



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2025 – 05:40 pm GMT

PDB ID : 8CA3 / pdb\_00008ca3  
EMDB ID : EMD-16516  
Title : Cryo-EM structure NDUFS4 knockout complex I from Mus musculus heart (Class 2).  
Authors : Yin, Z.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.  
Deposited on : 2023-01-24  
Resolution : 3.20 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](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:

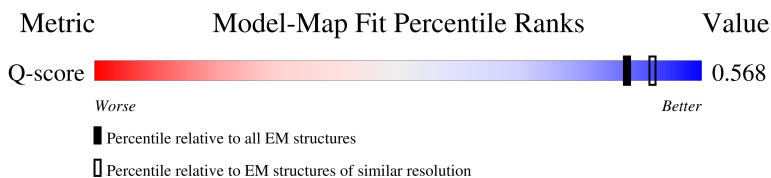
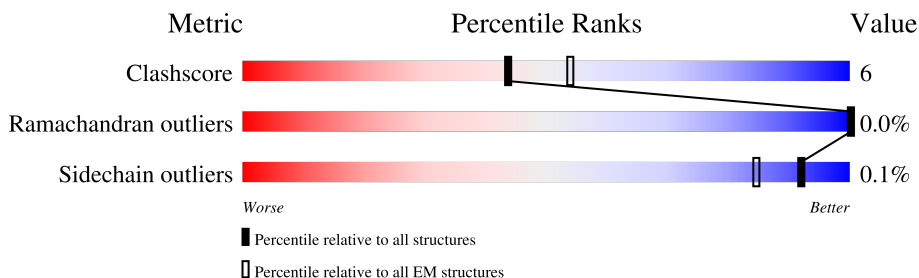
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.47

# 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 3.20 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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	 90% 10%
2	B	224	 56% 14% 30%
3	C	263	 69% 10% 21%
4	D	463	 77% 16% 7%



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Mol	Chain	Length	Quality of chain
5	E	245	
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	R	116	
18	S	99	
19	T	156	
19	U	156	
20	V	116	
21	W	131	
22	X	172	
23	Y	143	
24	Z	144	
25	a	70	
26	b	84	
27	c	76	
28	d	120	

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Mol	Chain	Length	Quality of chain
29	e	106	
30	f	57	
31	g	151	
32	h	189	
33	i	127	
34	j	105	
35	k	104	
36	l	186	
37	m	129	
38	n	179	
39	o	137	
40	p	176	
41	r	113	
42	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
43	SF4	I	201	-	-	X	-
46	FMN	F	502	-	X	-	-

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 63712 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	156	Total	C	N	O	S	0	0
			1247	796	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	N	O	S	0	0
			1721	1111	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	N	O	S	0	0
			3463	2215	595	629	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1639	1043	275	310	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
			3300	2080	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	N	O	S	0	0
			5248	3294	910	1003	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
			1431	898	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	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	325	Total	C	N	O	S	0	0
			2626	1702	456	461	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	55	Total	C	N	O	S	0	0
			413	258	74	78	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	82	Total	C	N	O	S	0	0
			594	374	108	110	2		

- Molecule 19 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	76	Total	C	N	O	S	0	0
			611	392	90	124	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	86	Total	C	N	O	S	0	0
			692	446	102	139	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			935	598	175	156	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

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

- Molecule 23 is a protein called MCG5603.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	68	Total	C	N	O	S	0	0
			556	360	99	93	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	94	Total	C	N	O	S	0	0
			787	515	134	135	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	62	Total	C	N	O	S	0	0
			537	355	88	93	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	75	Total	C	N	O	S	0	0
			609	404	103	100	2		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	154	Total	C	N	O	S	0	0
			1294	834	215	234	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	113	Total	C	N	O	S	0	0
			979	617	184	170	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	168	Total	C	N	O	S	0	0
			1424	896	256	264	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	61	Total	C	N	O	S	0	0
			487	311	87	86	3		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

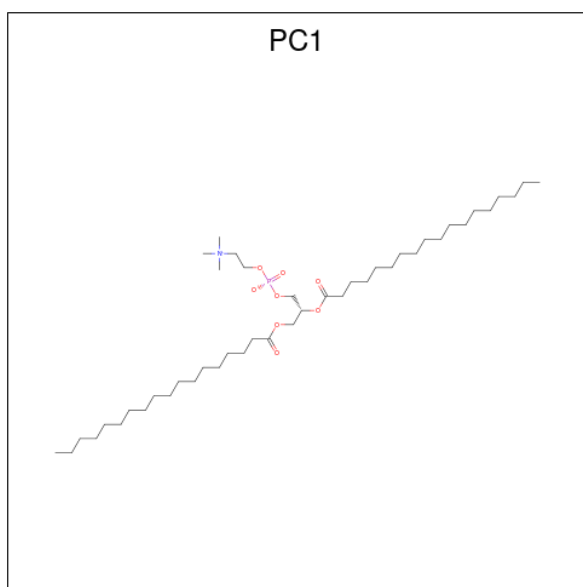
Mol	Chain	Residues	Atoms				AltConf	Trace
42	s	31	Total	C	N	O	0	0
			269	174	45	50		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



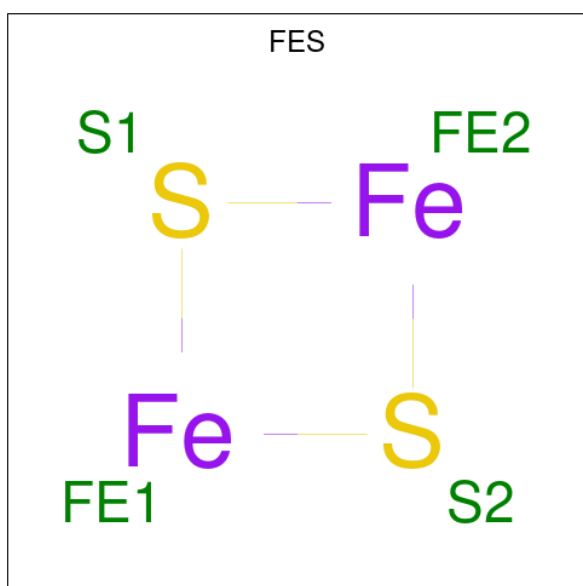
Mol	Chain	Residues	Atoms			AltConf
43	B	1	Total	Fe	S	0
			8	4	4	
43	F	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	

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



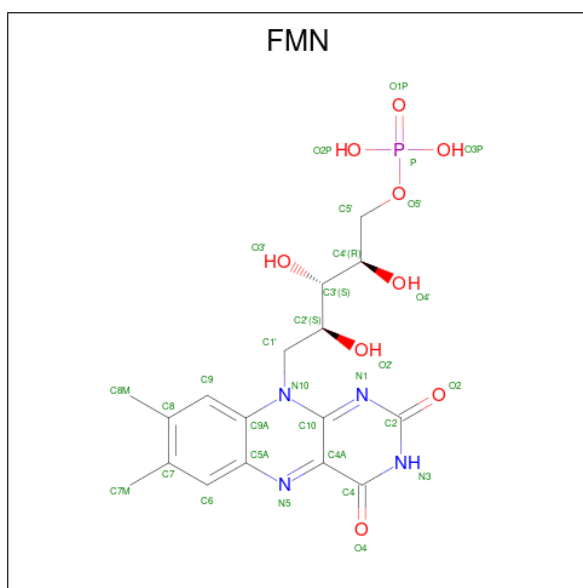
Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
44	H	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



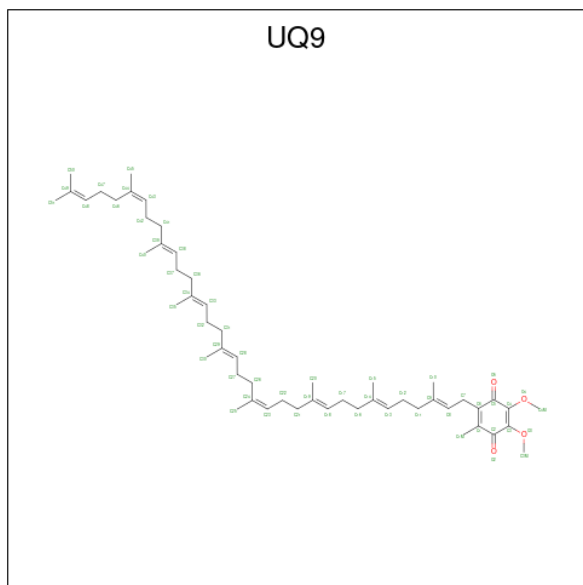
Mol	Chain	Residues	Atoms			AltConf
45	E	1	Total	Fe	S	0
			4	2	2	
45	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					AltConf
46	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

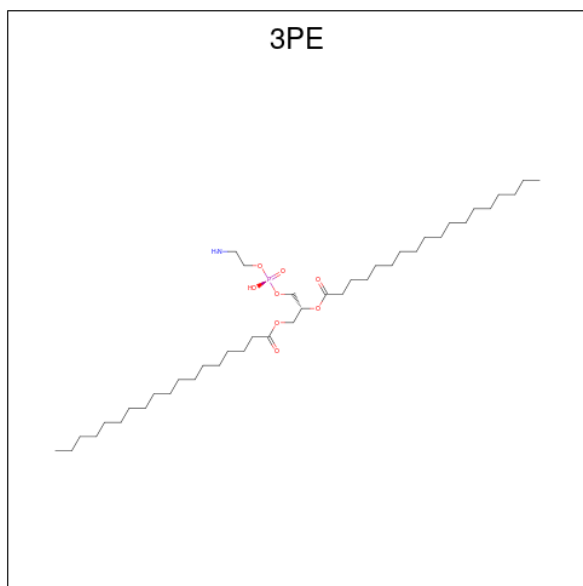
- Molecule 47 is Ubiquinone-9 (CCD ID: UQ9) (formula:  $C_{54}H_{82}O_4$ ).



Mol	Chain	Residues	Atoms		AltConf
47	H	1	Total	C	0
			45	45	

- Molecule 48 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
48	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	J	1	Total	C	N	O	P	0
			33	23	1	8	1	
48	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
48	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
48	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
48	i	1	Total	C	N	O	P	0
			42	32	1	8	1	

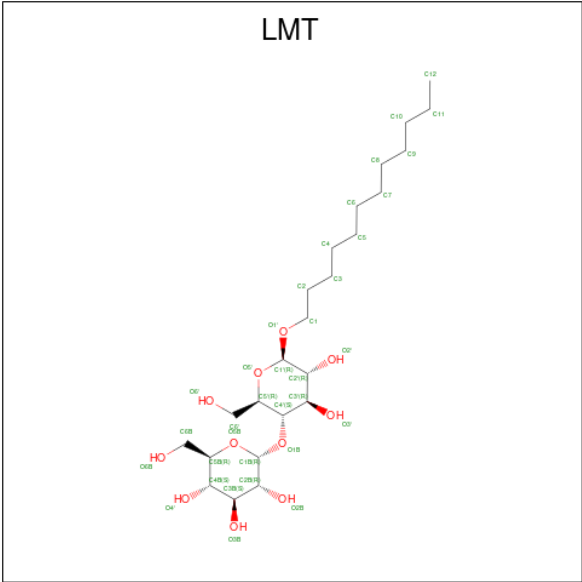
- Molecule 49 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
49	L	1	Total	C	O	P	0
			74	55	17	2	
49	M	1	Total	C	O	P	0
			59	41	16	2	
49	N	1	Total	C	O	P	0
			65	46	17	2	
49	N	1	Total	C	O	P	0
			63	44	17	2	
49	d	1	Total	C	O	P	0
			67	48	17	2	
49	h	1	Total	C	O	P	0
			70	51	17	2	

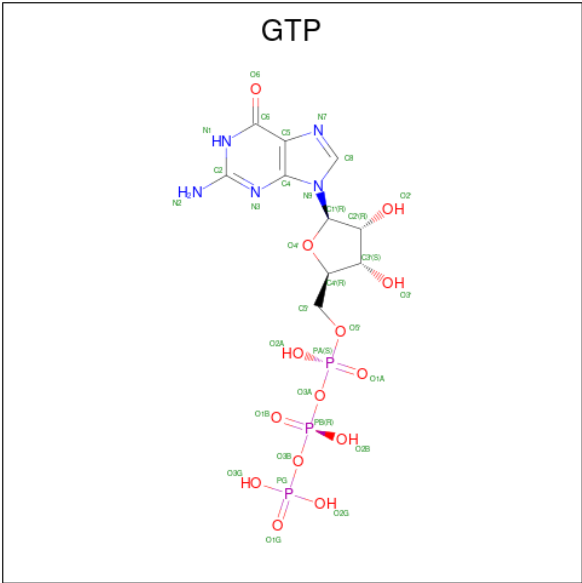
- Molecule 50 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).





Mol	Chain	Residues	Atoms			AltConf
50	L	1	Total	C	O	0
			35	24	11	
50	L	1	Total	C	O	0
			35	24	11	

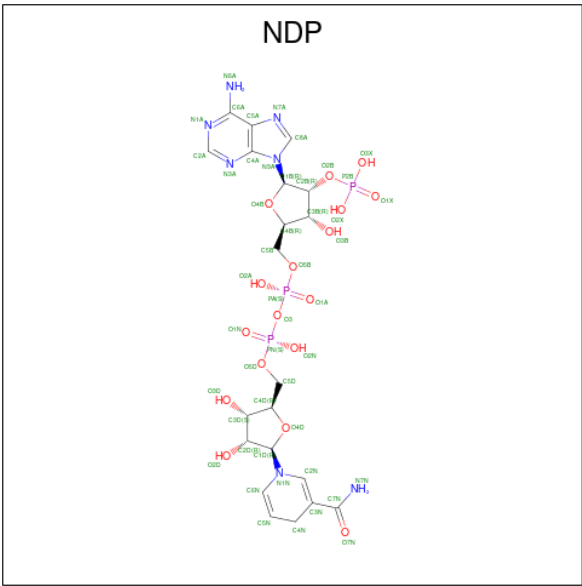
- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
51	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).

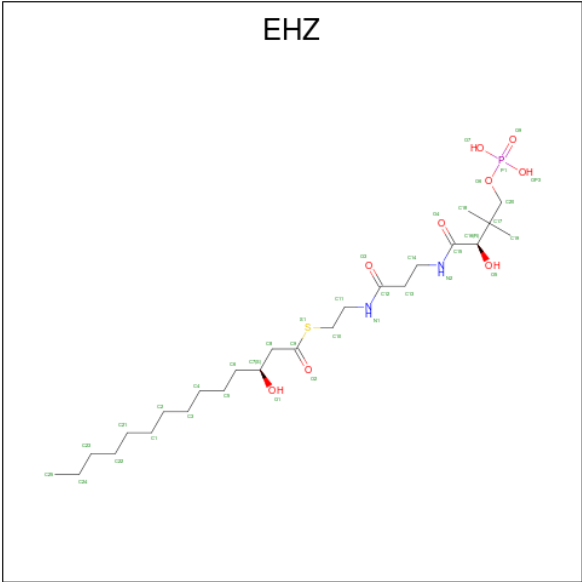


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

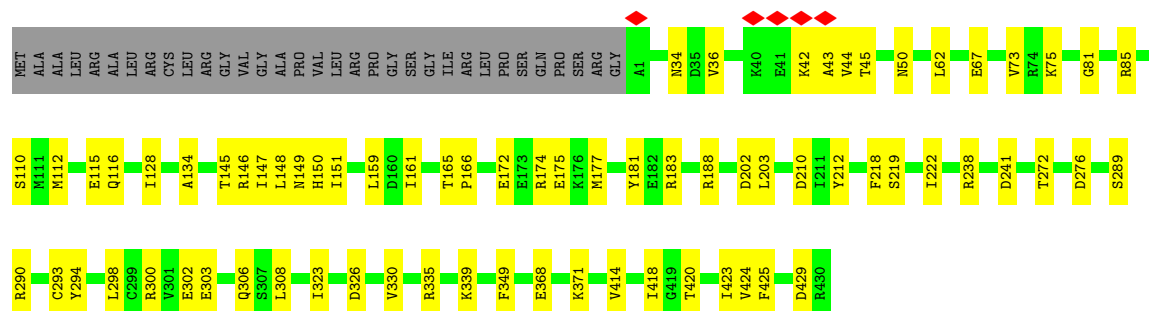
Mol	Chain	Residues	Atoms		AltConf
53	R	1	Total	Zn	0
			1	1	

- 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: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

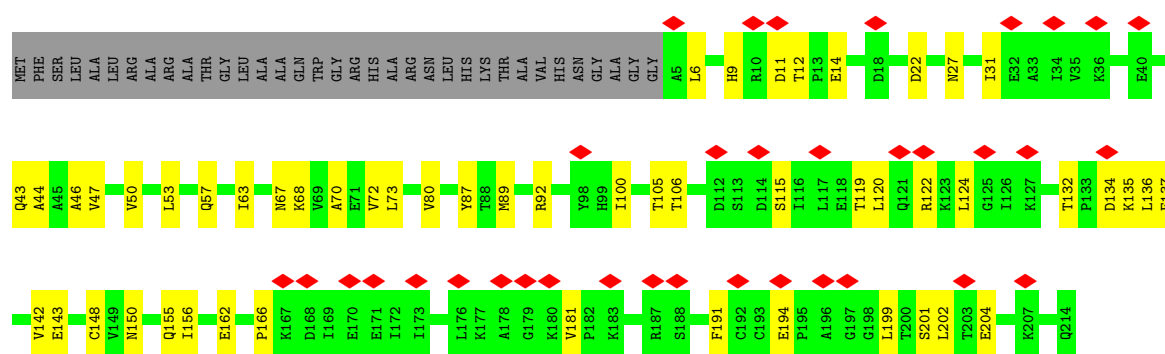


Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

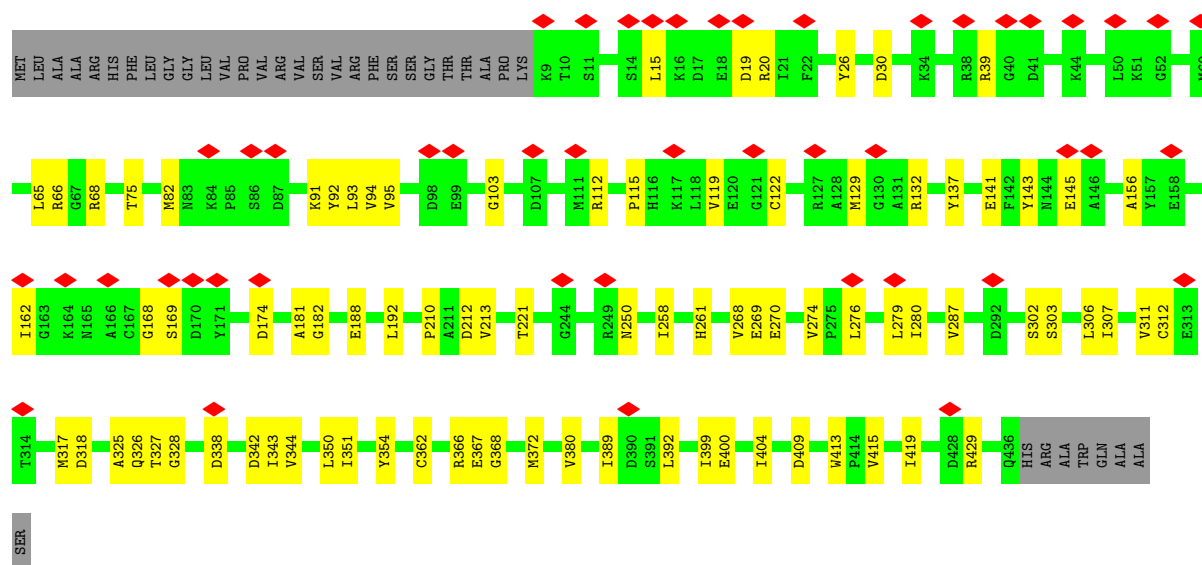
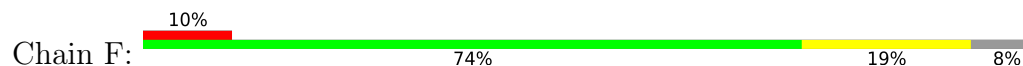




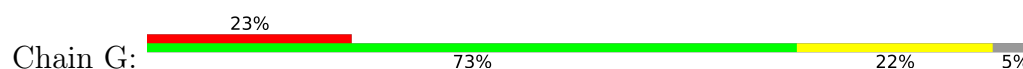
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

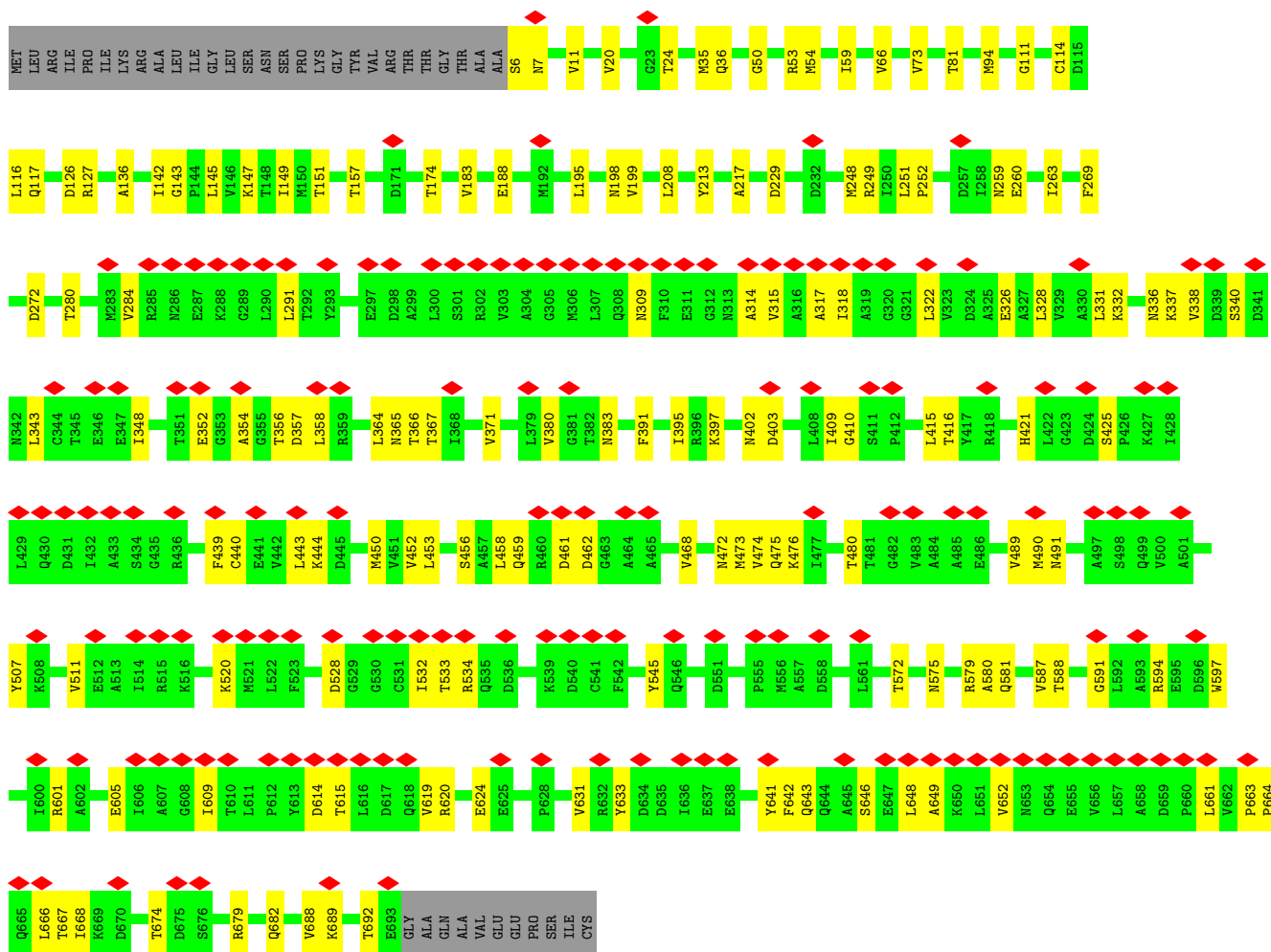


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

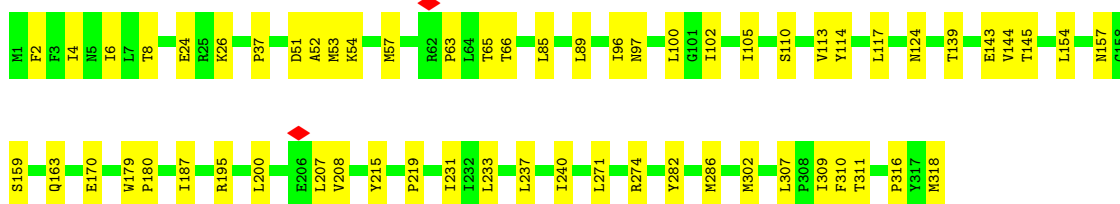
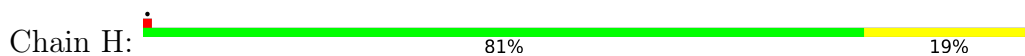


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

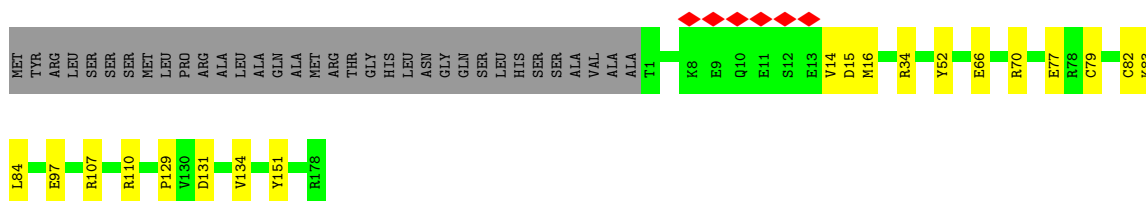
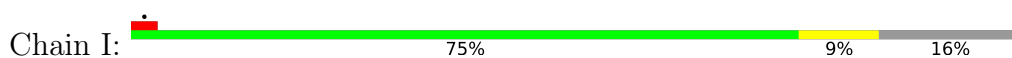





• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

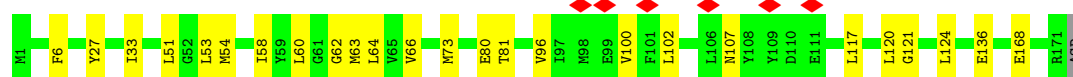


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  85% 15%




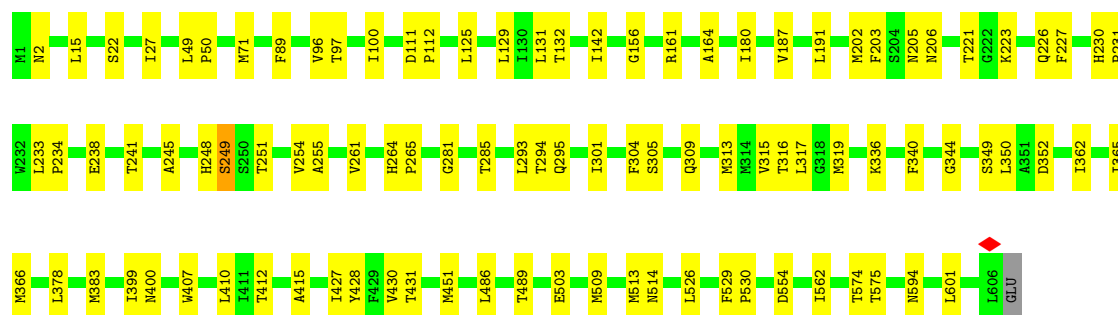
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  84% 16%




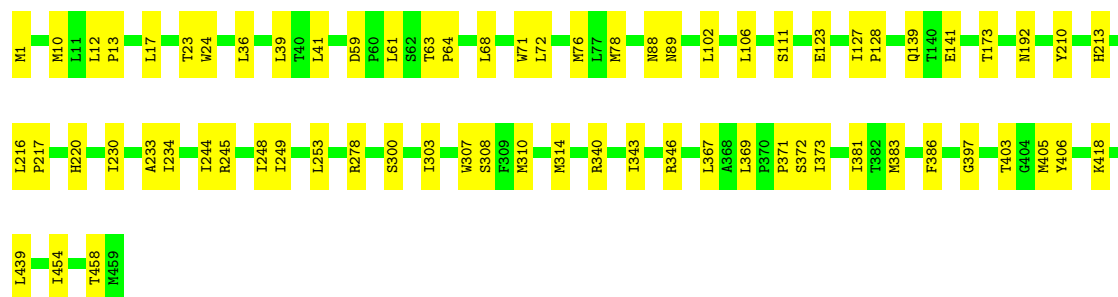
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  84% 16%




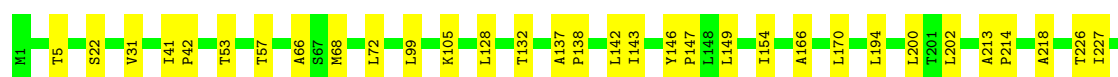
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  85% 15%



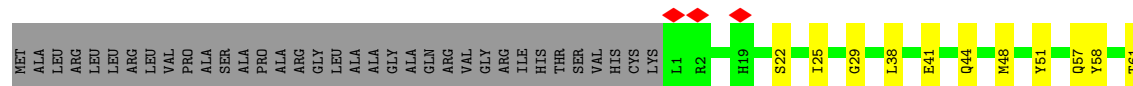
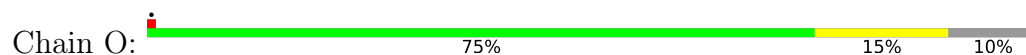
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  83% 17%

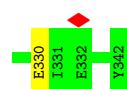
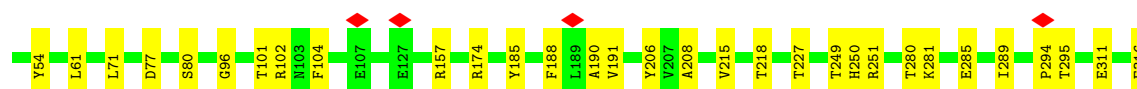
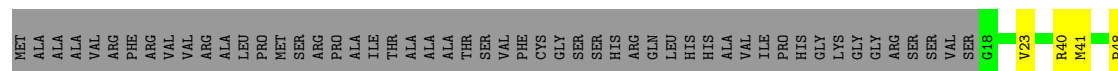
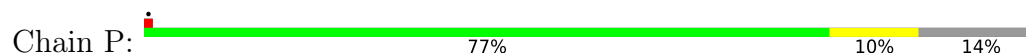




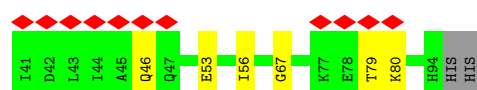
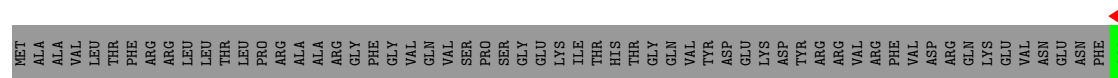
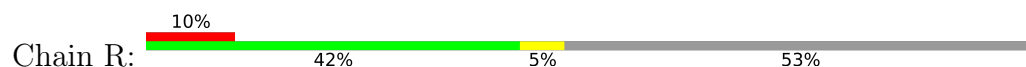
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



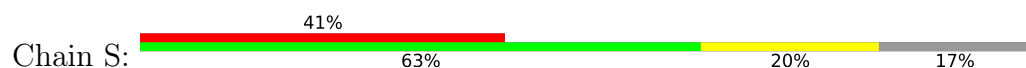
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



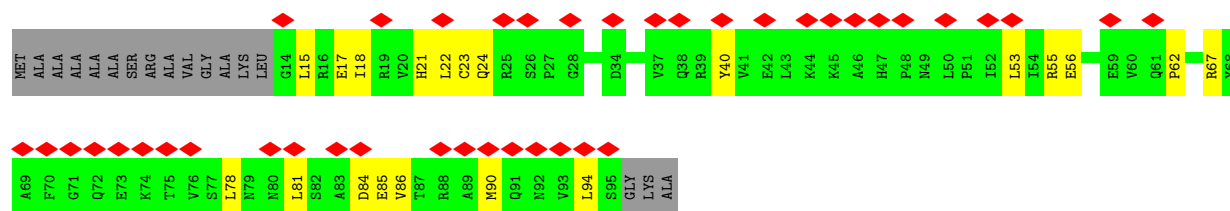
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



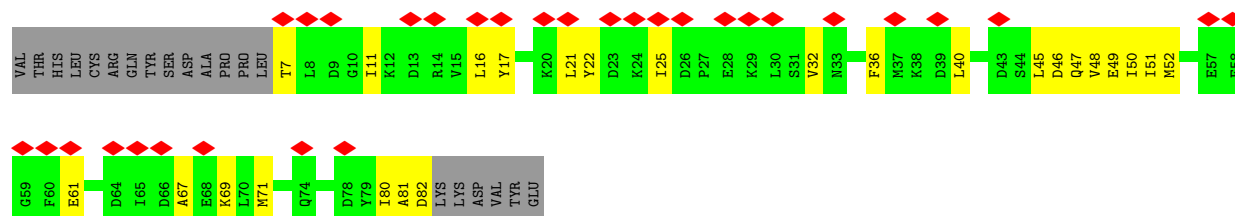
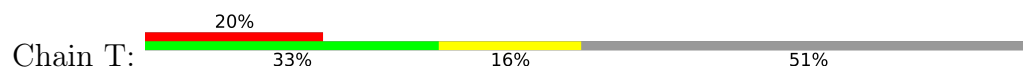
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



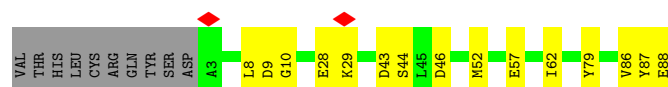




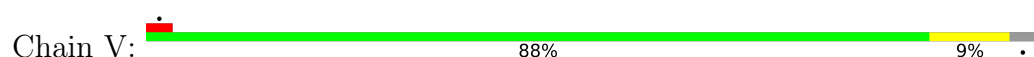
• Molecule 19: Acyl carrier protein, mitochondrial



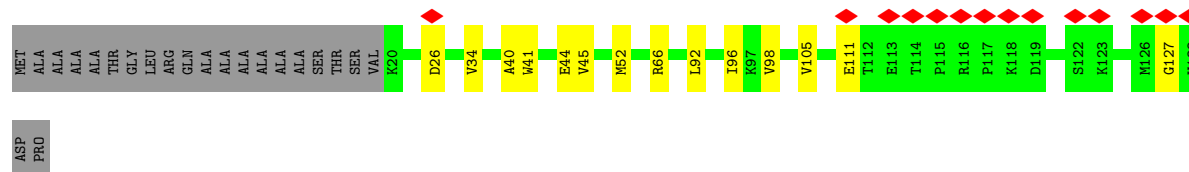
• Molecule 19: Acyl carrier protein, mitochondrial




• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

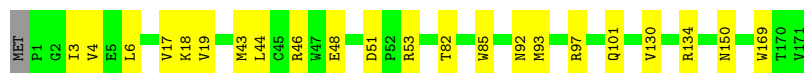


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6




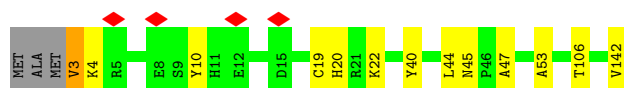
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  87% 13% .




- Molecule 23: MCG5603

Chain Y:  89% 8% ..



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  83% 15% .




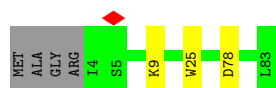
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  87% 10% .



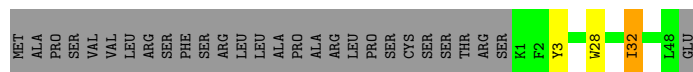
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  92% 5% .



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  59% 37% ..




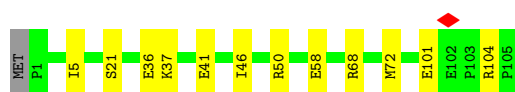
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  89% 11%




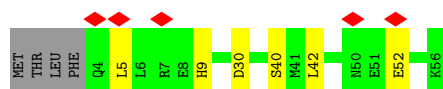
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e: 



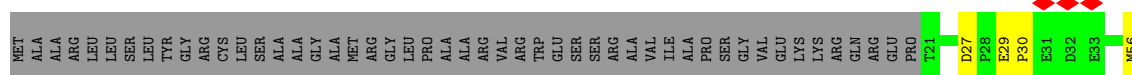
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f: 



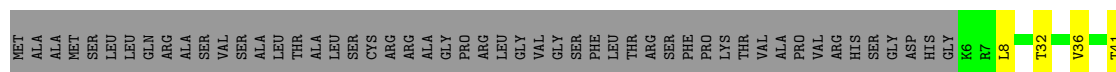
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g: 



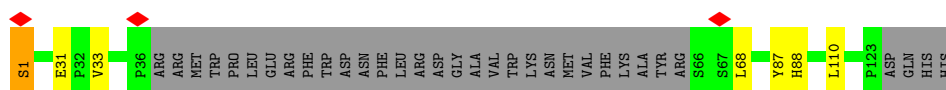
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 

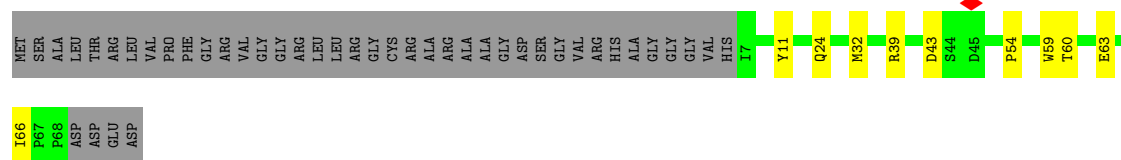


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 



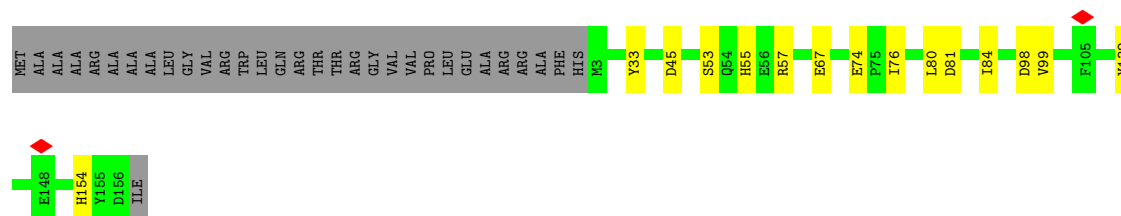
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



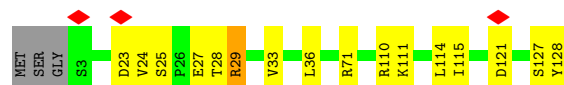
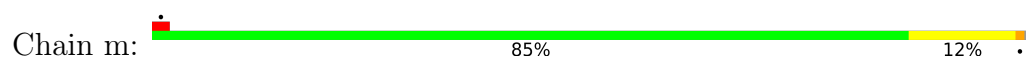
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



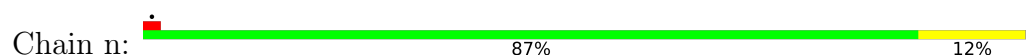
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4




- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

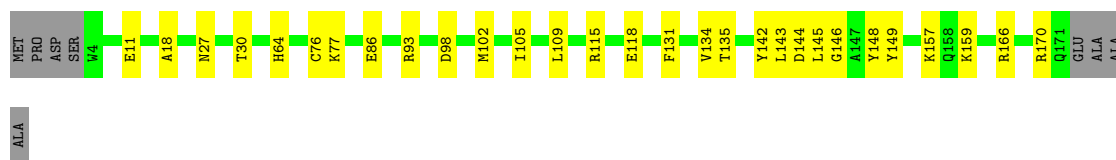


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



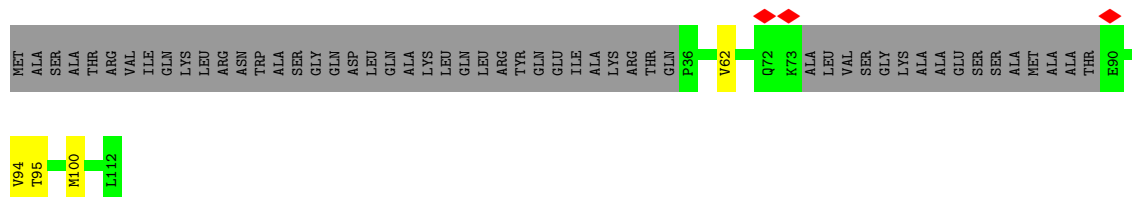
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  79% 16% 5%



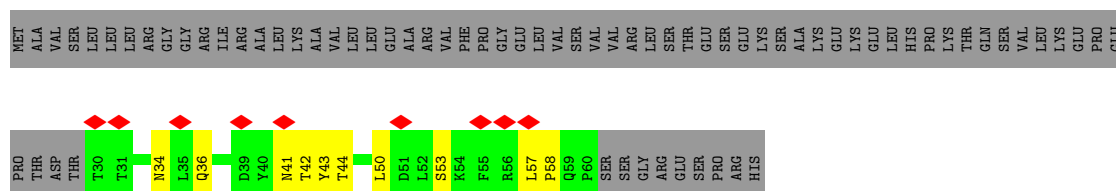
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:  50% 46%



- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:  9% 20% 10% 70%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10005	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.939	Depositor
Minimum map value	-4.972	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.422	Depositor
Recommended contour level	1.9	Depositor
Map size ( $\text{\AA}$ )	608.4, 608.4, 608.4	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.352, 1.352, 1.352	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EHZ, 2MR, PC1, UQ9, SAC, FME, GTP, 3PE, ZN, LMT, SF4, CDL, FES, NDP, FMN

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	0.16	0/949	0.30	0/1297
2	B	0.20	0/1278	0.39	0/1730
3	C	0.17	0/1771	0.30	0/2412
4	D	0.18	0/3539	0.30	0/4793
5	E	0.12	0/1679	0.31	0/2288
6	F	0.13	0/3374	0.29	0/4557
7	G	0.14	0/5335	0.30	0/7236
8	H	0.18	0/2607	0.33	0/3564
9	I	0.18	0/1461	0.30	0/1974
10	J	0.18	0/1322	0.33	0/1799
11	K	0.16	0/738	0.27	0/1002
12	L	0.17	0/4913	0.32	0/6686
13	M	0.18	0/3709	0.31	0/5052
14	N	0.18	0/2748	0.34	0/3741
15	O	0.16	0/2674	0.29	0/3626
16	P	0.14	0/2697	0.27	0/3658
17	R	0.17	0/420	0.30	0/566
18	S	0.10	0/604	0.27	0/827
19	T	0.13	0/620	0.33	0/836
19	U	0.16	0/704	0.36	0/951
20	V	0.15	0/937	0.25	0/1270
21	W	0.15	0/957	0.29	0/1284
22	X	0.16	0/1434	0.30	0/1937
23	Y	0.14	0/1061	0.26	0/1439
24	Z	0.18	0/1198	0.33	0/1616
25	a	0.18	0/569	0.29	0/766
26	b	0.23	0/651	0.31	0/895
27	c	0.17	0/409	0.26	0/555
28	d	0.17	0/1028	0.28	0/1387
29	e	0.15	0/900	0.27	0/1199
30	f	0.13	0/468	0.30	0/630
31	g	0.16	0/878	0.30	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	h	0.16	0/1197	0.28	0/1621
33	i	0.15	0/804	0.32	0/1094
34	j	0.14	0/561	0.27	0/768
35	k	0.14	0/629	0.26	0/851
36	l	0.15	0/1348	0.27	0/1840
37	m	0.18	0/1079	0.31	0/1463
38	n	0.17	0/1589	0.30	0/2152
39	o	0.14	0/1004	0.26	0/1348
40	p	0.16	0/1457	0.30	0/1969
41	r	0.13	0/502	0.27	0/680
42	s	0.09	0/277	0.23	0/377
All	All	0.16	0/64079	0.30	0/86932

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
37	m	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	m	29	ARG	Sidechain

## 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	9	0
2	B	1247	0	1255	22	0
3	C	1721	0	1680	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3463	0	3416	51	0
5	E	1639	0	1631	41	0
6	F	3300	0	3258	65	0
7	G	5248	0	5236	113	0
8	H	2540	0	2626	43	0
9	I	1431	0	1383	19	0
10	J	1300	0	1315	19	0
11	K	737	0	768	12	0
12	L	4800	0	4985	67	0
13	M	3632	0	3853	51	0
14	N	2696	0	2895	45	0
15	O	2607	0	2566	37	0
16	P	2626	0	2642	22	0
17	R	413	0	403	5	0
18	S	594	0	543	17	0
19	T	611	0	602	16	0
19	U	692	0	686	13	0
20	V	915	0	954	8	0
21	W	935	0	959	12	0
22	X	1396	0	1383	18	0
23	Y	1037	0	1024	9	0
24	Z	1167	0	1166	19	0
25	a	556	0	568	5	0
26	b	628	0	628	7	0
27	c	398	0	401	2	0
28	d	996	0	1001	14	0
29	e	877	0	871	9	0
30	f	456	0	452	6	0
31	g	850	0	783	14	0
32	h	1162	0	1163	14	0
33	i	787	0	797	6	0
34	j	537	0	495	9	0
35	k	609	0	603	3	0
36	l	1294	0	1186	13	0
37	m	1050	0	1061	14	0
38	n	1534	0	1466	20	0
39	o	979	0	963	12	0
40	p	1424	0	1393	24	0
41	r	487	0	502	3	0
42	s	269	0	256	8	0
43	B	8	0	0	0	0
43	F	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	G	16	0	0	1	0
43	I	16	0	0	3	0
44	B	41	0	59	0	0
44	H	42	0	58	0	0
45	E	4	0	0	0	0
45	G	4	0	0	1	0
46	F	31	0	18	1	0
47	H	45	0	71	3	0
48	H	51	0	82	1	0
48	J	33	0	40	0	0
48	L	91	0	136	1	0
48	Y	41	0	56	0	0
48	Z	44	0	65	1	0
48	i	42	0	61	0	0
49	L	74	0	92	0	0
49	M	59	0	68	0	0
49	N	128	0	147	0	0
49	d	67	0	81	0	0
49	h	70	0	87	0	0
50	L	70	0	90	1	0
51	O	31	0	10	2	0
52	P	48	0	26	1	0
53	R	1	0	0	0	0
54	T	37	0	0	2	0
54	U	37	0	0	1	0
All	All	63712	0	64034	803	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 6.

The worst 5 of 803 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)
40:p:131:PHE:O	40:p:135:THR:OG1	1.81	0.98
22:X:19:VAL:O	25:a:50:ARG:NH2	2.07	0.88
14:N:170:LEU:HD11	14:N:288:LEU:HD12	1.56	0.87
4:D:146:ARG:NH2	4:D:368:GLU:O	2.09	0.86
16:P:215:VAL:O	16:P:218:THR:OG1	1.93	0.86

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%)	108 (96%)	5 (4%)	0	100	100
2	B	154/224 (69%)	147 (96%)	7 (4%)	0	100	100
3	C	205/263 (78%)	196 (96%)	9 (4%)	0	100	100
4	D	427/463 (92%)	407 (95%)	20 (5%)	0	100	100
5	E	208/245 (85%)	193 (93%)	15 (7%)	0	100	100
6	F	426/464 (92%)	391 (92%)	35 (8%)	0	100	100
7	G	686/727 (94%)	631 (92%)	55 (8%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	176/212 (83%)	169 (96%)	7 (4%)	0	100	100
10	J	169/172 (98%)	155 (92%)	14 (8%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	572 (95%)	30 (5%)	2 (0%)	37	69
13	M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	N	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
15	O	318/355 (90%)	308 (97%)	10 (3%)	0	100	100
16	P	323/377 (86%)	301 (93%)	21 (6%)	1 (0%)	37	69
17	R	53/116 (46%)	52 (98%)	1 (2%)	0	100	100
18	S	80/99 (81%)	75 (94%)	5 (6%)	0	100	100
19	T	74/156 (47%)	70 (95%)	4 (5%)	0	100	100
19	U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
20	V	110/116 (95%)	108 (98%)	2 (2%)	0	100	100
21	W	107/131 (82%)	101 (94%)	6 (6%)	0	100	100
22	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
23	Y	138/143 (96%)	128 (93%)	10 (7%)	0	100	100
24	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	a	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
26	b	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
27	c	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
28	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
29	e	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
30	f	51/57 (90%)	47 (92%)	4 (8%)	0	100	100
31	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
32	h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
33	i	90/127 (71%)	84 (93%)	6 (7%)	0	100	100
34	j	60/105 (57%)	60 (100%)	0	0	100	100
35	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
36	l	152/186 (82%)	147 (97%)	5 (3%)	0	100	100
37	m	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
38	n	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
39	o	111/137 (81%)	107 (96%)	4 (4%)	0	100	100
40	p	166/176 (94%)	158 (95%)	8 (5%)	0	100	100
41	r	57/113 (50%)	55 (96%)	2 (4%)	0	100	100
42	s	29/104 (28%)	28 (97%)	1 (3%)	0	100	100
All	All	7708/8890 (87%)	7332 (95%)	373 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	P	250	HIS
12	L	249	SER
12	L	562	ILE

### 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	183/205 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	567/610 (93%)	566 (100%)	1 (0%)	92	97
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%)	548 (100%)	0	100	100
13	M	414/414 (100%)	413 (100%)	1 (0%)	92	97
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	286/325 (88%)	286 (100%)	0	100	100
17	R	43/96 (45%)	43 (100%)	0	100	100
18	S	56/80 (70%)	56 (100%)	0	100	100
19	T	70/135 (52%)	70 (100%)	0	100	100
19	U	79/135 (58%)	79 (100%)	0	100	100
20	V	100/102 (98%)	100 (100%)	0	100	100
21	W	103/114 (90%)	103 (100%)	0	100	100
22	X	153/154 (99%)	153 (100%)	0	100	100
23	Y	105/107 (98%)	104 (99%)	1 (1%)	73	87
24	Z	122/123 (99%)	122 (100%)	0	100	100
25	a	58/60 (97%)	58 (100%)	0	100	100
26	b	71/73 (97%)	71 (100%)	0	100	100
27	c	42/67 (63%)	41 (98%)	1 (2%)	44	71
28	d	107/107 (100%)	107 (100%)	0	100	100
29	e	93/94 (99%)	93 (100%)	0	100	100
30	f	49/53 (92%)	49 (100%)	0	100	100
31	g	92/129 (71%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	h	123/162 (76%)	123 (100%)	0	100	100
33	i	88/118 (75%)	88 (100%)	0	100	100
34	j	58/87 (67%)	58 (100%)	0	100	100
35	k	58/78 (74%)	58 (100%)	0	100	100
36	l	139/161 (86%)	139 (100%)	0	100	100
37	m	112/114 (98%)	112 (100%)	0	100	100
38	n	162/164 (99%)	162 (100%)	0	100	100
39	o	106/121 (88%)	106 (100%)	0	100	100
40	p	153/158 (97%)	153 (100%)	0	100	100
41	r	57/96 (59%)	57 (100%)	0	100	100
42	s	31/95 (33%)	31 (100%)	0	100	100
All	All	6809/7662 (89%)	6805 (100%)	4 (0%)	92	98

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

Mol	Chain	Res	Type
7	G	229	ASP
13	M	102	LEU
23	Y	3	VAL
27	c	32	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	63	GLN
37	m	125	ASN
16	P	67	GLN
37	m	116	GLN
31	g	109	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	0.92	0	7,9,11	0.89	0
1	FME	A	1	1	8,9,10	0.94	0	7,9,11	0.79	0
13	FME	M	1	13	8,9,10	0.94	0	7,9,11	0.70	0
4	2MR	D	85	4	10,12,13	1.83	1 (10%)	5,13,15	2.73	1 (20%)
12	FME	L	1	12	8,9,10	0.94	0	7,9,11	0.87	0
8	FME	H	1	8	8,9,10	0.91	0	7,9,11	1.23	0
33	SAC	i	1	33	7,8,9	1.01	0	8,9,11	1.55	1 (12%)
11	FME	K	1	11	8,9,10	0.96	0	7,9,11	1.25	1 (14%)
10	FME	J	1	10	8,9,10	0.95	0	7,9,11	0.94	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	-	1/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
13	FME	M	1	13	-	0/7/9/11	-
4	2MR	D	85	4	-	5/10/13/15	-
12	FME	L	1	12	-	1/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
33	SAC	i	1	33	-	6/7/8/10	-
11	FME	K	1	11	-	2/7/9/11	-
10	FME	J	1	10	-	5/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.13	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	85	2MR	NE-CZ-NH2	5.77	124.77	119.48
33	i	1	SAC	C2A-C1A-N	2.66	120.60	116.10
11	K	1	FME	C-CA-N	2.64	114.49	109.73

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	85	2MR	N-CA-CB-CG
4	D	85	2MR	C-CA-CB-CG
8	H	1	FME	O1-CN-N-CA
8	H	1	FME	CB-CA-N-CN
10	J	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
33	i	1	SAC	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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
49	CDL	N	401	-	64,64,99	1.11	7 (10%)	70,76,111	1.15	4 (5%)
43	SF4	G	801	7	0,12,12	-	-	-		
43	SF4	I	201	9	0,12,12	-	-	-		
50	LMT	L	705	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	1 (2%)
54	EHZ	U	201	19	29,36,37	1.89	5 (17%)	35,44,47	1.68	7 (20%)
43	SF4	I	202	9	0,12,12	-	-	-		
49	CDL	L	702	-	73,73,99	1.04	7 (9%)	79,85,111	1.13	4 (5%)
49	CDL	N	402	-	62,62,99	1.12	7 (11%)	68,74,111	1.14	4 (5%)
48	3PE	J	201	-	32,32,50	1.05	4 (12%)	35,37,55	1.13	2 (5%)
49	CDL	M	501	-	58,58,99	1.07	4 (6%)	63,69,111	1.06	3 (4%)
50	LMT	L	704	-	36,36,36	1.15	5 (13%)	47,47,47	1.02	3 (6%)
43	SF4	G	802	7	0,12,12	-	-	-		
44	PC1	H	402	-	41,41,53	1.42	6 (14%)	47,49,61	1.11	3 (6%)
48	3PE	Z	401	-	43,43,50	0.92	4 (9%)	46,48,55	1.11	2 (4%)
52	NDP	P	501	-	45,52,52	2.22	5 (11%)	53,80,80	1.68	10 (18%)
48	3PE	Y	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.03	2 (4%)
45	FES	G	803	7	0,4,4	-	-	-		
48	3PE	i	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.07	2 (4%)
48	3PE	H	403	-	50,50,50	0.86	4 (8%)	53,55,55	1.08	2 (3%)
43	SF4	F	501	6	0,12,12	-	-	-		
45	FES	E	301	5	0,4,4	-	-	-		
49	CDL	d	201	-	66,66,99	1.09	7 (10%)	72,78,111	1.17	4 (5%)
48	3PE	L	703	-	41,41,50	0.95	4 (9%)	44,46,55	1.08	2 (4%)
54	EHZ	T	201	19	29,36,37	1.87	5 (17%)	35,44,47	1.45	3 (8%)
46	FMN	F	502	-	33,33,33	4.64	19 (57%)	48,50,50	4.81	22 (45%)
47	UQ9	H	401	-	44,44,58	0.81	0	52,52,73	1.99	16 (30%)
51	GTP	O	401	-	26,33,34	2.65	10 (38%)	32,52,54	1.61	9 (28%)
43	SF4	B	201	2	0,12,12	-	-	-		
44	PC1	B	202	-	40,40,53	1.42	6 (15%)	46,48,61	1.07	2 (4%)
49	CDL	h	201	-	69,69,99	1.06	7 (10%)	75,81,111	1.17	5 (6%)
48	3PE	L	701	-	48,48,50	0.88	2 (4%)	51,53,55	1.03	2 (3%)

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	CDL	N	401	-	-	41/75/75/110	-
43	SF4	G	801	7	-	-	0/6/5/5
50	LMT	L	705	-	-	10/21/61/61	0/2/2/2
43	SF4	I	201	9	-	-	0/6/5/5
54	EHZ	U	201	19	-	17/42/44/45	-
49	CDL	L	702	-	-	32/84/84/110	-
43	SF4	I	202	9	-	-	0/6/5/5
49	CDL	N	402	-	-	34/73/73/110	-
48	3PE	J	201	-	-	10/36/36/54	-
49	CDL	M	501	-	-	42/67/67/110	-
50	LMT	L	704	-	-	13/21/61/61	0/2/2/2
44	PC1	H	402	-	-	17/45/45/57	-
43	SF4	G	802	7	-	-	0/6/5/5
48	3PE	Z	401	-	-	17/47/47/54	-
52	NDP	P	501	-	-	12/30/77/77	0/5/5/5
48	3PE	Y	401	-	-	14/44/44/54	-
48	3PE	i	201	-	-	16/45/45/54	-
45	FES	G	803	7	-	-	0/1/1/1
48	3PE	H	403	-	-	22/54/54/54	-
43	SF4	F	501	6	-	-	0/6/5/5
49	CDL	d	201	-	-	31/77/77/110	-
45	FES	E	301	5	-	-	0/1/1/1
48	3PE	L	703	-	-	18/45/45/54	-
54	EHZ	T	201	19	-	13/42/44/45	-
46	FMN	F	502	-	-	6/18/18/18	0/3/3/3
47	UQ9	H	401	-	-	15/50/50/81	-
51	GTP	O	401	-	-	4/18/34/38	0/3/3/3
43	SF4	B	201	2	-	-	0/6/5/5
44	PC1	B	202	-	-	19/44/44/57	-
49	CDL	h	201	-	-	41/80/80/110	-
48	3PE	L	701	-	-	16/52/52/54	-

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.31	1.82	1.59
46	F	502	FMN	C6-C5A	11.57	1.58	1.40
46	F	502	FMN	C9A-C5A	10.28	1.58	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	F	502	FMN	C9-C8	-9.89	1.25	1.39
46	F	502	FMN	O2-C2	8.65	1.40	1.24

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	F	502	FMN	C4-C4A-N5	15.31	140.02	118.23
46	F	502	FMN	C6-C5A-N5	15.30	145.22	118.51
46	F	502	FMN	C6-C5A-C9A	-12.12	101.79	118.94
46	F	502	FMN	C5A-N5-C4A	9.72	134.24	118.07
46	F	502	FMN	C9A-C5A-N5	-8.69	112.99	122.43

There are no chirality outliers.

5 of 460 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	202	PC1	C1-O11-P-O14
44	B	202	PC1	C12-C11-O13-P
44	B	202	PC1	O13-C11-C12-N
44	B	202	PC1	O11-C1-C2-O21
44	B	202	PC1	O22-C21-O21-C2

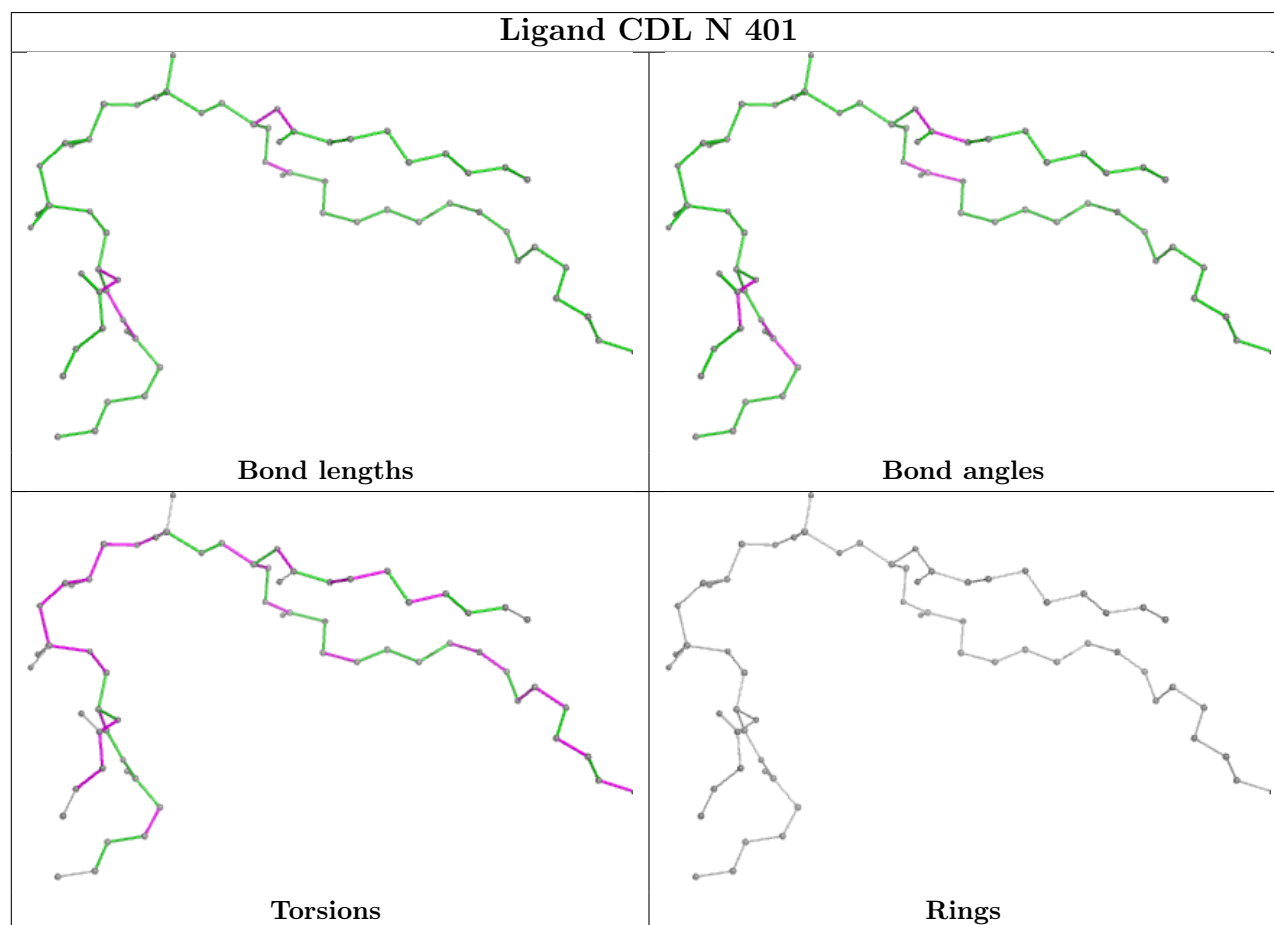
There are no ring outliers.

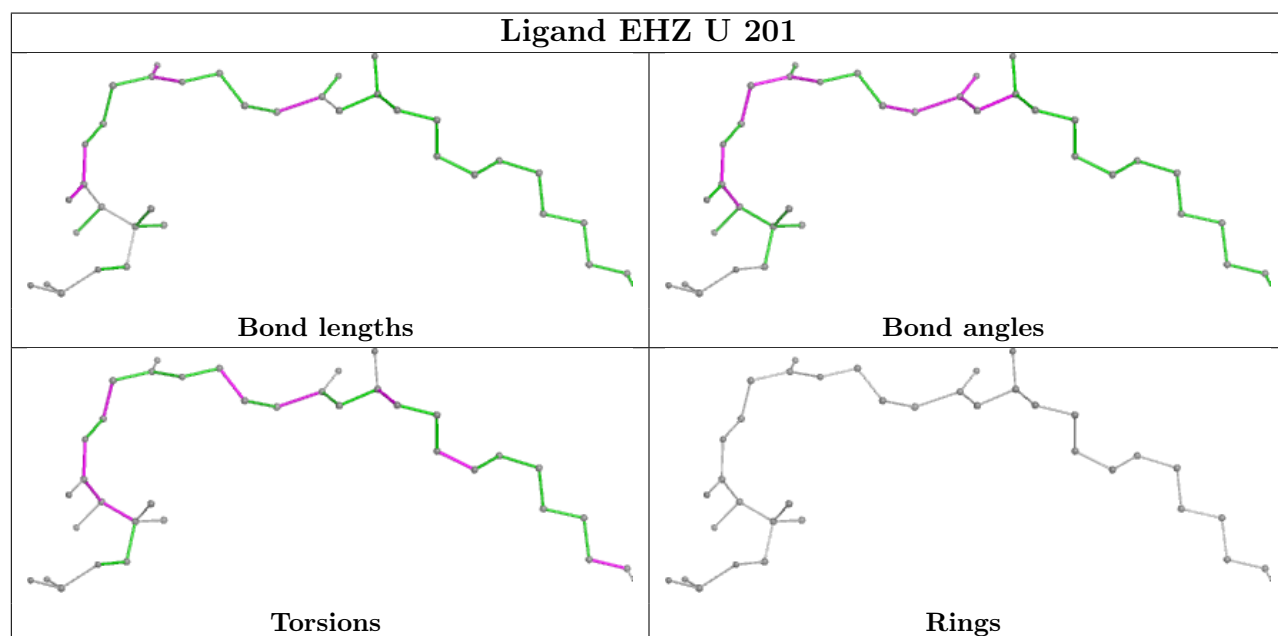
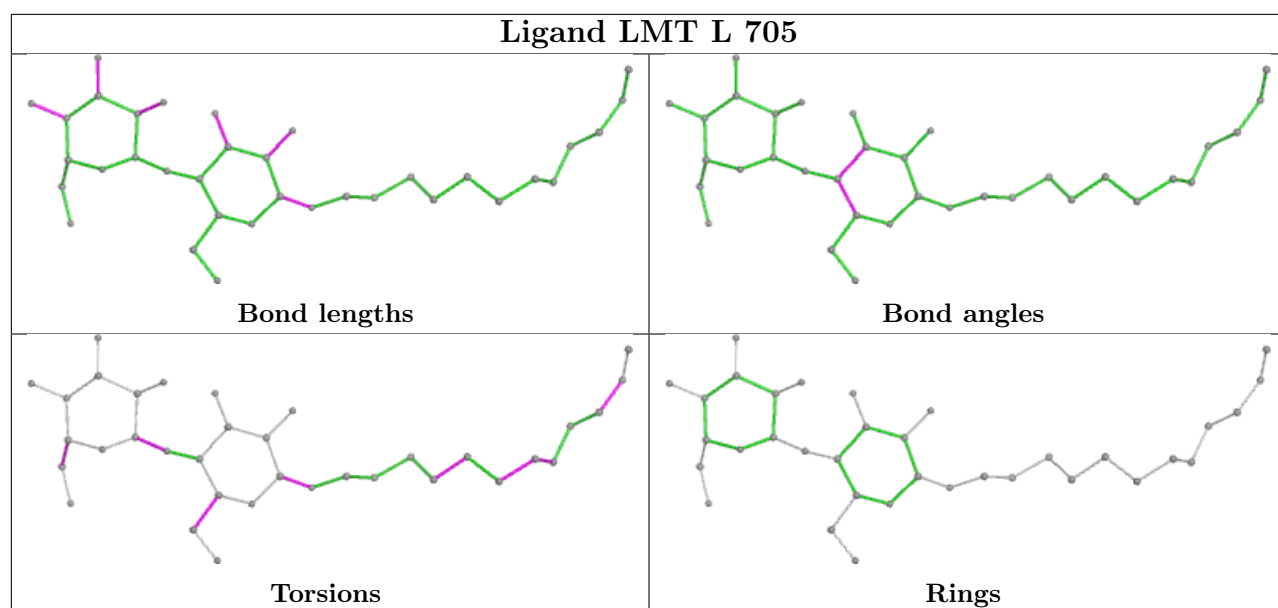
13 monomers are involved in 19 short contacts:

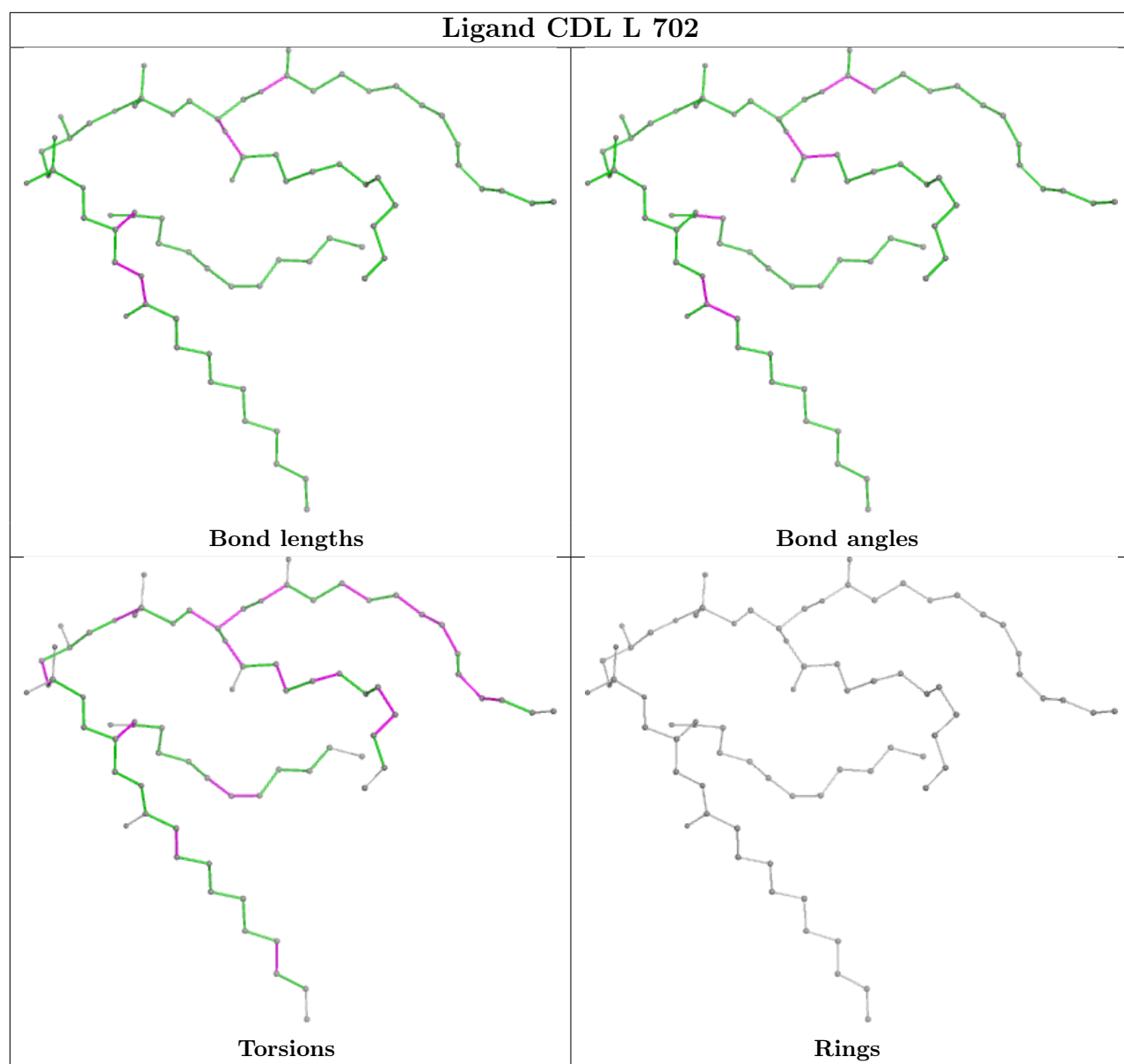
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	I	201	SF4	3	0
50	L	705	LMT	1	0
54	U	201	EHZ	1	0
43	G	802	SF4	1	0
48	Z	401	3PE	1	0
52	P	501	NDP	1	0
45	G	803	FES	1	0
48	H	403	3PE	1	0
48	L	703	3PE	1	0
54	T	201	EHZ	2	0
46	F	502	FMN	1	0
47	H	401	UQ9	3	0
51	O	401	GTP	2	0

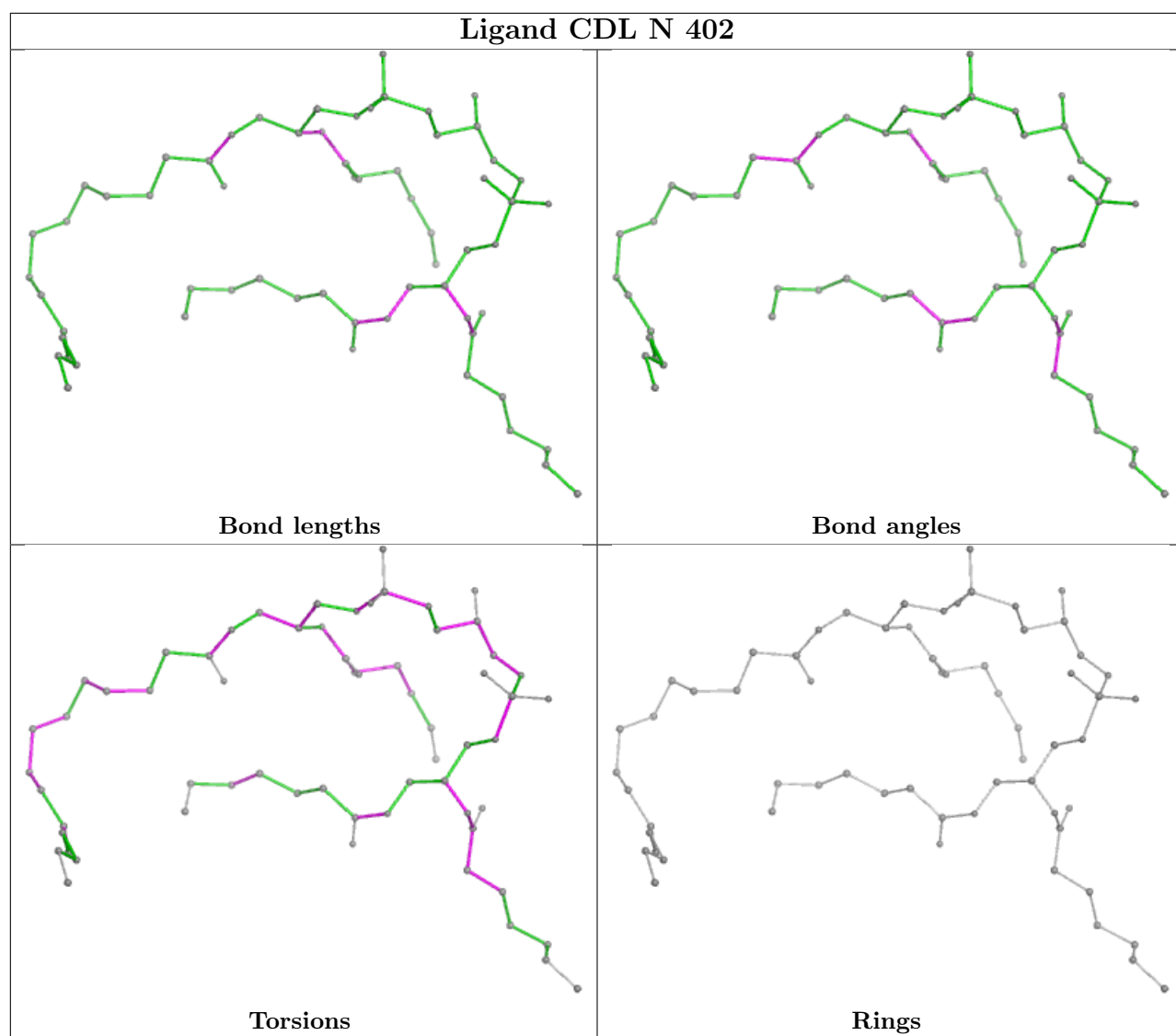
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

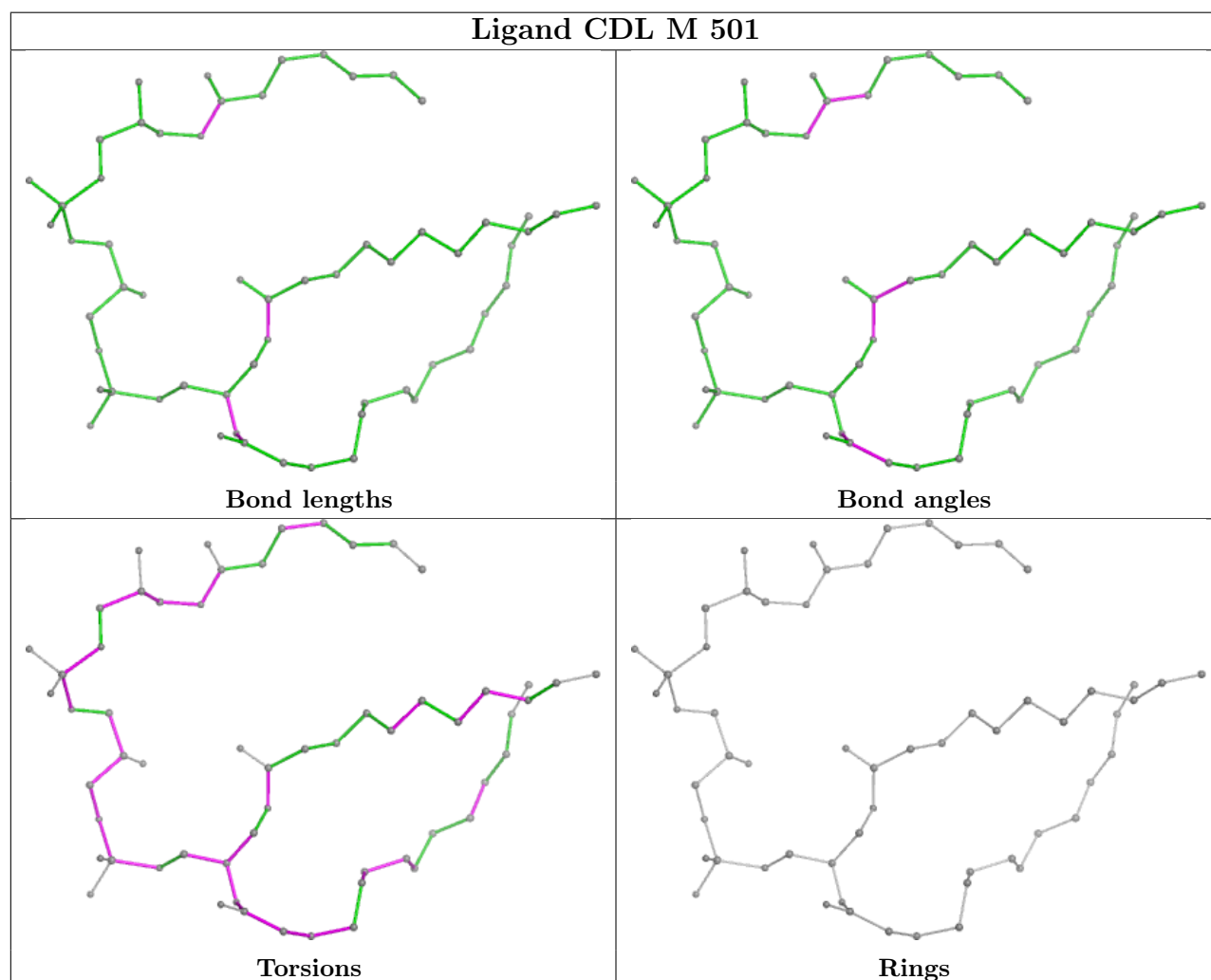
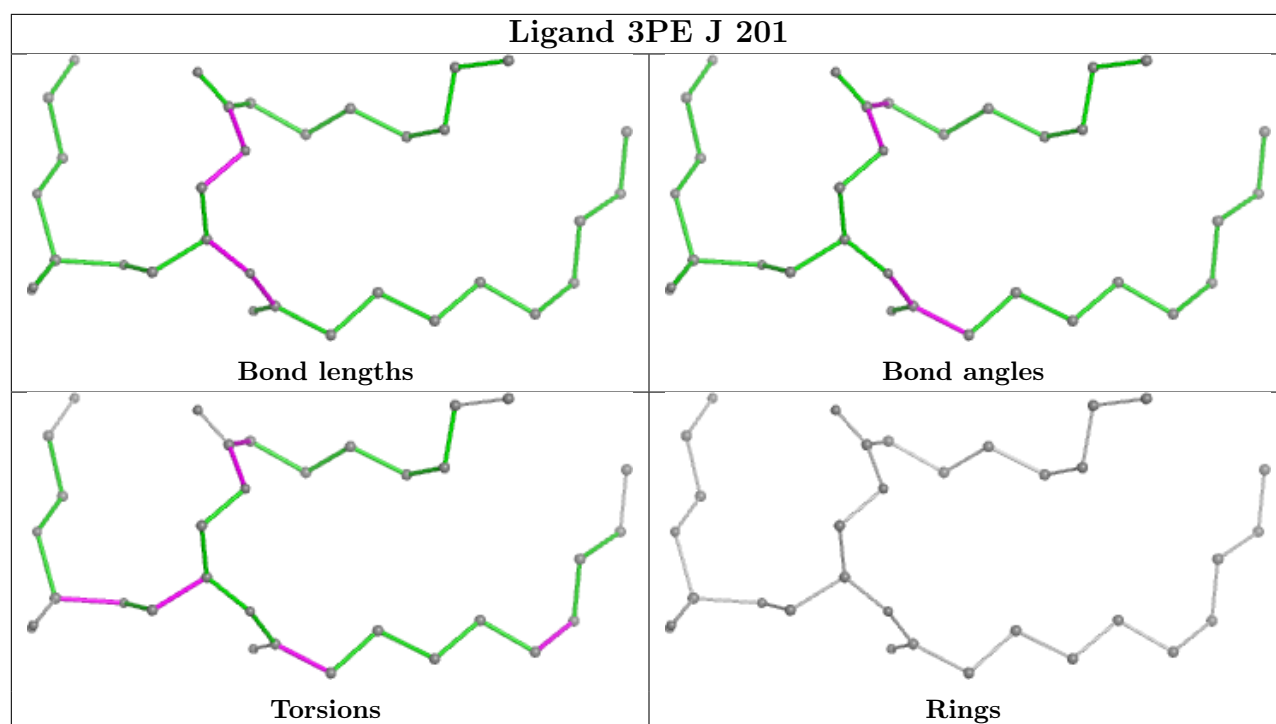
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



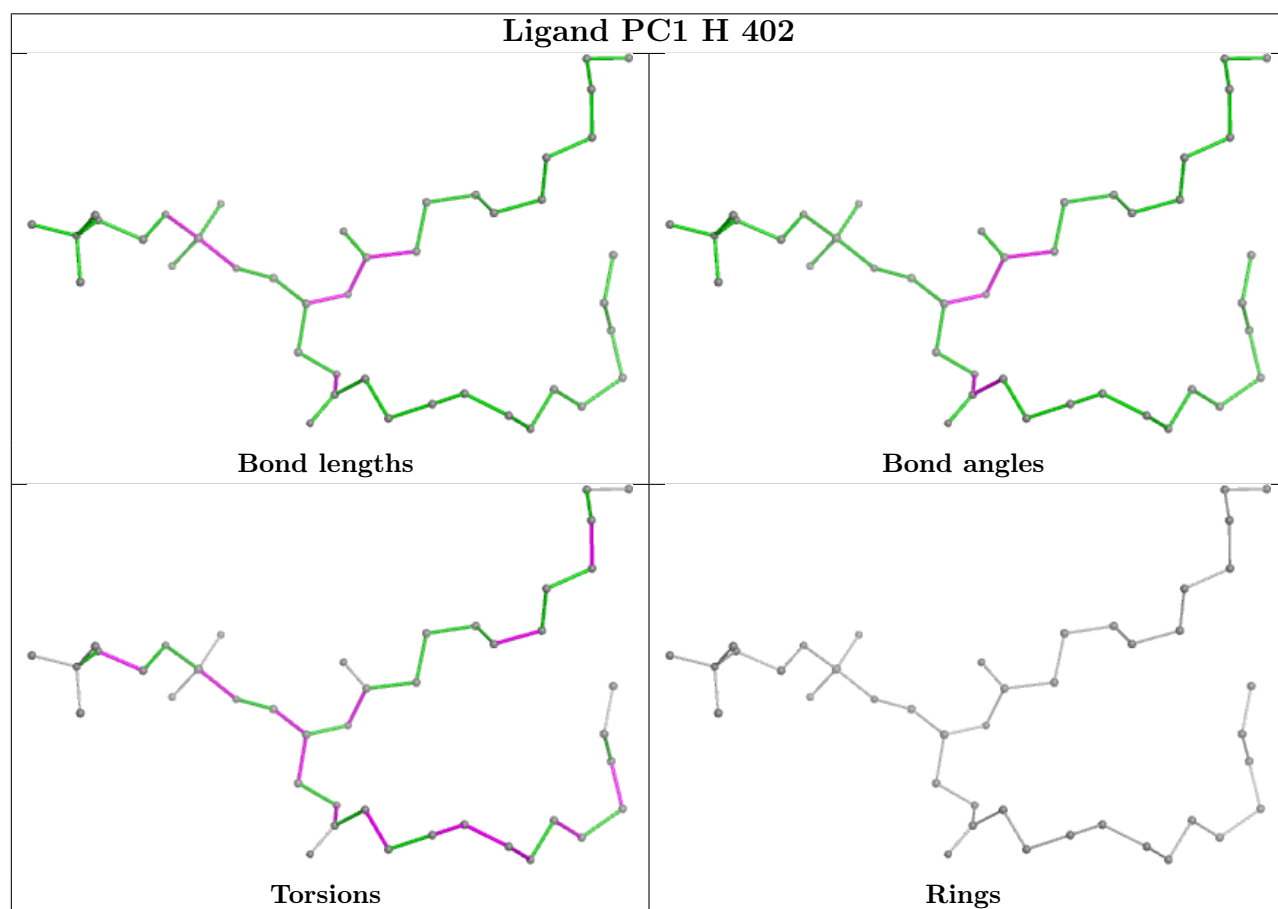
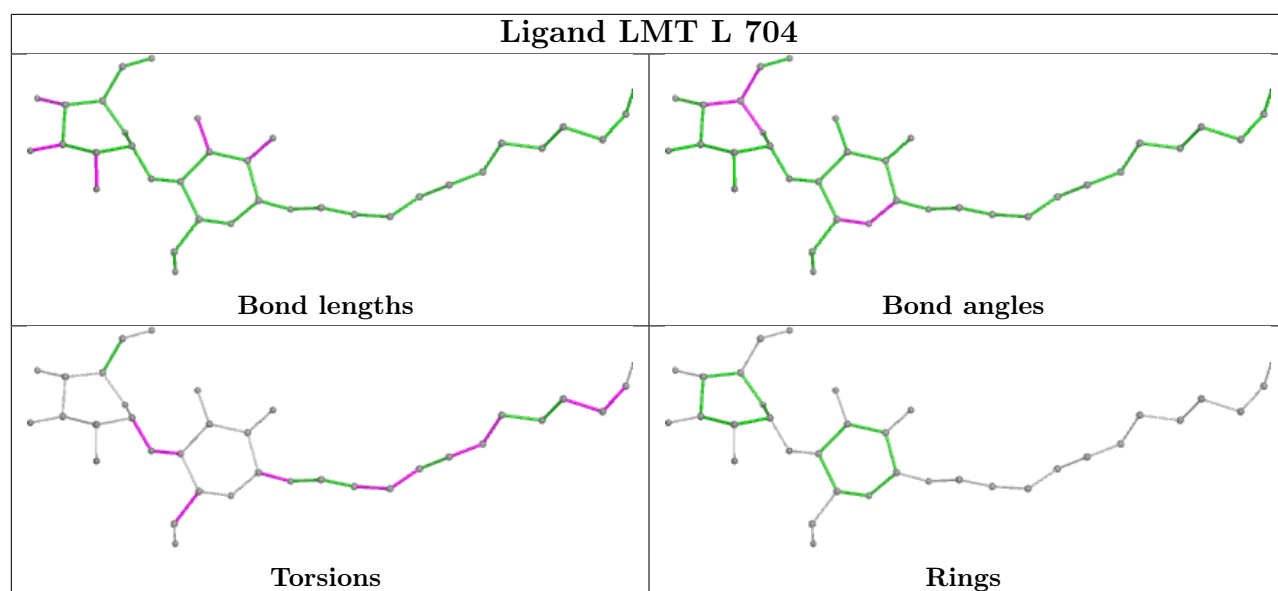


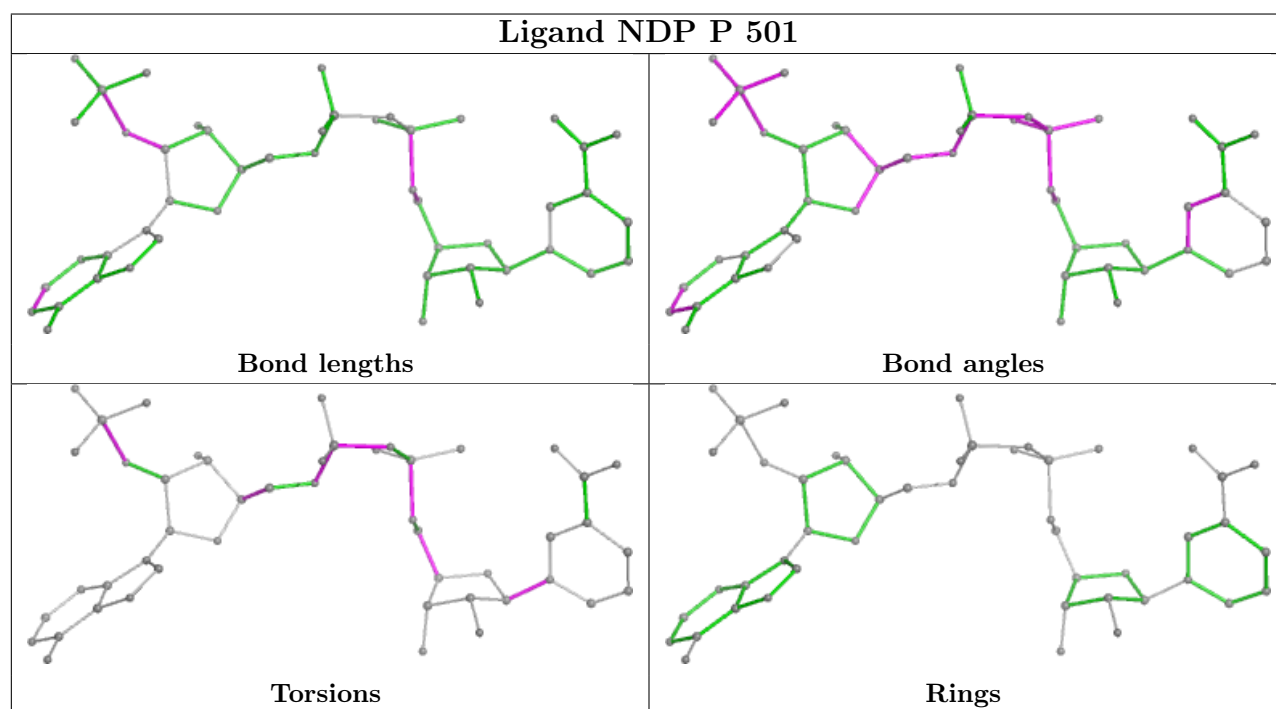
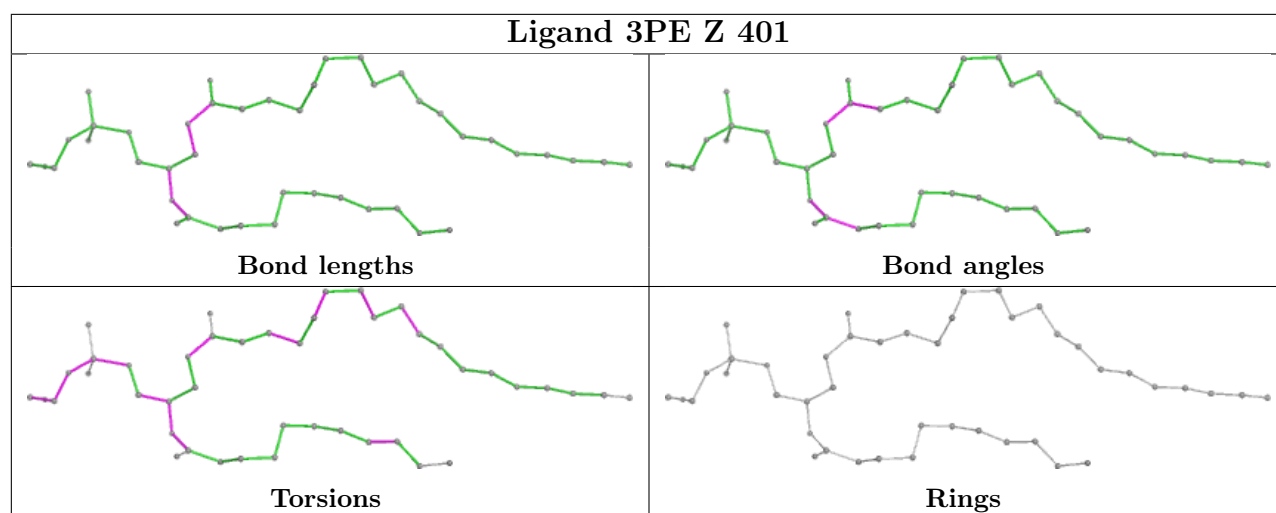


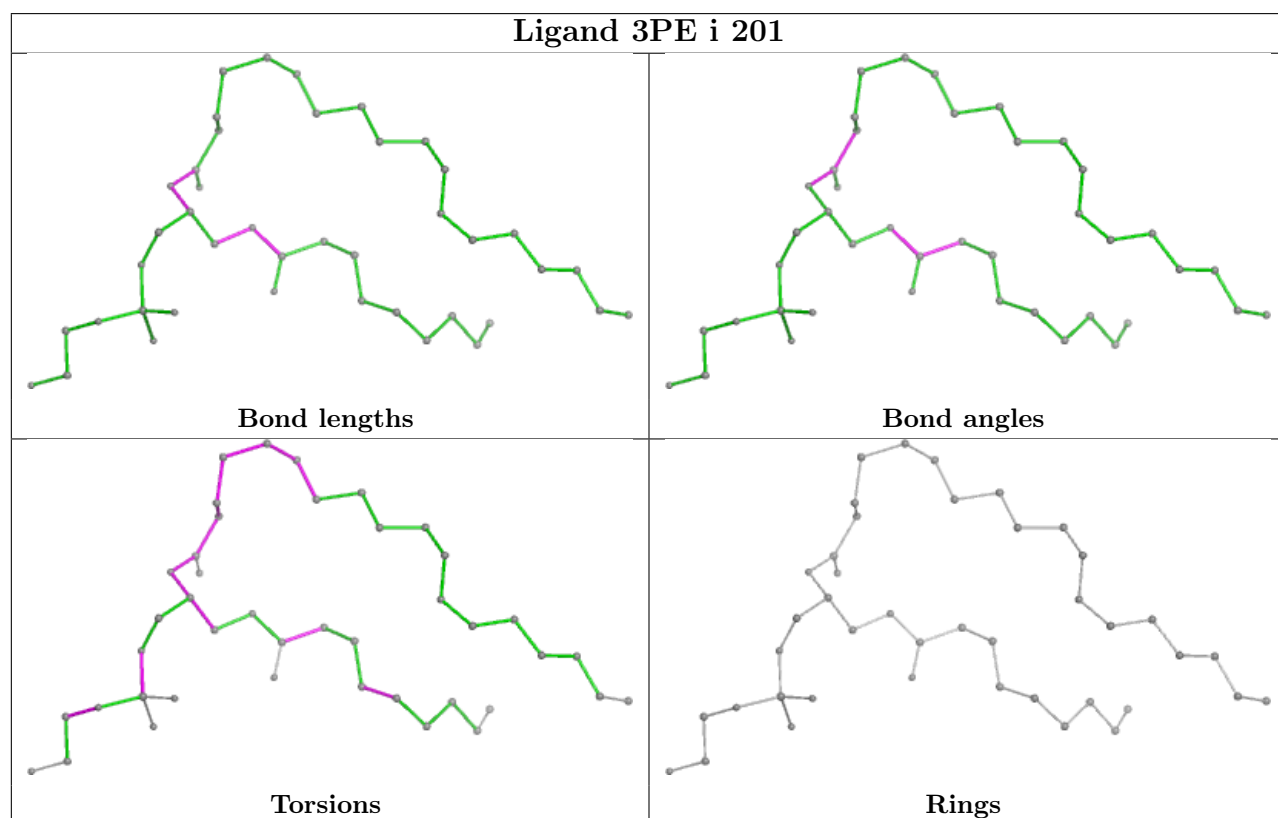
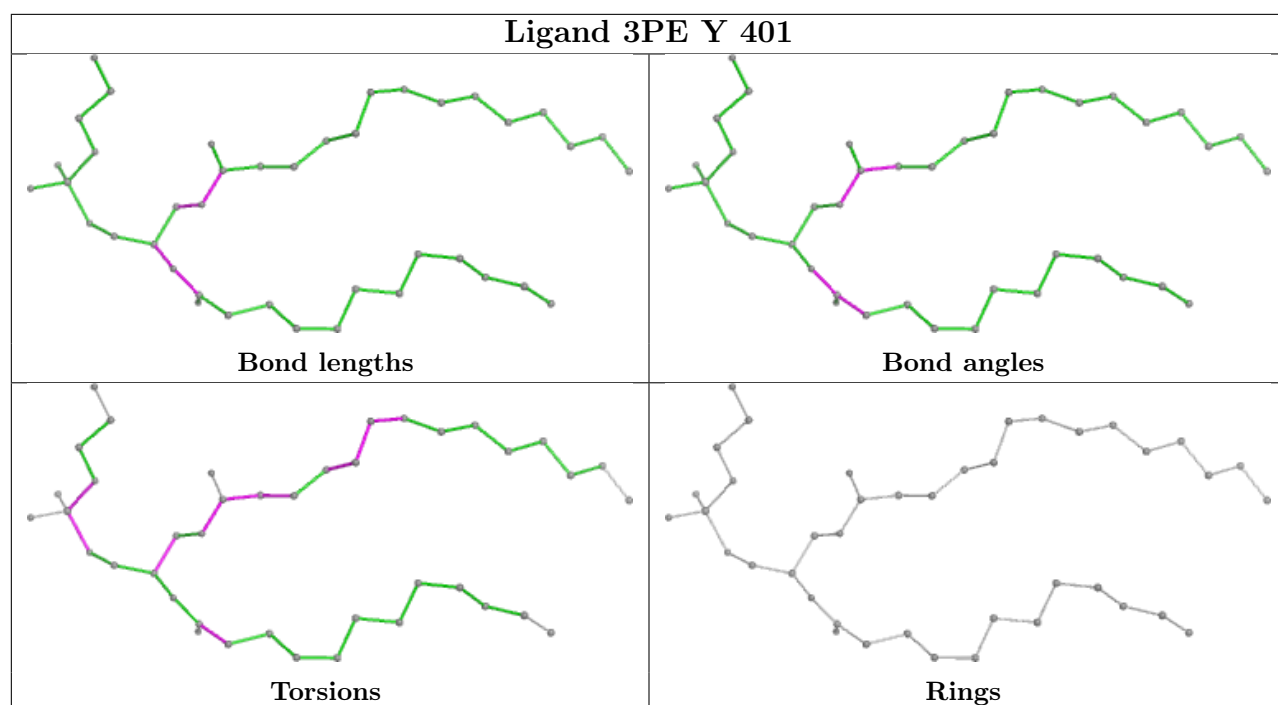


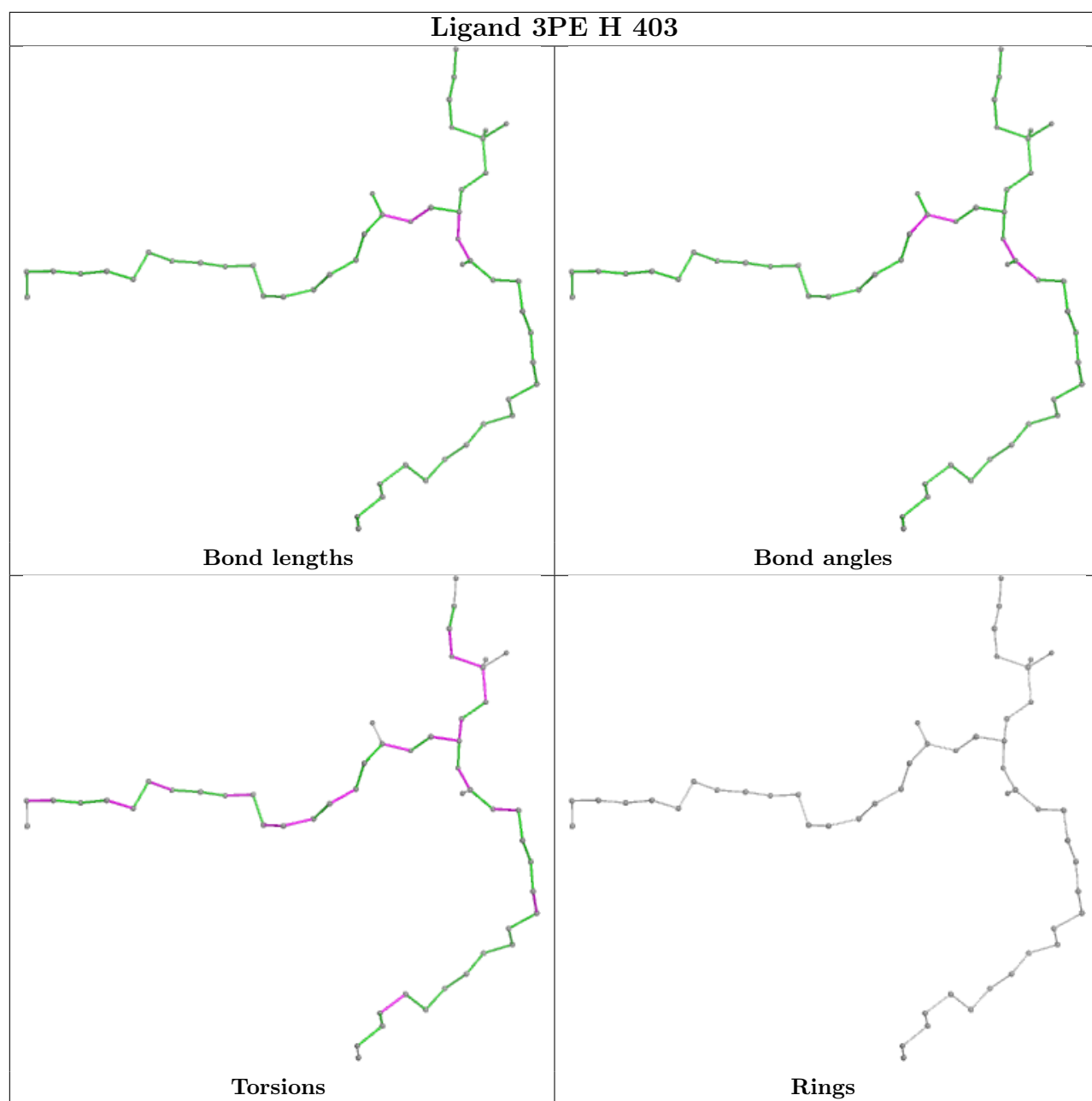


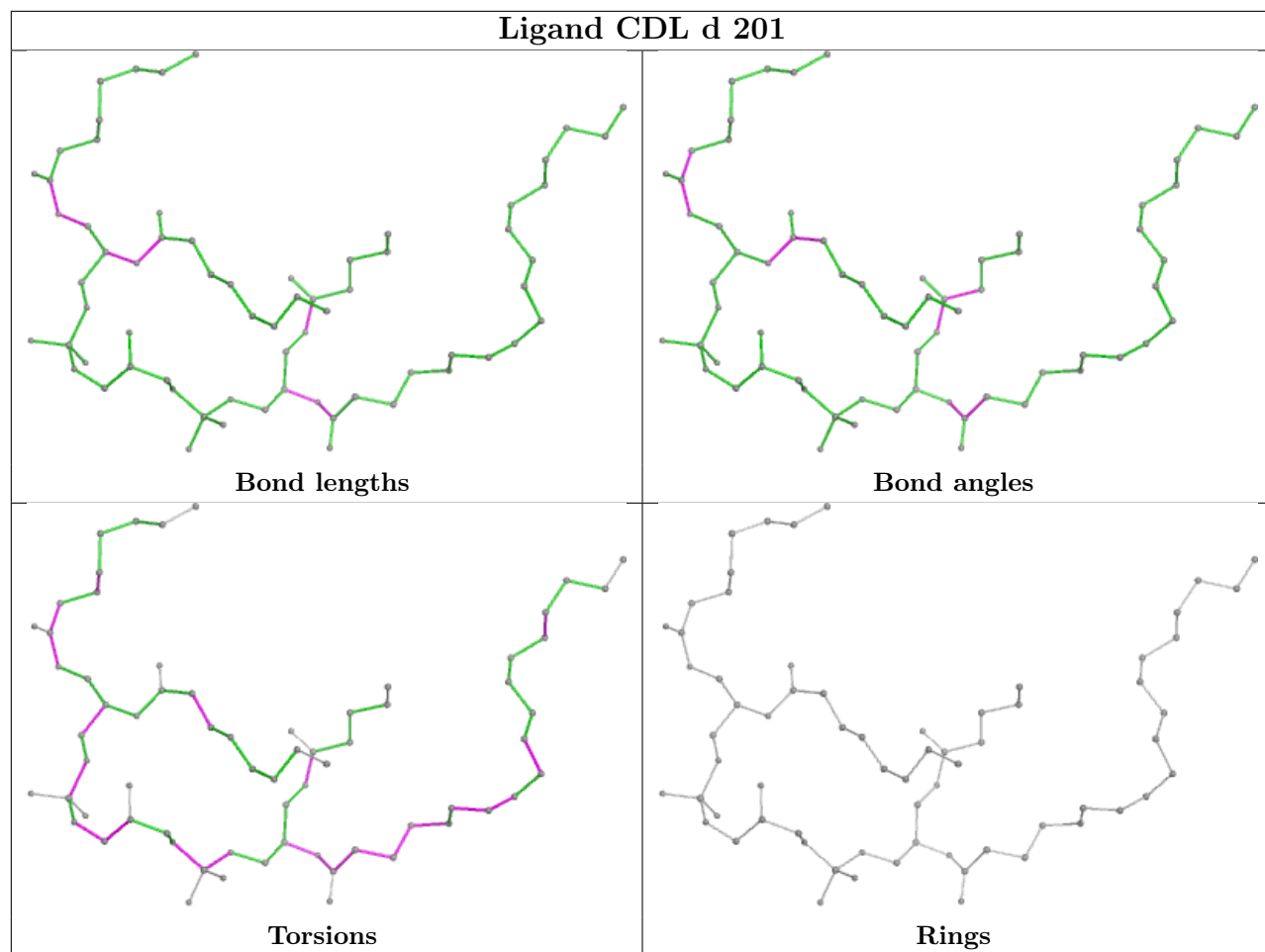


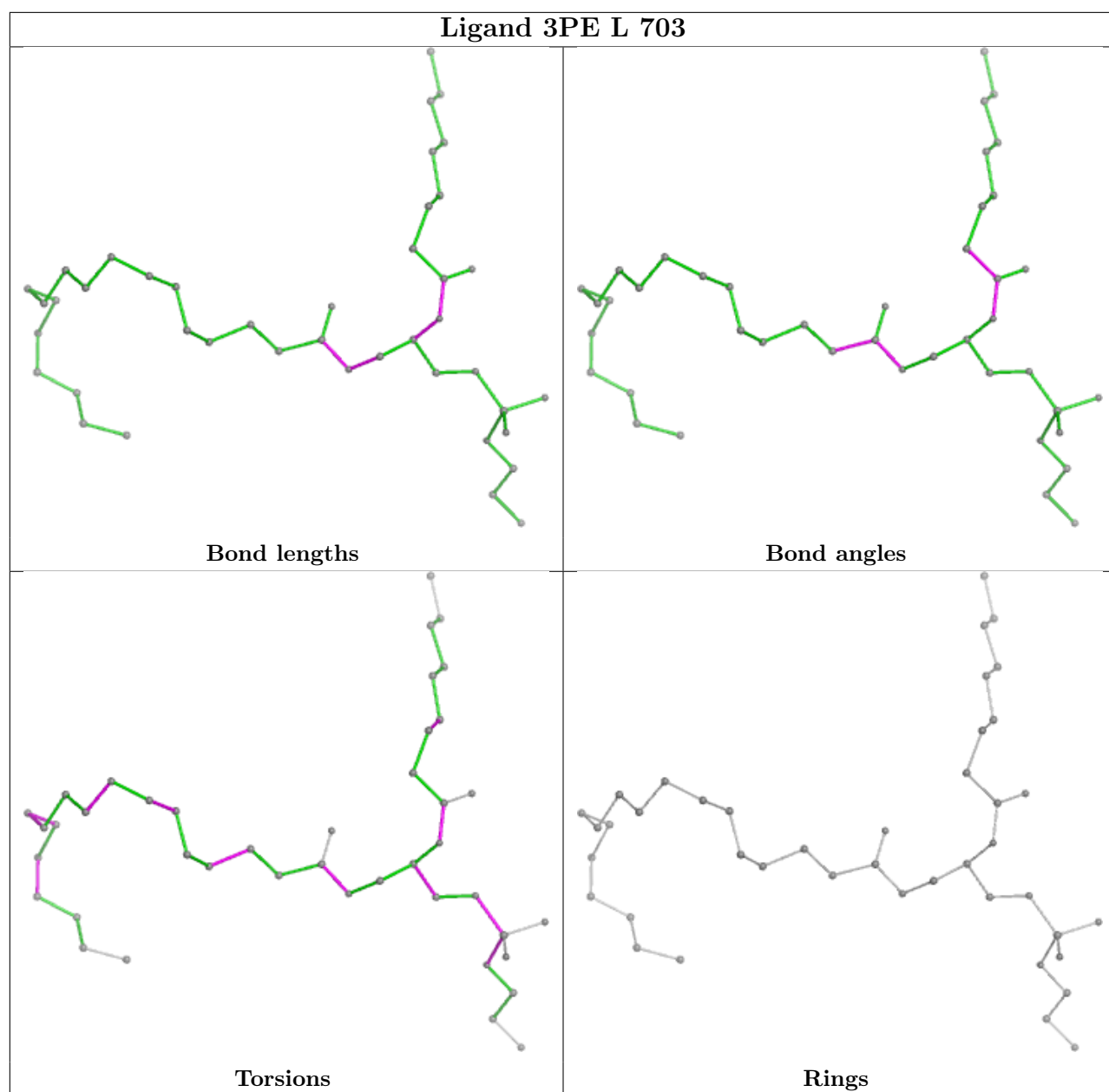




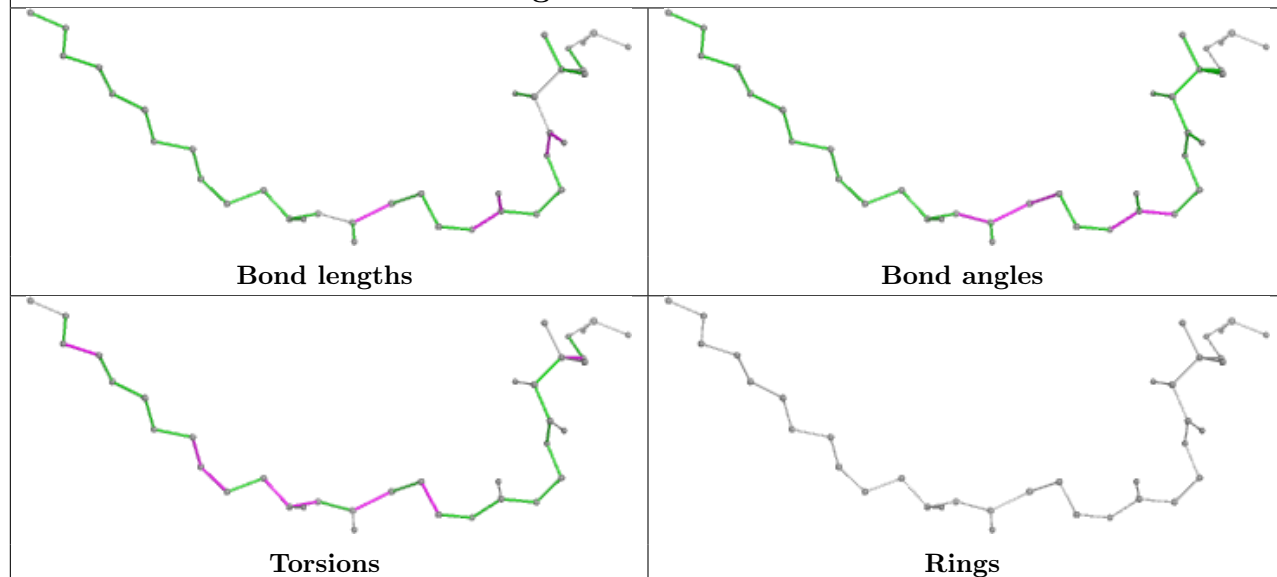




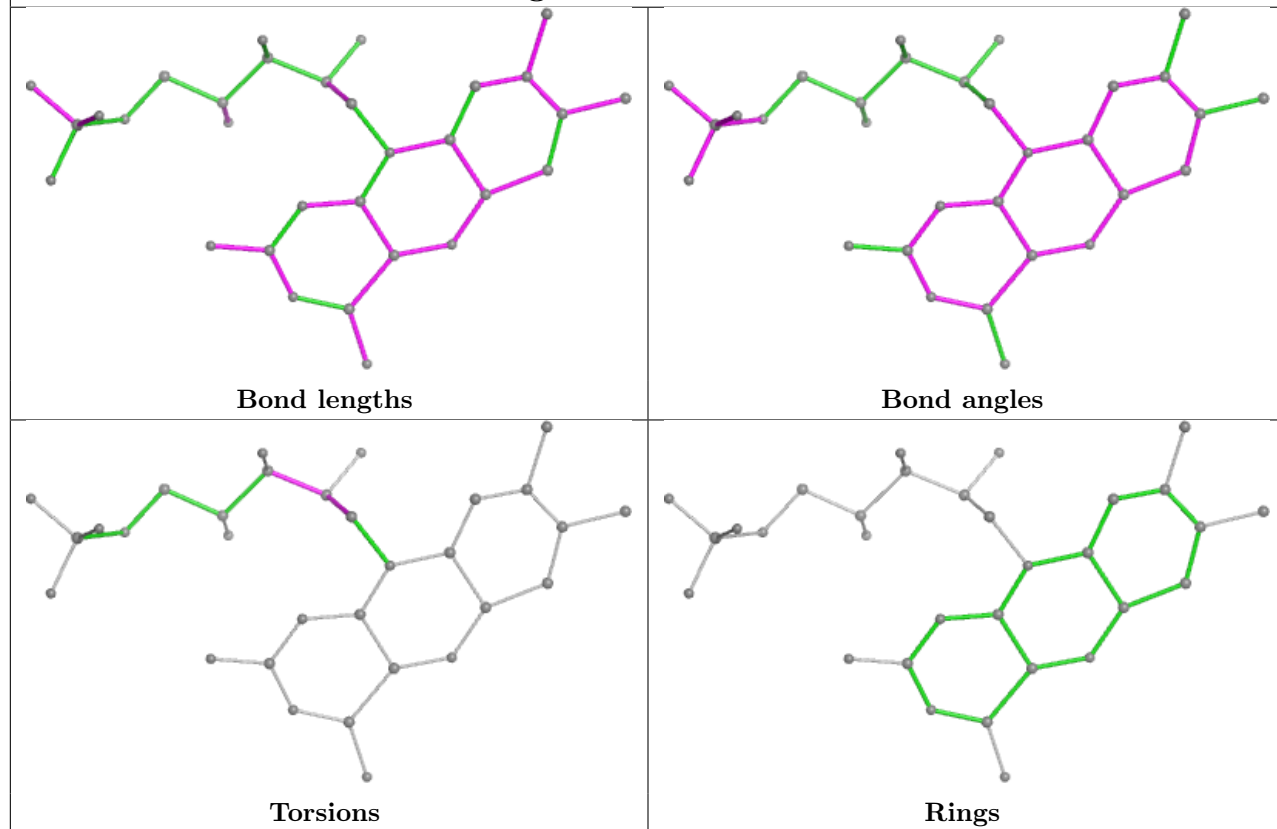


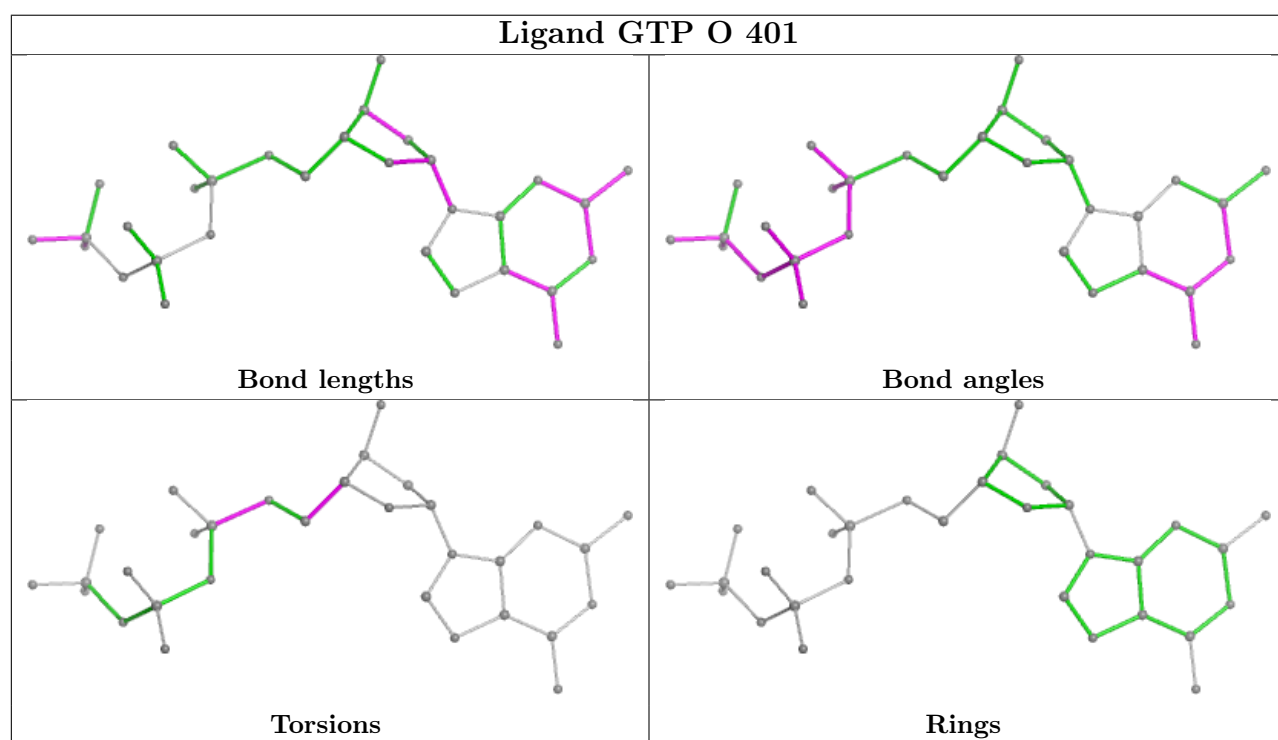
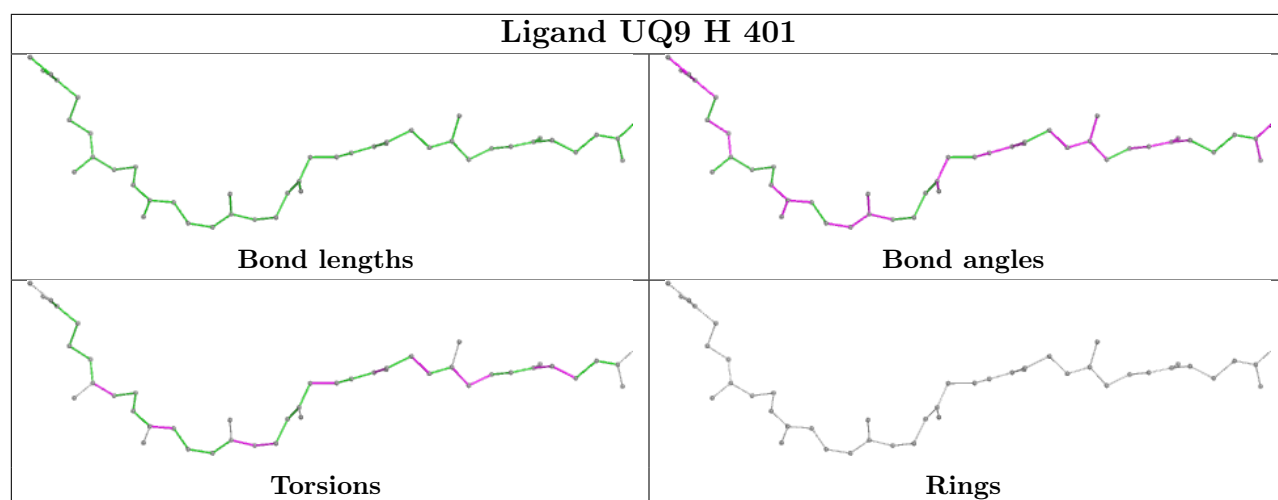


## Ligand EHZ T 201

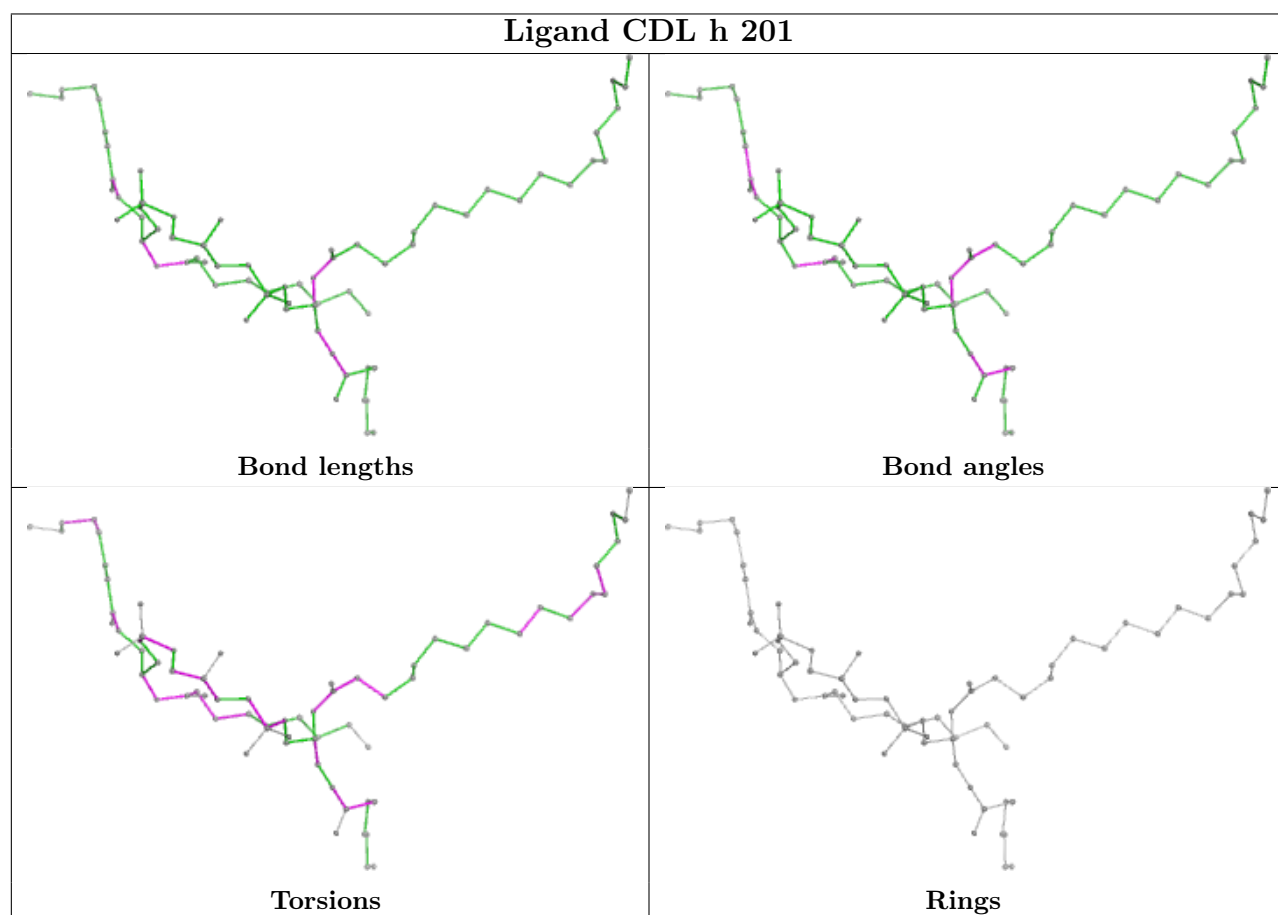
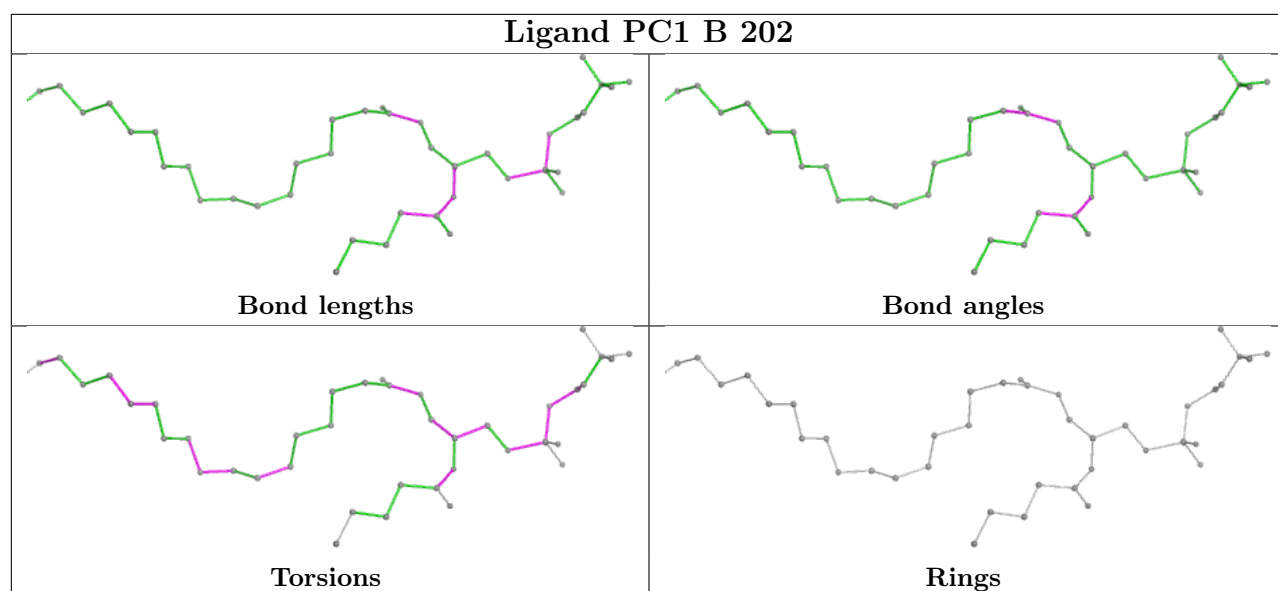


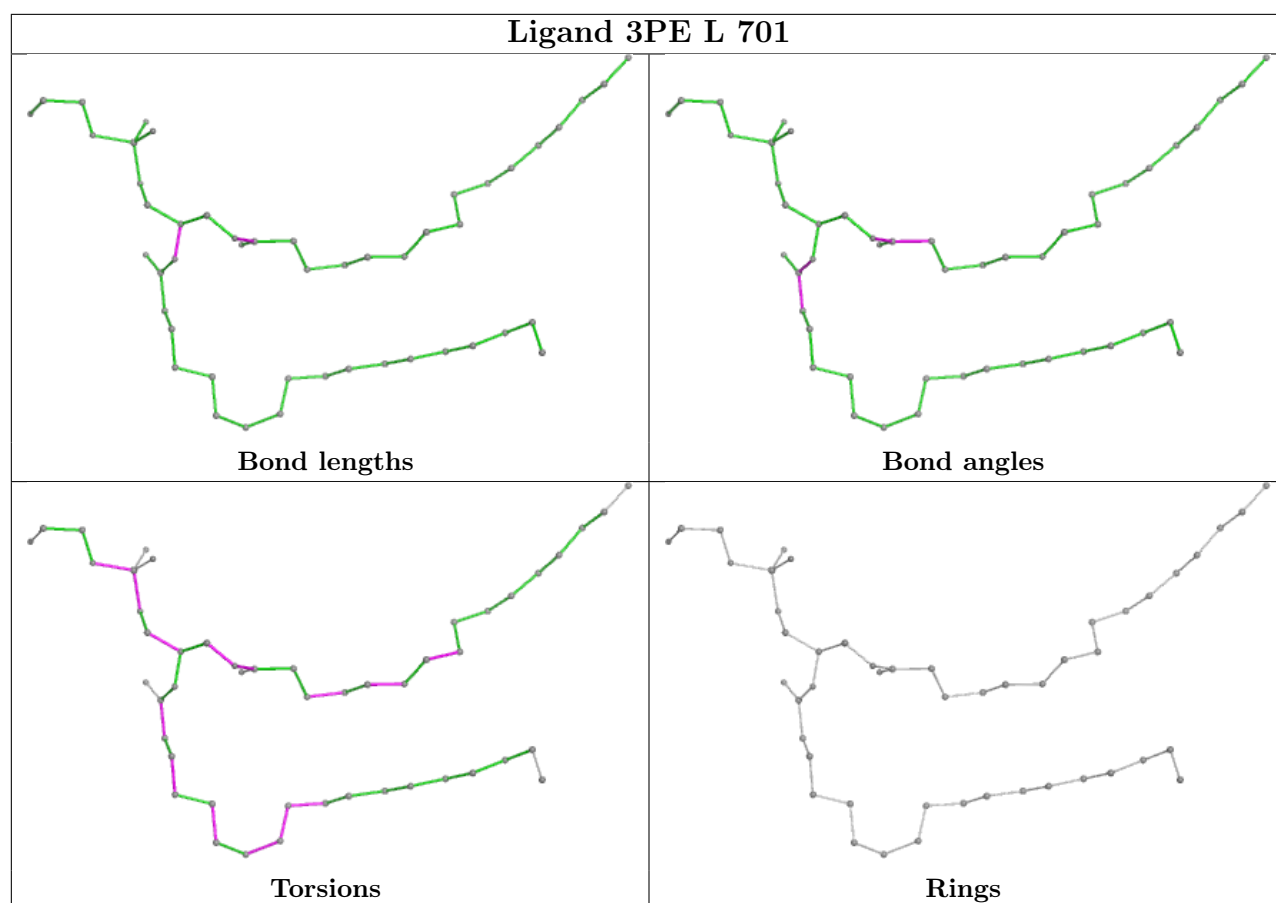
## Ligand FMN F 502











## 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.

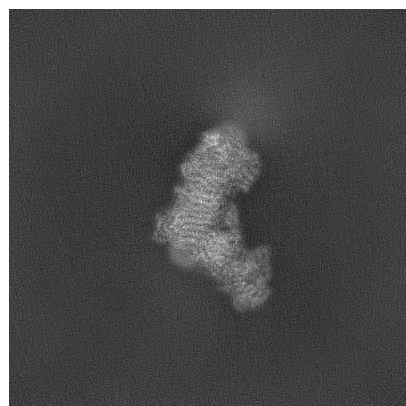
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16516. These allow visual inspection of the internal detail of the map and identification of artifacts.

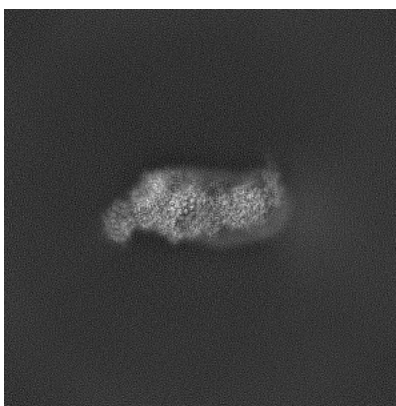
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

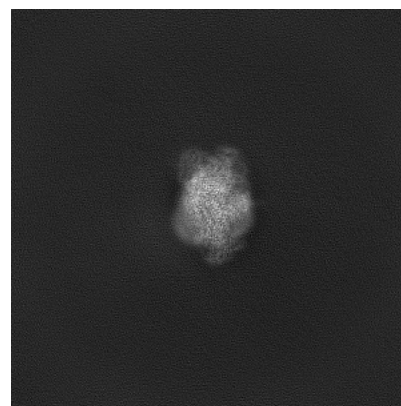
#### 6.1.1 Primary map



X

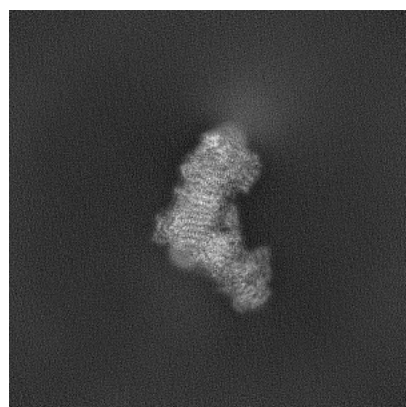


Y

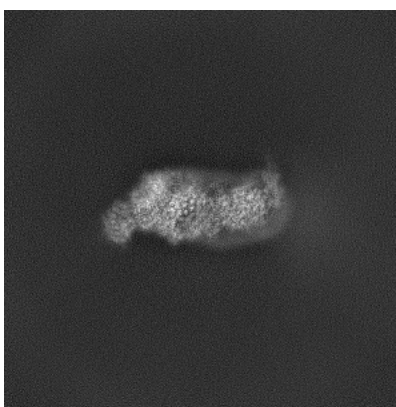


Z

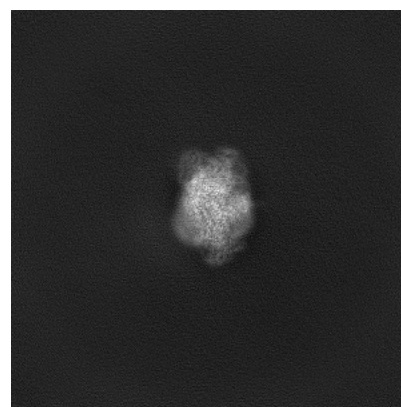
#### 6.1.2 Raw map



X



Y

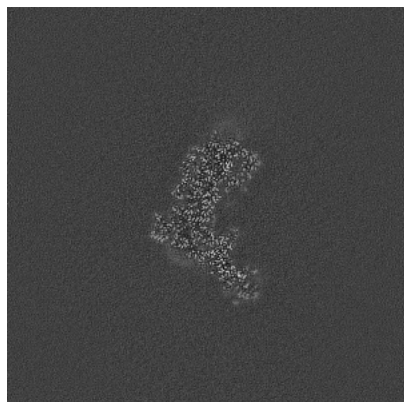


Z

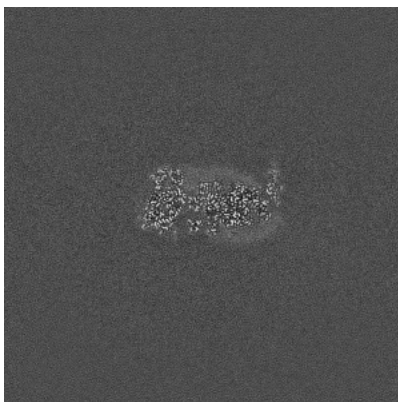
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

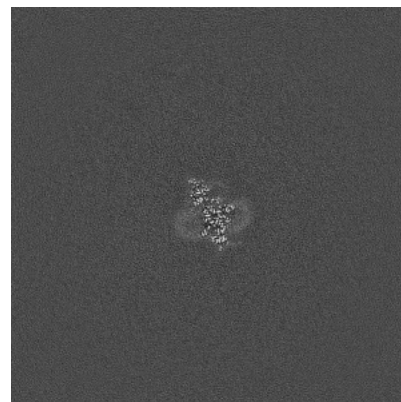
### 6.2.1 Primary map



X Index: 225

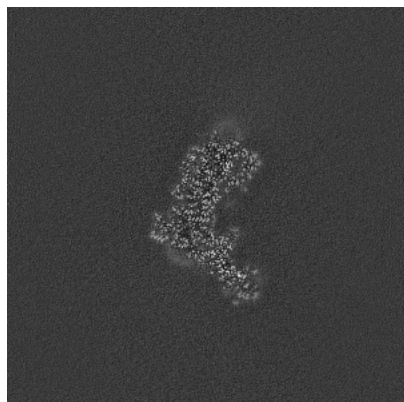


Y Index: 225

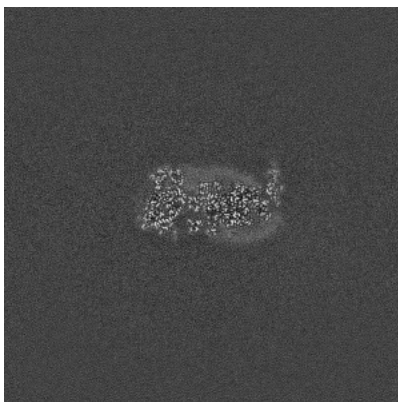


Z Index: 225

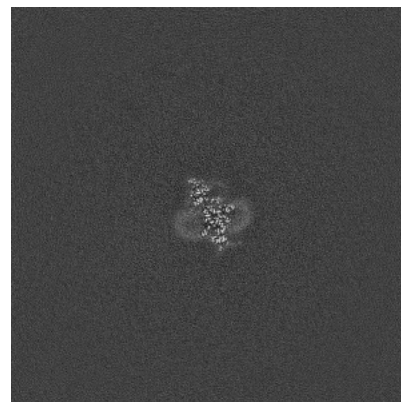
### 6.2.2 Raw map



X Index: 225



Y Index: 225

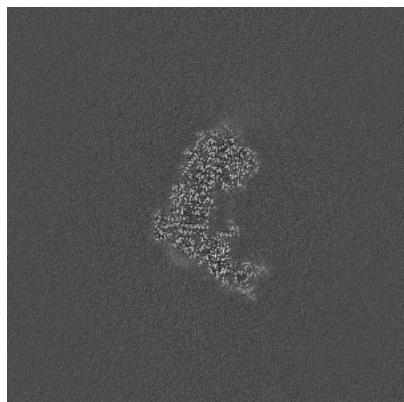


Z Index: 225

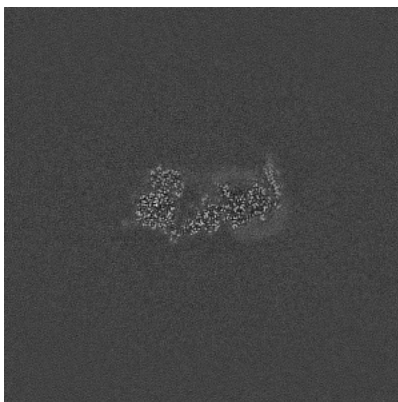
The images above show central slices of the map in three orthogonal directions.

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

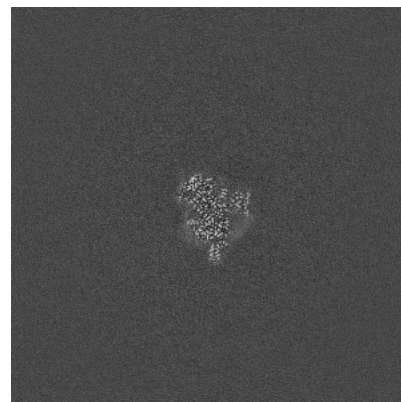
### 6.3.1 Primary map



X Index: 230

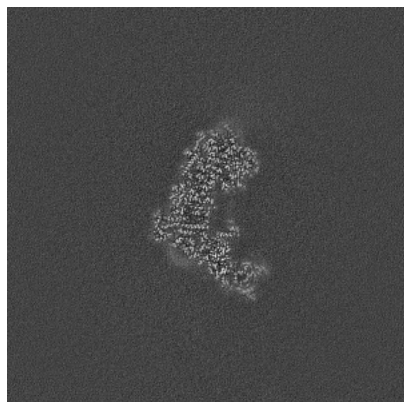


Y Index: 234



Z Index: 189

### 6.3.2 Raw map



X Index: 230



Y Index: 234



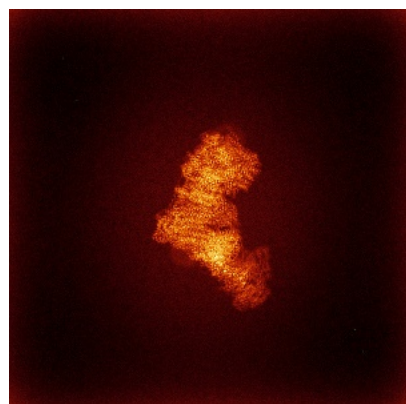
Z Index: 189

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

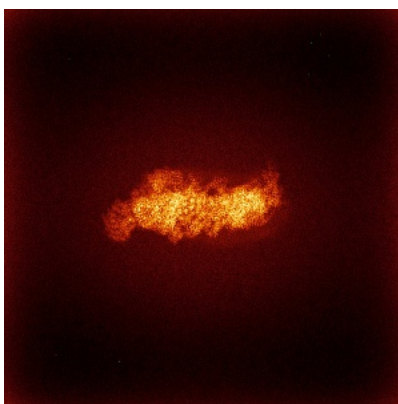


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

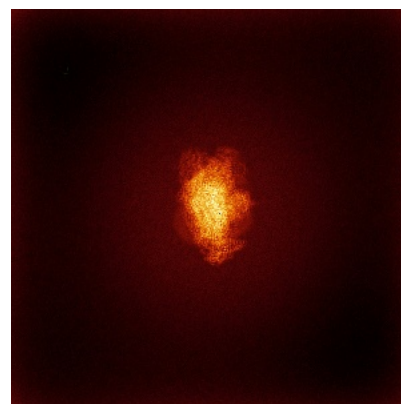
### 6.4.1 Primary map



X

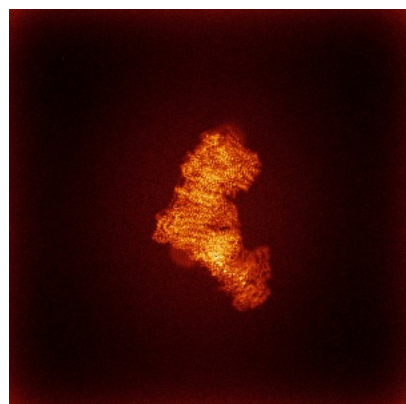


Y

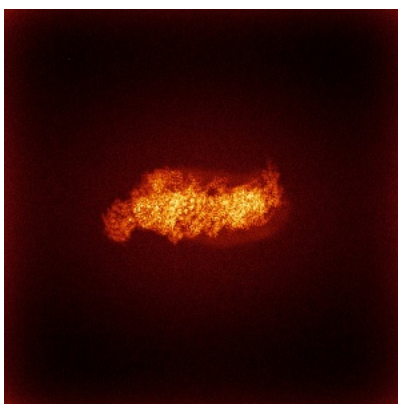


Z

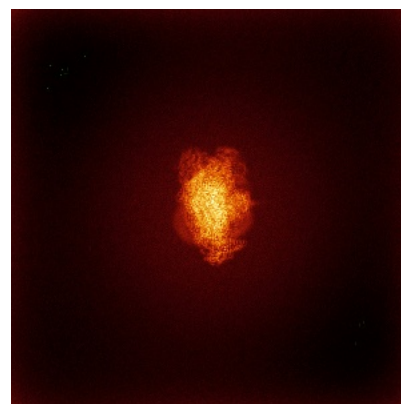
### 6.4.2 Raw map



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

### 6.5.2 Raw map



X



Y



Z

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

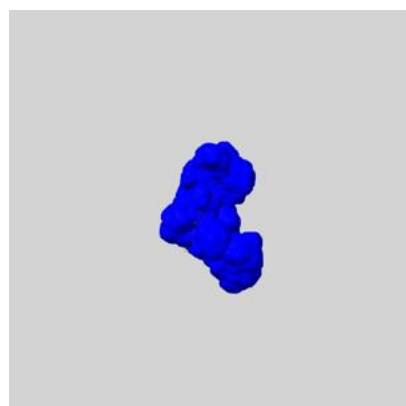
## 6.6 Mask visualisation [i](#)

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

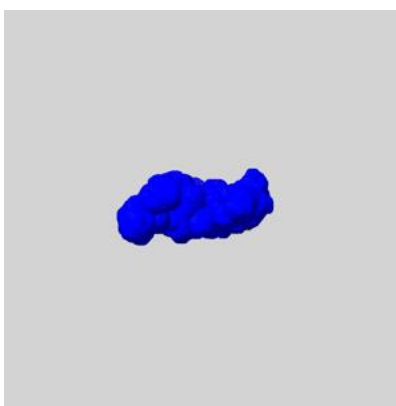
A mask typically either:

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

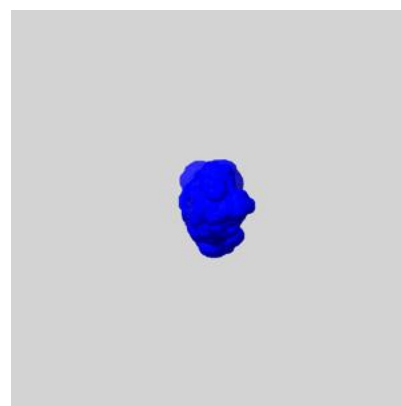
### 6.6.1 emd\_16516\_msk\_1.map [i](#)



X



Y



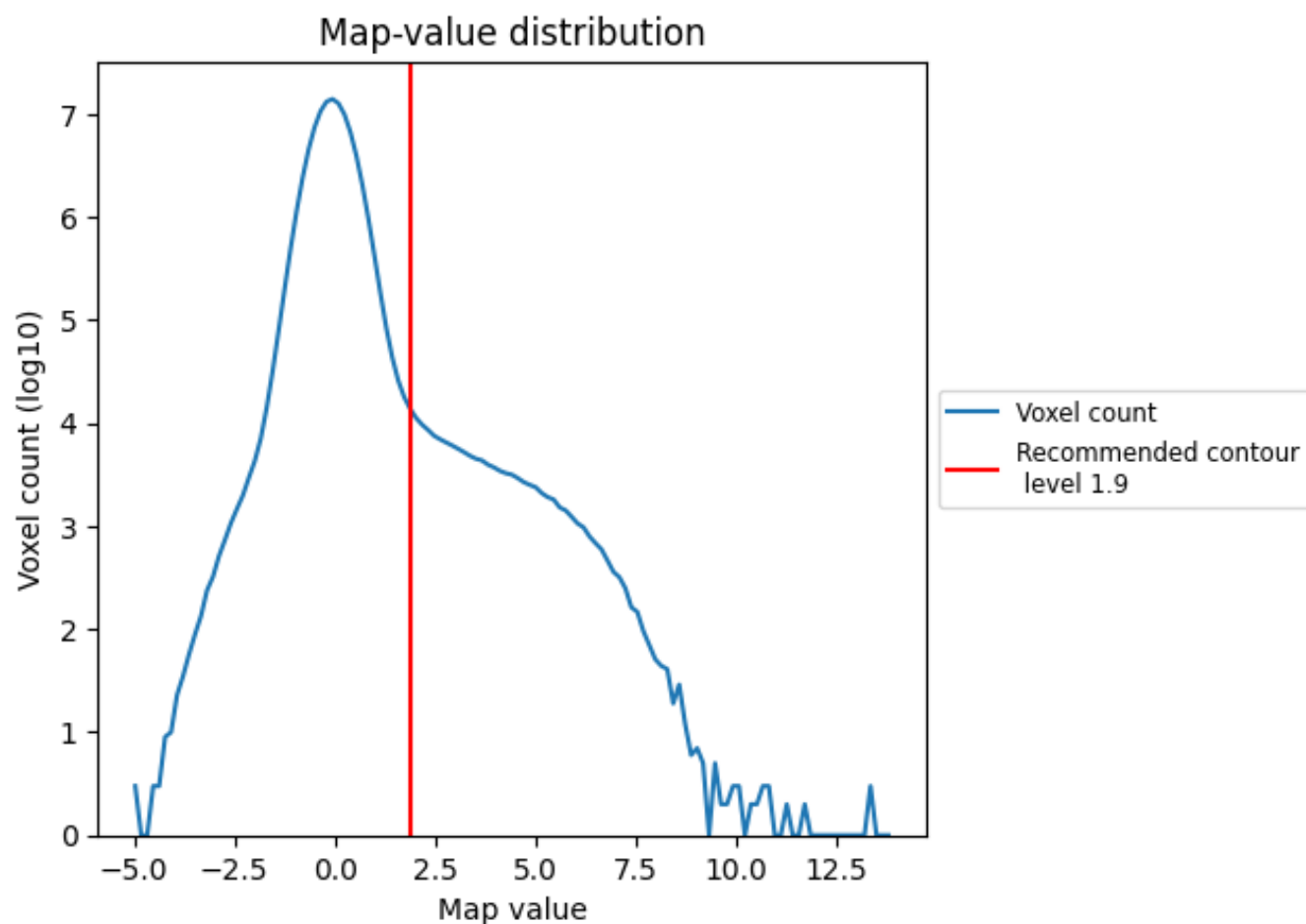
Z



## 7 Map analysis [i](#)

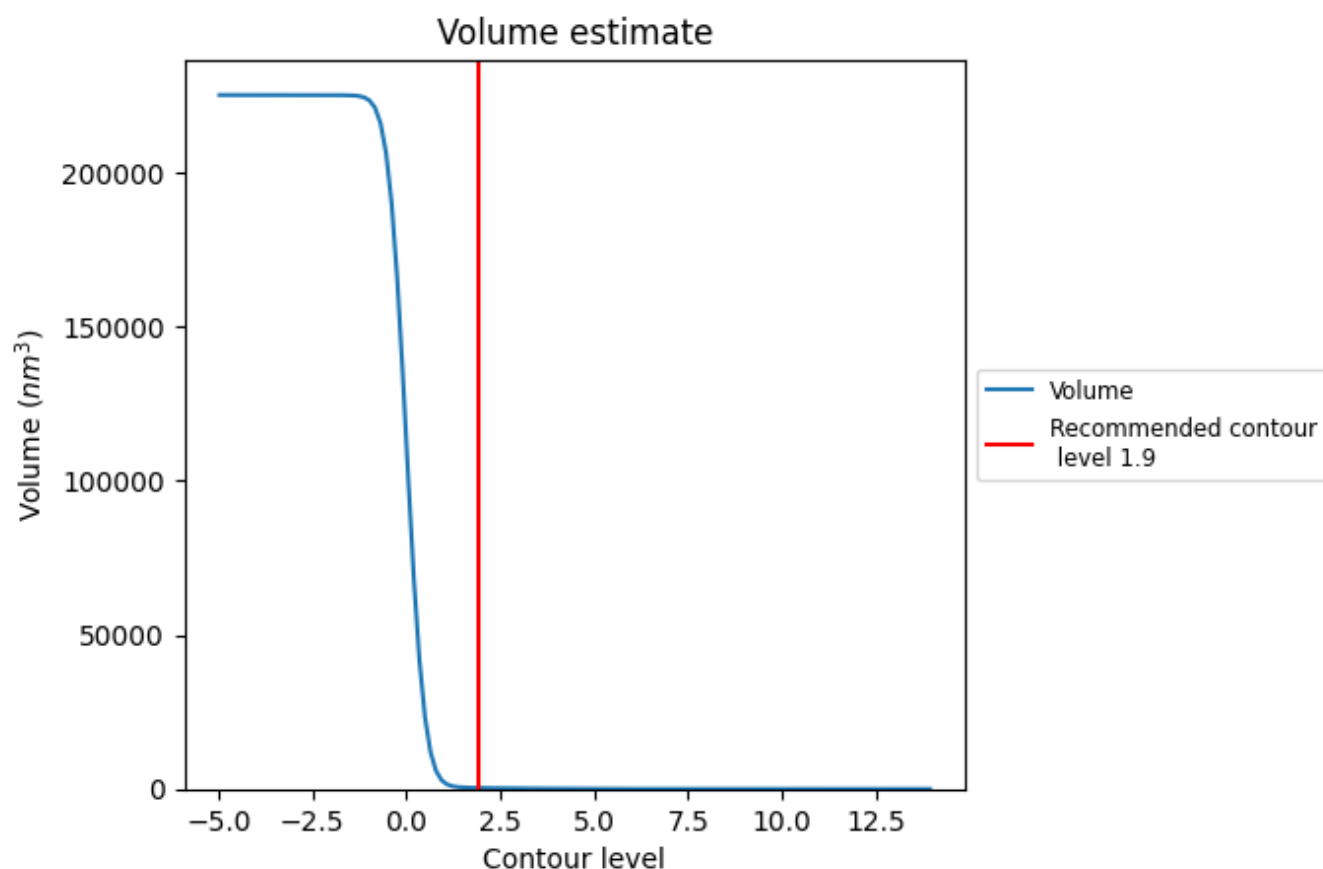
This section contains the results of statistical analysis of the map.

### 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.

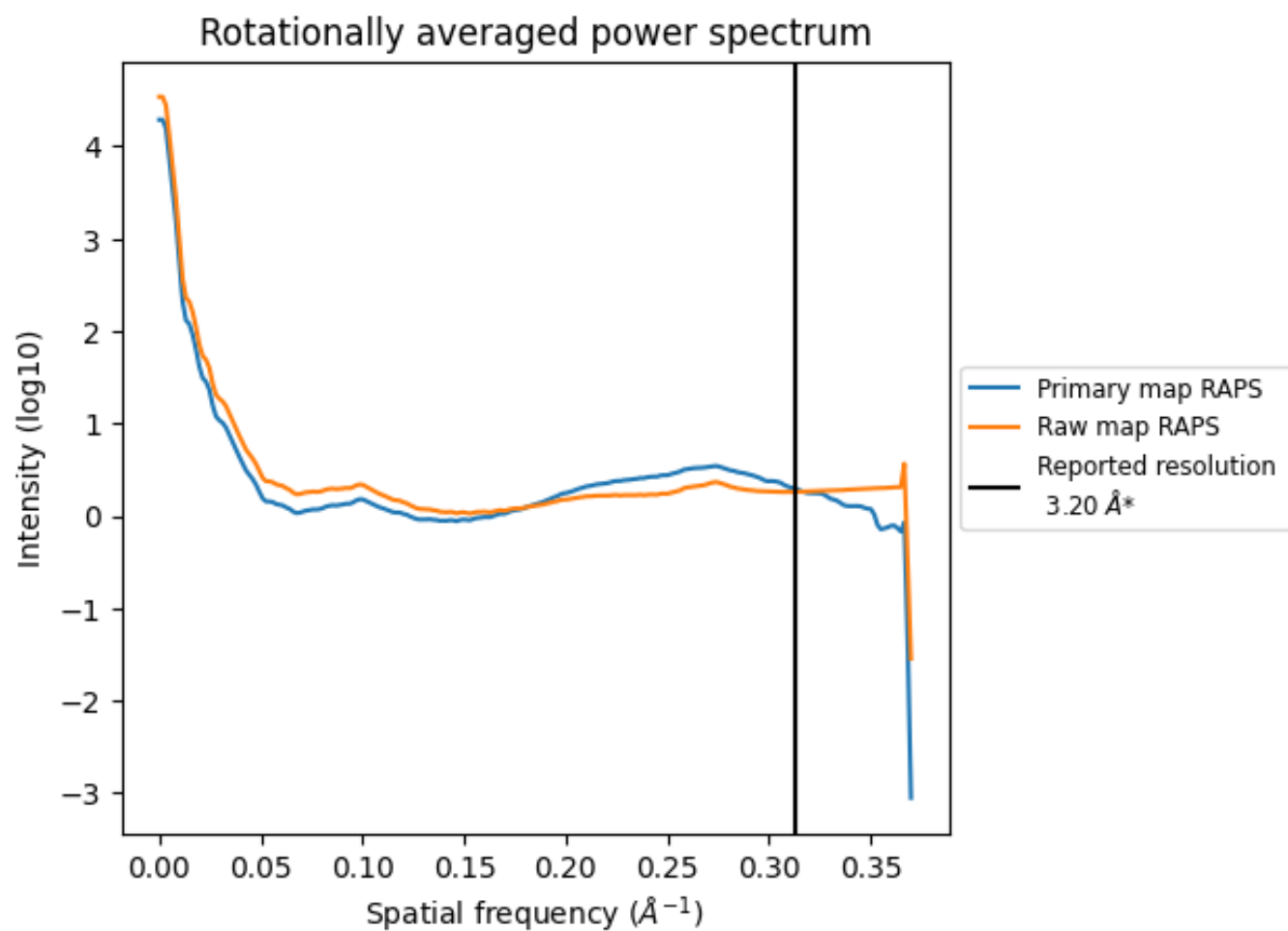
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339  $\text{nm}^3$ ; this corresponds to an approximate mass of 306 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 ⓘ

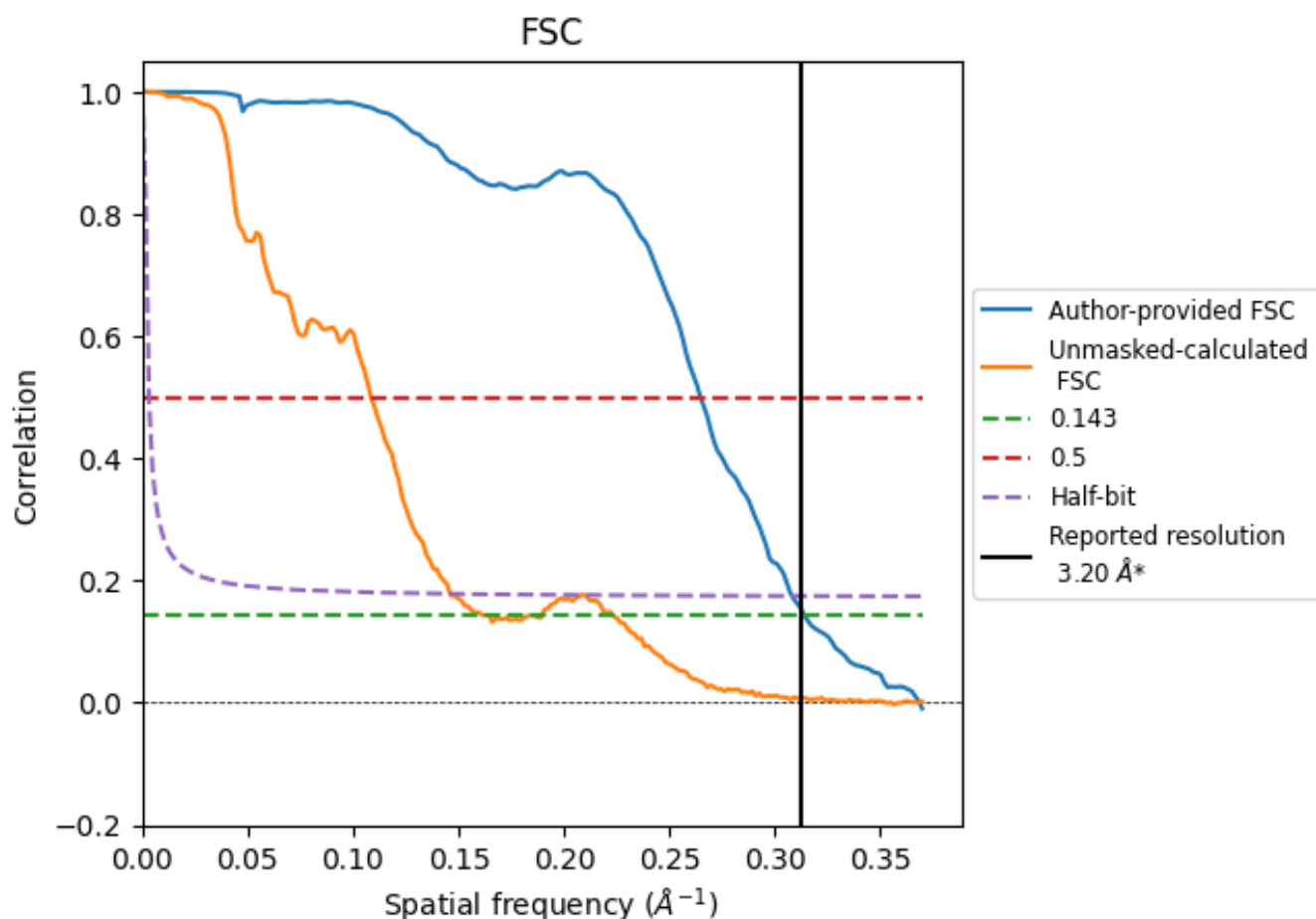


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

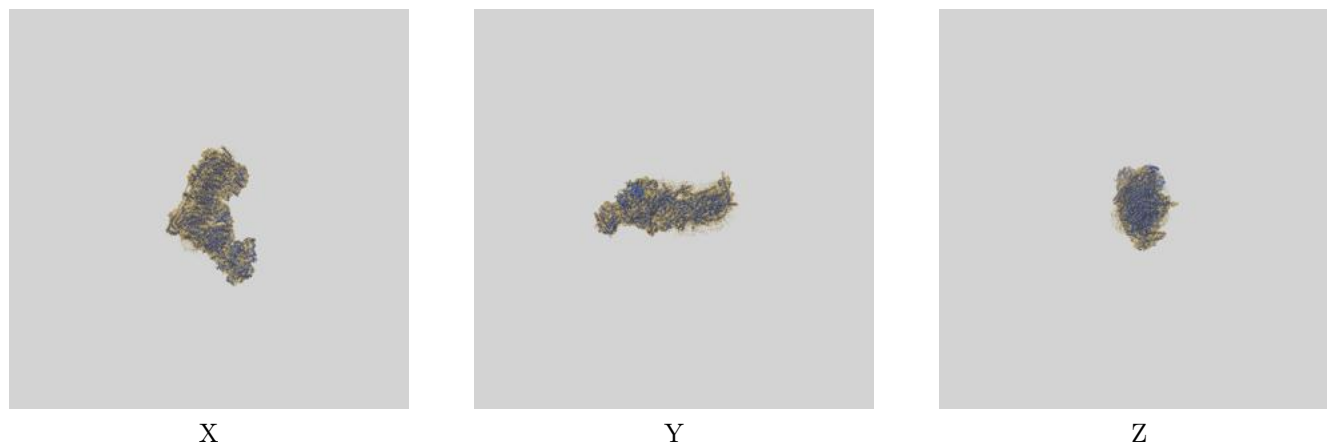
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.78	3.25
Unmasked-calculated*	6.17	9.22	6.85

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.17 differs from the reported value 3.2 by more than 10 %

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

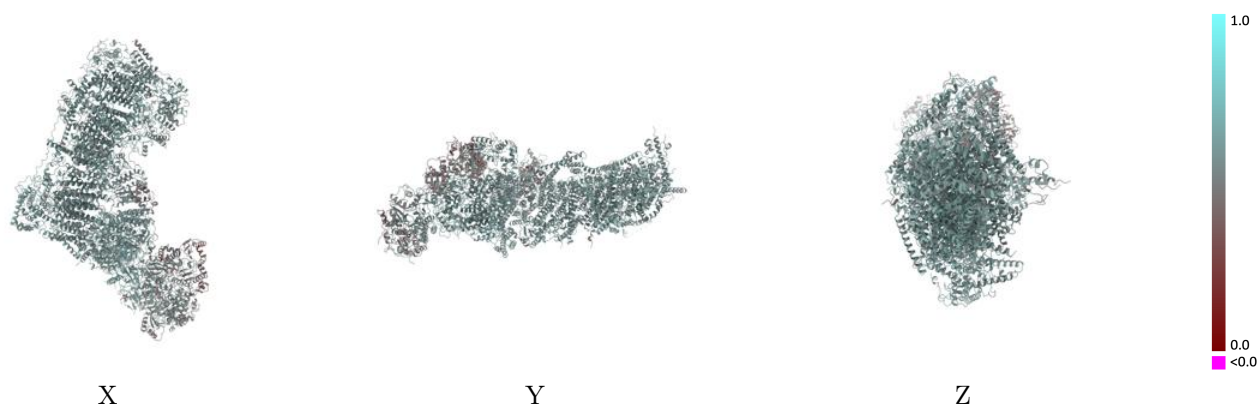
This section contains information regarding the fit between EMDB map EMD-16516 and PDB model 8CA3. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



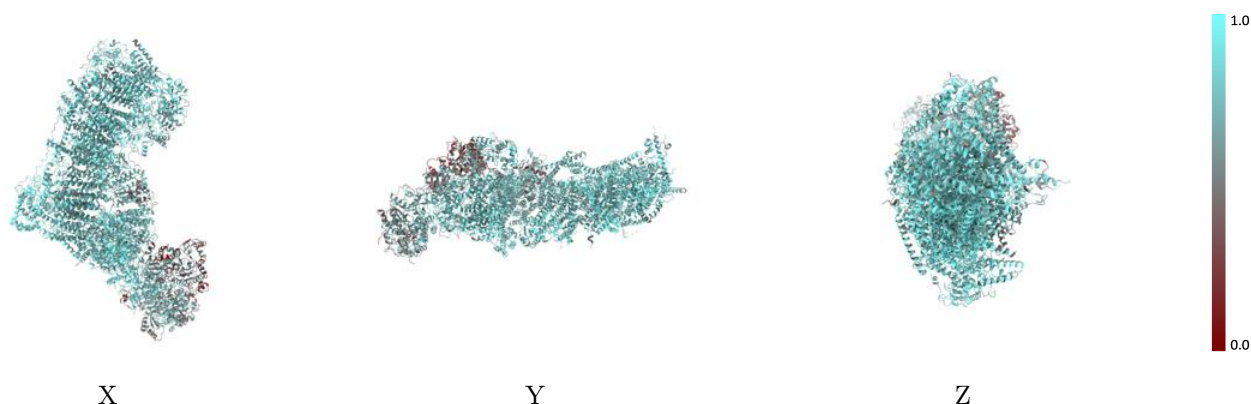
The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



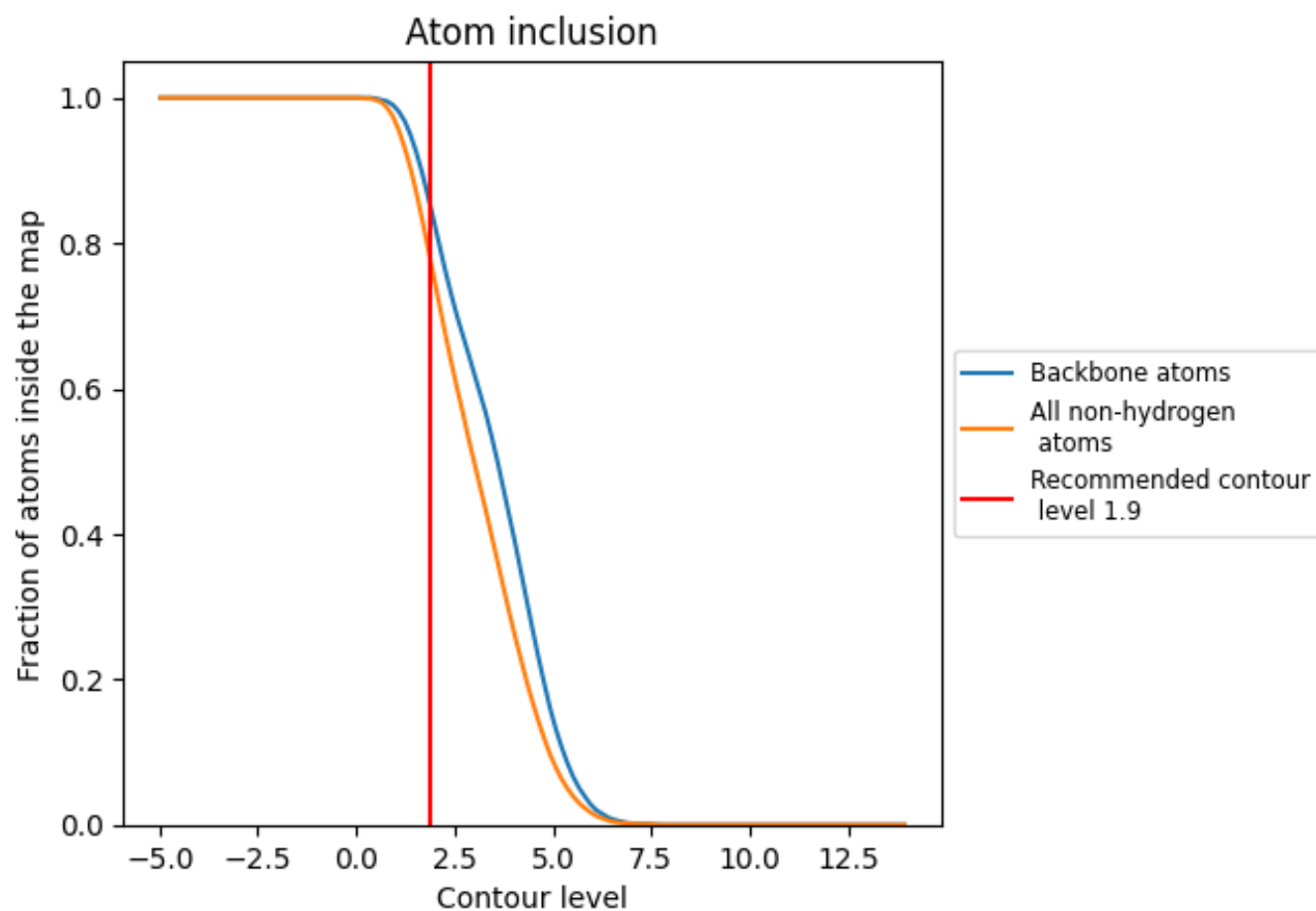
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.9).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 85% of all backbone atoms, 77% 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 (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5680
A	 0.8020	 0.5870
B	 0.8710	 0.6010
C	 0.8420	 0.6030
D	 0.8530	 0.6010
E	 0.6070	 0.5000
F	 0.6360	 0.5160
G	 0.5940	 0.5110
H	 0.8160	 0.5850
I	 0.8400	 0.5830
J	 0.7710	 0.5720
K	 0.8210	 0.5880
L	 0.8090	 0.5820
M	 0.8610	 0.5990
N	 0.8350	 0.5950
O	 0.8380	 0.5860
P	 0.7820	 0.5780
R	 0.6150	 0.5580
S	 0.4410	 0.4350
T	 0.4950	 0.4590
U	 0.7570	 0.5510
V	 0.7960	 0.5760
W	 0.7100	 0.5620
X	 0.8320	 0.5800
Y	 0.7610	 0.5640
Z	 0.8000	 0.5770
a	 0.8660	 0.5990
b	 0.8090	 0.5720
c	 0.7670	 0.5620
d	 0.8380	 0.5920
e	 0.8480	 0.5910
f	 0.7340	 0.5520
g	 0.8050	 0.5800
h	 0.8360	 0.5910
i	 0.7640	 0.5670



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
j	 0.7870	 0.5670
k	 0.7570	 0.5510
l	 0.8320	 0.5810
m	 0.8100	 0.5760
n	 0.8140	 0.5770
o	 0.7610	 0.5530
p	 0.8080	 0.5730
r	 0.7730	 0.5880
s	 0.5040	 0.4750