



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 03:19 pm GMT

PDB ID : 7ZM8  
EMDB ID : EMD-14792  
Title : CryoEM structure of mitochondrial complex I from *Chaetomium thermophilum* (inhibited by DDM) - membrane arm  
Authors : Laube, E.; Kuehlbrandt, W.  
Deposited on : 2022-04-19  
Resolution : 2.76 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

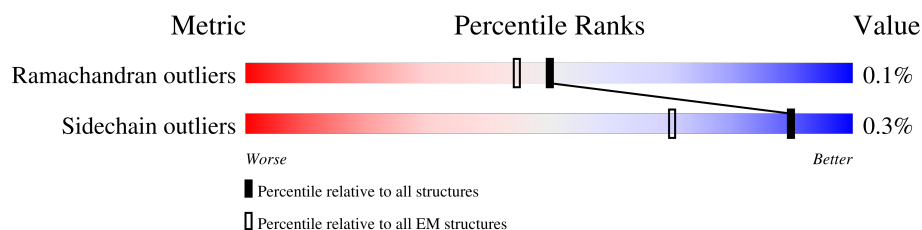
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 2.76 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	378	<div> <div>8%</div> <div>99%</div> <div>.</div> </div>
2	2	571	<div> <div>98%</div> <div>.</div> </div>
3	3	146	<div> <div>69%</div> <div>31%</div> </div>
4	4	542	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
5	5	679	<div> <div>98%</div> <div>.</div> </div>
6	6	224	<div> <div>84%</div> <div>16%</div> </div>
7	8	86	<div> <div>90%</div> <div>10%</div> </div>
8	9	785	<div> <div>13%</div> <div>87%</div> </div>
9	D	86	<div> <div>98%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
10	J	199	
11	L	89	
12	Q	141	
13	R	99	
14	S	143	
15	U	186	
16	W	121	
17	X	191	
18	a	815	
19	b	94	
20	c	93	
21	d	105	
22	e	46	
23	g	82	
24	i	93	
25	j	75	
26	n	184	

## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 37030 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
1	1	378	Total	C	N	O	S	0	0
			2848	1914	430	494	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	558	Total	C	N	O	S	0	0
			4456	2993	672	780	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	101	Total	C	N	O	S	0	0
			790	541	115	132	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	670	Total	C	N	O	S	0	0
			5276	3552	793	906	25		

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
6	6	189	Total	C	N	O	S	0	0
			1460	985	219	250	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			654	405	125	118	6		

- Molecule 8 is a protein called Subunit NDUF5 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	102	Total	C	N	O	S	0	0
			802	497	146	153	6		

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 NDUF1 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	188	Total	C	N	O	S	0	0
			1408	892	263	251	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
			670	421	109	139	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	72	Total	C	N	O	0	0
			598	393	96	109		

- 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
			1353	852	252	240	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	101	Total	C	N	O	S	0	0
			825	527	156	140	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	186	Total	C	N	O	S	0	0
			1467	934	266	259	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	143	Total	C	N	O	S	0	0
			1167	750	195	217	5		

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
19	b	80	Total	C	N	O	S	0	0
			675	440	124	109	2		

- Molecule 20 is a protein called Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	64	Total	C	N	O	S	0	0
			510	332	90	86	2		

- Molecule 21 is a protein called Subunit NDUF10 of NADH-ubiquinone oxidoreductase

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	100	Total	C	N	O	S	0	0
			827	526	146	151	4		

- Molecule 22 is a protein called Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	38	Total	C	N	O	S	0	0
			320	217	58	44	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	77	Total	C	N	O	S	0	0
			604	395	104	104	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	81	Total	C	N	O	S	0	0
			686	453	119	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	73	Total	C	N	O	S	0	0
			603	391	108	101	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	135	Total	C	N	O	S	0	0
			1068	683	189	195	1		

There are 52 discrepancies between the modelled and reference sequences:



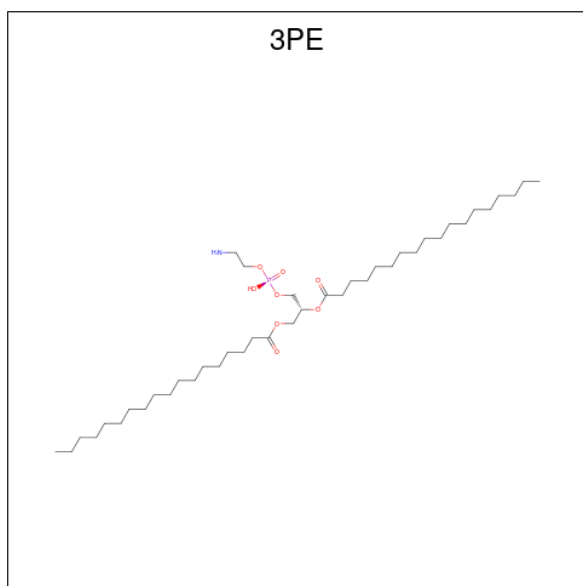
Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP 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:  $C_{41}H_{82}NO_8P$ ).



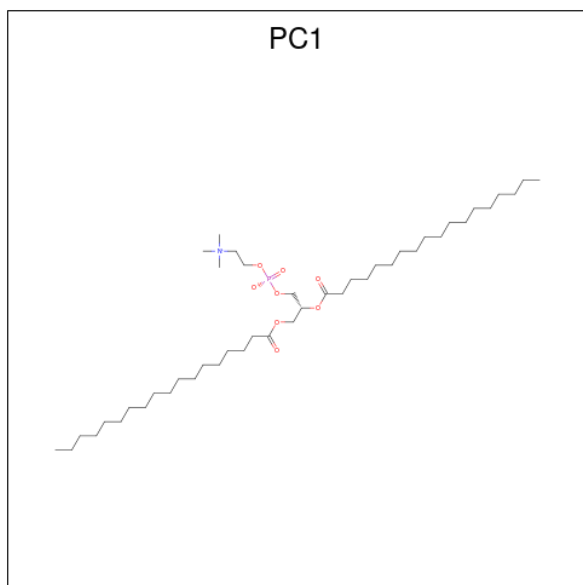
Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
27	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
27	5	1	Total	C	N	O	P	0
			44	34	1	8	1	
27	W	1	Total	C	N	O	P	0
			40	30	1	8	1	
27	W	1	Total	C	N	O	P	0
			36	26	1	8	1	

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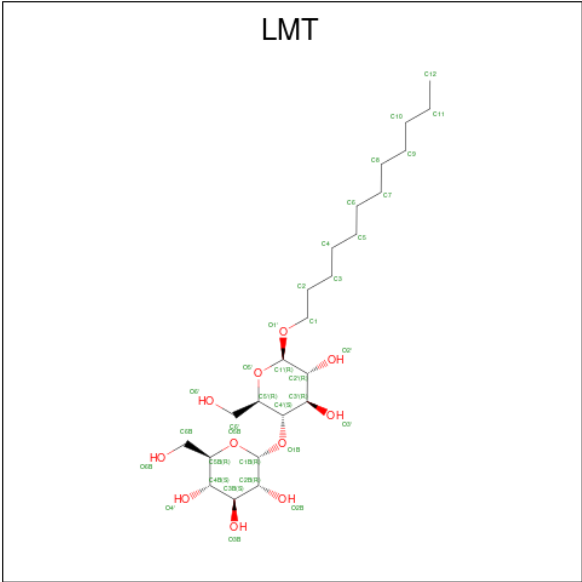
Mol	Chain	Residues	Atoms					AltConf
27	i	1	Total	C	N	O	P	0
			43	33	1	8	1	

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



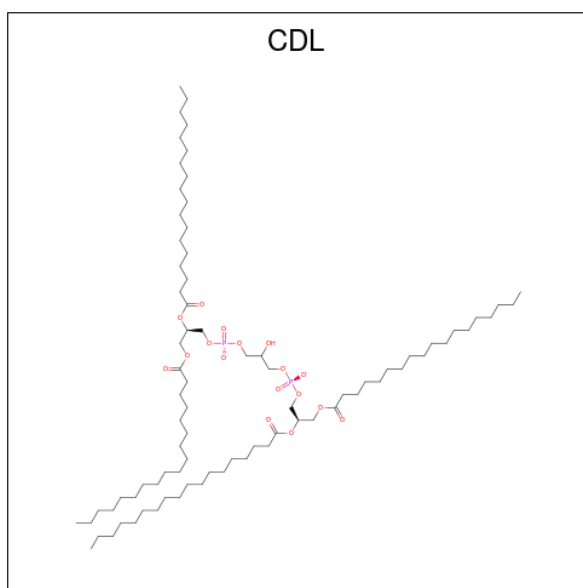
Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			33	23	1	8	1	
28	2	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			40	30	1	8	1	
28	5	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			35	24	11	
29	1	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	3	1	Total	C	O	0
			35	24	11	
29	3	1	Total	C	O	0
			35	24	11	
29	4	1	Total	C	O	0
			31	20	11	
29	5	1	Total	C	O	0
			35	24	11	
29	J	1	Total	C	O	0
			35	24	11	
29	J	1	Total	C	O	0
			35	24	11	
29	a	1	Total	C	O	0
			35	24	11	
29	g	1	Total	C	O	0
			34	23	11	

- Molecule 30 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
30	2	1	Total	C	O	P	0
			69	50	17	2	
30	D	1	Total	C	O	P	0
			65	46	17	2	
30	S	1	Total	C	O	P	0
			61	42	17	2	
30	X	1	Total	C	O	P	0
			53	34	17	2	
30	X	1	Total	C	O	P	0
			76	57	17	2	

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



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

- Molecule 32 is water.

Mol	Chain	Residues	Atoms	AltConf
32	1	36	Total O 36 36	0
32	2	122	Total O 122 122	0
32	3	6	Total O 6 6	0
32	4	96	Total O 96 96	0
32	5	71	Total O 71 71	0
32	6	21	Total O 21 21	0
32	9	18	Total O 18 18	0
32	D	23	Total O 23 23	0
32	J	3	Total O 3 3	0
32	L	5	Total O 5 5	0
32	Q	3	Total O 3 3	0

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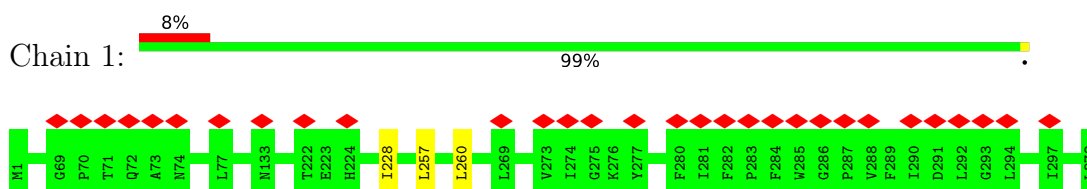
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Mol	Chain	Residues	Atoms		AltConf
32	R	16	Total 16	O 16	0
32	S	7	Total 7	O 7	0
32	U	19	Total 19	O 19	0
32	W	35	Total 35	O 35	0
32	X	37	Total 37	O 37	0
32	a	12	Total 12	O 12	0
32	b	6	Total 6	O 6	0
32	c	1	Total 1	O 1	0
32	d	18	Total 18	O 18	0
32	g	2	Total 2	O 2	0
32	i	5	Total 5	O 5	0
32	j	18	Total 18	O 18	0
32	n	28	Total 28	O 28	0

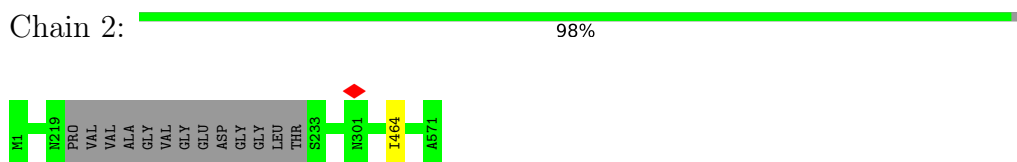
### 3 Residue-property plots

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.

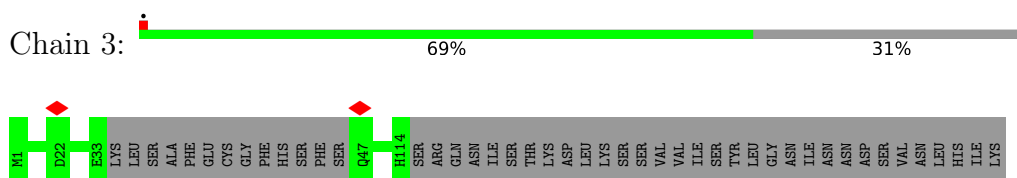
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



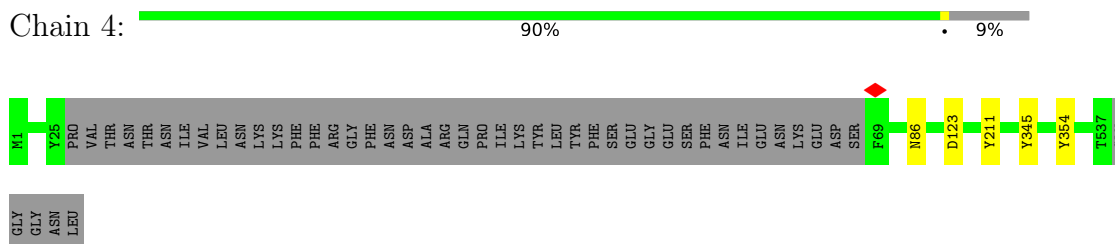
- Molecule 2: NADH dehydrogenase subunit 2



- Molecule 3: NADH-ubiquinone oxidoreductase chain 3



- Molecule 4: NADH-ubiquinone oxidoreductase chain 4



- Molecule 5: NADH-ubiquinone oxidoreductase chain 5








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

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

Chain D:  98% ..

MET P2 V81 X86

- Molecule 10: NADH-ubiquinone oxidoreductase-like protein

Chain J:  5% 94% 6%

MET ALA PRO ILE GLU GLU HIS HIS Y11 H12 D70 R105 S128 G132 V133 F134 K135 R136 D137 Q198 ALA

- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain L:  98% .

MET H2 Y88 LYS

- Molecule 12: Acyl carrier protein

Chain Q:  60% 40%

MET PHE ARG SER VAL LEU ARG SER ALA ALA ALA THR ARG THR THR ILE ARG SER ILE PRO PRO PRO ALA ALA ALA LYS LYS PHE ALA VAL ALA PRO VAL VAL SER SER ARG VAL THR THR PHE ILE PRO LYS THR ALA ALA TRP GLN VAL ILE ARG CYS TYR ALA ALA SER ASN E57 E63

A91 H141

- Molecule 13: Complex I-B22

Chain R:  99% .

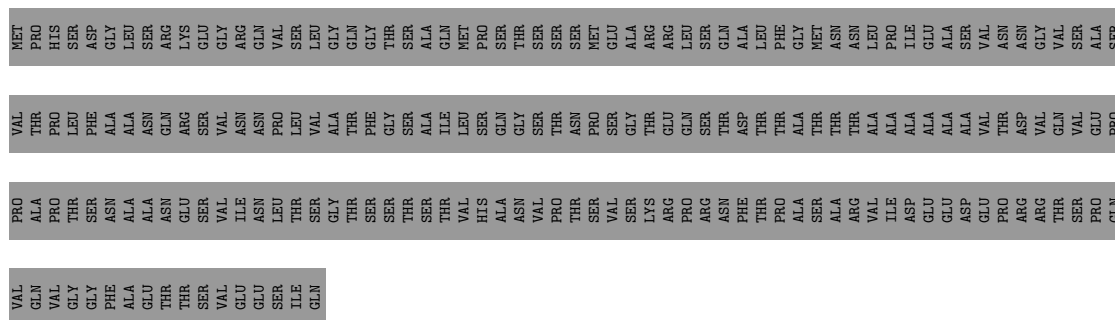
MET S2 F99

- Molecule 14: Complex I-ESSS

Chain S:  50% 50%

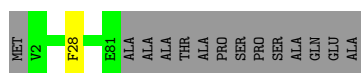
MET ASP GLY GLY PRO PRO THR PHE PHE ARG PRO THR ALA ALA GLN GLN ALA PRO PRO GLY LYS LEU SER SER ALA PRO VAL THR THR ARG LEU ALA ALA ALA LEU SER ARG ALA SER THR VAL SER LYS ALA LEU THR PRO ARG ARG PHE ARG PHE SER THR THR GLN ARG ARG





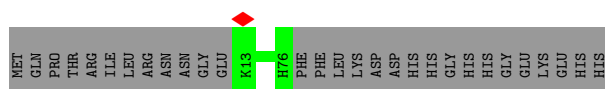
- Molecule 19: Subunit NDUFC2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain b: 84% 15%



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

Chain c: 69% 31%



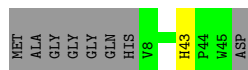
- Molecule 21: Subunit NDUF10 of NADH-ubiquinone oxidoreductase (Complex I)

Chain d: 95% 5%



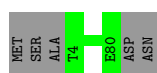
- Molecule 22: Subunit NDUF2 of NADH-ubiquinone oxidoreductase (Complex I)

Chain e: 80% 17%



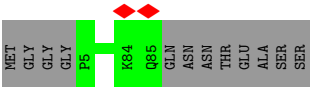
- Molecule 23: Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I)

Chain g: 94% 6%



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

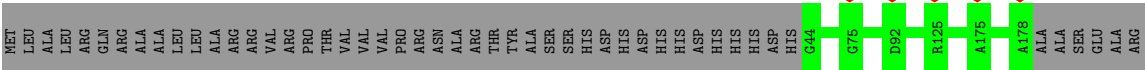
Chain i: 87% 13%



- 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	37767	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)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.887	Depositor
Minimum map value	-1.296	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	153.4554, 154.48529, 277.04364	wwPDB
Map dimensions	269, 150, 149	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.029902, 1.029902, 1.029902	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, PC1, ZMP, 3PE, LMT

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	0.49	0/2917	0.62	0/3991
2	2	0.50	0/4562	0.64	0/6205
3	3	0.47	0/811	0.57	0/1105
4	4	0.50	0/4002	0.66	0/5454
5	5	0.44	0/5418	0.58	0/7376
6	6	0.49	0/1487	0.63	0/2026
7	8	0.39	0/667	0.49	0/892
8	9	0.51	0/819	0.69	0/1105
9	D	0.44	0/674	0.66	0/911
10	J	0.38	0/1435	0.56	0/1940
11	L	0.48	0/680	0.62	0/921
12	Q	0.37	0/680	0.47	0/922
13	R	0.47	0/832	0.68	0/1133
14	S	0.48	0/622	0.59	0/850
15	U	0.51	1/1390 (0.1%)	0.73	0/1885
16	W	0.48	0/844	0.69	0/1139
17	X	0.51	0/1506	0.72	0/2036
18	a	0.36	0/1204	0.52	0/1632
19	b	0.42	0/693	0.60	0/929
20	c	0.37	0/529	0.52	0/720
21	d	0.44	0/845	0.62	0/1137
22	e	0.51	0/335	0.68	0/454
23	g	0.49	0/624	0.66	0/857
24	i	0.40	0/715	0.51	0/971
25	j	0.46	0/617	0.60	0/830
26	n	0.45	0/1100	0.63	0/1491
All	All	0.47	1/36008 (0.0%)	0.62	0/48912

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	90	HIS	C-N	5.03	1.45	1.34

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	1	376/378 (100%)	359 (96%)	16 (4%)	1 (0%)	37	55
2	2	554/571 (97%)	540 (98%)	14 (2%)	0	100	100
3	3	97/146 (66%)	95 (98%)	2 (2%)	0	100	100
4	4	490/542 (90%)	473 (96%)	17 (4%)	0	100	100
5	5	668/679 (98%)	637 (95%)	30 (4%)	1 (0%)	48	70
6	6	185/224 (83%)	180 (97%)	5 (3%)	0	100	100
7	8	75/86 (87%)	73 (97%)	2 (3%)	0	100	100
8	9	100/785 (13%)	98 (98%)	2 (2%)	0	100	100
9	D	79/86 (92%)	75 (95%)	4 (5%)	0	100	100
10	J	186/199 (94%)	183 (98%)	3 (2%)	0	100	100
11	L	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
12	Q	83/141 (59%)	82 (99%)	1 (1%)	0	100	100
13	R	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
14	S	70/143 (49%)	68 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	U	165/186 (89%)	163 (99%)	2 (1%)	0	100	100
16	W	99/121 (82%)	99 (100%)	0	0	100	100
17	X	184/191 (96%)	178 (97%)	6 (3%)	0	100	100
18	a	141/815 (17%)	137 (97%)	4 (3%)	0	100	100
19	b	78/94 (83%)	76 (97%)	1 (1%)	1 (1%)	10	17
20	c	62/93 (67%)	60 (97%)	2 (3%)	0	100	100
21	d	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
22	e	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
23	g	75/82 (92%)	72 (96%)	3 (4%)	0	100	100
24	i	79/93 (85%)	73 (92%)	6 (8%)	0	100	100
25	j	71/75 (95%)	69 (97%)	2 (3%)	0	100	100
26	n	133/184 (72%)	127 (96%)	6 (4%)	0	100	100
All	All	4365/6253 (70%)	4220 (97%)	142 (3%)	3 (0%)	50	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	b	28	PHE
1	1	228	ILE
5	5	350	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	1	297/326 (91%)	295 (99%)	2 (1%)	81	89
2	2	509/518 (98%)	508 (100%)	1 (0%)	92	96
3	3	83/128 (65%)	83 (100%)	0	100	100
4	4	431/477 (90%)	426 (99%)	5 (1%)	67	81
5	5	581/596 (98%)	579 (100%)	2 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	167/203 (82%)	166 (99%)	1 (1%)	84	90
7	8	68/75 (91%)	68 (100%)	0	100	100
8	9	84/687 (12%)	84 (100%)	0	100	100
9	D	68/69 (99%)	67 (98%)	1 (2%)	60	76
10	J	131/146 (90%)	131 (100%)	0	100	100
11	L	74/76 (97%)	74 (100%)	0	100	100
12	Q	74/119 (62%)	74 (100%)	0	100	100
13	R	87/89 (98%)	87 (100%)	0	100	100
14	S	58/111 (52%)	58 (100%)	0	100	100
15	U	148/167 (89%)	148 (100%)	0	100	100
16	W	84/102 (82%)	84 (100%)	0	100	100
17	X	143/152 (94%)	143 (100%)	0	100	100
18	a	123/697 (18%)	123 (100%)	0	100	100
19	b	66/74 (89%)	66 (100%)	0	100	100
20	c	47/80 (59%)	47 (100%)	0	100	100
21	d	87/94 (93%)	87 (100%)	0	100	100
22	e	30/35 (86%)	29 (97%)	1 (3%)	33	55
23	g	65/69 (94%)	65 (100%)	0	100	100
24	i	69/78 (88%)	69 (100%)	0	100	100
25	j	63/64 (98%)	63 (100%)	0	100	100
26	n	108/150 (72%)	108 (100%)	0	100	100
All	All	3745/5382 (70%)	3732 (100%)	13 (0%)	90	95

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	354	TYR
5	5	340	PHE
22	e	43	HIS
6	6	198	VAL
9	D	81	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
6	6	182	ASN
26	n	84	HIS
14	S	117	GLN
26	n	126	HIS
18	a	101	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](#)

31 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
28	PC1	1	402	-	32,32,53	0.34	0	38,40,61	0.39	0
27	3PE	i	101	-	42,42,50	0.92	4 (9%)	45,47,55	1.08	2 (4%)
29	LMT	2	603	-	36,36,36	0.40	0	47,47,47	0.74	0
28	PC1	2	606	-	44,44,53	1.00	3 (6%)	50,52,61	1.18	2 (4%)
30	CDL	2	601	-	68,68,99	0.34	0	74,80,111	0.42	0
29	LMT	J	201	-	36,36,36	1.13	2 (5%)	47,47,47	1.16	3 (6%)
29	LMT	g	101	-	35,35,36	1.10	2 (5%)	46,46,47	1.07	3 (6%)
29	LMT	4	601	-	32,32,36	1.19	2 (6%)	43,43,47	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMT	3	202	-	36,36,36	0.39	0	47,47,47	0.99	2 (4%)
30	CDL	D	101	-	64,64,99	0.33	0	70,76,111	0.41	0
27	3PE	5	704	-	41,41,50	0.94	4 (9%)	44,46,55	1.16	2 (4%)
27	3PE	W	202	-	35,35,50	1.00	4 (11%)	38,40,55	1.19	2 (5%)
30	CDL	X	201	-	52,52,99	0.37	0	58,64,111	0.45	0
30	CDL	S	201	-	60,60,99	0.31	0	66,72,111	0.42	0
28	PC1	5	702	-	39,39,53	0.40	0	45,47,61	0.54	0
28	PC1	5	703	-	44,44,53	0.33	0	50,52,61	0.36	0
29	LMT	J	202	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
29	LMT	5	705	-	36,36,36	1.10	2 (5%)	47,47,47	1.31	5 (10%)
29	LMT	2	605	-	36,36,36	0.39	0	47,47,47	0.69	0
29	LMT	2	602	-	36,36,36	0.36	0	47,47,47	0.72	1 (2%)
27	3PE	5	706	-	42,42,50	0.29	0	44,46,55	0.34	0
27	3PE	1	401	-	38,38,50	0.33	0	41,43,55	0.54	0
31	ZMP	Q	201	12	29,35,36	0.17	0	34,42,45	0.39	0
29	LMT	a	901	-	36,36,36	0.35	0	47,47,47	0.83	1 (2%)
30	CDL	X	202	-	75,75,99	0.33	0	81,87,111	0.35	0
29	LMT	3	201	-	36,36,36	0.37	0	47,47,47	0.69	0
29	LMT	2	604	-	36,36,36	0.39	0	47,47,47	0.82	0
27	3PE	W	201	-	39,39,50	0.30	0	42,44,55	0.34	0
29	LMT	1	404	-	36,36,36	1.13	2 (5%)	47,47,47	0.94	2 (4%)
27	3PE	5	701	-	40,40,50	0.94	4 (10%)	43,45,55	1.19	3 (6%)
29	LMT	1	403	-	36,36,36	1.10	2 (5%)	47,47,47	1.06	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
28	PC1	1	402	-	-	7/36/36/57	-
27	3PE	i	101	-	-	20/46/46/54	-
29	LMT	2	603	-	-	6/21/61/61	0/2/2/2
28	PC1	2	606	-	-	19/48/48/57	-
30	CDL	2	601	-	-	26/79/79/110	-
29	LMT	J	201	-	-	11/21/61/61	0/2/2/2
29	LMT	g	101	-	-	6/20/60/61	0/2/2/2
29	LMT	4	601	-	-	9/17/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	3	202	-	-	8/21/61/61	0/2/2/2
30	CDL	D	101	-	-	21/75/75/110	-
27	3PE	5	704	-	-	17/45/45/54	-
27	3PE	W	202	-	-	14/39/39/54	-
30	CDL	X	201	-	-	22/63/63/110	-
30	CDL	S	201	-	-	20/70/70/110	-
28	PC1	5	702	-	-	10/43/43/57	-
28	PC1	5	703	-	-	11/48/48/57	-
29	LMT	J	202	-	-	5/21/61/61	0/2/2/2
29	LMT	5	705	-	-	7/21/61/61	0/2/2/2
29	LMT	2	605	-	-	10/21/61/61	0/2/2/2
29	LMT	2	602	-	-	8/21/61/61	0/2/2/2
27	3PE	5	706	-	-	15/45/45/54	-
27	3PE	1	401	-	-	18/42/42/54	-
31	ZMP	Q	201	12	-	11/40/42/43	-
29	LMT	a	901	-	-	7/21/61/61	0/2/2/2
30	CDL	X	202	-	-	17/86/86/110	-
29	LMT	3	201	-	-	2/21/61/61	0/2/2/2
29	LMT	2	604	-	-	8/21/61/61	0/2/2/2
27	3PE	W	201	-	-	6/43/43/54	-
29	LMT	1	404	-	-	8/21/61/61	0/2/2/2
27	3PE	5	701	-	-	14/44/44/54	-
29	LMT	1	403	-	-	10/21/61/61	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	201	LMT	O5'-C1'	3.38	1.50	1.41
29	4	601	LMT	O5'-C1'	3.30	1.50	1.41
29	J	201	LMT	O5B-C1B	3.29	1.50	1.41
29	4	601	LMT	O5B-C1B	3.28	1.50	1.41
29	1	404	LMT	O5B-C1B	3.28	1.50	1.41

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	606	PC1	O21-C21-C22	4.76	121.77	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	704	3PE	O21-C21-C22	4.43	121.04	111.50
27	5	701	3PE	O21-C21-C22	4.11	120.35	111.50
27	W	202	3PE	O21-C21-C22	3.77	119.62	111.50
27	i	101	3PE	O21-C21-C22	3.64	119.35	111.50

There are no chirality outliers.

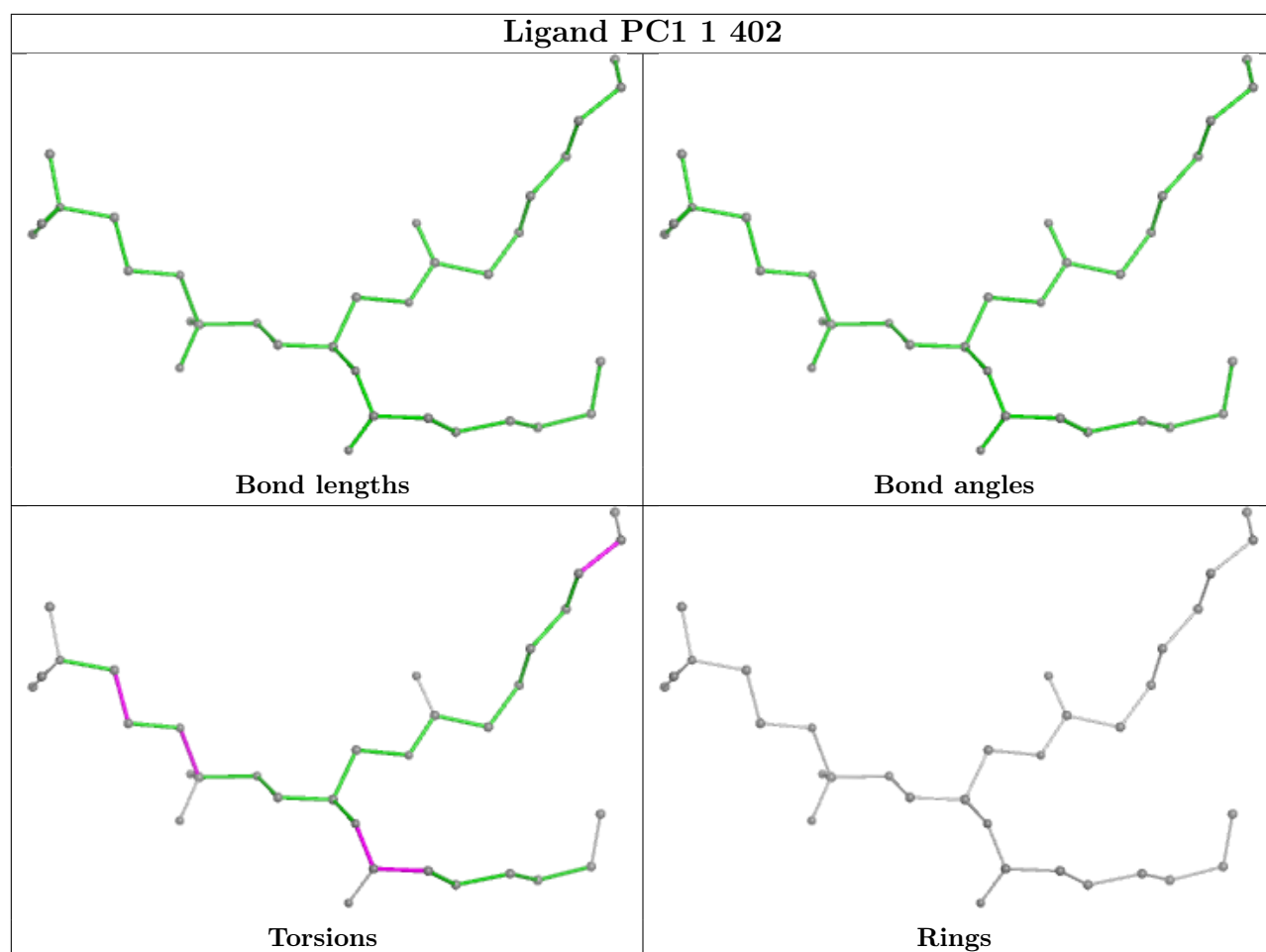
5 of 373 torsion outliers are listed below:

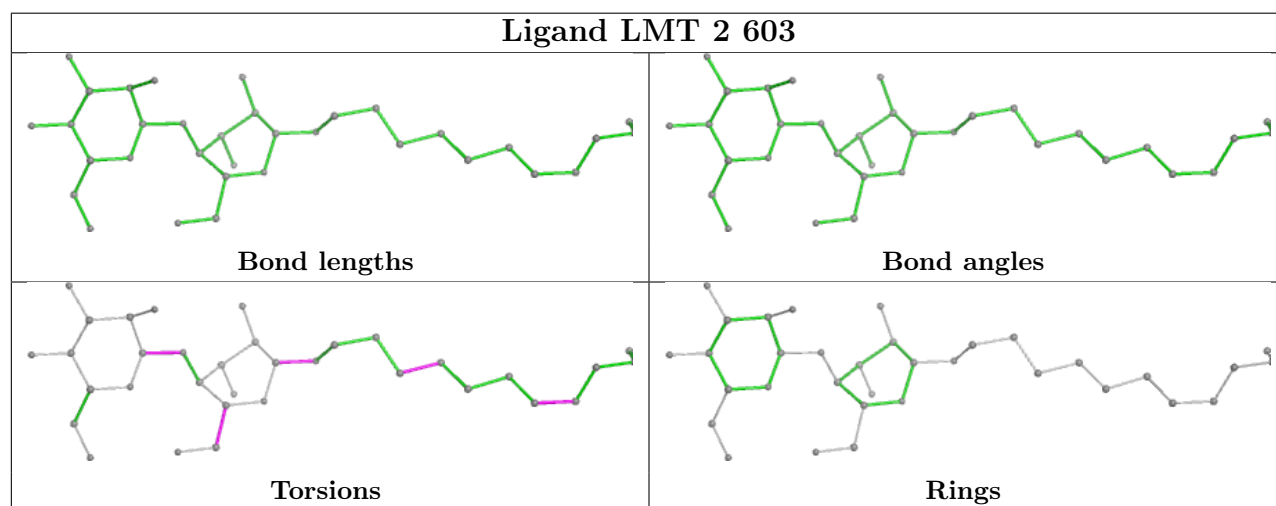
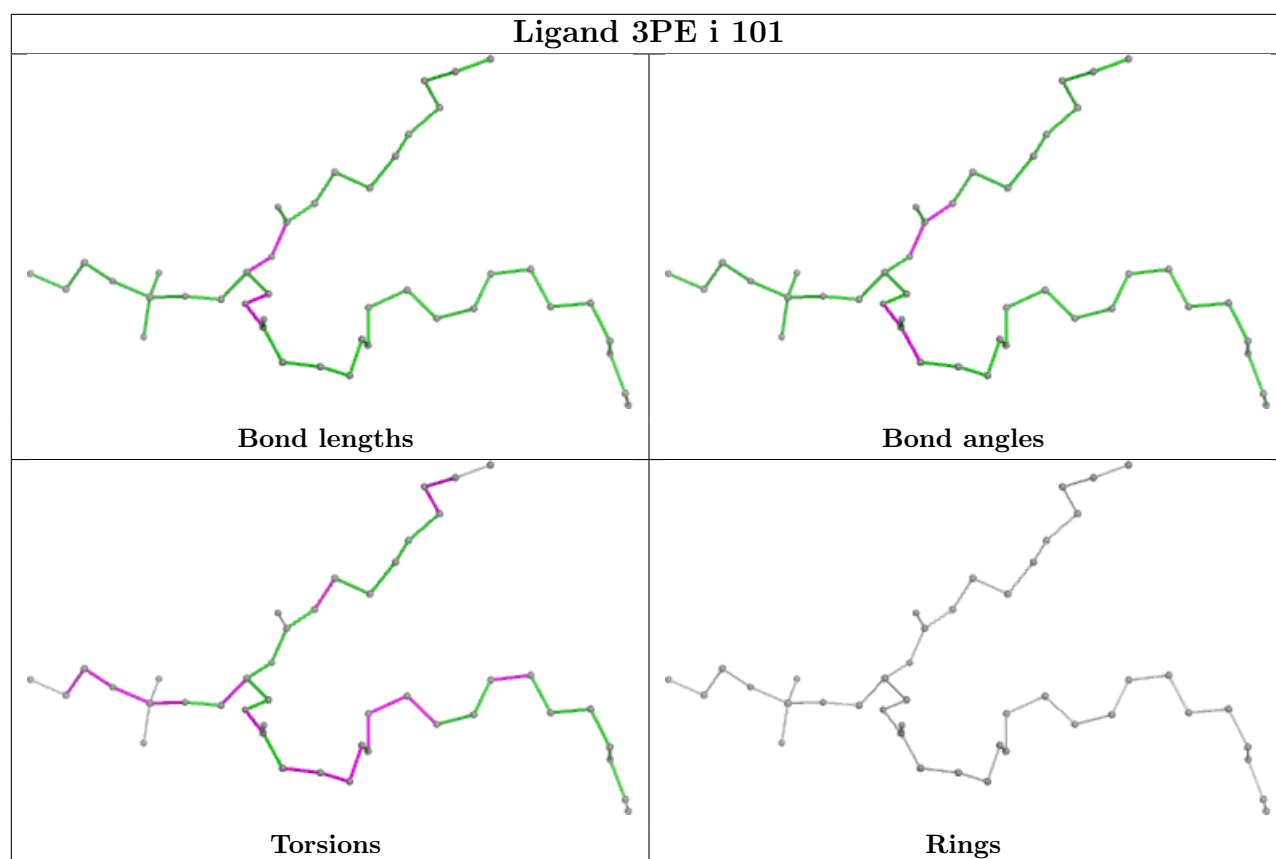
Mol	Chain	Res	Type	Atoms
27	1	401	3PE	C1-O11-P-O14
27	1	401	3PE	C11-O13-P-O12
27	5	701	3PE	O13-C11-C12-N
27	5	704	3PE	C1-O11-P-O14
27	5	704	3PE	C11-O13-P-O12

There are no ring outliers.

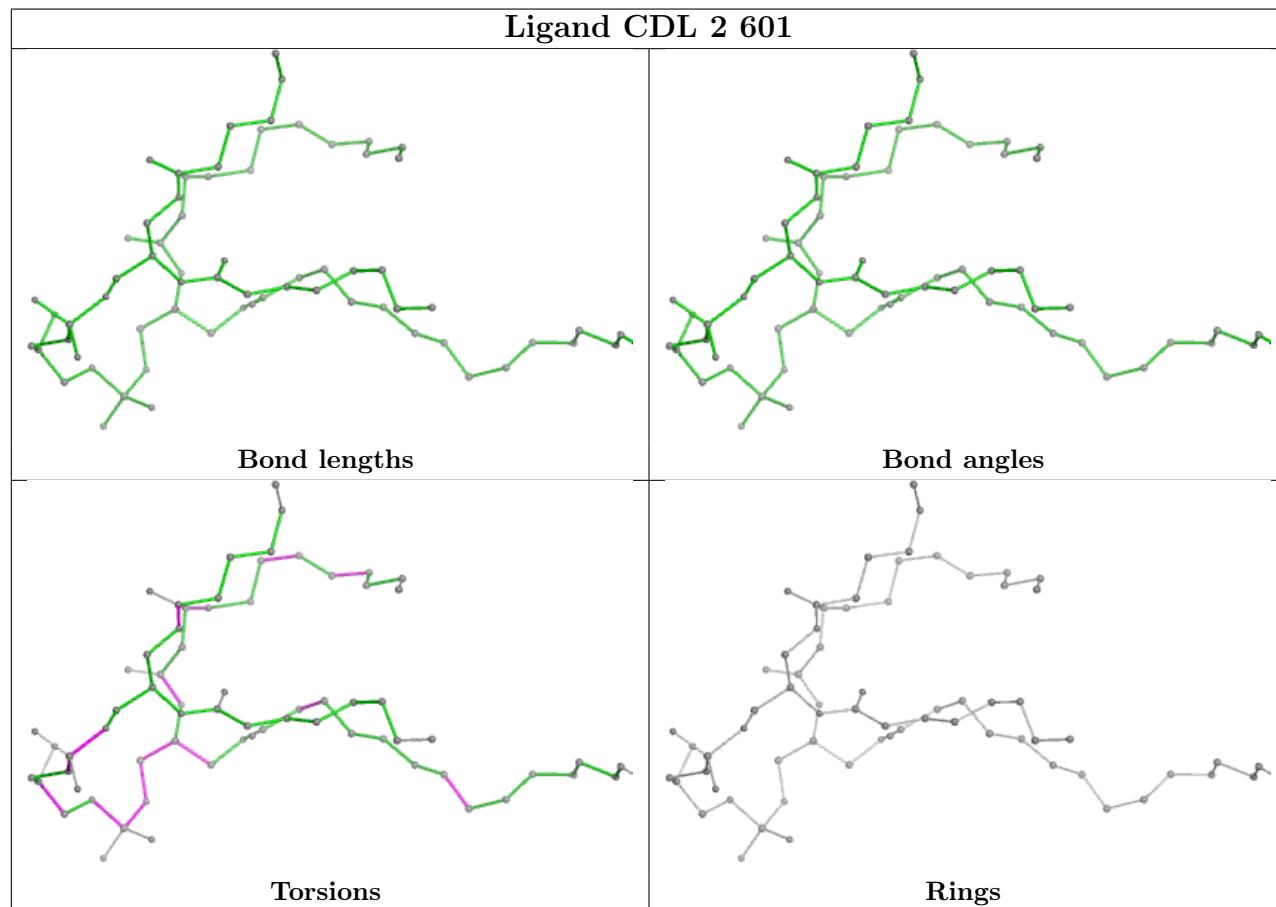
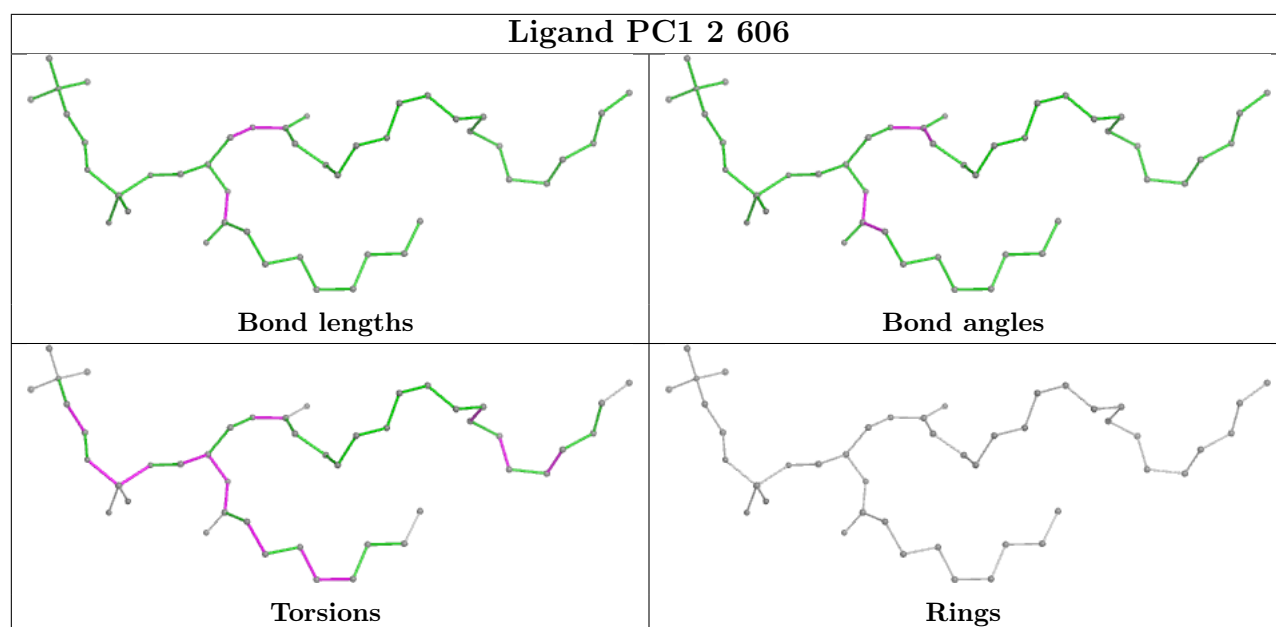
No monomer is involved in short contacts.

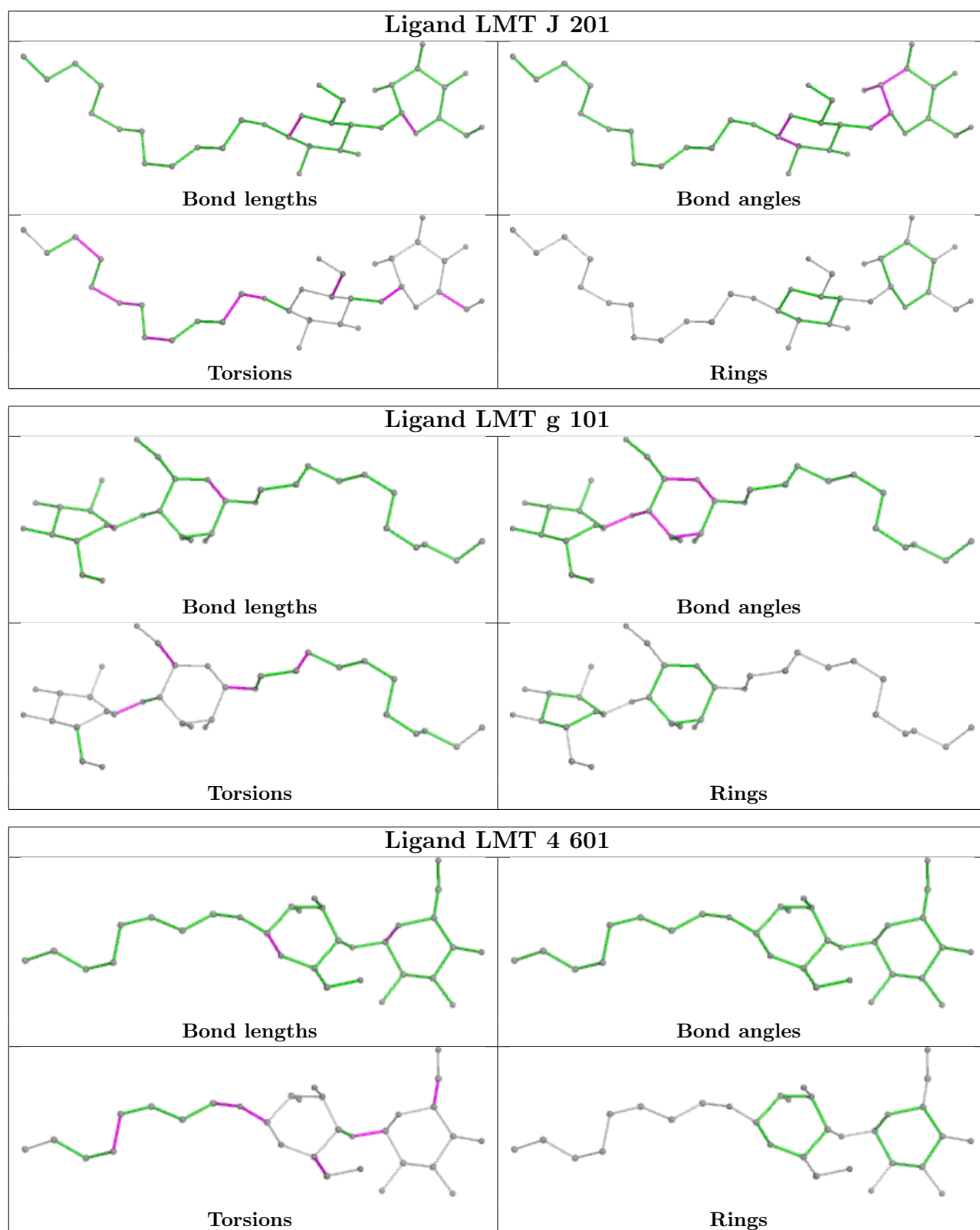
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

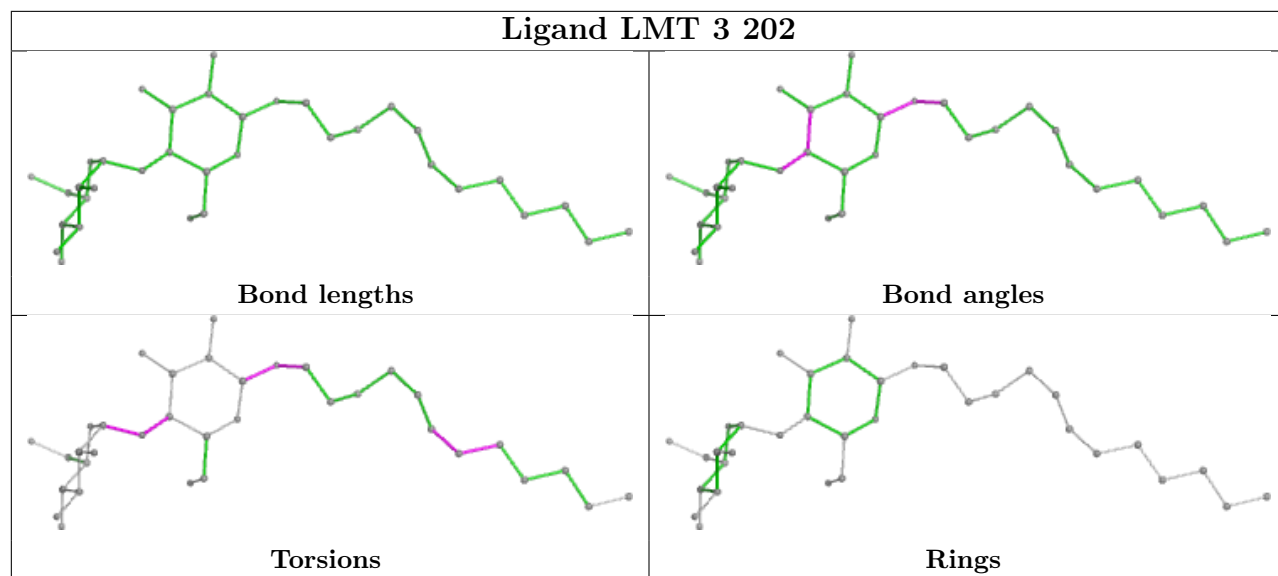


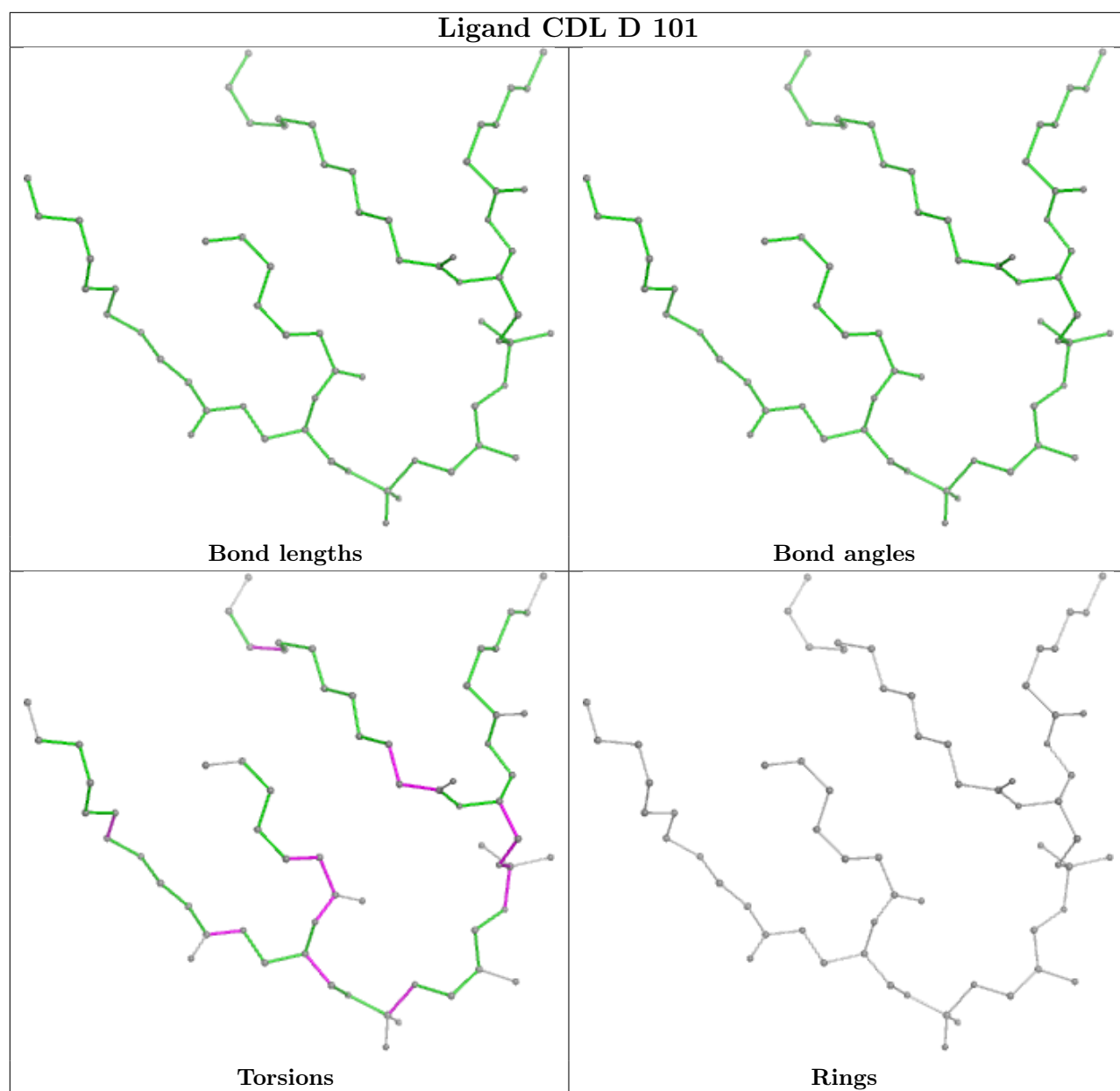


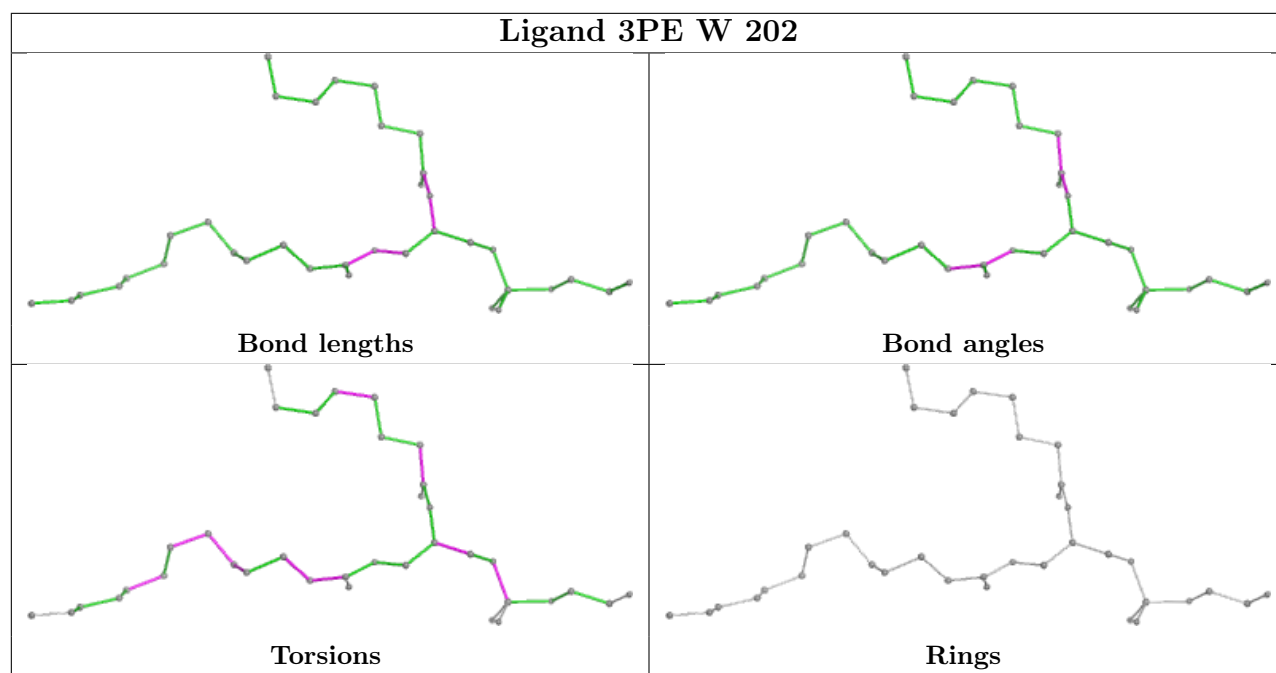
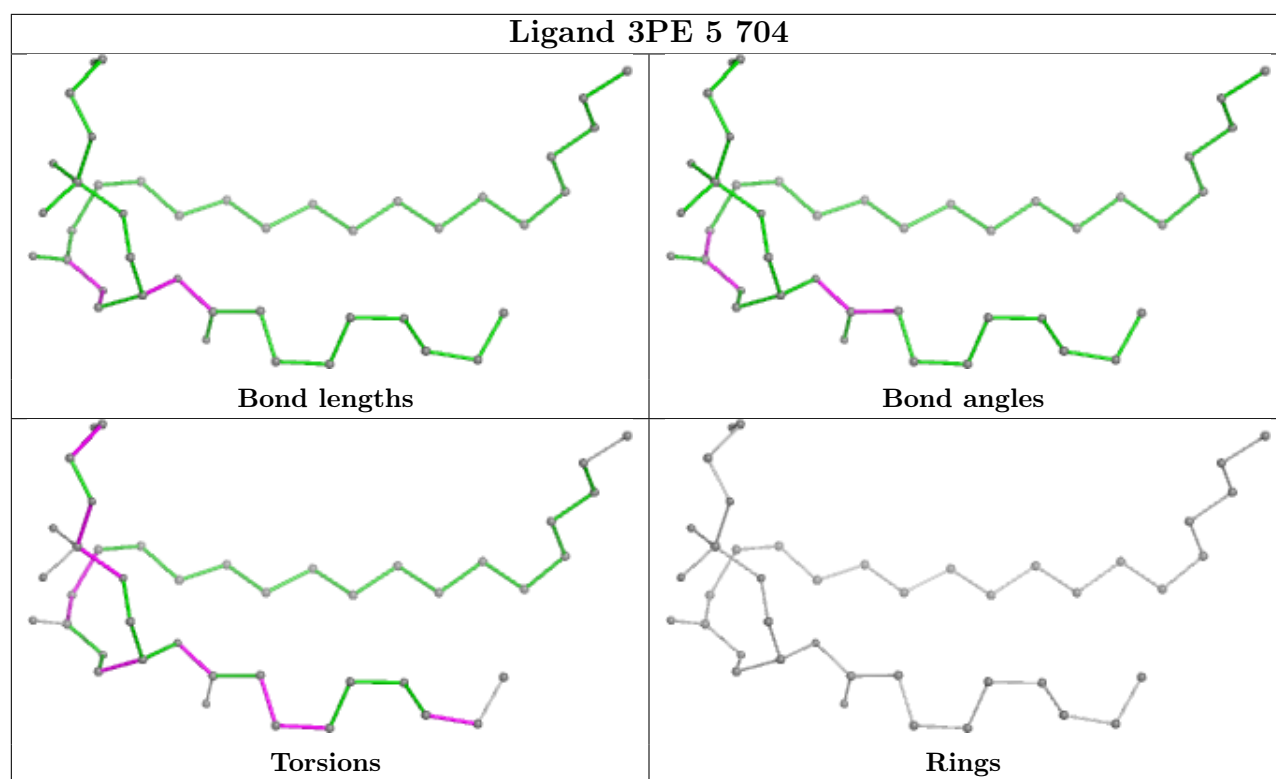


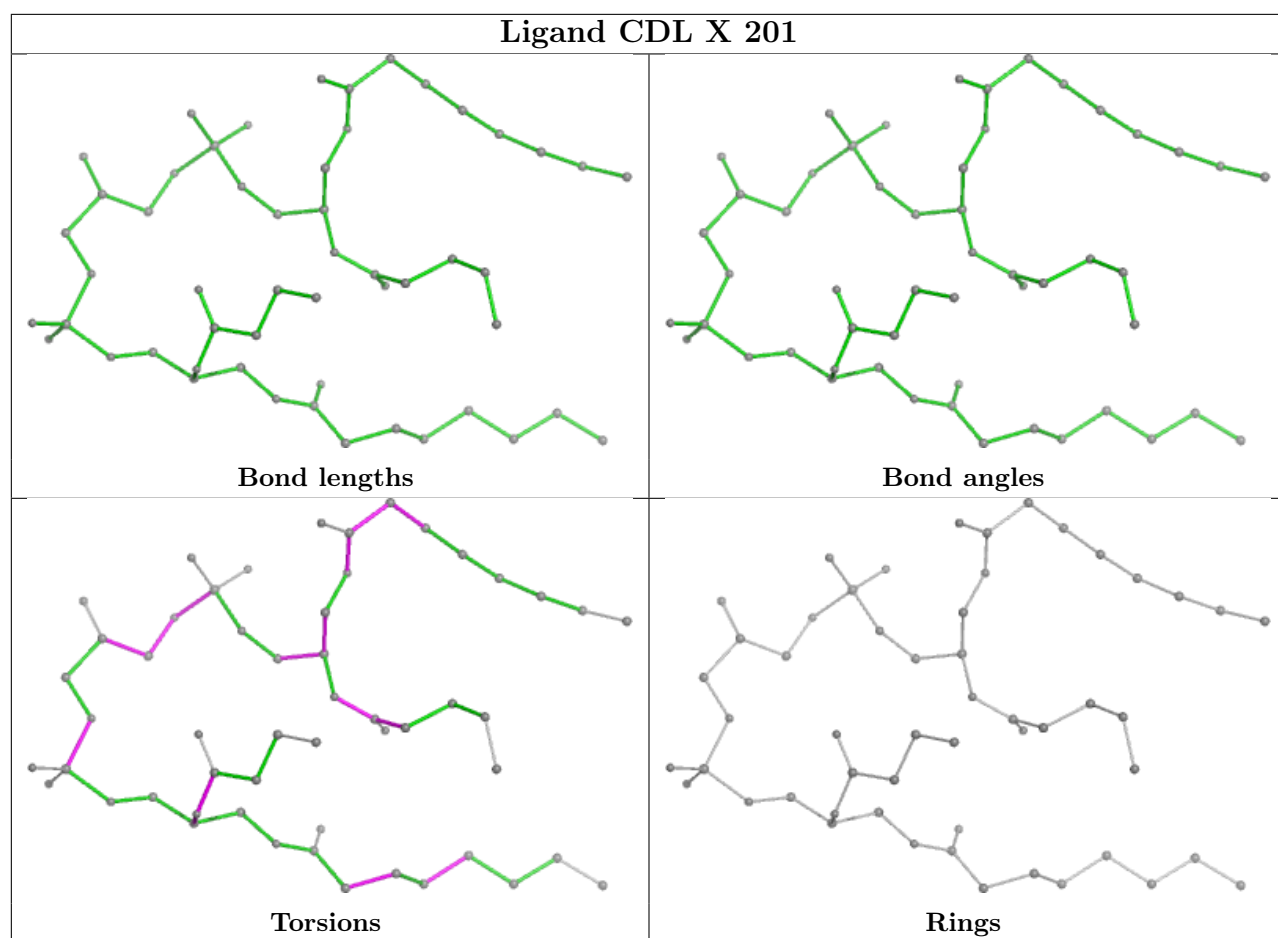




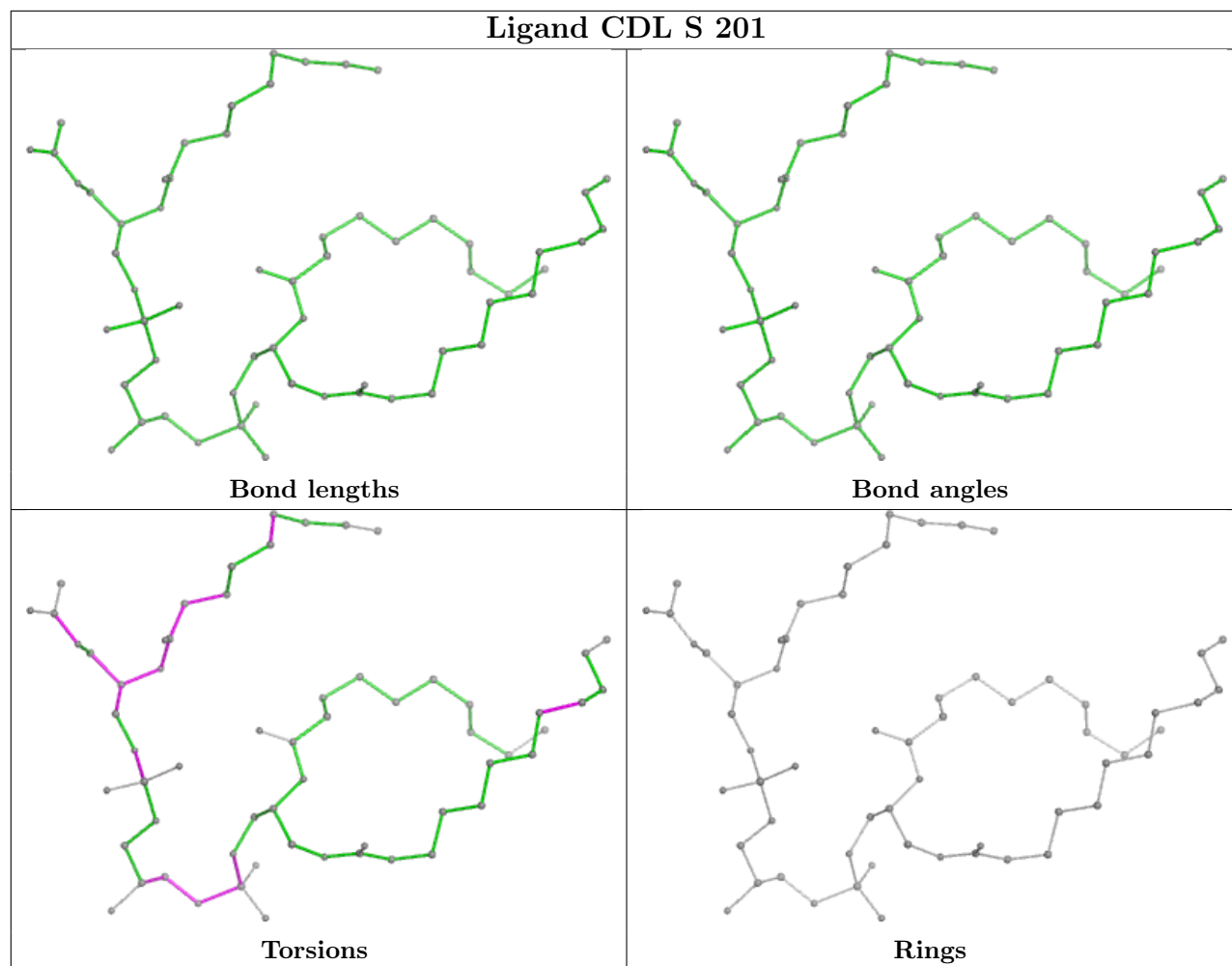




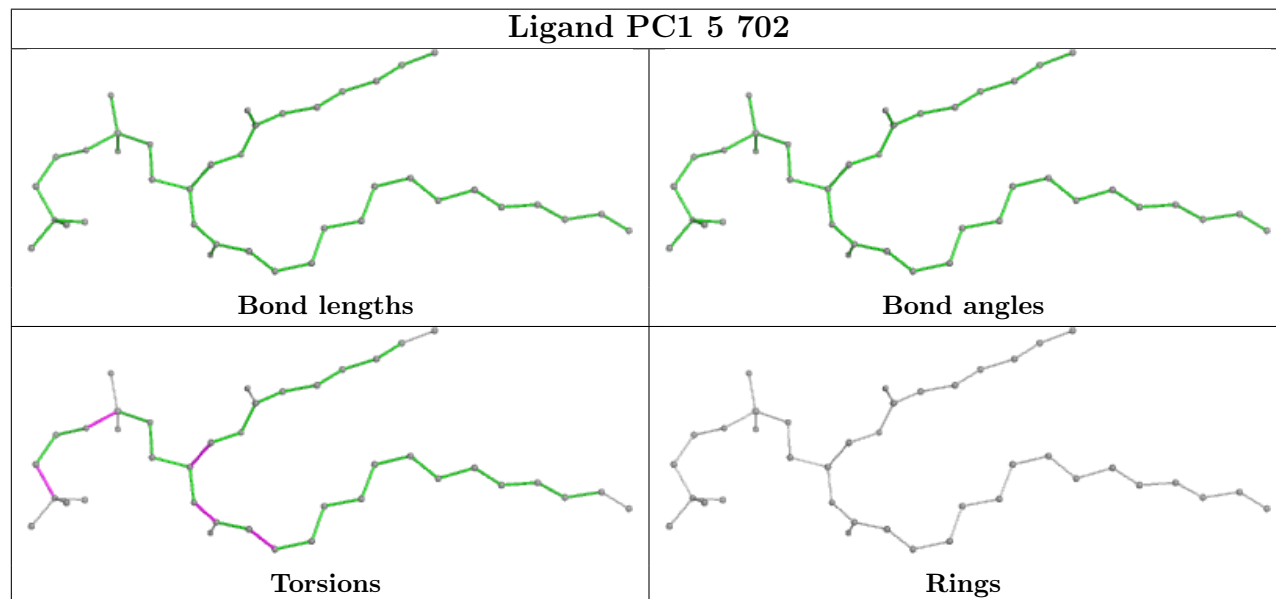


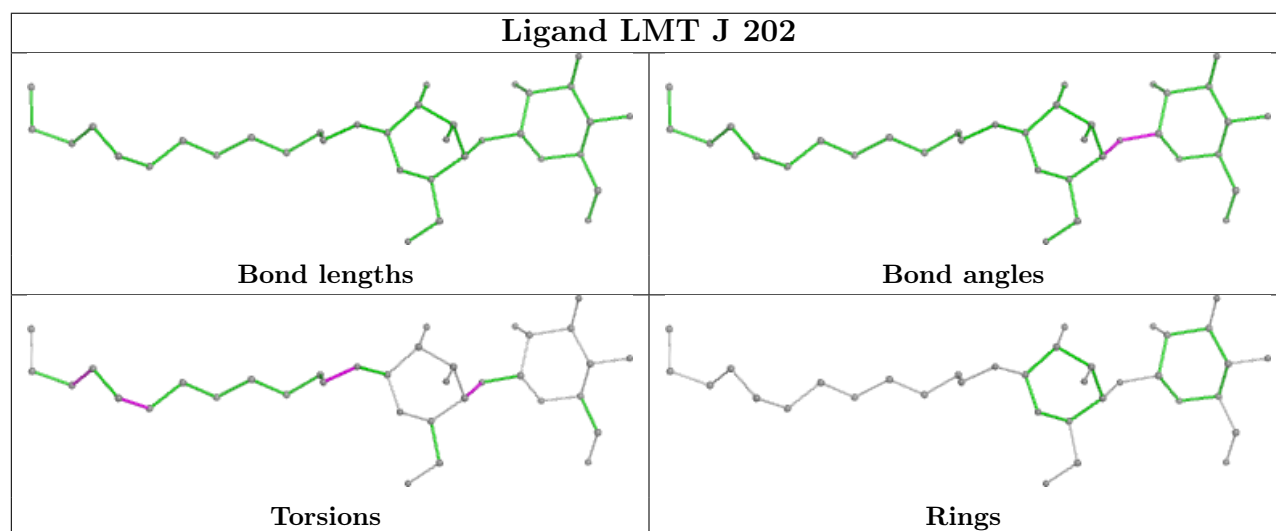
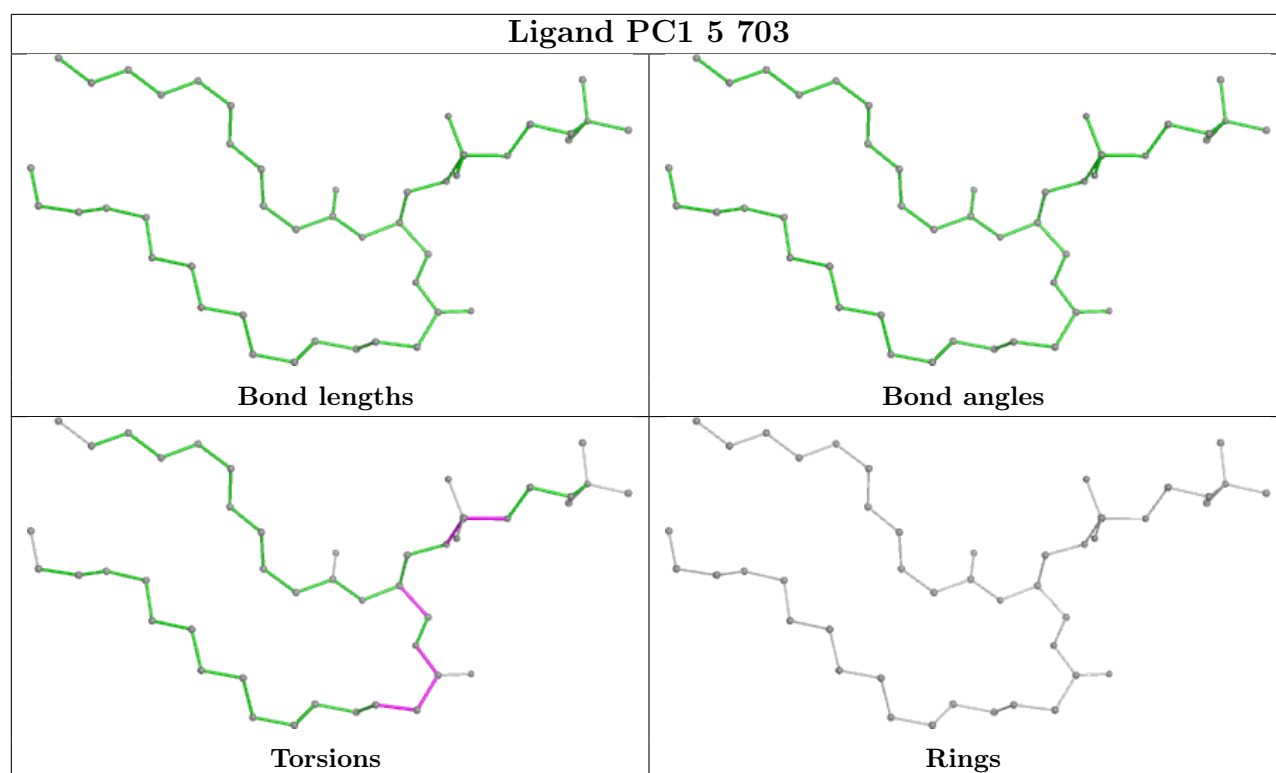


## Ligand CDL S 201

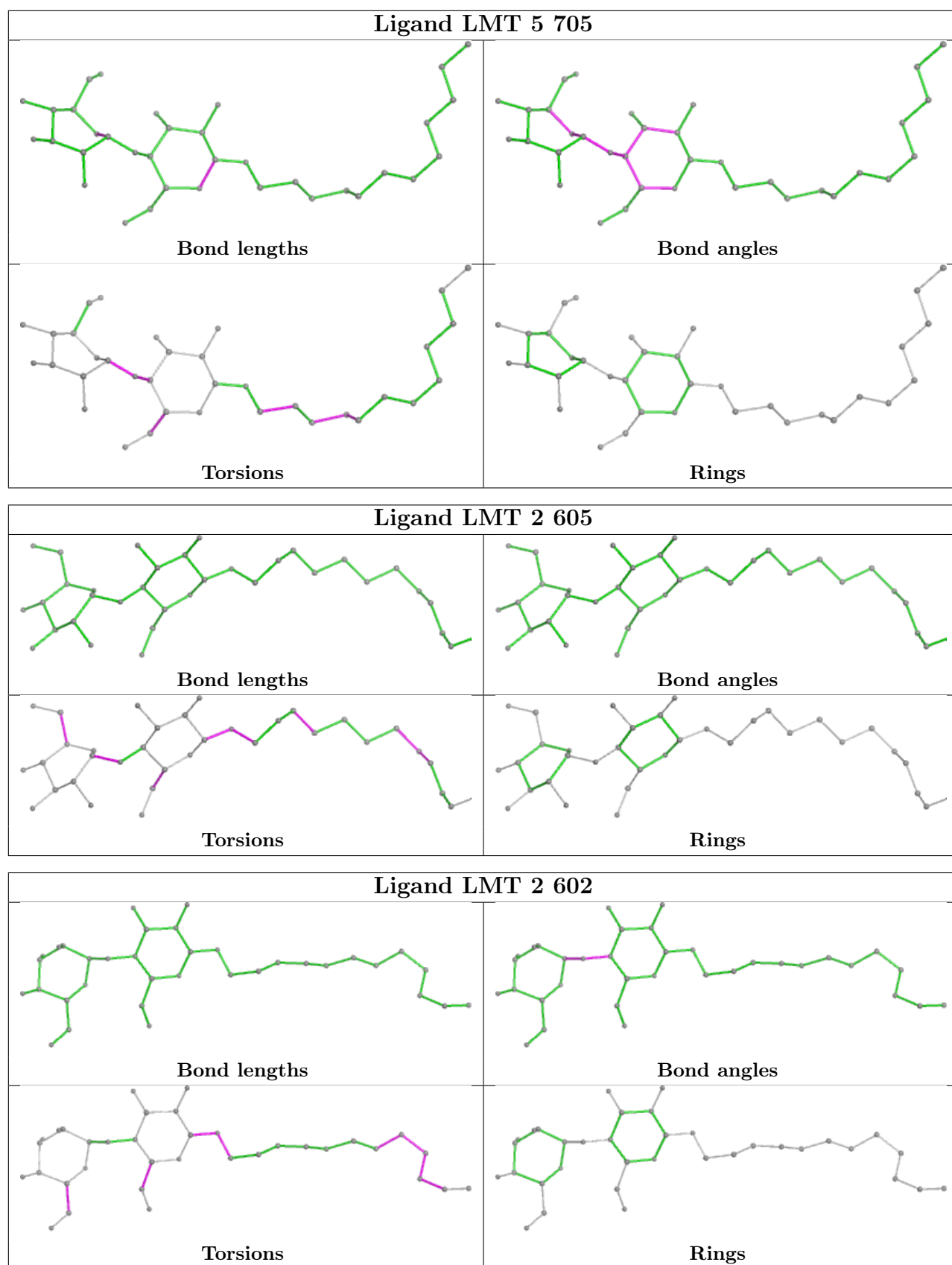


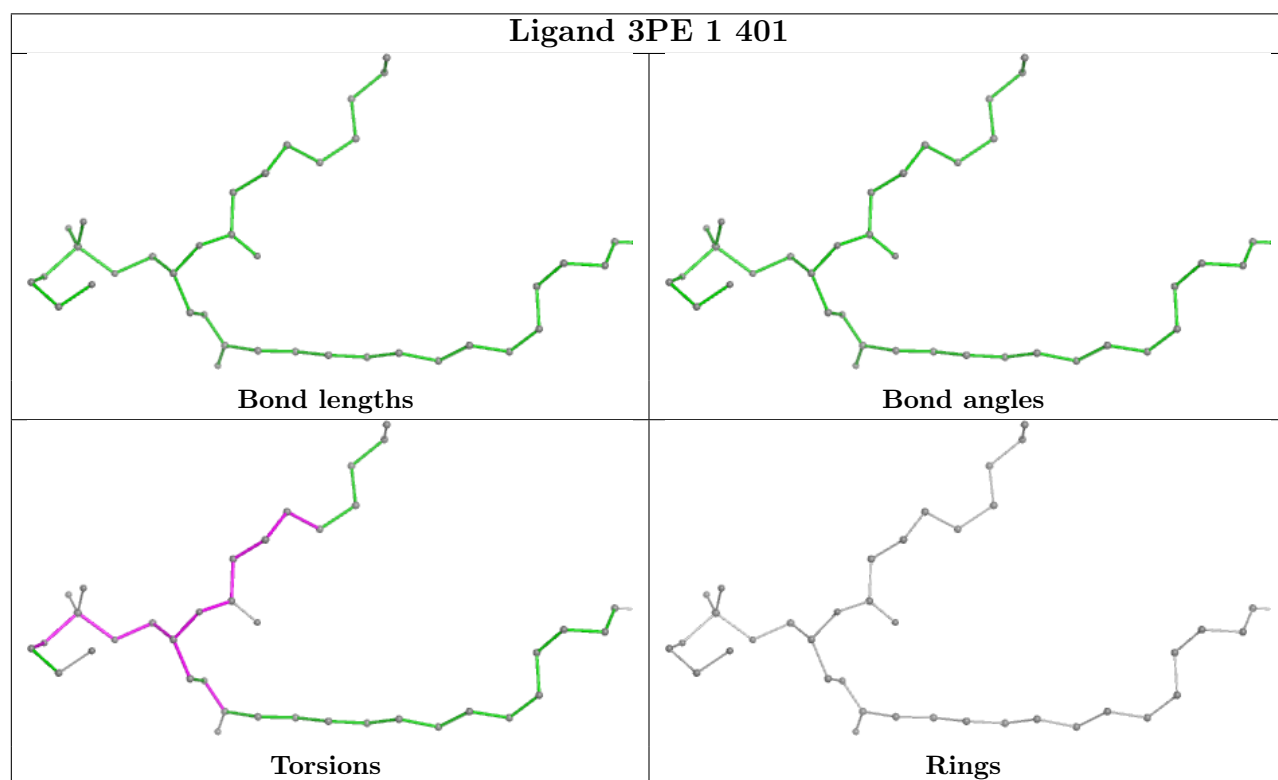
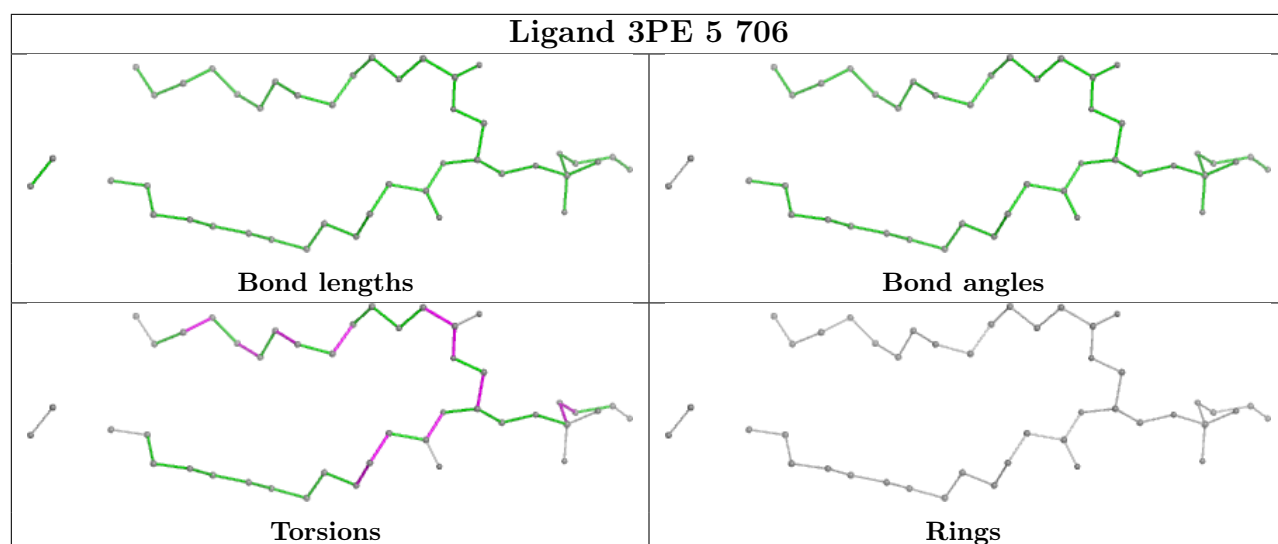
## Ligand PC1 5 702

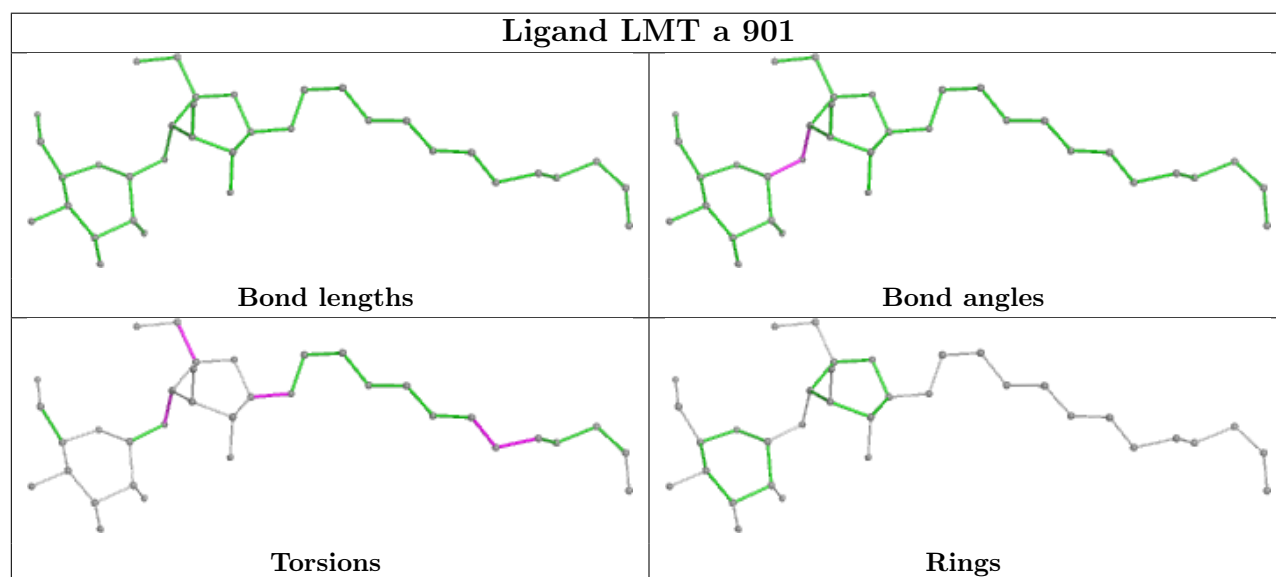
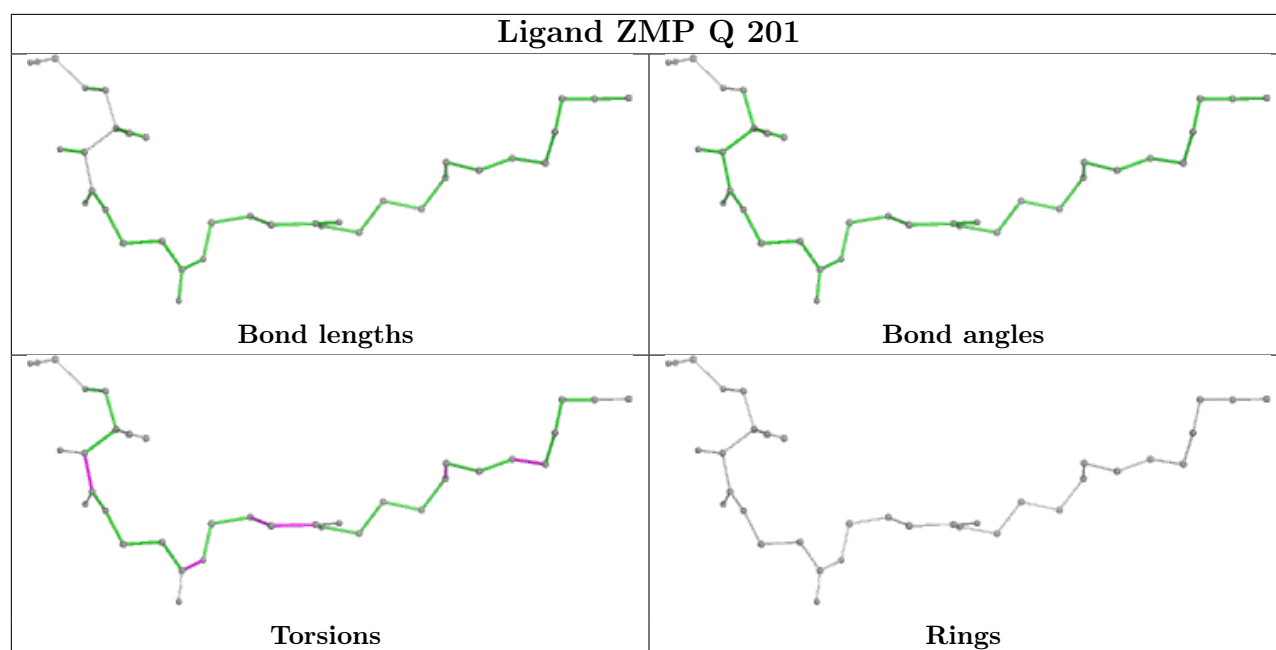


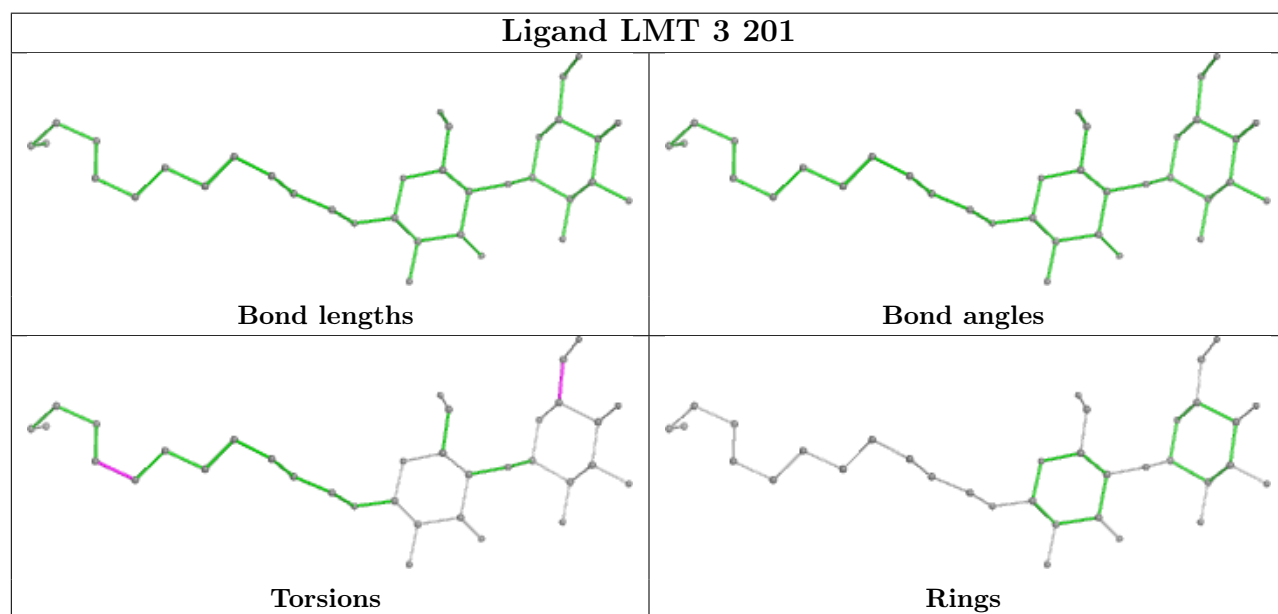
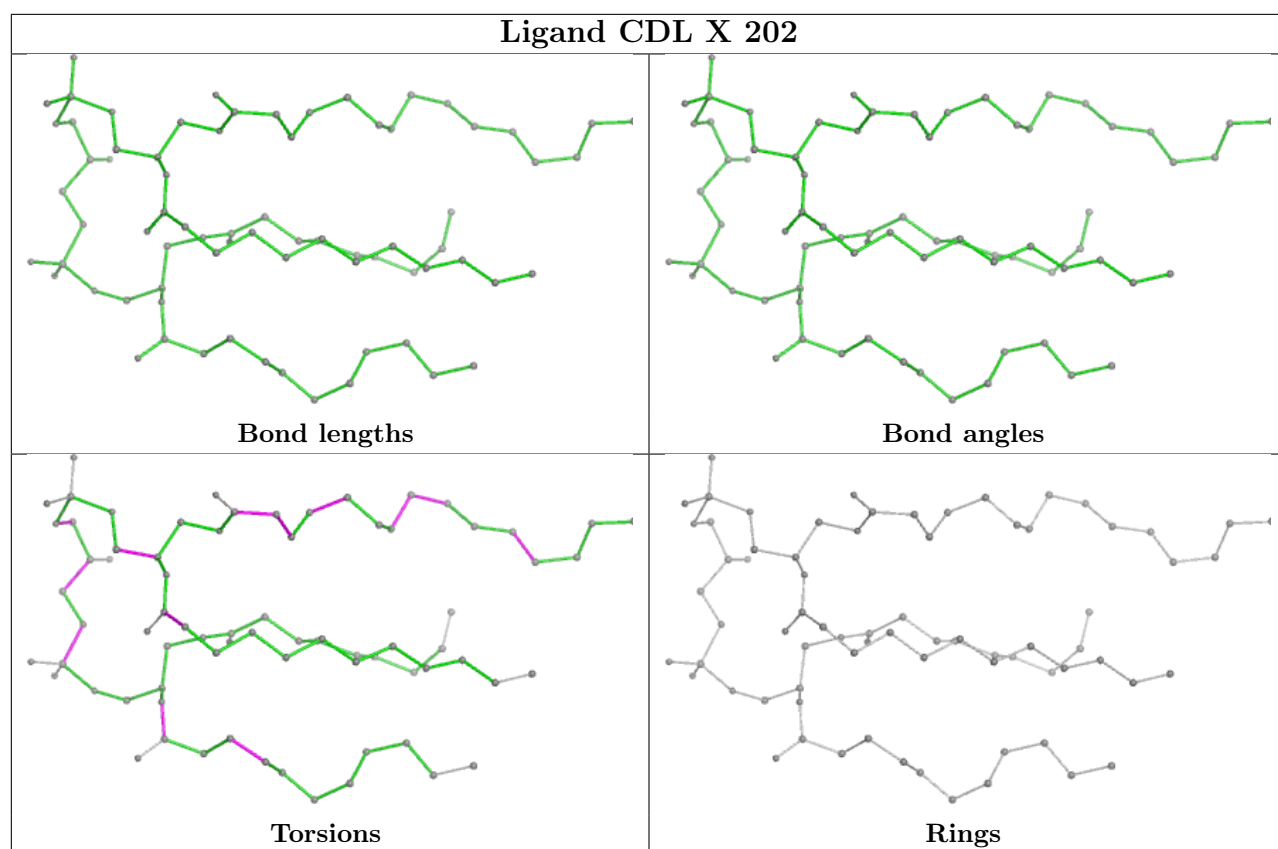


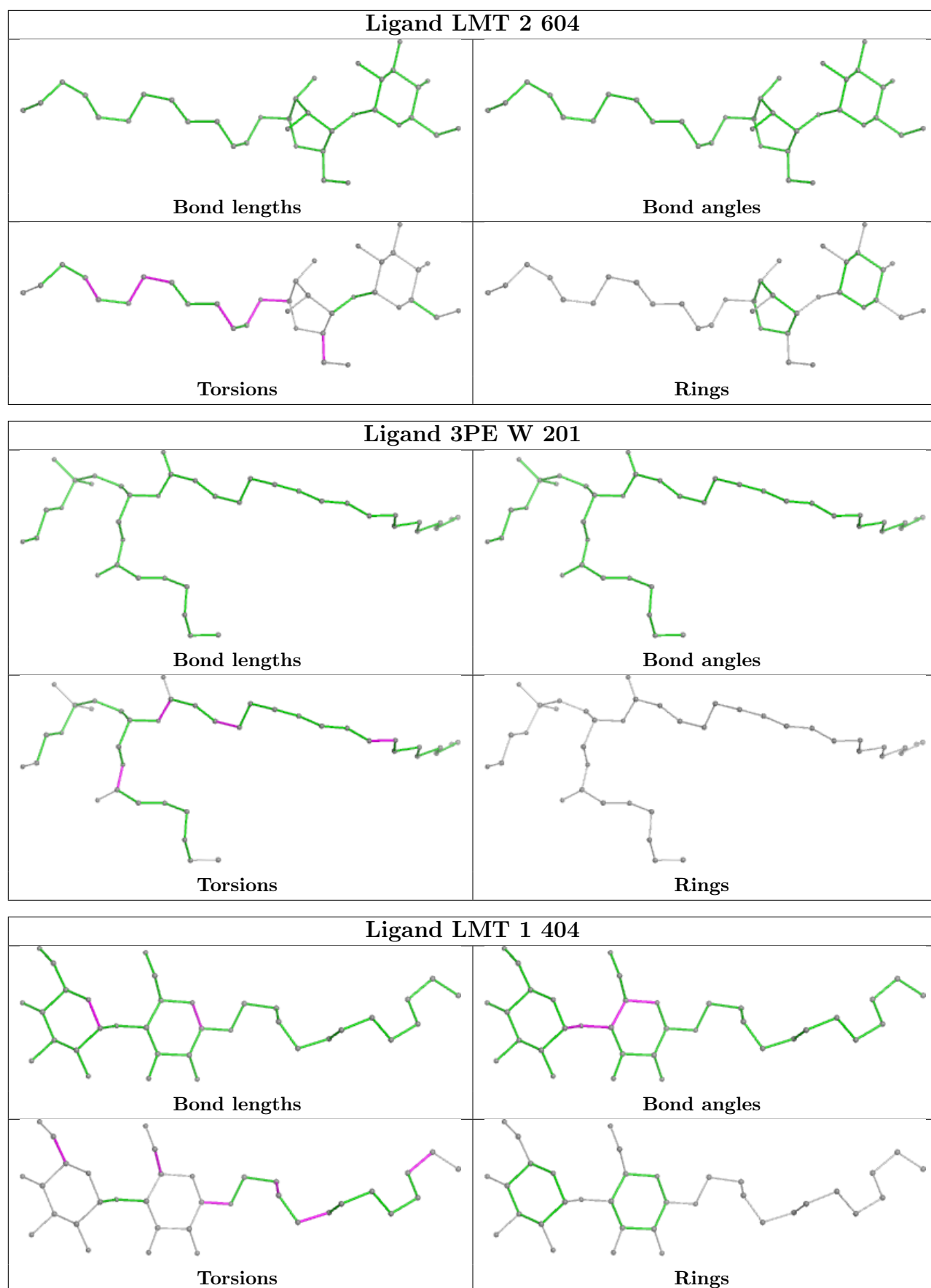


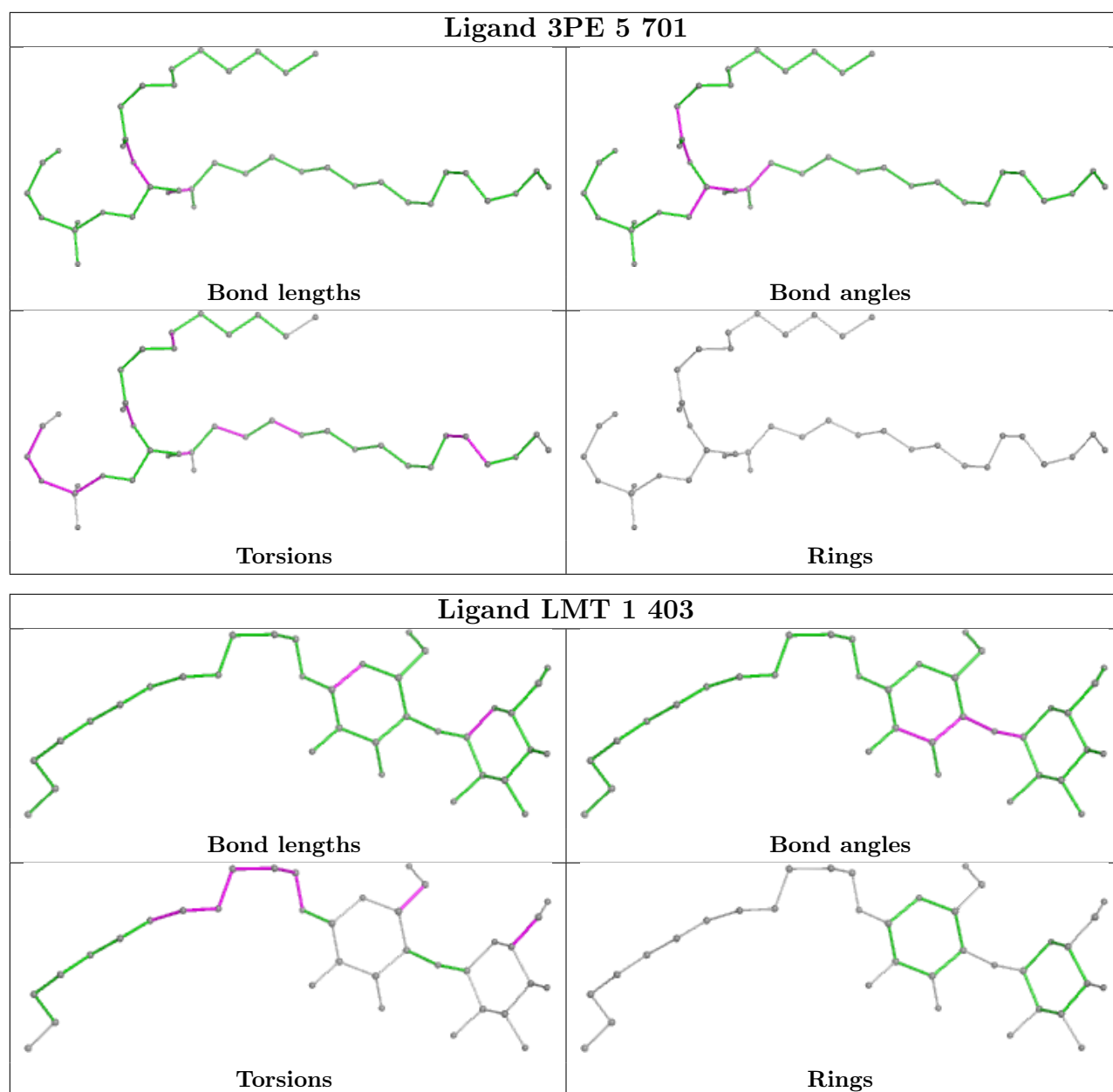












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

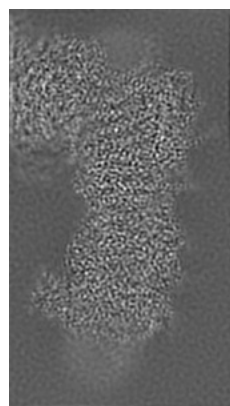
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14792. These allow visual inspection of the internal detail of the map and identification of artifacts.

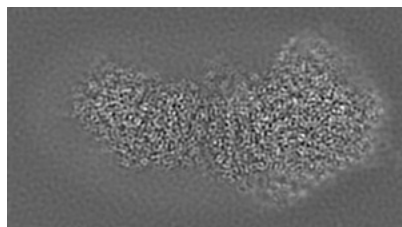
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

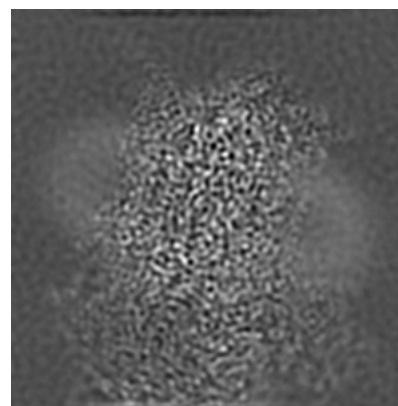
#### 6.1.1 Primary map



X

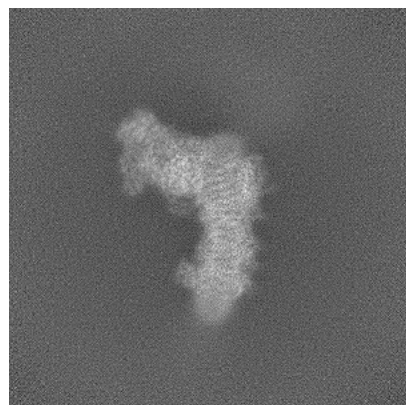


Y

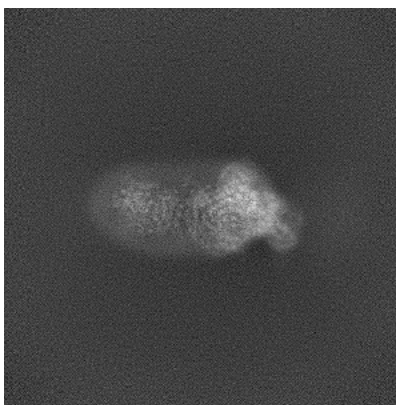


Z

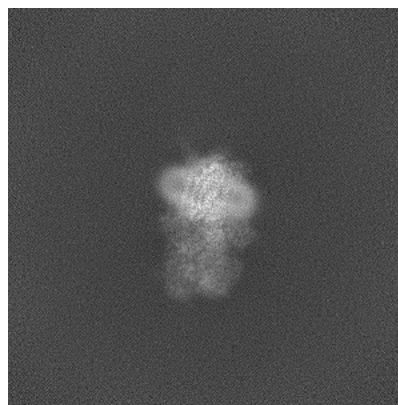
#### 6.1.2 Raw map



X



Y

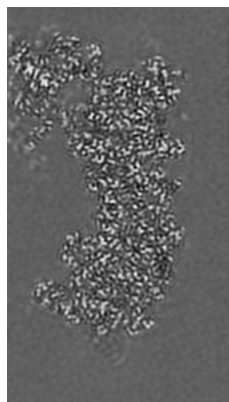


Z

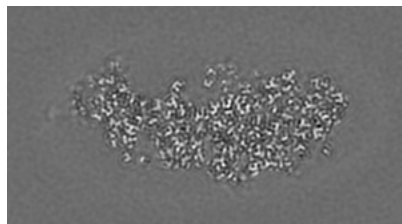
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

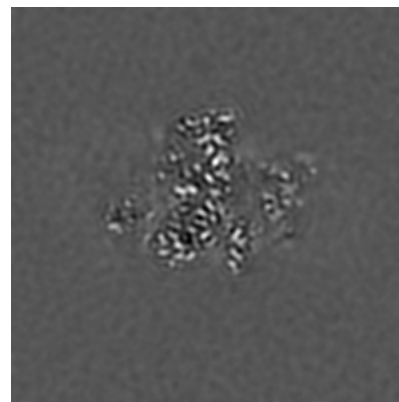
### 6.2.1 Primary map



X Index: 74

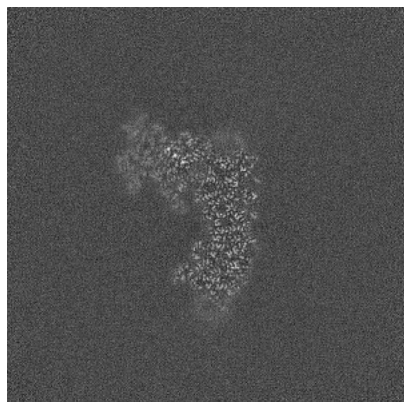


Y Index: 75

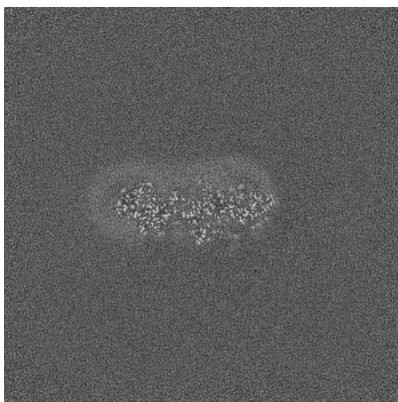


Z Index: 134

### 6.2.2 Raw map



X Index: 256



Y Index: 256



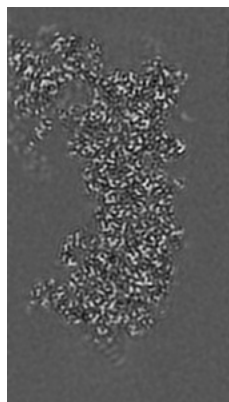
Z Index: 256

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

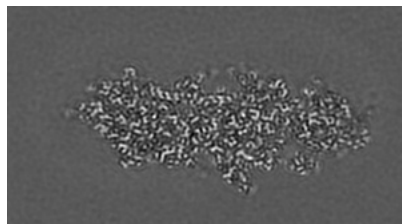


## 6.3 Largest variance slices [i](#)

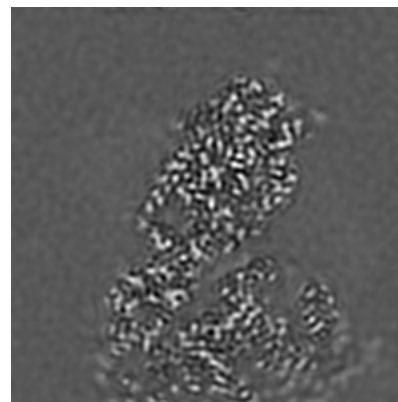
### 6.3.1 Primary map



X Index: 75

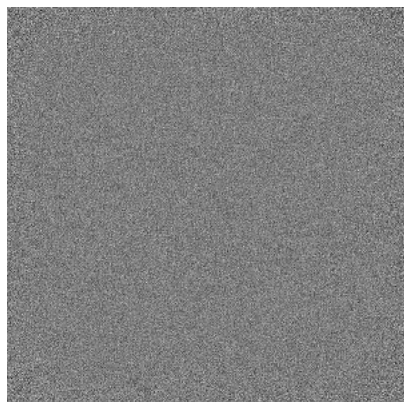


Y Index: 63

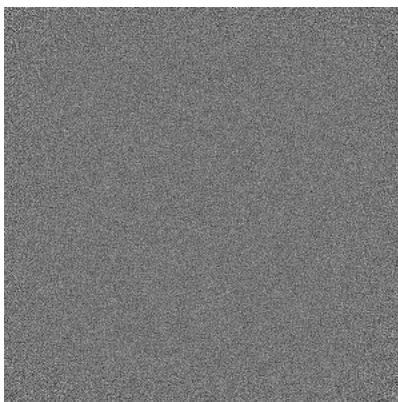


Z Index: 214

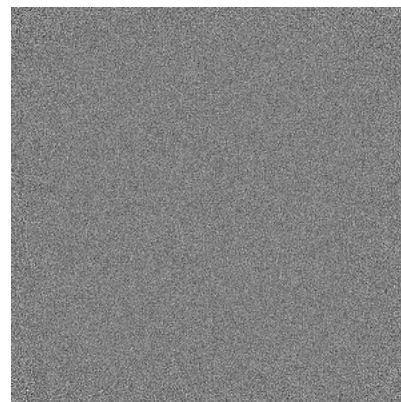
### 6.3.2 Raw map



X Index: 0



Y Index: 0

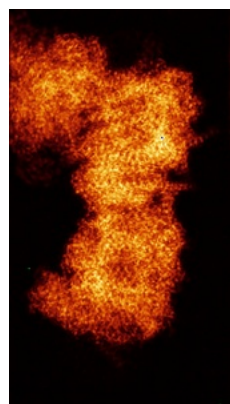


Z Index: 0

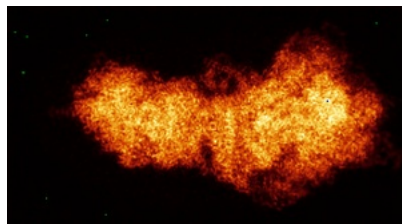
The images above show the largest variance slices of the map in three orthogonal directions.

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

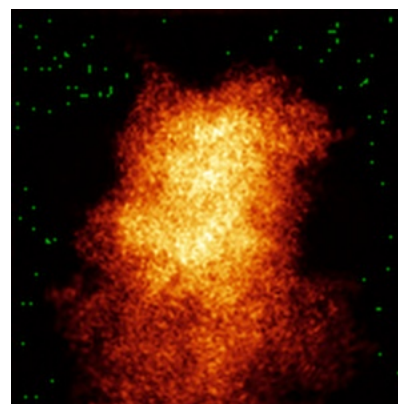
### 6.4.1 Primary map



X

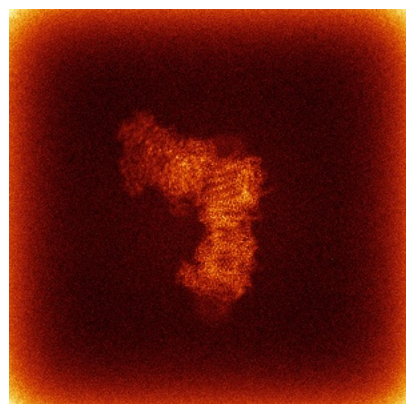


Y

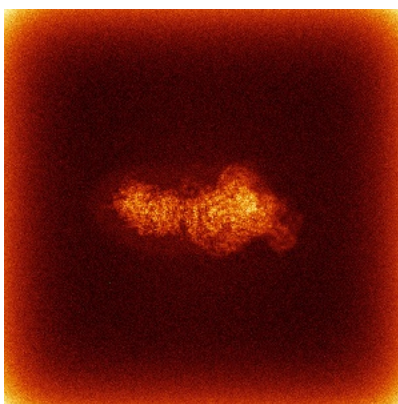


Z

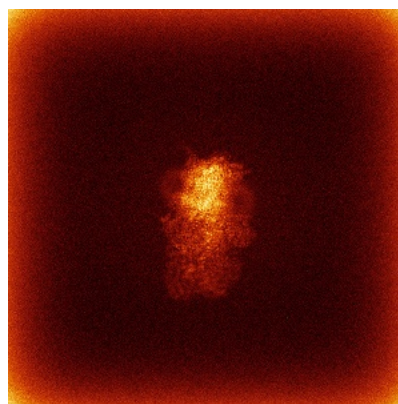
### 6.4.2 Raw map



X



Y

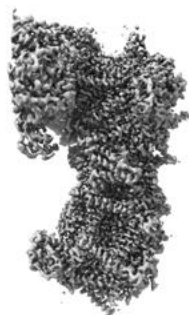


Z

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



X



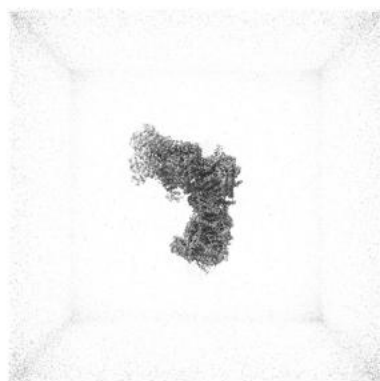
Y



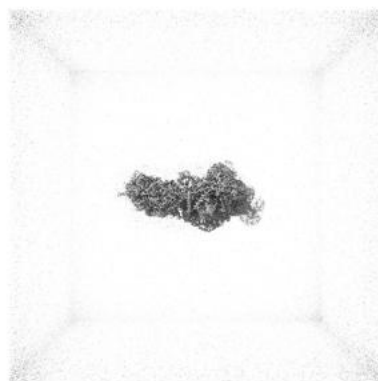
Z

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.

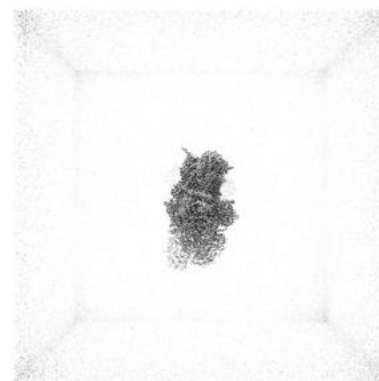
### 6.5.2 Raw map



X



Y



Z

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

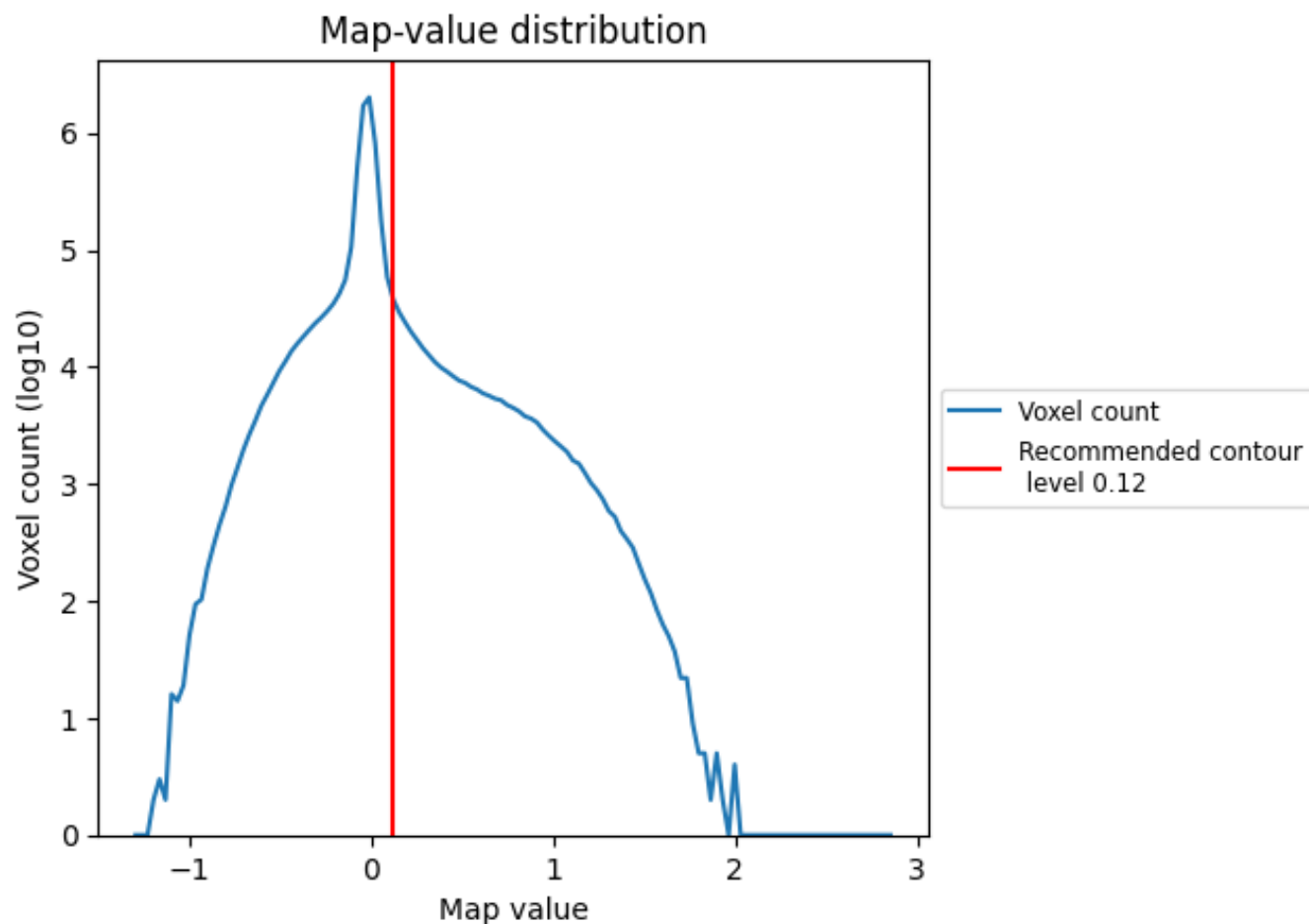
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

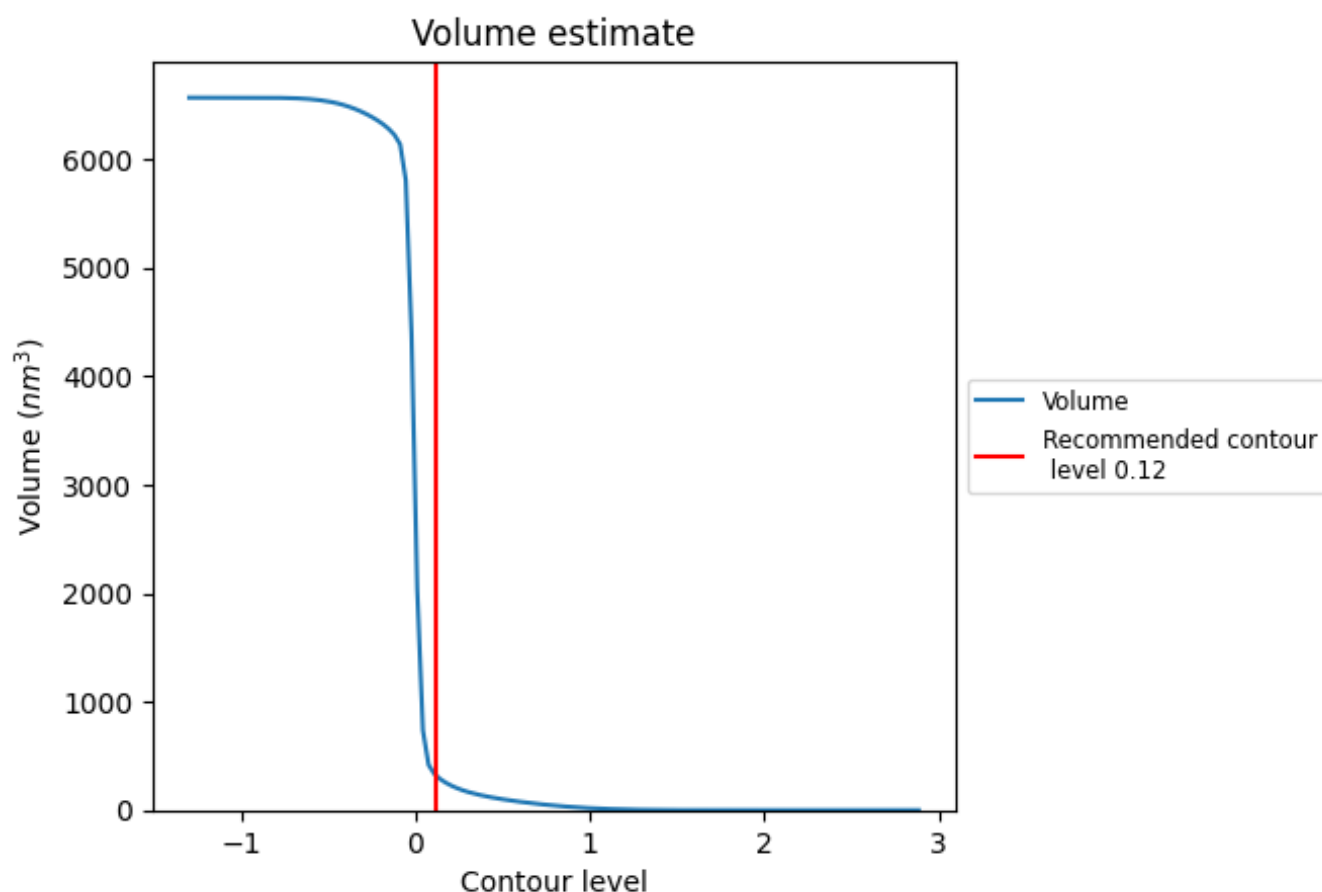
This section contains the results of statistical analysis of the map.

### 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 319 nm<sup>3</sup>; this corresponds to an approximate mass of 288 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

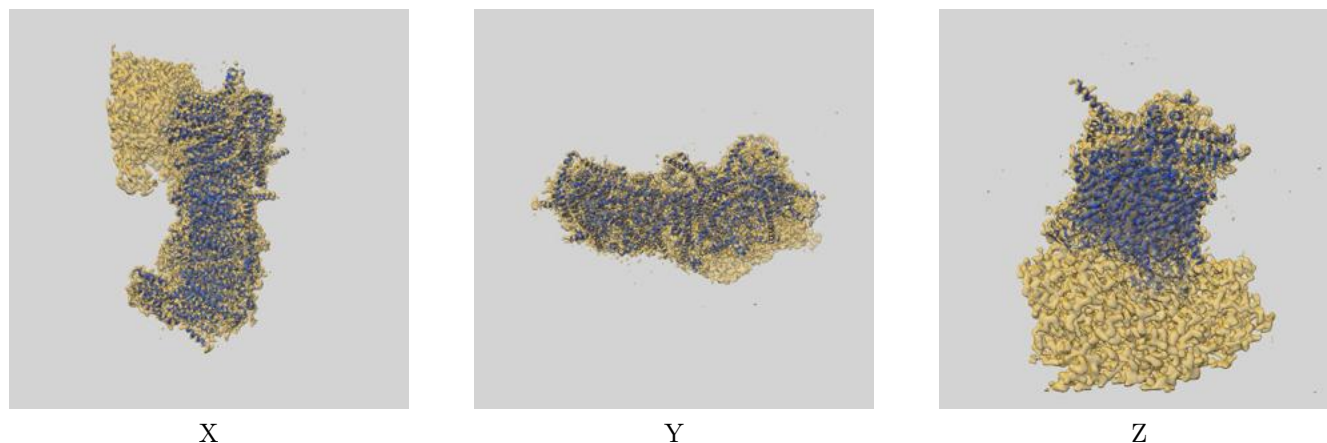
This section was not generated. No FSC curve or half-maps provided.



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

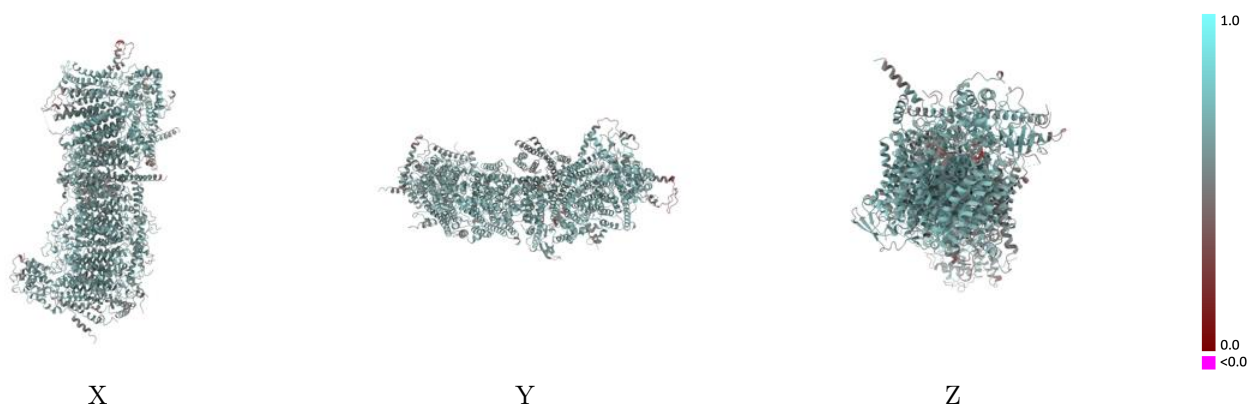
This section contains information regarding the fit between EMDB map EMD-14792 and PDB model 7ZM8. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

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



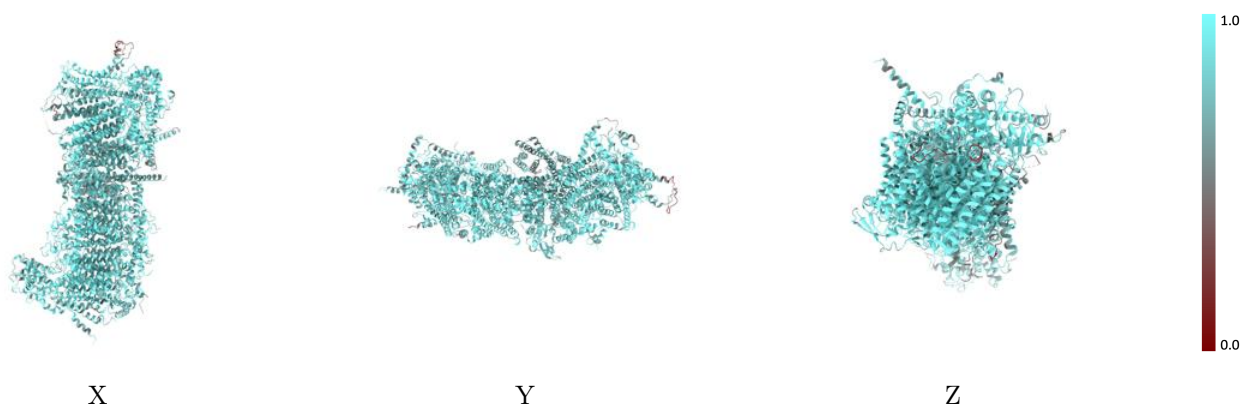
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

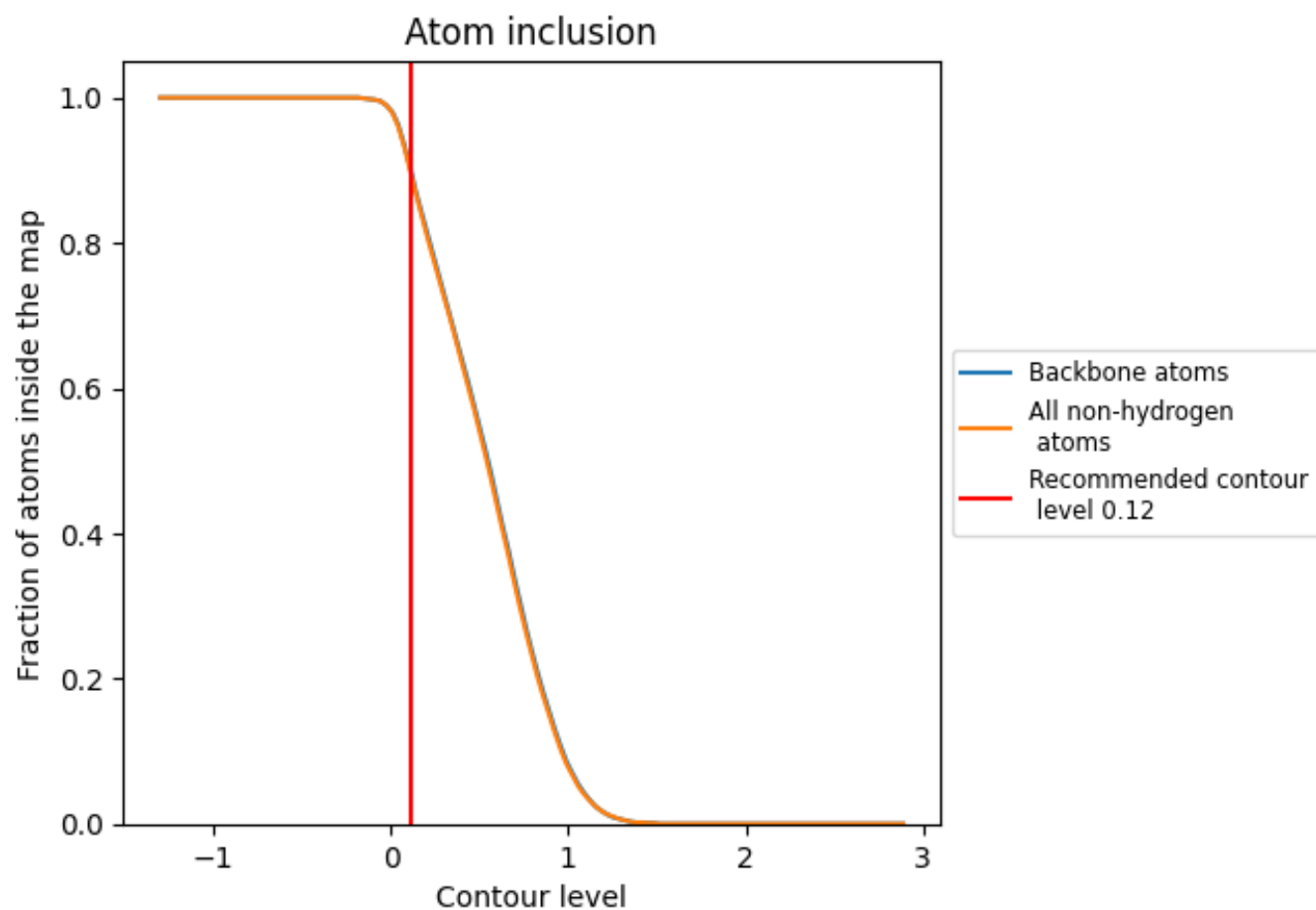
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 90% of all backbone atoms, 89% 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	 0.8900	 0.6040
1	 0.8440	 0.5810
2	 0.9370	 0.6370
3	 0.8260	 0.5680
4	 0.9600	 0.6430
5	 0.9220	 0.6160
6	 0.8880	 0.6040
8	 0.8320	 0.5480
9	 0.8420	 0.5700
D	 0.9250	 0.6300
J	 0.7420	 0.5350
L	 0.9430	 0.6260
Q	 0.8090	 0.5280
R	 0.8560	 0.5780
S	 0.9060	 0.5980
U	 0.9200	 0.6170
W	 0.8590	 0.6000
X	 0.9260	 0.6210
a	 0.8650	 0.5740
b	 0.8710	 0.6010
c	 0.8460	 0.5580
d	 0.9220	 0.6170
e	 0.8060	 0.5490
g	 0.8680	 0.5910
i	 0.8590	 0.5860
j	 0.9400	 0.6250
n	 0.8290	 0.5680

