



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 7PSA / pdb\_00007psa  
EMDB ID : EMD-13611  
Title : The acetogenin-bound complex I of Mus musculus resolved to 3.4 angstroms  
Authors : Grba, D.; Hirst, J.  
Deposited on : 2021-09-22  
Resolution : 3.40 Å(reported)  
Based on initial model : 6ZR2

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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 EMD 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

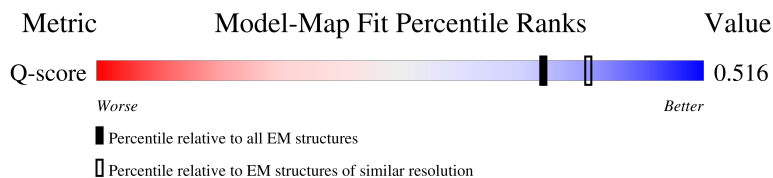
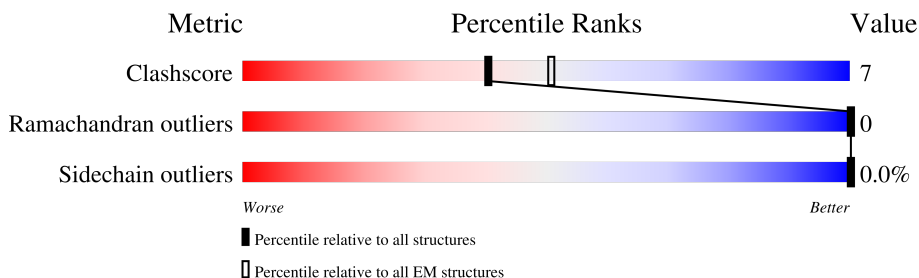
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	14717 ( 2.90 - 3.90 )

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

Mol	Chain	Length	Quality of chain
1	A	115	 80% 20%
2	B	224	 54% 16% 30%
3	C	263	 62% 17% 21%
4	D	463	 5% 75% 18% 7%

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

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
55	EHZ	T	201	X	-	-	-
55	EHZ	U	201	X	-	-	-

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 134755 atoms, of which 67673 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	115	Total	C	H	N	O	S	0	0
			1902	633	969	133	160	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	156	Total	C	H	N	O	S	0	0
			2502	796	1255	223	214	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	207	Total	C	H	N	O	S	0	0
			3402	1111	1681	296	311	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	430	Total	C	H	N	O	S	0	0
			6878	2215	3414	595	630	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	212	Total	C	H	N	O	S	0	0
			3287	1048	1639	277	312	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	428	Total	C	H	N	O	S	0	0
			6559	2080	3259	589	609	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	688	Total	C	H	N	O	S	0	0
			10618	3321	5322	919	1015	41		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	318	Total	C	H	N	O	S	0	0
			5166	1706	2626	384	428	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	178	Total	C	H	N	O	S	0	0
			2812	898	1381	245	276	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	171	Total	C	H	N	O	S	0	0
			2615	874	1315	185	226	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	98	Total	C	H	N	O	S	0	0
			1505	477	768	112	137	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	606	Total	C	H	N	O	S	0	0
			9785	3182	4985	746	827	45		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	459	Total	C	H	N	O	S	0	0
			7485	2408	3853	567	617	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	344	Total	C	H	N	O	S	0	0
			5591	1791	2895	416	452	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	320	Total	C	H	N	O	S	0	0
			5171	1674	2564	431	492	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	342	Total	C	H	N	O	S	0	0
			5514	1777	2766	483	481	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	125	Total	C	H	N	O	S	0	0
			2031	642	1016	179	190	4		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	94	Total	C	H	N	O	S	0	0
			1453	458	715	135	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	83	Total	C	H	N	O	S	0	0
			1353	419	686	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	76	Total	C	H	N	O	S	0	0
			1213	392	602	90	124	5		
20	U	86	Total	C	H	N	O	S	0	0
			1378	446	686	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	114	Total	C	H	N	O	S	0	0
			1895	604	968	154	166	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	W	114	Total	C	H	N	O	S	0	0
			1961	619	991	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	171	Total	C	H	N	O	S	0	0
			2773	889	1377	250	247	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	140	Total	C	H	N	O	S	0	0
			2062	662	1025	175	192	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	MET	-	variant	UNP Q9D8B4
Y	-1	ALA	-	variant	UNP Q9D8B4
Y	39	SER	ARG	conflict	UNP Q9D8B4

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 13.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	141	Total	C	H	N	O	S	0	0
			2333	750	1166	207	202	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	68	Total	C	H	N	O	S	0	0
			1124	360	568	99	93	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	80	Total	C	H	N	O	S	0	0
			1256	414	628	99	111	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
28	c	48	Total	C	H	N	O	S	0	0
			797	261	399	69	67	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	d	120	Total	C	H	N	O	S	0	0
			1997	651	1001	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e	105	Total	C	H	N	O	S	0	0
			1746	555	869	162	152	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	f	53	Total	C	H	N	O	S	0	0
			908	295	452	82	77	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	101	Total	C	H	N	O	S	0	0
			1633	549	783	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	h	138	Total	C	H	N	O	S	0	0
			2325	762	1163	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	i	94	Total	C	H	N	O	S	0	0
			1578	513	794	134	134	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	j	62	Total	C	H	N	O	S	0	0
			1033	355	496	88	93	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	k	75	Total	C	H	N	O	S	0	0
			1213	404	604	103	100	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	l	154	Total	C	H	N	O	S	0	0
			2481	834	1187	215	234	11		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	126	Total	C	H	N	O	0	0
			2111	676	1061	189	185		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	n	177	Total	C	H	N	O	S	0	0
			2998	981	1464	275	267	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	o	111	Total	C	H	N	O	S	0	0
			1894	605	937	176	168	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
41	p	169	Total	C	H	N	O	S	0	0
			2832	901	1399	257	267	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	q	144	Total	C	H	N	O	S	0	0
			2361	773	1158	213	212	5		

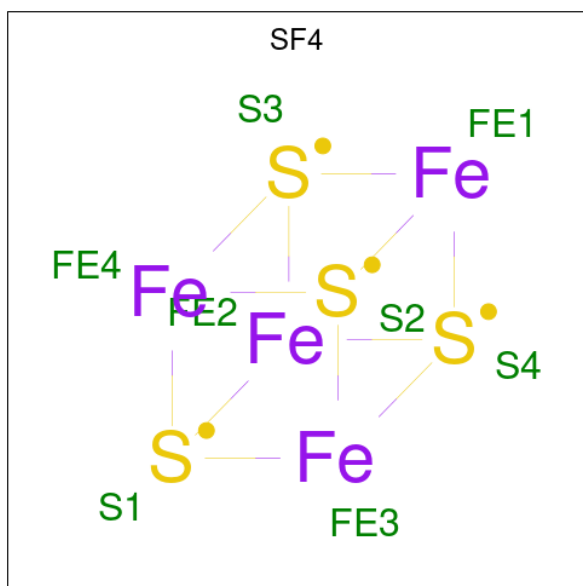
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	r	100	Total	C	H	N	O	S	0	0
			1638	507	836	149	143	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

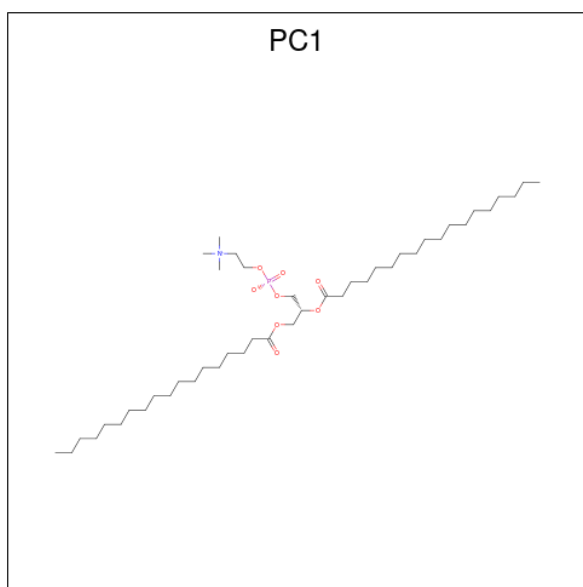
Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	41	Total	C	H	N	O	0	0
			668	215	324	61	68		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



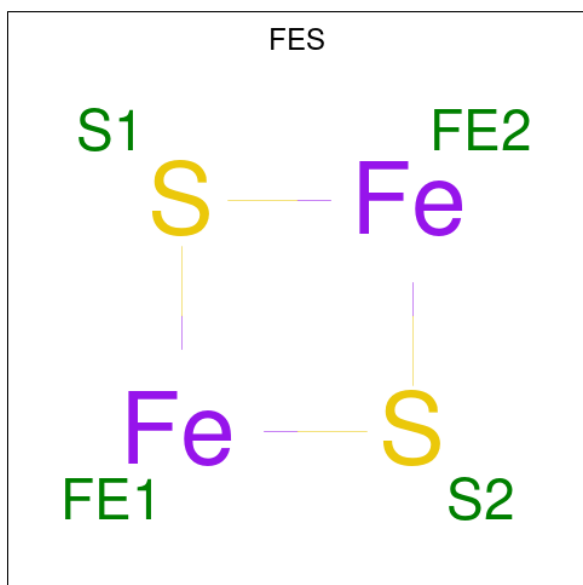
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$ ).



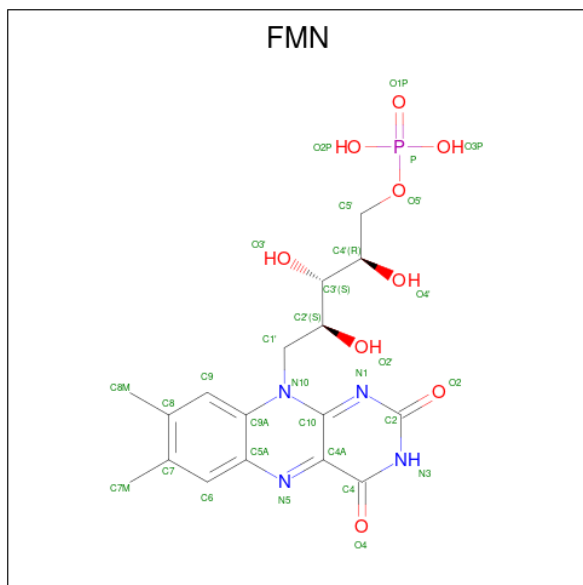
Mol	Chain	Residues	Atoms						AltConf
46	B	1	Total	C	H	N	O	P	0
			83	25	48	1	8	1	
46	B	1	Total	C	H	N	O	P	0
			108	33	65	1	8	1	
46	J	1	Total	C	H	N	O	P	0
			104	32	62	1	8	1	
46	Z	1	Total	C	H	N	O	P	0
			113	35	68	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



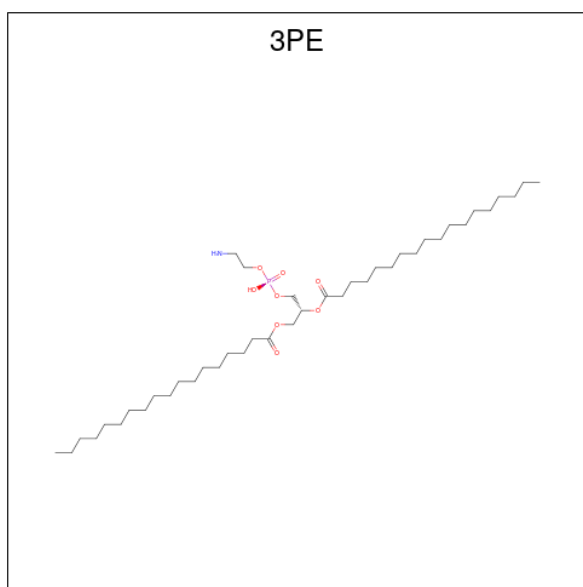
Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



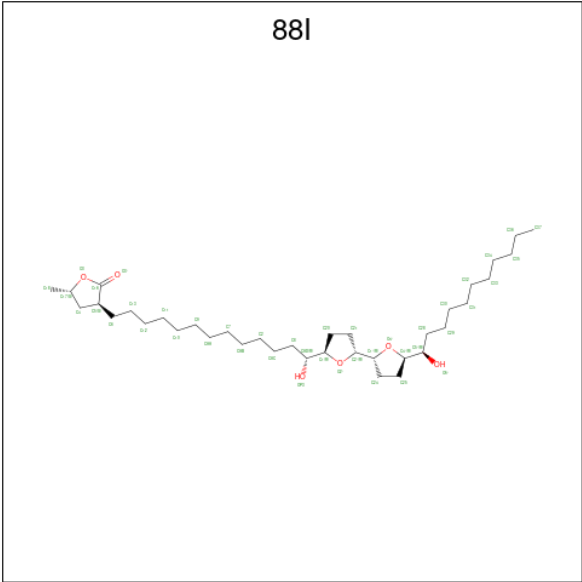
Mol	Chain	Residues	Atoms					AltConf	
48	F	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



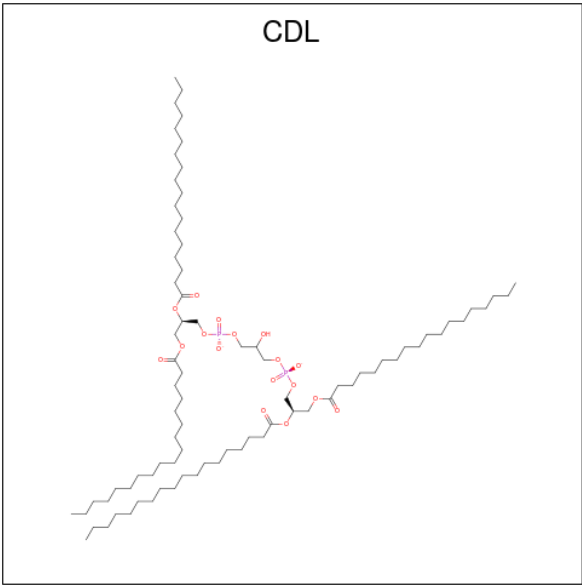
Mol	Chain	Residues	Atoms						AltConf
49	H	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
49	H	1	Total	C	H	N	O	P	0
			111	34	67	1	8	1	
49	K	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	
49	L	1	Total	C	H	N	O	P	0
			126	39	77	1	8	1	
49	L	1	Total	C	H	N	O	P	0
			105	32	63	1	8	1	
49	L	1	Total	C	H	N	O	P	0
			126	39	77	1	8	1	
49	M	1	Total	C	H	N	O	P	0
			89	27	52	1	8	1	
49	M	1	Total	C	H	N	O	P	0
			105	32	63	1	8	1	
49	Y	1	Total	C	H	N	O	P	0
			101	31	60	1	8	1	

- Molecule 50 is (3 {S},5 {S})-5-methyl-3-[(13 {R})-13-oxidanyl-13-[(2 {R},5 {R})-5-[(2 {R},5 {R})-5-[(1 {R})-1-oxidanylundecyl]oxolan-2-yl]oxolan-2-yl]tridecyl]oxolan-2-one (CCD ID: 88I) (formula: C<sub>37</sub>H<sub>68</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
50	H	1	109	37	66	6	0

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



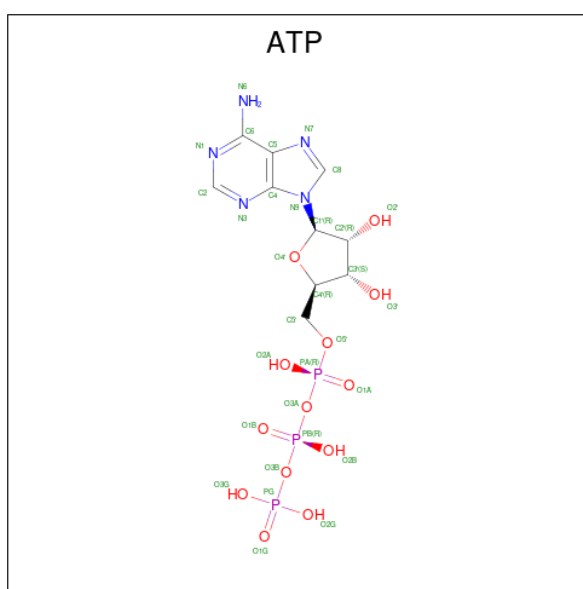
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
51	L	1	174	55	100	17	2	0
51	N	1	148	46	83	17	2	0
51	X	1	154	48	87	17	2	0

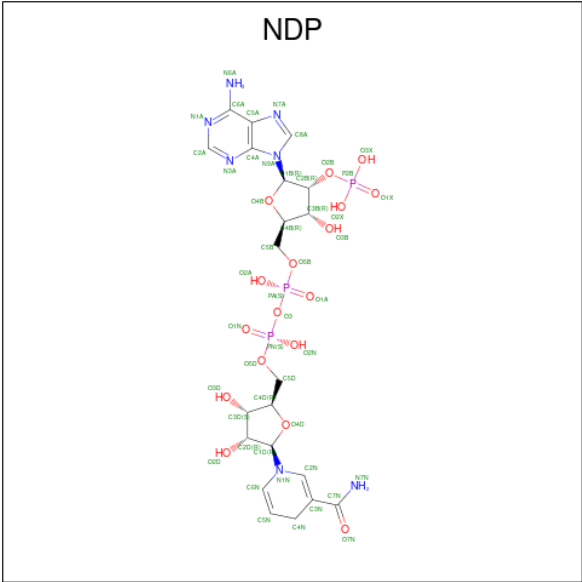
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Mol	Chain	Residues	Atoms					AltConf
51	d	1	Total	C	H	O	P	0
			133	41	74	16	2	
51	d	1	Total	C	H	O	P	0
			141	44	78	17	2	
51	i	1	Total	C	H	O	P	0
			163	51	93	17	2	
51	r	1	Total	C	H	O	P	0
			123	38	66	17	2	

- Molecule 52 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



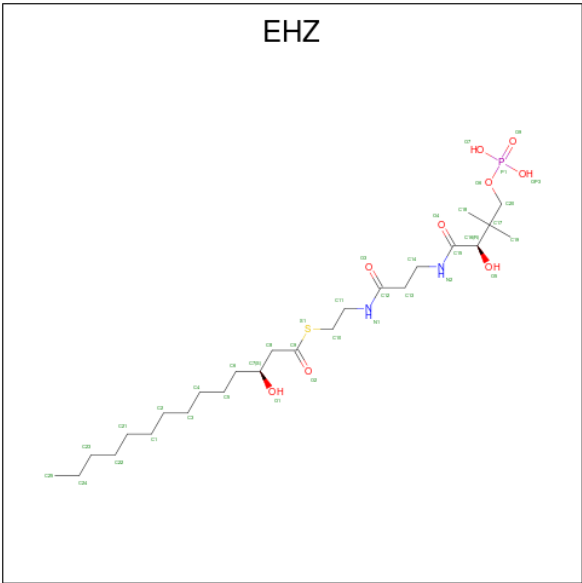


Mol	Chain	Residues	Atoms						AltConf
53	P	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 55 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

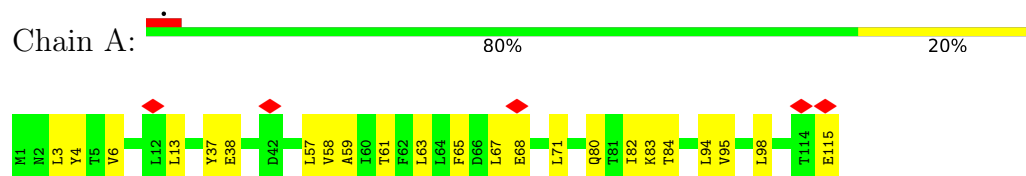


Mol	Chain	Residues	Atoms							AltConf
55	T	1	Total	C	H	N	O	P	S	0
			84	25	47	2	8	1	1	
55	U	1	Total	C	H	N	O	P	S	0
			84	25	47	2	8	1	1	

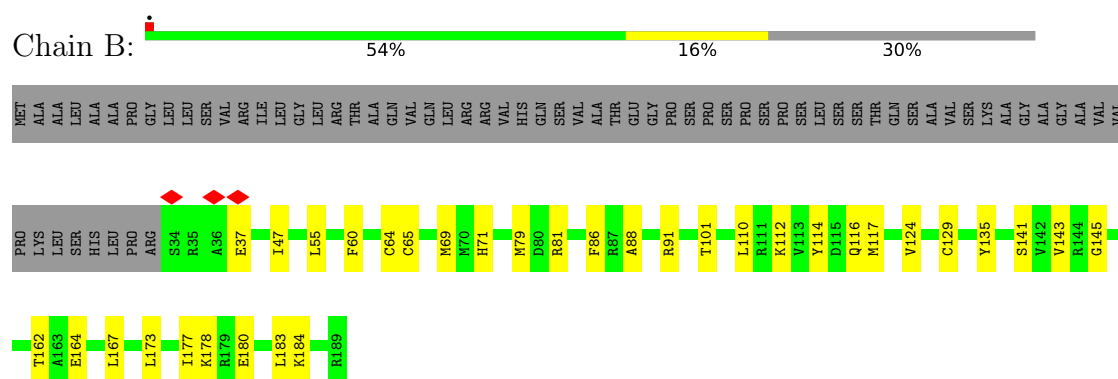
### 3 Residue-property plots

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.

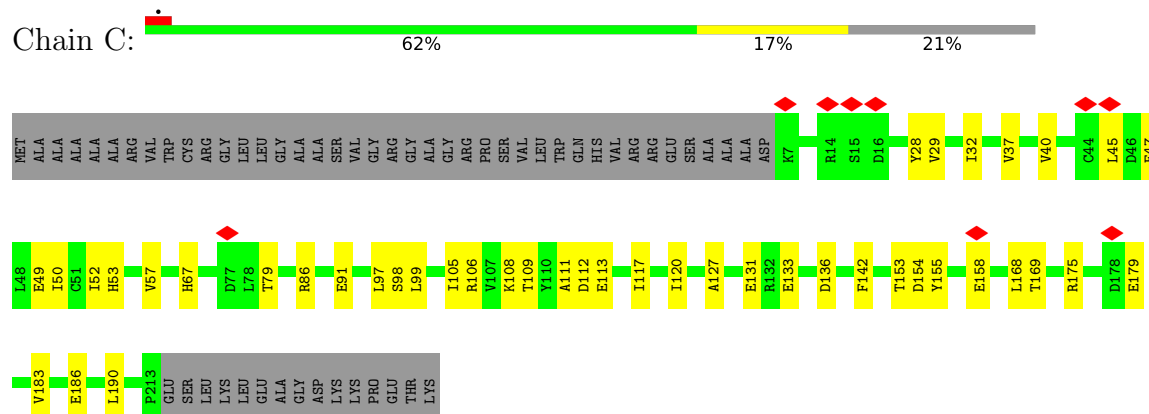
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



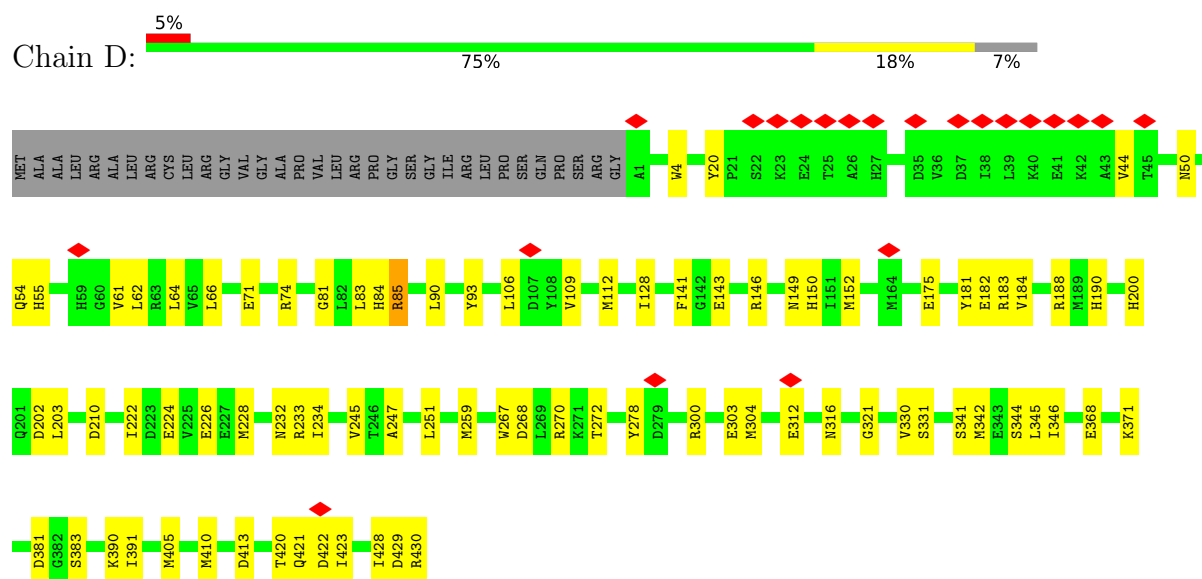
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



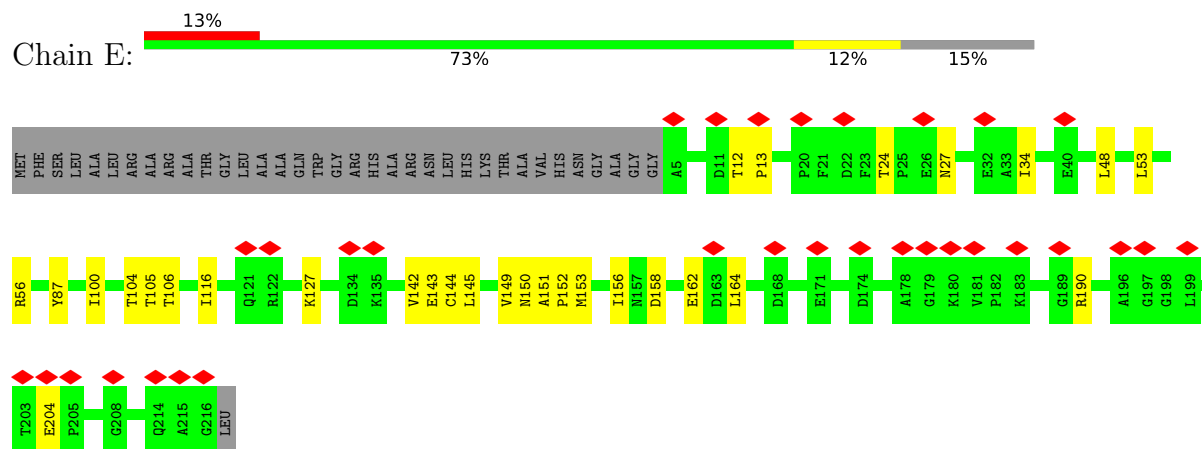
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



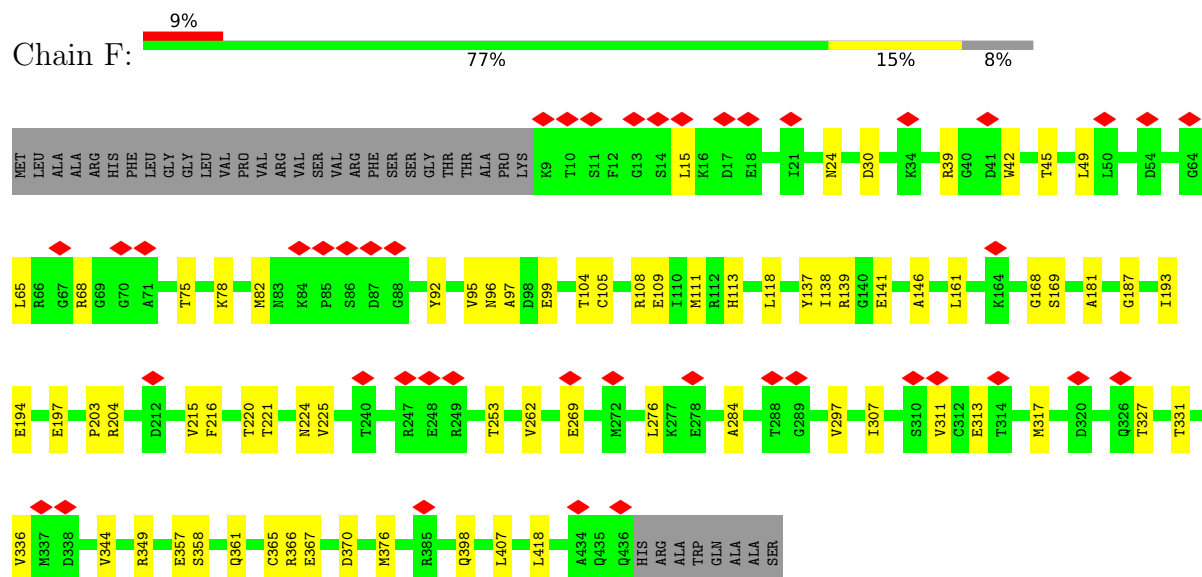
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

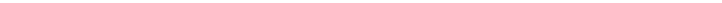


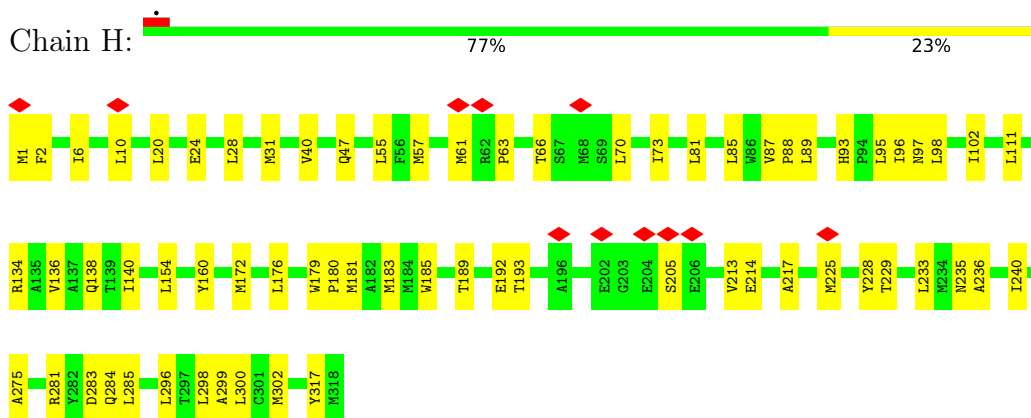
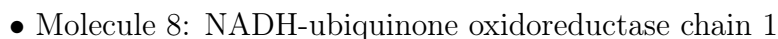
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



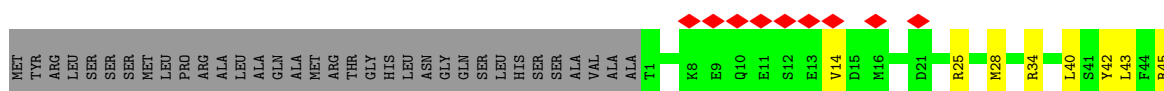
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

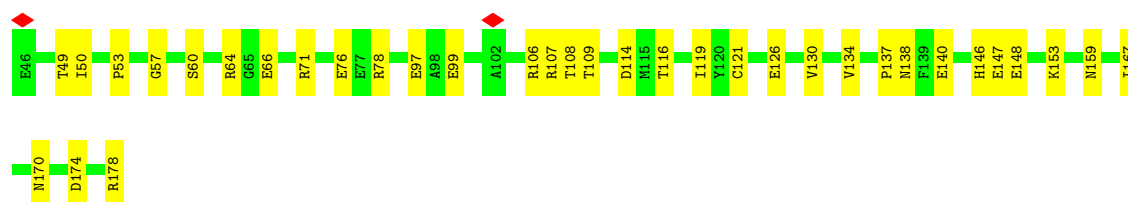


- Chain G:  9% 76% 19% 5%

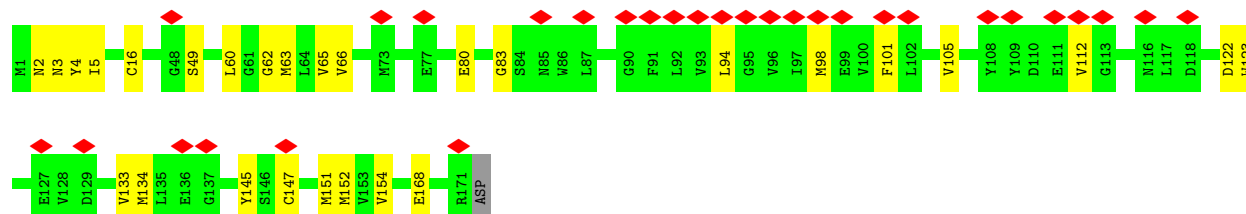
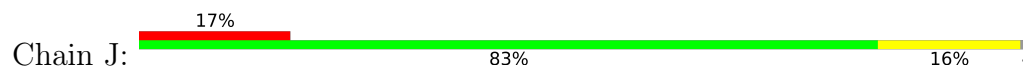


- Chain I: 

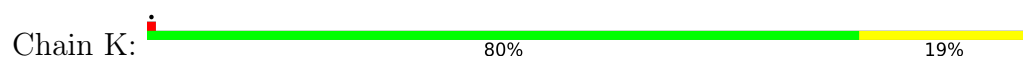




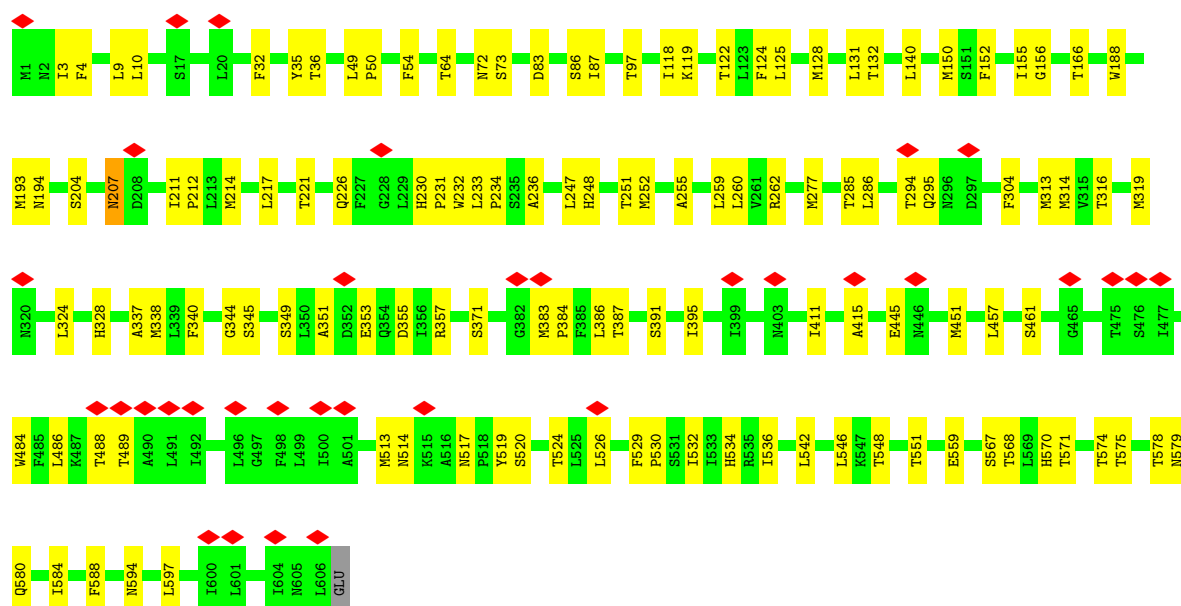
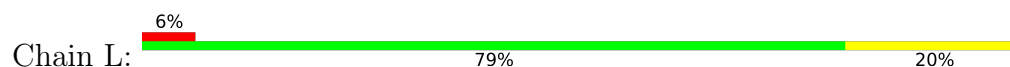
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6




- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

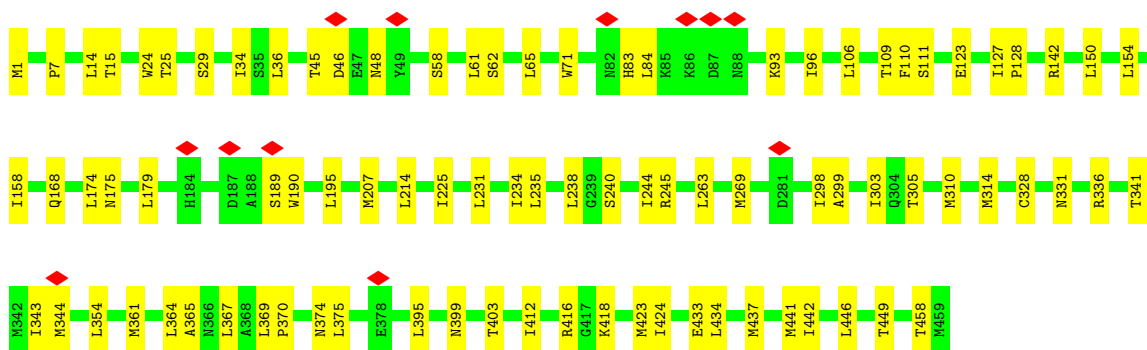


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5




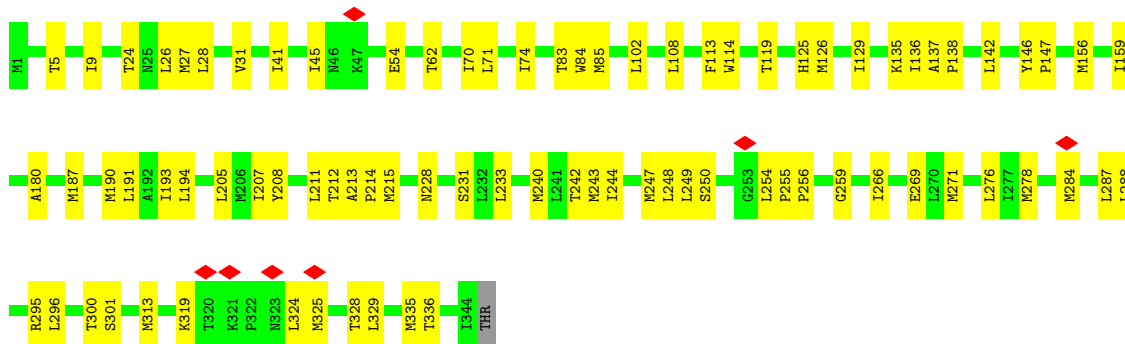
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  81% 19%




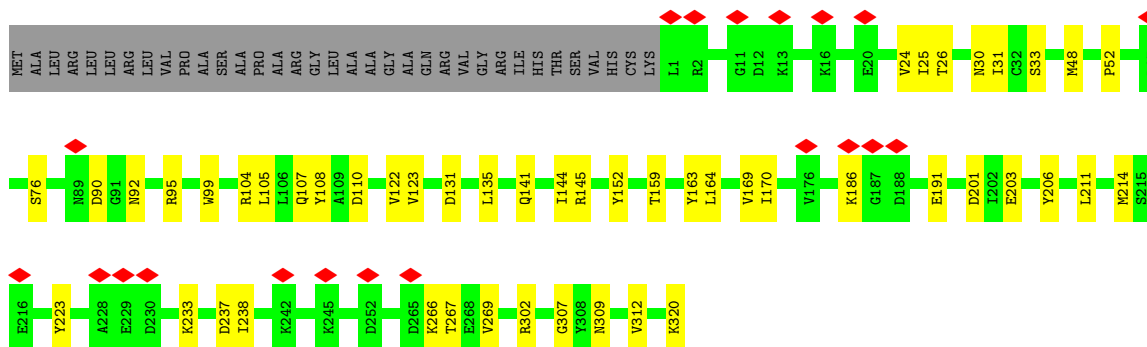
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  76% 24%




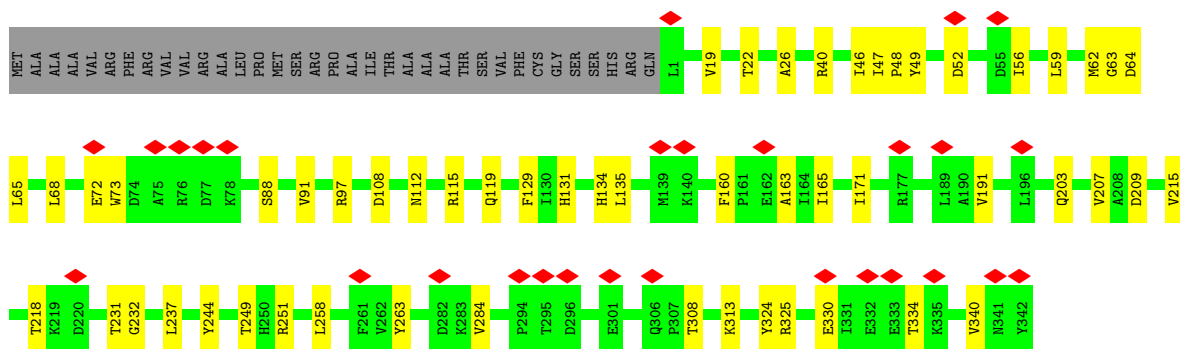
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  6% 76% 14% 10%

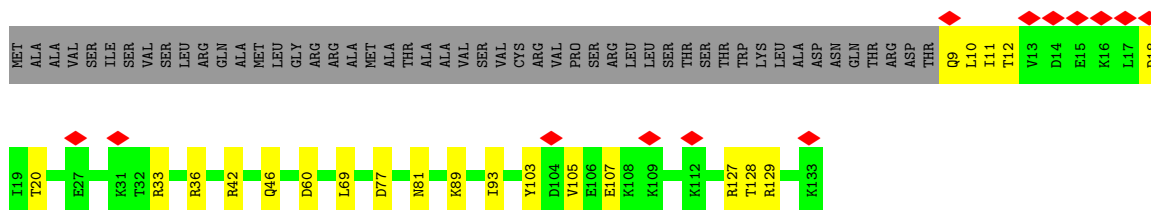


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

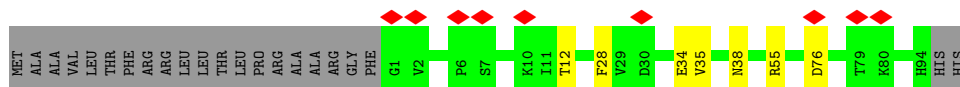
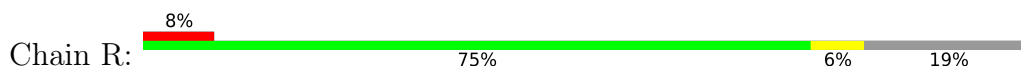
Chain P:  7% 76% 15% 9%



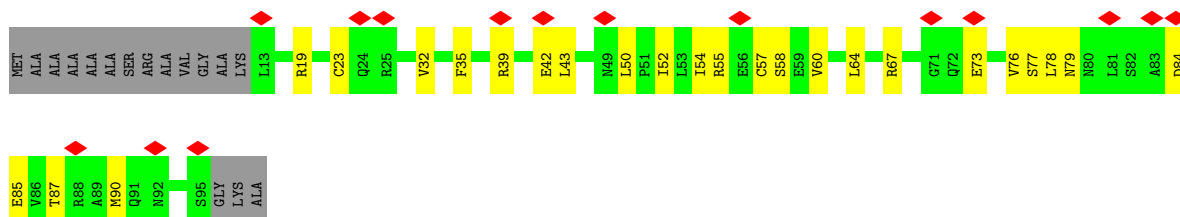
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



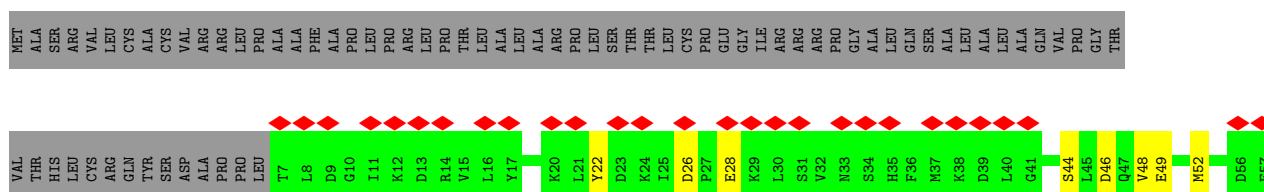
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

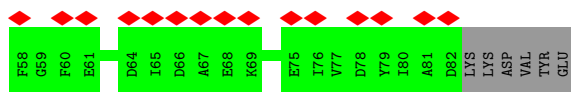


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

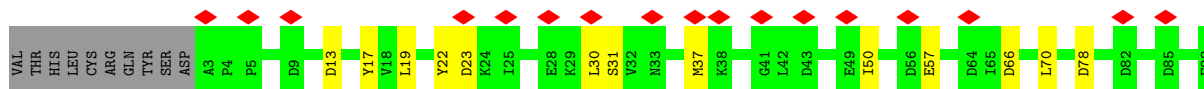


- Molecule 20: Acyl carrier protein, mitochondrial

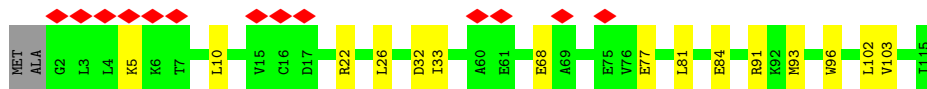
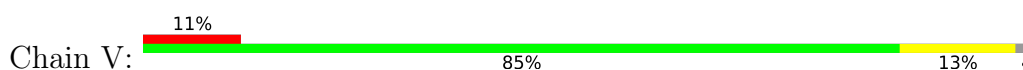




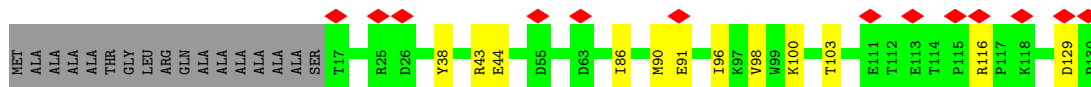
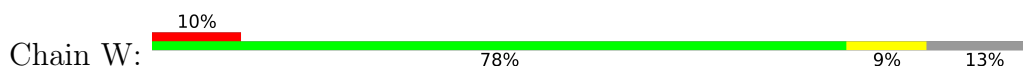
- Molecule 20: Acyl carrier protein, mitochondrial



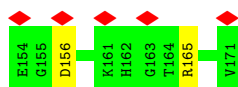
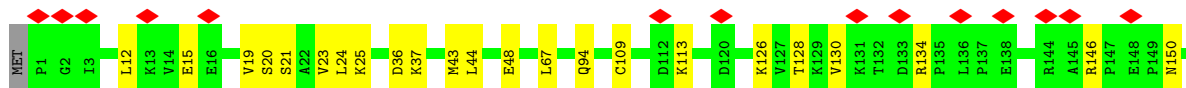
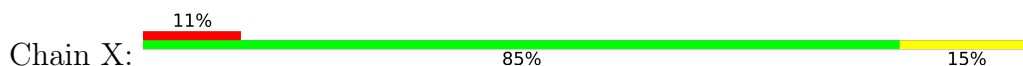
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



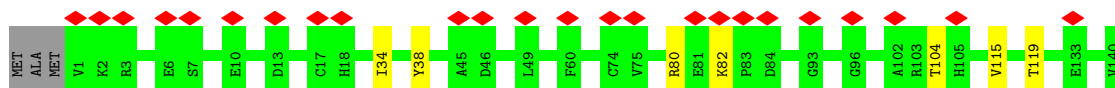
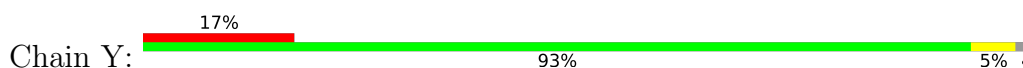
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



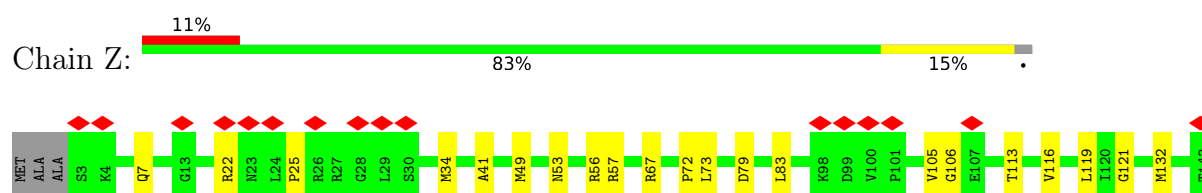
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



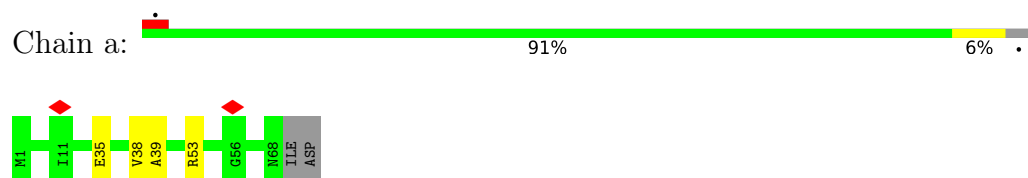
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



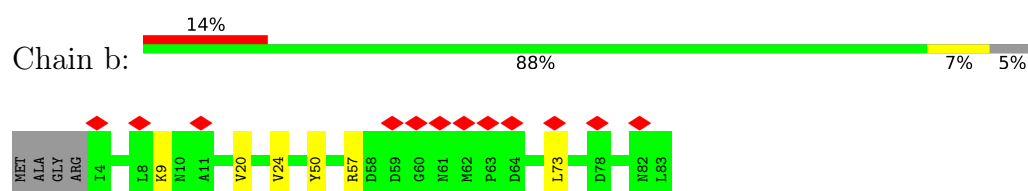
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



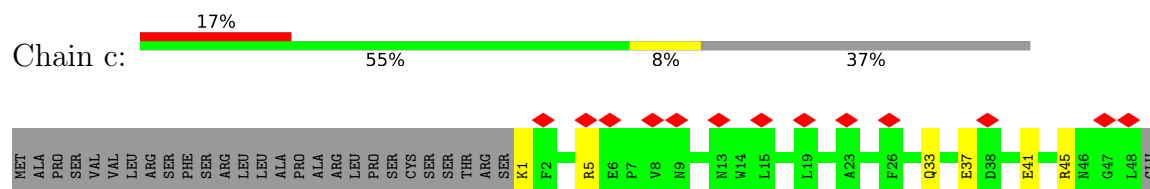
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



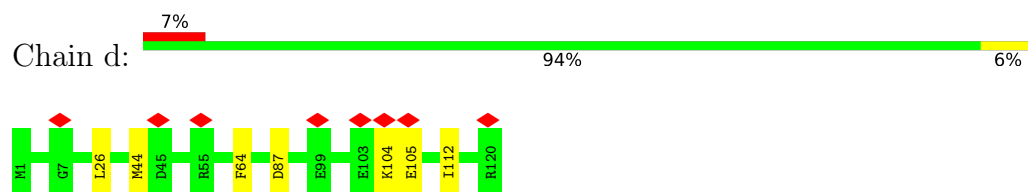
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



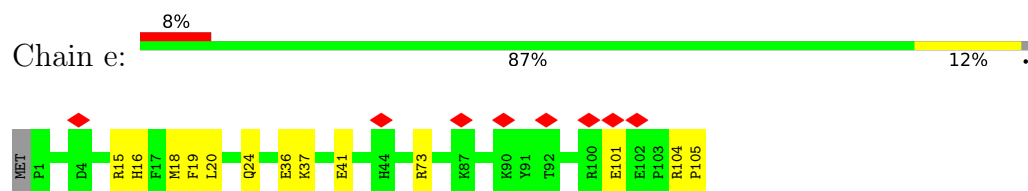
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



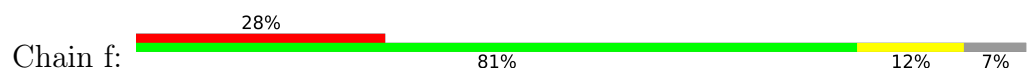
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

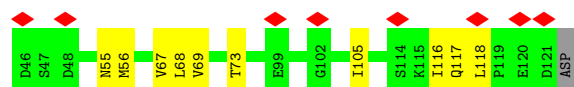
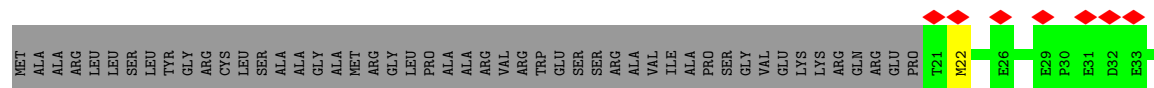


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

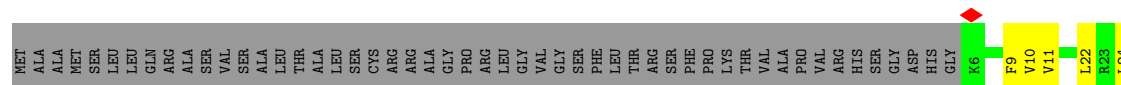




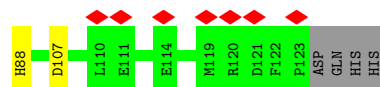
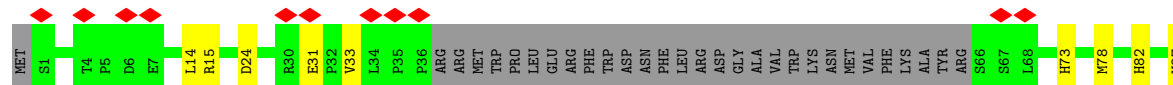
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



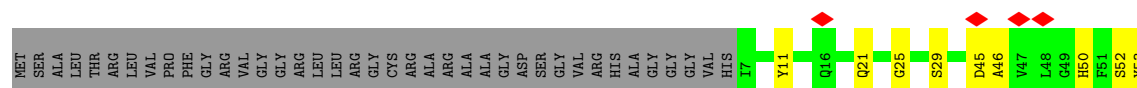
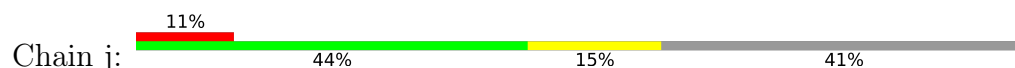
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

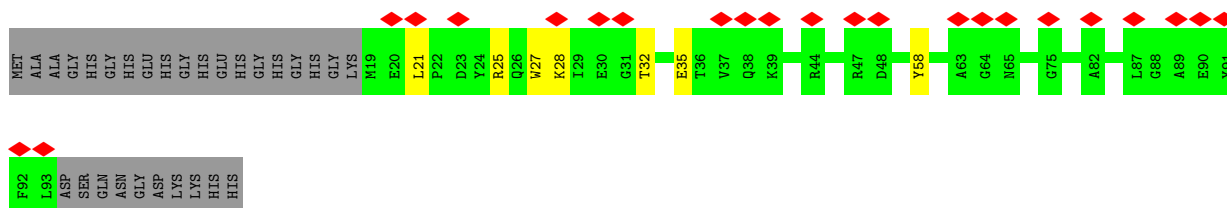


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

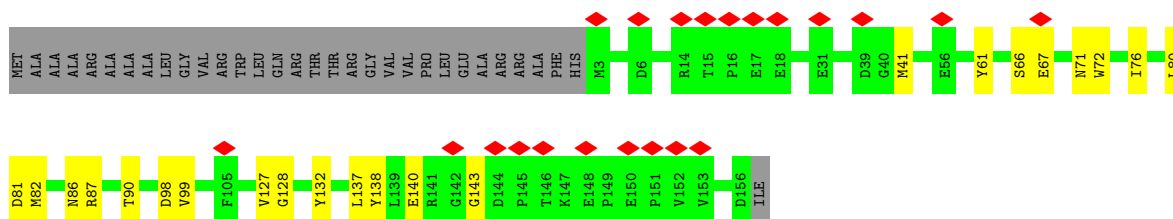




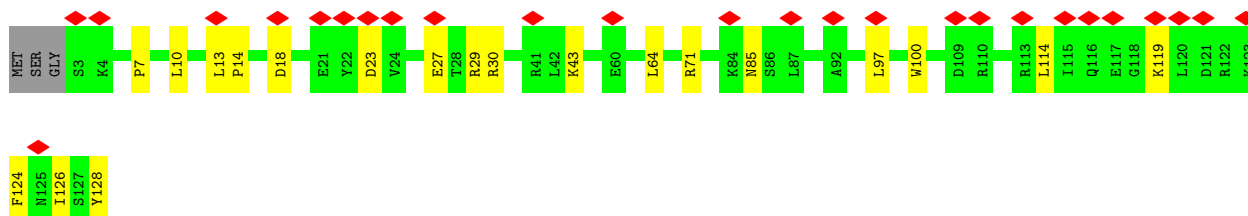
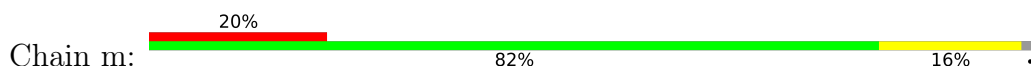
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



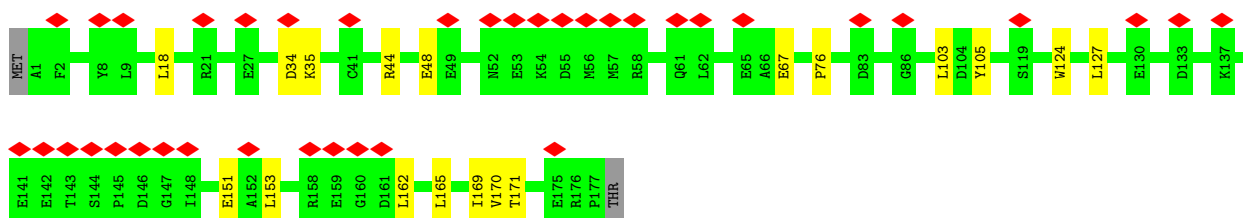
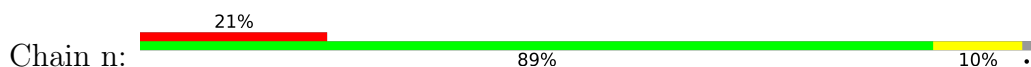
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



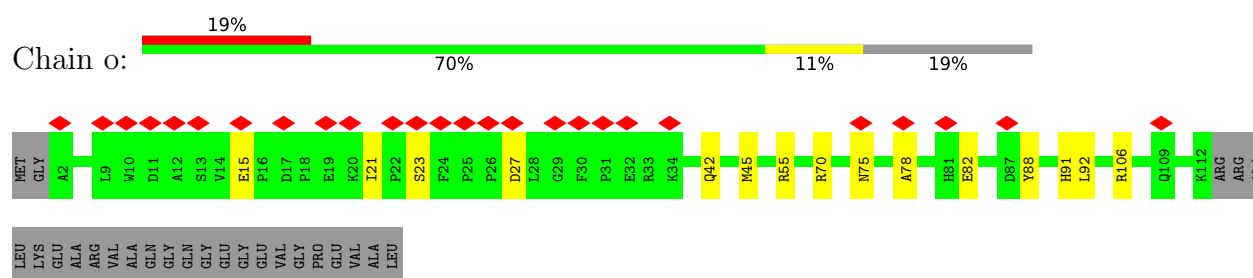
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



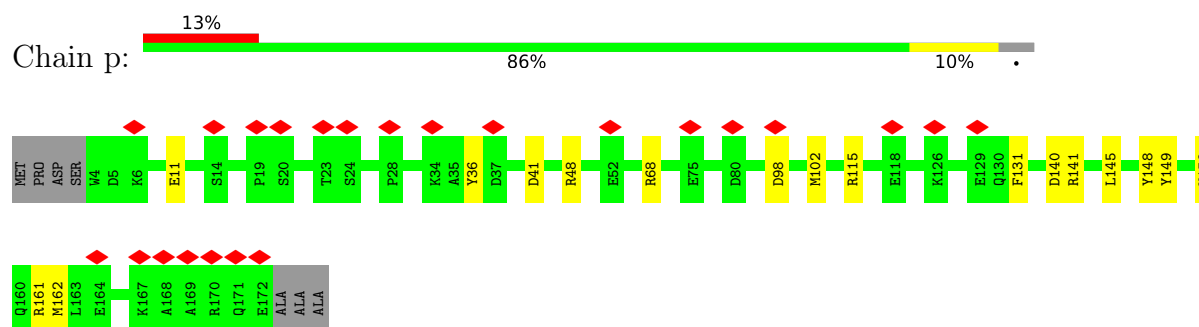
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



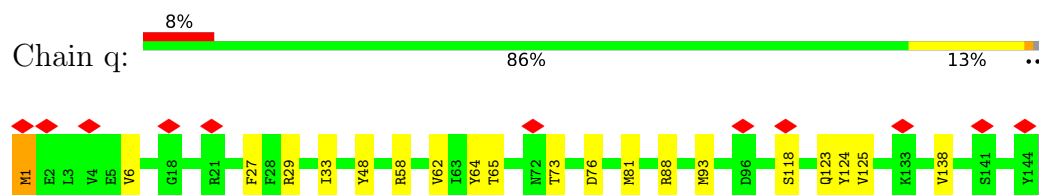
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



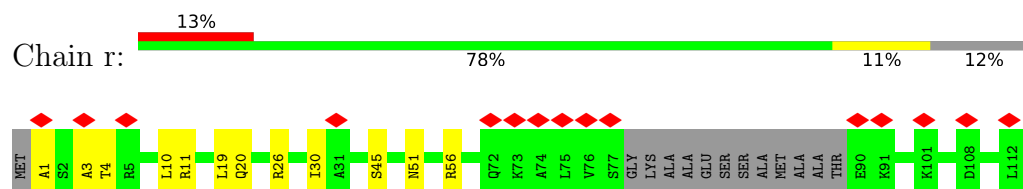
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



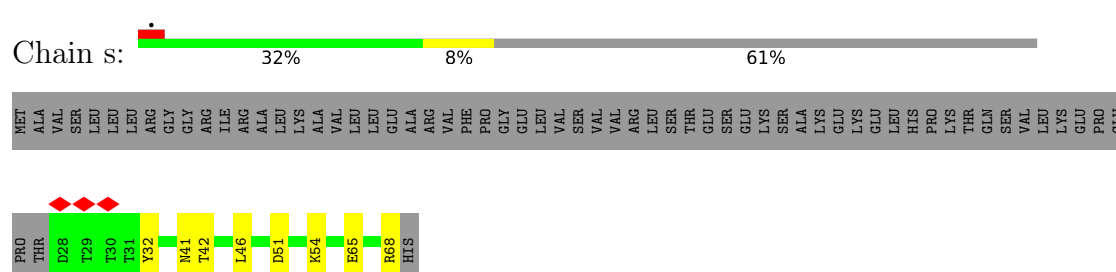
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	469.35, 469.35, 469.35	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.043, 1.043, 1.043	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, ATP, 88I, 3PE, FES, CDL, ZN, AME, AYA, EHZ, FME, SF4, NDP, FMN, 2MR

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	0.22	0/949	0.33	0/1297
2	B	0.32	0/1278	0.38	1/1730 (0.1%)
3	C	0.28	0/1771	0.37	0/2412
4	D	0.28	0/3540	0.35	0/4795
5	E	0.20	0/1688	0.36	0/2300
6	F	0.23	0/3374	0.35	0/4557
7	G	0.24	0/5383	0.34	0/7293
8	H	0.24	0/2607	0.38	0/3564
9	I	0.31	0/1461	0.40	0/1974
10	J	0.21	0/1322	0.34	0/1799
11	K	0.22	0/738	0.34	0/1002
12	L	0.23	0/4913	0.36	0/6686
13	M	0.24	0/3709	0.35	0/5052
14	N	0.24	0/2748	0.40	0/3741
15	O	0.21	0/2674	0.29	0/3626
16	P	0.23	0/2823	0.36	0/3828
17	Q	0.23	0/1038	0.30	0/1401
18	R	0.26	0/751	0.38	0/1011
19	S	0.18	0/678	0.34	0/915
20	T	0.14	0/620	0.32	0/836
20	U	0.20	0/704	0.36	0/951
21	V	0.20	0/949	0.35	0/1286
22	W	0.21	0/993	0.34	0/1335
23	X	0.21	0/1434	0.37	0/1937
24	Y	0.17	0/1061	0.26	0/1439
25	Z	0.21	0/1198	0.35	0/1616
26	a	0.21	0/569	0.32	0/766
27	b	0.18	0/651	0.30	0/895
28	c	0.17	0/409	0.25	0/555
29	d	0.22	0/1028	0.30	0/1387
30	e	0.21	0/900	0.32	0/1199
31	f	0.17	0/468	0.30	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	g	0.21	0/878	0.33	0/1196
33	h	0.22	0/1197	0.30	0/1621
34	i	0.21	0/810	0.35	0/1102
35	j	0.23	0/561	0.38	1/768 (0.1%)
36	k	0.16	0/629	0.31	0/851
37	l	0.21	0/1348	0.35	0/1840
38	m	0.19	0/1079	0.32	0/1463
39	n	0.19	0/1589	0.29	0/2152
40	o	0.18	0/982	0.37	0/1320
41	p	0.20	0/1466	0.32	0/1981
42	q	0.25	0/1234	0.34	0/1681
43	r	0.23	0/812	0.45	0/1098
44	s	0.19	0/353	0.31	0/479
All	All	0.23	0/67367	0.35	2/91367 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
42	q	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	56	PRO	CA-N-CD	-5.61	104.15	112.00
2	B	65	CYS	CA-CB-SG	5.13	126.19	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	q	1	AME	Mainchain

## 5.2 Too-close contacts

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	933	969	969	26	0
2	B	1247	1255	1255	30	0
3	C	1721	1681	1680	38	0
4	D	3464	3414	3417	73	0
5	E	1648	1639	1639	25	0
6	F	3300	3259	3258	53	0
7	G	5296	5322	5322	103	0
8	H	2540	2626	2626	60	0
9	I	1431	1381	1383	38	0
10	J	1300	1315	1315	29	0
11	K	737	768	768	18	0
12	L	4800	4985	4985	100	0
13	M	3632	3853	3853	75	0
14	N	2696	2895	2895	74	0
15	O	2607	2564	2566	35	0
16	P	2748	2766	2768	38	0
17	Q	1015	1016	1016	17	0
18	R	738	715	717	5	0
19	S	667	686	685	17	0
20	T	611	602	602	5	0
20	U	692	686	686	9	0
21	V	927	968	968	12	0
22	W	970	991	991	8	0
23	X	1396	1377	1381	19	0
24	Y	1037	1025	1027	5	0
25	Z	1167	1166	1166	19	0
26	a	556	568	568	4	0
27	b	628	628	628	6	0
28	c	398	399	401	4	0
29	d	996	1001	1001	8	0
30	e	877	869	871	12	0
31	f	456	452	452	5	0
32	g	850	783	783	13	0
33	h	1162	1163	1163	16	0
34	i	784	794	796	10	0
35	j	537	496	495	12	0
36	k	609	604	603	5	0
37	l	1294	1187	1186	21	0
38	m	1050	1061	1061	18	0
39	n	1534	1464	1466	16	0
40	o	957	937	937	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	p	1433	1399	1399	17	0
42	q	1203	1158	1158	19	0
43	r	802	836	836	8	0
44	s	344	324	324	6	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	B	78	113	107	0	0
46	J	42	62	58	2	0
46	Z	45	68	64	0	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	19	19	4	0
49	H	95	149	147	3	0
49	K	33	44	40	0	0
49	L	140	217	211	2	0
49	M	79	115	109	0	0
49	Y	41	60	56	0	0
50	H	43	66	0	0	0
51	L	74	100	92	0	0
51	N	65	83	77	1	0
51	X	67	87	81	0	0
51	d	122	152	138	1	0
51	i	70	93	87	1	0
51	r	57	66	58	0	0
52	O	31	12	12	1	0
53	P	48	26	26	2	0
54	R	1	0	0	0	0
55	T	37	47	0	2	0
55	U	37	47	0	1	0
All	All	67082	67673	67448	936	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 7.

The worst 5 of 936 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)
12:L:316:THR:HG22	12:L:395:ILE:HD12	1.48	0.94
14:N:243:MET:HE3	29:d:44:MET:HE3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HD11	4:D:90:LEU:HD12	1.56	0.88
12:L:128:MET:HE3	12:L:251:THR:HG22	1.55	0.87
7:G:258:ILE:HG22	7:G:368:ILE:HD12	1.57	0.87

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	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	12 (8%)	0	100	100
3	C	205/263 (78%)	191 (93%)	14 (7%)	0	100	100
4	D	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
5	E	210/248 (85%)	191 (91%)	19 (9%)	0	100	100
6	F	426/464 (92%)	392 (92%)	34 (8%)	0	100	100
7	G	686/727 (94%)	629 (92%)	57 (8%)	0	100	100
8	H	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
9	I	176/212 (83%)	164 (93%)	12 (7%)	0	100	100
10	J	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
11	K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
12	L	604/607 (100%)	559 (92%)	45 (8%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	324 (95%)	18 (5%)	0	100	100
15	O	318/355 (90%)	306 (96%)	12 (4%)	0	100	100
16	P	340/377 (90%)	302 (89%)	38 (11%)	0	100	100
17	Q	123/175 (70%)	116 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	92/116 (79%)	90 (98%)	2 (2%)	0	100	100
19	S	81/99 (82%)	68 (84%)	13 (16%)	0	100	100
20	T	74/156 (47%)	69 (93%)	5 (7%)	0	100	100
20	U	84/156 (54%)	78 (93%)	6 (7%)	0	100	100
21	V	112/116 (97%)	103 (92%)	9 (8%)	0	100	100
22	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
24	Y	138/143 (96%)	132 (96%)	6 (4%)	0	100	100
25	Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
26	a	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
27	b	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
28	c	46/76 (60%)	43 (94%)	3 (6%)	0	100	100
29	d	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
30	e	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
31	f	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
32	g	99/151 (66%)	91 (92%)	8 (8%)	0	100	100
33	h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	i	90/128 (70%)	84 (93%)	6 (7%)	0	100	100
35	j	60/105 (57%)	58 (97%)	2 (3%)	0	100	100
36	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
37	l	152/186 (82%)	133 (88%)	19 (12%)	0	100	100
38	m	124/129 (96%)	115 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
40	o	109/137 (80%)	97 (89%)	12 (11%)	0	100	100
41	p	167/176 (95%)	157 (94%)	10 (6%)	0	100	100
42	q	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
43	r	96/113 (85%)	86 (90%)	10 (10%)	0	100	100
44	s	39/104 (38%)	36 (92%)	3 (8%)	0	100	100
All	All	8087/9214 (88%)	7538 (93%)	549 (7%)	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	A	103/103 (100%)	103 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	189/227 (83%)	189 (100%)	0	100	100
4	D	370/394 (94%)	370 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	580/610 (95%)	580 (100%)	0	100	100
8	H	279/279 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/137 (99%)	136 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	547 (100%)	1 (0%)	87	85
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	299 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/96 (82%)	79 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	122/123 (99%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	58/60 (97%)	58 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	42/67 (63%)	42 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	49/53 (92%)	49 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	89/120 (74%)	89 (100%)	0	100	100
35	j	58/87 (67%)	58 (100%)	0	100	100
36	k	58/78 (74%)	58 (100%)	0	100	100
37	l	139/161 (86%)	139 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	104/121 (86%)	104 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	129/130 (99%)	129 (100%)	0	100	100
43	r	89/96 (93%)	89 (100%)	0	100	100
44	s	40/95 (42%)	40 (100%)	0	100	100
All	All	7177/7948 (90%)	7176 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	47	HIS
25	Z	111	HIS
41	p	55	HIS
21	V	36	HIS
23	X	29	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z  > 2$
42	AME	q	1	42	9,10,11	1.55	1 (11%)	9,11,13	1.37	2 (22%)
10	FME	J	1	10	8,9,10	0.92	0	8,9,11	0.94	0
4	2MR	D	85	4	10,12,13	2.43	2 (20%)	5,13,15	1.25	1 (20%)
11	FME	K	1	11	8,9,10	1.00	0	8,9,11	1.29	1 (12%)
12	FME	L	1	12	8,9,10	0.97	0	8,9,11	0.89	0
43	AYA	r	1	43	6,7,8	1.86	2 (33%)	6,8,10	1.29	1 (16%)
14	FME	N	1	14	8,9,10	0.99	0	8,9,11	0.78	0
13	FME	M	1	13	8,9,10	1.01	0	8,9,11	0.86	0
8	FME	H	1	8	8,9,10	0.87	0	8,9,11	1.44	1 (12%)
1	FME	A	1	1	8,9,10	1.00	0	8,9,11	0.98	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
42	AME	q	1	42	-	3/9/10/12	-
10	FME	J	1	10	-	2/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
11	FME	K	1	11	-	4/7/9/11	-
12	FME	L	1	12	-	5/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
14	FME	N	1	14	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	M	1	13	-	2/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
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)
4	D	85	2MR	CZ-NE	5.05	1.45	1.34
4	D	85	2MR	CZ-NH2	5.03	1.43	1.33
42	q	1	AME	CT1-N	3.56	1.45	1.34
43	r	1	AYA	CT-N	3.38	1.45	1.34
43	r	1	AYA	OT-CT	-2.05	1.18	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	FME	C-CA-N	3.09	115.45	109.50
11	K	1	FME	C-CA-N	2.79	114.89	109.50
4	D	85	2MR	CD-NE-CZ	2.63	128.31	123.36
42	q	1	AME	O-C-CA	-2.36	118.70	124.77
42	q	1	AME	CT2-CT1-N	2.22	119.80	116.12

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	85	2MR	2	0
11	K	1	FME	1	0
13	M	1	FME	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 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
45	SF4	G	803	7	0,12,12	-	-	-		
49	3PE	H	403	-	43,43,50	0.93	4 (9%)	46,48,55	1.15	2 (4%)
49	3PE	M	502	-	41,41,50	0.95	3 (7%)	44,46,55	1.11	2 (4%)
51	CDL	d	201	-	58,58,99	1.03	6 (10%)	63,69,111	1.06	3 (4%)
46	PC1	Z	201	-	44,44,53	1.05	4 (9%)	50,52,61	1.04	2 (4%)
49	3PE	L	701	-	48,48,50	0.89	4 (8%)	51,53,55	1.12	2 (3%)
51	CDL	d	202	-	62,62,99	1.10	8 (12%)	68,74,111	1.17	4 (5%)
55	EHZ	U	201	20	31,36,37	1.56	5 (16%)	36,44,47	1.68	9 (25%)
53	NDP	P	501	-	51,52,52	2.17	5 (9%)	71,80,80	1.53	17 (23%)
51	CDL	L	703	-	73,73,99	1.02	8 (10%)	79,85,111	1.14	4 (5%)
49	3PE	H	401	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)
45	SF4	G	801	7	0,12,12	-	-	-		
49	3PE	Y	401	-	40,40,50	0.97	4 (10%)	43,45,55	1.06	2 (4%)
48	FMN	F	502	-	33,33,33	1.13	3 (9%)	48,50,50	1.34	7 (14%)
46	PC1	B	202	-	34,34,53	1.17	4 (11%)	40,42,61	1.08	2 (5%)
49	3PE	K	201	-	32,32,50	1.07	4 (12%)	35,37,55	1.21	2 (5%)
45	SF4	F	501	6	0,12,12	-	-	-		
46	PC1	B	203	-	42,42,53	1.05	4 (9%)	48,50,61	1.06	2 (4%)
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	I	202	9	0,12,12	-	-	-		
51	CDL	r	201	-	56,56,99	1.16	8 (14%)	62,68,111	1.18	4 (6%)
49	3PE	L	704	-	48,48,50	0.89	4 (8%)	51,53,55	1.07	2 (3%)
49	3PE	M	501	-	36,36,50	1.03	4 (11%)	39,41,55	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
51	CDL	N	401	-	64,64,99	1.09	8 (12%)	70,76,111	1.16	4 (5%)
49	3PE	L	702	-	41,41,50	0.97	4 (9%)	44,46,55	1.16	2 (4%)
47	FES	G	802	7	0,4,4	-	-	-	-	-
45	SF4	I	201	9	0,12,12	-	-	-	-	-
51	CDL	i	201	-	69,69,99	1.04	7 (10%)	75,81,111	1.18	5 (6%)
46	PC1	J	201	-	41,41,53	1.06	4 (9%)	47,49,61	1.07	2 (4%)
50	88I	H	402	-	45,45,45	1.91	9 (20%)	55,56,56	1.73	13 (23%)
51	CDL	X	201	-	66,66,99	1.06	8 (12%)	72,78,111	1.16	4 (5%)
55	EHZ	T	201	20	31,36,37	1.54	5 (16%)	36,44,47	1.45	4 (11%)
52	ATP	O	401	-	32,33,33	0.32	0	48,52,52	0.70	0
47	FES	E	301	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	3PE	H	403	-	-	20/47/47/54	-
45	SF4	G	803	7	-	-	0/6/5/5
49	3PE	M	502	-	-	13/45/45/54	-
51	CDL	d	201	-	-	28/67/67/110	-
46	PC1	Z	201	-	-	18/48/48/57	-
49	3PE	L	701	-	-	16/52/52/54	-
55	EHZ	U	201	20	1/1/9/9	15/42/44/45	-
51	CDL	d	202	-	-	29/73/73/110	-
53	NDP	P	501	-	-	8/34/77/77	0/5/5/5
51	CDL	L	703	-	-	32/84/84/110	-
49	3PE	H	401	-	-	21/54/54/54	-
45	SF4	G	801	7	-	-	0/6/5/5
49	3PE	Y	401	-	-	14/44/44/54	-
48	FMN	F	502	-	-	11/18/18/18	0/3/3/3
46	PC1	B	202	-	-	14/38/38/57	-
49	3PE	K	201	-	-	14/36/36/54	-
45	SF4	F	501	6	-	-	0/6/5/5
46	PC1	B	203	-	-	12/46/46/57	-
45	SF4	B	201	2	-	-	0/6/5/5

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	I	202	9	-	-	0/6/5/5
51	CDL	r	201	-	-	25/67/67/110	-
49	3PE	L	704	-	-	23/52/52/54	-
49	3PE	M	501	-	-	15/40/40/54	-
51	CDL	N	401	-	-	34/75/75/110	-
49	3PE	L	702	-	-	16/45/45/54	-
51	CDL	i	201	-	-	29/80/80/110	-
45	SF4	I	201	9	-	-	0/6/5/5
47	FES	G	802	7	-	-	0/1/1/1
46	PC1	J	201	-	-	16/45/45/57	-
50	88I	H	402	-	-	17/37/67/67	0/3/3/3
55	EHZ	T	201	20	1/1/9/9	17/42/44/45	-
51	CDL	X	201	-	-	35/77/77/110	-
52	ATP	O	401	-	-	6/22/38/38	0/3/3/3
47	FES	E	301	5	-	-	0/1/1/1

The worst 5 of 131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	P2B-O2B	12.01	1.80	1.59
50	H	402	88I	C4-C5	-9.38	1.32	1.54
55	U	201	EHZ	C15-N2	5.10	1.45	1.33
55	U	201	EHZ	C12-N1	4.97	1.45	1.33
55	T	201	EHZ	C15-N2	4.96	1.45	1.33

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	T	201	EHZ	C8-C9-S1	6.01	121.14	113.56
55	U	201	EHZ	C8-C9-S1	5.40	120.38	113.56
50	H	402	88I	C29-C28-C5'	-5.40	105.27	114.11
49	L	701	3PE	O21-C21-C22	4.52	121.25	111.48
49	K	201	3PE	O21-C21-C22	4.48	121.17	111.48

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
55	T	201	EHZ	C16
55	U	201	EHZ	C16

5 of 498 torsion outliers are listed below:

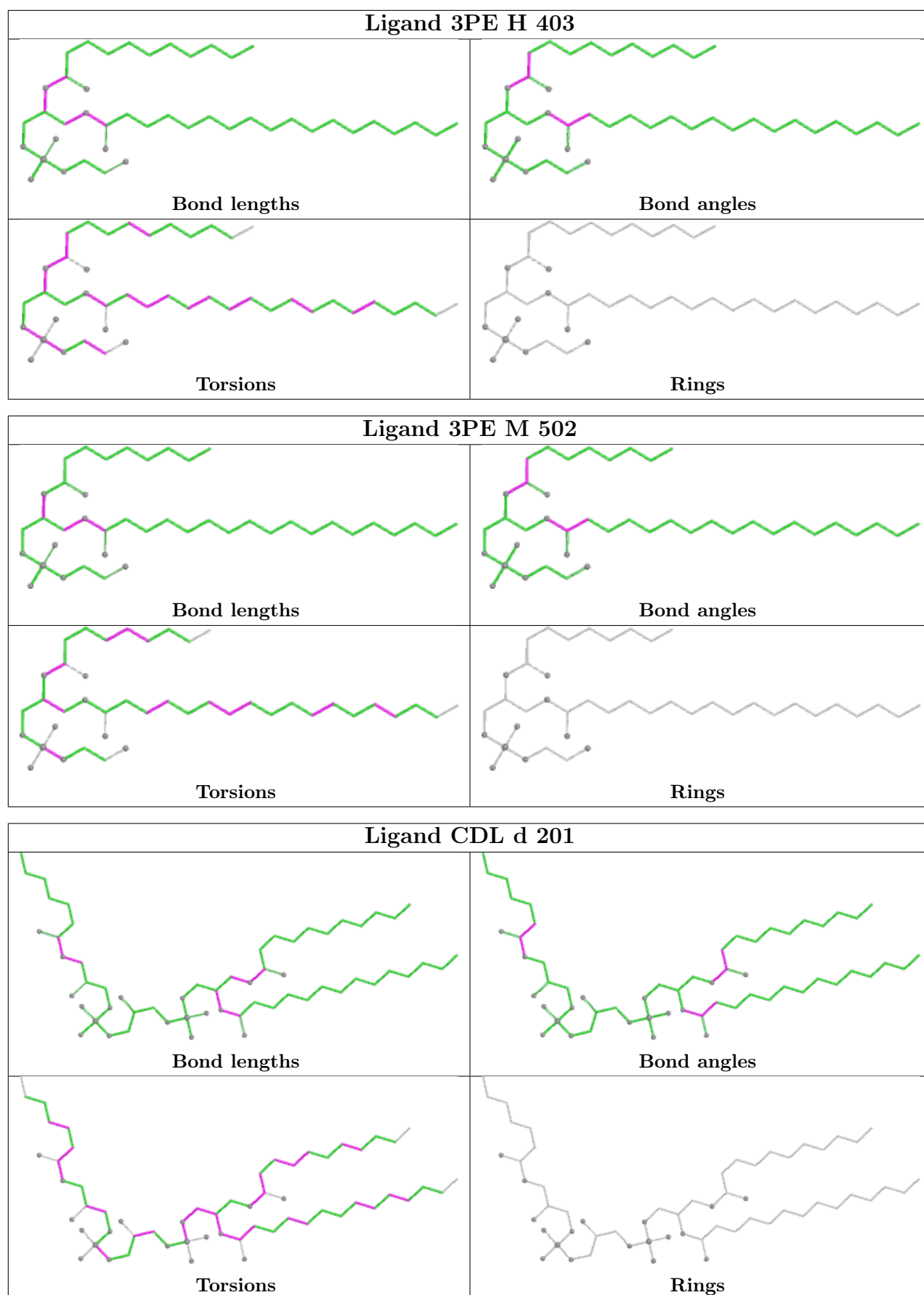
Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	O13-C11-C12-N
46	B	203	PC1	C11-O13-P-O14

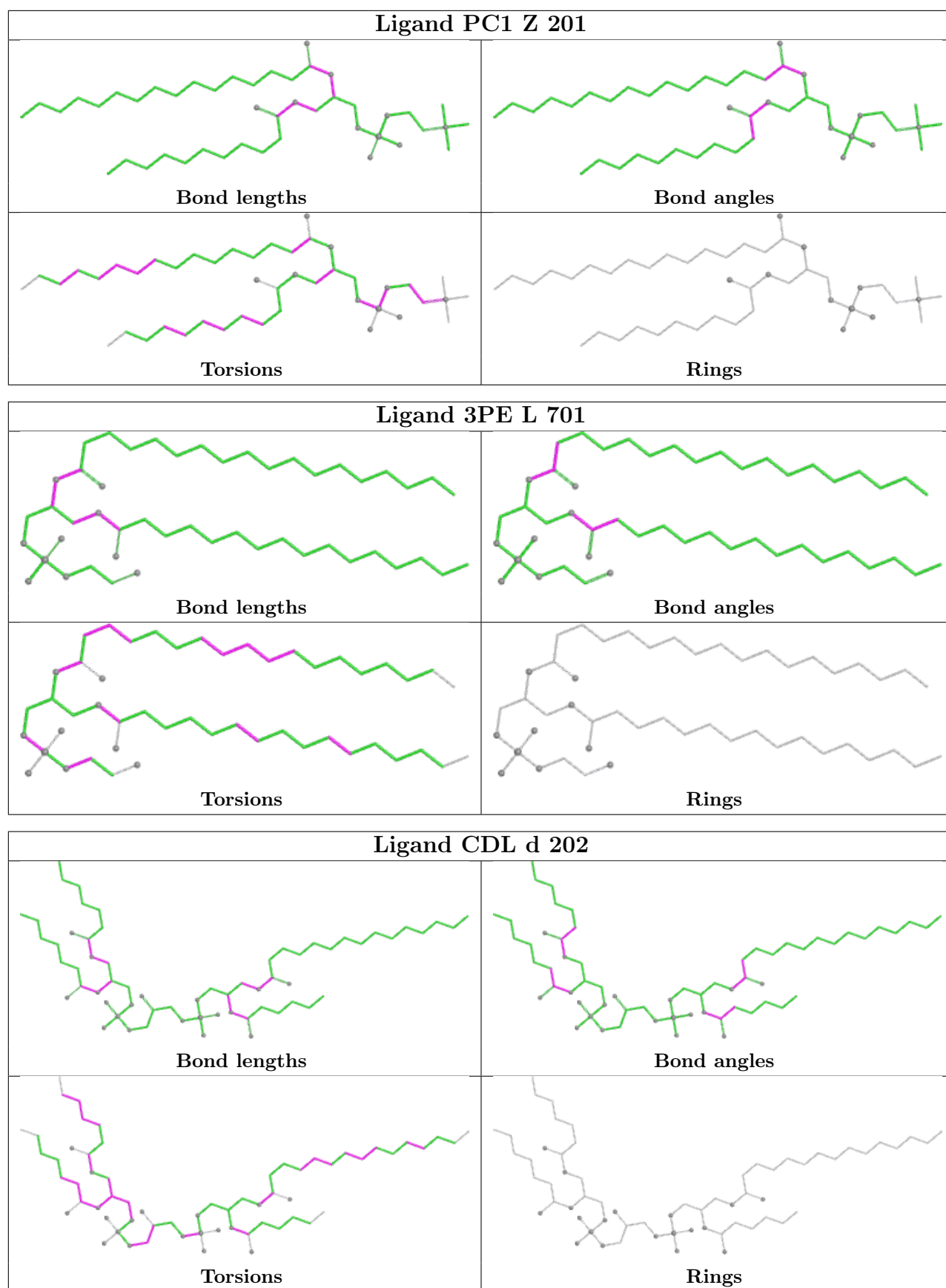
There are no ring outliers.

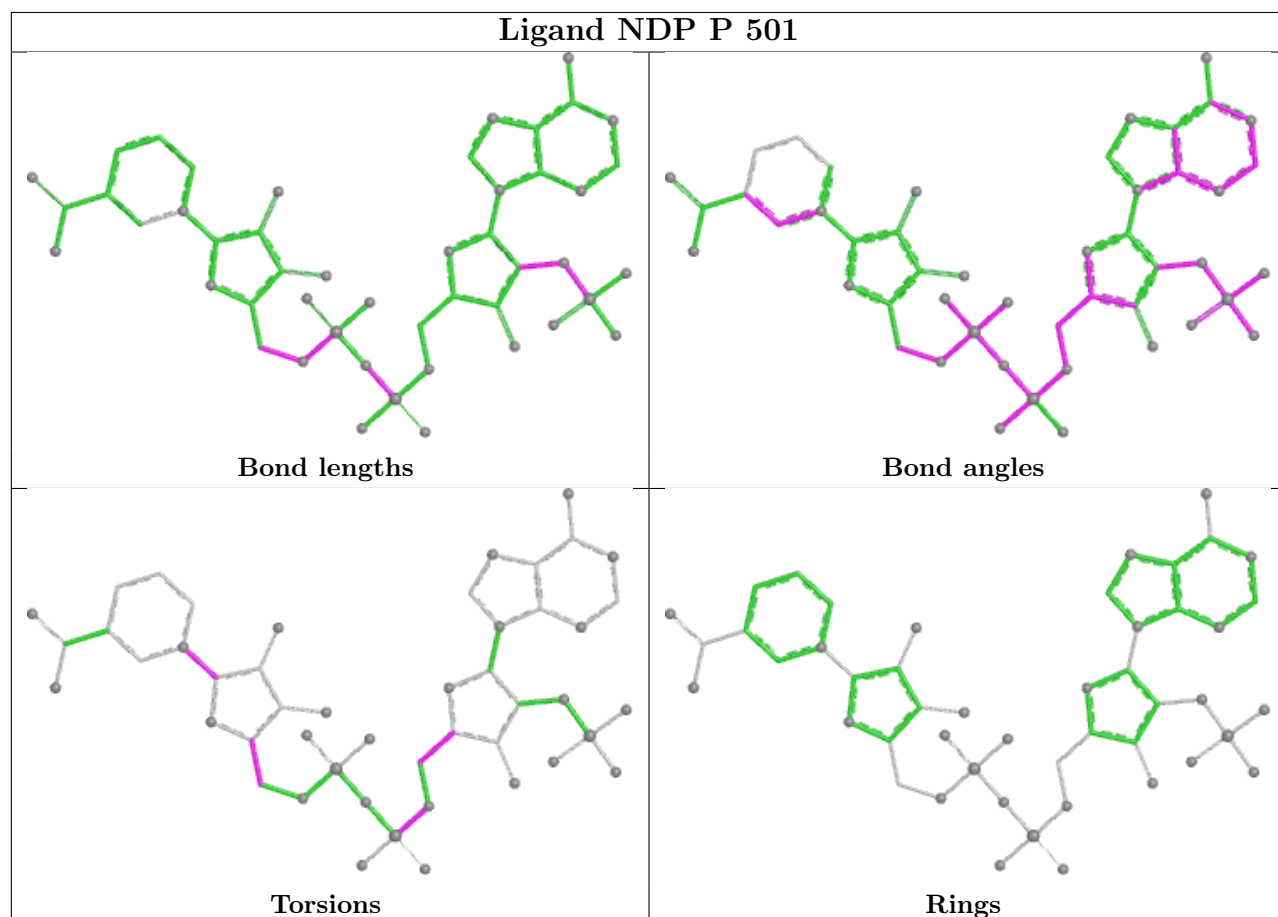
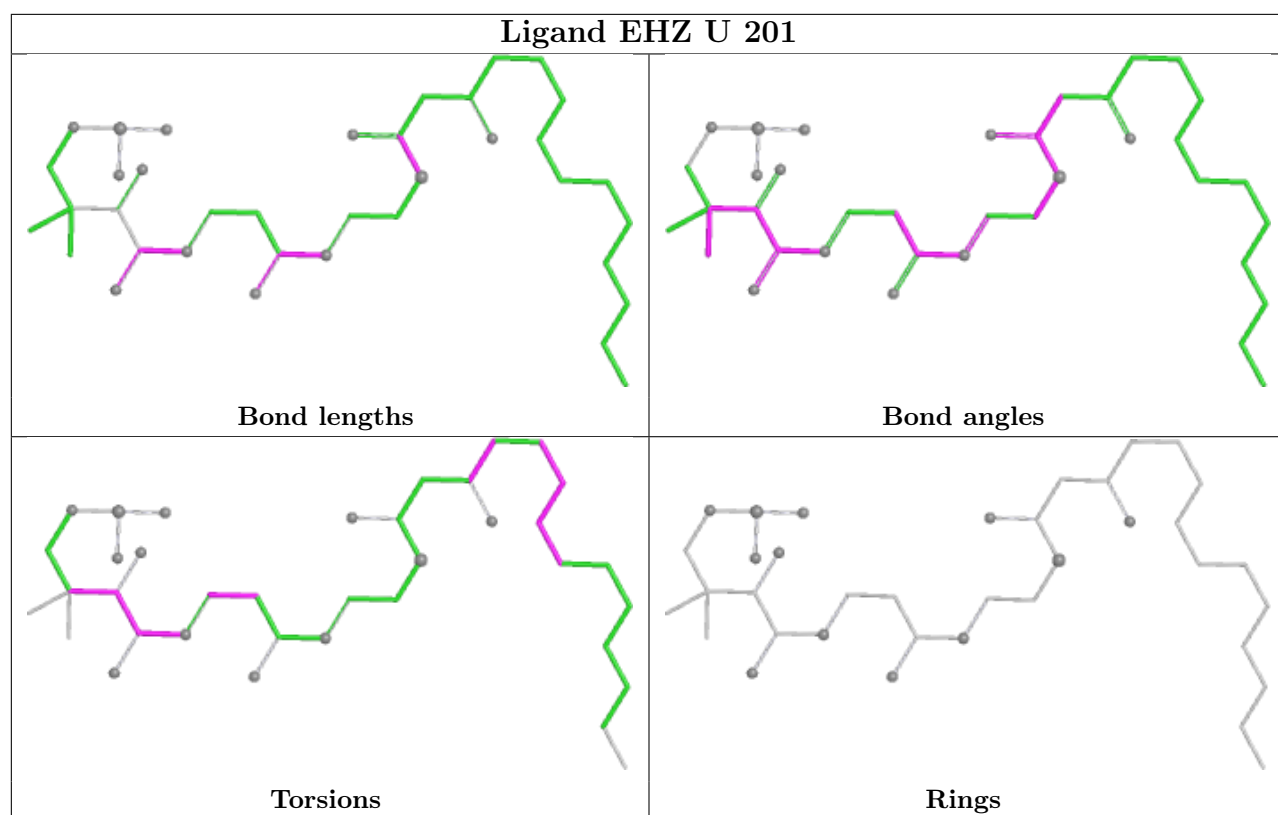
13 monomers are involved in 20 short contacts:

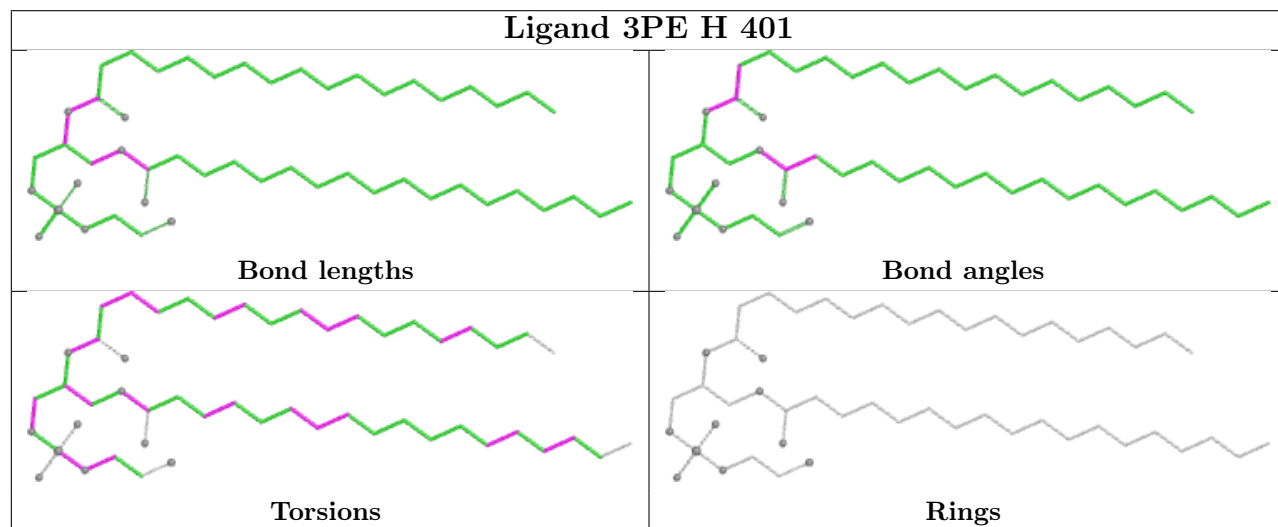
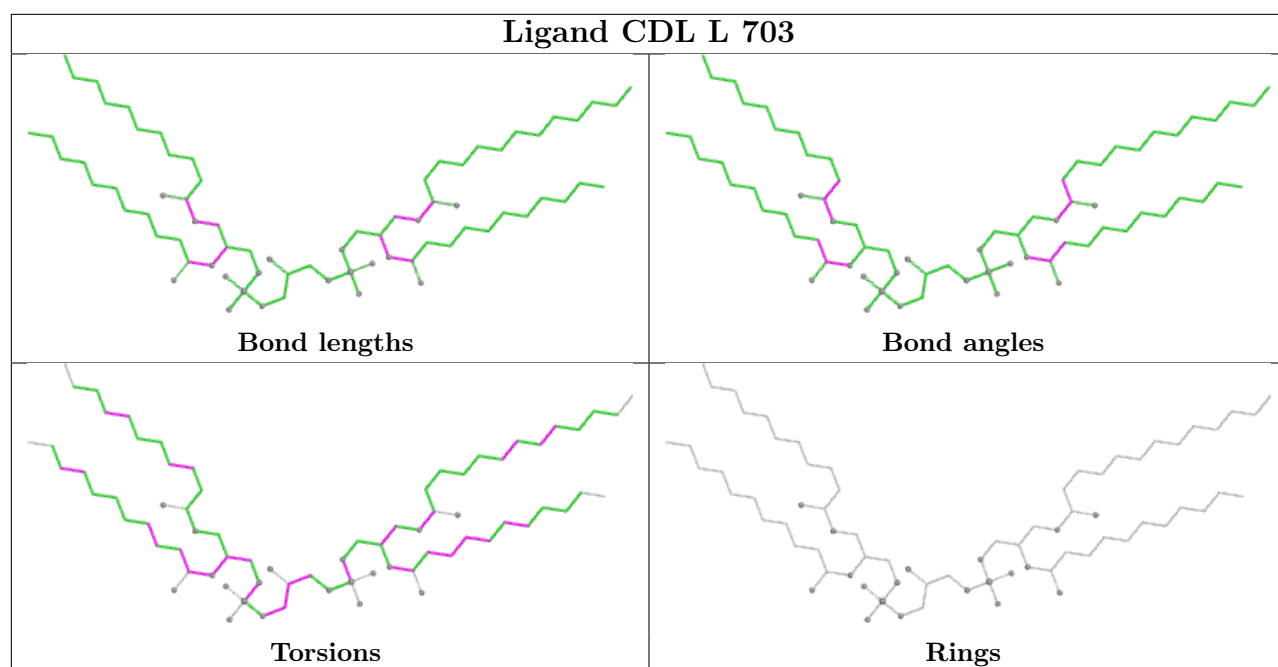
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	H	403	3PE	2	0
51	d	201	CDL	1	0
49	L	701	3PE	1	0
55	U	201	EHZ	1	0
53	P	501	NDP	2	0
49	H	401	3PE	1	0
48	F	502	FMN	4	0
51	N	401	CDL	1	0
49	L	702	3PE	1	0
51	i	201	CDL	1	0
46	J	201	PC1	2	0
55	T	201	EHZ	2	0
52	O	401	ATP	1	0

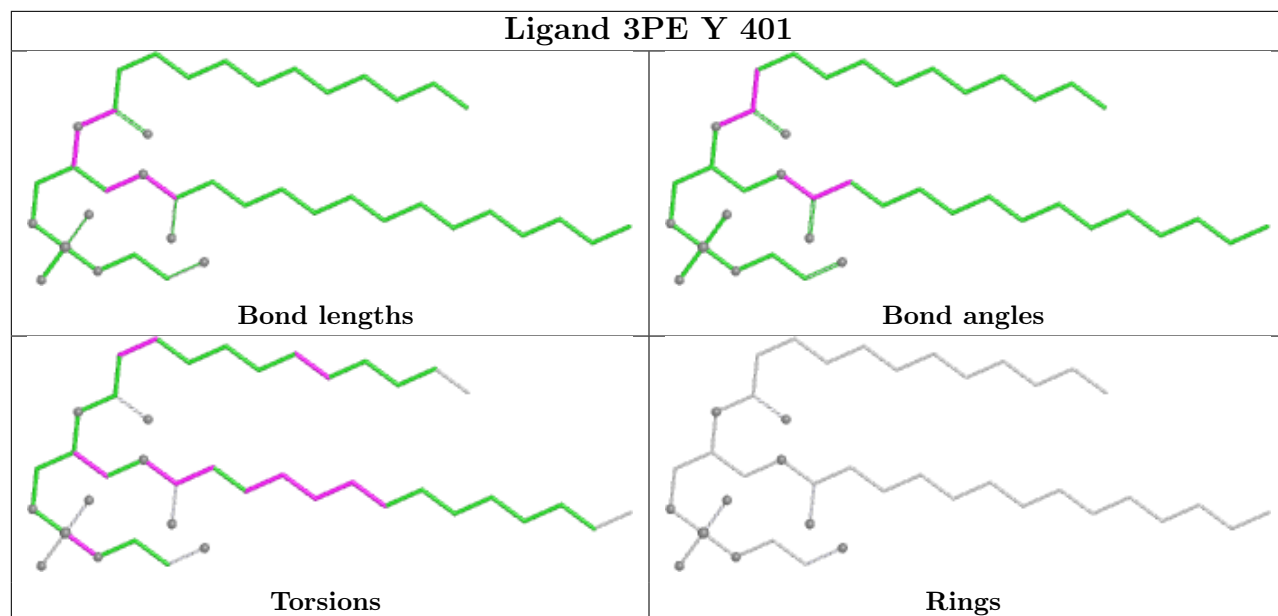
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

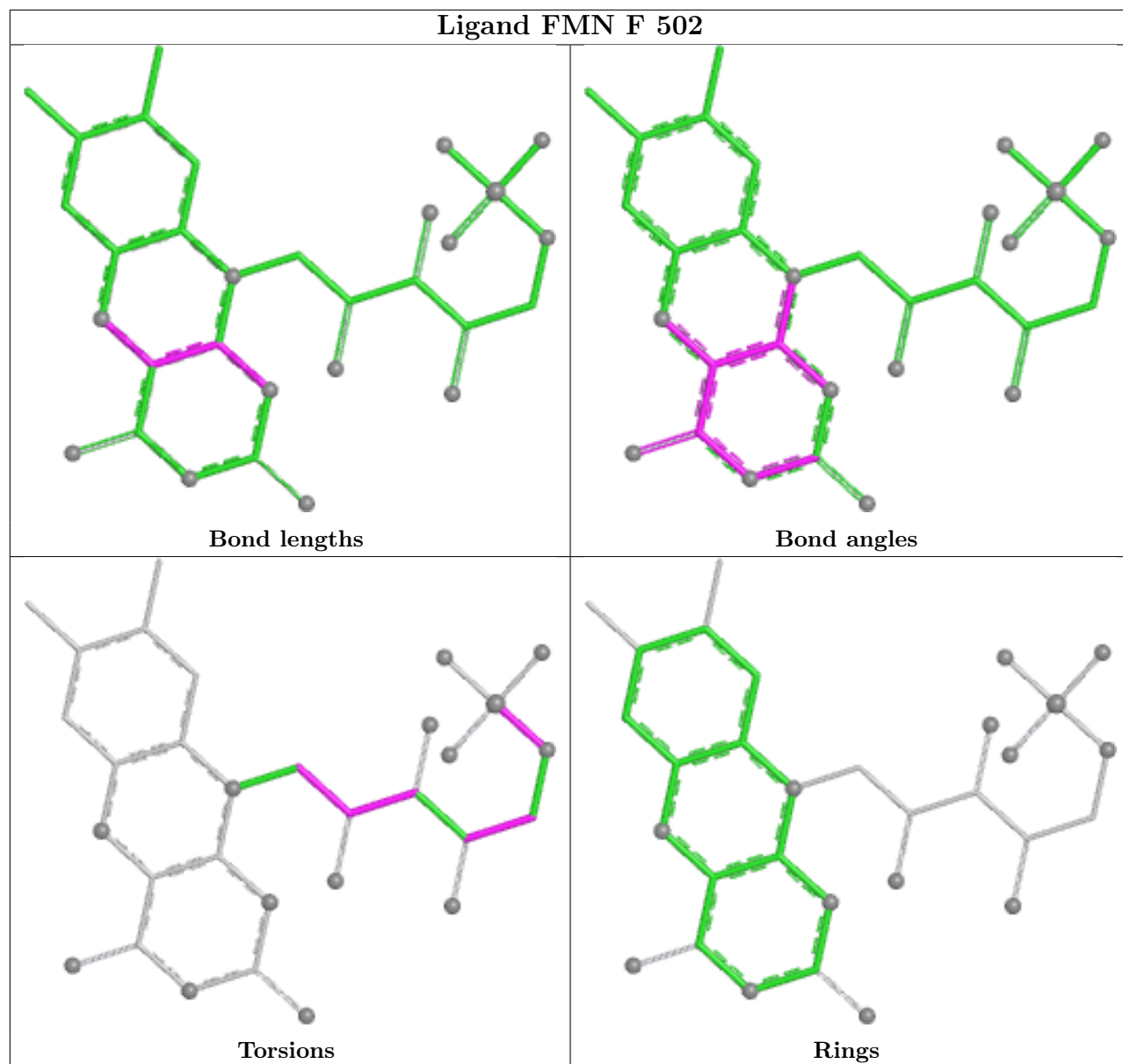


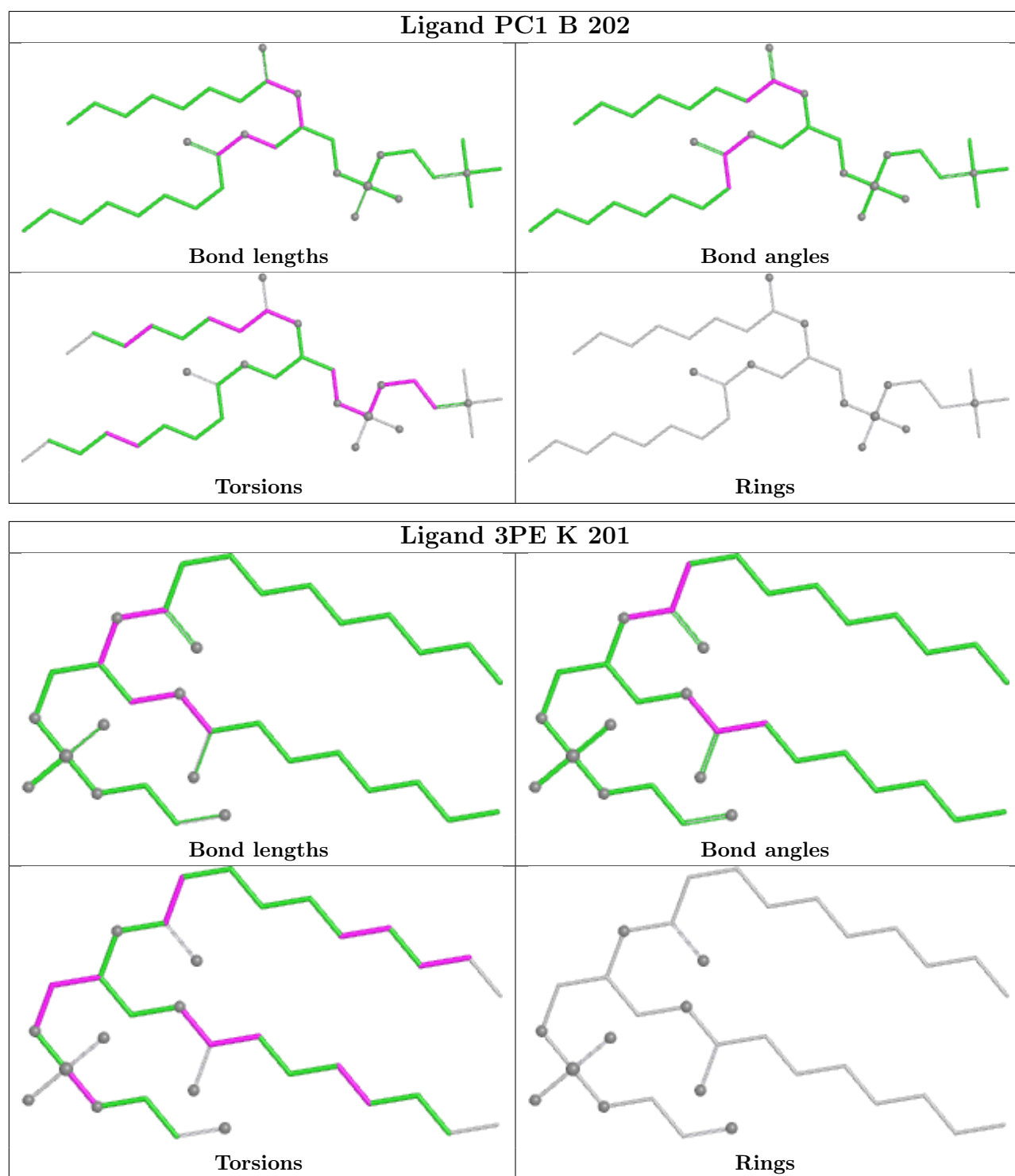


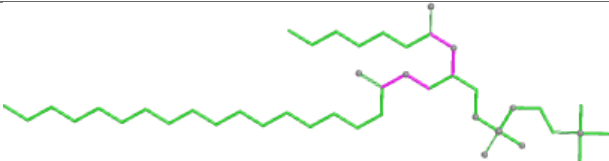
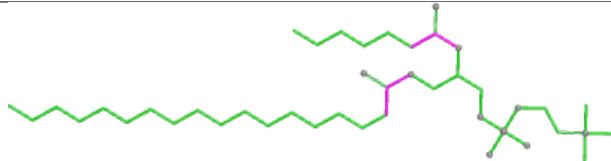
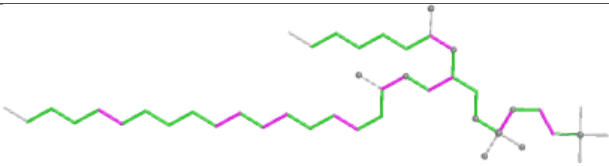
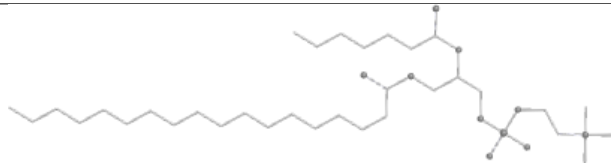


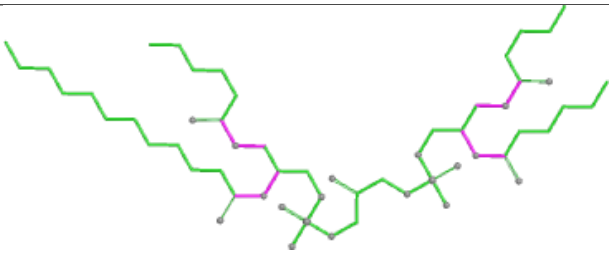
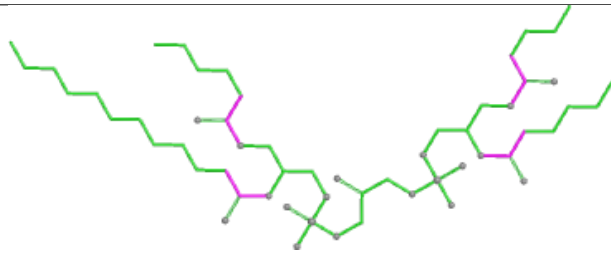
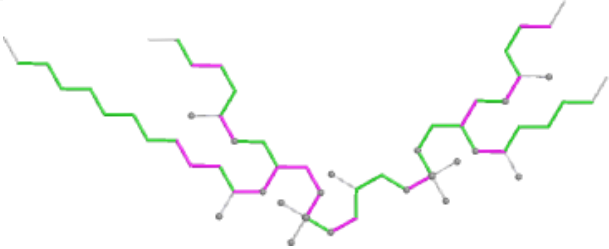
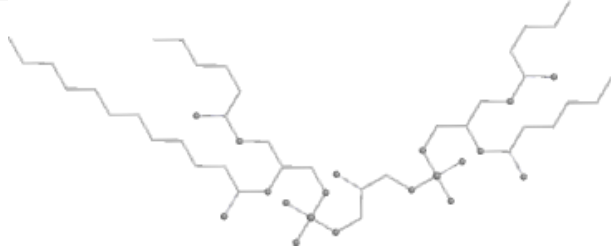


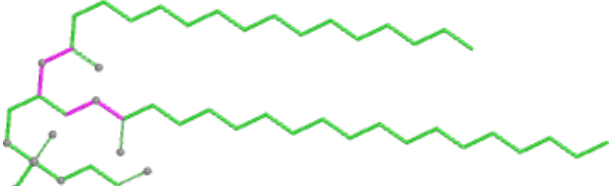
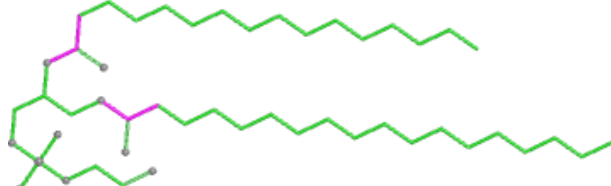
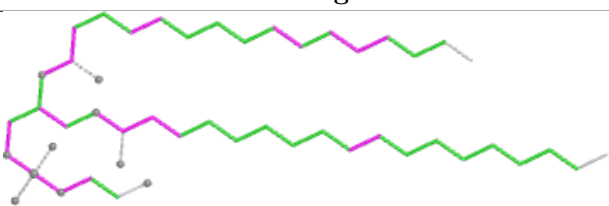
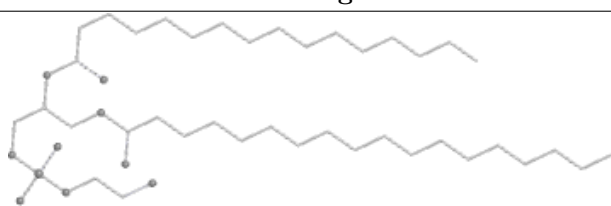


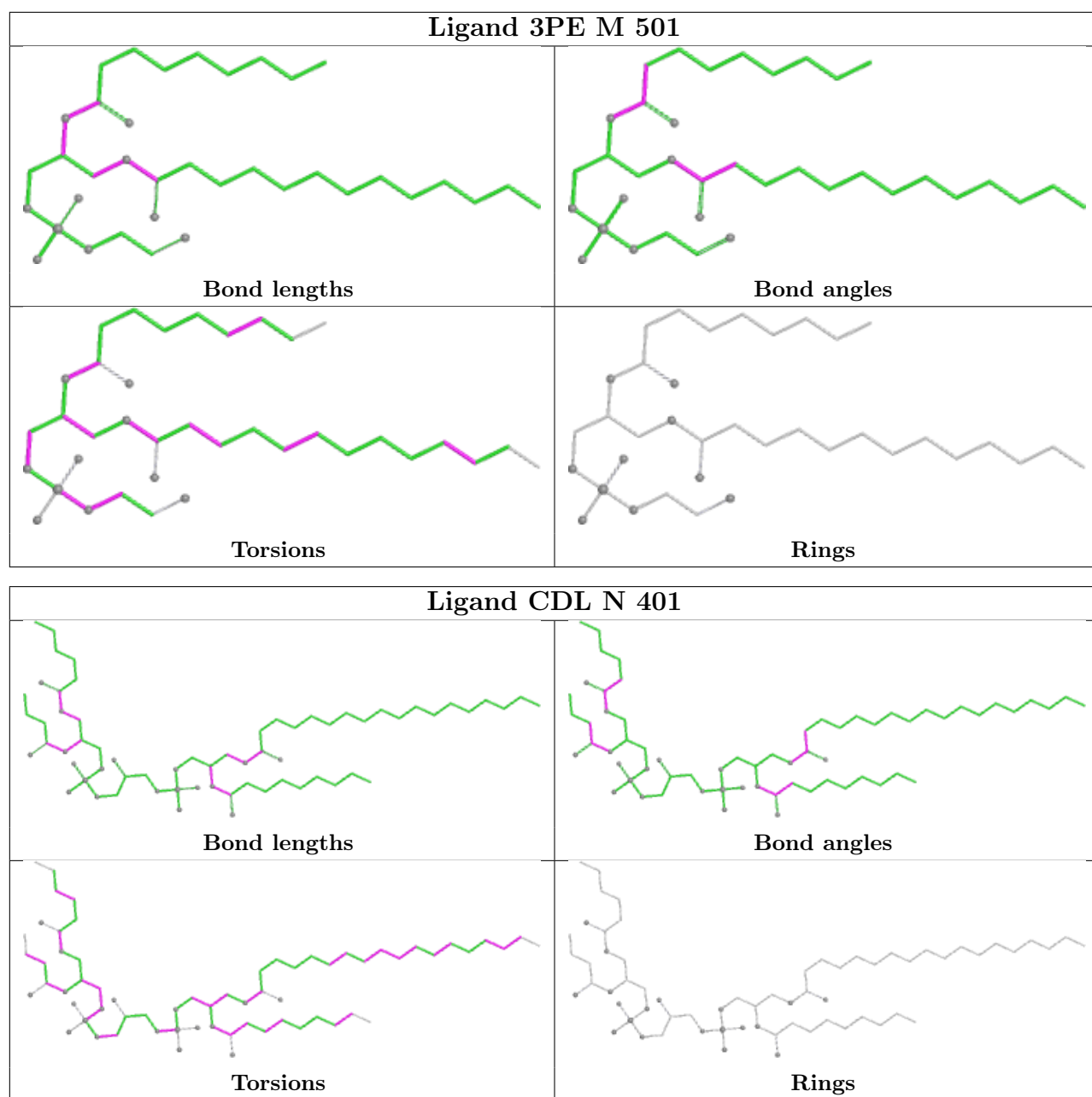


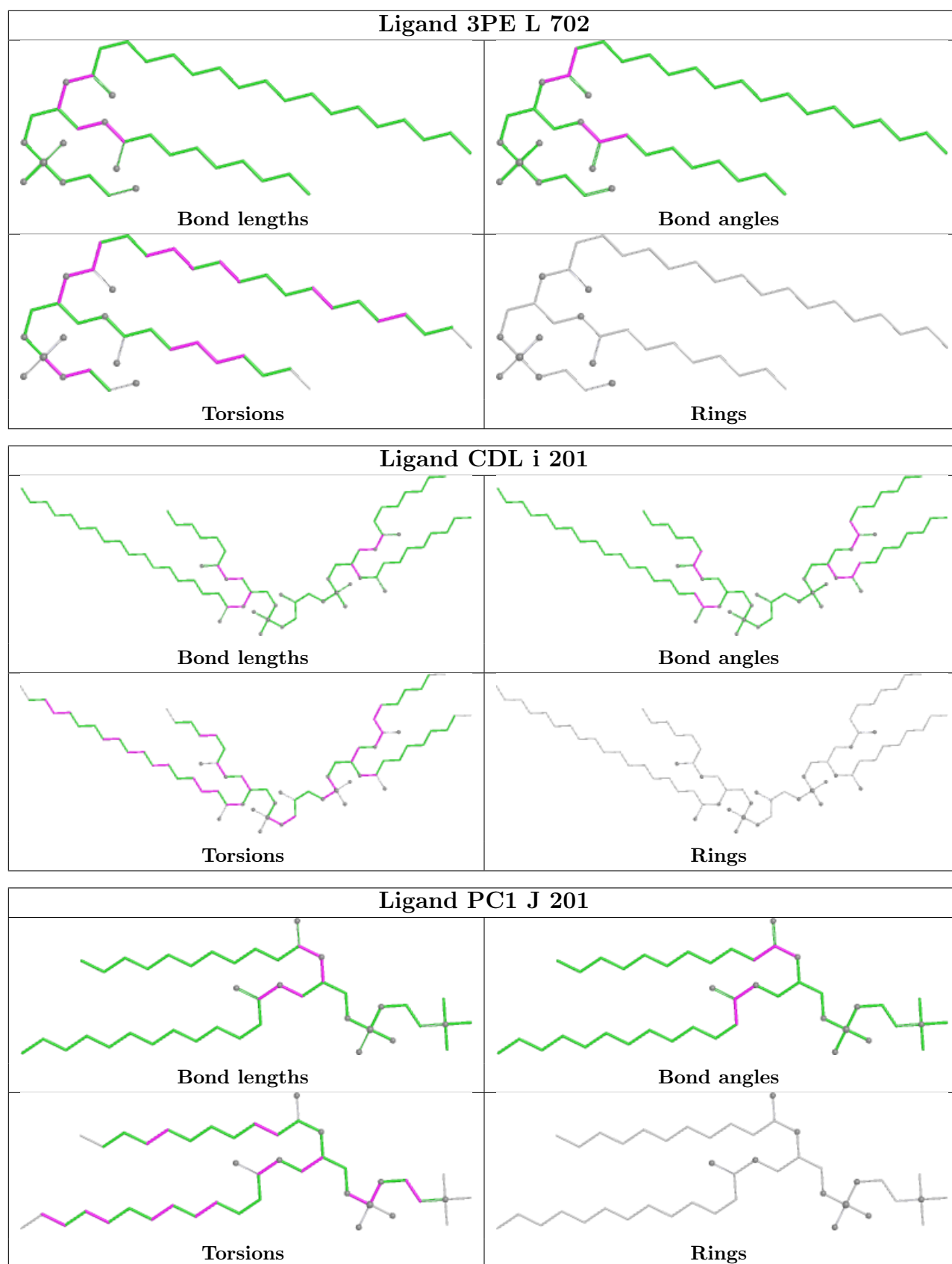


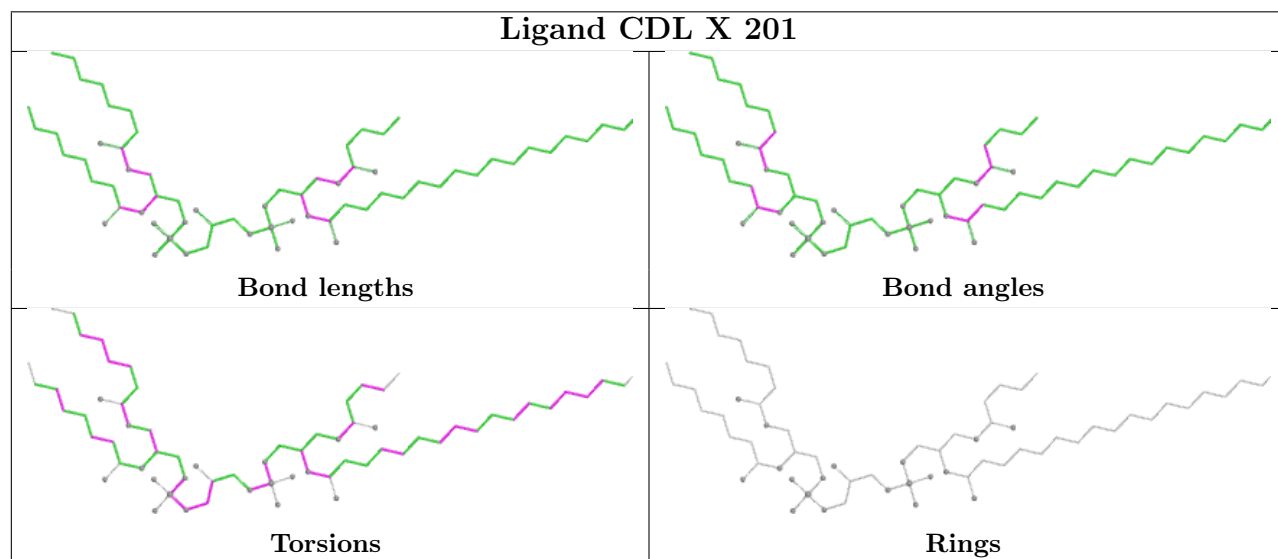
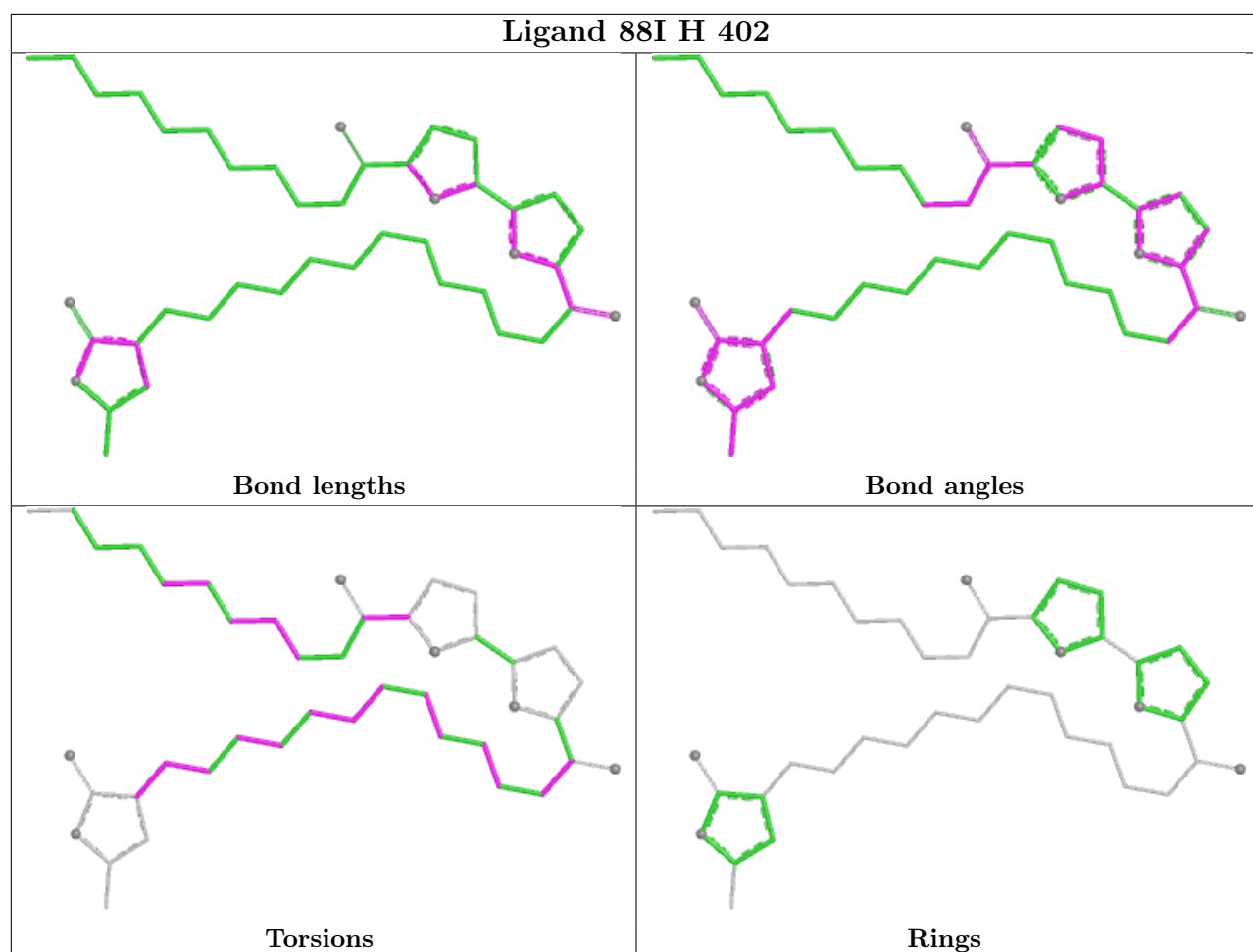
Ligand PC1 B 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

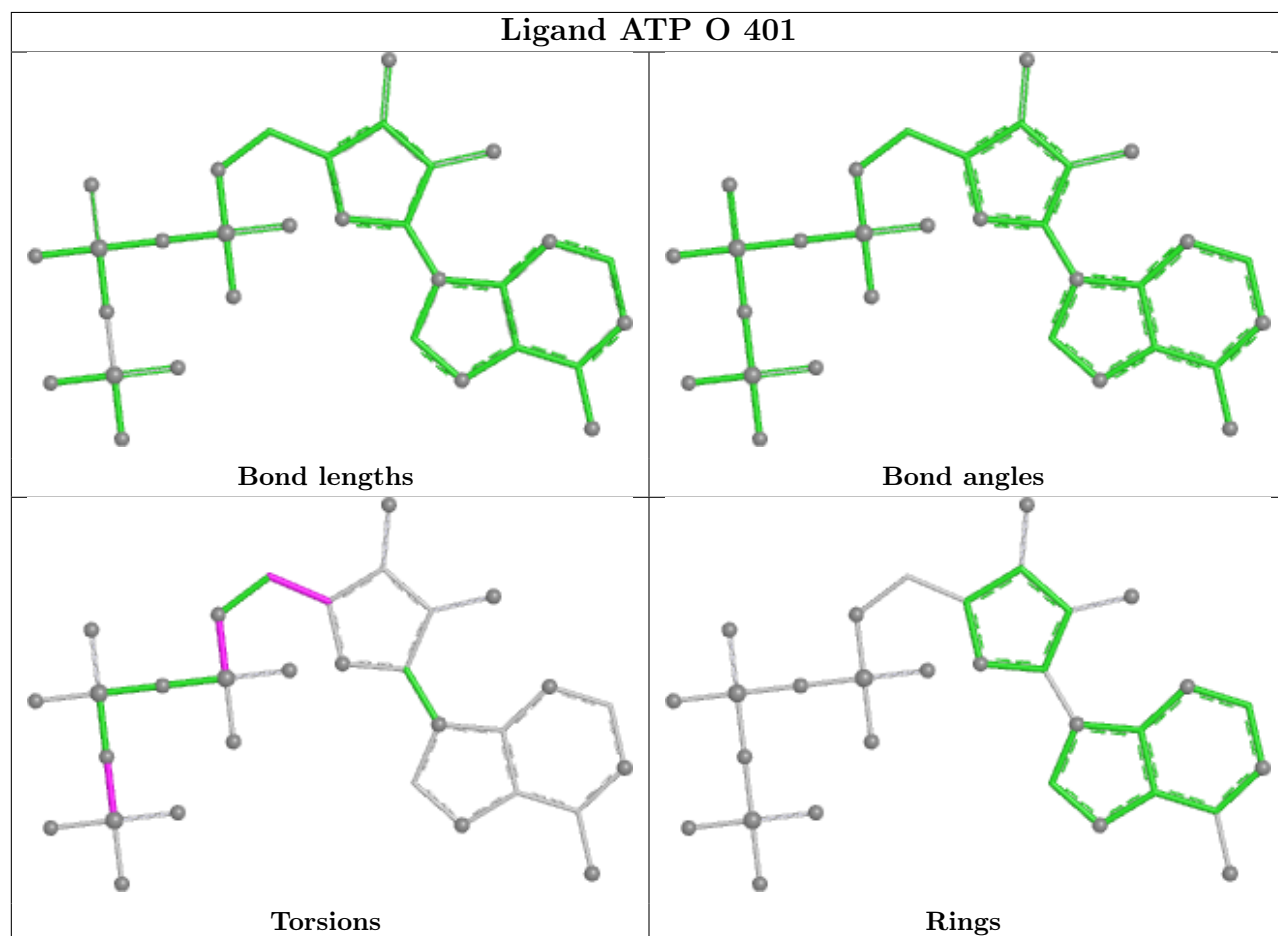
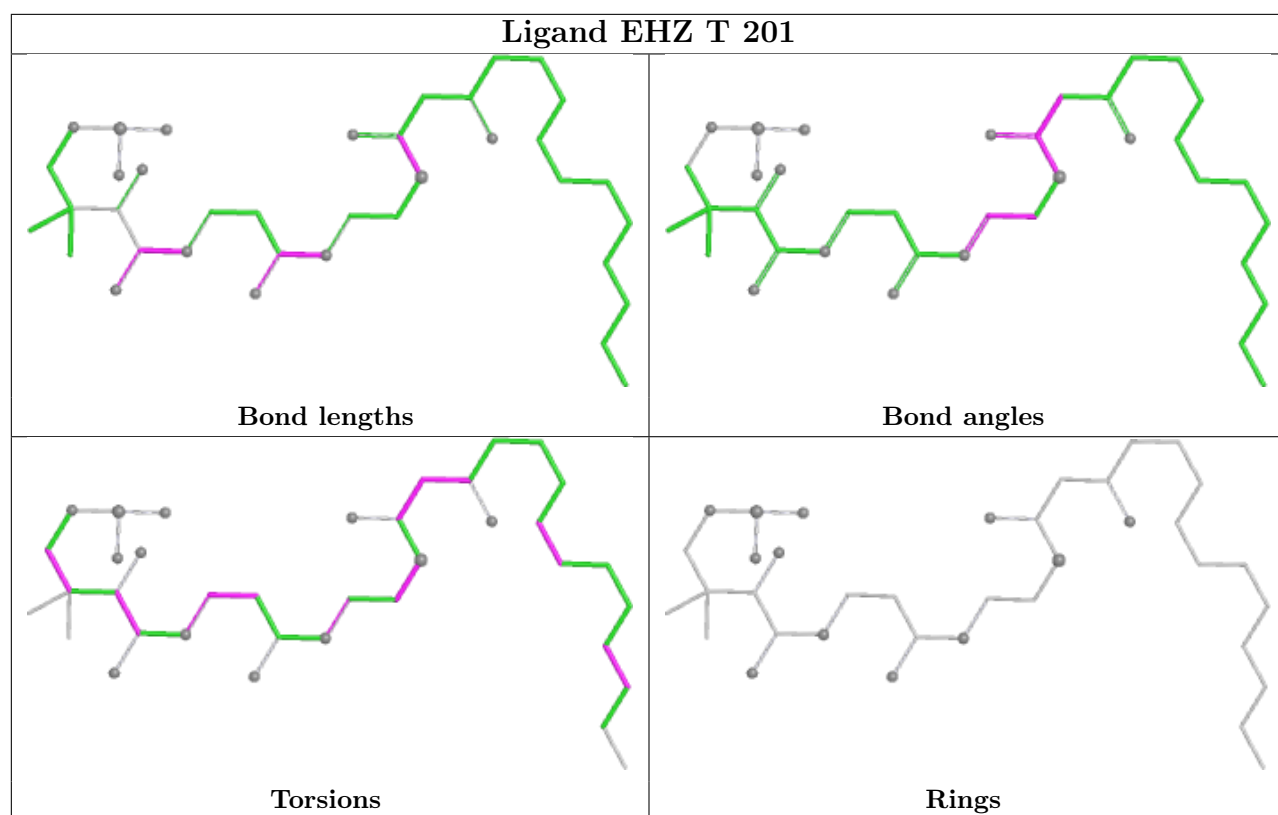
Ligand CDL r 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE L 704	
	
Bond lengths	Bond angles
	
Torsions	Rings









## 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.

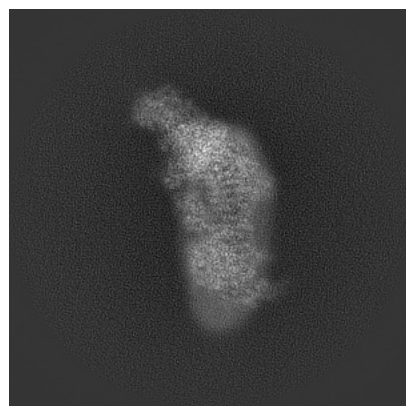
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13611. These allow visual inspection of the internal detail of the map and identification of artifacts.

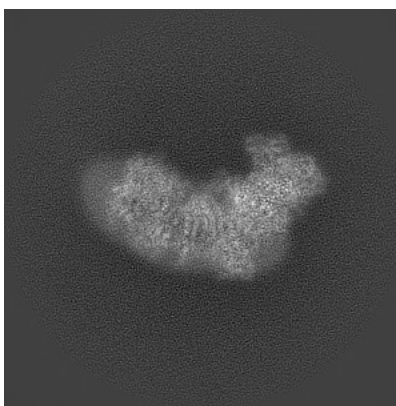
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

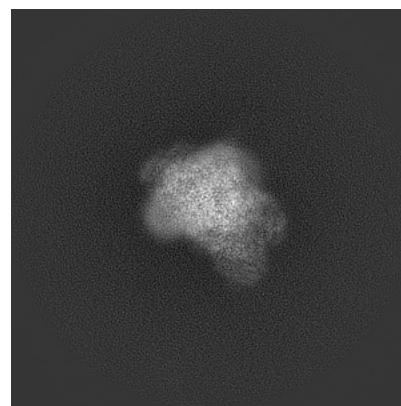
#### 6.1.1 Primary map



X

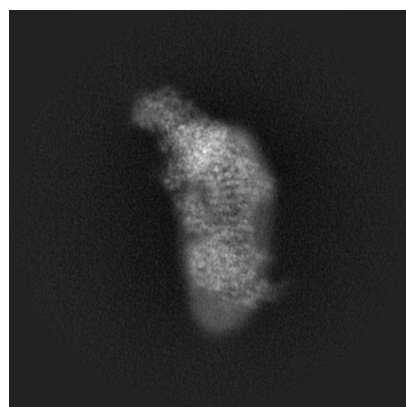


Y

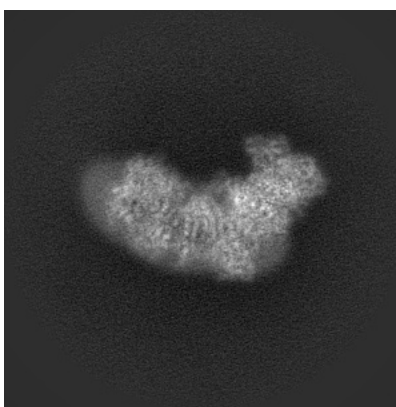


Z

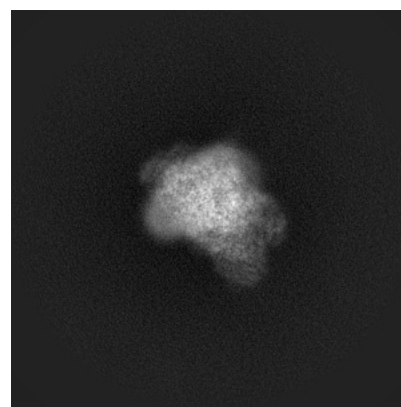
#### 6.1.2 Raw map



X



Y

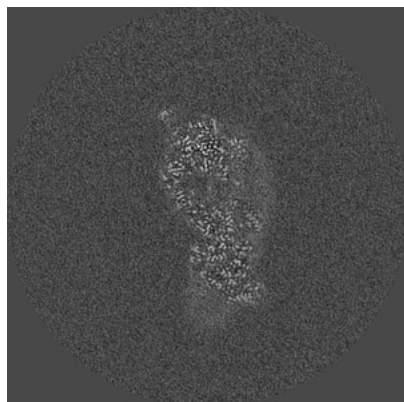


Z

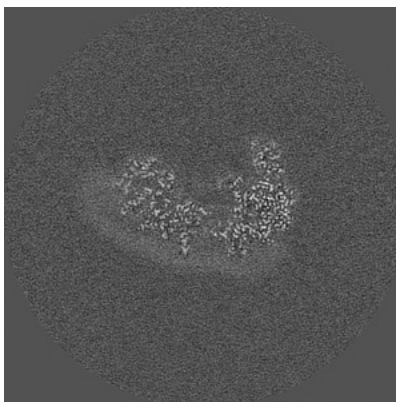
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

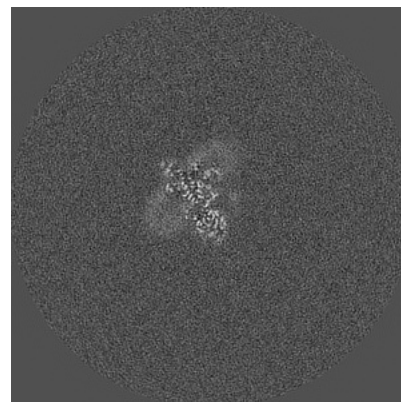
### 6.2.1 Primary map



X Index: 225

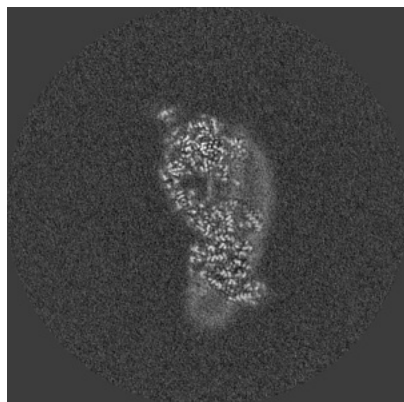


Y Index: 225

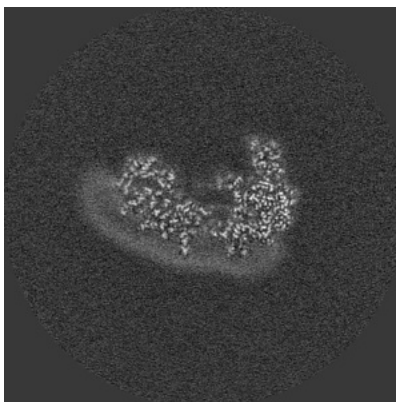


Z Index: 225

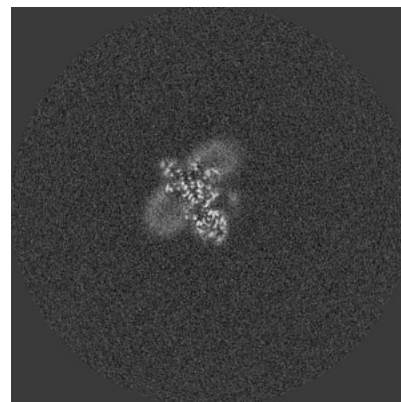
### 6.2.2 Raw map



X Index: 225



Y Index: 225

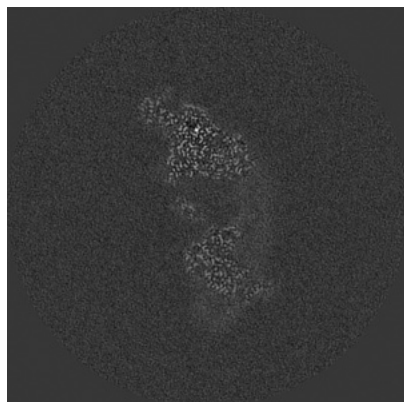


Z Index: 225

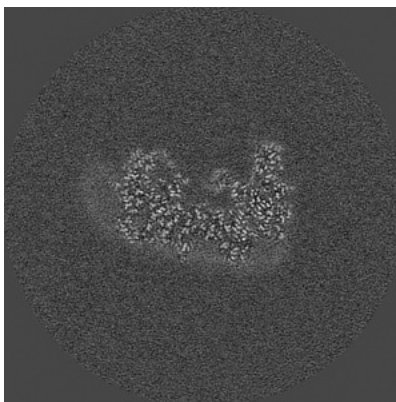
The images above show central slices of the map in three orthogonal directions.

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

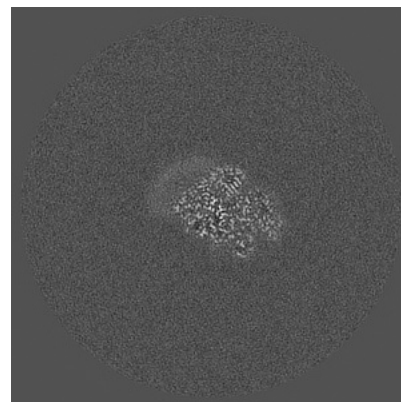
### 6.3.1 Primary map



X Index: 240

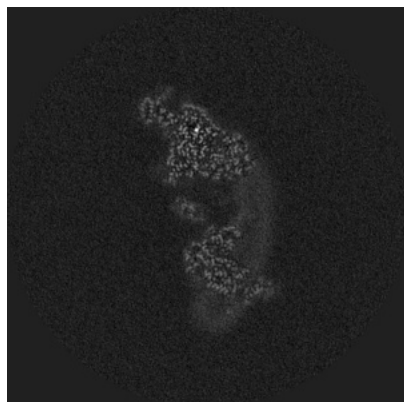


Y Index: 235

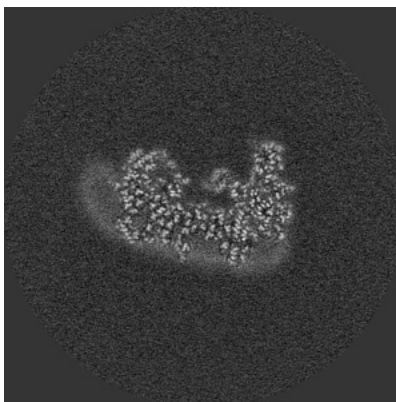


Z Index: 297

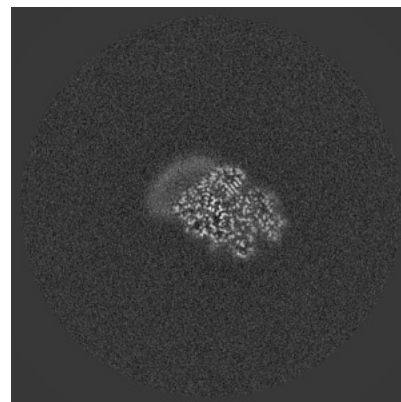
### 6.3.2 Raw map



X Index: 240



Y Index: 235

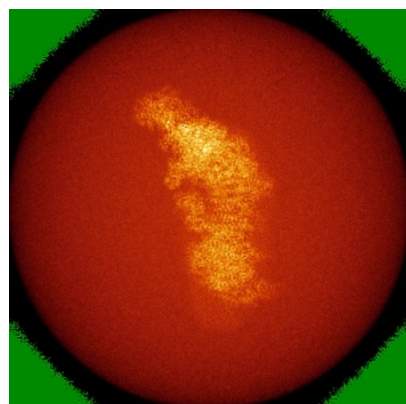


Z Index: 297

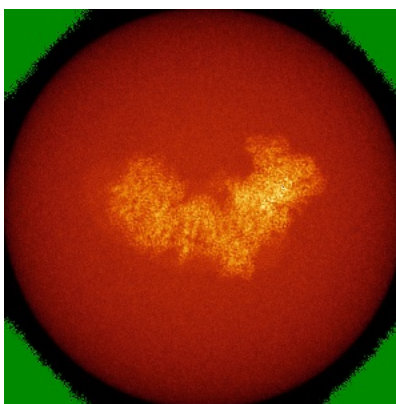
The images above show the largest variance slices of the map in three orthogonal directions.

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

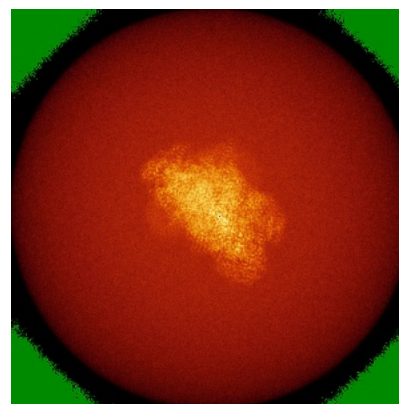
### 6.4.1 Primary map



X

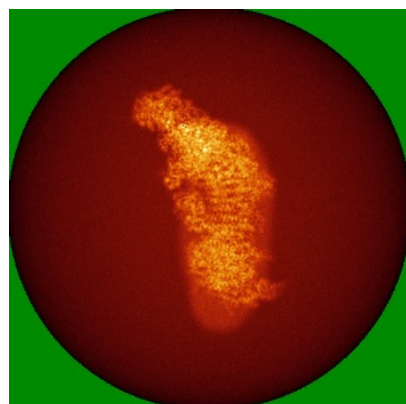


Y

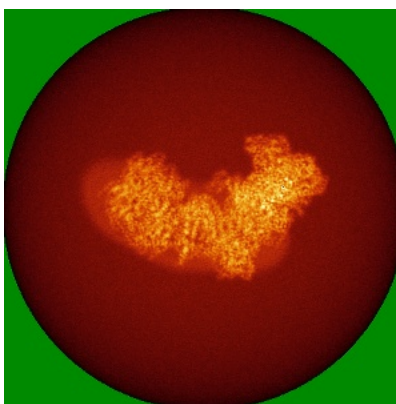


Z

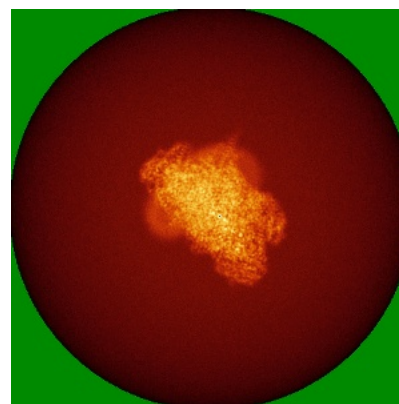
### 6.4.2 Raw map



X



Y

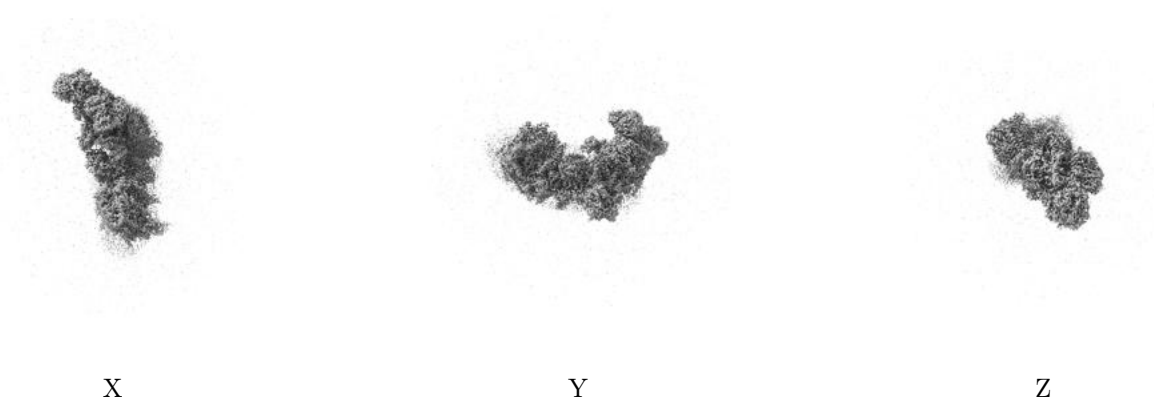


Z

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.

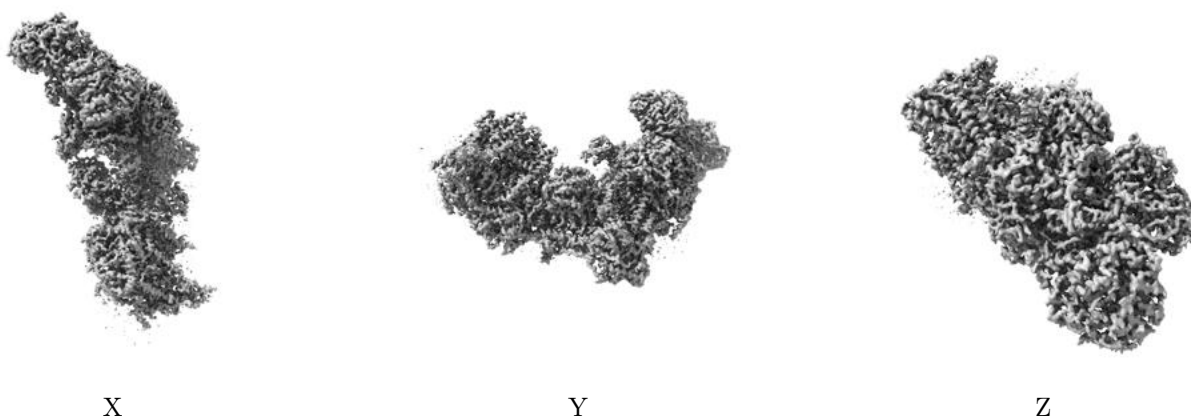
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

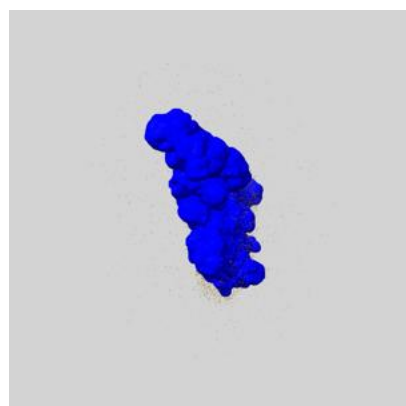
## 6.6 Mask visualisation [i](#)

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

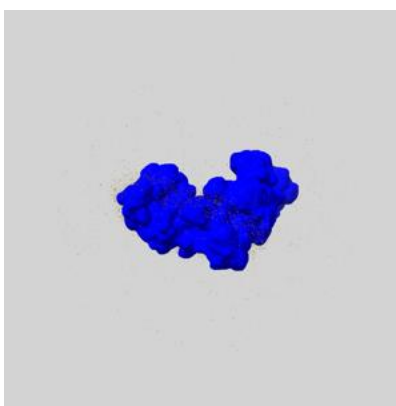
A mask typically either:

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

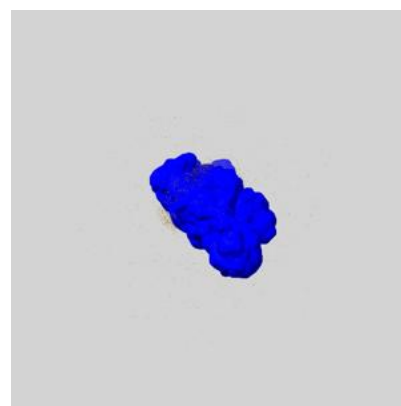
### 6.6.1 emd\_13611\_msk\_1.map [i](#)



X



Y

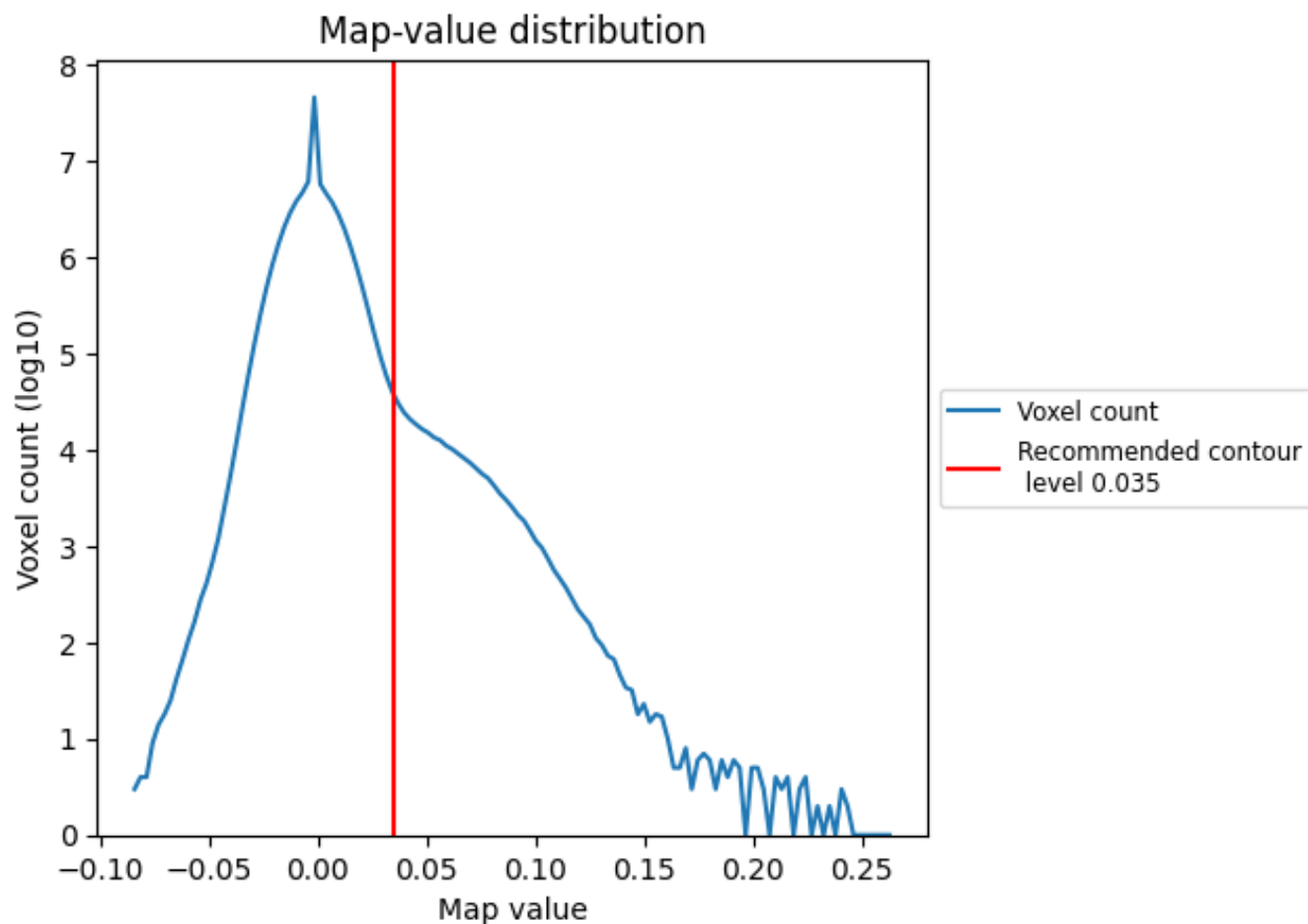


Z

## 7 Map analysis [i](#)

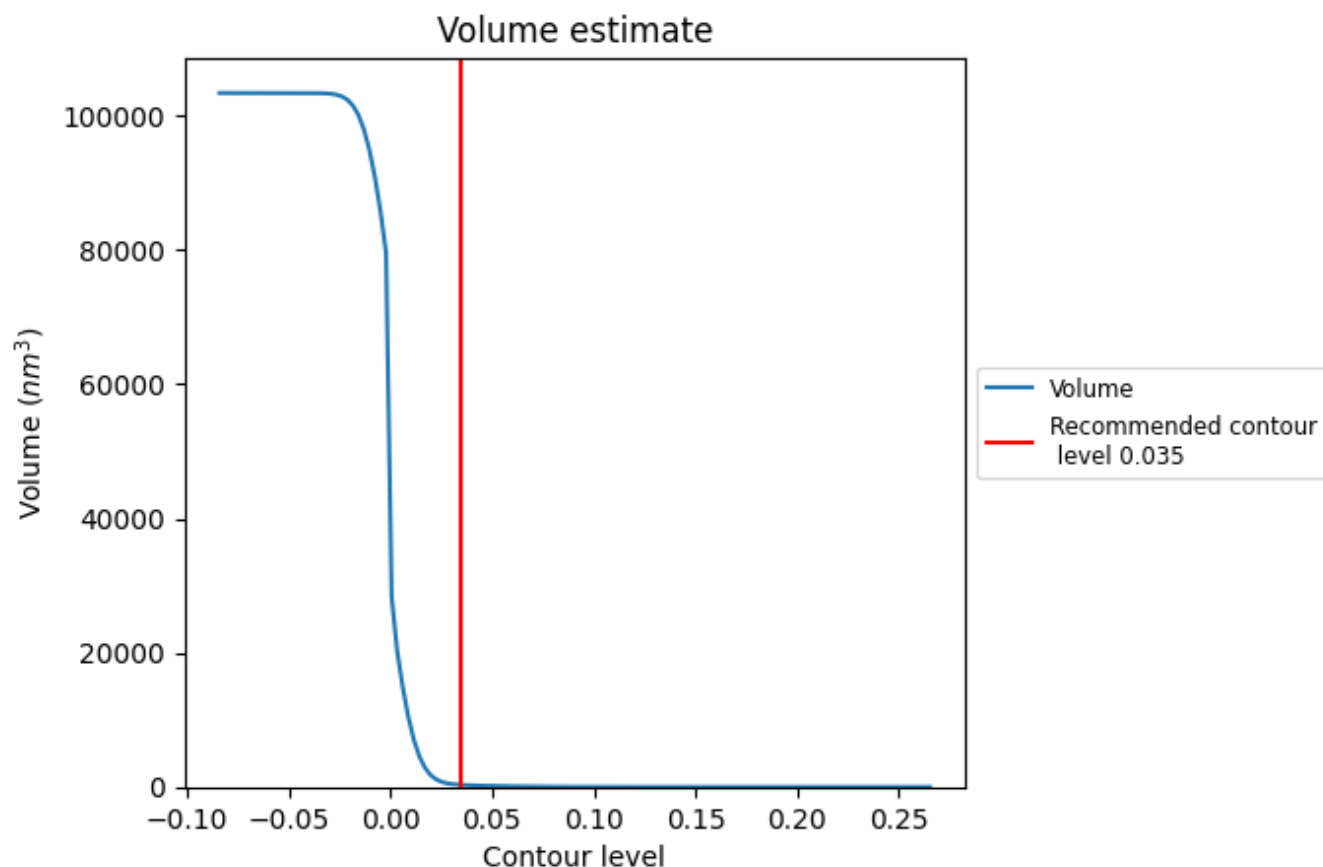
This section contains the results of statistical analysis of the map.

### 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.

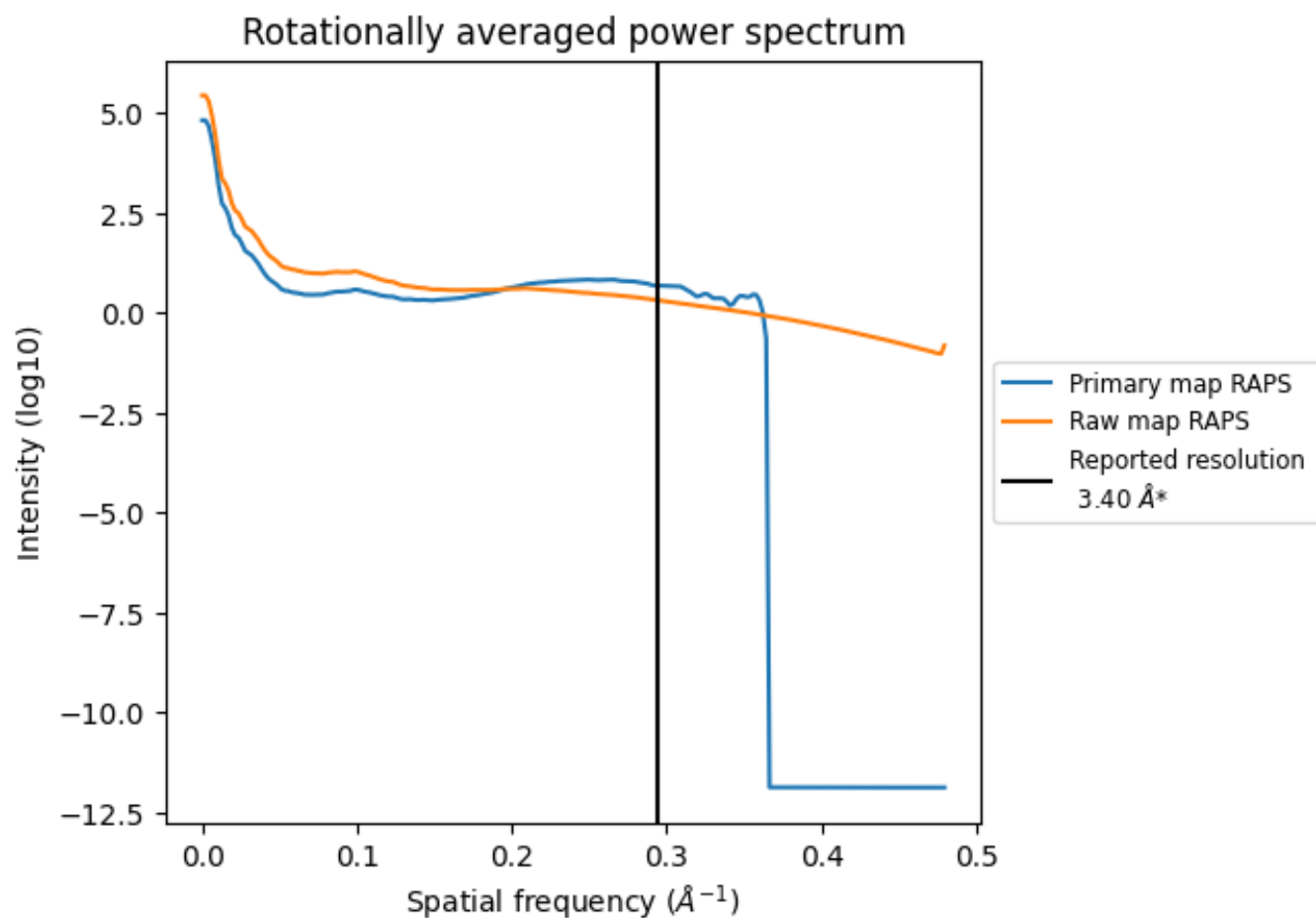
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306  $\text{nm}^3$ ; this corresponds to an approximate mass of 276 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 ⓘ

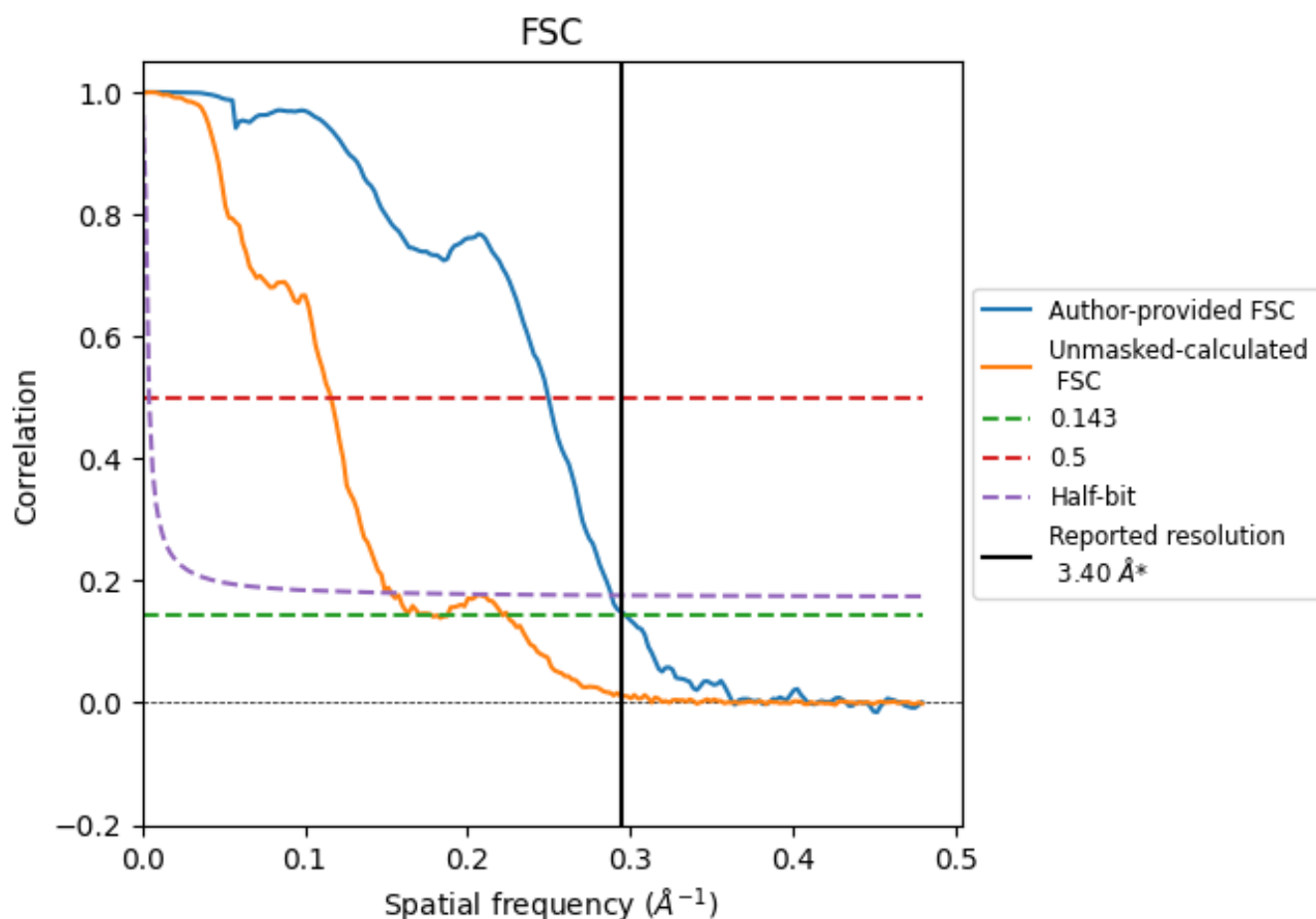


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

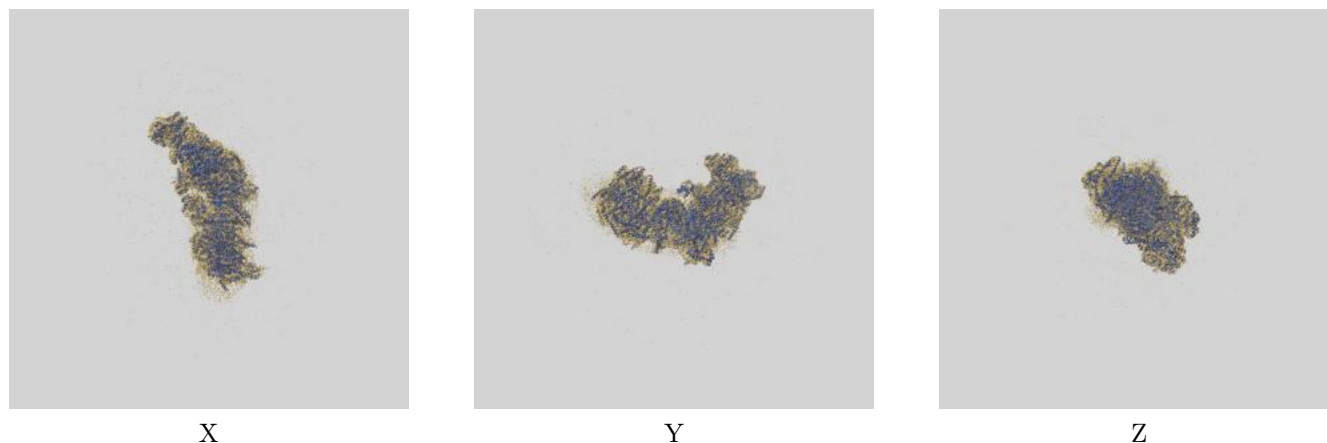
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.01	3.47
Unmasked-calculated*	5.62	8.64	6.54

\*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 5.62 differs from the reported value 3.4 by more than 10 %

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

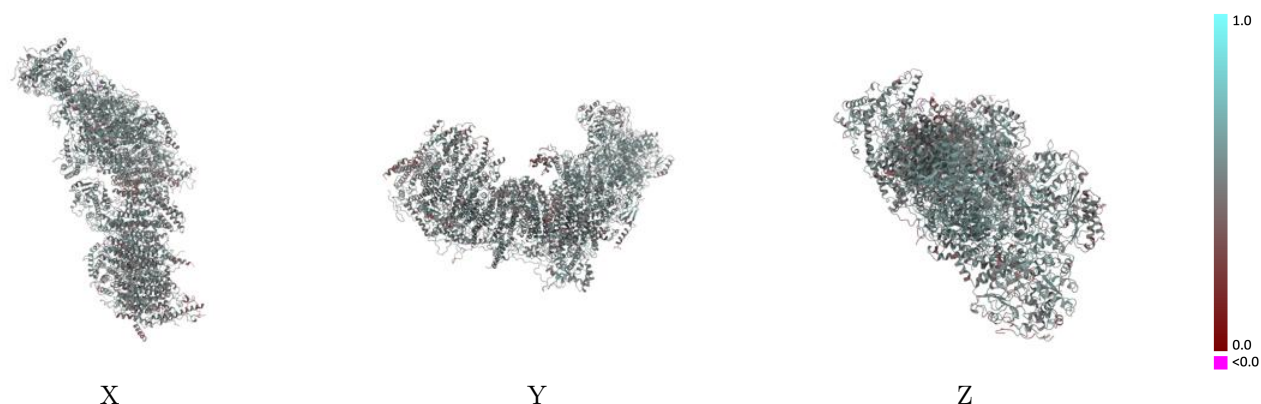
This section contains information regarding the fit between EMDB map EMD-13611 and PDB model 7PSA. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



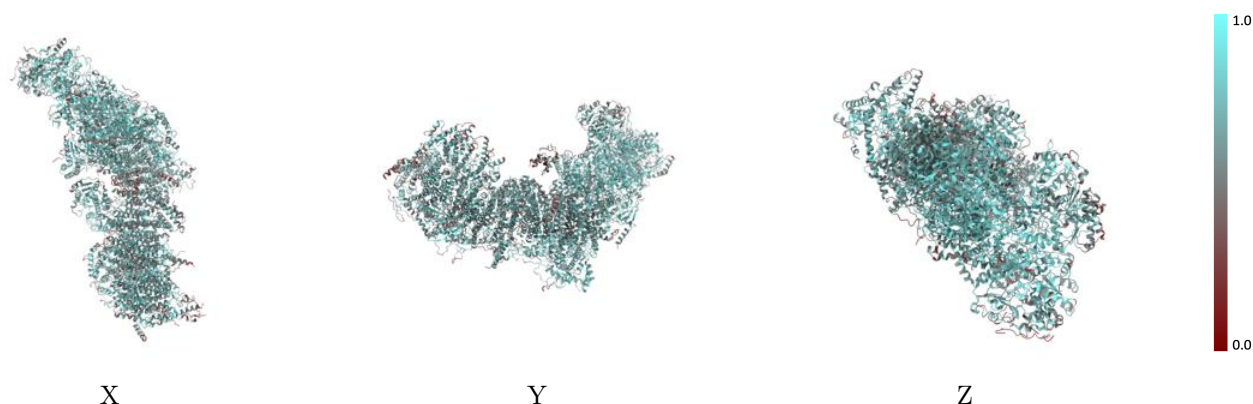
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



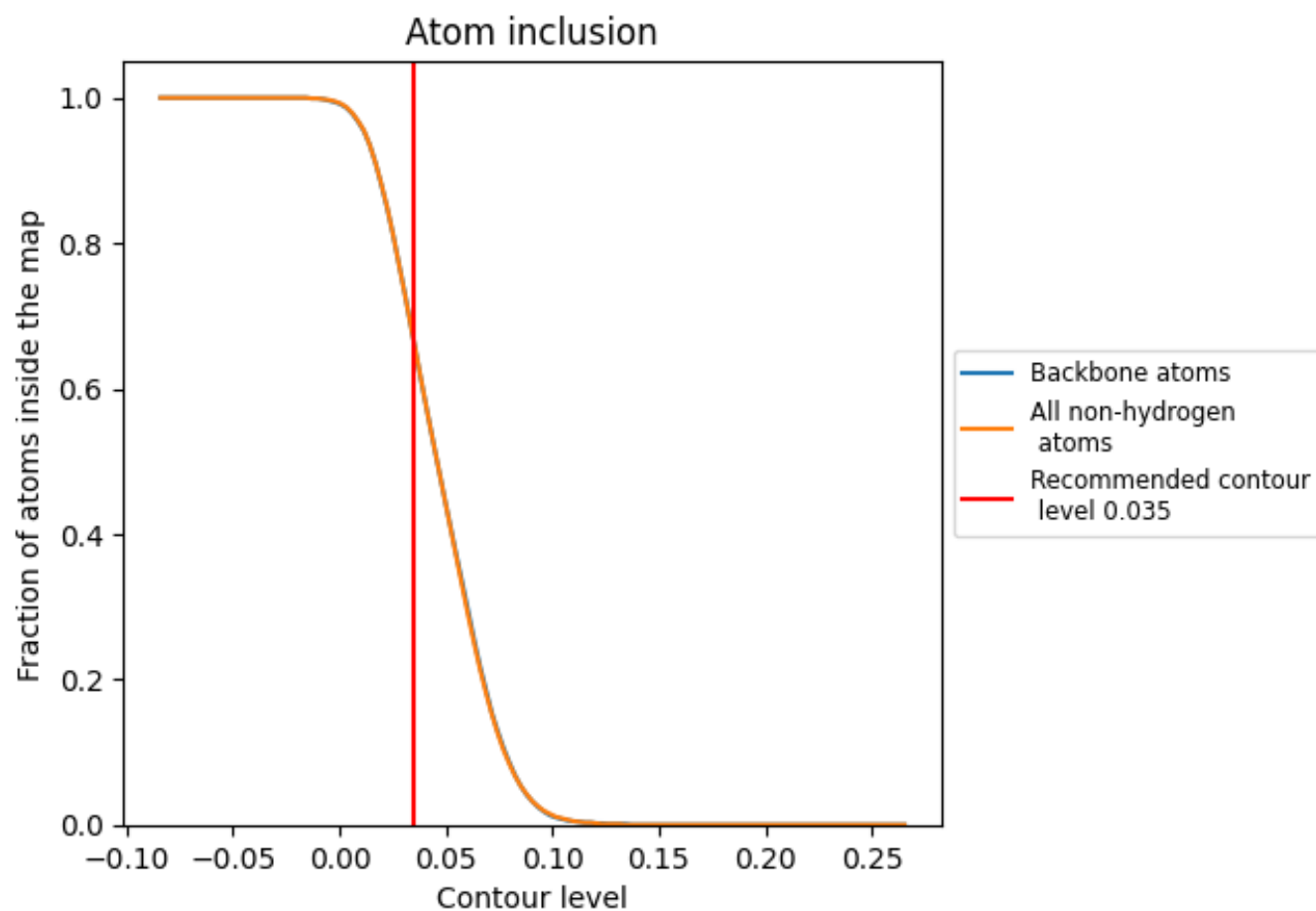
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.5160
A	 0.6680	 0.5230
B	 0.7740	 0.5590
C	 0.7680	 0.5570
D	 0.7380	 0.5470
E	 0.6500	 0.4990
F	 0.6760	 0.5100
G	 0.6890	 0.5230
H	 0.6920	 0.5320
I	 0.7640	 0.5460
J	 0.6080	 0.4800
K	 0.6770	 0.5360
L	 0.6550	 0.5180
M	 0.6990	 0.5390
N	 0.6860	 0.5340
O	 0.6980	 0.5290
P	 0.6870	 0.5250
Q	 0.6920	 0.5360
R	 0.7160	 0.5480
S	 0.6020	 0.4820
T	 0.3890	 0.4050
U	 0.5980	 0.4740
V	 0.6320	 0.5060
W	 0.6760	 0.5230
X	 0.6400	 0.4970
Y	 0.5700	 0.4840
Z	 0.6690	 0.5070
a	 0.7260	 0.5320
b	 0.6320	 0.5050
c	 0.5690	 0.4670
d	 0.6520	 0.5160
e	 0.6600	 0.5130
f	 0.5530	 0.4620
g	 0.6260	 0.5080
h	 0.7040	 0.5300



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Chain	Atom inclusion	Q-score
i	 0.5900	 0.4940
j	 0.5650	 0.4560
k	 0.5590	 0.4620
l	 0.6590	 0.5050
m	 0.6140	 0.4750
n	 0.6300	 0.4940
o	 0.5650	 0.4490
p	 0.6450	 0.4930
q	 0.7040	 0.5310
r	 0.6230	 0.5010
s	 0.6330	 0.5040