



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:47 AM UTC

PDB ID : 6YNX / pdb_00006ynx
EMDB ID : EMD-10859
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- Fo-subcomplex
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 2.50 Å(reported)

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:

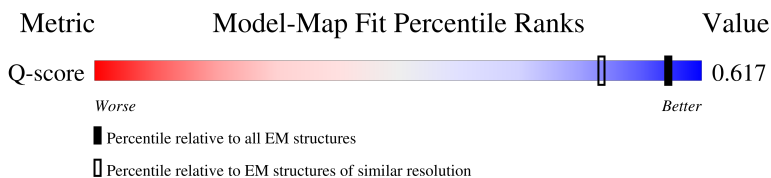
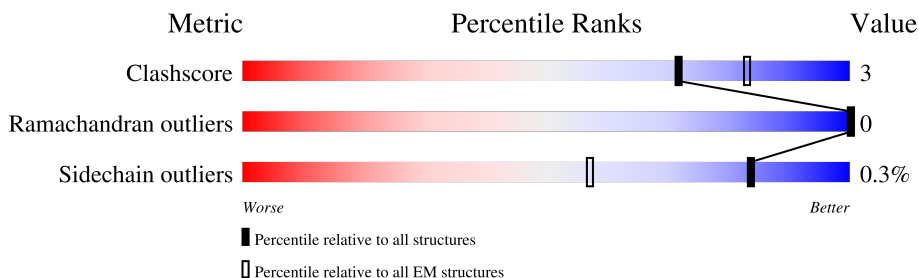
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 Å.

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









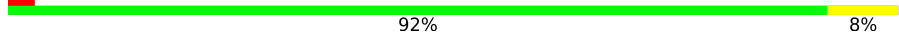
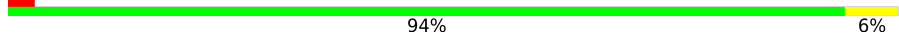
















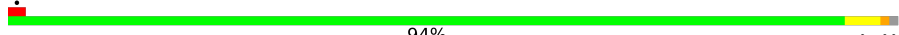
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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

Mol	Chain	Length	Quality of chain
1	A	446	87% 10% .
1	a	446	89% 8% .
2	B	381	36% 6% 58%
2	b	381	38% . 58%

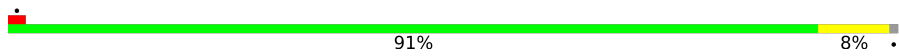


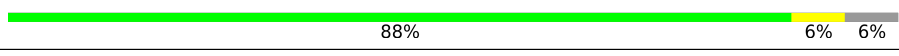
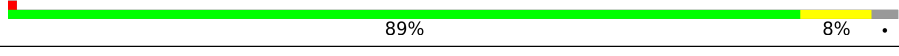



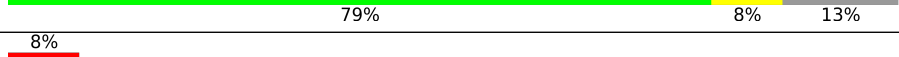
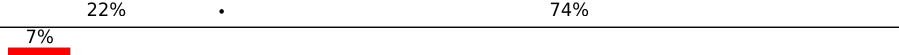

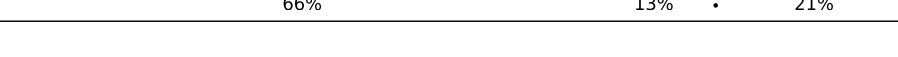
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Mol	Chain	Length	Quality of chain
3	D	234	 45% 53%
3	d	234	 44% 53%
4	F	204	 90% 8%
4	f	204	 89% 8%
5	I	209	 90% 10%
5	i	209	 89% 11%
6	K	179	 92% 8%
6	k	179	 94% 6%
7	C	100	 85% 11%
7	c	100	 84% 12%
8	G	286	 82% 7% 10%
8	g	286	 83% 7% 10%
9	H	268	 82% 5% 14%
9	h	268	 81% 5% 14%
10	J	273	 93% 5%
10	j	273	 93% 5%
11	L	247	 89% 11%
11	l	247	 90% 10%
12	M	221	 90% 10%
12	m	221	 90% 10%
13	N	179	 61% 5% 34%
13	n	179	 63% 34%
14	O	154	 62% 36%
14	o	154	 61% 36%
15	P	152	 94%

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Mol	Chain	Length	Quality of chain
15	p	152	 91% 8%
16	Q	152	 64% 7% 29%
16	q	152	 65% 6% 29%
17	R	149	 88% 6% 6%
17	r	149	 89% 8%
18	S	145	 70% 27%
18	s	145	 61% 11% 28%
19	E	480	 77% 10% 13%
19	e	480	 79% 8% 13%
20	i1	108	 8% 22% 74%
20	i2	108	 7% 25% 5% 70%
21	t	460	 66% 13% 21%

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 139915 atoms, of which 70075 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 subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	a	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	b	161	Total	C	H	N	O	S	0	0
			2678	903	1310	223	232	10		
2	B	161	Total	C	H	N	O	S	0	0
			2675	903	1307	223	232	10		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	d	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		
3	D	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	i	209	Total 3461	C 1121	H 1741	N 304	O 285	S 10	0	0
5	I	209	Total 3461	C 1121	H 1741	N 304	O 285	S 10	0	0

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	k	179	Total 2903	C 939	H 1430	N 257	O 266	S 11	0	0
6	K	179	Total 2903	C 939	H 1430	N 257	O 266	S 11	0	0

- Molecule 7 is a protein called subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	c	96	Total 1671	C 565	H 830	N 131	O 143	S 2	0	0
7	C	96	Total 1671	C 565	H 830	N 131	O 143	S 2	0	0

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	g	256	Total 4338	C 1474	H 2118	N 348	O 388	S 10	0	0
8	G	256	Total 4338	C 1474	H 2118	N 348	O 388	S 10	0	0

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	h	231	Total 3836	C 1236	H 1883	N 361	O 350	S 6	0	0
9	H	231	Total 3836	C 1236	H 1883	N 361	O 350	S 6	0	0

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	j	269	Total 4346	C 1381	H 2147	N 406	O 404	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	269	Total	C	H	N	O	S	0	0
			4344	1381	2145	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	I	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		

- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	s	105	Total	C	H	N	O	S	0	0
			1714	552	849	148	160	5		
18	S	106	Total	C	H	N	O	S	0	0
			1728	556	856	149	162	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

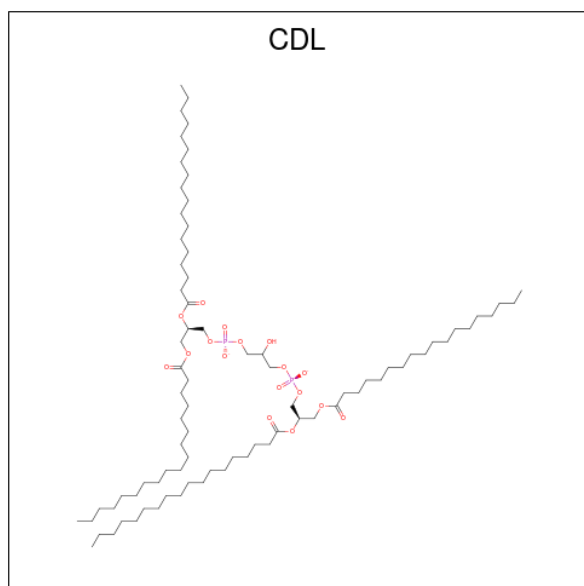
- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	H	N			O
20	i1	28	Total	C	H	N	O	0	0
			474	154	236	39	45		
20	i2	32	Total	C	H	N	O	0	0
			529	171	262	45	51		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	t	365	5889	1925	2876	533	544	11	0	0

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



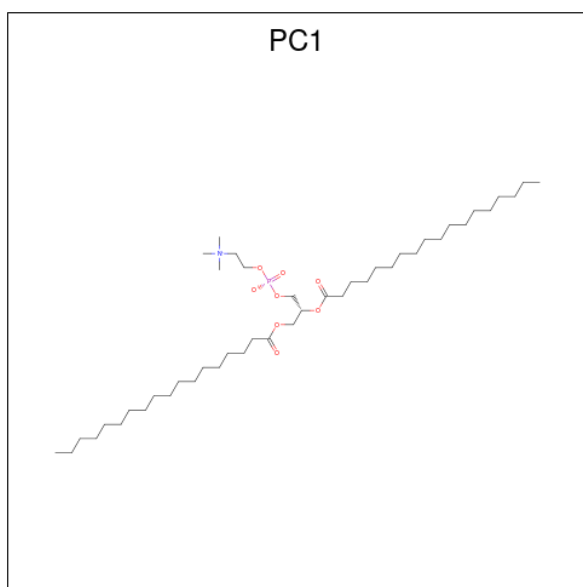
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
22	a	1	256	81	156	17	2	0
22	b	1	256	81	156	17	2	0
22	b	1	256	81	156	17	2	0
22	f	1	256	81	156	17	2	0
22	f	1	256	81	156	17	2	0
22	f	1	256	81	156	17	2	0
22	i	1	256	81	156	17	2	0
22	k	1	256	81	156	17	2	0
22	k	1	256	81	156	17	2	0
22	k	1	256	81	156	17	2	0
22	j	1	256	81	156	17	2	0

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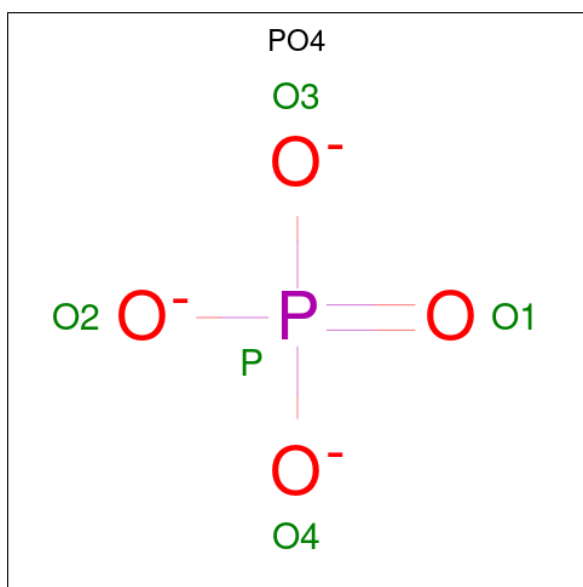
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
22	j	1	256	81	156	17	2	0
22	l	1	256	81	156	17	2	0
22	l	1	256	81	156	17	2	0
22	p	1	256	81	156	17	2	0
22	r	1	256	81	156	17	2	0
22	A	1	256	81	156	17	2	0
22	B	1	256	81	156	17	2	0
22	B	1	256	81	156	17	2	0
22	B	1	256	81	156	17	2	0
22	B	1	256	81	156	17	2	0
22	B	1	256	81	156	17	2	0
22	I	1	256	81	156	17	2	0
22	I	1	256	81	156	17	2	0
22	K	1	256	81	156	17	2	0
22	K	1	256	81	156	17	2	0
22	J	1	256	81	156	17	2	0
22	J	1	256	81	156	17	2	0
22	L	1	256	81	156	17	2	0
22	P	1	256	81	156	17	2	0

- Molecule 23 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



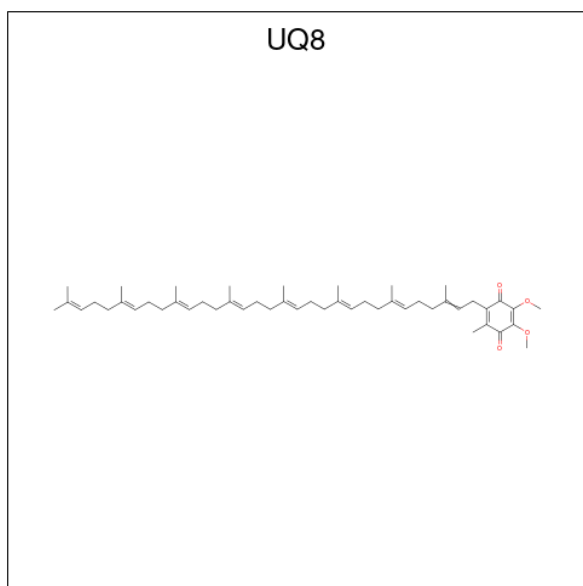
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
23	d	1	142	44	88	1	8	1	0
23	i	1	142	44	88	1	8	1	0
23	g	1	142	44	88	1	8	1	0
23	D	1	142	44	88	1	8	1	0
23	G	1	142	44	88	1	8	1	0
23	G	1	142	44	88	1	8	1	0

- Molecule 24 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



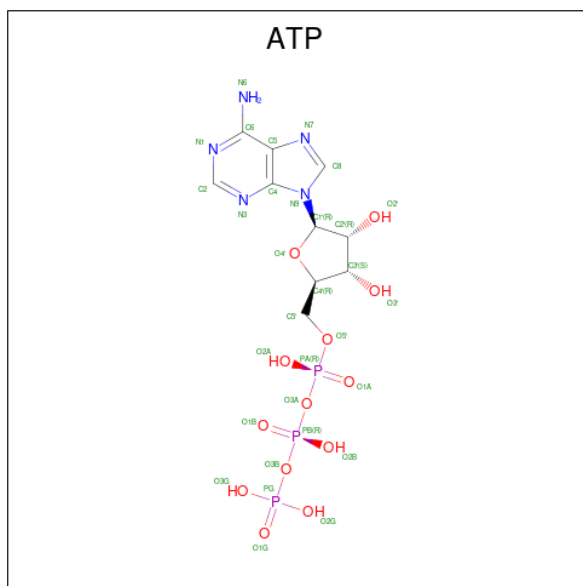
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
24	f	1	5	4	1	0
24	F	1	5	4	1	0

- Molecule 25 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
25	i	1	127	49	74	4	0
25	I	1	127	49	74	4	0

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

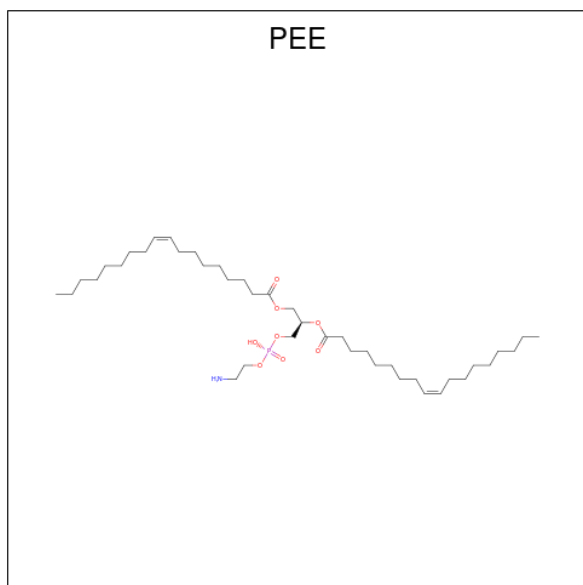


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
26	g	1	42	10	11	5	13	3	0
26	G	1	42	10	11	5	13	3	0

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

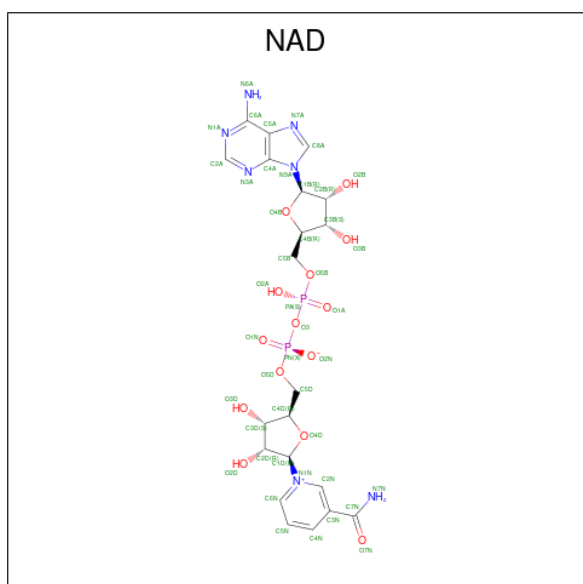
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
27	g	1	1	1	0
27	G	1	1	1	0

- Molecule 28 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
28	1	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
28	1	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
28	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 29 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

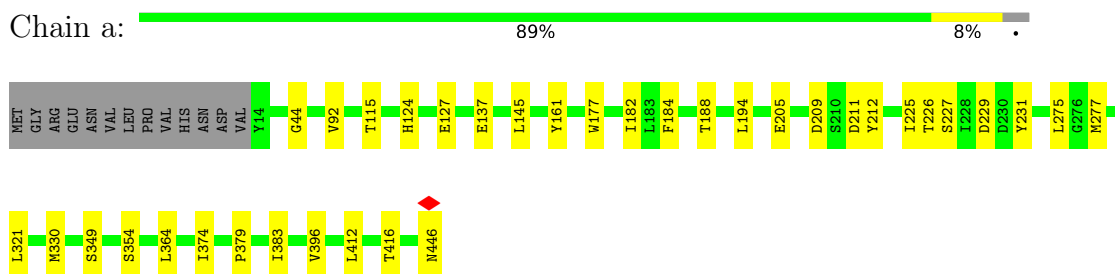


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
29	e	1	70	21	26	7	14	2	0
29	E	1	70	21	26	7	14	2	0

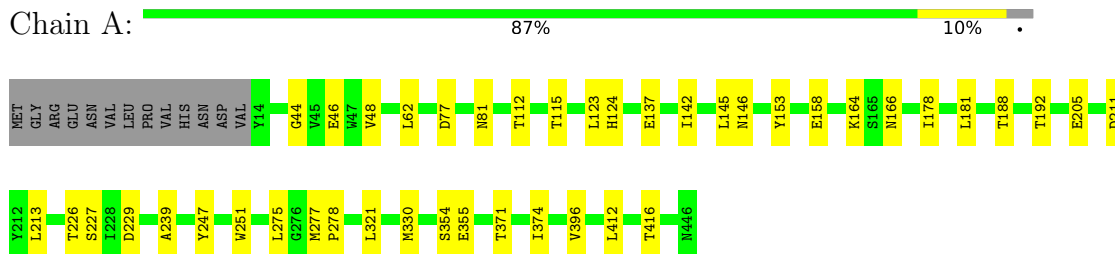
3 Residue-property plots [i](#)

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.

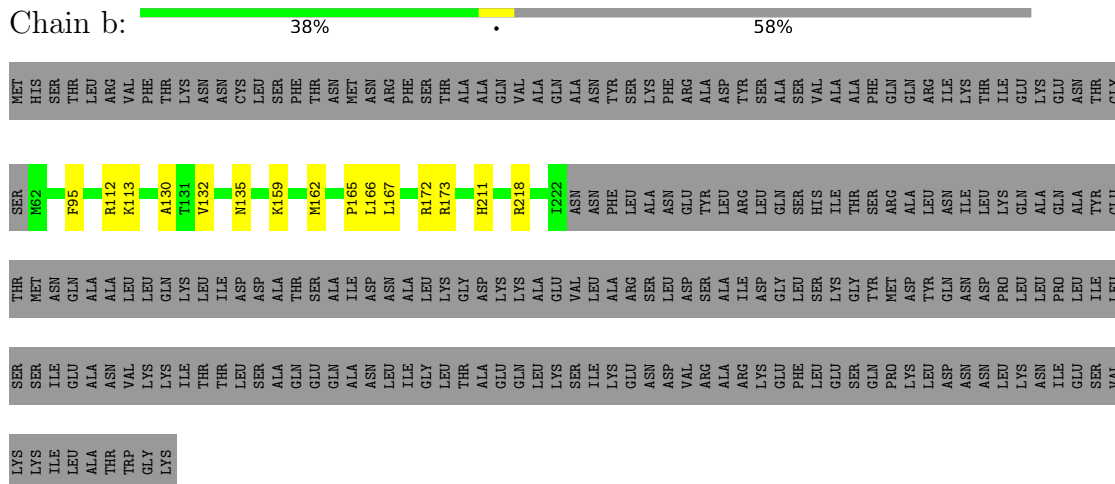
- Molecule 1: subunit a



- Molecule 1: subunit a

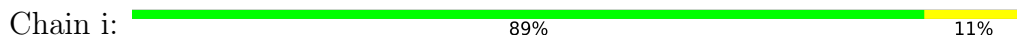


- Molecule 2: subunit b

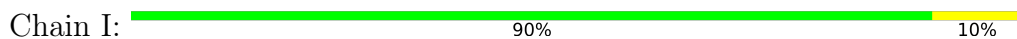




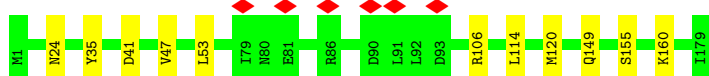
• Molecule 5: subunit i/j



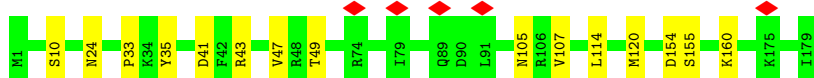
• Molecule 5: subunit i/j



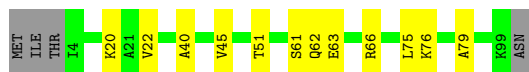
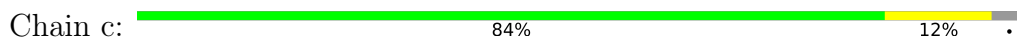
• Molecule 6: subunit k



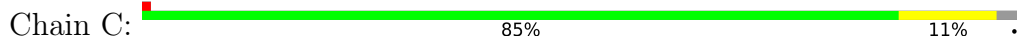
• Molecule 6: subunit k



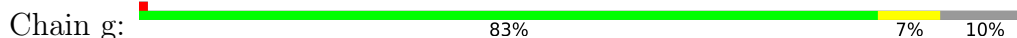
• Molecule 7: subunit 8

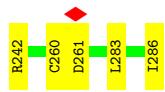


• Molecule 7: subunit 8

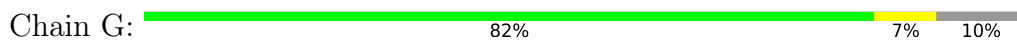


• Molecule 8: ATPTT3

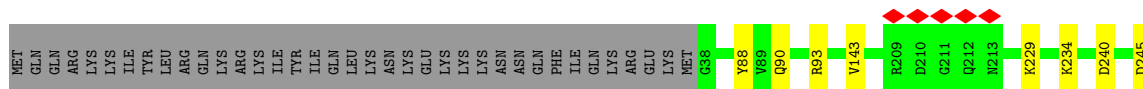
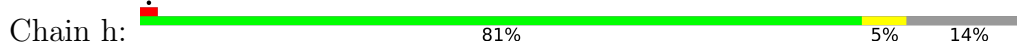




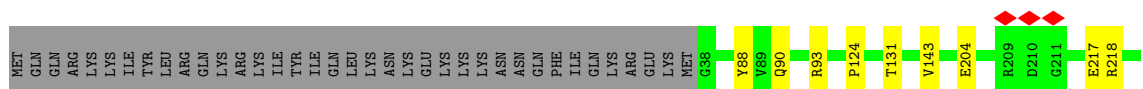
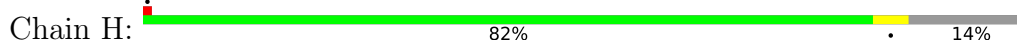
• Molecule 8: ATPTT3



• Molecule 9: ATPTT4



• Molecule 9: ATPTT4



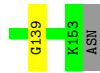
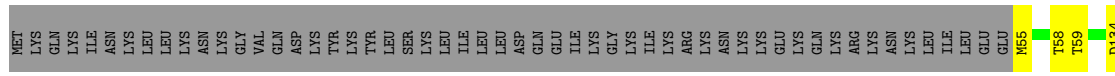
• Molecule 10: ATPTT5



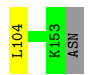
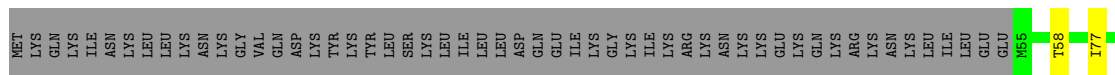
• Molecule 10: ATPTT5



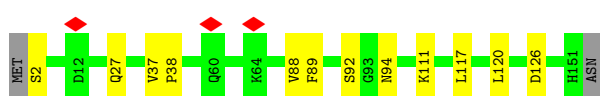
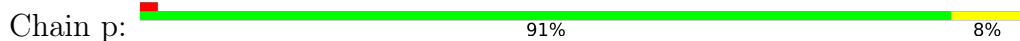
• Molecule 14: ATPTT9



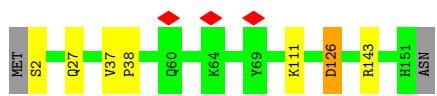
• Molecule 14: ATPTT9



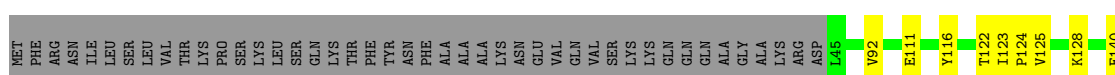
• Molecule 15: ATPTT10



• Molecule 15: ATPTT10

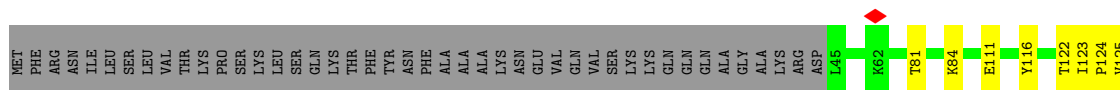


• Molecule 16: ATPTT11

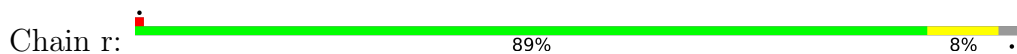


• Molecule 16: ATPTT11

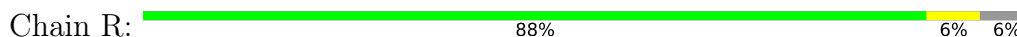




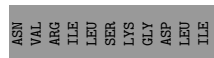
• Molecule 17: ATPTT12



• Molecule 17: ATPTT12



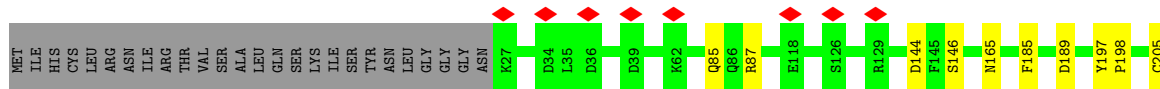
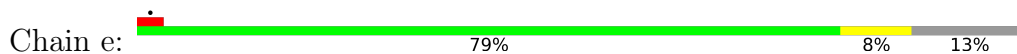
• Molecule 18: ATPTT13

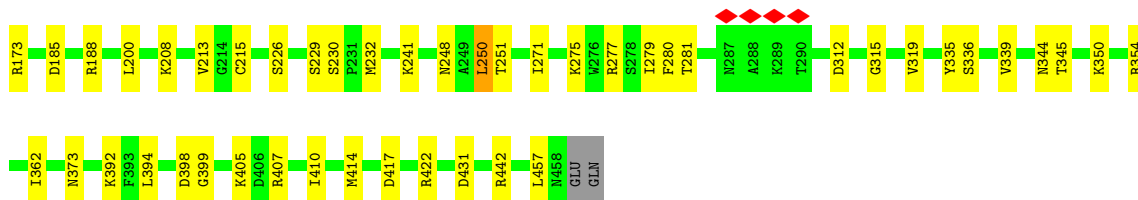


• Molecule 18: ATPTT13



• Molecule 19: ATPTT1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, PC1, ATP, MG, CDL, NAD, PEE, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/3752	0.30	0/5109
1	a	0.28	0/3752	0.30	0/5109
2	B	0.30	0/1417	0.34	0/1915
2	b	0.30	0/1417	0.33	0/1915
3	D	0.29	0/944	0.29	0/1278
3	d	0.29	0/944	0.30	0/1278
4	F	0.30	0/1733	0.34	0/2327
4	f	0.30	0/1733	0.32	0/2327
5	I	0.29	0/1771	0.34	0/2394
5	i	0.29	0/1771	0.33	0/2394
6	K	0.23	0/1508	0.30	0/2024
6	k	0.23	0/1508	0.29	0/2024
7	C	0.28	0/866	0.33	0/1176
7	c	0.28	0/866	0.34	0/1176
8	G	0.26	0/2302	0.31	0/3115
8	g	0.26	0/2302	0.31	0/3115
9	H	0.28	0/2006	0.32	0/2704
9	h	0.28	0/2006	0.32	0/2704
10	J	0.27	0/2256	0.31	0/3069
10	j	0.27	0/2256	0.31	0/3069
11	L	0.29	0/2140	0.32	0/2903
11	l	0.28	0/2140	0.32	0/2903
12	M	0.30	0/1912	0.31	0/2598
12	m	0.30	0/1912	0.32	0/2598
13	N	0.30	0/1030	0.32	0/1393
13	n	0.30	0/1030	0.32	0/1393
14	O	0.24	0/821	0.29	0/1104
14	o	0.24	0/821	0.28	0/1104
15	P	0.20	0/1249	0.25	0/1695
15	p	0.20	0/1249	0.25	0/1695
16	Q	0.24	0/888	0.26	0/1200
16	q	0.24	0/888	0.27	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.28	0/1185	0.31	0/1594
17	r	0.27	0/1225	0.32	0/1649
18	S	0.27	0/892	0.34	0/1209
18	s	0.28	0/885	0.33	0/1199
19	E	0.17	0/3492	0.26	0/4720
19	e	0.17	0/3492	0.26	0/4720
20	i1	0.60	0/242	1.02	0/328
20	i2	0.13	0/272	0.26	0/370
21	t	0.27	0/3103	0.34	0/4200
All	All	0.27	0/67978	0.31	0/91997

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	3529	3529	37	0
1	a	3628	3529	3529	35	0
2	B	1368	1307	1307	20	0
2	b	1368	1310	1310	17	0
3	D	918	846	846	4	0
3	d	918	846	846	7	0
4	F	1682	1692	1692	14	0
4	f	1682	1691	1691	16	0
5	I	1720	1741	1740	14	0
5	i	1720	1741	1741	18	0
6	K	1473	1430	1430	10	0
6	k	1473	1430	1430	9	0
7	C	841	830	830	8	0
7	c	841	830	830	9	0
8	G	2220	2118	2118	14	0
8	g	2220	2118	2118	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	1953	1883	1882	9	0
9	h	1953	1883	1882	11	0
10	J	2199	2145	2145	13	0
10	j	2199	2147	2147	12	0
11	L	2071	1999	2000	25	0
11	l	2071	1999	2000	20	0
12	M	1861	1835	1835	18	0
12	m	1861	1835	1835	16	0
13	N	998	962	962	10	0
13	n	998	962	962	5	0
14	O	805	794	794	4	0
14	o	805	794	794	4	0
15	P	1217	1196	1196	6	0
15	p	1217	1196	1196	8	0
16	Q	875	874	874	6	0
16	q	875	874	874	5	0
17	R	1154	1134	1134	9	0
17	r	1193	1180	1180	11	0
18	S	872	856	856	4	0
18	s	865	849	849	14	0
19	E	3395	3286	3285	25	0
19	e	3395	3286	3285	22	0
20	i1	238	236	236	12	0
20	i2	267	262	262	13	0
21	t	3013	2876	2876	44	0
22	A	100	156	156	4	0
22	B	500	780	780	28	0
22	I	200	312	312	6	0
22	J	200	312	312	3	0
22	K	200	312	312	2	0
22	L	100	156	156	11	0
22	P	100	156	156	0	0
22	a	100	156	156	4	0
22	b	200	312	312	8	0
22	f	300	468	468	17	0
22	i	100	156	156	1	0
22	j	200	312	312	3	0
22	k	300	468	468	6	0
22	l	200	312	312	14	0
22	p	100	156	156	0	0
22	r	100	156	156	3	0
23	D	54	88	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	G	108	176	176	2	0
23	d	54	88	88	1	0
23	g	54	88	88	0	0
23	i	54	88	88	1	0
24	F	5	0	0	0	0
24	f	5	0	0	0	0
25	I	53	74	74	5	0
25	i	53	74	74	8	0
26	G	31	11	12	1	0
26	g	31	11	12	1	0
27	G	1	0	0	0	0
27	g	1	0	0	0	0
28	J	99	157	155	4	0
28	l	99	157	155	3	0
29	E	44	26	25	1	0
29	e	44	26	25	0	0
All	All	69840	70075	70068	481	0

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

The worst 5 of 481 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:203:CDL:O1	11:L:32:LYS:NZ	1.99	0.95
11:l:32:LYS:NZ	22:l:304:CDL:O1	2.03	0.89
17:r:31:GLU:OE1	22:r:201:CDL:O1	1.96	0.84
1:a:374:ILE:O	11:L:128:TYR:OH	1.98	0.82
18:s:36:VAL:O	21:t:407:ARG:NH2	2.13	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
1	a	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
2	B	159/381 (42%)	153 (96%)	6 (4%)	0	100	100
2	b	159/381 (42%)	154 (97%)	5 (3%)	0	100	100
3	D	108/234 (46%)	106 (98%)	2 (2%)	0	100	100
3	d	108/234 (46%)	107 (99%)	1 (1%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
5	i	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
6	K	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k	177/179 (99%)	168 (95%)	9 (5%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
8	G	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
9	H	229/268 (85%)	223 (97%)	6 (3%)	0	100	100
9	h	229/268 (85%)	227 (99%)	2 (1%)	0	100	100
10	J	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
10	j	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	240 (98%)	4 (2%)	0	100	100
12	M	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
13	N	117/179 (65%)	113 (97%)	4 (3%)	0	100	100
13	n	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
15	p	148/152 (97%)	143 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	106/152 (70%)	104 (98%)	2 (2%)	0	100	100
16	q	106/152 (70%)	103 (97%)	3 (3%)	0	100	100
17	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	r	143/149 (96%)	141 (99%)	2 (1%)	0	100	100
18	S	104/145 (72%)	101 (97%)	3 (3%)	0	100	100
18	s	103/145 (71%)	100 (97%)	3 (3%)	0	100	100
19	E	415/480 (86%)	408 (98%)	7 (2%)	0	100	100
19	e	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
20	i1	26/108 (24%)	26 (100%)	0	0	100	100
20	i2	30/108 (28%)	30 (100%)	0	0	100	100
21	t	363/460 (79%)	356 (98%)	7 (2%)	0	100	100
All	All	7847/9594 (82%)	7667 (98%)	180 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	397/409 (97%)	397 (100%)	0	100	100
1	a	397/409 (97%)	396 (100%)	1 (0%)	86	94
2	B	143/331 (43%)	142 (99%)	1 (1%)	76	89
2	b	143/331 (43%)	143 (100%)	0	100	100
3	D	95/206 (46%)	95 (100%)	0	100	100
3	d	95/206 (46%)	95 (100%)	0	100	100
4	F	175/178 (98%)	175 (100%)	0	100	100
4	f	175/178 (98%)	173 (99%)	2 (1%)	65	84
5	I	182/182 (100%)	180 (99%)	2 (1%)	65	84
5	i	182/182 (100%)	181 (100%)	1 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	152/152 (100%)	151 (99%)	1 (1%)	76	89
6	k	152/152 (100%)	152 (100%)	0	100	100
7	C	93/97 (96%)	93 (100%)	0	100	100
7	c	93/97 (96%)	93 (100%)	0	100	100
8	G	235/262 (90%)	234 (100%)	1 (0%)	84	93
8	g	235/262 (90%)	234 (100%)	1 (0%)	84	93
9	H	208/245 (85%)	208 (100%)	0	100	100
9	h	208/245 (85%)	208 (100%)	0	100	100
10	J	235/239 (98%)	235 (100%)	0	100	100
10	j	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	218 (100%)	1 (0%)	81	92
11	l	219/220 (100%)	218 (100%)	1 (0%)	81	92
12	M	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	202 (100%)	0	100	100
13	N	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	104 (100%)	0	100	100
14	O	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	130 (99%)	1 (1%)	73	88
15	p	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100
16	q	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	120 (100%)	0	100	100
17	r	125/129 (97%)	125 (100%)	0	100	100
18	S	95/131 (72%)	94 (99%)	1 (1%)	65	84
18	s	94/131 (72%)	94 (100%)	0	100	100
19	E	359/414 (87%)	358 (100%)	1 (0%)	86	94
19	e	359/414 (87%)	358 (100%)	1 (0%)	86	94
20	i1	26/101 (26%)	26 (100%)	0	100	100
20	i2	29/101 (29%)	29 (100%)	0	100	100
21	t	325/414 (78%)	321 (99%)	4 (1%)	63	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7046/8554 (82%)	7026 (100%)	20 (0%)	84 94

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	62	LYS
21	t	101	ARG
21	t	250	LEU
21	t	173	ARG
19	e	398	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
19	E	221	HIS
19	E	370	GLN
19	e	165	ASN
19	e	54	HIS
21	t	254	ASN

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](#)

Of 50 ligands modelled in this entry, 2 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	b	402	-	99,99,99	0.90	7 (7%)	105,111,111	0.94	4 (3%)
22	CDL	i	302	-	99,99,99	0.91	8 (8%)	105,111,111	0.95	4 (3%)
22	CDL	I	302	-	99,99,99	0.90	8 (8%)	105,111,111	0.99	4 (3%)
26	ATP	G	301	27	32,33,33	3.48	12 (37%)	48,52,52	2.18	12 (25%)
22	CDL	f	303	-	99,99,99	0.91	8 (8%)	105,111,111	1.13	6 (5%)
22	CDL	P	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	5 (4%)
24	PO4	F	900	-	4,4,4	1.11	0	6,6,6	0.49	0
23	PC1	G	304	-	53,53,53	0.98	3 (5%)	59,61,61	1.05	2 (3%)
22	CDL	B	404	-	99,99,99	0.90	8 (8%)	105,111,111	0.96	4 (3%)
29	NAD	e	900	-	46,48,48	4.04	22 (47%)	64,73,73	2.08	13 (20%)
29	NAD	E	900	-	46,48,48	4.03	22 (47%)	64,73,73	2.07	14 (21%)
24	PO4	f	301	-	4,4,4	1.11	0	6,6,6	0.45	0
22	CDL	p	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.01	4 (3%)
22	CDL	I	301	-	99,99,99	0.89	6 (6%)	105,111,111	0.96	4 (3%)
28	PEE	J	304	-	50,50,50	1.18	6 (12%)	53,55,55	1.14	4 (7%)
22	CDL	L	301	-	99,99,99	0.90	8 (8%)	105,111,111	0.99	4 (3%)
22	CDL	K	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
22	CDL	B	405	-	99,99,99	0.89	8 (8%)	105,111,111	1.11	5 (4%)
22	CDL	j	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.08	5 (4%)
22	CDL	b	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
25	UQ8	i	303	-	53,53,53	1.86	7 (13%)	66,67,67	1.57	15 (22%)
22	CDL	k	203	-	99,99,99	0.90	8 (8%)	105,111,111	1.00	4 (3%)
22	CDL	l	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.02	4 (3%)
23	PC1	i	301	-	53,53,53	0.98	4 (7%)	59,61,61	0.97	2 (3%)
28	PEE	J	303	-	47,47,50	1.20	6 (12%)	50,52,55	1.14	4 (8%)
22	CDL	B	403	-	99,99,99	0.88	7 (7%)	105,111,111	1.10	4 (3%)
22	CDL	B	402	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
22	CDL	K	202	-	99,99,99	0.90	7 (7%)	105,111,111	1.07	5 (4%)
28	PEE	l	302	-	47,47,50	1.21	6 (12%)	50,52,55	1.10	4 (8%)
22	CDL	J	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.08	4 (3%)
22	CDL	l	304	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PC1	G	303	-	53,53,53	0.99	4 (7%)	59,61,61	0.95	2 (3%)
28	PEE	l	303	-	50,50,50	1.17	6 (12%)	53,55,55	1.14	4 (7%)
22	CDL	r	201	-	99,99,99	0.88	6 (6%)	105,111,111	0.98	4 (3%)
23	PC1	D	301	-	53,53,53	0.96	4 (7%)	59,61,61	1.10	3 (5%)
22	CDL	A	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.02	6 (5%)
22	CDL	J	302	-	99,99,99	0.89	7 (7%)	105,111,111	1.00	4 (3%)
23	PC1	g	303	-	53,53,53	0.98	4 (7%)	59,61,61	1.05	3 (5%)
22	CDL	k	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.08	5 (4%)
22	CDL	B	401	-	99,99,99	0.90	8 (8%)	105,111,111	1.00	5 (4%)
25	UQ8	I	303	-	53,53,53	1.86	7 (13%)	66,67,67	1.55	13 (19%)
23	PC1	d	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.09	3 (5%)
26	ATP	g	301	27	32,33,33	3.47	13 (40%)	48,52,52	2.16	12 (25%)
22	CDL	f	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.07	5 (4%)
22	CDL	k	202	-	99,99,99	0.90	7 (7%)	105,111,111	1.04	5 (4%)
22	CDL	f	304	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	5 (4%)
22	CDL	a	501	-	99,99,99	0.90	7 (7%)	105,111,111	1.02	3 (2%)
22	CDL	j	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	4 (3%)

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
22	CDL	b	402	-	-	42/110/110/110	-
22	CDL	i	302	-	-	40/110/110/110	-
22	CDL	I	302	-	-	38/110/110/110	-
26	ATP	G	301	27	-	0/22/38/38	0/3/3/3
22	CDL	f	303	-	-	42/110/110/110	-
22	CDL	P	201	-	-	39/110/110/110	-
23	PC1	G	304	-	-	19/57/57/57	-
22	CDL	B	404	-	-	38/110/110/110	-
29	NAD	e	900	-	-	7/30/62/62	0/5/5/5
29	NAD	E	900	-	-	7/30/62/62	0/5/5/5
22	CDL	p	201	-	-	33/110/110/110	-
22	CDL	I	301	-	-	50/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PEE	J	304	-	-	24/54/54/54	-
22	CDL	L	301	-	-	44/110/110/110	-
22	CDL	K	201	-	-	33/110/110/110	-
22	CDL	B	405	-	-	40/110/110/110	-
22	CDL	j	301	-	-	40/110/110/110	-
22	CDL	b	401	-	-	55/110/110/110	-
25	UQ8	i	303	-	-	8/51/75/75	0/1/1/1
22	CDL	k	203	-	-	45/110/110/110	-
22	CDL	l	301	-	-	36/110/110/110	-
23	PC1	i	301	-	-	16/57/57/57	-
28	PEE	J	303	-	-	23/51/51/54	-
22	CDL	B	403	-	-	42/110/110/110	-
22	CDL	B	402	-	-	53/110/110/110	-
22	CDL	K	202	-	-	39/110/110/110	-
28	PEE	l	302	-	-	26/51/51/54	-
22	CDL	J	301	-	-	33/110/110/110	-
22	CDL	l	304	-	-	40/110/110/110	-
23	PC1	G	303	-	-	17/57/57/57	-
28	PEE	l	303	-	-	24/54/54/54	-
22	CDL	r	201	-	-	45/110/110/110	-
23	PC1	D	301	-	-	14/57/57/57	-
22	CDL	A	501	-	-	49/110/110/110	-
22	CDL	J	302	-	-	36/110/110/110	-
23	PC1	g	303	-	-	16/57/57/57	-
22	CDL	k	201	-	-	35/110/110/110	-
22	CDL	B	401	-	-	51/110/110/110	-
25	UQ8	I	303	-	-	11/51/75/75	0/1/1/1
23	PC1	d	301	-	-	17/57/57/57	-
26	ATP	g	301	27	-	0/22/38/38	0/3/3/3
22	CDL	f	302	-	-	43/110/110/110	-
22	CDL	k	202	-	-	42/110/110/110	-
22	CDL	f	304	-	-	58/110/110/110	-
22	CDL	a	501	-	-	47/110/110/110	-
22	CDL	j	302	-	-	37/110/110/110	-

The worst 5 of 356 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	900	NAD	O4D-C1D	-10.29	1.27	1.40
29	E	900	NAD	O4D-C1D	-10.21	1.27	1.40
25	i	303	UQ8	C6-C1	9.99	1.53	1.35
25	I	303	UQ8	C6-C1	9.94	1.53	1.35
29	e	900	NAD	PN-O3	9.64	1.69	1.59

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	900	NAD	C4A-N9A-C1B	-6.28	111.94	126.63
29	E	900	NAD	C4A-N9A-C1B	-6.09	112.38	126.63
26	G	301	ATP	C1'-N9-C8	-5.67	114.51	127.09
29	e	900	NAD	N3A-C2A-N1A	-5.56	120.17	128.58
26	g	301	ATP	C1'-N9-C8	-5.52	114.85	127.09

There are no chirality outliers.

5 of 1494 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	a	501	CDL	CB3-OB5-PB2-OB2
22	a	501	CDL	CB3-OB5-PB2-OB3
22	a	501	CDL	CB3-OB5-PB2-OB4
22	a	501	CDL	OB7-CB5-OB6-CB4
22	a	501	CDL	C51-CB5-OB6-CB4

There are no ring outliers.

40 monomers are involved in 124 short contacts:

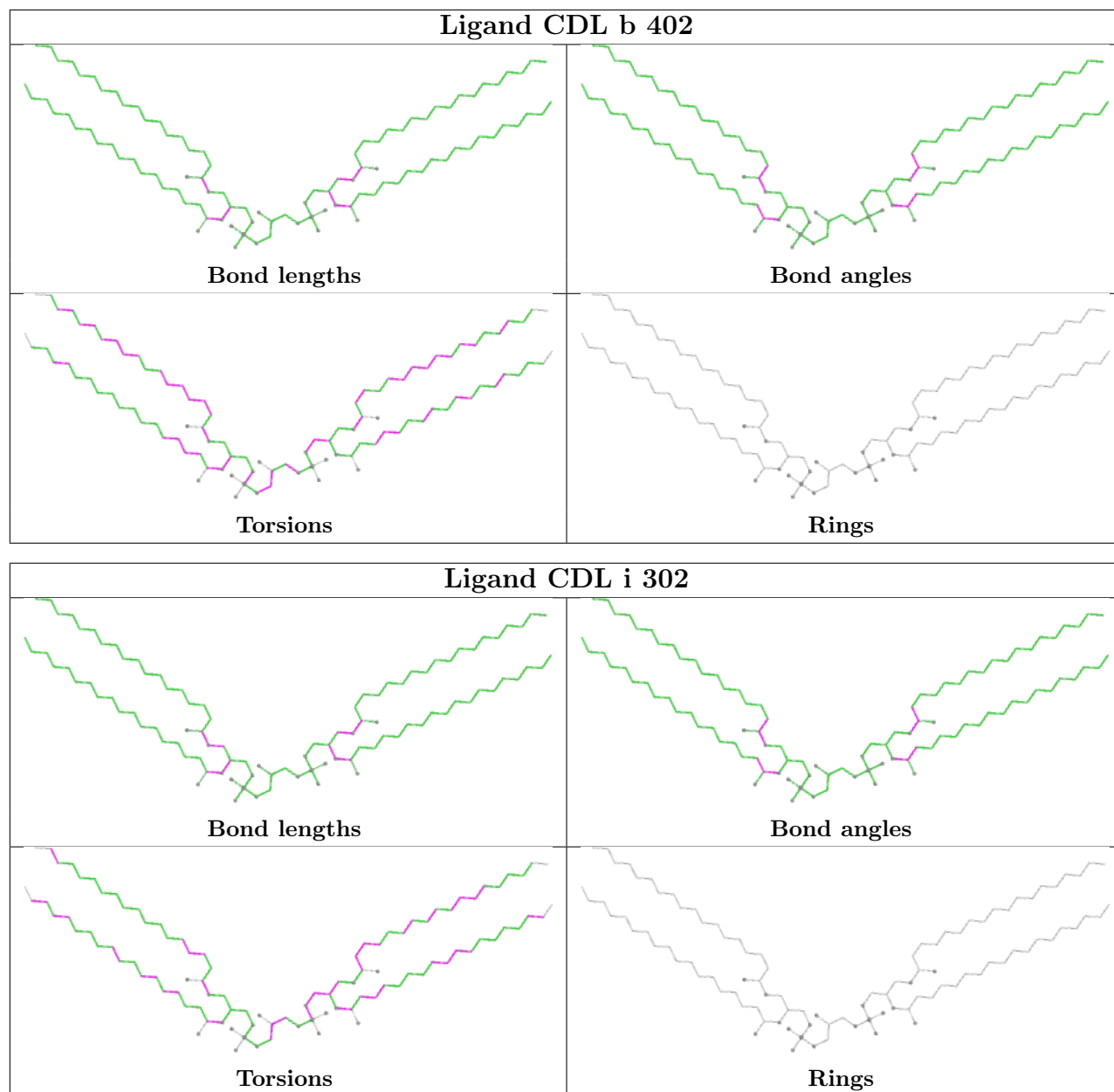
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	402	CDL	1	0
22	i	302	CDL	1	0
22	I	302	CDL	1	0
26	G	301	ATP	1	0
22	f	303	CDL	8	0
23	G	304	PC1	1	0
22	B	404	CDL	1	0
29	E	900	NAD	1	0
22	I	301	CDL	5	0
22	L	301	CDL	11	0
22	K	201	CDL	1	0

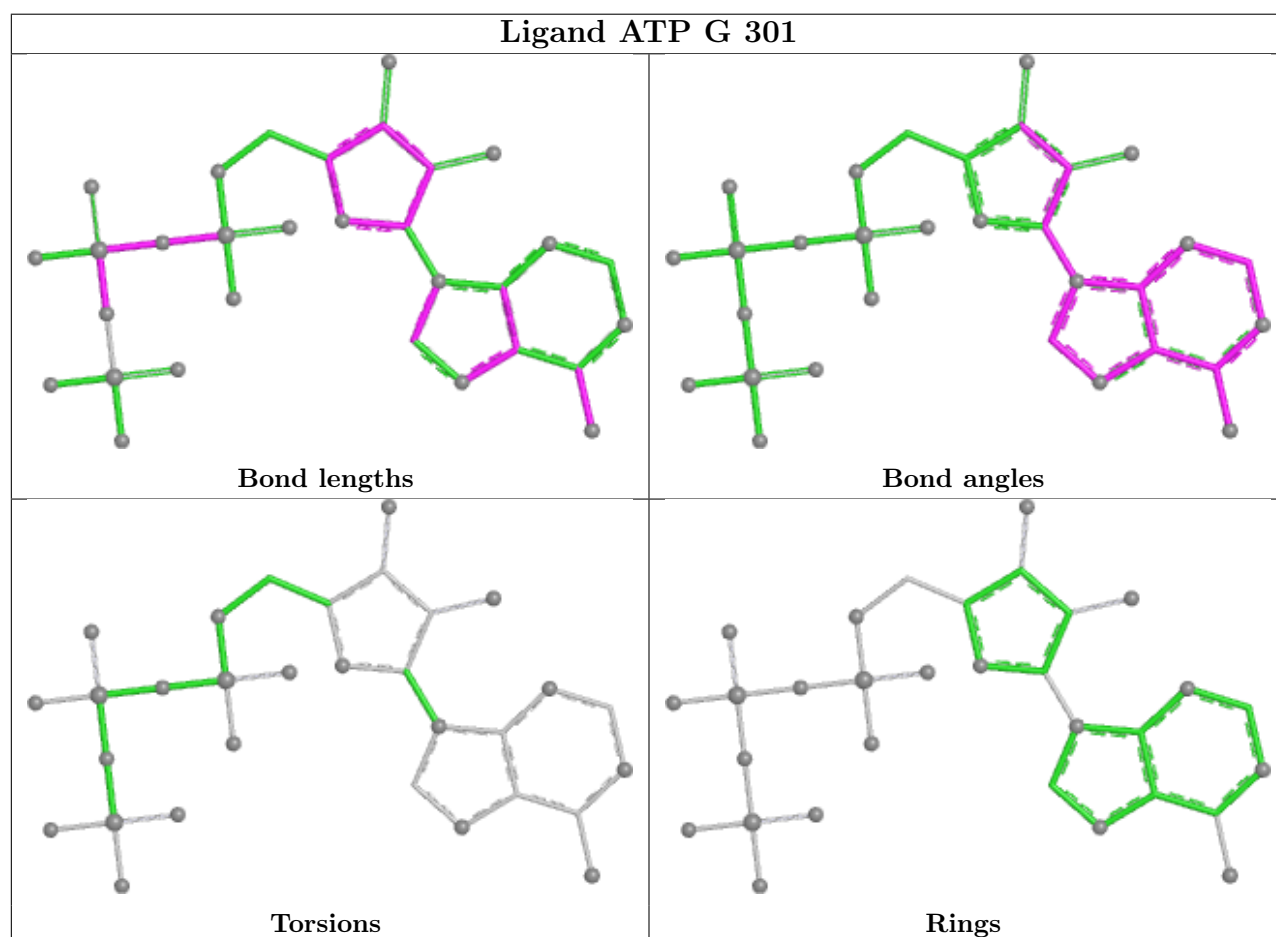
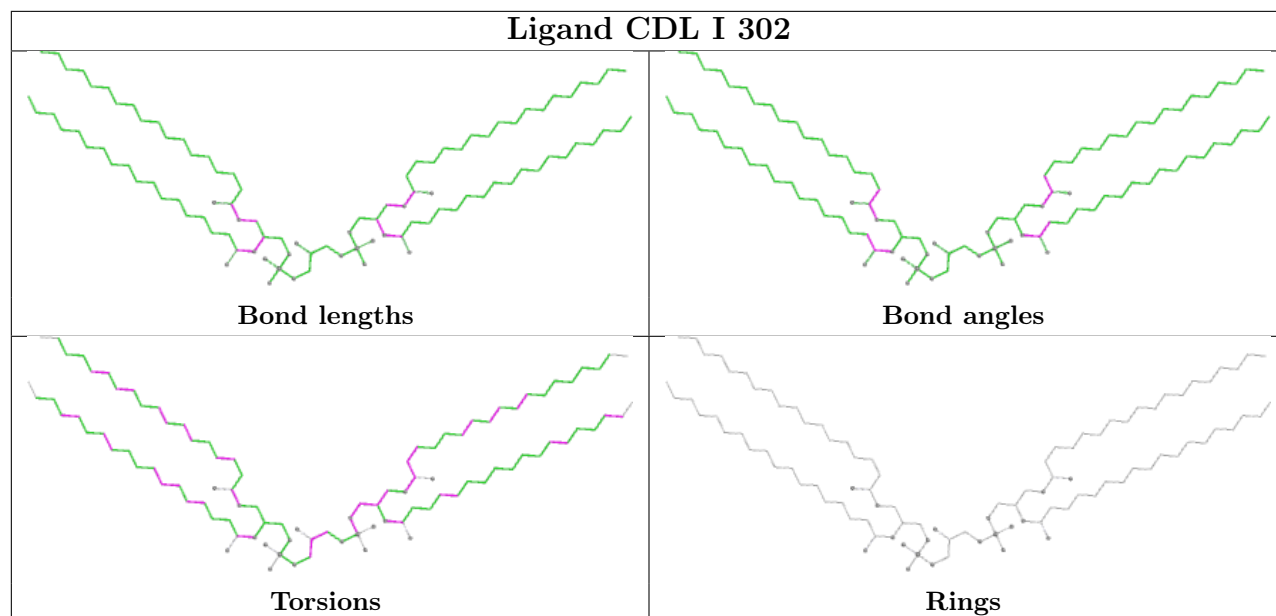
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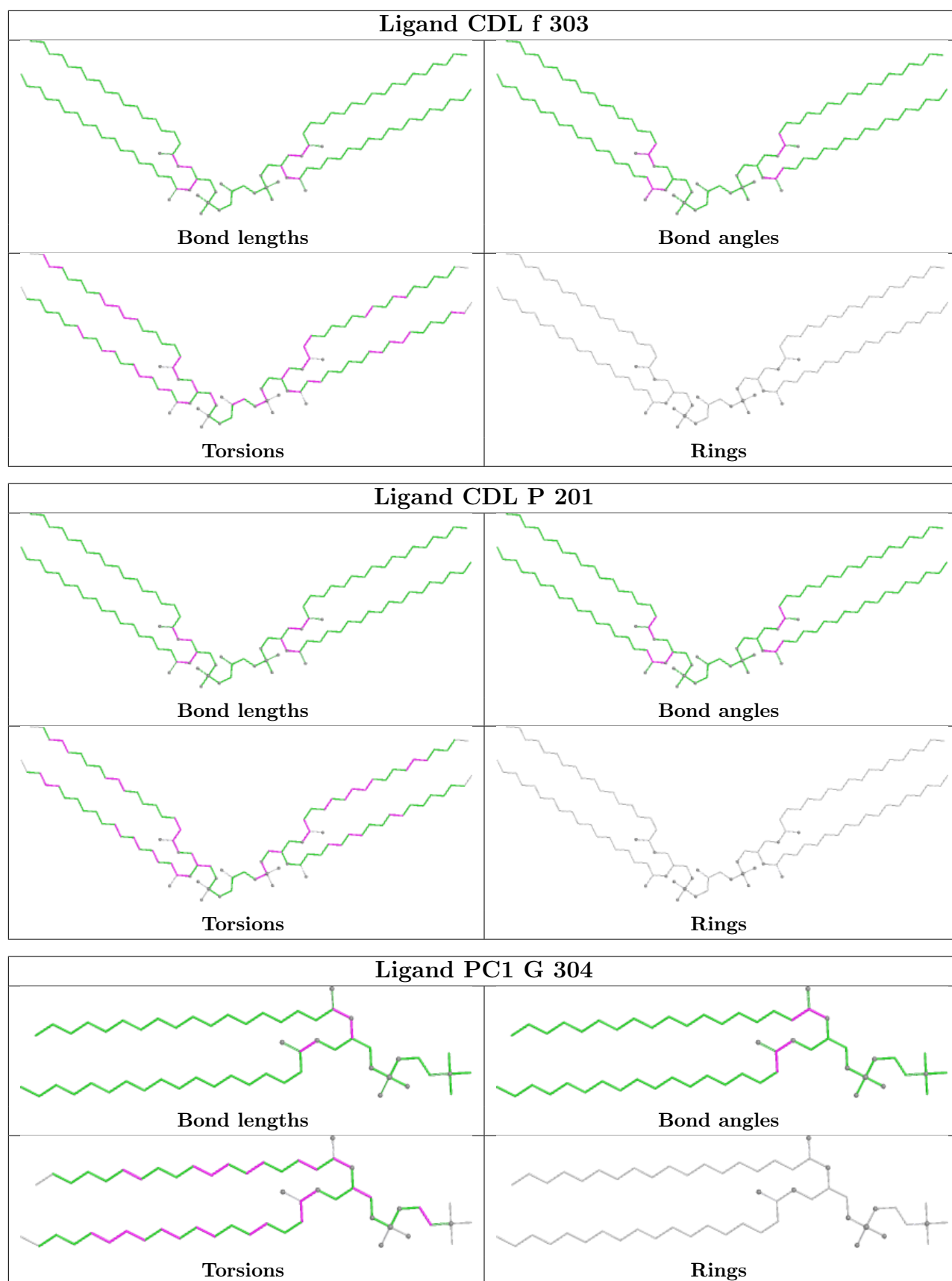
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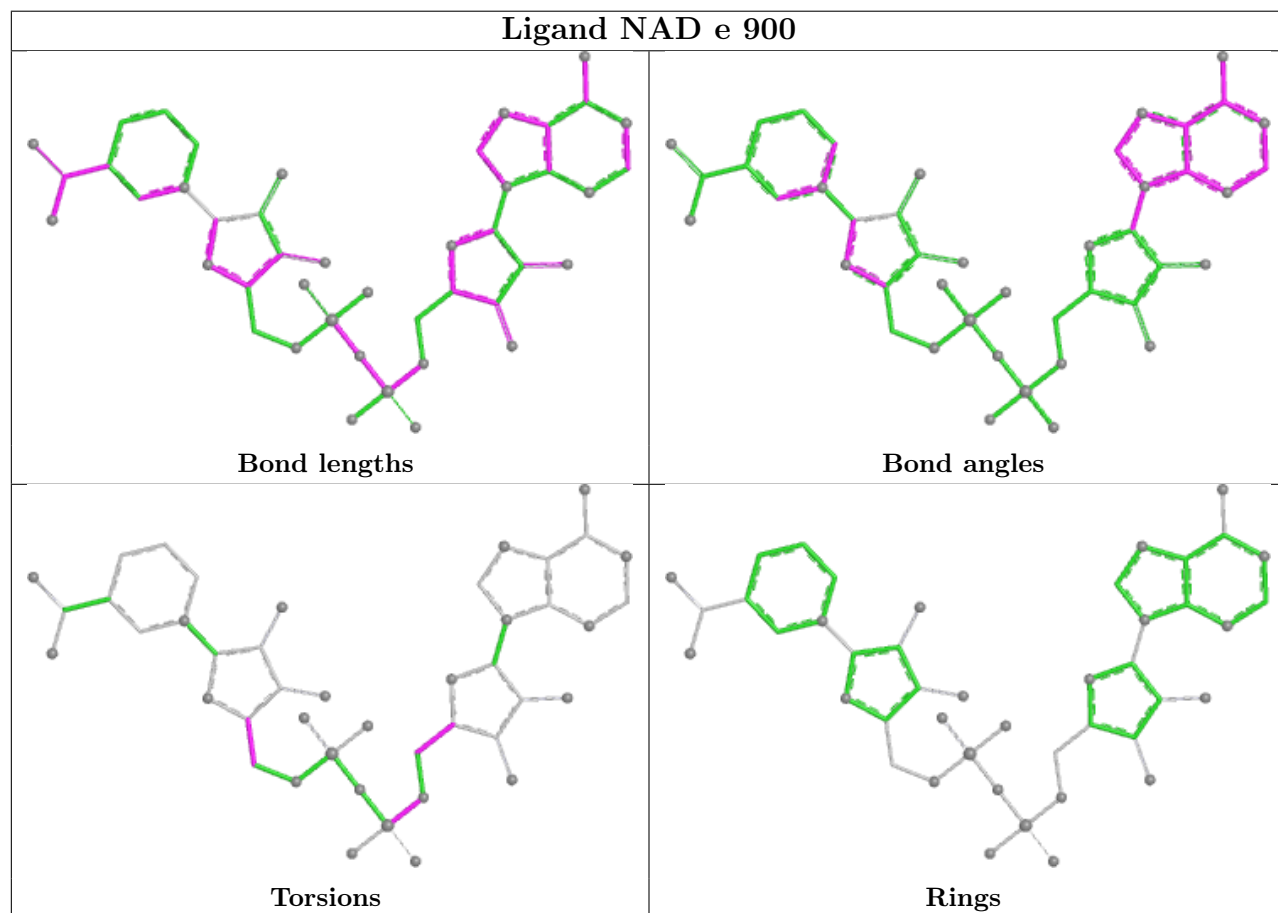
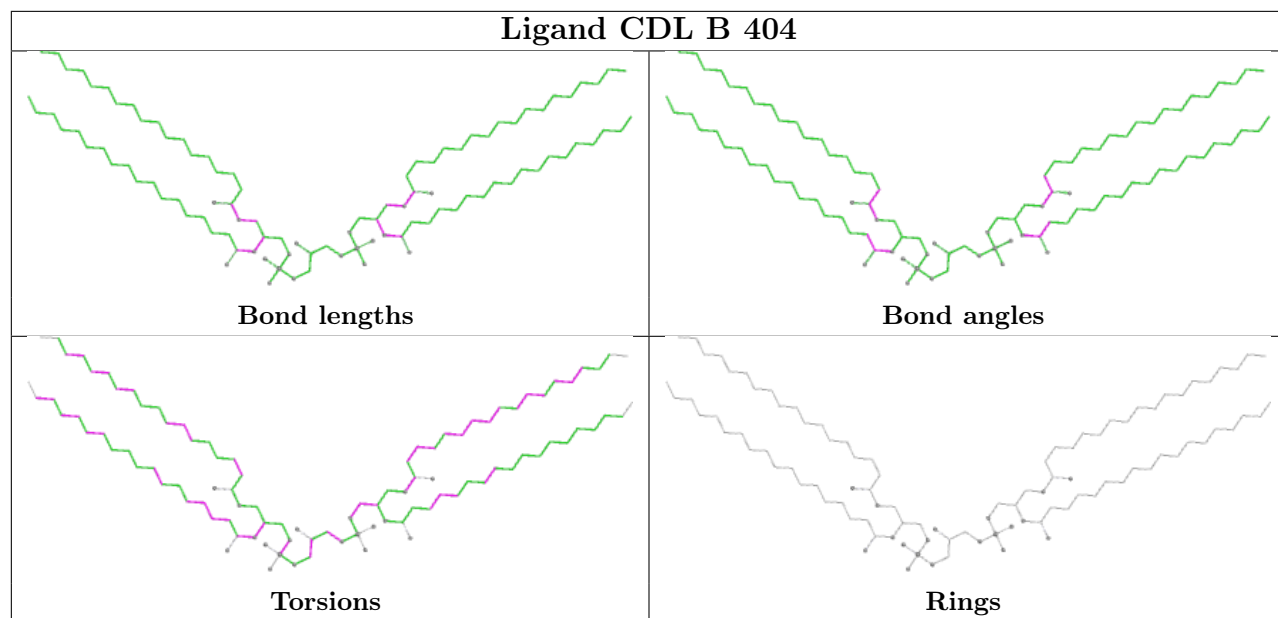
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	405	CDL	6	0
22	j	301	CDL	2	0
22	b	401	CDL	7	0
25	i	303	UQ8	8	0
22	k	203	CDL	4	0
22	l	301	CDL	11	0
23	i	301	PC1	1	0
28	J	303	PEE	4	0
22	B	403	CDL	7	0
22	B	402	CDL	6	0
22	K	202	CDL	1	0
28	l	302	PEE	2	0
22	J	301	CDL	2	0
22	l	304	CDL	3	0
23	G	303	PC1	1	0
28	l	303	PEE	1	0
22	r	201	CDL	3	0
23	D	301	PC1	4	0
22	A	501	CDL	4	0
22	J	302	CDL	1	0
22	B	401	CDL	9	0
25	I	303	UQ8	5	0
23	d	301	PC1	1	0
26	g	301	ATP	1	0
22	f	302	CDL	7	0
22	k	202	CDL	2	0
22	f	304	CDL	2	0
22	a	501	CDL	4	0
22	j	302	CDL	1	0

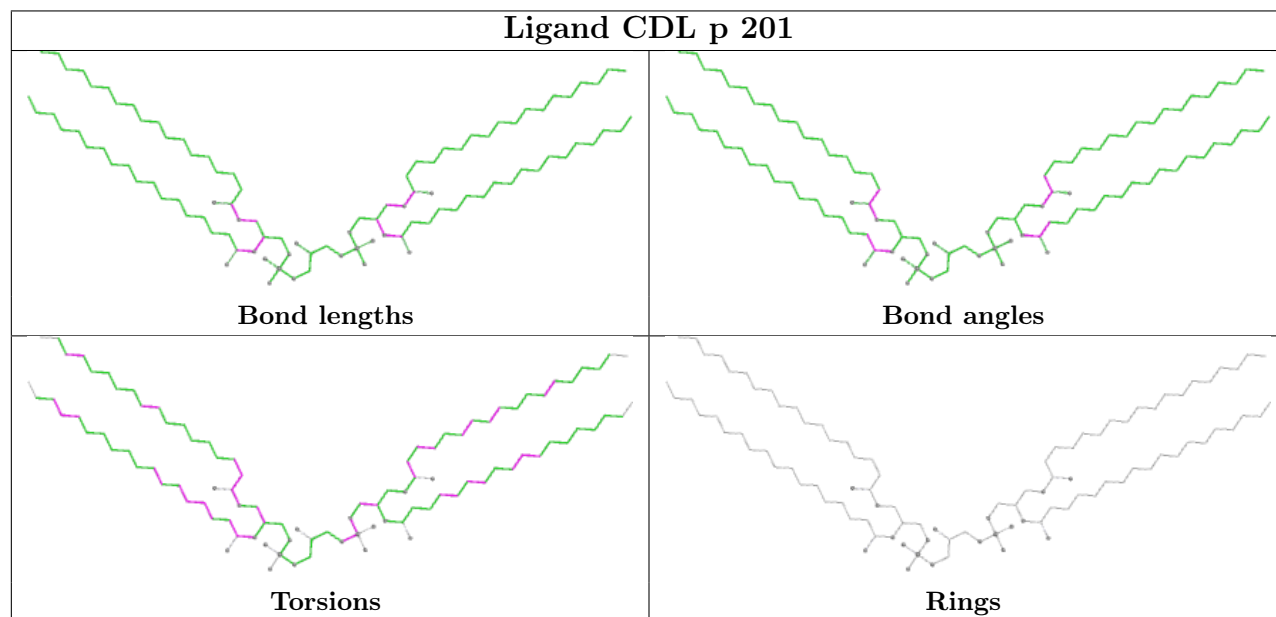
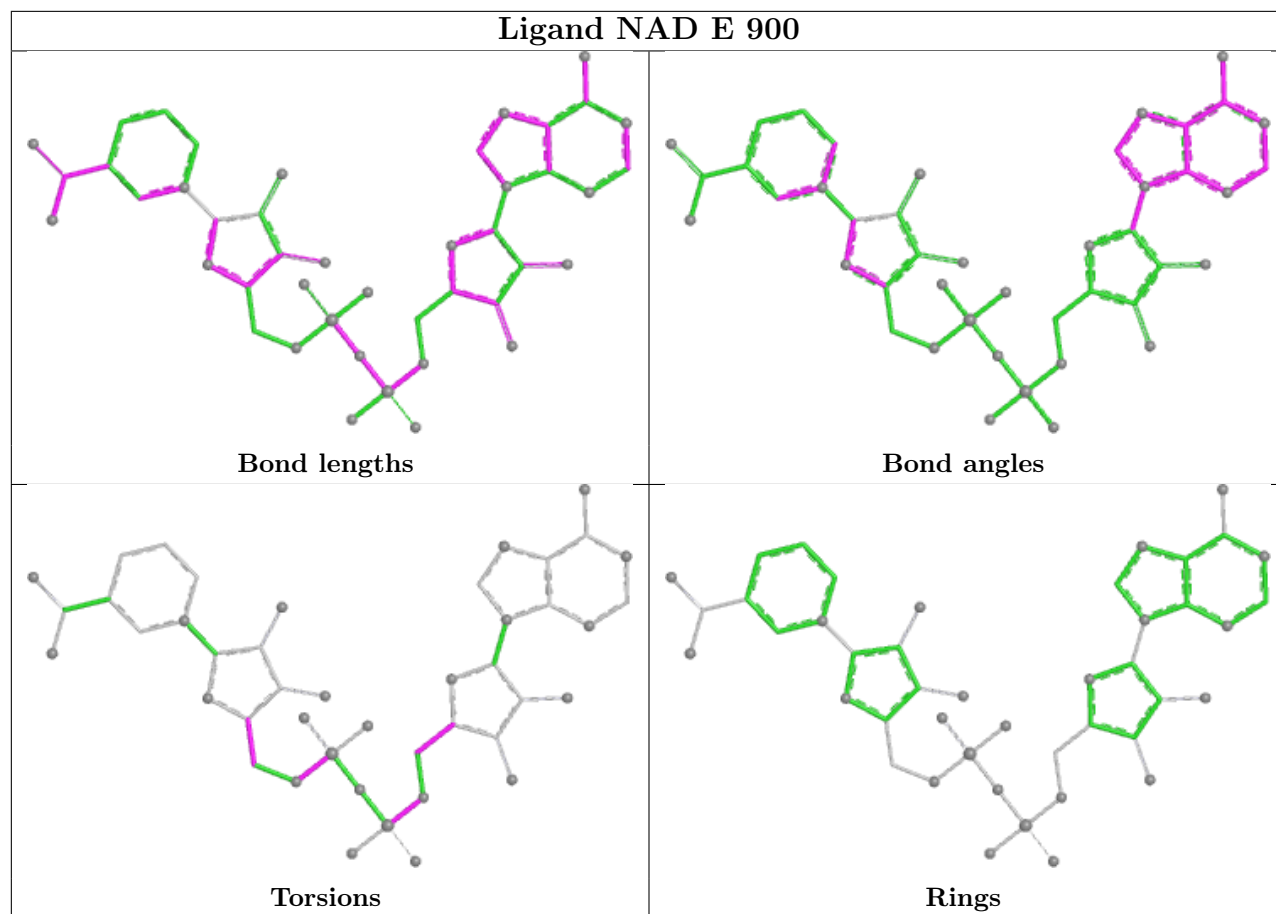
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

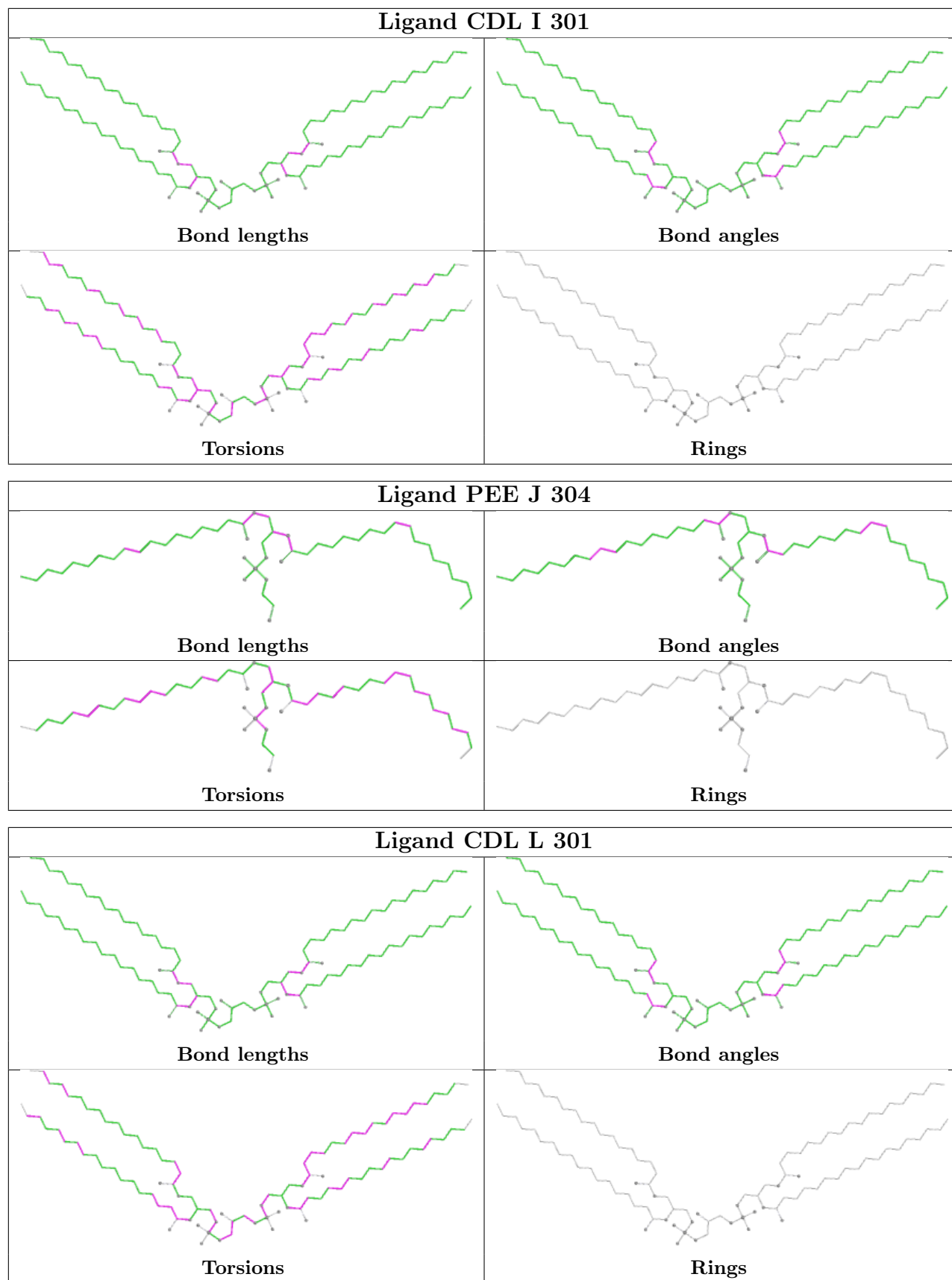


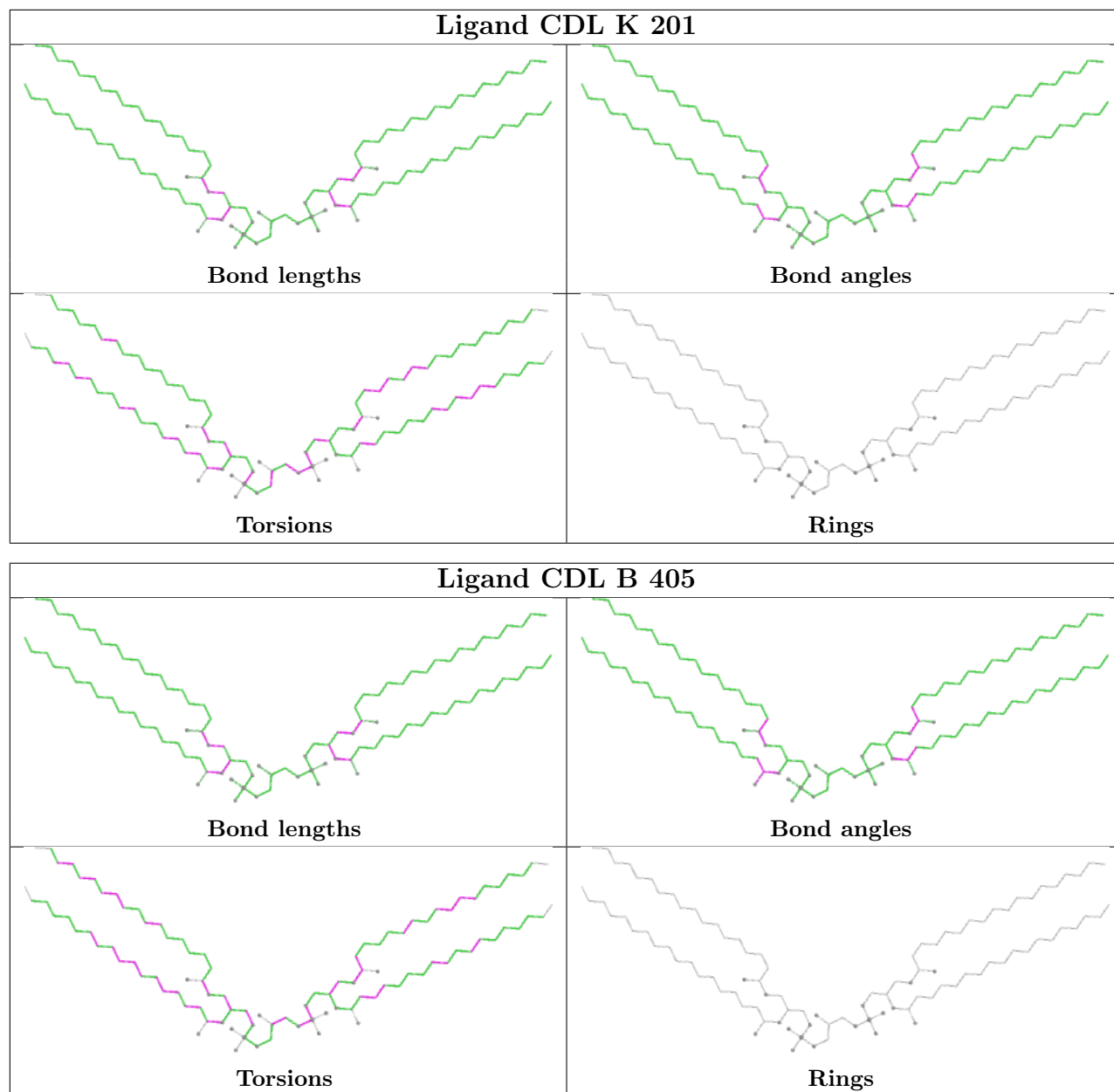


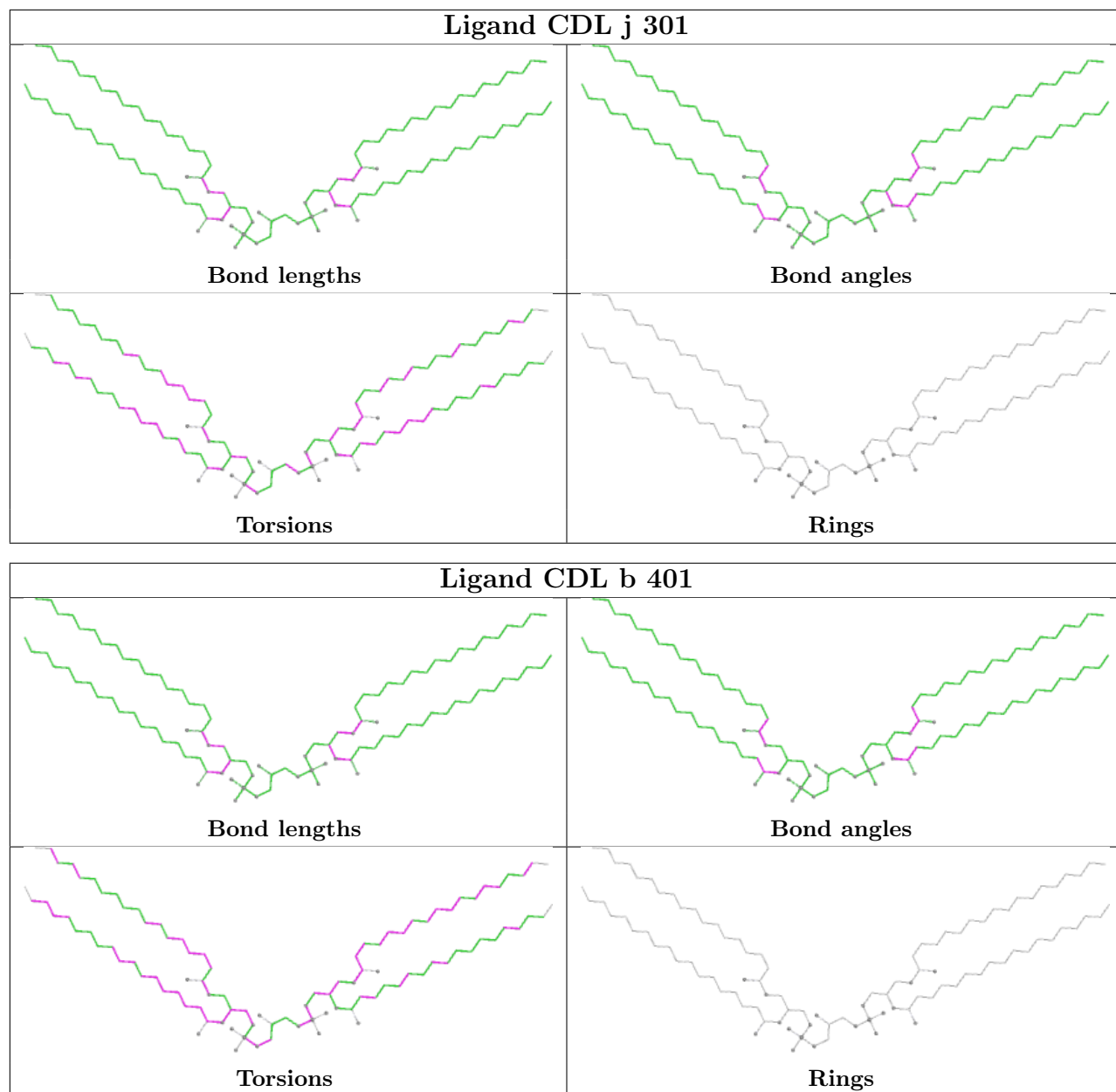


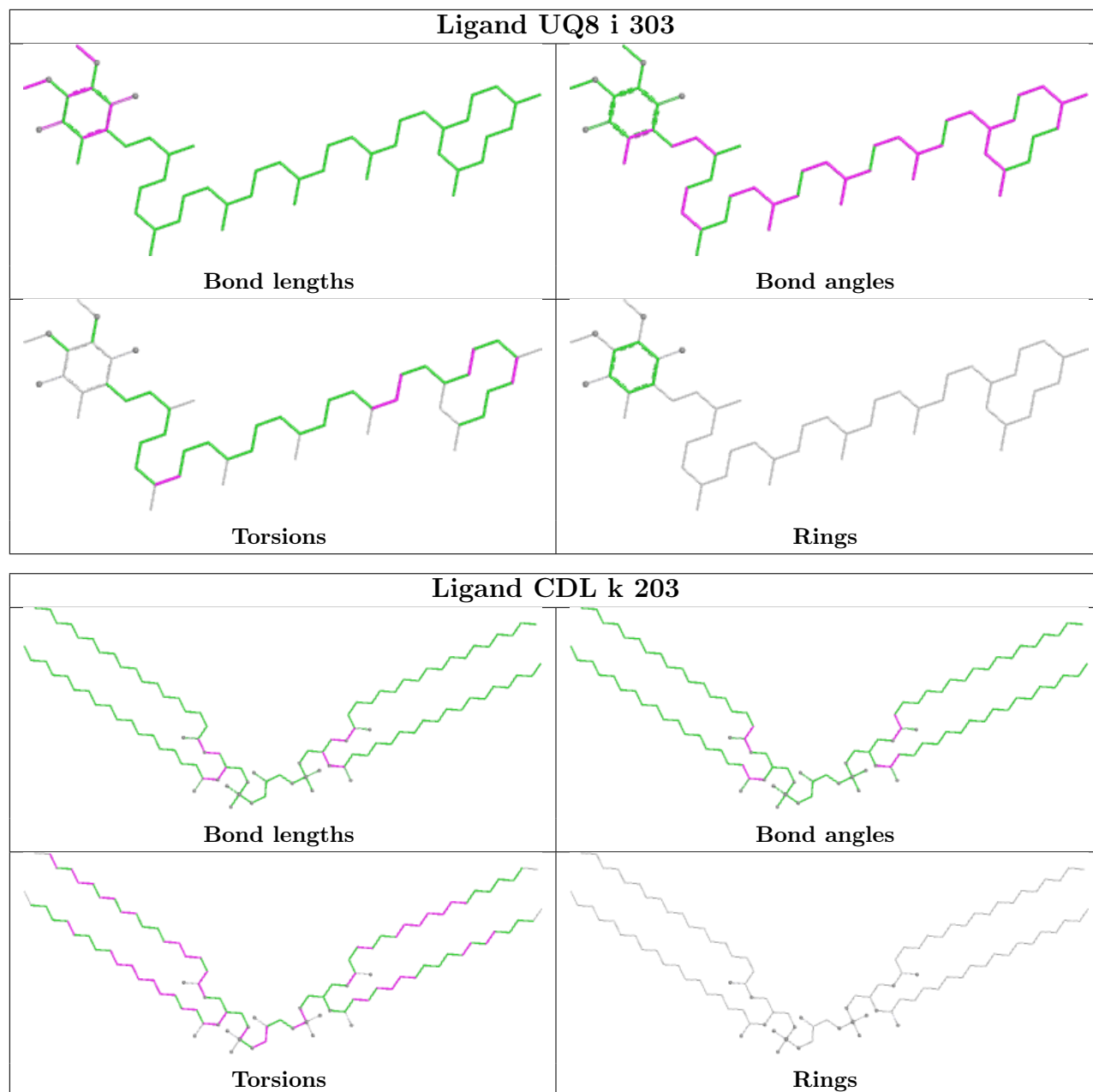


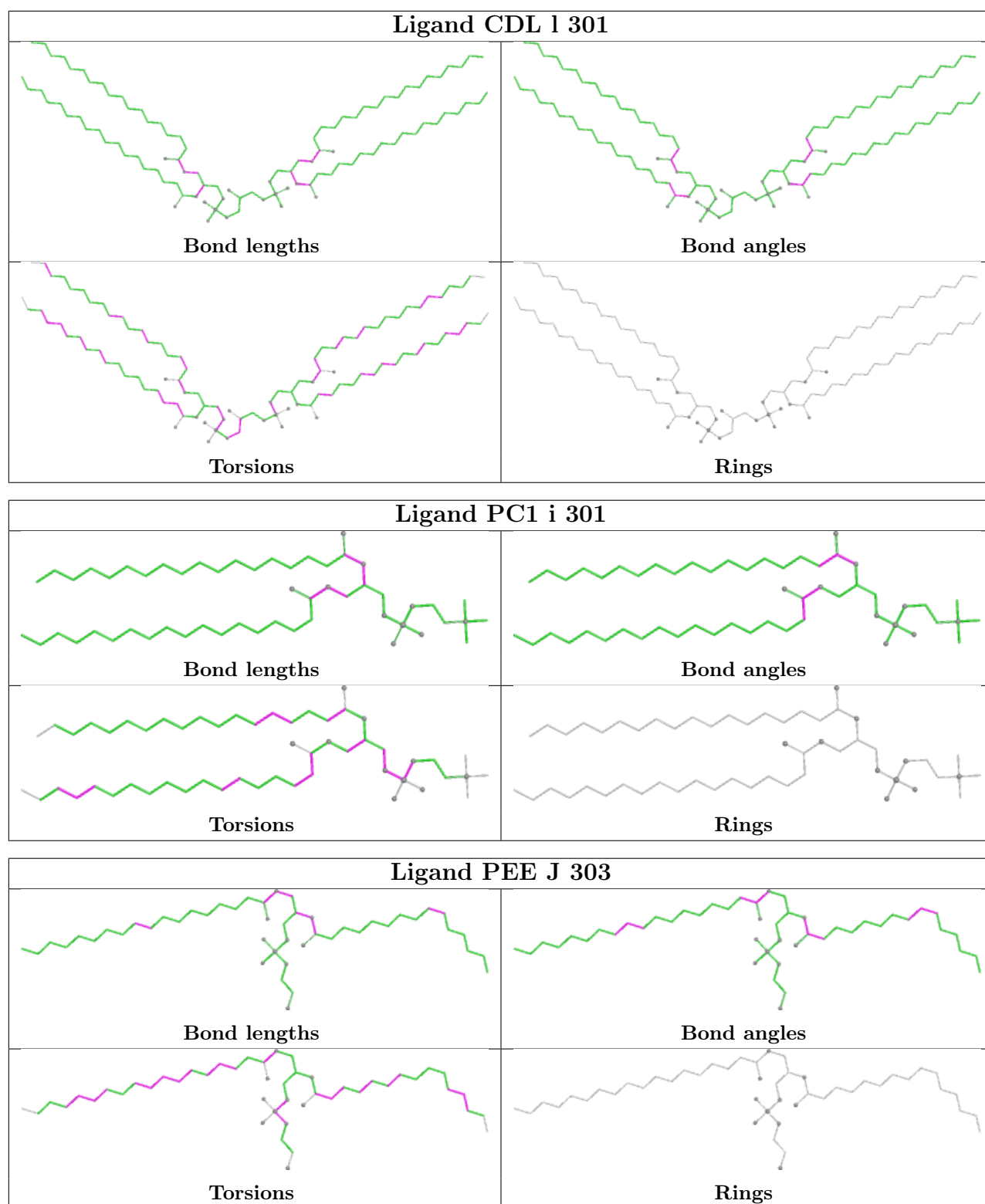


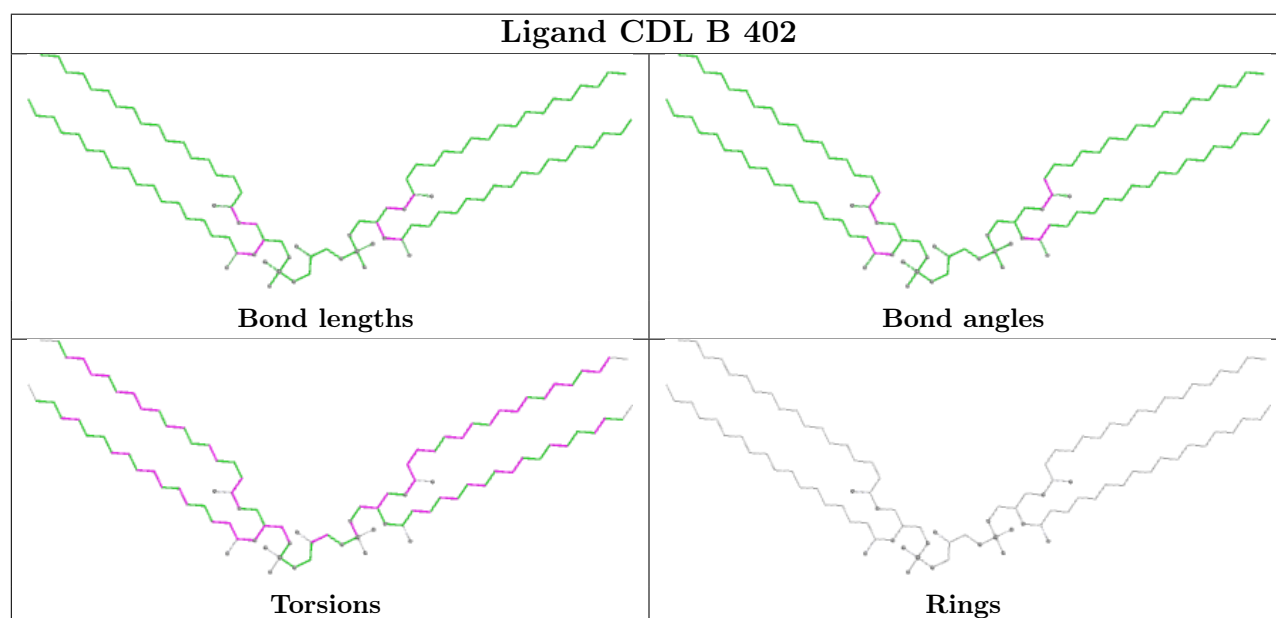
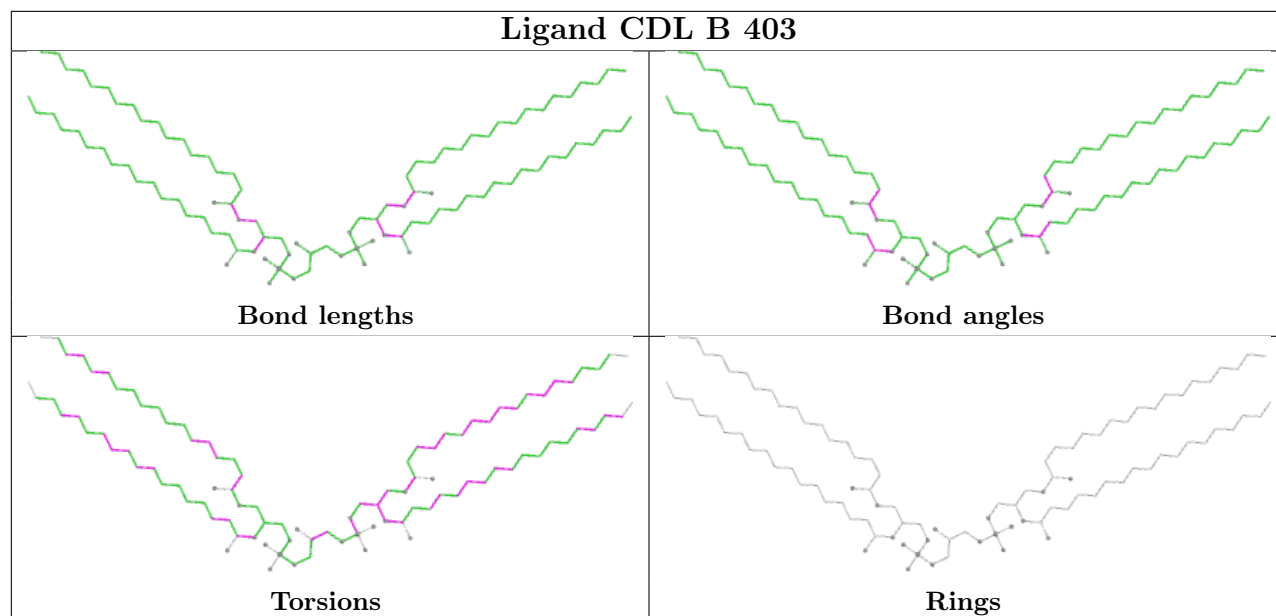


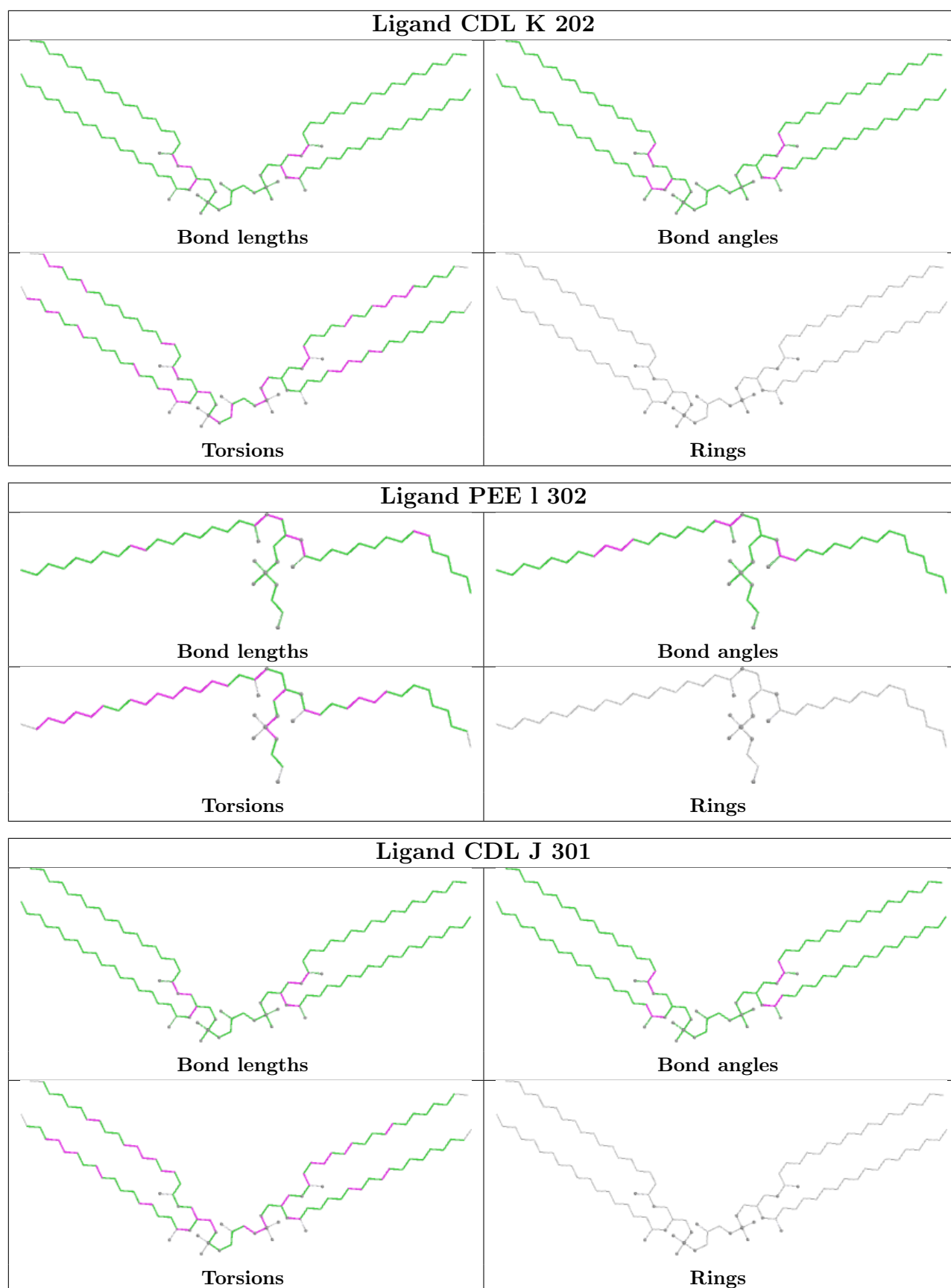


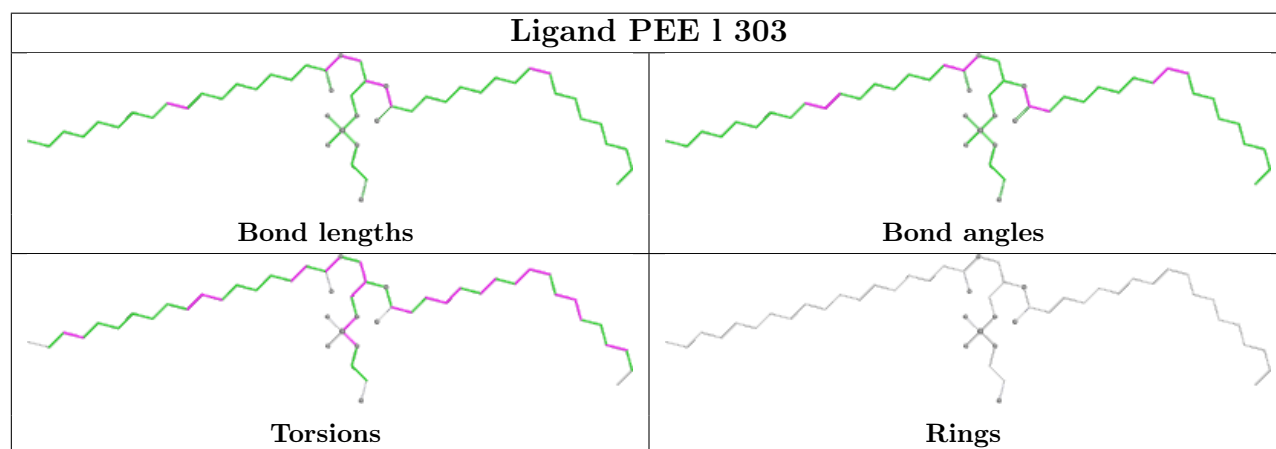
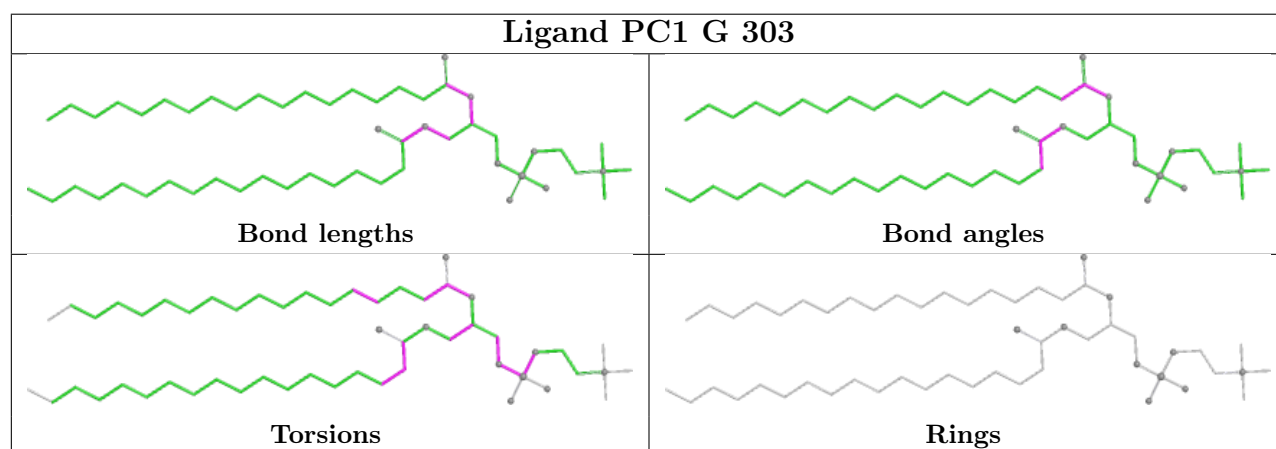
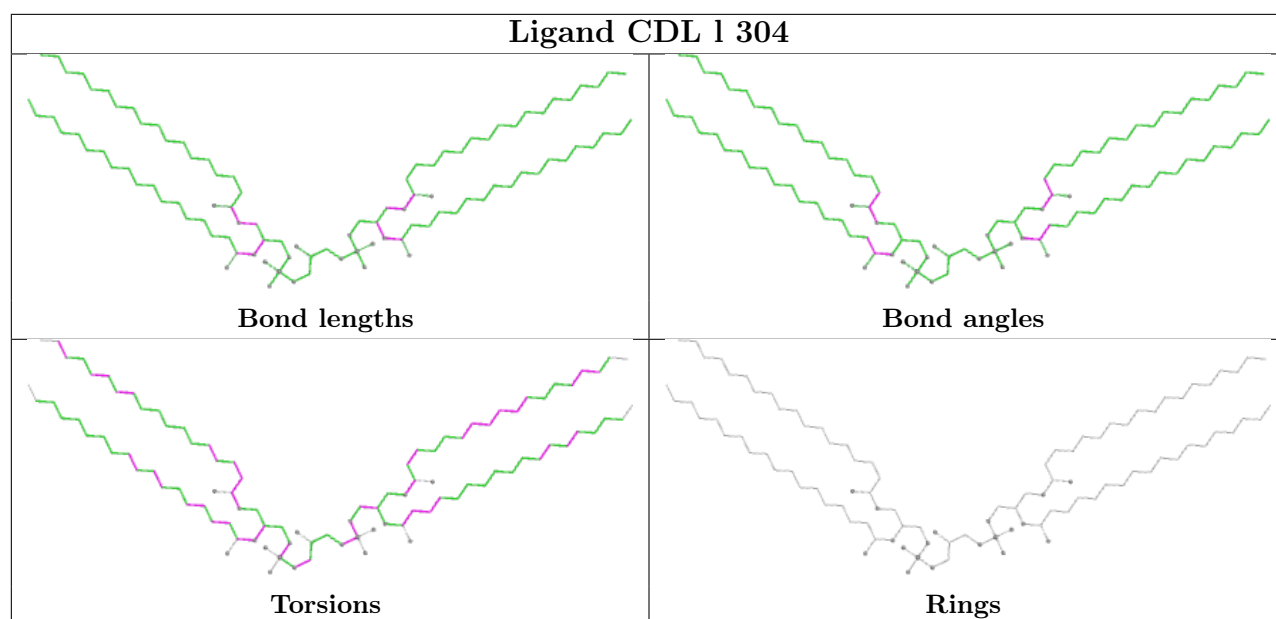


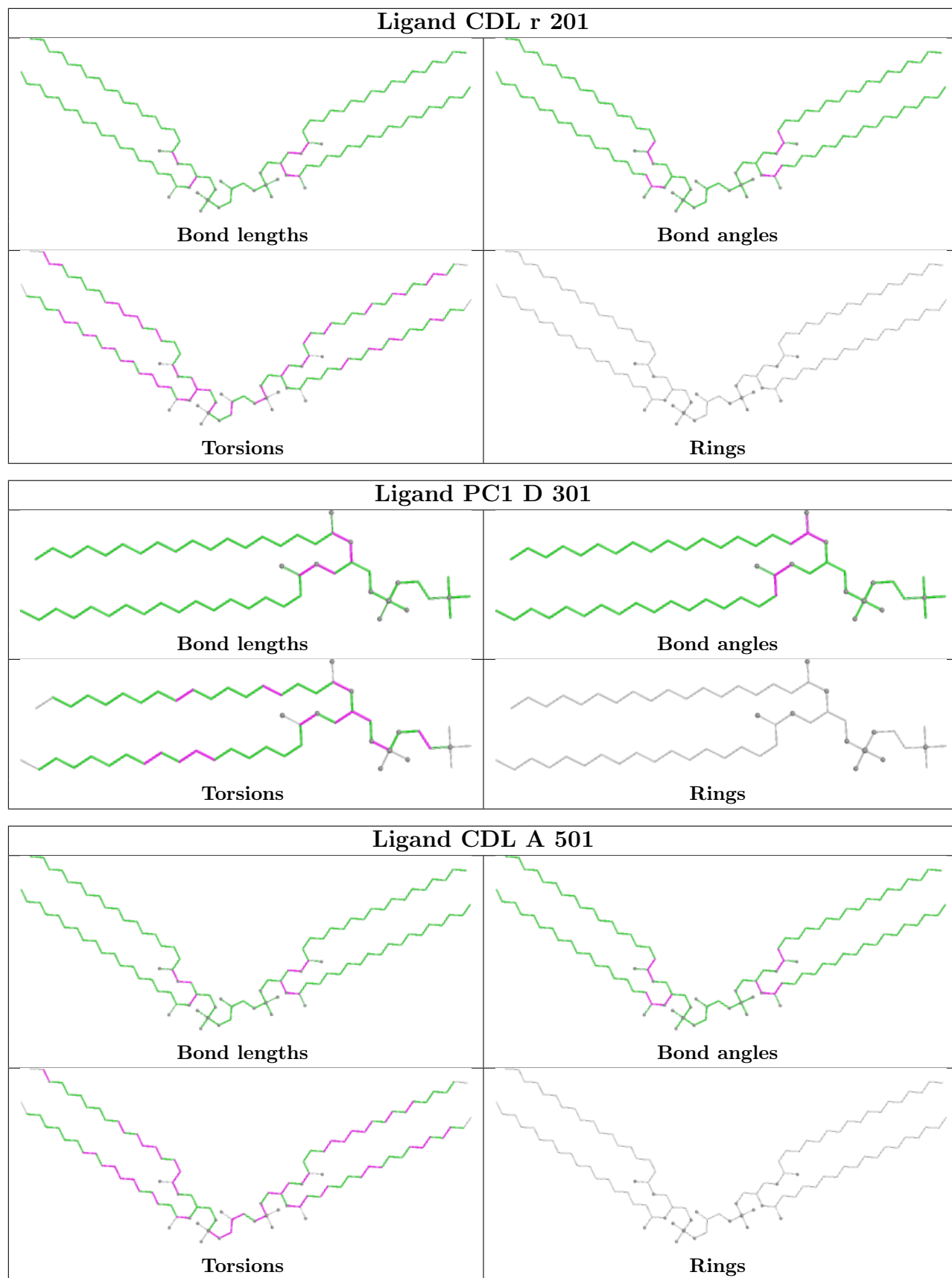


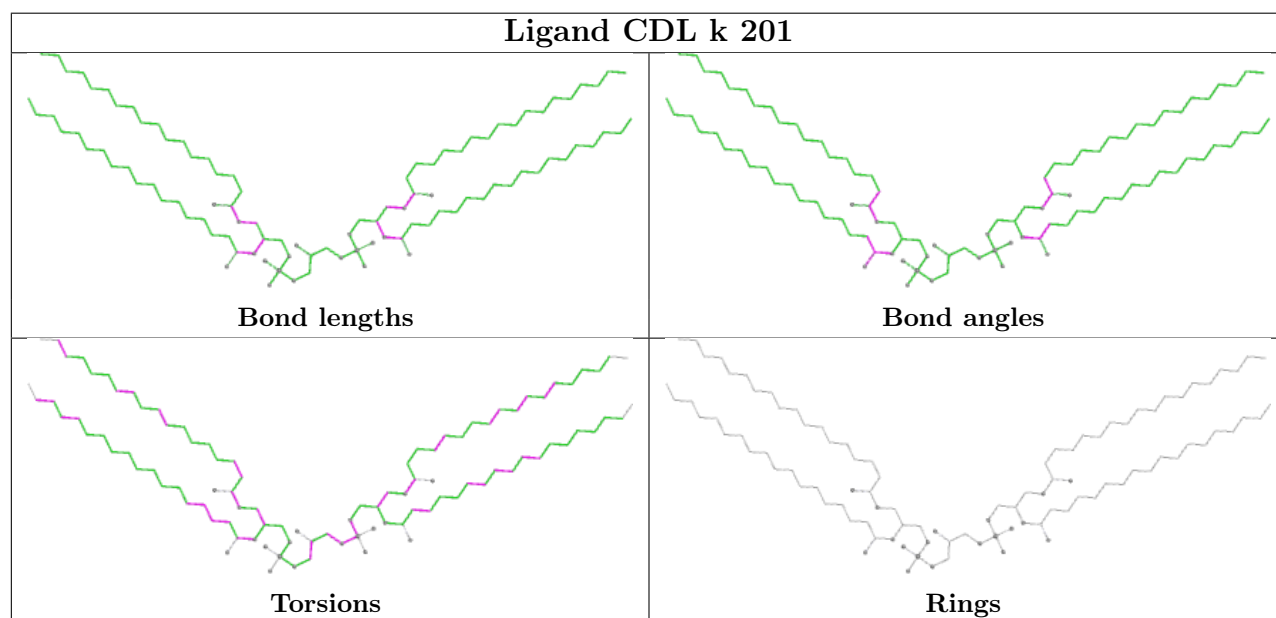
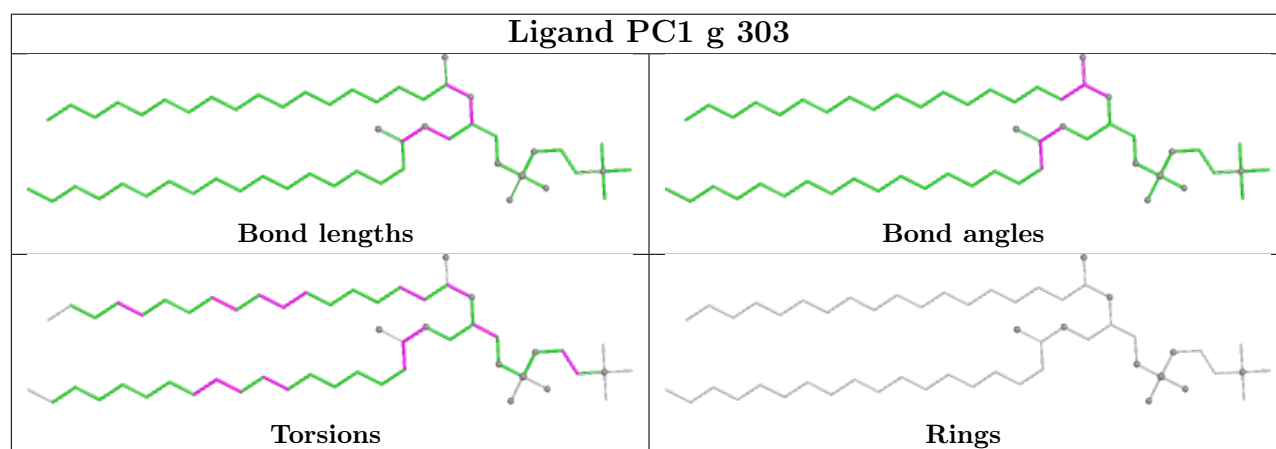
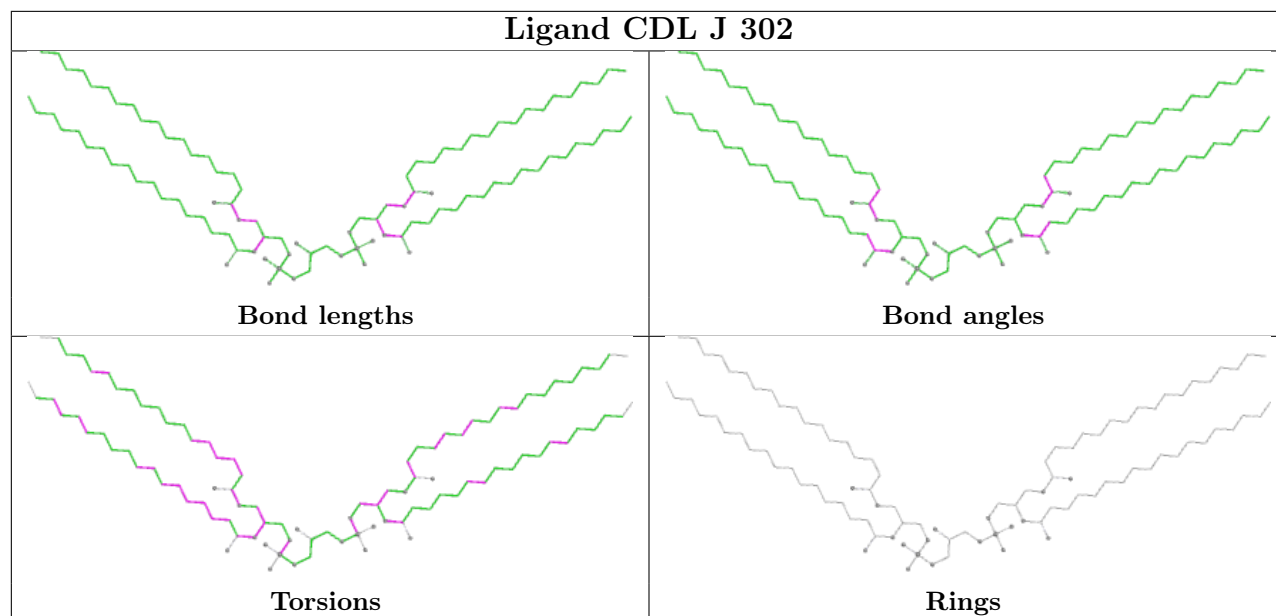


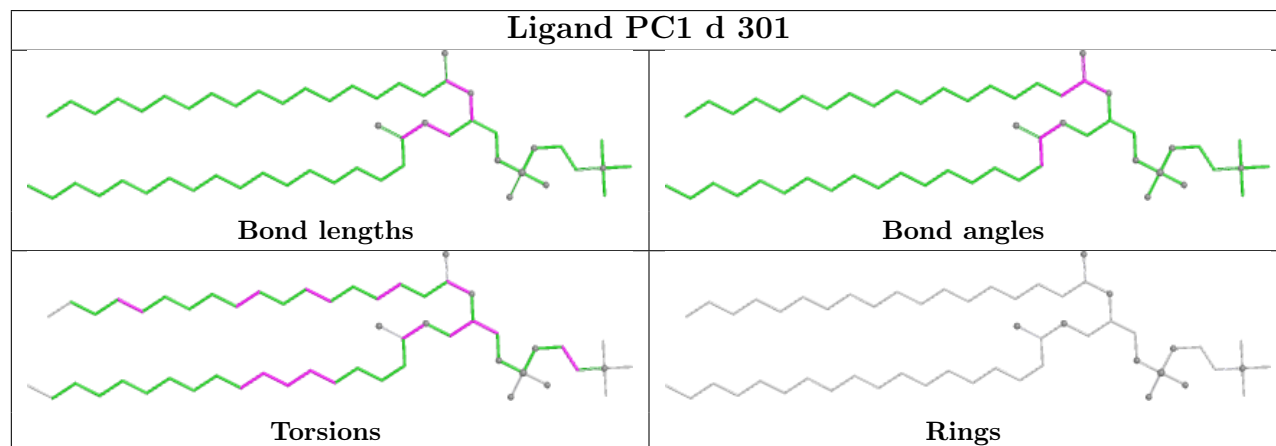
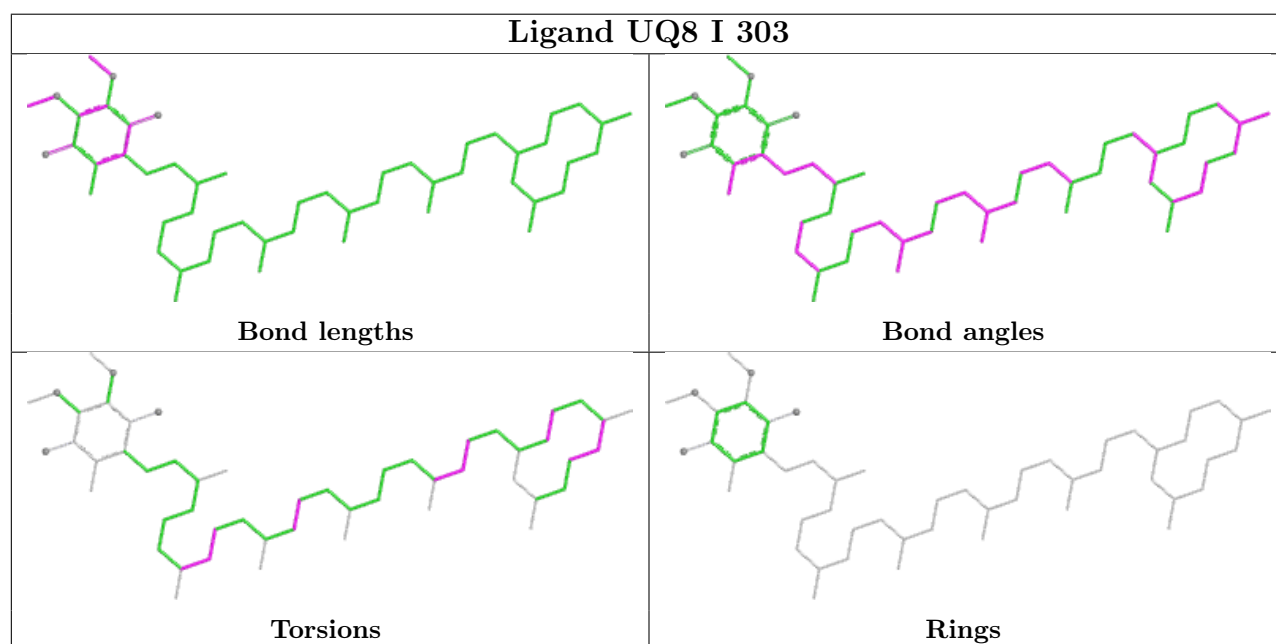
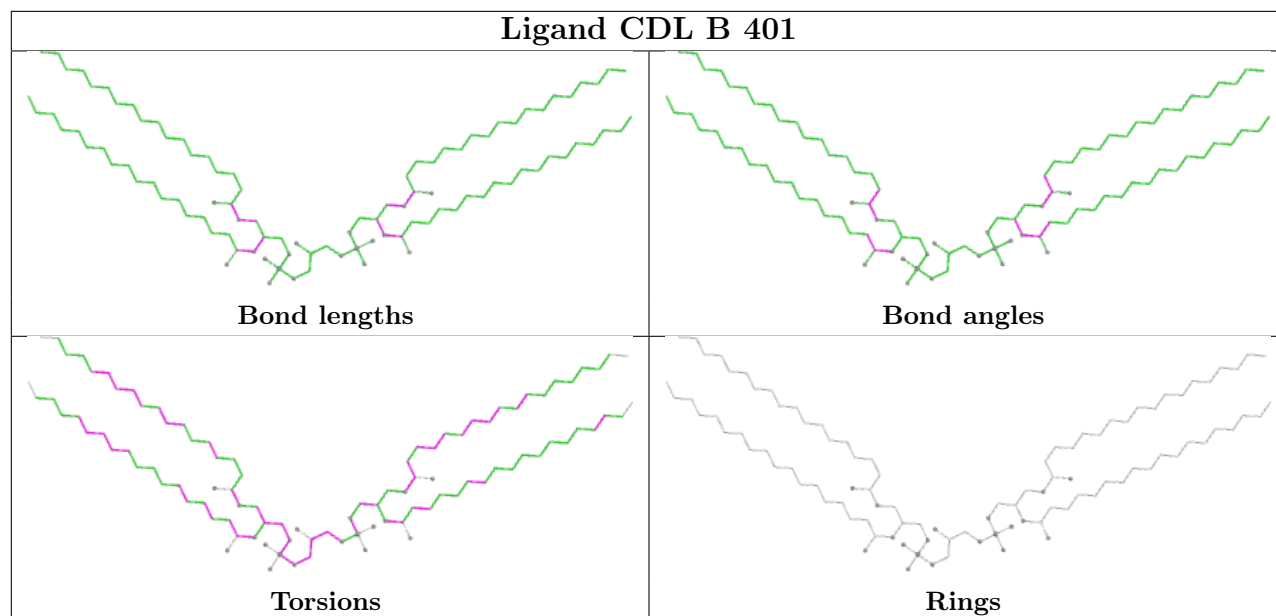


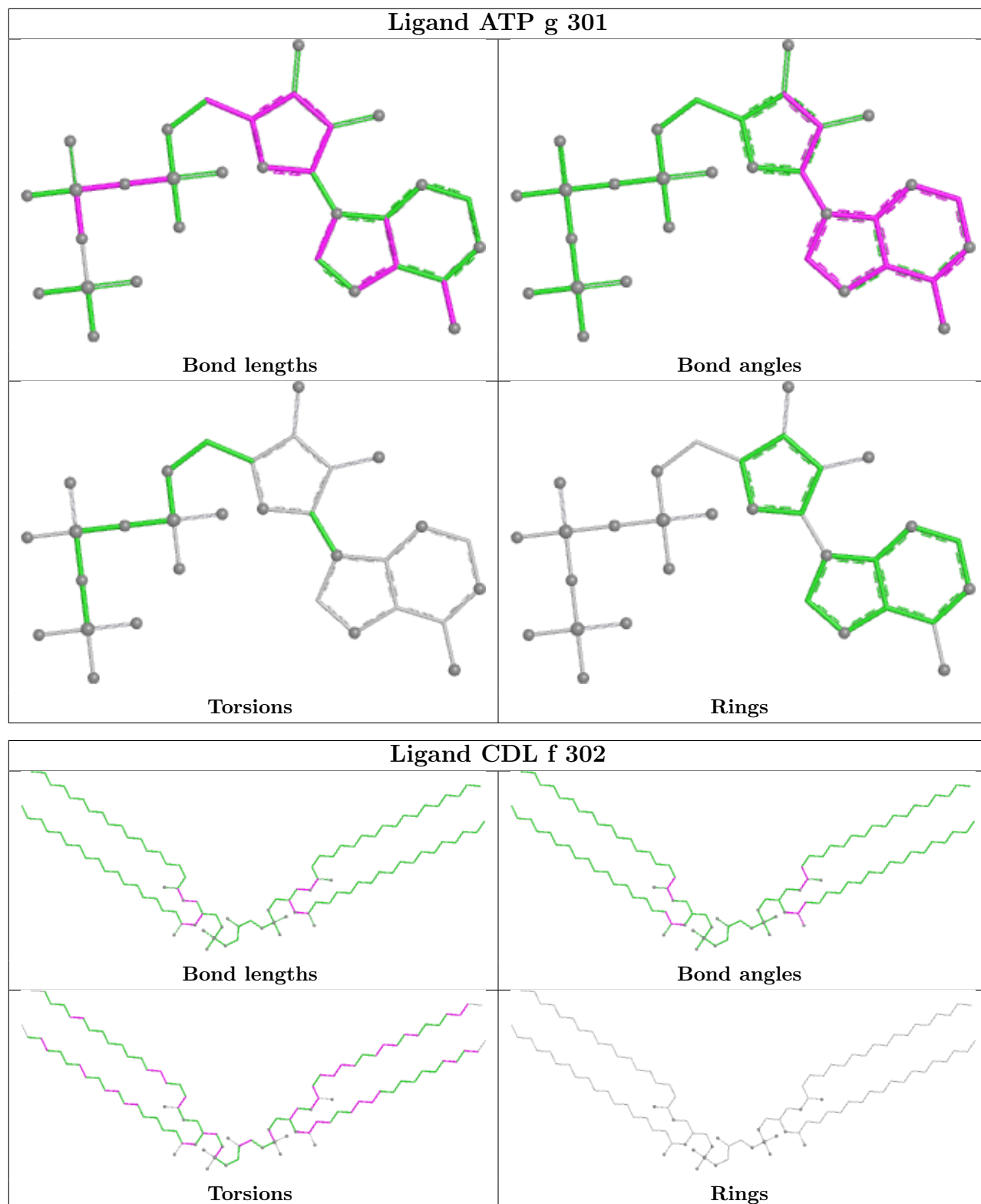


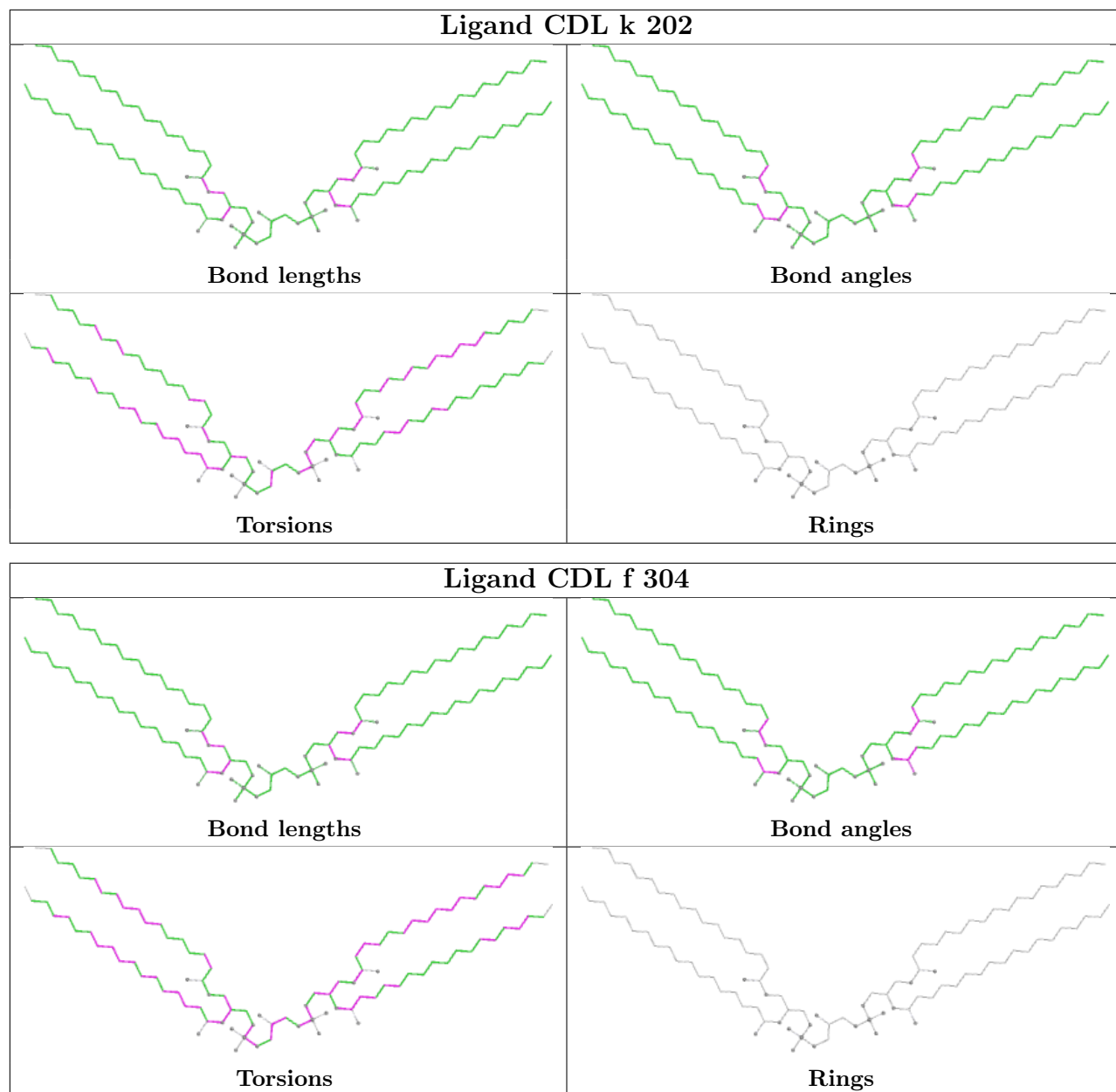


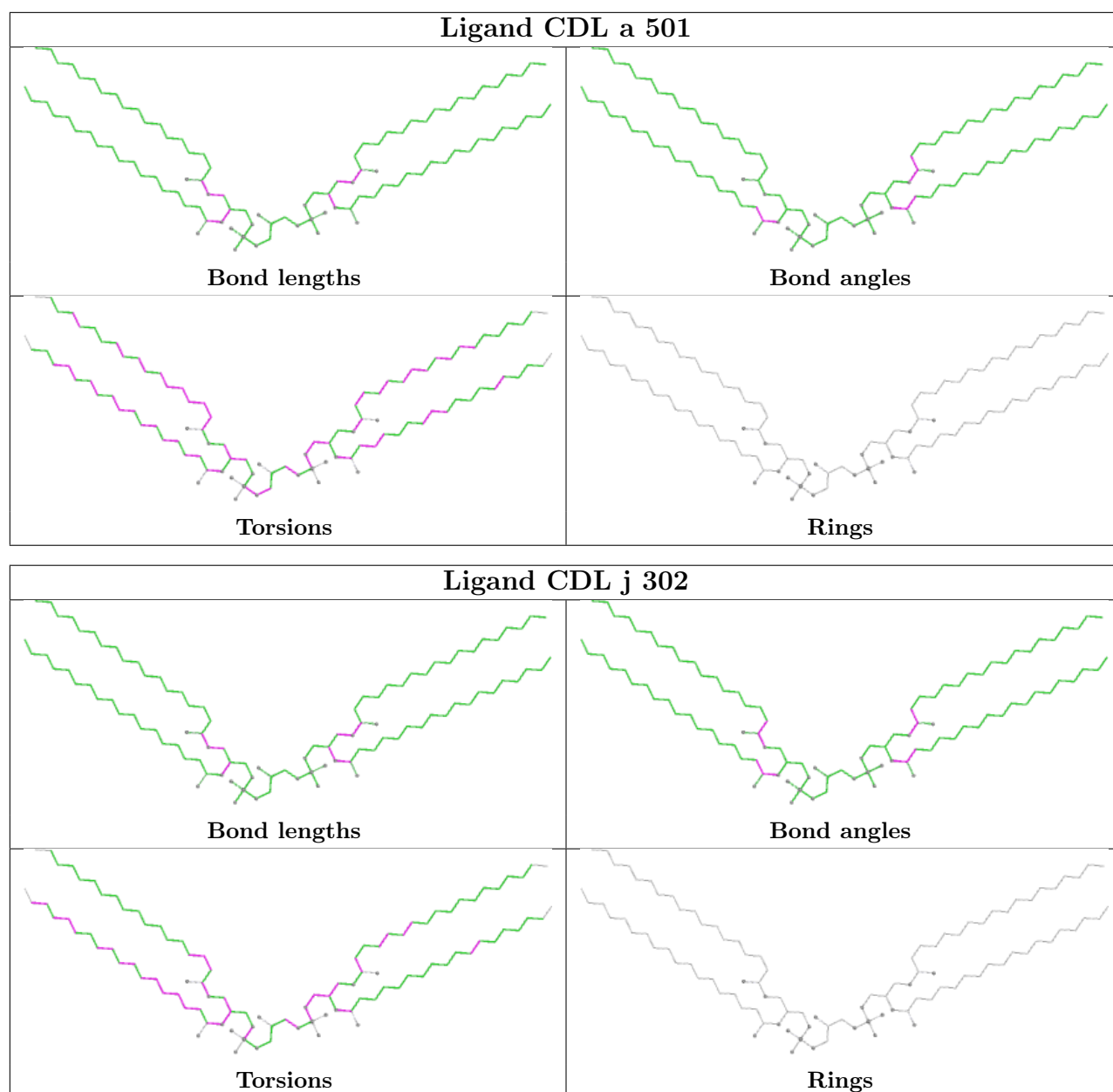












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

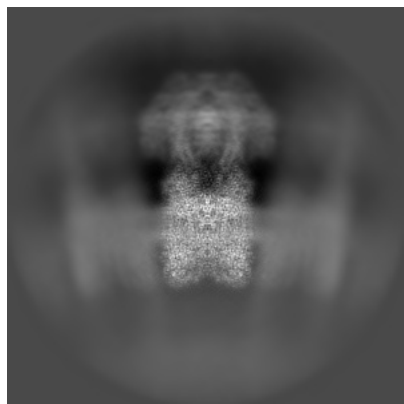
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10859. These allow visual inspection of the internal detail of the map and identification of artifacts.

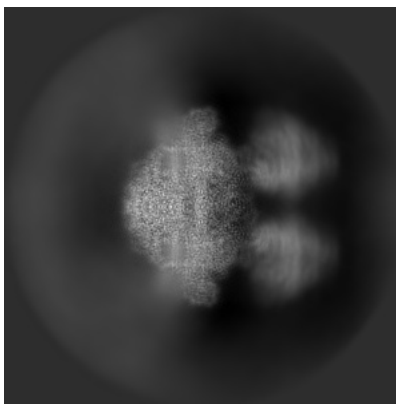
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

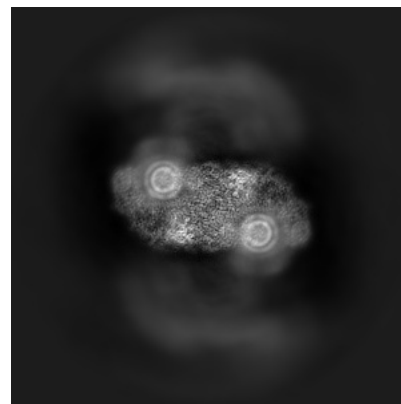
6.1.1 Primary map



X

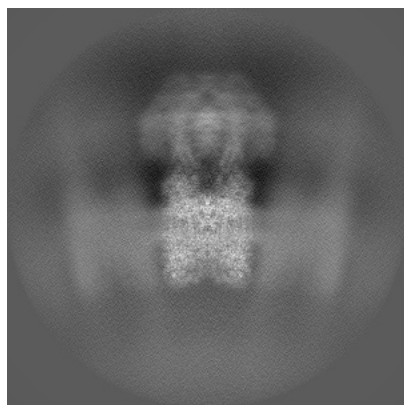


Y

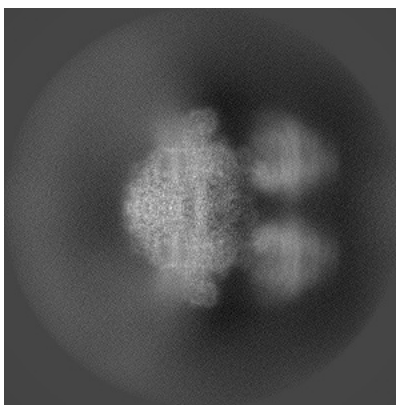


Z

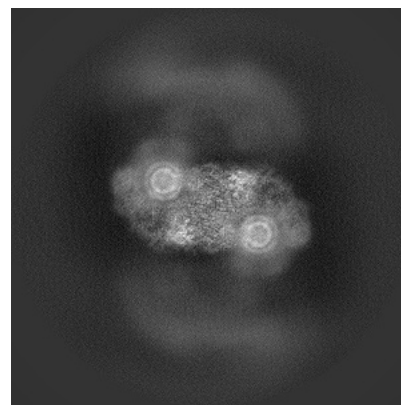
6.1.2 Raw map



X



Y

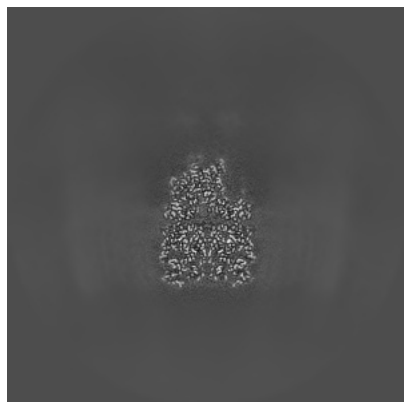


Z

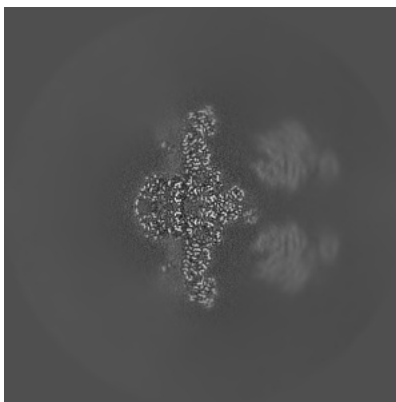
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

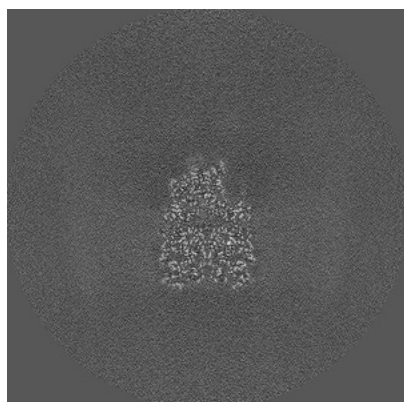


Y Index: 300

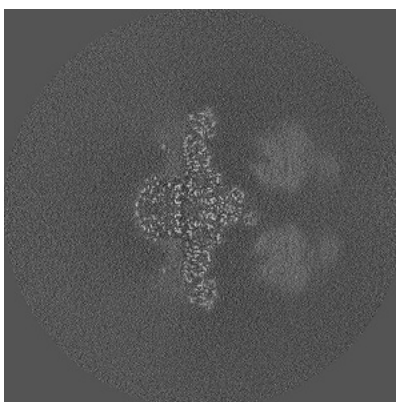


Z Index: 300

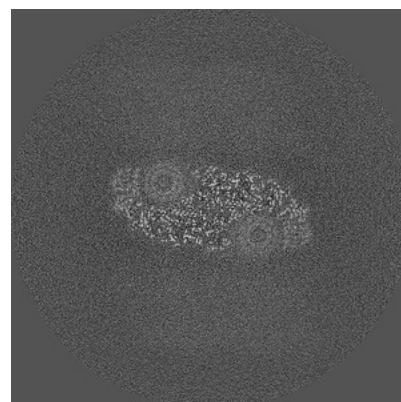
6.2.2 Raw map



X Index: 300



Y Index: 300

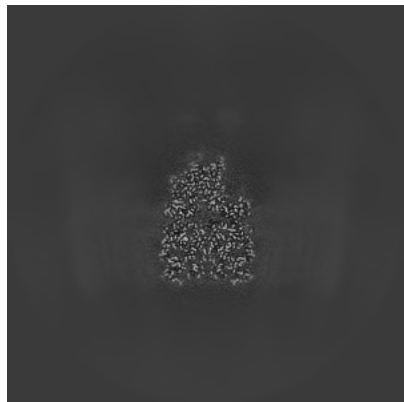


Z Index: 300

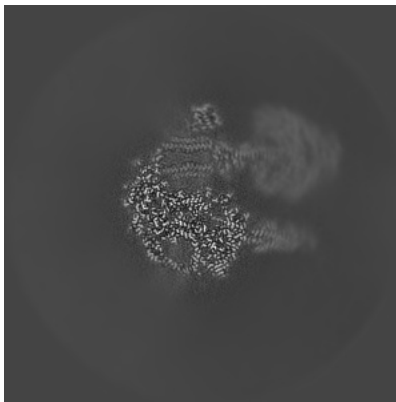
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 299

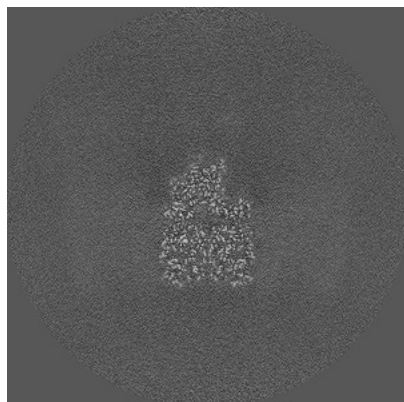


Y Index: 259

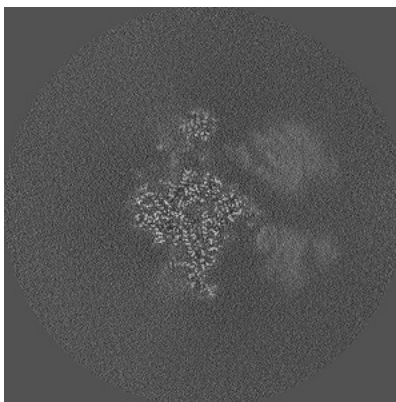


Z Index: 292

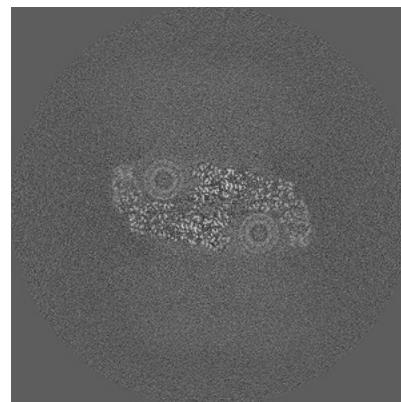
6.3.2 Raw map



X Index: 299



Y Index: 290

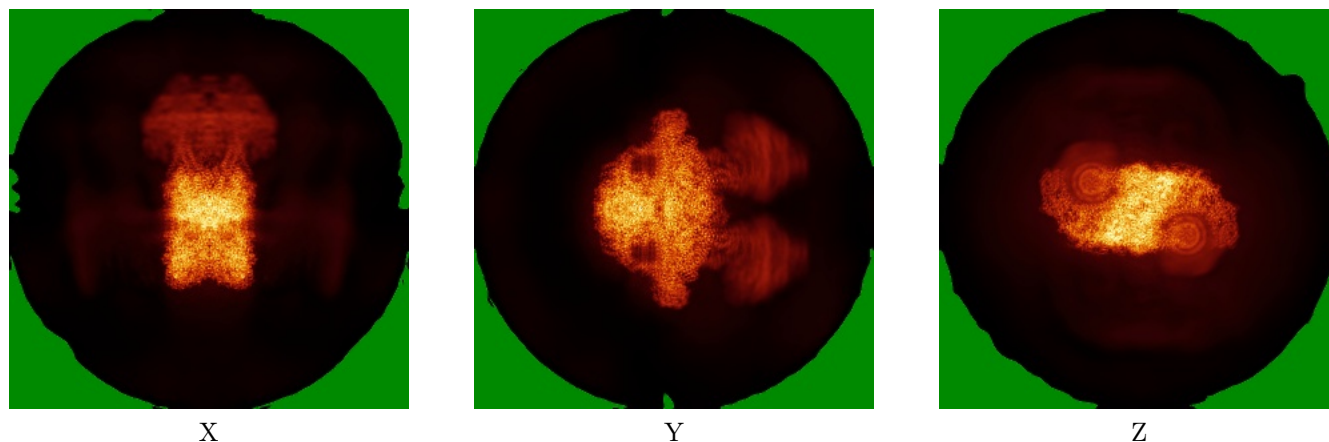


Z Index: 292

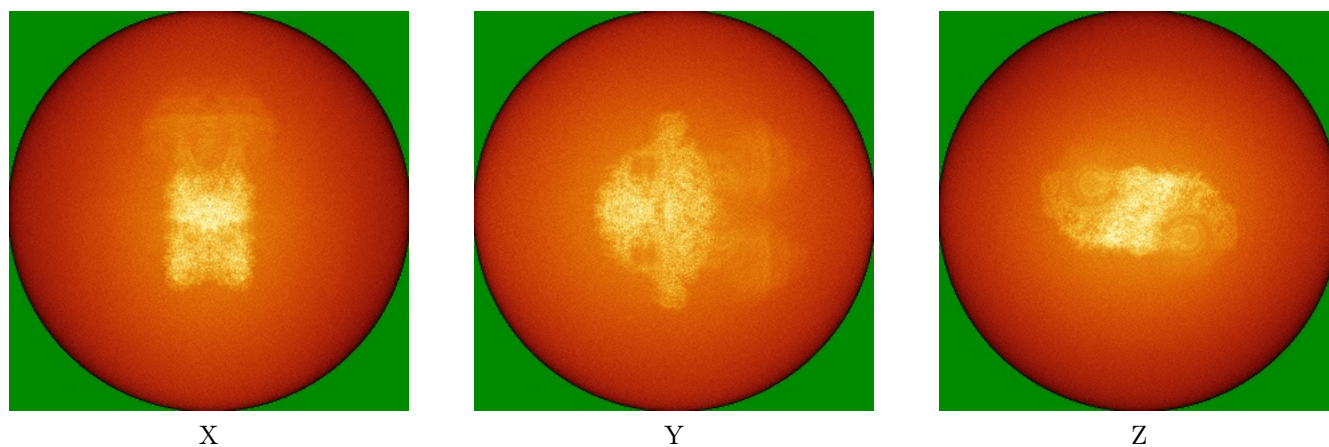
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

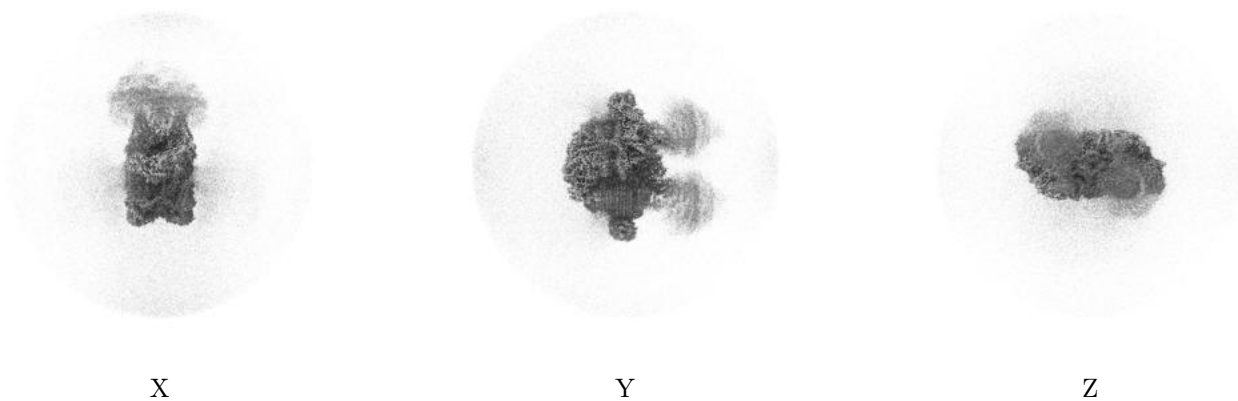
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

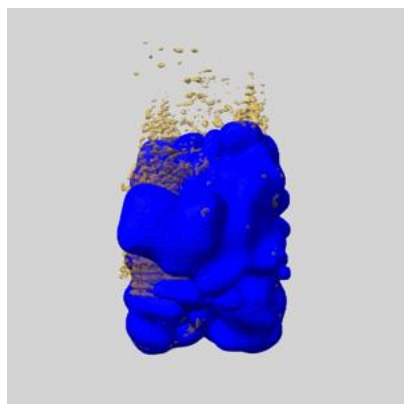
6.6 Mask visualisation [i](#)

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

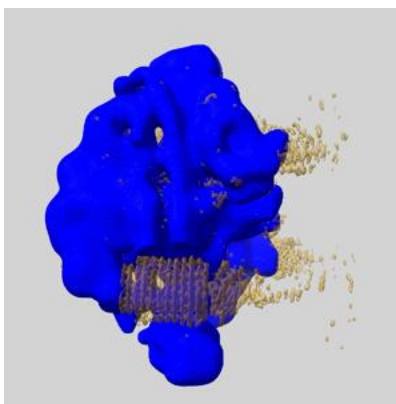
A mask typically either:

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

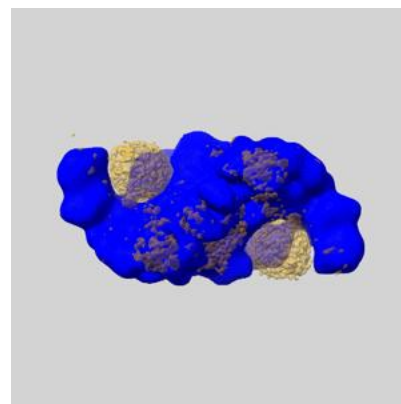
6.6.1 emd_10859_msk_1.map [i](#)



X



Y

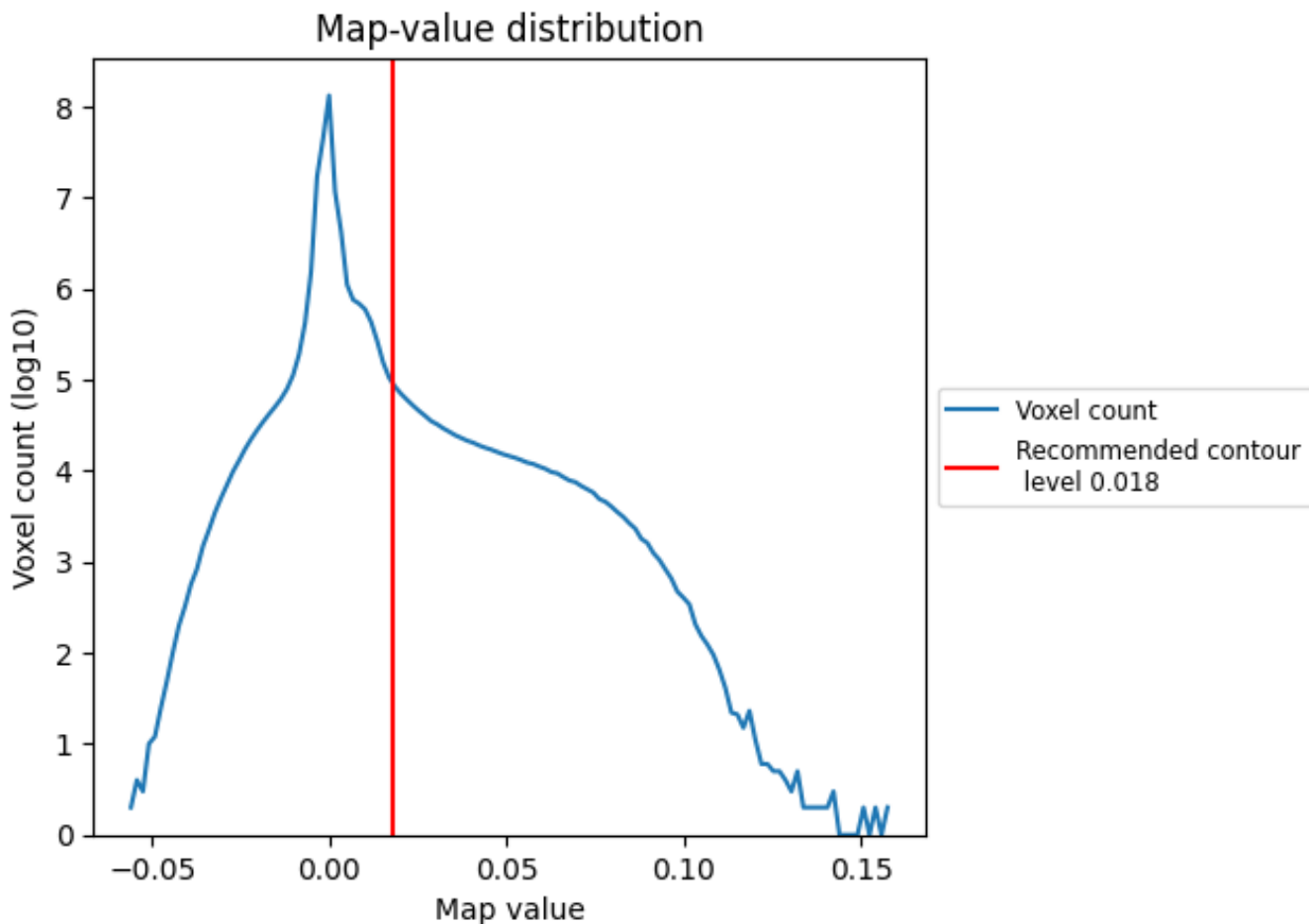


Z

7 Map analysis [i](#)

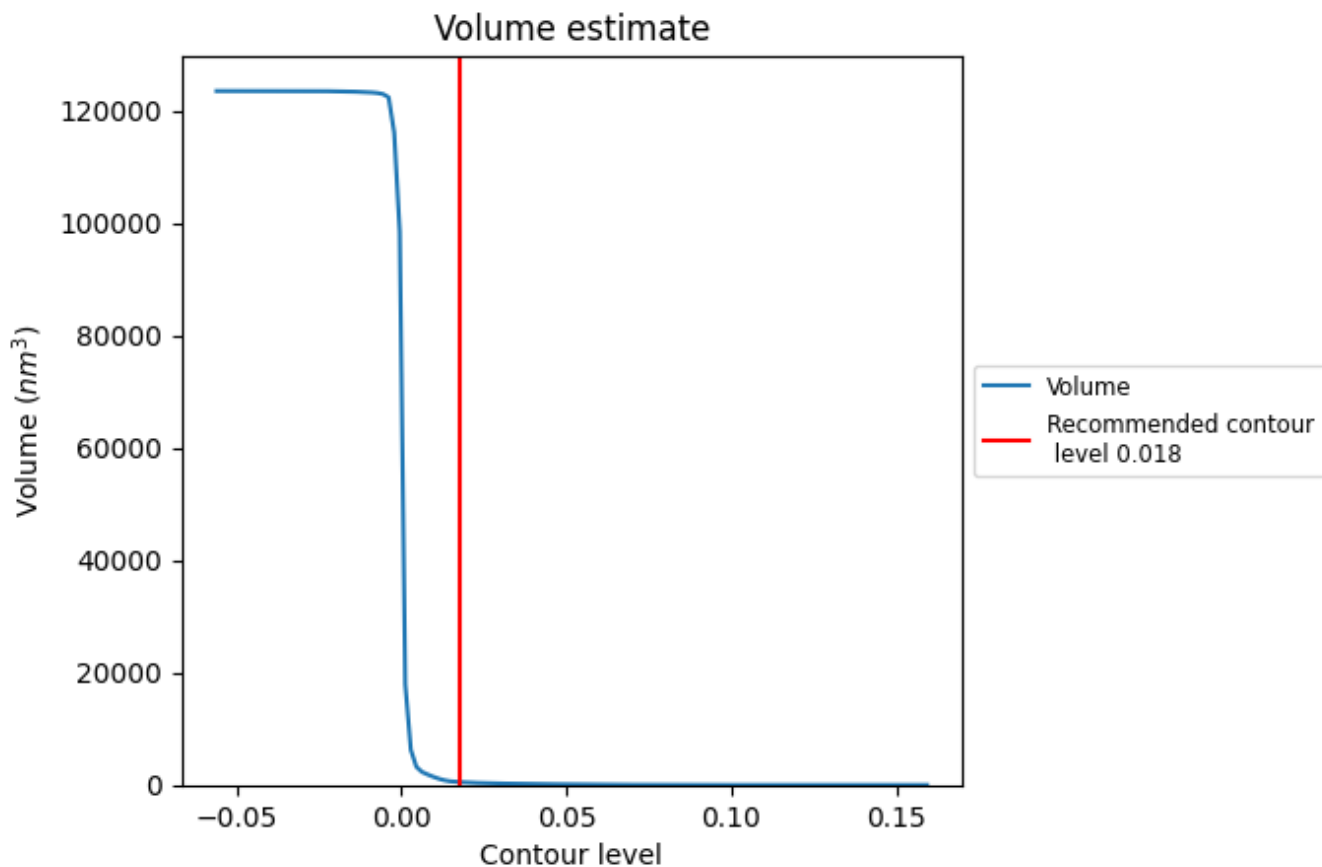
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

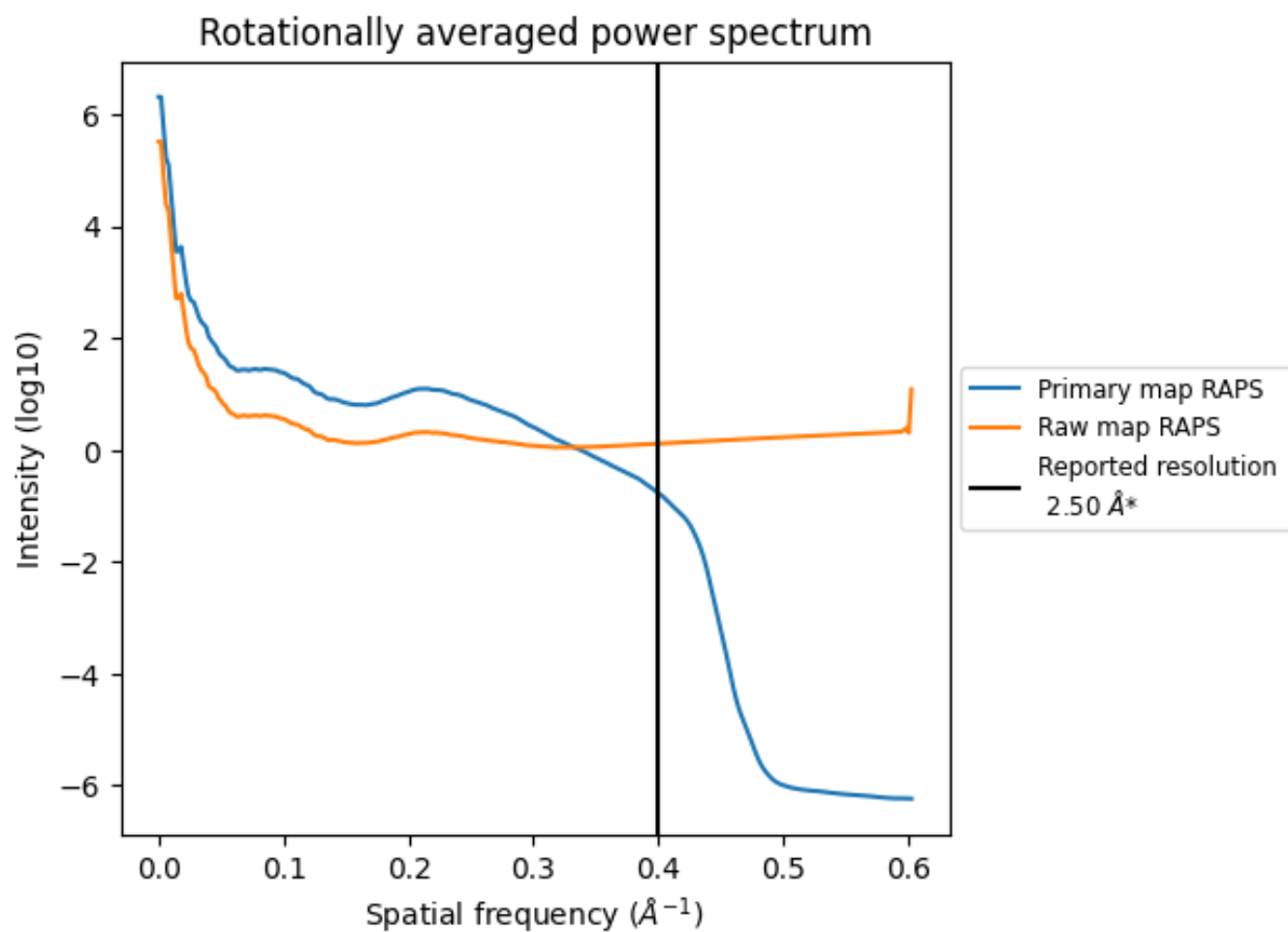
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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

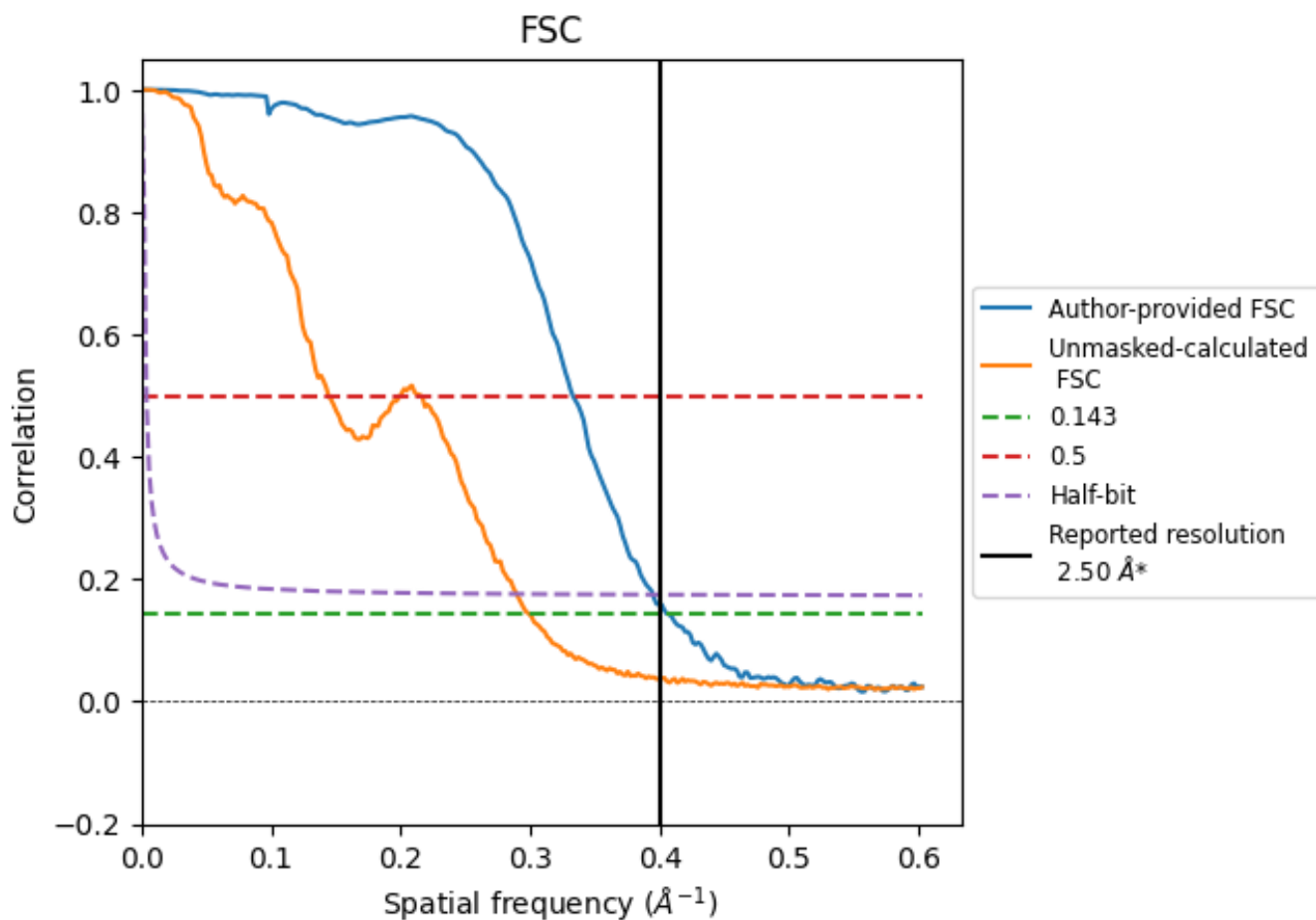


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

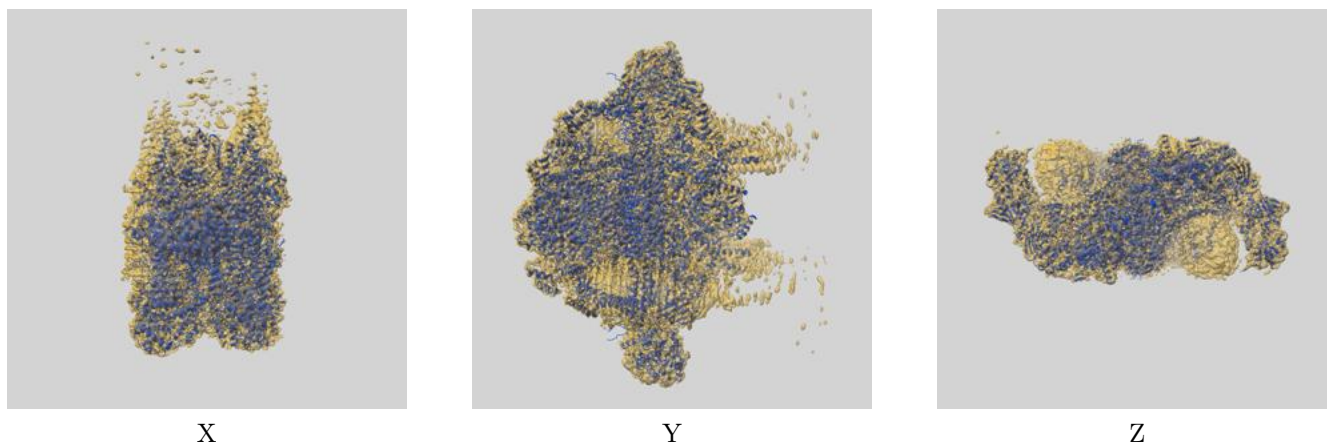
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.46	3.00	2.53
Unmasked-calculated*	3.34	6.92	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

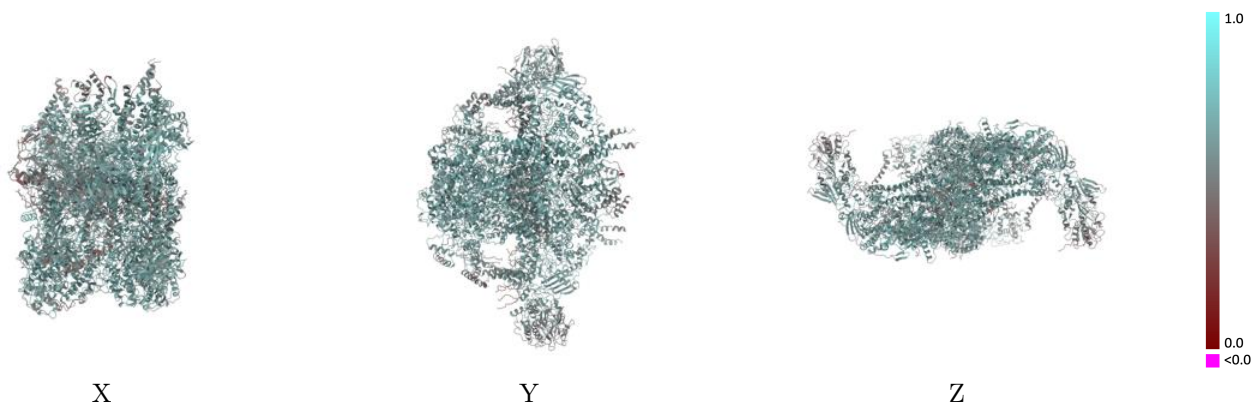
This section contains information regarding the fit between EMDB map EMD-10859 and PDB model 6YNX. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



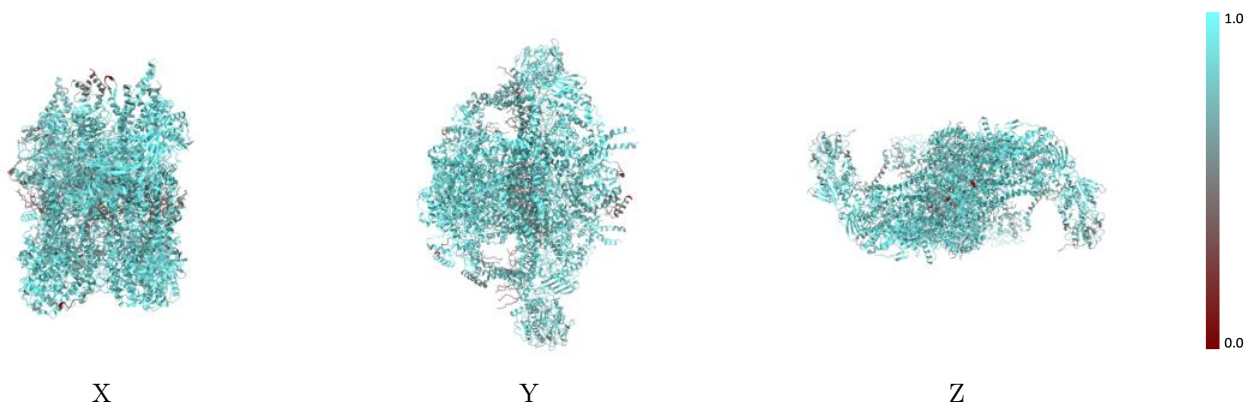
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



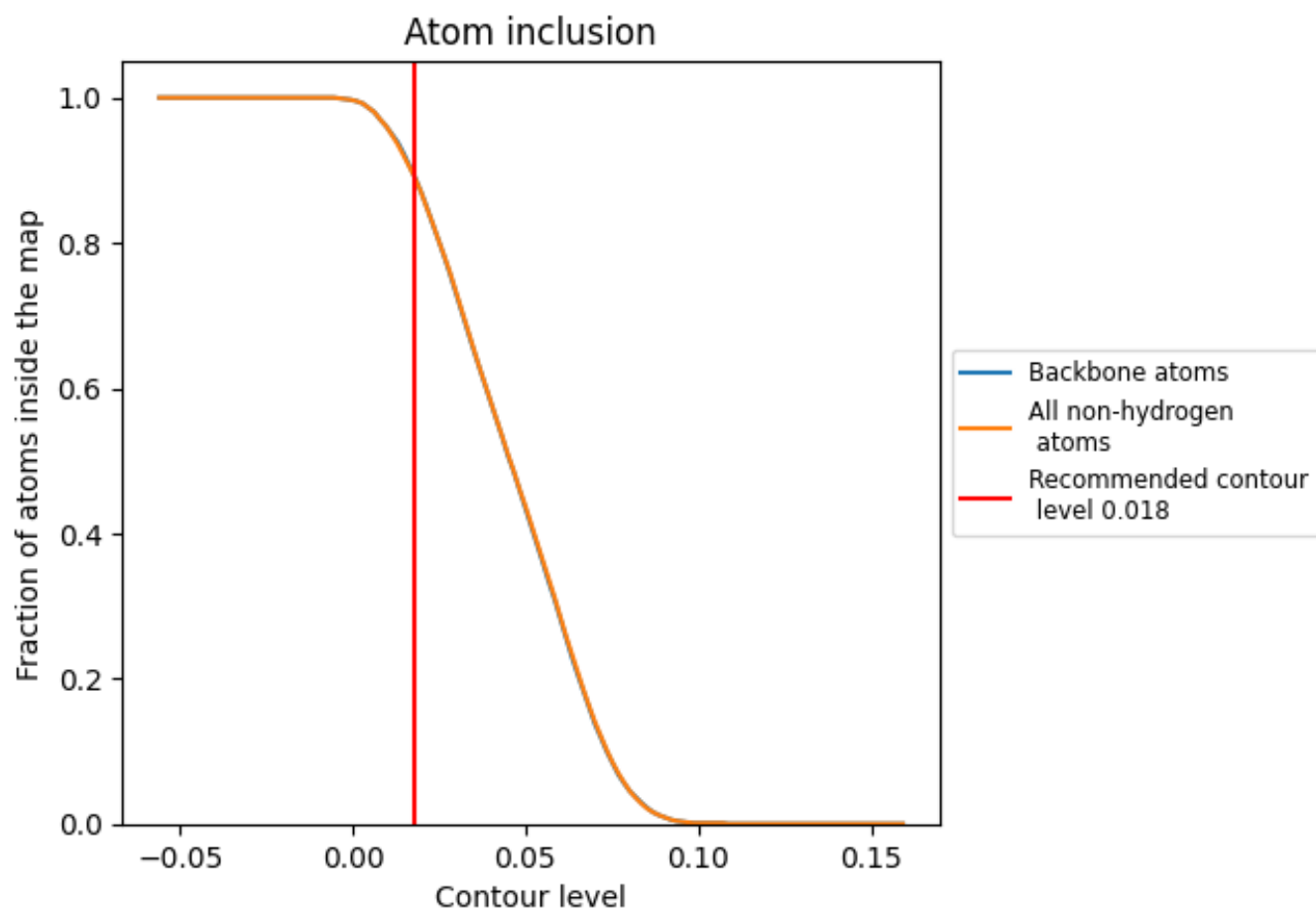
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.6170
A	0.9410	0.6470
B	0.8590	0.6150
C	0.9720	0.6630
D	0.9470	0.6500
E	0.7790	0.5230
F	0.9700	0.6710
G	0.9030	0.6150
H	0.9170	0.6300
I	0.8920	0.6220
J	0.8580	0.6070
K	0.8170	0.5610
L	0.9280	0.6450
M	0.9640	0.6530
N	0.9630	0.6550
O	0.9300	0.6230
P	0.7830	0.5660
Q	0.9060	0.6210
R	0.9350	0.6420
S	0.9270	0.6240
a	0.9430	0.6470
b	0.8970	0.6280
c	0.9710	0.6650
d	0.9510	0.6560
e	0.7880	0.5250
f	0.9220	0.6510
g	0.9170	0.6200
h	0.9230	0.6370
i	0.8890	0.6240
i1	0.5450	0.4790
i2	0.5300	0.4990
j	0.8640	0.6130
k	0.7810	0.5550
l	0.9020	0.6320
m	0.9680	0.6550



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Chain	Atom inclusion	Q-score
n	 0.9550	 0.6560
o	 0.9220	 0.6200
p	 0.7930	 0.5660
q	 0.9180	 0.6240
r	 0.9270	 0.6350
s	 0.9130	 0.6170
t	 0.9230	 0.6310