



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2024 – 08:52 am BST

PDB ID : 8Q0Q
EMDB ID : EMD-18059
Title : Outward-facing, slack proteoliposome complex I at 3.6 Å. Initially purified in DDM
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-07-28
Resolution : 3.60 Å (reported)
Based on initial model : 7QSO

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:

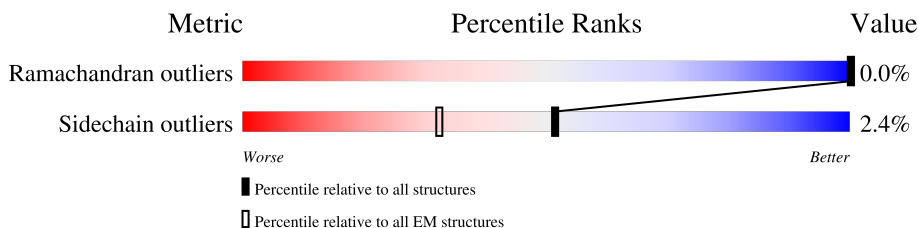
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.60 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	87% 10%
2	B	216	72% 27%
3	C	266	77% 21%
4	D	463	82% 16%
5	E	249	84% 14%
6	F	464	91% 7%
7	G	727	93% 5%
8	H	318	97%
9	I	212	83% 17%

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Mol	Chain	Length	Quality of chain
10	J	175	5% 90% 9%
11	K	98	81% 7% 12%
12	L	606	30% 89% 10%
13	M	459	9% 98%
14	N	347	99%
15	O	343	40% 92% 7%
16	P	380	82% 16%
17	Q	175	69% 29%
18	R	124	5% 77% 23%
19	S	99	87% 12%
20	T	156	52% 46%
20	U	156	35% 54% 44%
21	V	116	97%
22	W	128	87% 10%
23	X	172	97%
24	Y	141	12% 23% 77%
25	Z	144	97%
26	a	70	100%
27	b	84	96%
28	c	76	16% 63% 37%
29	d	120	9% 98%
30	e	106	92% 7%
31	f	57	25% 96%
32	g	154	12% 57% 42%
33	h	189	13% 75% 24%

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Mol	Chain	Length	Quality of chain
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

2 Entry composition i

There are 58 unique types of molecules in this entry. The entry contains 65579 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
			Total	C	N	O	S		
1	A	104	842	575	119	143	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	158	1260	803	227	216	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	210	1743	1123	299	318	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	388	3110	1984	538	564	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1659	1059	278	312	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	432	3324	2094	594	616	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	689	5284	3310	921	1014	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	318	2509	1681	385	420	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	176	1414	889	243	270	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	160	1219	823	172	212	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	86	647	425	96	111	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	547	4334	2880	667	746	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3654	2436	570	609	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	347	2733	1817	416	457	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	320	2560	1652	452	451	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	125	1016	641	181	191	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			701	439	133	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	84	Total	C	N	O	S	0	0
			681	439	100	137	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	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	113	Total	C	N	O	S	0	0
			919	595	155	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			977	625	181	167	4		

- 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
			1402	887	253	252	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	33	248	162	39	46	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	142	1157	743	202	203	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	70	569	365	104	95	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	83	654	427	109	116	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	48	405	268	69	68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	120	999	650	172	172	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	99	829	523	158	142	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	57	492	322	86	82	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	90	750	483	124	139	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	143	1186	776	203	205	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	127	1097	722	191	183	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	70	592	387	98	106	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	81	653	427	110	114	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	156	1314	850	216	240	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	128	1070	686	188	196		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	171	1487	952	272	256	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	120	1035	645	199	183	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	173	1455	912	268	267	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	145	1212	780	216	211	5	0	0

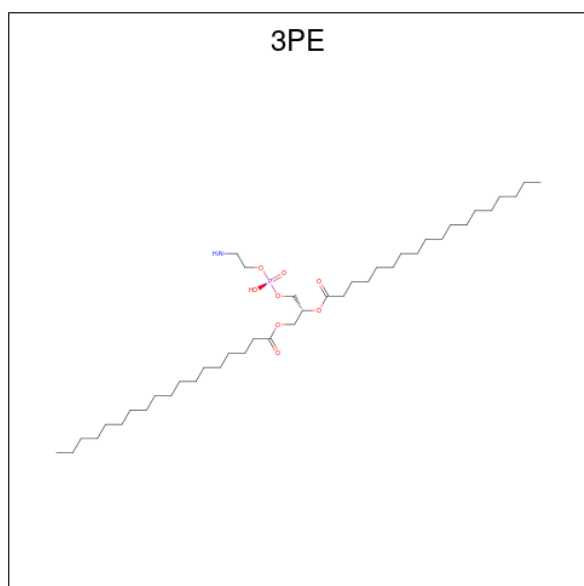
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	96	785	496	146	140	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	45	380	238	67	74	1	0	0

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



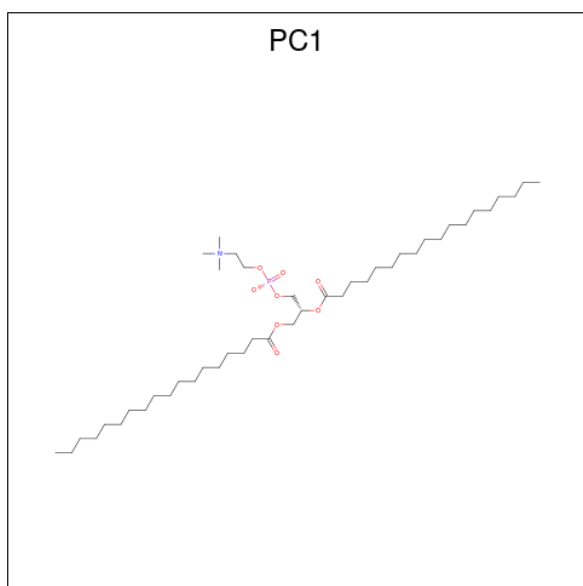
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	A	1	43	33	1	8	1	0
45	I	1	51	41	1	8	1	0
45	I	1	33	23	1	8	1	0
45	J	1	39	29	1	8	1	0
45	M	1	38	28	1	8	1	0
45	M	1	39	29	1	8	1	0
45	O	1	35	25	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	Z	1	Total 49	C 39	N 1	O 8	P 1	0
45	d	1	Total 49	C 39	N 1	O 8	P 1	0
45	h	1	Total 32	C 22	N 1	O 8	P 1	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	Total 50	C 40	N 1	O 8	P 1	0
46	B	1	Total 51	C 41	N 1	O 8	P 1	0
46	H	1	Total 43	C 33	N 1	O 8	P 1	0
46	d	1	Total 33	C 23	N 1	O 8	P 1	0
46	q	1	Total 37	C 27	N 1	O 8	P 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



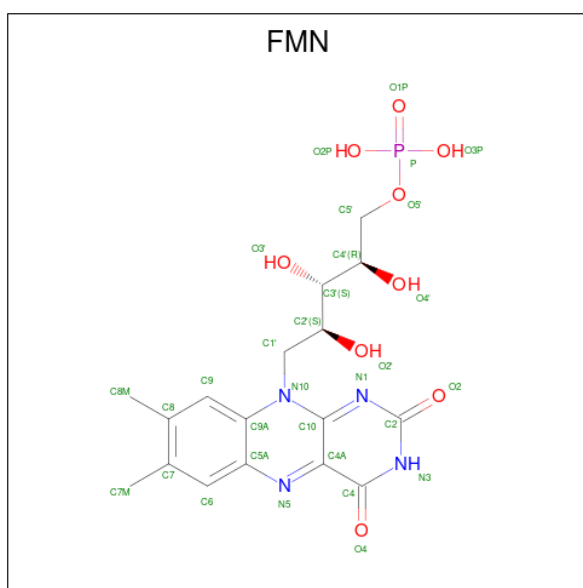
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	8	4	4	0
47	F	1	8	4	4	0
47	G	1	8	4	4	0
47	G	1	8	4	4	0
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

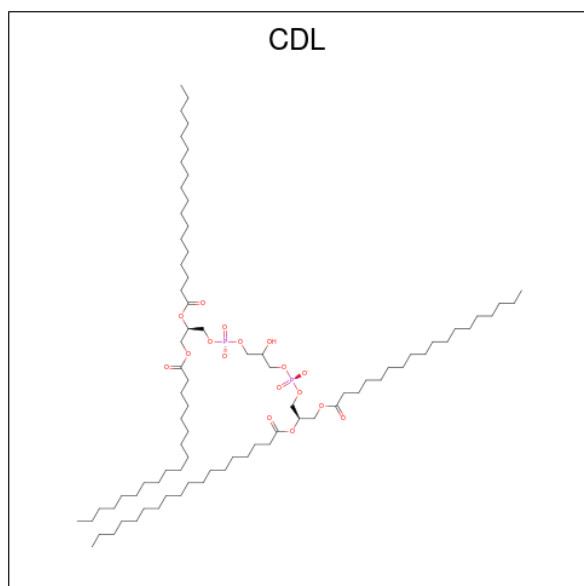


Mol	Chain	Residues	Atoms				AltConf	
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

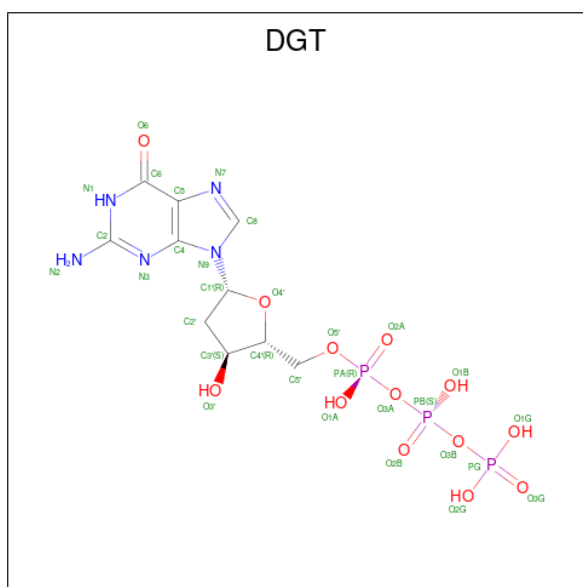
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	N	1	73	54	17	2	0
51	X	1	79	60	17	2	0
51	d	1	65	46	17	2	0
51	q	1	60	41	17	2	0

- Molecule 52 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

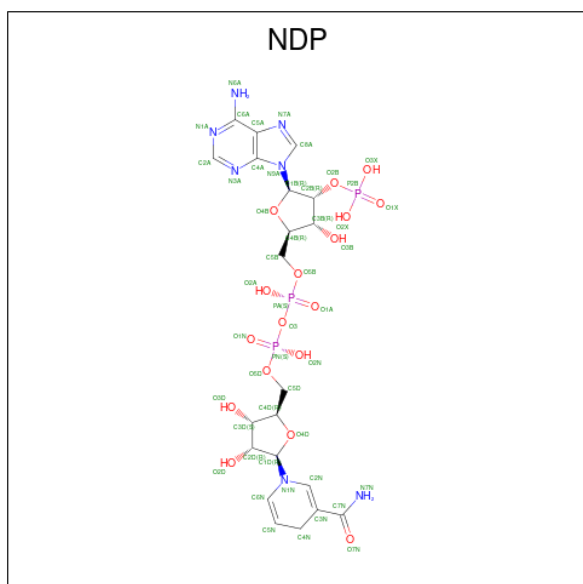


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	O	1	31	10	5	13	3	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
53	O	1	1	1	0

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

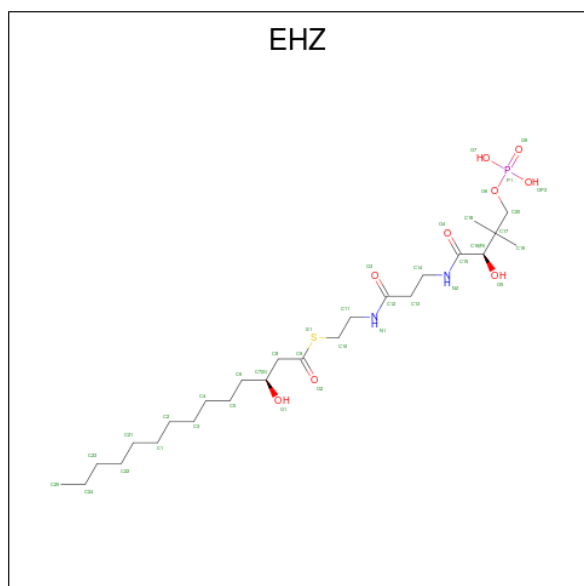


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	P	1	48	21	7	17	3	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

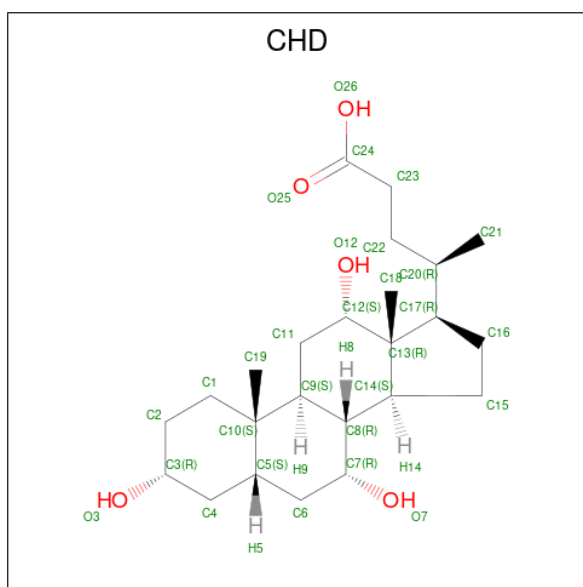
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	R	1	1	1	0

- Molecule 56 is {S}-[2-[3-[[2 {R}]-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



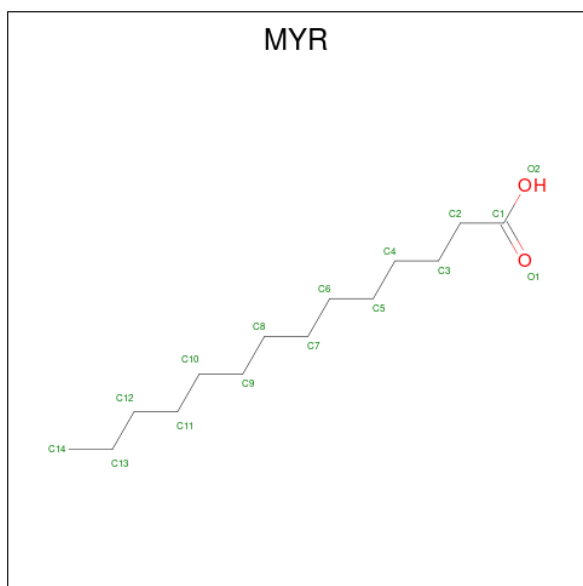
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
56	T	1	37	25	2	8	1	1	0
56	U	1	37	25	2	8	1	1	0

- Molecule 57 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
57	i	1	Total	C	O	0
			29	24	5	

- Molecule 58 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).




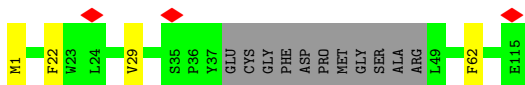
Mol	Chain	Residues	Atoms			AltConf
58	o	1	Total	C	O	0
			15	14	1	

3 Residue-property plots [i](#)

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

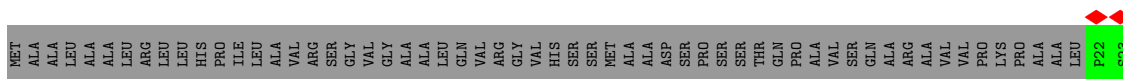
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:  87% 10%




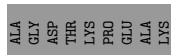
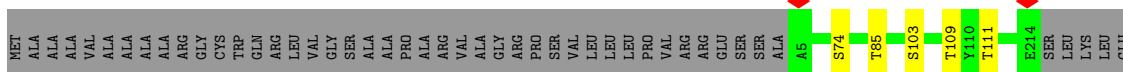
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:  72% 27%




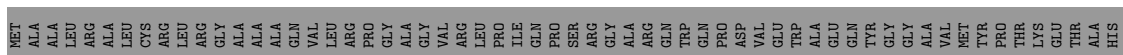
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

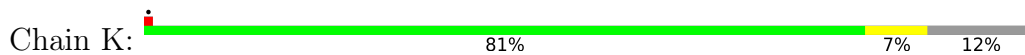
Chain C:  77% 21%



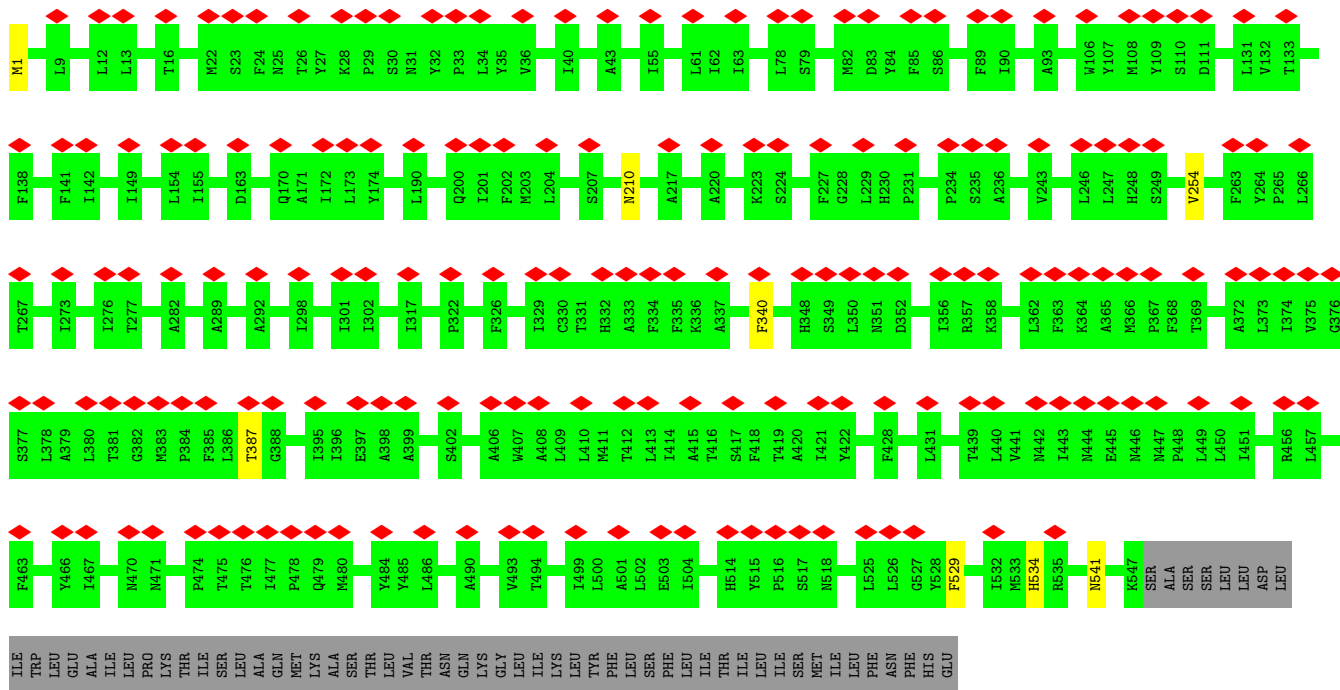
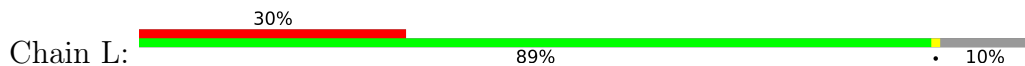
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  82% 16%

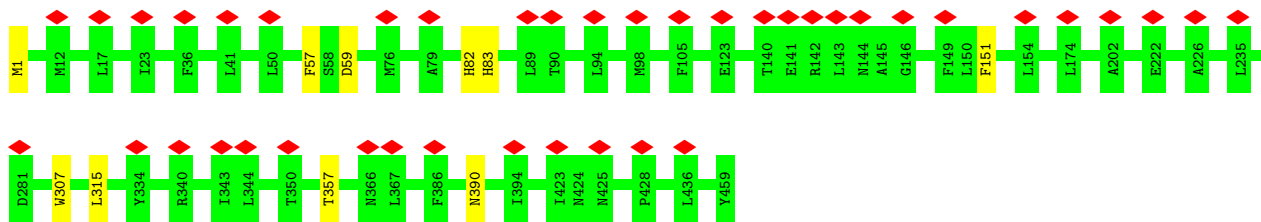




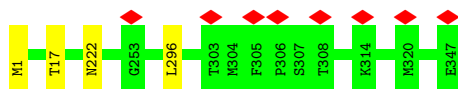
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



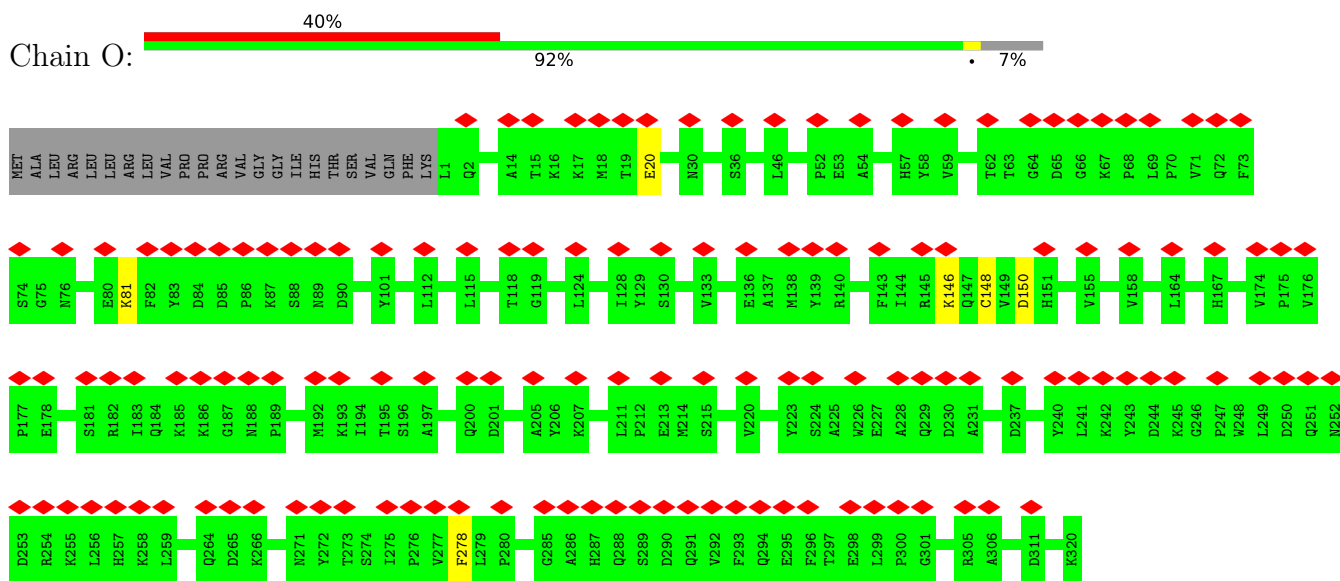
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



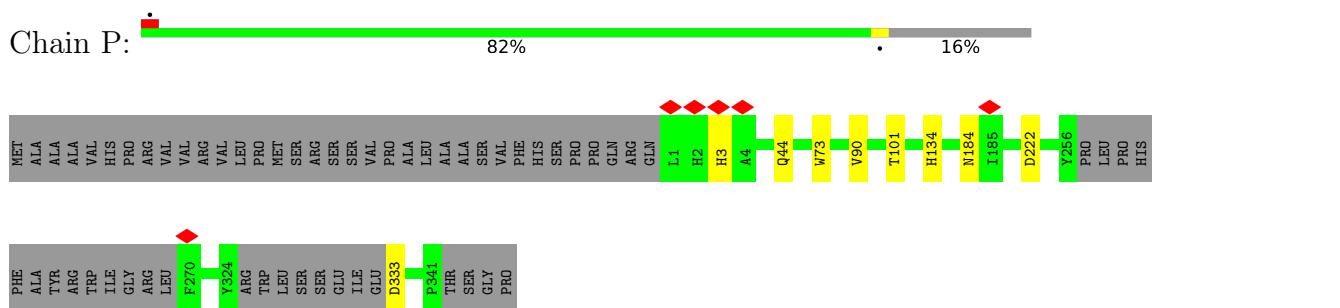
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



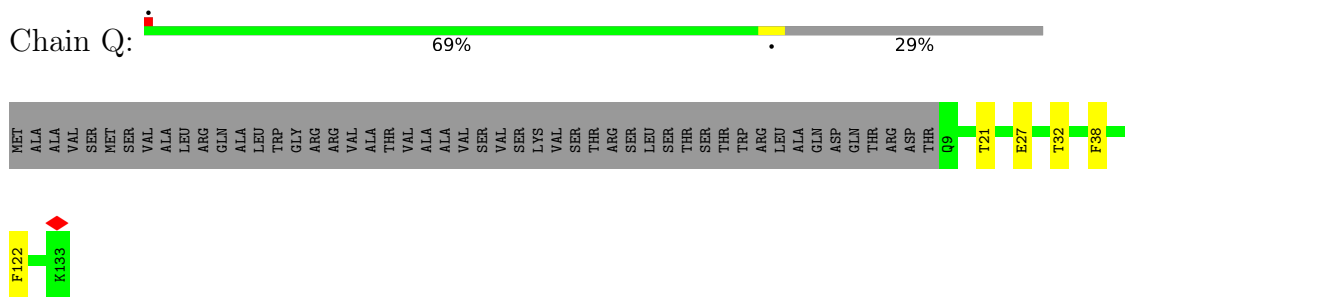
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



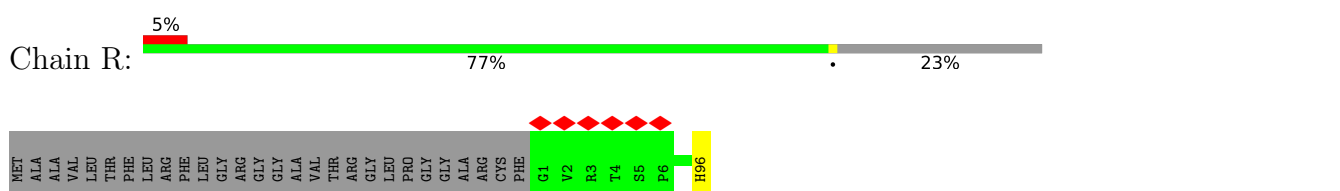
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



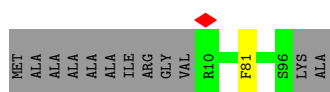
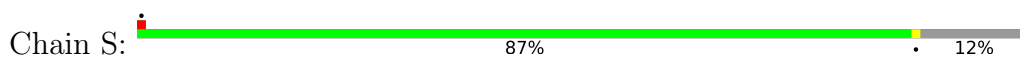
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



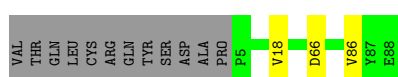
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



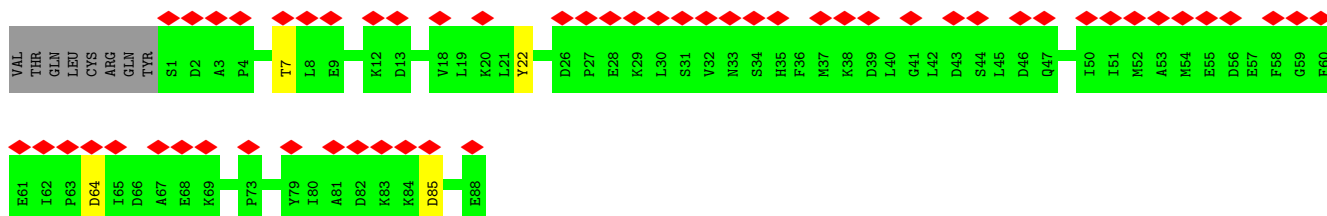
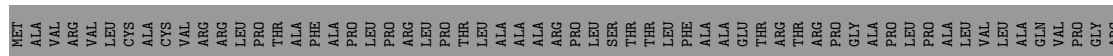
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



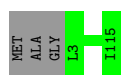
- Molecule 20: Acyl carrier protein, mitochondrial



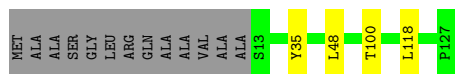
- Molecule 20: Acyl carrier protein, mitochondrial



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



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

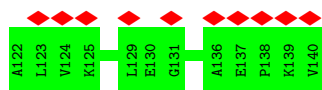
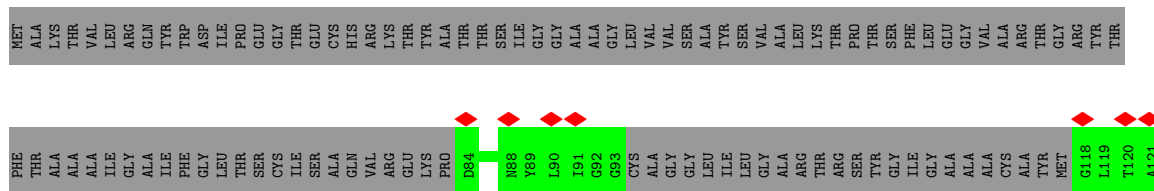


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8





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



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



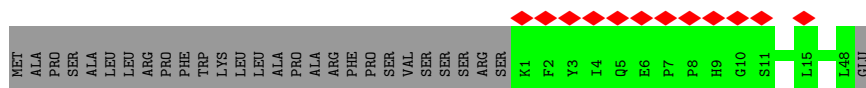
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



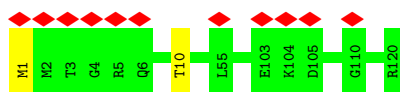
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



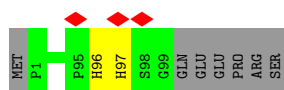
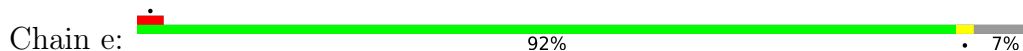
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



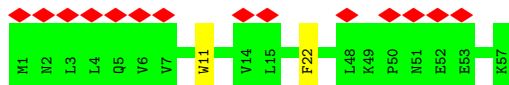
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



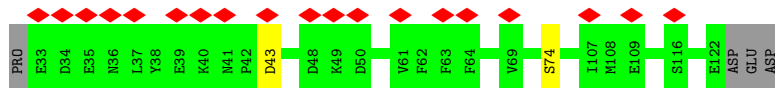
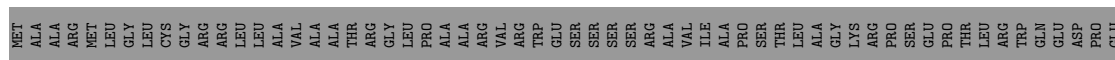
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



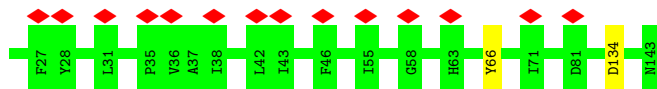
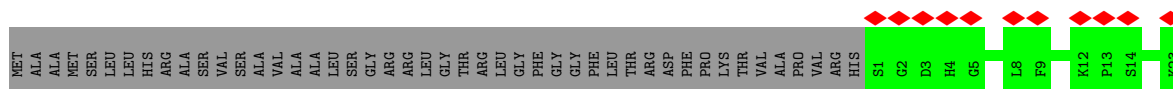
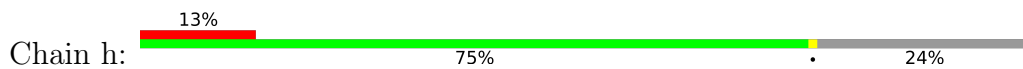
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



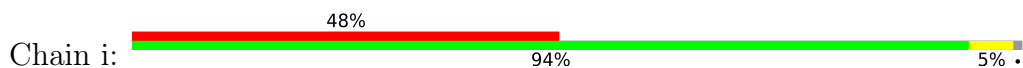
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

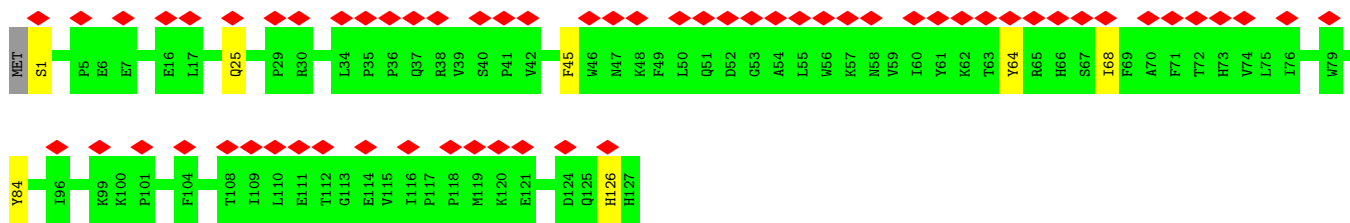


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

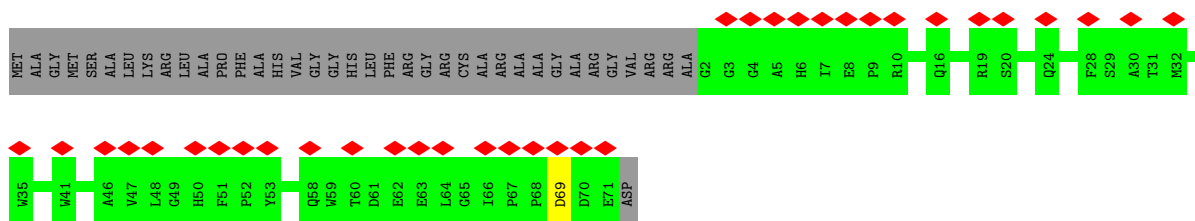


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

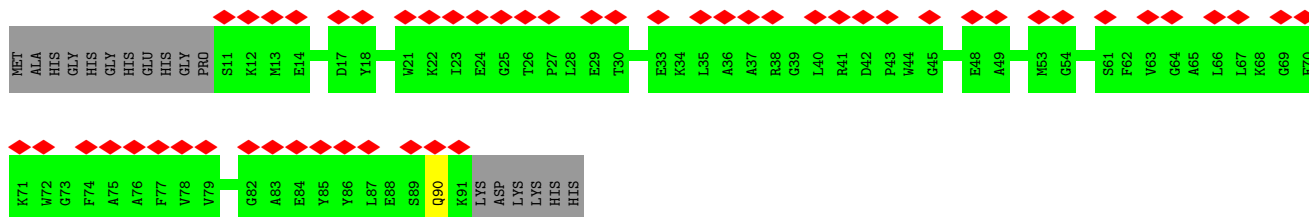
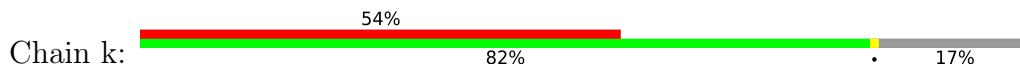




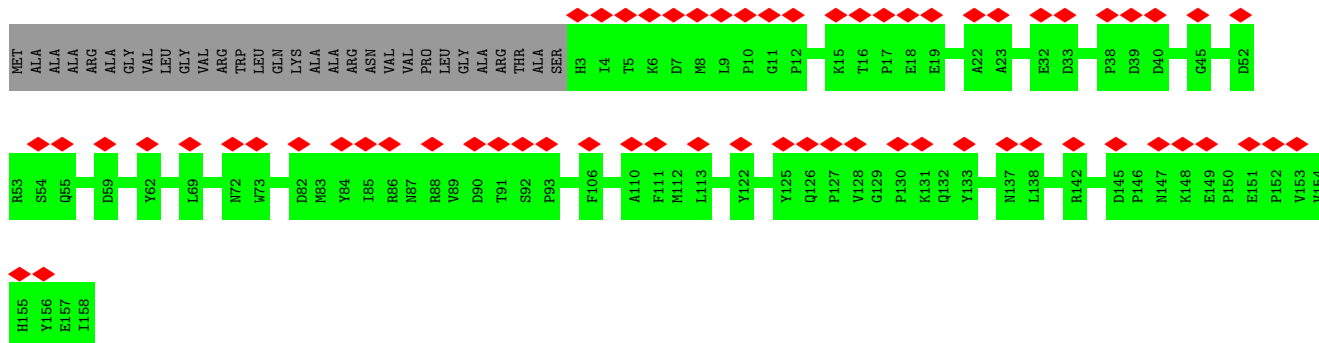
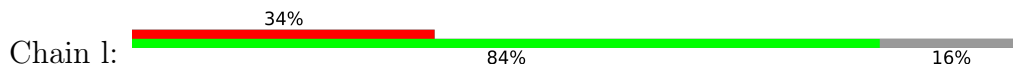
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



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

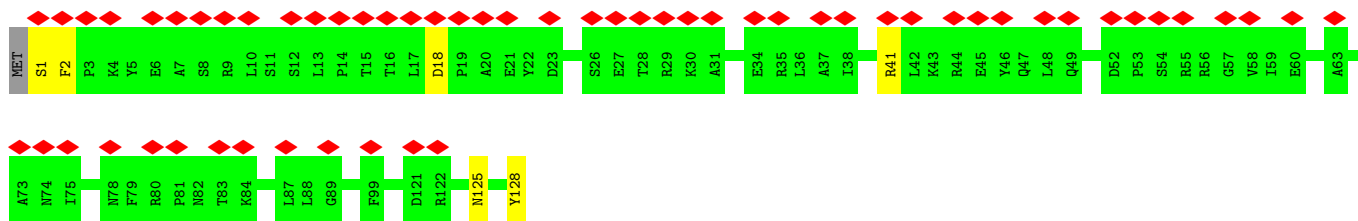


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



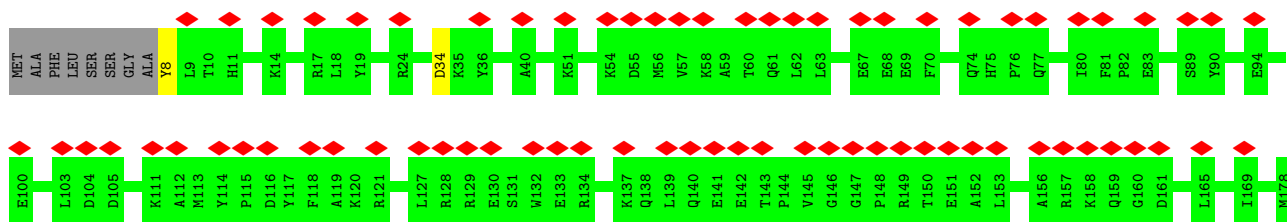
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4





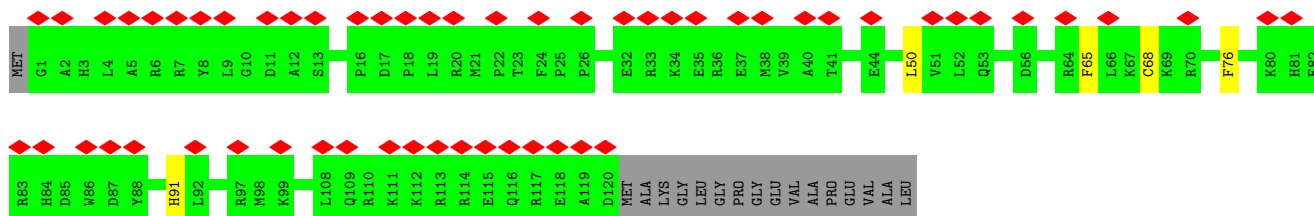
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 40% 94%



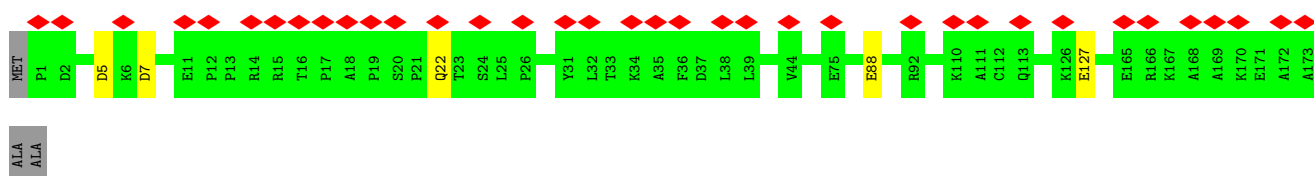
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 42% 84% 12%



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

Chain p: 20% 95%



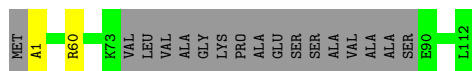
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 94% 6%

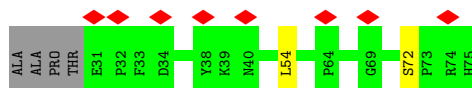


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r: 83% 15%



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45544	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 ($e^-/\text{\AA}^2$)	39.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, 2MR, SF4, EHZ, AME, 3PE, AYA, NDP, FME, CDL, MG, SAC, PC1, FMN, K, ZN, MYR, DGT, CHD

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	0.31	0/854	0.41	0/1170
2	B	0.48	0/1292	0.54	0/1747
3	C	0.43	0/1794	0.52	0/2443
4	D	0.43	0/3170	0.51	0/4285
5	E	0.31	0/1699	0.46	0/2312
6	F	0.30	0/3398	0.50	0/4591
7	G	0.35	0/5372	0.50	0/7281
8	H	0.37	0/2571	0.44	0/3513
9	I	0.49	0/1445	0.53	0/1956
10	J	0.35	0/1239	0.43	0/1677
11	K	0.30	0/646	0.42	0/872
12	L	0.26	0/4443	0.41	0/6047
13	M	0.26	0/3738	0.42	0/5097
14	N	0.29	0/2792	0.42	0/3800
15	O	0.27	0/2651	0.43	0/3587
16	P	0.32	0/2626	0.49	0/3557
17	Q	0.37	0/1039	0.51	0/1404
18	R	0.35	0/753	0.51	0/1014
19	S	0.27	0/712	0.53	0/957
20	T	0.27	0/692	0.40	0/932
20	U	0.25	0/719	0.40	0/971
21	V	0.30	0/939	0.41	0/1272
22	W	0.33	0/1001	0.51	0/1345
23	X	0.29	0/1439	0.48	0/1942
24	Y	0.25	0/252	0.39	0/340
25	Z	0.31	0/1186	0.51	0/1599
26	a	0.34	0/584	0.50	0/786
27	b	0.30	0/667	0.45	0/916
28	c	0.27	0/418	0.41	0/567
29	d	0.30	0/1018	0.48	0/1375
30	e	0.29	0/850	0.50	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.27	0/505	0.47	0/681
32	g	0.27	0/772	0.45	0/1046
33	h	0.27	0/1221	0.47	0/1651
34	i	0.25	0/1127	0.47	0/1534
35	j	0.26	0/619	0.44	0/848
36	k	0.25	0/672	0.43	0/906
37	l	0.26	0/1369	0.43	0/1873
38	m	0.26	0/1088	0.53	0/1472
39	n	0.25	0/1540	0.47	0/2085
40	o	0.25	0/1060	0.52	0/1420
41	p	0.26	0/1489	0.49	0/2008
42	q	0.39	0/1242	0.51	0/1688
43	r	0.35	0/798	0.50	0/1079
44	s	0.26	0/392	0.45	0/531
All	All	0.32	0/65893	0.47	0/89313

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	100/115 (87%)	87 (87%)	12 (12%)	1 (1%)	15	55
2	B	156/216 (72%)	147 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	208/266 (78%)	185 (89%)	23 (11%)	0	100	100
4	D	385/463 (83%)	359 (93%)	26 (7%)	0	100	100
5	E	212/249 (85%)	195 (92%)	17 (8%)	0	100	100
6	F	430/464 (93%)	403 (94%)	27 (6%)	0	100	100
7	G	687/727 (94%)	632 (92%)	55 (8%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	174/212 (82%)	160 (92%)	14 (8%)	0	100	100
10	J	156/175 (89%)	132 (85%)	24 (15%)	0	100	100
11	K	84/98 (86%)	79 (94%)	4 (5%)	1 (1%)	13	51
12	L	545/606 (90%)	518 (95%)	27 (5%)	0	100	100
13	M	457/459 (100%)	432 (94%)	25 (6%)	0	100	100
14	N	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
15	O	318/343 (93%)	305 (96%)	13 (4%)	0	100	100
16	P	314/380 (83%)	288 (92%)	26 (8%)	0	100	100
17	Q	123/175 (70%)	113 (92%)	10 (8%)	0	100	100
18	R	94/124 (76%)	82 (87%)	12 (13%)	0	100	100
19	S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	T	82/156 (53%)	80 (98%)	2 (2%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	111/116 (96%)	105 (95%)	6 (5%)	0	100	100
22	W	113/128 (88%)	104 (92%)	9 (8%)	0	100	100
23	X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
24	Y	29/141 (21%)	27 (93%)	2 (7%)	0	100	100
25	Z	140/144 (97%)	133 (95%)	7 (5%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
30	e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
32	g	88/154 (57%)	79 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	141/189 (75%)	131 (93%)	10 (7%)	0	100	100
34	i	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
35	j	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
36	k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	138 (90%)	16 (10%)	0	100	100
38	m	126/129 (98%)	118 (94%)	8 (6%)	0	100	100
39	n	169/179 (94%)	160 (95%)	9 (5%)	0	100	100
40	o	118/137 (86%)	109 (92%)	9 (8%)	0	100	100
41	p	171/176 (97%)	162 (95%)	9 (5%)	0	100	100
42	q	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
43	r	92/113 (81%)	79 (86%)	13 (14%)	0	100	100
44	s	43/109 (39%)	42 (98%)	1 (2%)	0	100	100
All	All	7901/9213 (86%)	7377 (93%)	522 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	2	SER
1	A	29	VAL

5.3.2 Protein sidechains [i](#)

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	92/100 (92%)	90 (98%)	2 (2%)	52	77
2	B	134/175 (77%)	132 (98%)	2 (2%)	65	84
3	C	190/228 (83%)	185 (97%)	5 (3%)	46	74
4	D	334/392 (85%)	326 (98%)	8 (2%)	49	75
5	E	183/205 (89%)	178 (97%)	5 (3%)	44	73
6	F	345/368 (94%)	336 (97%)	9 (3%)	46	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	578/608 (95%)	564 (98%)	14 (2%)	49	75
8	H	274/274 (100%)	266 (97%)	8 (3%)	42	72
9	I	151/175 (86%)	150 (99%)	1 (1%)	84	93
10	J	127/141 (90%)	125 (98%)	2 (2%)	62	83
11	K	73/85 (86%)	68 (93%)	5 (7%)	16	50
12	L	479/533 (90%)	472 (98%)	7 (2%)	65	84
13	M	412/412 (100%)	403 (98%)	9 (2%)	52	77
14	N	315/315 (100%)	312 (99%)	3 (1%)	76	88
15	O	283/303 (93%)	277 (98%)	6 (2%)	53	78
16	P	276/327 (84%)	267 (97%)	9 (3%)	38	69
17	Q	112/153 (73%)	107 (96%)	5 (4%)	27	62
18	R	79/97 (81%)	78 (99%)	1 (1%)	69	86
19	S	77/82 (94%)	76 (99%)	1 (1%)	69	86
20	T	78/135 (58%)	75 (96%)	3 (4%)	33	66
20	U	81/135 (60%)	77 (95%)	4 (5%)	25	59
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	104 (96%)	4 (4%)	34	66
23	X	154/155 (99%)	149 (97%)	5 (3%)	39	70
24	Y	25/102 (24%)	25 (100%)	0	100	100
25	Z	120/121 (99%)	118 (98%)	2 (2%)	60	82
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	70 (99%)	1 (1%)	67	85
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	105/105 (100%)	104 (99%)	1 (1%)	76	88
30	e	89/96 (93%)	87 (98%)	2 (2%)	52	77
31	f	54/54 (100%)	52 (96%)	2 (4%)	34	66
32	g	81/131 (62%)	79 (98%)	2 (2%)	47	75
33	h	124/158 (78%)	122 (98%)	2 (2%)	62	83
34	i	120/121 (99%)	114 (95%)	6 (5%)	24	59
35	j	61/84 (73%)	60 (98%)	1 (2%)	62	83
36	k	63/76 (83%)	62 (98%)	1 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	l	140/159 (88%)	140 (100%)	0	100	100
38	m	113/114 (99%)	108 (96%)	5 (4%)	28	63
39	n	156/161 (97%)	154 (99%)	2 (1%)	69	86
40	o	109/120 (91%)	104 (95%)	5 (5%)	27	61
41	p	156/157 (99%)	151 (97%)	5 (3%)	39	70
42	q	130/130 (100%)	123 (95%)	7 (5%)	22	57
43	r	86/97 (89%)	85 (99%)	1 (1%)	71	87
44	s	44/92 (48%)	42 (96%)	2 (4%)	27	62
All	All	6986/7891 (88%)	6821 (98%)	165 (2%)	51	75

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	X	120	ASP
39	n	8	TYR
25	Z	51	LYS
34	i	25	GLN
41	p	5	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
12	L	56	HIS
36	k	47	ASN
37	l	87	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

14 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	1.51	1 (12%)	7,9,11	1.64	2 (28%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	7,9,11	1.75	2 (28%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	7,9,11	1.76	3 (42%)
27	AYA	b	1	27	6,7,8	1.84	1 (16%)	5,8,10	1.38	1 (20%)
4	2MR	D	85	4	10,12,13	2.31	2 (20%)	5,13,15	1.64	2 (40%)
42	AME	q	1	42	9,10,11	1.45	1 (11%)	9,11,13	1.71	3 (33%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.75	3 (42%)
11	FME	K	1	11	8,9,10	1.53	1 (12%)	7,9,11	1.60	2 (28%)
38	SAC	m	1	38	7,8,9	1.71	1 (14%)	8,9,11	1.67	1 (12%)
29	AME	d	1	29	9,10,11	1.44	1 (11%)	9,11,13	1.38	1 (11%)
34	SAC	i	1	34	7,8,9	1.64	1 (14%)	8,9,11	1.31	1 (12%)
43	AYA	r	1	43	6,7,8	1.77	1 (16%)	5,8,10	1.36	1 (20%)
10	FME	J	1	10	8,9,10	1.52	1 (12%)	7,9,11	1.72	2 (28%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	7,9,11	1.75	2 (28%)

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	-	4/7/9/11	-
12	FME	L	1	12	-	3/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
27	AYA	b	1	27	-	0/4/6/8	-
4	2MR	D	85	4	-	0/10/13/15	-
42	AME	q	1	42	-	1/9/10/12	-
1	FME	A	1	1	-	3/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
38	SAC	m	1	38	-	3/7/8/10	-
29	AME	d	1	29	-	1/9/10/12	-
34	SAC	i	1	34	-	2/7/8/10	-
43	AYA	r	1	43	-	0/4/6/8	-
10	FME	J	1	10	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	M	1	13	-	3/7/9/11	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.96	1.44	1.33
4	D	85	2MR	CZ-NE	4.84	1.44	1.34
11	K	1	FME	CN-N	3.82	1.46	1.33
10	J	1	FME	CN-N	3.68	1.45	1.33
14	N	1	FME	CN-N	3.68	1.45	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	1	SAC	C2A-C1A-N	3.61	122.21	116.10
8	H	1	FME	CE-SD-CG	2.99	110.68	100.40
10	J	1	FME	CE-SD-CG	2.83	110.11	100.40
13	M	1	FME	CE-SD-CG	2.82	110.08	100.40
14	N	1	FME	CE-SD-CG	2.78	109.96	100.40

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 37 ligands modelled in this entry, 3 are monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	EHZ	T	101	20	29,36,37	1.75	5 (17%)	35,44,47	1.79	8 (22%)
45	3PE	d	201	-	48,48,50	0.87	4 (8%)	51,53,55	1.09	2 (3%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-
51	CDL	d	203	-	64,64,99	1.06	6 (9%)	70,76,111	1.13	5 (7%)
45	3PE	Z	201	-	48,48,50	0.86	4 (8%)	51,53,55	1.06	2 (3%)
45	3PE	A	201	-	42,42,50	0.91	3 (7%)	45,47,55	1.14	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
49	FMN	F	501	-	33,33,33	2.71	10 (30%)	48,50,50	1.70	12 (25%)
56	EHZ	U	101	20	29,36,37	1.72	5 (17%)	35,44,47	1.66	7 (20%)
54	NDP	P	501	-	45,52,52	4.23	23 (51%)	53,80,80	2.12	5 (9%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
45	3PE	h	201	-	31,31,50	1.08	4 (12%)	34,36,55	1.20	2 (5%)
46	PC1	A	202	-	49,49,53	0.99	3 (6%)	55,57,61	0.99	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
47	SF4	F	502	6	0,12,12	-	-	-	-	-
46	PC1	B	201	-	50,50,53	0.99	4 (8%)	56,58,61	1.01	2 (3%)
46	PC1	q	701	-	36,36,53	1.11	4 (11%)	42,44,61	1.02	2 (4%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
51	CDL	N	401	-	72,72,99	1.01	8 (11%)	78,84,111	1.08	4 (5%)
45	3PE	J	201	-	38,38,50	0.99	4 (10%)	41,43,55	1.10	2 (4%)
58	MYR	o	201	40	14,14,15	0.46	0	13,13,15	0.87	0
57	CHD	i	201	-	32,32,32	3.22	10 (31%)	51,51,51	2.14	19 (37%)
45	3PE	M	502	-	38,38,50	0.97	4 (10%)	41,43,55	1.13	2 (4%)
47	SF4	B	202	2	0,12,12	-	-	-	-	-
47	SF4	I	203	9	0,12,12	-	-	-	-	-
45	3PE	O	401	-	34,34,50	1.02	4 (11%)	37,39,55	1.13	2 (5%)
52	DGT	O	402	53	26,33,33	2.65	8 (30%)	32,52,52	1.69	10 (31%)
45	3PE	I	201	-	50,50,50	0.85	2 (4%)	53,55,55	1.14	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	CDL	X	201	-	78,78,99	0.98	7 (8%)	84,90,111	1.13	6 (7%)
46	PC1	d	202	-	32,32,53	1.19	3 (9%)	38,40,61	1.09	2 (5%)
45	3PE	M	501	-	37,37,50	0.98	4 (10%)	40,42,55	1.22	2 (5%)
51	CDL	q	702	-	59,59,99	1.10	6 (10%)	65,71,111	1.14	4 (6%)
46	PC1	H	401	-	42,42,53	1.06	4 (9%)	48,50,61	1.09	2 (4%)
45	3PE	I	204	-	32,32,50	1.05	4 (12%)	35,37,55	1.12	2 (5%)

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
56	EHZ	T	101	20	-	16/42/44/45	-
45	3PE	d	201	-	-	18/52/52/54	-
47	SF4	I	202	9	-	-	0/6/5/5
51	CDL	d	203	-	-	24/75/75/110	-
45	3PE	Z	201	-	-	22/52/52/54	-
45	3PE	A	201	-	-	18/46/46/54	-
47	SF4	G	801	7	-	-	0/6/5/5
49	FMN	F	501	-	-	9/18/18/18	0/3/3/3
56	EHZ	U	101	20	-	23/42/44/45	-
54	NDP	P	501	-	-	8/30/77/77	0/5/5/5
48	FES	E	301	5	-	-	0/1/1/1
45	3PE	h	201	-	-	19/35/35/54	-
46	PC1	A	202	-	-	20/53/53/57	-
48	FES	G	803	7	-	-	0/1/1/1
47	SF4	F	502	6	-	-	0/6/5/5
46	PC1	B	201	-	-	20/54/54/57	-
46	PC1	q	701	-	-	20/40/40/57	-
51	CDL	N	401	-	-	39/83/83/110	-
47	SF4	G	802	7	-	-	0/6/5/5
45	3PE	J	201	-	-	20/42/42/54	-
58	MYR	o	201	40	-	6/11/12/13	-
57	CHD	i	201	-	-	3/9/74/74	0/4/4/4
45	3PE	M	502	-	-	21/42/42/54	-
47	SF4	B	202	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	I	203	9	-	-	0/6/5/5
45	3PE	O	401	-	-	13/38/38/54	-
52	DGT	O	402	53	-	6/18/34/34	0/3/3/3
45	3PE	I	201	-	-	19/54/54/54	-
51	CDL	X	201	-	-	36/89/89/110	-
46	PC1	d	202	-	-	20/36/36/57	-
45	3PE	M	501	-	-	20/41/41/54	-
51	CDL	q	702	-	-	36/70/70/110	-
46	PC1	H	401	-	-	13/46/46/57	-
45	3PE	I	204	-	-	18/36/36/54	-

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	O4B-C1B	14.45	1.61	1.41
54	P	501	NDP	C6N-C5N	12.08	1.54	1.33
57	i	201	CHD	C11-C12	9.04	1.68	1.53
54	P	501	NDP	C7N-N7N	8.29	1.55	1.33
52	O	402	DGT	O6-C6	8.26	1.40	1.23

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	P	501	NDP	C5A-C6A-N6A	8.68	133.55	120.35
54	P	501	NDP	C1B-N9A-C4A	-7.64	113.22	126.64
57	i	201	CHD	C17-C13-C12	6.50	123.60	117.67
54	P	501	NDP	N6A-C6A-N1A	-6.22	105.66	118.57
56	U	101	EHZ	C8-C9-S1	5.76	120.76	113.63

There are no chirality outliers.

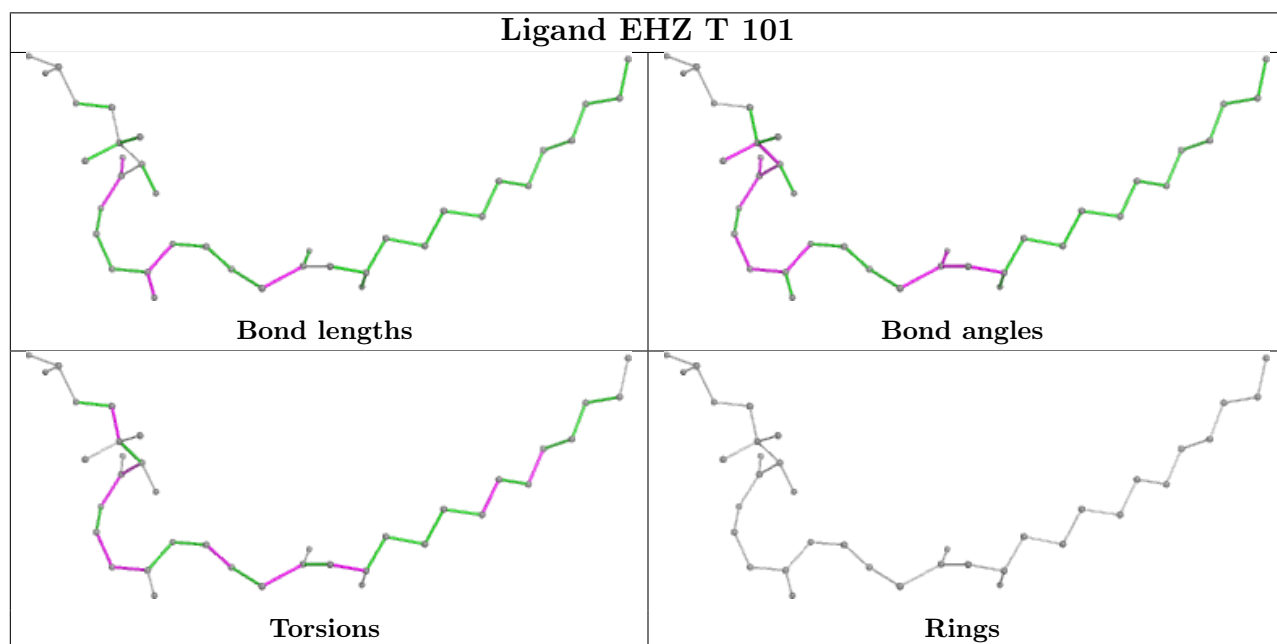
5 of 487 torsion outliers are listed below:

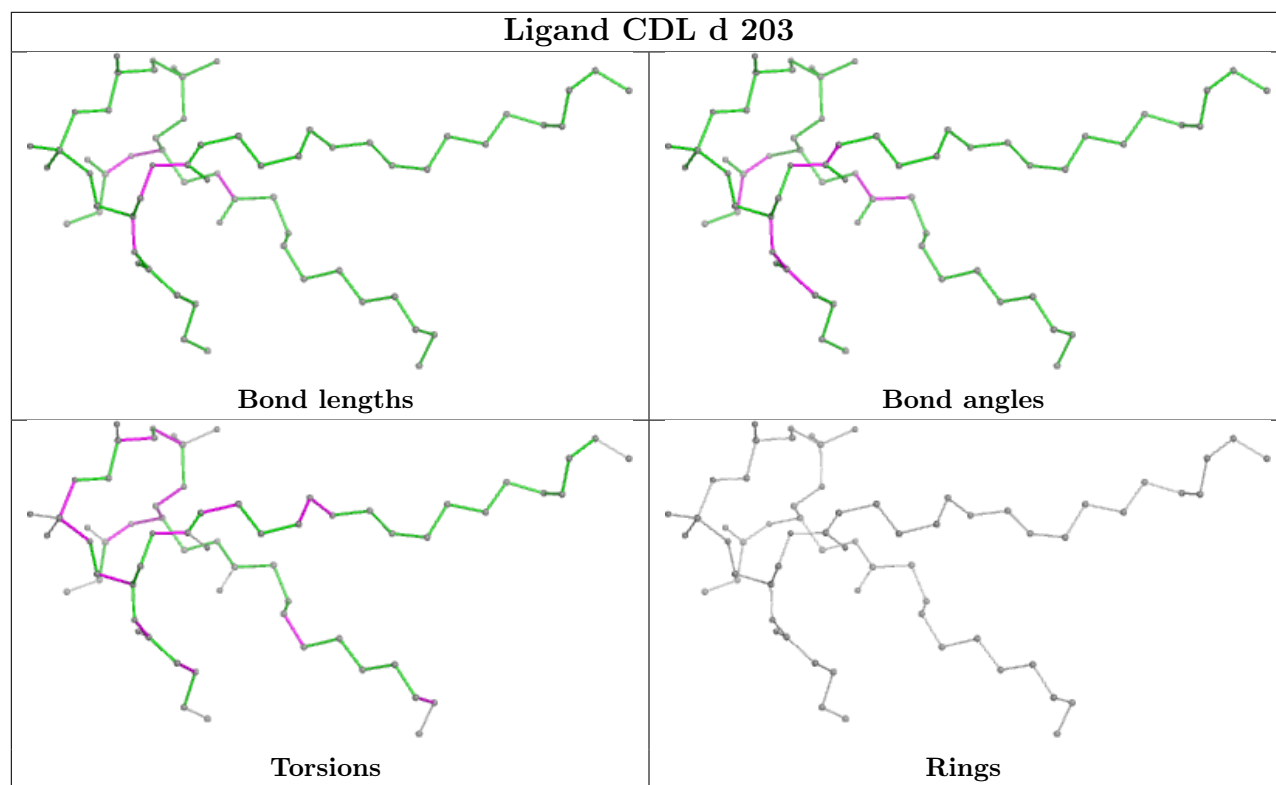
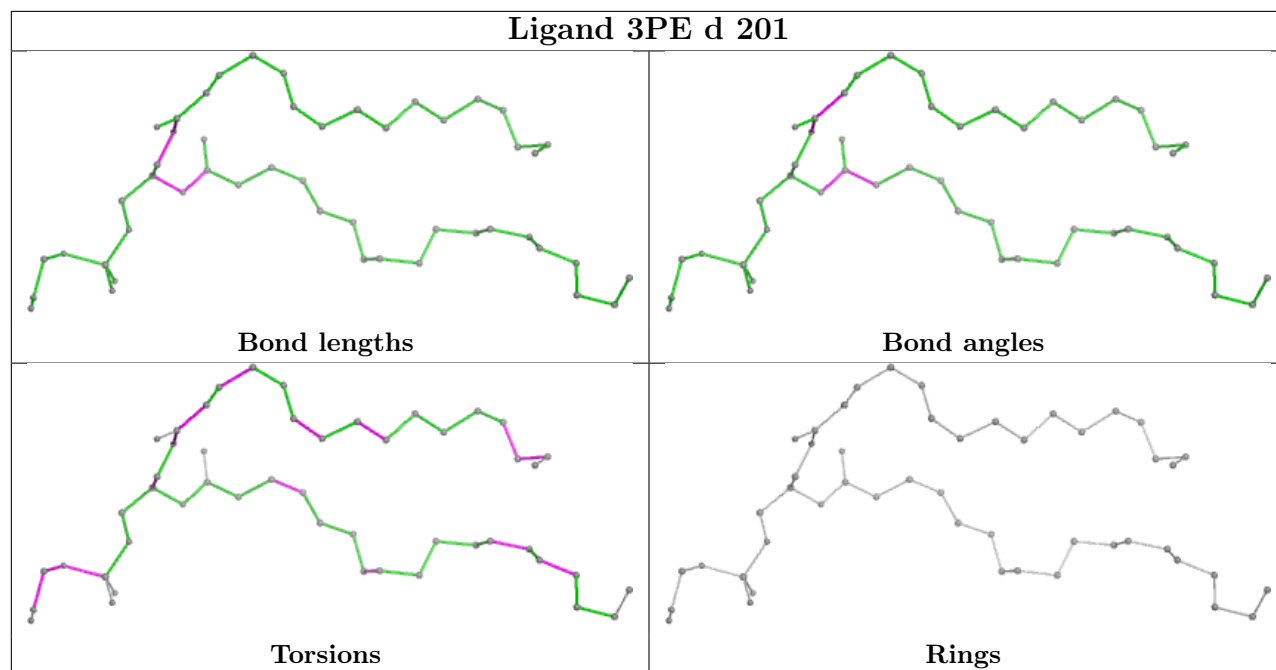
Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O14
45	A	201	3PE	C12-C11-O13-P
45	A	201	3PE	O21-C2-C3-O31
45	I	201	3PE	C1-O11-P-O13
45	I	201	3PE	C1-O11-P-O14

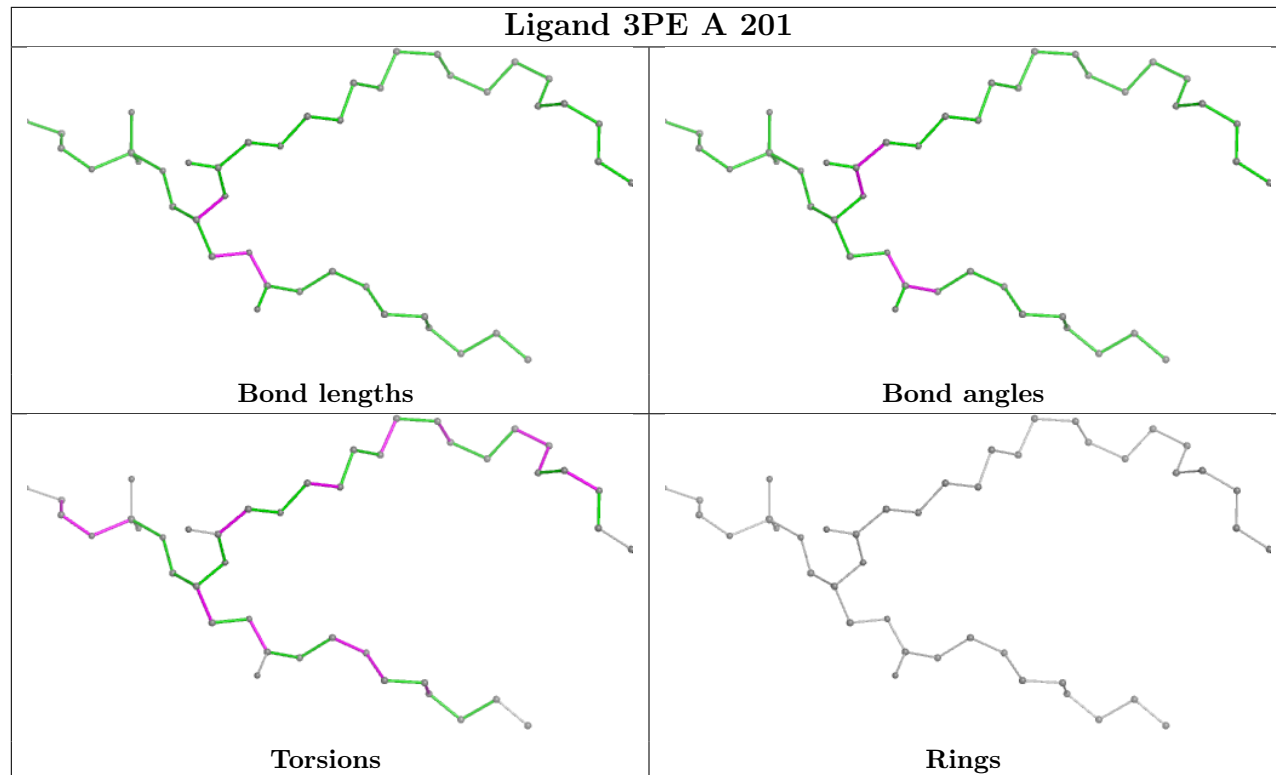
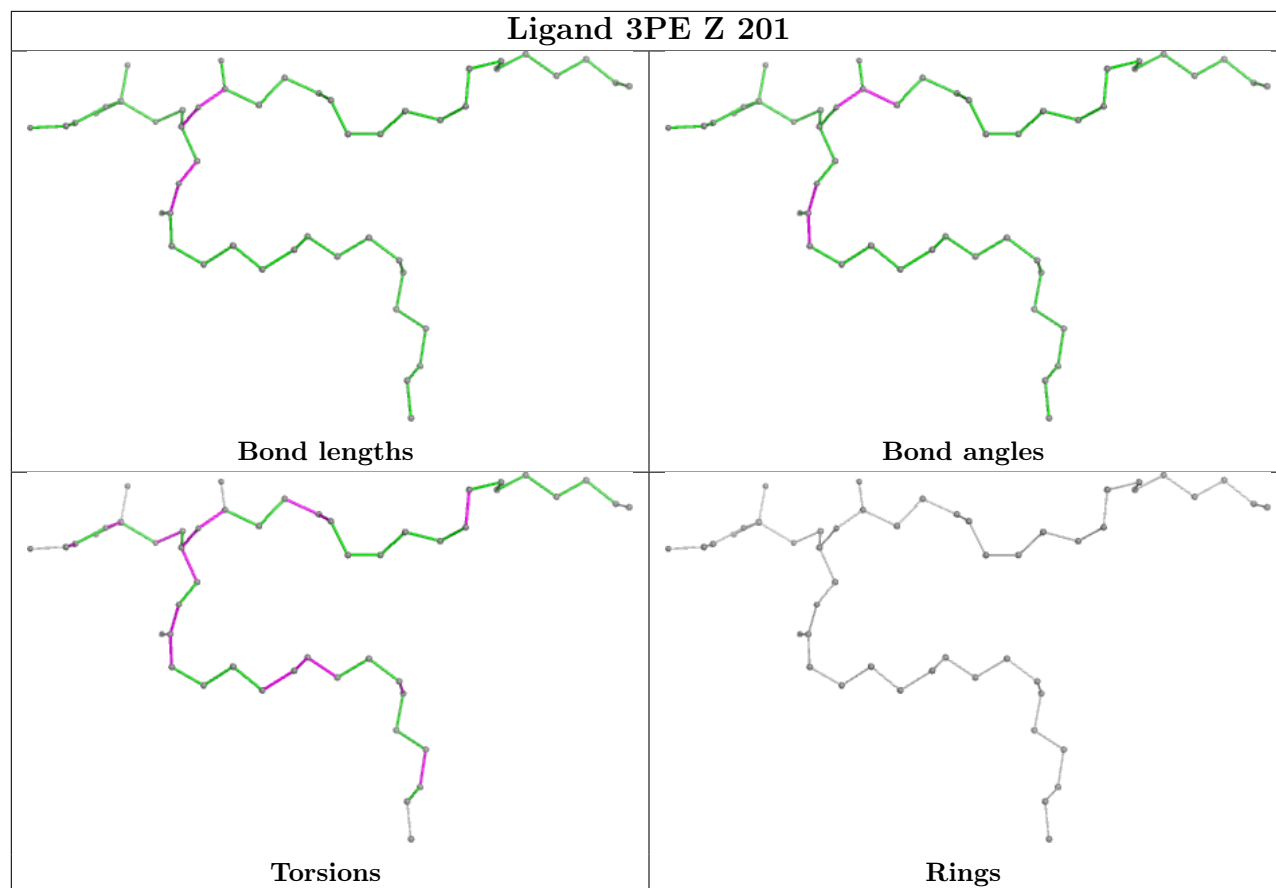
There are no ring outliers.

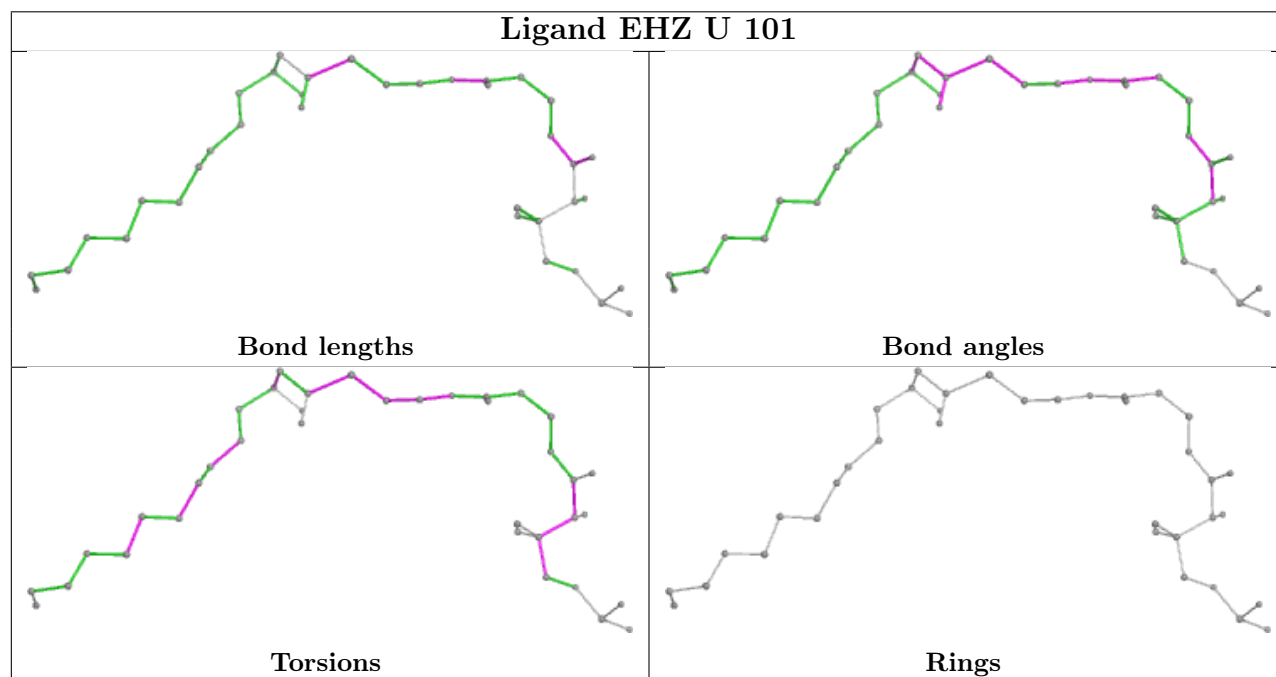
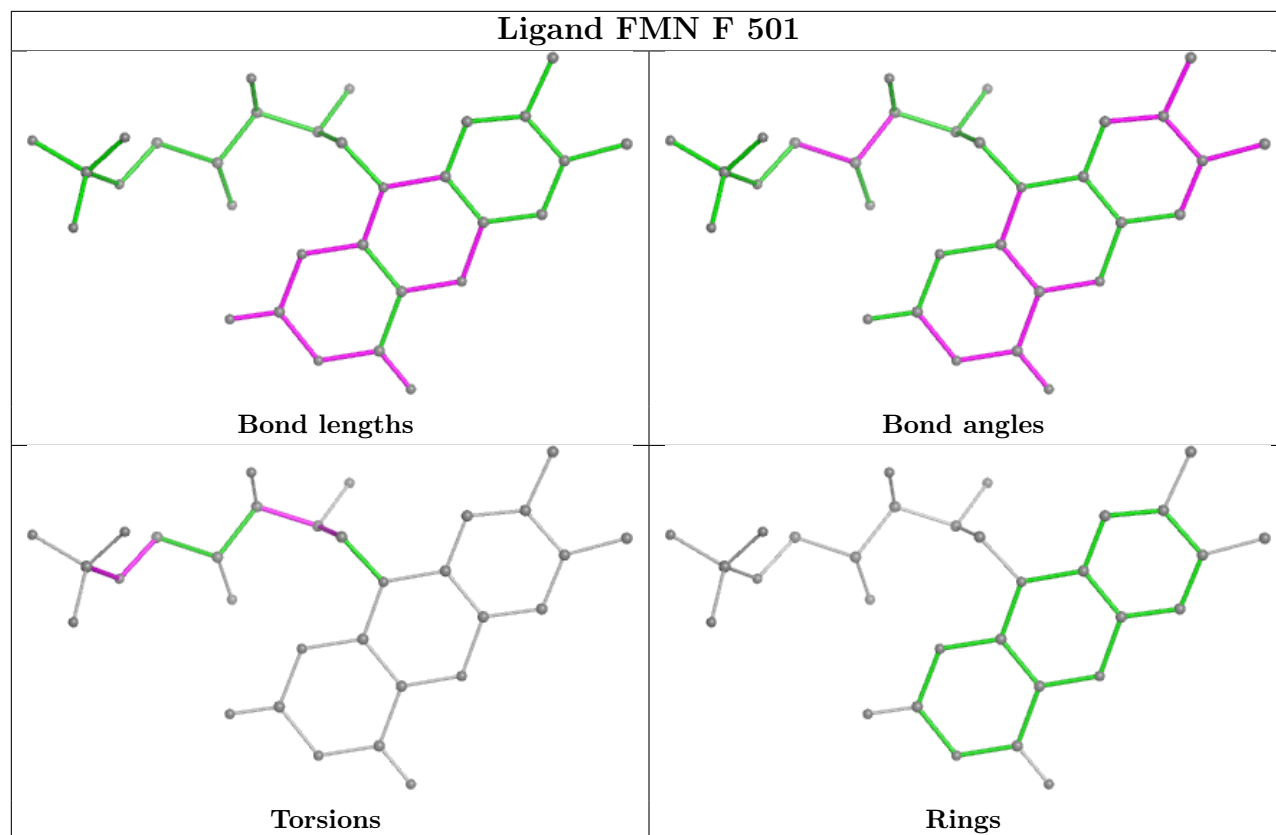
No monomer is involved in short contacts.

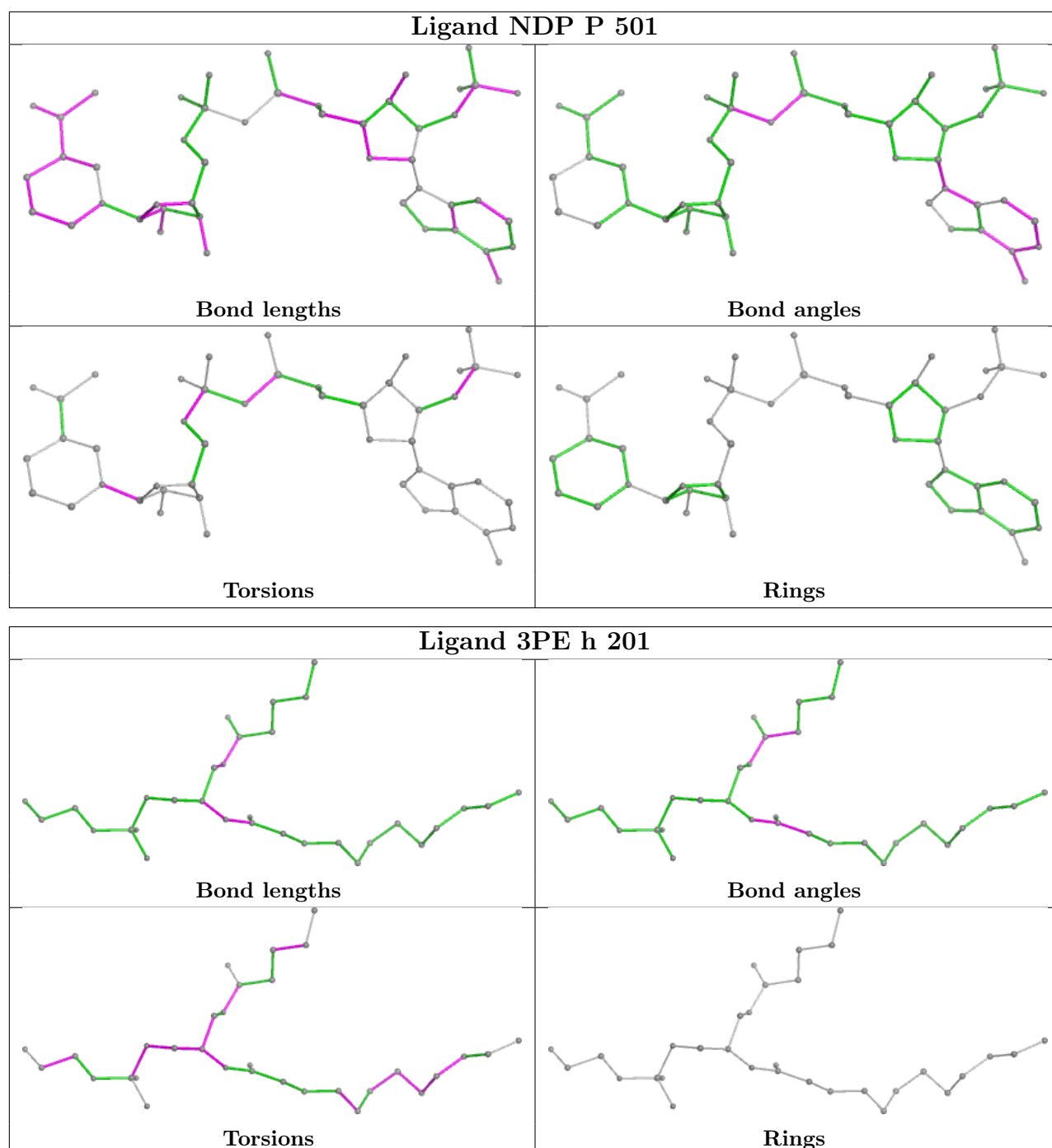
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

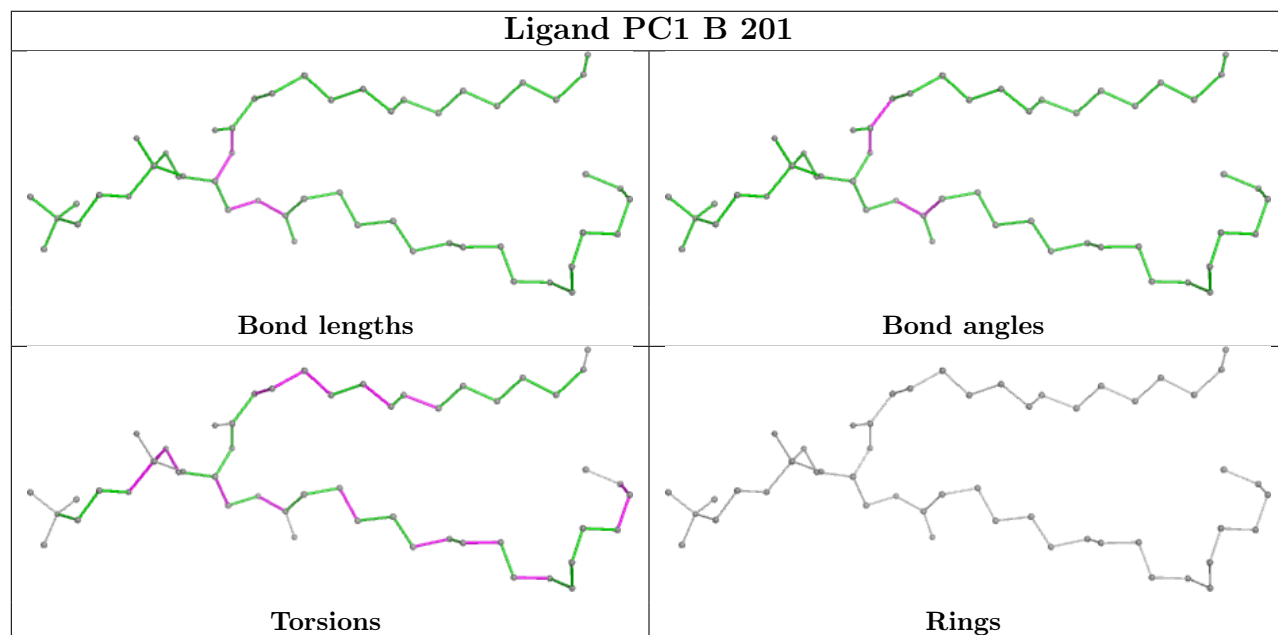
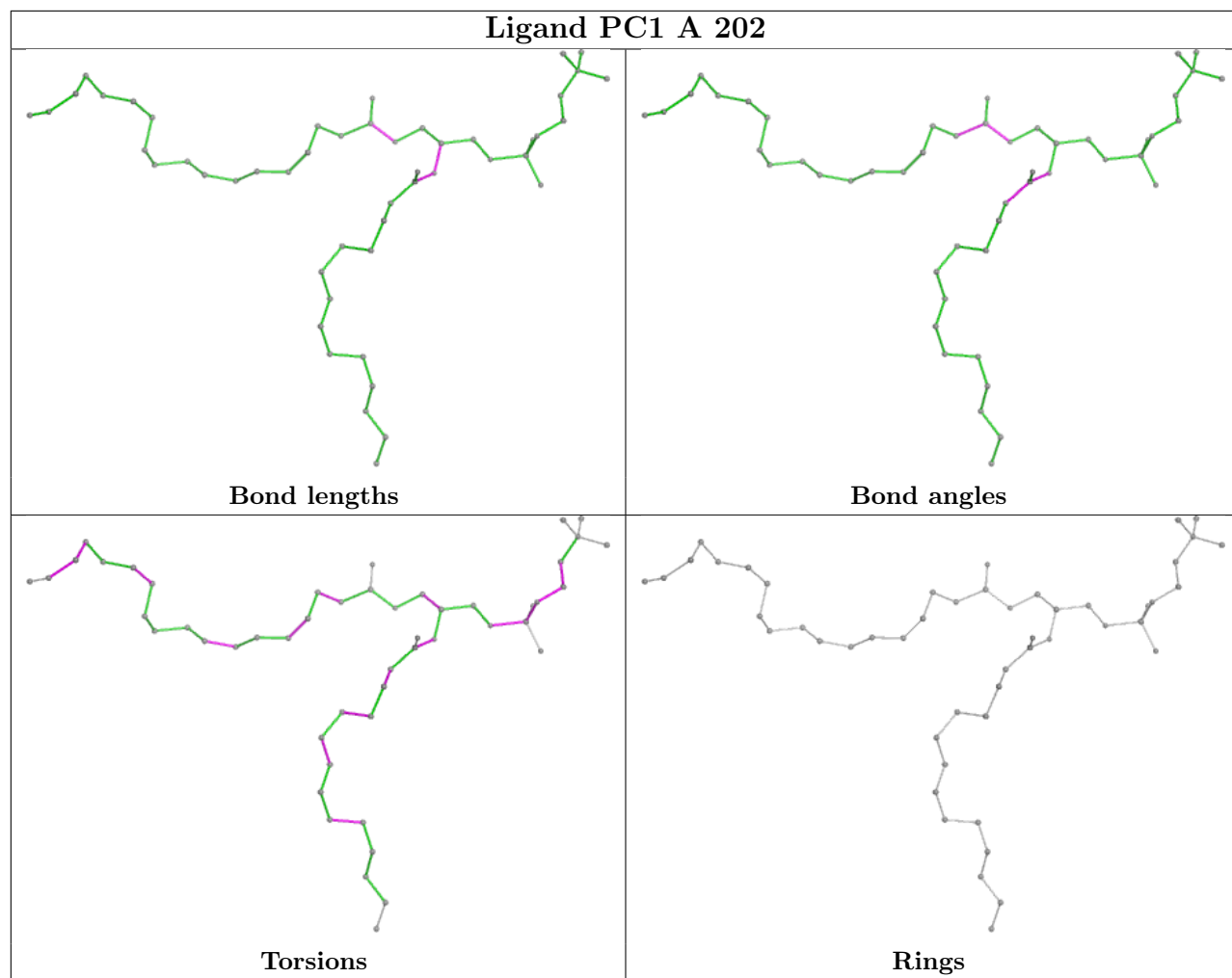


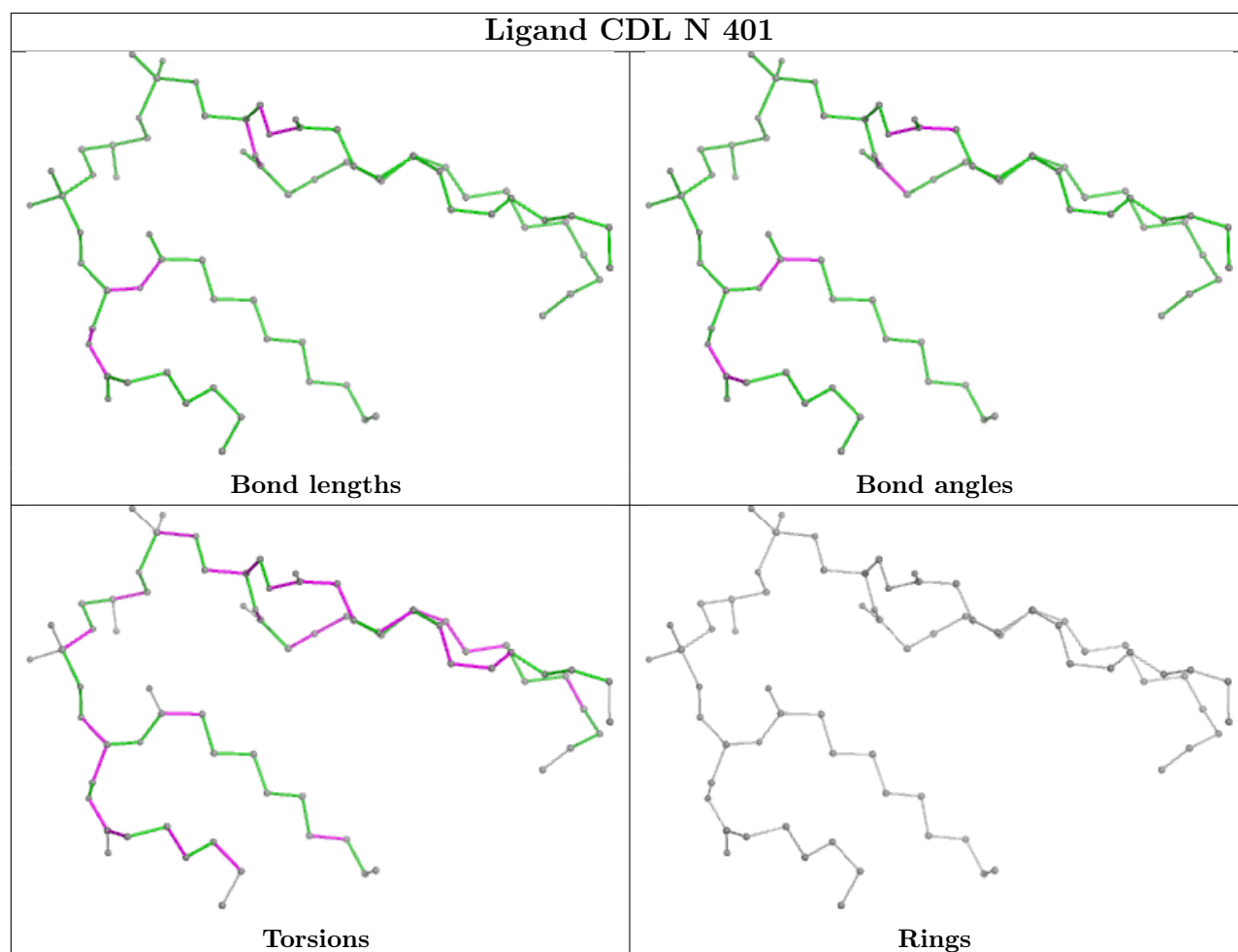
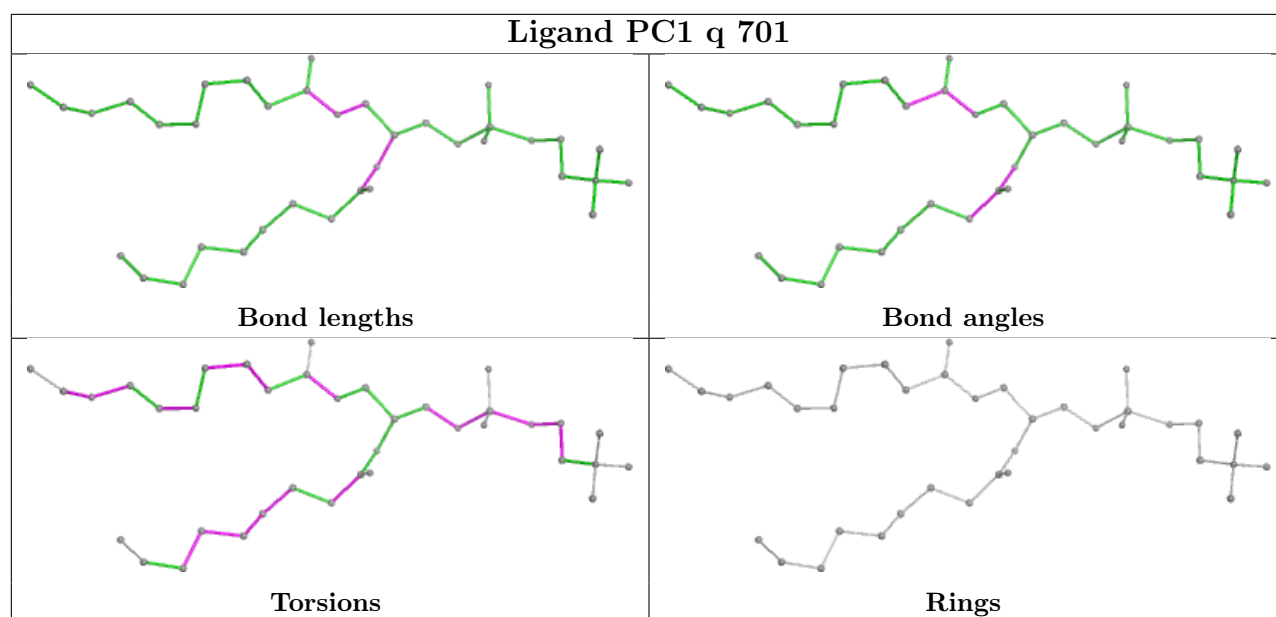


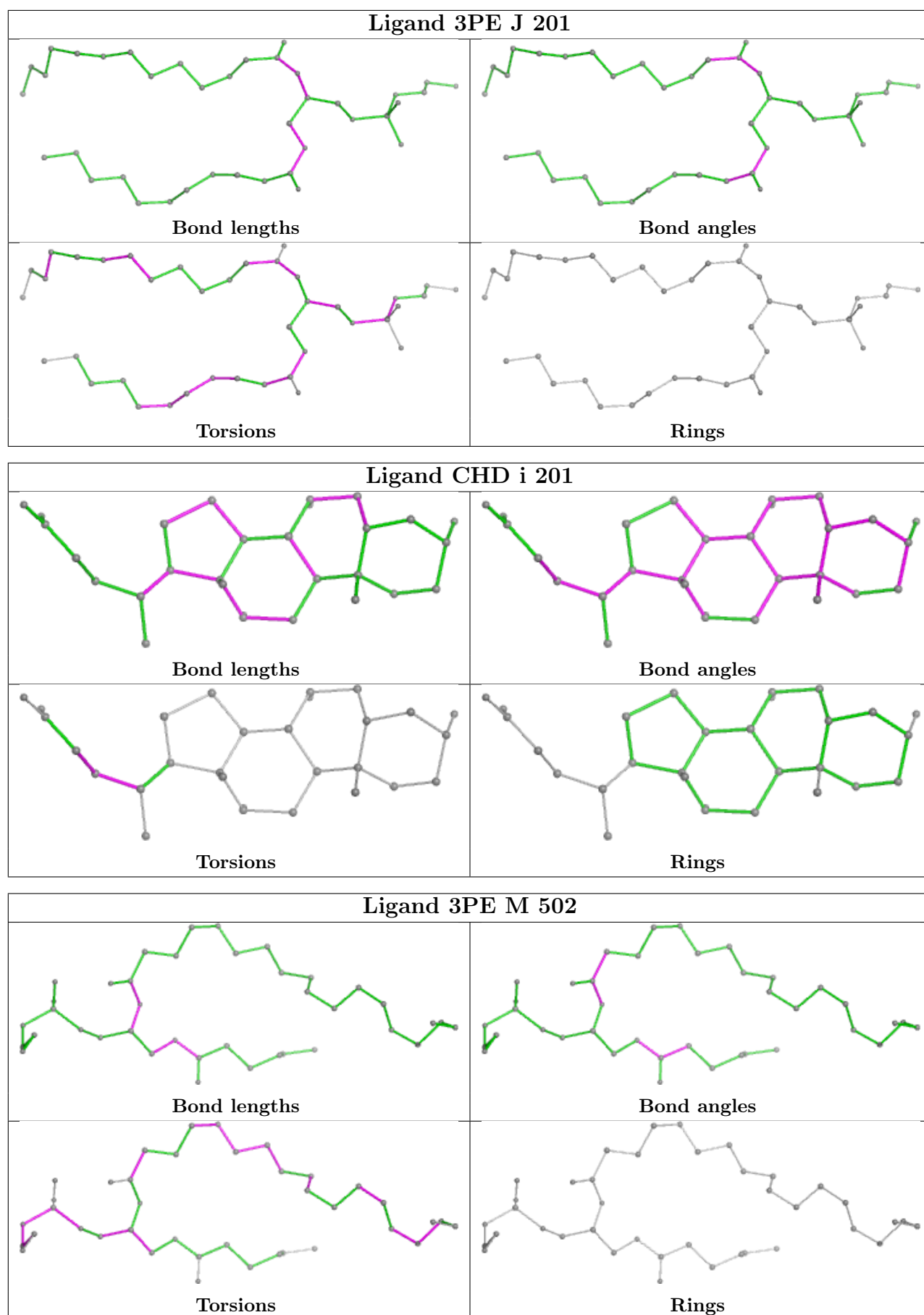


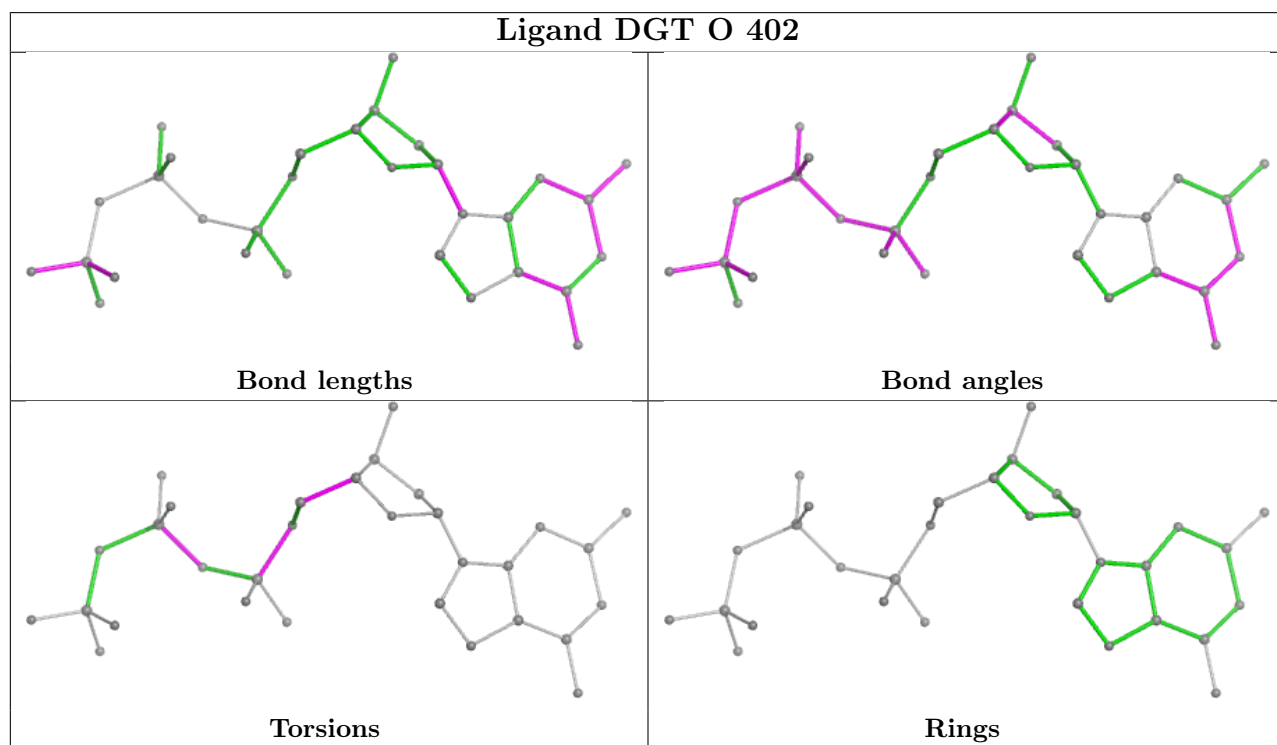
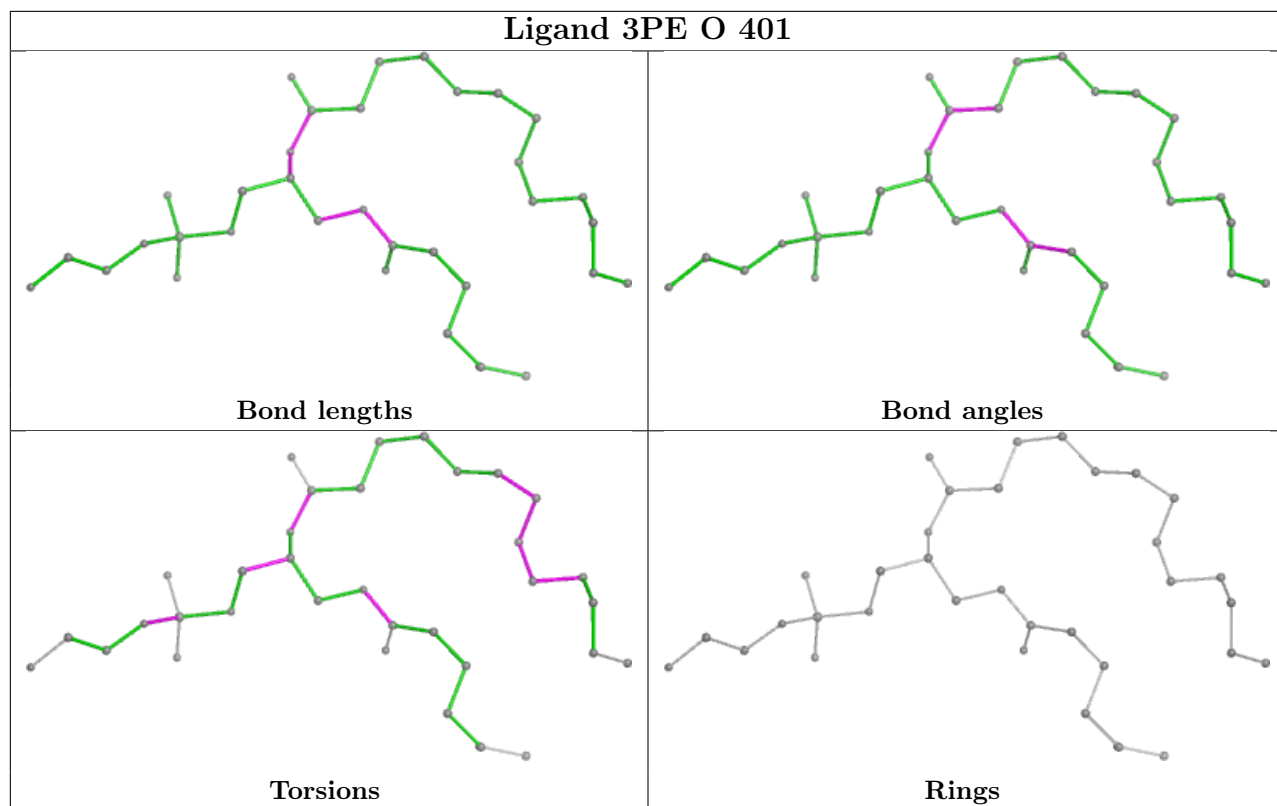


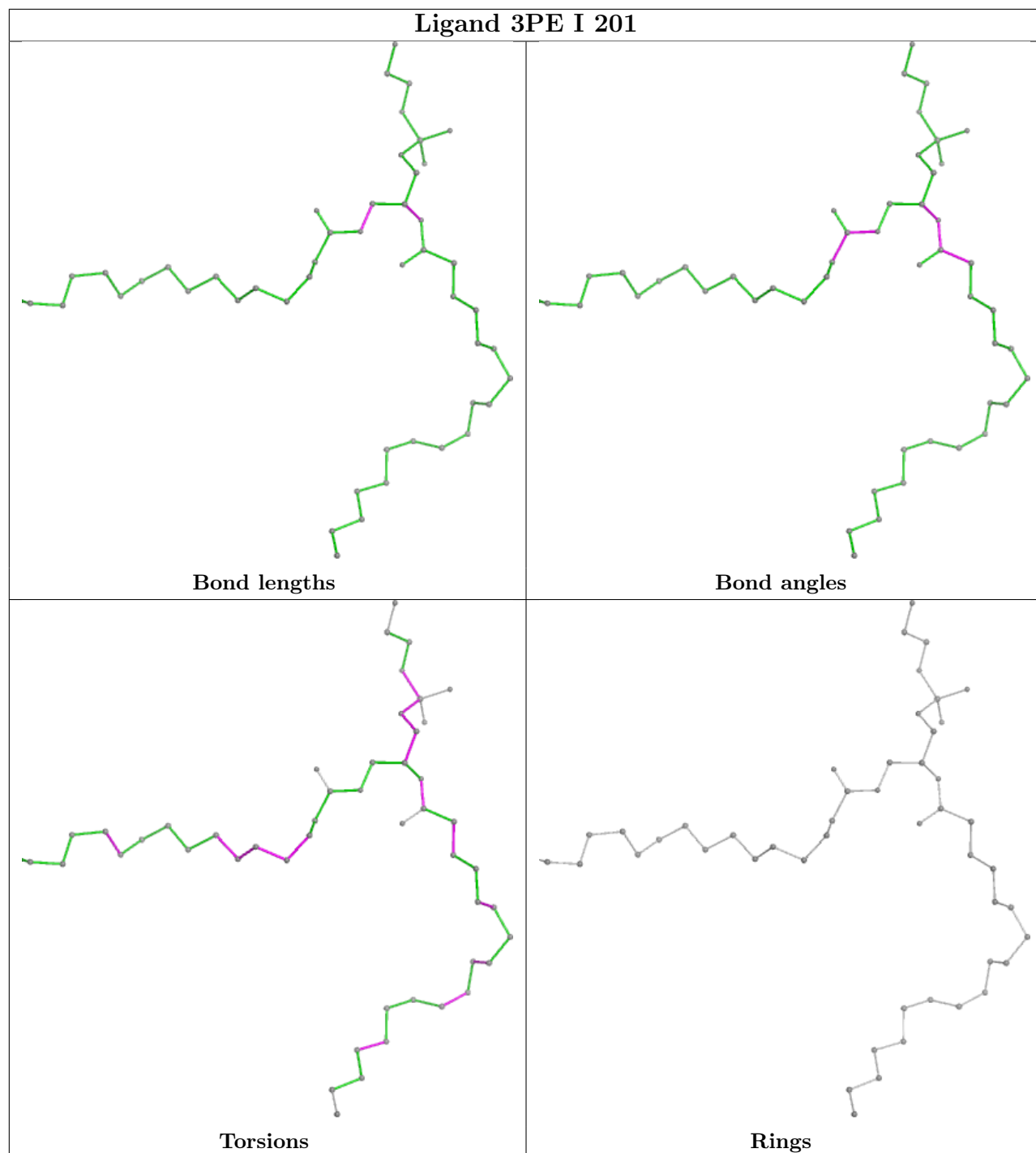


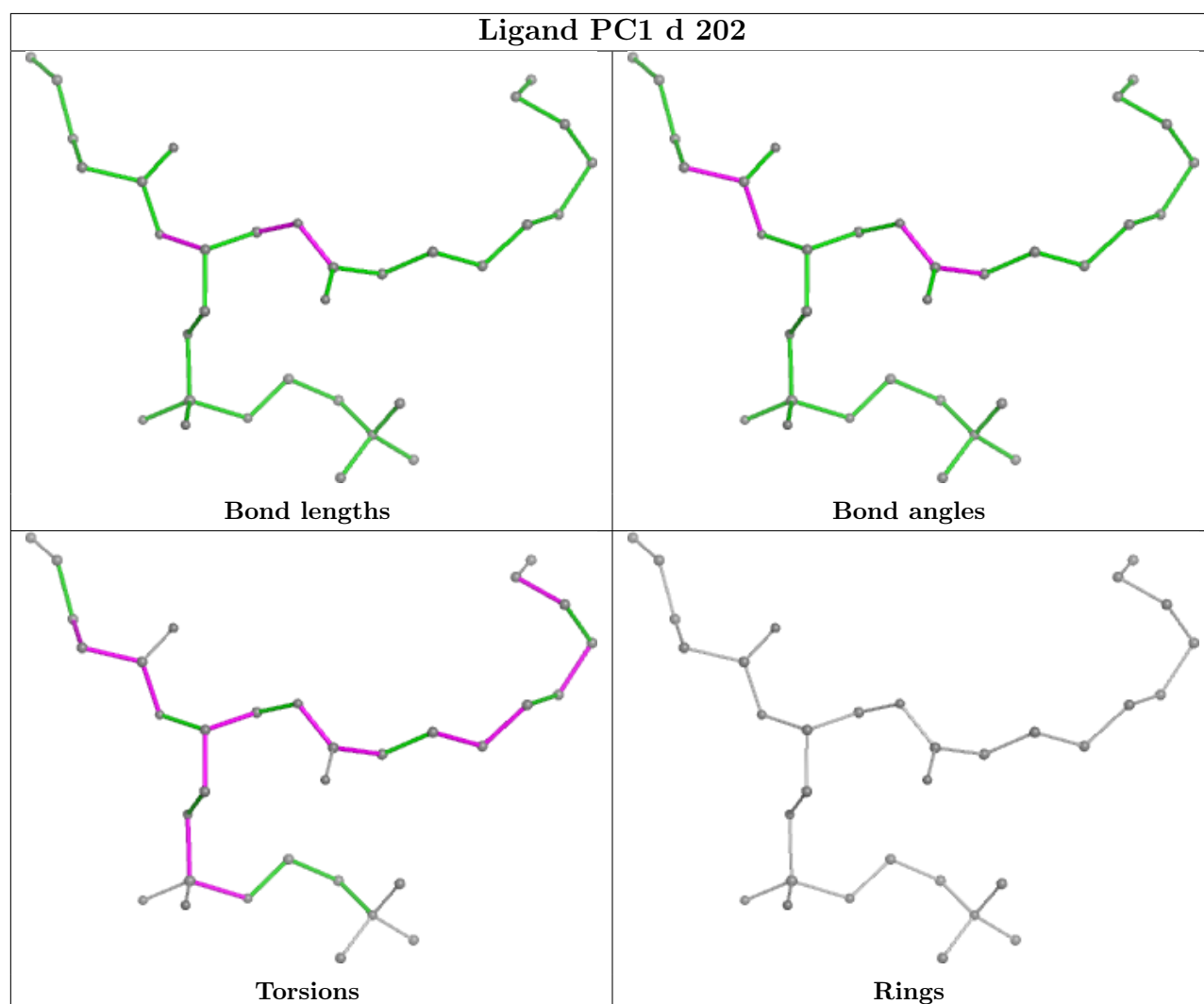
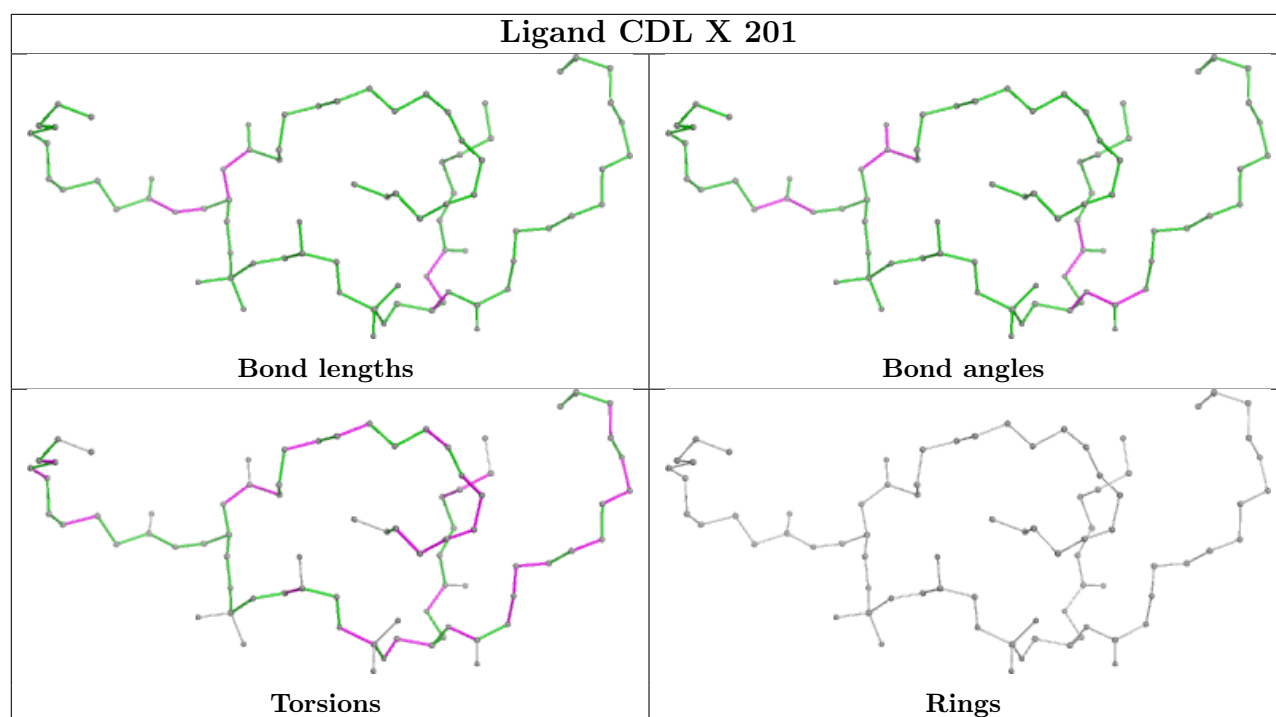


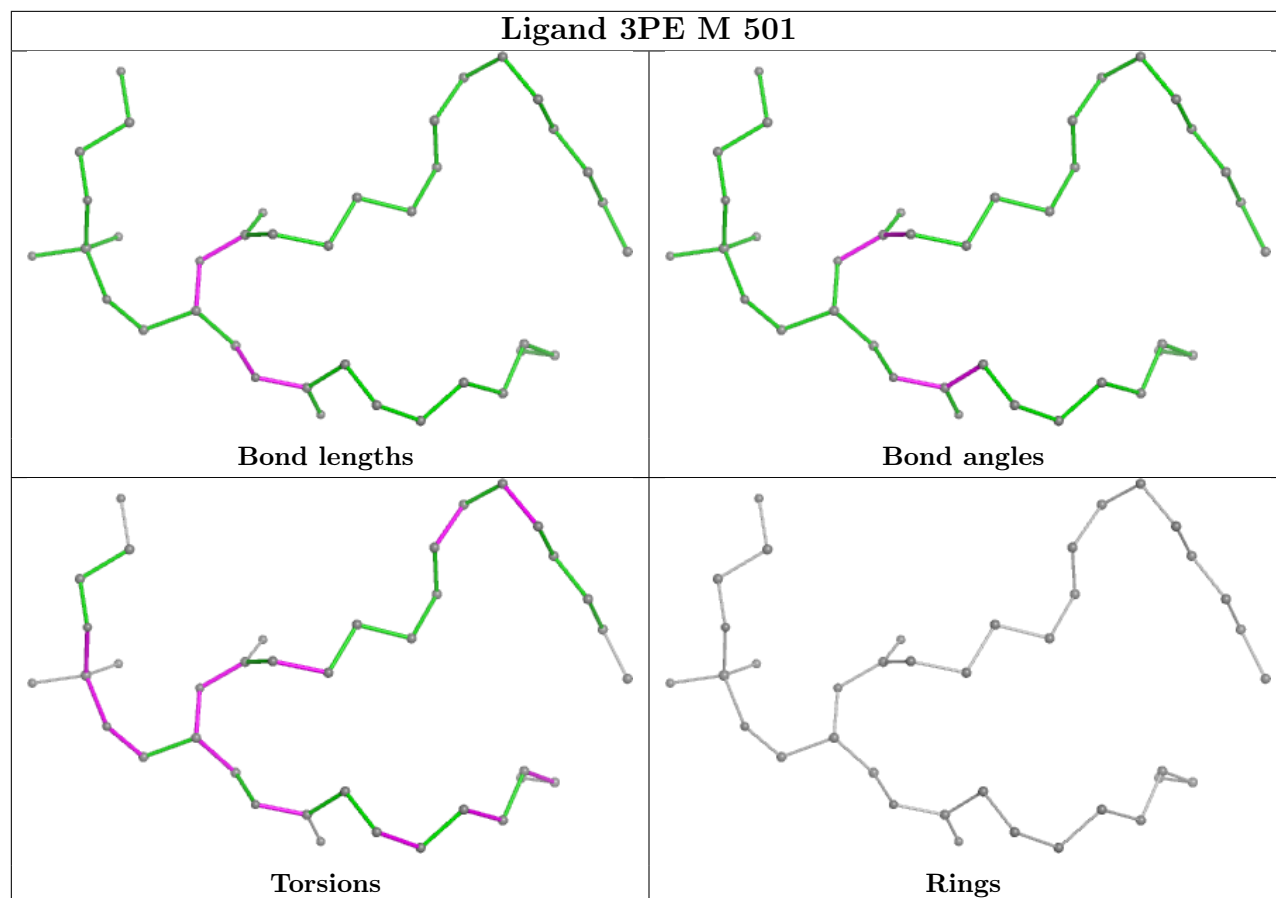


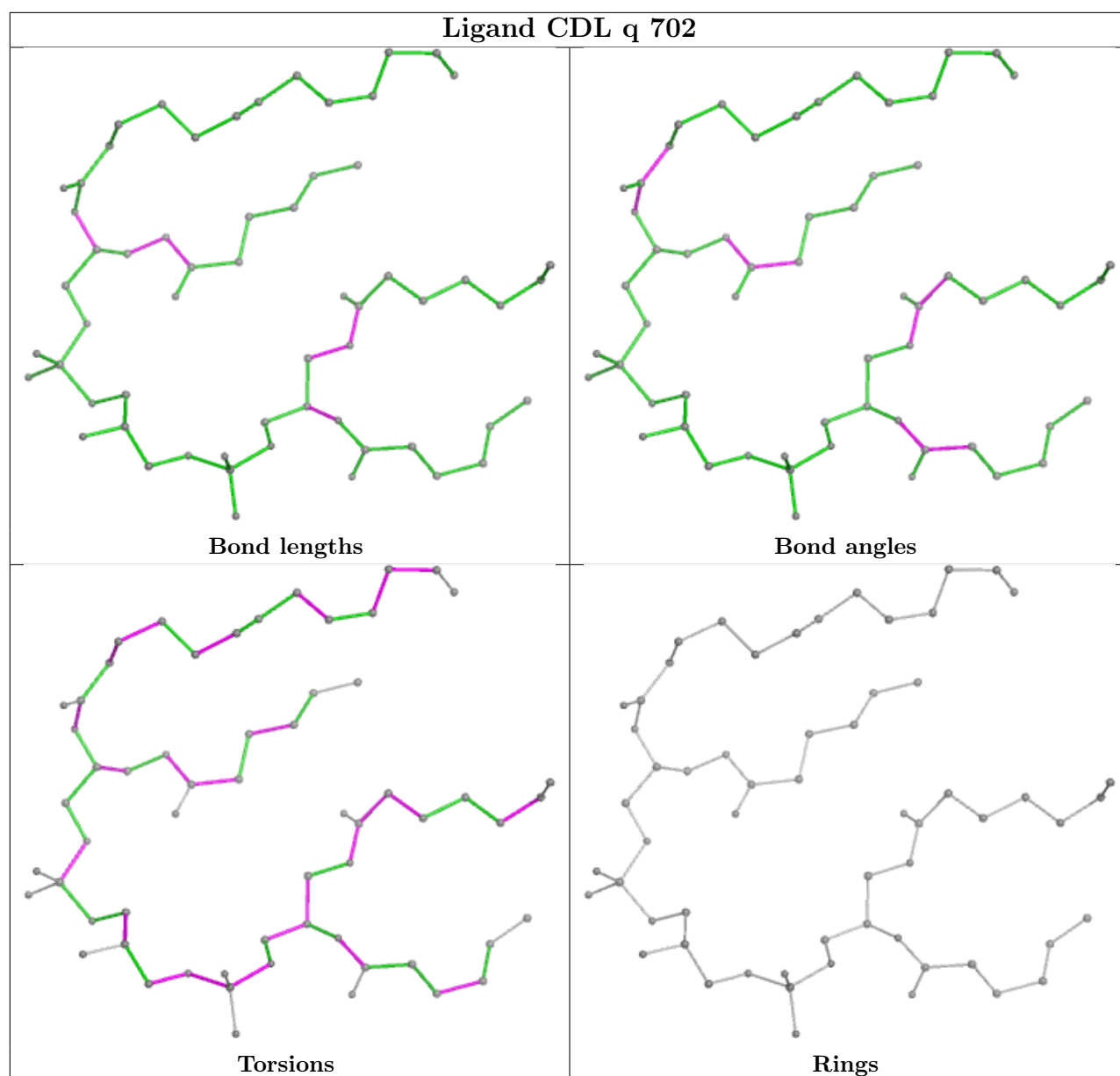


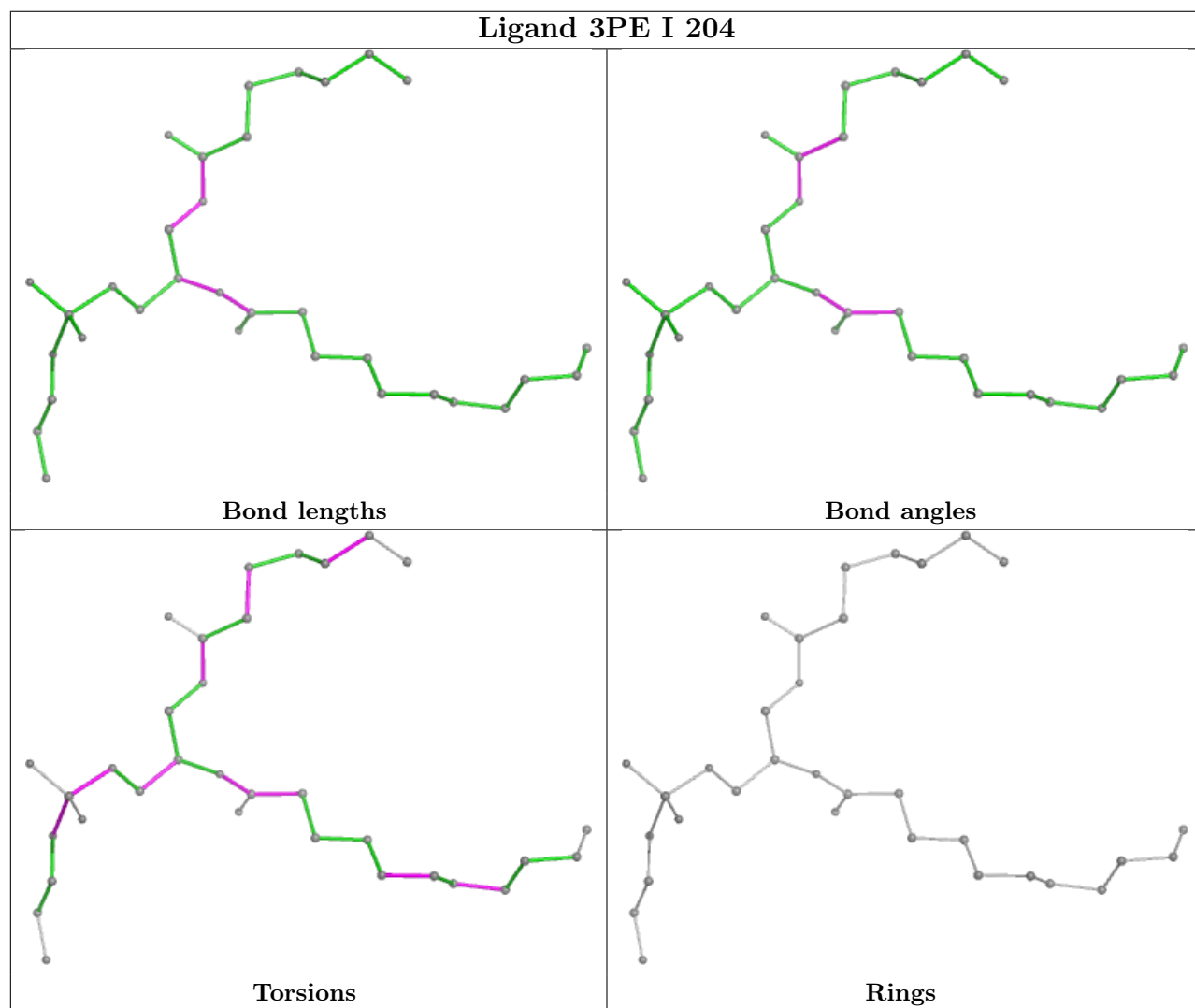
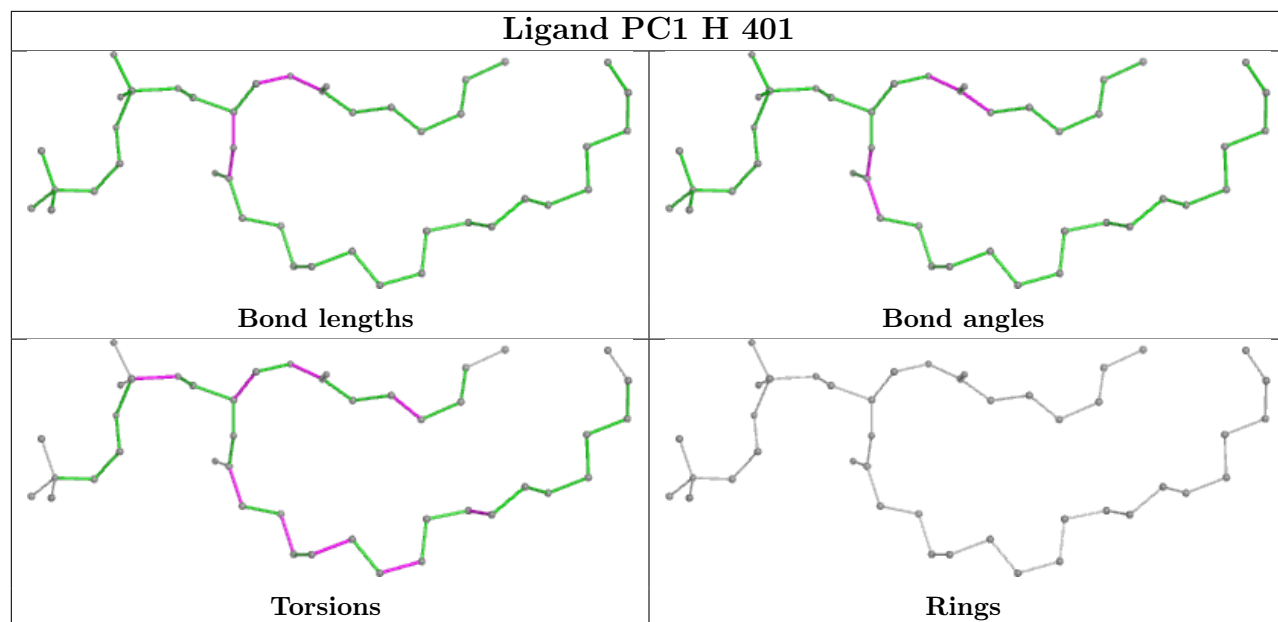












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

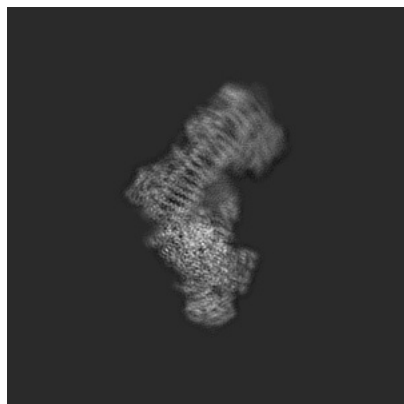
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18059. These allow visual inspection of the internal detail of the map and identification of artifacts.

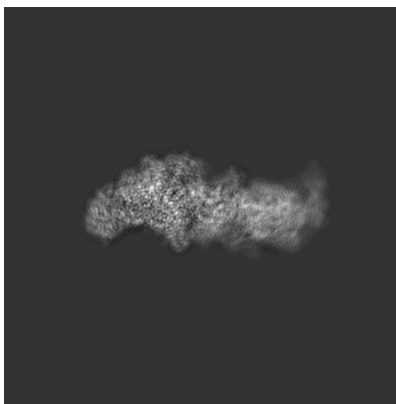
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

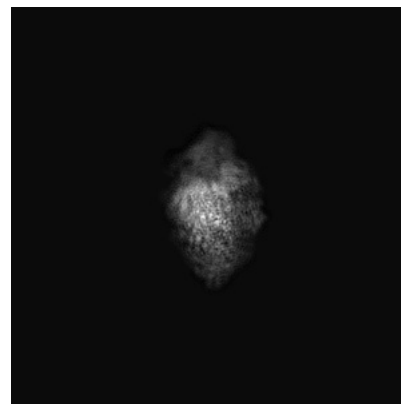
6.1.1 Primary map



X

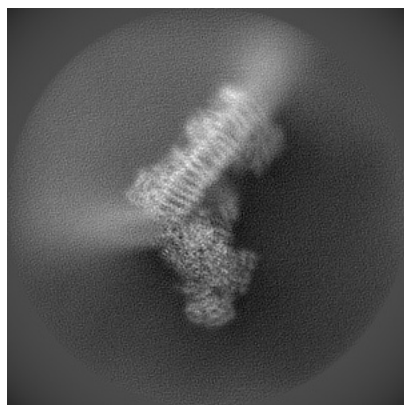


Y

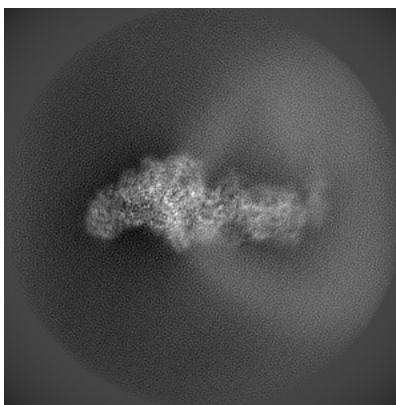


Z

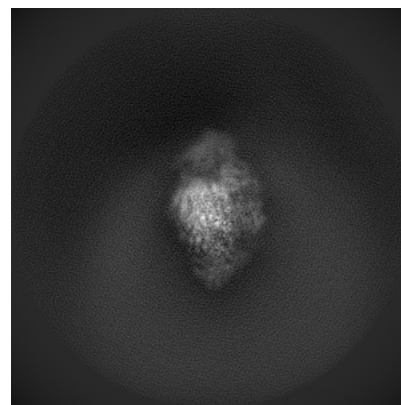
6.1.2 Raw map



X



Y

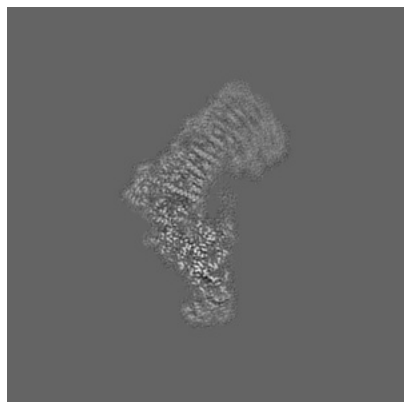


Z

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

6.2 Central slices [i](#)

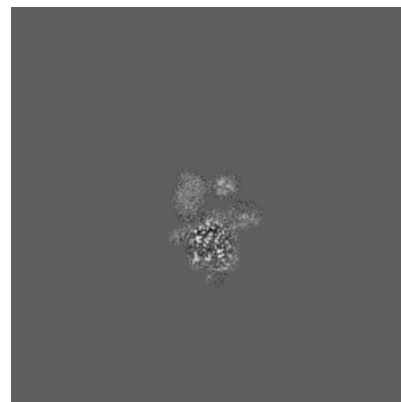
6.2.1 Primary map



X Index: 180

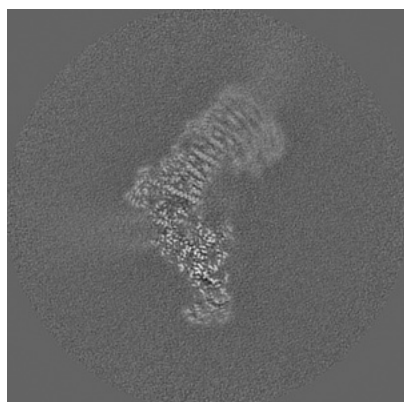


Y Index: 180

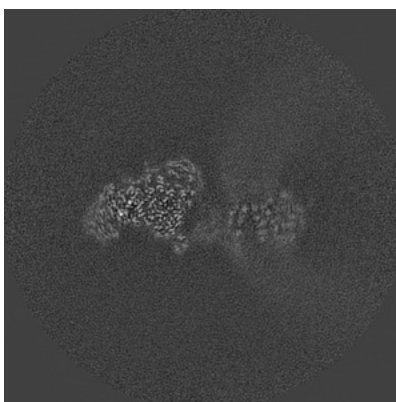


Z Index: 180

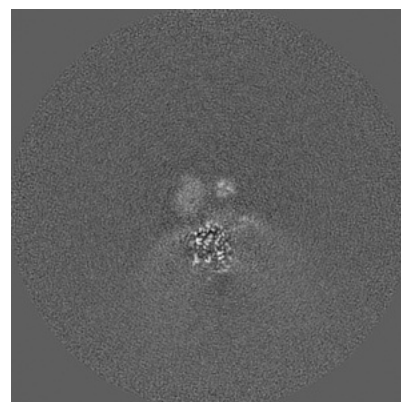
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

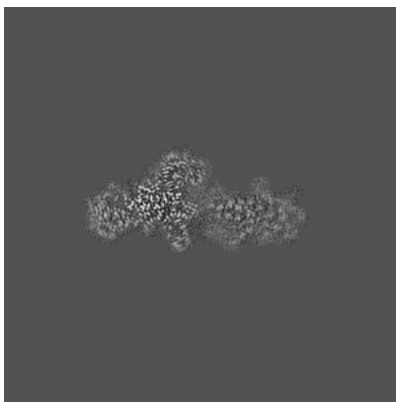
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

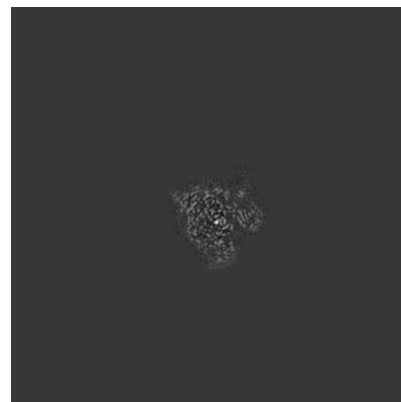
6.3.1 Primary map



X Index: 186

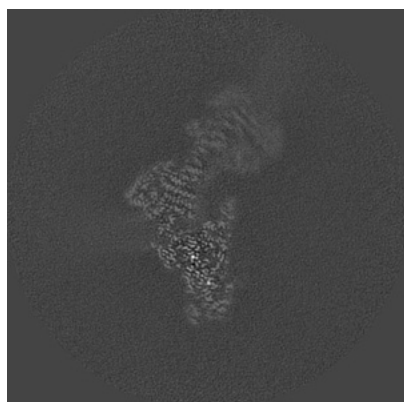


Y Index: 172

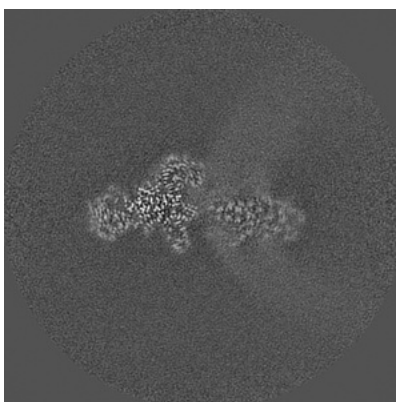


Z Index: 146

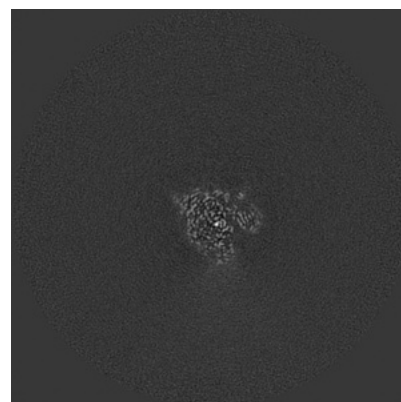
6.3.2 Raw map



X Index: 186



Y Index: 172

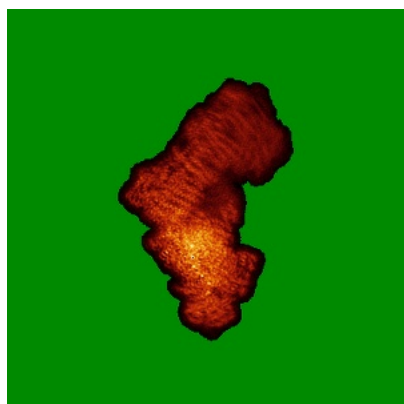


Z Index: 146

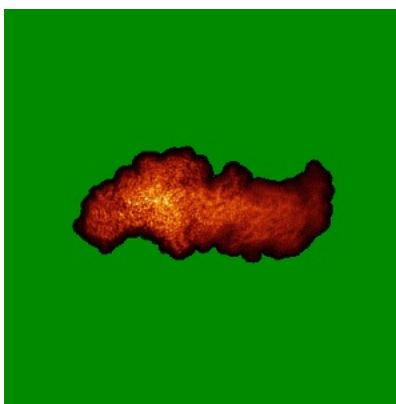
The images above show the largest variance slices of the map in three orthogonal directions.

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

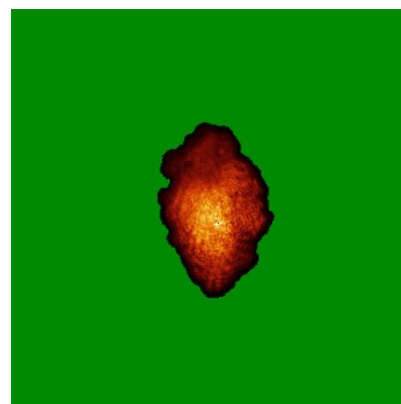
6.4.1 Primary map



X

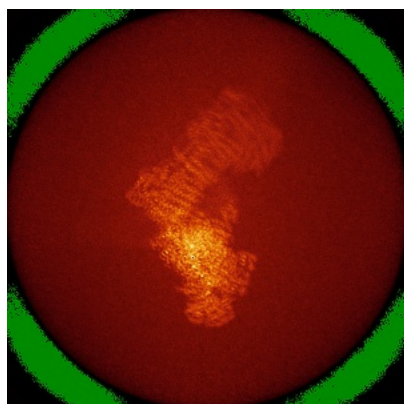


Y

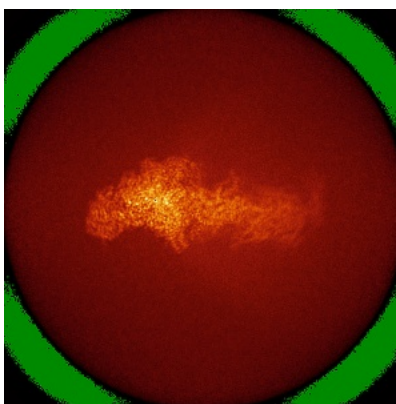


Z

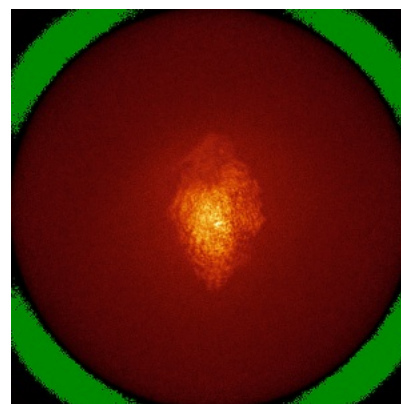
6.4.2 Raw map



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



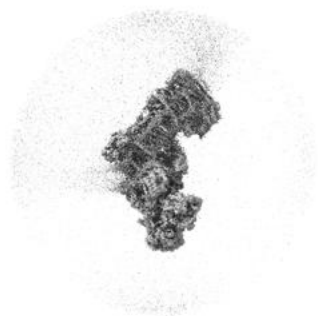
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

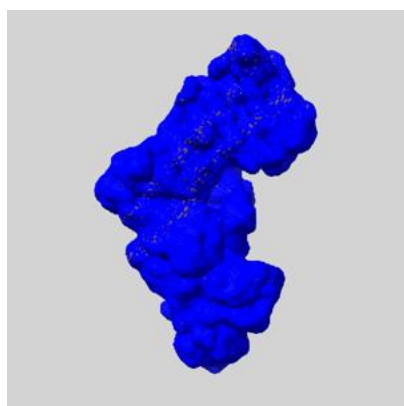
6.6 Mask visualisation [i](#)

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

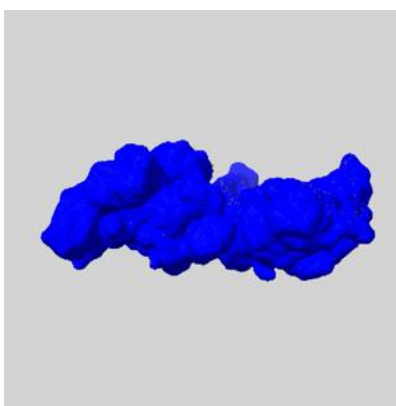
A mask typically either:

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

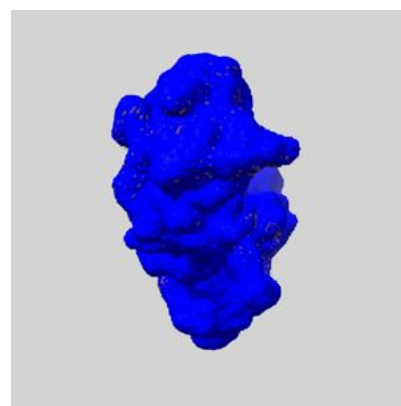
6.6.1 emd_18059_msk_1.map [i](#)



X



Y

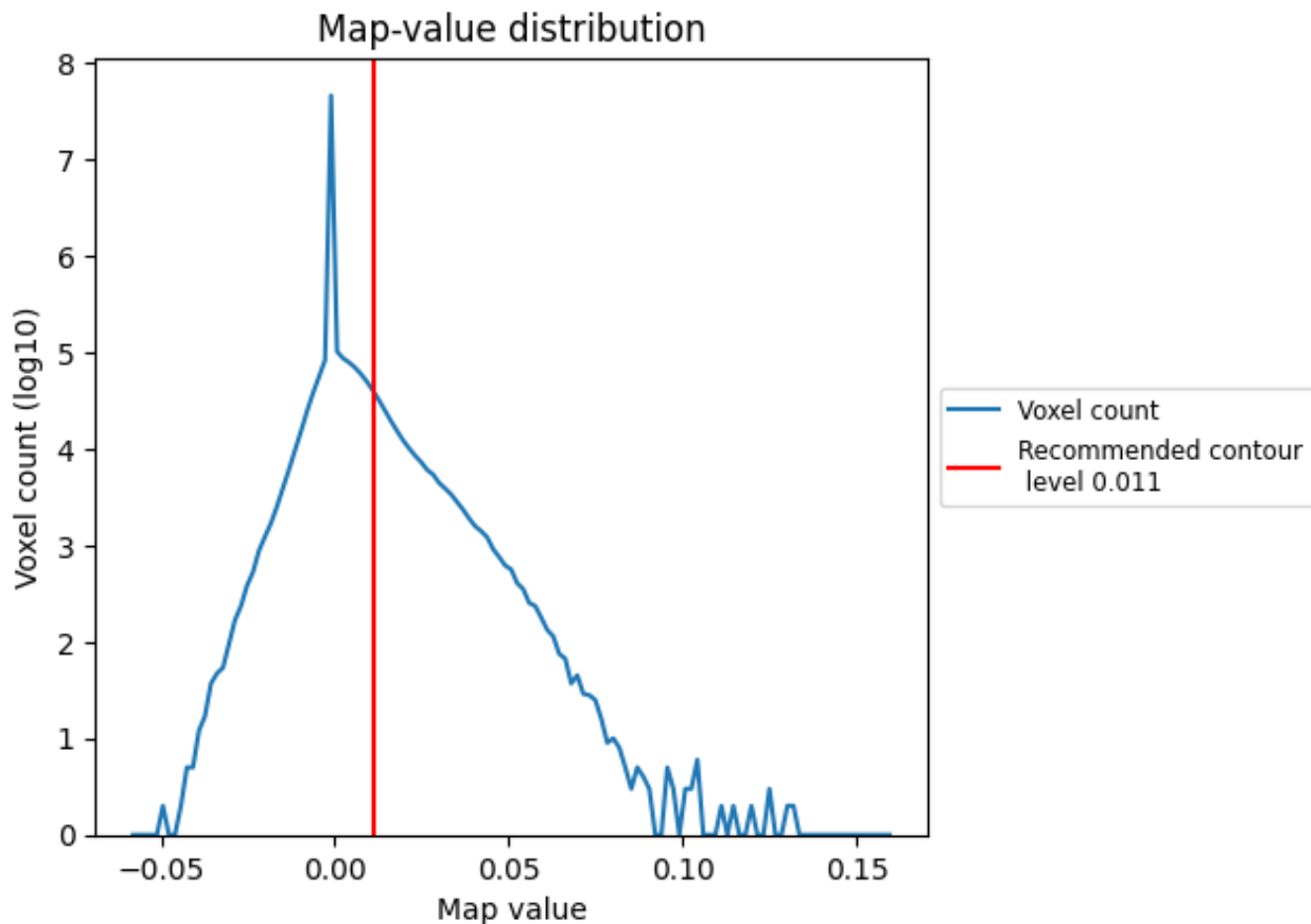


Z

7 Map analysis [i](#)

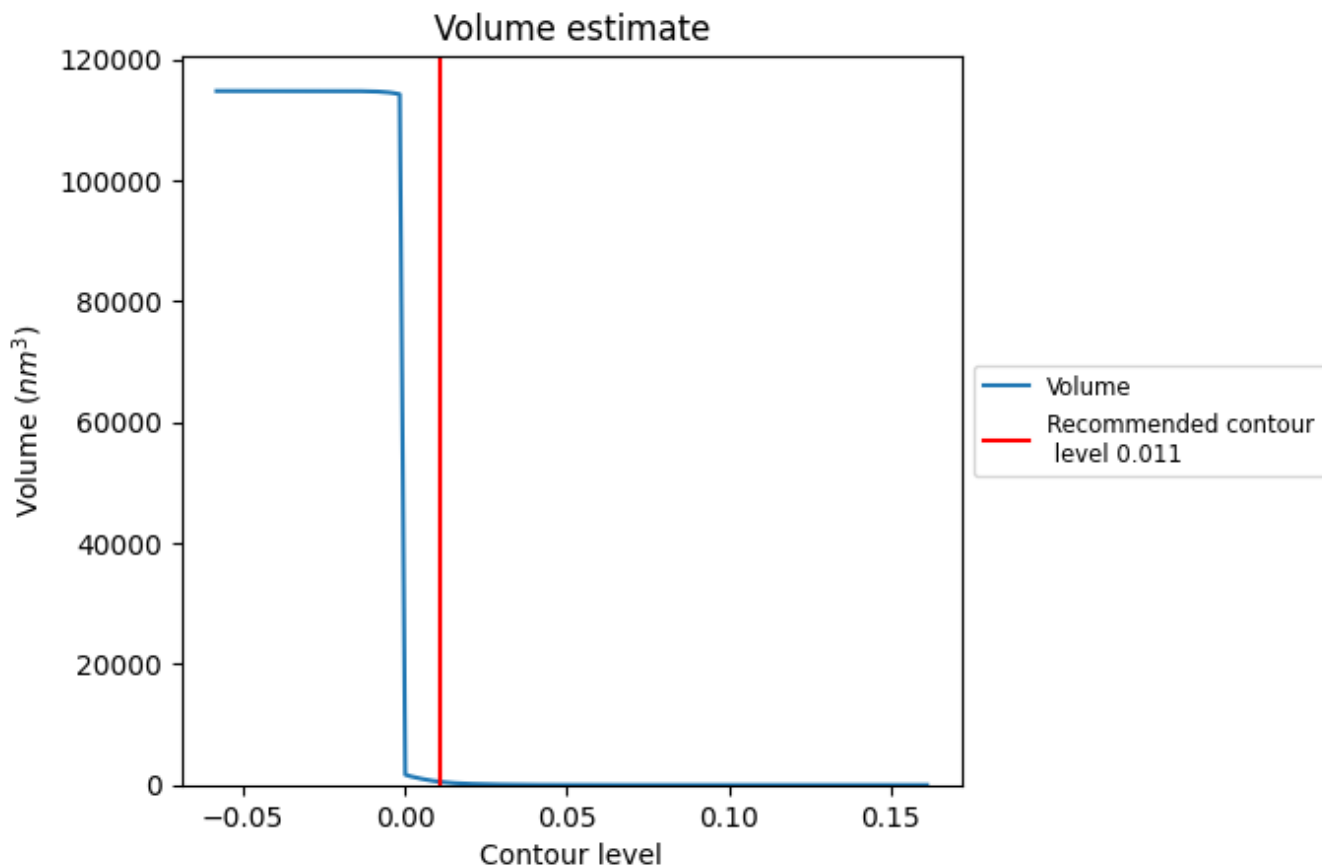
This section contains the results of statistical analysis of the map.

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.

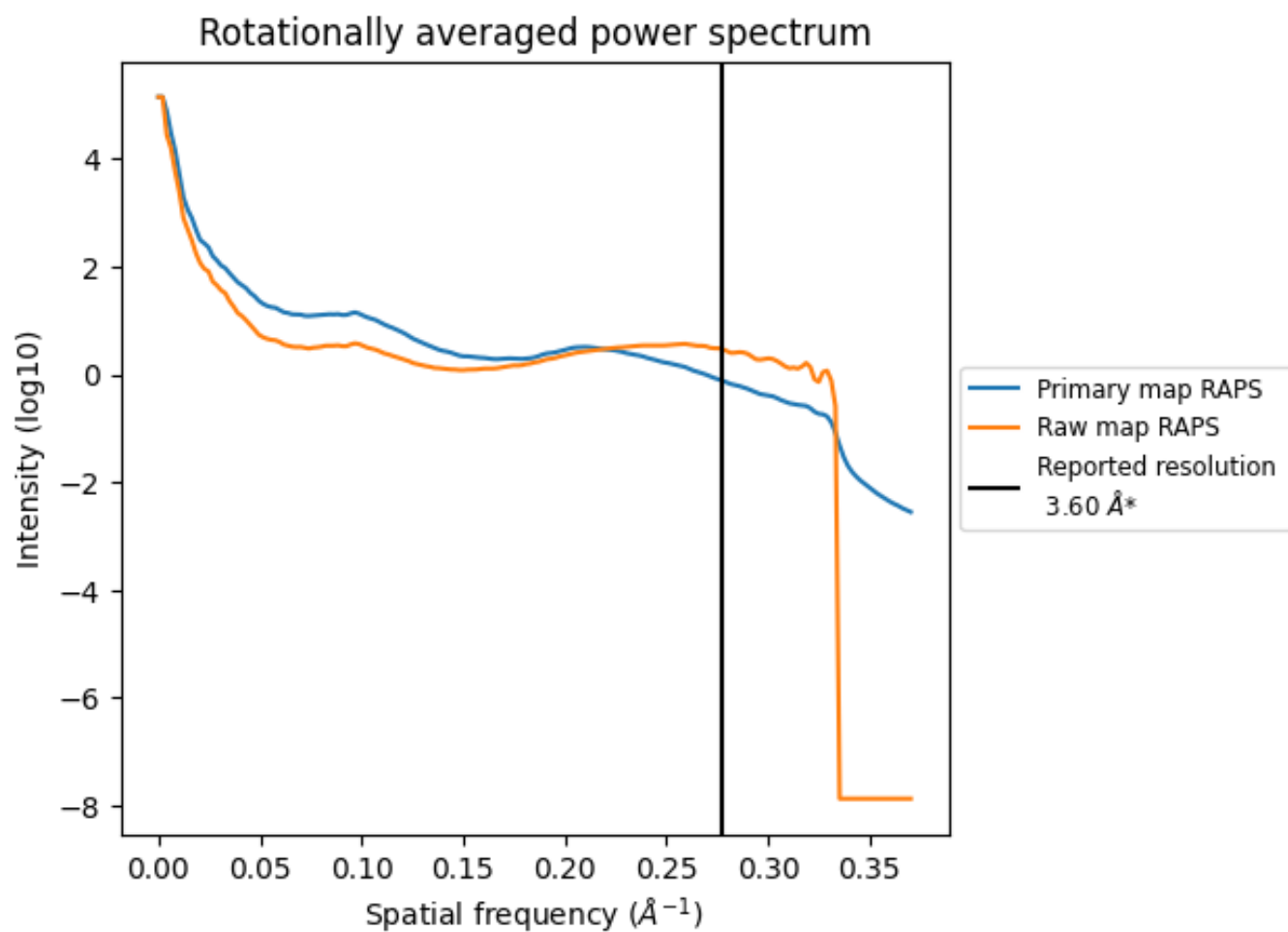
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 515 nm³; this corresponds to an approximate mass of 466 kDa.

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

7.3 Rotationally averaged power spectrum i

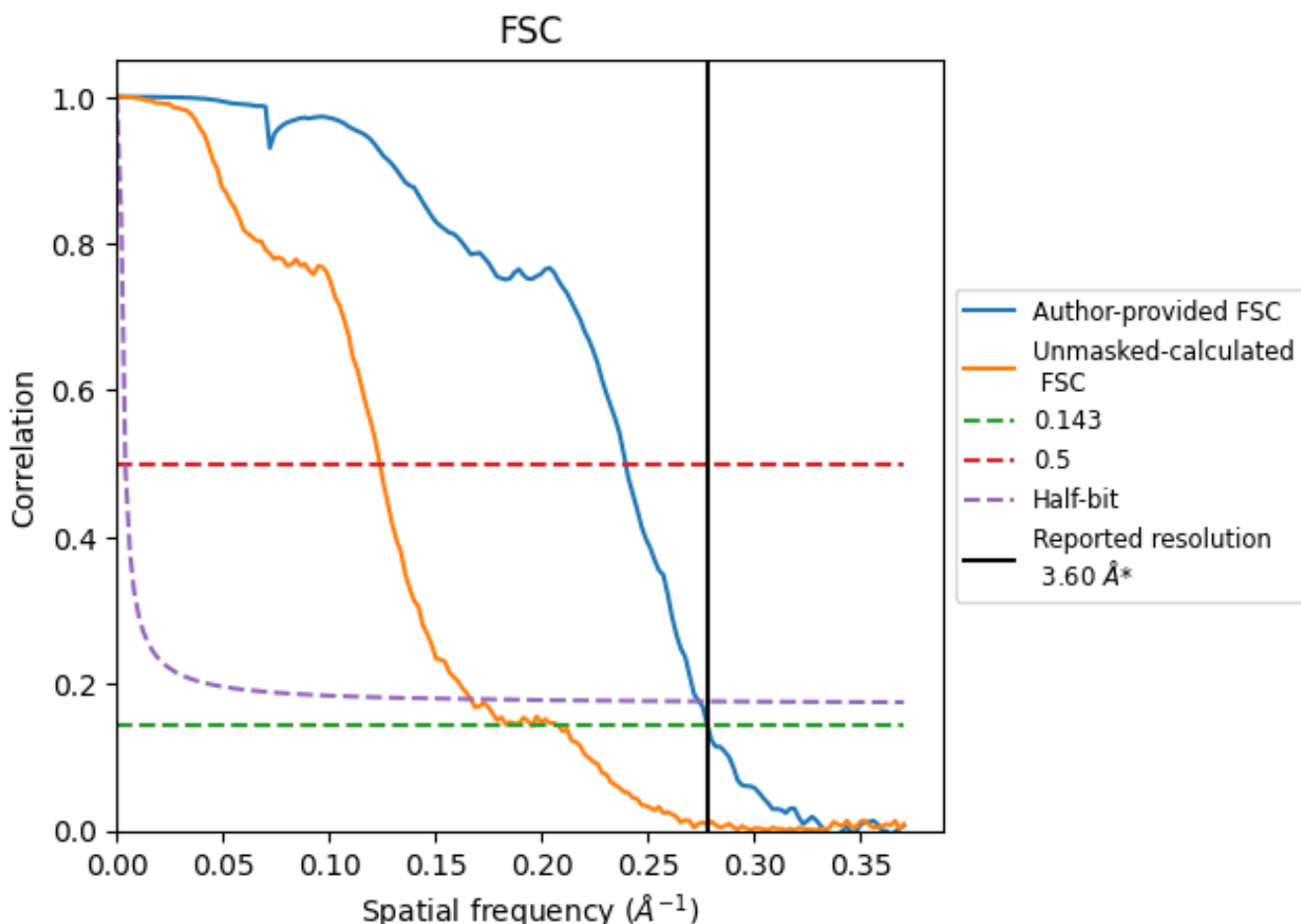


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

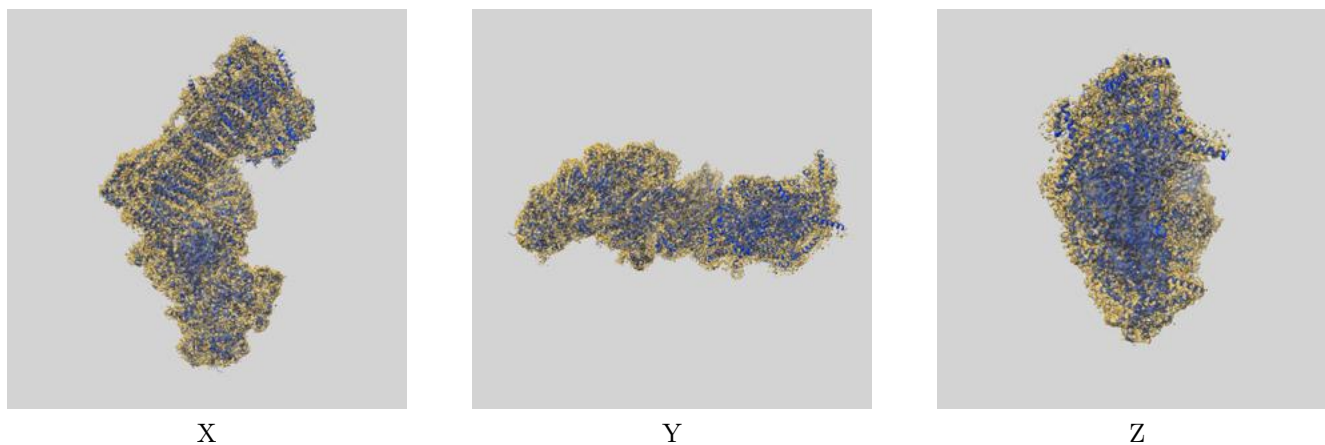
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.18	3.65
Unmasked-calculated*	5.12	8.08	6.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.12 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

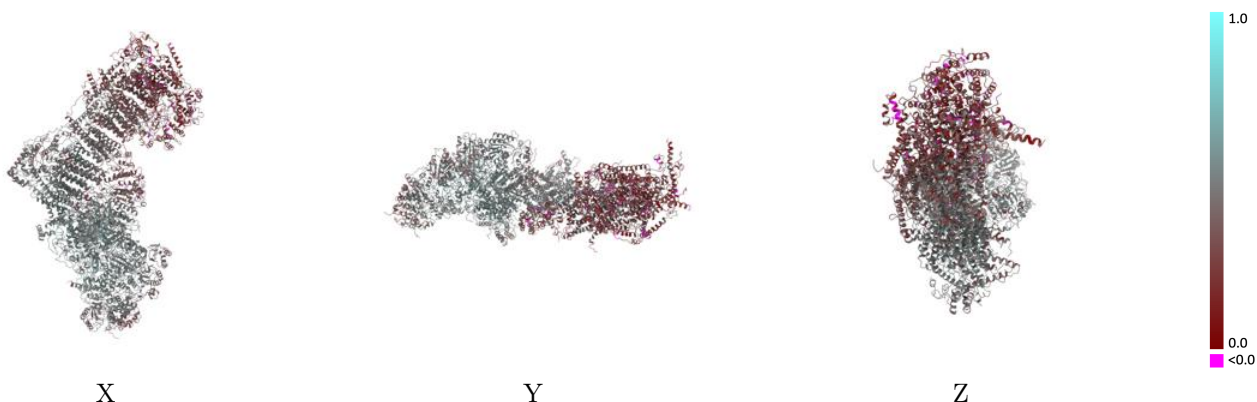
This section contains information regarding the fit between EMDB map EMD-18059 and PDB model 8Q0Q. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



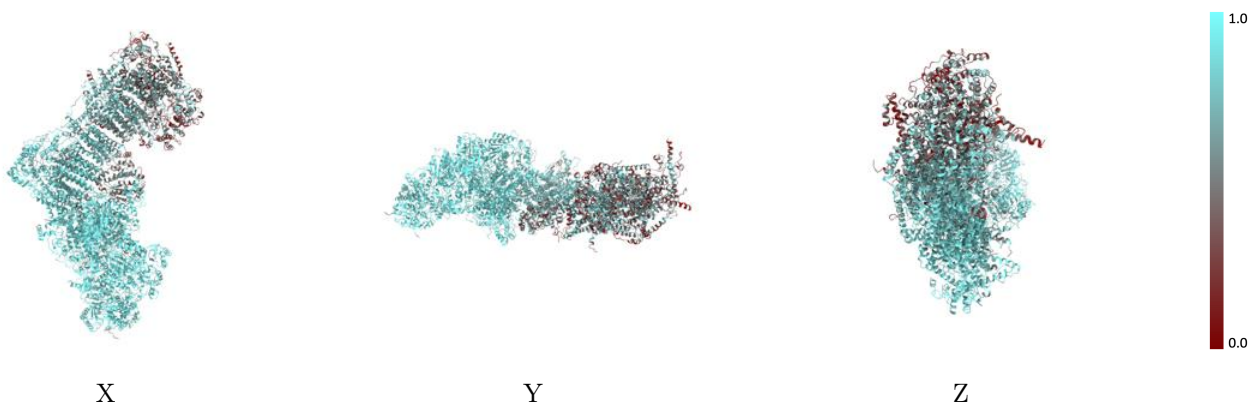
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



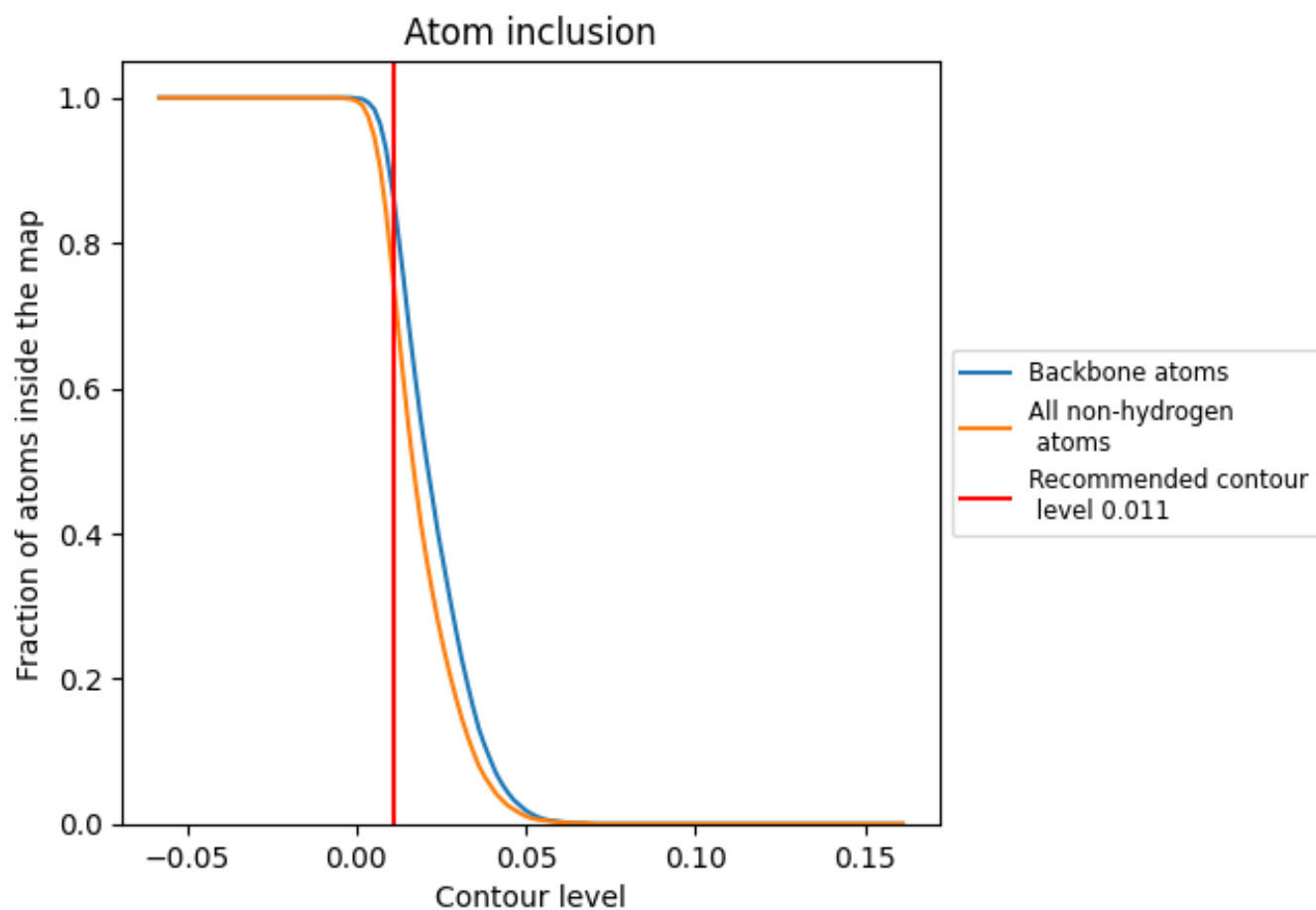
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 74% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.4190
A	0.7840	0.4890
B	0.9070	0.5450
C	0.9380	0.5450
D	0.9240	0.5490
E	0.8980	0.4510
F	0.8820	0.4490
G	0.9040	0.5050
H	0.8850	0.5170
I	0.9360	0.5500
J	0.7610	0.4460
K	0.8240	0.4900
L	0.5030	0.2710
M	0.6710	0.3620
N	0.7890	0.4510
O	0.4490	0.2780
P	0.8620	0.4830
Q	0.9010	0.5330
R	0.8520	0.5080
S	0.8500	0.4300
T	0.8270	0.4090
U	0.3510	0.2220
V	0.8960	0.4670
W	0.8900	0.4970
X	0.8190	0.4580
Y	0.3860	0.3270
Z	0.8290	0.4700
a	0.9000	0.5080
b	0.8560	0.4630
c	0.5760	0.3200
d	0.7090	0.4010
e	0.8250	0.4600
f	0.6080	0.3670
g	0.6120	0.3190
h	0.6800	0.3480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.3950	 0.2140
j	 0.4060	 0.2610
k	 0.3420	 0.2420
l	 0.4780	 0.2620
m	 0.4520	 0.2890
n	 0.4760	 0.2440
o	 0.4790	 0.2640
p	 0.6400	 0.3360
q	 0.8930	 0.5280
r	 0.9050	 0.5190
s	 0.6680	 0.3900