



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 07:59 pm BST

PDB ID : 7B0N
EMDB ID : EMD-11969
Title : A 3.7-angstrom structure of Yarrowia lipolytica complex I with an R121M mutation in NUCM.
Authors : Hirst, J.; Grba, D.
Deposited on : 2020-11-20
Resolution : 3.70 Å(reported)
Based on initial model : 6YJ4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

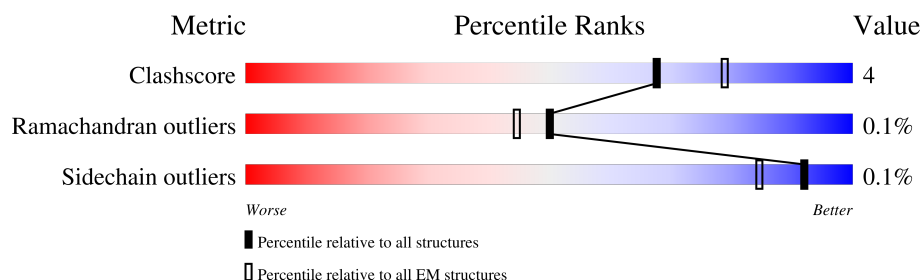
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY








The reported resolution of this entry is 3.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	128	
2	B	210	
3	C	293	
4	D	466	
5	E	243	
6	F	488	
7	G	728	
8	H	341	

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Mol	Chain	Length	Quality of chain
9	I	193	
10	J	185	
11	K	89	
12	L	655	
13	M	486	
14	N	469	
15	O	169	
16	P	355	
17	Q	161	
18	R	118	
19	S	87	
20	T	81	
21	U	88	
22	V	144	
23	W	124	
24	X	172	
25	Y	180	
26	Z	122	
27	a	86	
28	b	78	
29	c	182	
30	d	73	
31	e	89	
32	f	138	
33	g	249	

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Mol	Chain	Length	Quality of chain
34	h	139	
35	i	90	
36	j	67	
37	k	60	
38	l	149	
39	m	93	
40	n	109	
41	o	99	
42	p	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	FMN	F	501	-	X	-	-
47	3PE	H	6401	X	-	-	-
47	3PE	I	501	X	-	-	-
47	3PE	M	502	X	-	-	-
47	3PE	g	301	X	-	-	-
51	EHZ	T	201	X	-	-	-
52	LMT	Y	1401	X	-	-	-
52	LMT	Y	1402	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 131131 atoms, of which 65779 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 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	94	Total	C	H	N	O	S	0	0
			1593	528	827	111	125	2		

- Molecule 2 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	177	Total	C	H	N	O	S	0	0
			2766	885	1373	246	249	13		

- Molecule 3 is a protein called NUGM protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	242	Total	C	H	N	O	S	0	0
			3924	1285	1925	339	371	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	282	ALA	-	expression tag	UNP Q9UUU0
C	283	ALA	-	expression tag	UNP Q9UUU0
C	284	ALA	-	expression tag	UNP Q9UUU0
C	285	ALA	-	expression tag	UNP Q9UUU0
C	286	ALA	-	expression tag	UNP Q9UUU0
C	287	ALA	-	expression tag	UNP Q9UUU0
C	288	HIS	-	expression tag	UNP Q9UUU0
C	289	HIS	-	expression tag	UNP Q9UUU0
C	290	HIS	-	expression tag	UNP Q9UUU0
C	291	HIS	-	expression tag	UNP Q9UUU0
C	292	HIS	-	expression tag	UNP Q9UUU0
C	293	HIS	-	expression tag	UNP Q9UUU0

- Molecule 4 is a protein called NUCM protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	437	Total	C	H	N	O	S	0	0
			6788	2181	3354	586	645	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	MET	ARG	engineered mutation	UNP Q9UUU1

- Molecule 5 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	216	Total	C	H	N	O	S	0	0
			3348	1060	1660	284	326	18		

- Molecule 6 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	460	Total	C	H	N	O	S	0	0
			7072	2248	3513	629	658	24		

- Molecule 7 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	694	Total	C	H	N	O	S	0	0
			10447	3275	5173	928	1042	29		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	341	Total	C	H	N	O	S	0	0
			5463	1828	2774	394	460	7		

- Molecule 9 is a protein called Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	191	Total	C	H	N	O	S	0	0
			2997	972	1471	255	289	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	185	Total	C	H	N	O	S	0	0
			3044	990	1582	209	254	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	FME	-	initiating methionine	UNP S5U3X7

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	89	Total	C	H	N	O	S	0	0
			1446	465	753	109	116	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	655	Total	C	H	N	O	S	0	0
			10571	3485	5364	786	907	29		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	486	Total	C	H	N	O	S	0	0
			7910	2601	4053	586	655	15		

- Molecule 14 is a protein called NADH dehydrogenase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	469	Total	C	H	N	O	S	0	0
			7780	2558	4004	550	656	12		

- Molecule 15 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	168	Total	C	H	N	O	S	0	0
			2586	845	1281	223	233	4		

- Molecule 16 is a protein called Epimerase domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	355	Total	C	H	N	O	S	0	0
			5575	1785	2763	493	524	10		

- Molecule 17 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	125	Total	C	H	N	O	S	0	0
			2031	659	994	190	186	2		

- Molecule 18 is a protein called zf-CHCC domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	118	Total	C	H	N	O	S	0	0
			1798	574	876	166	177	5		

- Molecule 19 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	86	Total	C	H	N	O	S	0	0
			1351	418	684	126	122	1		

- Molecule 20 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	81	Total	C	H	N	O		0	0
			1234	391	614	98	131			

- Molecule 21 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	88	Total	C	H	N	O	S	0	0
			1322	416	655	106	143	2		

- Molecule 22 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	126	Total	C	H	N	O	S	0	0
			2049	653	1021	173	200	2		

- Molecule 23 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	123	Total	C	H	N	O	S	0	0
			2054	667	1018	182	185	2		

- Molecule 24 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	171	Total	C	H	N	O	S	0	0
			2678	847	1333	236	252	10		

- Molecule 25 is a protein called Complex I-B14.7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	179	Total	C	H	N	O	S	0	0
			2638	842	1311	240	240	5		

- Molecule 26 is a protein called GRIM-19.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	122	Total	C	H	N	O	S	0	0
			1983	629	1000	180	169	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	86	Total	C	H	N	O	S	0	0
			1353	432	672	127	119	3		

- Molecule 28 is a protein called subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	78	Total	C	H	N	O	S	0	0
			1257	418	618	115	105	1		

- Molecule 29 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	182	Total	C	H	N	O	S	0	0
			2804	898	1407	241	256	2		

- Molecule 30 is a protein called subunit NEBM of protein NADH:Ubiquinone Oxidoreductase (Complex I) [*Yarrowia lipolytica*].

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	67	Total	C	H	N	O		0	0
			1042	339	532	86	85			

- Molecule 31 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	e	68	Total	C	H	N	O	S	0	0
			1082	336	536	102	102	6		

- Molecule 32 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	f	137	Total	C	H	N	O	S	0	0
			2225	730	1089	194	210	2		

- Molecule 33 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	g	198	Total	C	H	N	O	S	0	0
			3188	1019	1603	273	291	2		

- Molecule 34 is a protein called subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	h	113	Total	C	H	N	O	S	0	0
			1786	585	877	153	170	1		

- Molecule 35 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
35	i	86	Total	C	H	N	O	S	0	0
			1300	420	641	120	118	1		

- Molecule 36 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
36	j	53	Total	C	H	N	O	S	0	0
			884	299	439	77	66	3		

- Molecule 37 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
37	k	47	Total	C	H	N	O		0	0
			734	242	361	70	61			

- Molecule 38 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
38	l	125	Total	C	H	N	O	S	0	0
			2012	674	973	166	197	2		

- Molecule 39 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
39	m	92	Total	C	H	N	O		0	0
			1453	472	718	134	129			

- Molecule 40 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
40	n	108	Total	C	H	N	O	S	0	0
			1804	571	904	172	154	3		

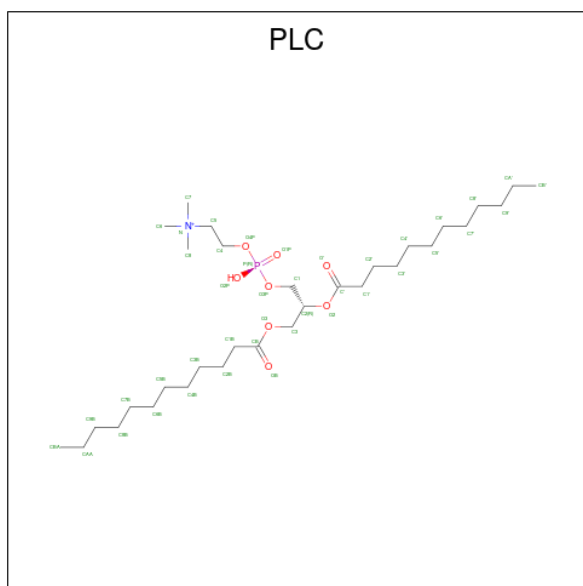
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
41	o	83	Total	C	H	N	O	S	0	0
			1366	431	685	123	119	8		

- Molecule 42 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms						AltConf	Trace
42	p	91	Total	C	H	N	O	S	0	0
			1492	475	726	138	150	3		

- Molecule 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
43	D	1	Total	C	H	N	O	P	0
			61	17	34	1	8	1	
43	H	1	Total	C	H	N	O	P	0
			64	18	36	1	8	1	
43	L	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
43	L	1	Total	C	H	N	O	P	0
			82	24	48	1	8	1	
43	N	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
43	d	1	Total	C	H	N	O	P	0
			61	17	34	1	8	1	

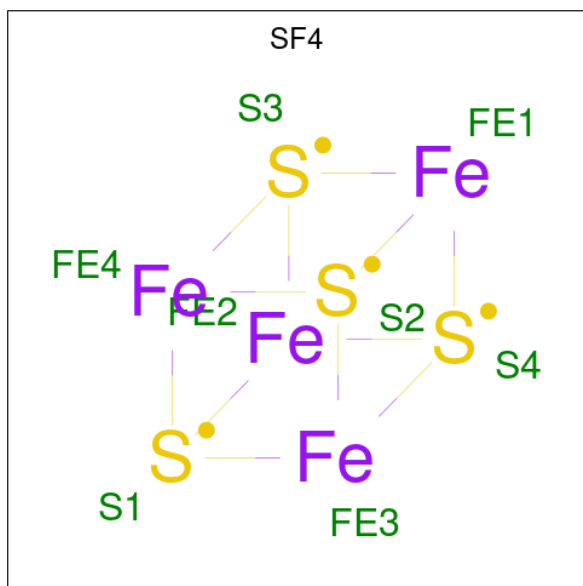
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- Diagram illustrating the structure of a ferredoxin center (FES). The structure shows two iron atoms (Fe1 and Fe2) and two sulfur atoms (S1 and S2) arranged in a square geometry. The bonds between the atoms are represented by lines, indicating the coordination of the iron atoms by the sulfur atoms.

Mol	Chain	Residues	Atoms			AltConf
44	E	1	Total 4	Fe 2	S 2	0
44	G	1	Total 4	Fe 2	S 2	0

-
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5, and two carbonyl groups, C2=O2 and C4=O4). The ring is substituted with a ribitol chain at the C10 position (N10). The ribitol chain is a five-carbon chain (C1' to C5') with hydroxyl groups at C1' (OH), C2' (OH), C3' (OH), and C4' (OH). The C5' carbon is attached to a phosphate group (O3P) via an oxygen atom (O5'). The phosphate group is shown as a phosphorus atom (P) double-bonded to an oxygen atom (O1P) and single-bonded to three hydroxyl groups (OH) and an oxygen atom (O3P).

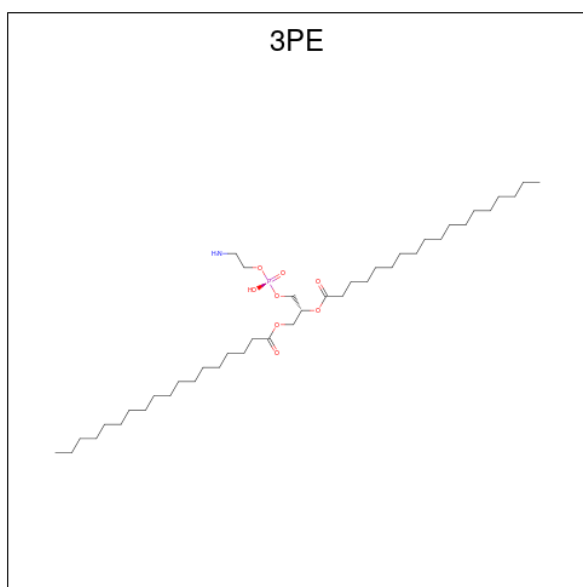
Mol	Chain	Residues	Atoms					AltConf	
45	F	1	Total	C	H	N	O	P	0
			49	17	18	4	9	1	

- Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$).



Mol	Chain	Residues	Atoms						AltConf
47	H	1	Total	C	H	N	O	P	0
			44	12	22	1	8	1	
47	H	1	Total	C	H	N	O	P	0
			118	36	72	1	8	1	
47	I	1	Total	C	H	N	O	P	0
			74	22	42	1	8	1	
47	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	L	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	M	1	Total	C	H	N	O	P	0
			69	20	39	1	8	1	
47	N	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
47	Y	1	Total	C	H	N	O	P	0
			79	23	46	1	8	1	
47	Z	1	Total	C	H	N	O	P	0
			109	33	66	1	8	1	
47	b	1	Total	C	H	N	O	P	0
			109	33	66	1	8	1	
47	d	1	Total	C	H	N	O	P	0
			52	14	28	1	8	1	
47	g	1	Total	C	H	N	O	P	0
			68	20	38	1	8	1	

- Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
48	M	1	Total	C	H	O	P	0
			205	64	122	17	2	
48	O	1	Total	C	H	O	P	0
			145	44	82	17	2	
48	Z	1	Total	C	H	O	P	0
			123	38	66	17	2	
48	a	1	Total	C	H	O	P	0
			108	33	56	17	2	
48	b	1	Total	C	H	O	P	0
			100	29	52	17	2	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						AltConf
49	P	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

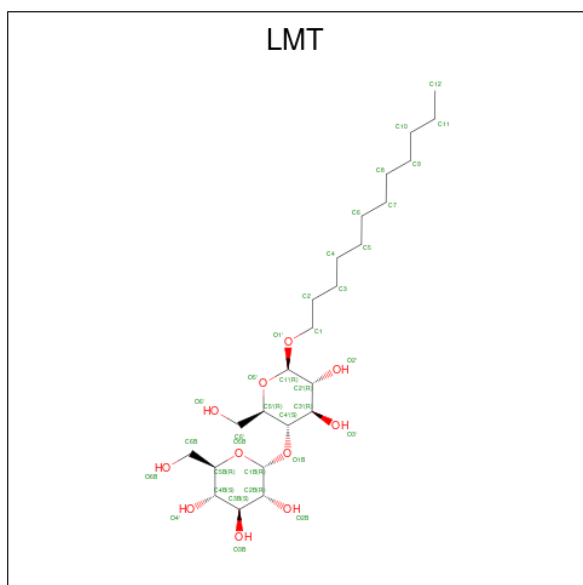
Mol	Chain	Residues	Atoms	AltConf
50	R	1	Total Zn 1 1	0

- Molecule 51 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



Mol	Chain	Residues	Atoms							AltConf
51	T	1	Total	C	H	N	O	P	S	0
			75	22	40	2	9	1	1	
51	U	1	Total	C	H	N	O	P	S	0
			77	23	41	2	9	1	1	

- Molecule 52 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

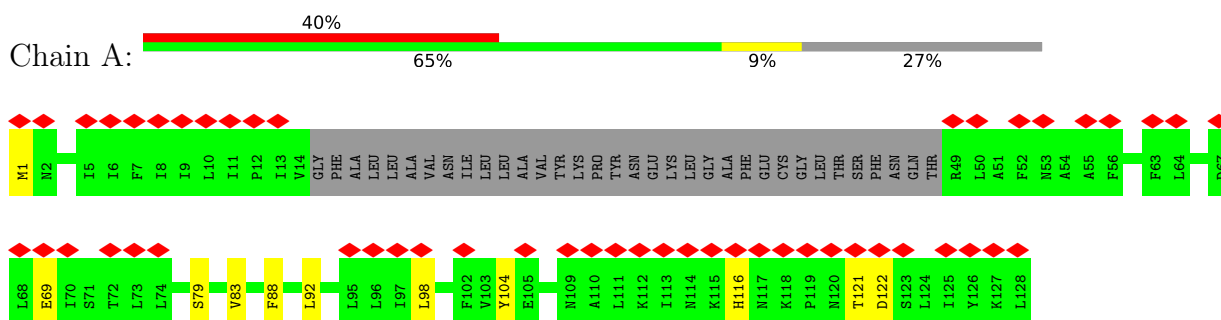


Mol	Chain	Residues	Atoms				AltConf
52	Y	1	Total	C	H	O	0
			81	24	46	11	
52	Y	1	Total	C	H	O	0
			81	24	46	11	

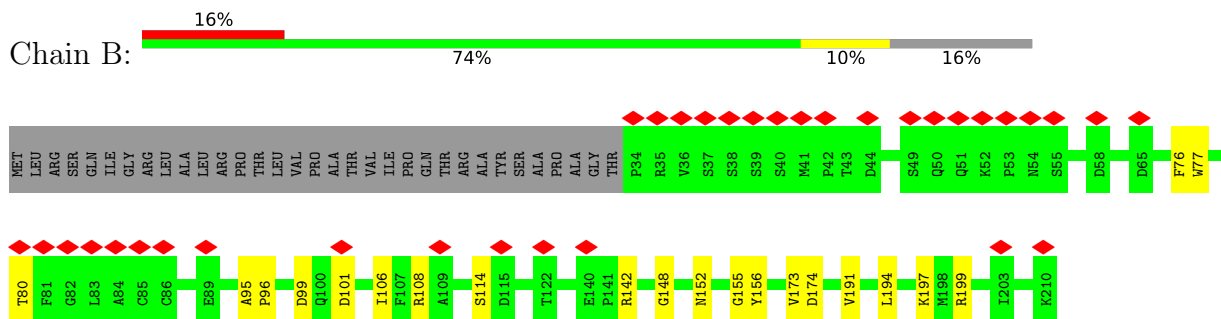
3 Residue-property plots

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.

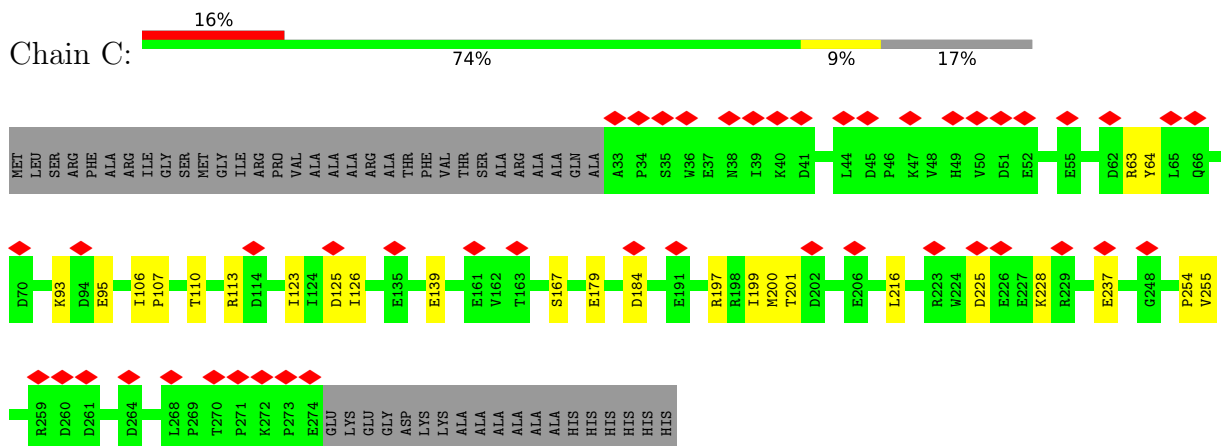
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



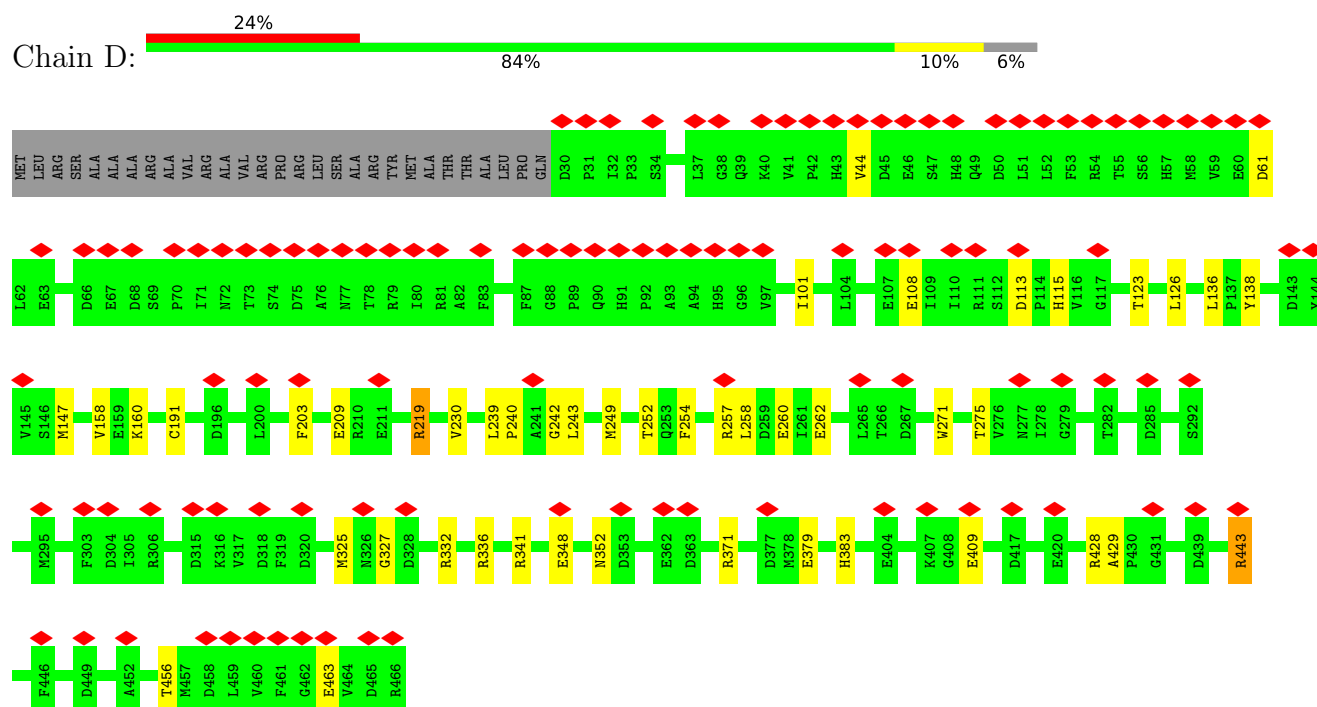
- Molecule 2: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)



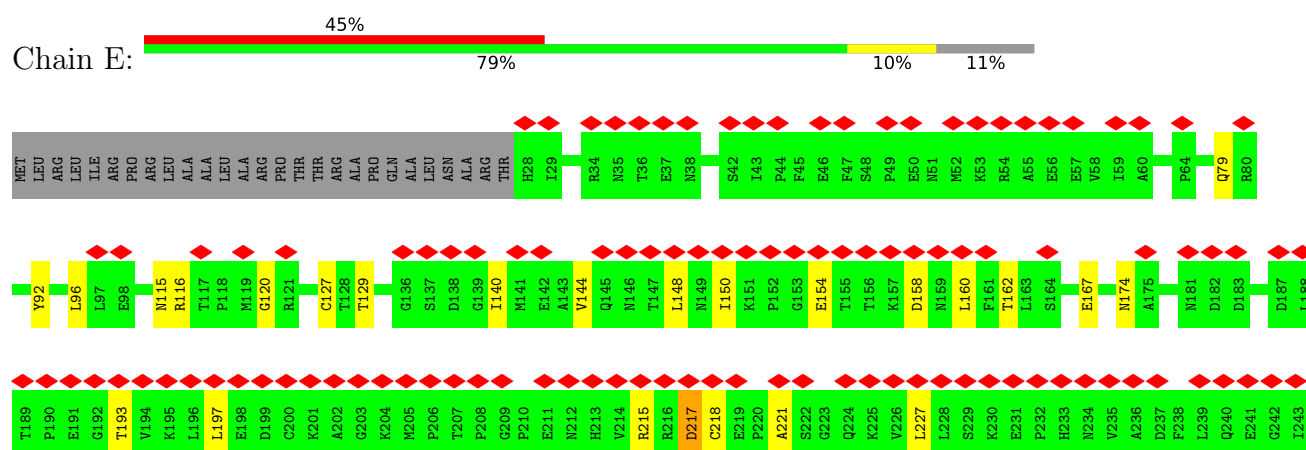
- Molecule 3: NUGM protein



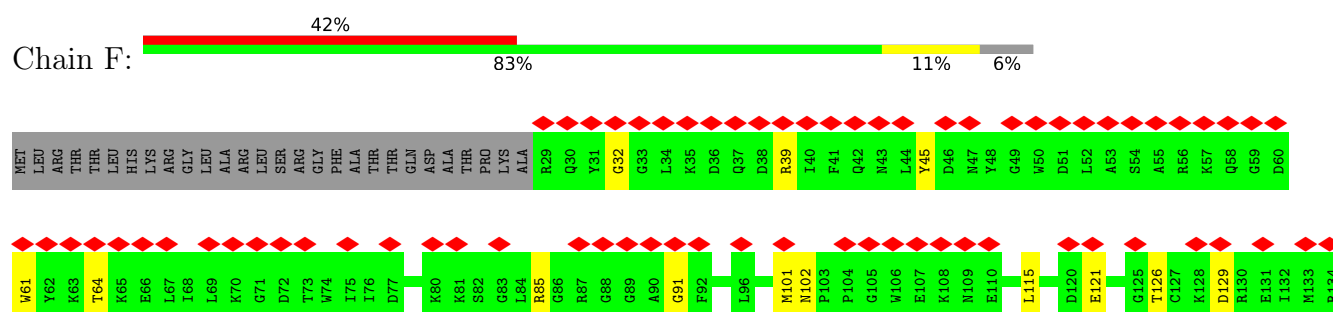
- Molecule 4: NUCM protein

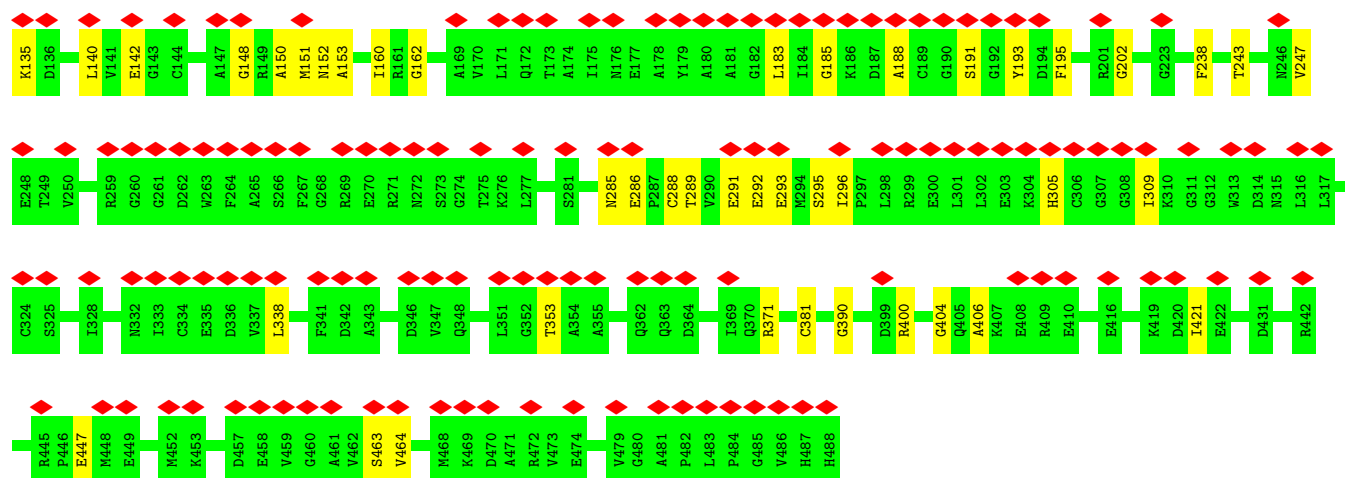


- Molecule 5: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

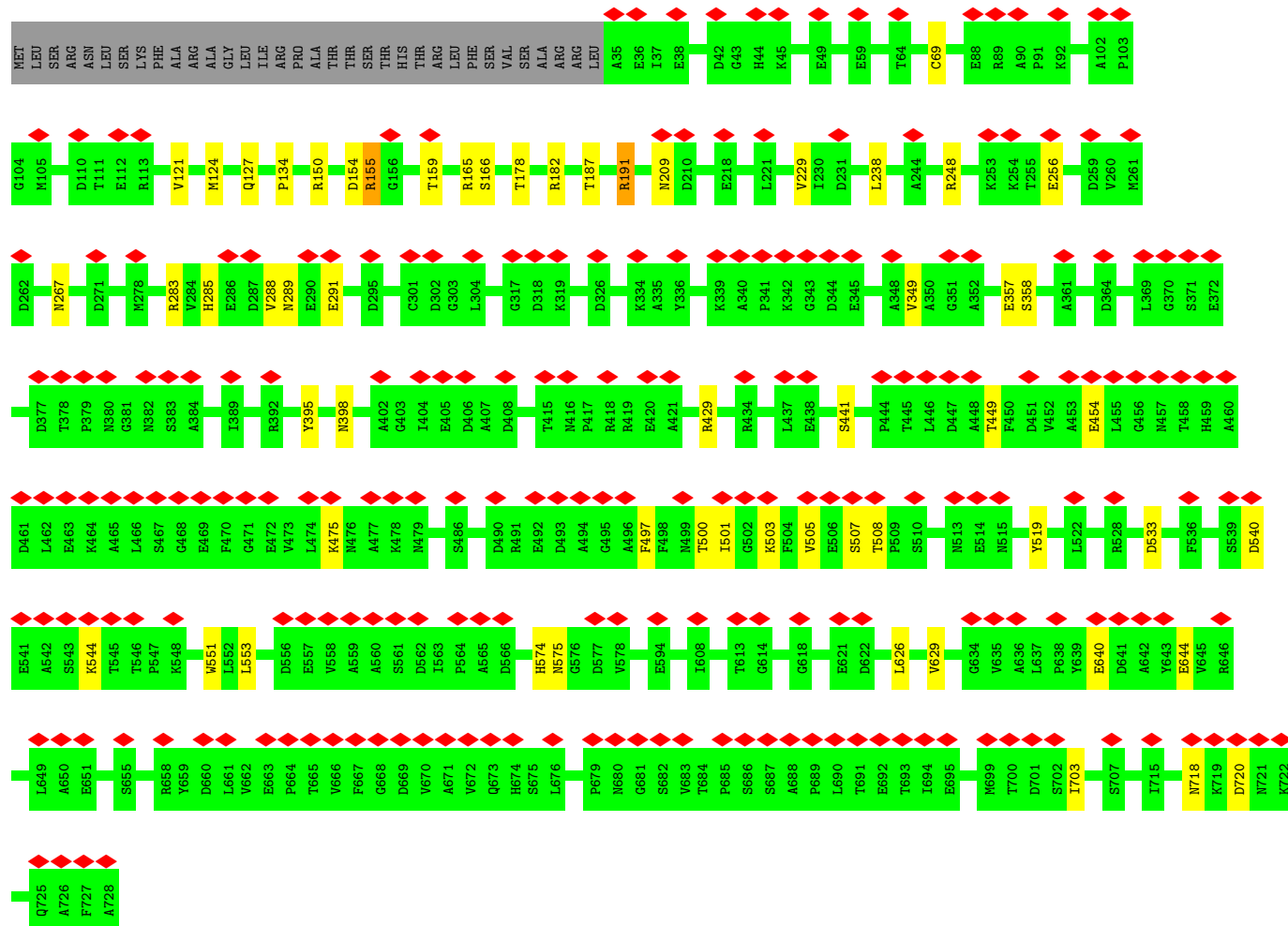
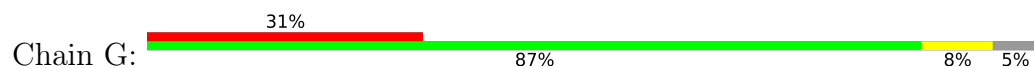


- Molecule 6: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)





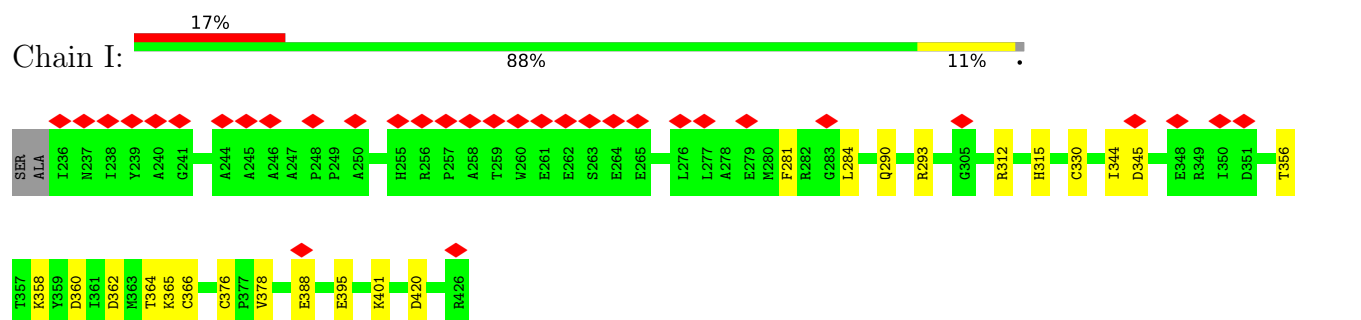
• Molecule 7: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)



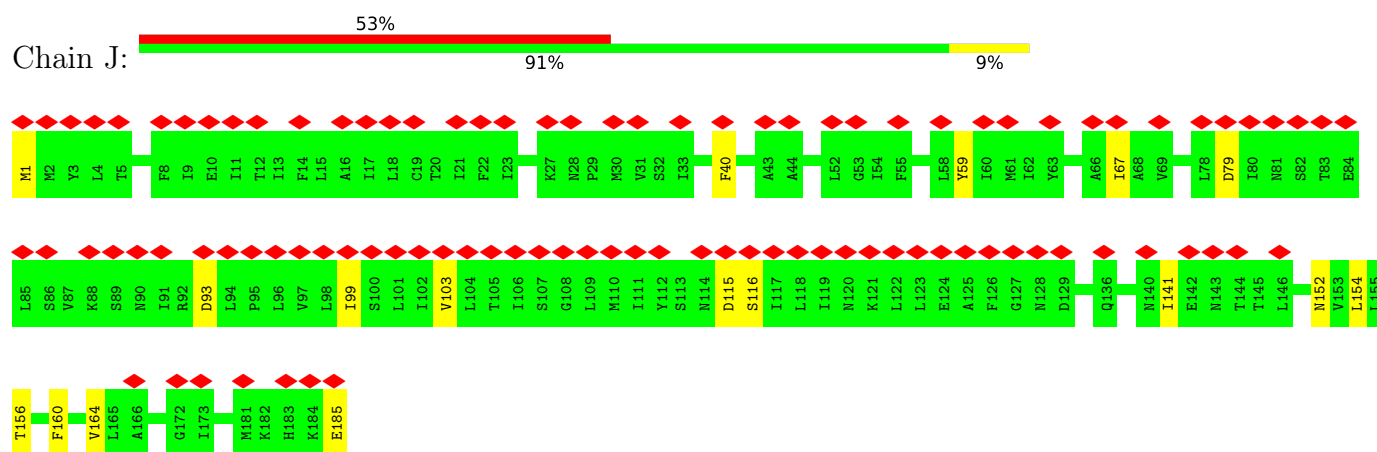
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



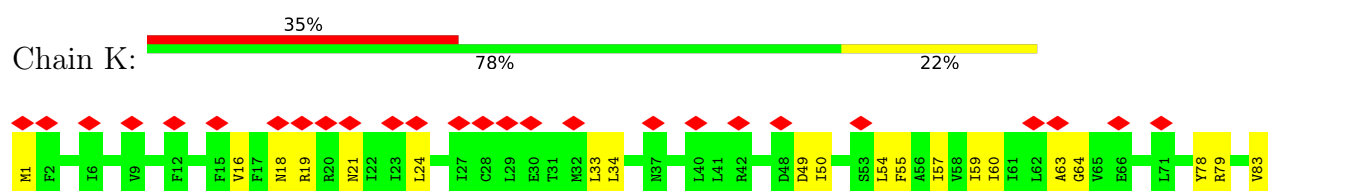
- Molecule 9: Subunit NUIM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

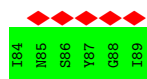


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

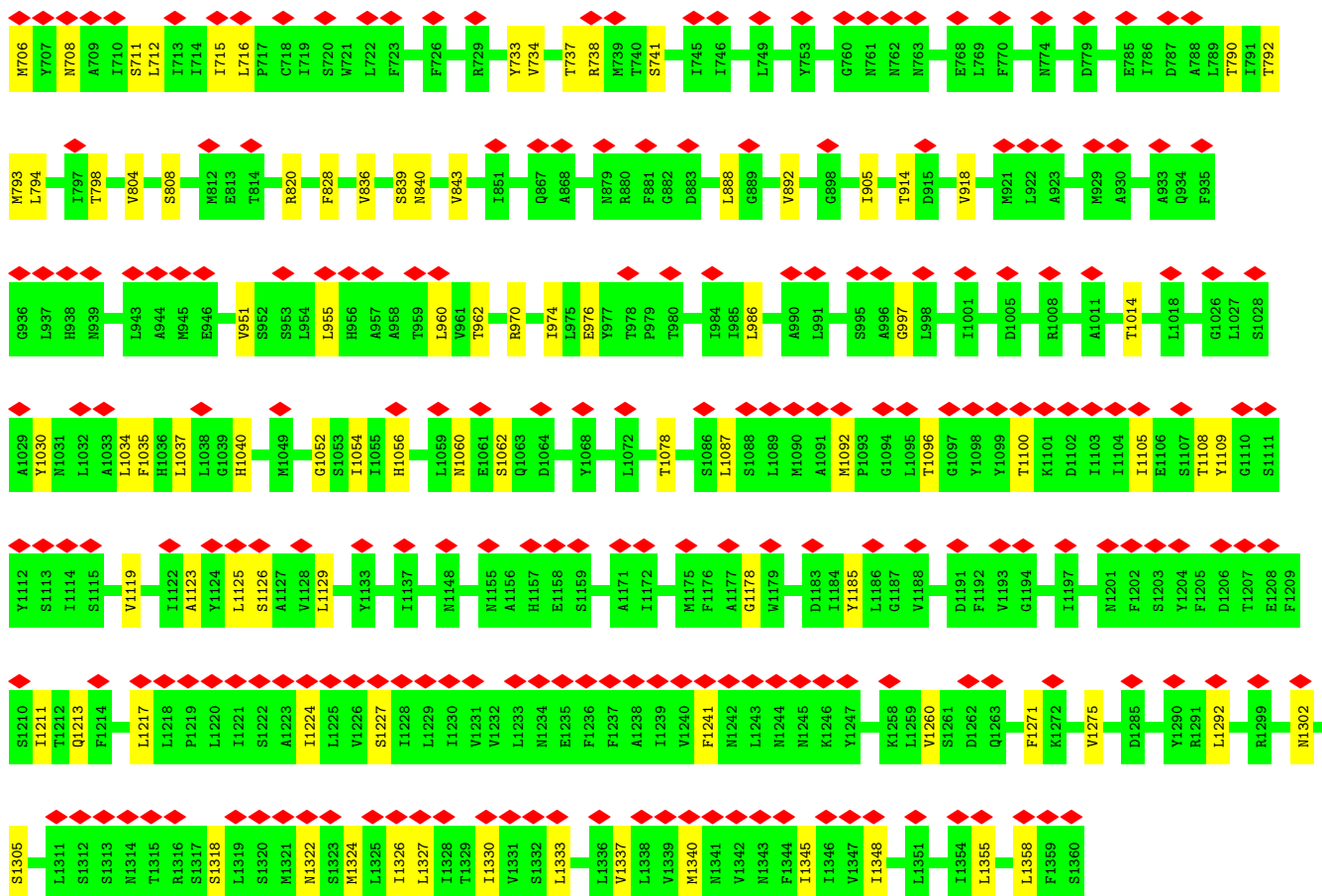
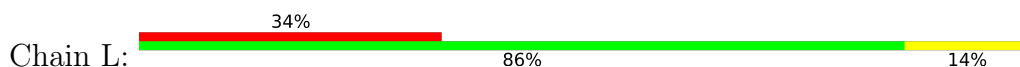


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

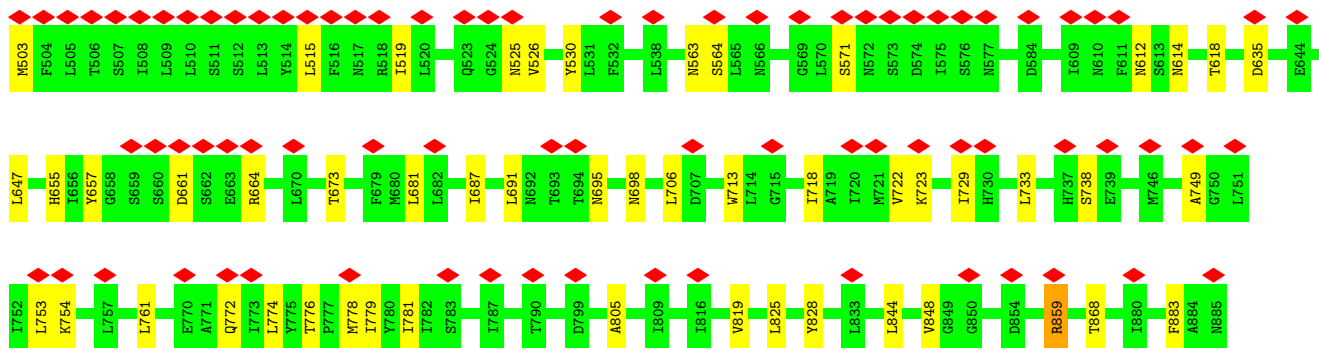
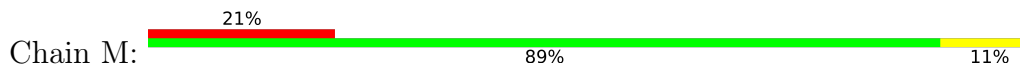


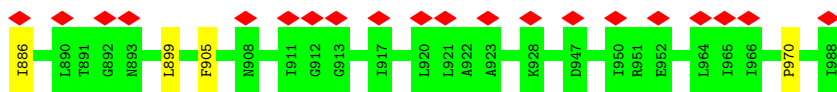


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

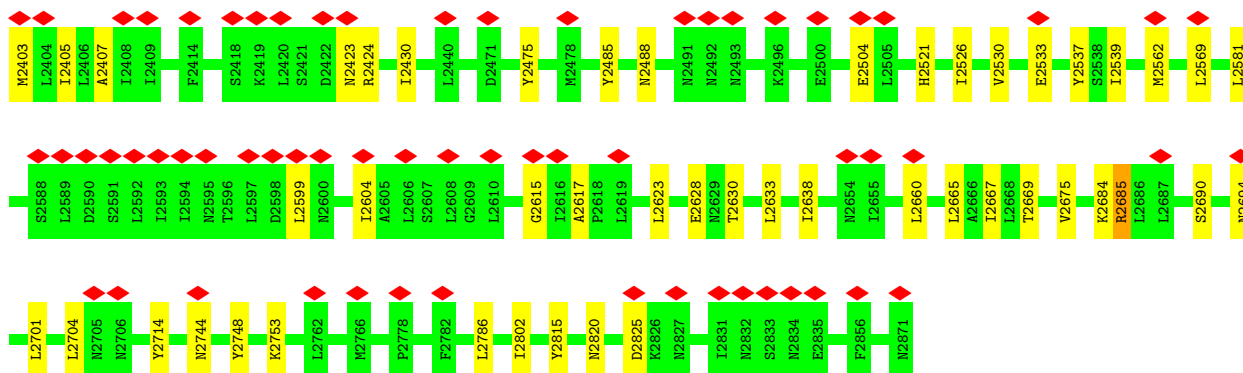
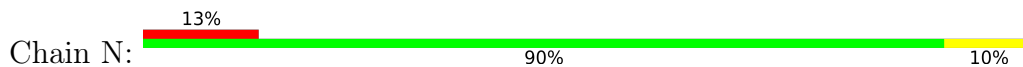


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

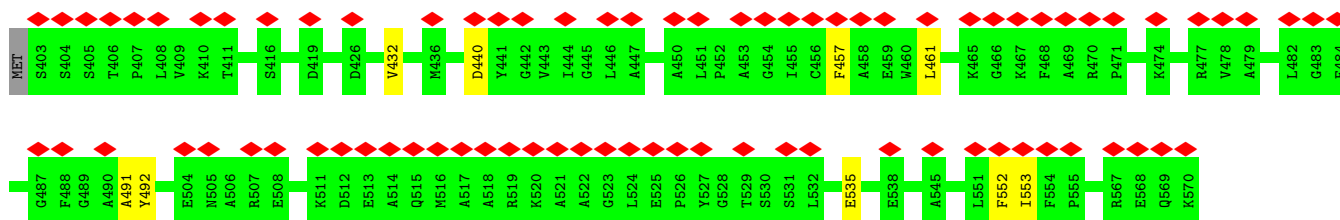




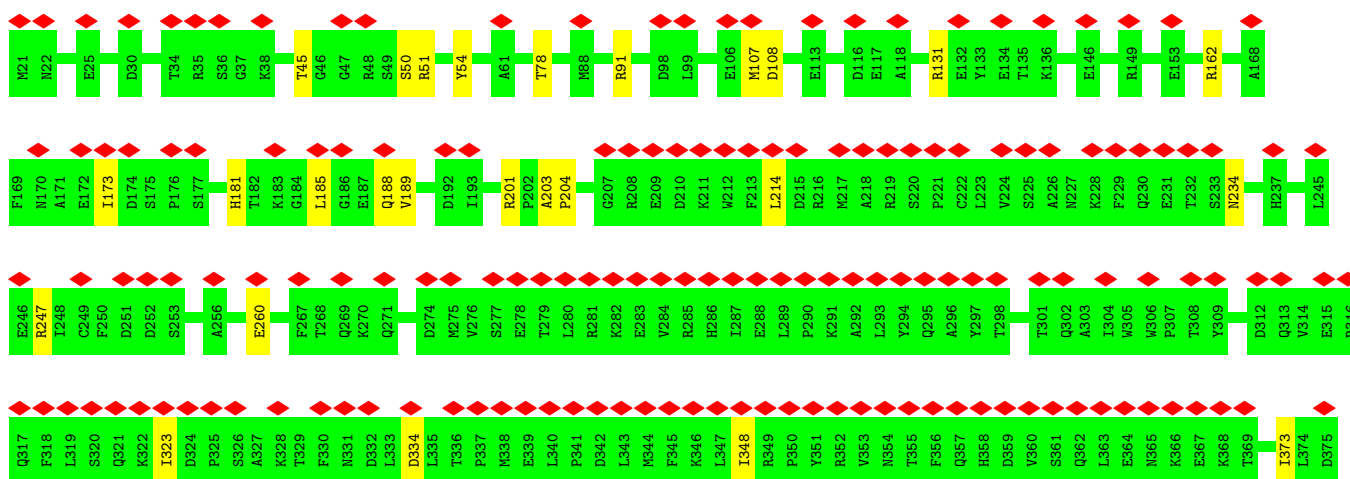
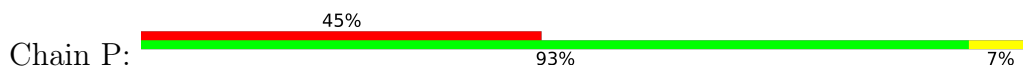
• Molecule 14: NADH dehydrogenase subunit 2



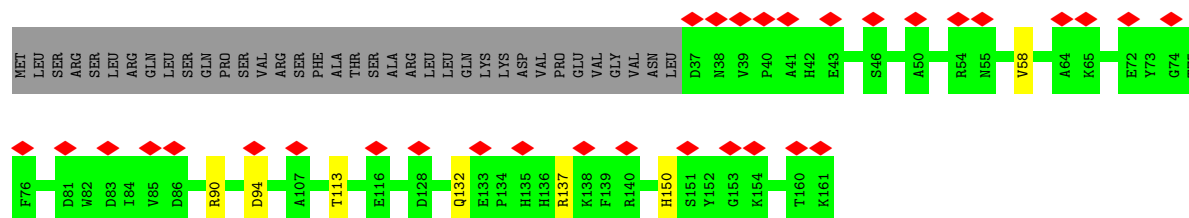
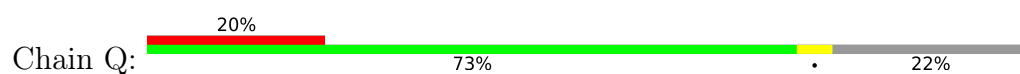
• Molecule 15: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)



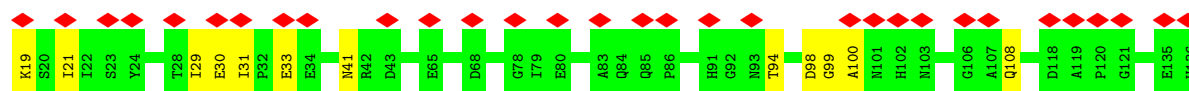
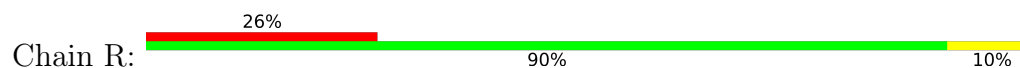
• Molecule 16: Epimerase domain-containing protein



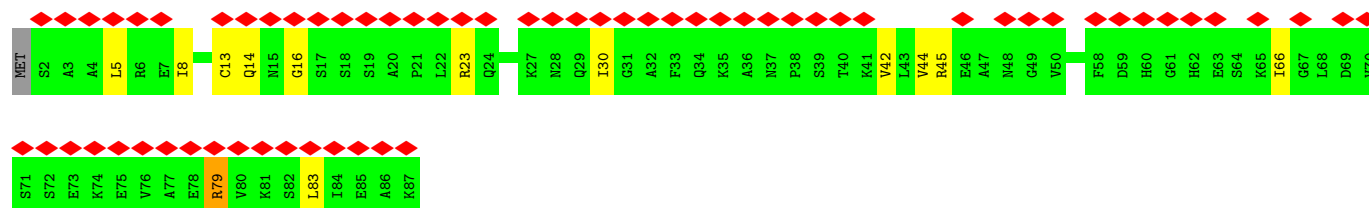
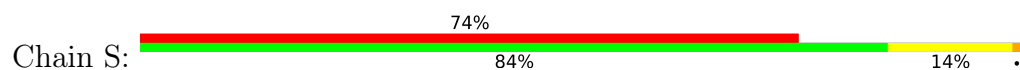
• Molecule 17: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)



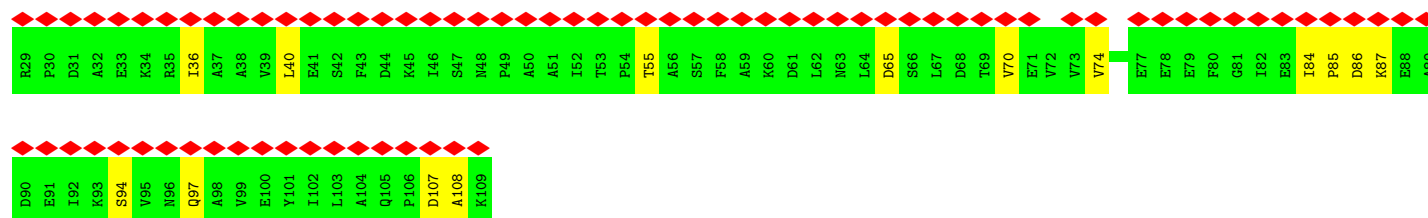
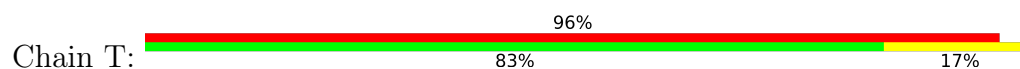
- Molecule 18: zf-CHCC domain-containing protein



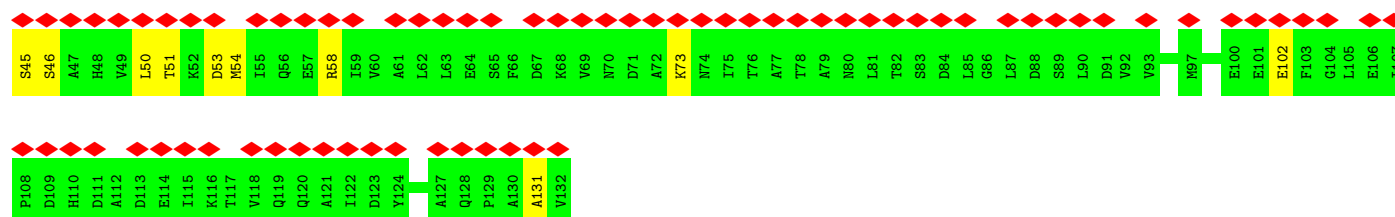
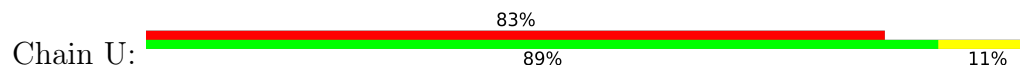
- Molecule 19: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



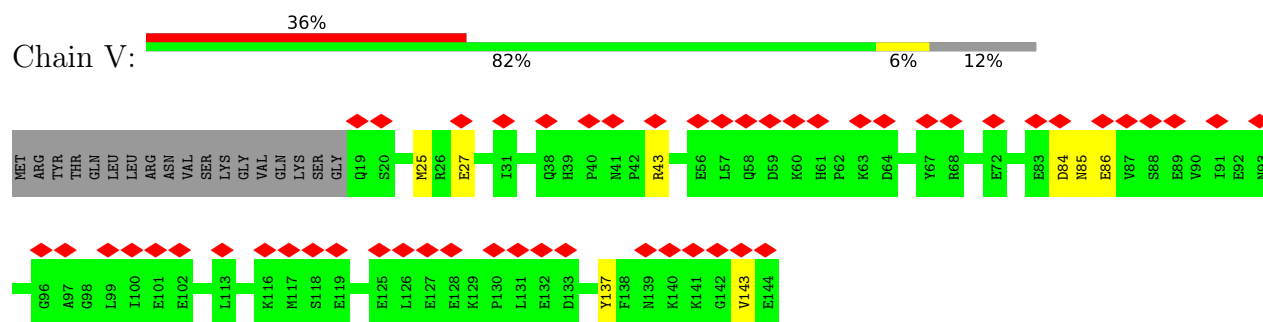
- Molecule 20: Acyl carrier protein



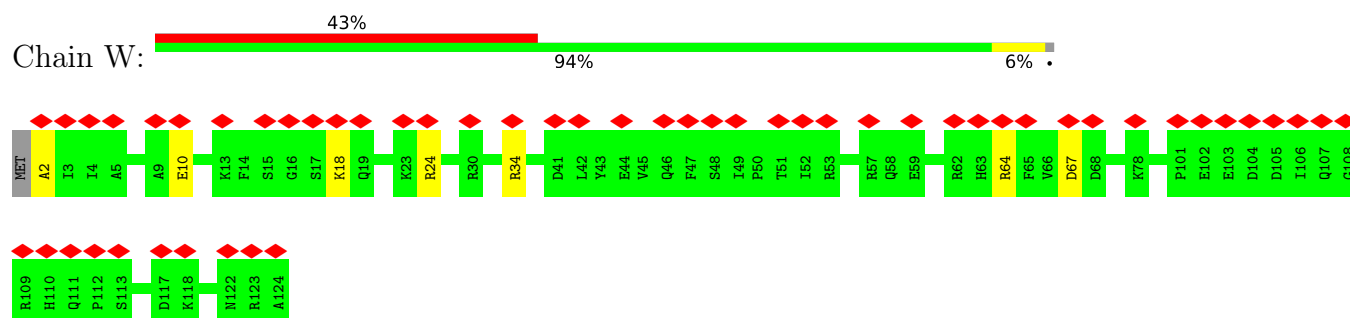
- Molecule 21: Acyl carrier protein



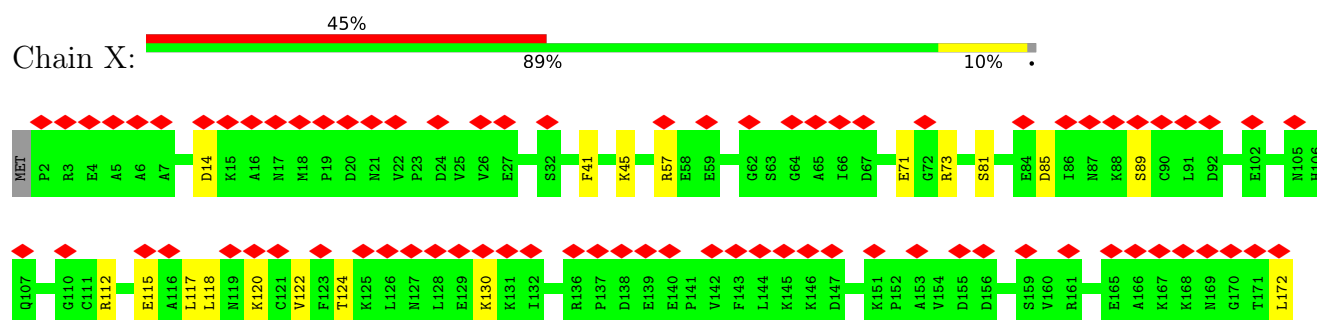
- Molecule 22: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



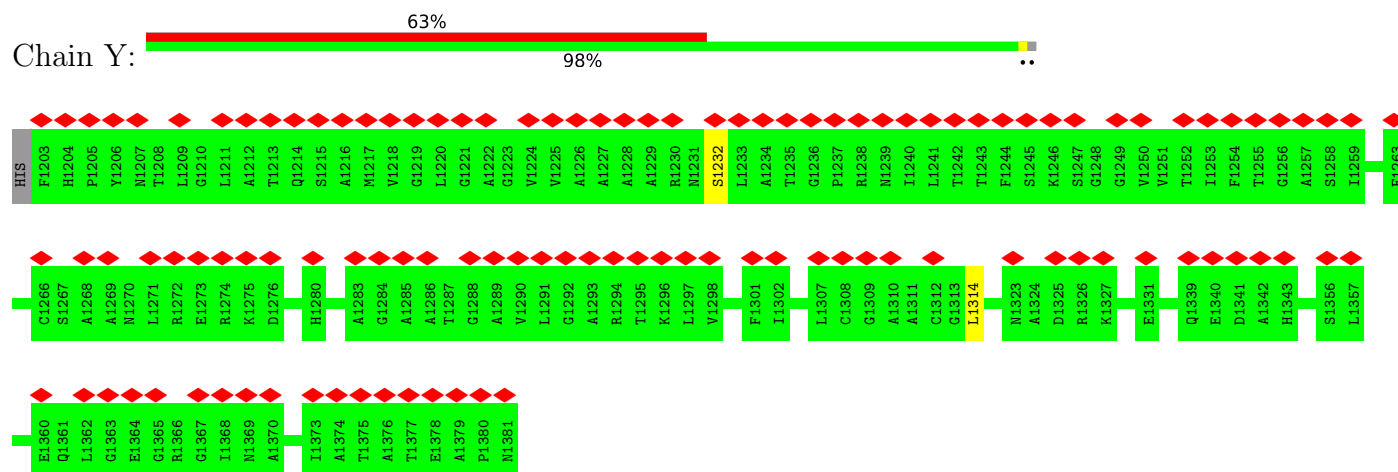
- Molecule 23: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



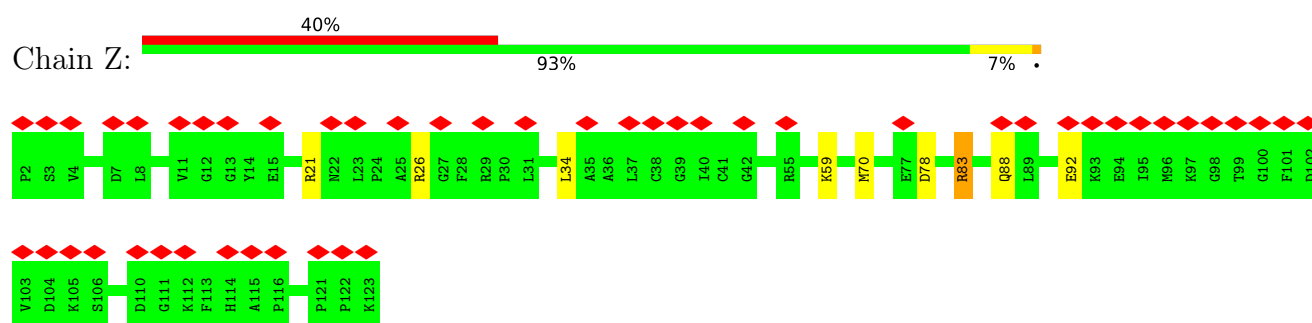
- Molecule 24: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



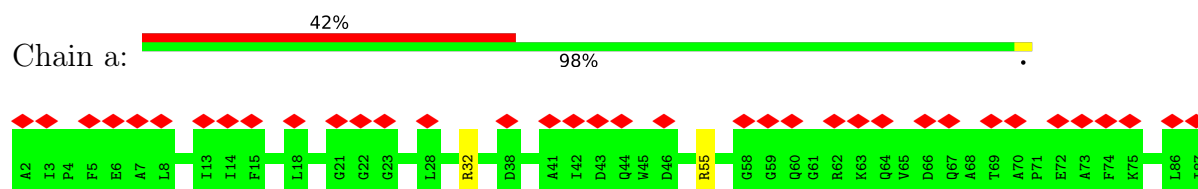
- Molecule 25: Complex I-B14.7



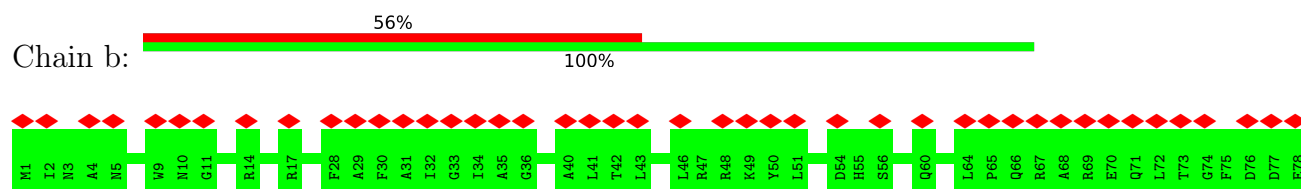
- Molecule 26: GRIM-19



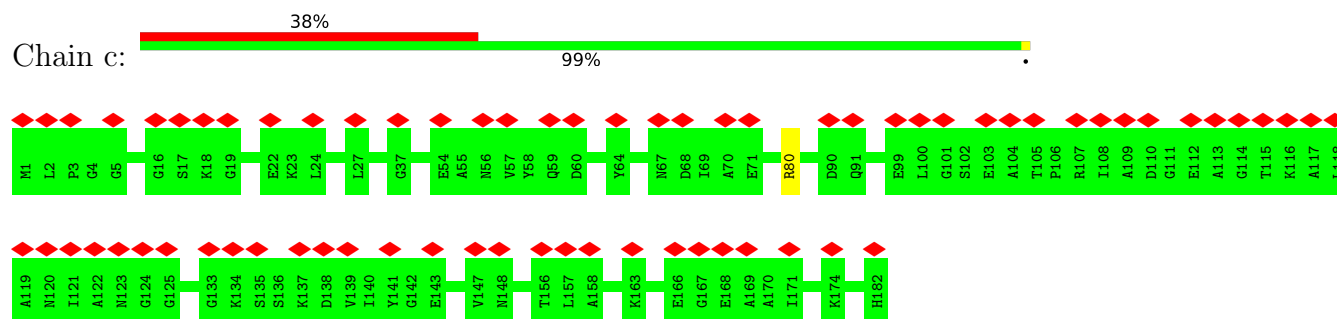
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



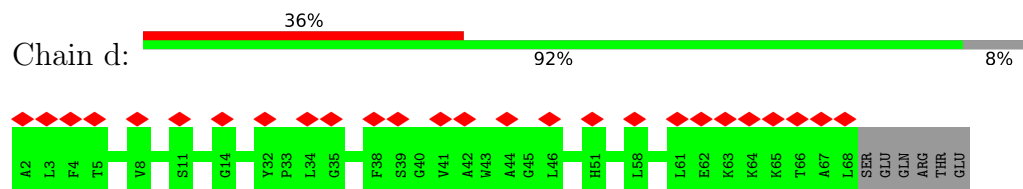
- Molecule 28: subunit NI9M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



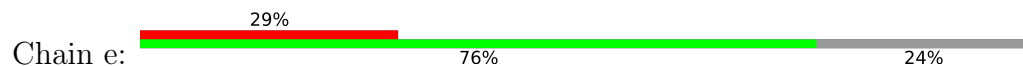
- Molecule 29: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

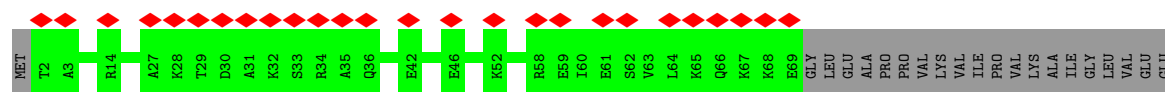


- Molecule 30: subunit NEBM of protein NADH:Ubiquinone Oxidoreductase (Complex I) [Yarrowia lipolytica]

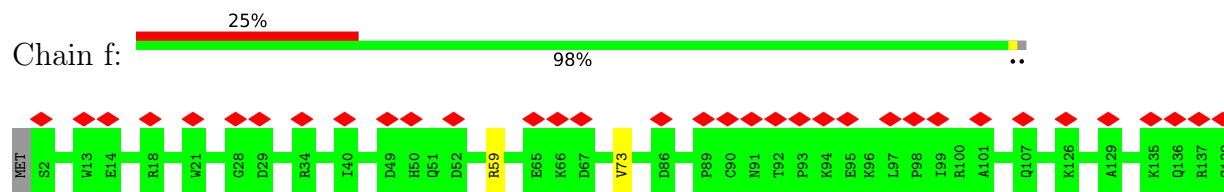


- Molecule 31: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

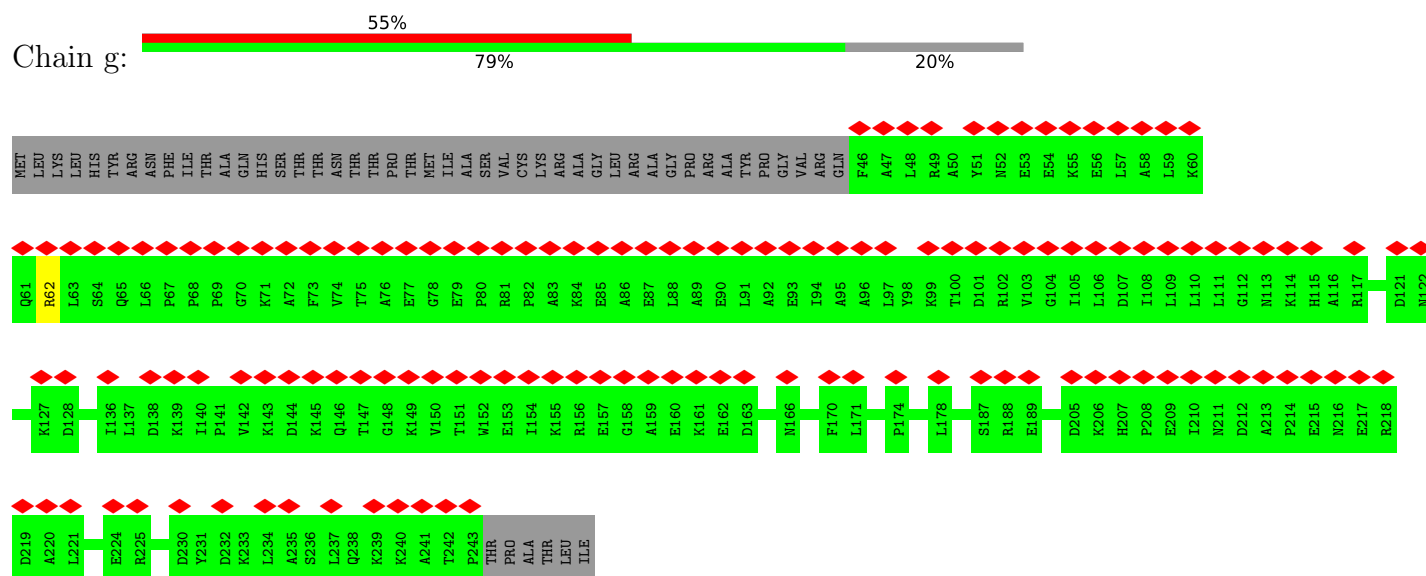




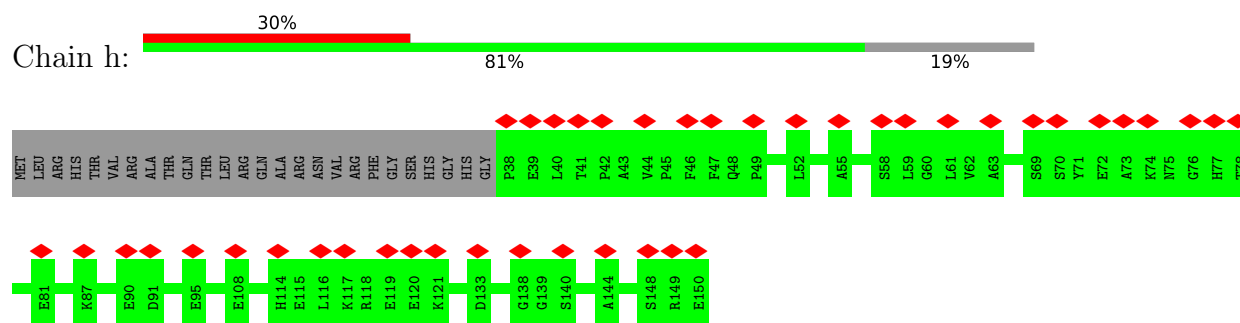
- Molecule 32: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



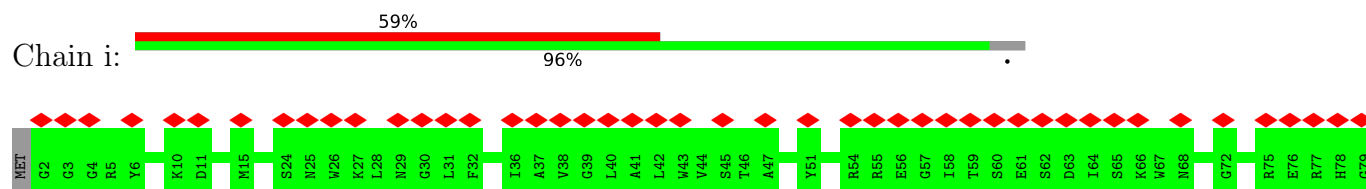
- Molecule 33: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

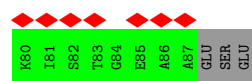


- Molecule 34: subunit NUNM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

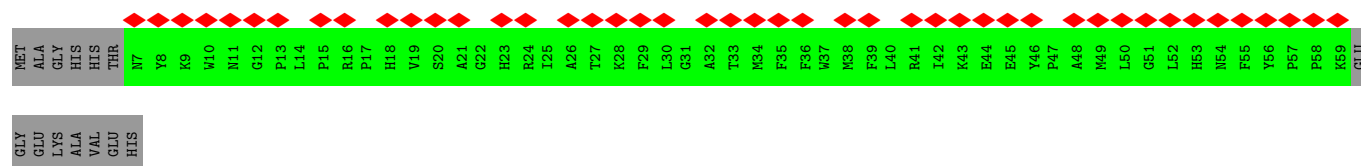
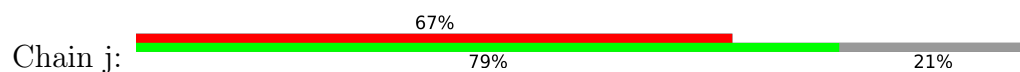


- Molecule 35: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

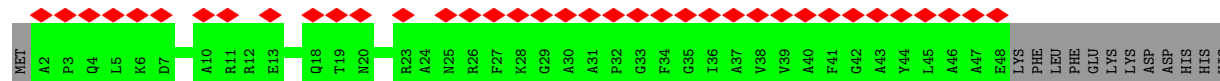
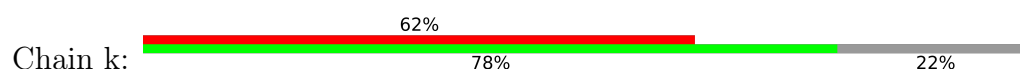




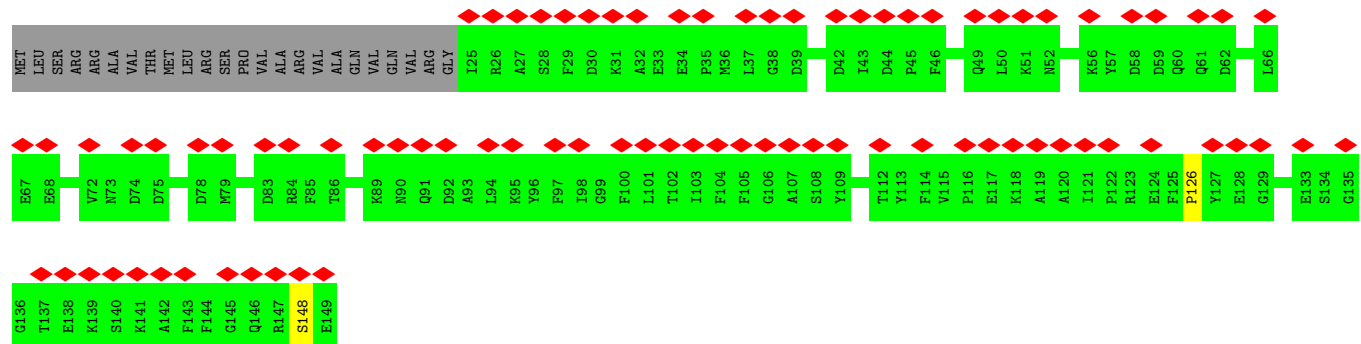
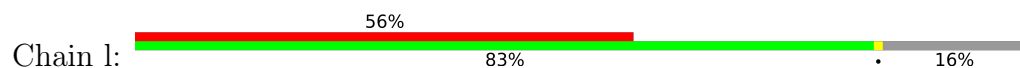
- Molecule 36: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



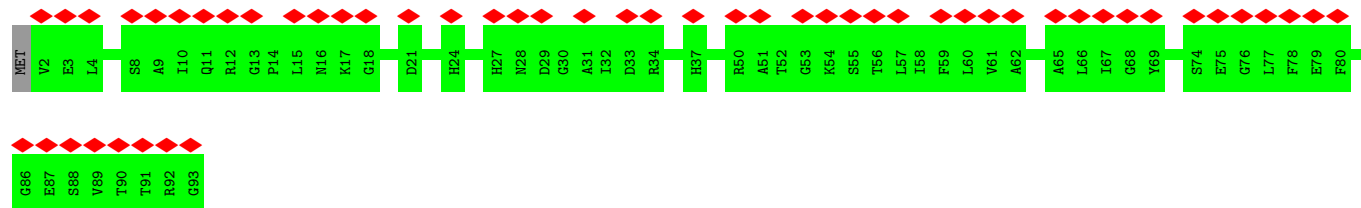
- Molecule 37: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 38: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)

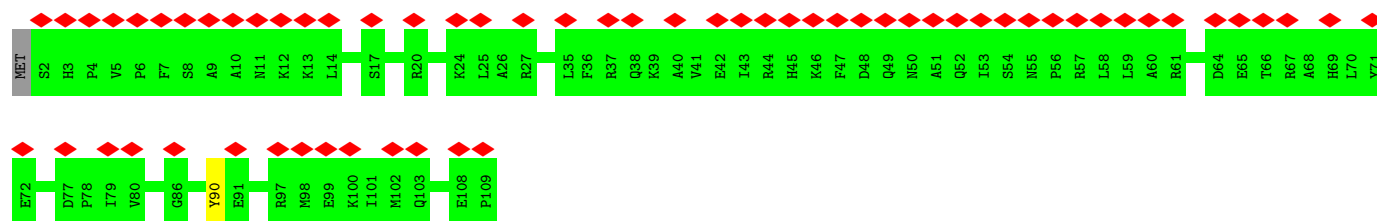


- Molecule 39: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

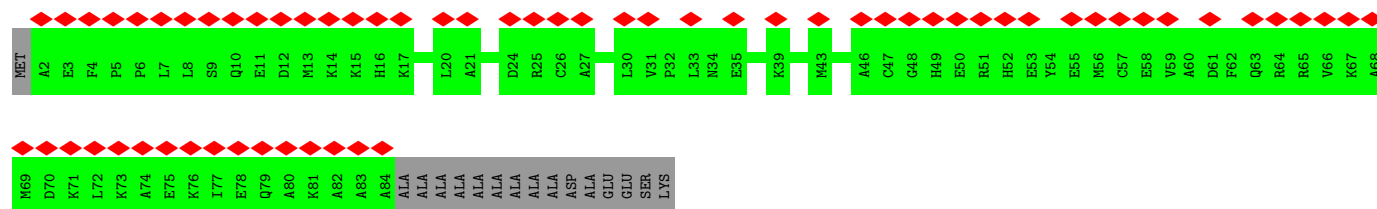
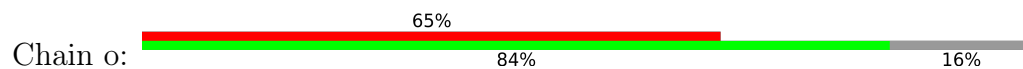


- Molecule 40: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

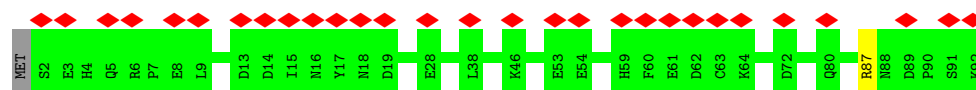




- Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 42: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21013	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, NDP, SF4, FMN, 3PE, PLC, EHZ, ZN, FES, CDL, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/773	0.68	0/1054
2	B	1.01	4/1432 (0.3%)	0.72	2/1948 (0.1%)
3	C	0.97	0/2062	0.70	1/2813 (0.0%)
4	D	0.92	1/3513 (0.0%)	0.73	2/4763 (0.0%)
5	E	0.73	0/1725	0.67	1/2343 (0.0%)
6	F	0.72	1/3638 (0.0%)	0.67	1/4910 (0.0%)
7	G	0.85	3/5368 (0.1%)	0.71	3/7285 (0.0%)
8	H	0.76	1/2751 (0.0%)	0.66	1/3758 (0.0%)
9	I	1.12	4/1564 (0.3%)	0.74	1/2121 (0.0%)
10	J	0.66	0/1477	0.62	0/2015
11	K	0.76	0/692	0.71	0/937
12	L	0.74	0/5327	0.63	1/7273 (0.0%)
13	M	0.86	0/3941	0.65	1/5382 (0.0%)
14	N	0.93	0/3846	0.62	1/5242 (0.0%)
15	O	0.75	0/1344	0.63	0/1822
16	P	0.73	0/2873	0.67	1/3894 (0.0%)
17	Q	0.90	1/1067 (0.1%)	0.71	1/1442 (0.1%)
18	R	0.84	0/946	0.60	0/1283
19	S	0.64	0/677	0.67	1/907 (0.1%)
20	T	0.49	0/628	0.65	1/854 (0.1%)
21	U	0.53	0/673	0.60	0/916
22	V	0.68	0/1049	0.59	0/1420
23	W	0.79	0/1061	0.65	0/1427
24	X	0.71	0/1374	0.70	3/1856 (0.2%)
25	Y	0.66	0/1359	0.63	0/1851
26	Z	0.80	0/1007	0.72	1/1357 (0.1%)
27	a	0.68	0/697	0.72	2/940 (0.2%)
28	b	0.72	0/665	0.62	0/909
29	c	0.78	0/1438	0.65	1/1965 (0.1%)
30	d	0.75	0/523	0.58	0/707
31	e	0.67	0/555	0.61	0/740
32	f	0.94	1/1174 (0.1%)	0.67	1/1597 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.61	0/1614	0.66	0/2182
34	h	0.70	0/937	0.63	0/1270
35	i	0.66	0/679	0.66	0/924
36	j	0.60	0/465	0.64	0/630
37	k	0.58	0/385	0.71	0/522
38	l	0.67	0/1073	0.60	0/1451
39	m	0.70	0/756	0.66	0/1021
40	n	0.63	0/926	0.67	0/1253
41	o	0.59	0/695	0.62	0/930
42	p	0.78	0/782	0.69	1/1051 (0.1%)
All	All	0.80	16/65531 (0.0%)	0.67	28/88965 (0.0%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	366	CYS	CB-SG	-7.20	1.70	1.82
17	Q	58	VAL	CB-CG2	-6.42	1.39	1.52
9	I	330	CYS	CB-SG	-6.34	1.71	1.82
7	G	229	VAL	CB-CG1	-6.27	1.39	1.52
8	H	194	VAL	CB-CG1	-5.84	1.40	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	2685	ARG	NE-CZ-NH1	-6.29	117.15	120.30
7	G	191	ARG	NE-CZ-NH1	5.97	123.28	120.30
6	F	400	ARG	NE-CZ-NH2	5.96	123.28	120.30
24	X	112	ARG	NE-CZ-NH1	5.89	123.25	120.30
42	p	87	ARG	NE-CZ-NH1	5.86	123.23	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	766	827	826	8	0
2	B	1393	1373	1373	10	0
3	C	1999	1925	1925	16	0
4	D	3434	3354	3354	34	0
5	E	1688	1660	1660	19	0
6	F	3559	3513	3513	33	0
7	G	5274	5173	5173	34	0
8	H	2689	2774	2774	22	0
9	I	1526	1471	1471	14	0
10	J	1462	1582	1582	13	0
11	K	693	753	753	18	0
12	L	5207	5364	5364	61	0
13	M	3857	4053	4053	37	0
14	N	3776	4004	4004	33	0
15	O	1305	1281	1281	6	0
16	P	2812	2763	2763	18	0
17	Q	1037	994	994	5	0
18	R	922	876	876	8	0
19	S	667	684	684	7	0
20	T	620	614	614	7	0
21	U	667	655	655	5	0
22	V	1028	1021	1021	5	0
23	W	1036	1018	1018	5	0
24	X	1345	1333	1333	10	0
25	Y	1327	1311	1310	2	0
26	Z	983	1000	1000	8	0
27	a	681	672	671	0	0
28	b	639	618	620	0	0
29	c	1397	1407	1407	0	0
30	d	510	532	532	0	0
31	e	546	536	536	0	0
32	f	1136	1089	1089	0	0
33	g	1585	1603	1603	0	0
34	h	909	877	877	0	0
35	i	659	641	641	0	0
36	j	445	439	439	0	0
37	k	373	361	361	0	0
38	l	1039	973	973	0	0
39	m	735	718	718	0	0
40	n	900	904	904	0	0
41	o	681	685	685	0	0
42	p	766	726	726	0	0
43	D	27	34	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	H	28	36	27	0	0
43	L	76	112	106	3	0
43	N	42	64	64	0	0
43	d	27	34	28	0	0
44	E	4	0	0	1	0
44	G	4	0	0	0	0
45	F	31	18	18	1	0
46	F	8	0	0	0	0
46	G	16	0	0	0	0
46	I	16	0	0	1	0
47	H	68	94	87	1	0
47	I	32	42	38	0	0
47	L	153	246	246	3	0
47	M	30	39	34	0	0
47	N	51	82	82	3	0
47	Y	33	46	40	1	0
47	Z	43	66	60	0	0
47	b	43	66	63	0	0
47	d	24	28	22	0	0
47	g	30	38	34	0	0
48	M	83	122	113	0	0
48	O	63	82	73	1	0
48	Z	57	66	58	1	0
48	a	52	56	48	0	0
48	b	48	52	40	0	0
49	P	48	26	26	2	0
50	R	1	0	0	0	0
51	T	35	40	0	3	0
51	U	36	41	0	0	0
52	Y	70	92	92	0	0
All	All	65352	65779	65583	386	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 4.

The worst 5 of 386 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)
14:N:2539:ILE:HD11	14:N:2638:ILE:HG22	1.44	0.97
3:C:216:LEU:HD11	4:D:126:LEU:HD23	1.58	0.84
51:T:201:EHZ:N2	51:T:201:EHZ:O3	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:131:ARG:NH2	49:P:401:NDP:O2X	2.15	0.80
16:P:247:ARG:NH1	16:P:334:ASP:O	2.16	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/128 (70%)	85 (94%)	5 (6%)	0	100	100
2	B	175/210 (83%)	168 (96%)	7 (4%)	0	100	100
3	C	240/293 (82%)	221 (92%)	18 (8%)	1 (0%)	30	62
4	D	435/466 (93%)	410 (94%)	25 (6%)	0	100	100
5	E	214/243 (88%)	199 (93%)	14 (6%)	1 (0%)	25	57
6	F	458/488 (94%)	425 (93%)	33 (7%)	0	100	100
7	G	692/728 (95%)	639 (92%)	53 (8%)	0	100	100
8	H	339/341 (99%)	321 (95%)	18 (5%)	0	100	100
9	I	189/193 (98%)	181 (96%)	8 (4%)	0	100	100
10	J	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
11	K	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
12	L	653/655 (100%)	616 (94%)	36 (6%)	1 (0%)	44	72
13	M	484/486 (100%)	464 (96%)	20 (4%)	0	100	100
14	N	467/469 (100%)	452 (97%)	15 (3%)	0	100	100
15	O	166/169 (98%)	156 (94%)	10 (6%)	0	100	100
16	P	353/355 (99%)	337 (96%)	16 (4%)	0	100	100
17	Q	123/161 (76%)	118 (96%)	5 (4%)	0	100	100
18	R	116/118 (98%)	106 (91%)	9 (8%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
20	T	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	10	40
21	U	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
22	V	124/144 (86%)	119 (96%)	5 (4%)	0	100	100
23	W	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
24	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
25	Y	177/180 (98%)	171 (97%)	6 (3%)	0	100	100
26	Z	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
27	a	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
28	b	76/78 (97%)	67 (88%)	9 (12%)	0	100	100
29	c	180/182 (99%)	166 (92%)	14 (8%)	0	100	100
30	d	65/73 (89%)	65 (100%)	0	0	100	100
31	e	66/89 (74%)	65 (98%)	1 (2%)	0	100	100
32	f	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
33	g	196/249 (79%)	187 (95%)	9 (5%)	0	100	100
34	h	111/139 (80%)	106 (96%)	5 (4%)	0	100	100
35	i	84/90 (93%)	82 (98%)	2 (2%)	0	100	100
36	j	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
37	k	45/60 (75%)	41 (91%)	4 (9%)	0	100	100
38	l	123/149 (83%)	112 (91%)	9 (7%)	2 (2%)	8	37
39	m	90/93 (97%)	84 (93%)	6 (7%)	0	100	100
40	n	106/109 (97%)	99 (93%)	6 (6%)	1 (1%)	14	47
41	o	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
42	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
All	All	8006/8568 (93%)	7557 (94%)	441 (6%)	8 (0%)	50	78

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	1260	VAL
5	E	217	ASP
38	l	148	SER
40	n	90	TYR
3	C	254	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	A	86/113 (76%)	86 (100%)	0	100	100
2	B	152/180 (84%)	152 (100%)	0	100	100
3	C	218/251 (87%)	218 (100%)	0	100	100
4	D	367/394 (93%)	367 (100%)	0	100	100
5	E	191/212 (90%)	191 (100%)	0	100	100
6	F	367/389 (94%)	367 (100%)	0	100	100
7	G	566/595 (95%)	565 (100%)	1 (0%)	92	96
8	H	293/301 (97%)	293 (100%)	0	100	100
9	I	157/158 (99%)	157 (100%)	0	100	100
10	J	166/166 (100%)	166 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	579/579 (100%)	578 (100%)	1 (0%)	92	96
13	M	433/433 (100%)	433 (100%)	0	100	100
14	N	432/432 (100%)	431 (100%)	1 (0%)	92	96
15	O	132/133 (99%)	132 (100%)	0	100	100
16	P	299/311 (96%)	299 (100%)	0	100	100
17	Q	107/140 (76%)	107 (100%)	0	100	100
18	R	98/98 (100%)	98 (100%)	0	100	100
19	S	72/73 (99%)	72 (100%)	0	100	100
20	T	68/68 (100%)	68 (100%)	0	100	100
21	U	75/75 (100%)	74 (99%)	1 (1%)	65	77
22	V	113/129 (88%)	111 (98%)	2 (2%)	54	71
23	W	109/110 (99%)	109 (100%)	0	100	100
24	X	147/148 (99%)	147 (100%)	0	100	100
25	Y	130/131 (99%)	130 (100%)	0	100	100
26	Z	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	68/68 (100%)	68 (100%)	0	100	100
28	b	65/65 (100%)	65 (100%)	0	100	100
29	c	148/148 (100%)	148 (100%)	0	100	100
30	d	52/58 (90%)	52 (100%)	0	100	100
31	e	59/76 (78%)	59 (100%)	0	100	100
32	f	122/123 (99%)	122 (100%)	0	100	100
33	g	161/211 (76%)	160 (99%)	1 (1%)	84	90
34	h	98/119 (82%)	98 (100%)	0	100	100
35	i	64/68 (94%)	64 (100%)	0	100	100
36	j	45/55 (82%)	45 (100%)	0	100	100
37	k	32/45 (71%)	32 (100%)	0	100	100
38	l	109/129 (84%)	109 (100%)	0	100	100
39	m	72/73 (99%)	72 (100%)	0	100	100
40	n	99/100 (99%)	99 (100%)	0	100	100
41	o	70/76 (92%)	70 (100%)	0	100	100
42	p	84/85 (99%)	84 (100%)	0	100	100
All	All	6882/7295 (94%)	6875 (100%)	7 (0%)	92	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	U	73	LYS
22	V	25	MET
33	g	62	ARG
22	V	27	GLU
14	N	2488	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	185	ASN
14	N	2706	ASN
16	P	234	ASN
41	o	16	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

7 non-standard protein/DNA/RNA residues 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
13	FME	M	503	13	8,9,10	0.88	0	7,9,11	1.07	1 (14%)
11	FME	K	1	11	8,9,10	1.03	1 (12%)	7,9,11	1.23	1 (14%)
12	FME	L	706	12	8,9,10	1.01	1 (12%)	7,9,11	1.04	0
8	FME	H	1	8	8,9,10	1.17	1 (12%)	7,9,11	1.07	0
10	FME	J	1	10	8,9,10	0.97	0	7,9,11	1.02	1 (14%)
14	FME	N	2403	14	8,9,10	1.45	1 (12%)	7,9,11	0.55	0
1	FME	A	1	1	8,9,10	1.07	1 (12%)	7,9,11	1.27	1 (14%)

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
13	FME	M	503	13	-	0/7/9/11	-
11	FME	K	1	11	-	2/7/9/11	-
12	FME	L	706	12	-	2/7/9/11	-
8	FME	H	1	8	-	1/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-
14	FME	N	2403	14	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	2403	FME	CA-N	-3.69	1.41	1.46
8	H	1	FME	CA-N	-2.42	1.42	1.46
11	K	1	FME	CA-N	-2.17	1.43	1.46
1	A	1	FME	CA-N	-2.16	1.43	1.46
12	L	706	FME	CN-N	2.05	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	2.75	114.70	109.73
11	K	1	FME	C-CA-N	2.32	113.92	109.73
10	J	1	FME	CE-SD-CG	2.25	108.13	100.40
13	M	503	FME	C-CA-N	2.11	113.55	109.73

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O-C-CA-CB
8	H	1	FME	O1-CN-N-CA
11	K	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 1 is monoatomic - leaving 37 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	3PE	N	2402	-	50,50,50	0.90	2 (4%)	53,55,55	1.09	2 (3%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-
45	FMN	F	501	-	33,33,33	3.26	13 (39%)	48,50,50	2.57	21 (43%)
46	SF4	G	801	7	0,12,12	-	-	-	-	-
47	3PE	L	705	-	50,50,50	0.89	4 (8%)	53,55,55	1.30	3 (5%)
47	3PE	g	301	-	29,29,50	1.21	3 (10%)	32,34,55	1.30	5 (15%)
48	CDL	M	501	-	82,82,99	1.33	8 (9%)	88,94,111	1.11	5 (5%)
43	PLC	D	501	-	26,26,41	1.48	6 (23%)	32,34,49	1.15	3 (9%)
47	3PE	L	703	-	50,50,50	0.86	4 (8%)	53,55,55	1.02	2 (3%)
47	3PE	Y	1403	-	32,32,50	1.16	5 (15%)	35,37,55	1.11	3 (8%)
46	SF4	I	502	9	0,12,12	-	-	-	-	-
43	PLC	H	6402	-	26,26,41	1.48	5 (19%)	30,32,49	1.88	4 (13%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
47	3PE	I	501	-	31,31,50	1.14	3 (9%)	34,36,55	1.21	3 (8%)
44	FES	E	301	5	0,4,4	-	-	-	-	-
47	3PE	L	704	-	50,50,50	0.87	4 (8%)	53,55,55	1.09	3 (5%)
48	CDL	O	601	-	62,62,99	1.19	7 (11%)	68,74,111	1.20	7 (10%)
47	3PE	Z	202	-	42,42,50	0.97	3 (7%)	45,47,55	1.03	3 (6%)
43	PLC	L	701	-	41,41,41	1.30	6 (14%)	47,49,49	1.14	4 (8%)
49	NDP	P	401	-	45,52,52	2.54	9 (20%)	53,80,80	1.76	11 (20%)
51	EHZ	T	201	20	30,34,37	2.15	8 (26%)	40,44,47	1.51	8 (20%)
47	3PE	b	402	-	42,42,50	1.21	6 (14%)	45,47,55	1.12	3 (6%)
48	CDL	a	101	-	51,51,99	1.27	9 (17%)	57,63,111	1.45	6 (10%)
47	3PE	d	502	-	23,23,50	1.33	3 (13%)	26,28,55	1.26	3 (11%)
47	3PE	H	6401	-	21,21,50	1.28	2 (9%)	24,26,55	1.18	2 (8%)
46	SF4	I	503	9	0,12,12	-	-	-	-	-
51	EHZ	U	201	21	31,35,37	2.12	7 (22%)	41,45,47	1.40	4 (9%)
47	3PE	M	502	-	29,29,50	1.20	4 (13%)	32,34,55	1.21	4 (12%)
48	CDL	b	401	-	47,47,99	1.33	7 (14%)	53,59,111	1.35	6 (11%)
43	PLC	N	2401	-	41,41,41	1.12	5 (12%)	47,49,49	1.08	3 (6%)
44	FES	G	803	7	0,4,4	-	-	-	-	-
52	LMT	Y	1401	-	36,36,36	0.92	2 (5%)	47,47,47	1.11	2 (4%)
43	PLC	L	702	-	33,33,41	1.36	2 (6%)	39,41,49	1.10	2 (5%)
47	3PE	H	6403	-	45,45,50	1.19	3 (6%)	48,50,55	1.10	3 (6%)
48	CDL	Z	201	-	56,56,99	1.20	7 (12%)	62,68,111	1.21	7 (11%)
43	PLC	d	501	-	26,26,41	1.46	5 (19%)	32,34,49	1.30	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	LMT	Y	1402	-	36,36,36	0.89	0	47,47,47	1.18	6 (12%)

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
47	3PE	N	2402	-	-	23/54/54/54	-
46	SF4	G	802	7	-	-	0/6/5/5
45	FMN	F	501	-	-	12/18/18/18	0/3/3/3
47	3PE	L	705	-	-	22/54/54/54	-
47	3PE	g	301	-	1/1/4/4	9/33/33/54	-
48	CDL	M	501	-	-	45/93/93/110	-
46	SF4	G	801	7	-	-	0/6/5/5
43	PLC	D	501	-	-	11/30/30/45	-
47	3PE	L	703	-	-	23/54/54/54	-
47	3PE	Y	1403	-	-	16/36/36/54	-
46	SF4	I	502	9	-	-	0/6/5/5
43	PLC	H	6402	-	-	13/30/30/45	-
46	SF4	F	502	6	-	-	0/6/5/5
47	3PE	I	501	-	1/1/4/4	21/35/35/54	-
44	FES	E	301	5	-	-	0/1/1/1
47	3PE	L	704	-	-	21/54/54/54	-
48	CDL	O	601	-	-	28/73/73/110	-
47	3PE	Z	202	-	-	12/46/46/54	-
43	PLC	L	701	-	-	23/45/45/45	-
49	NDP	P	401	-	-	11/30/77/77	0/5/5/5
51	EHZ	T	201	20	1/1/9/9	15/42/42/45	-
47	3PE	b	402	-	-	15/46/46/54	-
48	CDL	a	101	-	-	23/62/62/110	-
47	3PE	d	502	-	-	14/27/27/54	-
47	3PE	H	6401	-	1/1/4/4	12/24/24/54	-
51	EHZ	U	201	21	-	8/43/43/45	-
46	SF4	I	503	9	-	-	0/6/5/5
47	3PE	M	502	-	1/1/4/4	18/33/33/54	-
48	CDL	b	401	-	-	20/58/58/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	PLC	N	2401	-	-	17/45/45/45	-
52	LMT	Y	1401	-	4/4/10/10	9/21/61/61	0/2/2/2
44	FES	G	803	7	-	-	0/1/1/1
43	PLC	L	702	-	-	18/37/37/45	-
47	3PE	H	6403	-	-	18/49/49/54	-
48	CDL	Z	201	-	-	38/67/67/110	-
43	PLC	d	501	-	-	11/30/30/45	-
52	LMT	Y	1402	-	4/4/10/10	11/21/61/61	0/2/2/2

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	401	NDP	P2B-O2B	14.28	1.86	1.59
45	F	501	FMN	O3'-C3'	-10.24	1.18	1.43
45	F	501	FMN	O2-C2	8.34	1.39	1.24
45	F	501	FMN	O4-C4	8.24	1.39	1.23
51	T	201	EHZ	C15-N2	6.41	1.47	1.33

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	F	501	FMN	C9-C9A-N10	7.99	132.64	121.84
43	H	6402	PLC	C7-N-C6	-7.08	91.43	109.73
47	L	705	3PE	O21-C21-C22	6.85	126.27	111.50
49	P	401	NDP	PN-O3-PA	-6.70	109.82	132.83
45	F	501	FMN	C10-N1-C2	6.25	129.40	116.90

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	H	6401	3PE	C2
47	I	501	3PE	C2
47	M	502	3PE	C2
47	g	301	3PE	C2
51	T	201	EHZ	C16

5 of 537 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	D	501	PLC	C1-O3P-P-O2P

Continued on next page...

Continued from previous page...

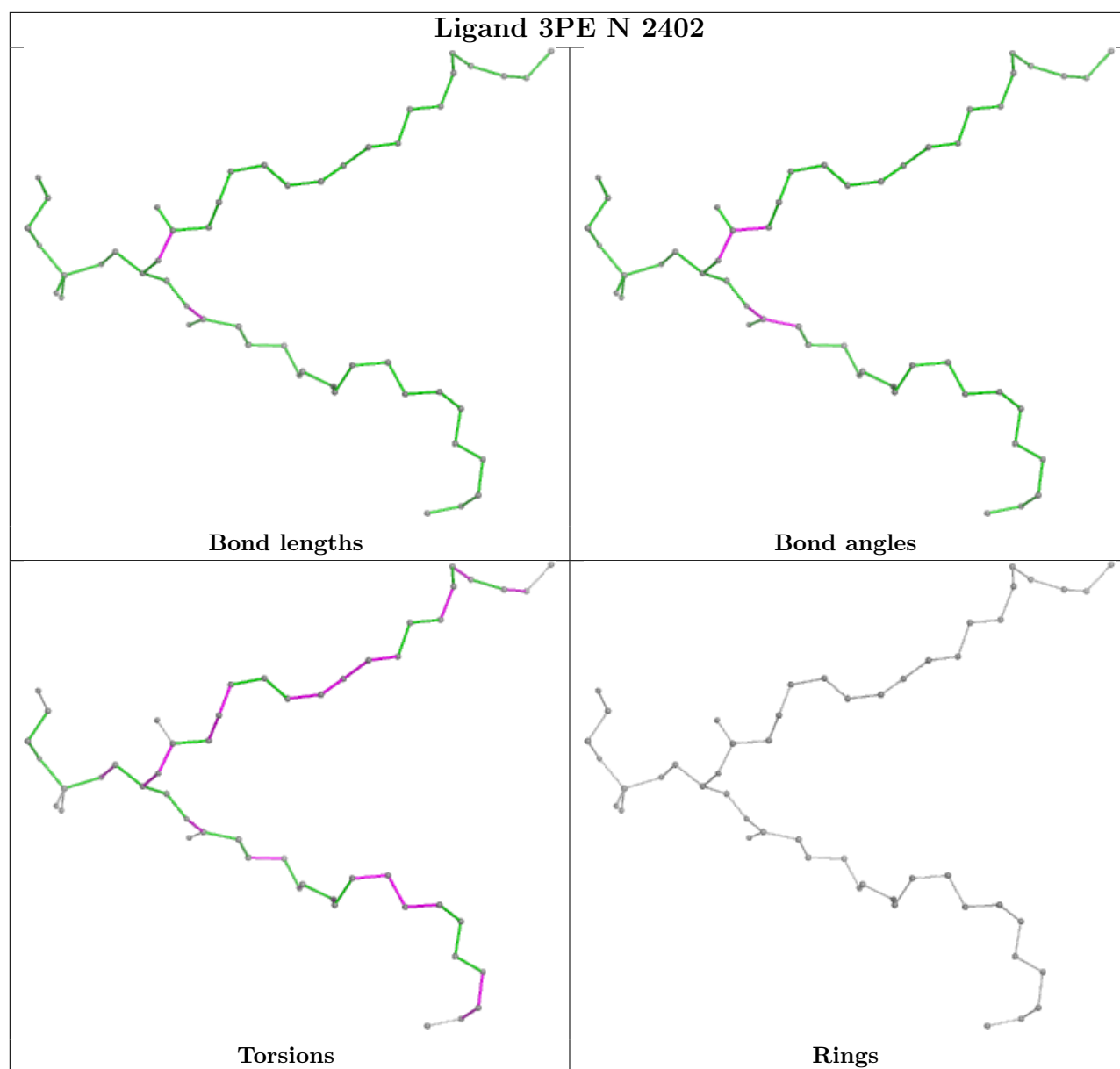
Mol	Chain	Res	Type	Atoms
43	H	6402	PLC	O3P-C1-C2-O2
43	H	6402	PLC	C4-O4P-P-O1P
43	H	6402	PLC	C4-O4P-P-O2P
43	L	701	PLC	O4P-C4-C5-N

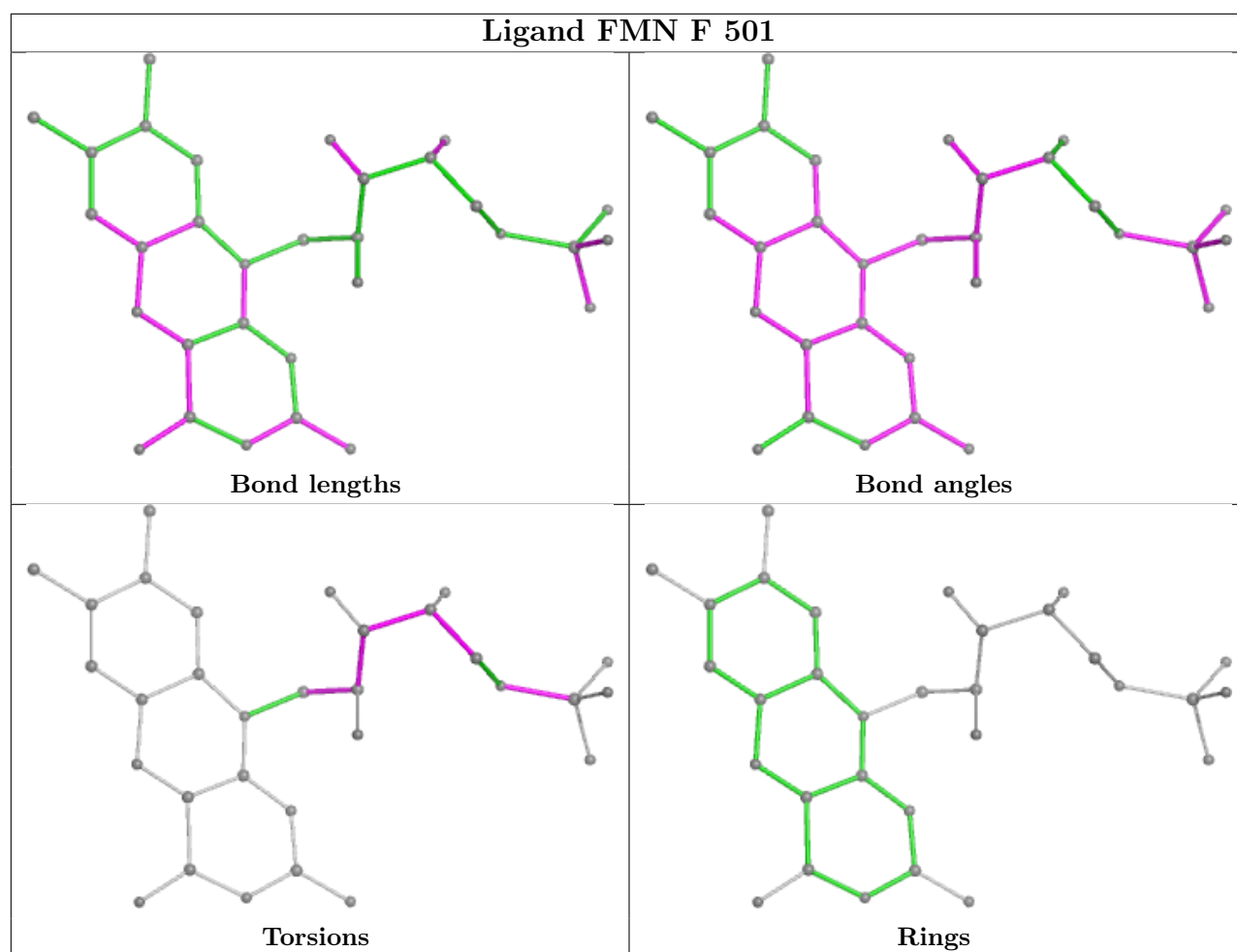
There are no ring outliers.

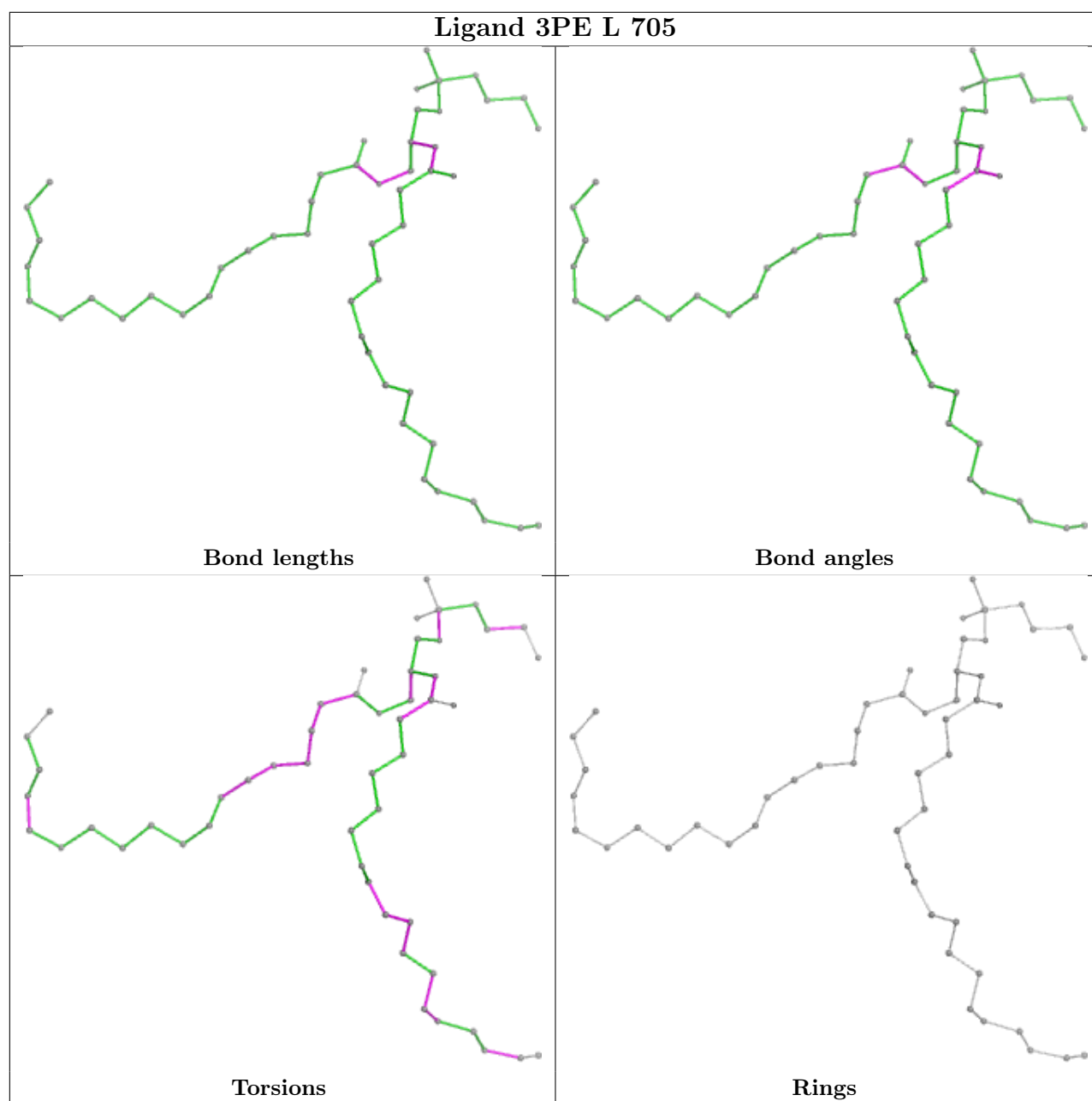
13 monomers are involved in 21 short contacts:

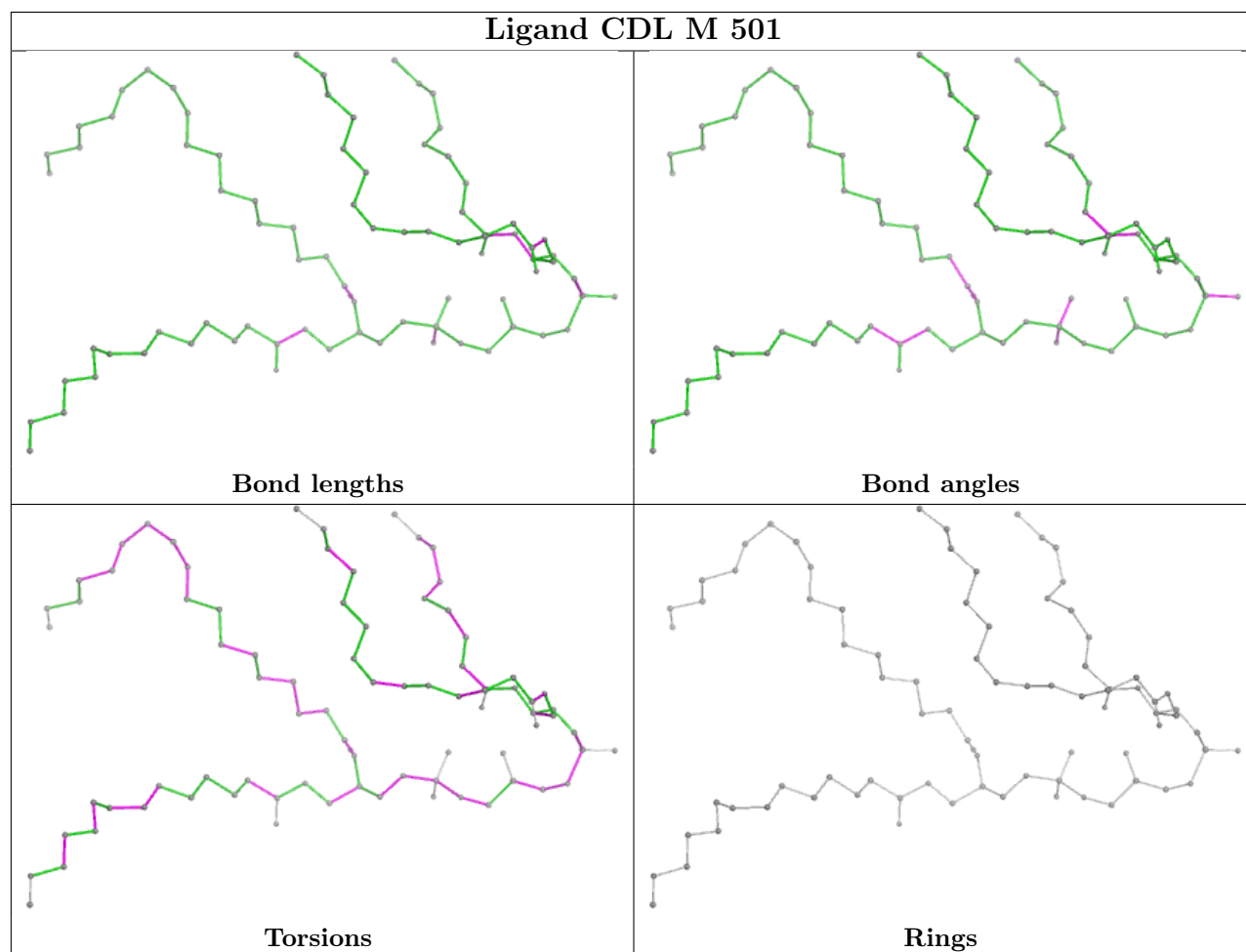
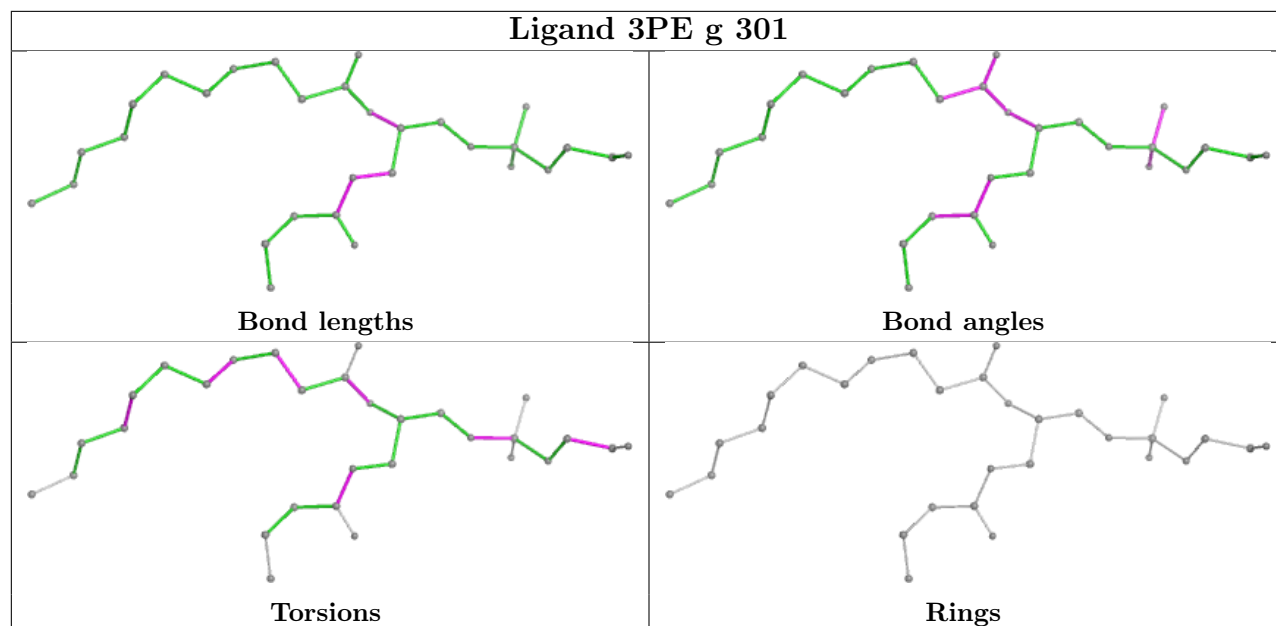
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	N	2402	3PE	3	0
45	F	501	FMN	1	0
47	L	705	3PE	3	0
47	Y	1403	3PE	1	0
44	E	301	FES	1	0
48	O	601	CDL	1	0
43	L	701	PLC	2	0
49	P	401	NDP	2	0
51	T	201	EHZ	3	0
46	I	503	SF4	1	0
43	L	702	PLC	1	0
47	H	6403	3PE	1	0
48	Z	201	CDL	1	0

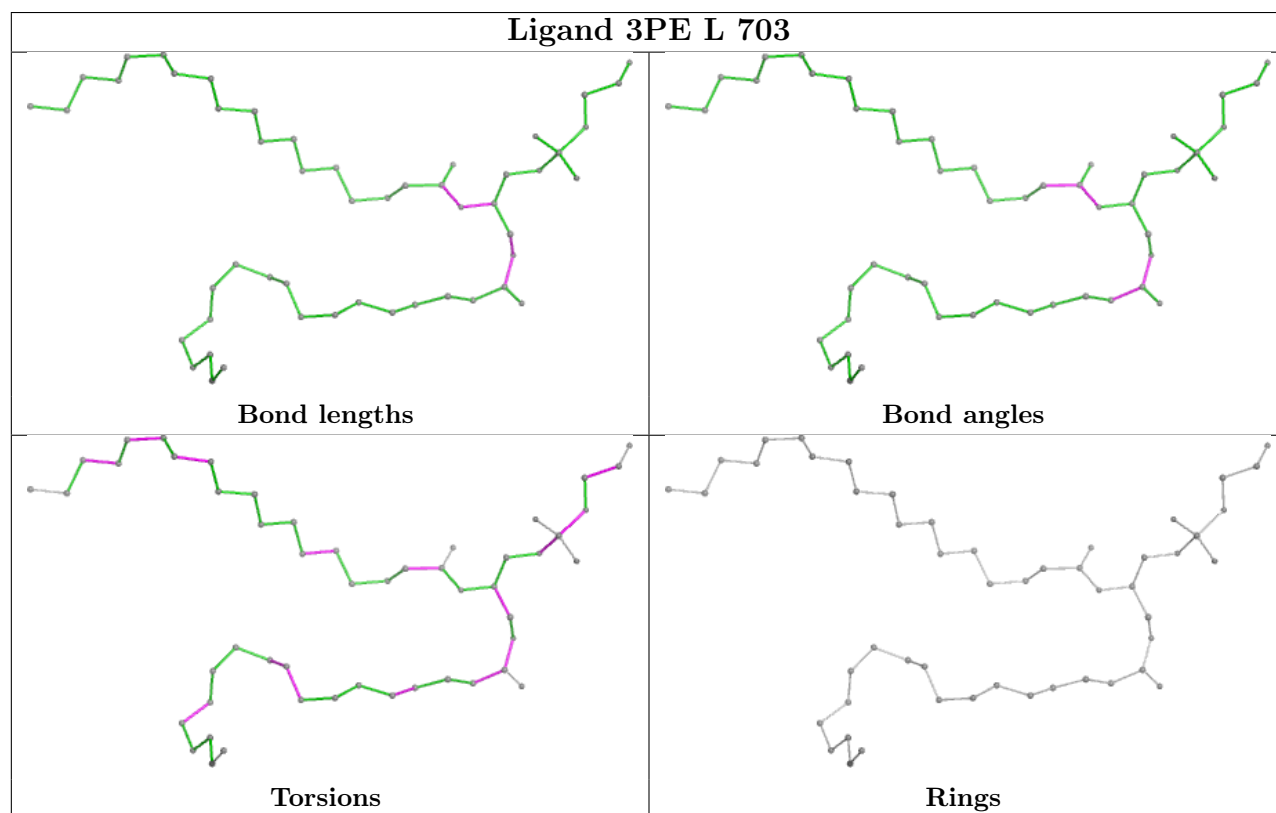
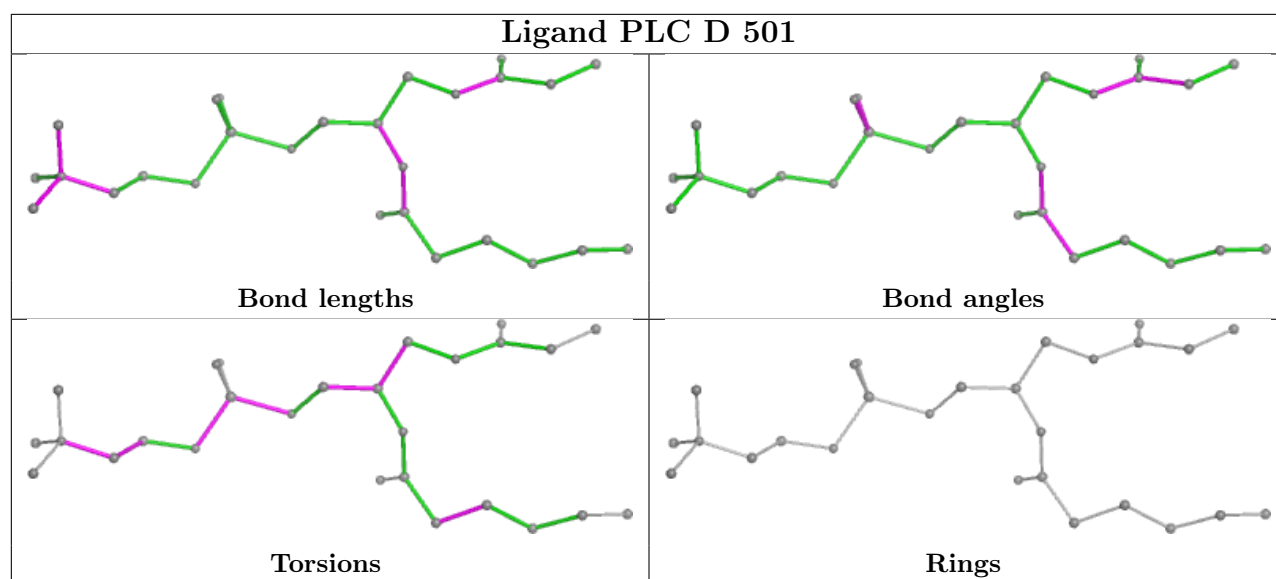
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

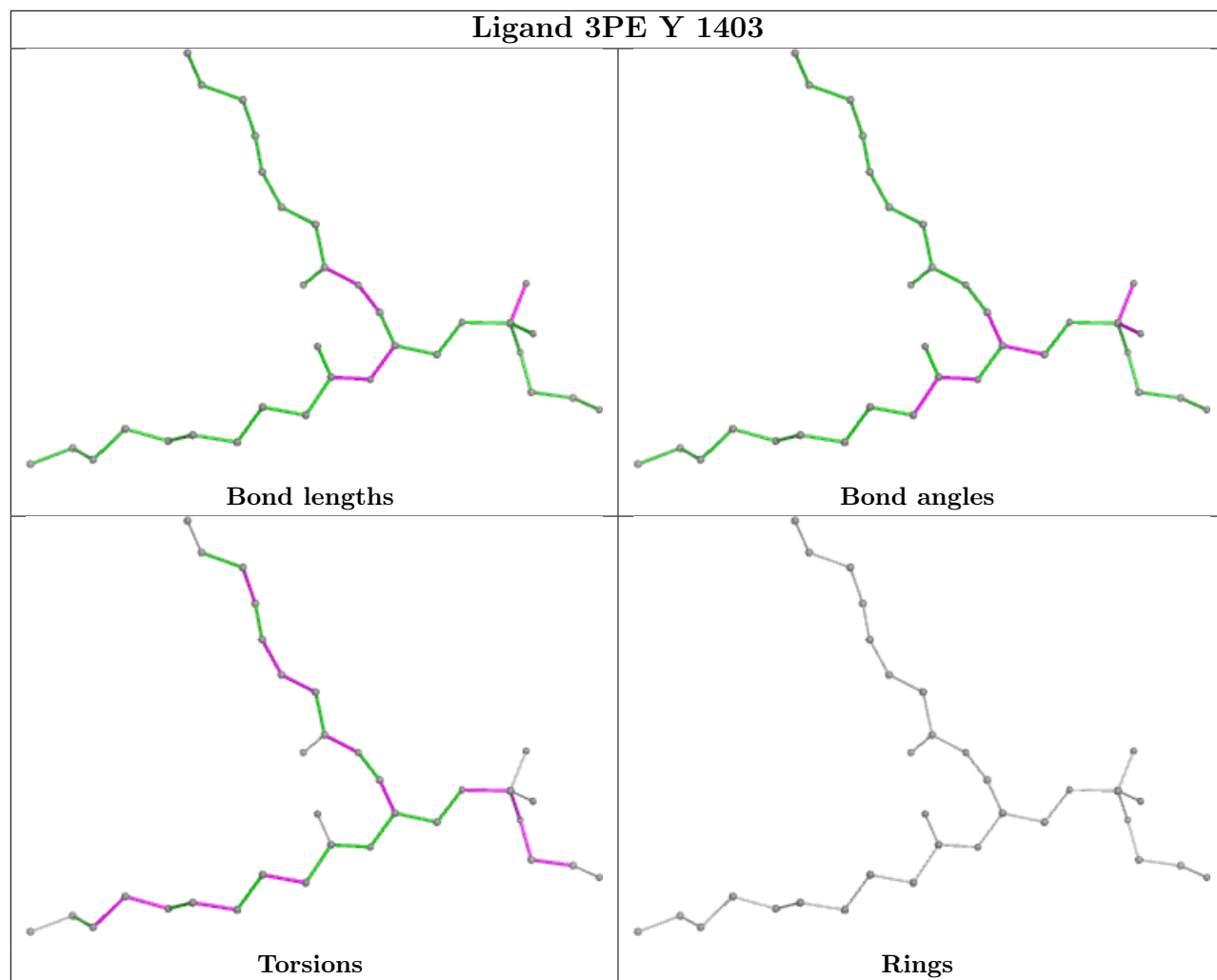




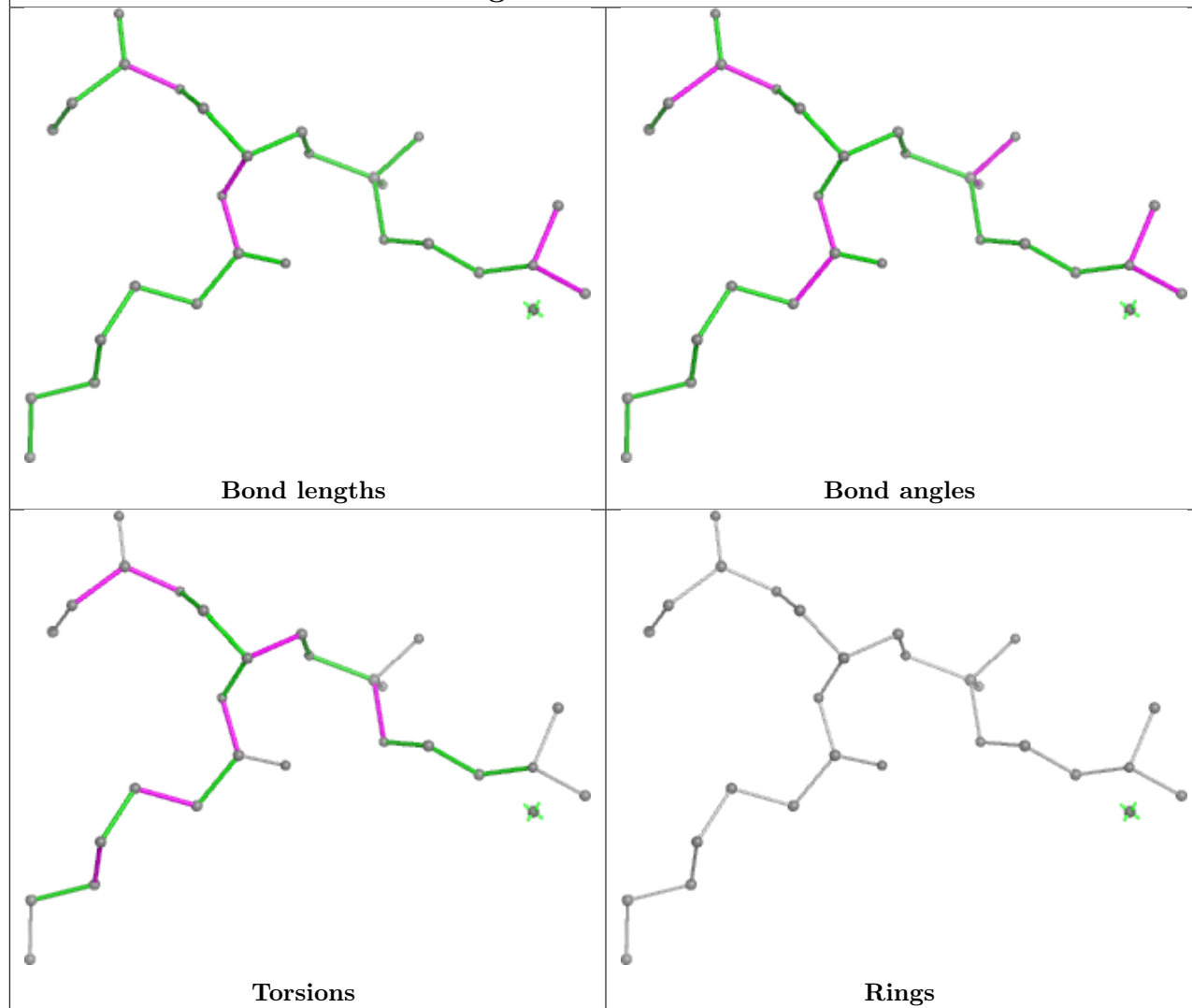




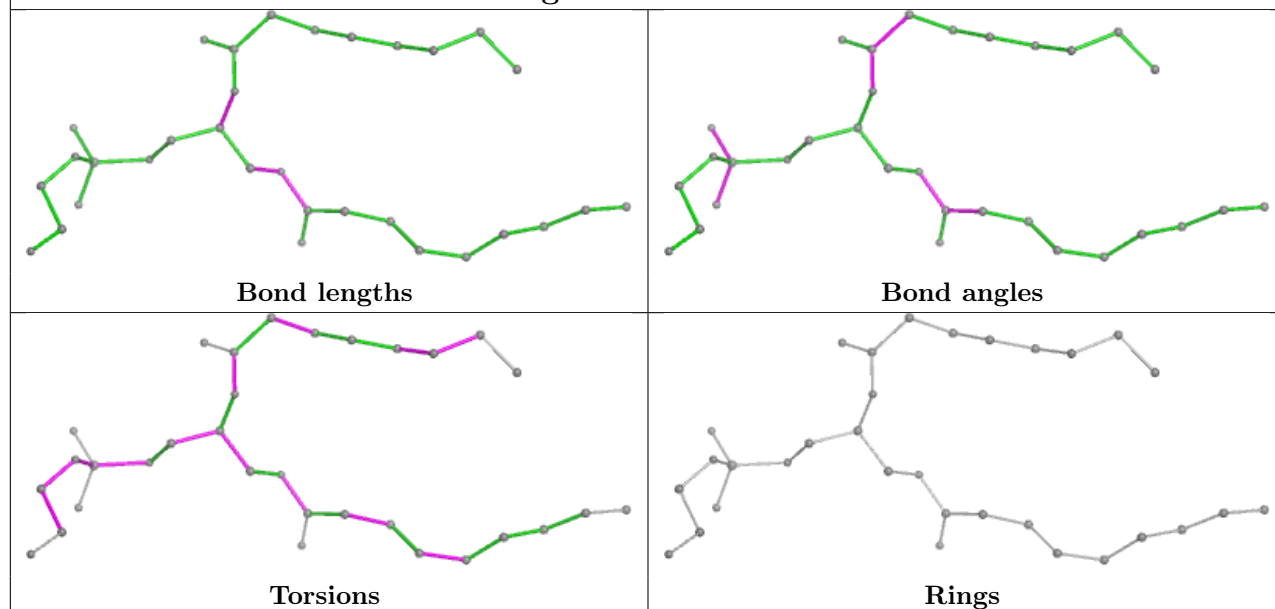


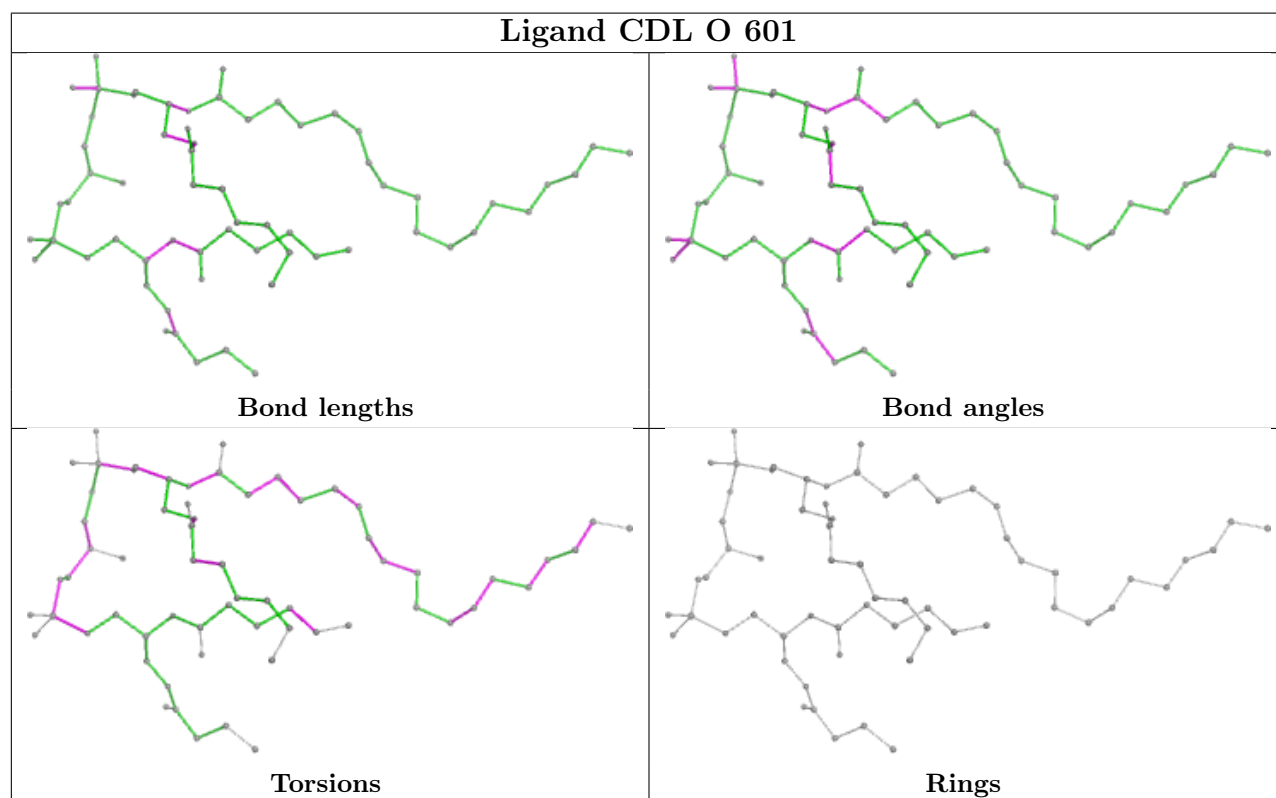
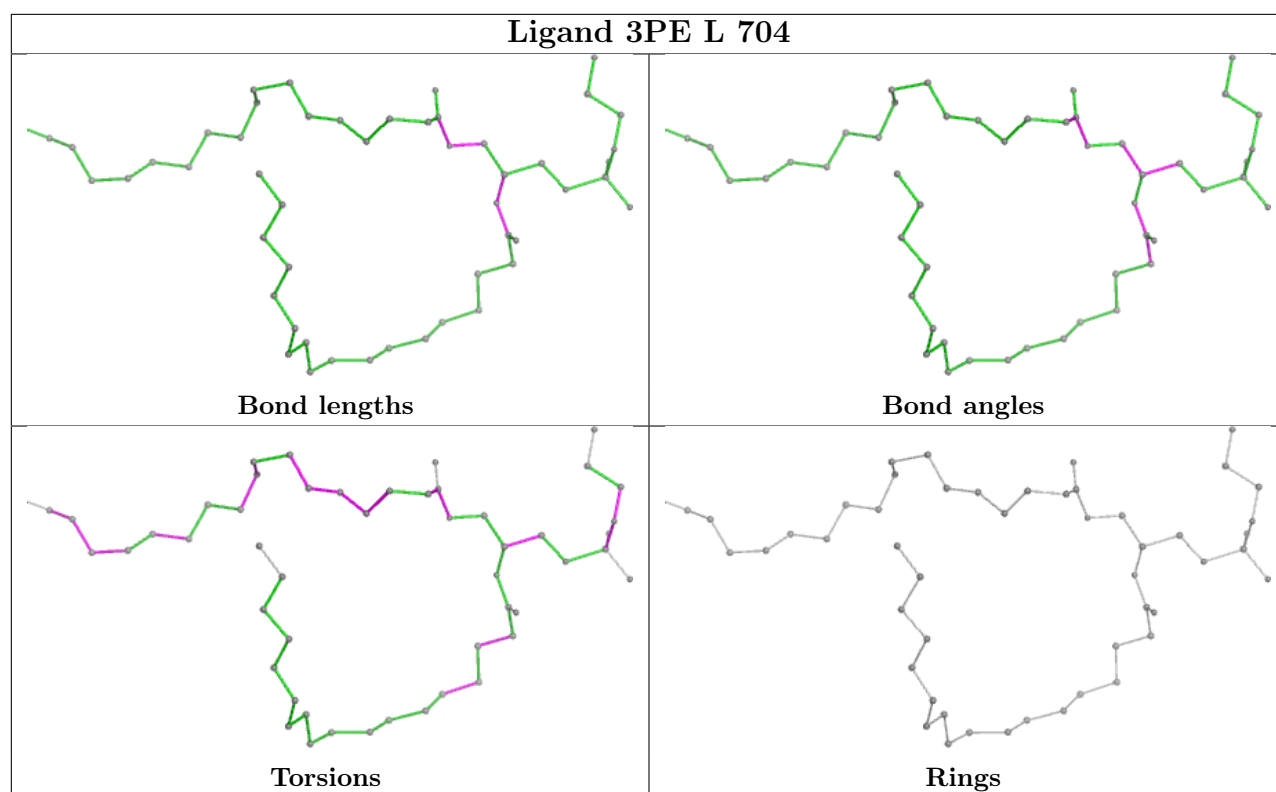


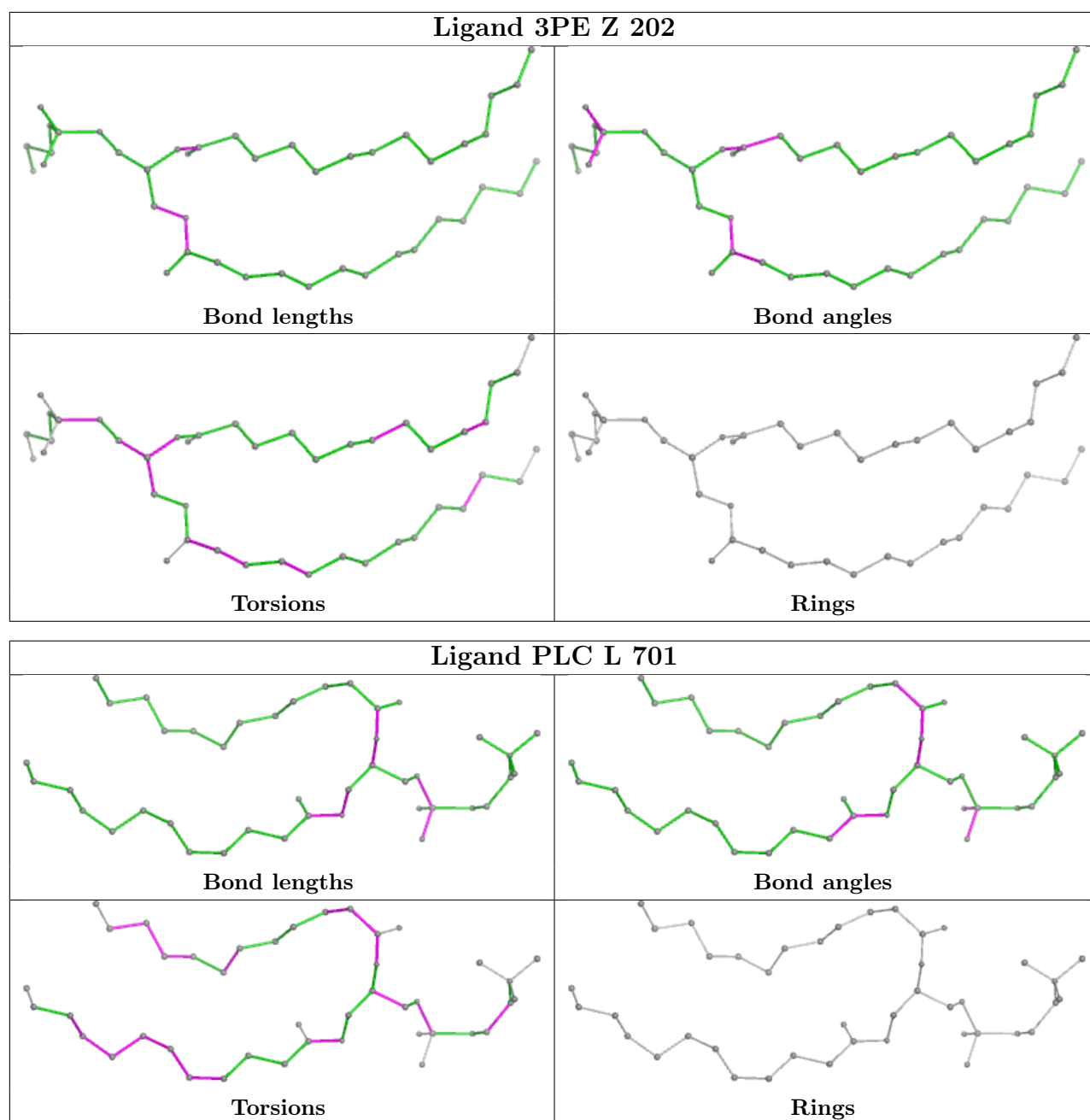
Ligand PLC H 6402

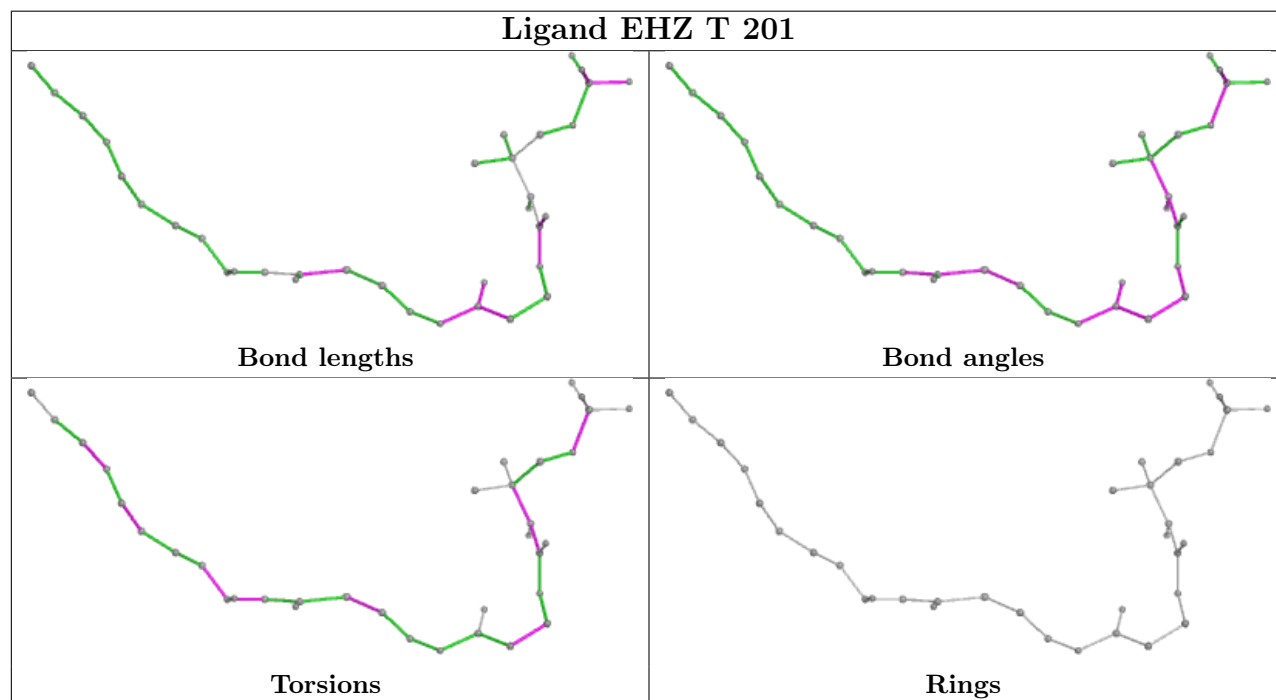
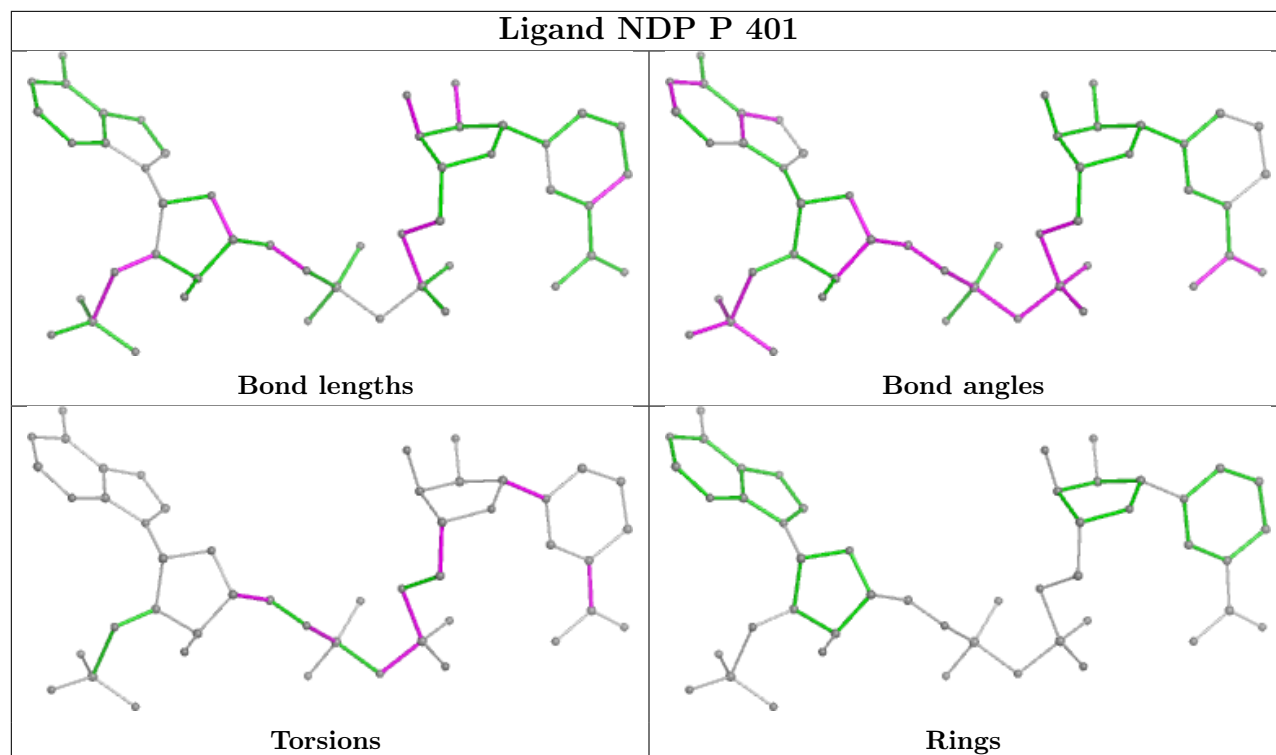


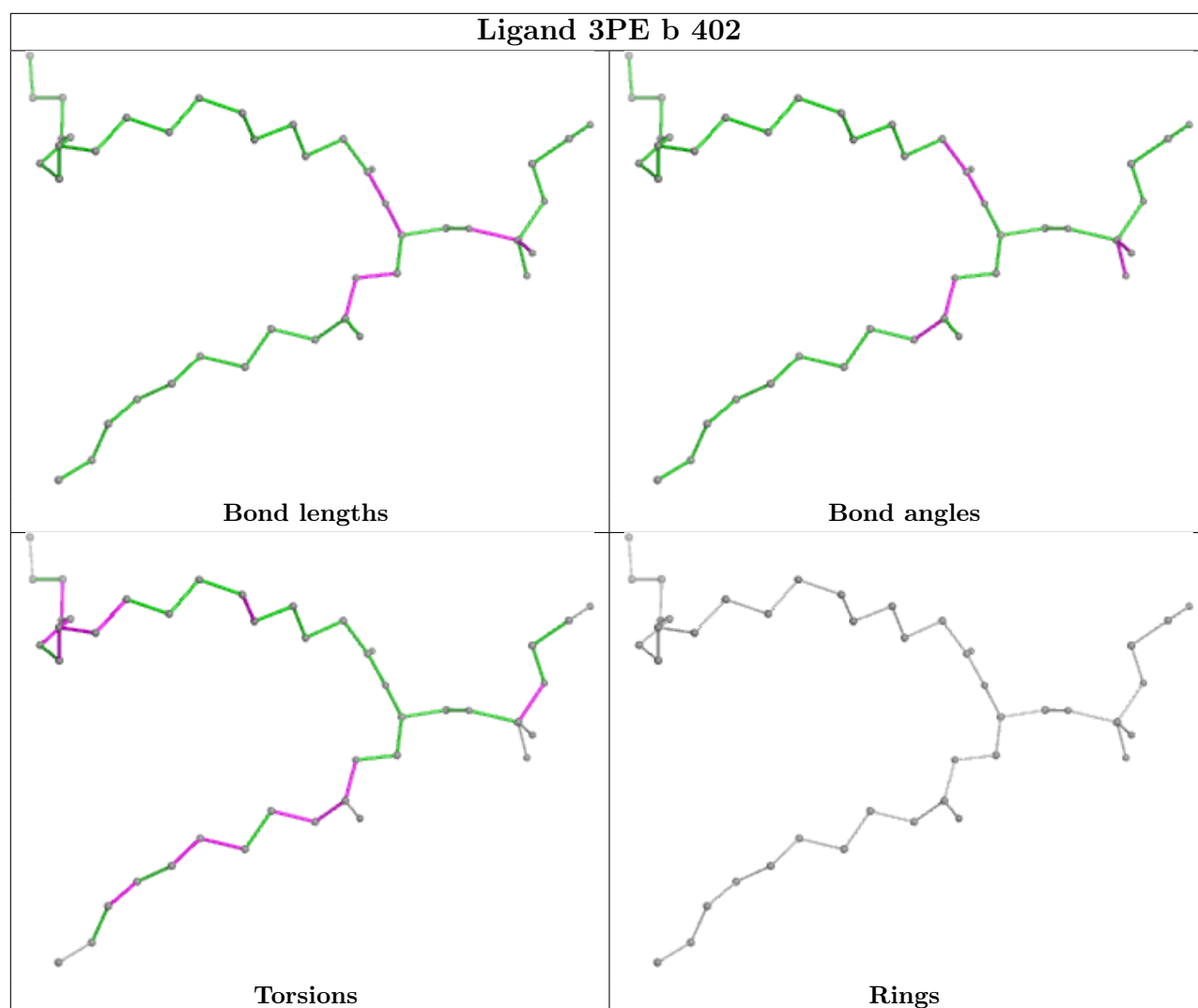
Ligand 3PE I 501

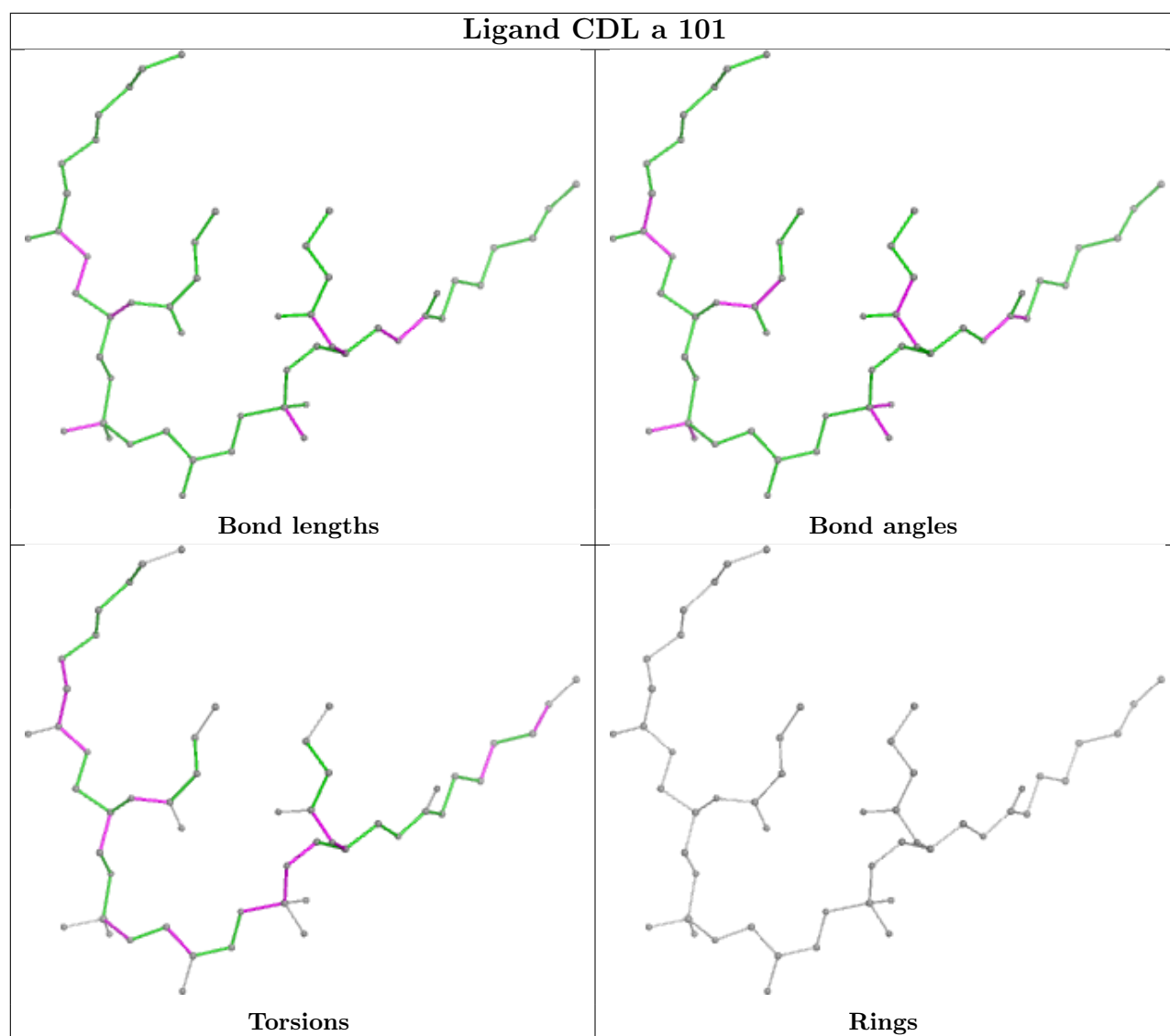


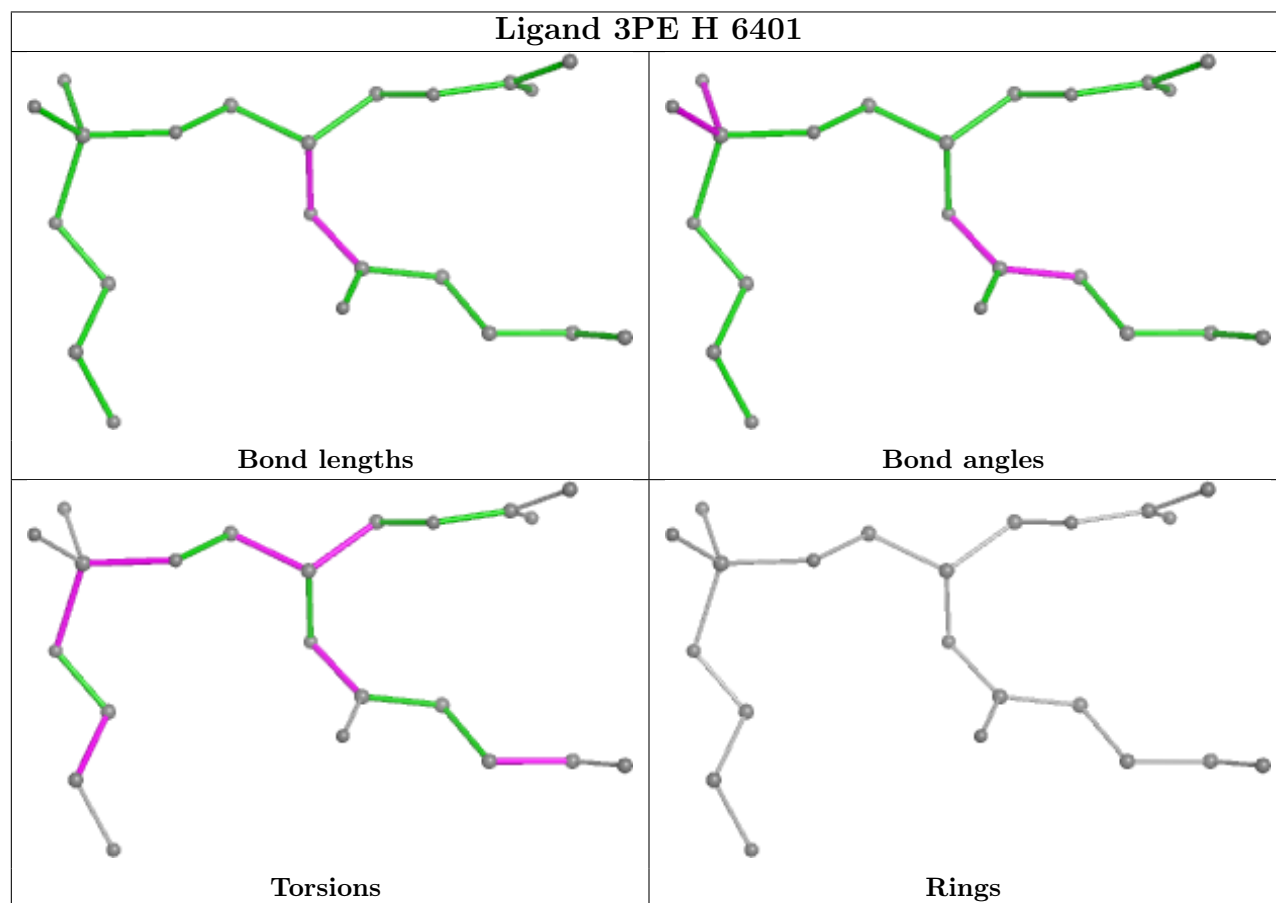
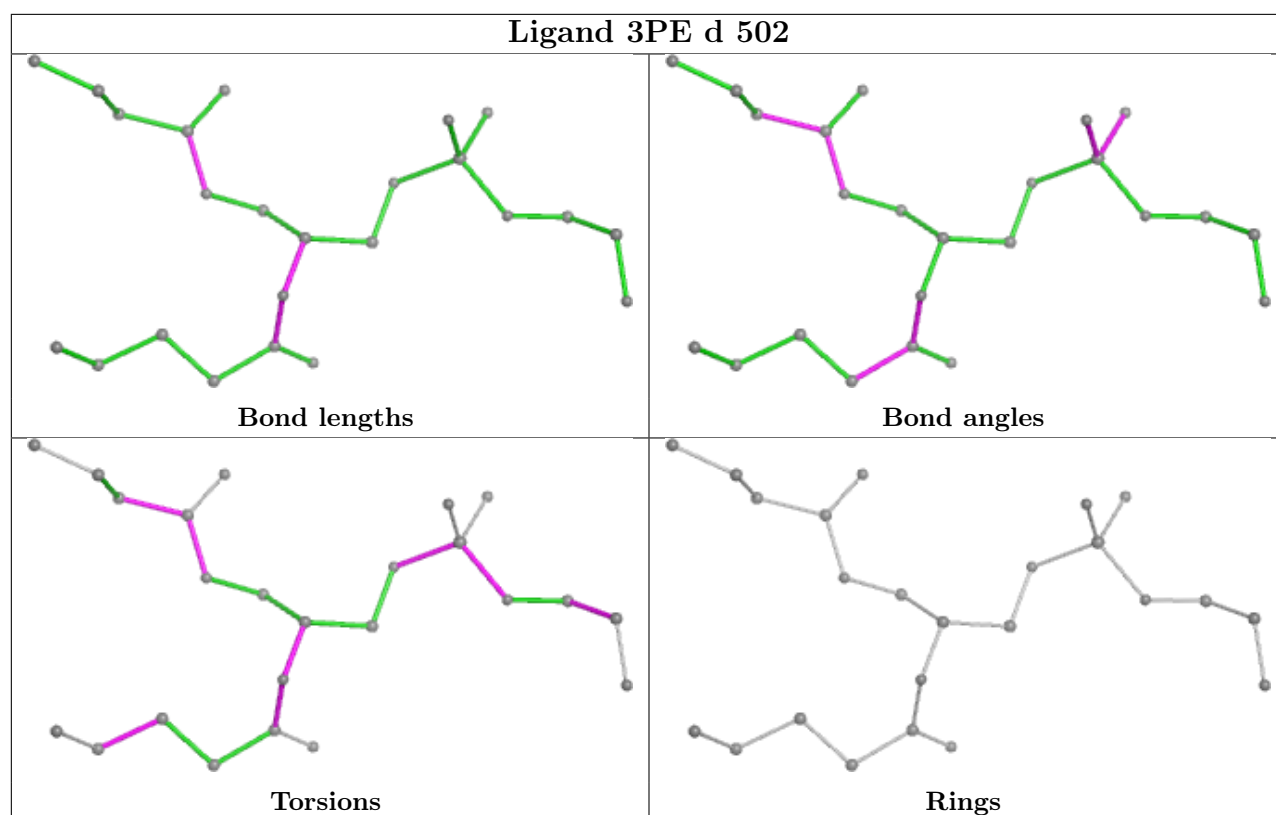


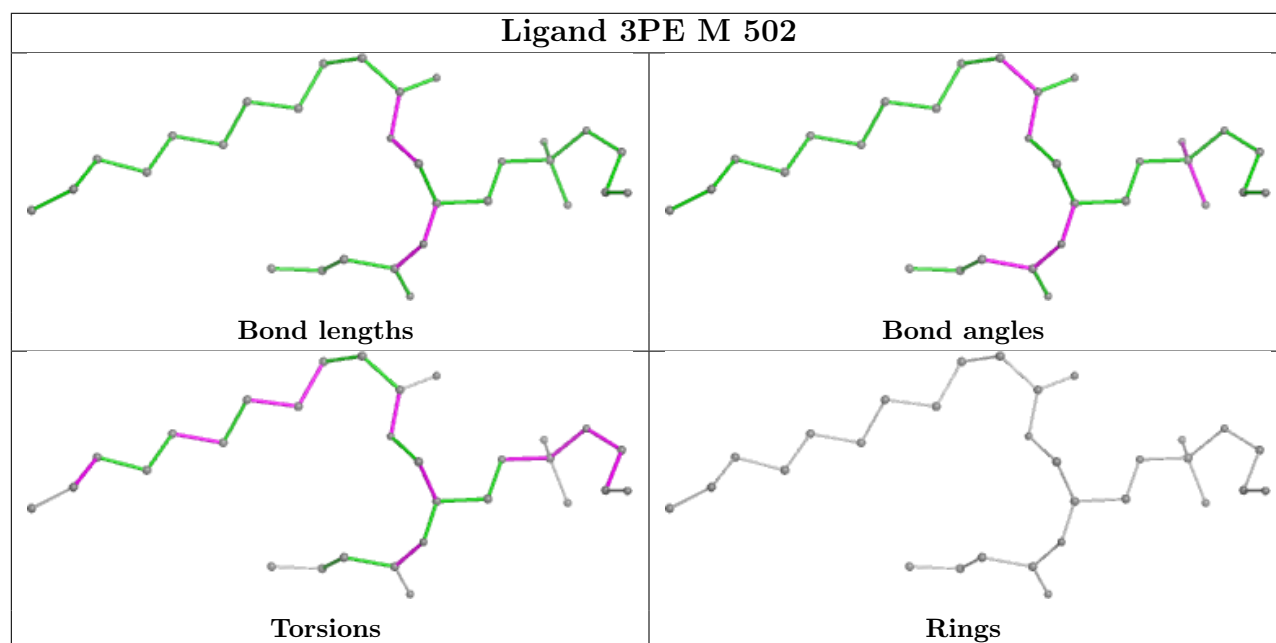
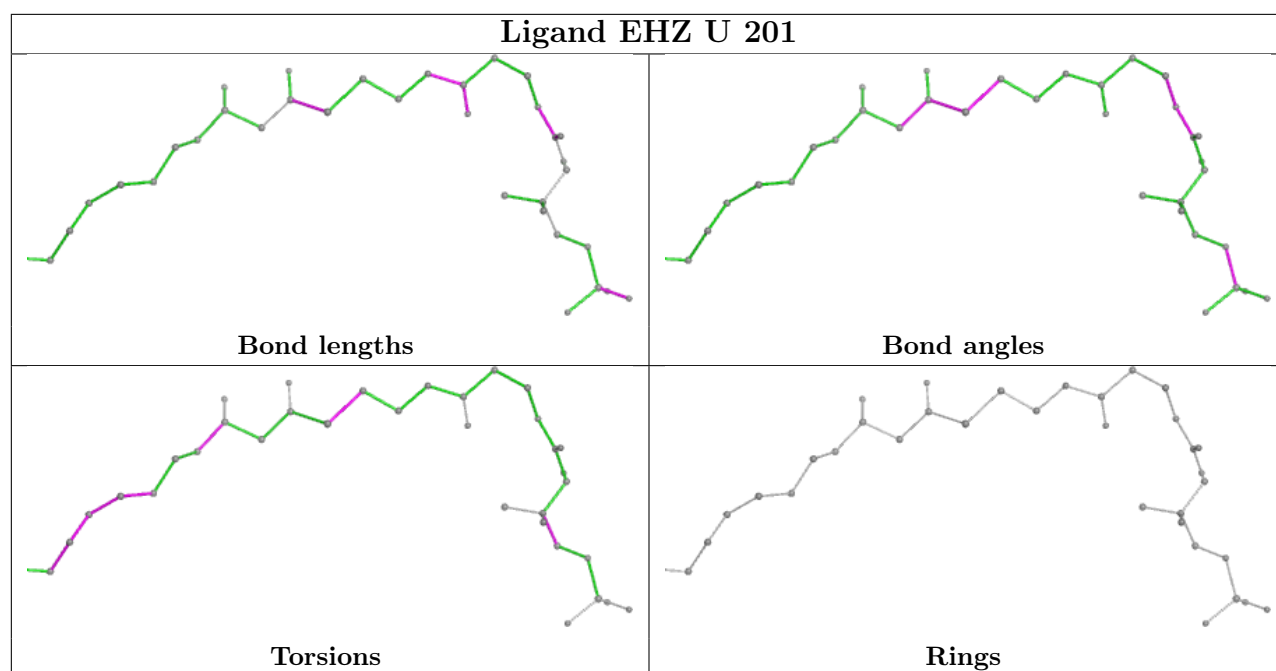


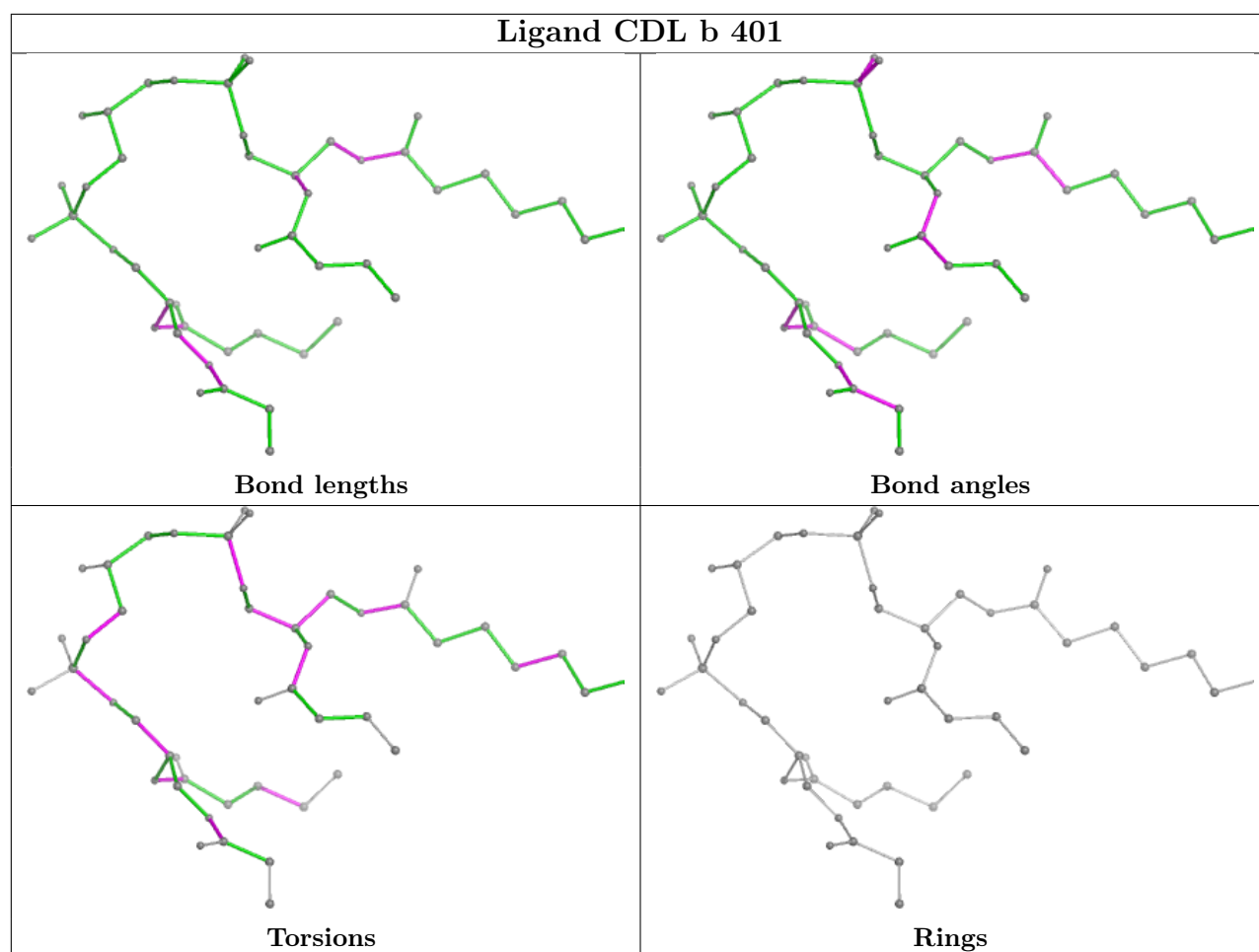


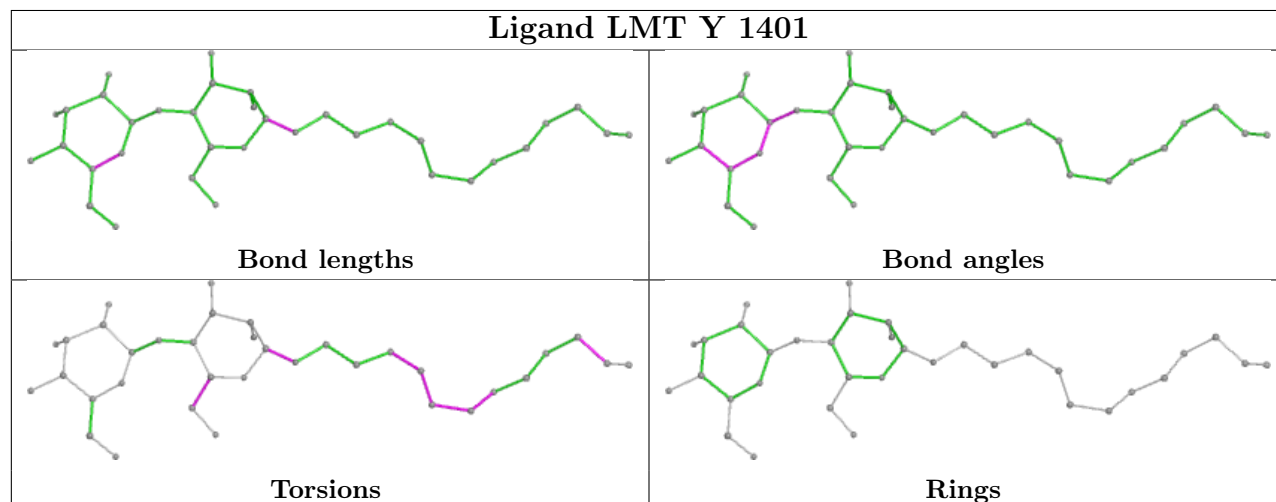
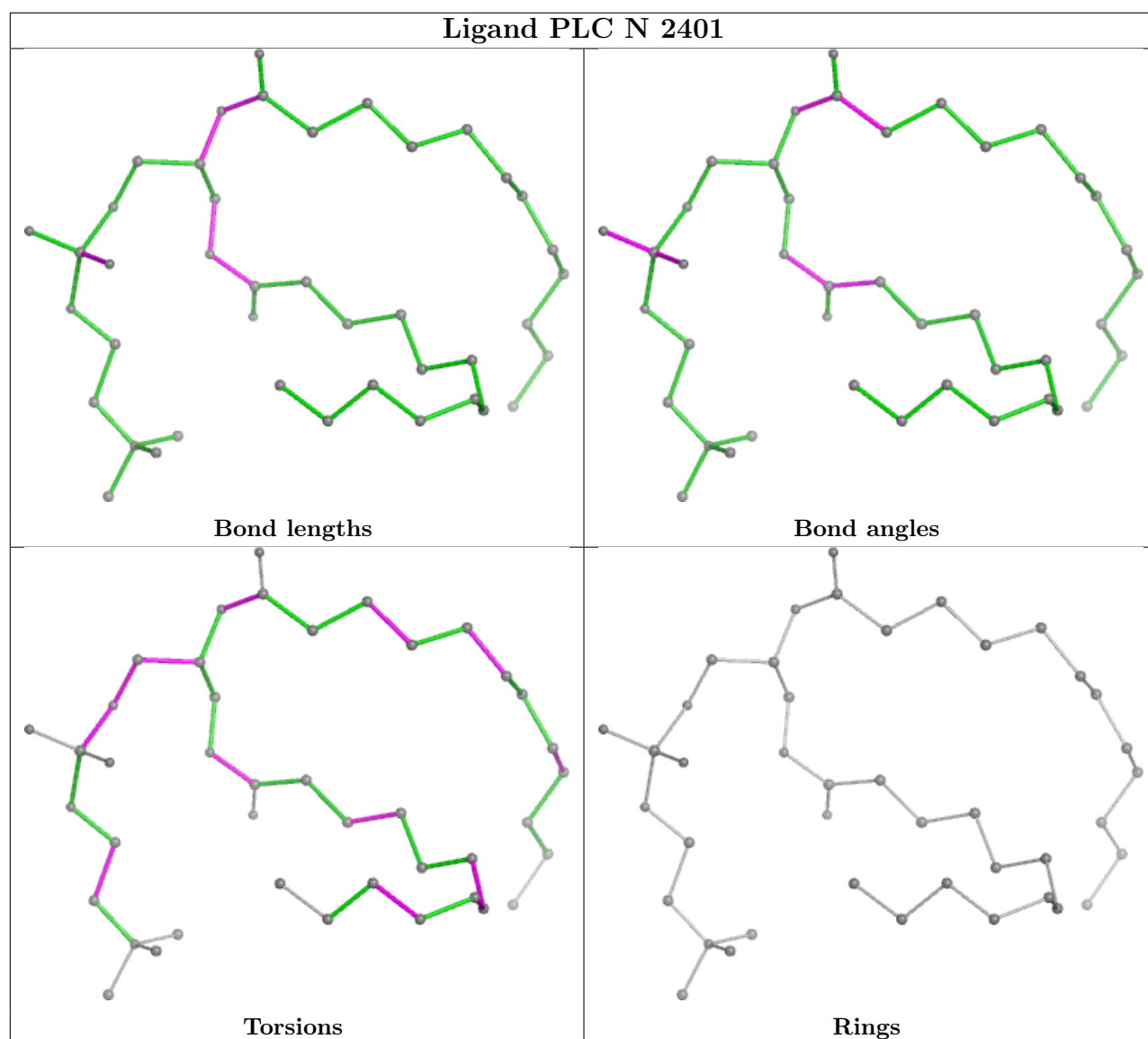


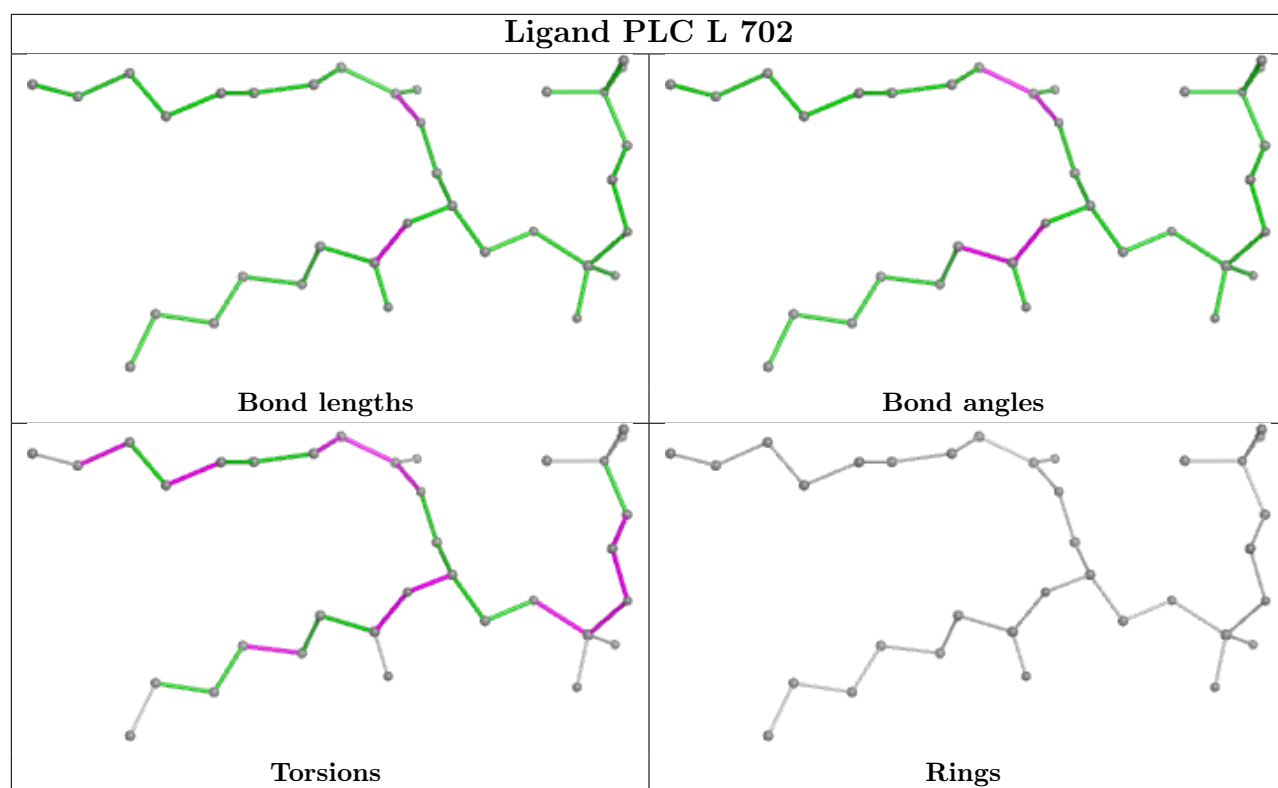


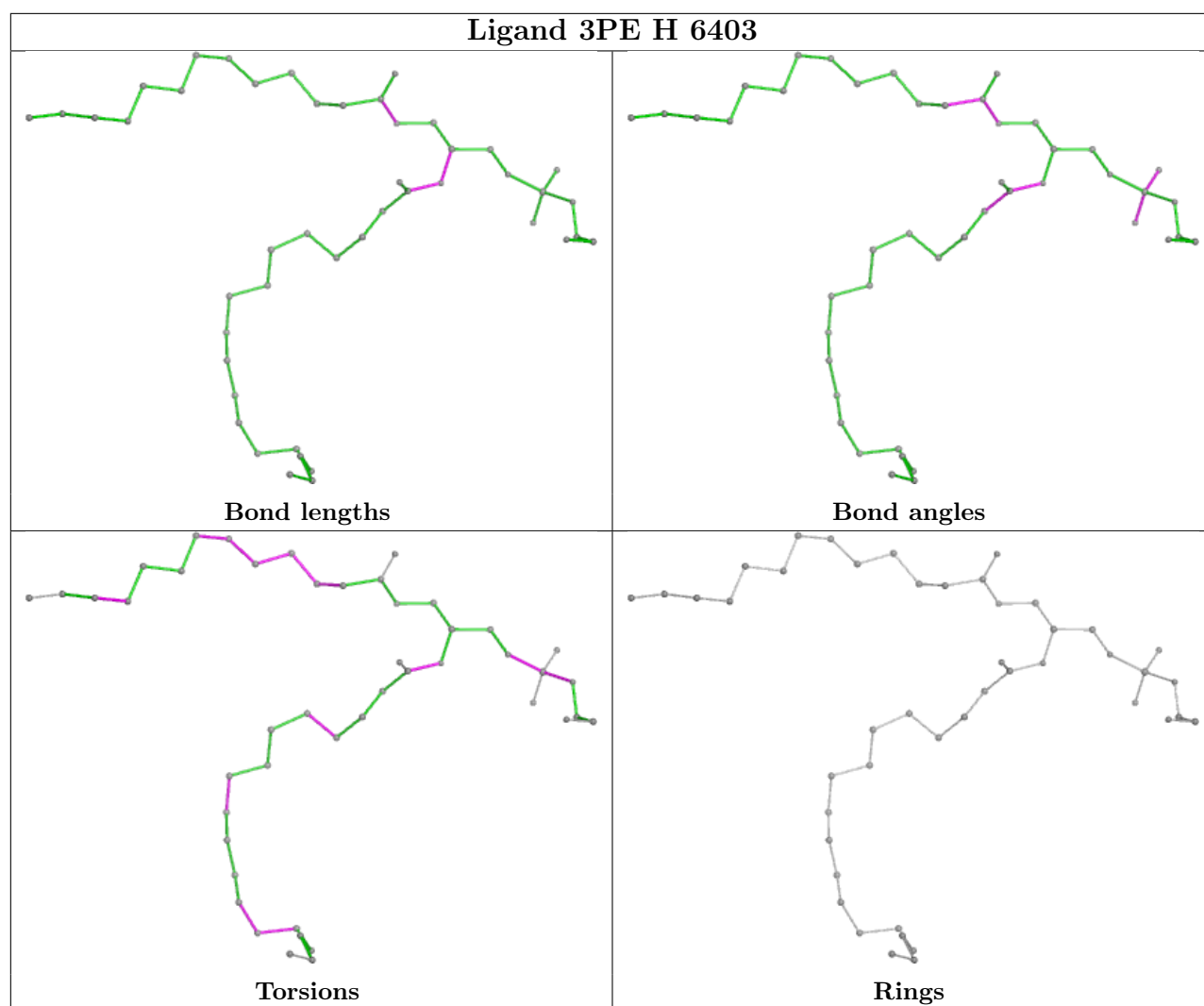


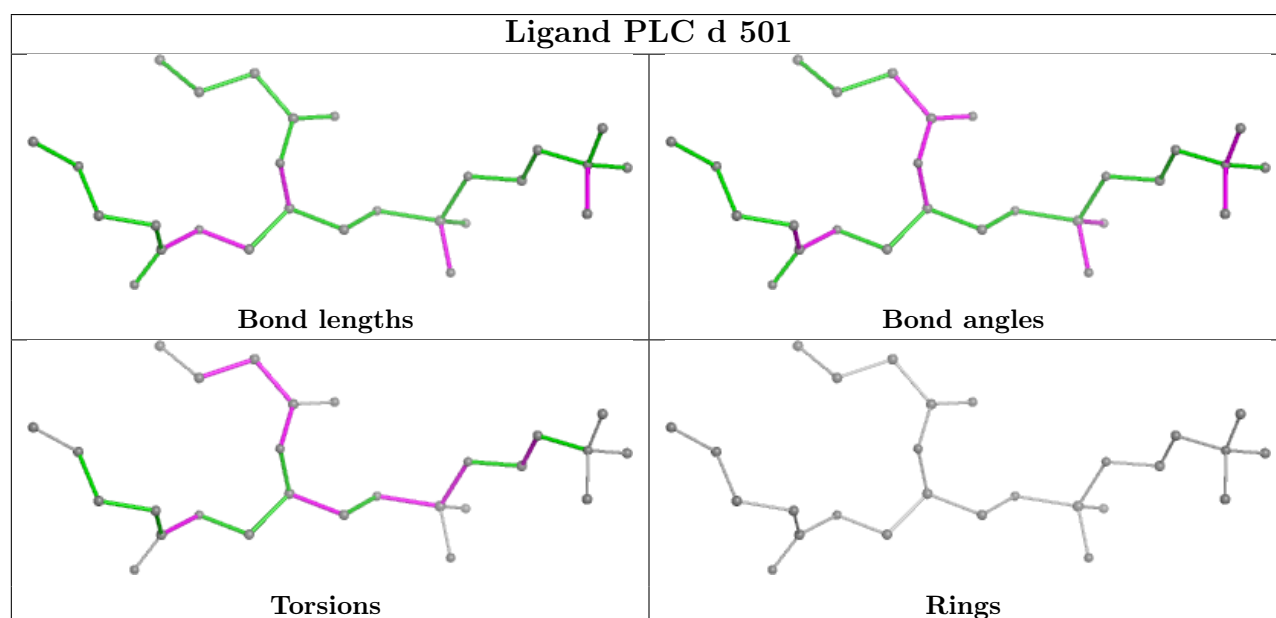
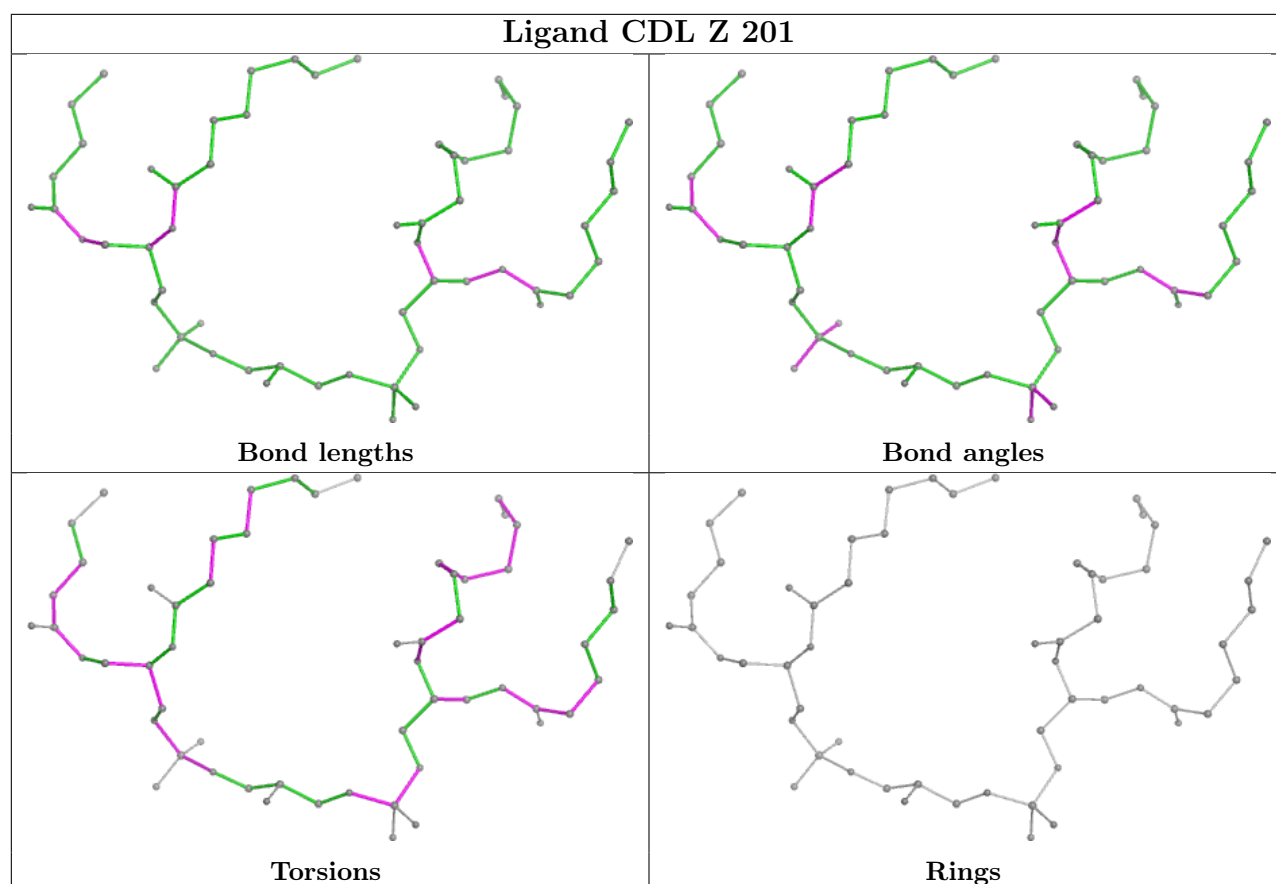


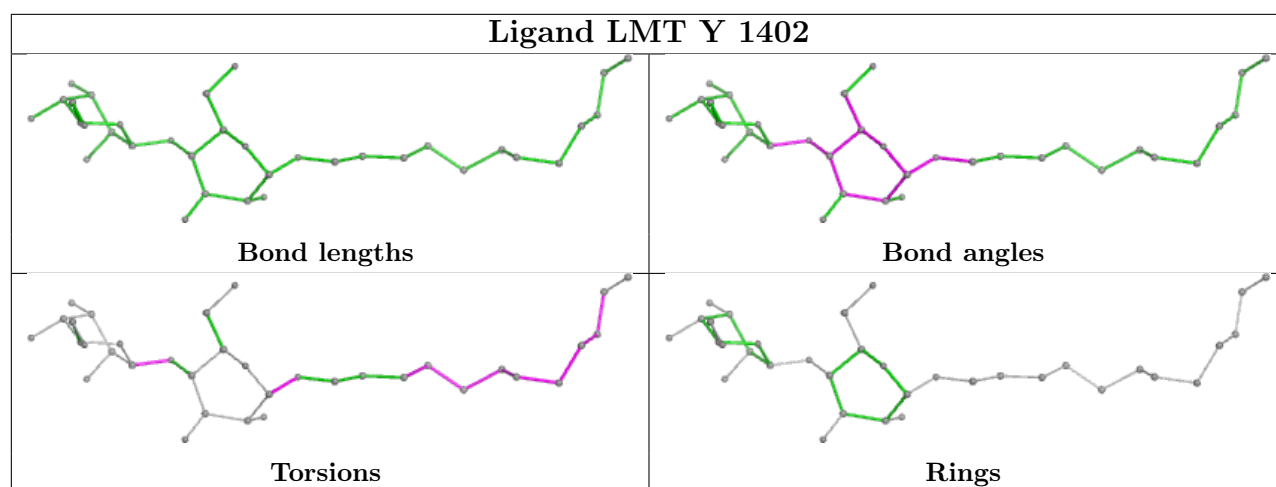












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

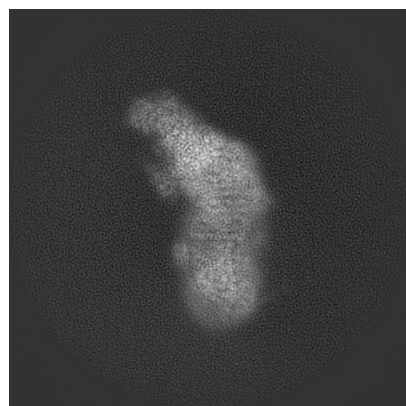
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11969. These allow visual inspection of the internal detail of the map and identification of artifacts.

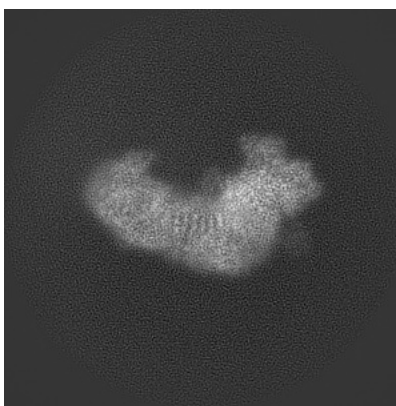
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

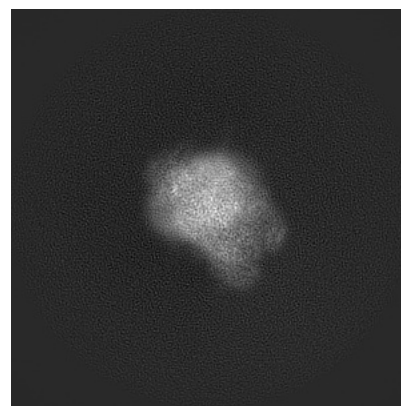
6.1.1 Primary map



X

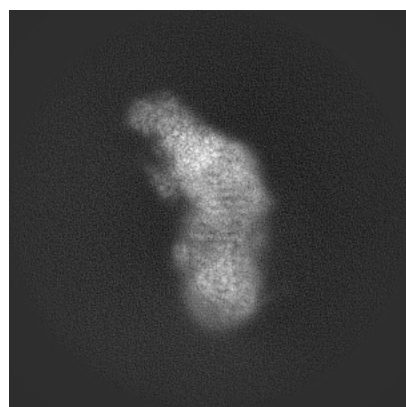


Y

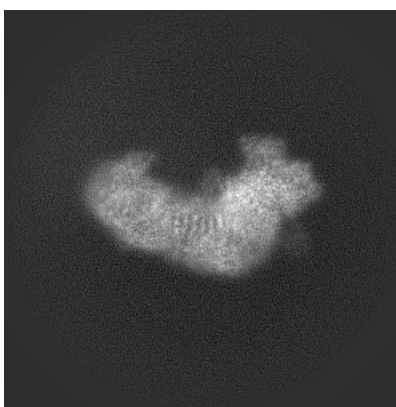


Z

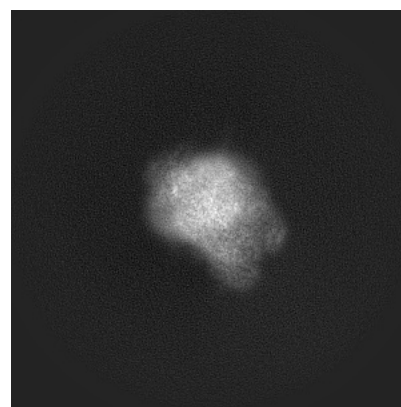
6.1.2 Raw map



X



Y

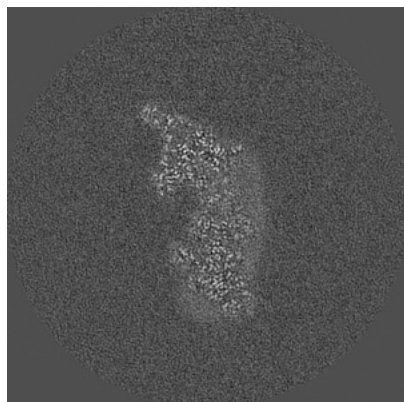


Z

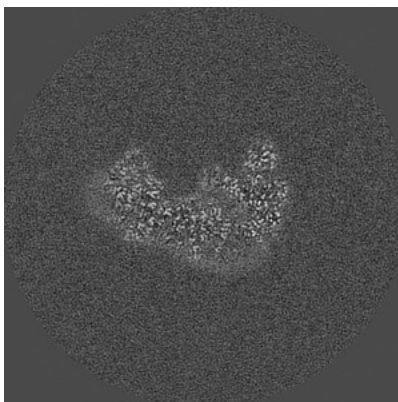
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

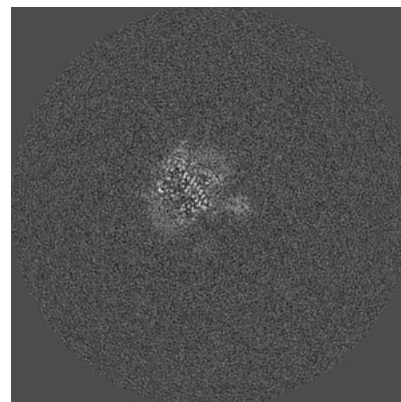
6.2.1 Primary map



X Index: 225

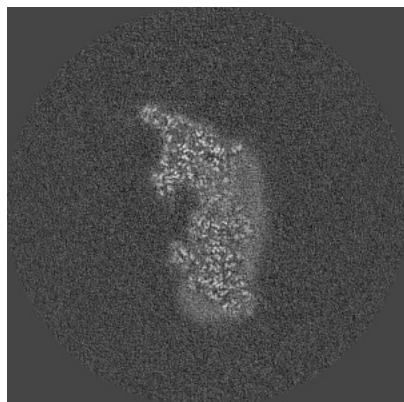


Y Index: 225

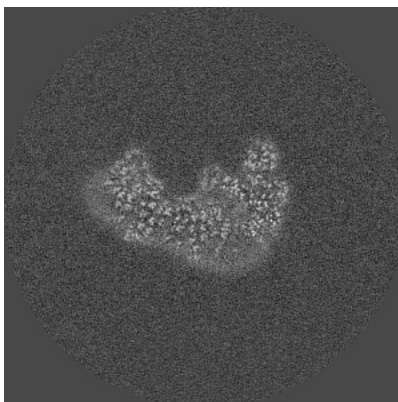


Z Index: 225

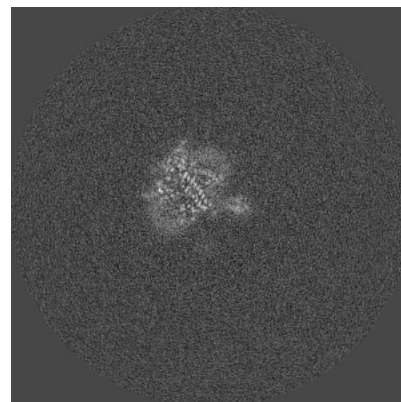
6.2.2 Raw map



X Index: 225



Y Index: 225

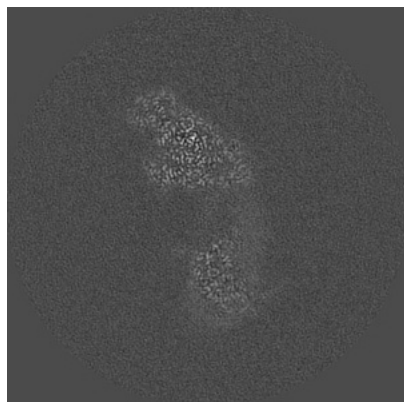


Z Index: 225

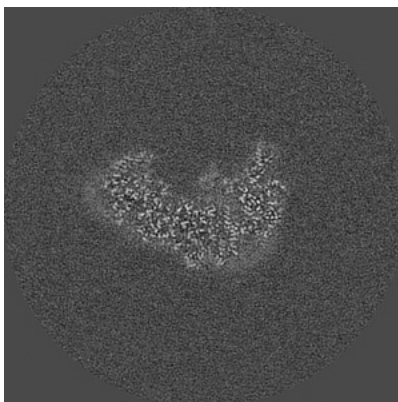
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

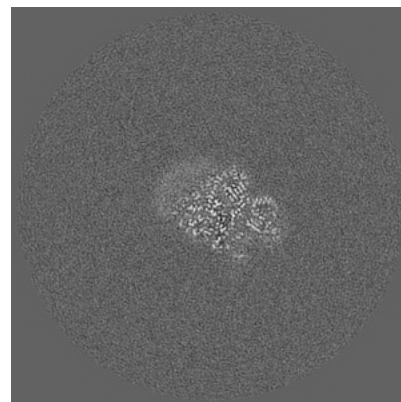
6.3.1 Primary map



X Index: 241

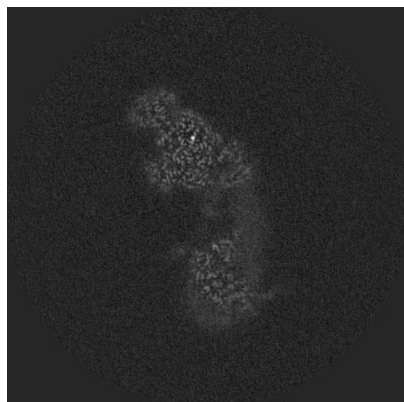


Y Index: 231

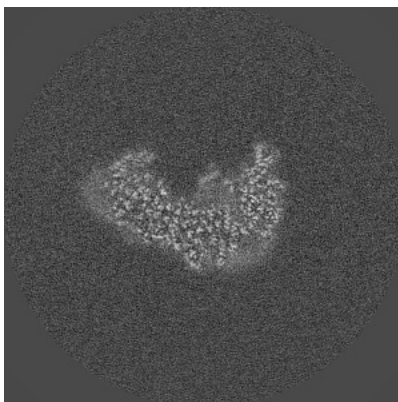


Z Index: 286

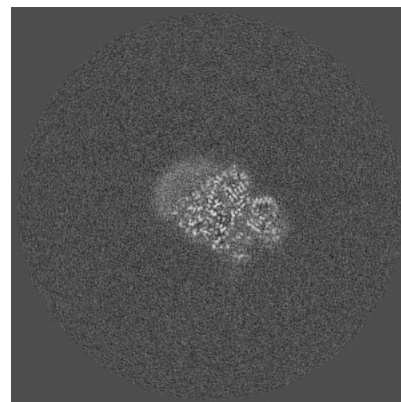
6.3.2 Raw map



X Index: 240



Y Index: 232

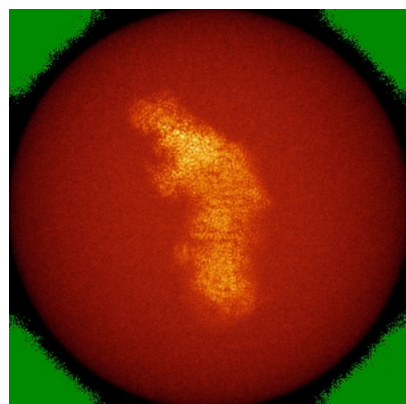


Z Index: 286

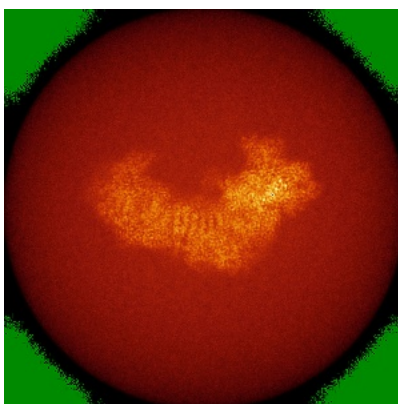
The images above show the largest variance slices of the map in three orthogonal directions.

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

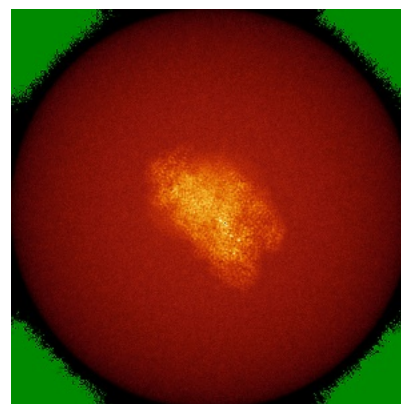
6.4.1 Primary map



X

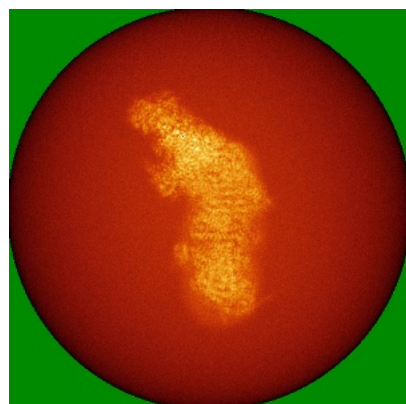


Y

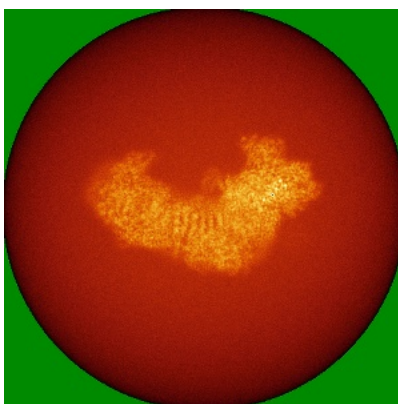


Z

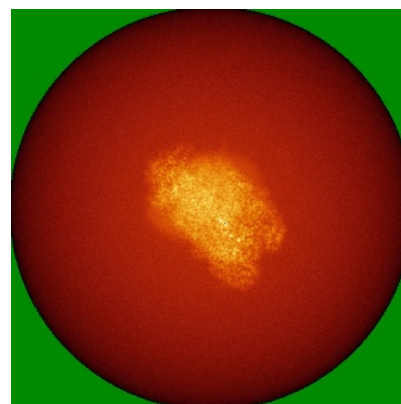
6.4.2 Raw map



X



Y



Z

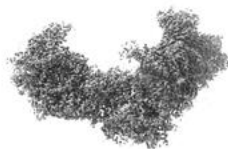
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

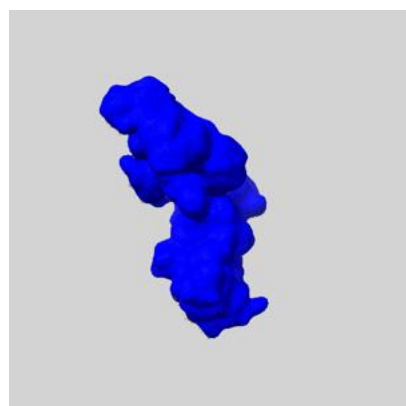
6.6 Mask visualisation [i](#)

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

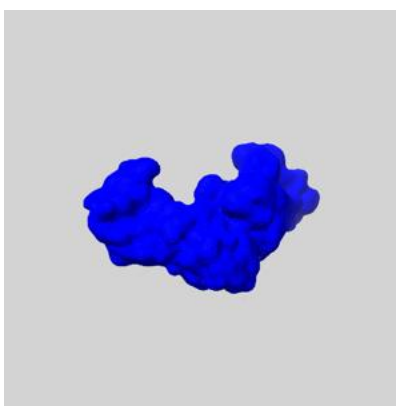
A mask typically either:

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

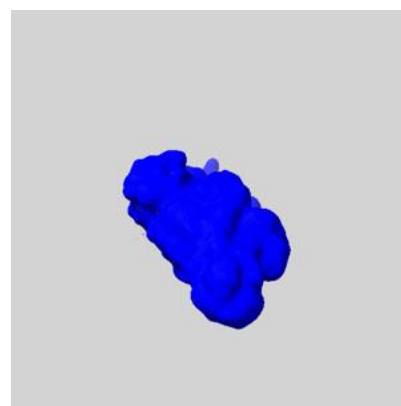
6.6.1 emd_11969_msk_1.map [i](#)



X



Y

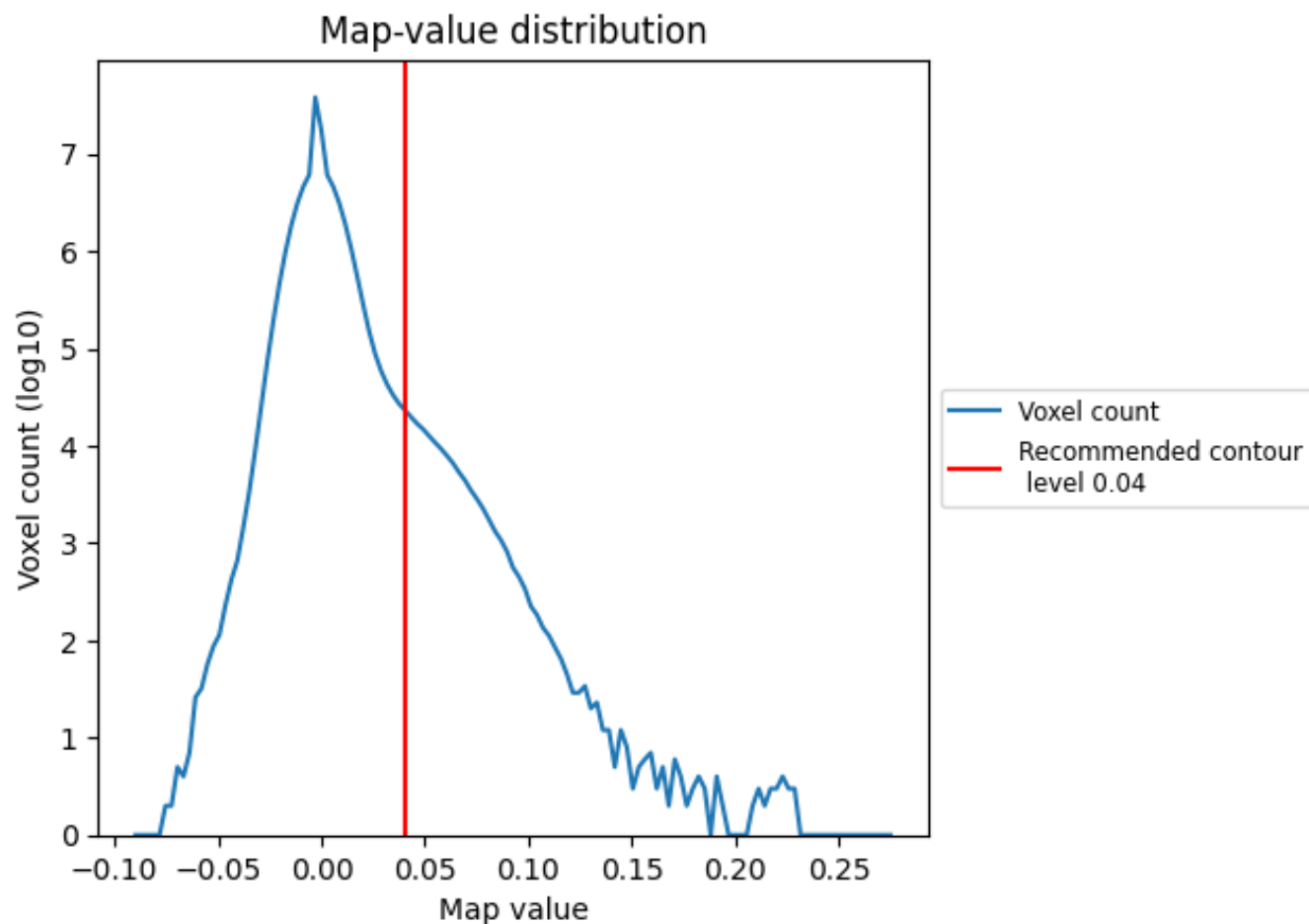


Z

7 Map analysis [i](#)

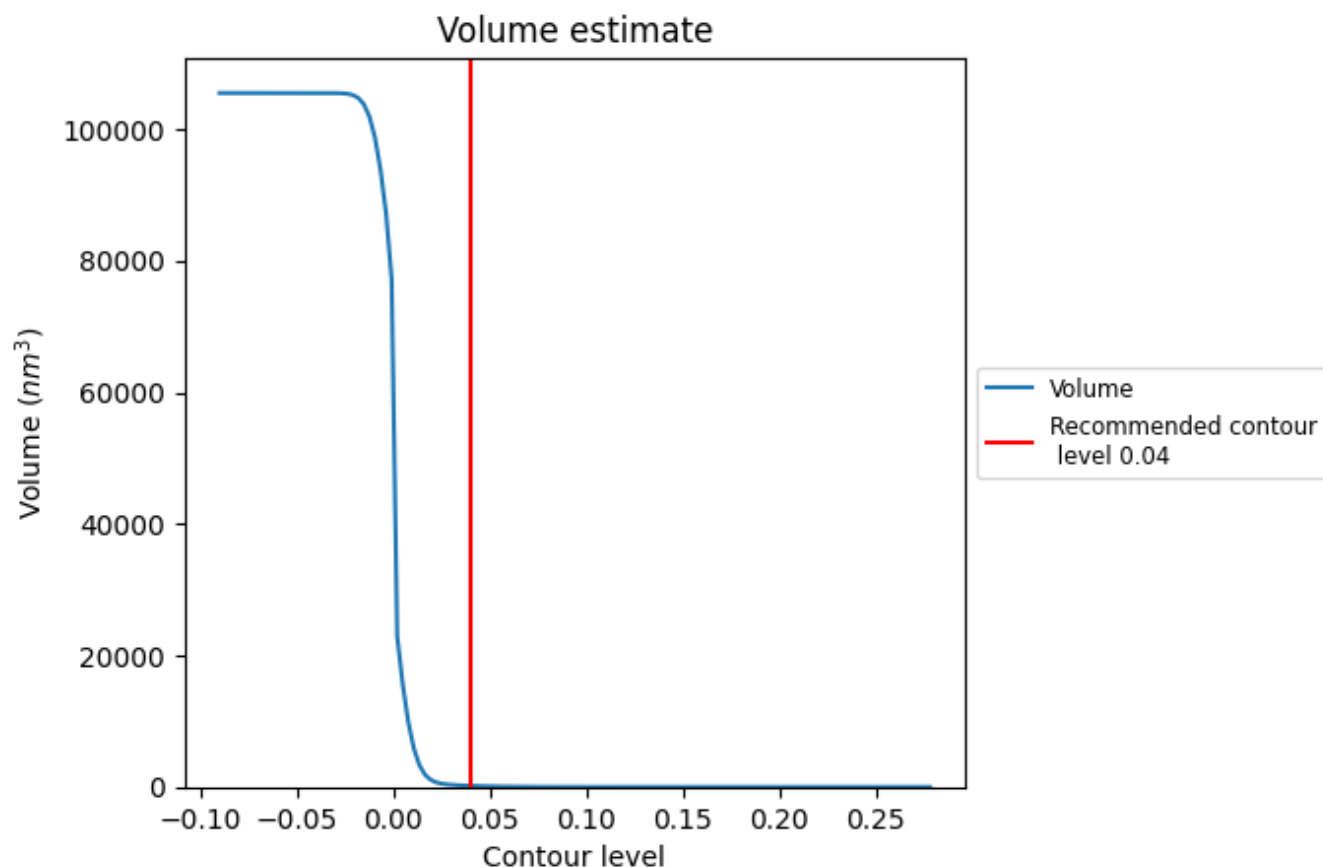
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

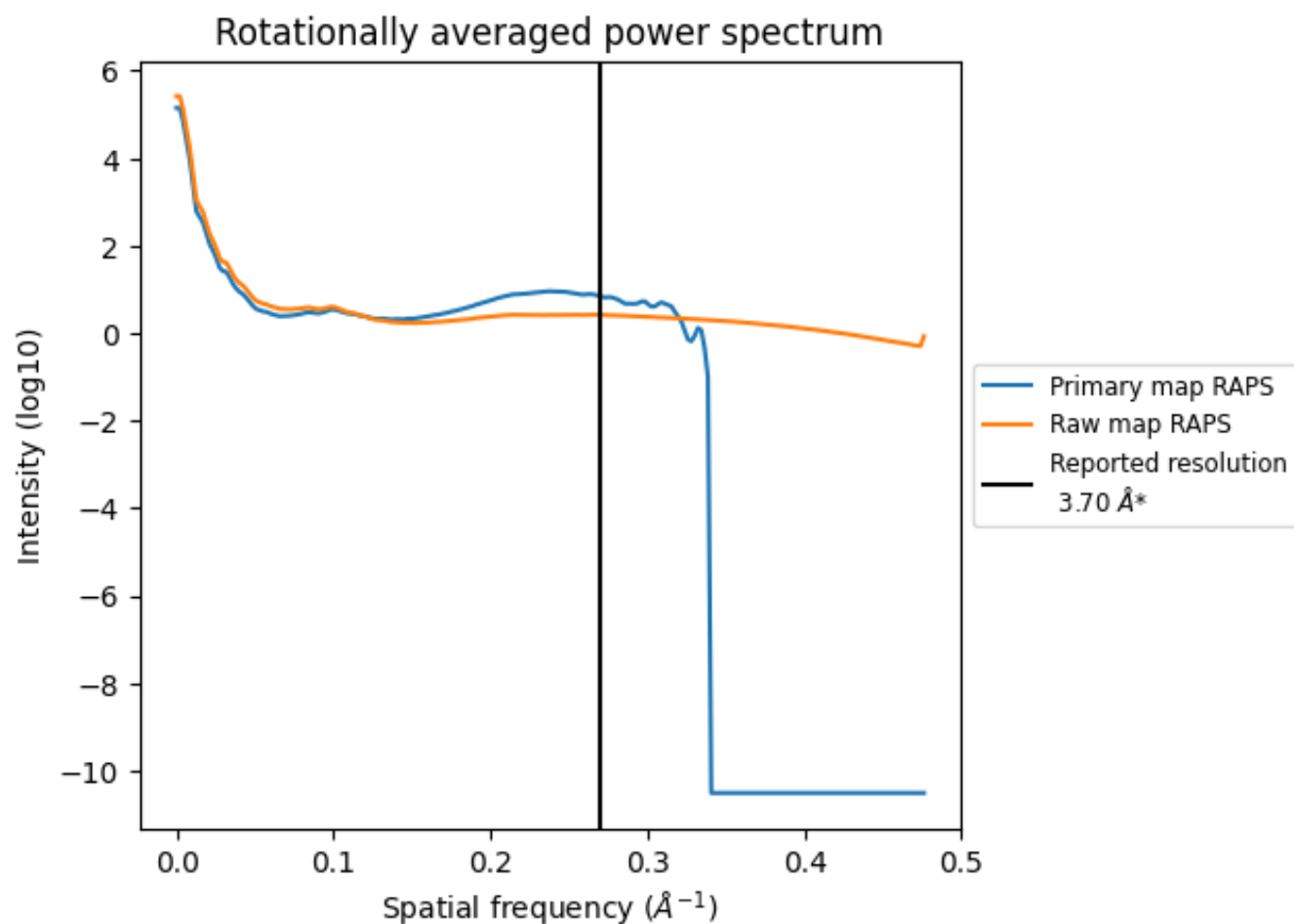
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 ⓘ

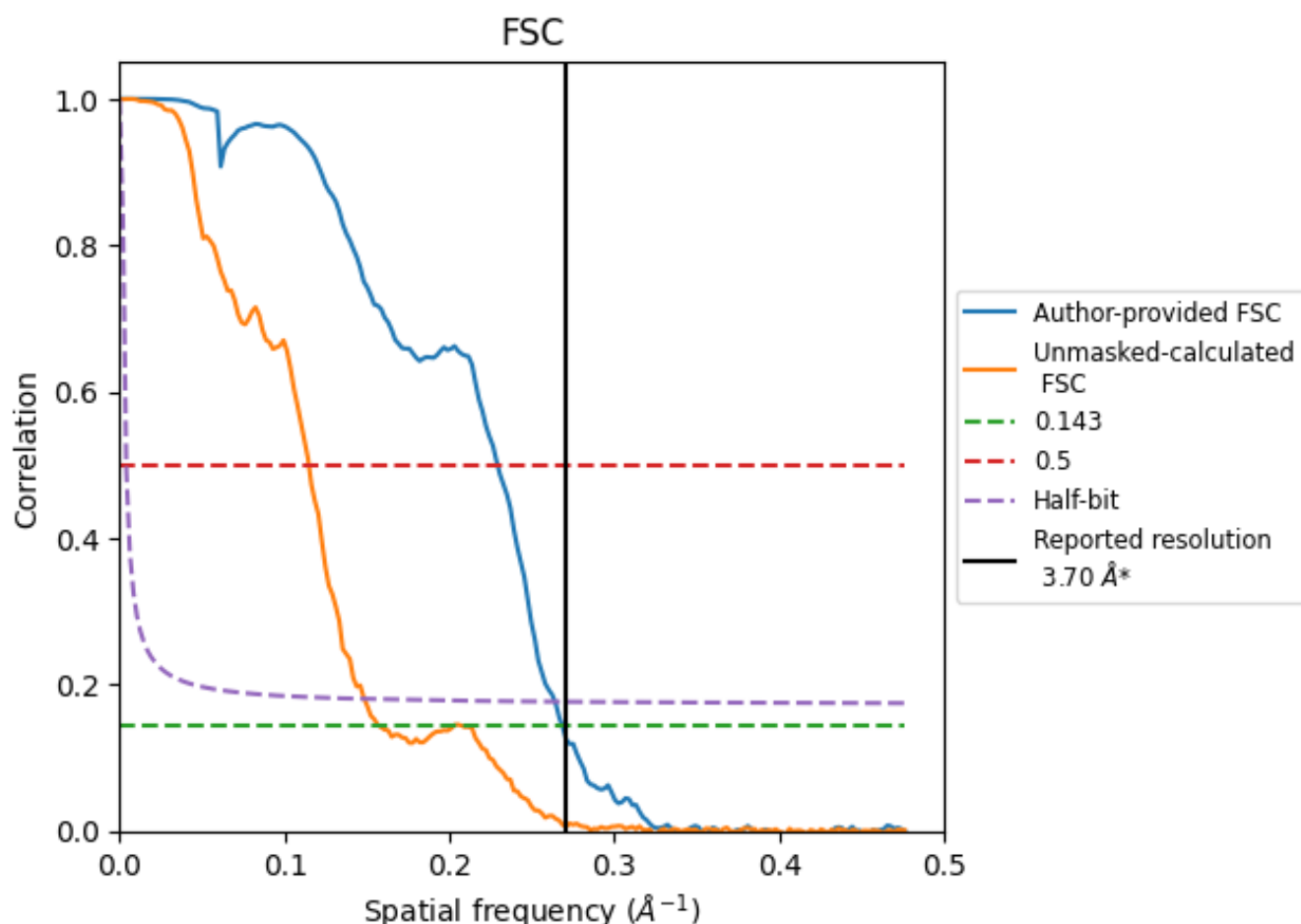


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

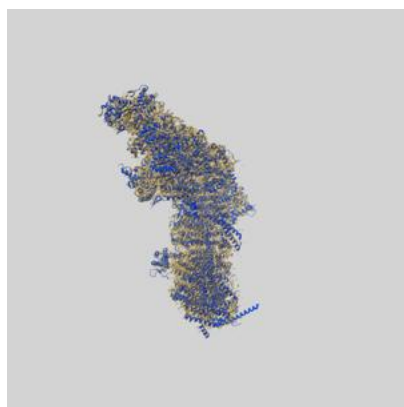
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.36	3.79
Unmasked-calculated*	6.35	8.71	6.73

*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 6.35 differs from the reported value 3.7 by more than 10 %

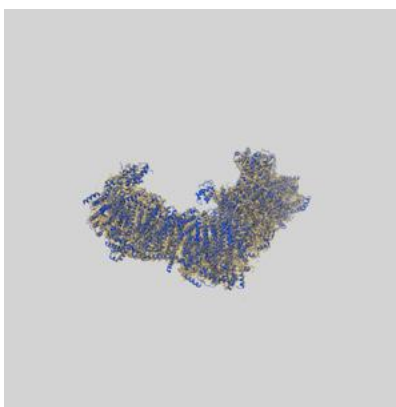
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11969 and PDB model 7B0N. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

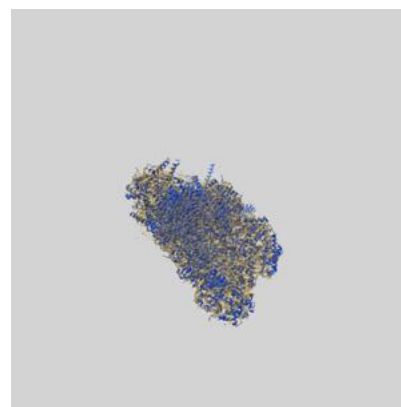
9.1 Map-model overlay [i](#)



X



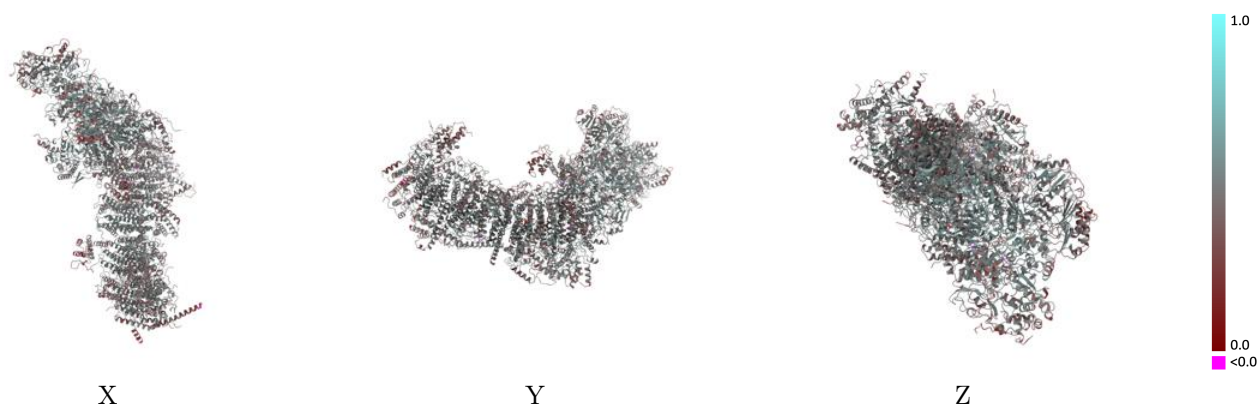
Y



Z

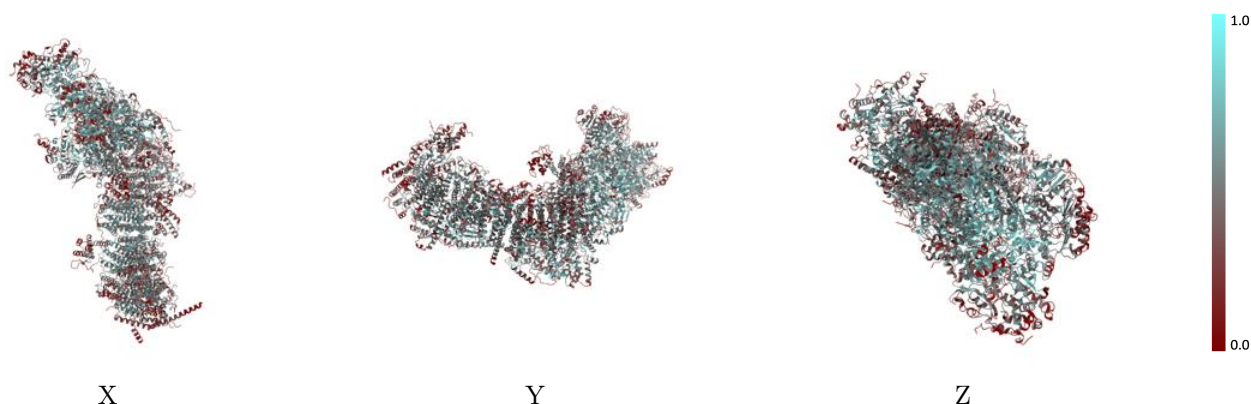
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



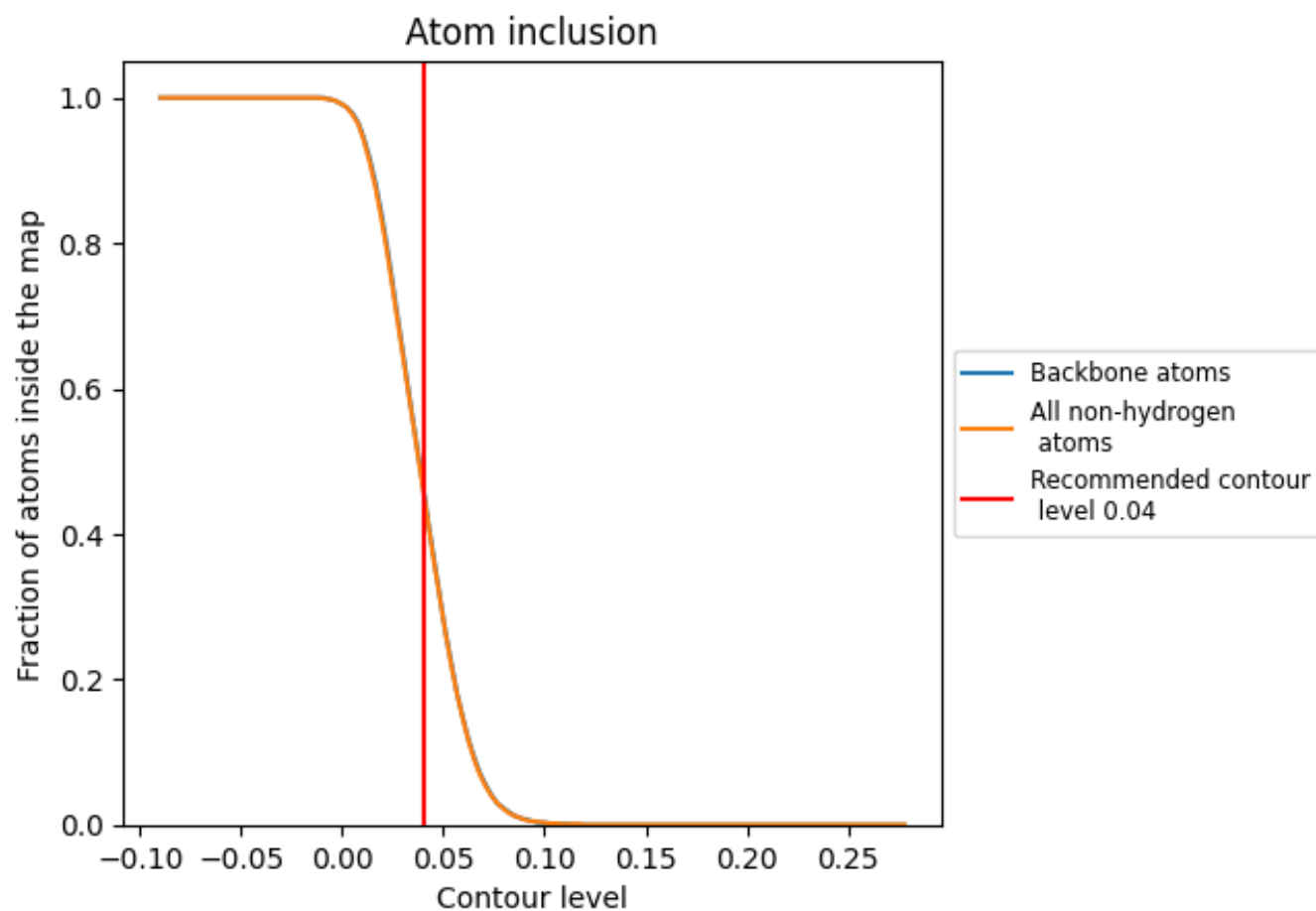
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 46% of all backbone atoms, 46% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4600	 0.4670
A	 0.3680	 0.4450
B	 0.5880	 0.5110
C	 0.5970	 0.5190
D	 0.5490	 0.4970
E	 0.4060	 0.4400
F	 0.4410	 0.4530
G	 0.5200	 0.4860
H	 0.4430	 0.4580
I	 0.6290	 0.5180
J	 0.3720	 0.4470
K	 0.4600	 0.4680
L	 0.4680	 0.4730
M	 0.5430	 0.4950
N	 0.5780	 0.5130
O	 0.4170	 0.4500
P	 0.4430	 0.4580
Q	 0.5520	 0.5010
R	 0.5480	 0.5010
S	 0.3110	 0.3990
T	 0.0880	 0.3100
U	 0.1940	 0.3840
V	 0.4310	 0.4720
W	 0.4530	 0.4540
X	 0.4270	 0.4400
Y	 0.3190	 0.4390
Z	 0.4450	 0.4680
a	 0.4270	 0.4650
b	 0.3600	 0.4570
c	 0.4790	 0.4840
d	 0.4180	 0.4600
e	 0.4570	 0.4530
f	 0.5470	 0.4960
g	 0.2850	 0.3810
h	 0.4510	 0.4660



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Chain	Atom inclusion	Q-score
i	 0.3770	 0.4280
j	 0.2400	 0.3850
k	 0.2810	 0.3820
l	 0.3390	 0.4380
m	 0.3860	 0.4420
n	 0.3780	 0.4180
o	 0.2760	 0.3770
p	 0.5310	 0.4730