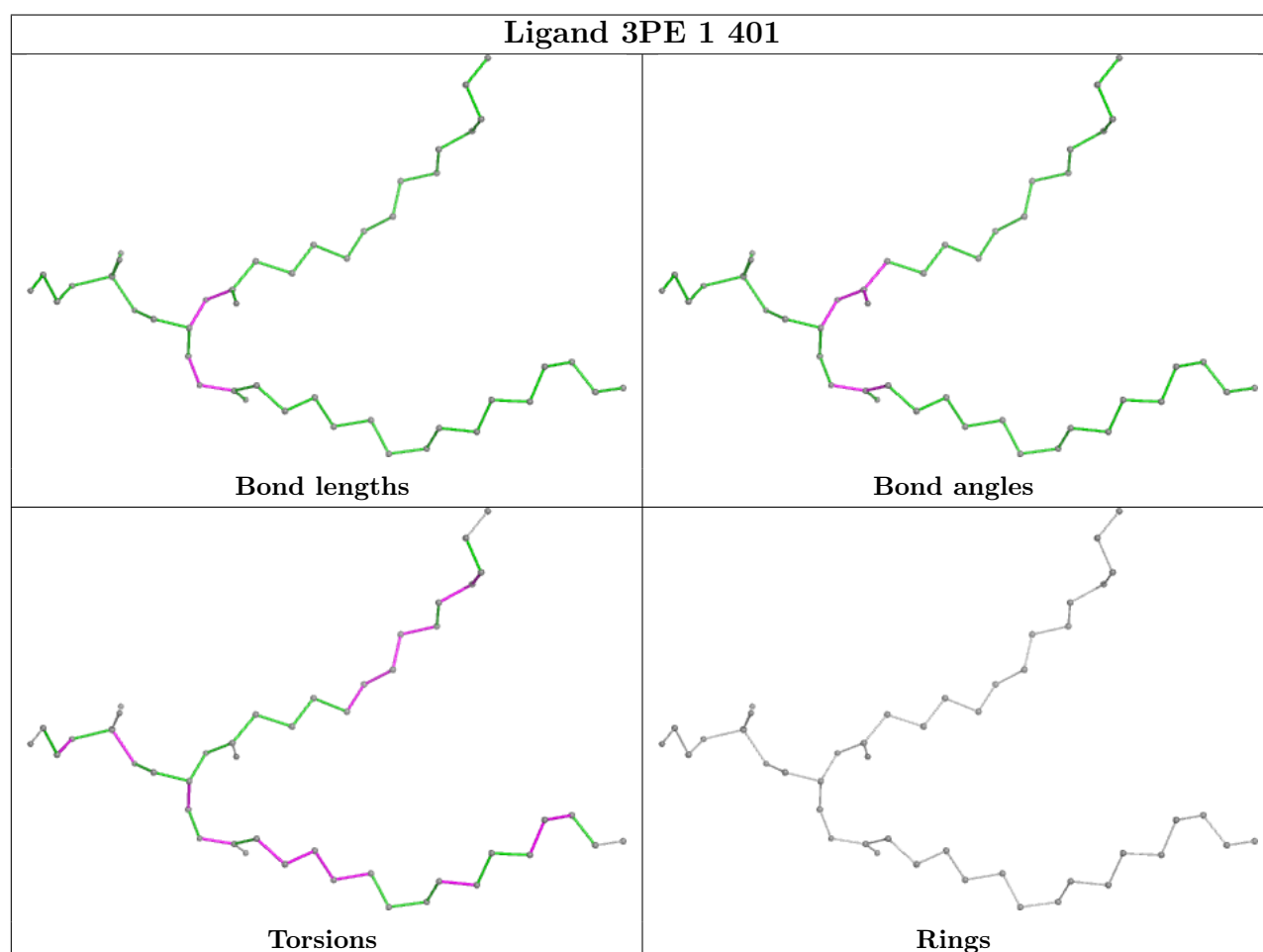
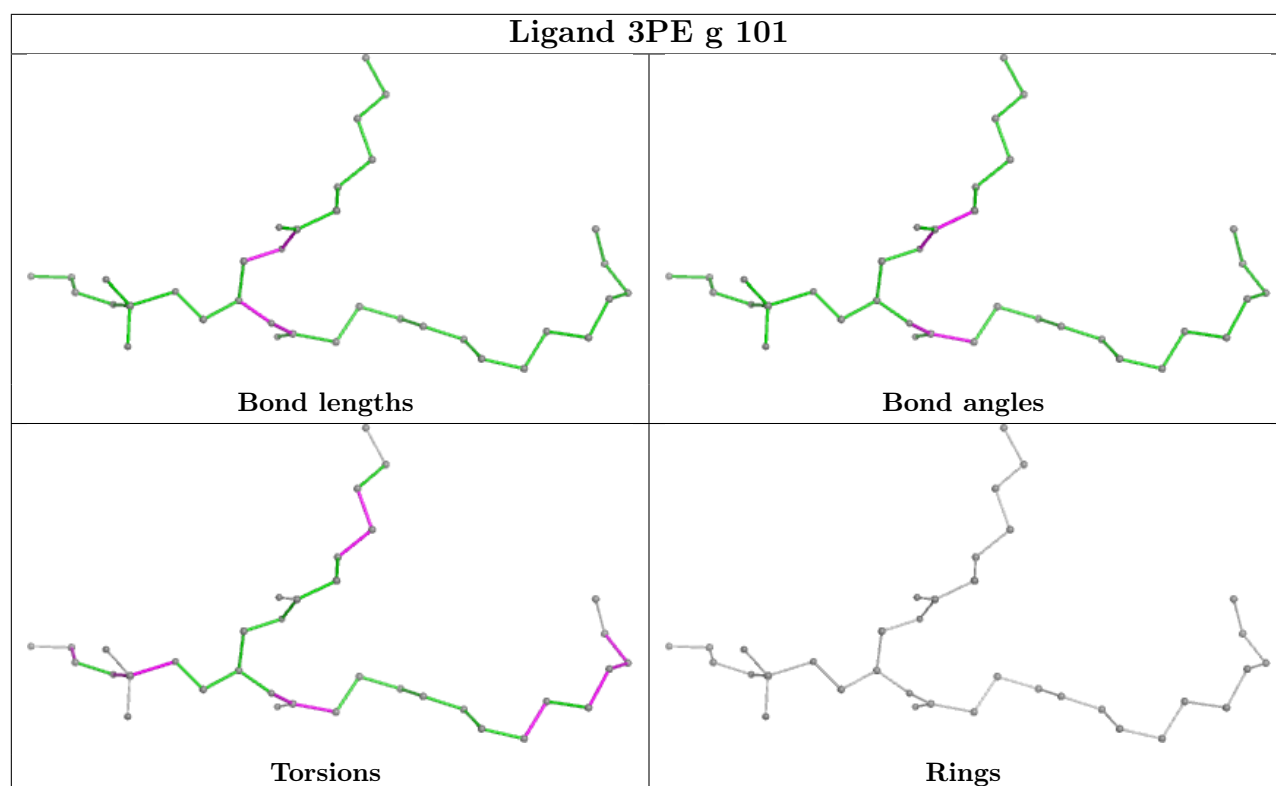


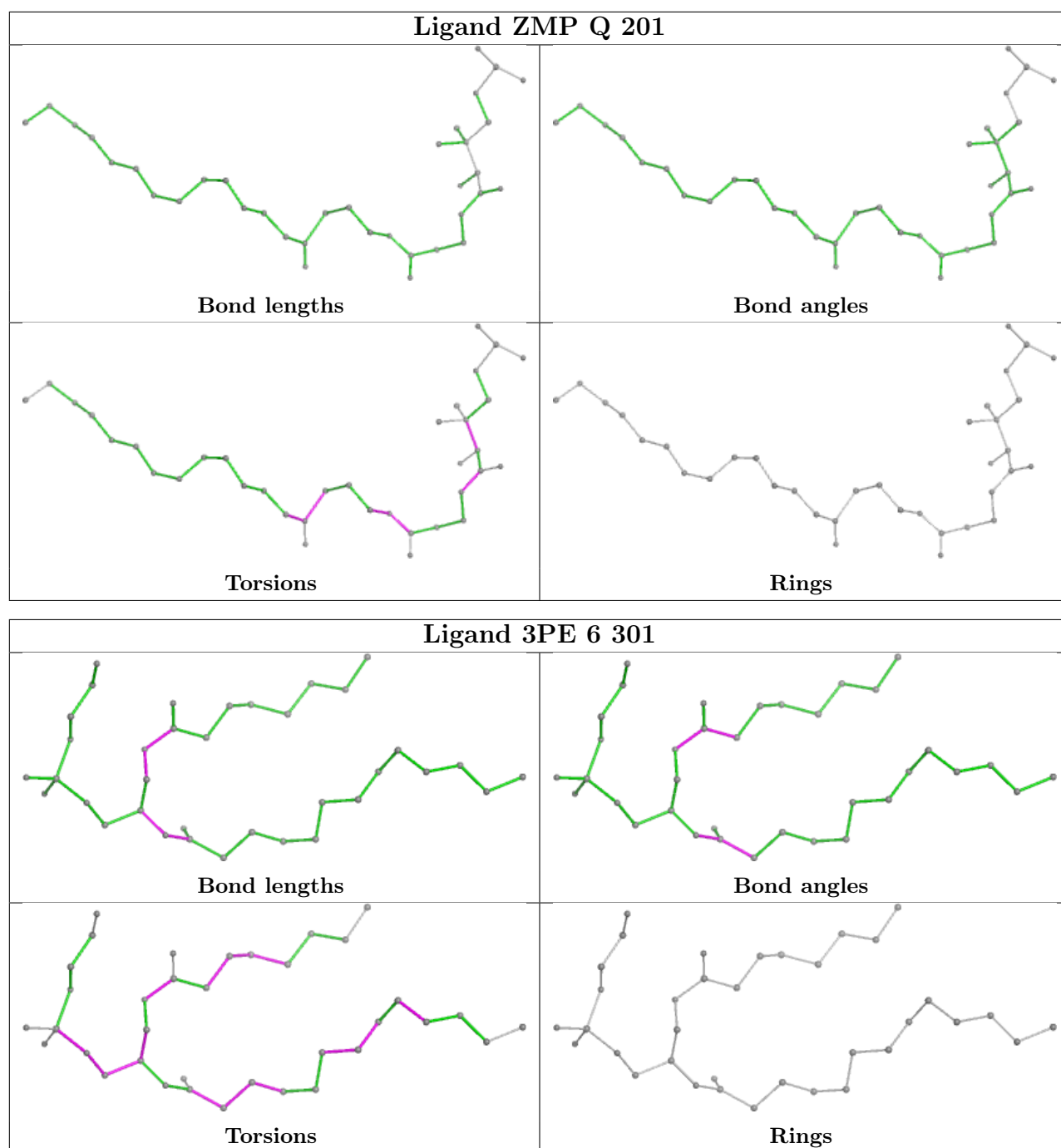


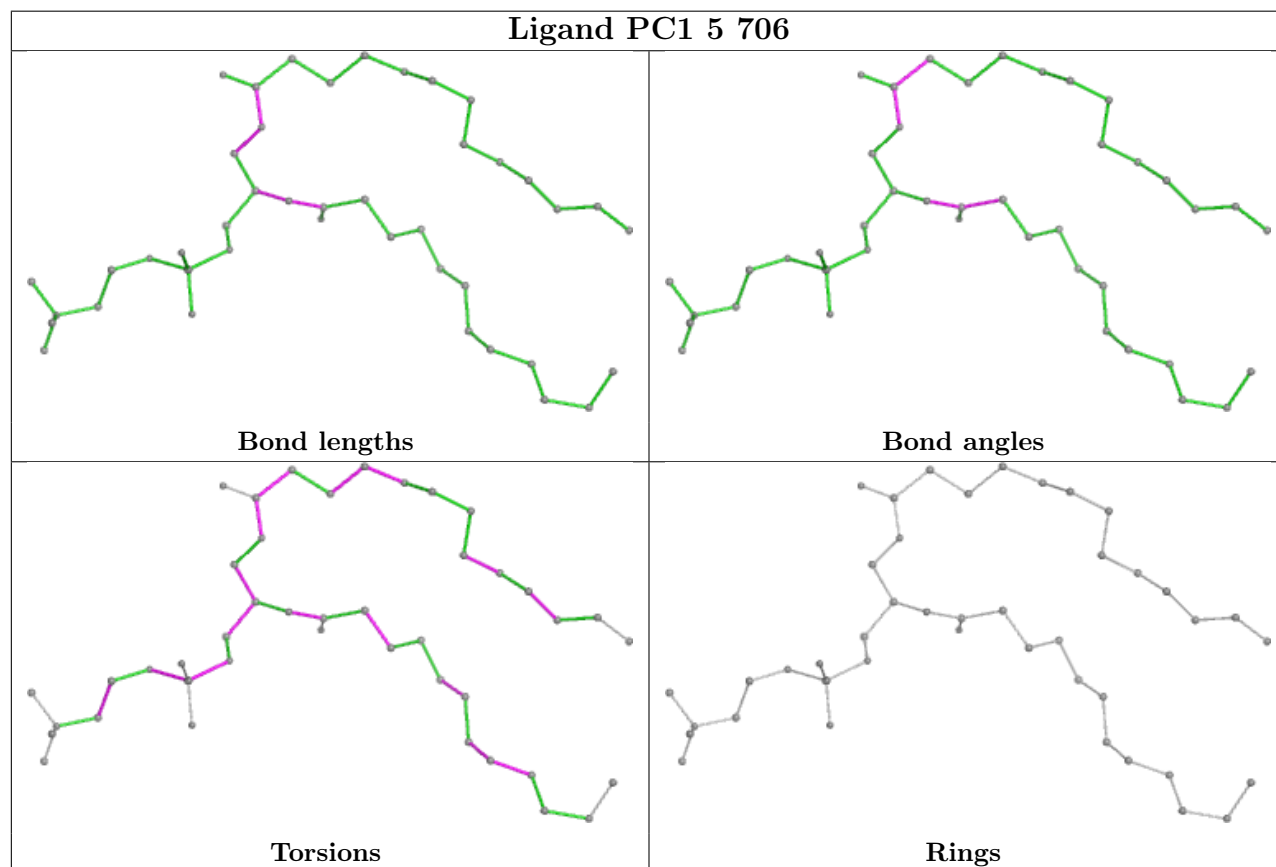
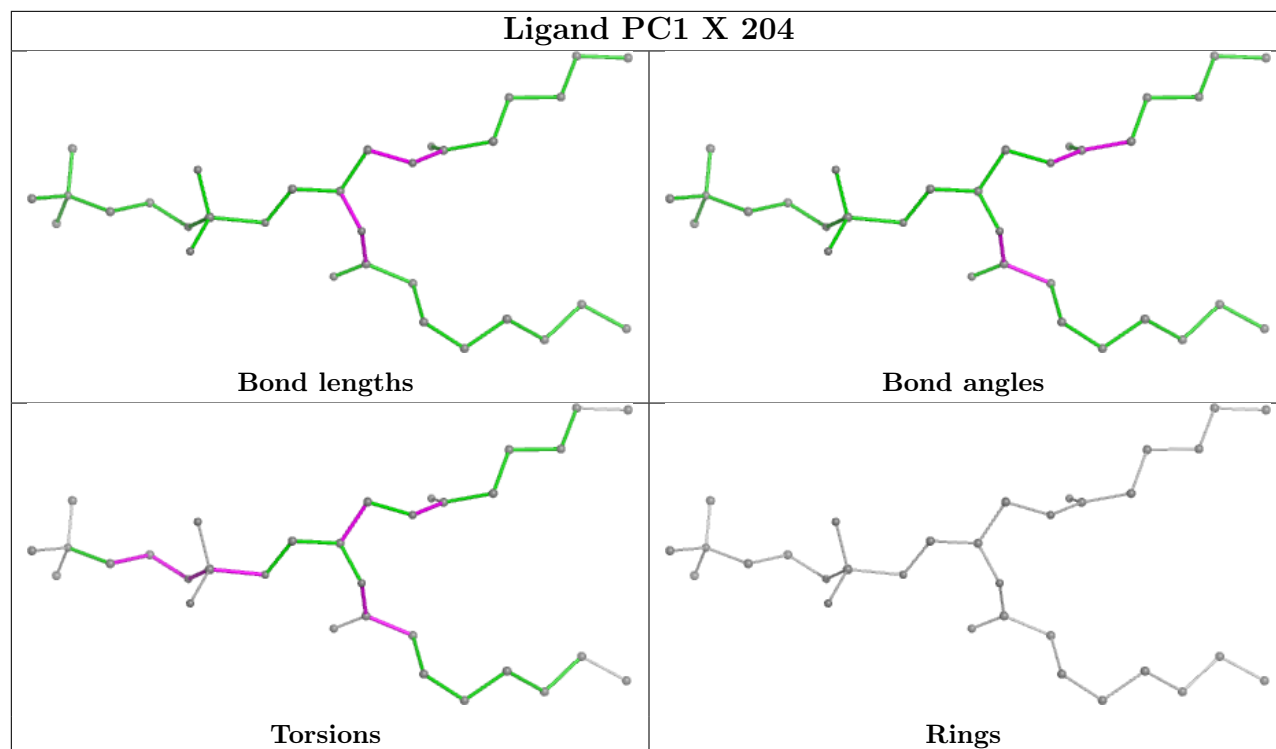


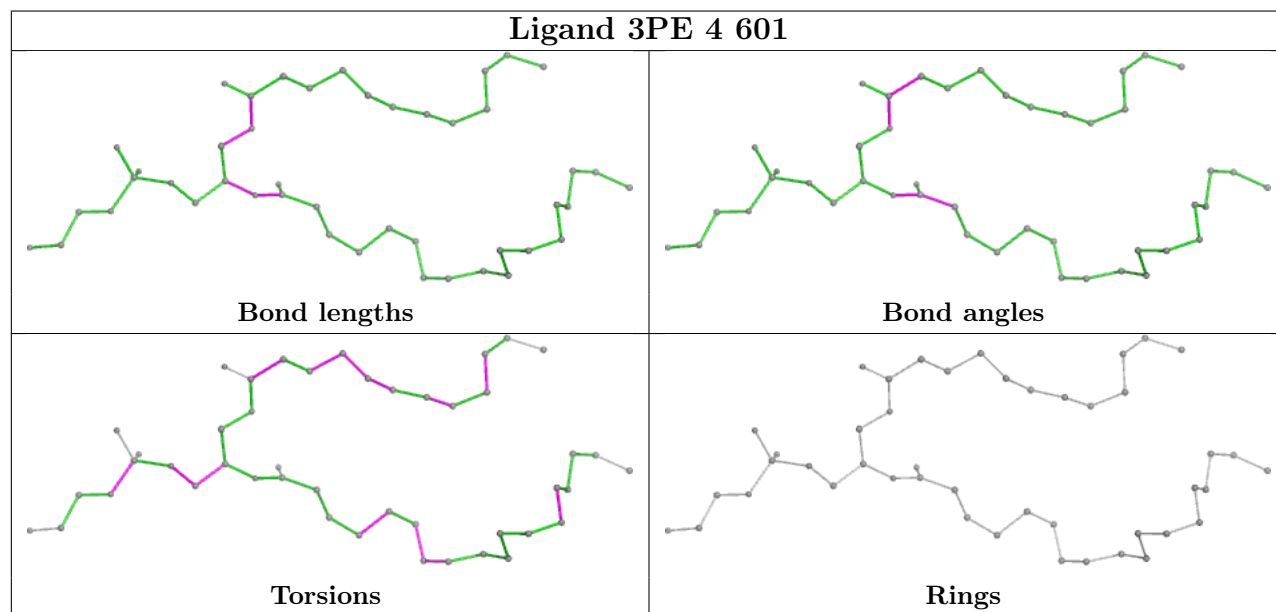
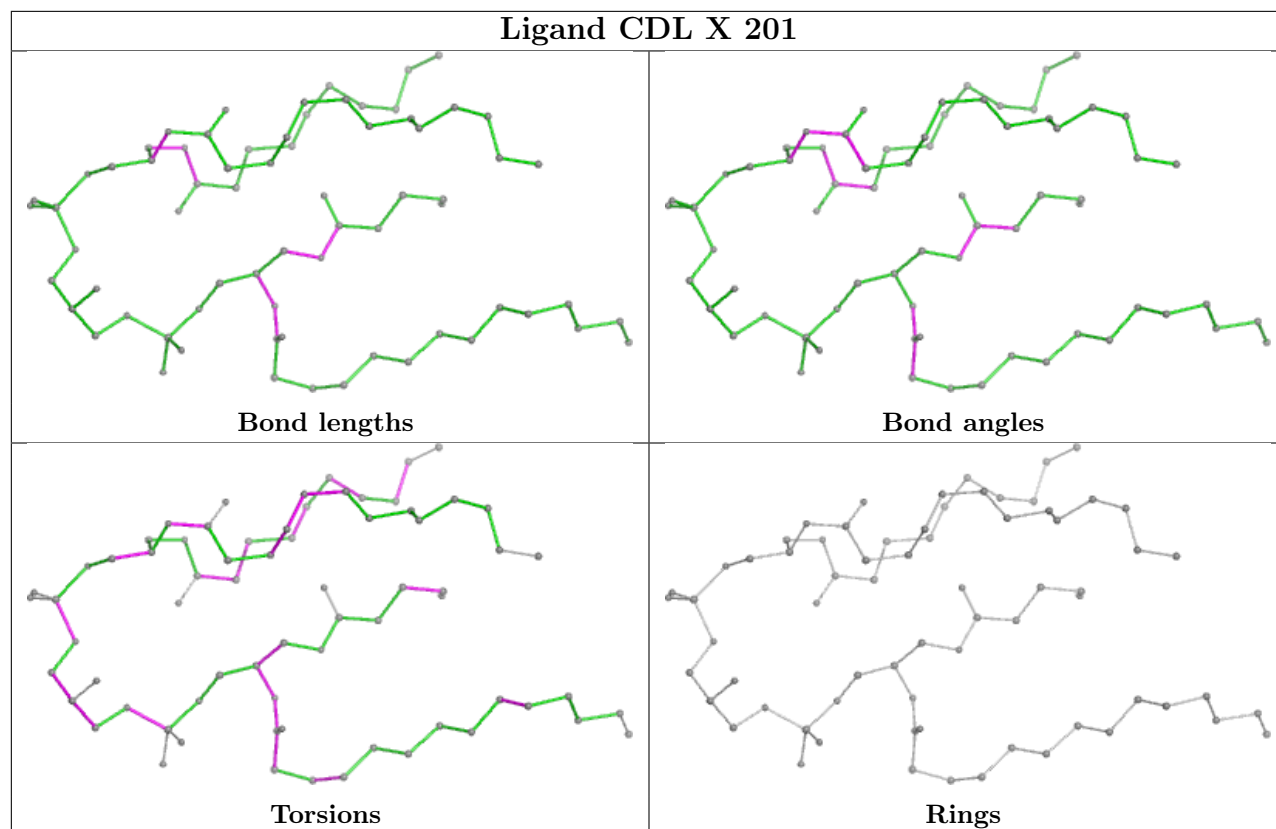


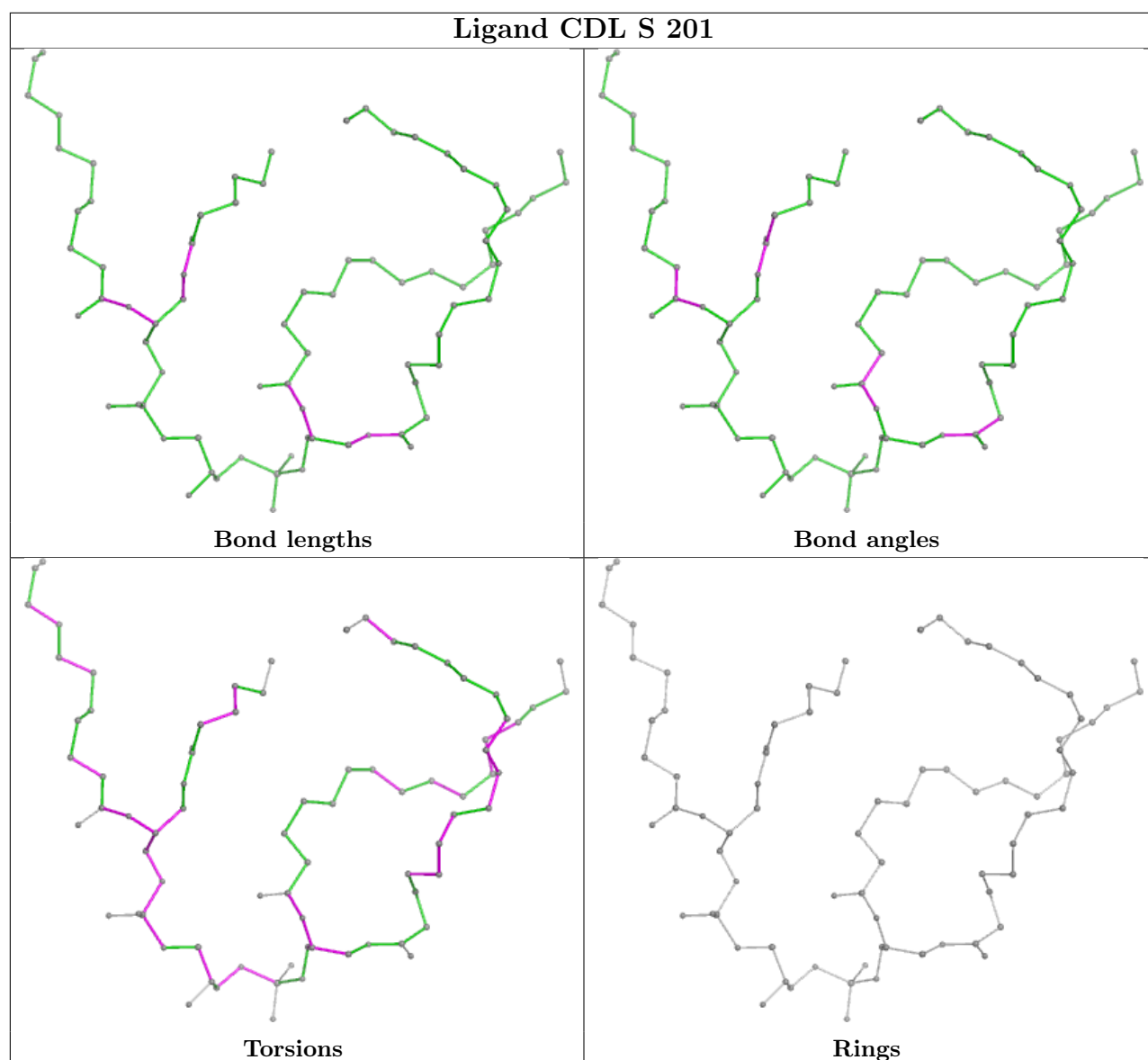












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

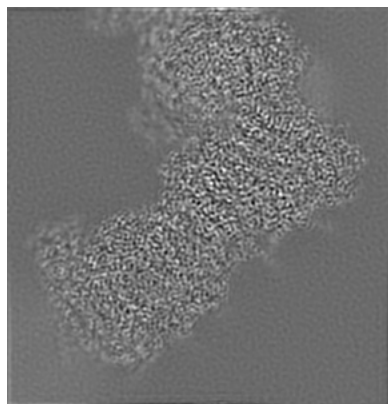
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14798. These allow visual inspection of the internal detail of the map and identification of artifacts.

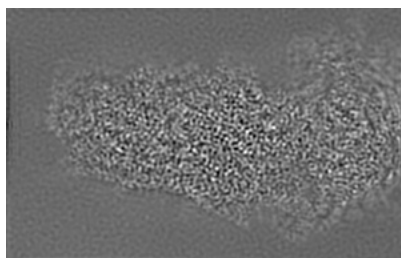
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

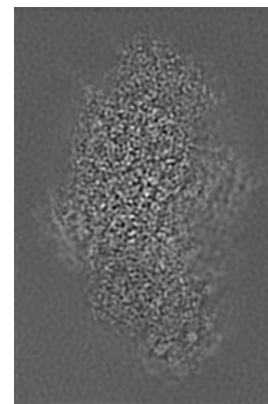
6.1.1 Primary map



X

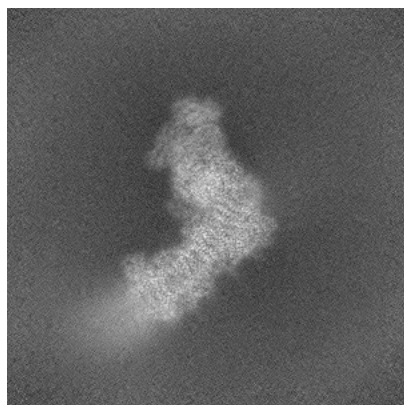


Y

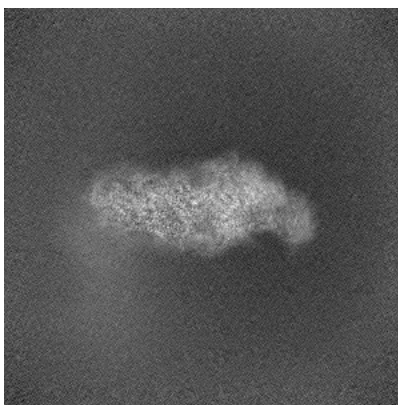


Z

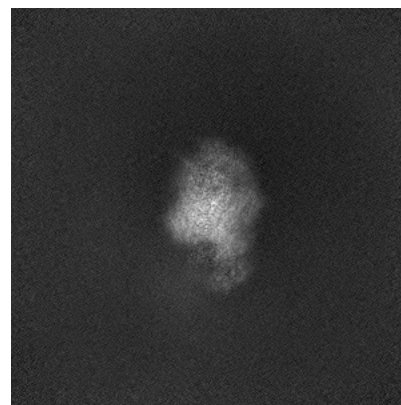
6.1.2 Raw map



X



Y

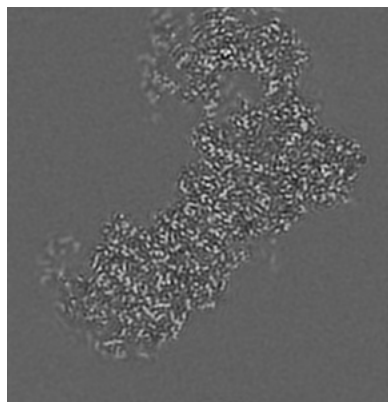


Z

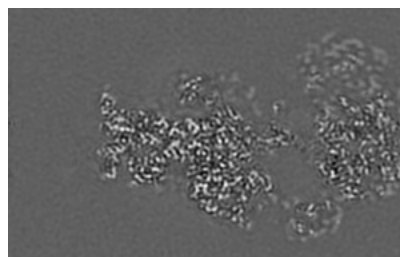
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

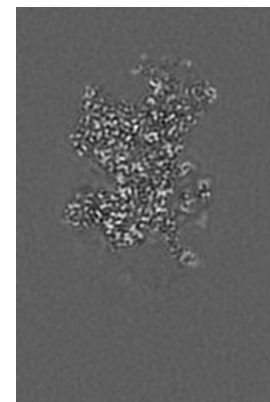
6.2.1 Primary map



X Index: 86

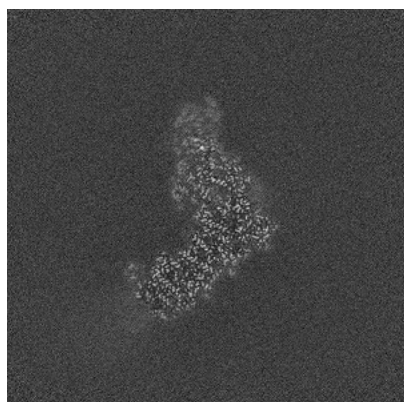


Y Index: 130

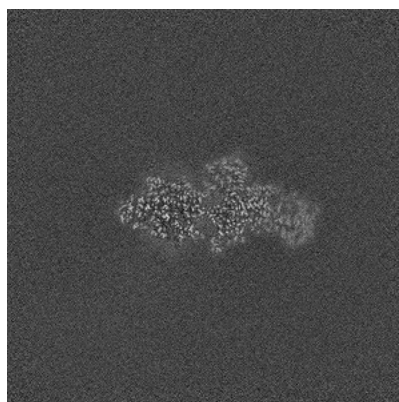


Z Index: 136

6.2.2 Raw map



X Index: 294



Y Index: 294

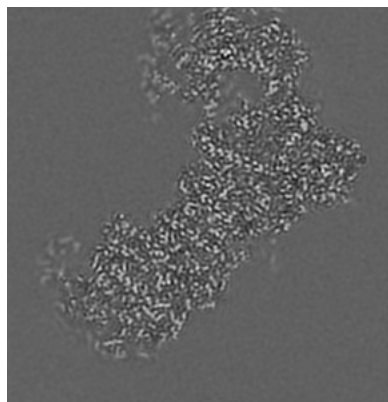


Z Index: 294

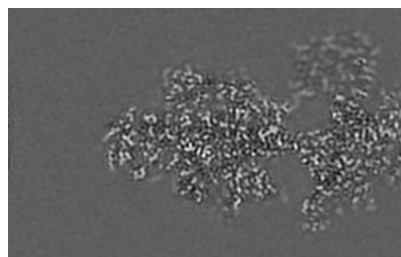
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

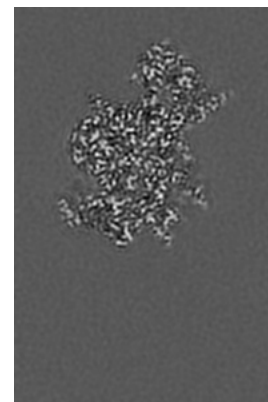
6.3.1 Primary map



X Index: 86

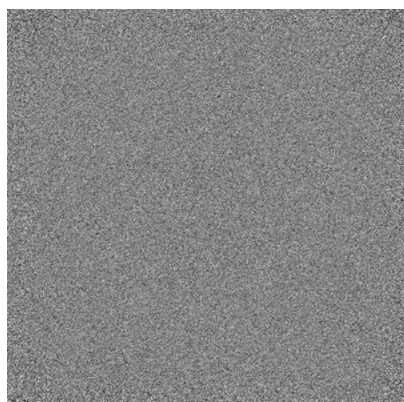


Y Index: 140

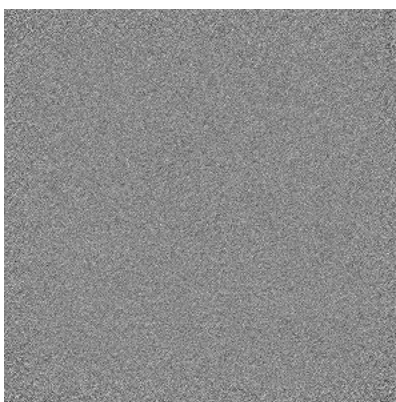


Z Index: 145

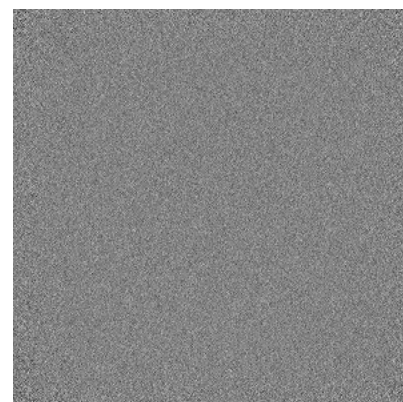
6.3.2 Raw map



X Index: 0



Y Index: 0

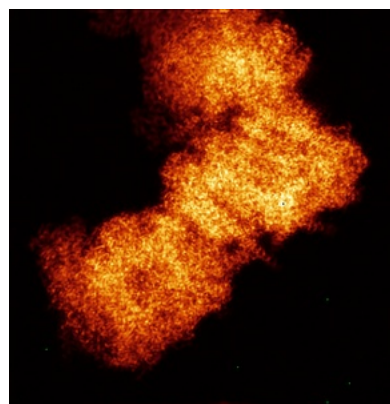


Z Index: 0

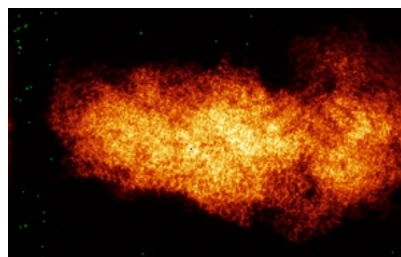
The images above show the largest variance slices of the map in three orthogonal directions.

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

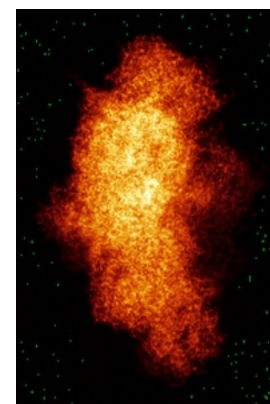
6.4.1 Primary map



X

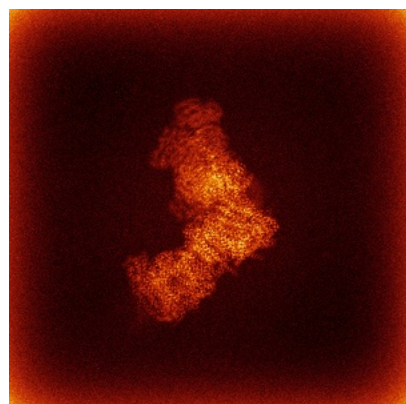


Y

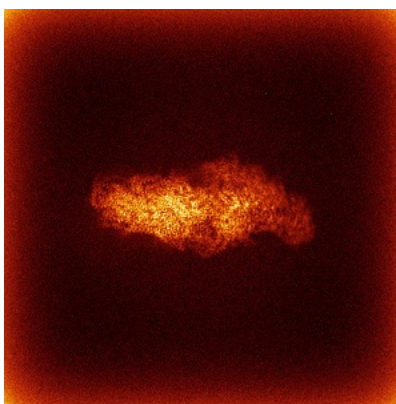


Z

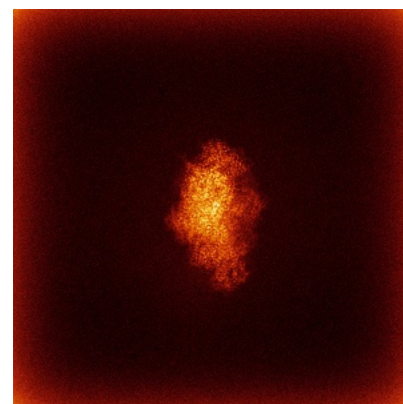
6.4.2 Raw map



X



Y

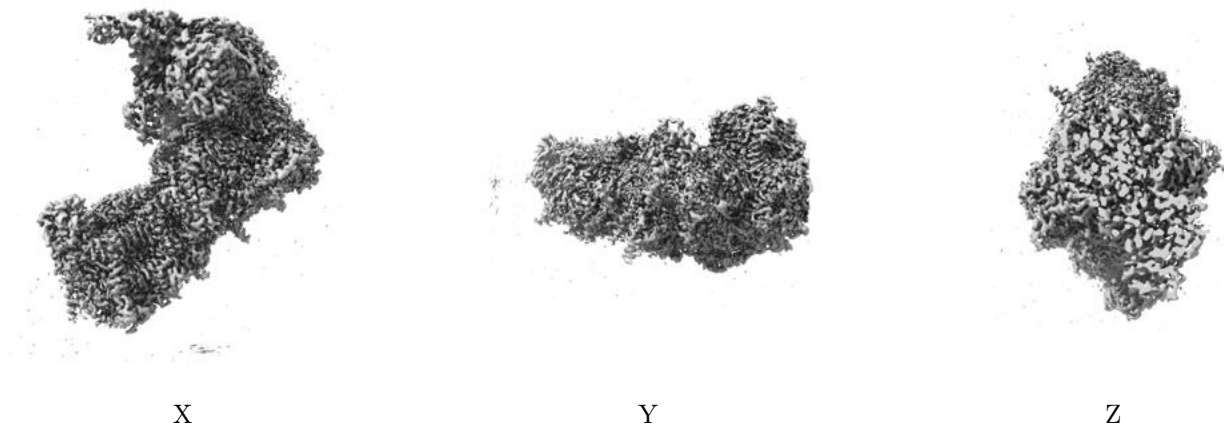


Z

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

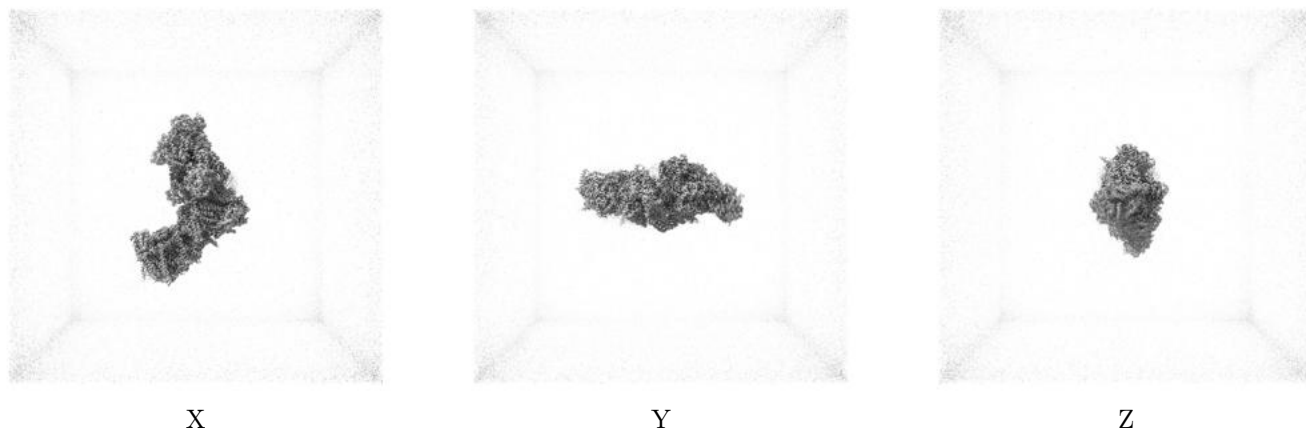
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

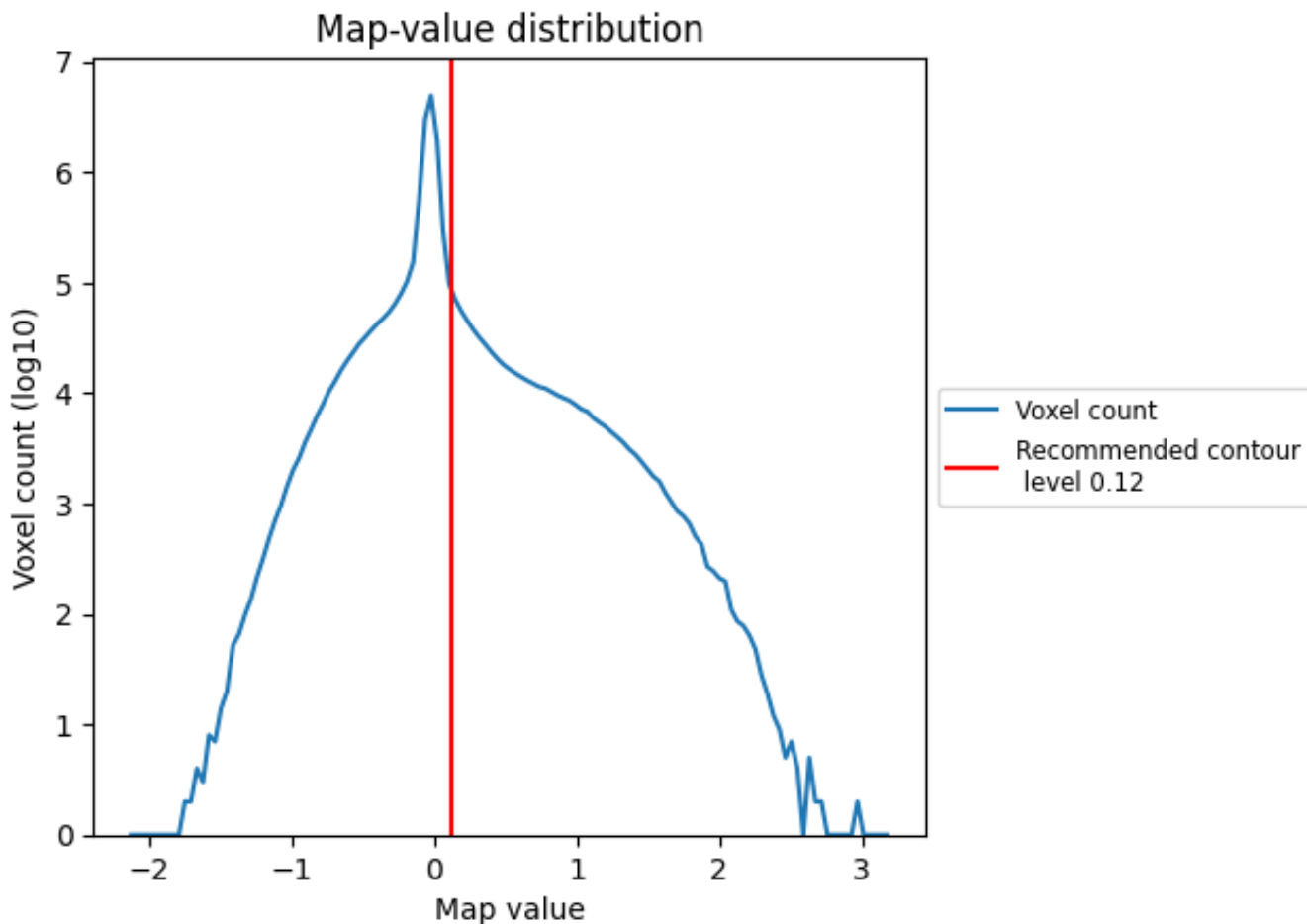
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

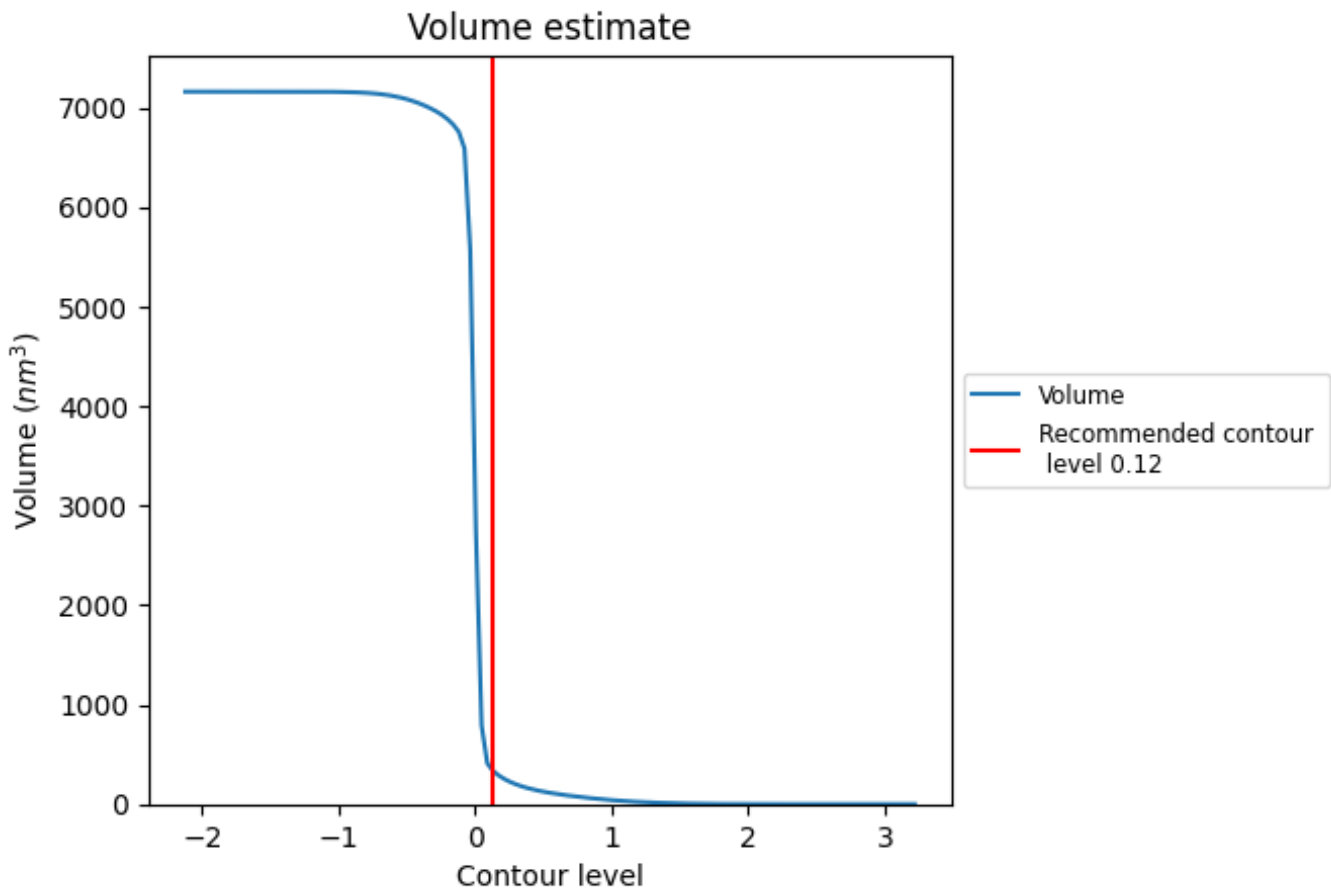
This section contains the results of statistical analysis of the map.

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 354 nm³; this corresponds to an approximate mass of 319 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

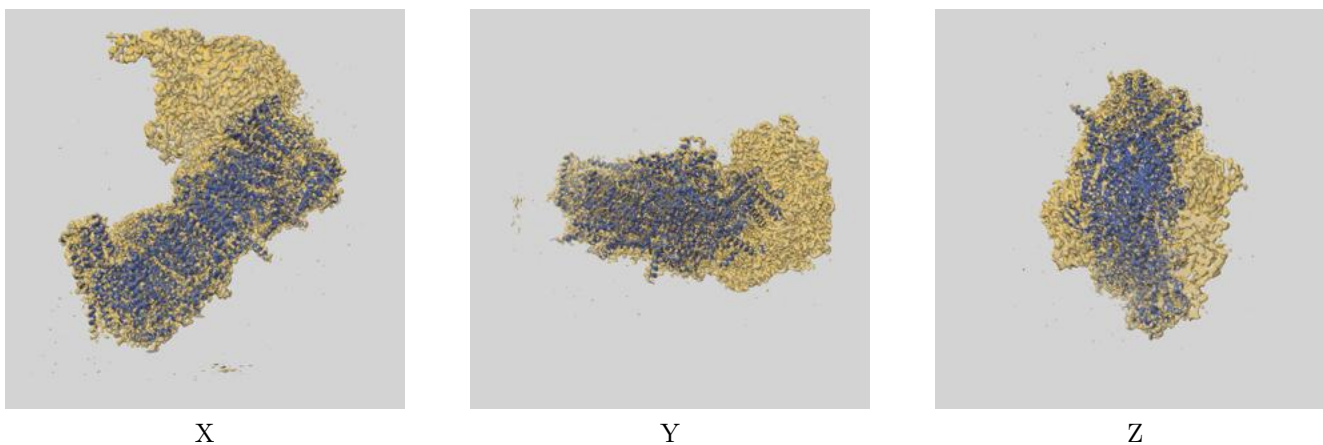
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

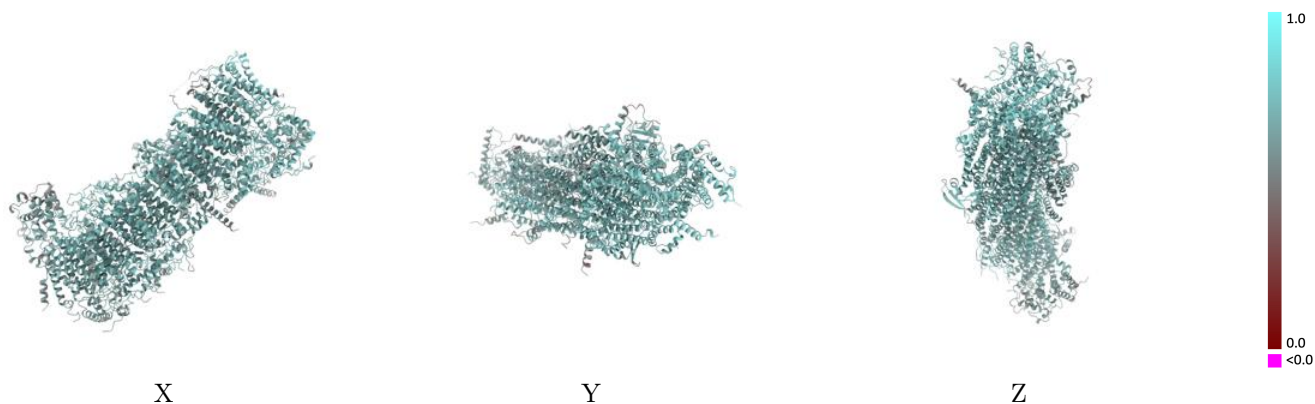
This section contains information regarding the fit between EMDB map EMD-14798 and PDB model 7ZMH. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



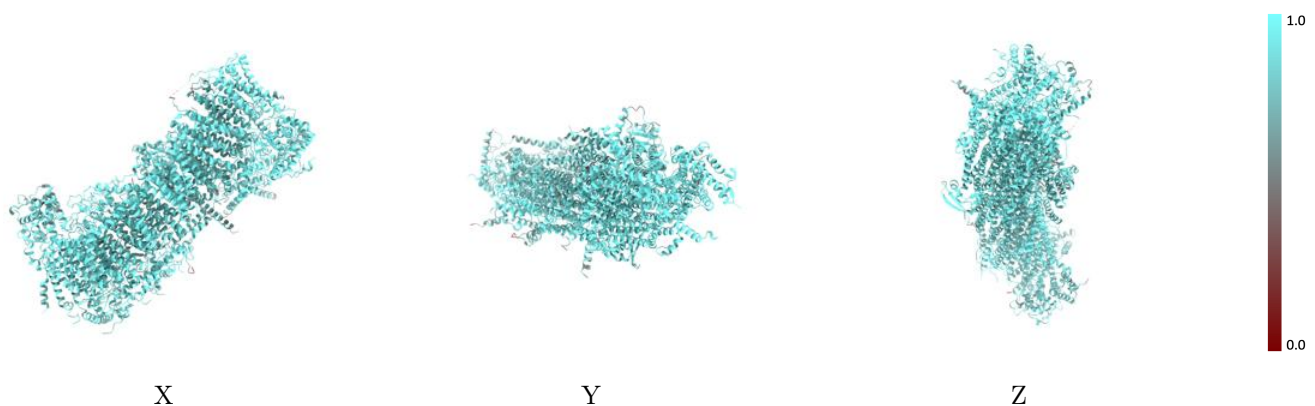
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



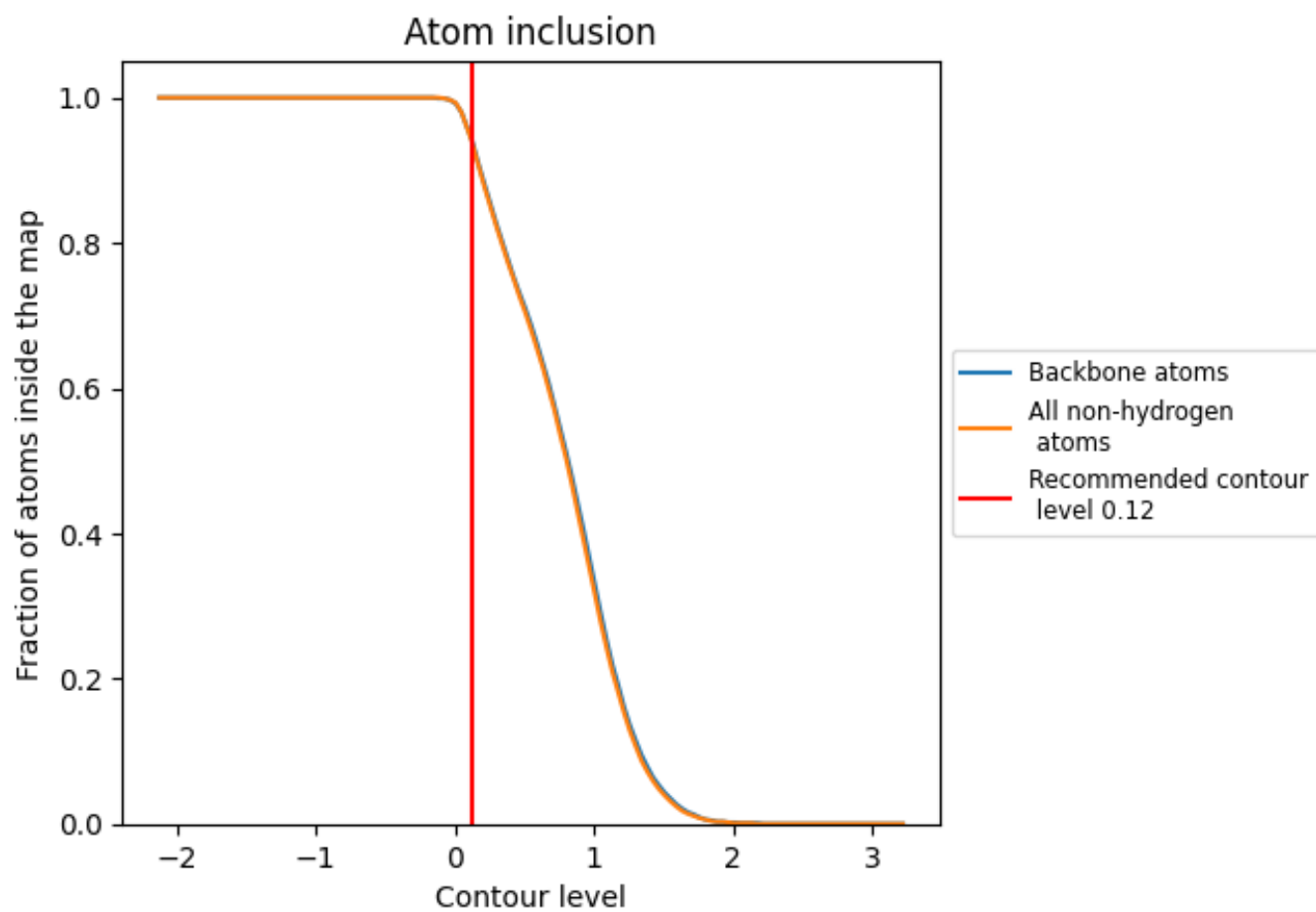
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.6720
1	 0.9560	 0.6940
2	 0.9720	 0.7080
3	 0.9260	 0.6630
4	 0.9740	 0.7030
5	 0.9660	 0.6790
6	 0.9380	 0.6790
8	 0.8910	 0.5970
9	 0.8910	 0.6450
D	 0.9920	 0.7050
J	 0.8880	 0.6120
L	 0.9760	 0.7070
Q	 0.8060	 0.5640
R	 0.9000	 0.6270
S	 0.9300	 0.6450
U	 0.9660	 0.6880
W	 0.9440	 0.6790
X	 0.9490	 0.6820
a	 0.9150	 0.6300
b	 0.9210	 0.6620
c	 0.8910	 0.5780
d	 0.9420	 0.6730
e	 0.9060	 0.6070
g	 0.9510	 0.6660
i	 0.8990	 0.6460
j	 0.9380	 0.6700
n	 0.8610	 0.6280

