



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:41 PM UTC

PDB ID : 6G2J / pdb_00006g2j
EMDB ID : EMD-4345
Title : Mouse mitochondrial complex I in the active state
Authors : Agip, A.N.A.; Blaza, J.N.; Bridges, H.R.; Viscomi, C.; Rawson, S.; Muench, S.P.; Hirst, J.
Deposited on : 2018-03-23
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

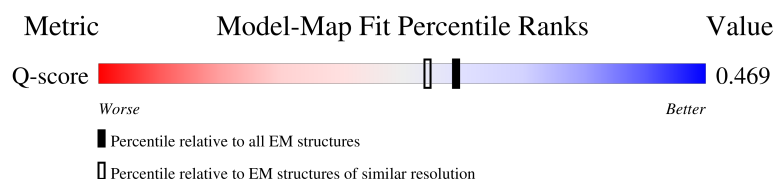
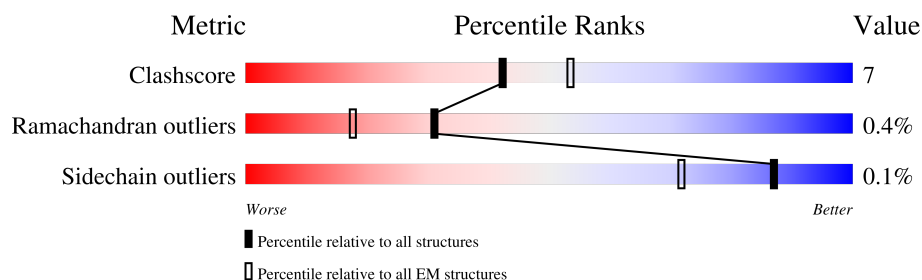
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	115	17% 82% 18%
2	B	224	7% 55% 13% 31%
3	C	263	13% 65% 13% 22%
4	D	463	11% 69% 24% 7%

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	428	
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	67	
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	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 66810 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			933	633	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	155	Total	C	N	O	S	0	0
			1241	793	222	212	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1712	1105	294	310	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	N	O	S	0	0
			3452	2207	593	628	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1648	1048	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	N	O	S	0	0
			3301	2080	590	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	N	O	S	0	0
			5296	3321	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	N	O	S	0	0
			2540	1706	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	N	O	S	0	0
			1408	885	243	268	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1300	874	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	N	O	S	0	0
			737	477	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	N	O	S	0	0
			4800	3182	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	N	O	S	0	0
			3632	2408	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	N	O	S	0	0
			2696	1791	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	N	O	S	0	0
			2607	1674	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	N	O	S	0	0
			2748	1777	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	N	O	S	0	0
			1015	642	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	95	Total	C	N	O	S	0	0
			748	464	138	143	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	N	O	S	0	0
			667	419	126	119	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			985	645	167	164	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			870	550	161	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			433	278	78	75	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	N	O	S	0	0
			850	549	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	137	Total	C	N	O	S	0	0
			1154	758	192	201	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	101	Total	C	N	O	S	0	0
			820	534	141	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	60	Total	C	N	O	S	0	0
			525	345	88	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	72	Total	C	N	O	S	0	0
			582	384	100	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	152	Total	C	N	O	S	0	0
			1274	821	213	229	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	124	Total	C	N	O		0	0
			1035	667	186	182			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	176	Total	C	N	O	S	0	0
			1527	976	274	266	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	105	Total	C	N	O	S	0	0
			898	565	167	158	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	170	Total	C	N	O	S	0	0
			1438	903	258	269	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	N	O	S	0	0
			1203	773	213	212	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	1	AME	MET	conflict	UNP Q7TMF3

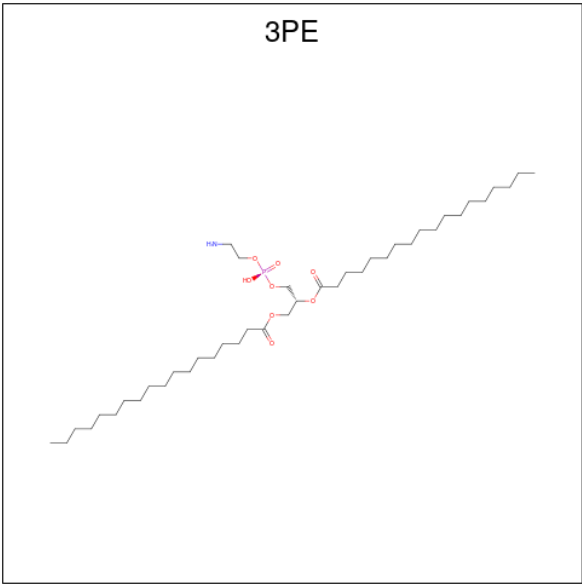
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	99	Total	C	N	O	S	0	0
			796	504	148	141	3		

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

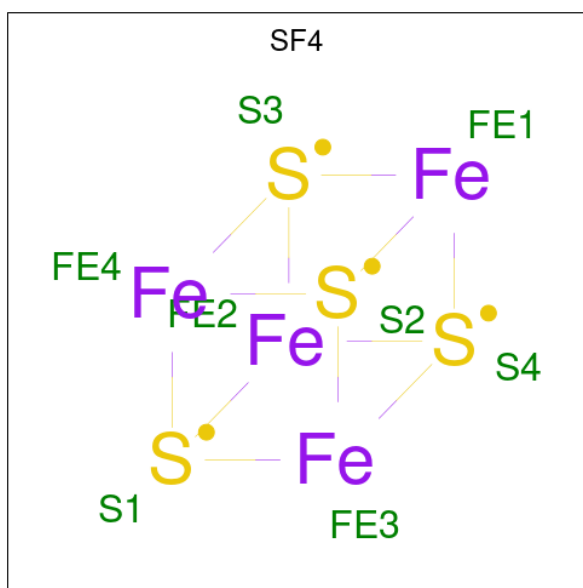
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	40	Total	C	N	O	0	0
			336	211	60	65		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



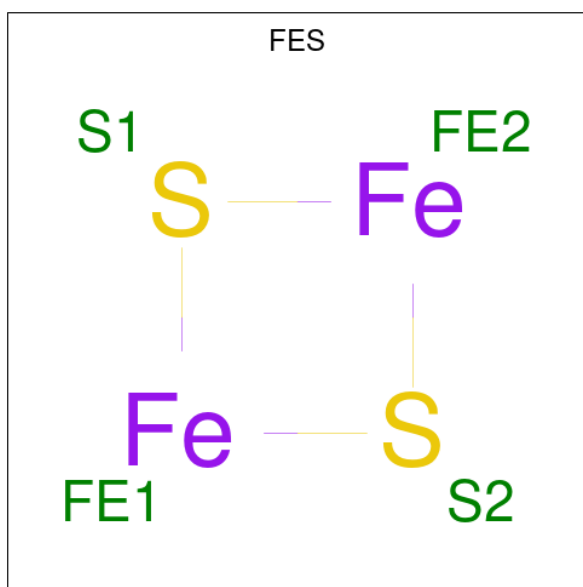
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	O	P		0
			42	33	8	1		
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	M	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	N	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



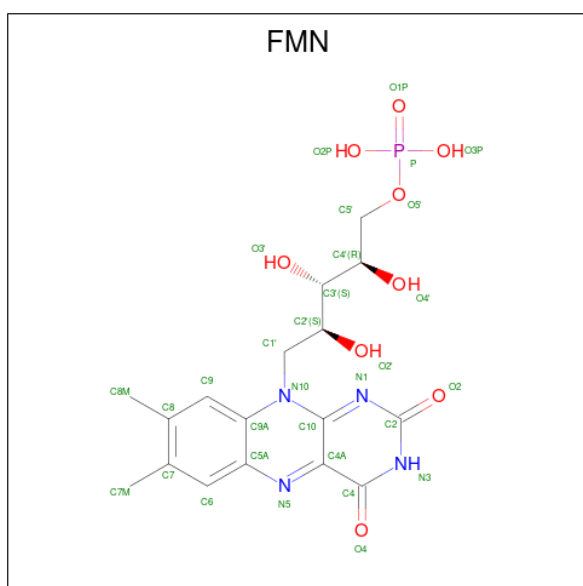
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	
46	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

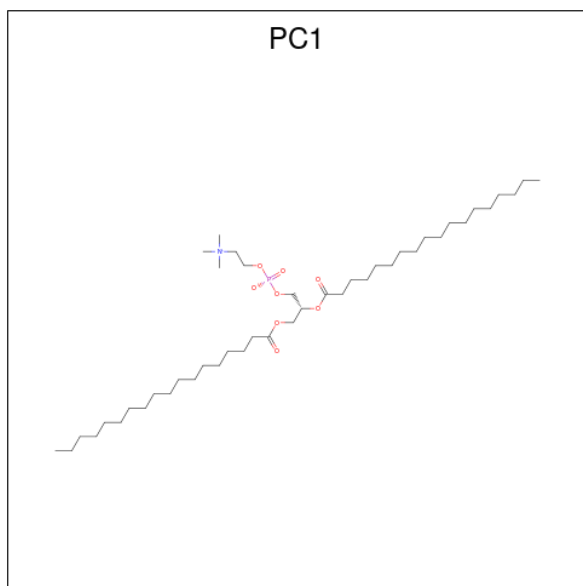


Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

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

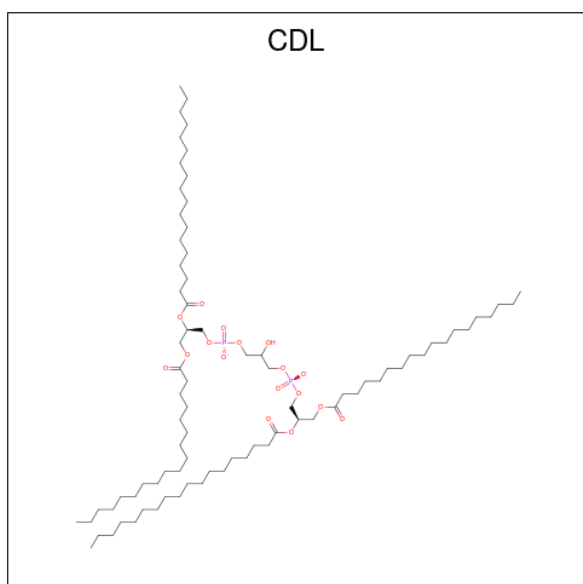


(formula: $C_{44}H_{88}NO_8P$).



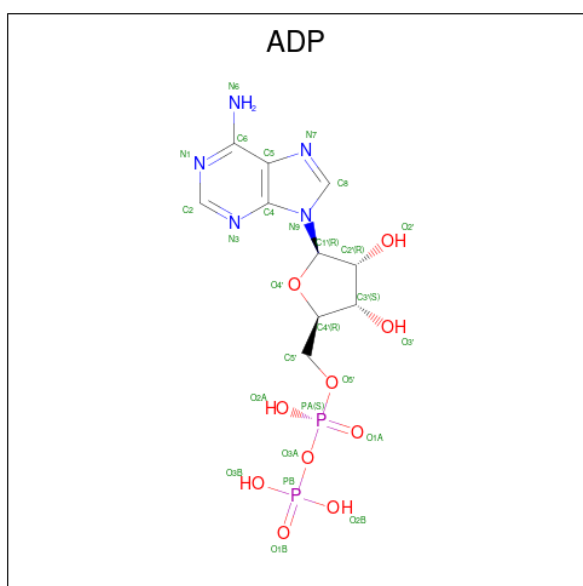
Mol	Chain	Residues	Atoms					AltConf
49	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
49	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
49	H	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	P	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
50	H	1	Total 57	C 38	O 17	P 2	0
50	L	1	Total 78	C 59	O 17	P 2	0
50	L	1	Total 70	C 51	O 17	P 2	0
50	M	1	Total 67	C 48	O 17	P 2	0

- Molecule 51 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total 48	C 21	N 7	O 17	P 3	0

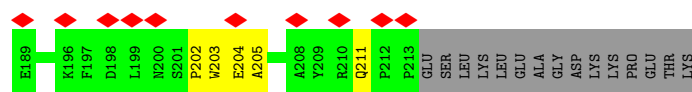
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

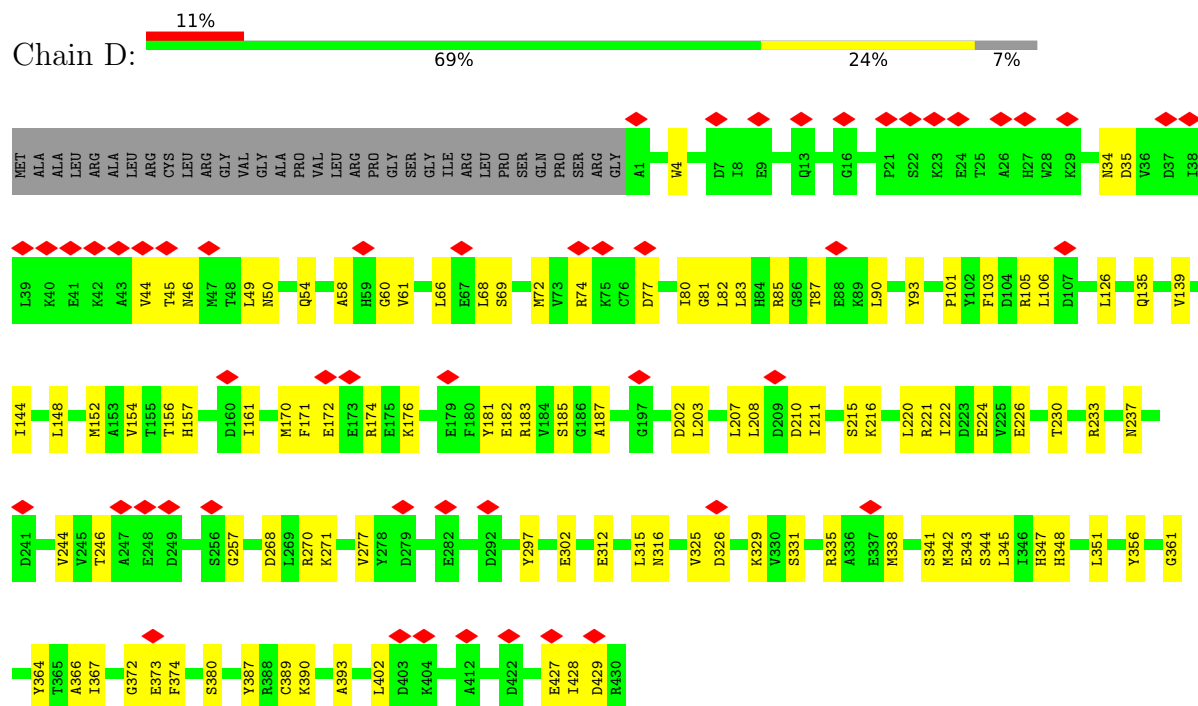
- Molecule 54 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



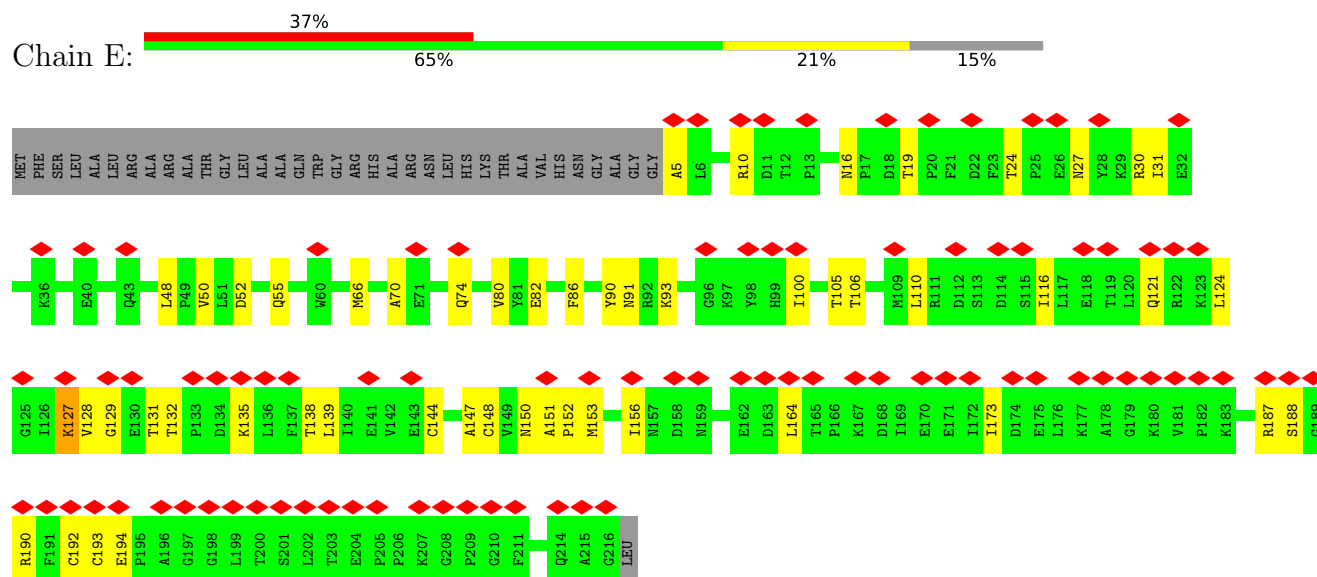
Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			34	22	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	



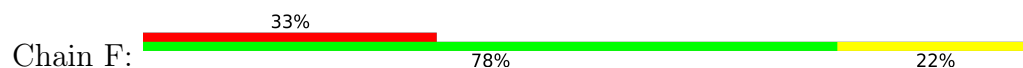
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

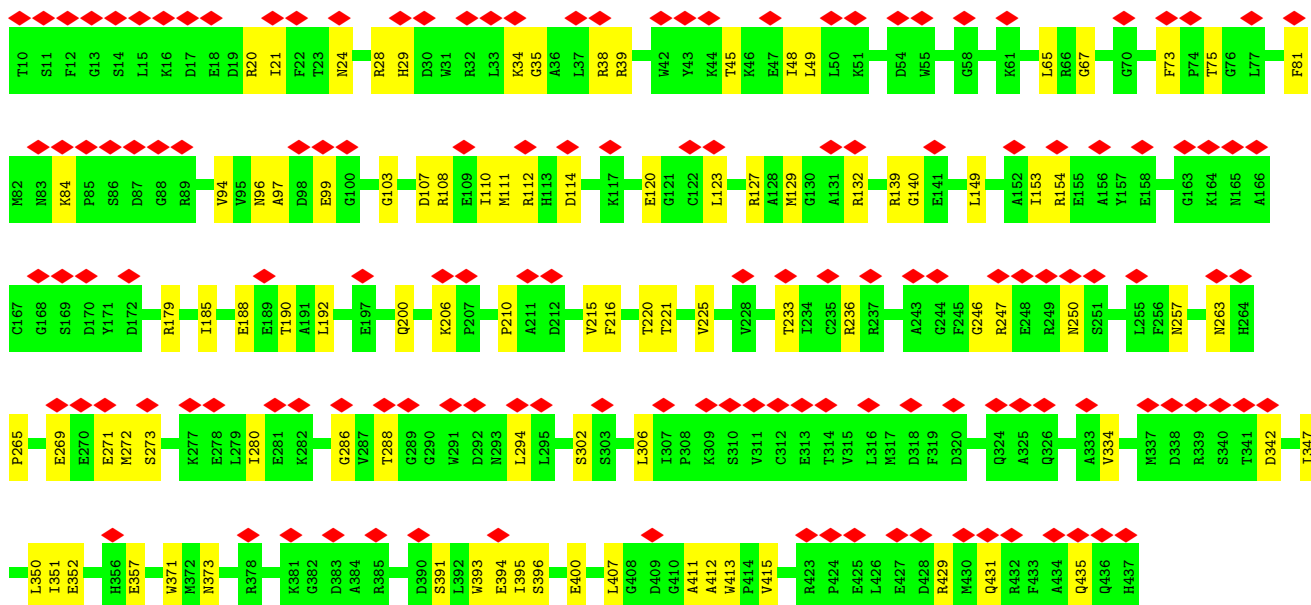


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

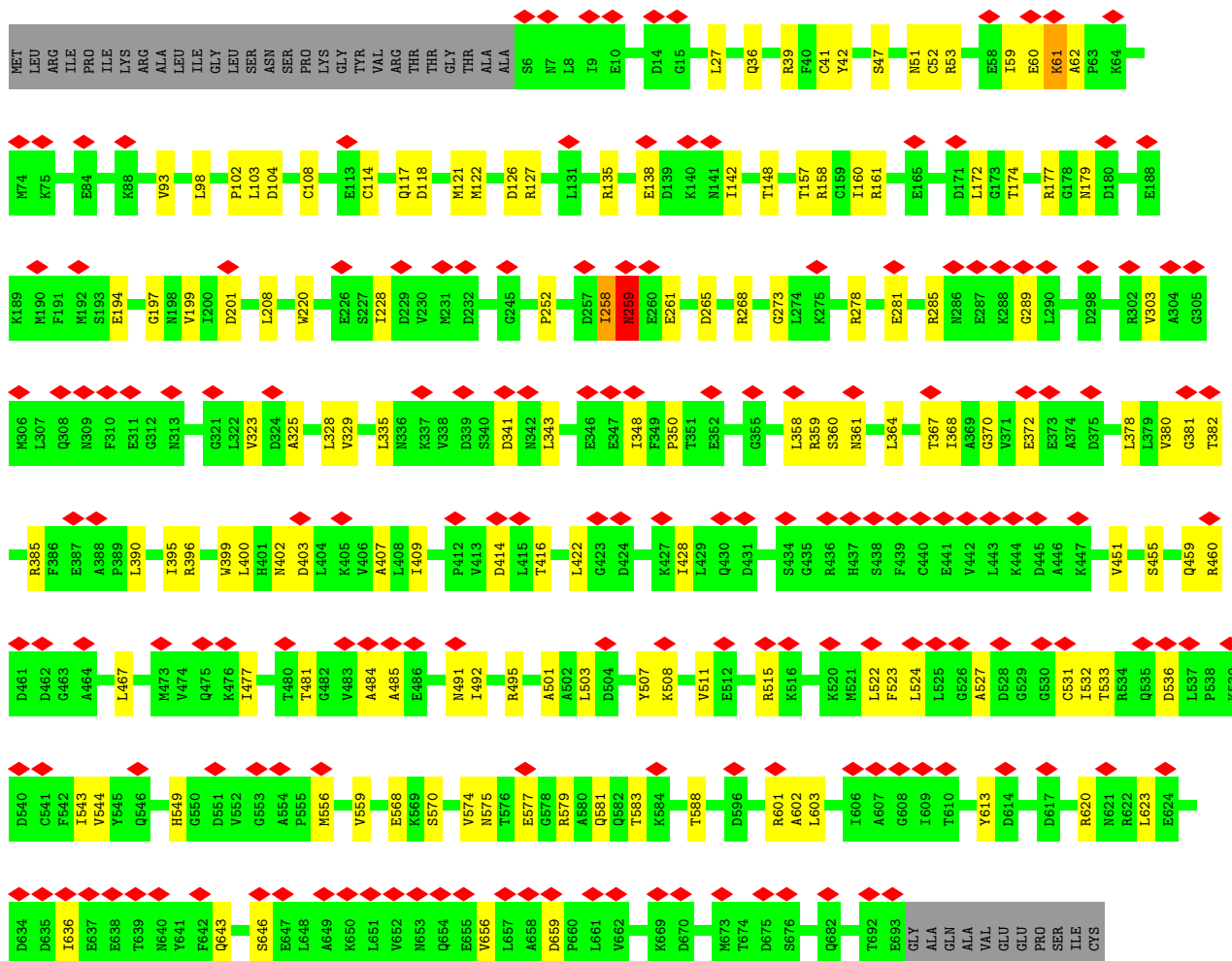
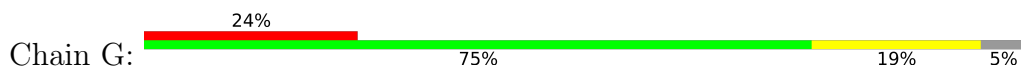


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

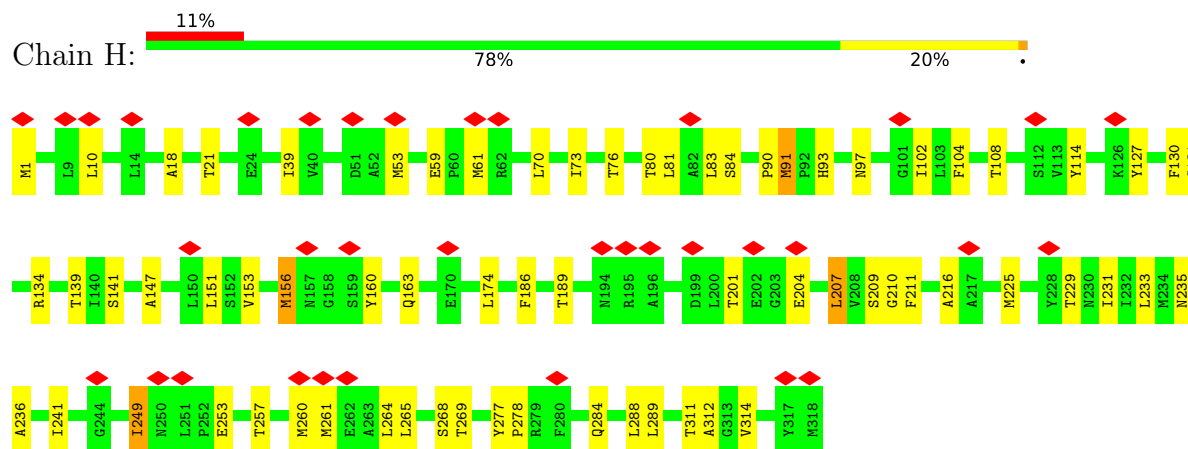




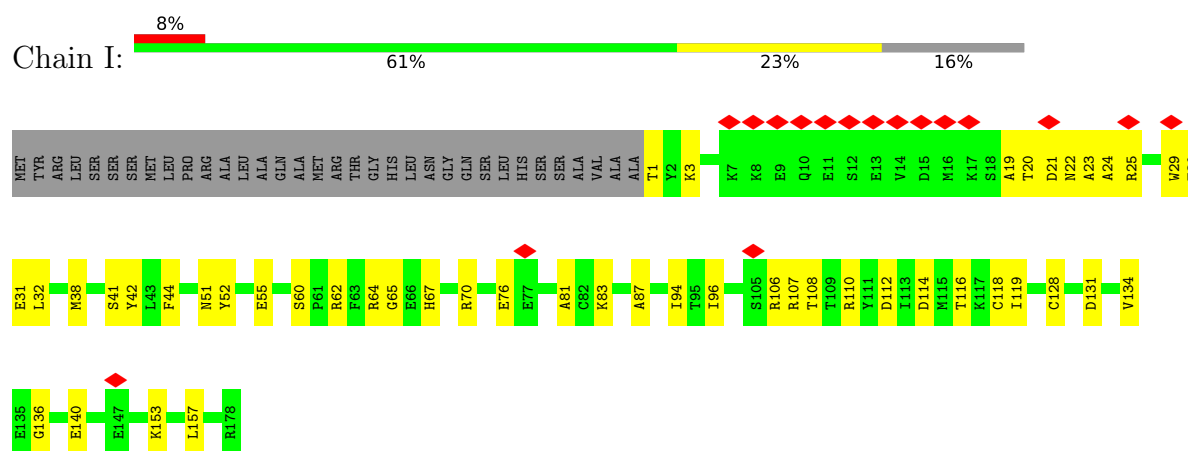
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



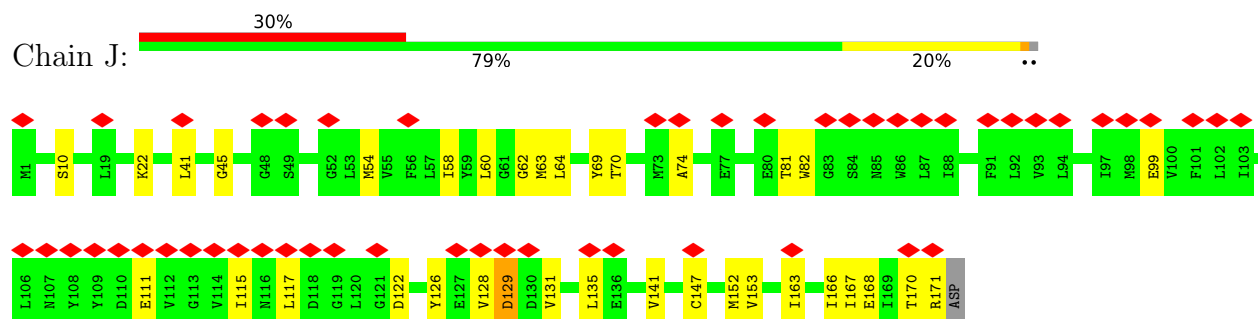
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



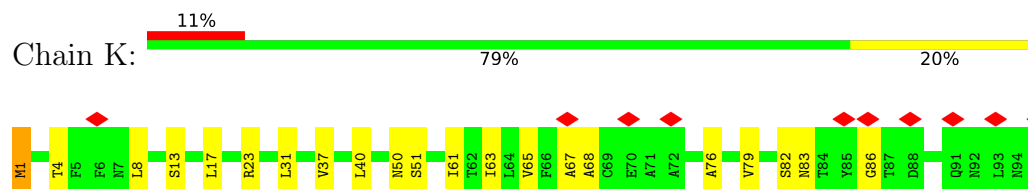
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



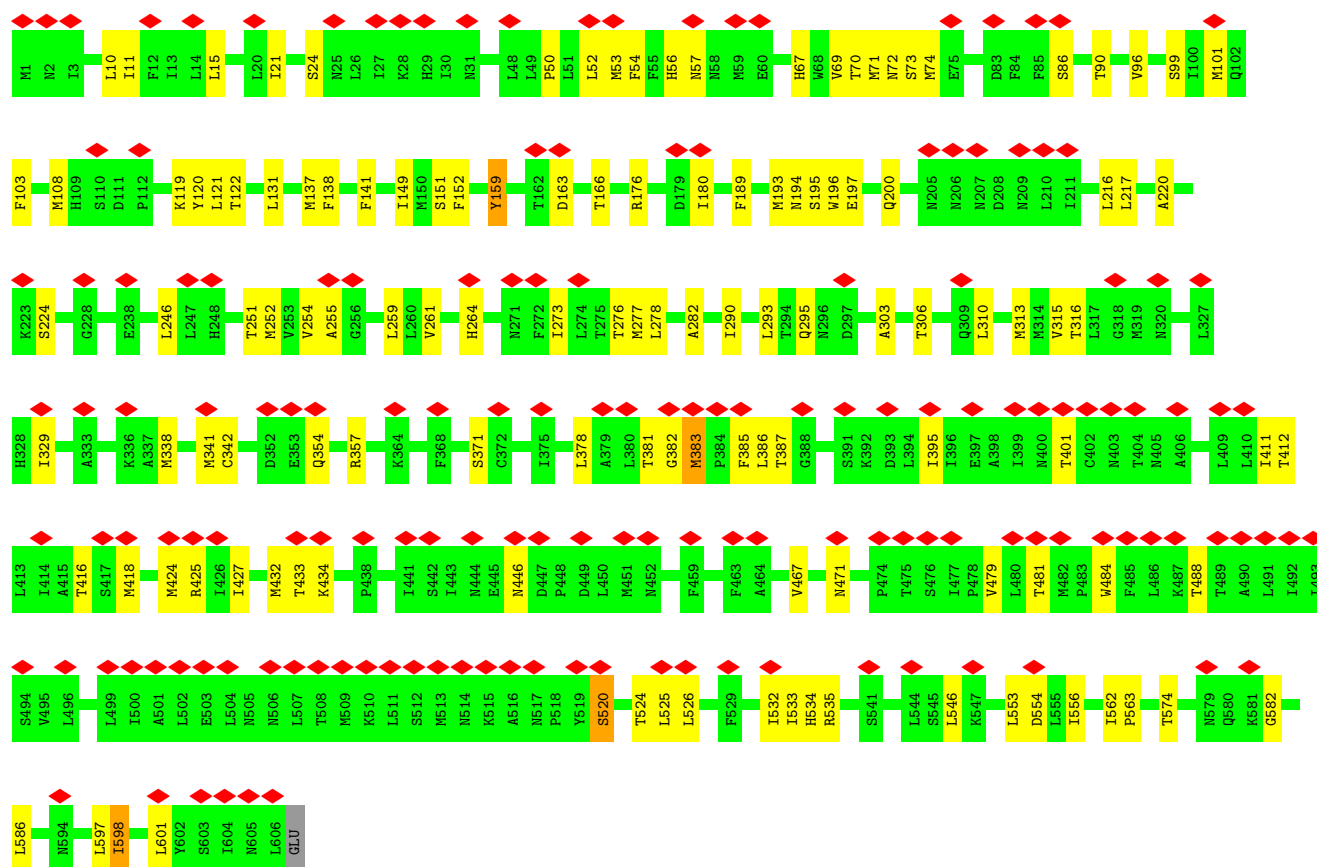
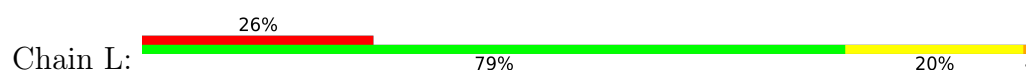
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



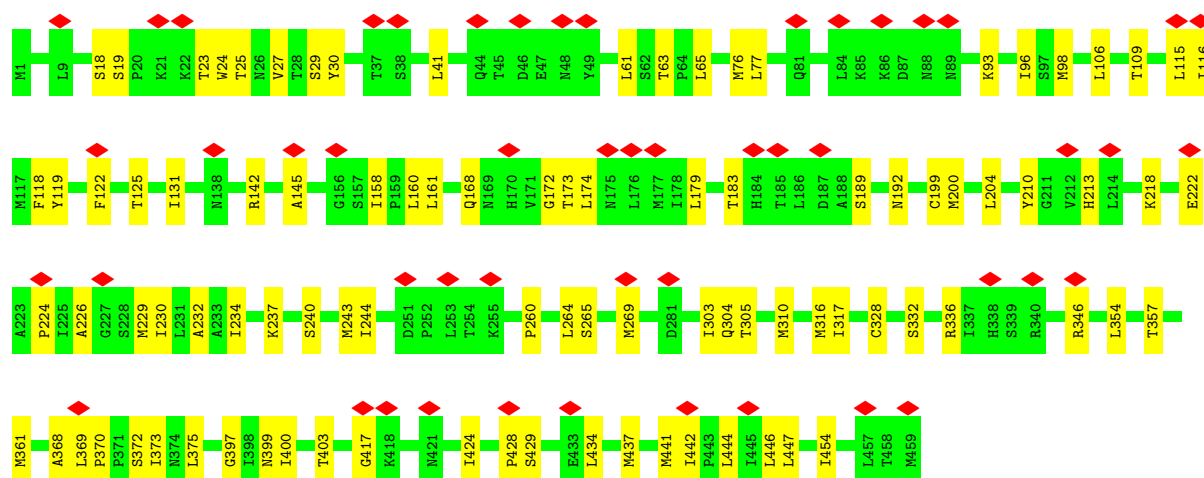
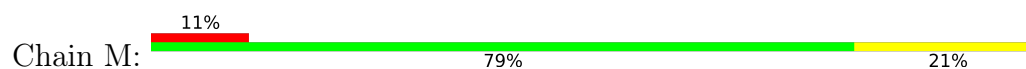
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



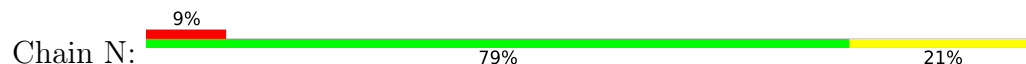
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

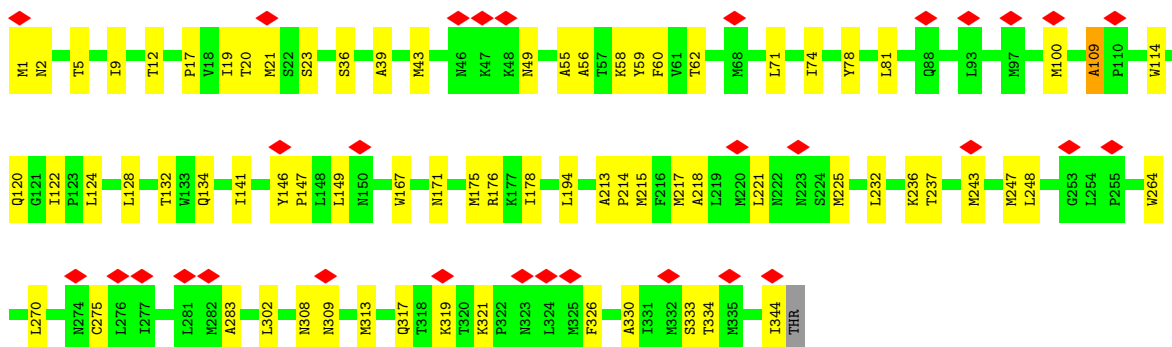


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

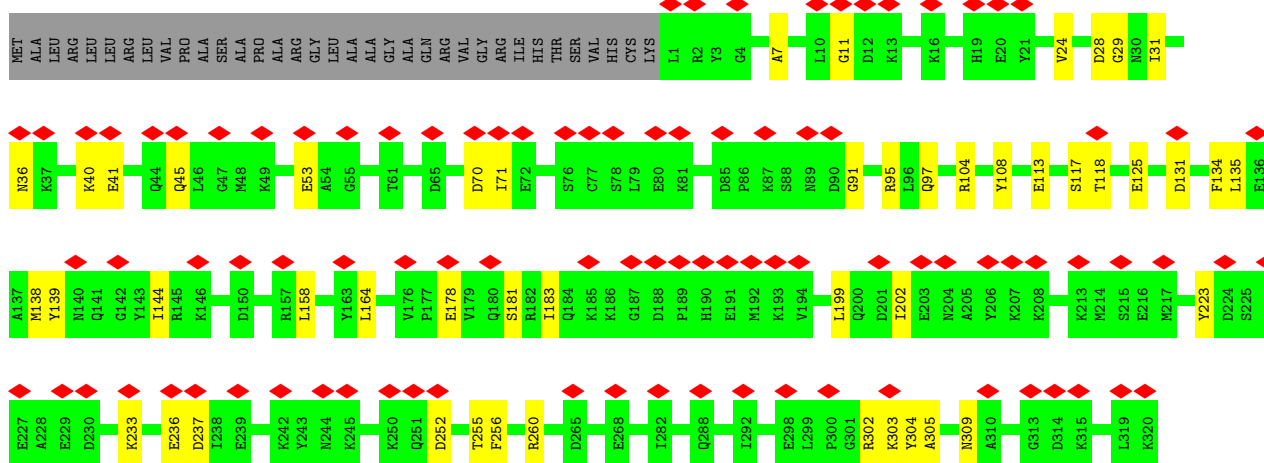
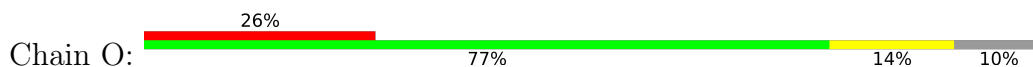


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

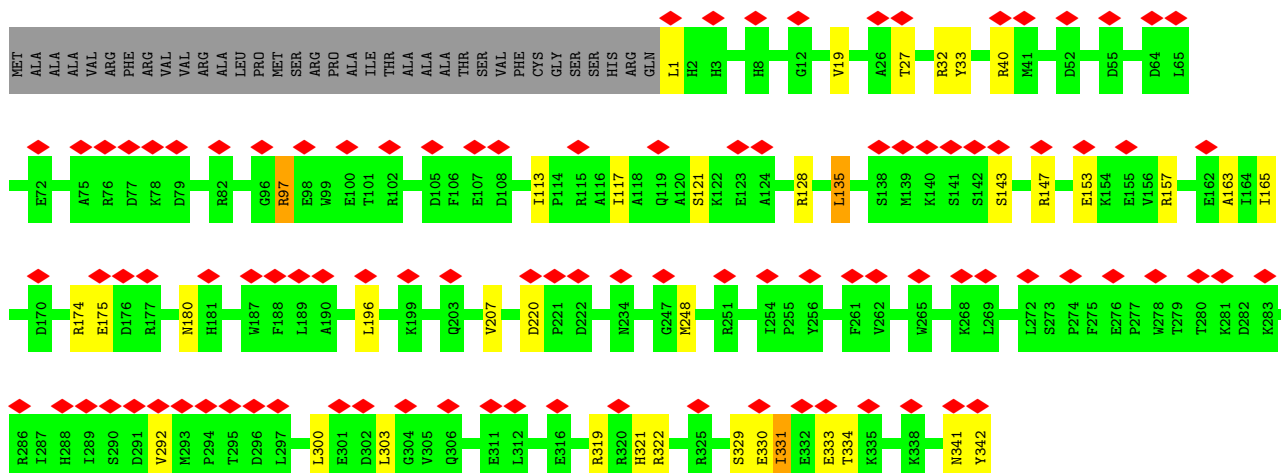
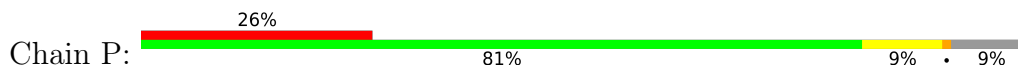




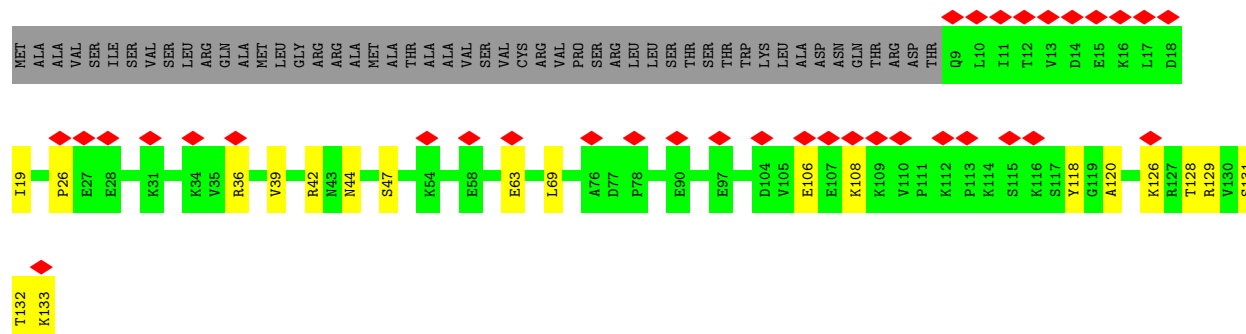
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



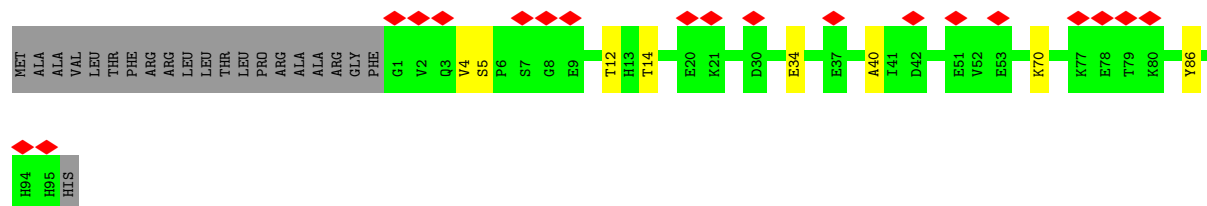
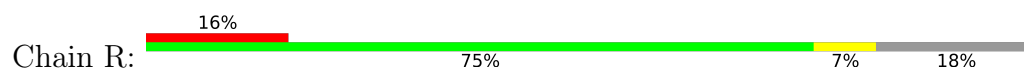
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



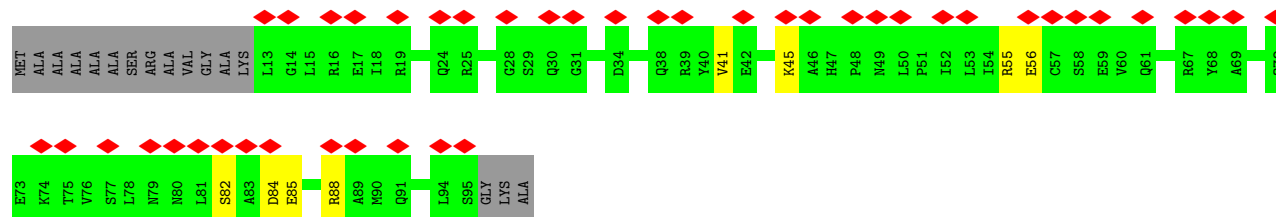
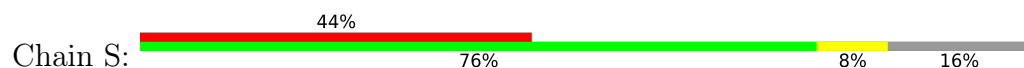
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



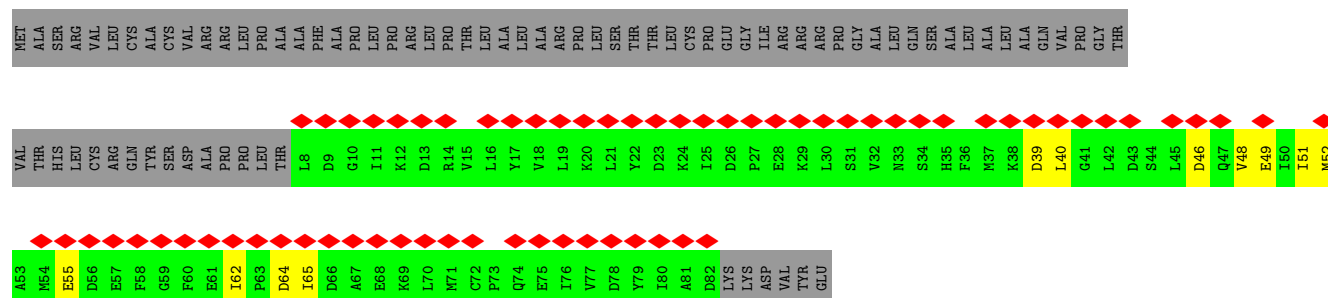
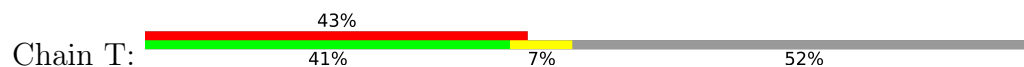
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



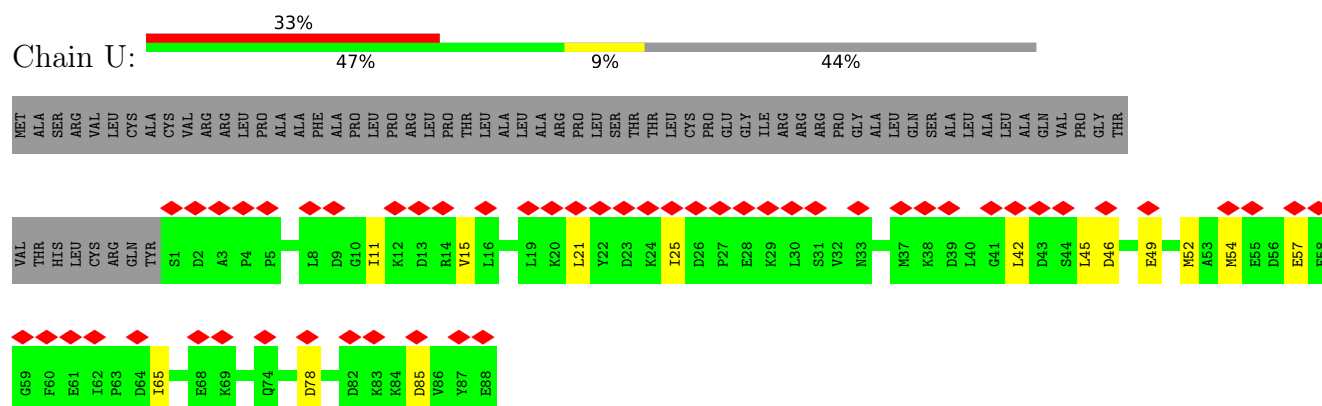
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



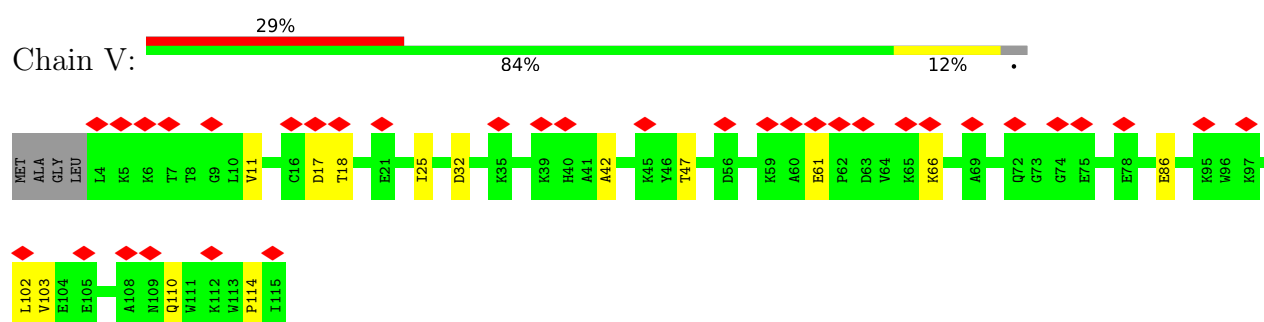
- Molecule 20: Acyl carrier protein, mitochondrial



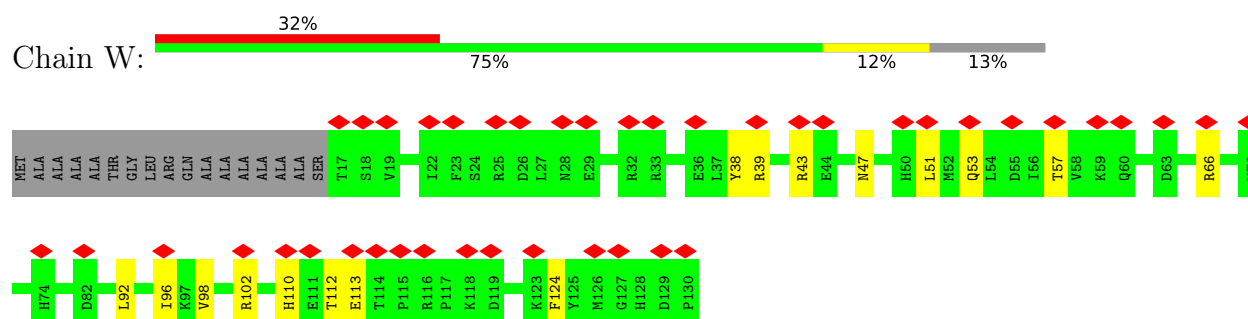
- Molecule 20: Acyl carrier protein, mitochondrial



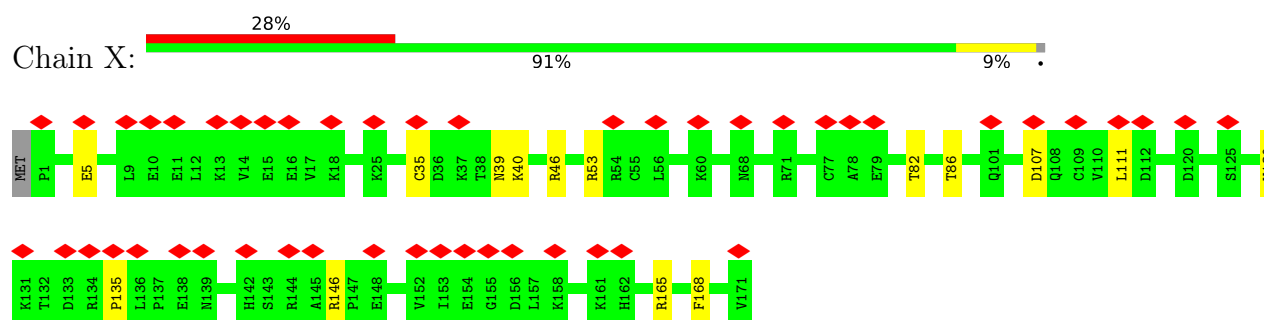
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



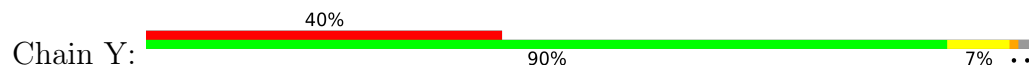
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

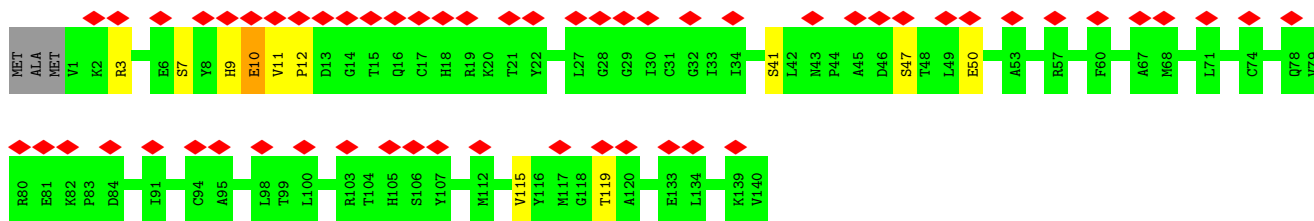


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

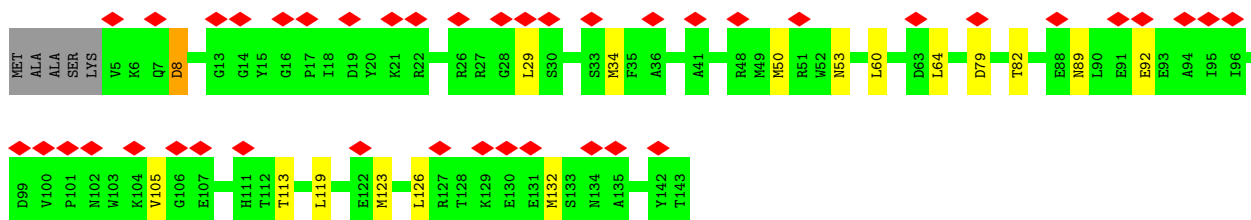
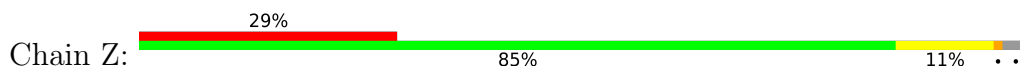


- Molecule 24: MCG5603

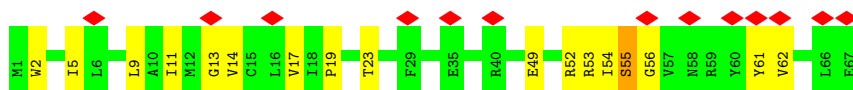
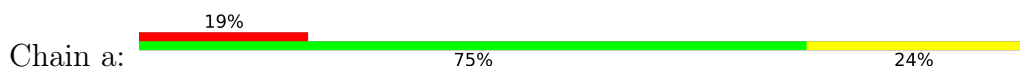




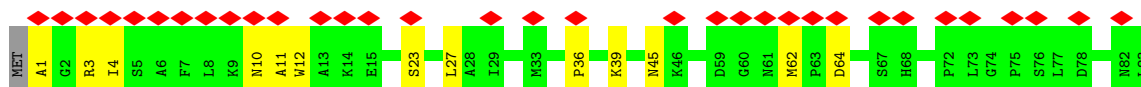
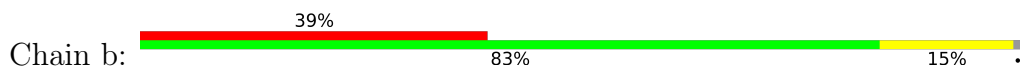
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



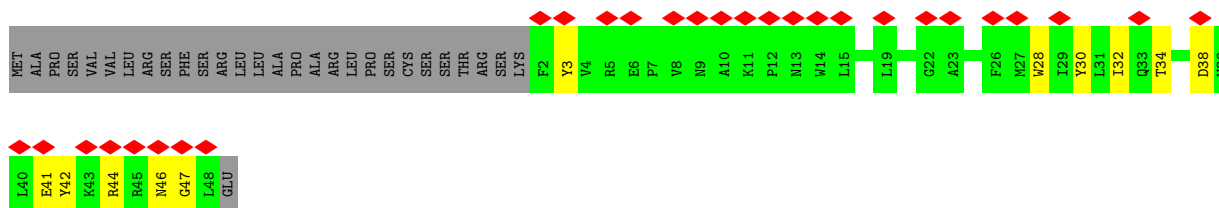
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



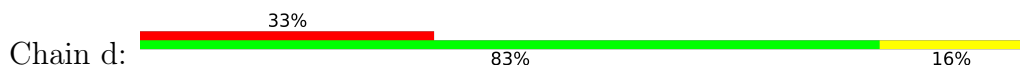
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

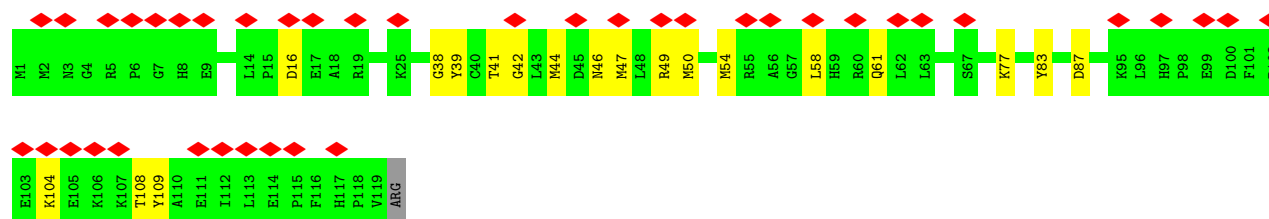


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



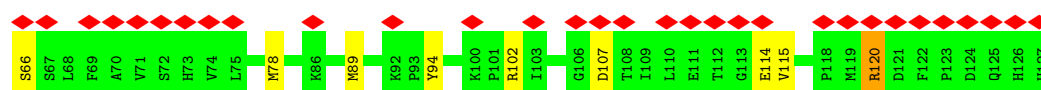
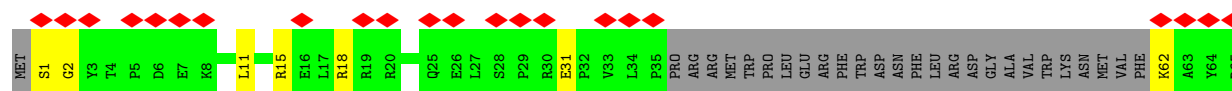
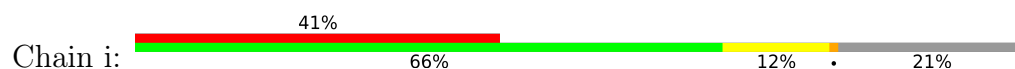
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



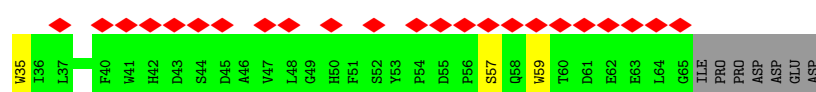
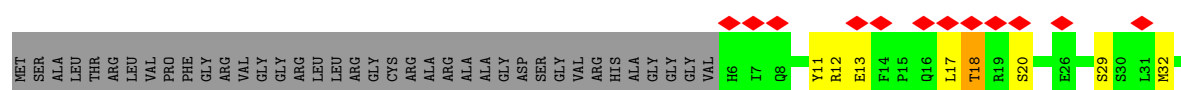




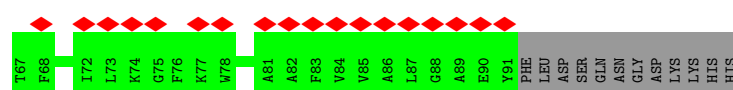
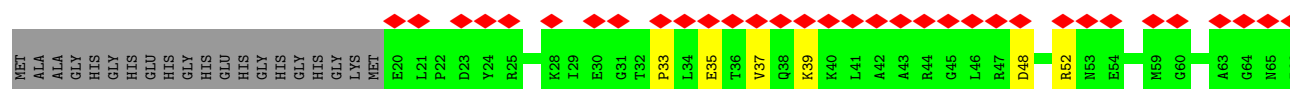
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



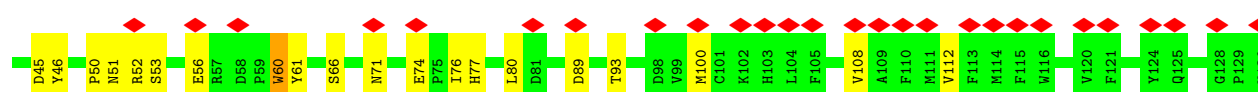
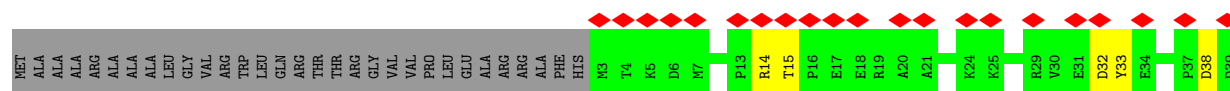
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

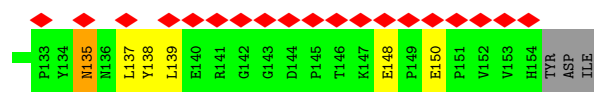


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

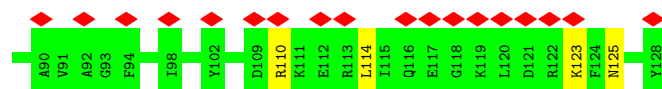
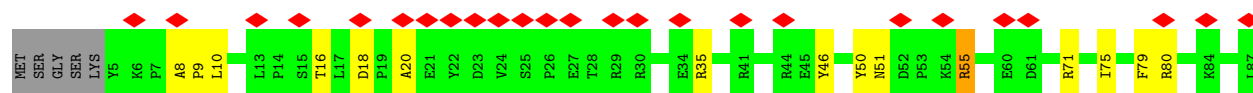
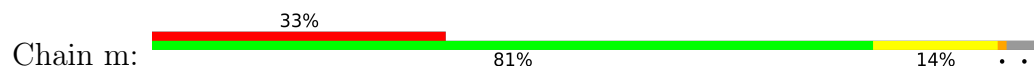


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

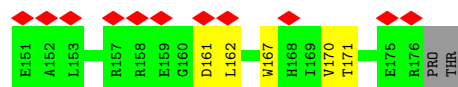
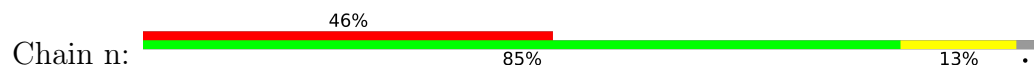




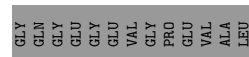
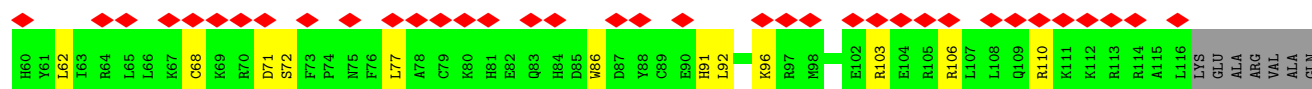
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



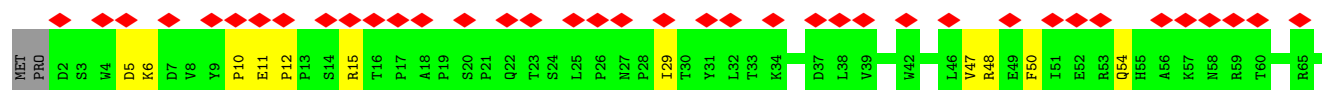
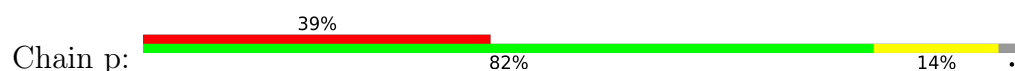
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

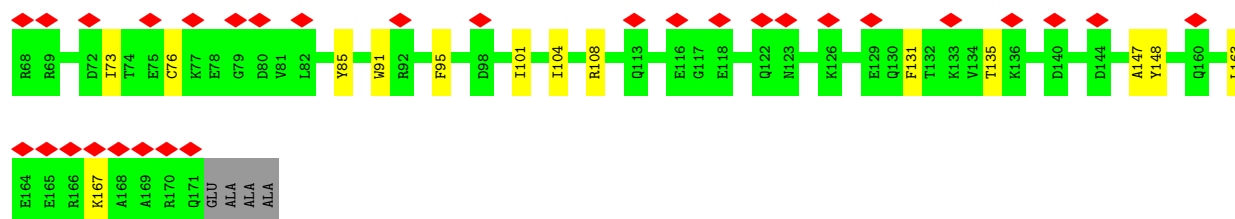


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

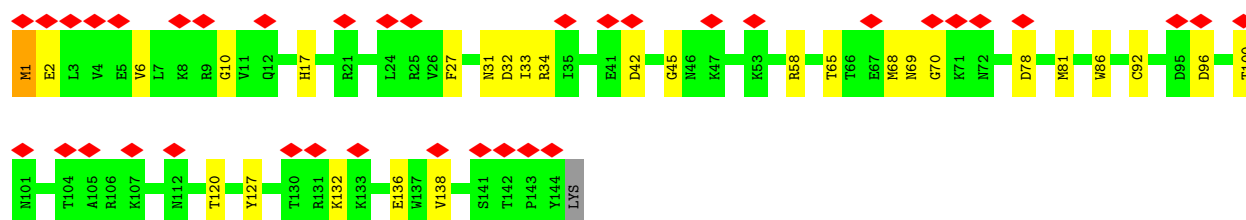
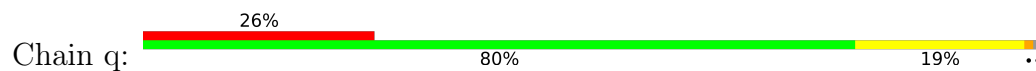


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

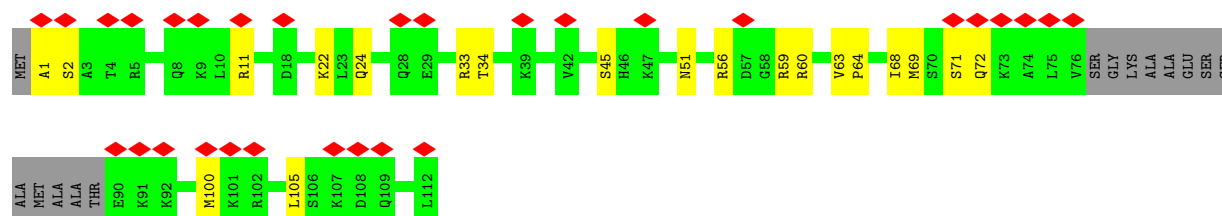




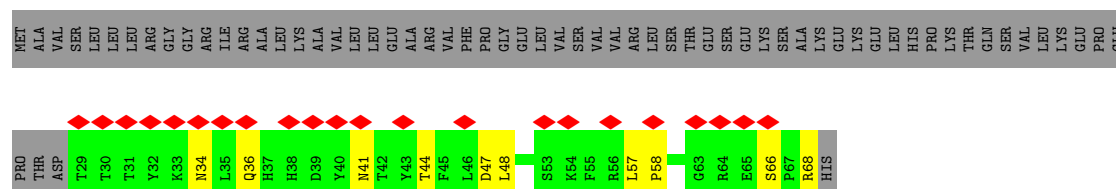
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	20370	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	47600	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.450	Depositor
Minimum map value	-0.156	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.075	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: CDL, NDP, 3PE, SAC, AYA, 2MR, ZN, FES, FMN, AME, PC1, ADP, FME, EHZ, SF4

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	0.35	0/949	0.67	0/1297
2	B	0.43	0/1272	0.61	0/1722
3	C	0.38	0/1762	0.58	0/2401
4	D	0.39	0/3528	0.57	0/4782
5	E	0.32	0/1688	0.64	0/2300
6	F	0.32	0/3376	0.57	0/4561
7	G	0.34	0/5383	0.58	0/7293
8	H	0.37	0/2607	0.60	0/3564
9	I	0.42	0/1438	0.68	0/1946
10	J	0.33	0/1322	0.57	0/1799
11	K	0.36	0/738	0.54	0/1002
12	L	0.35	0/4913	0.60	0/6686
13	M	0.37	0/3709	0.58	0/5052
14	N	0.37	0/2748	0.59	0/3741
15	O	0.31	0/2674	0.56	0/3626
16	P	0.31	0/2823	0.56	0/3828
17	Q	0.34	0/1038	0.53	0/1401
18	R	0.32	0/762	0.51	0/1026
19	S	0.30	0/678	0.58	0/915
20	T	0.21	0/613	0.42	0/826
20	U	0.30	0/718	0.56	0/970
21	V	0.29	0/937	0.65	0/1270
22	W	0.32	0/993	0.60	0/1335
23	X	0.30	0/1434	0.57	0/1937
24	Y	0.27	0/1061	0.50	0/1439
25	Z	0.32	0/1183	0.60	0/1597
26	a	0.33	0/561	0.68	1/755 (0.1%)
27	b	0.33	0/666	0.59	0/914
28	c	0.26	0/400	0.54	0/544
29	d	0.32	0/1017	0.55	0/1373
30	e	0.29	0/892	0.64	0/1187
31	f	0.32	0/443	0.60	0/596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.28	0/878	0.59	0/1196
33	h	0.31	0/1189	0.53	0/1610
34	i	0.30	0/836	0.59	0/1138
35	j	0.31	0/548	0.70	0/748
36	k	0.27	0/601	0.54	0/814
37	l	0.31	0/1327	0.65	0/1811
38	m	0.32	0/1064	0.61	0/1444
39	n	0.31	0/1581	0.56	0/2140
40	o	0.29	0/919	0.60	0/1232
41	p	0.31	0/1471	0.59	0/1988
42	q	0.34	0/1234	0.59	1/1681 (0.1%)
43	r	0.34	0/806	0.64	0/1090
44	s	0.27	0/345	0.50	0/468
All	All	0.34	0/67125	0.59	2/91045 (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
2	B	0	2
3	C	0	1
4	D	0	2
5	E	0	1
6	F	0	1
7	G	0	5
8	H	0	5
10	J	0	2
12	L	0	7
13	M	0	1
14	N	0	2
16	P	0	3
17	Q	0	1
20	U	0	1
22	W	0	1
23	X	0	1
25	Z	0	1
26	a	0	2
29	d	0	2
30	e	0	1
31	f	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	g	0	2
34	i	0	3
35	j	0	2
37	l	0	3
38	m	0	1
40	o	0	2
41	p	0	3
42	q	0	1
All	All	0	60

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	11	ILE	N-CA-C	-6.19	106.77	112.96
42	q	132	LYS	N-CA-CB	-5.78	107.58	114.17

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	119	GLU	Peptide
2	B	134	GLY	Peptide
3	C	8	ARG	Peptide
4	D	171	PHE	Peptide
4	D	87	THR	Peptide

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	0	969	22	0
2	B	1241	0	1250	23	0
3	C	1712	0	1667	27	0
4	D	3452	0	3390	86	0
5	E	1648	0	1639	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	3301	0	3252	64	0
7	G	5296	0	5322	105	0
8	H	2540	0	2626	49	0
9	I	1408	0	1344	40	0
10	J	1300	0	1315	27	0
11	K	737	0	768	16	0
12	L	4800	0	4985	91	0
13	M	3632	0	3853	77	0
14	N	2696	0	2895	48	0
15	O	2607	0	2566	30	0
16	P	2748	0	2768	26	0
17	Q	1015	0	1016	13	0
18	R	748	0	724	6	0
19	S	667	0	685	7	0
20	T	604	0	595	10	0
20	U	706	0	698	13	0
21	V	915	0	954	10	0
22	W	970	0	991	13	0
23	X	1396	0	1379	7	0
24	Y	1037	0	1027	6	0
25	Z	1152	0	1148	15	0
26	a	548	0	562	12	0
27	b	651	0	653	9	0
28	c	389	0	385	7	0
29	d	985	0	988	13	0
30	e	870	0	864	13	0
31	f	433	0	429	5	0
32	g	850	0	783	9	0
33	h	1154	0	1157	14	0
34	i	820	0	809	12	0
35	j	525	0	477	9	0
36	k	582	0	574	4	0
37	l	1274	0	1173	18	0
38	m	1035	0	1043	16	0
39	n	1527	0	1459	20	0
40	o	898	0	887	15	0
41	p	1438	0	1402	20	0
42	q	1203	0	1157	16	0
43	r	796	0	831	19	0
44	s	336	0	320	7	0
45	A	41	0	59	0	0
45	H	102	0	164	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	L	93	0	143	1	0
45	M	277	0	424	2	0
45	N	51	0	82	0	0
46	B	8	0	0	0	0
46	F	8	0	0	0	0
46	G	16	0	0	1	0
46	I	16	0	0	0	0
47	E	4	0	0	1	0
47	G	4	0	0	0	0
48	F	31	0	19	1	0
49	H	124	0	173	2	0
49	P	43	0	63	0	0
50	H	57	0	58	2	0
50	L	148	0	187	3	0
50	M	67	0	81	0	0
51	O	27	0	12	0	0
52	P	48	0	26	5	0
53	R	1	0	0	0	0
54	T	34	0	0	1	0
54	U	35	0	0	0	0
All	All	66810	0	67270	900	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 900 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)
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.41	0.97
12:L:371:SER:HG	35:j:29:SER:HG	1.13	0.95
7:G:228:ILE:HG22	7:G:583:THR:HG22	1.55	0.87
45:M:505:3PE:H271	29:d:47:MET:HE3	1.57	0.86
50:H:405:CDL:H1O1	43:r:2:SER:HG	1.17	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	90 (80%)	22 (20%)	1 (1%)	14	43
2	B	153/224 (68%)	134 (88%)	19 (12%)	0	100	100
3	C	204/263 (78%)	172 (84%)	30 (15%)	2 (1%)	12	40
4	D	427/463 (92%)	372 (87%)	55 (13%)	0	100	100
5	E	210/248 (85%)	169 (80%)	40 (19%)	1 (0%)	24	55
6	F	426/428 (100%)	360 (84%)	66 (16%)	0	100	100
7	G	686/727 (94%)	593 (86%)	90 (13%)	3 (0%)	30	60
8	H	316/318 (99%)	272 (86%)	44 (14%)	0	100	100
9	I	176/212 (83%)	145 (82%)	31 (18%)	0	100	100
10	J	169/172 (98%)	148 (88%)	20 (12%)	1 (1%)	21	52
11	K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
12	L	604/607 (100%)	508 (84%)	96 (16%)	0	100	100
13	M	457/459 (100%)	413 (90%)	43 (9%)	1 (0%)	43	71
14	N	342/345 (99%)	309 (90%)	31 (9%)	2 (1%)	21	52
15	O	318/355 (90%)	273 (86%)	44 (14%)	1 (0%)	36	65
16	P	340/377 (90%)	280 (82%)	59 (17%)	1 (0%)	36	65
17	Q	123/175 (70%)	109 (89%)	13 (11%)	1 (1%)	16	45
18	R	93/116 (80%)	80 (86%)	13 (14%)	0	100	100
19	S	81/99 (82%)	69 (85%)	12 (15%)	0	100	100
20	T	73/156 (47%)	66 (90%)	7 (10%)	0	100	100
20	U	86/156 (55%)	69 (80%)	17 (20%)	0	100	100
21	V	110/116 (95%)	92 (84%)	18 (16%)	0	100	100
22	W	112/131 (86%)	101 (90%)	11 (10%)	0	100	100
23	X	169/172 (98%)	140 (83%)	27 (16%)	2 (1%)	10	37
24	Y	138/143 (96%)	120 (87%)	16 (12%)	2 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	137/144 (95%)	114 (83%)	22 (16%)	1 (1%)	18	49
26	a	65/67 (97%)	55 (85%)	9 (14%)	1 (2%)	8	32
27	b	81/84 (96%)	63 (78%)	18 (22%)	0	100	100
28	c	45/76 (59%)	42 (93%)	3 (7%)	0	100	100
29	d	117/120 (98%)	98 (84%)	19 (16%)	0	100	100
30	e	102/106 (96%)	84 (82%)	17 (17%)	1 (1%)	12	40
31	f	49/57 (86%)	37 (76%)	11 (22%)	1 (2%)	6	27
32	g	99/151 (66%)	76 (77%)	22 (22%)	1 (1%)	12	40
33	h	135/189 (71%)	113 (84%)	21 (16%)	1 (1%)	18	49
34	i	97/128 (76%)	76 (78%)	19 (20%)	2 (2%)	5	26
35	j	58/105 (55%)	41 (71%)	16 (28%)	1 (2%)	7	30
36	k	70/104 (67%)	54 (77%)	16 (23%)	0	100	100
37	l	150/186 (81%)	112 (75%)	35 (23%)	3 (2%)	6	27
38	m	122/129 (95%)	102 (84%)	20 (16%)	0	100	100
39	n	174/179 (97%)	149 (86%)	25 (14%)	0	100	100
40	o	103/137 (75%)	85 (82%)	18 (18%)	0	100	100
41	p	168/176 (96%)	142 (84%)	26 (16%)	0	100	100
42	q	142/145 (98%)	108 (76%)	32 (22%)	2 (1%)	9	33
43	r	95/113 (84%)	77 (81%)	18 (19%)	0	100	100
44	s	38/104 (36%)	32 (84%)	6 (16%)	0	100	100
All	All	8069/9175 (88%)	6833 (85%)	1204 (15%)	32 (0%)	31	60

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	g	107	GLU
35	j	13	GLU
37	l	61	TYR
7	G	259	ASN
15	O	303	LYS

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	131/185 (71%)	130 (99%)	1 (1%)	73	79
3	C	188/227 (83%)	188 (100%)	0	100	100
4	D	367/394 (93%)	367 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100
6	F	343/343 (100%)	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	145/178 (82%)	145 (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%)	548 (100%)	0	100	100
13	M	414/414 (100%)	413 (100%)	1 (0%)	87	88
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%)	298 (100%)	1 (0%)	86	86
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	80/96 (83%)	80 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	100/102 (98%)	100 (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	120/123 (98%)	120 (100%)	0	100	100
26	a	57/57 (100%)	57 (100%)	0	100	100
27	b	72/73 (99%)	72 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	92/94 (98%)	92 (100%)	0	100	100
31	f	47/53 (89%)	46 (98%)	1 (2%)	47	67
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	122/162 (75%)	122 (100%)	0	100	100
34	i	87/119 (73%)	87 (100%)	0	100	100
35	j	56/87 (64%)	56 (100%)	0	100	100
36	k	55/78 (70%)	55 (100%)	0	100	100
37	l	137/161 (85%)	137 (100%)	0	100	100
38	m	110/114 (96%)	110 (100%)	0	100	100
39	n	161/164 (98%)	161 (100%)	0	100	100
40	o	98/121 (81%)	98 (100%)	0	100	100
41	p	155/158 (98%)	155 (100%)	0	100	100
42	q	129/130 (99%)	129 (100%)	0	100	100
43	r	88/96 (92%)	88 (100%)	0	100	100
44	s	39/95 (41%)	39 (100%)	0	100	100
All	All	7139/7917 (90%)	7135 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	CYS
13	M	434	LEU
16	P	135	LEU
31	f	50	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
34	i	12	GLN
37	l	103	HIS
42	q	135	HIS
12	L	444	ASN
12	L	332	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z > 2$
14	FME	N	1	14	8,9,10	0.98	0	8,9,11	1.28	1 (12%)
27	AYA	b	1	27	6,7,8	1.25	1 (16%)	6,8,10	1.05	1 (16%)
43	AYA	r	1	43	6,7,8	1.22	1 (16%)	6,8,10	1.13	1 (16%)
34	SAC	i	1	34	7,8,9	1.04	0	7,9,11	1.09	0
4	2MR	D	85	4	10,12,13	2.60	3 (30%)	5,13,15	1.69	1 (20%)
1	FME	A	1	1	8,9,10	1.01	1 (12%)	8,9,11	1.01	0
12	FME	L	1	12	8,9,10	0.98	0	8,9,11	0.73	0
42	AME	q	1	42	9,10,11	1.79	2 (22%)	9,11,13	1.83	4 (44%)
13	FME	M	1	13	8,9,10	1.01	0	8,9,11	0.79	0
11	FME	K	1	11	8,9,10	1.08	1 (12%)	8,9,11	1.20	1 (12%)
8	FME	H	1	8	8,9,10	0.97	0	8,9,11	1.21	1 (12%)
10	FME	J	1	10	8,9,10	0.95	0	8,9,11	0.86	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
14	FME	N	1	14	-	3/7/9/11	-
27	AYA	b	1	27	-	1/5/6/8	-
43	AYA	r	1	43	-	1/5/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
4	2MR	D	85	4	-	4/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	3/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
42	AME	q	1	42	-	4/9/10/12	-
13	FME	M	1	13	-	1/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
10	FME	J	1	10	-	2/7/9/11	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.62	1.46	1.34
4	D	85	2MR	CZ-NH2	5.20	1.44	1.33
42	q	1	AME	CT1-N	4.15	1.47	1.34
43	r	1	AYA	CA-N	-2.36	1.44	1.46
27	b	1	AYA	CA-N	-2.23	1.44	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	CD-NE-CZ	3.52	129.97	123.36
42	q	1	AME	CT2-CT1-N	3.13	121.31	116.12
8	H	1	FME	C-CA-N	2.96	115.21	109.50
14	N	1	FME	C-CA-N	2.64	114.60	109.50
43	r	1	AYA	CB-CA-N	2.41	112.40	109.68

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	O-C-CA-CB
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	i	1	SAC	1	0
42	q	1	AME	1	0
11	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 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	3PE	H	403	-	50,50,50	0.88	3 (6%)	53,55,55	1.11	2 (3%)
49	PC1	H	406	-	34,34,53	1.19	4 (11%)	40,42,61	1.10	2 (5%)
50	CDL	M	507	-	66,66,99	1.06	8 (12%)	72,78,111	1.24	5 (6%)
46	SF4	I	202	9	0,12,12	-	-	-	-	-
46	SF4	G	801	7	0,12,12	-	-	-	-	-
45	3PE	L	701	-	50,50,50	0.86	4 (8%)	53,55,55	1.01	2 (3%)
49	PC1	H	402	-	41,41,53	1.08	3 (7%)	47,49,61	0.93	2 (4%)
46	SF4	B	201	2	0,12,12	-	-	-	-	-
54	EHZ	T	201	20	28,33,37	1.68	5 (17%)	33,41,47	1.40	4 (12%)
45	3PE	M	505	-	50,50,50	0.88	3 (6%)	53,55,55	1.03	3 (5%)
45	3PE	M	503	-	50,50,50	0.88	3 (6%)	53,55,55	1.07	2 (3%)
45	3PE	A	201	-	40,40,50	0.97	4 (10%)	43,45,55	1.07	2 (4%)
48	FMN	F	501	-	33,33,33	1.12	2 (6%)	48,50,50	1.42	7 (14%)
54	EHZ	U	201	20	29,34,37	1.66	5 (17%)	34,42,47	1.23	4 (11%)
51	ADP	O	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.98	10 (23%)
45	3PE	L	704	-	41,41,50	0.96	4 (9%)	44,46,55	1.02	2 (4%)
46	SF4	F	502	6	0,12,12	-	-	-	-	-
52	NDP	P	501	-	51,52,52	2.36	8 (15%)	71,80,80	1.57	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	N	401	-	50,50,50	0.90	4 (8%)	53,55,55	1.10	3 (5%)
50	CDL	L	703	-	69,69,99	1.04	8 (11%)	75,81,111	1.09	4 (5%)
50	CDL	L	702	-	77,77,99	1.00	8 (10%)	83,89,111	1.14	4 (4%)
45	3PE	M	501	-	50,50,50	0.88	4 (8%)	53,55,55	0.98	2 (3%)
49	PC1	H	404	-	46,46,53	1.04	4 (8%)	52,54,61	1.03	2 (3%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-
45	3PE	M	502	-	41,41,50	1.05	4 (9%)	44,46,55	1.24	3 (6%)
45	3PE	H	401	-	50,50,50	0.86	4 (8%)	53,55,55	0.99	2 (3%)
47	FES	E	301	5	0,4,4	-	-	-	-	-
49	PC1	P	401	-	42,42,53	1.08	4 (9%)	48,50,61	1.04	2 (4%)
45	3PE	M	506	-	30,30,50	1.11	4 (13%)	33,35,55	1.15	2 (6%)
45	3PE	M	504	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
46	SF4	I	201	9	0,12,12	-	-	-	-	-
47	FES	G	803	7	0,4,4	-	-	-	-	-
50	CDL	H	405	-	56,56,99	1.15	7 (12%)	62,68,111	1.12	4 (6%)

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
45	3PE	H	403	-	-	24/54/54/54	-
49	PC1	H	406	-	-	18/38/38/57	-
50	CDL	M	507	-	-	32/77/77/110	-
46	SF4	I	202	9	-	-	0/6/5/5
46	SF4	G	801	7	-	-	0/6/5/5
45	3PE	L	701	-	-	19/54/54/54	-
49	PC1	H	402	-	-	25/45/45/57	-
46	SF4	B	201	2	-	-	0/6/5/5
54	EHZ	T	201	20	-	8/39/41/45	-
45	3PE	M	505	-	-	25/54/54/54	-
45	3PE	M	503	-	-	21/54/54/54	-
45	3PE	A	201	-	-	18/44/44/54	-
48	FMN	F	501	-	-	7/18/18/18	0/3/3/3
54	EHZ	U	201	20	-	16/40/42/45	-
51	ADP	O	401	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	L	704	-	-	17/45/45/54	-
46	SF4	F	502	6	-	-	0/6/5/5
52	NDP	P	501	-	-	5/34/77/77	0/5/5/5
45	3PE	N	401	-	-	25/54/54/54	-
50	CDL	L	703	-	-	39/80/80/110	-
50	CDL	L	702	-	-	42/88/88/110	-
45	3PE	M	501	-	-	29/54/54/54	-
49	PC1	H	404	-	-	22/50/50/57	-
46	SF4	G	802	7	-	-	0/6/5/5
45	3PE	M	502	-	-	16/43/43/54	-
45	3PE	H	401	-	-	26/54/54/54	-
47	FES	E	301	5	-	-	0/1/1/1
49	PC1	P	401	-	-	26/46/46/57	-
45	3PE	M	506	-	-	14/34/34/54	-
45	3PE	M	504	-	-	23/54/54/54	-
46	SF4	I	201	9	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
50	CDL	H	405	-	-	37/67/67/110	-

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	13.04	1.82	1.59
54	U	201	EHZ	C15-N2	5.15	1.45	1.33
54	T	201	EHZ	C15-N2	5.13	1.45	1.33
54	U	201	EHZ	C12-N1	5.10	1.45	1.33
54	T	201	EHZ	C12-N1	5.10	1.45	1.33

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	O	401	ADP	C5-C4-N3	-6.23	118.14	126.72
54	T	201	EHZ	C8-C9-S1	4.99	119.86	113.56
52	P	501	NDP	P2B-O2B-C2B	-4.92	110.30	123.43
51	O	401	ADP	N3-C4-N9	4.80	135.34	127.17
45	M	502	3PE	O31-C31-C32	4.77	126.36	111.83

There are no chirality outliers.

5 of 537 torsion outliers are listed below:

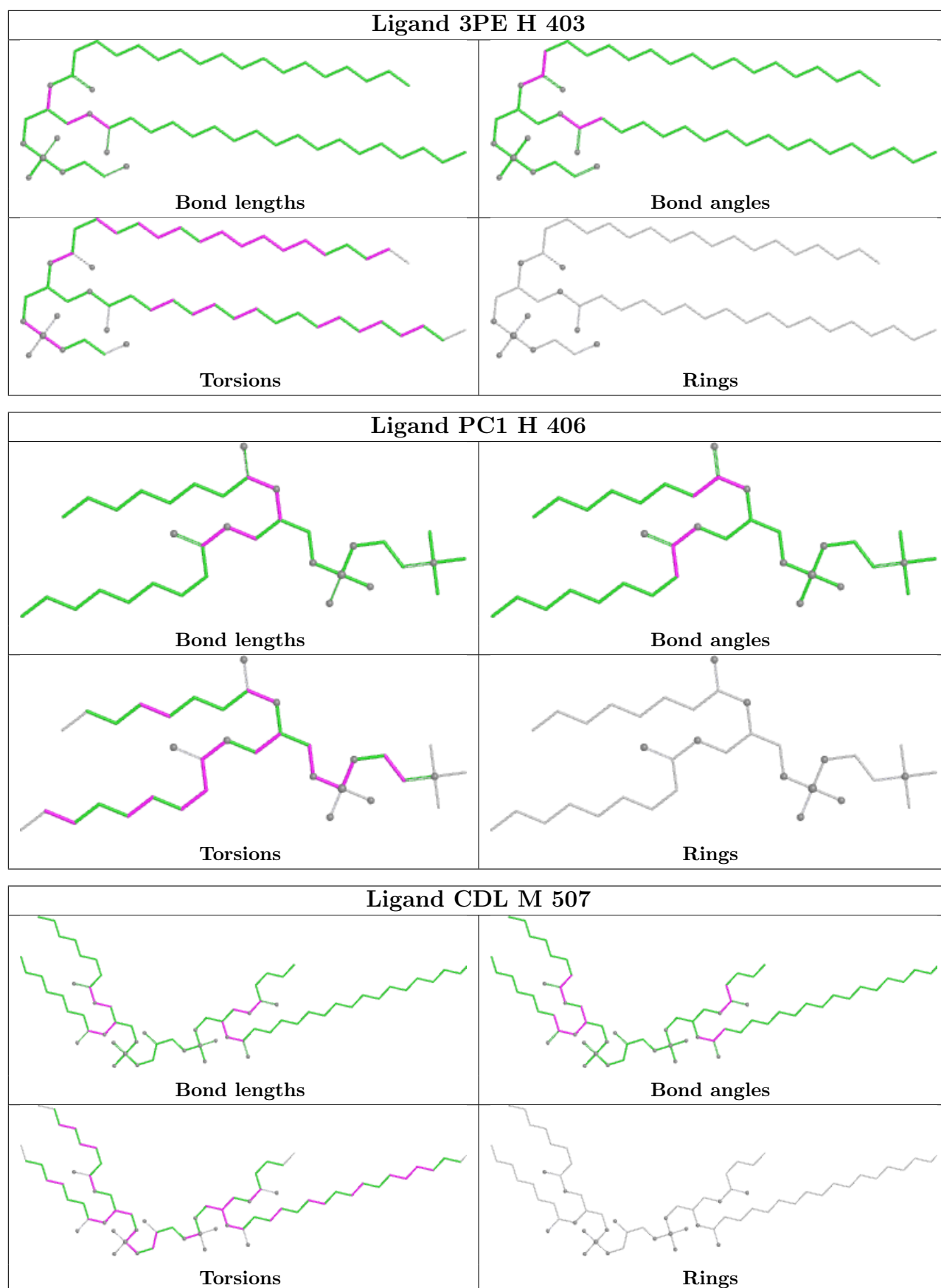
Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C1-O11-P-O14
45	H	401	3PE	C11-O13-P-O11
45	H	401	3PE	C11-O13-P-O12
45	H	401	3PE	O13-C11-C12-N
45	H	401	3PE	C22-C21-O21-C2

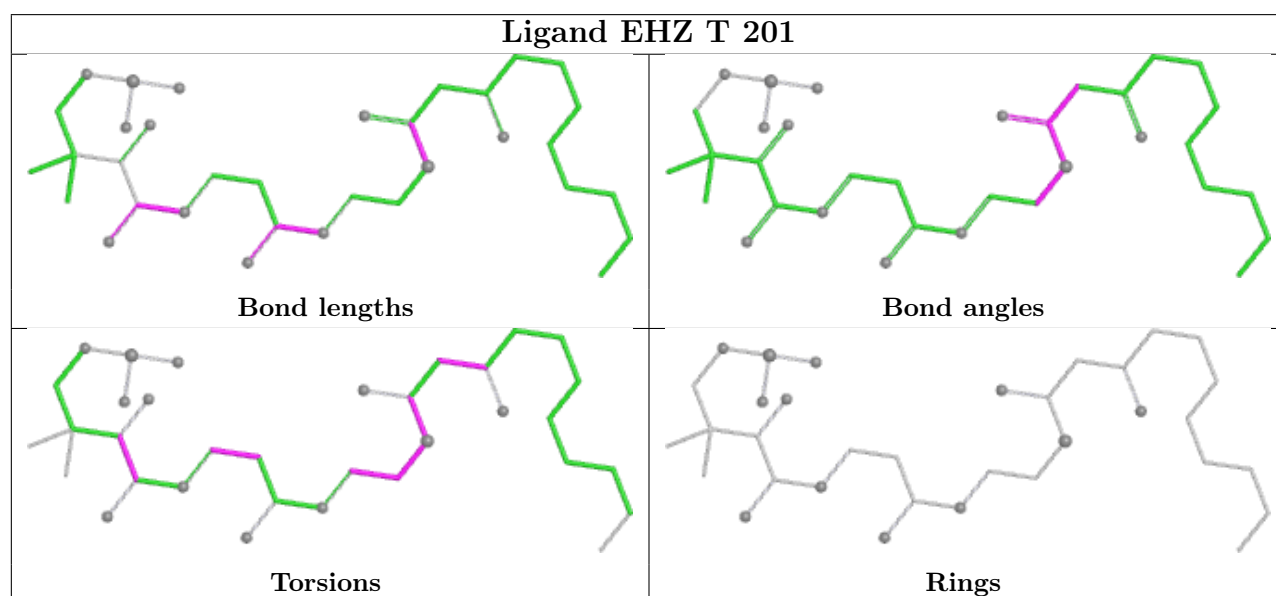
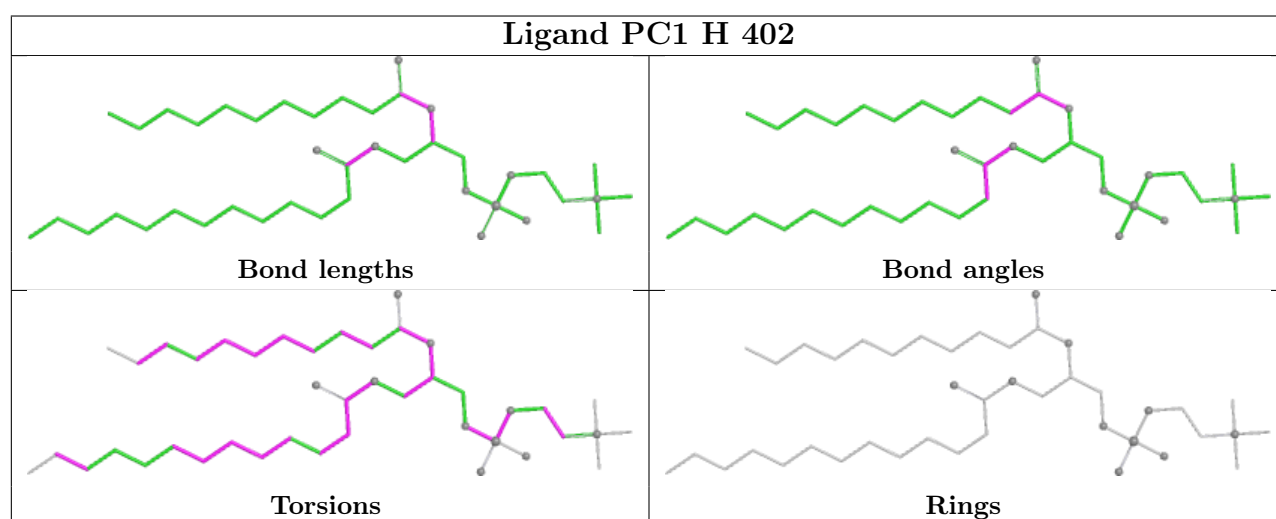
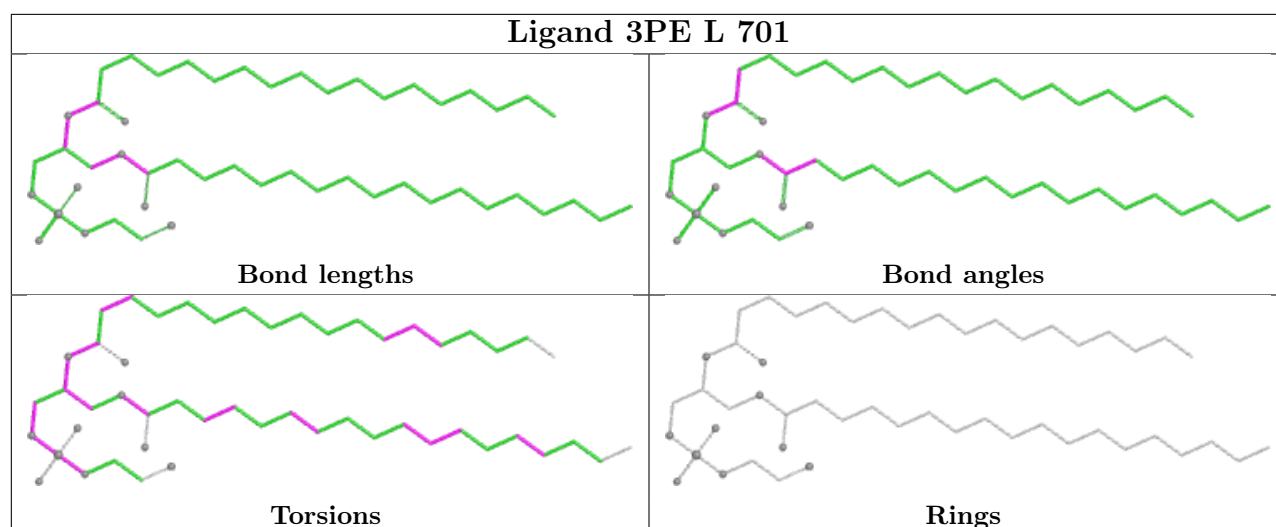
There are no ring outliers.

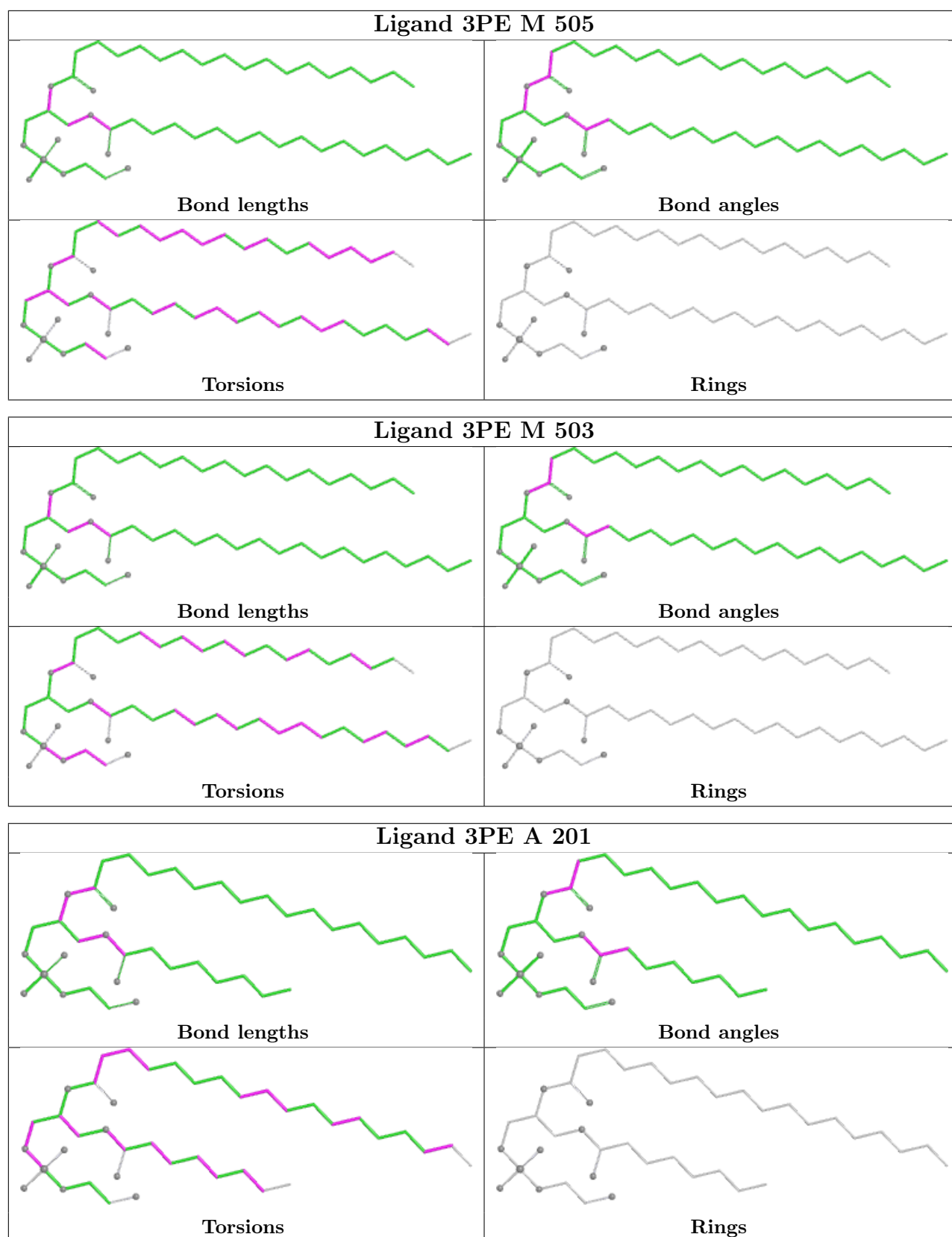
13 monomers are involved in 20 short contacts:

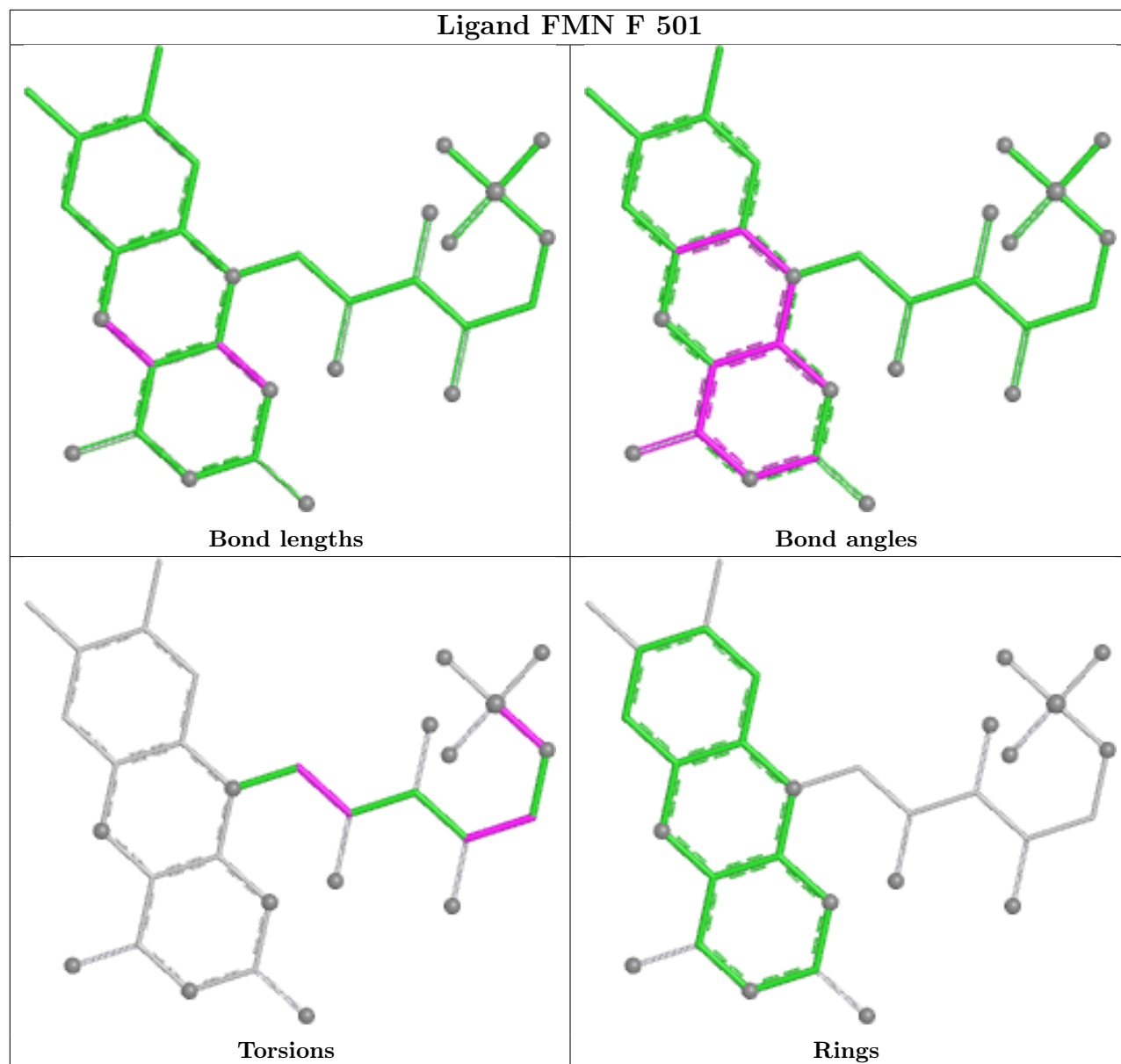
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	H	403	3PE	1	0
49	H	406	PC1	1	0
46	G	801	SF4	1	0
45	L	701	3PE	1	0
54	T	201	EHZ	1	0
45	M	505	3PE	2	0
48	F	501	FMN	1	0
52	P	501	NDP	5	0
50	L	703	CDL	2	0
50	L	702	CDL	1	0
49	H	404	PC1	1	0
47	E	301	FES	1	0
50	H	405	CDL	2	0

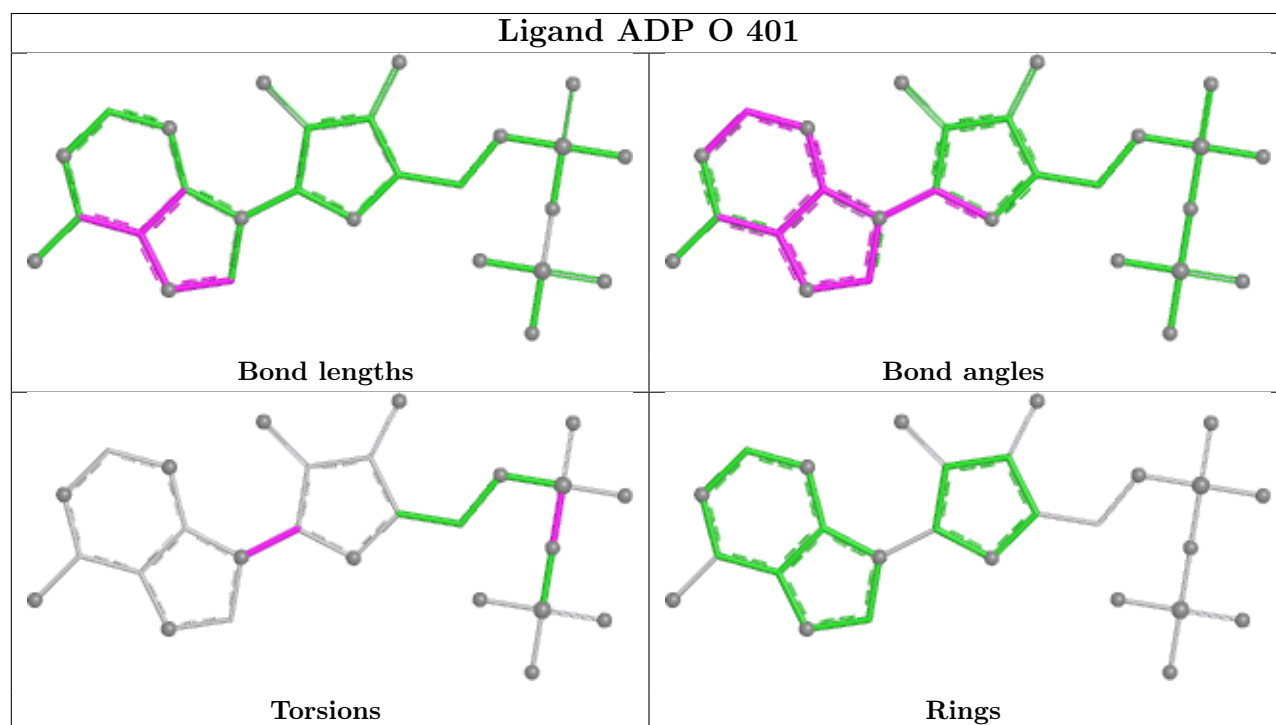
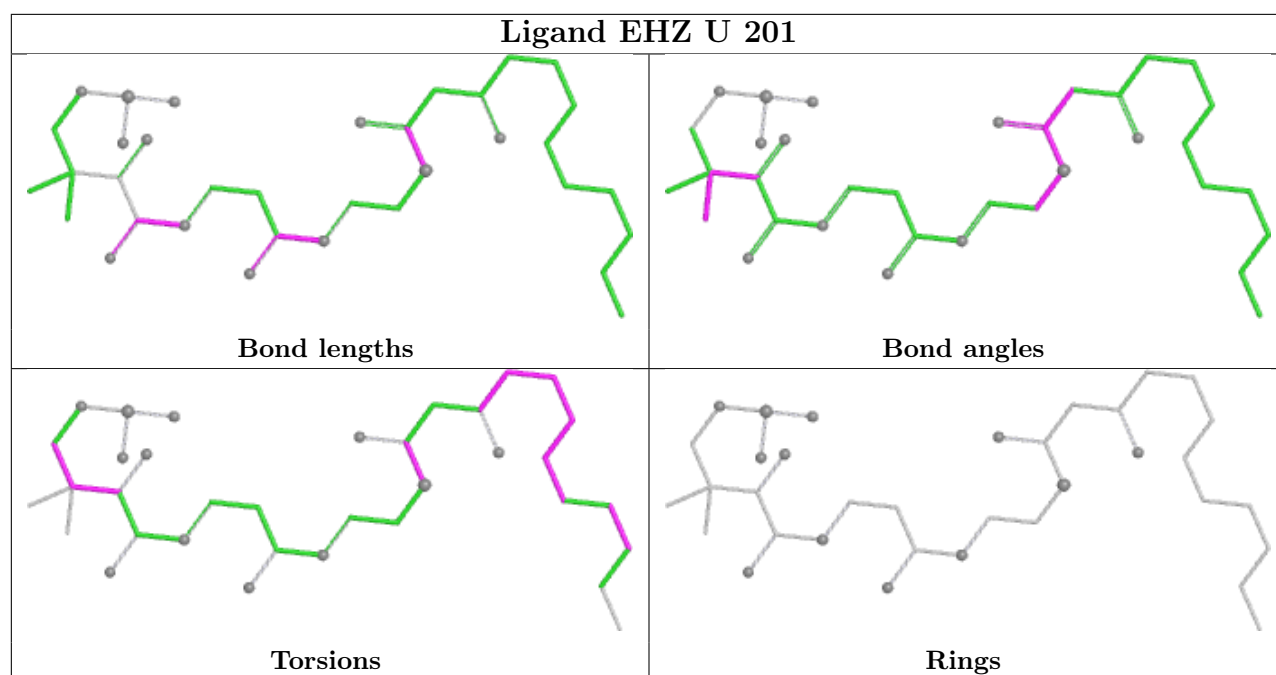
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

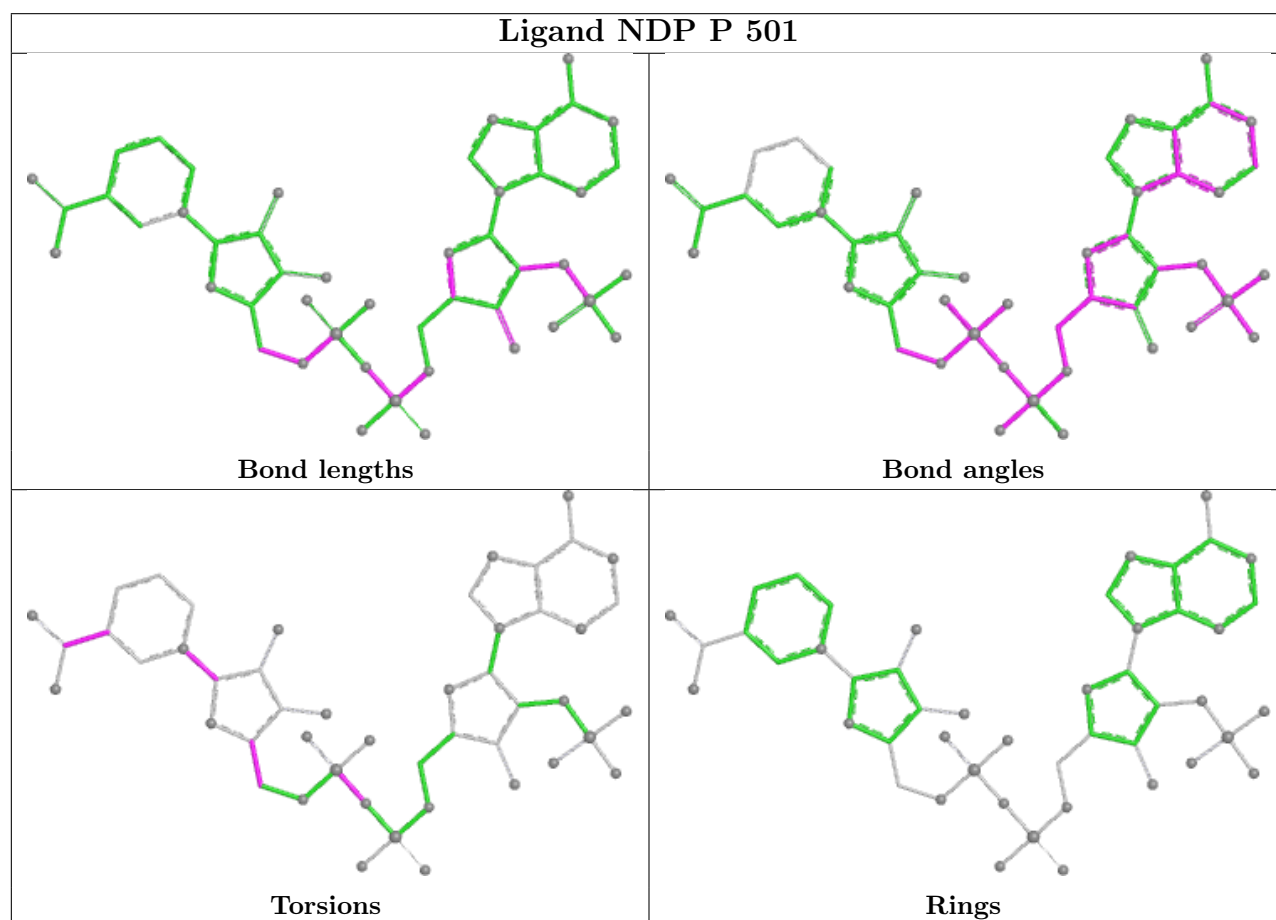
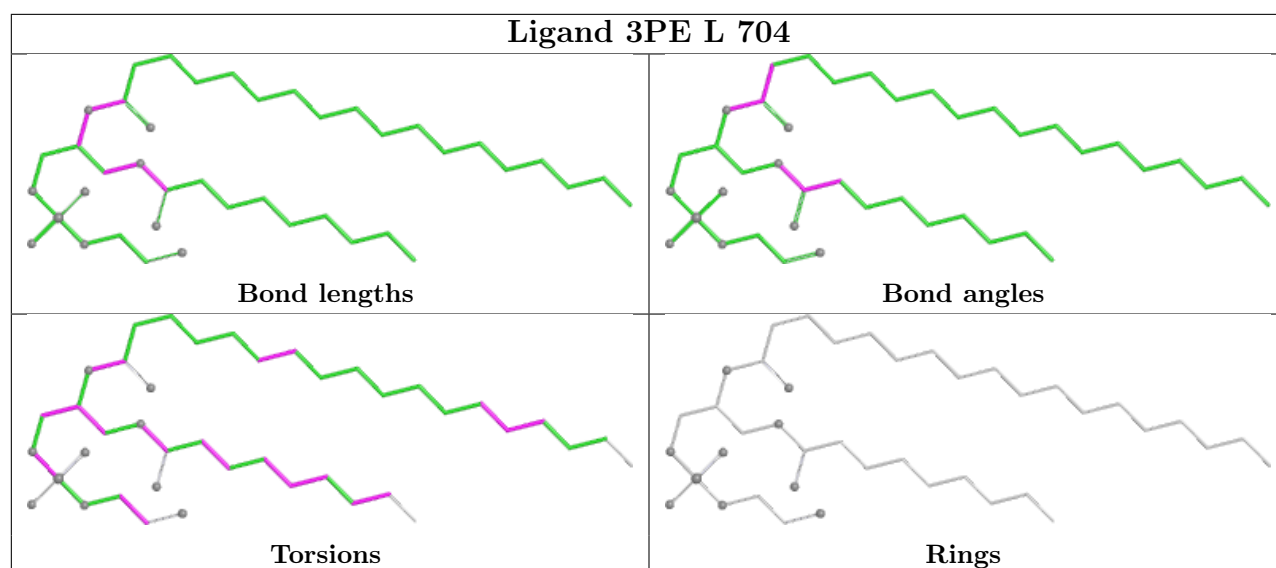


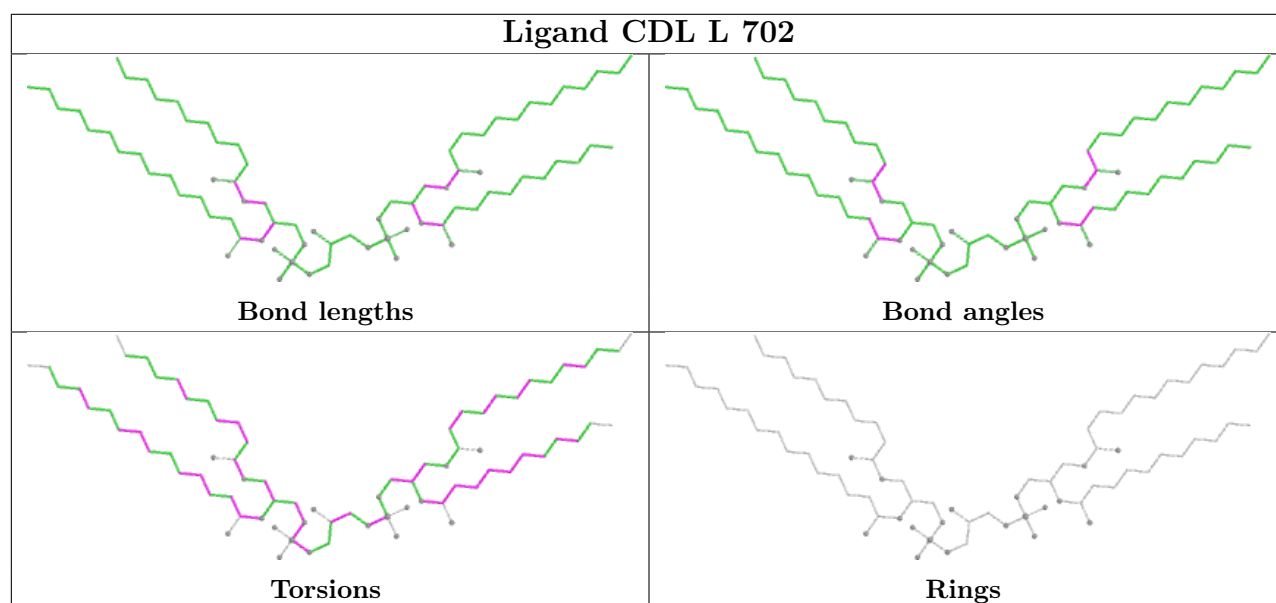
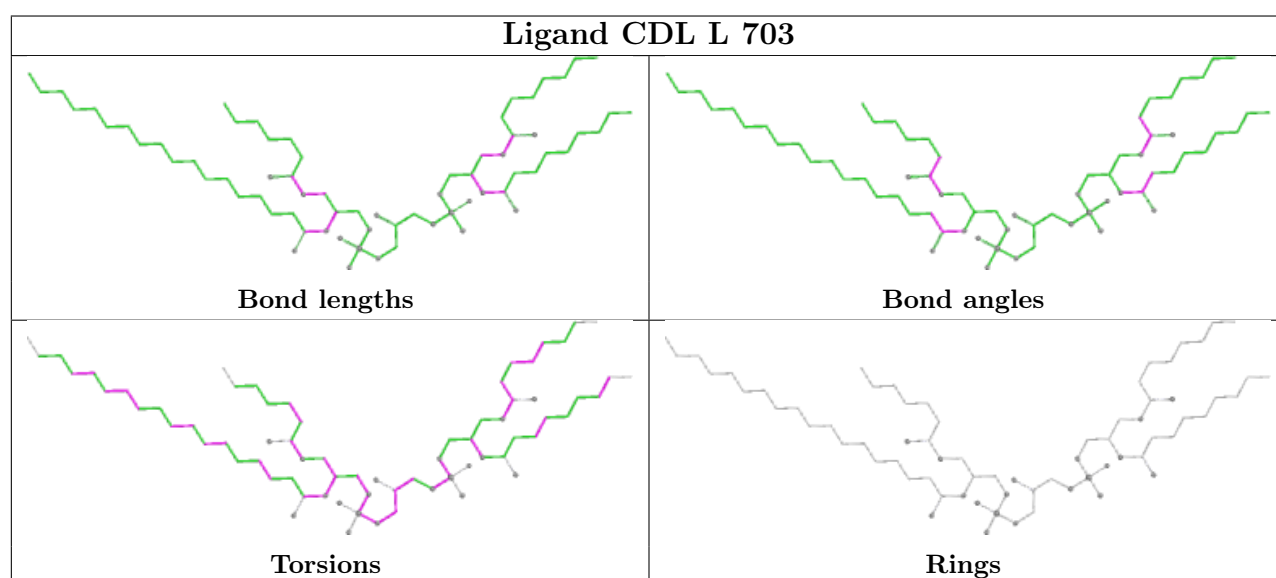
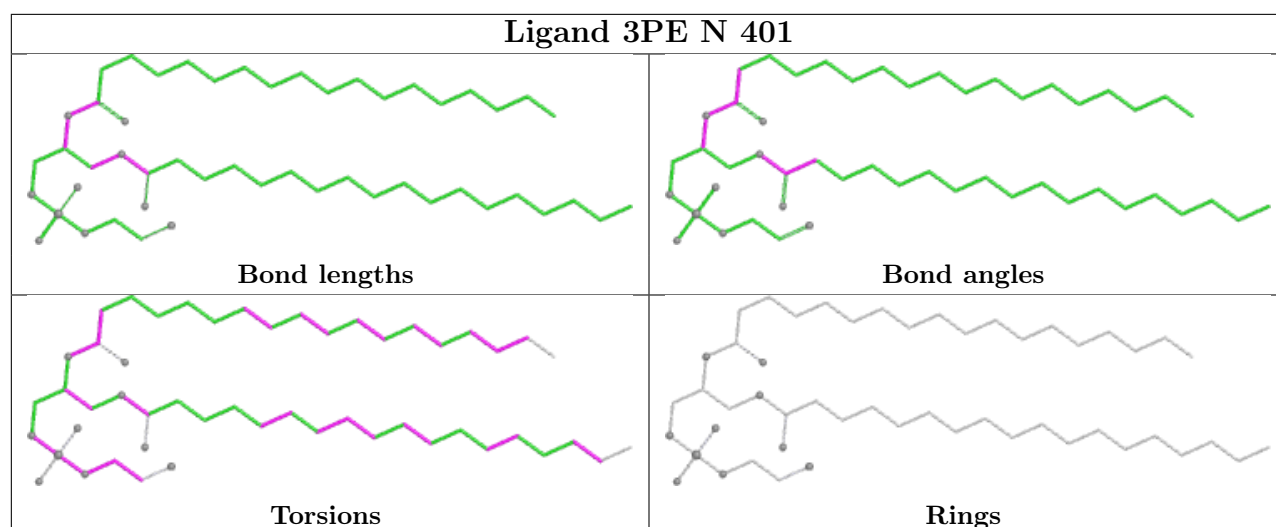


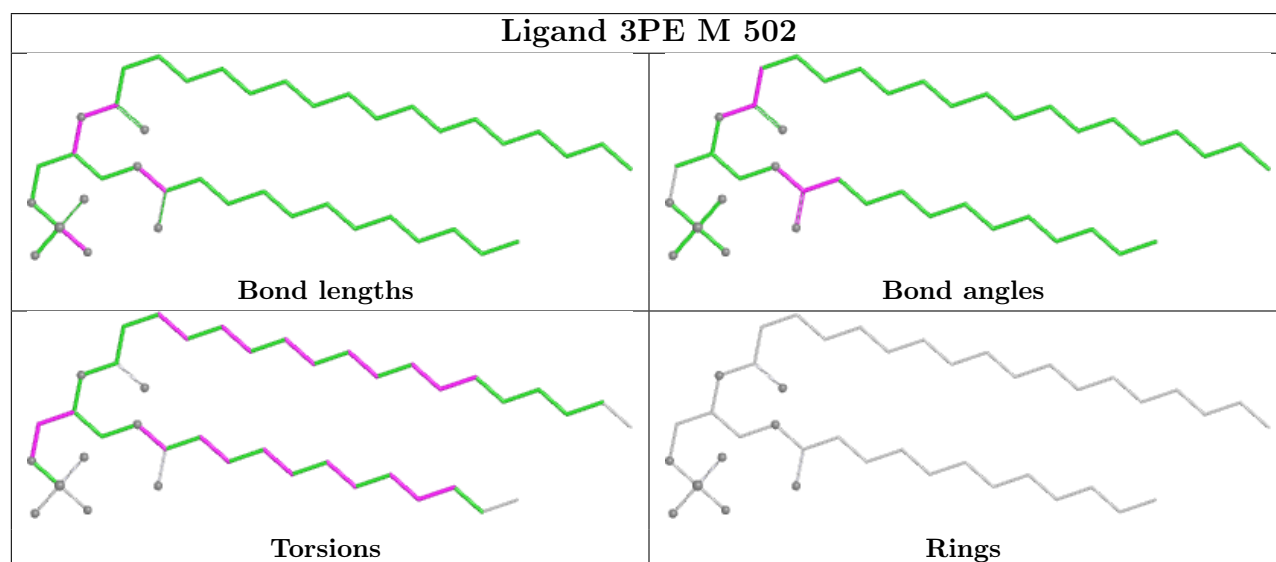
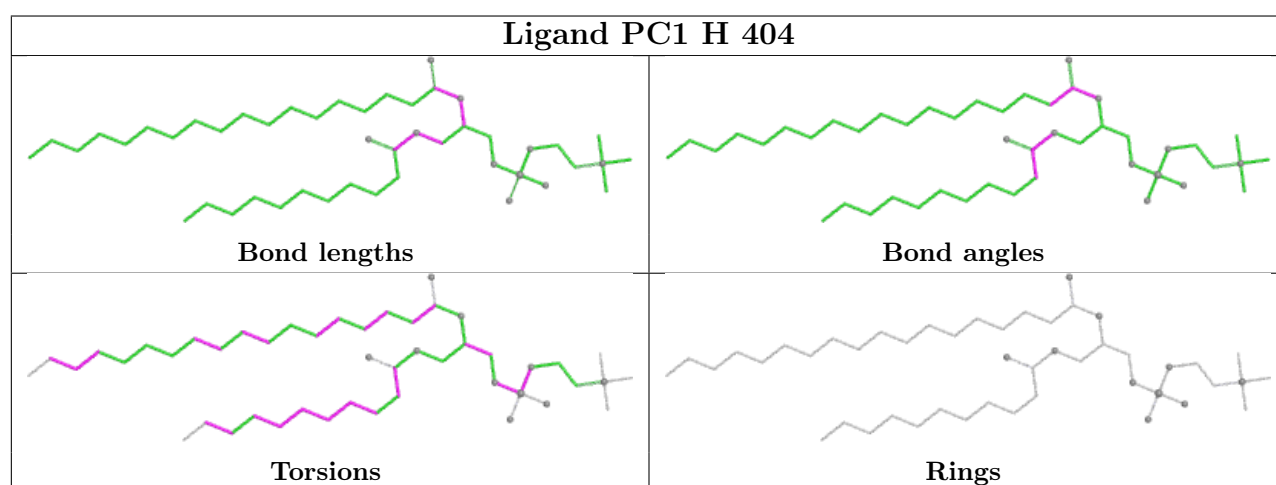
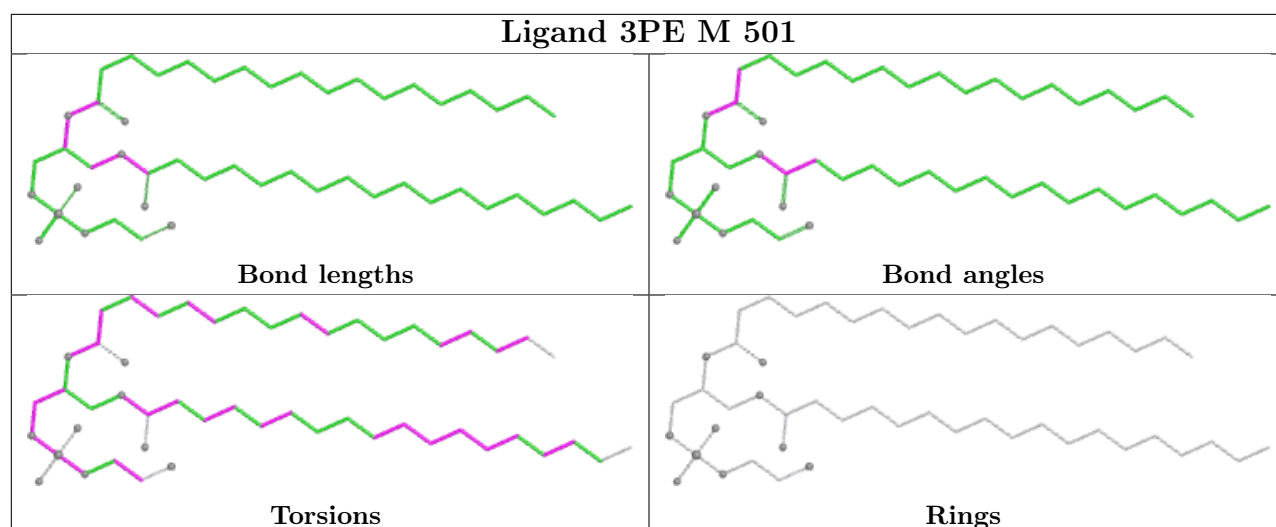


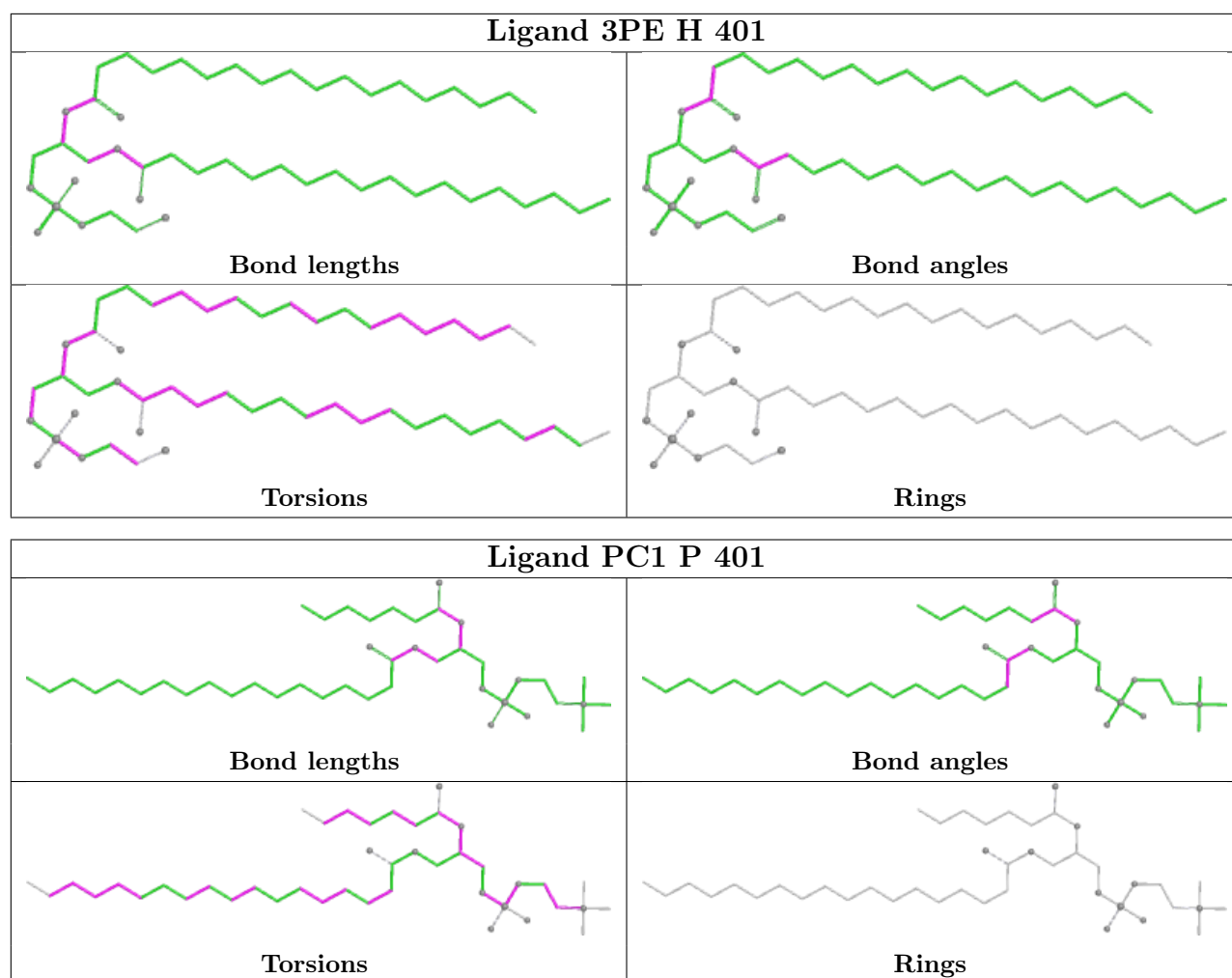


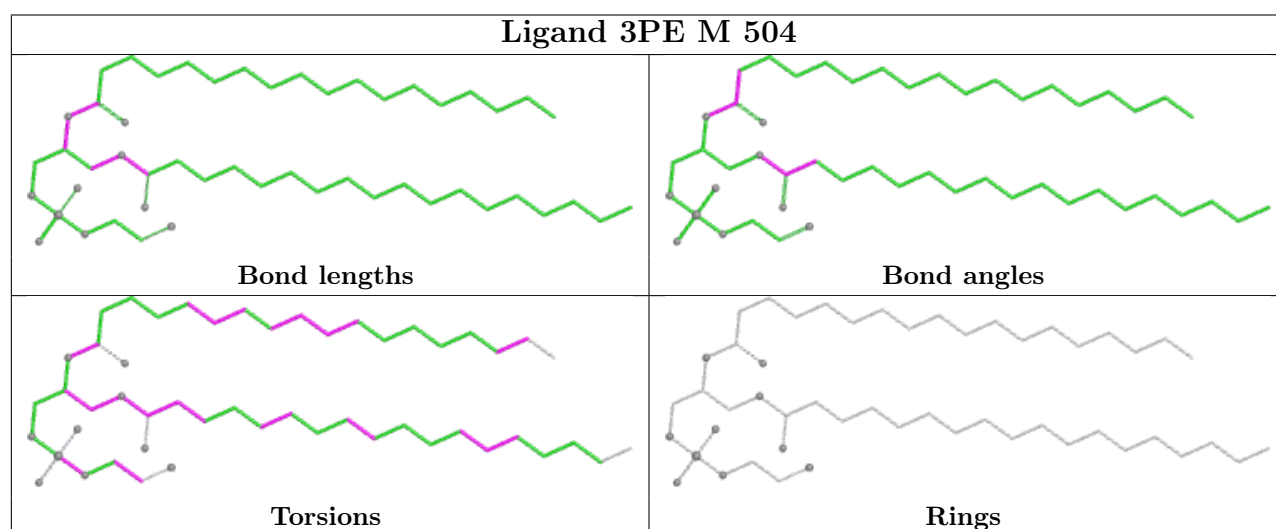
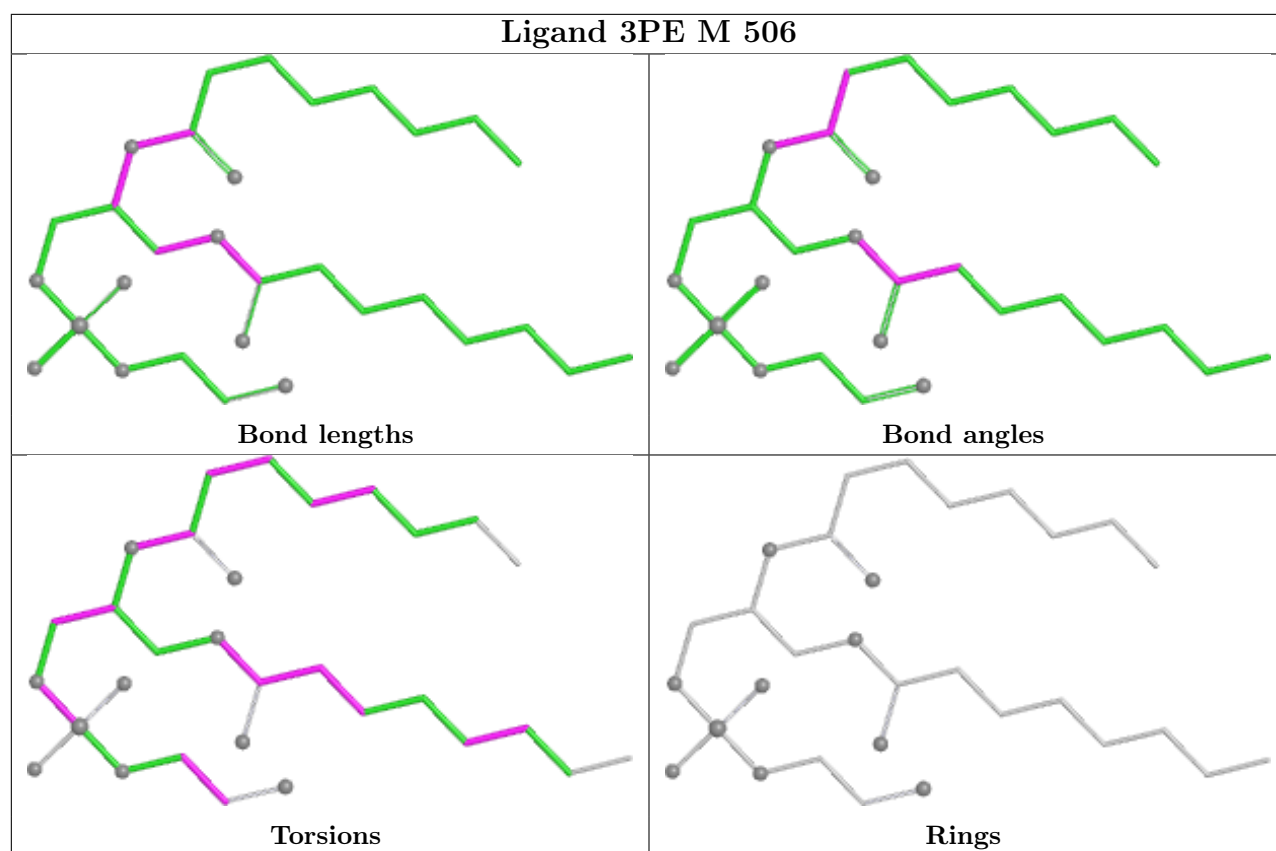


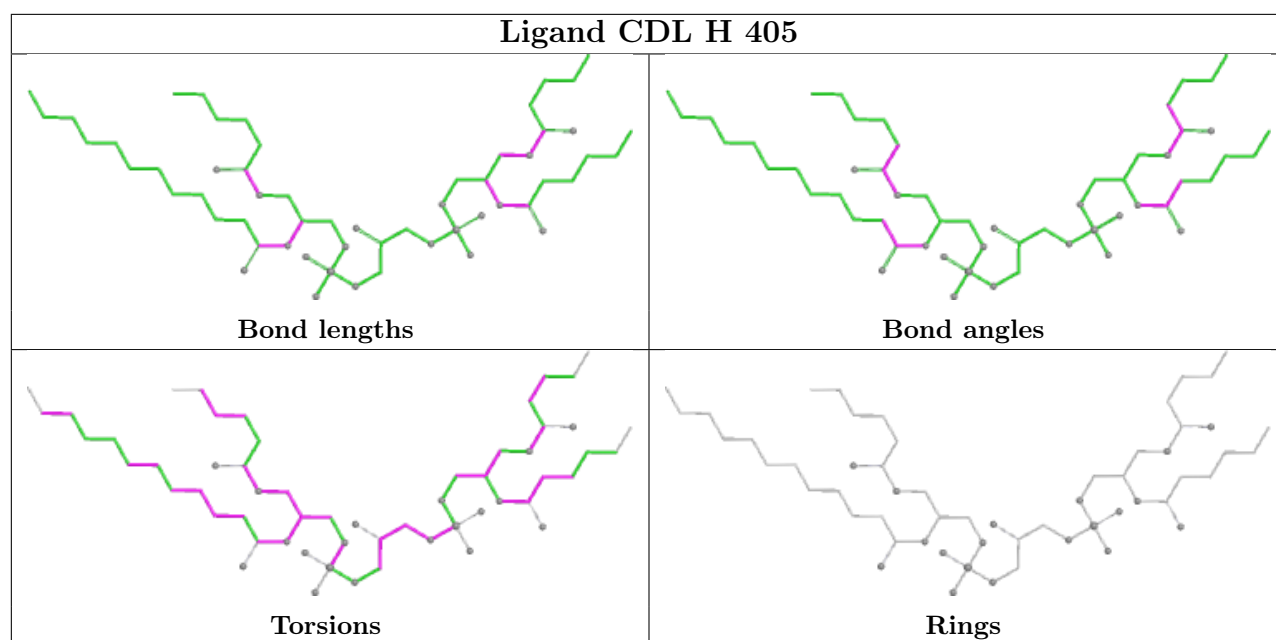












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

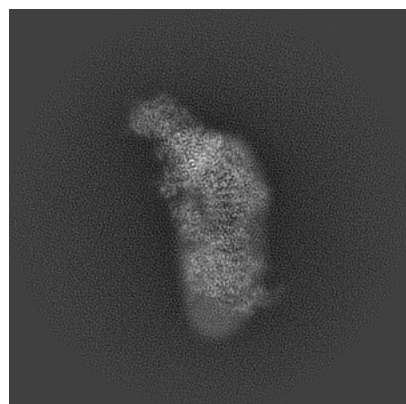
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4345. These allow visual inspection of the internal detail of the map and identification of artifacts.

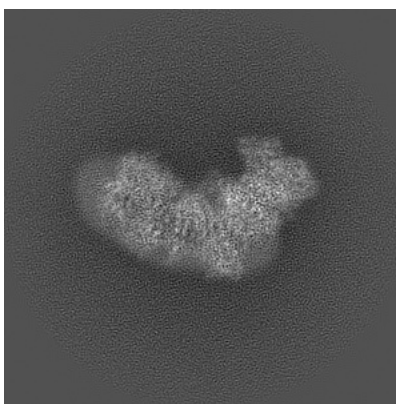
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

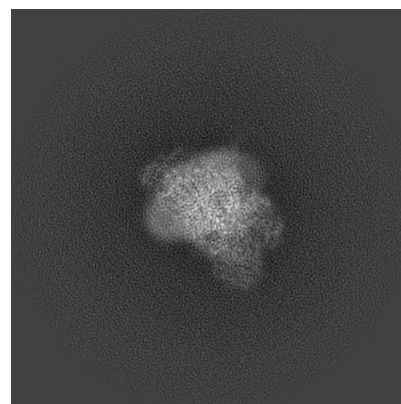
6.1.1 Primary map



X

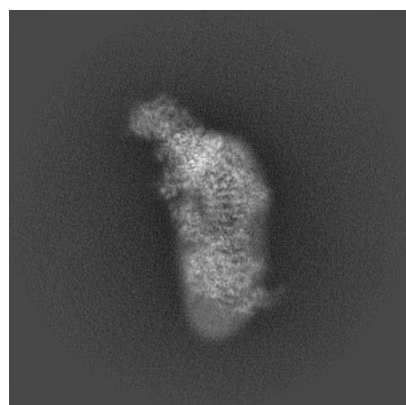


Y

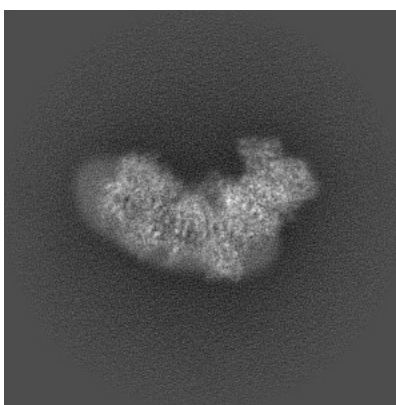


Z

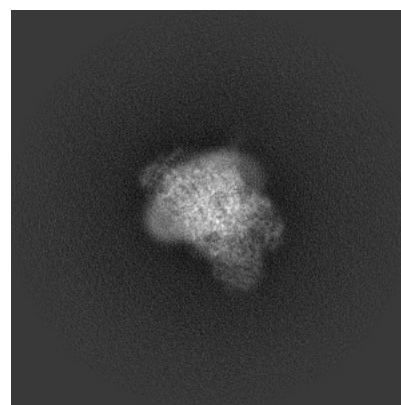
6.1.2 Raw map



X



Y

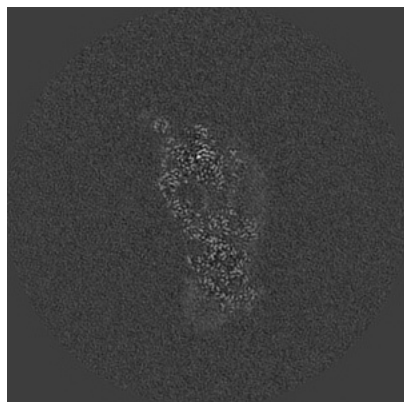


Z

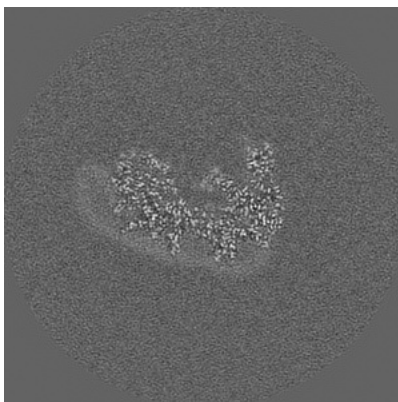
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

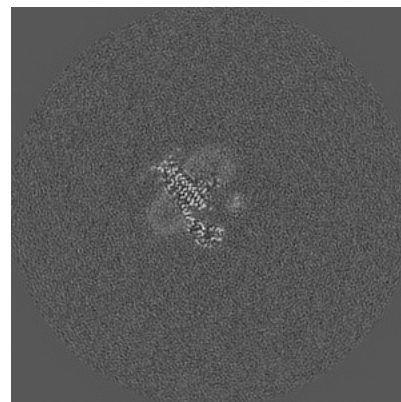
6.2.1 Primary map



X Index: 225

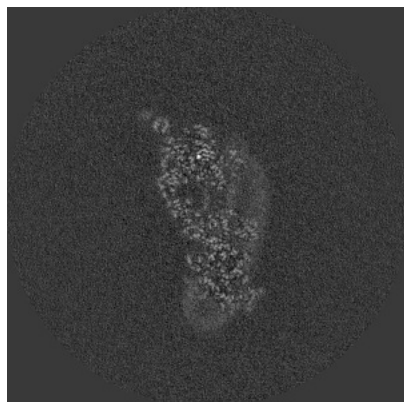


Y Index: 225

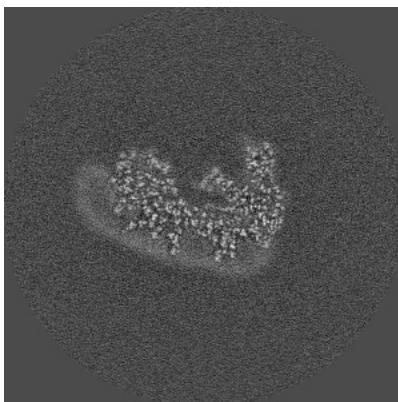


Z Index: 225

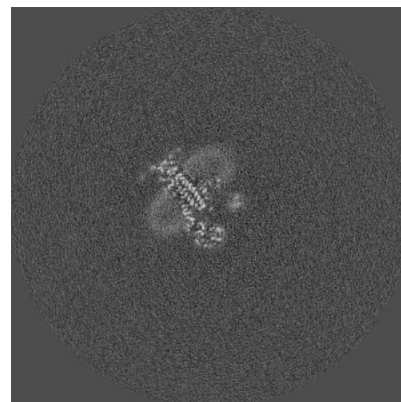
6.2.2 Raw map



X Index: 225



Y Index: 225

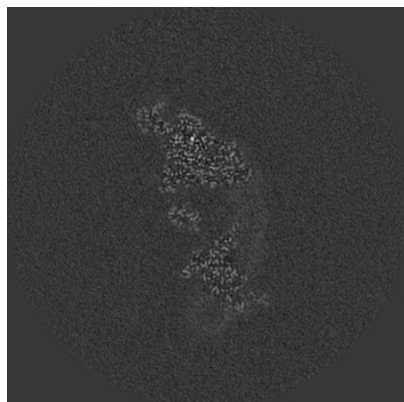


Z Index: 225

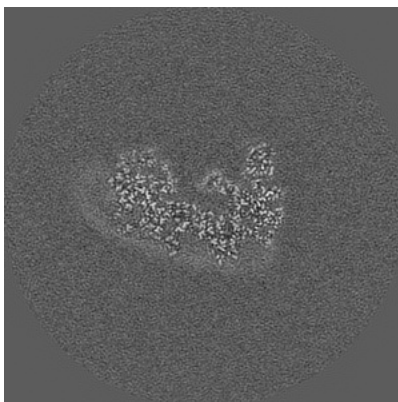
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

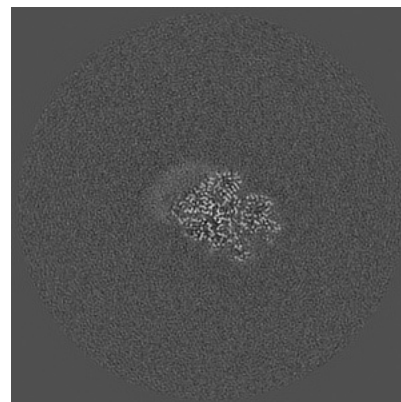
6.3.1 Primary map



X Index: 237

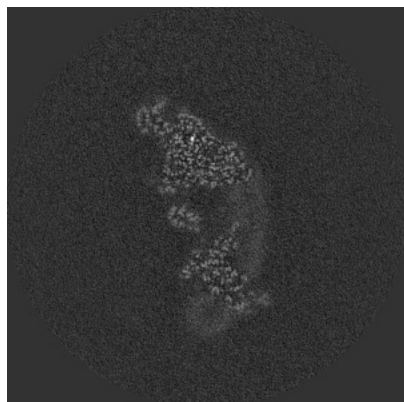


Y Index: 227

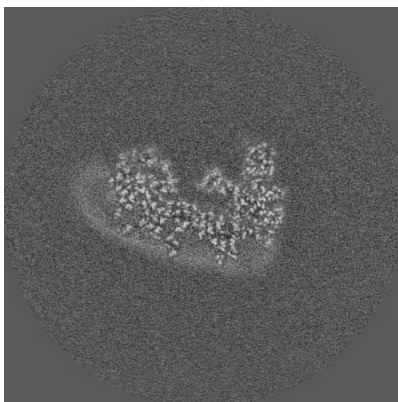


Z Index: 287

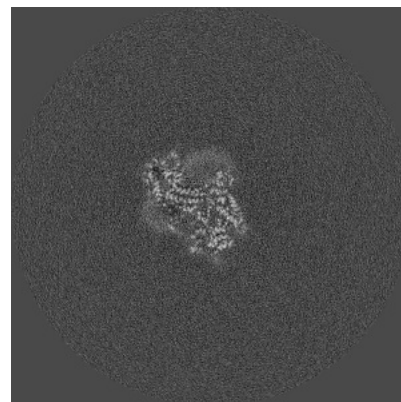
6.3.2 Raw map



X Index: 237



Y Index: 227

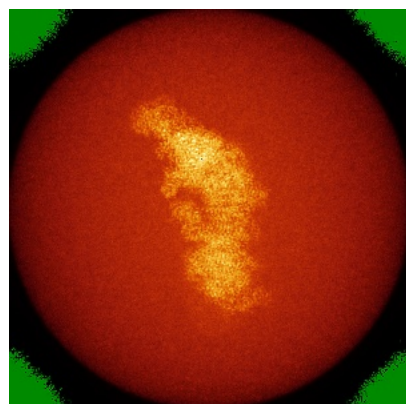


Z Index: 252

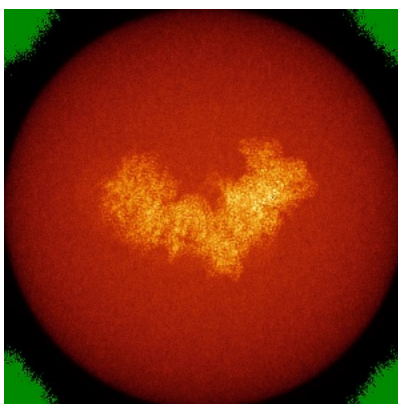
The images above show the largest variance slices of the map in three orthogonal directions.

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

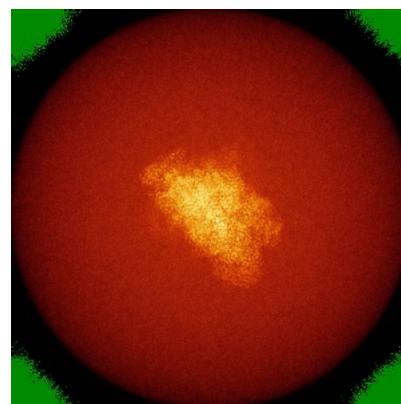
6.4.1 Primary map



X

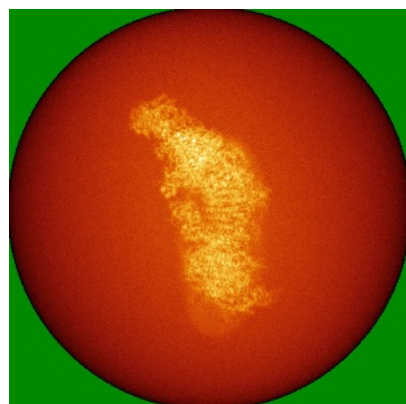


Y

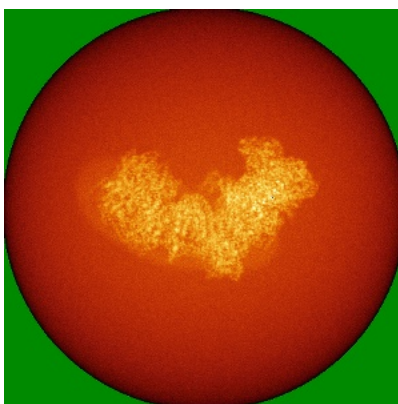


Z

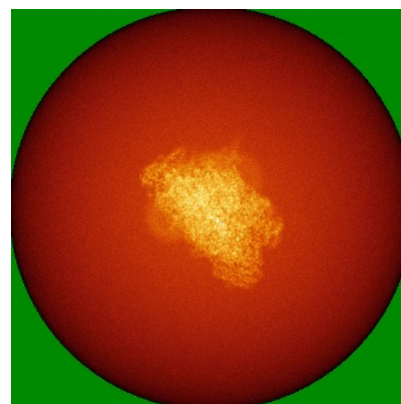
6.4.2 Raw map



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 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

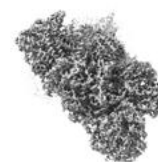
6.5.2 Raw map



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.

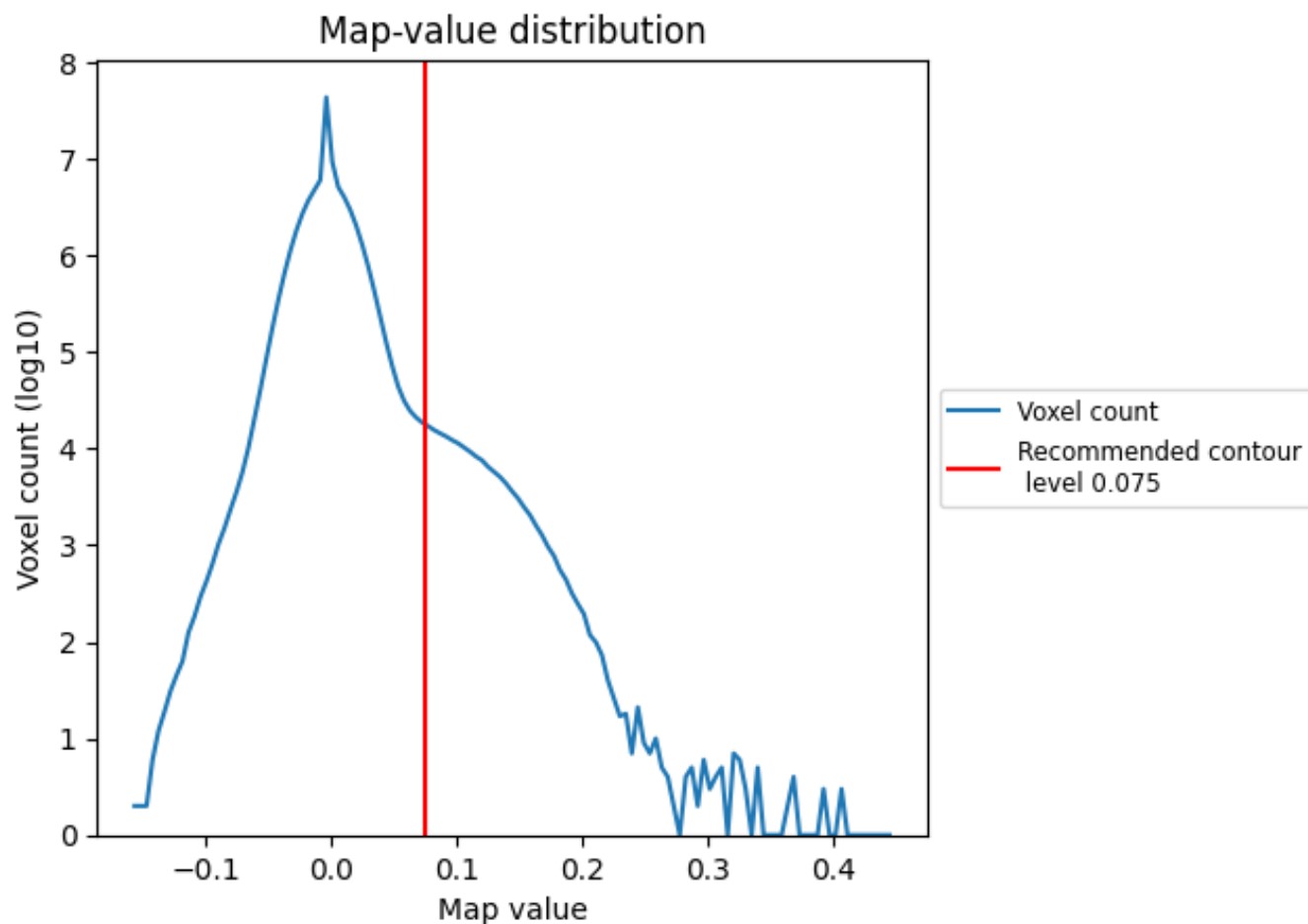
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

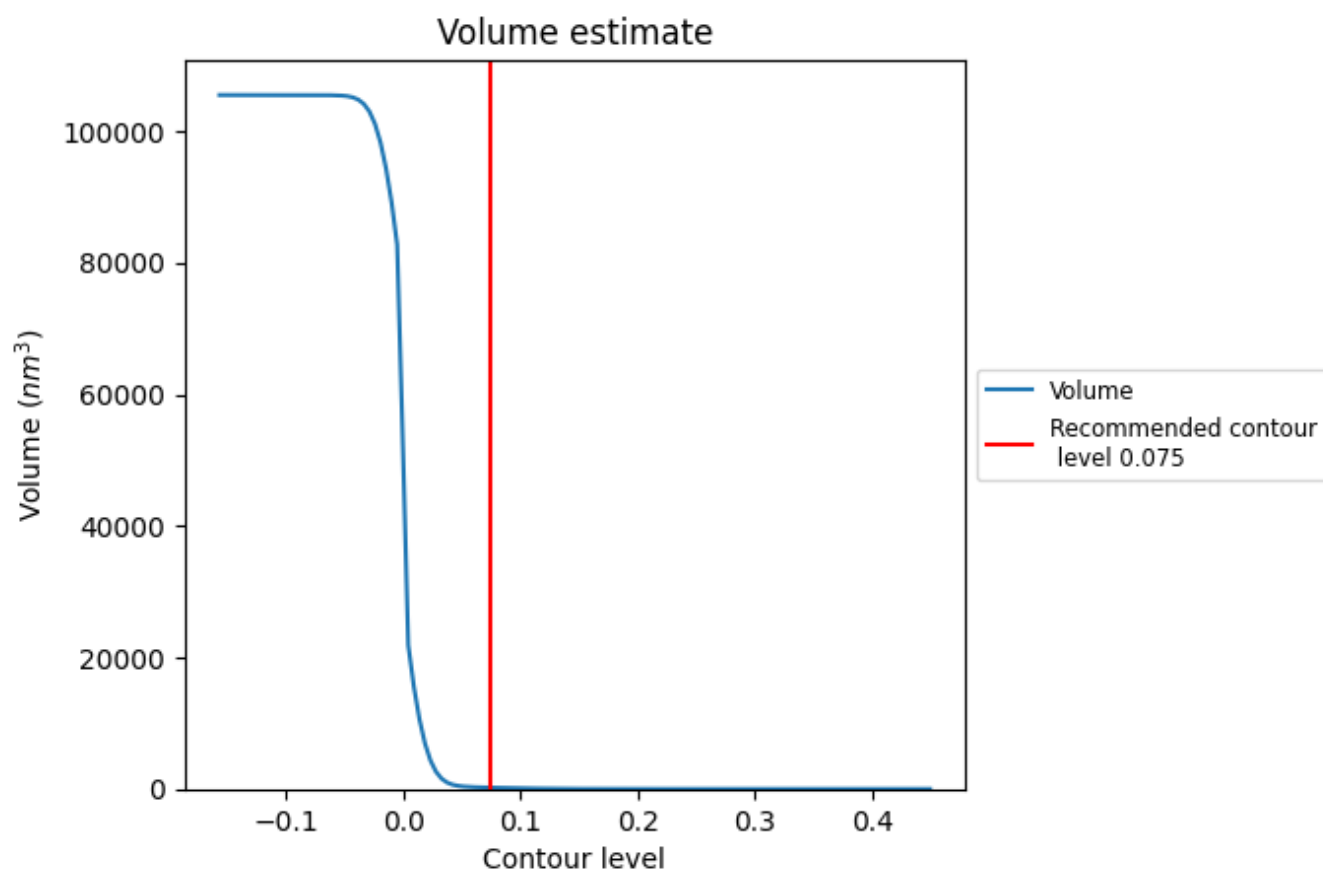
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

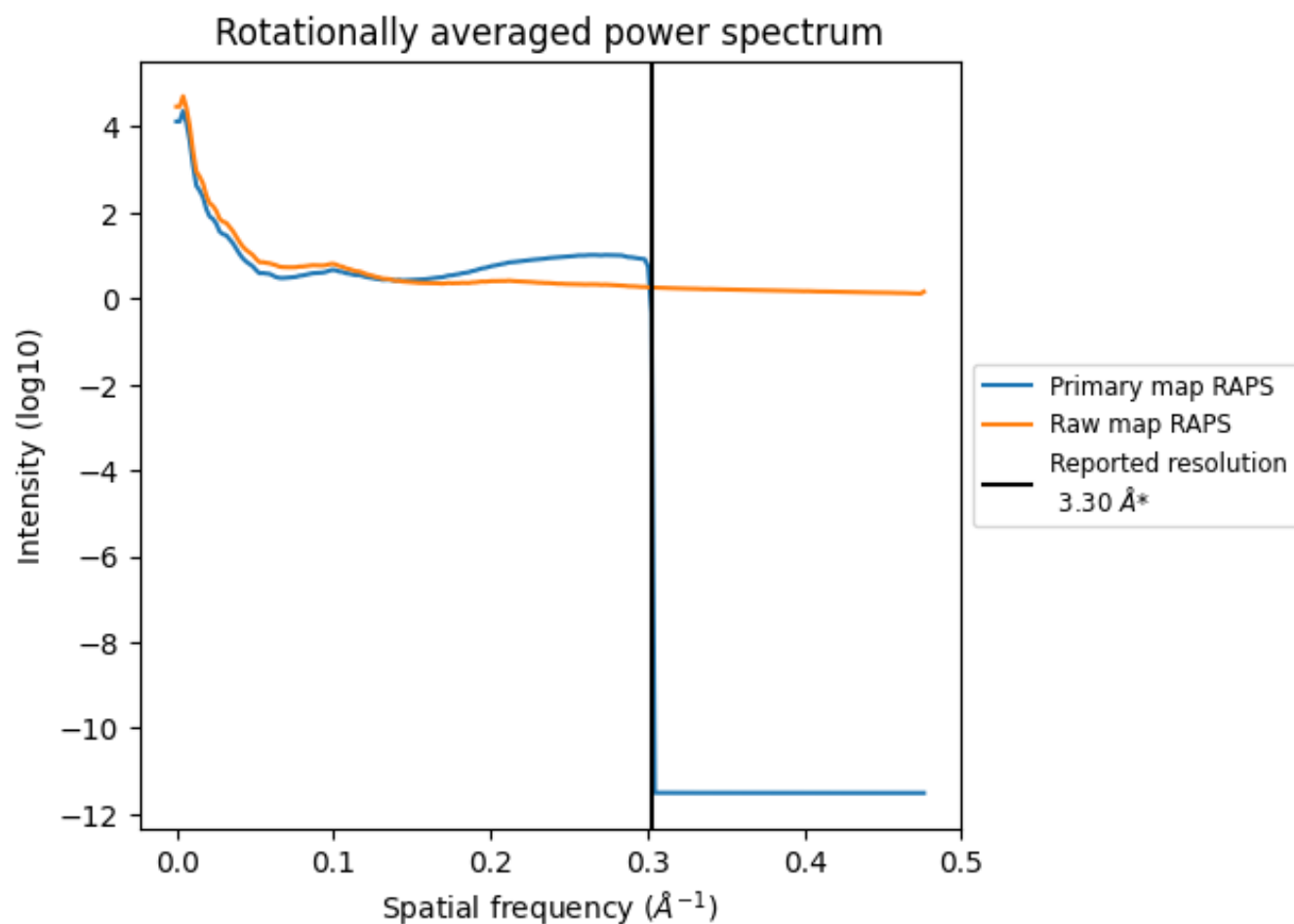
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm^3 ; this corresponds to an approximate mass of 176 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

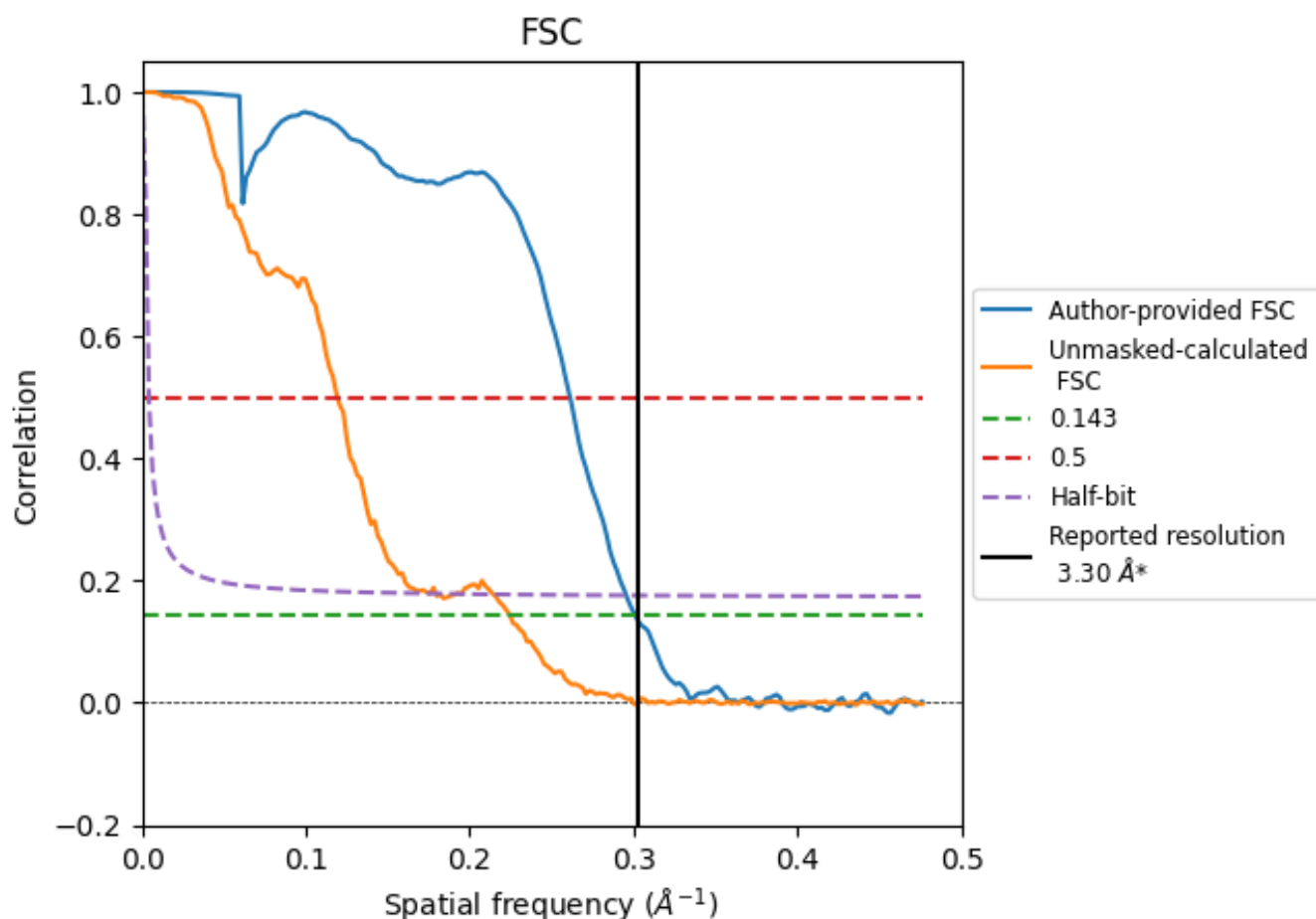


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

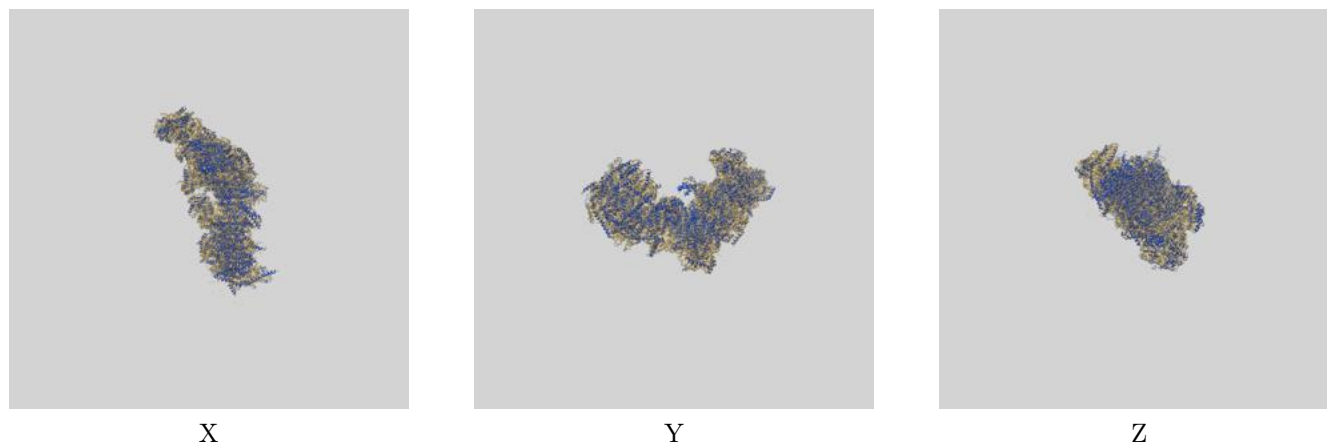
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.83	3.38
Unmasked-calculated*	4.45	8.39	5.70

*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 4.45 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

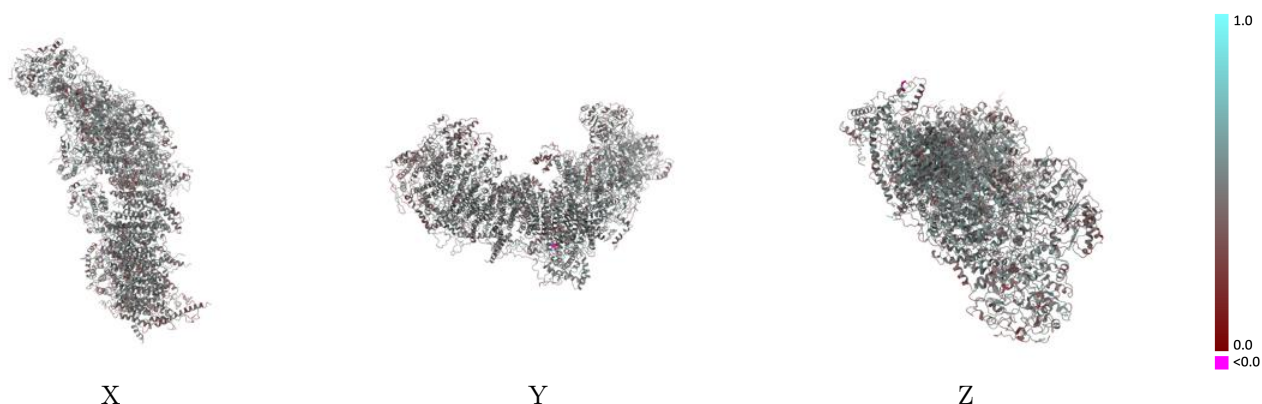
This section contains information regarding the fit between EMDB map EMD-4345 and PDB model 6G2J. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



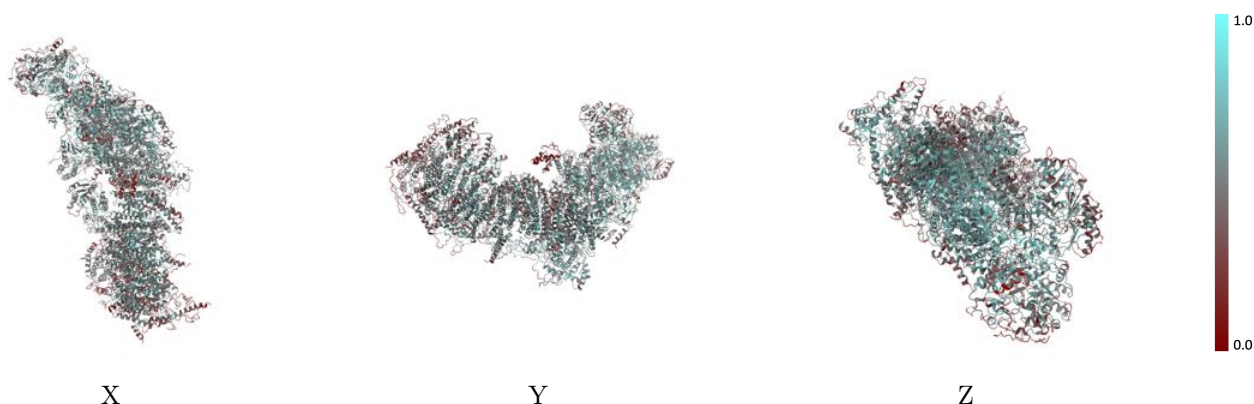
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



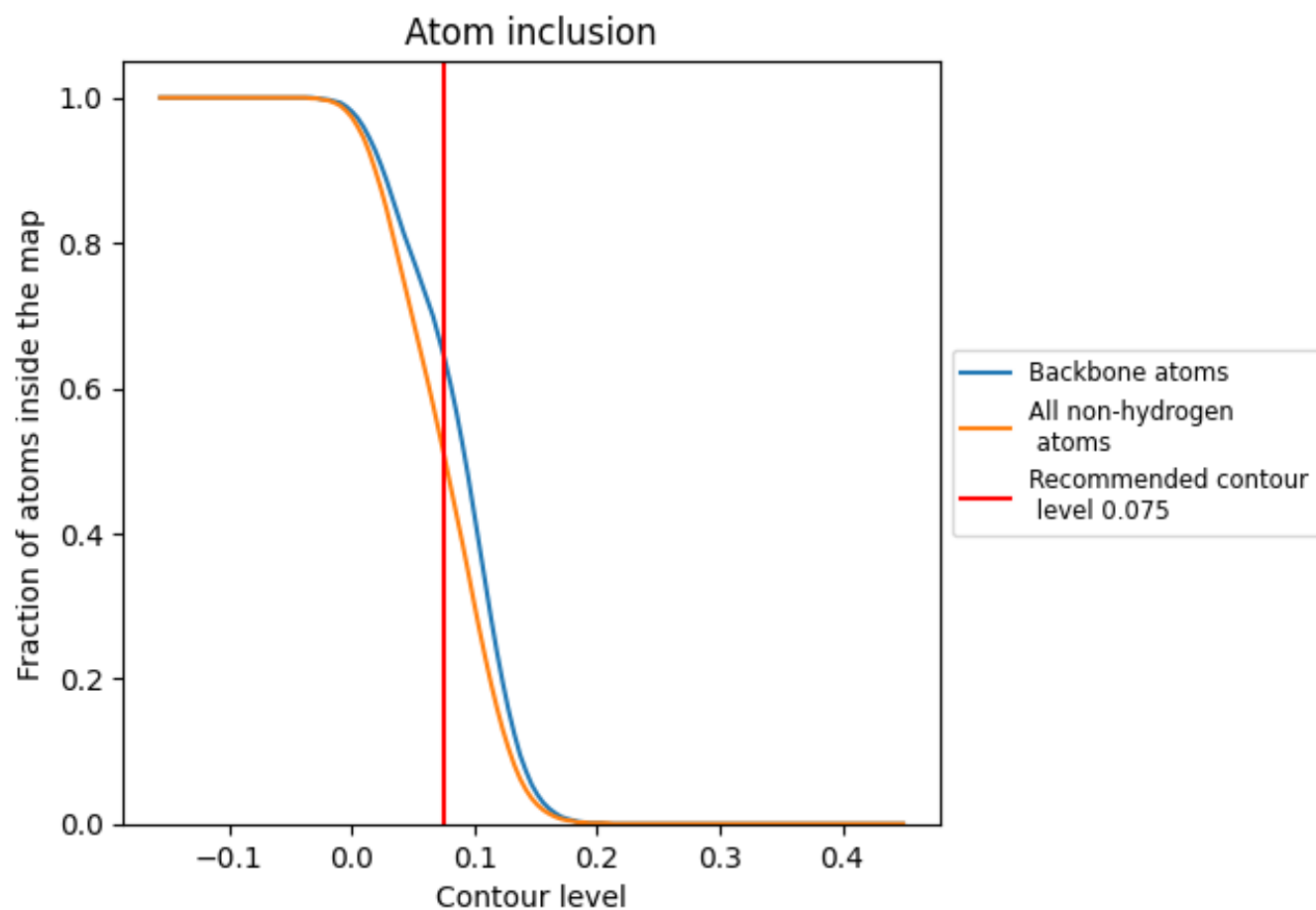
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5100	0.4690
A	0.5090	0.4820
B	0.6560	0.5030
C	0.6030	0.4980
D	0.6180	0.5020
E	0.4470	0.4570
F	0.4940	0.4600
G	0.5380	0.4760
H	0.5600	0.4960
I	0.6520	0.5070
J	0.4830	0.4650
K	0.5650	0.4900
L	0.4970	0.4760
M	0.5580	0.5020
N	0.5770	0.4920
O	0.5030	0.4640
P	0.5170	0.4680
Q	0.5330	0.4850
R	0.5400	0.4850
S	0.4140	0.4400
T	0.1780	0.3630
U	0.3540	0.4140
V	0.4730	0.4550
W	0.4950	0.4640
X	0.5180	0.4720
Y	0.4350	0.4490
Z	0.5160	0.4500
a	0.5670	0.4960
b	0.4630	0.4310
c	0.3810	0.4180
d	0.4960	0.4650
e	0.5200	0.4630
f	0.4180	0.4250
g	0.4330	0.4570
h	0.5140	0.4690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.3730	 0.4220
j	 0.3510	 0.3870
k	 0.3260	 0.4250
l	 0.4560	 0.4470
m	 0.4630	 0.4640
n	 0.4240	 0.4110
o	 0.3220	 0.3870
p	 0.4600	 0.4440
q	 0.5570	 0.4780
r	 0.4950	 0.4560
s	 0.3850	 0.4410