



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 07:55 PM JST

PDB ID : 7VY1
EMDB ID : EMD-32191
Title : Membrane arm of deactive state CI from Q10 dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-13
Resolution : 3.30 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:

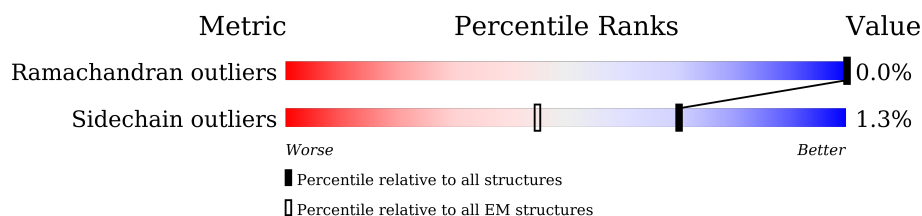
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	Q	473	
2	S	70	
3	U	84	
4	V	141	
5	W	144	
6	X	156	
7	Y	105	
8	Z	98	
9	a	189	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	b	128	
11	c	186	
12	d	176	
13	e	154	
14	f	76	
15	g	122	
16	h	106	
17	i	347	
18	j	113	
19	k	98	
20	l	603	
21	m	175	
22	n	58	
23	o	129	
24	p	179	
25	r	459	
26	s	318	
27	u	172	
28	v	136	
29	w	357	

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 38899 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 dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	40	Total	C	N	O	S	0	0
			333	217	56	59	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			699	450	103	141	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	70	Total	C	N	O	S	0	0
			597	392	98	106	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

- Molecule 10 is a protein called NADH dehydrogenase 1 beta subcomplex 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total	C	N	O	S	0	0
			875	571	158	145	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	156	Total	C	N	O	S	0	0
			1299	843	211	237	8		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	CYS	deletion	UNP A0A287BMW6
e	?	-	MET	deletion	UNP A0A287BMW6
e	?	-	GLY	deletion	UNP A0A287BMW6
e	?	-	CYS	deletion	UNP A0A287BMW6
e	?	-	PRO	deletion	UNP A0A287BMW6
e	?	-	ARG	deletion	UNP A0A287BMW6
e	?	-	GLU	deletion	UNP A0A287BMW6
e	?	-	TRP	deletion	UNP A0A287BMW6
e	?	-	GLY	deletion	UNP A0A287BMW6
e	?	-	GLY	deletion	UNP A0A287BMW6

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			344	227	58	59		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 18 is a protein called ND3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 23 is a protein called Complex I-B15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

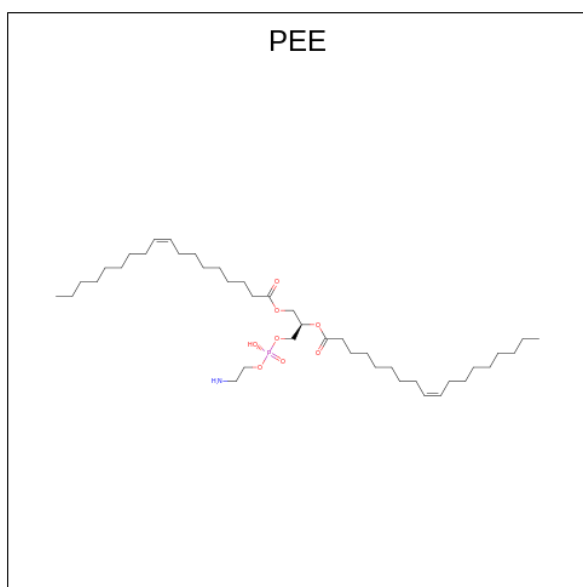
- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

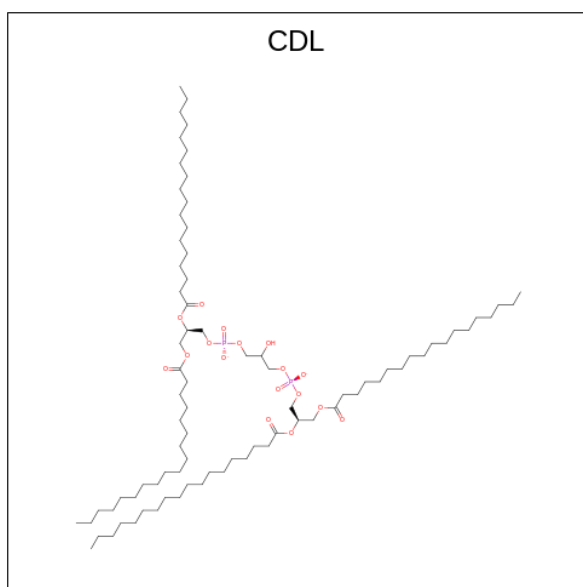
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2581	1645	437	489	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	l	1	Total	C	N	O	P	0
			86	66	2	16	2	
30	l	1	Total	C	N	O	P	0
			86	66	2	16	2	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 31 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



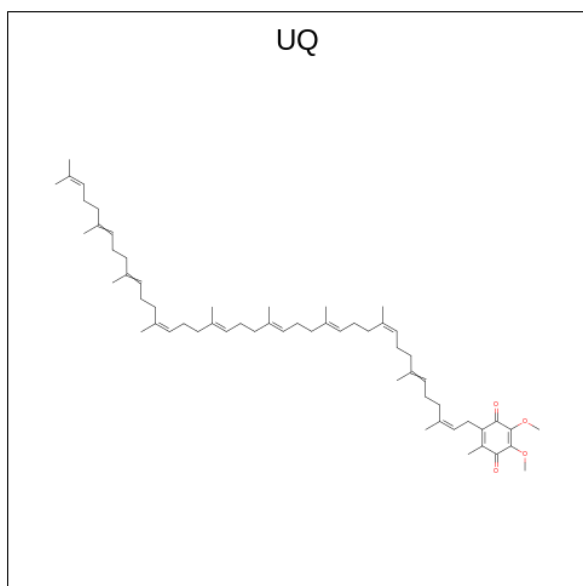
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	a	1	Total	C	O	P	0
			91	72	17	2	
31	g	1	Total	C	O	P	0
			95	76	17	2	
31	i	1	Total	C	O	P	0
			66	47	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	
31	o	1	Total	C	O	P	0
			68	49	17	2	
31	r	1	Total	C	O	P	0
			99	80	17	2	
31	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).

Continued from previous page...

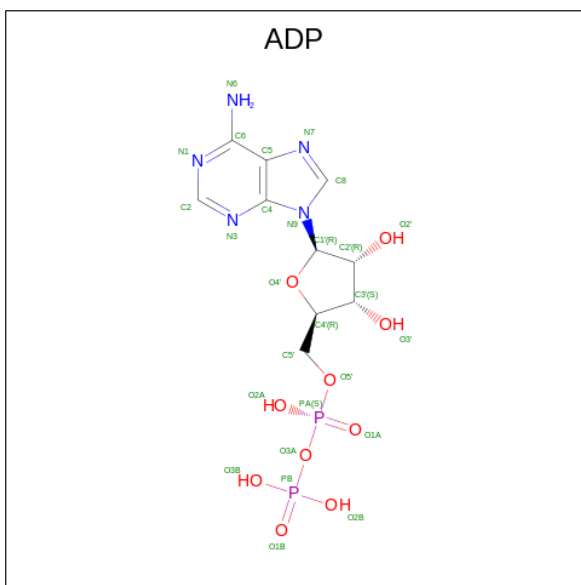
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			104	84	2	16	2	
33	r	1	Total	C	N	O	P	0
			104	84	2	16	2	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).

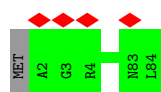


Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			28	24	4	

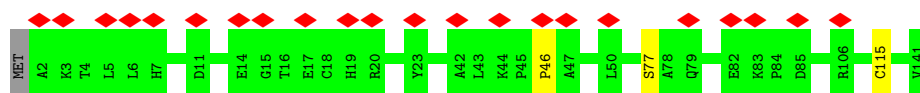
- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



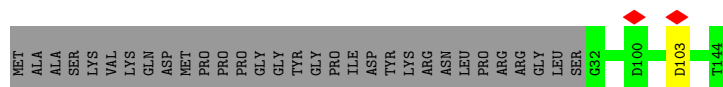
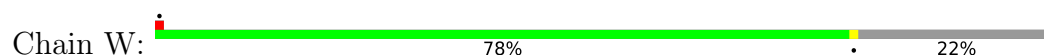
Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	



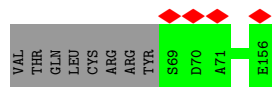
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



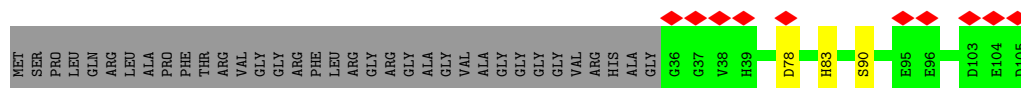
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



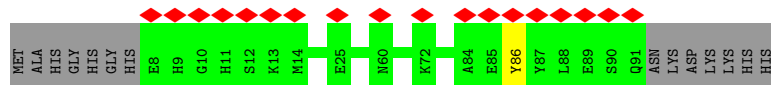
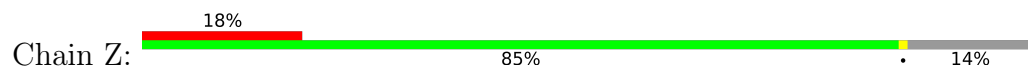
- Molecule 6: Acyl carrier protein



- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

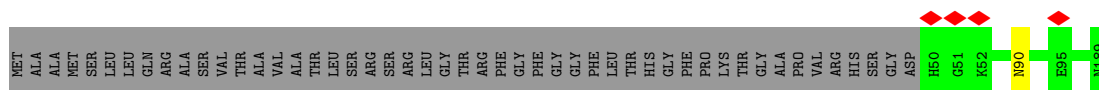


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

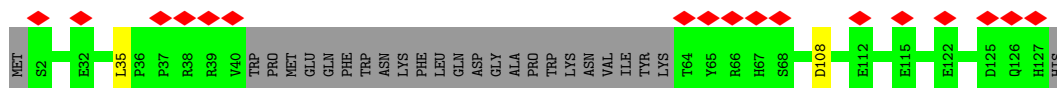
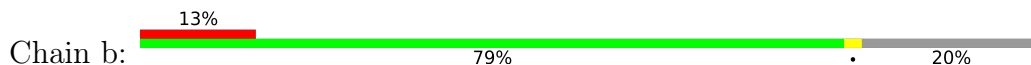


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

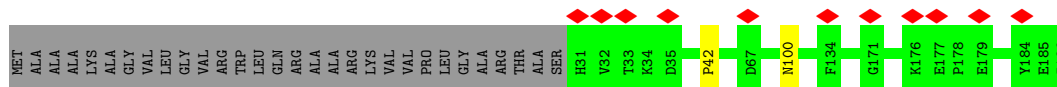
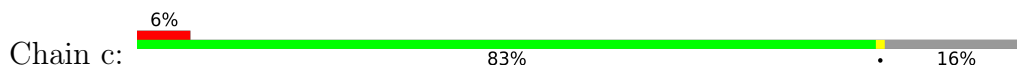




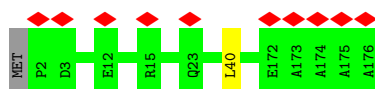
- Molecule 10: NADH dehydrogenase 1 beta subcomplex 6



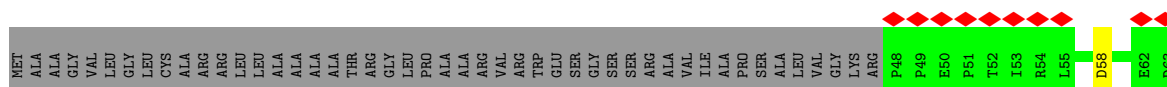
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



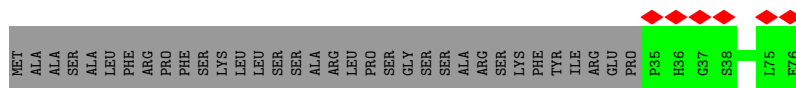
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 13: Complex I-ESSS

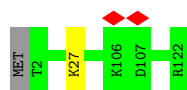


- Molecule 14: Complex I-KFYI

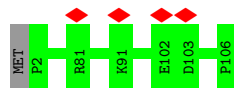


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

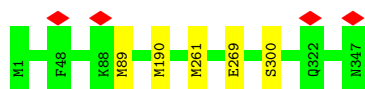




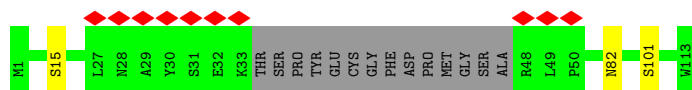
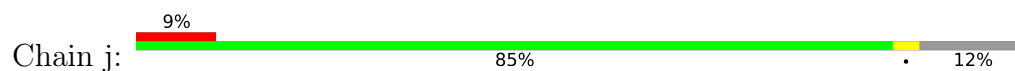
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



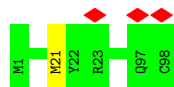
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



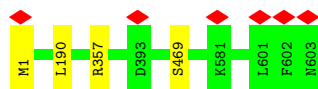
- Molecule 18: ND3



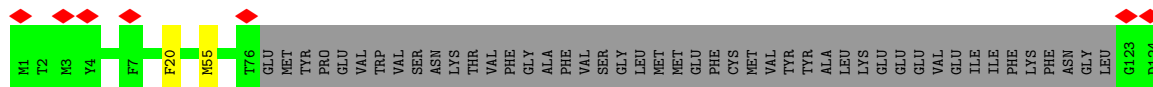
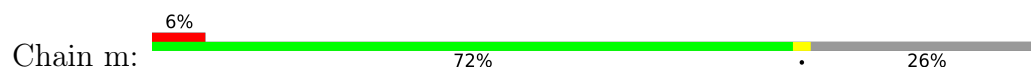
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

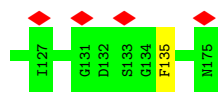


- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

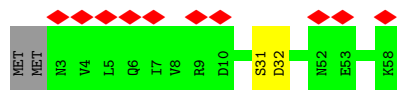


- Molecule 21: NADH-ubiquinone oxidoreductase chain 6

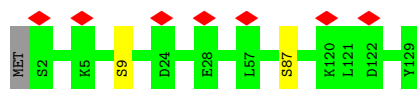




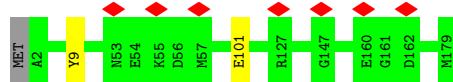
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 23: Complex I-B15



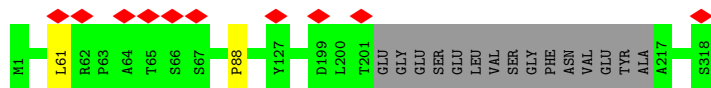
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



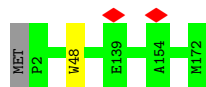
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4



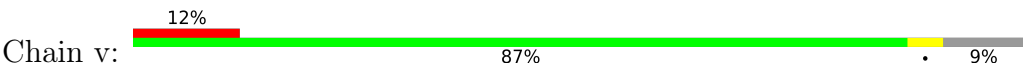
- Molecule 26: NADH-ubiquinone oxidoreductase chain 1



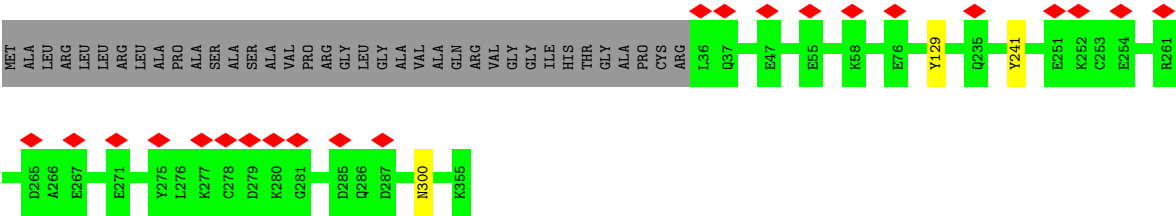
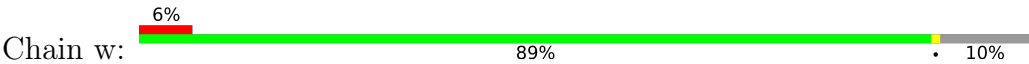
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0238	Depositor
Map size (Å)	354.48602, 354.48602, 354.48602	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8Q1, ADP, PLX, CDL, PEE, UQ

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	Q	0.28	0/350	0.45	0/483
2	S	0.27	0/582	0.48	0/783
3	U	0.26	0/664	0.44	0/912
4	V	0.27	0/1042	0.48	0/1411
5	W	0.29	0/973	0.50	0/1312
6	X	0.27	0/711	0.44	0/963
7	Y	0.26	0/623	0.45	0/853
8	Z	0.25	0/695	0.47	0/939
9	a	0.29	0/1199	0.48	0/1623
10	b	0.27	0/902	0.51	0/1227
11	c	0.29	0/1355	0.48	0/1857
12	d	0.28	0/1494	0.51	0/2015
13	e	0.26	0/916	0.53	2/1246 (0.2%)
14	f	0.25	0/353	0.43	0/477
15	g	0.29	0/1031	0.47	0/1394
16	h	0.26	0/889	0.47	0/1190
17	i	0.27	0/2773	0.45	0/3768
18	j	0.27	0/819	0.46	0/1117
19	k	0.27	0/759	0.44	0/1029
20	l	0.28	0/4914	0.45	0/6683
21	m	0.30	0/973	0.50	0/1320
22	n	0.25	0/491	0.50	0/663
23	o	0.28	0/1092	0.51	0/1481
24	p	0.28	0/1590	0.51	0/2155
25	r	0.28	0/3723	0.46	0/5078
26	s	0.28	0/2464	0.47	0/3369
27	u	0.27	0/1436	0.48	0/1938
28	v	0.28	0/1052	0.55	0/1411
29	w	0.28	0/2641	0.47	0/3577
All	All	0.28	0/38506	0.48	2/52274 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	83	ASP	CB-CG-OD1	5.88	123.59	118.30
13	e	83	ASP	CB-CG-OD2	-5.08	113.72	118.30

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	Q	38/473 (8%)	37 (97%)	1 (3%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
4	V	138/141 (98%)	129 (94%)	8 (6%)	1 (1%)	22	54
5	W	111/144 (77%)	109 (98%)	2 (2%)	0	100	100
6	X	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/105 (65%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/98 (84%)	79 (96%)	3 (4%)	0	100	100
9	a	138/189 (73%)	134 (97%)	4 (3%)	0	100	100
10	b	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
11	c	154/186 (83%)	142 (92%)	11 (7%)	1 (1%)	25	57
12	d	173/176 (98%)	169 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	e	105/154 (68%)	102 (97%)	3 (3%)	0	100	100
14	f	40/76 (53%)	39 (98%)	1 (2%)	0	100	100
15	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
16	h	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
17	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
18	j	95/113 (84%)	88 (93%)	7 (7%)	0	100	100
19	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
20	l	601/603 (100%)	568 (94%)	33 (6%)	0	100	100
21	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
22	n	54/58 (93%)	54 (100%)	0	0	100	100
23	o	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
24	p	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
25	r	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
26	s	299/318 (94%)	288 (96%)	11 (4%)	0	100	100
27	u	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
28	v	122/136 (90%)	118 (97%)	4 (3%)	0	100	100
29	w	318/357 (89%)	302 (95%)	16 (5%)	0	100	100
All	All	4586/5552 (83%)	4384 (96%)	200 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	c	42	PRO
4	V	46	PRO

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	Q	34/401 (8%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	58/58 (100%)	58 (100%)	0	100	100
3	U	69/70 (99%)	69 (100%)	0	100	100
4	V	101/102 (99%)	99 (98%)	2 (2%)	55	76
5	W	99/124 (80%)	98 (99%)	1 (1%)	76	86
6	X	78/132 (59%)	78 (100%)	0	100	100
7	Y	62/84 (74%)	59 (95%)	3 (5%)	25	56
8	Z	65/76 (86%)	64 (98%)	1 (2%)	65	81
9	a	122/158 (77%)	121 (99%)	1 (1%)	81	89
10	b	97/121 (80%)	95 (98%)	2 (2%)	53	75
11	c	137/160 (86%)	136 (99%)	1 (1%)	84	90
12	d	155/156 (99%)	154 (99%)	1 (1%)	86	91
13	e	99/129 (77%)	97 (98%)	2 (2%)	55	76
14	f	36/66 (54%)	36 (100%)	0	100	100
15	g	108/109 (99%)	107 (99%)	1 (1%)	78	87
16	h	93/94 (99%)	93 (100%)	0	100	100
17	i	311/311 (100%)	306 (98%)	5 (2%)	62	79
18	j	88/99 (89%)	85 (97%)	3 (3%)	37	65
19	k	85/85 (100%)	84 (99%)	1 (1%)	71	83
20	l	537/537 (100%)	533 (99%)	4 (1%)	84	90
21	m	99/141 (70%)	96 (97%)	3 (3%)	41	68
22	n	53/55 (96%)	51 (96%)	2 (4%)	33	62
23	o	113/114 (99%)	111 (98%)	2 (2%)	59	78
24	p	159/160 (99%)	157 (99%)	2 (1%)	69	82
25	r	410/410 (100%)	407 (99%)	3 (1%)	84	90
26	s	263/275 (96%)	261 (99%)	2 (1%)	81	89
27	u	153/154 (99%)	152 (99%)	1 (1%)	84	90
28	v	104/119 (87%)	98 (94%)	6 (6%)	20	50
29	w	281/307 (92%)	278 (99%)	3 (1%)	73	85
All	All	4069/4807 (85%)	4017 (99%)	52 (1%)	70	82

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	m	20	PHE
24	p	9	TYR
29	w	129	TYR
21	m	55	MET
22	n	32	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
12	d	124	ASN
20	l	59	GLN
26	s	287	HIS
28	v	47	ASN
28	v	110	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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
30	PEE	j	201	-	50,50,50	1.15	6 (12%)	53,55,55	0.96	2 (3%)
31	CDL	V	201	-	93,93,99	1.11	8 (8%)	99,105,111	0.85	4 (4%)
32	8Q1	X	201	-	31,34,34	1.68	6 (19%)	40,43,43	1.60	6 (15%)
33	PLX	g	201	-	51,51,51	1.13	3 (5%)	55,59,59	0.62	1 (1%)
33	PLX	a	202	-	51,51,51	0.63	0	55,59,59	0.66	0
30	PEE	l	703	-	45,45,50	1.22	6 (13%)	48,50,55	0.97	2 (4%)
33	PLX	r	503	-	51,51,51	1.13	3 (5%)	55,59,59	0.59	1 (1%)
31	CDL	l	702	-	99,99,99	1.08	9 (9%)	105,111,111	0.85	4 (3%)
31	CDL	i	401	-	65,65,99	1.26	8 (12%)	71,77,111	1.03	4 (5%)
30	PEE	b	201	-	45,45,50	1.22	5 (11%)	48,50,55	0.98	2 (4%)
30	PEE	U	401	-	50,50,50	1.15	6 (12%)	53,55,55	0.97	2 (3%)
34	UQ	s	401	-	28,28,63	0.52	0	34,37,79	0.97	2 (5%)
30	PEE	W	201	-	40,40,50	1.13	5 (12%)	43,45,55	1.02	2 (4%)
31	CDL	r	504	-	98,98,99	1.08	8 (8%)	104,110,111	0.91	4 (3%)
33	PLX	r	502	-	51,51,51	1.12	4 (7%)	55,59,59	0.64	1 (1%)
35	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.43	4 (13%)
31	CDL	o	201	-	67,67,99	1.24	8 (11%)	73,79,111	1.01	4 (5%)
33	PLX	j	202	-	51,51,51	1.14	3 (5%)	55,59,59	0.60	1 (1%)
30	PEE	r	501	-	50,50,50	1.16	6 (12%)	53,55,55	0.98	2 (3%)
31	CDL	a	201	-	90,90,99	1.12	8 (8%)	96,102,111	0.94	4 (4%)
30	PEE	l	701	-	39,39,50	1.31	6 (15%)	41,44,55	1.05	2 (4%)
31	CDL	u	201	-	77,77,99	1.20	8 (10%)	83,89,111	0.96	4 (4%)
31	CDL	g	202	-	94,94,99	1.10	8 (8%)	100,106,111	0.88	4 (4%)
30	PEE	i	402	-	46,46,50	1.19	6 (13%)	49,51,55	1.00	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
30	PEE	j	201	-	-	26/54/54/54	-
31	CDL	V	201	-	-	50/104/104/110	-
32	8Q1	X	201	-	-	17/41/41/41	-
33	PLX	g	201	-	-	23/55/55/55	-
33	PLX	a	202	-	-	12/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PEE	l	703	-	-	23/49/49/54	-
33	PLX	r	503	-	-	34/55/55/55	-
31	CDL	l	702	-	-	55/110/110/110	-
31	CDL	i	401	-	-	41/76/76/110	-
30	PEE	b	201	-	-	28/49/49/54	-
30	PEE	U	401	-	-	24/54/54/54	-
34	UQ	s	401	-	-	8/21/45/87	0/1/1/1
30	PEE	W	201	-	-	20/44/44/54	-
31	CDL	r	504	-	-	53/109/109/110	-
33	PLX	r	502	-	-	23/55/55/55	-
35	ADP	w	401	-	-	4/12/32/32	0/3/3/3
31	CDL	o	201	-	-	42/78/78/110	-
33	PLX	j	202	-	-	28/55/55/55	-
30	PEE	r	501	-	-	29/54/54/54	-
31	CDL	a	201	-	-	47/101/101/110	-
30	PEE	l	701	-	-	30/43/43/54	-
31	CDL	u	201	-	-	38/88/88/110	-
31	CDL	g	202	-	-	60/105/105/110	-
30	PEE	i	402	-	-	19/50/50/54	-

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	w	401	ADP	C3'-C4'	-8.89	1.30	1.53
35	w	401	ADP	O4'-C4'	7.66	1.62	1.45
35	w	401	ADP	O4'-C1'	-6.92	1.31	1.41
32	X	201	8Q1	C34-N36	5.37	1.45	1.33
32	X	201	8Q1	C39-N41	5.30	1.45	1.33

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	201	8Q1	C6-C1-S44	6.25	120.74	113.46
35	w	401	ADP	N3-C2-N1	-4.40	121.80	128.68
31	a	201	CDL	OA6-CA5-C11	4.31	120.78	111.50
31	r	504	CDL	OB6-CB5-C51	4.22	120.59	111.50
31	u	201	CDL	OB6-CB5-C51	4.14	120.43	111.50

There are no chirality outliers.

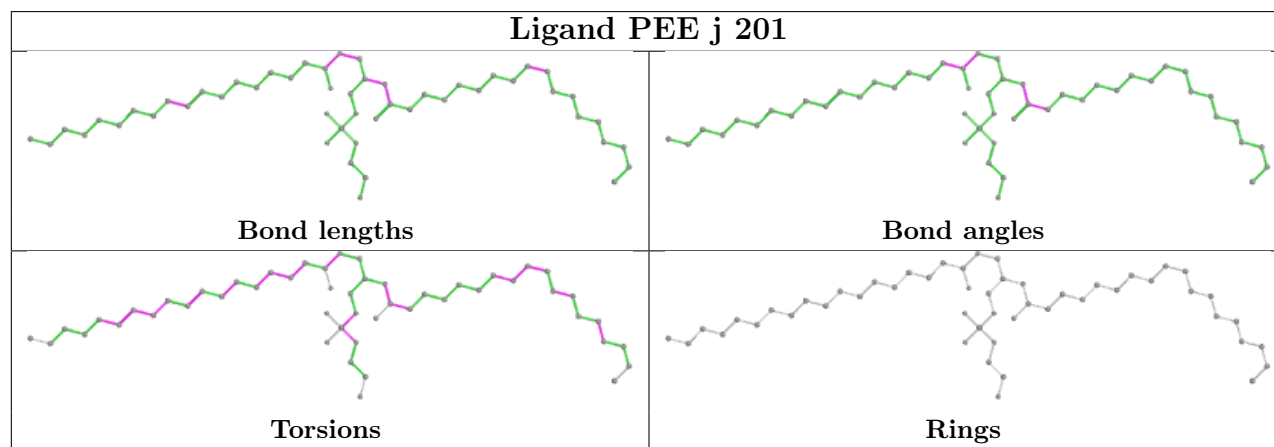
5 of 734 torsion outliers are listed below:

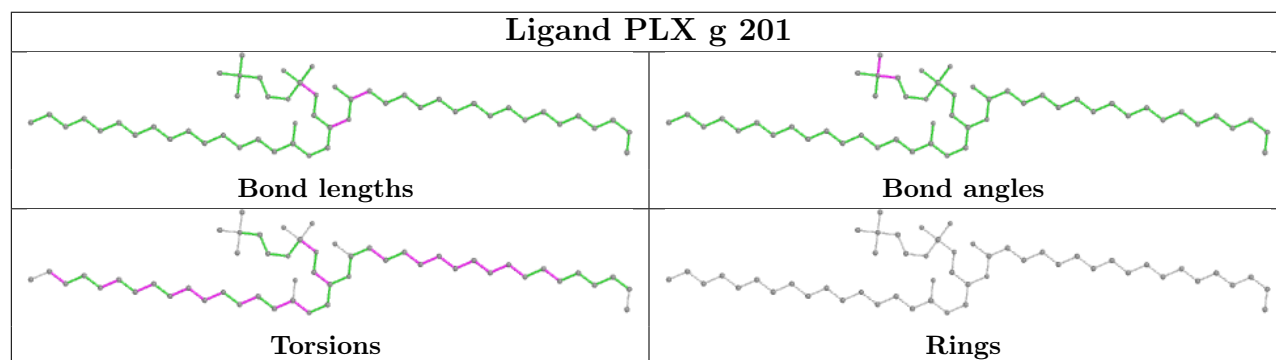
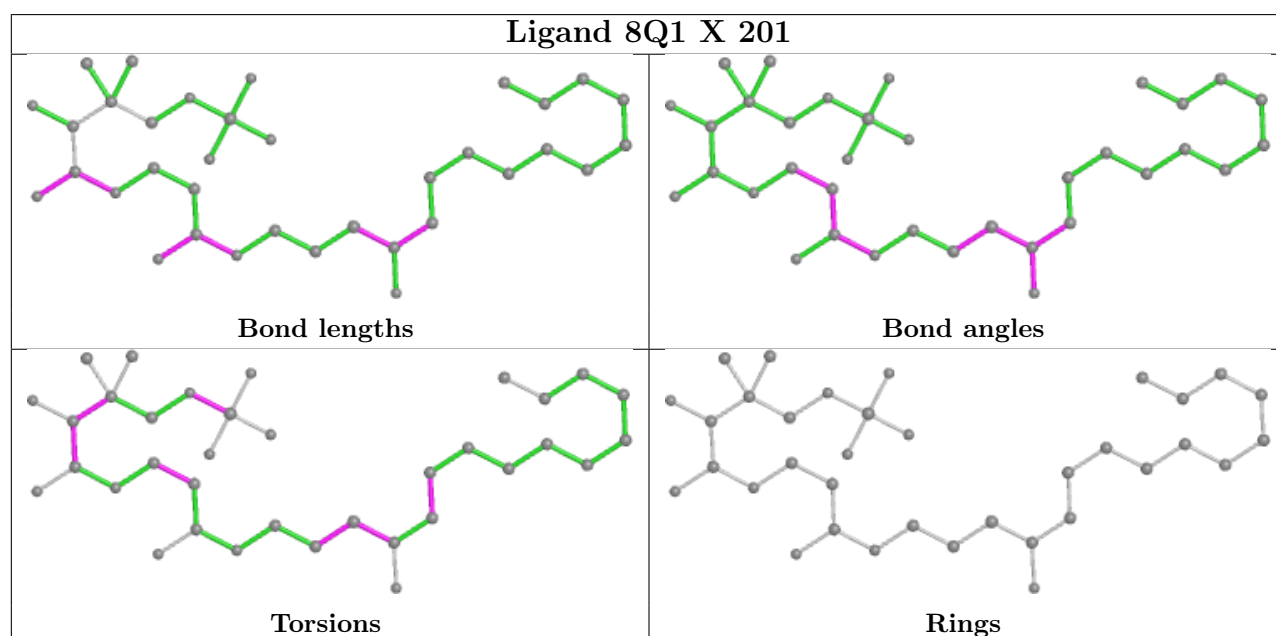
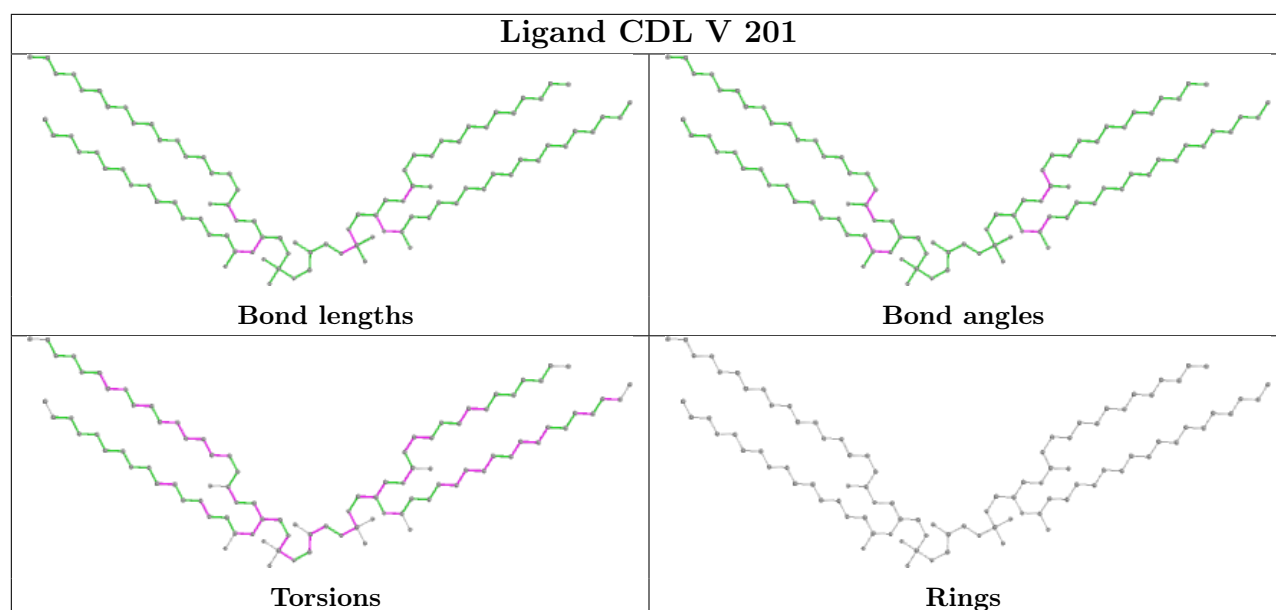
Mol	Chain	Res	Type	Atoms
30	W	201	PEE	C4-O4P-P-O1P
30	b	201	PEE	C37-C38-C39-C40
30	i	402	PEE	C11-C10-O2-C2
30	j	201	PEE	C1-O3P-P-O2P
30	j	201	PEE	C1-O3P-P-O1P

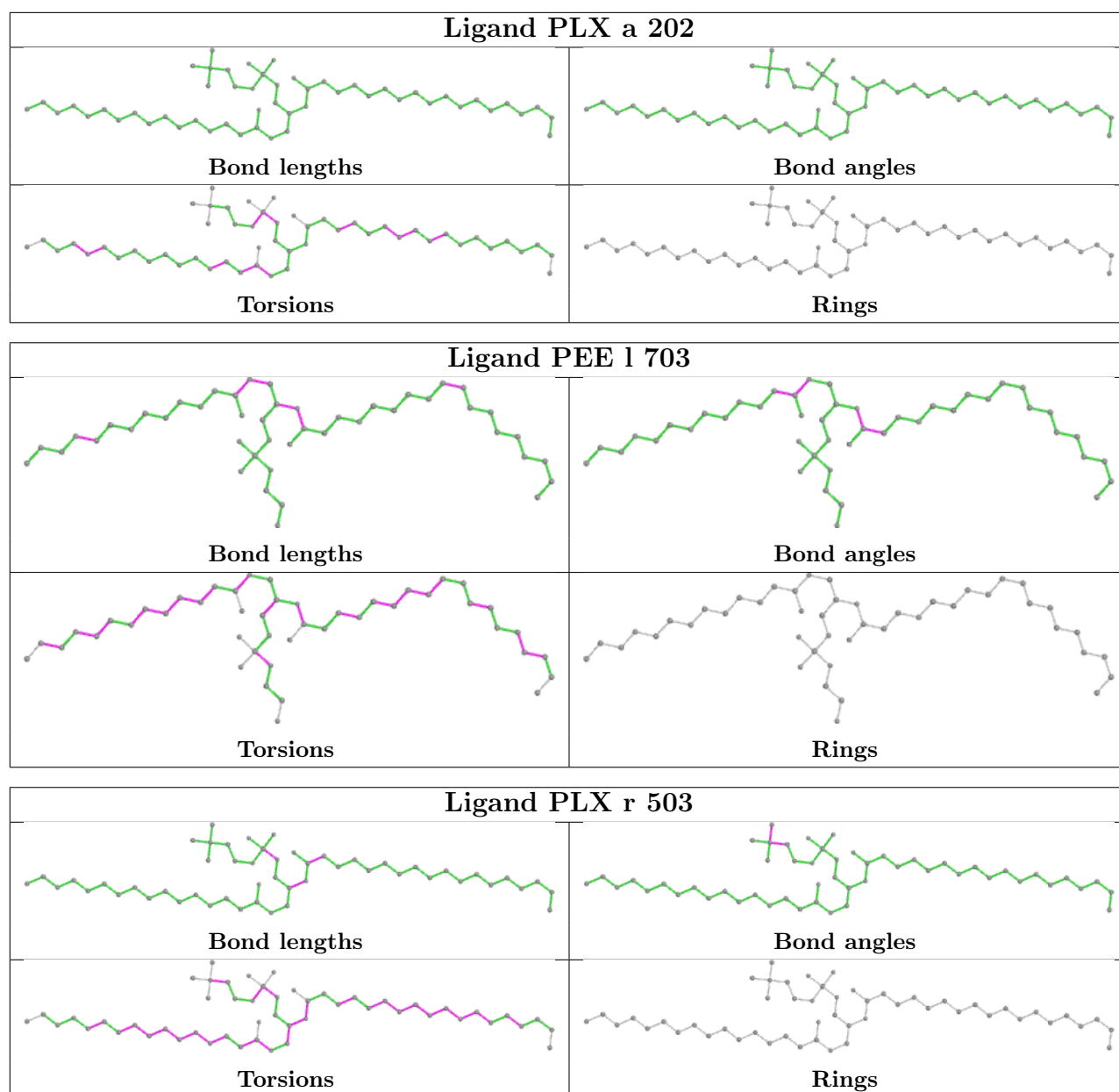
There are no ring outliers.

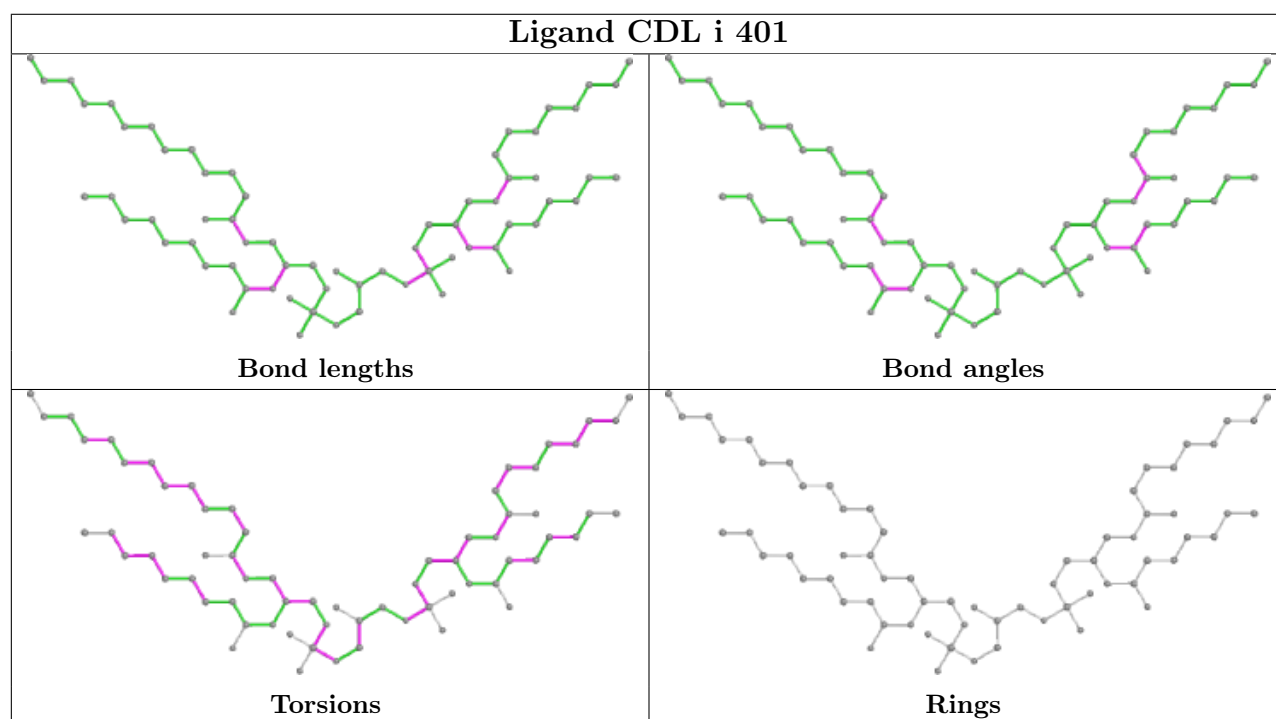
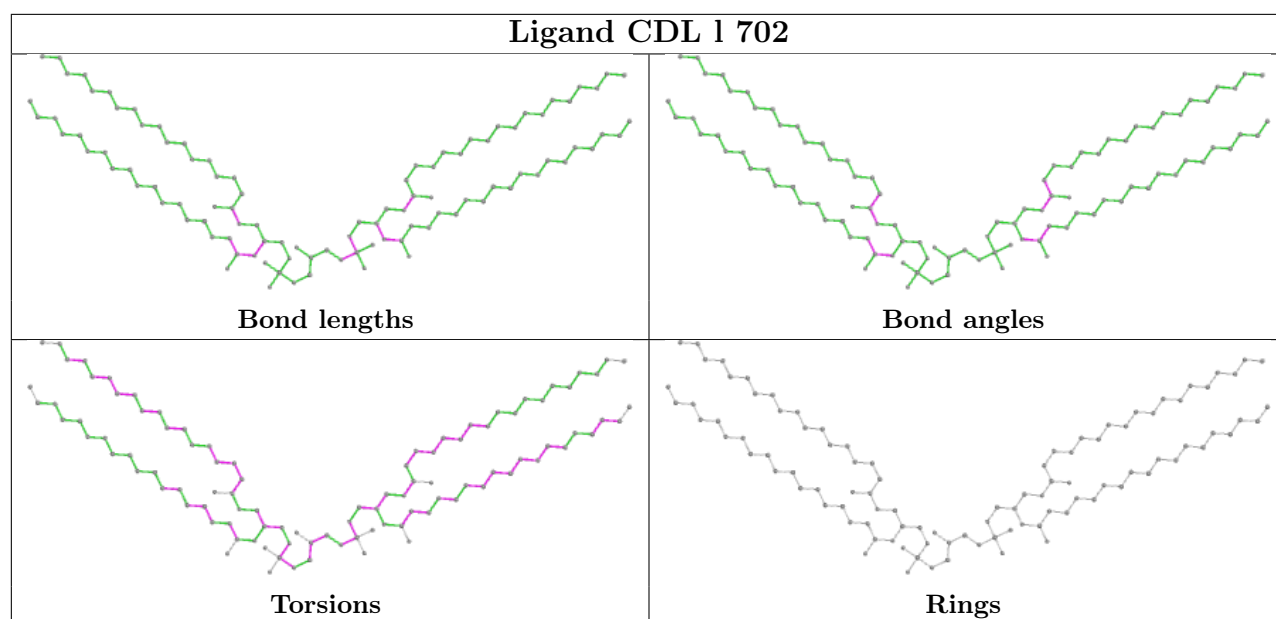
No monomer is involved in short contacts.

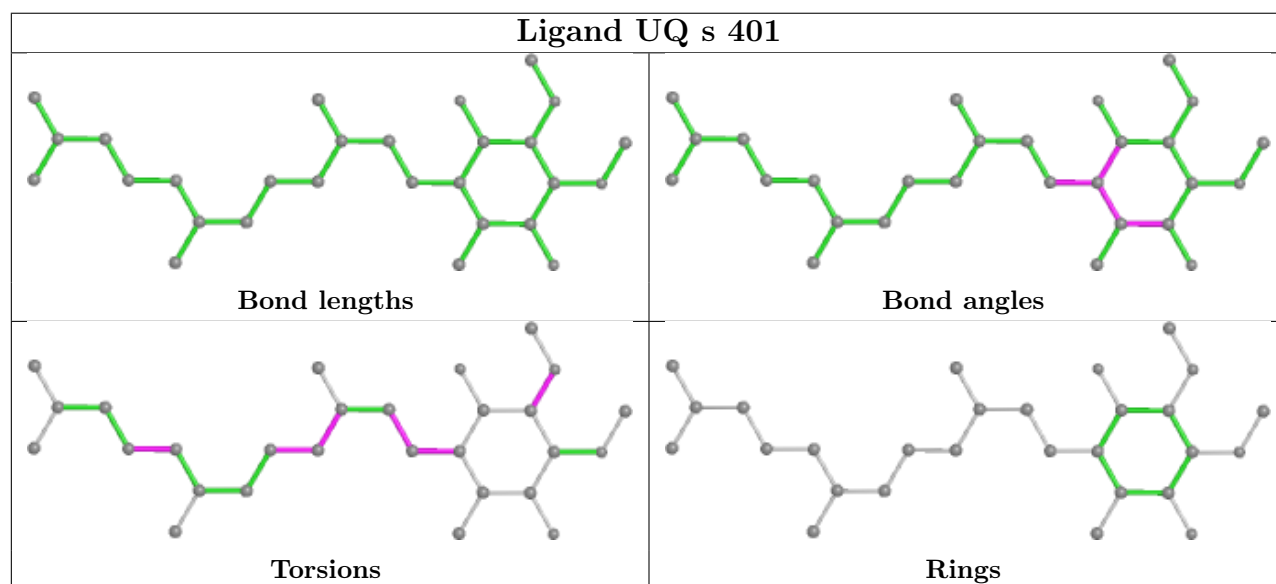
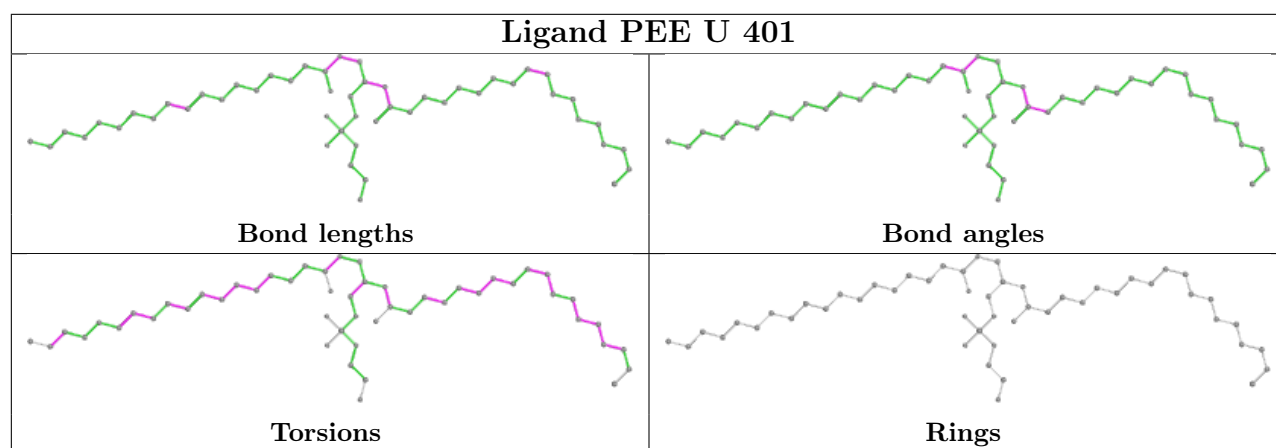
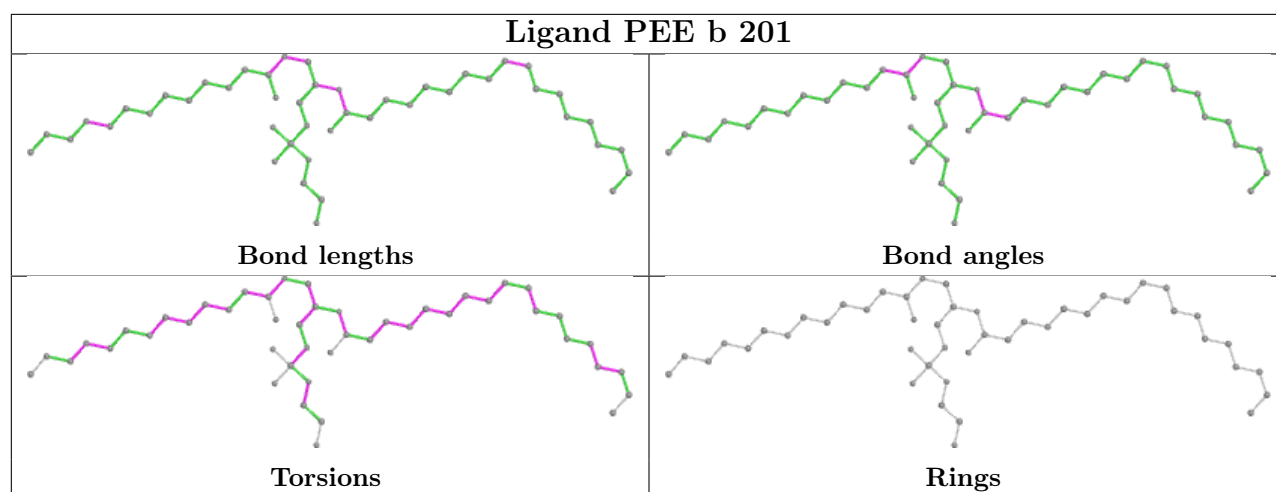
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

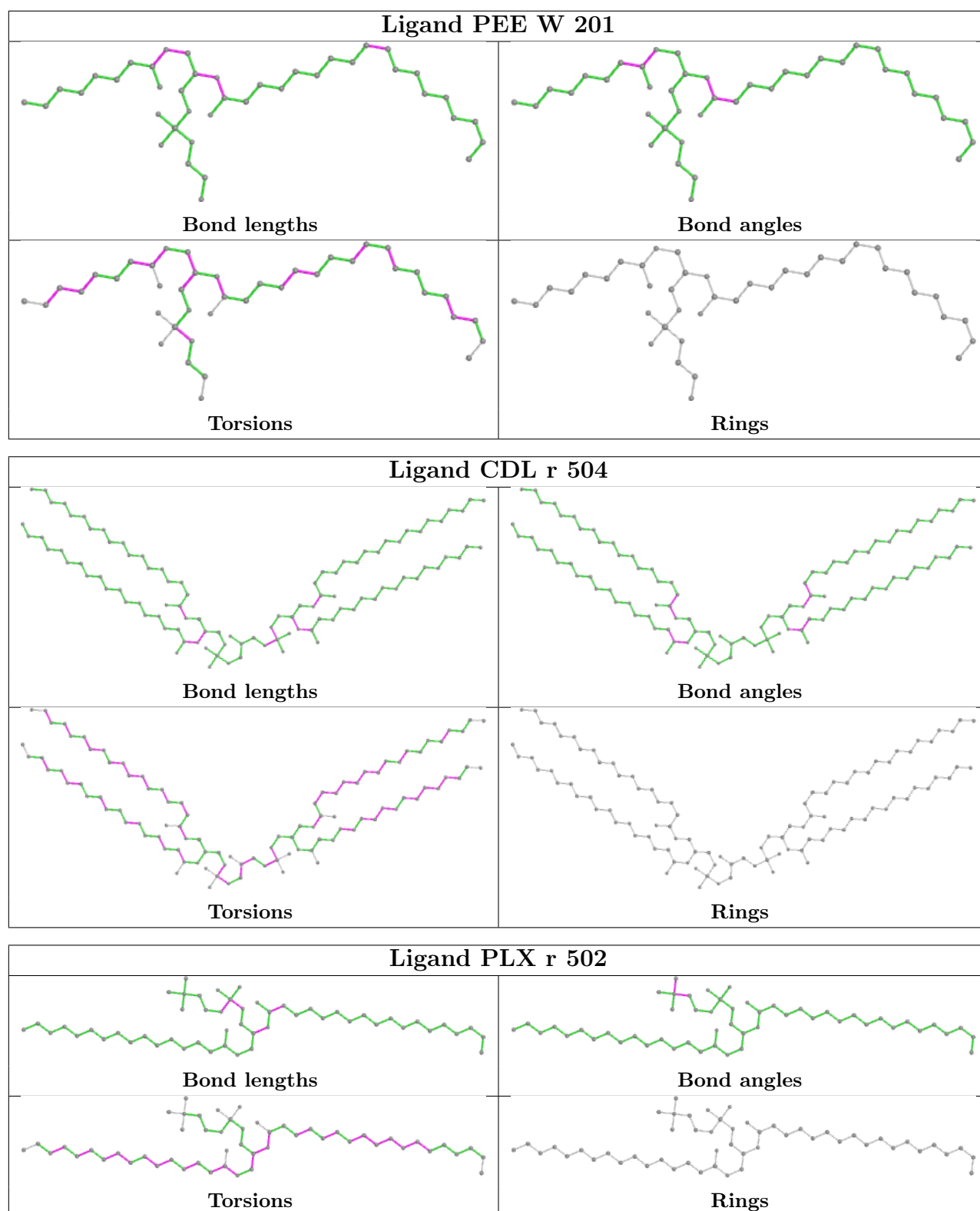


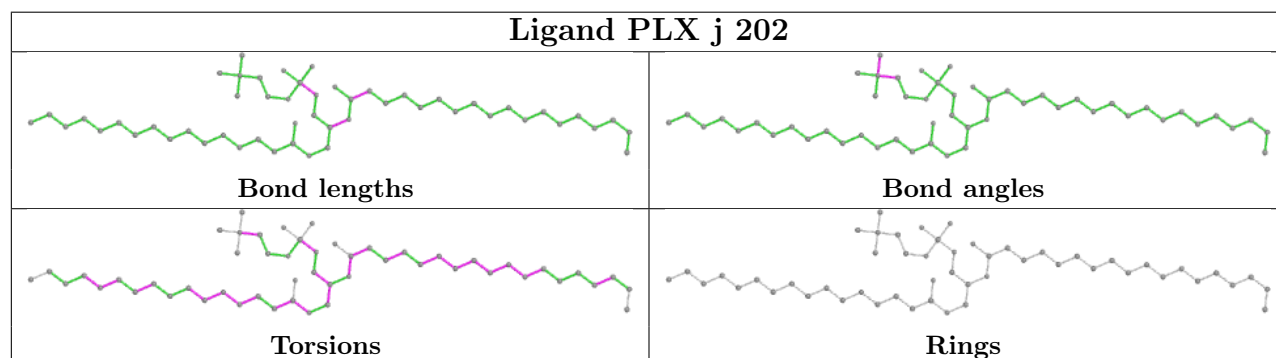
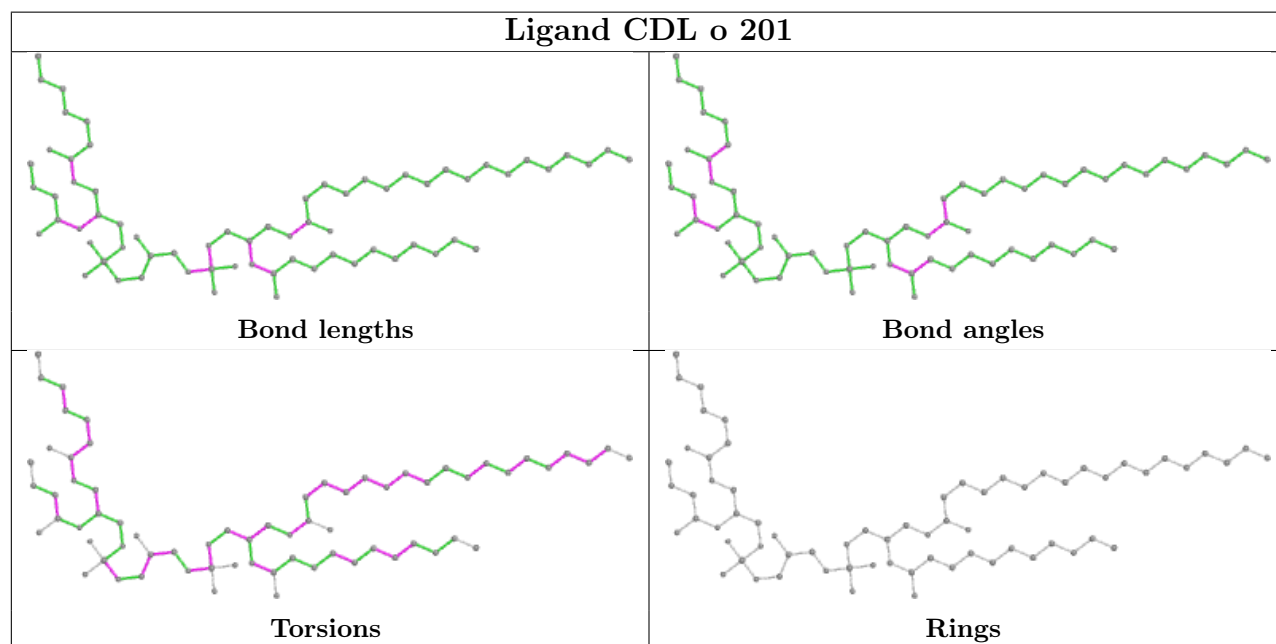
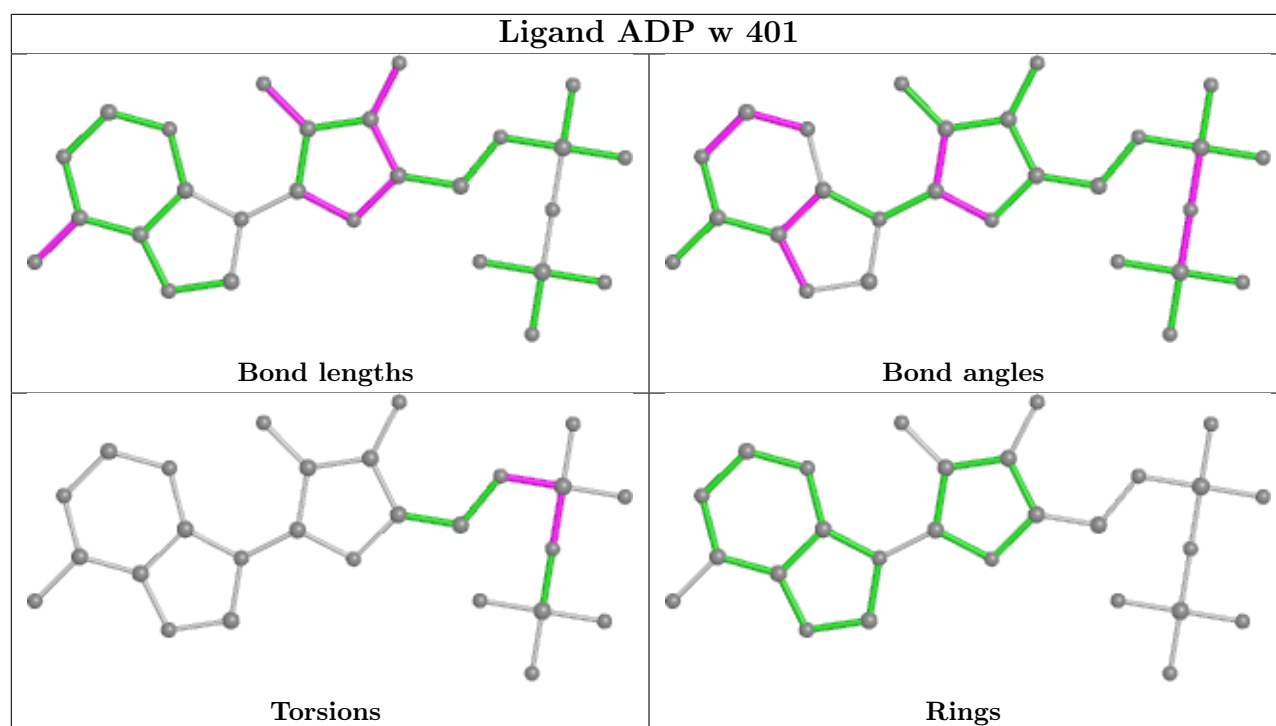


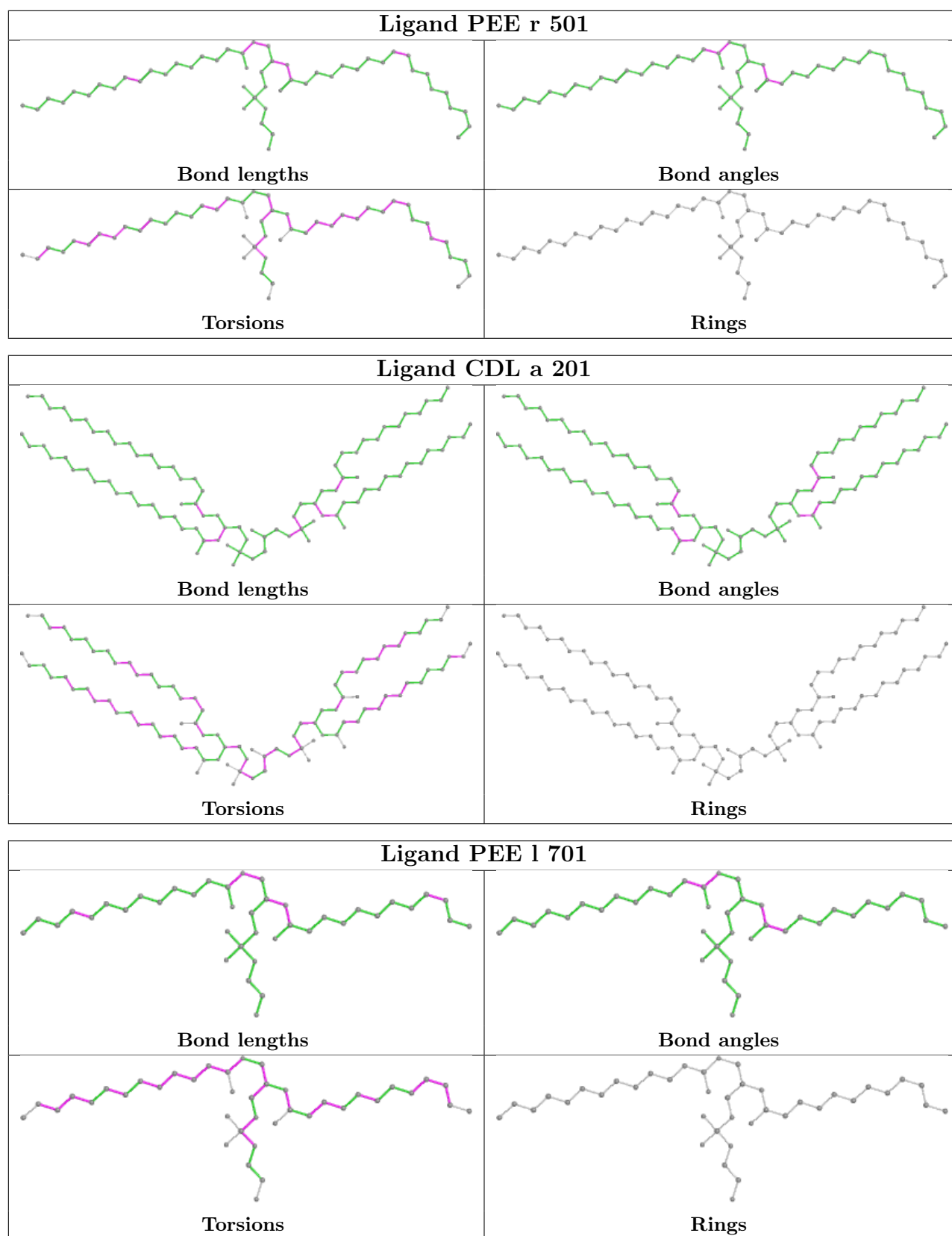


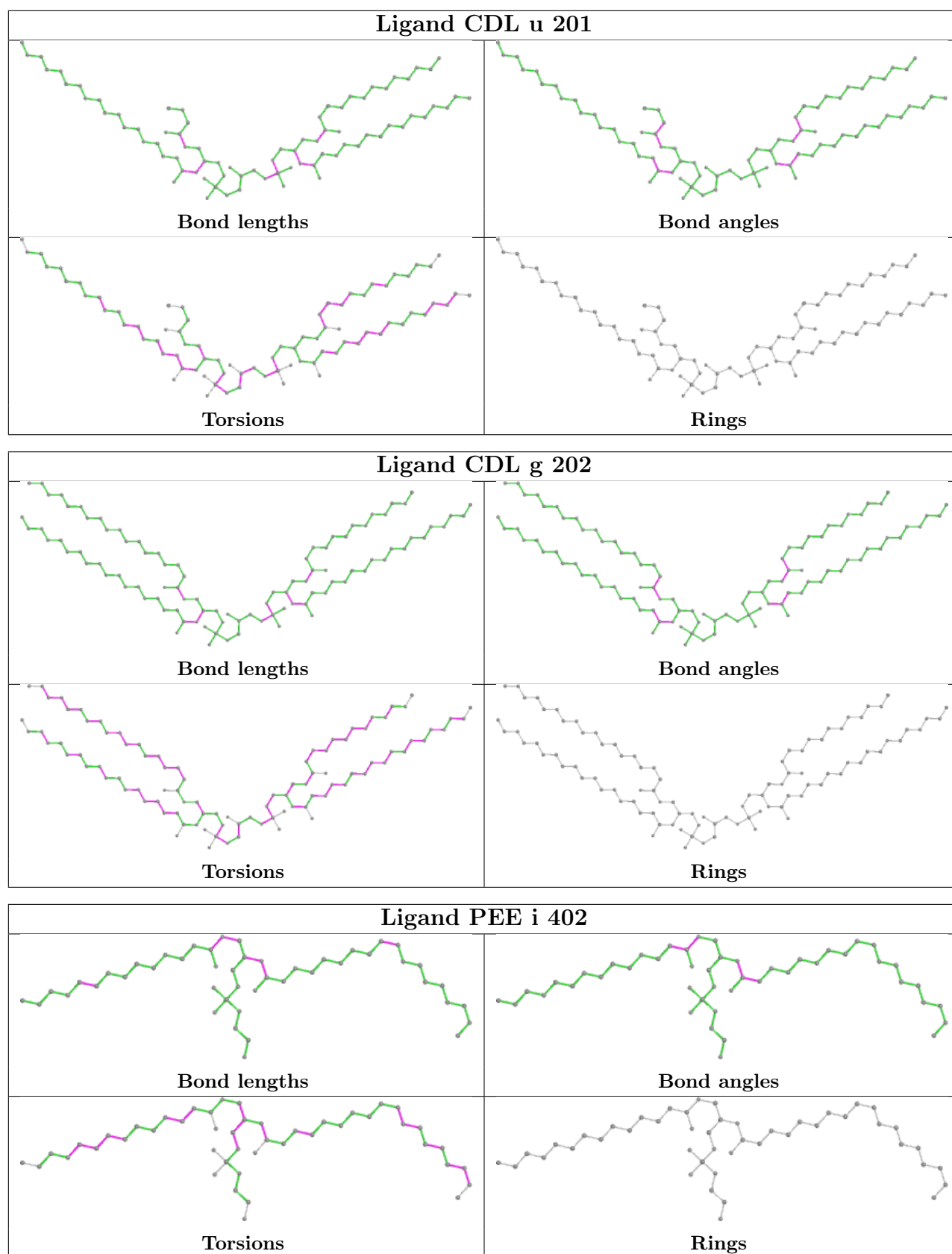












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

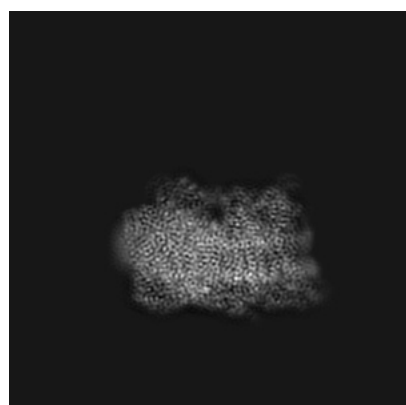
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32191. These allow visual inspection of the internal detail of the map and identification of artifacts.

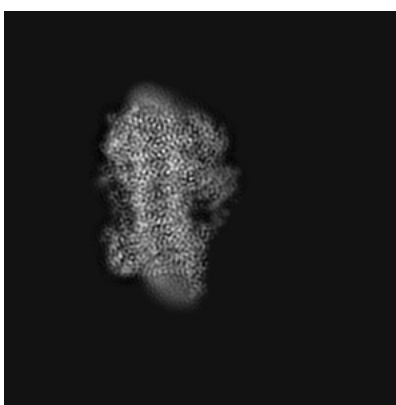
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

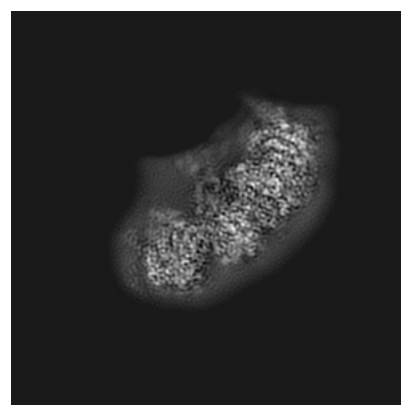
6.1.1 Primary map



X



Y

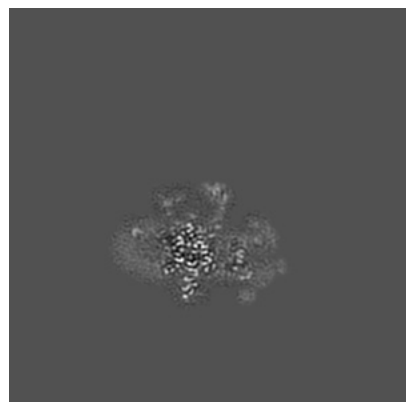


Z

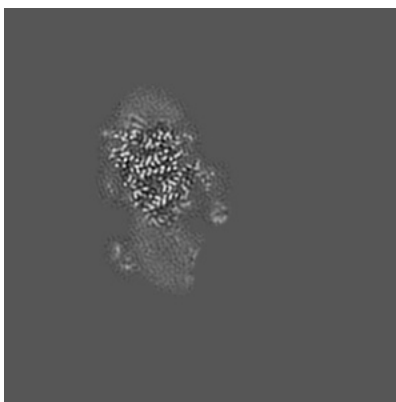
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

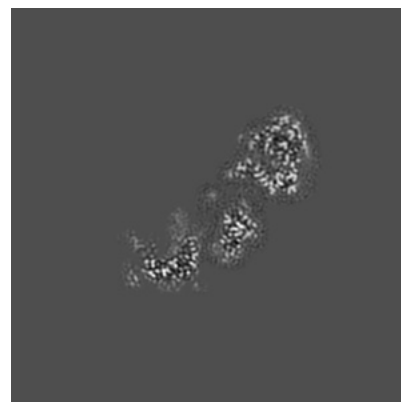
6.2.1 Primary map



X Index: 165



Y Index: 165

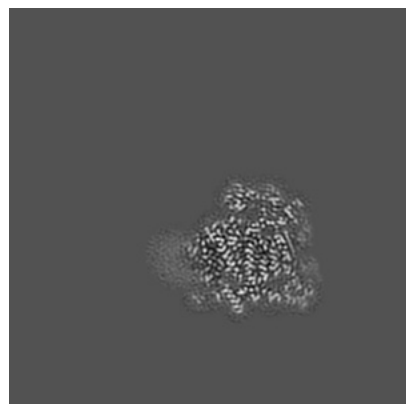


Z Index: 165

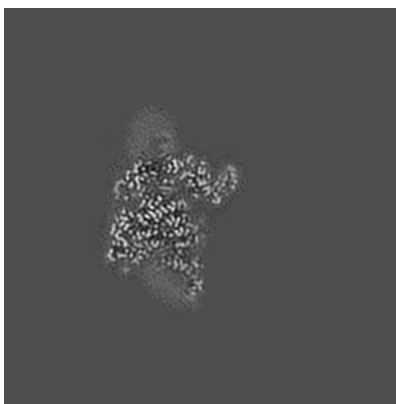
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

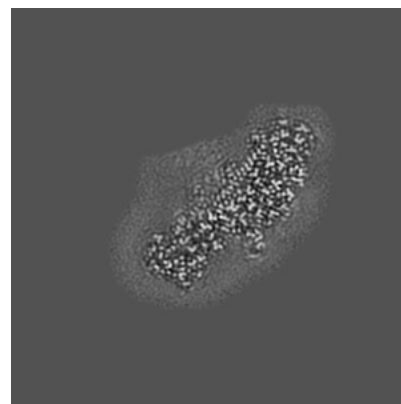
6.3.1 Primary map



X Index: 219



Y Index: 142



Z Index: 136

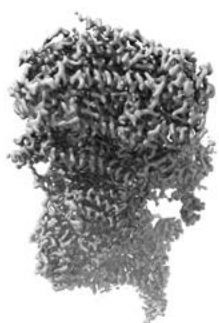
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

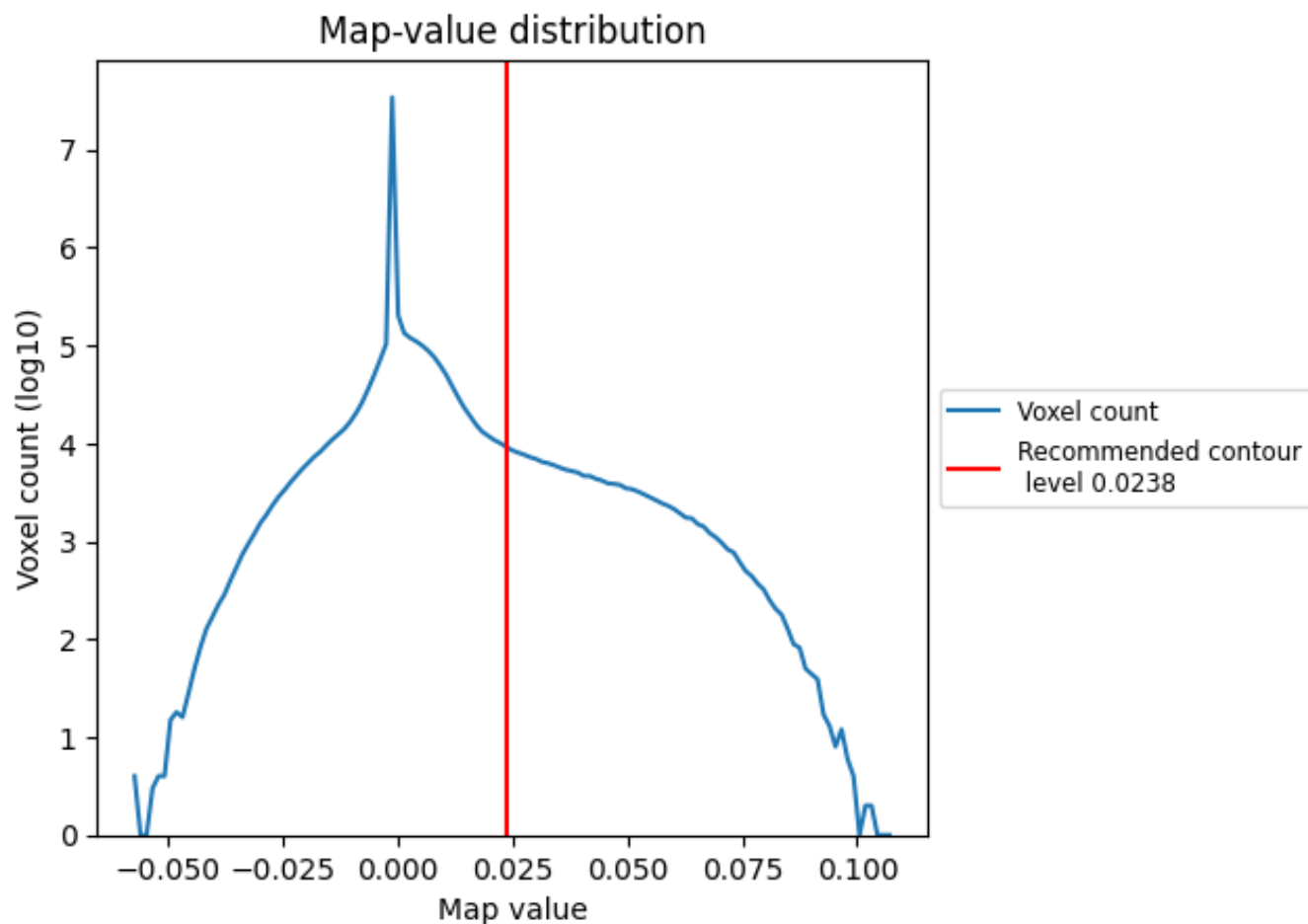
6.5 Mask visualisation

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

7 Map analysis [i](#)

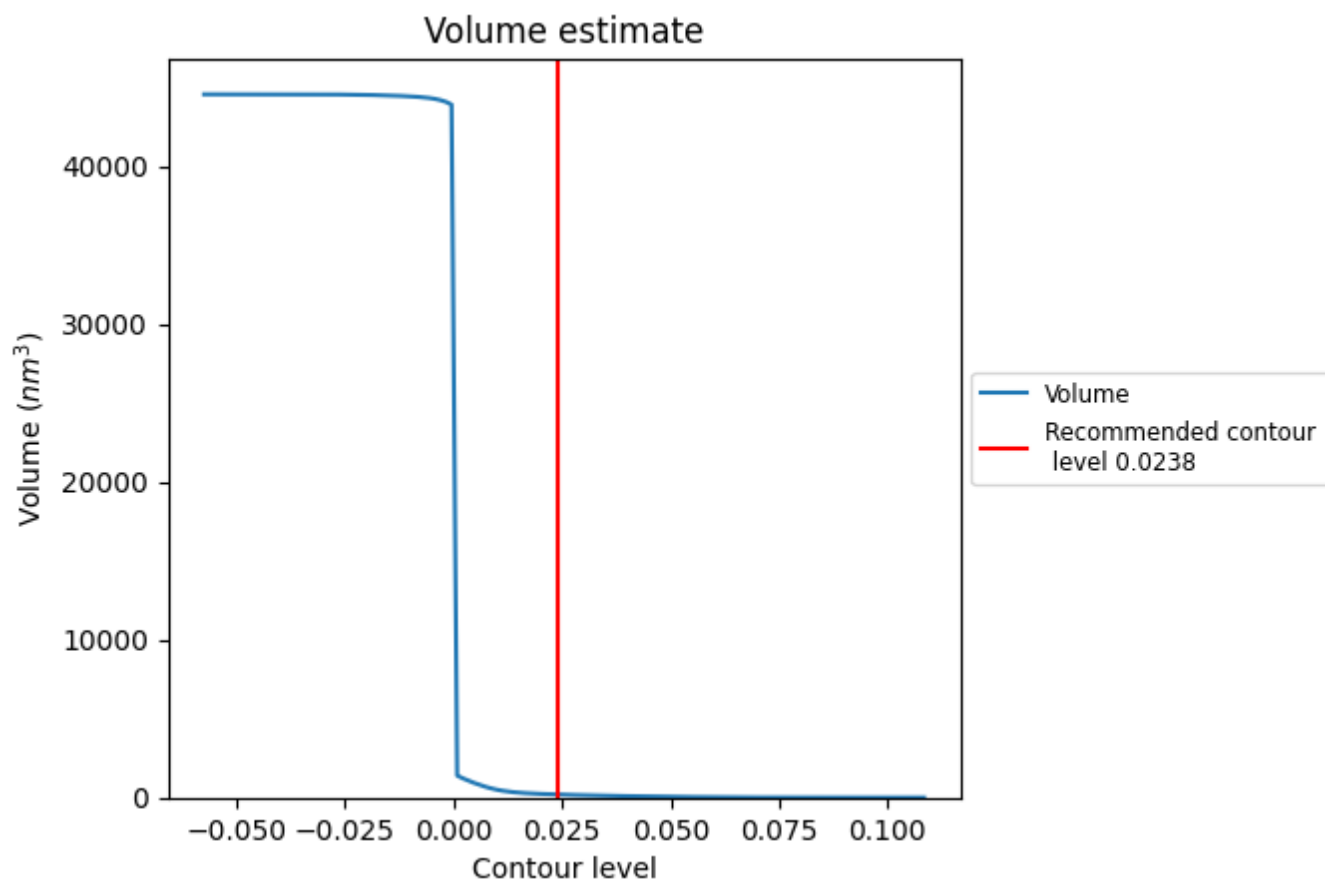
This section contains the results of statistical analysis of the map.

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.

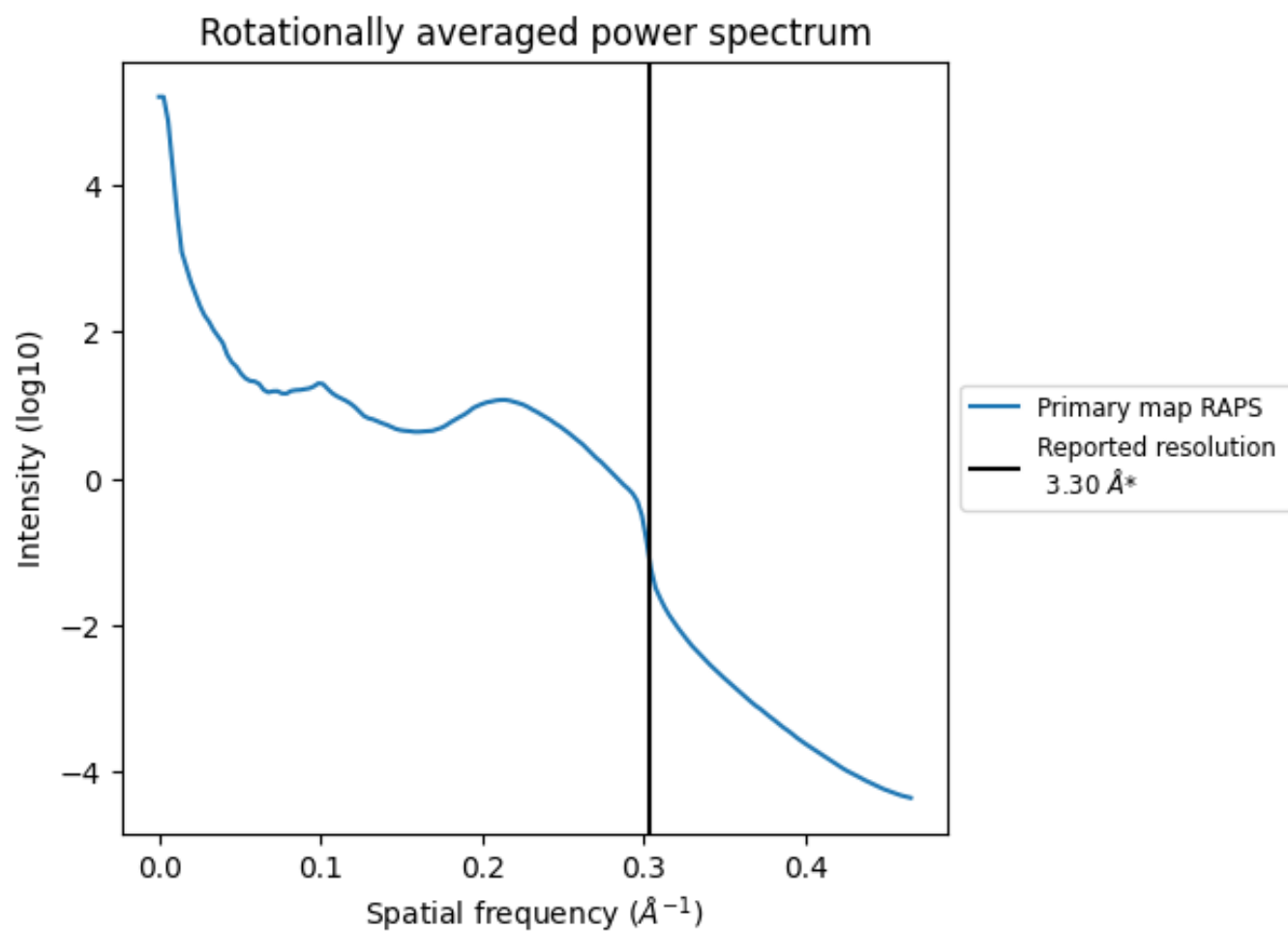
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

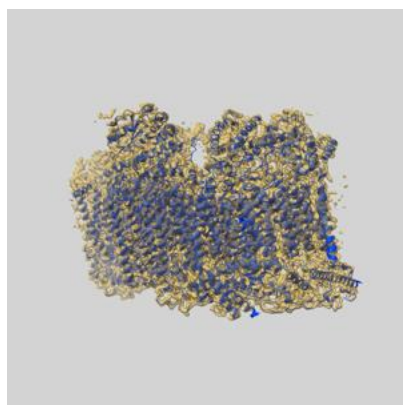
8 Fourier-Shell correlation ⓘ

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

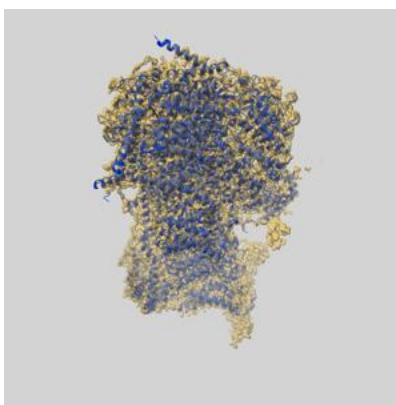
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32191 and PDB model 7VY1. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

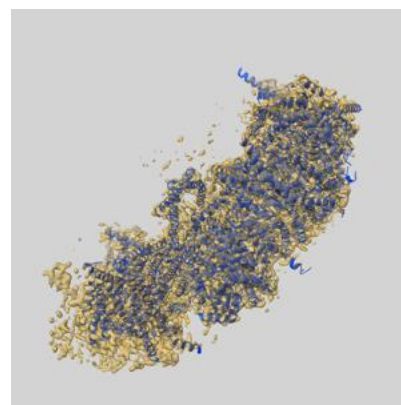
9.1 Map-model overlay [i](#)



X



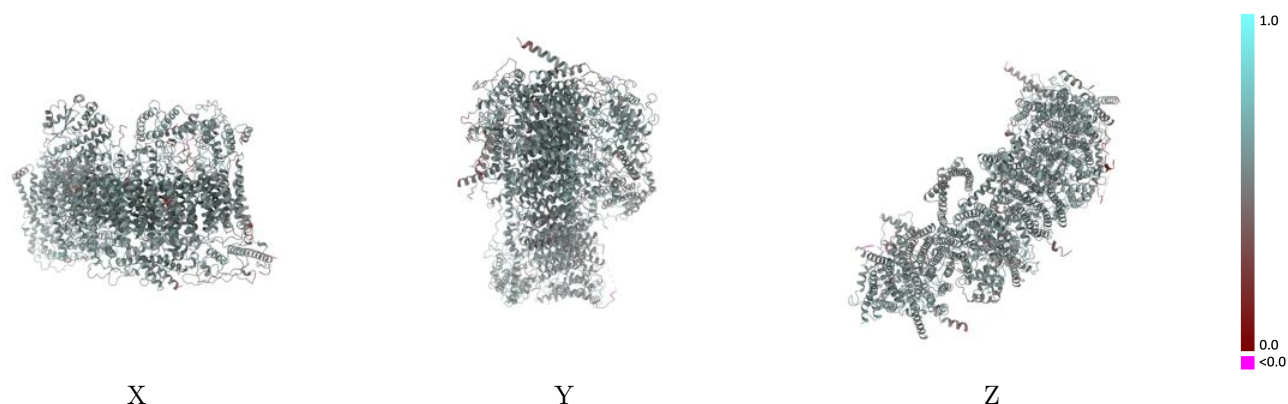
Y



Z

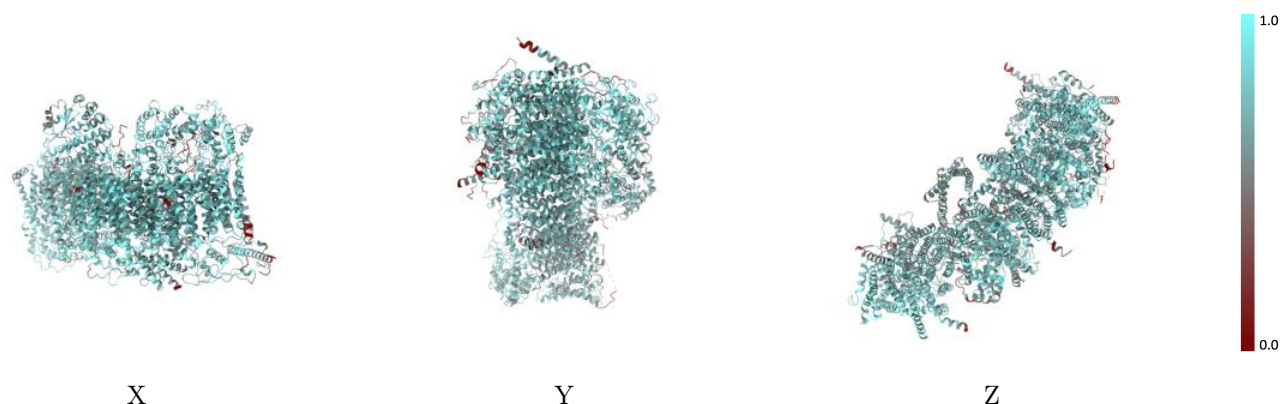
The images above show the 3D surface view of the map at the recommended contour level 0.0238 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



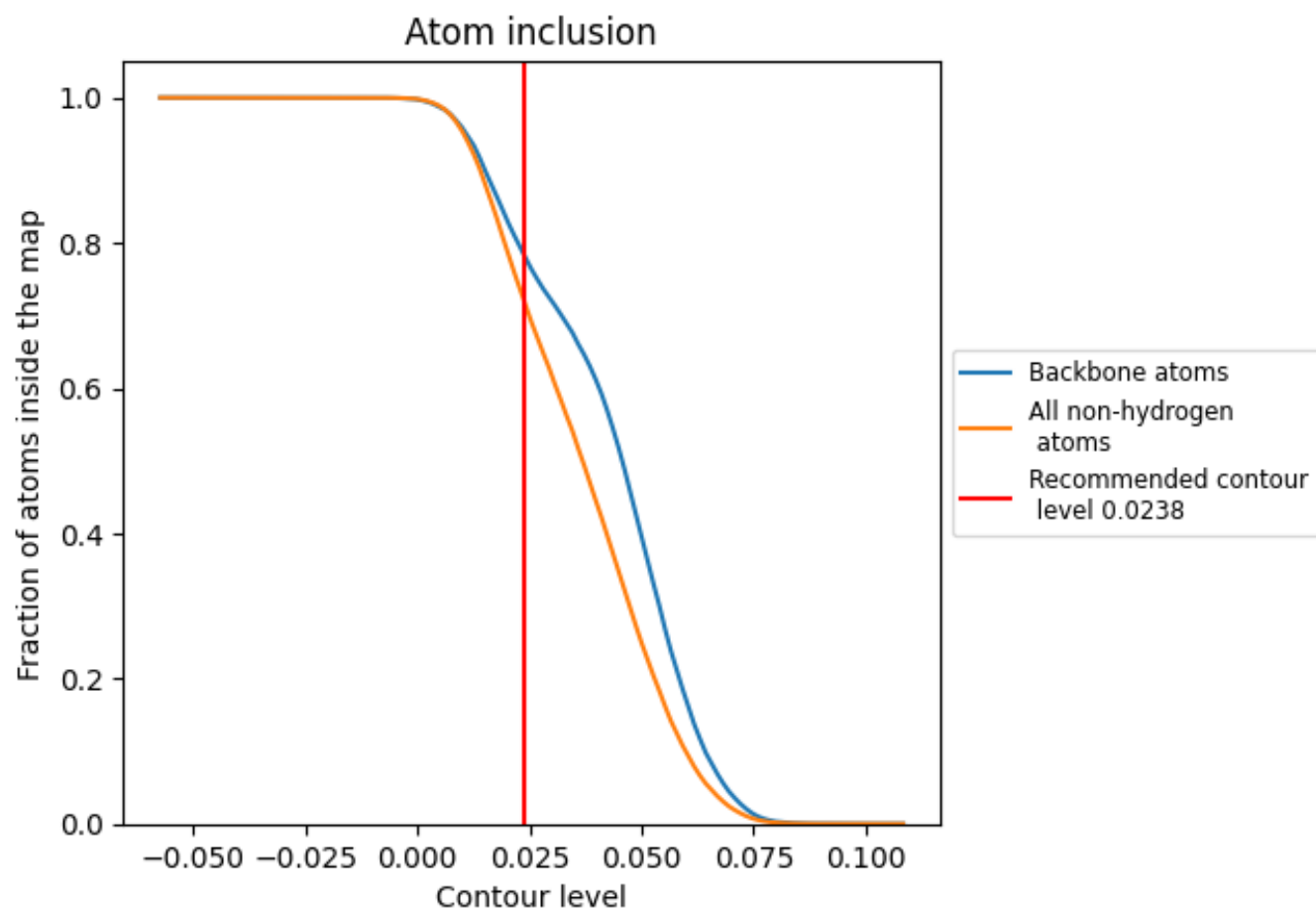
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0238).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.0238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7192	 0.5380
Q	 0.6227	 0.5400
S	 0.7884	 0.5560
U	 0.7529	 0.5410
V	 0.5388	 0.5080
W	 0.7688	 0.5520
X	 0.7088	 0.5240
Y	 0.6735	 0.5130
Z	 0.5836	 0.4800
a	 0.7475	 0.5540
b	 0.6319	 0.5140
c	 0.7427	 0.5370
d	 0.7173	 0.5290
e	 0.6674	 0.5230
f	 0.6577	 0.5210
g	 0.7410	 0.5560
h	 0.7376	 0.5480
i	 0.7666	 0.5560
j	 0.6201	 0.5130
k	 0.6927	 0.5350
l	 0.7438	 0.5470
m	 0.6872	 0.5200
n	 0.6379	 0.5180
o	 0.6764	 0.5360
p	 0.7481	 0.5400
r	 0.7682	 0.5570
s	 0.7565	 0.5450
u	 0.7514	 0.5450
v	 0.6606	 0.5010
w	 0.6980	 0.5280

