



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:34 PM UTC

PDB ID : 7ZME / pdb_00007zme
EMDB ID : EMD-14796
Title : CryoEM structure of mitochondrial complex I from Chaetomium thermophilum (state 2) - membrane arm
Authors : Laube, E.; Kuehlbrandt, W.
Deposited on : 2022-04-19
Resolution : 2.83 Å (reported)
Based on initial models : 6RFR, 6RFQ

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

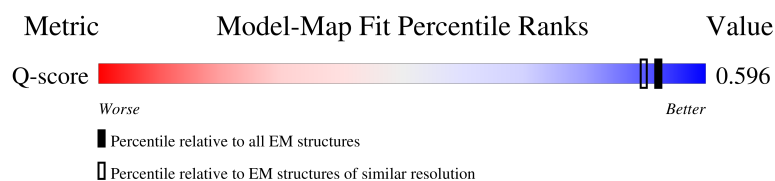
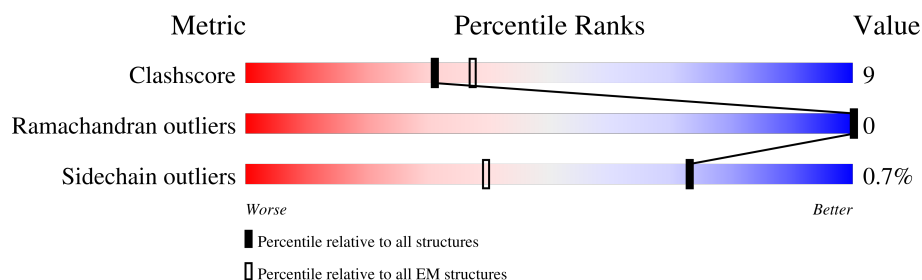
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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.



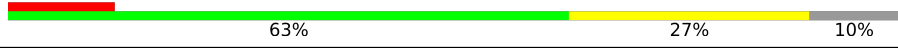
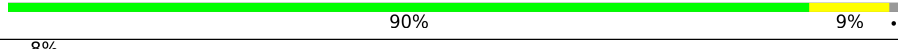
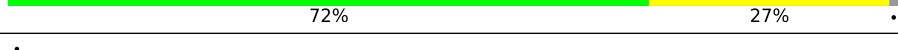
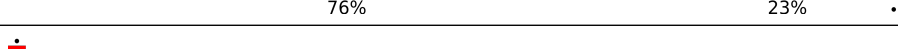
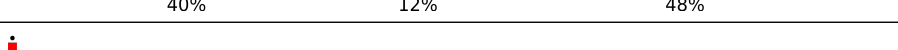
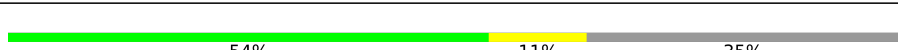
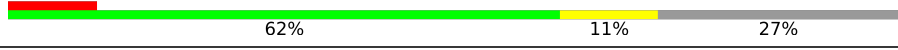
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

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

Mol	Chain	Length	Quality of chain
1	1	378	 69% 18% • 12%
2	2	571	 77% 19% ••
3	3	146	 62% 15% • 22%
4	4	542	 69% 22% 9%

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Mol	Chain	Length	Quality of chain
5	5	679	
6	6	224	
7	8	86	
8	9	785	
9	D	86	
10	J	199	
11	L	89	
12	Q	141	
13	R	99	
14	S	143	
15	U	186	
16	W	121	
17	X	191	
18	a	815	
19	b	94	
20	c	93	
21	d	105	
22	e	46	
23	g	82	
24	i	93	
25	j	75	
26	n	184	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 36964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	334	Total	C	N	O	S	0	0
			2573	1728	388	446	11		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	114	Total	C	N	O	S	0	0
			907	619	132	153	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	670	Total	C	N	O	S	0	0
			5272	3551	792	904	25		

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	190	Total	C	N	O	S	0	0
			1454	981	219	248	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	77	Total	C	N	O	S	0	0
			658	408	126	118	6		

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 9 is a protein called Subunit NDUF1 of NADH-ubiquinone oxidoreductase (Complex I).

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	186	Total	C	N	O	S	0	0
			1375	872	259	242	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	88	Total	C	N	O	S	0	0
			671	450	103	115	3		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	85	Total	C	N	O	S	0	0
			663	418	109	135	1		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	74	Total	C	N	O	0	0
			610	401	98	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	169	Total	C	N	O	S	0	0
			1365	860	254	242	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	99	Total	C	N	O	S	0	0
			812	519	154	137	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	187	Total	C	N	O	S	0	0
			1480	941	268	263	8		

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	60	Total	C	N	O	S	0	0
			490	320	86	82	2		

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

(Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	98	Total	C	N	O	S	0	0
			817	520	144	149	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	37	Total	C	N	O	S	0	0
			309	211	54	43	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	80	Total	C	N	O	S	0	0
			677	447	117	111	2		

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

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

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

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

There are 52 discrepancies between the modelled and reference sequences:

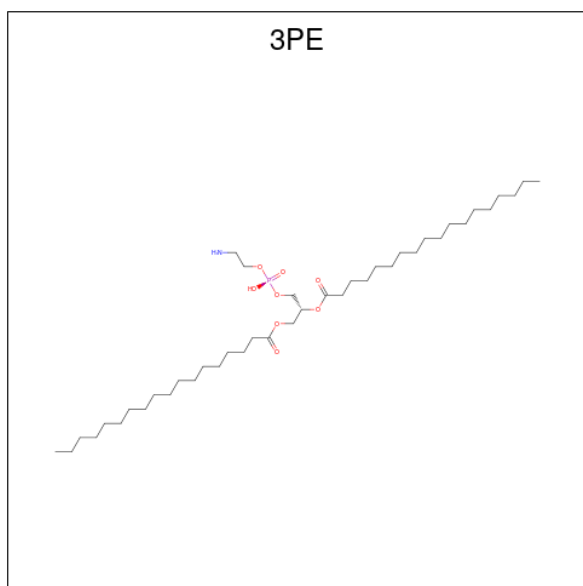
Chain	Residue	Modelled	Actual	Comment	Reference
n	1	MET	-	initiating methionine	UNP G0S086
n	2	LEU	-	insertion	UNP G0S086
n	3	ALA	-	insertion	UNP G0S086
n	4	LEU	-	insertion	UNP G0S086
n	5	ARG	-	insertion	UNP G0S086
n	6	GLN	-	insertion	UNP G0S086
n	7	ARG	-	insertion	UNP G0S086
n	8	ALA	-	insertion	UNP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

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

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



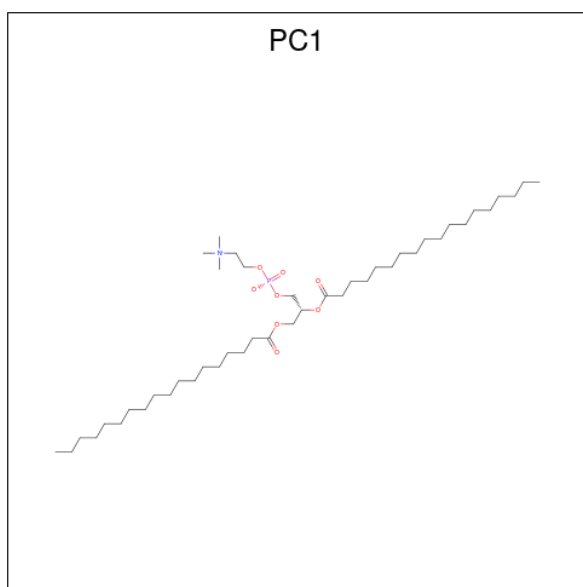
Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	N	O	P	0
			41	31	1	8	1	
27	1	1	Total	C	N	O	P	0
			27	18	1	7	1	
27	4	1	Total	C	N	O	P	0
			34	24	1	8	1	
27	4	1	Total	C	N	O	P	0
			33	23	1	8	1	
27	4	1	Total	C	N	O	P	0
			28	18	1	8	1	
27	5	1	Total	C	N	O	P	0
			40	30	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
27	5	1	Total	C	N	O	P	0
			28	18	1	8	1	
27	8	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	J	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
27	g	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	g	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	n	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	n	1	Total	C	N	O	P	0
			39	29	1	8	1	

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



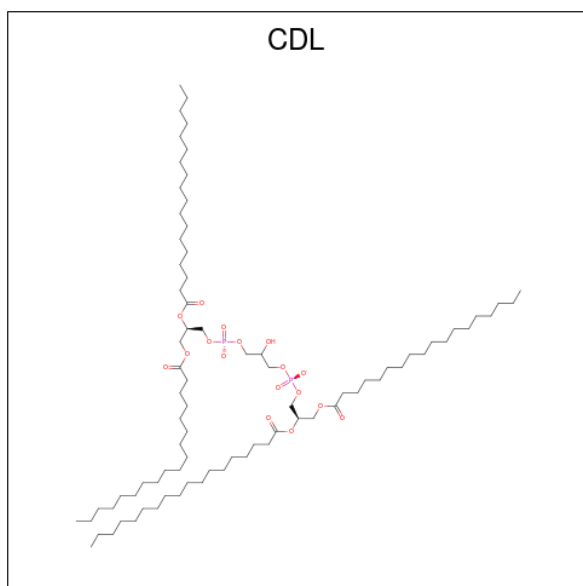
Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	N	O	P	0
			30	20	1	8	1	

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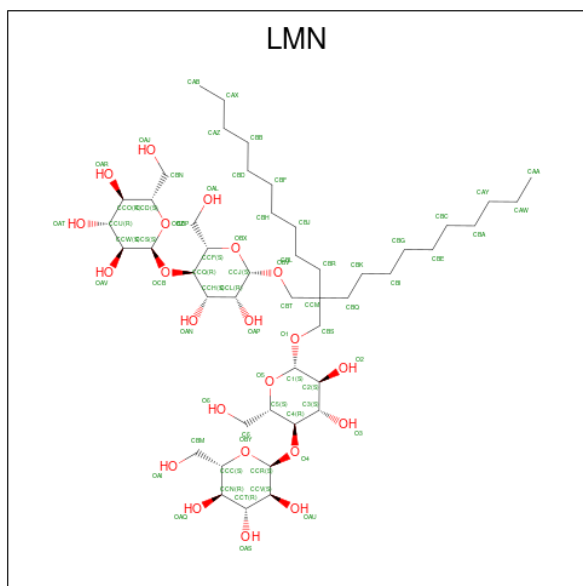
Mol	Chain	Residues	Atoms					AltConf
28	2	1	Total	C	N	O	P	0
			31	21	1	8	1	
28	3	1	Total	C	N	O	P	0
			36	26	1	8	1	
28	4	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			45	35	1	8	1	
28	5	1	Total	C	N	O	P	0
			41	31	1	8	1	
28	n	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



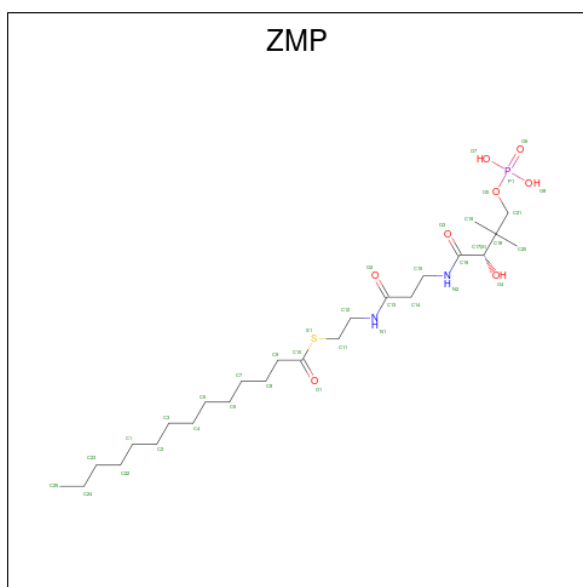
Mol	Chain	Residues	Atoms				AltConf
29	2	1	Total	C	O	P	0
			84	65	17	2	
29	4	1	Total	C	O	P	0
			86	67	17	2	
29	D	1	Total	C	O	P	0
			59	40	17	2	
29	X	1	Total	C	O	P	0
			79	60	17	2	
29	g	1	Total	C	O	P	0
			56	37	17	2	

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



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

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



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

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	1	62	Total	O	0
			62	62	
32	2	141	Total	O	0
			141	141	
32	3	24	Total	O	0
			24	24	
32	4	84	Total	O	0
			84	84	
32	5	49	Total	O	0
			49	49	
32	6	35	Total	O	0
			35	35	
32	9	19	Total	O	0
			19	19	
32	D	27	Total	O	0
			27	27	
32	J	1	Total	O	0
			1	1	
32	L	11	Total	O	0
			11	11	
32	R	4	Total	O	0
			4	4	
32	S	1	Total	O	0
			1	1	
32	U	36	Total	O	0
			36	36	
32	W	29	Total	O	0
			29	29	
32	X	45	Total	O	0
			45	45	
32	a	11	Total	O	0
			11	11	
32	b	4	Total	O	0
			4	4	
32	d	9	Total	O	0
			9	9	
32	g	10	Total	O	0
			10	10	

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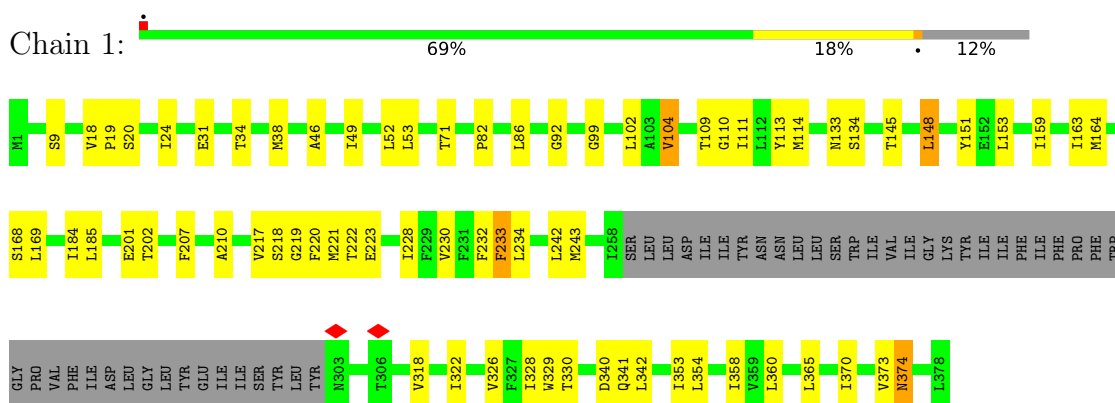
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Mol	Chain	Residues	Atoms		AltConf
32	i	4	Total 4	O 4	0
32	j	4	Total 4	O 4	0
32	n	23	Total 23	O 23	0

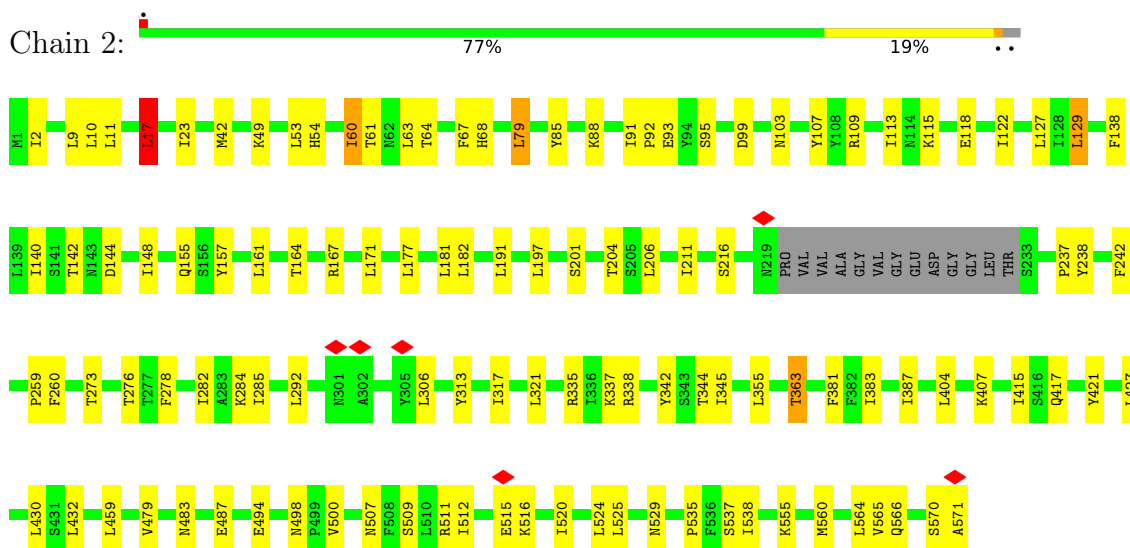
3 Residue-property plots

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 1

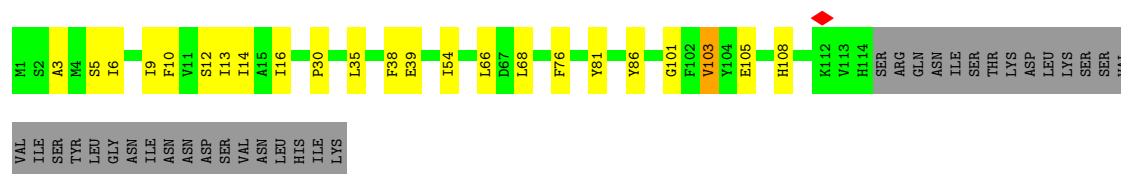


- Molecule 2: NADH dehydrogenase subunit 2

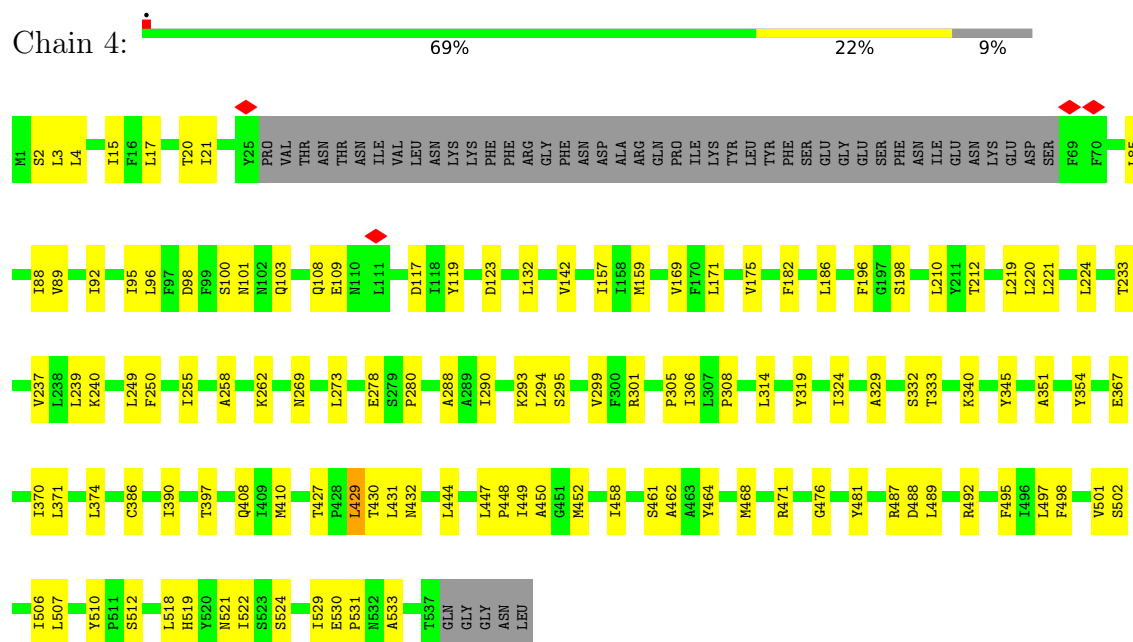


- Molecule 3: NADH-ubiquinone oxidoreductase chain 3

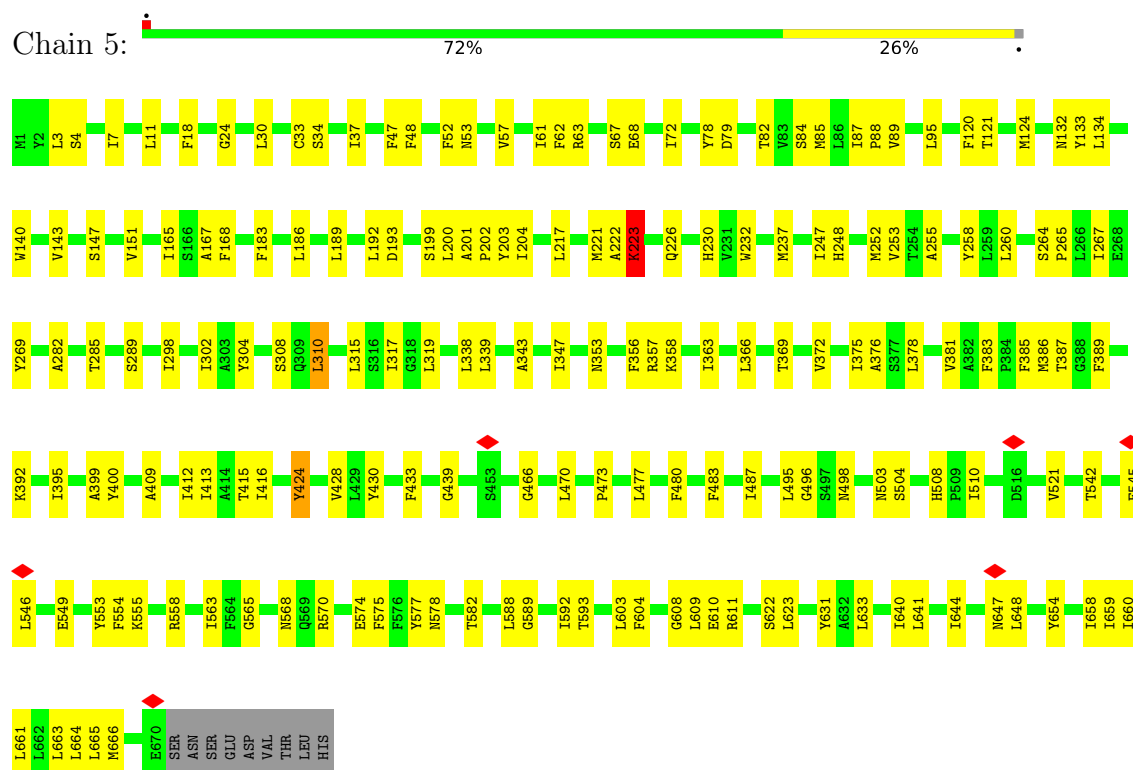




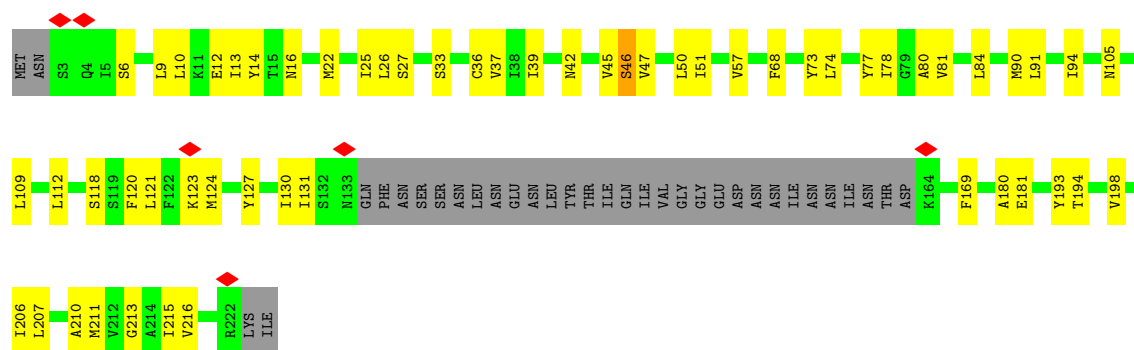
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4



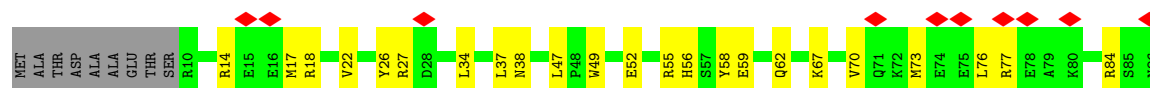
• Molecule 5: NADH-ubiquinone oxidoreductase chain 5



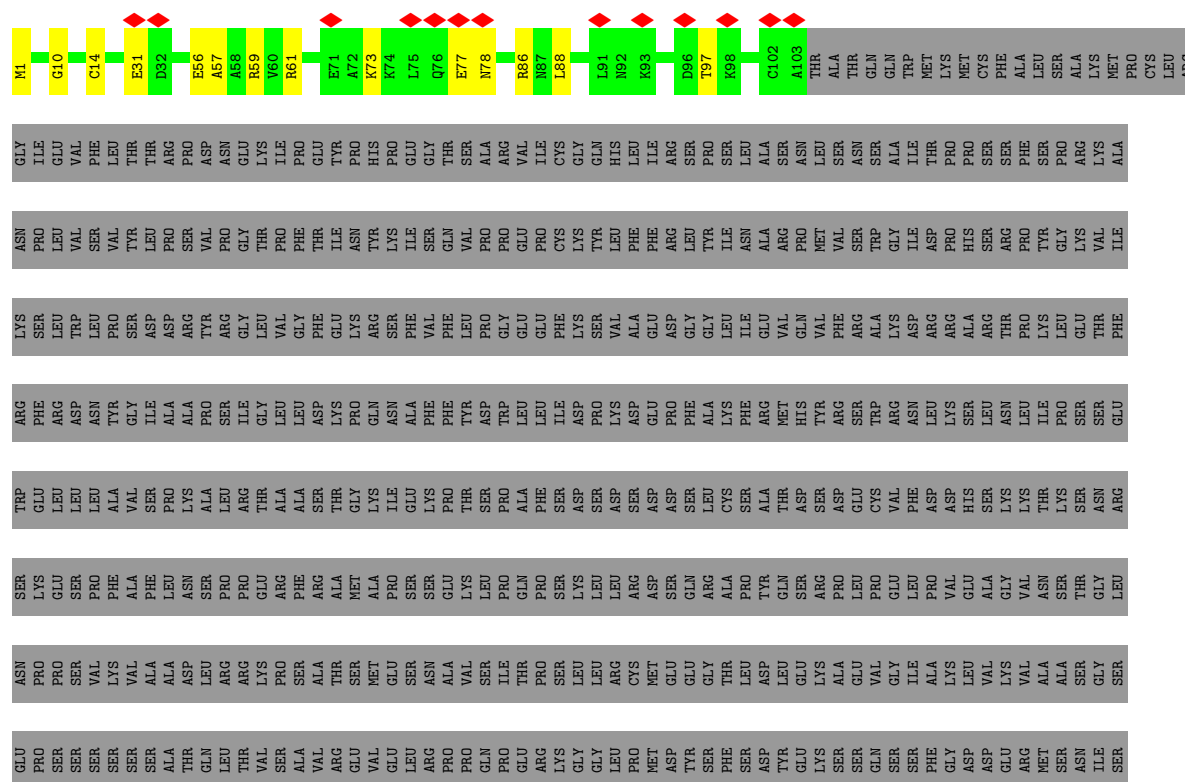
Chain 6: 59% 25% 15%



Chain 8:



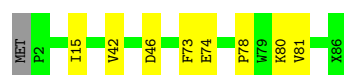
Chain 9: 11% 87%



ASP	MET	GLU	PRO	GLY	LYS	PRO	PHE	PRO	ARG	ALA	PRO	PRO	PRO	PRO	THR	CYS	TYR	LEU	PRO	THR	THR	GLY	GLY	LEU	GLU	ARG	GLY	LEU	GLY	LEU	ALA	MET	PHE	ASP	LYS	LEU	LEU	LEU	GLY	GLN	ALA	ASN	ASN	LYS	ASP	PRO	VAL	ARG	SER	VAL	GLU	PRO	GLY	GLU	PRO	THR	THR	THR	ASN	PRO	ARG	SER	LYS	ASN	LEU	VAL	ALA	SER	GLY	PRO	PRO	ALA	ARG	VAL	VAL	GLY	THR	PRO	GLY	GLU	THR	PRO	THR	THR	ASP	LEU	THR	VAL	SER	SER	PRO	THR	ASP	LEU	THR	VAL	GLY	LYS	LYS	THR	THR	GLY	GLY	GLY	GLU	GLU	GLY	LYS	PRO	PRO	GLY	SER
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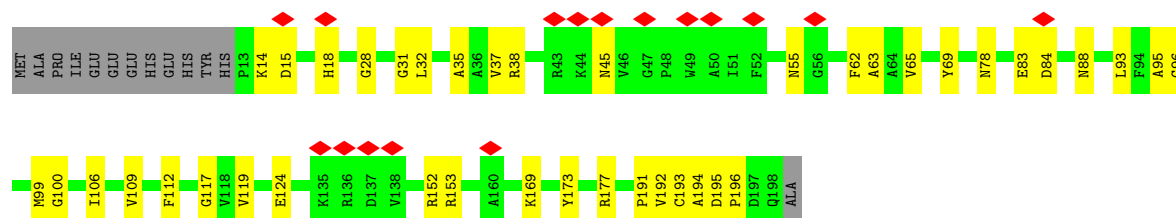
- Molecule 9: Subunit NDUFA1 of NADH-ubiquinone oxidoreductase (Complex I)

Chain D:  90% 9% .



- Molecule 10: NADH-ubiquinone oxidoreductase-like protein

Chain J:  8% 73% 21% 7% .



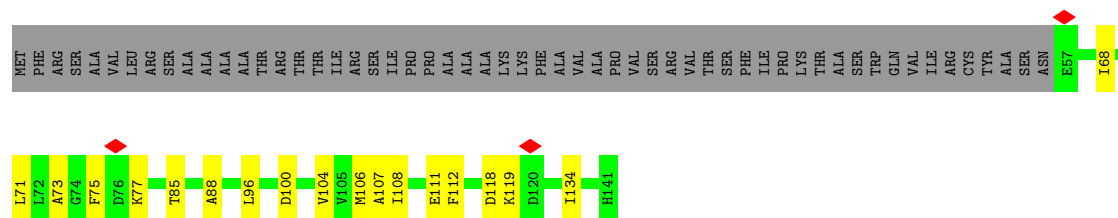
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain L:  72% 27% .



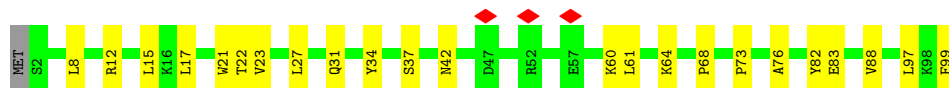
- Molecule 12: Acyl carrier protein

Chain Q:  48% 13% 40% .

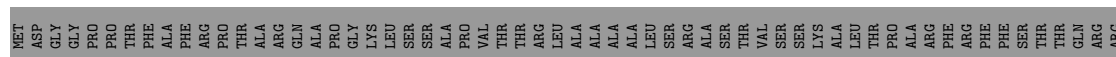


- Molecule 13: Complex I-B22

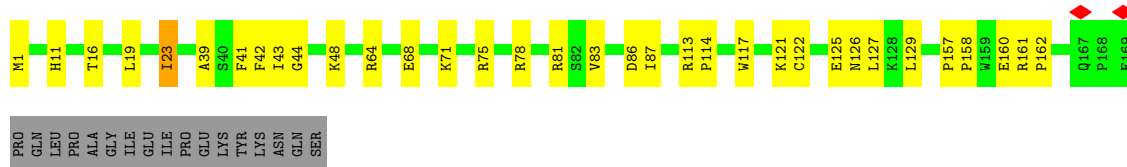
Chain R:  76% 23% .



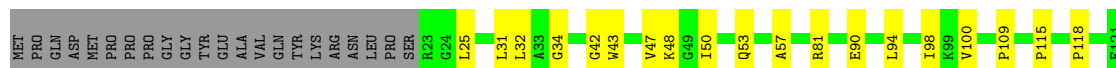
- Molecule 14: Complex I-ESSS



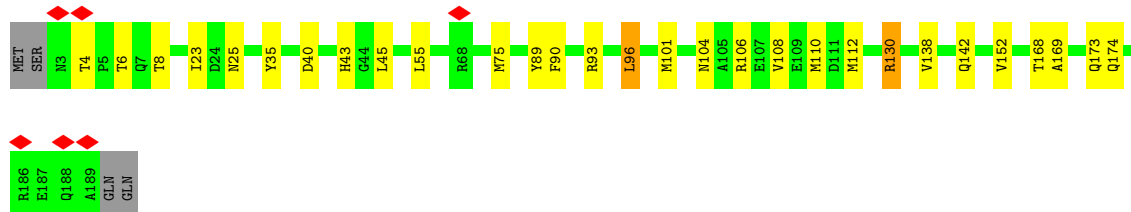
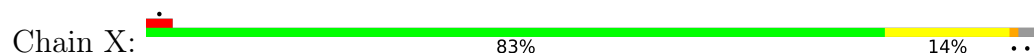
- Molecule 15: NADH-ubiquinone oxidoreductase



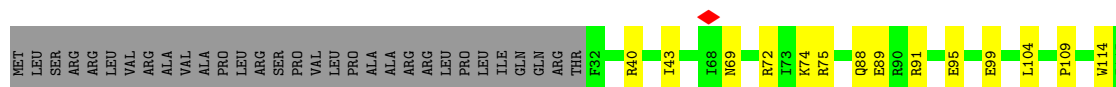
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

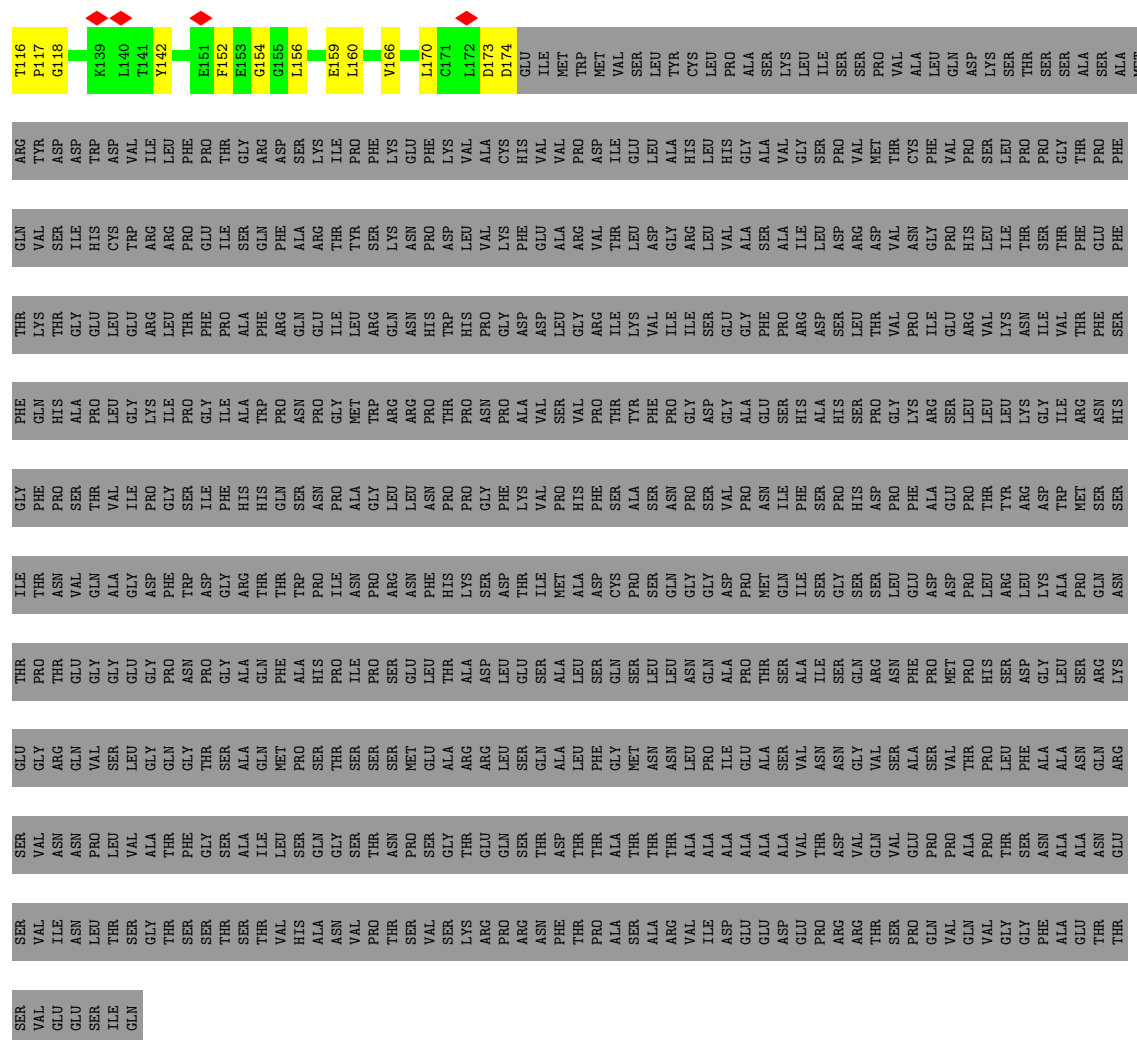


- Molecule 17: NADH-ubiquinone oxidoreductase-like protein

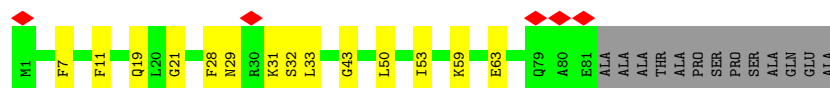


- Molecule 18: NADH dehydrogenase (Ubiquinone)-like protein





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

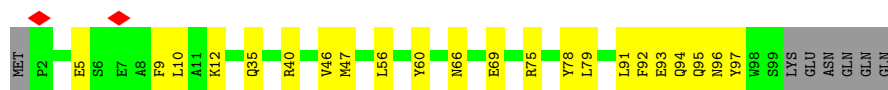


- Molecule 20: Subunit NDUF3 of NADH-ubiquinone oxidoreductase (Complex I)



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

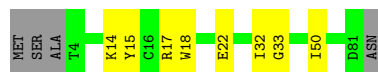
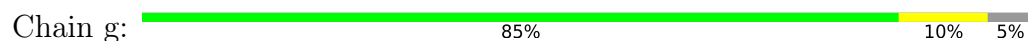




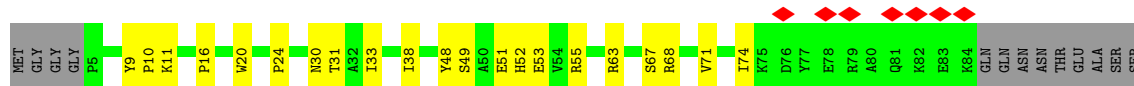
- Molecule 22: Subunit NDUFB2 of NADH-ubiquinone oxidoreductase (Complex I)



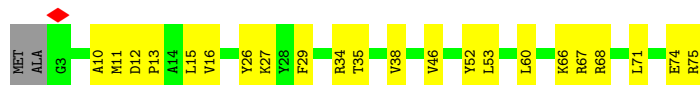
- Molecule 23: Subunit NDUFA3 of NADH-ubiquinone oxidoreductase (Complex I)



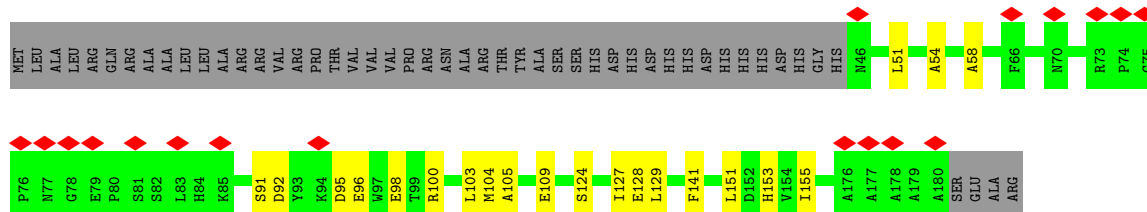
- Molecule 24: Subunit NDUFB6 of NADH-ubiquinone oxidoreductase (Complex I)



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.226	Depositor
Minimum map value	-1.186	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	143.964, 218.457, 227.664	wwPDB
Map dimensions	272, 261, 172	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, LMN, 3PE, CDL, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.62	1/2633 (0.0%)	0.91	3/3593 (0.1%)
2	2	0.64	1/4562 (0.0%)	0.94	9/6205 (0.1%)
3	3	0.53	0/934	0.88	2/1269 (0.2%)
4	4	0.49	0/4002	0.76	4/5454 (0.1%)
5	5	0.43	2/5414 (0.0%)	0.68	4/7371 (0.1%)
6	6	0.79	4/1481 (0.3%)	0.99	2/2020 (0.1%)
7	8	0.19	0/671	0.43	0/896
8	9	0.54	0/824	0.82	0/1112
9	D	0.79	1/674 (0.1%)	1.12	0/911
10	J	0.33	0/1400	0.56	0/1892
11	L	0.60	0/677	0.86	0/917
12	Q	0.25	0/673	0.56	1/913 (0.1%)
13	R	0.40	0/832	0.62	0/1133
14	S	0.32	0/635	0.57	0/869
15	U	0.73	1/1403 (0.1%)	1.10	2/1904 (0.1%)
16	W	0.69	0/830	1.17	2/1120 (0.2%)
17	X	0.73	0/1519	1.06	3/2053 (0.1%)
18	a	0.35	0/1204	0.55	0/1632
19	b	0.25	0/701	0.45	0/939
20	c	0.21	0/509	0.42	0/691
21	d	0.31	0/835	0.56	0/1123
22	e	0.48	2/324 (0.6%)	0.50	0/440
23	g	0.58	0/631	0.86	0/868
24	i	0.32	0/706	0.61	2/960 (0.2%)
25	j	0.21	0/617	0.37	0/830
26	n	0.66	2/1092 (0.2%)	0.93	0/1481
All	All	0.54	14/35783 (0.0%)	0.81	34/48596 (0.1%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	6	181	GLU	C-N	9.50	1.46	1.33
2	2	122	ILE	C-N	8.67	1.45	1.33
6	6	45	VAL	C-N	-8.59	1.21	1.33
5	5	222	ALA	C-N	-8.35	1.22	1.34
6	6	46	SER	C-N	8.22	1.43	1.34

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	130	ARG	N-CA-C	-7.72	103.66	113.23
16	W	25	LEU	N-CA-C	-7.47	103.62	112.89
4	4	182	PHE	CA-CB-CG	6.86	120.66	113.80
2	2	122	ILE	O-C-N	6.63	130.26	122.83
4	4	427	THR	CB-CA-C	6.55	118.90	109.26

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	1	2573	0	2696	45	0
2	2	4456	0	4650	81	0
3	3	907	0	922	22	0
4	4	3904	0	4056	92	0
5	5	5272	0	5396	142	0
6	6	1454	0	1538	49	0
7	8	658	0	648	17	0
8	9	807	0	778	10	0
9	D	678	0	642	5	0
10	J	1375	0	1386	37	0
11	L	671	0	737	24	0
12	Q	663	0	638	13	0
13	R	807	0	823	25	0
14	S	610	0	557	18	0
15	U	1365	0	1333	20	0
16	W	812	0	833	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X	1480	0	1432	21	0
18	a	1167	0	1104	23	0
19	b	683	0	690	13	0
20	c	490	0	451	12	0
21	d	817	0	810	24	0
22	e	309	0	300	5	0
23	g	610	0	620	6	0
24	i	677	0	653	19	0
25	j	603	0	623	17	0
26	n	1061	0	1022	17	0
27	1	68	0	93	2	0
27	4	95	0	112	8	0
27	5	142	0	183	7	0
27	8	36	0	46	1	0
27	J	30	0	34	3	0
27	W	34	0	47	1	0
27	g	75	0	101	6	0
27	n	78	0	110	2	0
28	1	30	0	34	2	0
28	2	31	0	36	0	0
28	3	36	0	46	0	0
28	4	45	0	64	4	0
28	5	86	0	123	8	0
28	n	51	0	76	5	0
29	2	84	0	115	8	0
29	4	86	0	119	8	0
29	D	59	0	62	1	0
29	X	79	0	105	4	0
29	g	56	0	56	3	0
30	2	58	0	77	2	0
30	4	58	0	77	5	0
30	J	69	0	88	0	0
31	Q	36	0	47	5	0
32	1	62	0	0	1	0
32	2	141	0	0	2	0
32	3	24	0	0	1	0
32	4	84	0	0	4	0
32	5	49	0	0	2	0
32	6	35	0	0	0	0
32	9	19	0	0	0	0
32	D	27	0	0	0	0
32	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	11	0	0	1	0
32	R	4	0	0	0	0
32	S	1	0	0	0	0
32	U	36	0	0	0	0
32	W	29	0	0	0	0
32	X	45	0	0	0	0
32	a	11	0	0	0	0
32	b	4	0	0	0	0
32	d	9	0	0	0	0
32	g	10	0	0	0	0
32	i	4	0	0	0	0
32	j	4	0	0	0	0
32	n	23	0	0	0	0
All	All	36964	0	37189	649	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 9.

The worst 5 of 649 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)
9:D:42:VAL:HG13	9:D:46:ASP:HB2	1.48	0.94
4:4:408:GLN:HA	28:5:701:PC1:H131	1.55	0.87
6:6:127:TYR:O	6:6:131:ILE:HG12	1.76	0.85
5:5:72:ILE:HG23	5:5:132:ASN:HD21	1.43	0.84
28:4:605:PC1:H241	5:5:610:GLU:HG2	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	330/378 (87%)	317 (96%)	13 (4%)	0	100	100
2	2	554/571 (97%)	545 (98%)	9 (2%)	0	100	100
3	3	112/146 (77%)	108 (96%)	4 (4%)	0	100	100
4	4	490/542 (90%)	479 (98%)	11 (2%)	0	100	100
5	5	668/679 (98%)	638 (96%)	30 (4%)	0	100	100
6	6	186/224 (83%)	178 (96%)	8 (4%)	0	100	100
7	8	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
8	9	101/785 (13%)	100 (99%)	1 (1%)	0	100	100
9	D	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
10	J	184/199 (92%)	179 (97%)	5 (3%)	0	100	100
11	L	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
12	Q	83/141 (59%)	83 (100%)	0	0	100	100
13	R	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
14	S	72/143 (50%)	68 (94%)	4 (6%)	0	100	100
15	U	167/186 (90%)	162 (97%)	5 (3%)	0	100	100
16	W	97/121 (80%)	97 (100%)	0	0	100	100
17	X	185/191 (97%)	182 (98%)	3 (2%)	0	100	100
18	a	141/815 (17%)	136 (96%)	5 (4%)	0	100	100
19	b	79/94 (84%)	78 (99%)	1 (1%)	0	100	100
20	c	58/93 (62%)	50 (86%)	8 (14%)	0	100	100
21	d	96/105 (91%)	92 (96%)	4 (4%)	0	100	100
22	e	35/46 (76%)	35 (100%)	0	0	100	100
23	g	76/82 (93%)	74 (97%)	2 (3%)	0	100	100
24	i	78/93 (84%)	75 (96%)	3 (4%)	0	100	100
25	j	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
26	n	133/184 (72%)	129 (97%)	4 (3%)	0	100	100
All	All	4332/6253 (69%)	4198 (97%)	134 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	284/326 (87%)	275 (97%)	9 (3%)	34	59
2	2	509/518 (98%)	502 (99%)	7 (1%)	59	78
3	3	97/128 (76%)	97 (100%)	0	100	100
4	4	431/477 (90%)	431 (100%)	0	100	100
5	5	579/596 (97%)	578 (100%)	1 (0%)	87	95
6	6	162/203 (80%)	160 (99%)	2 (1%)	63	80
7	8	69/75 (92%)	69 (100%)	0	100	100
8	9	84/687 (12%)	84 (100%)	0	100	100
9	D	68/69 (99%)	67 (98%)	1 (2%)	57	77
10	J	126/146 (86%)	126 (100%)	0	100	100
11	L	73/76 (96%)	72 (99%)	1 (1%)	59	78
12	Q	72/119 (60%)	72 (100%)	0	100	100
13	R	87/89 (98%)	87 (100%)	0	100	100
14	S	59/111 (53%)	59 (100%)	0	100	100
15	U	149/167 (89%)	148 (99%)	1 (1%)	76	88
16	W	82/102 (80%)	82 (100%)	0	100	100
17	X	145/152 (95%)	144 (99%)	1 (1%)	76	88
18	a	123/697 (18%)	122 (99%)	1 (1%)	73	86
19	b	67/74 (90%)	67 (100%)	0	100	100
20	c	47/80 (59%)	47 (100%)	0	100	100
21	d	87/94 (93%)	87 (100%)	0	100	100
22	e	29/35 (83%)	29 (100%)	0	100	100
23	g	65/69 (94%)	65 (100%)	0	100	100
24	i	68/78 (87%)	68 (100%)	0	100	100
25	j	63/64 (98%)	63 (100%)	0	100	100
26	n	106/150 (71%)	105 (99%)	1 (1%)	70	84
All	All	3731/5382 (69%)	3706 (99%)	25 (1%)	73	88

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	164	THR
6	6	73	TYR
26	n	103	LEU
5	5	223	LYS
6	6	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
16	W	54	ASN
24	i	29	GLN
17	X	65	GLN
20	c	39	HIS
5	5	503	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](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	3PE	n	201	-	38,38,50	1.00	4 (10%)	41,43,55	1.15	2 (4%)
29	CDL	X	201	-	78,78,99	0.32	0	84,90,111	0.41	0
27	3PE	5	702	-	39,39,50	0.31	0	42,44,55	0.37	0
28	PC1	2	603	-	30,30,53	0.34	0	36,38,61	0.37	0
28	PC1	4	605	-	44,44,53	1.04	4 (9%)	50,52,61	1.07	2 (4%)
29	CDL	4	601	-	85,85,99	0.29	0	91,97,111	0.35	0
27	3PE	4	602	-	33,33,50	1.06	4 (12%)	36,38,55	1.14	2 (5%)
28	PC1	5	701	-	44,44,53	0.46	0	50,52,61	0.47	0
28	PC1	n	202	-	50,50,53	0.98	4 (8%)	56,58,61	1.09	2 (3%)
29	CDL	D	101	-	58,58,99	0.34	0	64,70,111	0.45	0
29	CDL	2	601	-	83,83,99	0.32	0	89,95,111	0.37	0
27	3PE	1	401	-	40,40,50	0.41	0	43,45,55	0.44	0
28	PC1	1	403	-	29,29,53	1.28	4 (13%)	35,37,61	1.28	3 (8%)
27	3PE	5	703	-	31,31,50	1.10	4 (12%)	34,36,55	1.17	2 (5%)
27	3PE	4	606	-	27,27,50	1.17	4 (14%)	30,32,55	1.19	2 (6%)
27	3PE	J	201	-	29,29,50	1.13	4 (13%)	32,34,55	1.19	2 (6%)
27	3PE	5	706	-	27,27,50	1.10	3 (11%)	30,32,55	1.17	1 (3%)
27	3PE	W	201	-	33,33,50	0.32	0	34,37,55	0.41	0
27	3PE	n	203	-	38,38,50	0.99	4 (10%)	41,43,55	1.13	2 (4%)
30	LMN	2	602	-	60,60,72	0.21	0	74,80,98	0.41	0
31	ZMP	Q	201	12	30,35,36	0.21	0	34,42,45	0.45	0
27	3PE	1	402	-	26,26,50	0.35	0	28,30,55	0.55	0
28	PC1	3	201	-	35,35,53	0.34	0	41,43,61	0.39	0
27	3PE	5	704	-	41,41,50	0.96	4 (9%)	44,46,55	1.10	2 (4%)
29	CDL	g	101	-	55,55,99	0.35	0	61,67,111	0.56	0
30	LMN	J	202	-	72,72,72	0.17	0	92,98,98	0.29	0
28	PC1	5	705	-	40,40,53	1.10	3 (7%)	46,48,61	1.16	3 (6%)
30	LMN	4	604	-	60,60,72	0.20	0	74,80,98	0.29	0
27	3PE	g	103	-	38,38,50	0.36	0	41,43,55	0.38	0
27	3PE	4	603	-	32,32,50	1.07	4 (12%)	35,37,55	1.18	2 (5%)
27	3PE	8	101	-	35,35,50	1.03	4 (11%)	38,40,55	1.15	2 (5%)
27	3PE	g	102	-	35,35,50	0.34	0	38,40,55	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	3PE	n	201	-	-	14/42/42/54	-
29	CDL	X	201	-	-	23/89/89/110	-
27	3PE	5	702	-	-	13/43/43/54	-
28	PC1	2	603	-	-	7/34/34/57	-
28	PC1	4	605	-	-	29/48/48/57	-
29	CDL	4	601	-	-	21/96/96/110	-
27	3PE	4	602	-	-	12/37/37/54	-
28	PC1	5	701	-	-	19/48/48/57	-
28	PC1	n	202	-	-	19/54/54/57	-
29	CDL	D	101	-	-	25/69/69/110	-
29	CDL	2	601	-	-	21/94/94/110	-
27	3PE	1	401	-	-	6/44/44/54	-
28	PC1	1	403	-	-	16/32/32/57	-
27	3PE	5	703	-	-	8/35/35/54	-
27	3PE	4	606	-	-	7/31/31/54	-
27	3PE	J	201	-	-	14/33/33/54	-
27	3PE	5	706	-	-	8/30/30/54	-
27	3PE	W	201	-	-	12/36/36/54	-
27	3PE	n	203	-	-	19/42/42/54	-
30	LMN	2	602	-	-	18/44/104/130	0/3/3/4
31	ZMP	Q	201	12	-	8/40/42/43	-
27	3PE	1	402	-	-	8/29/29/54	-
28	PC1	3	201	-	-	10/39/39/57	-
27	3PE	5	704	-	-	14/45/45/54	-
29	CDL	g	101	-	-	15/66/66/110	-
30	LMN	J	202	-	-	11/50/130/130	0/4/4/4
28	PC1	5	705	-	-	22/44/44/57	-
30	LMN	4	604	-	-	15/44/104/130	0/3/3/4
27	3PE	g	103	-	-	15/42/42/54	-
27	3PE	4	603	-	-	20/36/36/54	-
27	3PE	8	101	-	-	16/39/39/54	-
27	3PE	g	102	-	-	15/39/39/54	-

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	705	PC1	O21-C2	-2.86	1.39	1.46
27	n	201	3PE	O21-C2	-2.71	1.40	1.46
27	4	606	3PE	O21-C2	-2.67	1.40	1.46
27	5	704	3PE	O21-C2	-2.67	1.40	1.46
27	4	602	3PE	O21-C2	-2.67	1.40	1.46

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	403	PC1	O21-C21-C22	5.03	120.05	111.09
27	n	201	3PE	O21-C21-C22	4.14	120.44	111.48
28	4	605	PC1	O21-C21-C22	4.13	120.41	111.48
28	n	202	PC1	O21-C21-C22	4.12	120.39	111.48
27	5	706	3PE	O21-C21-C22	4.11	120.37	111.48

There are no chirality outliers.

5 of 480 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	402	3PE	C11-O13-P-O14
27	4	602	3PE	C1-O11-P-O13
27	4	603	3PE	C1-O11-P-O12
27	4	603	3PE	C1-O11-P-O13
27	4	603	3PE	C1-O11-P-O14

There are no ring outliers.

26 monomers are involved in 84 short contacts:

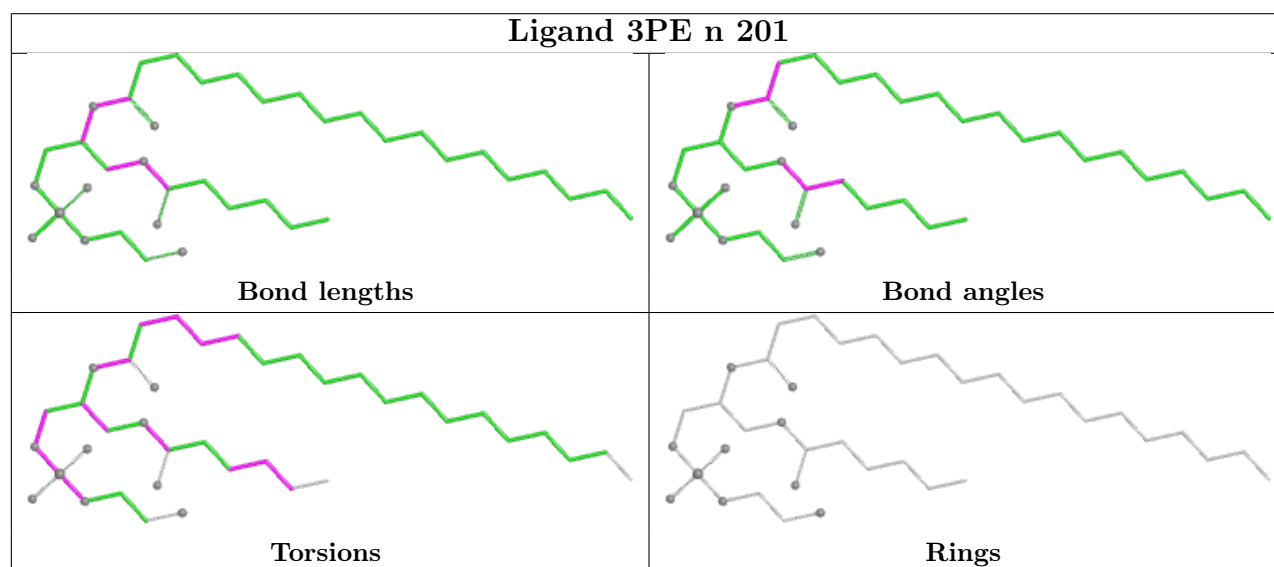
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	201	CDL	4	0
27	5	702	3PE	3	0
28	4	605	PC1	4	0
29	4	601	CDL	8	0
27	4	602	3PE	5	0
28	5	701	PC1	6	0
28	n	202	PC1	5	0
29	D	101	CDL	1	0
29	2	601	CDL	8	0
27	1	401	3PE	1	0
28	1	403	PC1	2	0
27	5	703	3PE	3	0
27	J	201	3PE	3	0

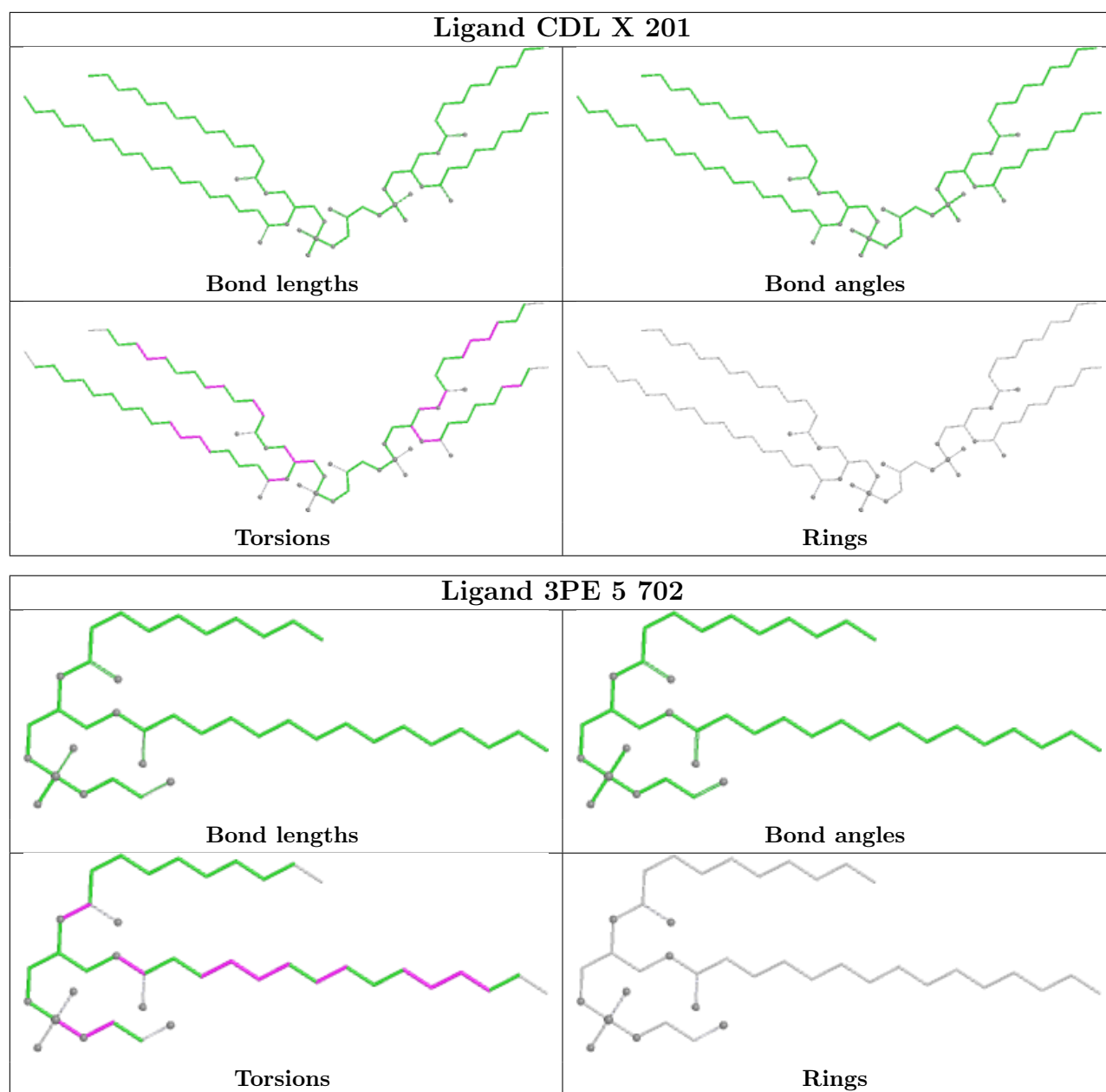
Continued on next page...

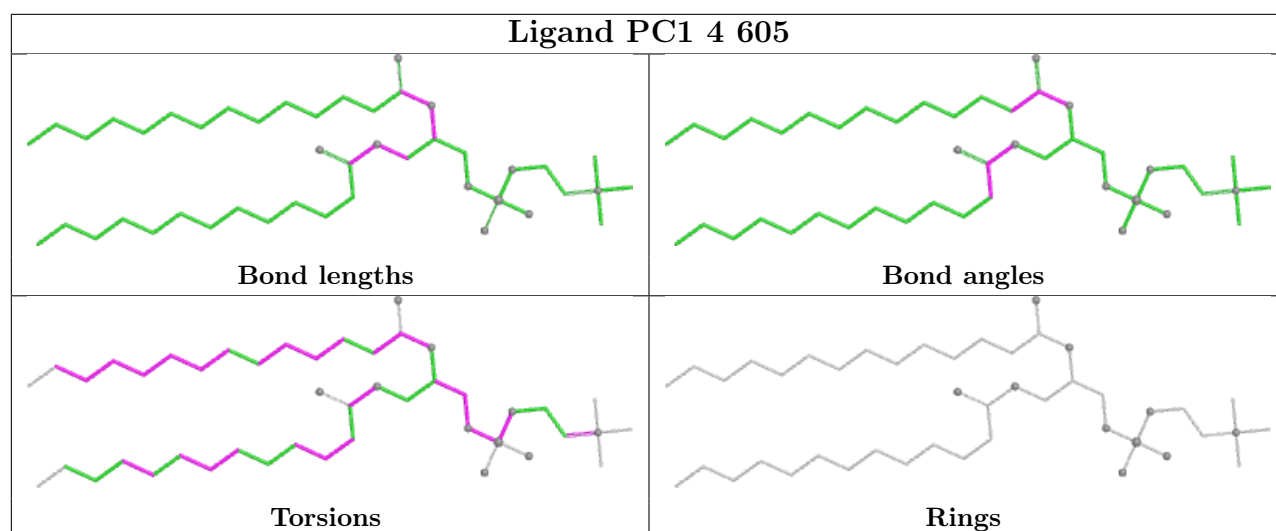
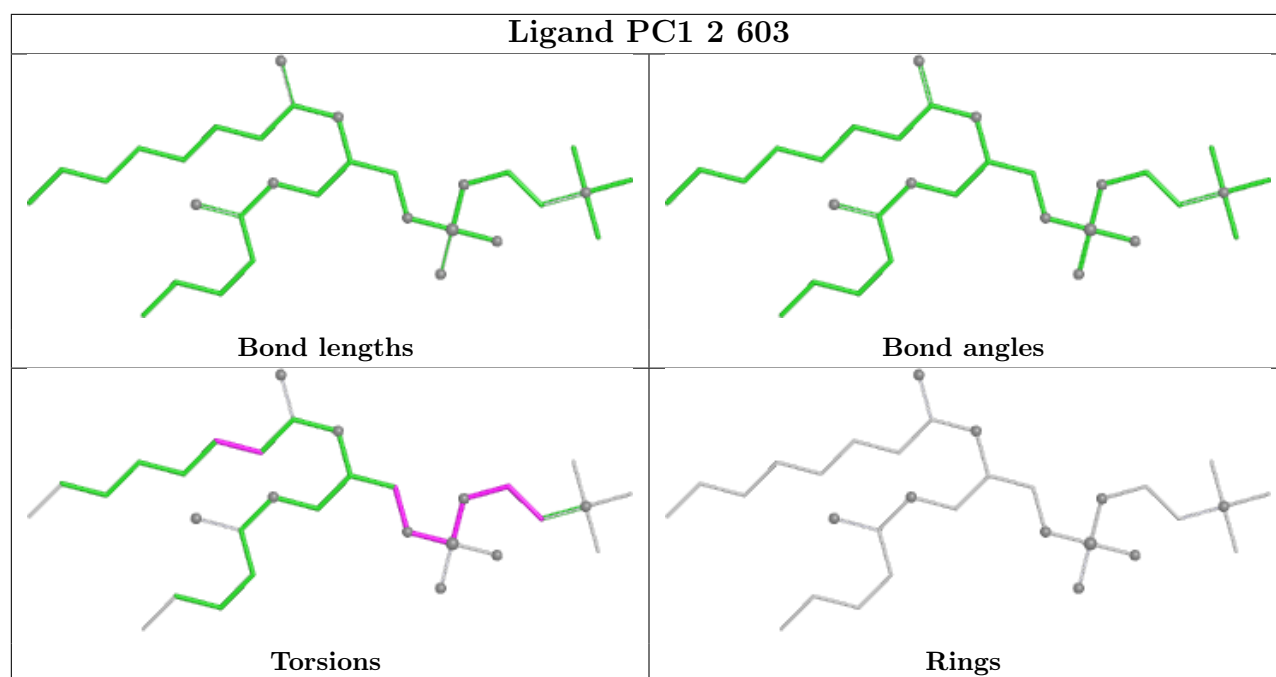
Continued from previous page...

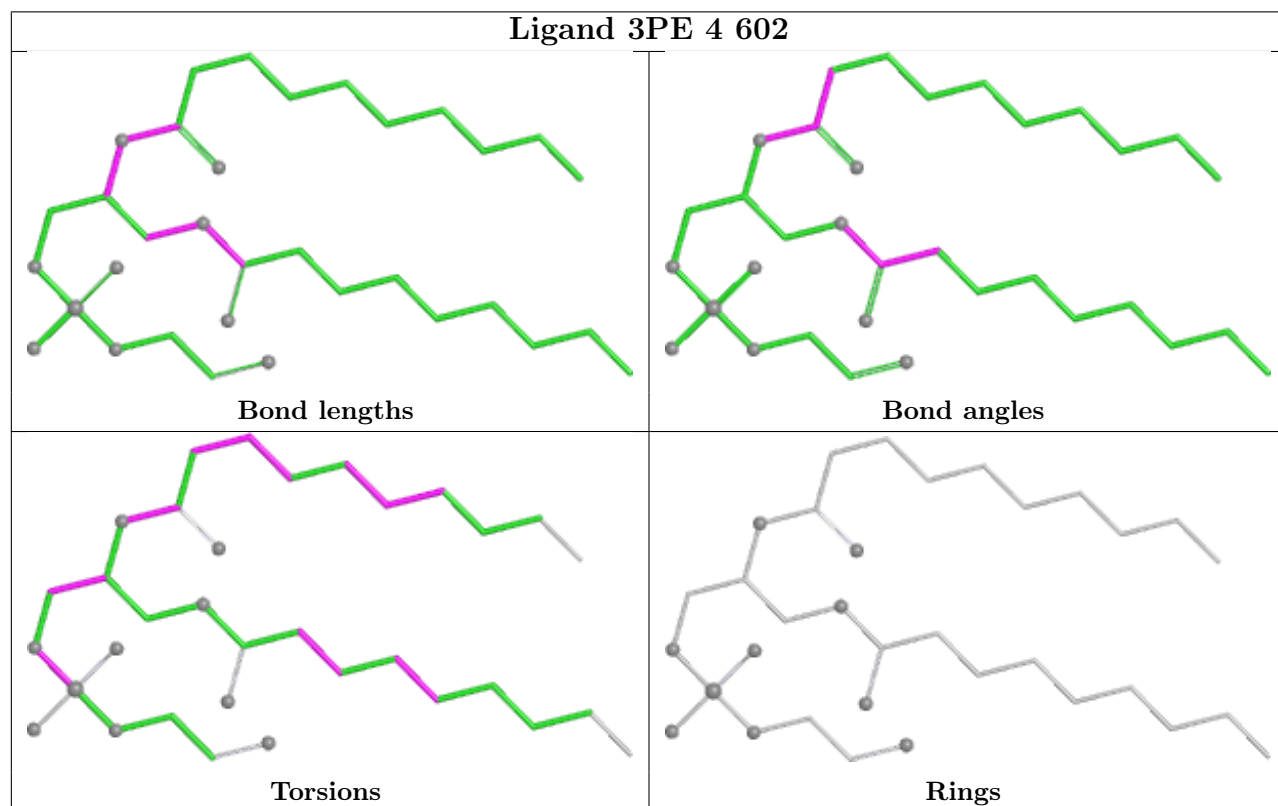
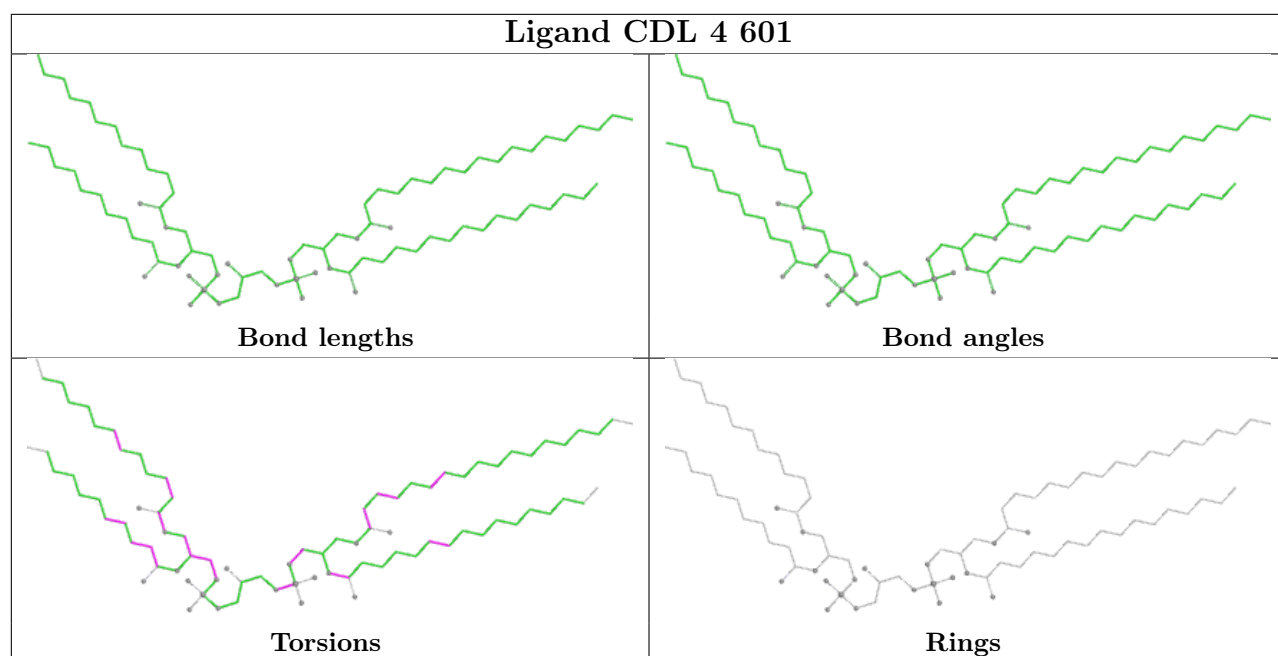
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	W	201	3PE	1	0
27	n	203	3PE	2	0
30	2	602	LMN	2	0
31	Q	201	ZMP	5	0
27	1	402	3PE	1	0
27	5	704	3PE	1	0
29	g	101	CDL	3	0
28	5	705	PC1	2	0
30	4	604	LMN	5	0
27	g	103	3PE	3	0
27	4	603	3PE	3	0
27	8	101	3PE	1	0
27	g	102	3PE	3	0

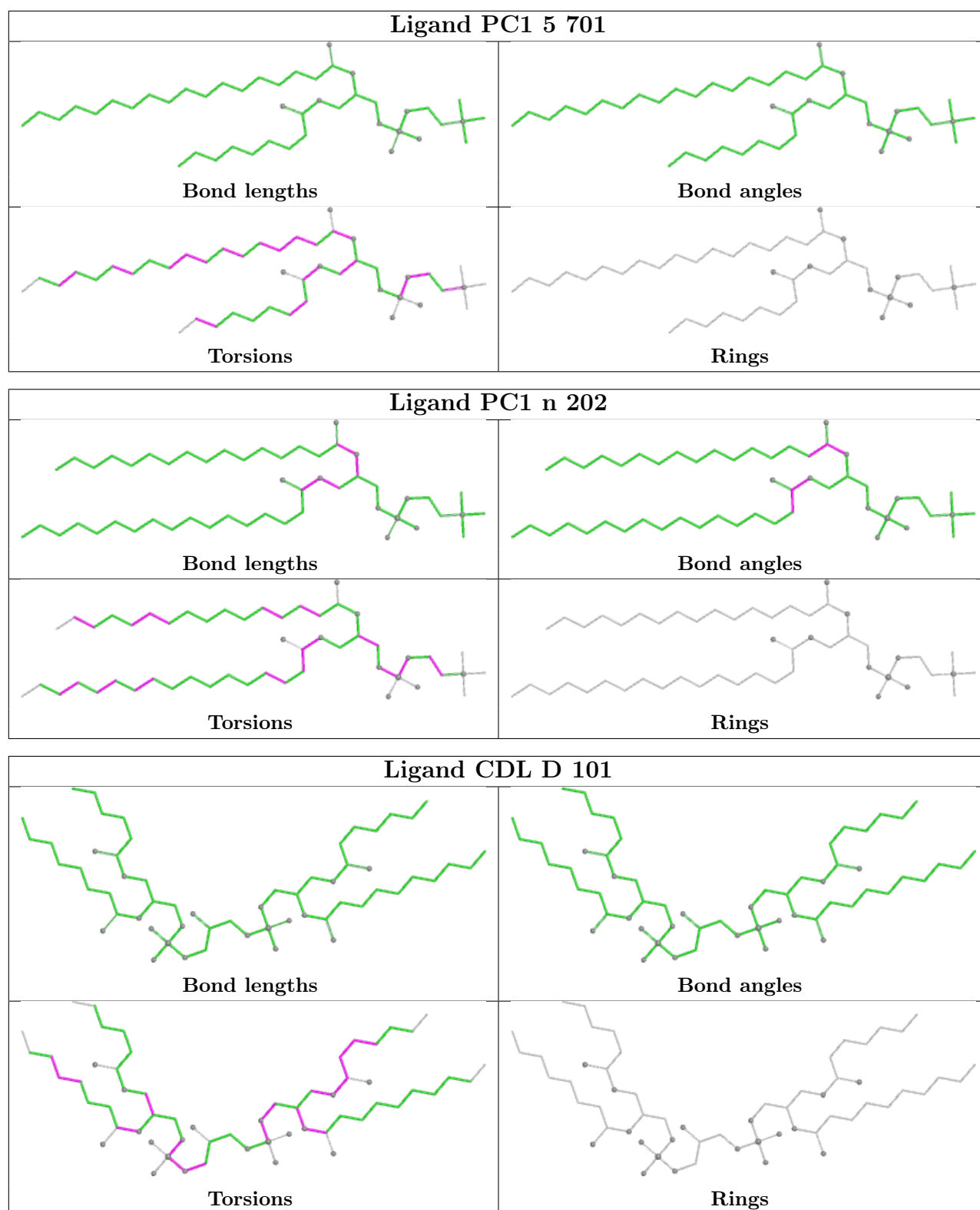
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

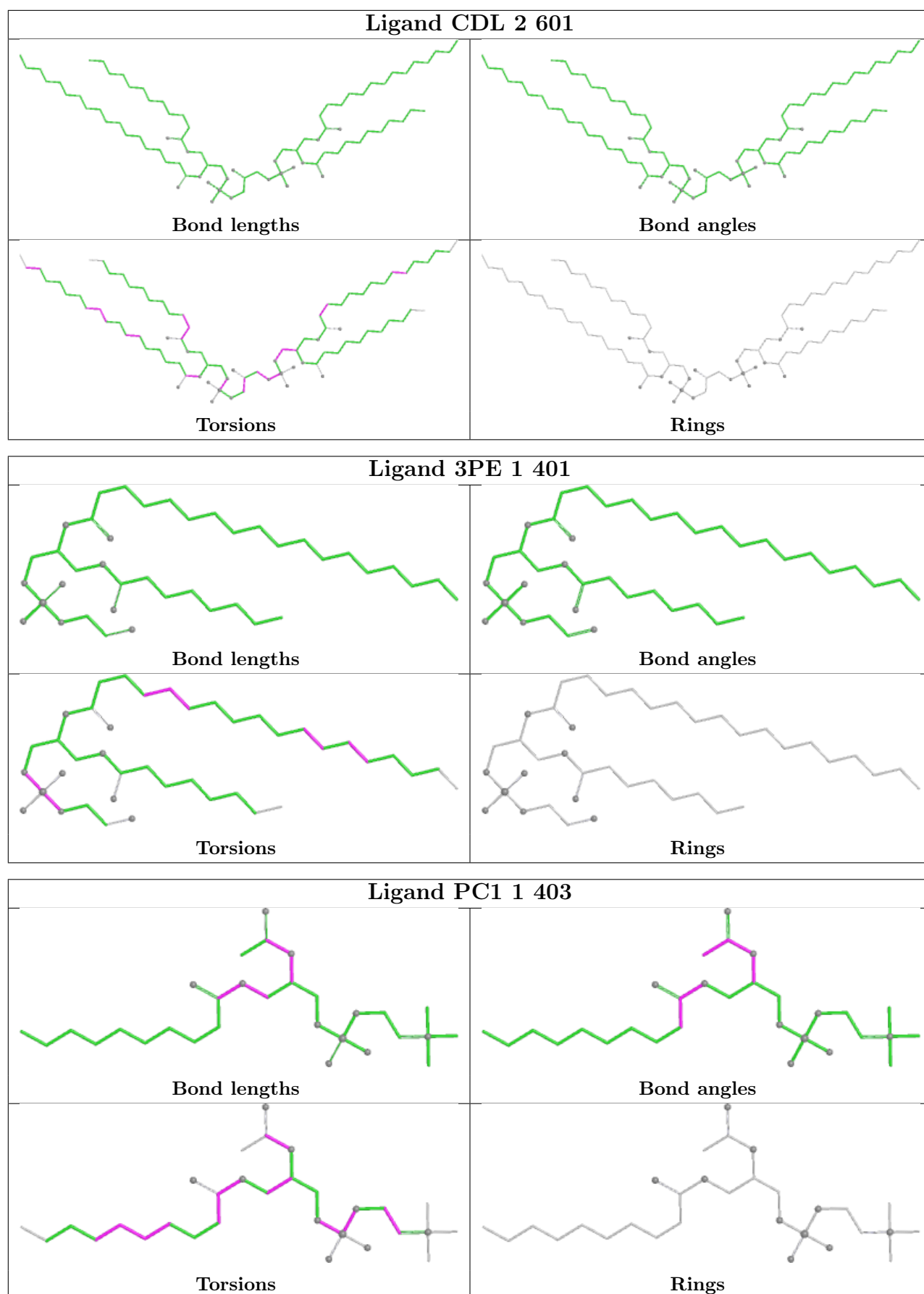


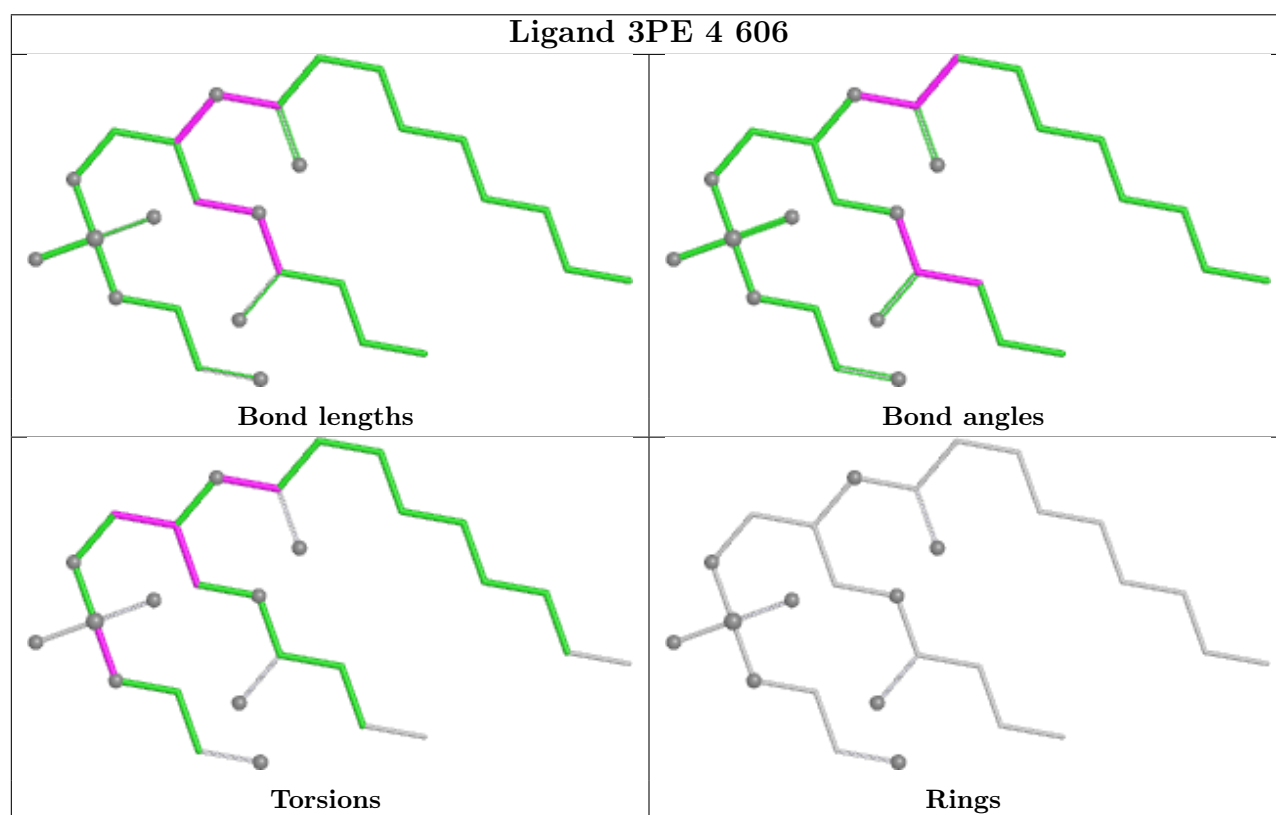
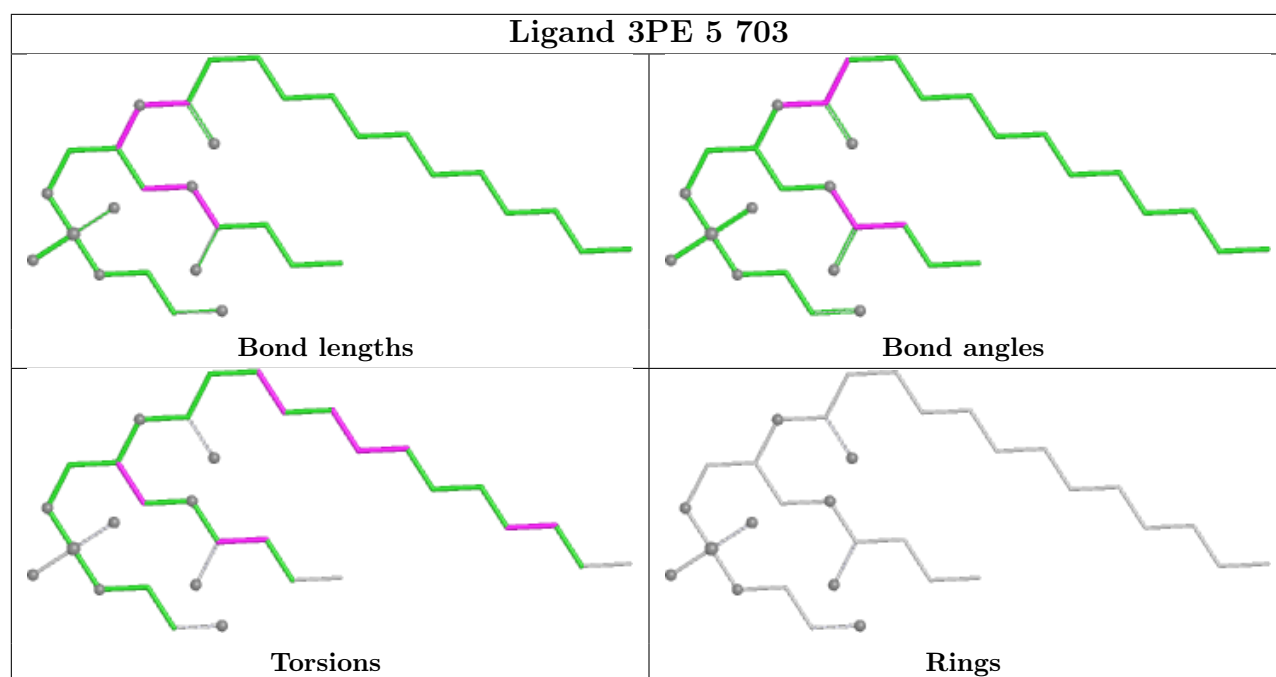




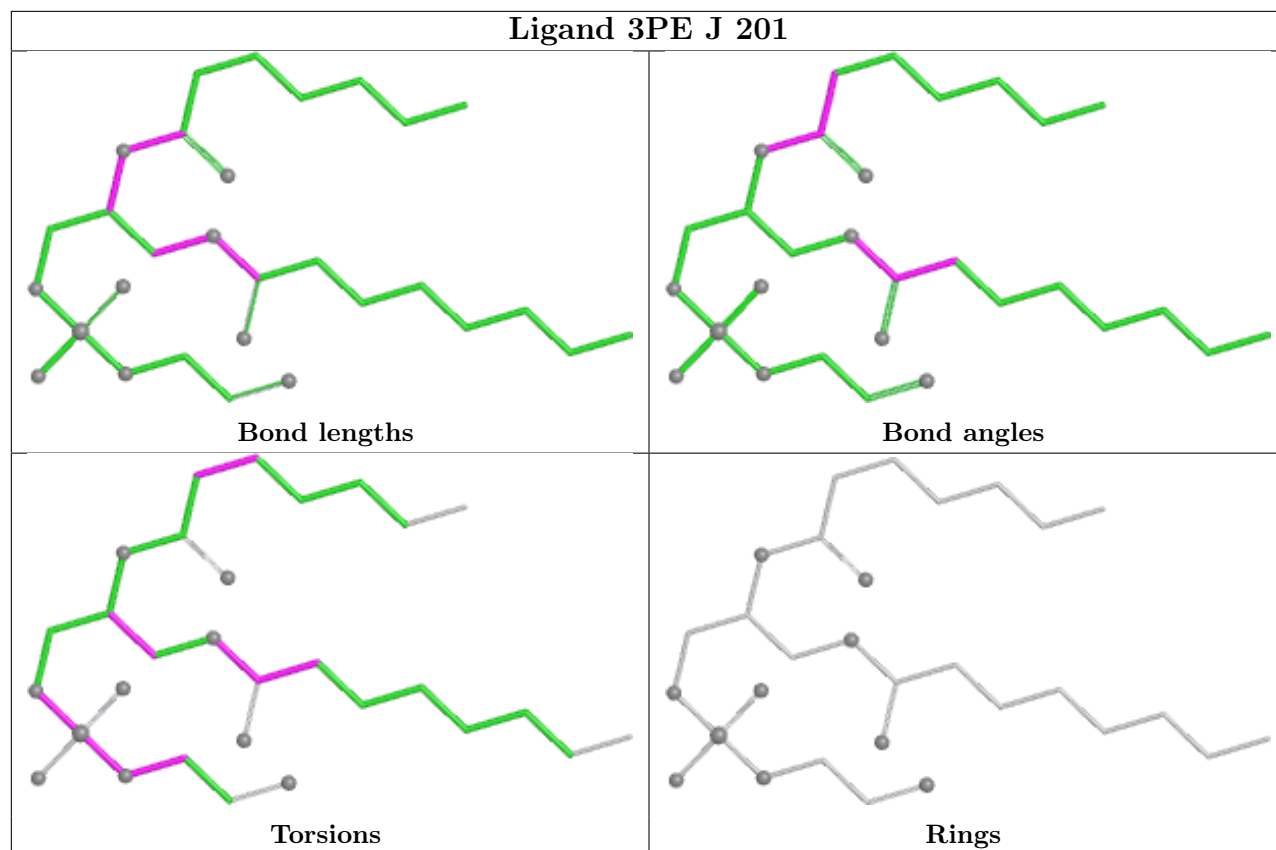




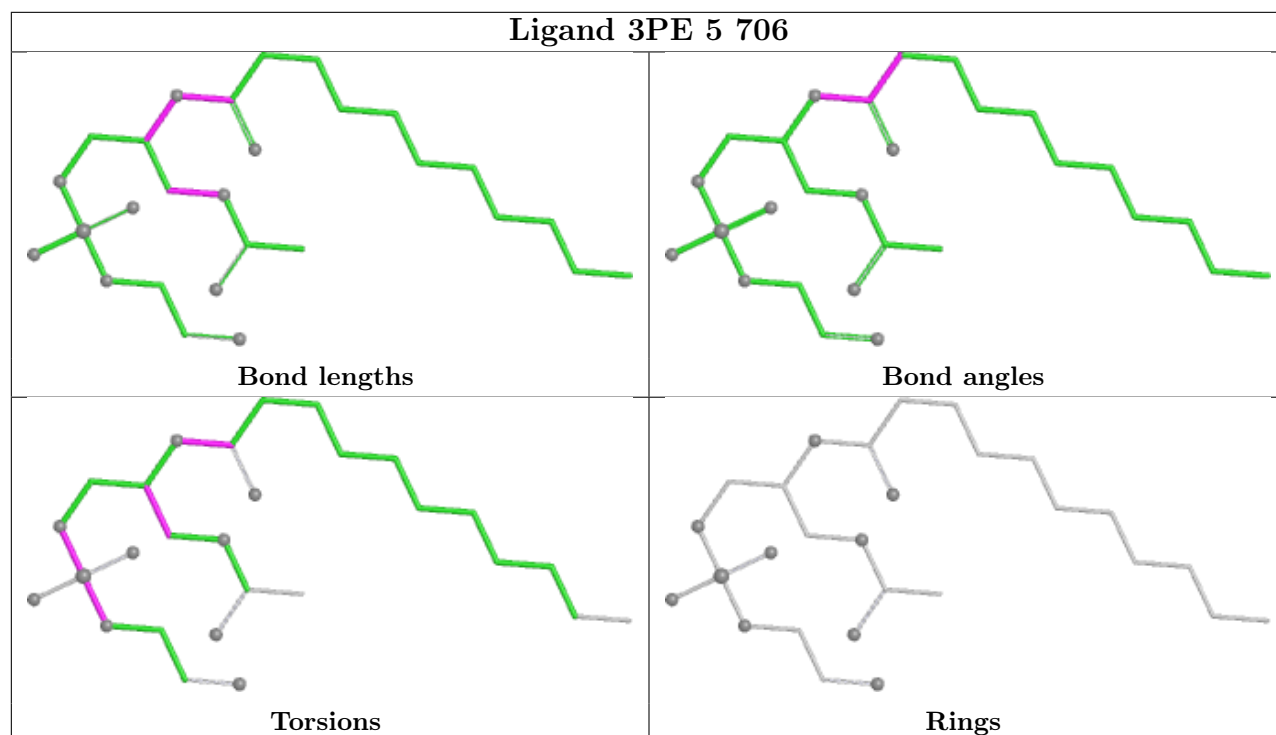


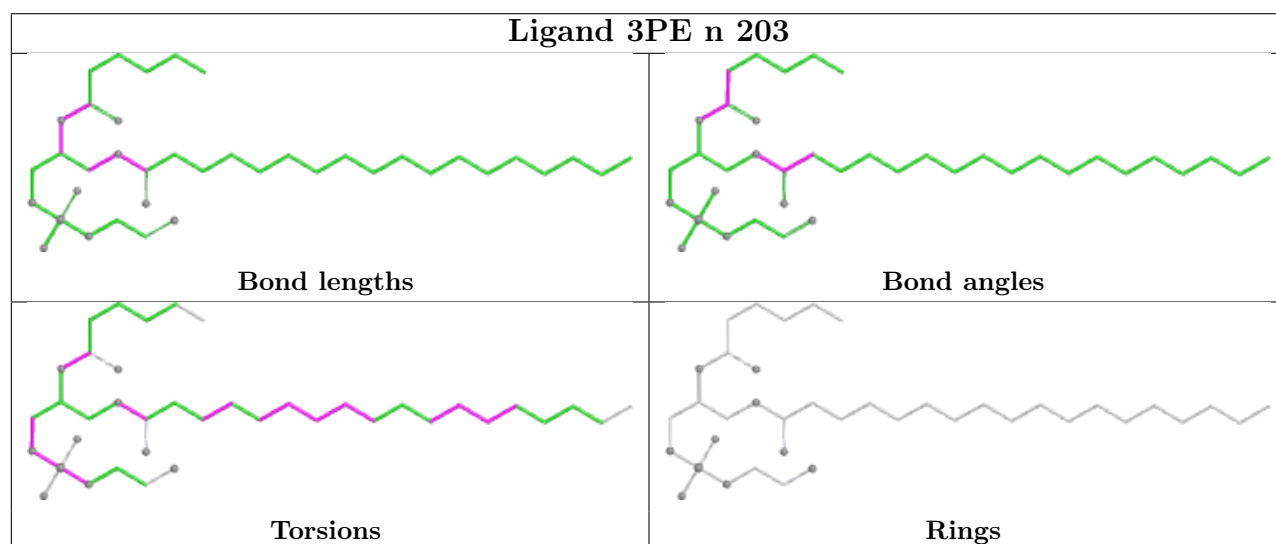
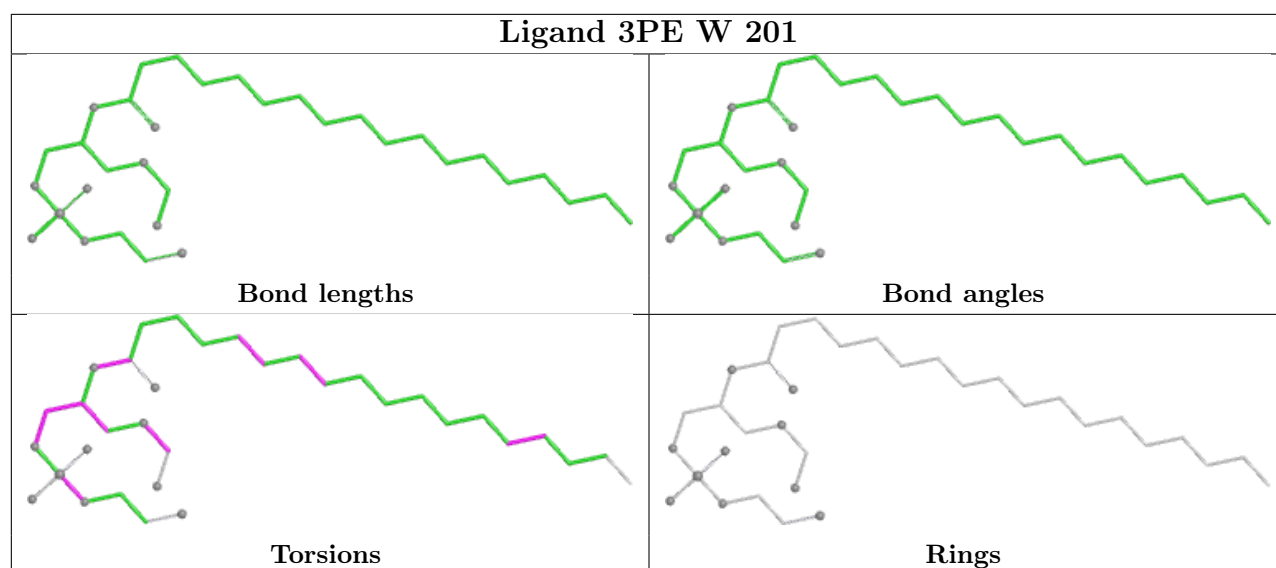


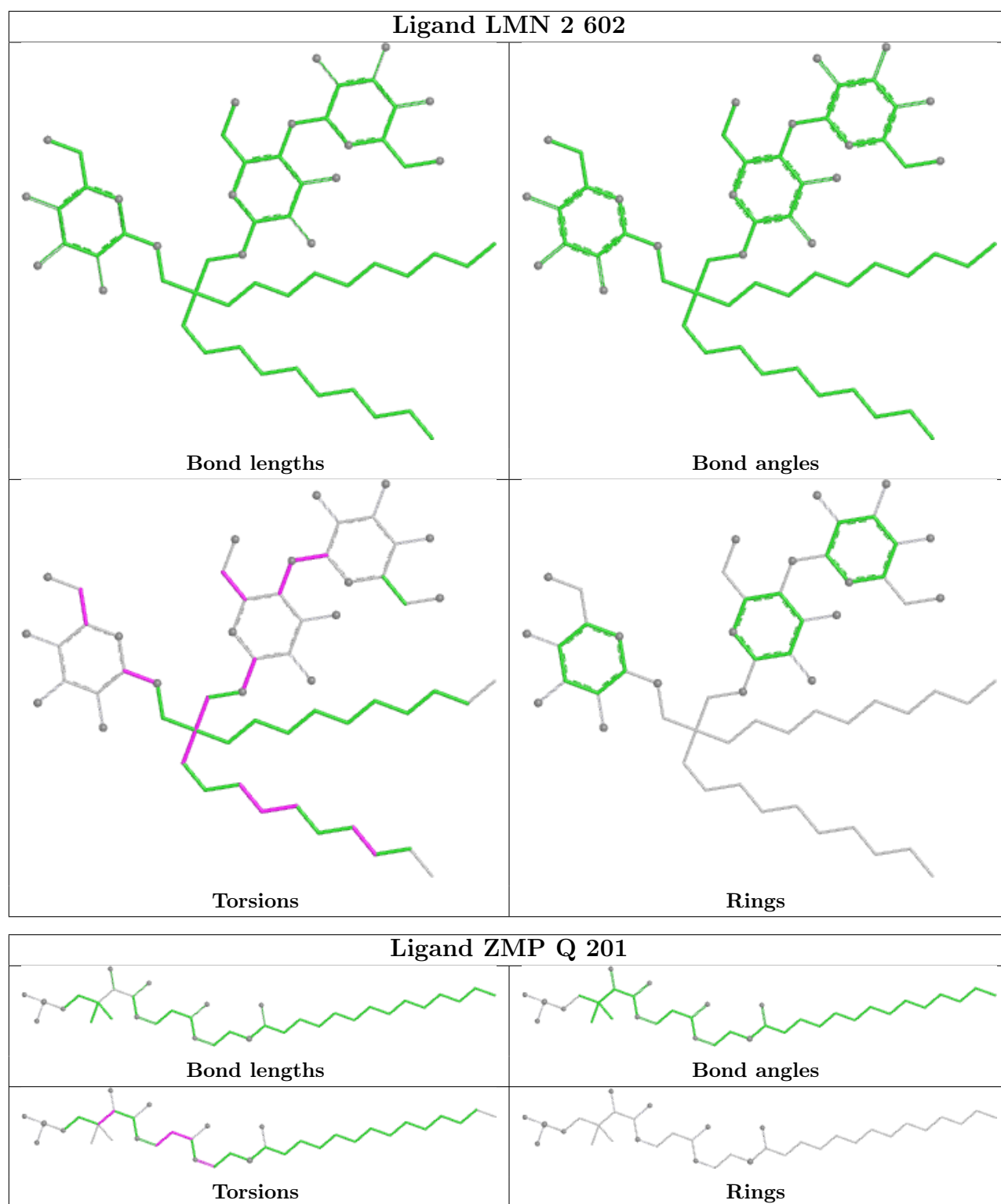
Ligand 3PE J 201

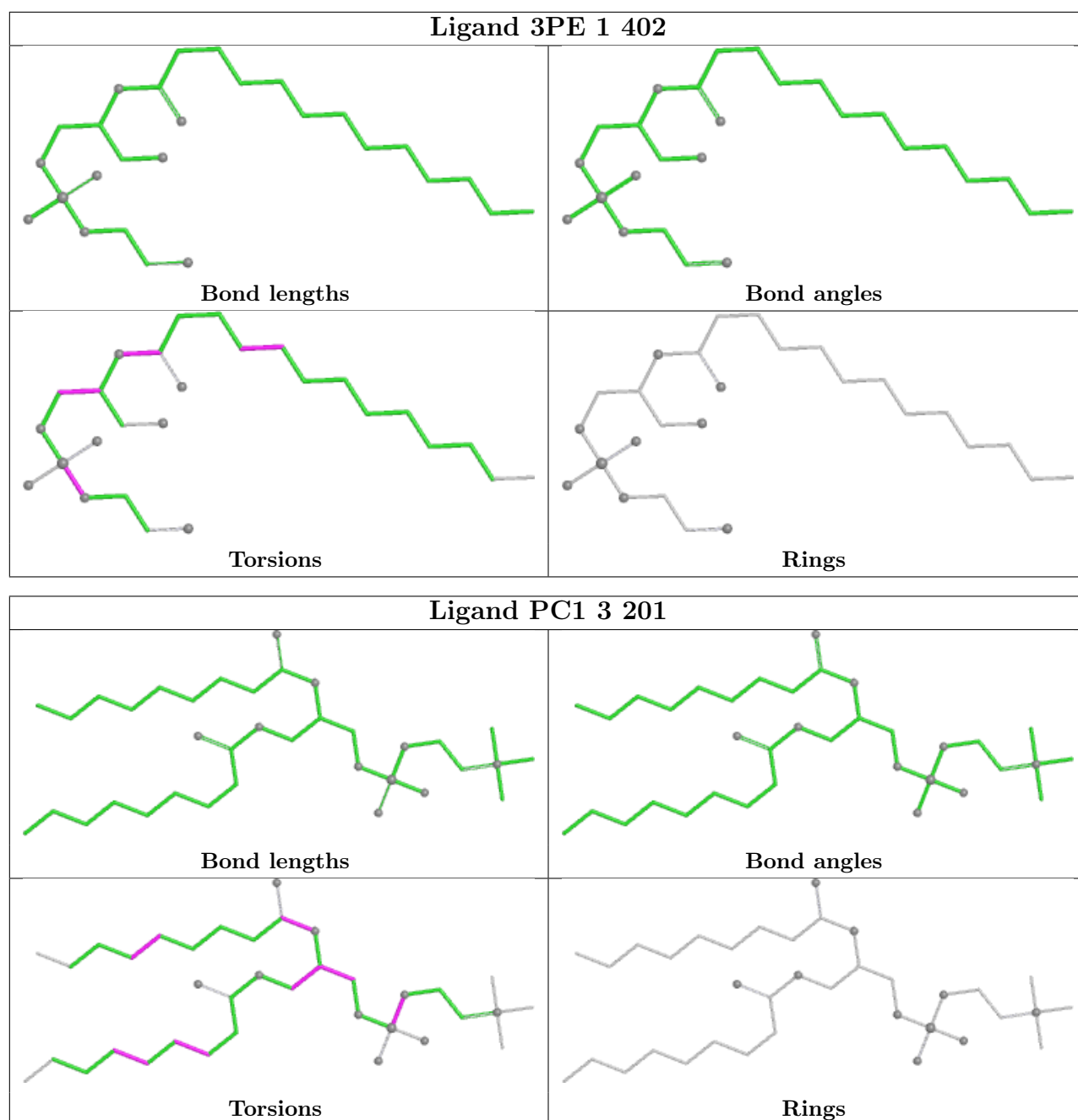


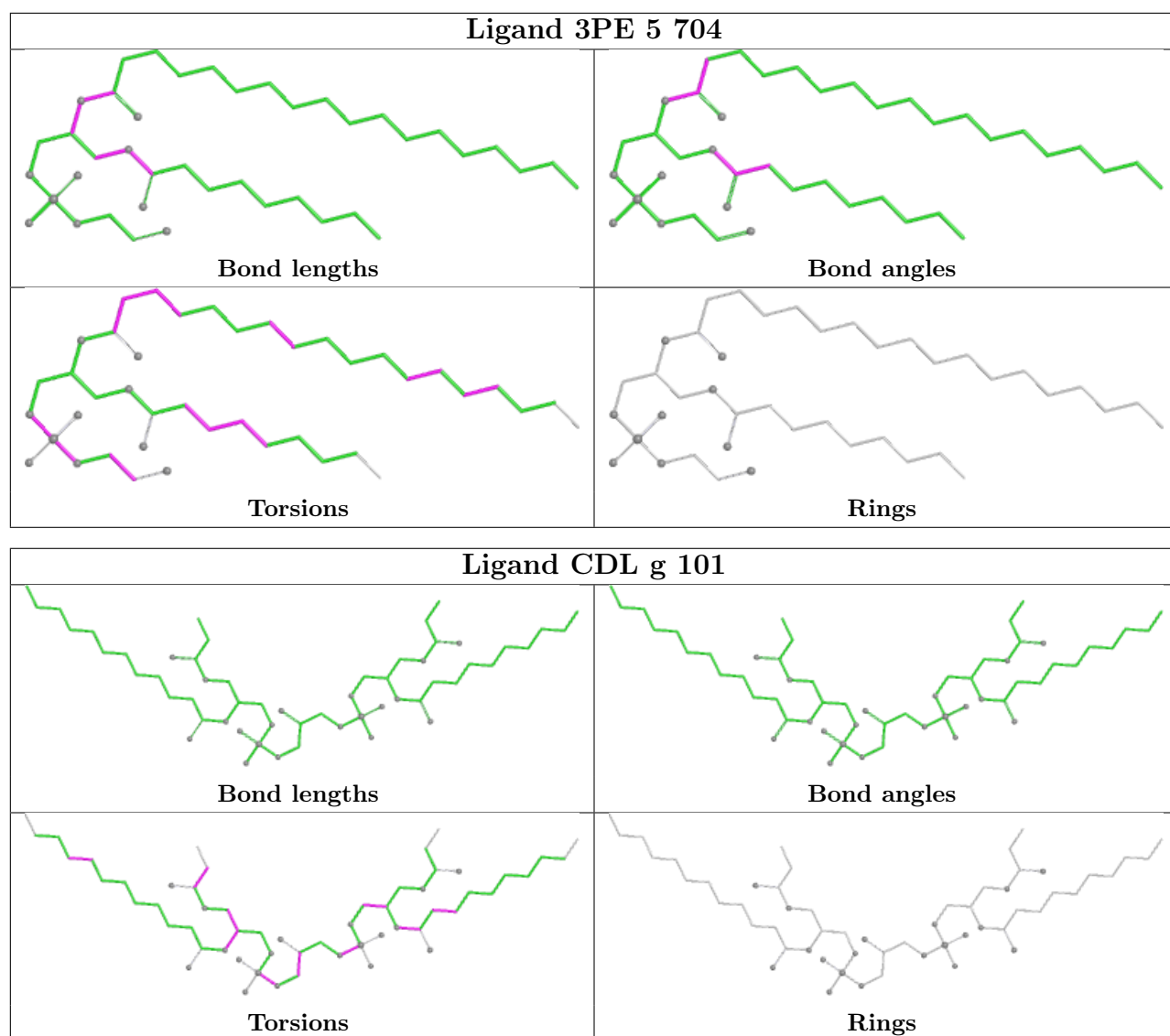
Ligand 3PE 5 706

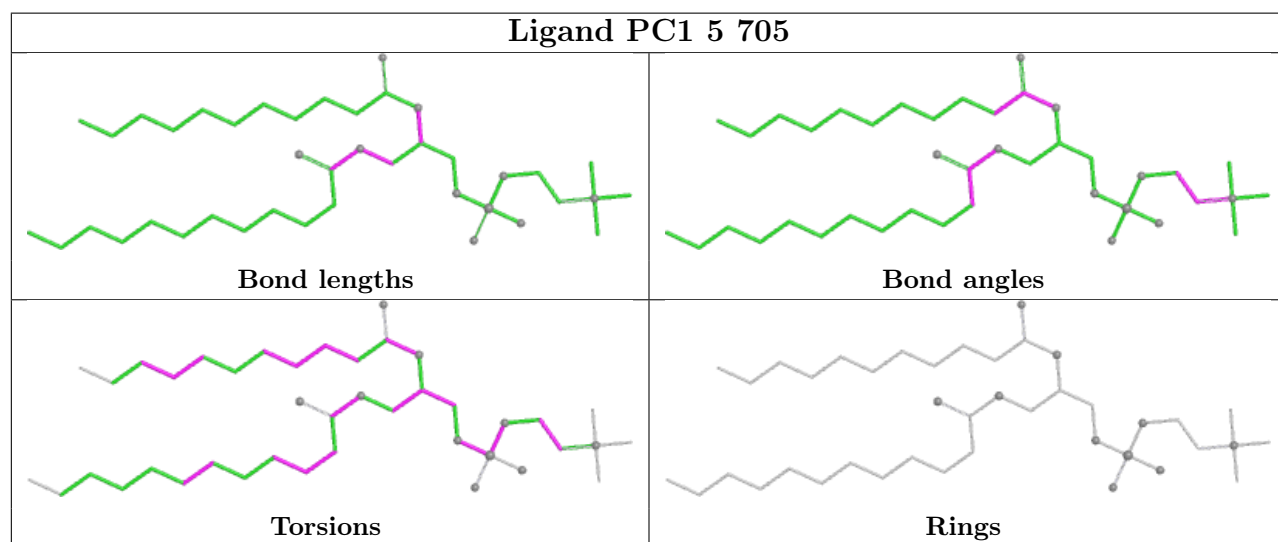
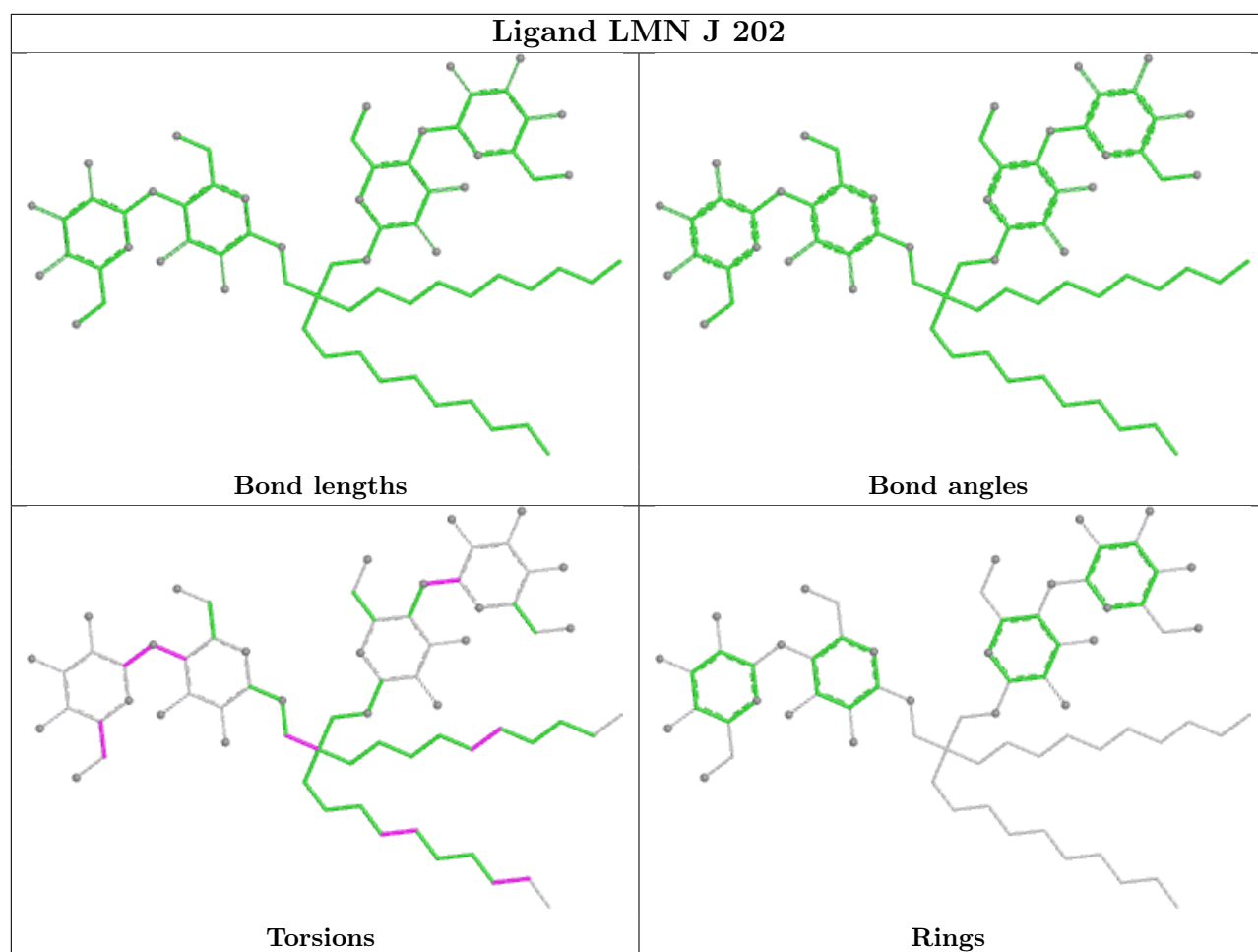


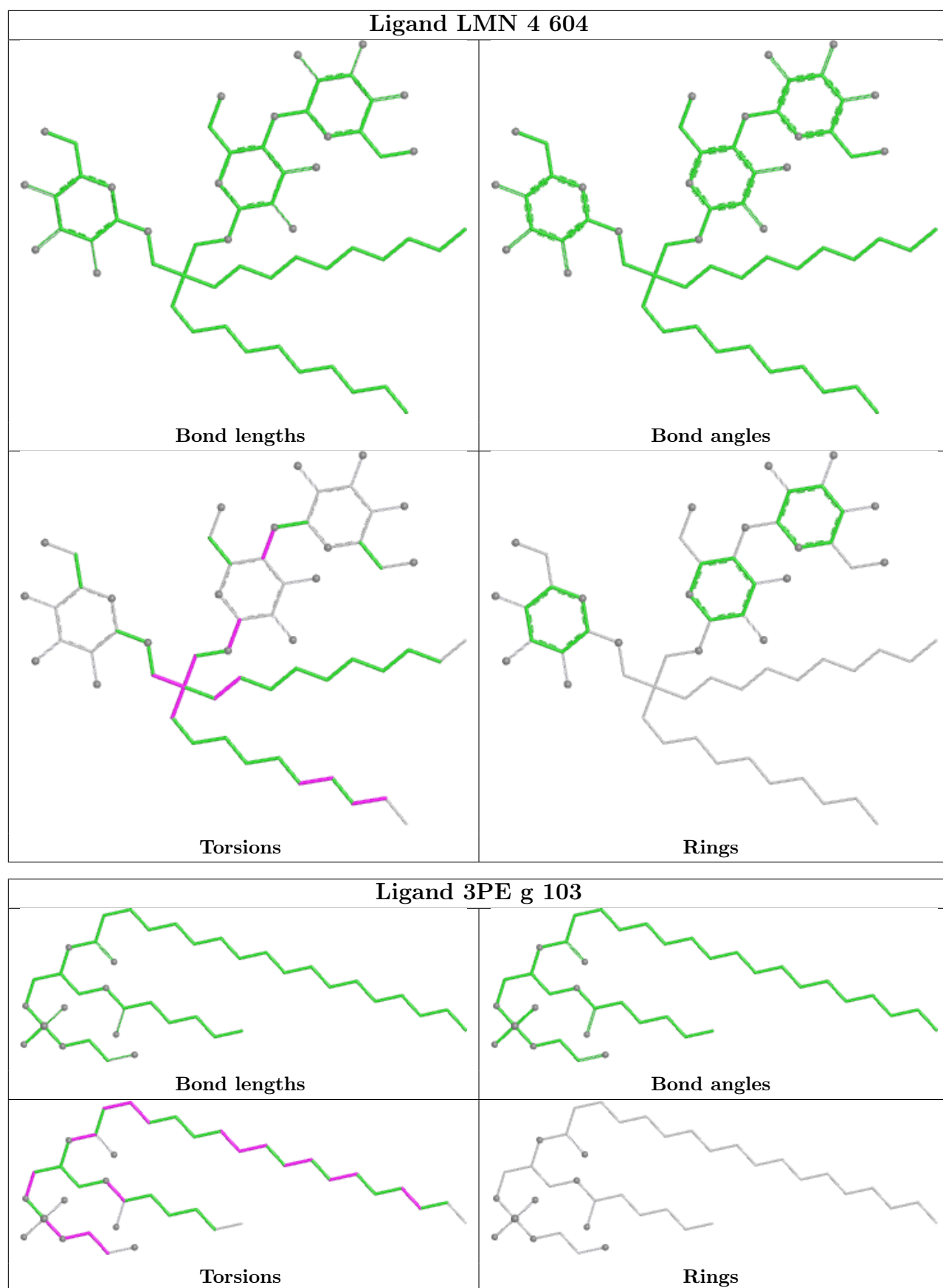


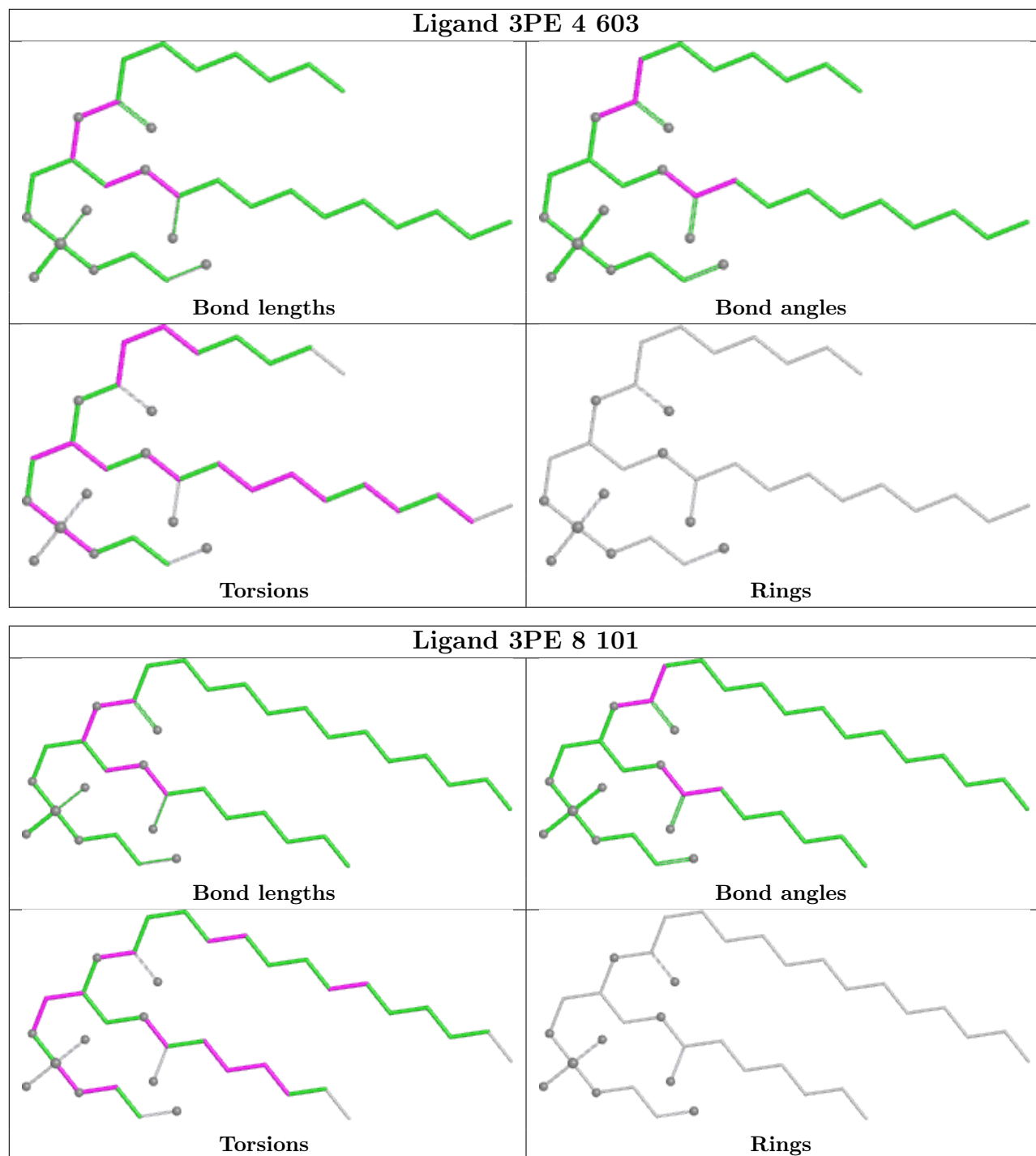


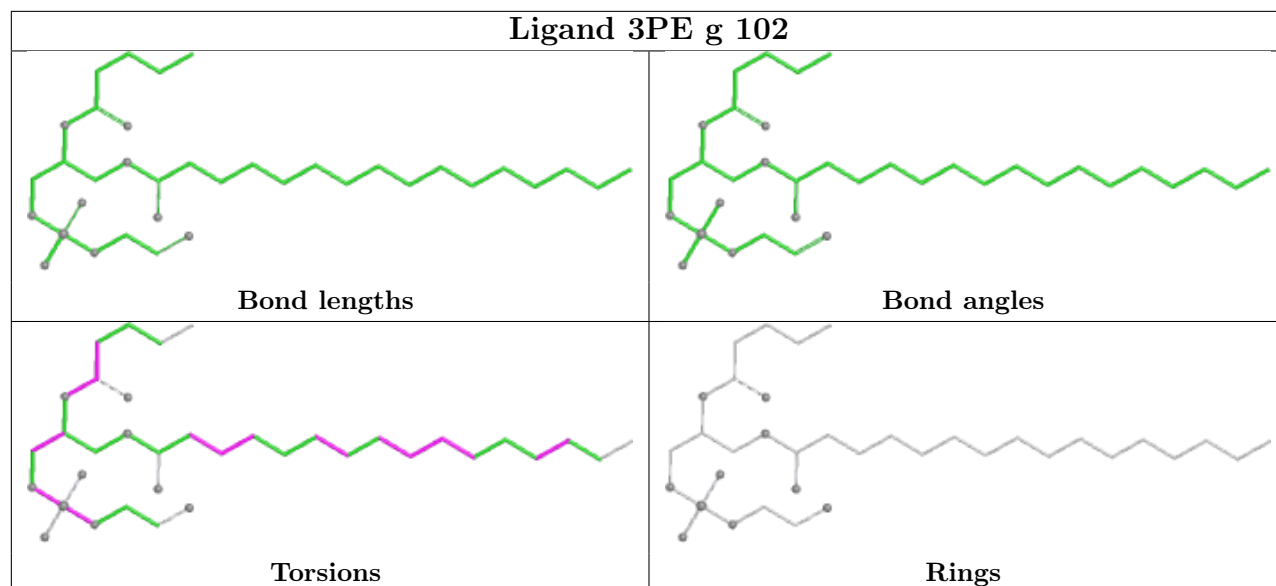












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

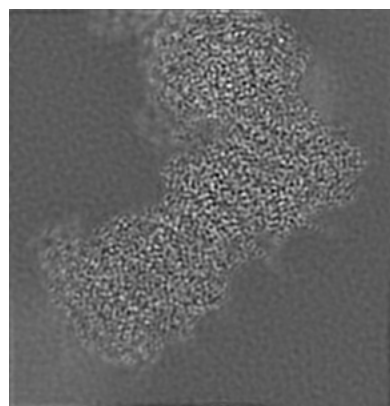
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14796. These allow visual inspection of the internal detail of the map and identification of artifacts.

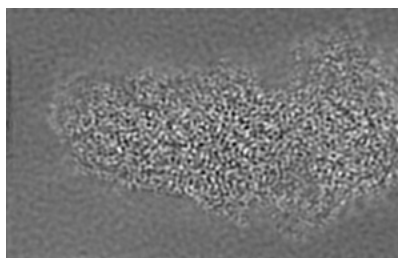
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

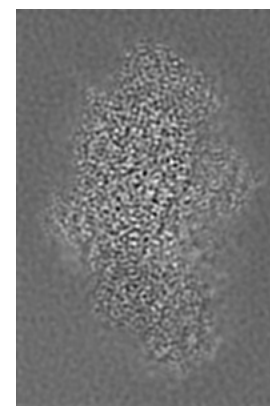
6.1.1 Primary map



X

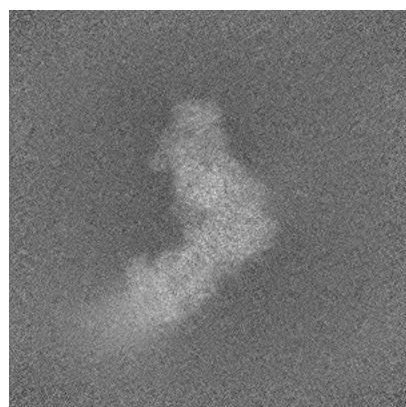


Y

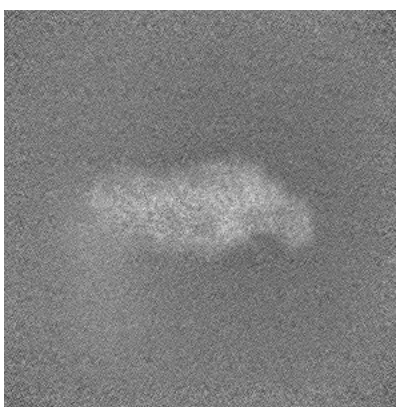


Z

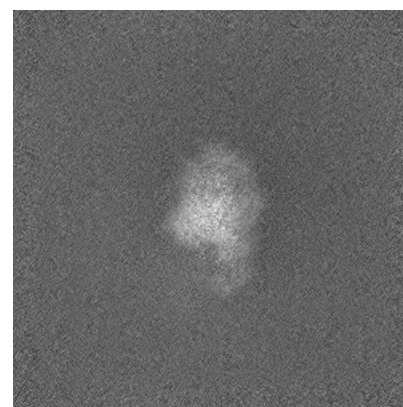
6.1.2 Raw map



X



Y

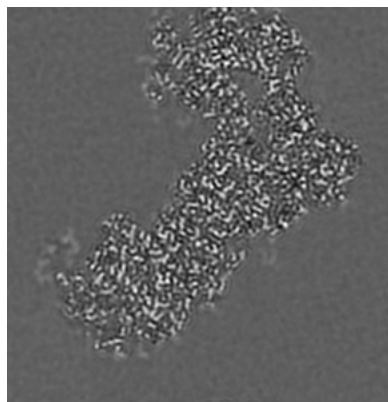


Z

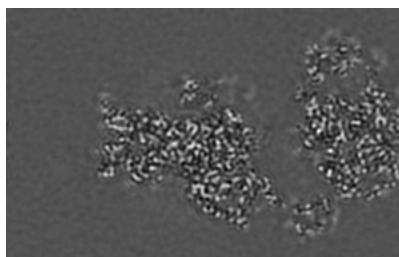
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

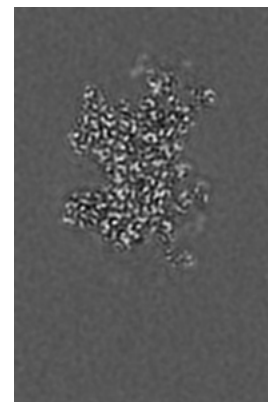
6.2.1 Primary map



X Index: 86

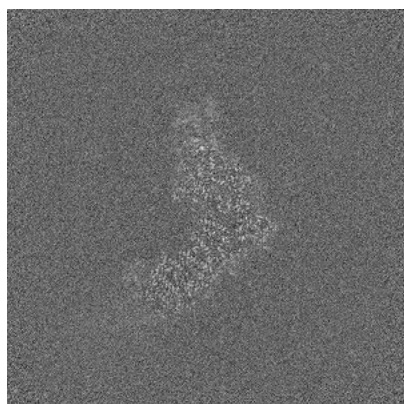


Y Index: 130

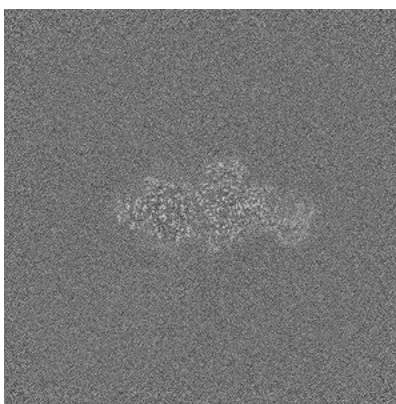


Z Index: 136

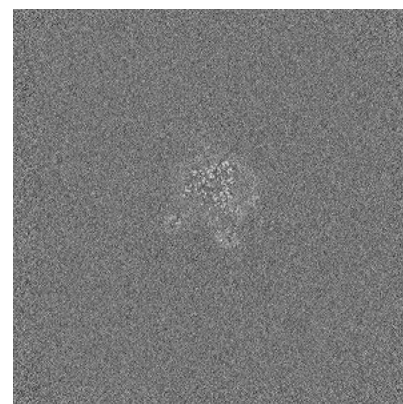
6.2.2 Raw map



X Index: 294



Y Index: 294

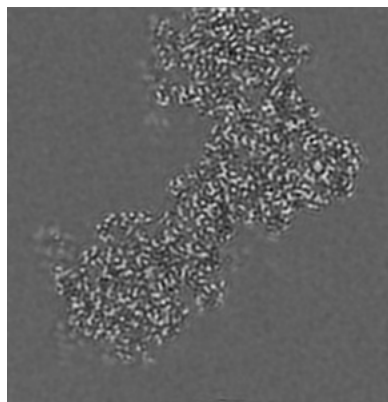


Z Index: 294

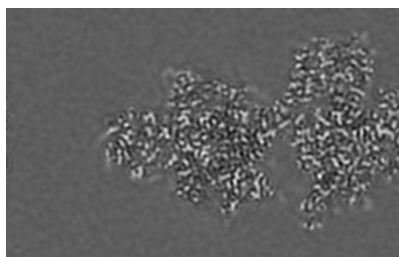
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

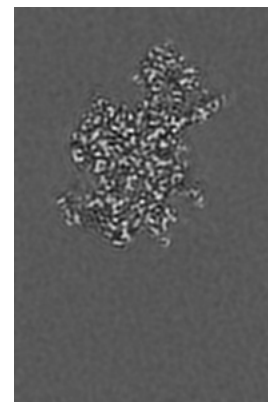
6.3.1 Primary map



X Index: 92

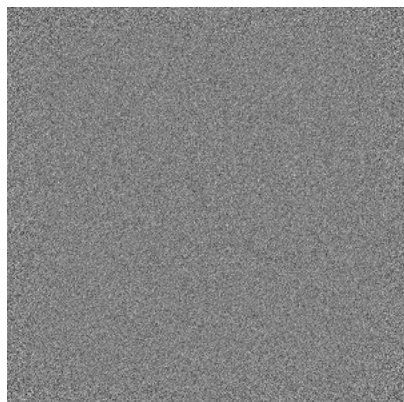


Y Index: 140

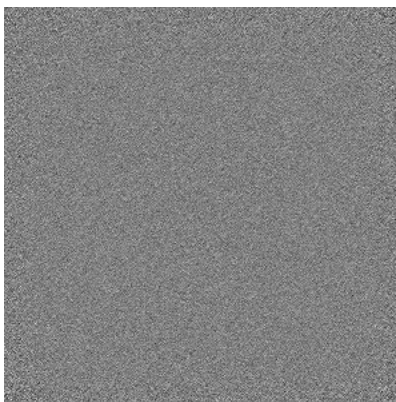


Z Index: 145

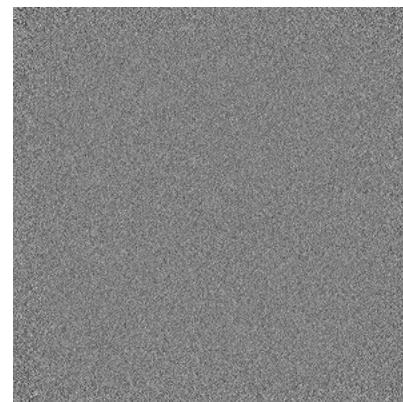
6.3.2 Raw map



X Index: 0



Y Index: 0

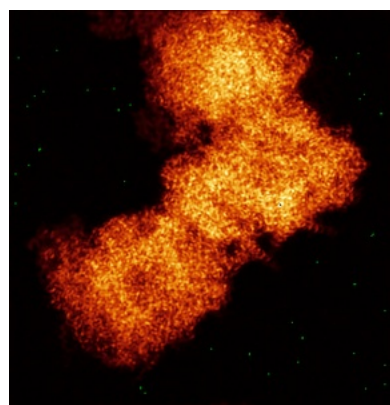


Z Index: 0

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

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

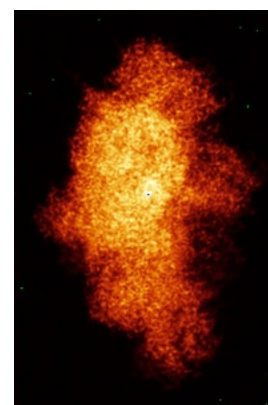
6.4.1 Primary map



X

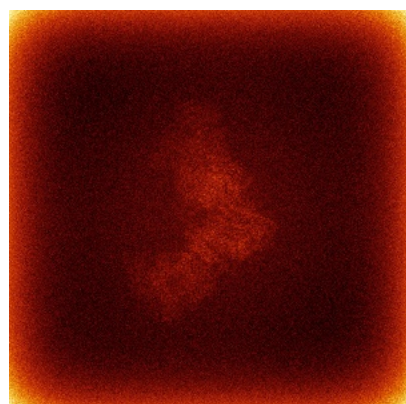


Y

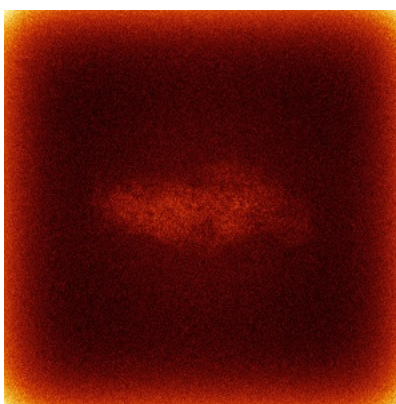


Z

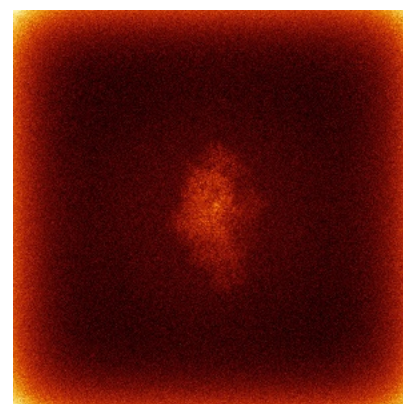
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

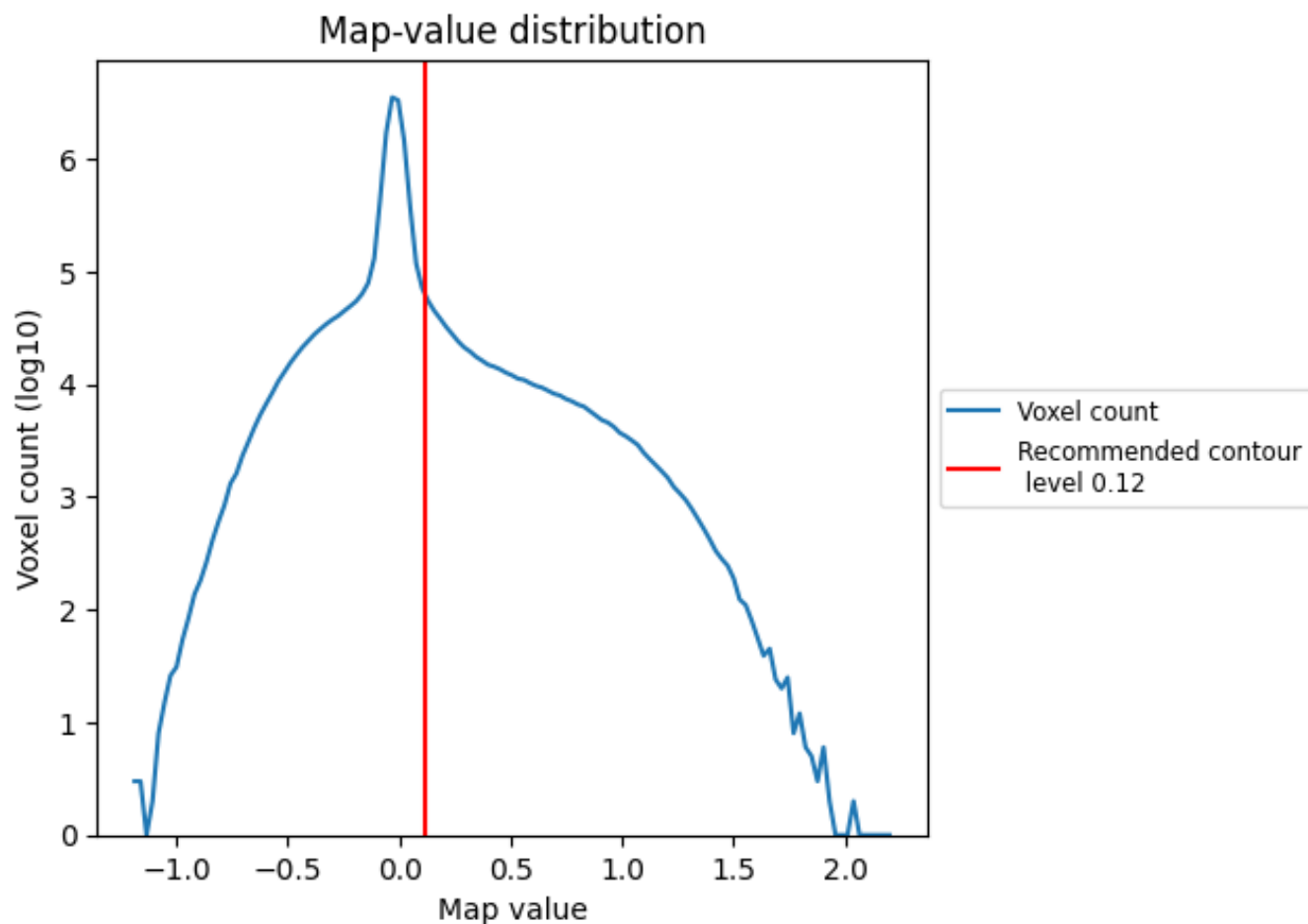
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

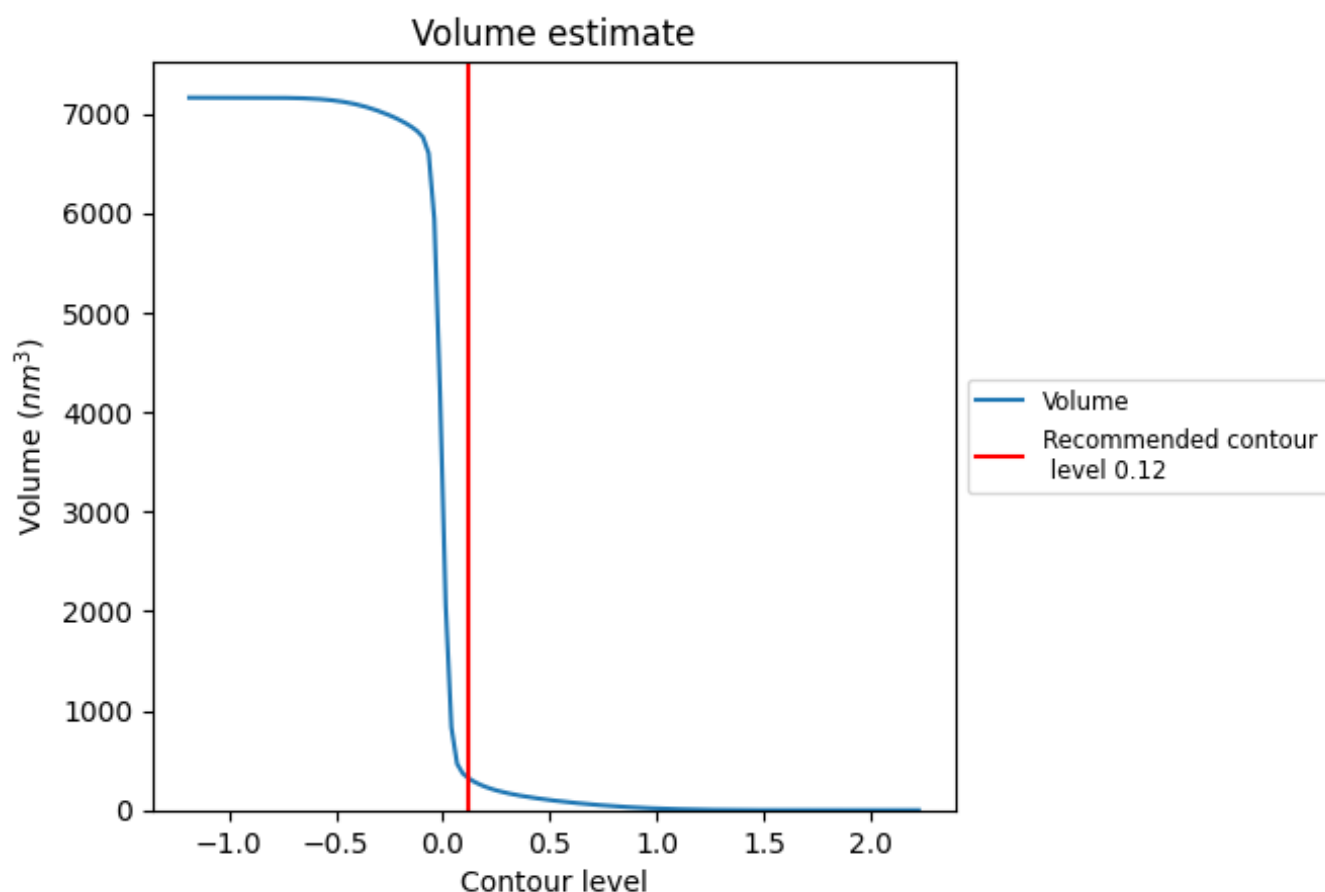
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm³; this corresponds to an approximate mass of 289 kDa.

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

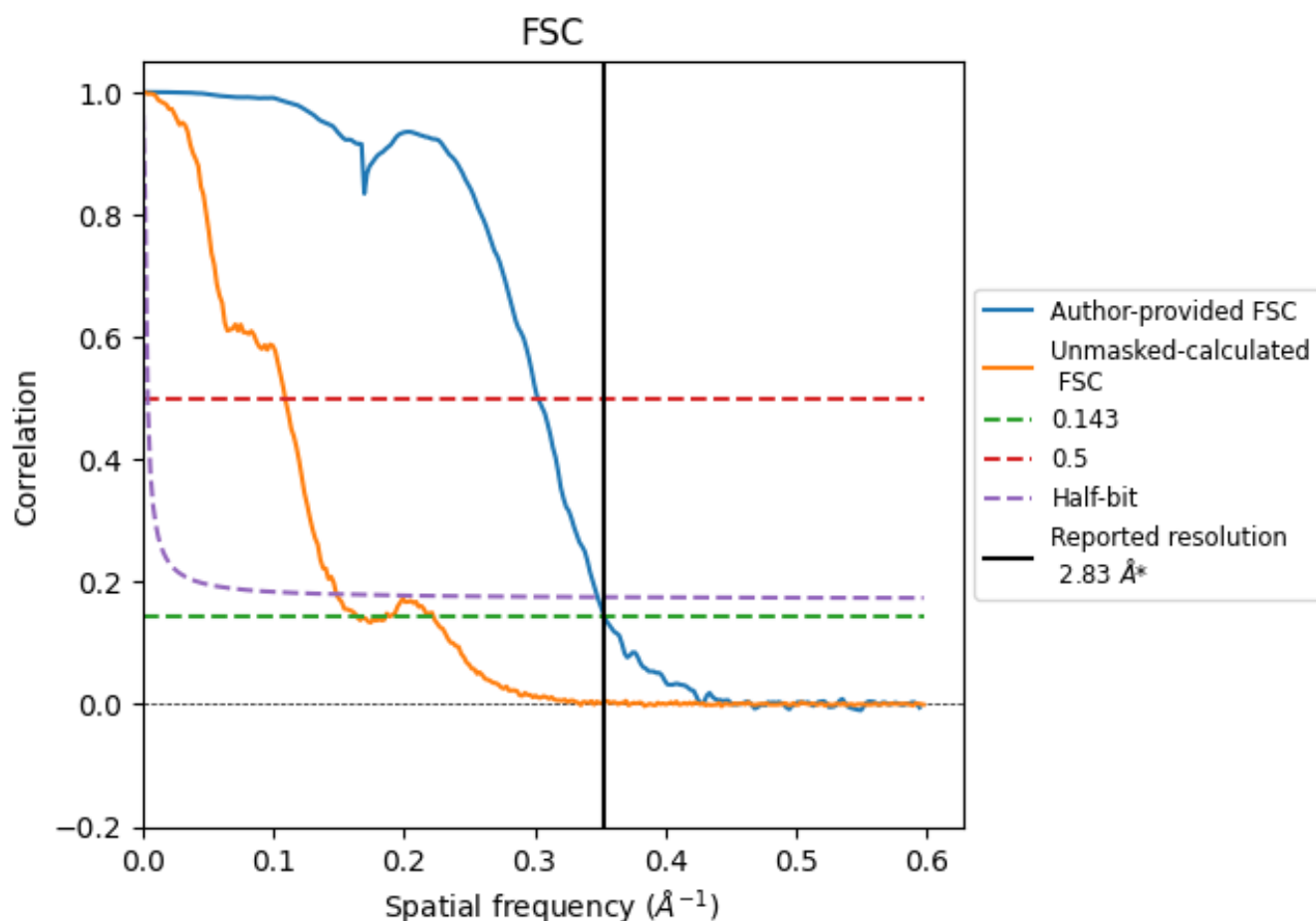
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [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 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.31	2.87
Unmasked-calculated*	6.09	9.16	6.74

*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 6.09 differs from the reported value 2.83 by more than 10 %

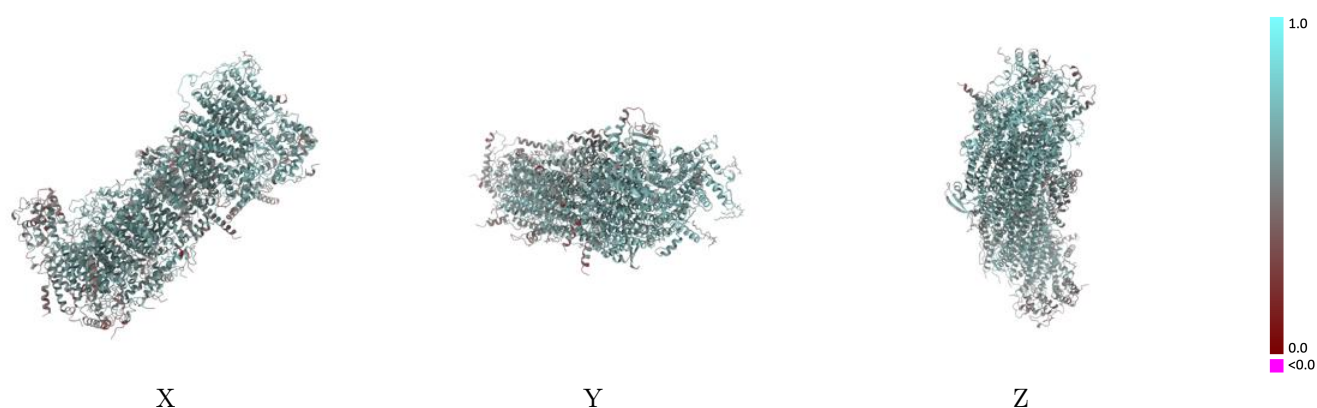
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14796 and PDB model 7ZME. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

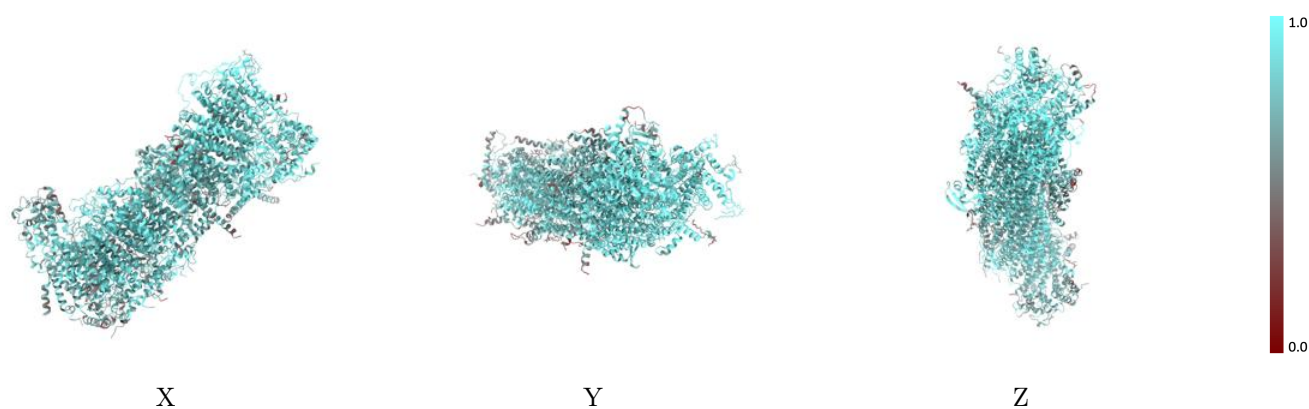
This section was not generated.

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



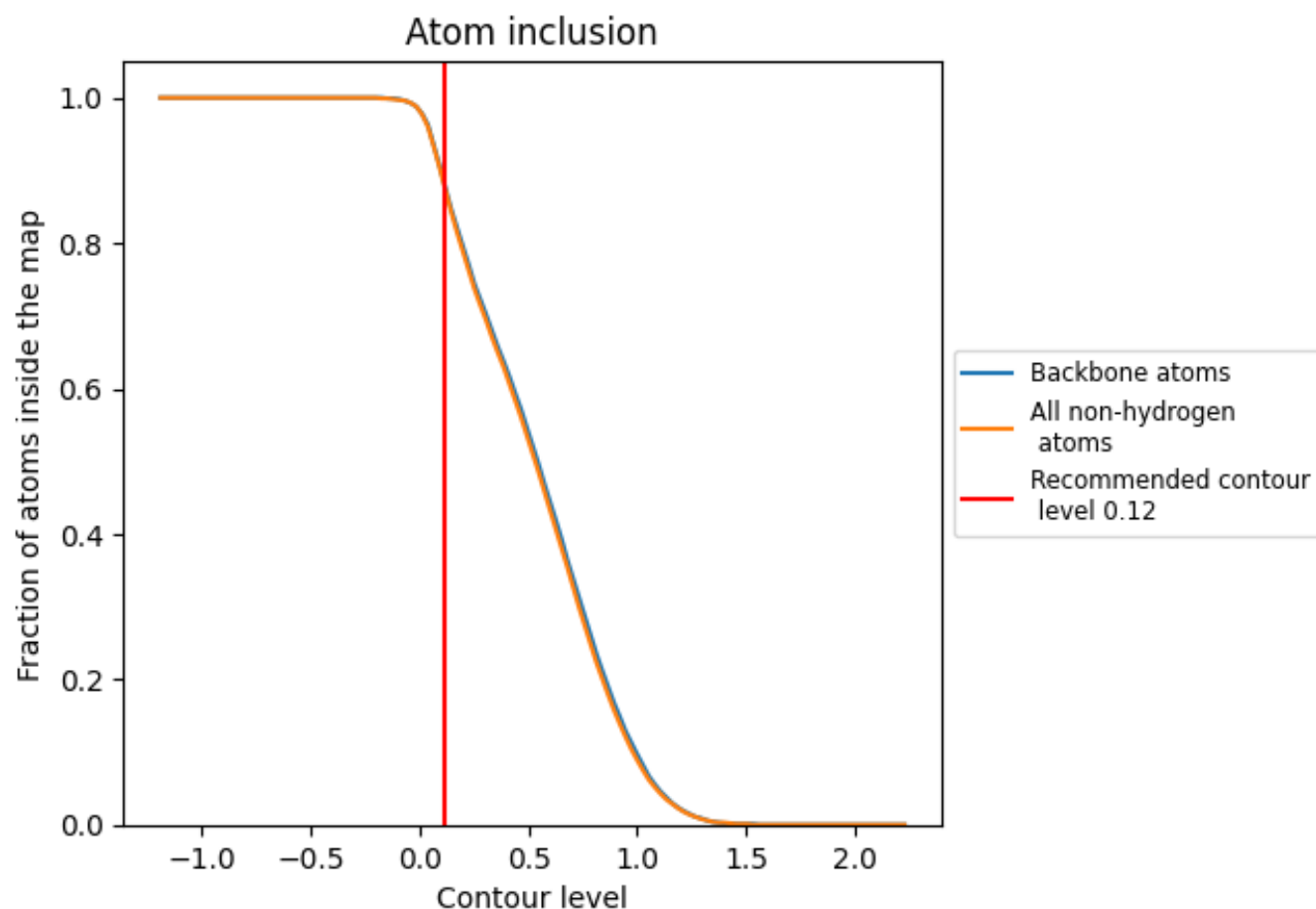
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.8730	 0.5960
1	 0.9560	 0.6450
2	 0.9400	 0.6410
3	 0.9260	 0.6270
4	 0.9260	 0.6290
5	 0.9000	 0.6030
6	 0.8990	 0.6080
8	 0.6260	 0.4540
9	 0.8030	 0.5620
D	 0.9370	 0.6340
J	 0.6970	 0.5030
L	 0.9330	 0.6310
Q	 0.6460	 0.4580
R	 0.7840	 0.5400
S	 0.8510	 0.5740
U	 0.9220	 0.6120
W	 0.9000	 0.6230
X	 0.9160	 0.6160
a	 0.8090	 0.5430
b	 0.8450	 0.5780
c	 0.7230	 0.4780
d	 0.8650	 0.5840
e	 0.7400	 0.5080
g	 0.9010	 0.5920
i	 0.7920	 0.5460
j	 0.9000	 0.5970
n	 0.7100	 0.5340

