



## wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 10:16 PM UTC

PDB ID : 7V30 / pdb\_00007v30  
EMDB ID : EMD-31648  
Title : Deactive state complex I from Q1-NADH dataset  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-08-10  
Resolution : 2.70 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>.

---

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

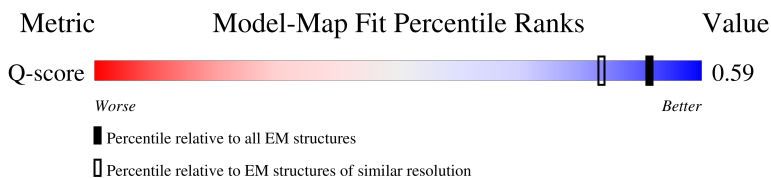
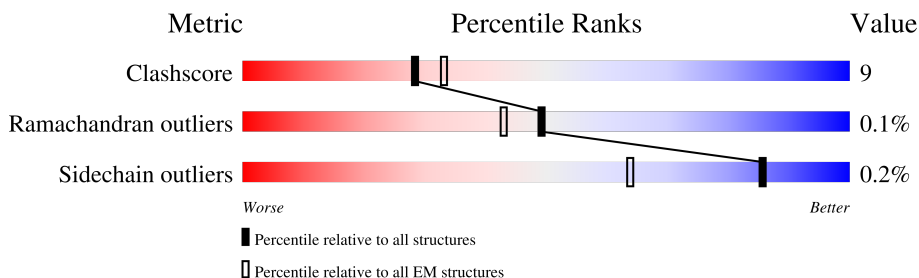
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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	431	75% 24%
2	B	176	78% 22%
3	C	156	86% 14%
4	E	115	77% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	86	9% 85% 15%
6	G	88	27% 61% 38%
6	X	88	7% 66% 33%
7	H	112	78% 22%
8	I	112	71% 15% 13%
9	J	341	8% 68% 19% 13%
10	K	42	17% 69% 31%
11	L	125	6% 83% 17%
12	M	690	83% 17%
13	N	144	84% 16%
14	O	217	11% 74% 26%
15	P	208	85% 15%
16	Q	430	79% 18%
17	S	70	87% 13%
18	T	96	92% 8%
19	U	83	5% 93% 7%
20	V	140	14% 84% 16%
21	W	142	80% 20%
22	Y	70	17% 79% 21%
23	Z	84	20% 89% 11%
24	a	140	83% 17%
25	b	126	10% 64% 17% 18%
26	c	156	78% 22%
27	d	175	5% 87% 13%
28	e	107	11% 81% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	f	42	
30	g	121	
31	h	105	
32	i	347	
33	j	113	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	131	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
54	CDL	a	201	-	-	X	-
57	ADP	w	401	-	-	X	-

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66820 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	176	1412	887	243	269	13	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	691	434	129	126	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			696	449	103	139	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	297	Total	C	N	O	S	0	0
			2359	1514	421	416	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5296	3320	923	1014	39	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	144	1204	770	218	212	4	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	217	1671	1065	281	315	10	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	208	1738	1124	298	314	2	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	419	3377	2162	578	613	24	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	70	567	364	104	94	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	96	741	452	140	146	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	83	643	417	110	115	1	0	0

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	140	1021	651	174	190	6	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1173	755	203	206	9	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Y	70	597	392	98	106	1	0	0

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	84	674	437	116	120	1	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	a	140	1165	762	199	201	3	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b	103	879	573	158	147	1	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	c	156	1315	853	213	241	8	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	d	175	1461	916	265	272	8	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	e	107	890	568	145	173	4	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	42	342	225	58	59	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	121	1000	650	173	171	6	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	105	867	550	161	150	6	0	0

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	i	347	2710	1782	420	462	46	0	0

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	99	800	545	118	132	5	0	0

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	98	748	493	113	128	14	0	0

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	603	4782	3172	740	819	51	0	0

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	129	948	636	138	166	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	n	56	479	311	88	79	1	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		
38	o	128	1062	691	182	189	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	p	178	1534	982	279	265	8	0	0

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3631	2412	572	609	38	0	0

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	s	303	2394	1607	369	397	21	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	u	171	1398	887	250	251	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1028	642	195	182	9	0	0

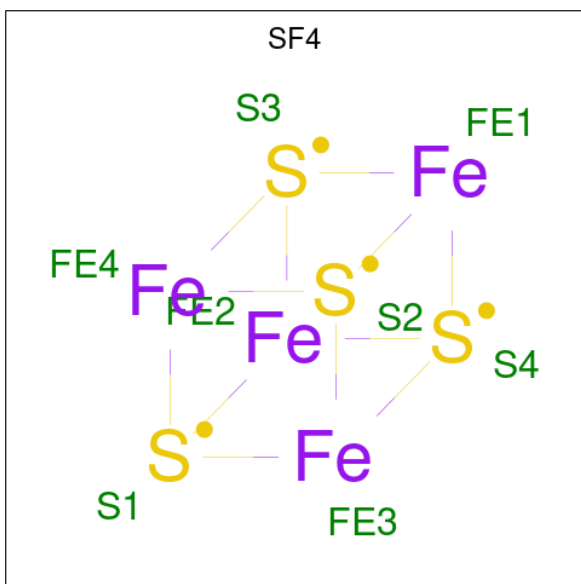
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

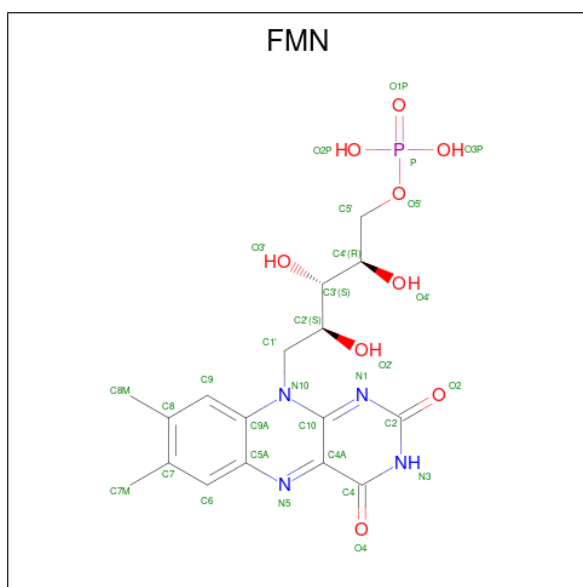
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2582	1643	438	491	10	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



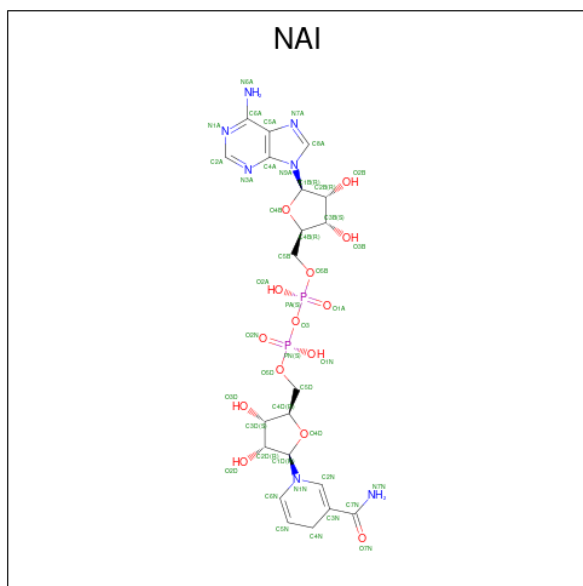
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	8	4	4	0
45	B	1	8	4	4	0
45	C	1	8	4	4	0
45	M	1	8	4	4	0
45	M	1	8	4	4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



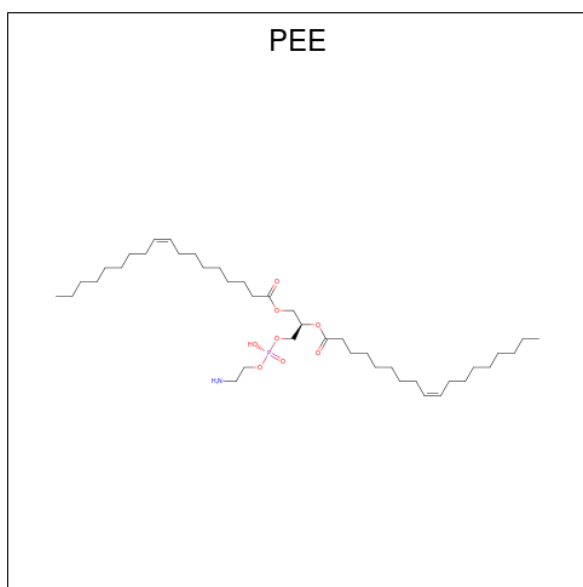
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



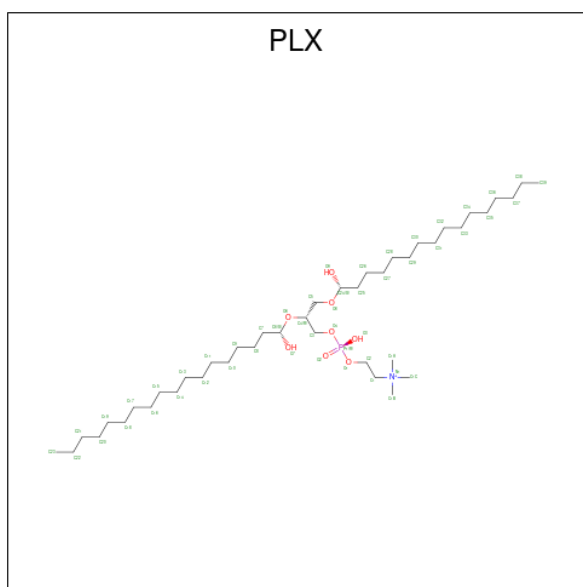
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



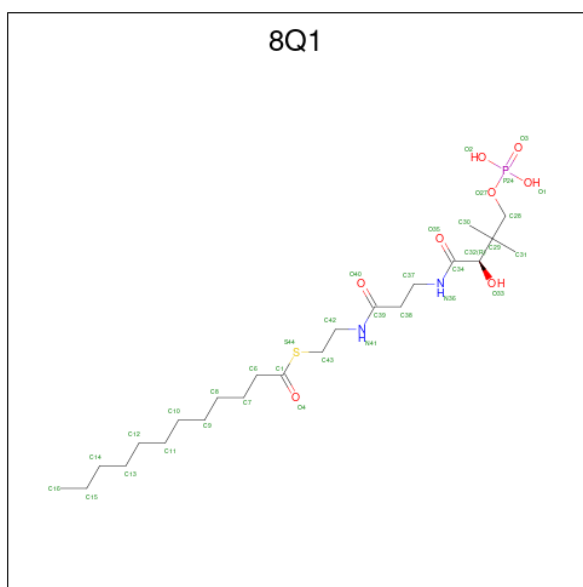
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	C	1	Total 47	37	1	8	1	0
48	U	1	Total 51	41	1	8	1	0
48	V	1	Total 51	41	1	8	1	0
48	l	1	Total 47	37	1	8	1	0
48	l	1	Total 46	36	1	8	1	0
48	l	1	Total 46	36	1	8	1	0
48	m	1	Total 41	31	1	8	1	0
48	s	1	Total 51	41	1	8	1	0

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



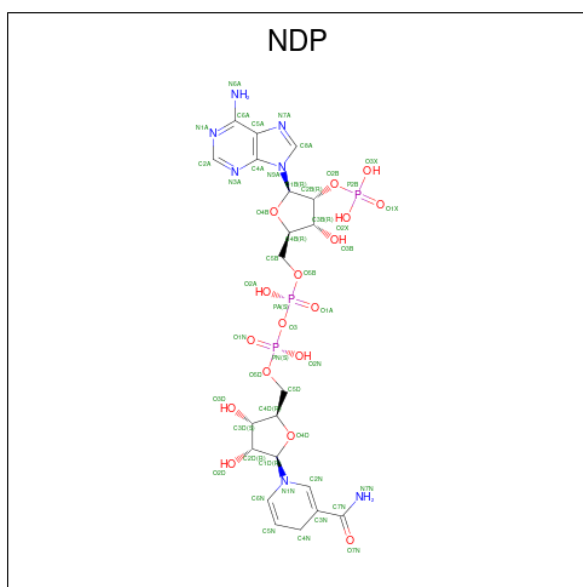
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	Total 52	42	1	8	1	0
49	V	1	Total 52	42	1	8	1	0
49	e	1	Total 52	42	1	8	1	0
49	i	1	Total 52	42	1	8	1	0
49	j	1	Total 52	42	1	8	1	0
49	n	1	Total 52	42	1	8	1	0

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



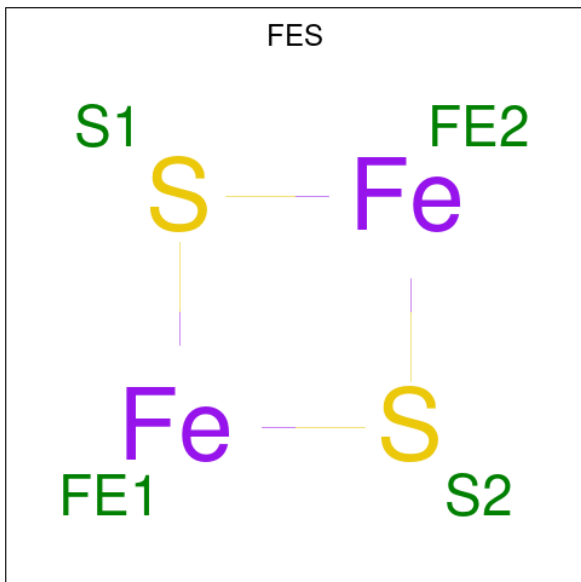
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

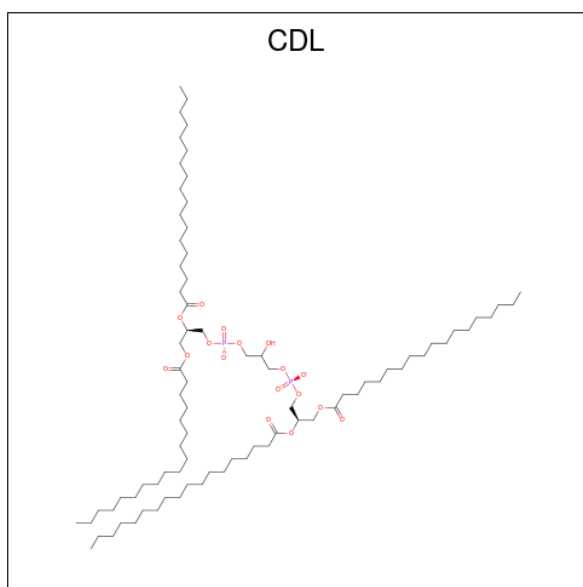


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
52	M	1	4	2	2	0
52	O	1	4	2	2	0

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula:  $\text{Mg}$ ) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

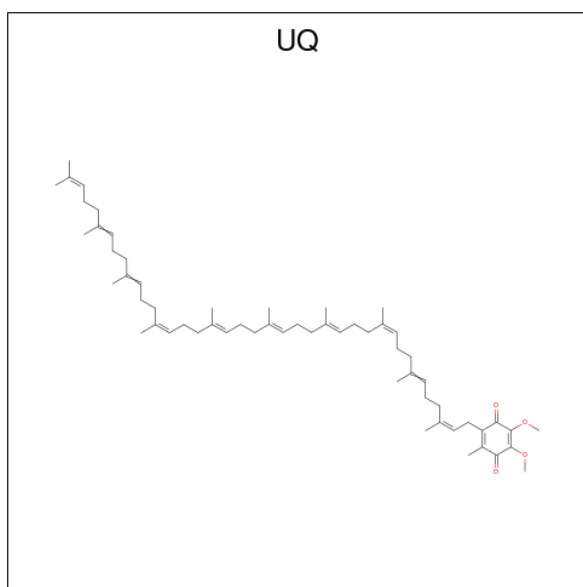


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
54	N	1	51	32	17	2	0
54	V	1	71	52	17	2	0
54	a	1	91	72	17	2	0
54	i	1	66	47	17	2	0
54	l	1	99	80	17	2	0
54	l	1	100	81	17	2	0
54	n	1	78	59	17	2	0
54	r	1	100	81	17	2	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

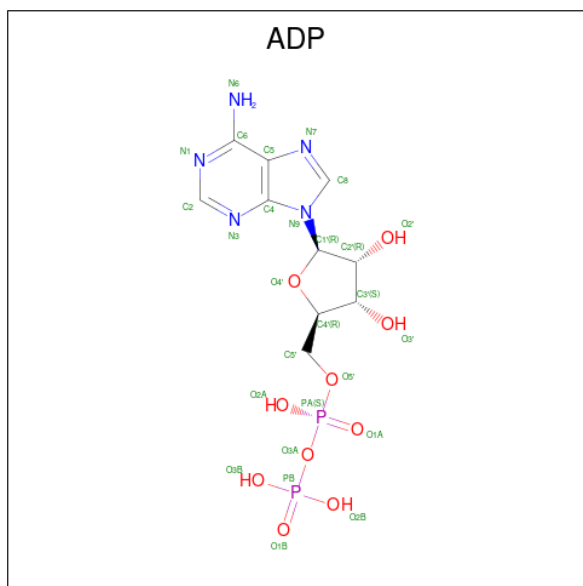
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	T	1	1	1	0

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	s	1	28	24	4	0

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

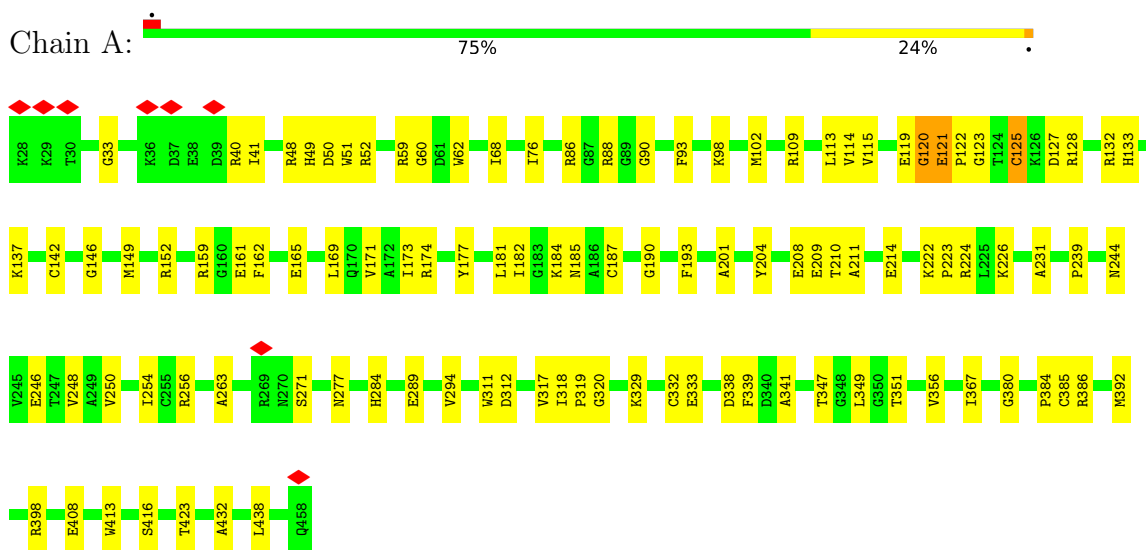


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

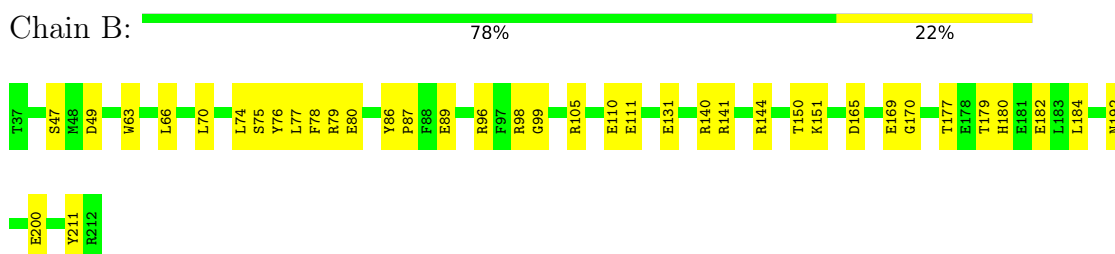
### 3 Residue-property plots [i](#)

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.

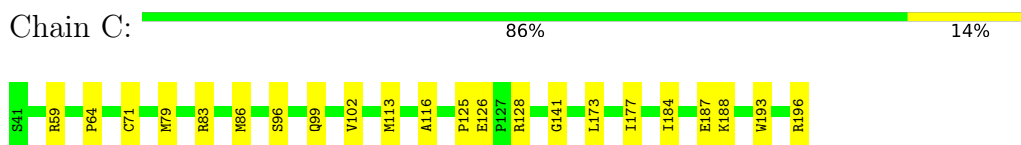
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



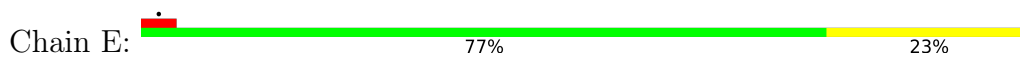
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



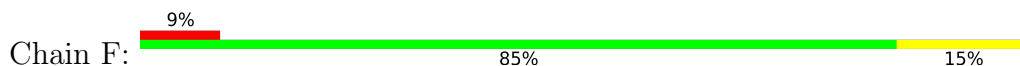
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



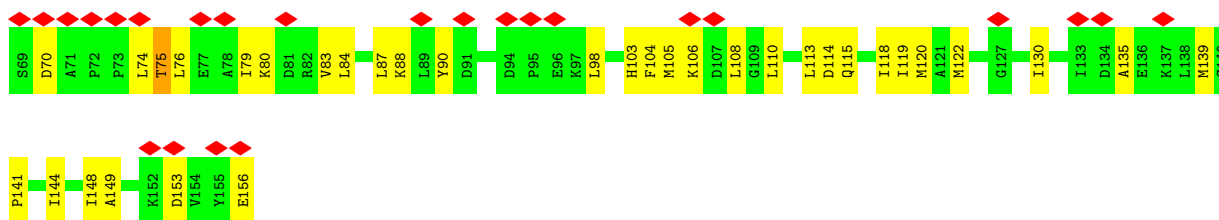
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



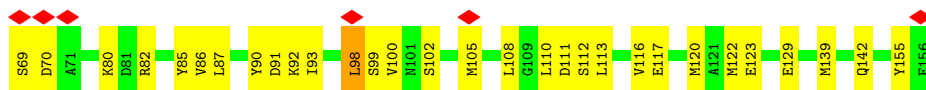
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



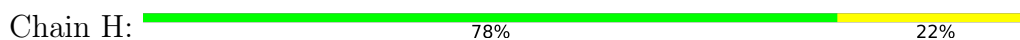
- Molecule 6: Acyl carrier protein, mitochondrial



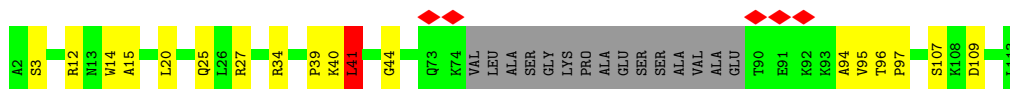
- Molecule 6: Acyl carrier protein, mitochondrial



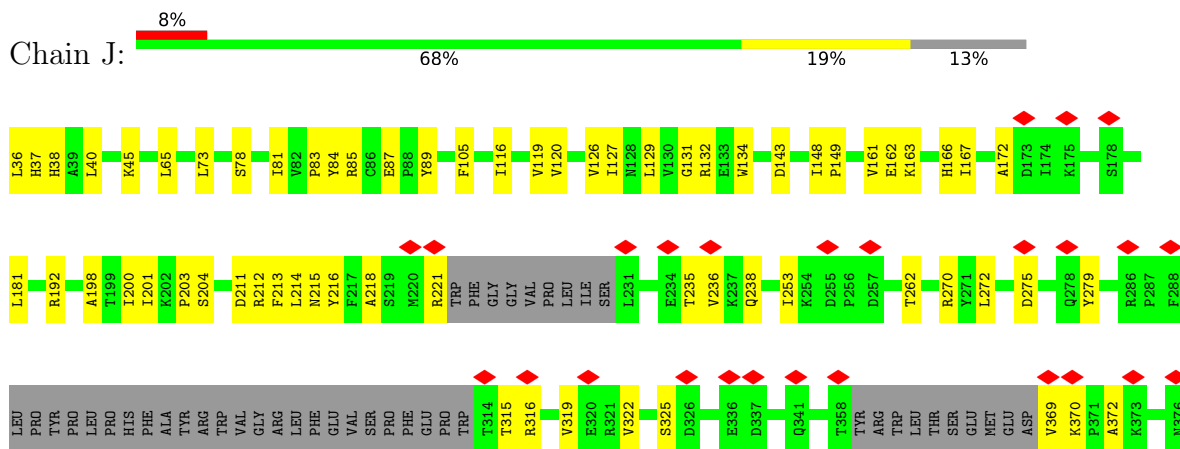
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



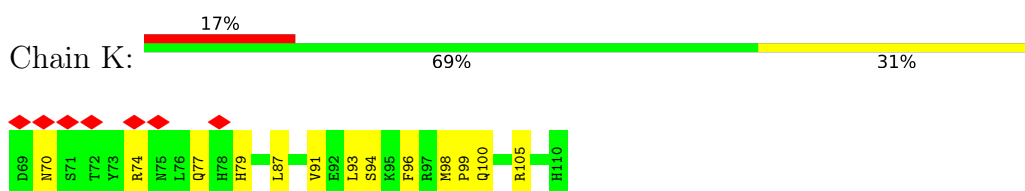
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



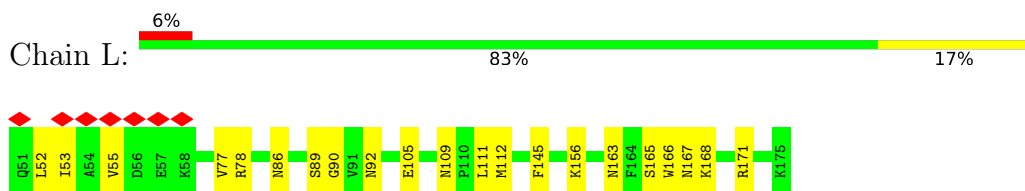
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



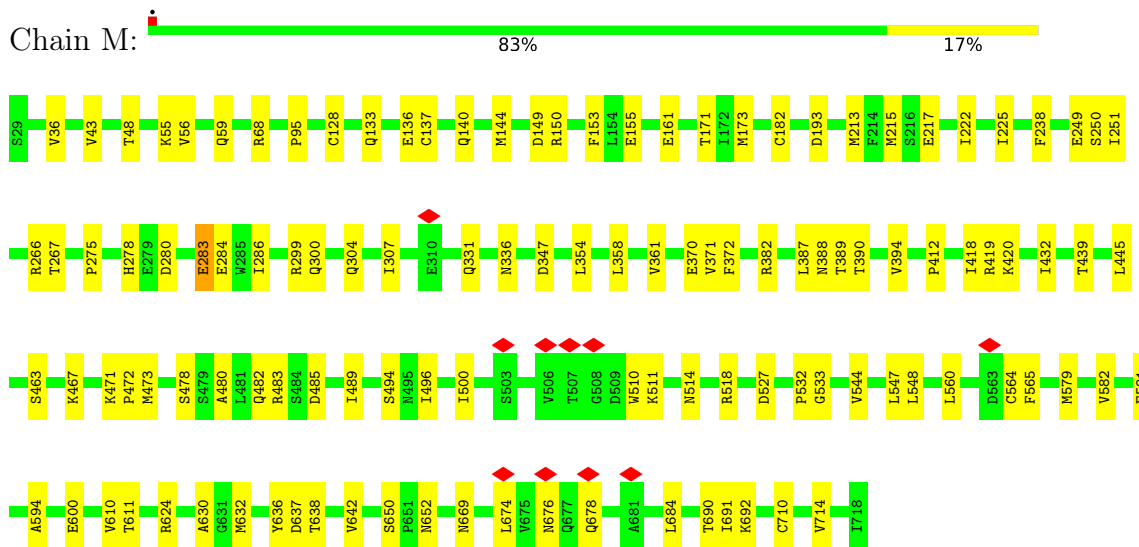
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



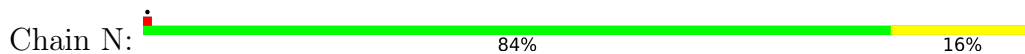
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

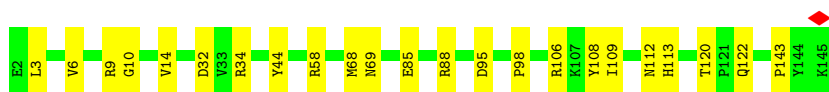


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

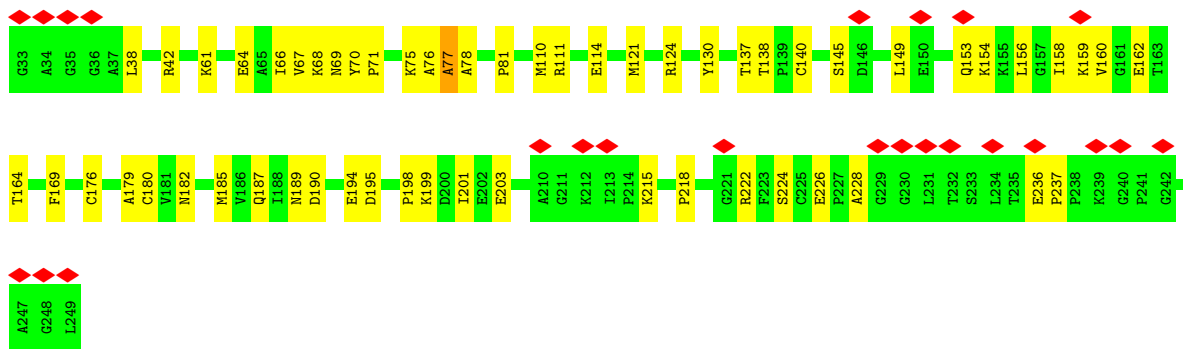
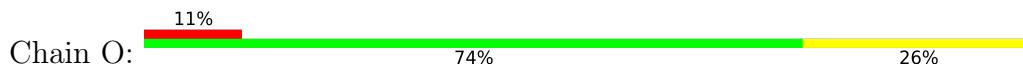


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

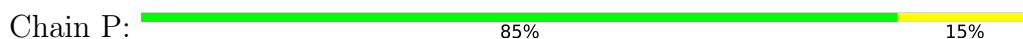




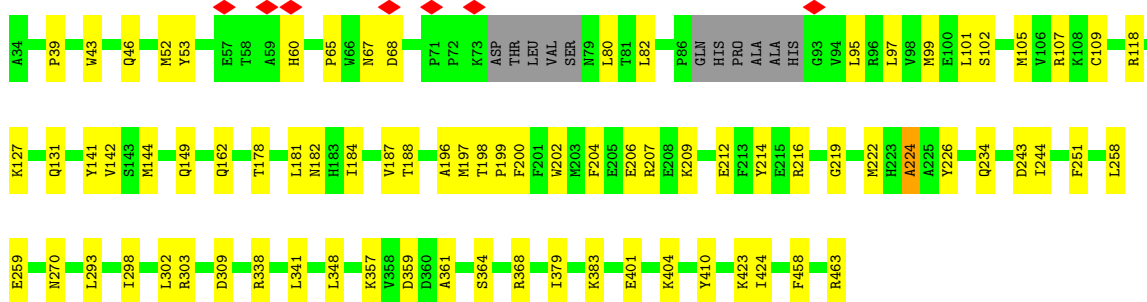
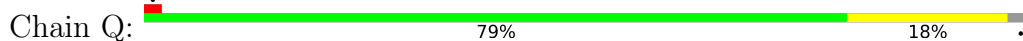
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



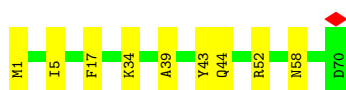
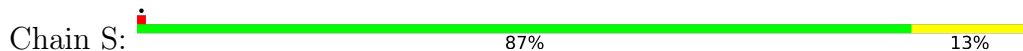
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



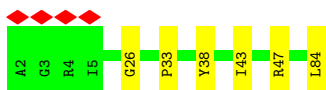
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  92% 8%




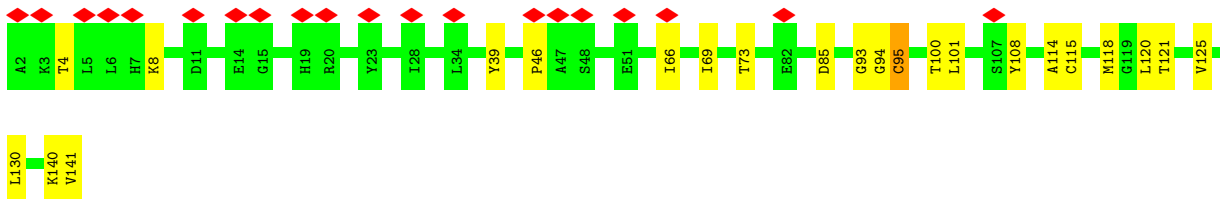
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  5% 93% 7%




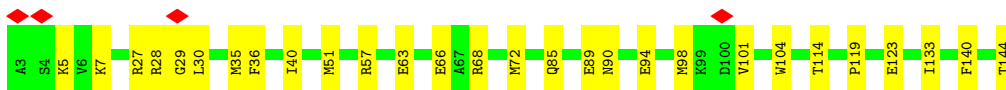
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  14% 84% 16%




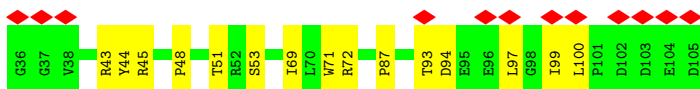
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  80% 20%




- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  17% 79% 21%

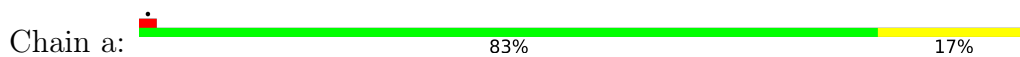


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

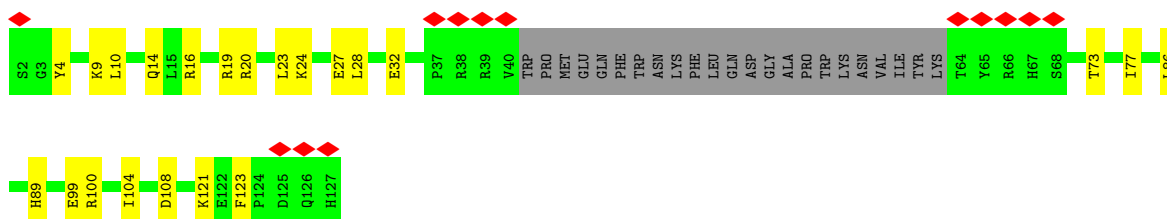
Chain Z:  20% 89% 11%



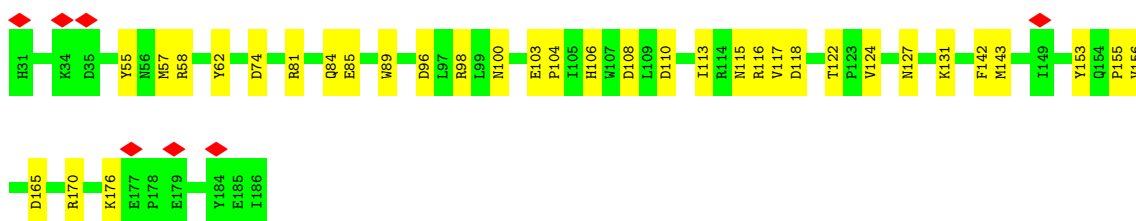
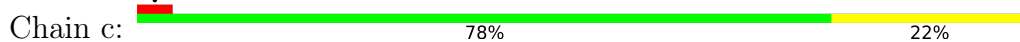
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



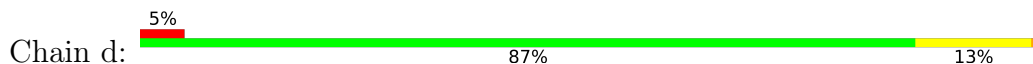
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



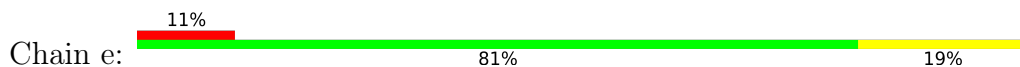
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



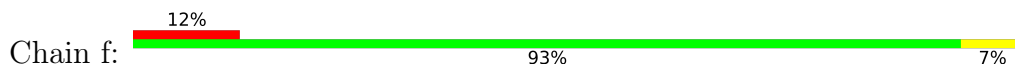
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

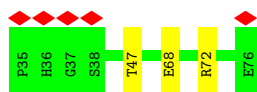


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

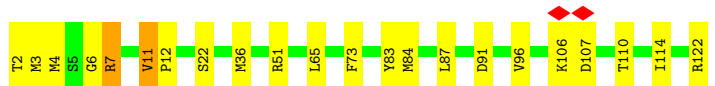
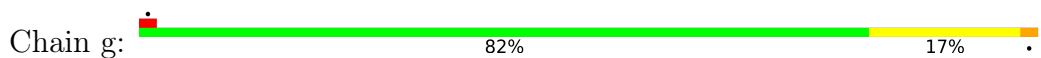


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

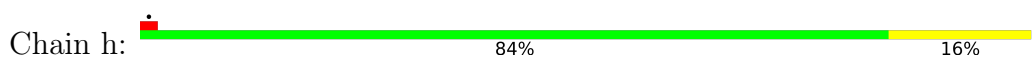




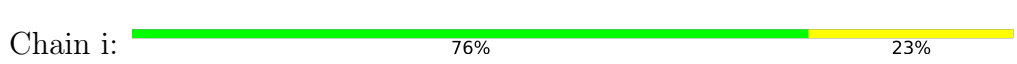
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



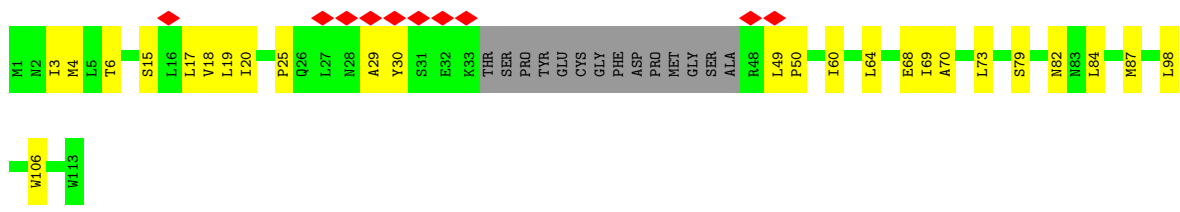
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



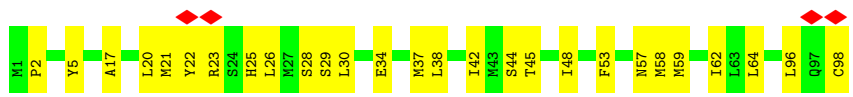
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2



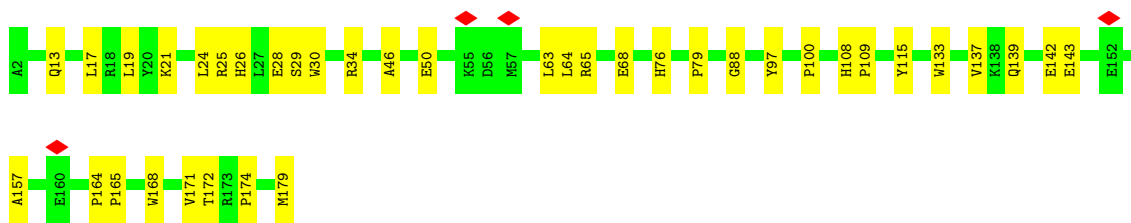
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

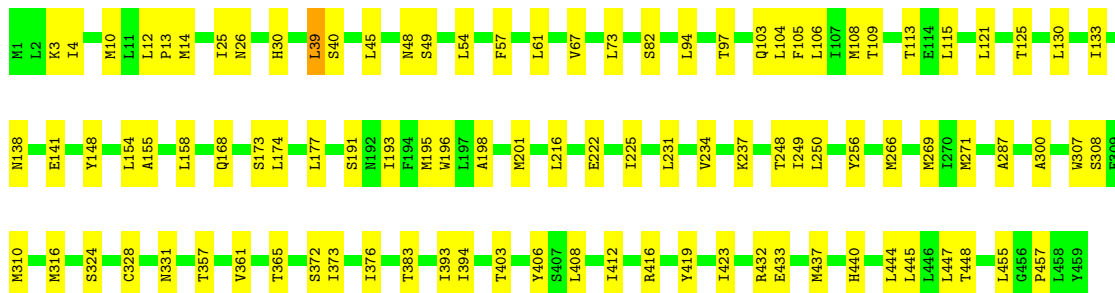






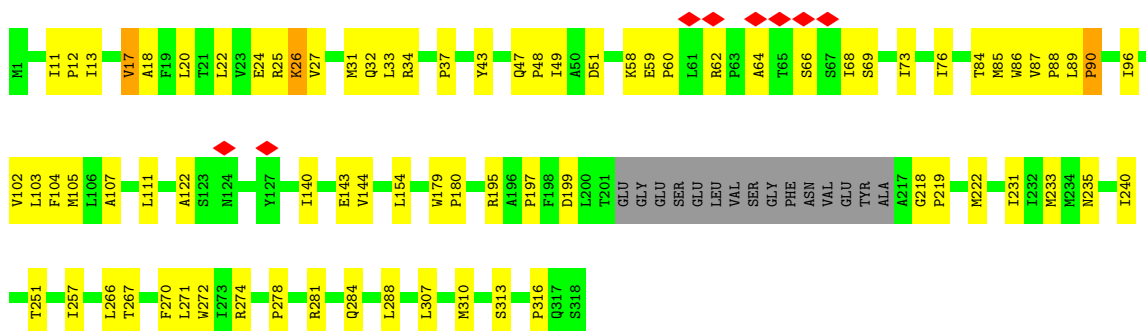
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 79% 21%



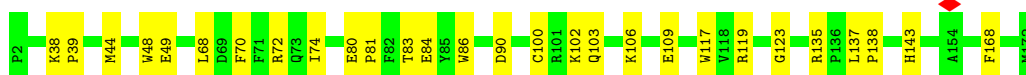
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 71% 24% 5%



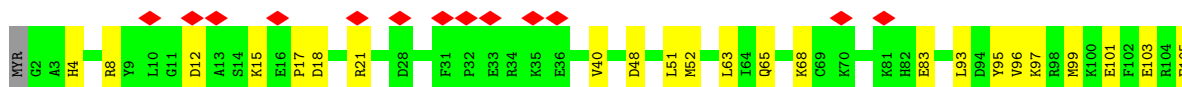
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

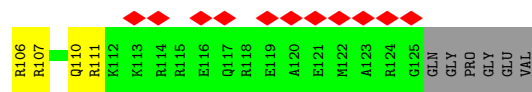
Chain u: 84% 16%



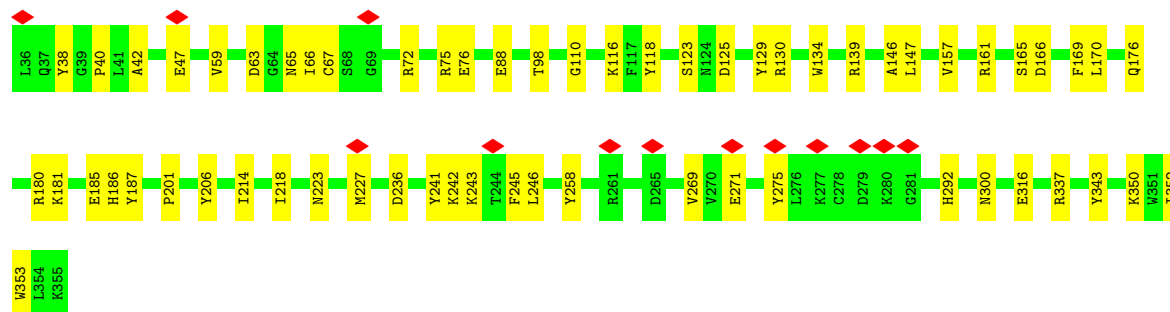
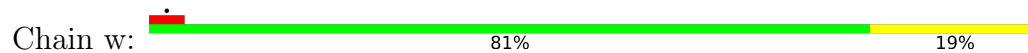
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 18% 74% 21% 5%





- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0239	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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, PEE, NDP, ADP, 8Q1, PLX, MG, ZN, NAI, FMN, UQ, CDL, SF4, 2MR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.18	0/3393	0.48	6/4584 (0.1%)
2	B	0.15	0/1443	0.34	0/1952
3	C	0.13	0/1279	0.33	0/1730
4	E	0.12	0/995	0.31	0/1340
5	F	0.11	0/702	0.34	0/945
6	G	0.15	0/705	0.39	0/956
6	X	0.16	0/708	0.45	0/959
7	H	0.12	0/929	0.32	0/1258
8	I	0.21	0/798	0.54	2/1079 (0.2%)
9	J	0.12	0/2411	0.33	0/3254
10	K	0.09	0/365	0.30	0/493
11	L	0.13	0/1039	0.31	0/1403
12	M	0.14	0/5384	0.34	1/7295 (0.0%)
13	N	0.28	1/1245 (0.1%)	0.49	3/1694 (0.2%)
14	O	0.16	0/1711	0.43	0/2328
15	P	0.14	0/1789	0.40	1/2436 (0.0%)
16	Q	0.17	0/3451	0.40	1/4672 (0.0%)
17	S	0.16	0/582	0.39	0/783
18	T	0.09	0/755	0.27	0/1018
19	U	0.11	0/664	0.33	0/912
20	V	0.19	0/1042	0.47	3/1411 (0.2%)
21	W	0.13	0/1204	0.30	0/1624
22	Y	0.13	0/623	0.30	0/853
23	Z	0.10	0/695	0.27	0/939
24	a	0.13	0/1199	0.33	0/1623
25	b	0.17	0/906	0.36	0/1232
26	c	0.17	0/1371	0.34	0/1875
27	d	0.17	0/1494	0.39	2/2015 (0.1%)
28	e	0.18	0/916	0.48	1/1246 (0.1%)
29	f	0.13	0/350	0.31	0/473
30	g	0.16	0/1031	0.49	4/1394 (0.3%)
31	h	0.11	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	i	0.17	0/2773	0.38	0/3768
33	j	0.16	0/819	0.37	0/1117
34	k	0.14	0/759	0.38	0/1029
35	l	0.18	0/4911	0.40	1/6679 (0.0%)
36	m	0.15	0/970	0.37	0/1316
37	n	0.21	0/491	0.66	1/663 (0.2%)
38	o	0.12	0/1092	0.32	0/1481
39	p	0.13	0/1590	0.31	0/2155
40	r	0.18	0/3723	0.44	0/5078
41	s	0.24	0/2464	0.54	4/3369 (0.1%)
42	u	0.13	0/1436	0.36	0/1938
43	v	0.14	0/1052	0.44	0/1411
44	w	0.14	0/2642	0.39	1/3580 (0.0%)
All	All	0.16	1/66790 (0.0%)	0.40	31/90550 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	143	PRO	CG-CD	-8.16	1.23	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	143	PRO	N-CD-CG	-11.44	86.05	103.20
13	N	143	PRO	CA-N-CD	-8.28	100.40	112.00
44	w	243	LYS	N-CA-C	7.87	119.94	111.36
1	A	120	GLY	N-CA-C	7.38	121.59	112.73
1	A	318	ILE	CA-C-N	7.33	126.83	118.85

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3280	95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1412	0	1363	36	0
3	C	1248	0	1254	16	0
4	E	971	0	975	20	0
5	F	691	0	704	9	0
6	G	693	0	671	27	0
6	X	696	0	680	33	0
7	H	910	0	950	16	0
8	I	780	0	808	18	0
9	J	2359	0	2402	40	0
10	K	355	0	329	15	0
11	L	1016	0	1016	18	0
12	M	5296	0	5326	78	0
13	N	1204	0	1162	14	0
14	O	1671	0	1673	48	0
15	P	1738	0	1693	22	0
16	Q	3377	0	3319	69	0
17	S	567	0	565	8	0
18	T	741	0	702	7	0
19	U	643	0	642	6	0
20	V	1021	0	1027	20	0
21	W	1173	0	1166	23	0
22	Y	597	0	537	11	0
23	Z	674	0	643	11	0
24	a	1165	0	1174	23	0
25	b	879	0	899	27	0
26	c	1315	0	1208	26	0
27	d	1461	0	1429	17	0
28	e	890	0	837	16	0
29	f	342	0	341	3	0
30	g	1000	0	994	23	0
31	h	867	0	871	13	0
32	i	2710	0	2874	84	0
33	j	800	0	855	26	0
34	k	748	0	799	22	0
35	l	4782	0	4929	117	0
36	m	948	0	960	24	0
37	n	479	0	486	11	0
38	o	1062	0	1072	11	0
39	p	1534	0	1470	29	0
40	r	3631	0	3839	77	0
41	s	2394	0	2508	77	0
42	u	1398	0	1378	22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1028	0	980	23	0
44	w	2582	0	2531	68	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	0	0
45	M	16	0	0	0	0
46	A	31	0	19	4	0
47	A	44	0	27	4	0
48	C	47	0	71	5	0
48	U	51	0	82	4	0
48	V	51	0	82	11	0
48	l	139	0	209	35	0
48	m	41	0	59	13	0
48	s	51	0	82	3	0
49	C	52	0	88	4	0
49	V	52	0	88	4	0
49	e	52	0	88	8	0
49	i	52	0	88	6	0
49	j	52	0	88	3	0
49	n	52	0	88	7	0
50	G	35	0	0	2	0
50	X	35	0	0	1	0
51	J	48	0	23	3	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	N	51	0	46	4	0
54	V	71	0	92	14	0
54	a	91	0	132	26	0
54	i	66	0	76	11	0
54	l	199	0	307	16	0
54	n	78	0	103	12	0
54	r	100	0	156	14	0
55	T	1	0	0	0	0
56	s	28	0	31	8	0
57	w	27	0	11	10	0
All	All	66820	0	67457	1272	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 9.

The worst 5 of 1272 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)
54:n:102:CDL:C82	54:r:714:CDL:H852	1.45	1.43
37:n:30:ARG:NE	54:n:102:CDL:OA4	1.70	1.23
1:A:48:ARG:HD2	10:K:70:ASN:O	1.41	1.21
6:X:93:ILE:CG2	6:X:108:LEU:HD23	1.71	1.20
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.19

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
6	G	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
7	H	110/112 (98%)	103 (94%)	7 (6%)	0	100	100
8	I	93/112 (83%)	81 (87%)	11 (12%)	1 (1%)	11	29
9	J	289/341 (85%)	278 (96%)	10 (4%)	1 (0%)	36	60
10	K	40/42 (95%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	668 (97%)	19 (3%)	1 (0%)	48	73
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	203 (94%)	11 (5%)	1 (0%)	24	48
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	41
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
29	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	115 (97%)	3 (2%)	1 (1%)	16	37
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	338 (98%)	7 (2%)	0	100	100
33	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
34	k	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
35	l	601/603 (100%)	578 (96%)	23 (4%)	0	100	100
36	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
39	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	21	44
40	r	457/459 (100%)	445 (97%)	12 (3%)	0	100	100
41	s	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	36	60
42	u	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
43	v	122/131 (93%)	112 (92%)	10 (8%)	0	100	100
44	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	8029/8315 (97%)	7720 (96%)	301 (4%)	8 (0%)	49	73

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	77	ALA
8	I	41	LEU
12	M	283	GLU
30	g	3	MET
9	J	38	HIS

### 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	345/345 (100%)	344 (100%)	1 (0%)	86	94
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	76/76 (100%)	76 (100%)	0	100	100
6	G	76/81 (94%)	75 (99%)	1 (1%)	61	83
6	X	77/81 (95%)	76 (99%)	1 (1%)	61	83
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	86 (99%)	1 (1%)	65	85
9	J	255/295 (86%)	255 (100%)	0	100	100
10	K	41/41 (100%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	87
12	M	580/580 (100%)	579 (100%)	1 (0%)	87	95
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	183/183 (100%)	183 (100%)	0	100	100
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	361/370 (98%)	361 (100%)	0	100	100
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	101/101 (100%)	101 (100%)	0	100	100
21	W	123/123 (100%)	123 (100%)	0	100	100
22	Y	62/63 (98%)	62 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	122 (100%)	0	100	100
25	b	98/119 (82%)	98 (100%)	0	100	100
26	c	141/141 (100%)	141 (100%)	0	100	100
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	99/99 (100%)	99 (100%)	0	100	100
29	f	35/38 (92%)	35 (100%)	0	100	100
30	g	108/108 (100%)	108 (100%)	0	100	100
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	310 (100%)	1 (0%)	86	94
33	j	88/99 (89%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	536/537 (100%)	533 (99%)	3 (1%)	78	91
36	m	98/141 (70%)	98 (100%)	0	100	100
37	n	53/53 (100%)	52 (98%)	1 (2%)	50	77
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	159 (100%)	0	100	100
40	r	410/410 (100%)	409 (100%)	1 (0%)	87	95
41	s	263/275 (96%)	260 (99%)	3 (1%)	65	85
42	u	153/153 (100%)	153 (100%)	0	100	100
43	v	104/115 (90%)	104 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	7065/7238 (98%)	7050 (100%)	15 (0%)	85	95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	l	70	THR
41	s	22	LEU
35	l	71	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
41	s	26	LYS
40	r	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
40	r	251	ASN
40	r	390	ASN
43	v	84	GLN
16	Q	160	ASN
15	P	196	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
16	2MR	Q	118	16	10,12,13	2.00	1 (10%)	5,13,15	6.08	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.73	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.32	130.78	119.48
16	Q	118	2MR	CD-NE-CZ	4.53	131.87	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.28	130.70	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
45	SF4	A	501	1	0,12,12	-	-	-	-	-
45	SF4	B	301	2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.08	7 (7%)
54	CDL	r	714	-	99,99,99	1.11	9 (9%)	105,111,111	0.87	4 (3%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
45	SF4	B	302	2	0,12,12	-	-	-	-	-
54	CDL	V	203	-	70,70,99	1.09	4 (5%)	76,82,111	1.13	7 (9%)
49	PLX	e	201	-	51,51,51	1.20	5 (9%)	53,59,59	0.63	1 (1%)
48	PEE	U	101	-	50,50,50	1.17	6 (12%)	53,55,55	0.98	2 (3%)
54	CDL	n	102	-	77,77,99	1.03	4 (5%)	83,89,111	1.12	4 (4%)
50	8Q1	X	201	-	32,34,34	2.35	7 (21%)	39,43,43	1.69	10 (25%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
52	FES	M	803	12	0,4,4	-	-	-	-	-
48	PEE	l	719	-	45,45,50	1.24	6 (13%)	48,50,55	1.01	2 (4%)
48	PEE	l	720	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
48	PEE	V	202	-	50,50,50	1.17	6 (12%)	53,55,55	1.02	2 (3%)
48	PEE	l	718	-	46,46,50	1.22	6 (13%)	49,51,55	1.03	2 (4%)
51	NDP	J	401	-	51,52,52	4.26	24 (47%)	71,80,80	2.23	14 (19%)
49	PLX	C	312	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
54	CDL	N	202	-	50,50,99	1.28	4 (8%)	56,62,111	1.35	7 (12%)
54	CDL	l	712	-	98,98,99	1.11	8 (8%)	104,110,111	0.89	4 (3%)
56	UQ	s	403	-	28,28,63	3.32	8 (28%)	36,37,79	2.68	11 (30%)
48	PEE	C	311	-	46,46,50	1.23	6 (13%)	49,51,55	0.95	2 (4%)
50	8Q1	G	201	-	32,34,34	2.31	7 (21%)	39,43,43	1.76	12 (30%)
54	CDL	l	713	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
47	NAI	A	503	-	47,48,48	3.99	22 (46%)	64,73,73	1.71	12 (18%)
57	ADP	w	401	-	28,29,29	3.19	9 (32%)	43,45,45	1.88	8 (18%)
49	PLX	n	101	-	51,51,51	0.60	0	53,59,59	0.70	0
49	PLX	i	705	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
49	PLX	V	205	-	51,51,51	1.20	5 (9%)	53,59,59	0.62	1 (1%)
46	FMN	A	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.20	7 (14%)
54	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.21	5 (7%)
52	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	s	401	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
48	PEE	m	202	-	40,40,50	1.16	5 (12%)	43,45,55	0.99	2 (4%)
49	PLX	j	203	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CDL	a	201	-	-	26/101/101/110	-
45	SF4	A	501	1	-	-	0/6/5/5
54	CDL	r	714	-	-	66/110/110/110	-
45	SF4	B	301	2	-	-	0/6/5/5
54	CDL	V	203	-	-	43/81/81/110	-
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
49	PLX	e	201	-	-	36/55/55/55	-
48	PEE	U	101	-	-	25/54/54/54	-
54	CDL	n	102	-	-	27/88/88/110	-
50	8Q1	X	201	-	-	26/41/41/41	-
45	SF4	M	801	12	-	-	0/6/5/5
52	FES	M	803	12	-	-	0/1/1/1
48	PEE	l	719	-	-	21/49/49/54	-
48	PEE	l	720	-	-	24/49/49/54	-
48	PEE	V	202	-	-	23/54/54/54	-
48	PEE	l	718	-	-	19/50/50/54	-
51	NDP	J	401	-	-	7/34/77/77	0/5/5/5
49	PLX	C	312	-	-	25/55/55/55	-
54	CDL	N	202	-	-	25/61/61/110	-
54	CDL	l	712	-	-	57/109/109/110	-
56	UQ	s	403	-	-	8/21/45/87	0/1/1/1
48	PEE	C	311	-	-	19/50/50/54	-
50	8Q1	G	201	-	-	16/41/41/41	-
54	CDL	l	713	-	-	55/110/110/110	-
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
49	PLX	n	101	-	-	17/55/55/55	-
49	PLX	i	705	-	-	25/55/55/55	-
49	PLX	V	205	-	-	27/55/55/55	-
46	FMN	A	502	-	-	5/18/18/18	0/3/3/3
54	CDL	i	401	-	-	25/76/76/110	-
52	FES	O	301	14	-	-	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	s	401	-	-	25/54/54/54	-
48	PEE	m	202	-	-	22/44/44/54	-
49	PLX	j	203	-	-	27/55/55/55	-
45	SF4	C	301	3	-	-	0/6/5/5

The worst 5 of 194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-12.71	1.25	1.53
51	J	401	NDP	O4D-C4D	10.71	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.52	1.26	1.53
51	J	401	NDP	C3D-C4D	-10.05	1.27	1.53
56	s	403	UQ	C13-C14	9.65	1.55	1.33

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	403	UQ	C7-C8-C9	-9.15	111.06	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.98	111.49	123.20
51	J	401	NDP	C6N-N1N-C2N	-6.83	112.01	119.32
51	J	401	NDP	C1D-N1N-C2N	-6.33	110.70	121.14
56	s	403	UQ	C12-C13-C14	-6.14	113.56	127.62

There are no chirality outliers.

5 of 731 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
47	A	503	NAI	C5B-O5B-PA-O1A
48	C	311	PEE	C1-O3P-P-O1P
48	C	311	PEE	C1-O3P-P-O4P

There are no ring outliers.

30 monomers are involved in 213 short contacts:

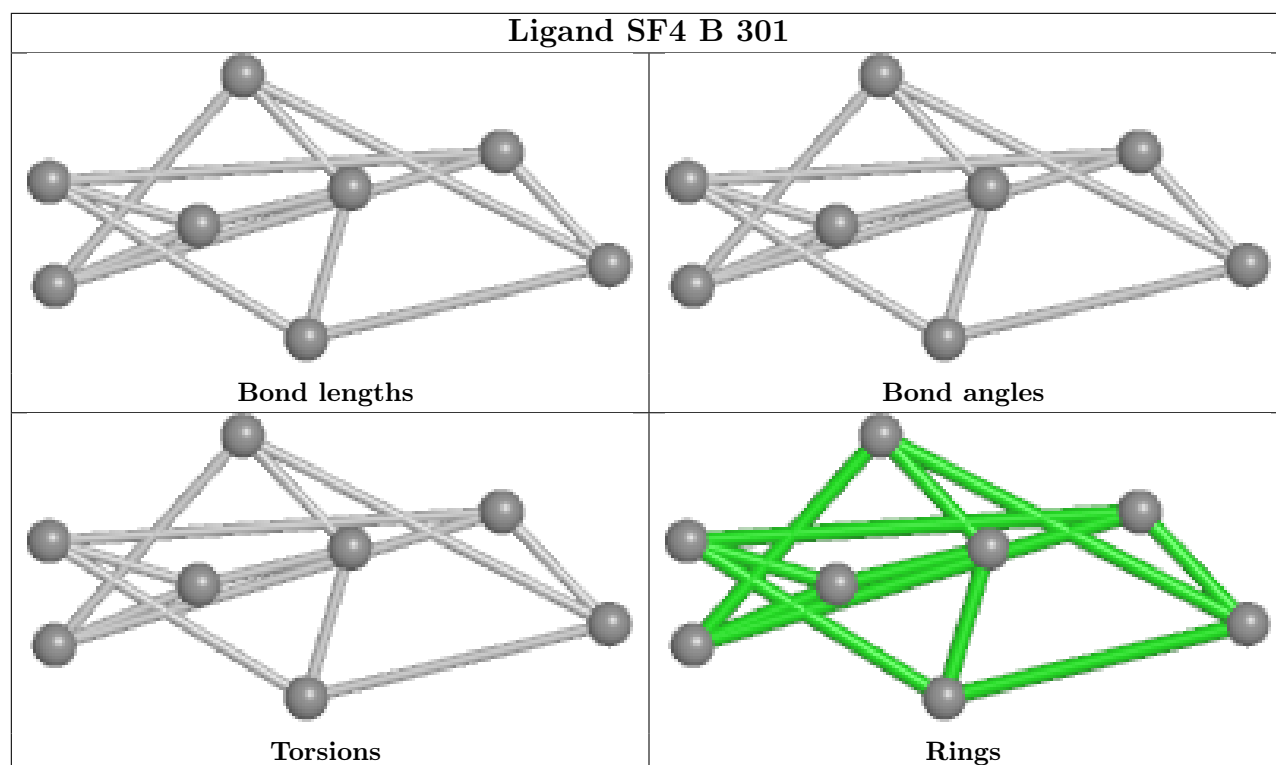
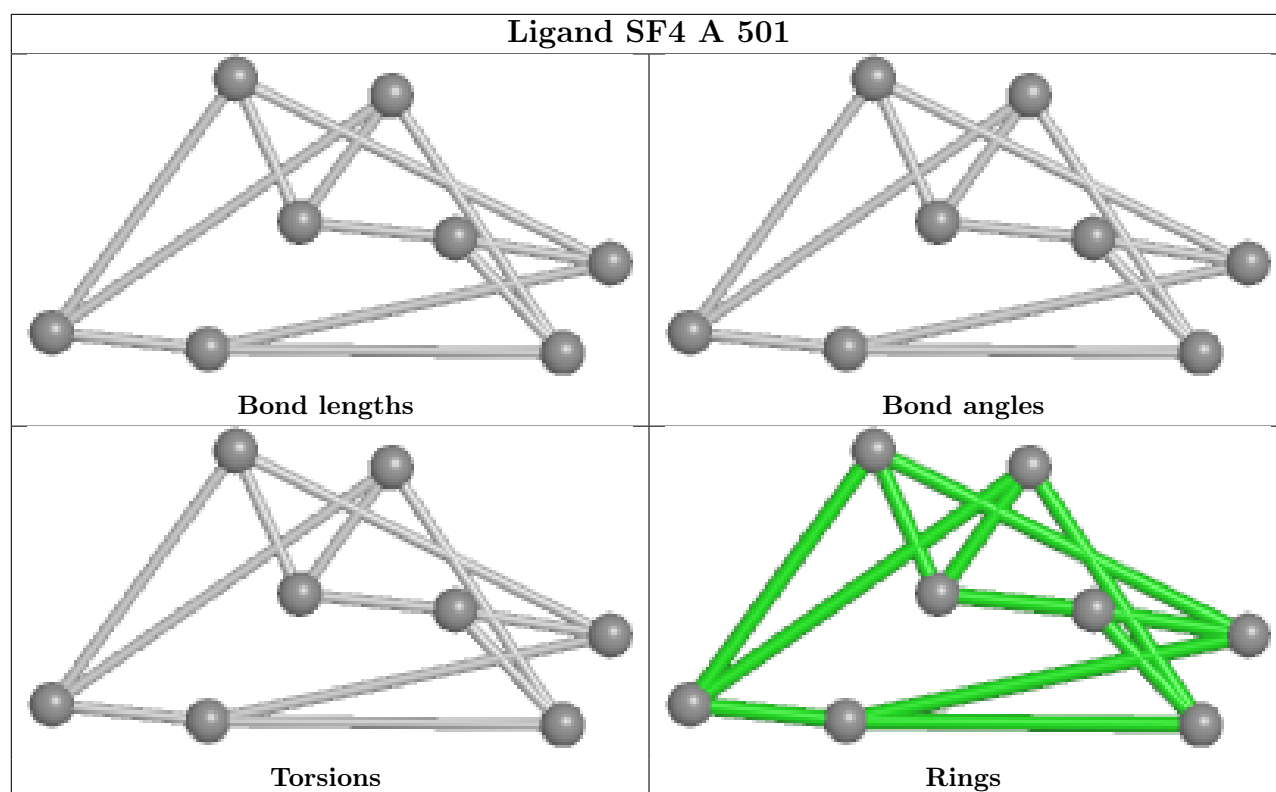
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	501	SF4	2	0
54	a	201	CDL	26	0
54	r	714	CDL	14	0

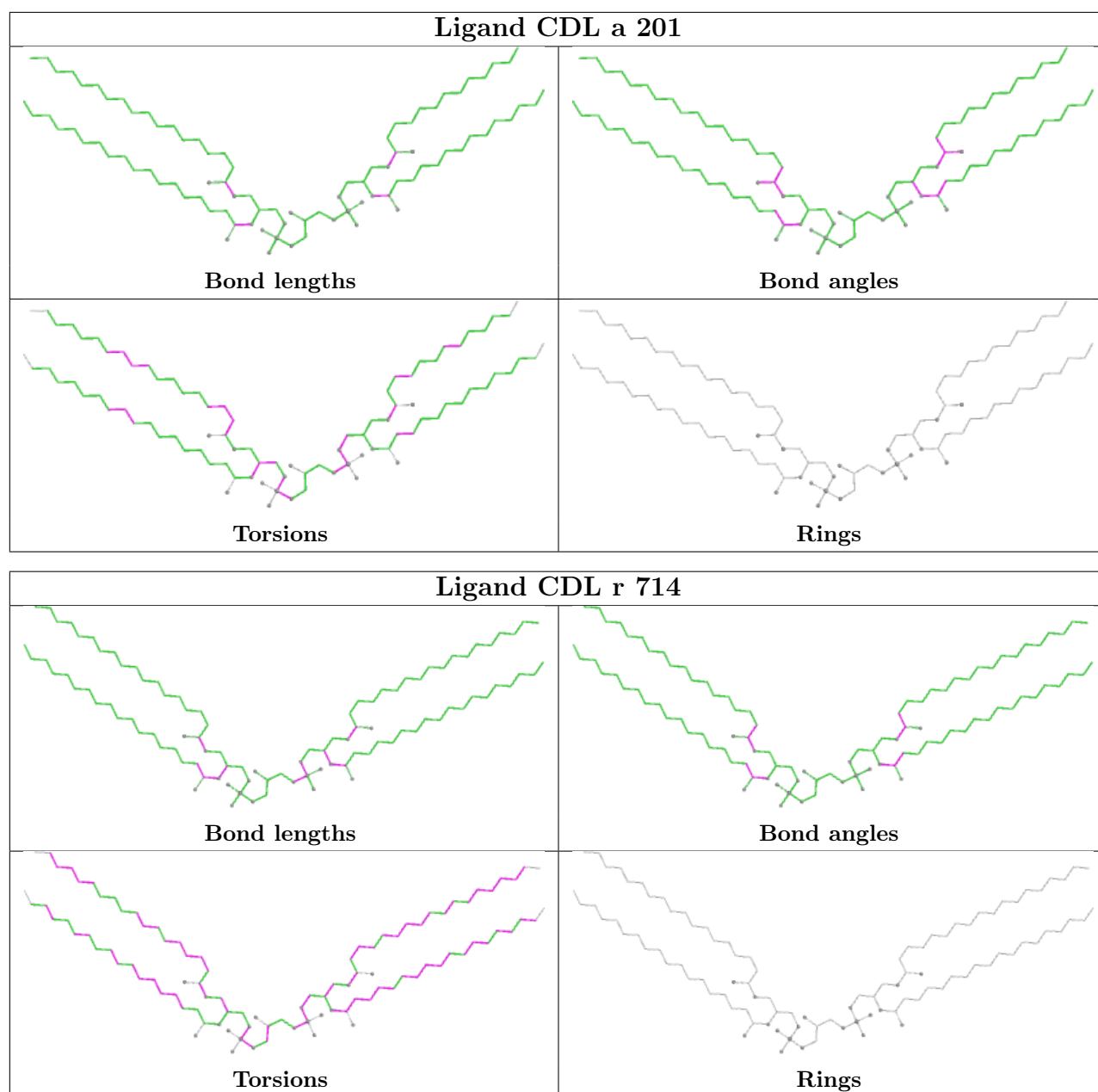
Continued on next page...

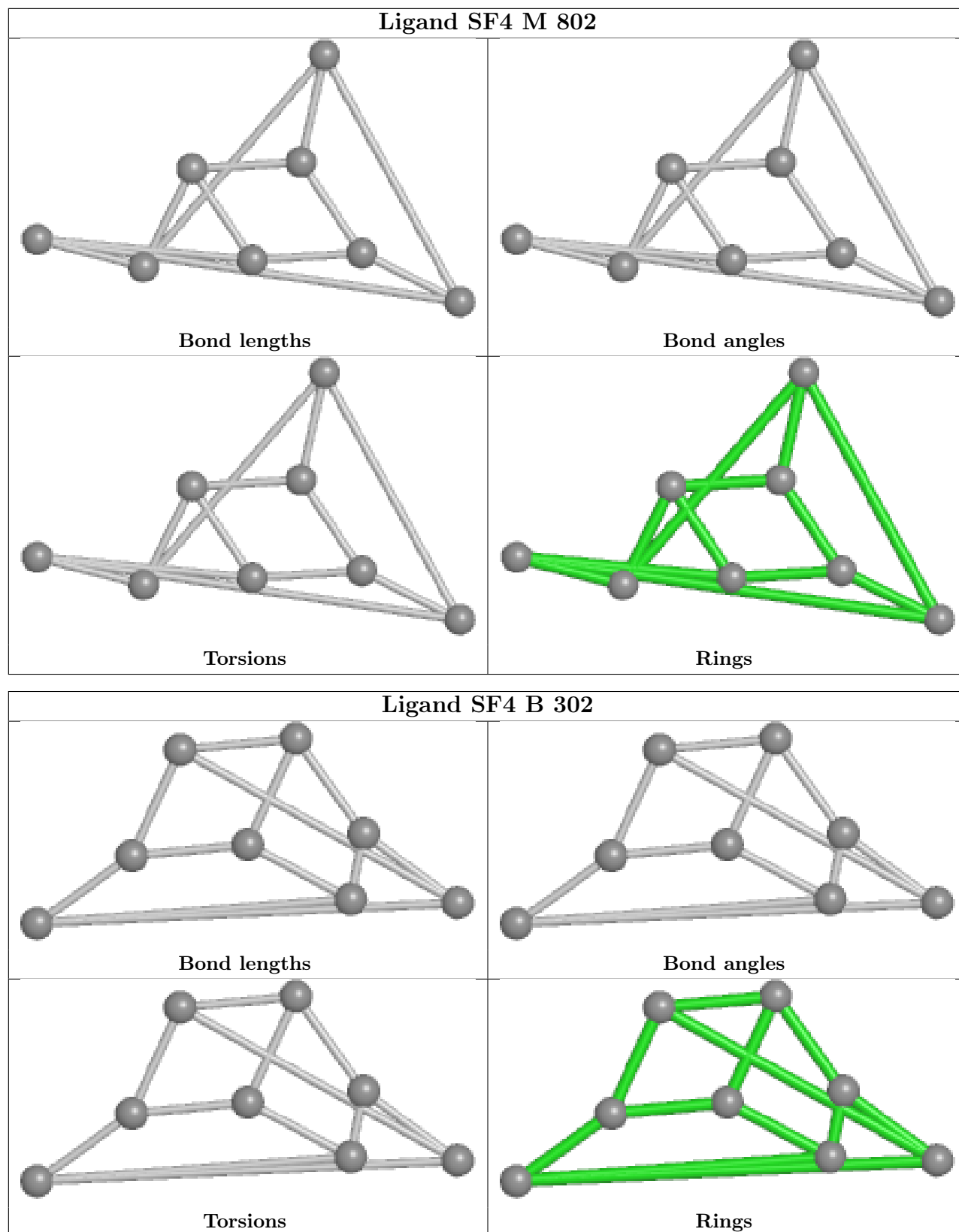
*Continued from previous page...*

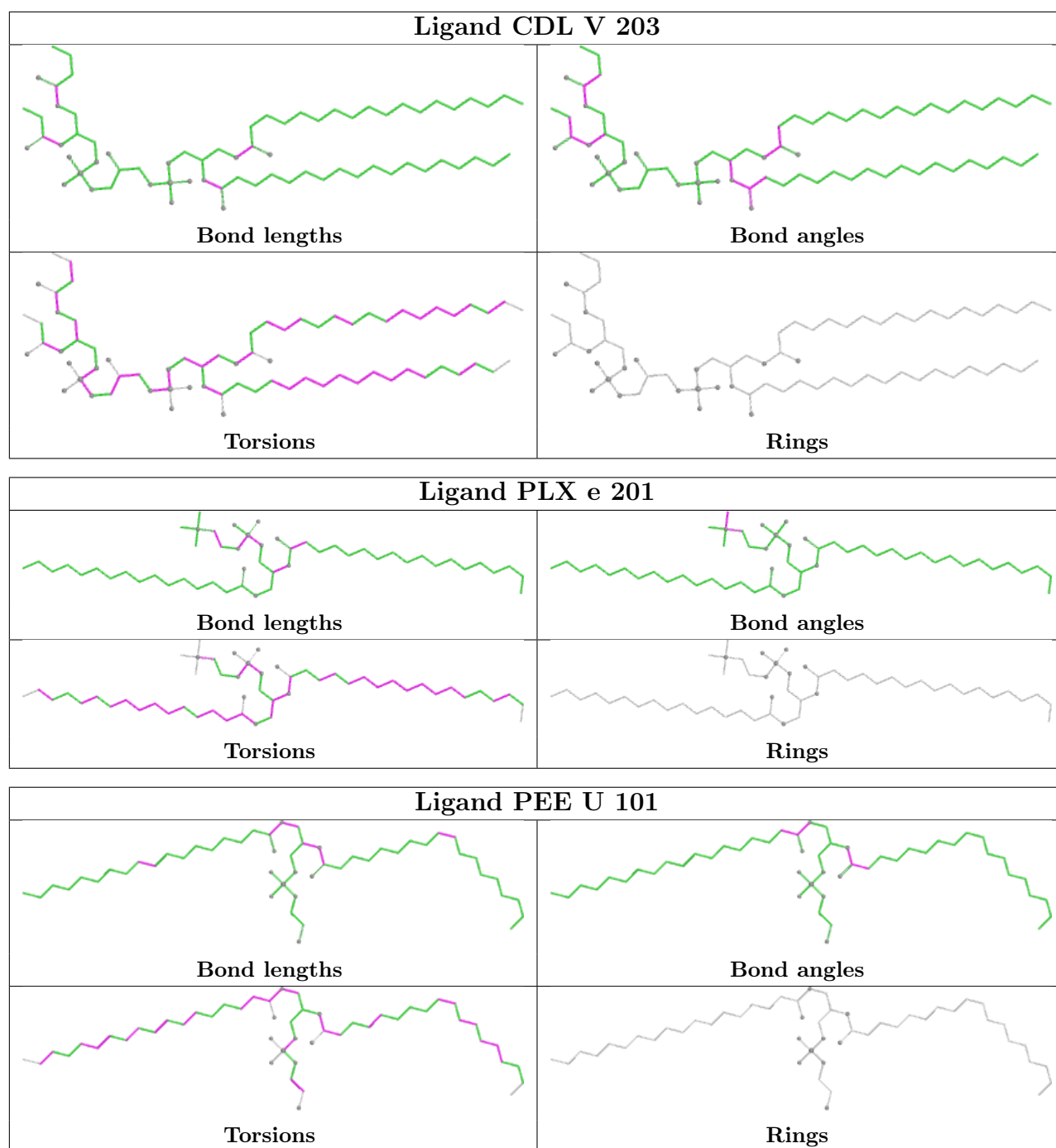
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	V	203	CDL	14	0
49	e	201	PLX	8	0
48	U	101	PEE	4	0
54	n	102	CDL	12	0
50	X	201	8Q1	1	0
48	l	719	PEE	2	0
48	l	720	PEE	15	0
48	V	202	PEE	11	0
48	l	718	PEE	18	0
51	J	401	NDP	3	0
49	C	312	PLX	4	0
54	N	202	CDL	4	0
54	l	712	CDL	12	0
56	s	403	UQ	8	0
48	C	311	PEE	5	0
50	G	201	8Q1	2	0
54	l	713	CDL	4	0
47	A	503	NAI	4	0
57	w	401	ADP	10	0
49	n	101	PLX	7	0
49	i	705	PLX	6	0
49	V	205	PLX	4	0
46	A	502	FMN	4	0
54	i	401	CDL	11	0
48	s	401	PEE	3	0
48	m	202	PEE	13	0
49	j	203	PLX	3	0

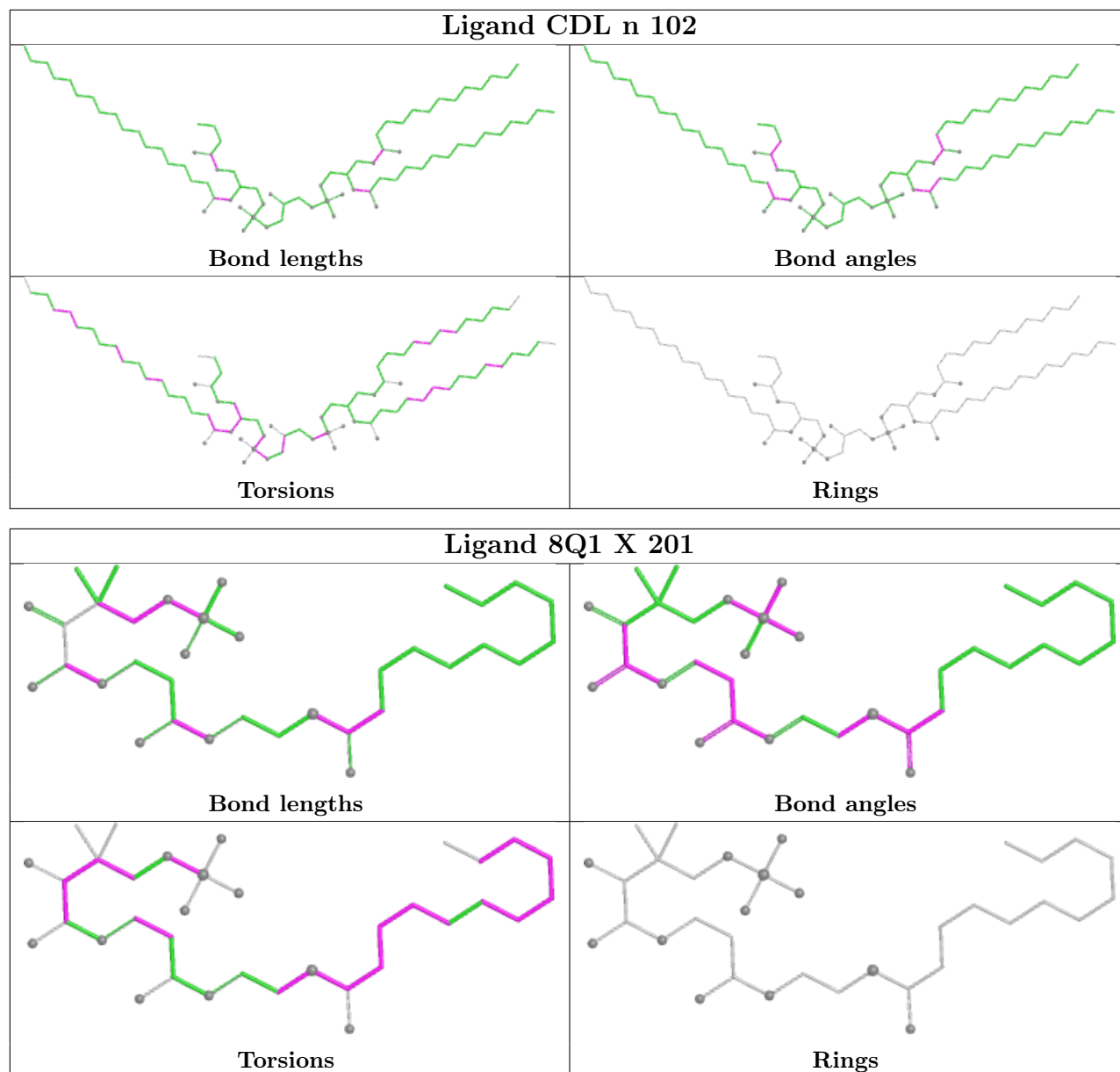
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

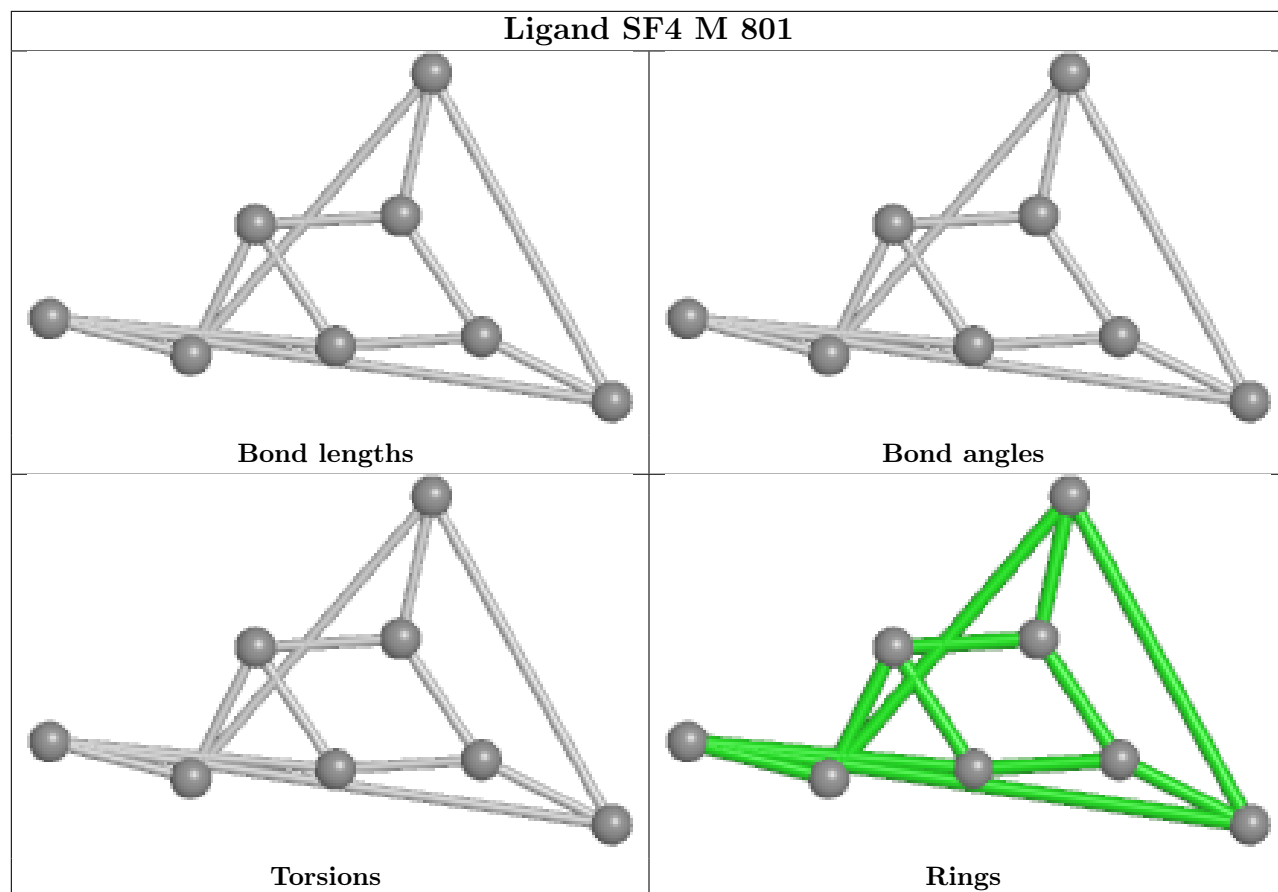


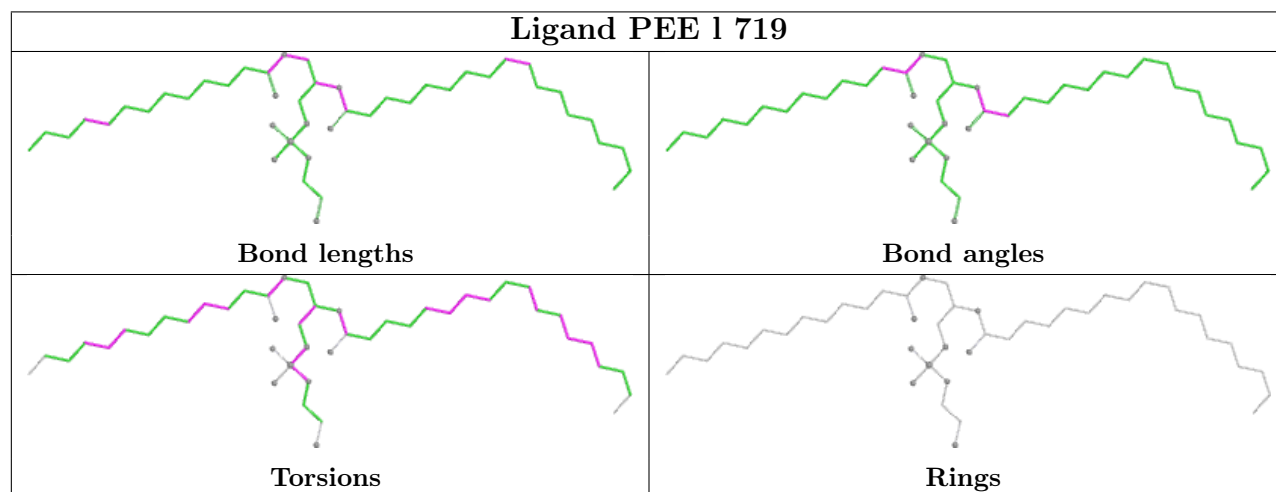
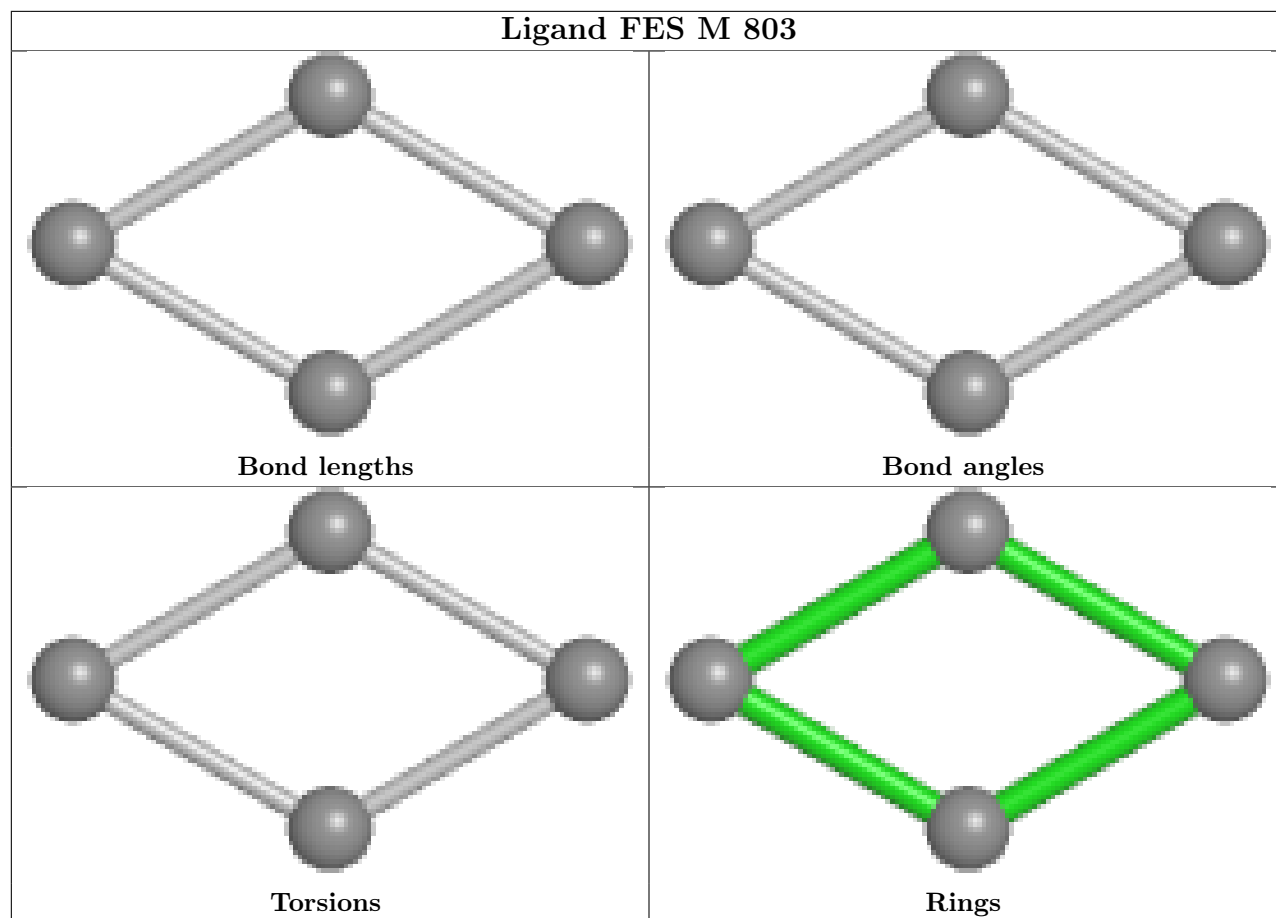


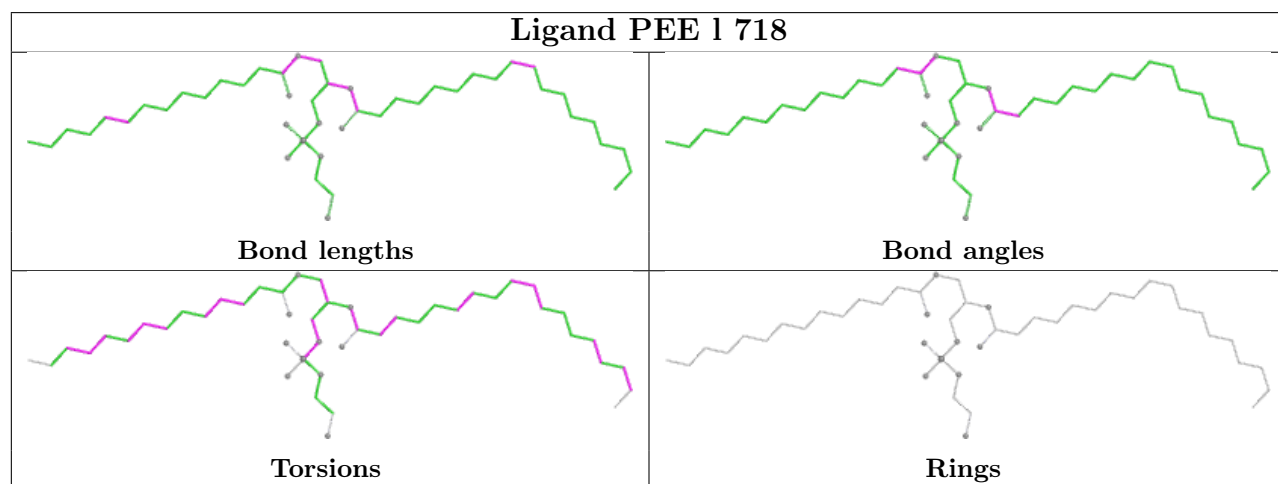
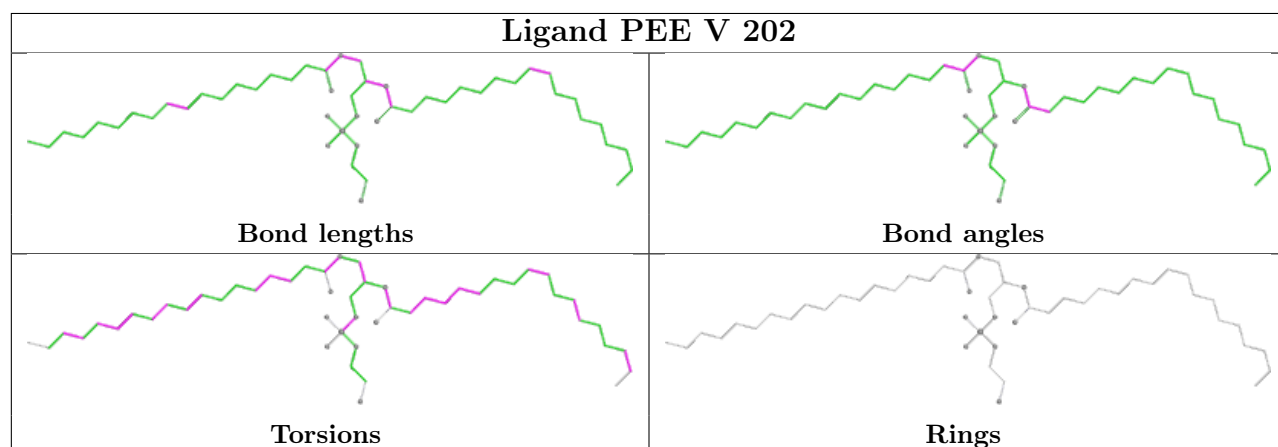
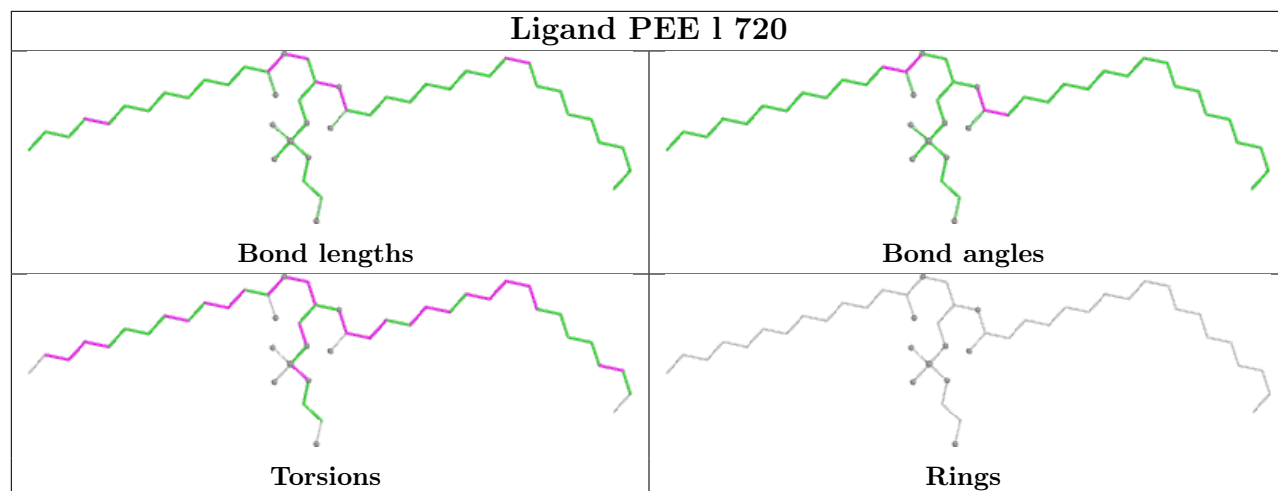


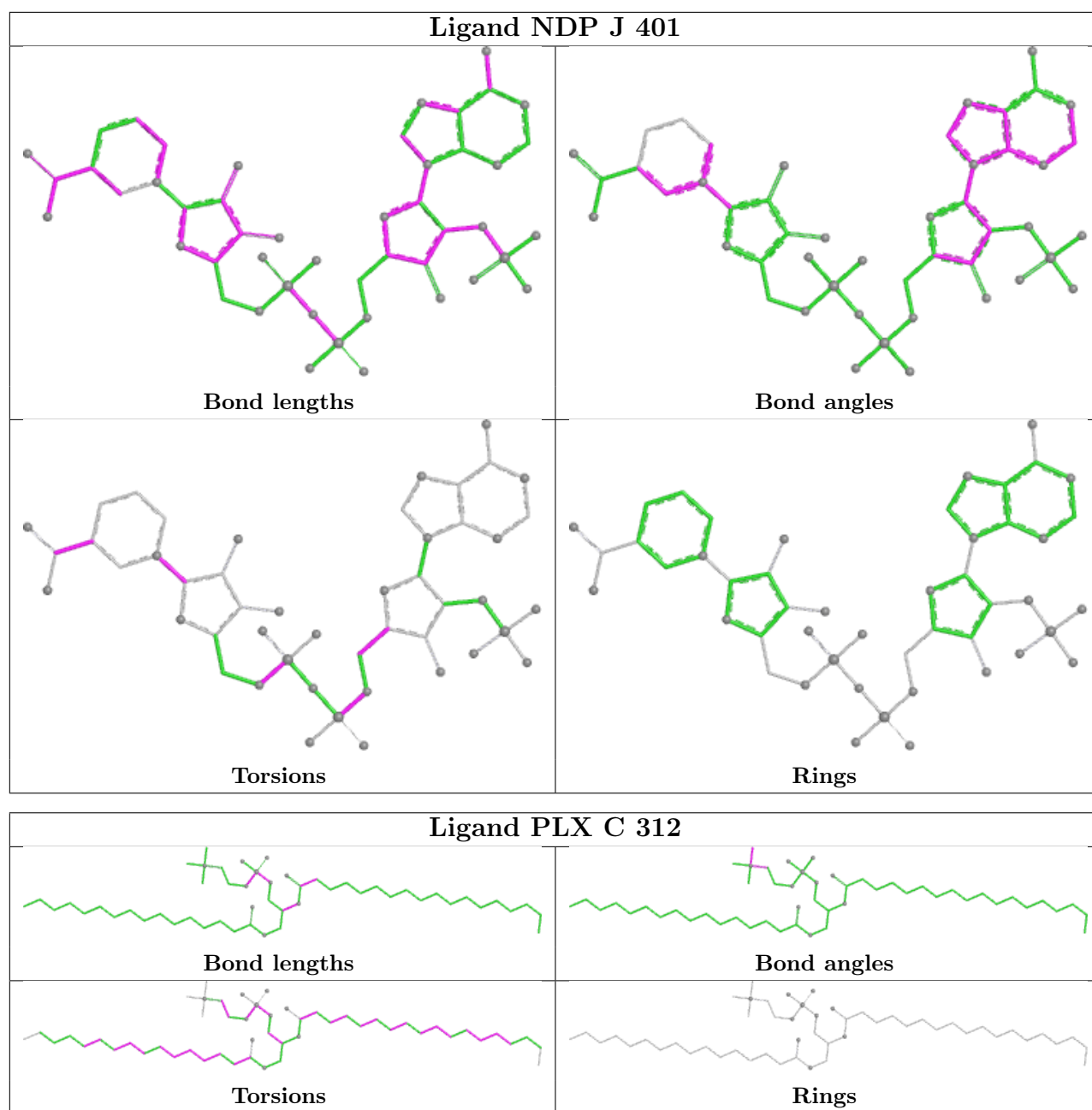


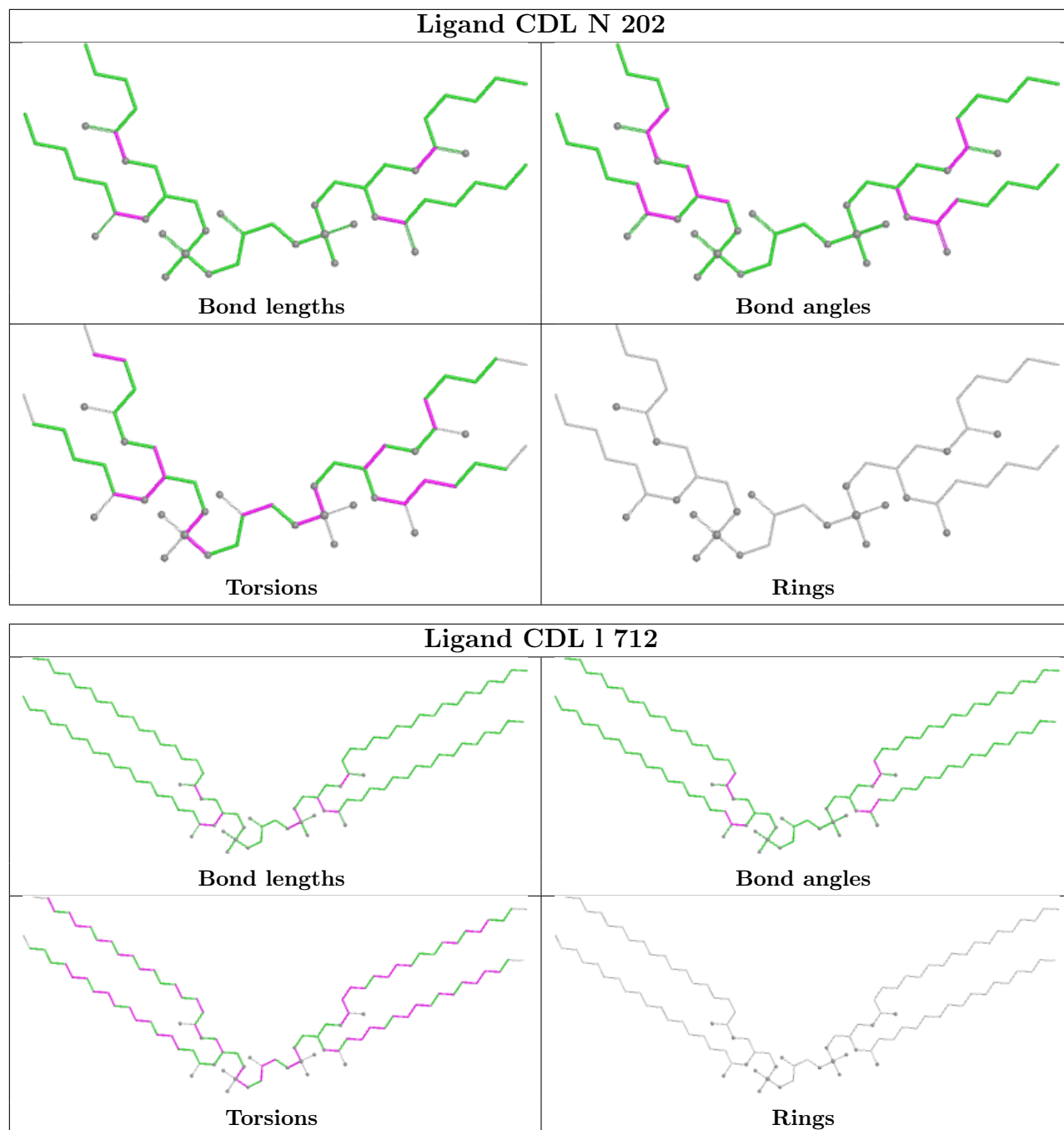


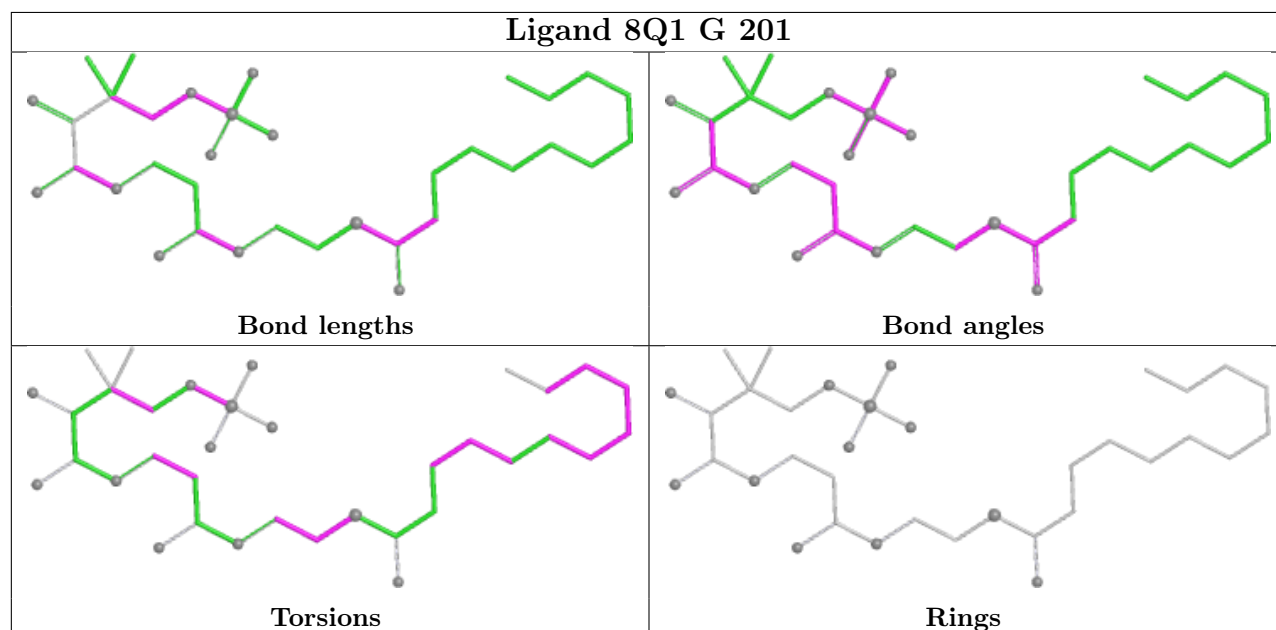
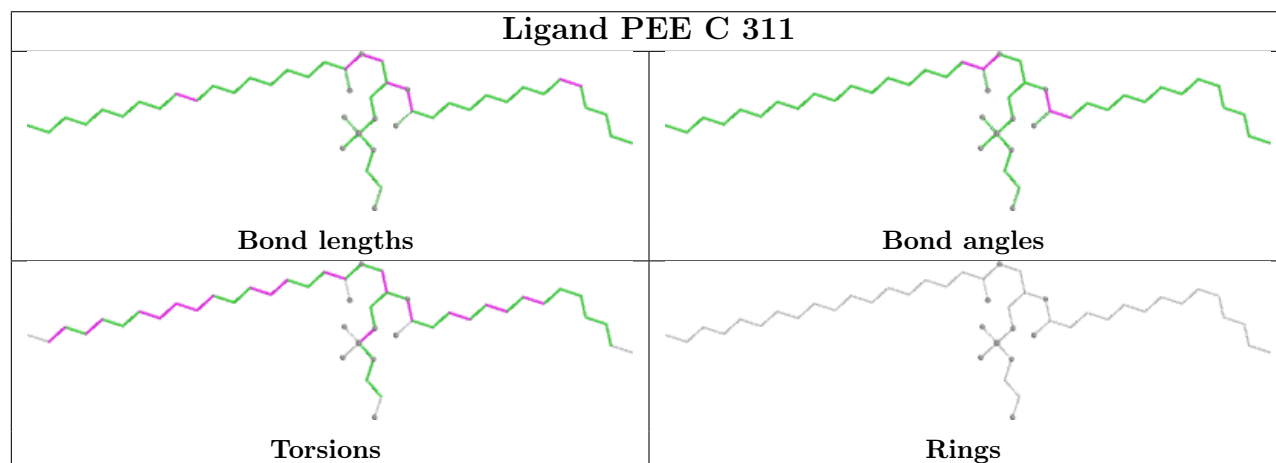
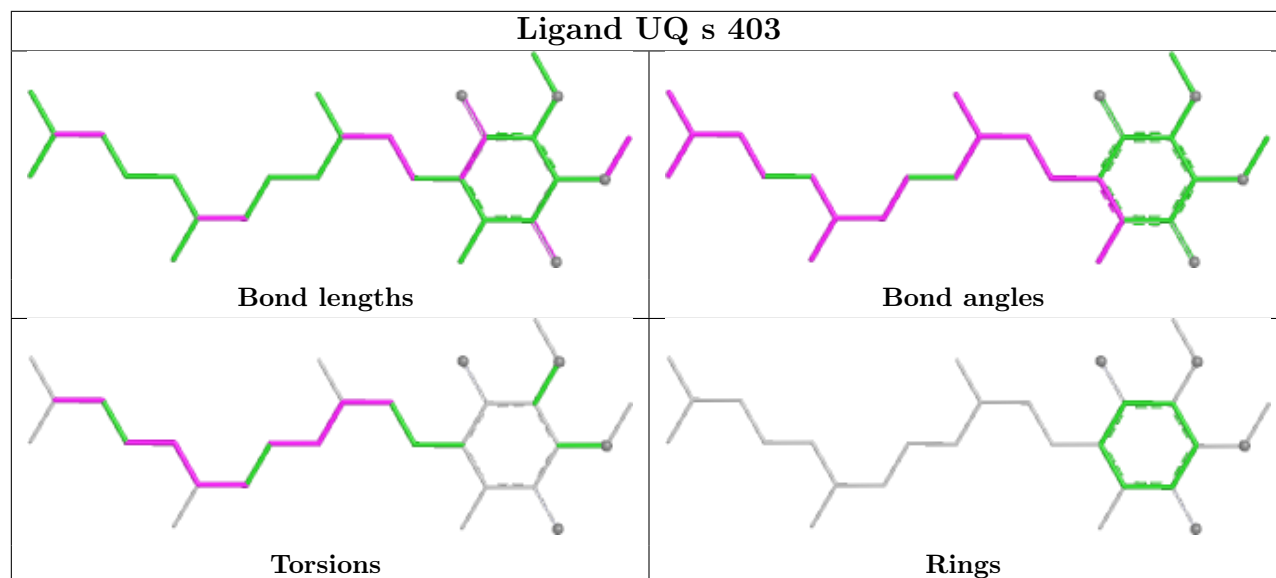


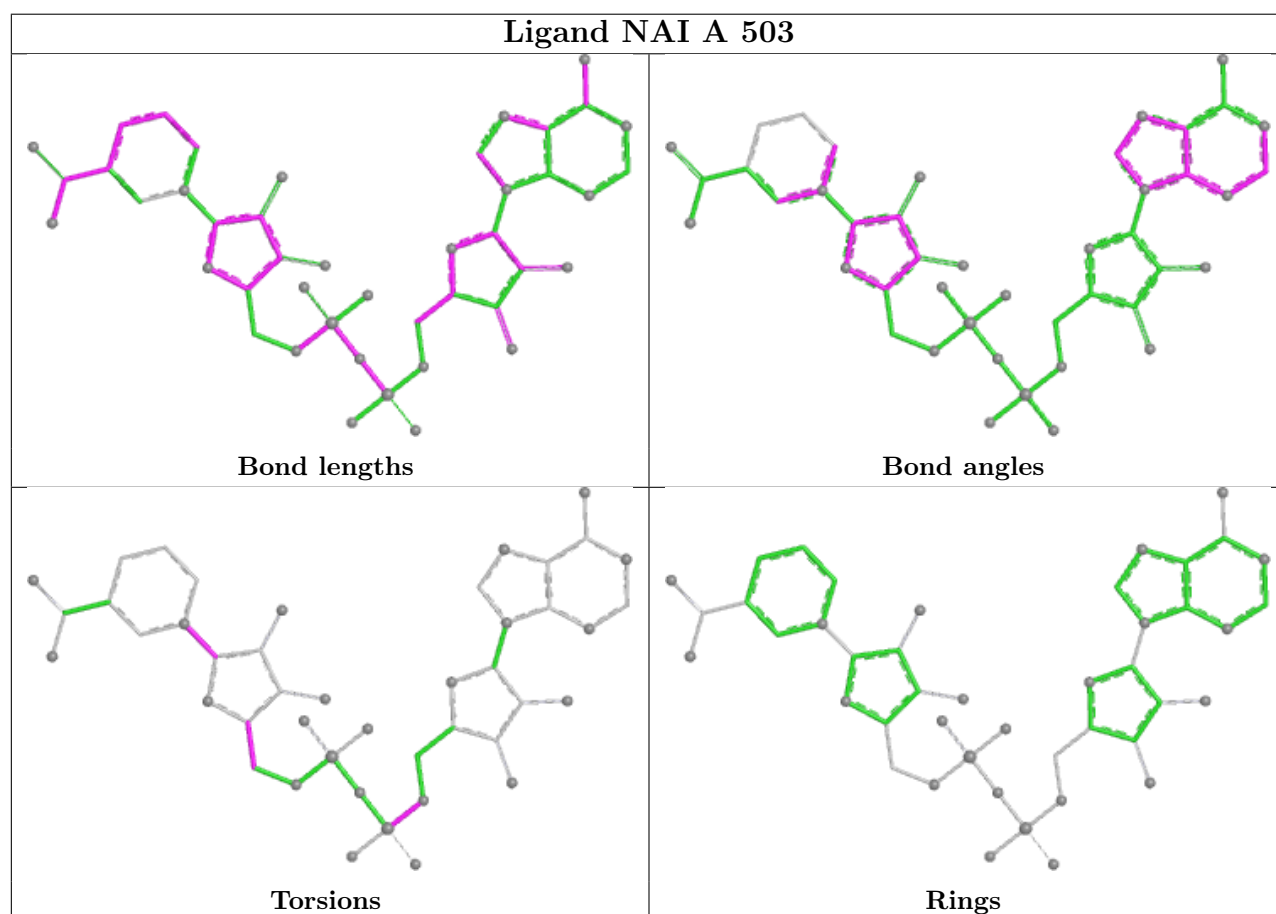
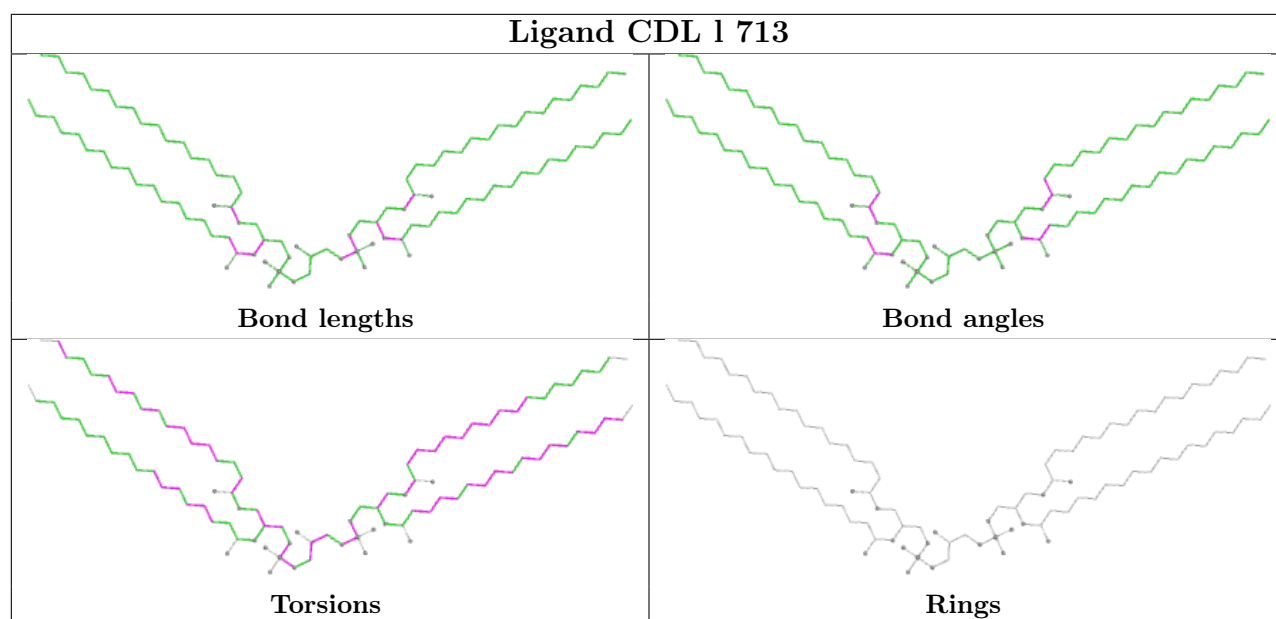


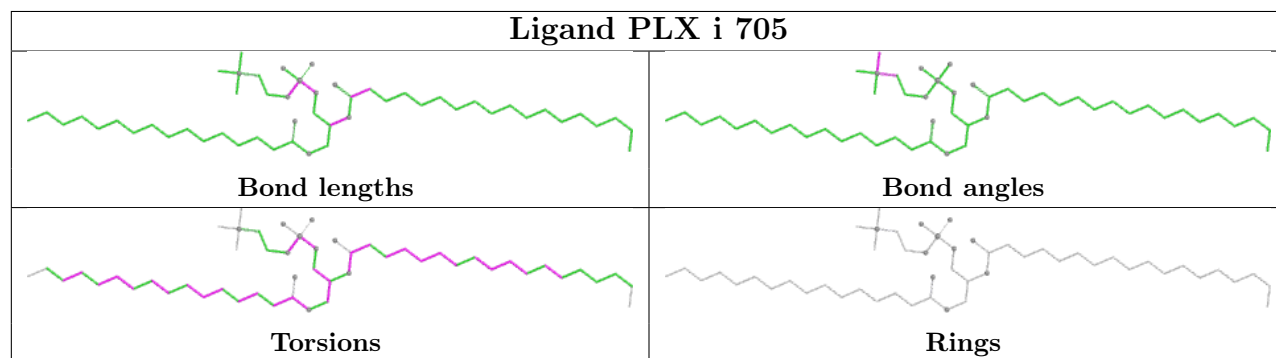
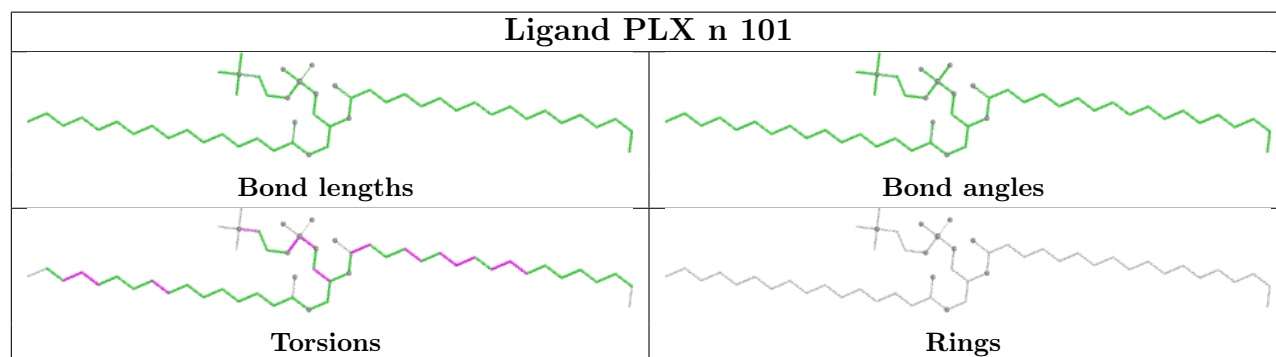
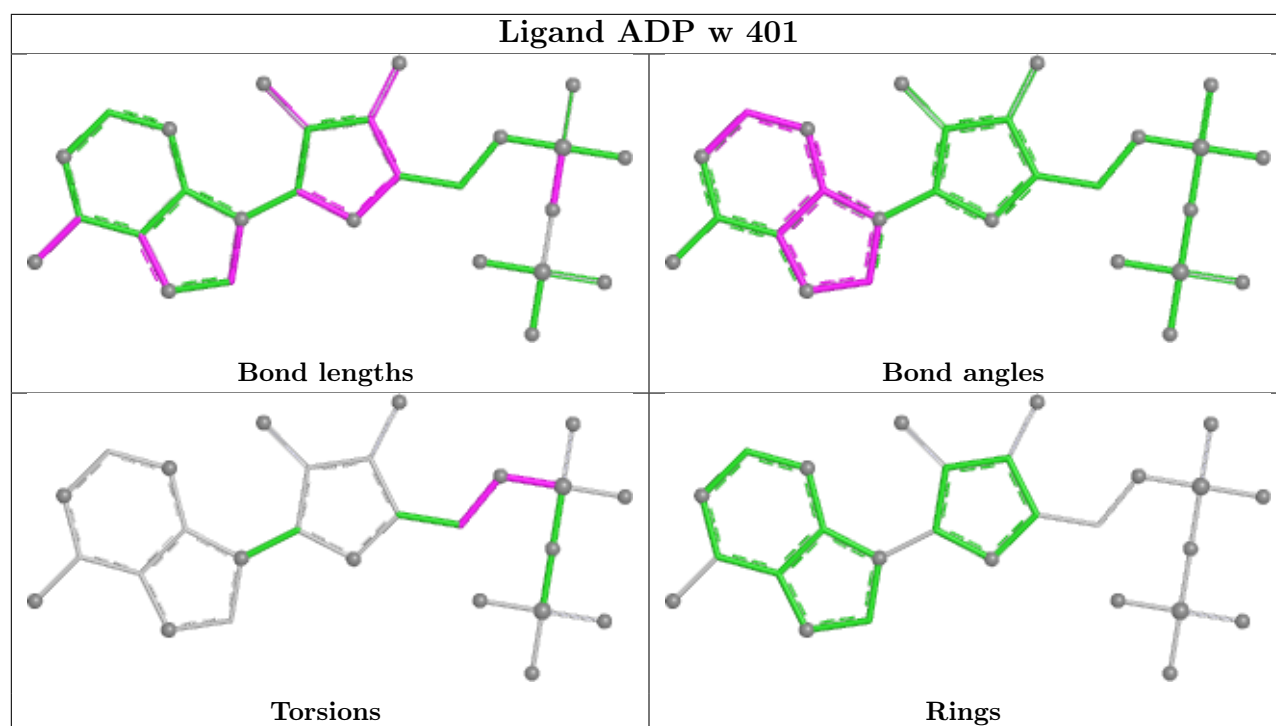


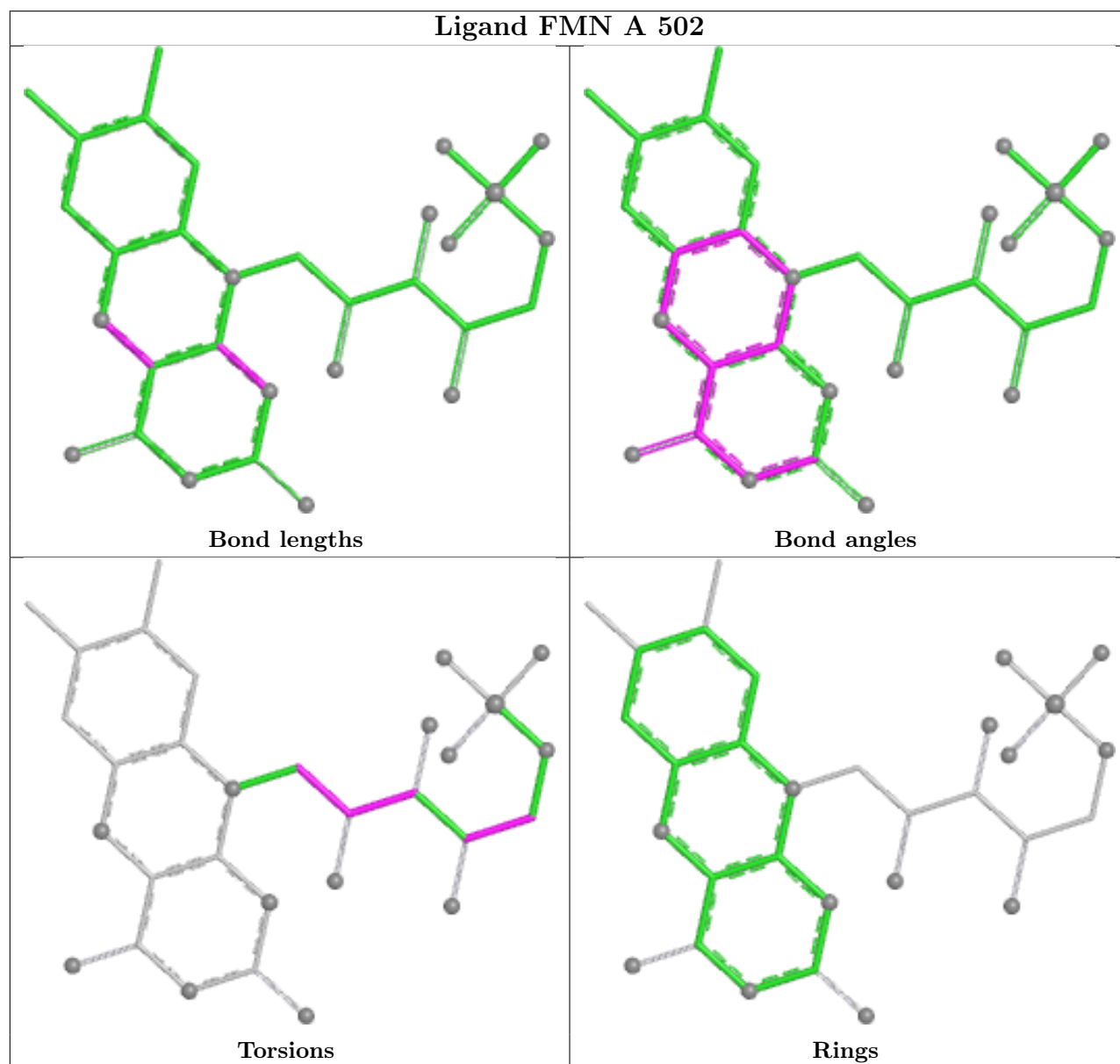
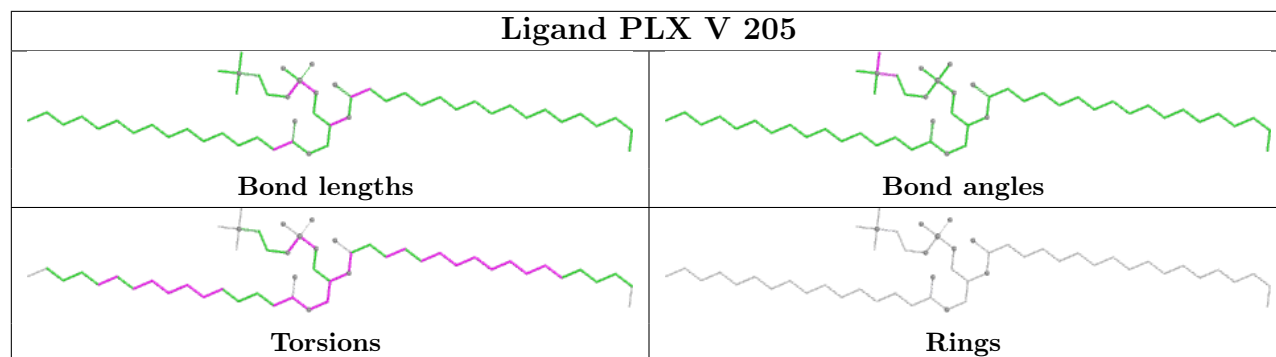


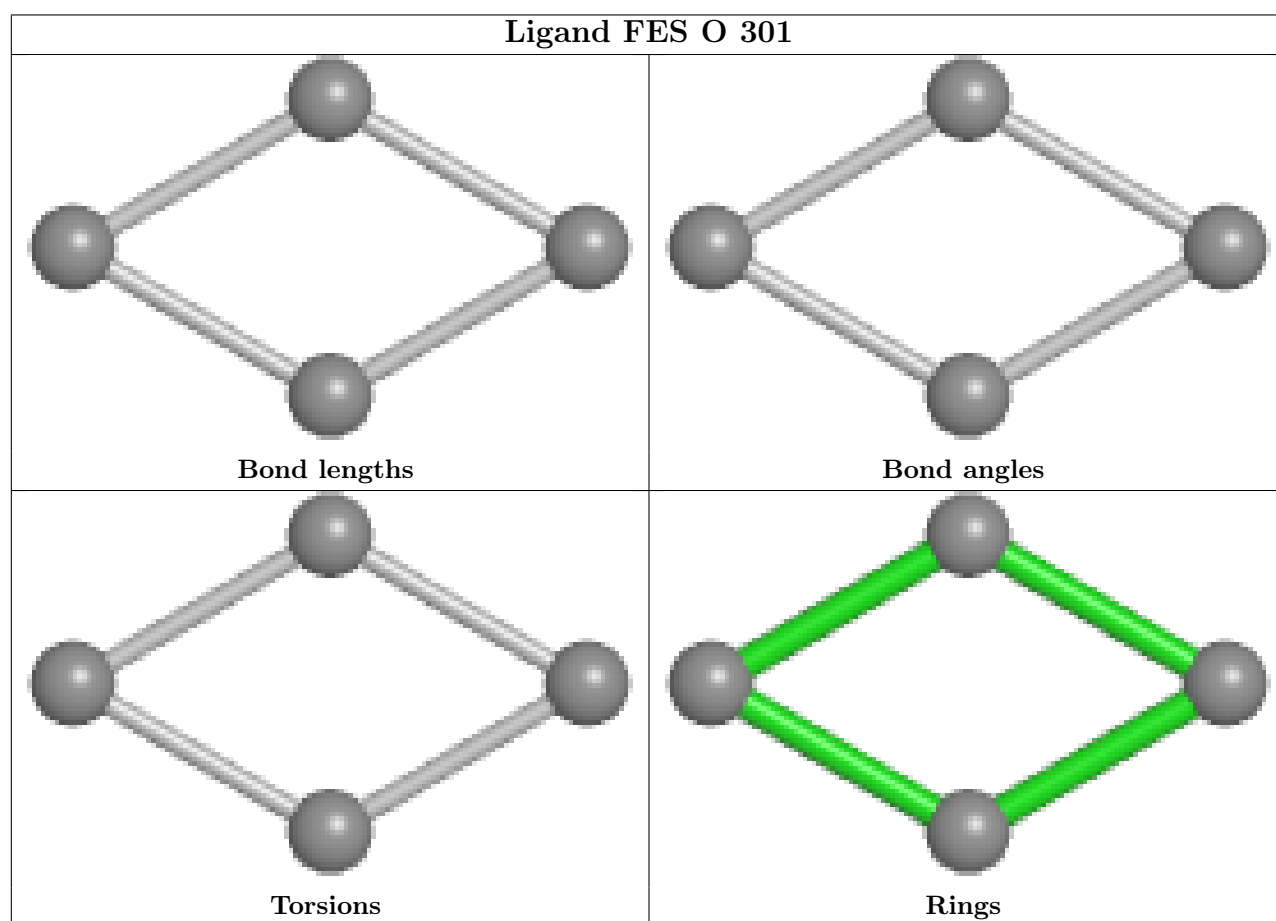
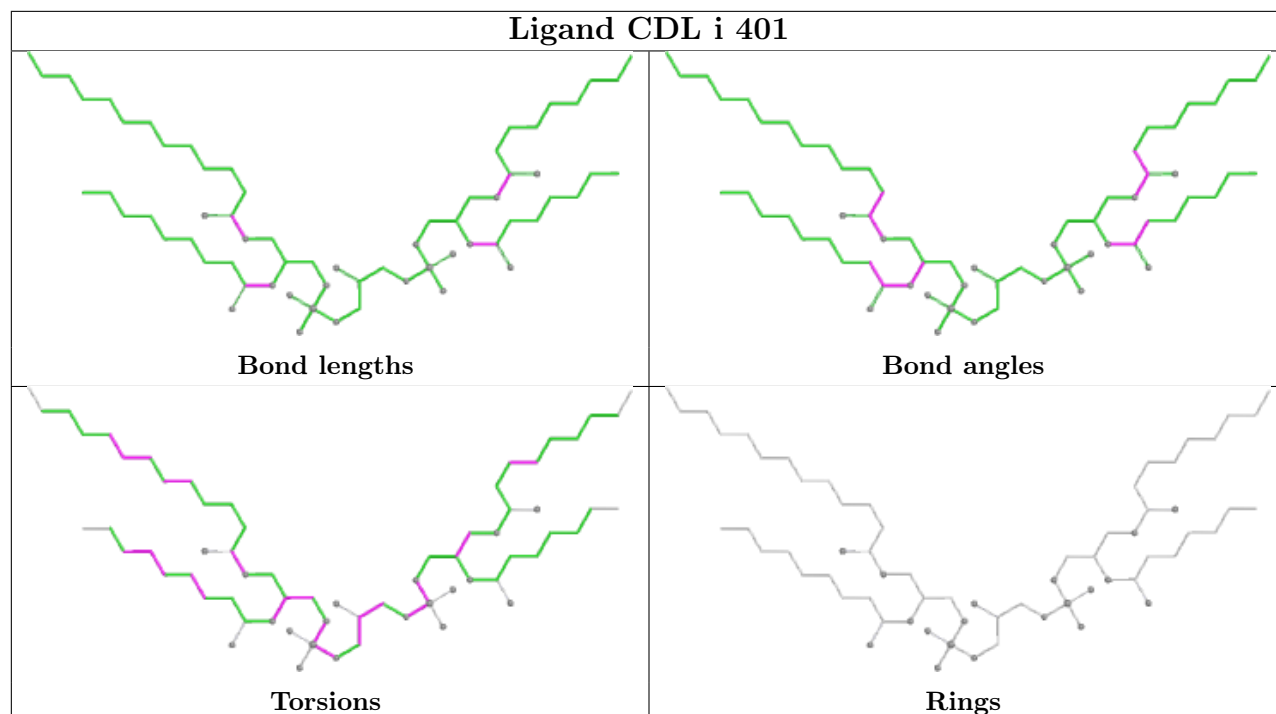


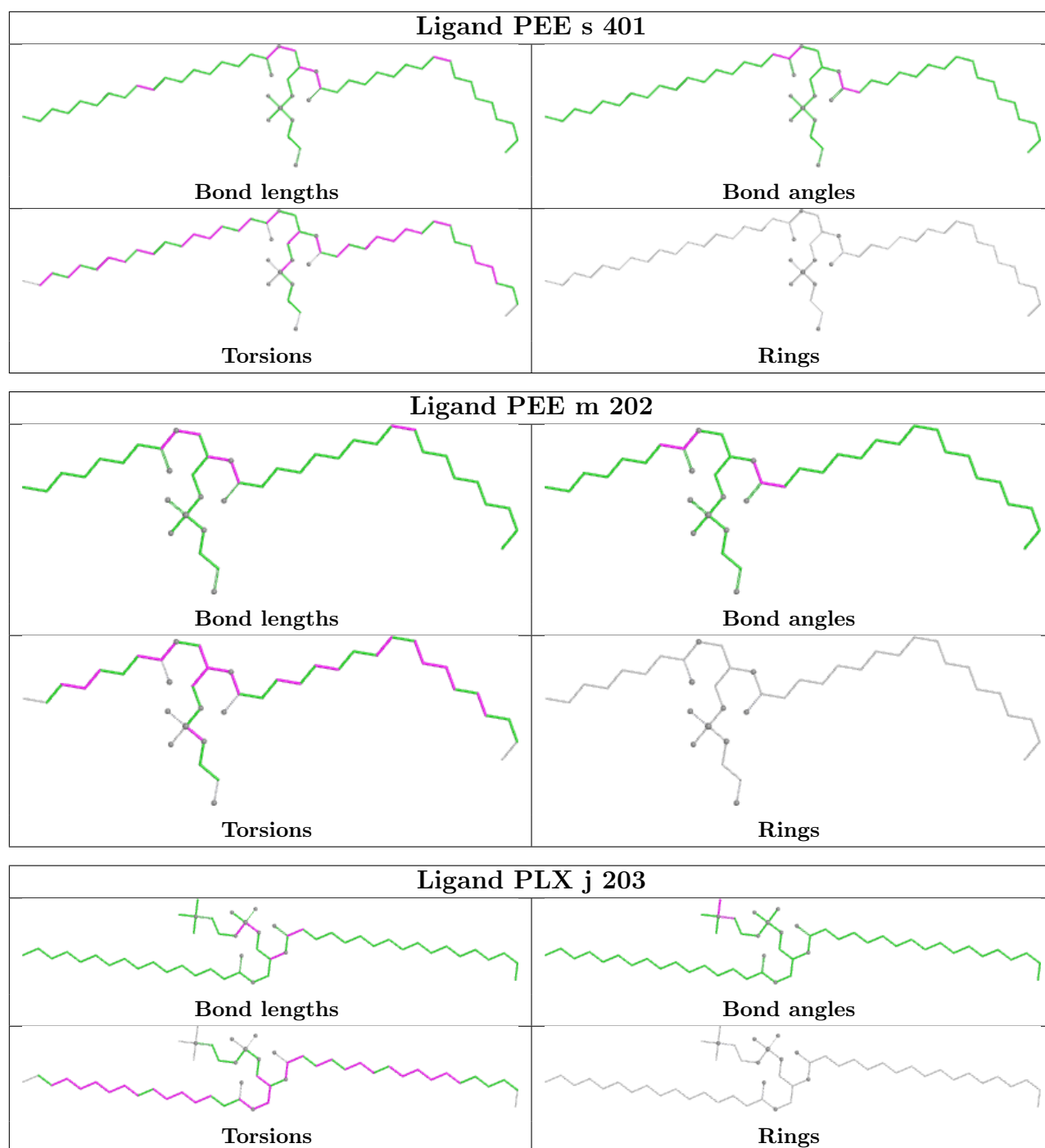


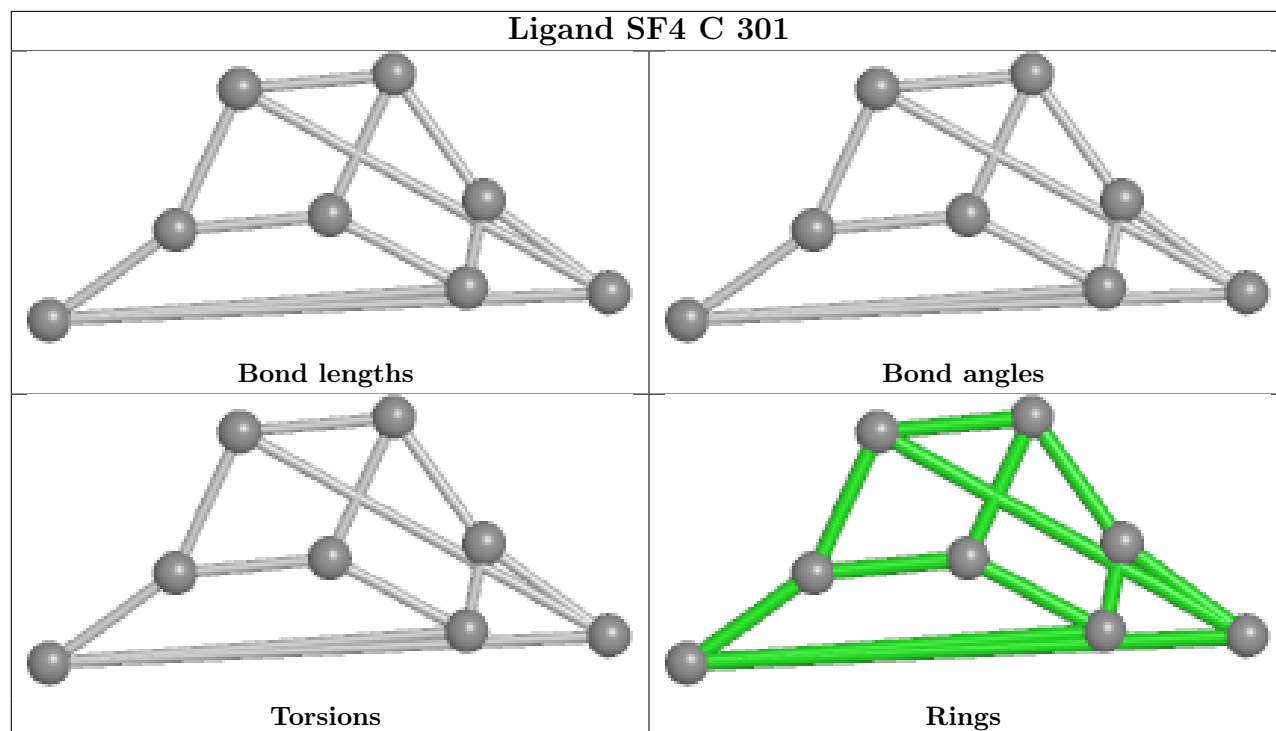












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

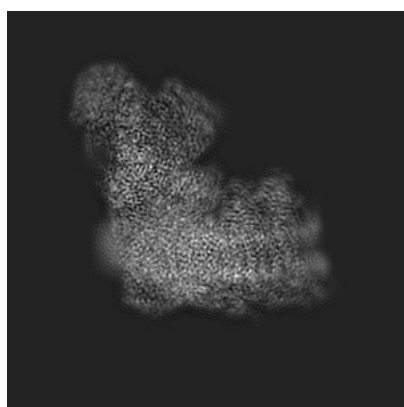
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31648. These allow visual inspection of the internal detail of the map and identification of artifacts.

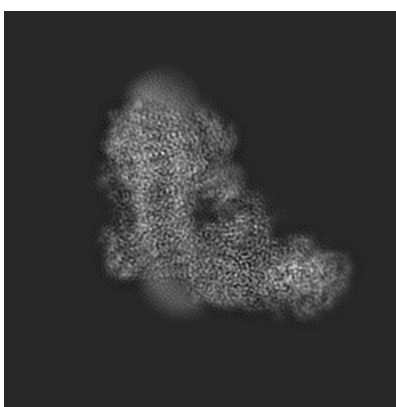
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

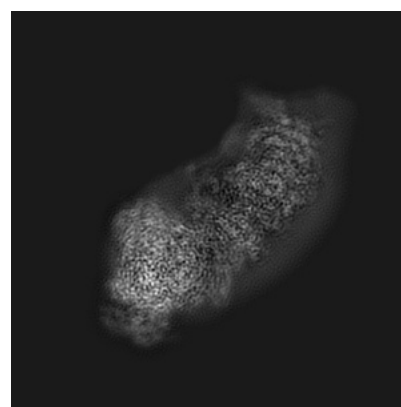
#### 6.1.1 Primary map



X



Y

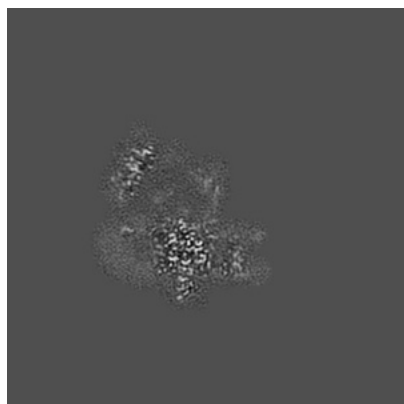


Z

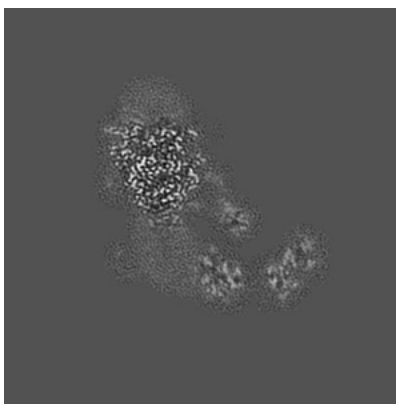
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

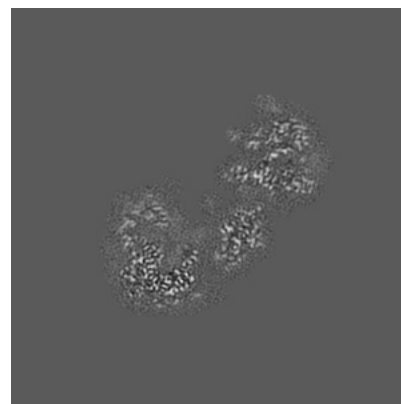
#### 6.2.1 Primary map



X Index: 152



Y Index: 152

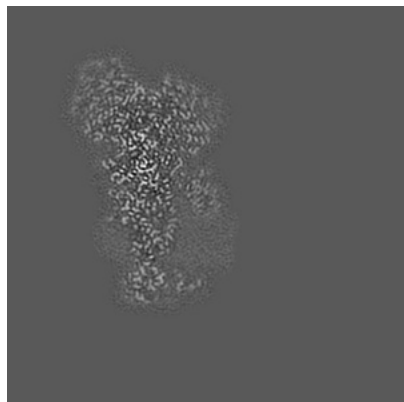


Z Index: 152

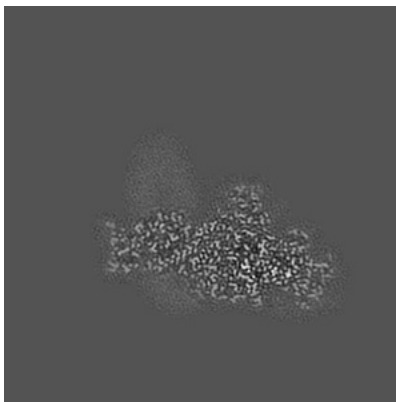
The images above show central slices of the map in three orthogonal directions.

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

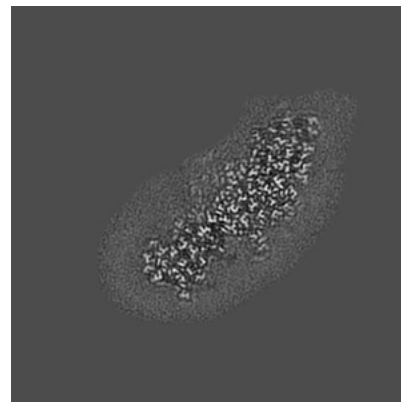
### 6.3.1 Primary map



X Index: 106



Y Index: 98

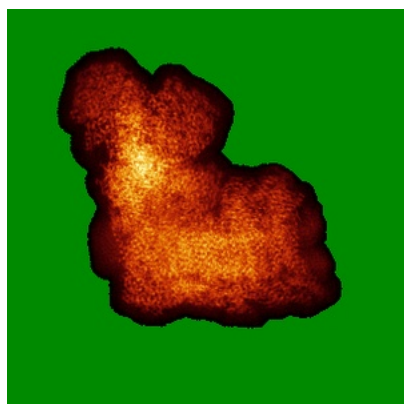


Z Index: 128

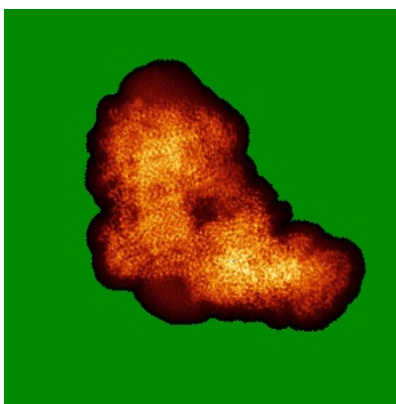
The images above show the largest variance slices of the map in three orthogonal directions.

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

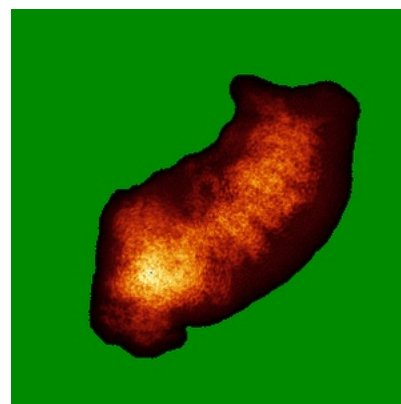
### 6.4.1 Primary map



X



Y

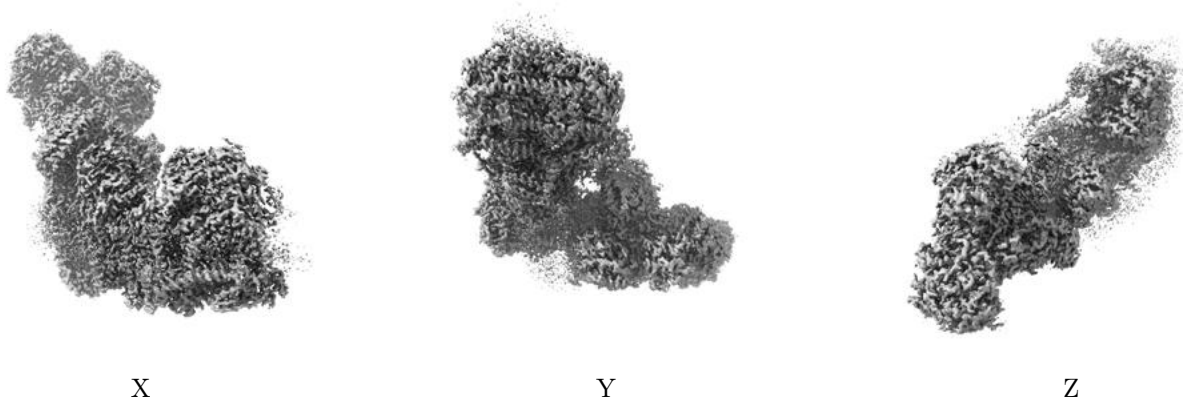


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0239. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

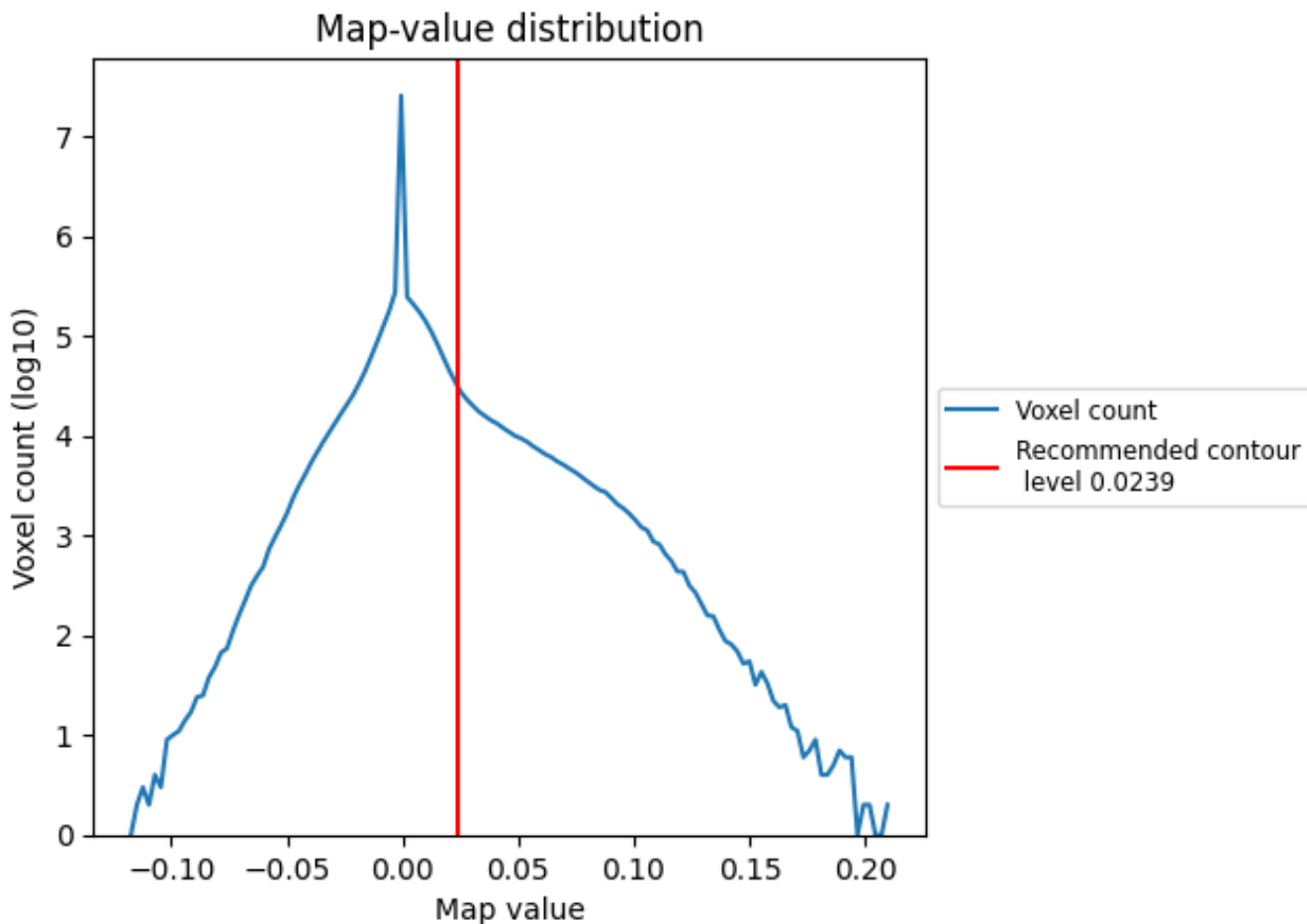
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

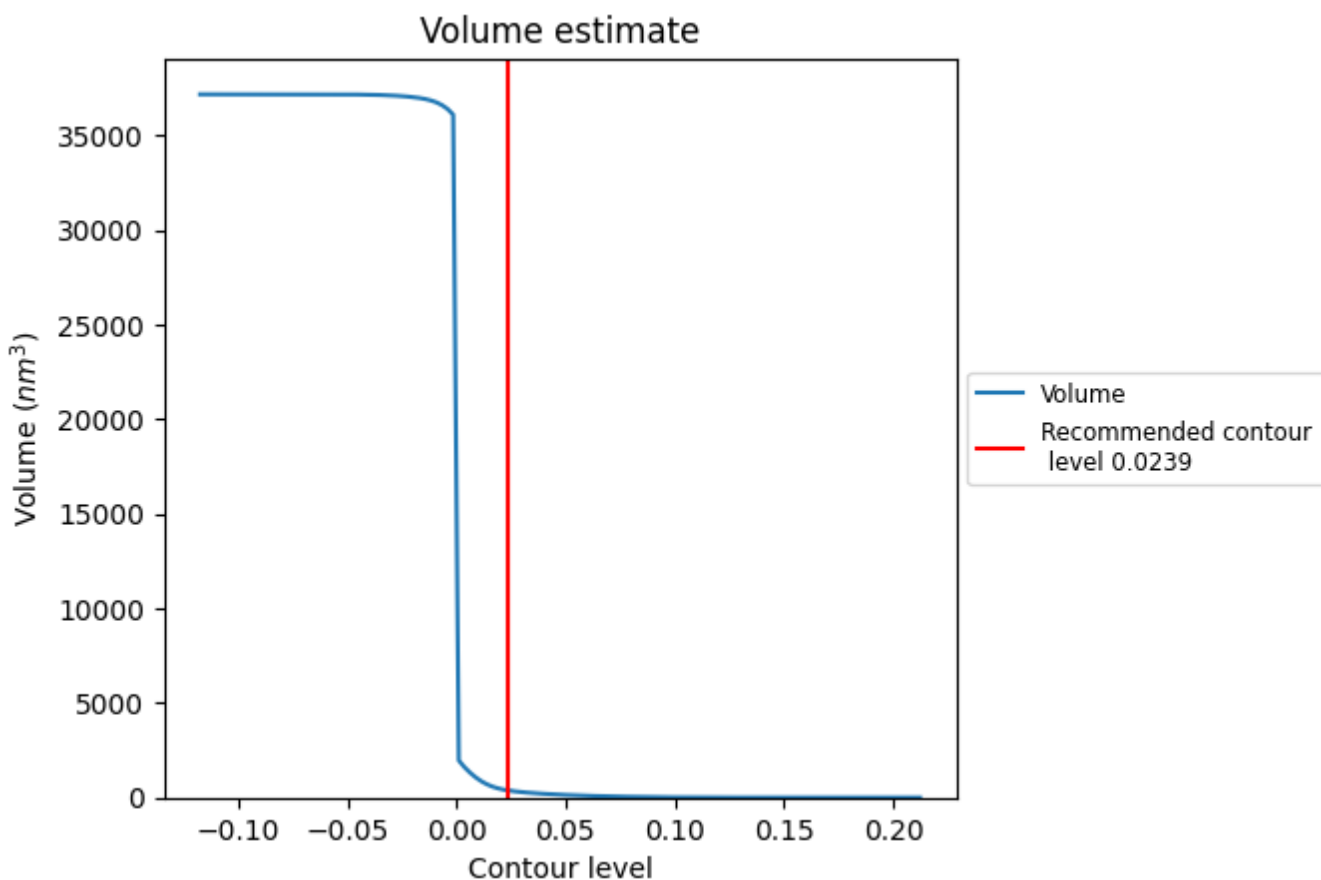
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

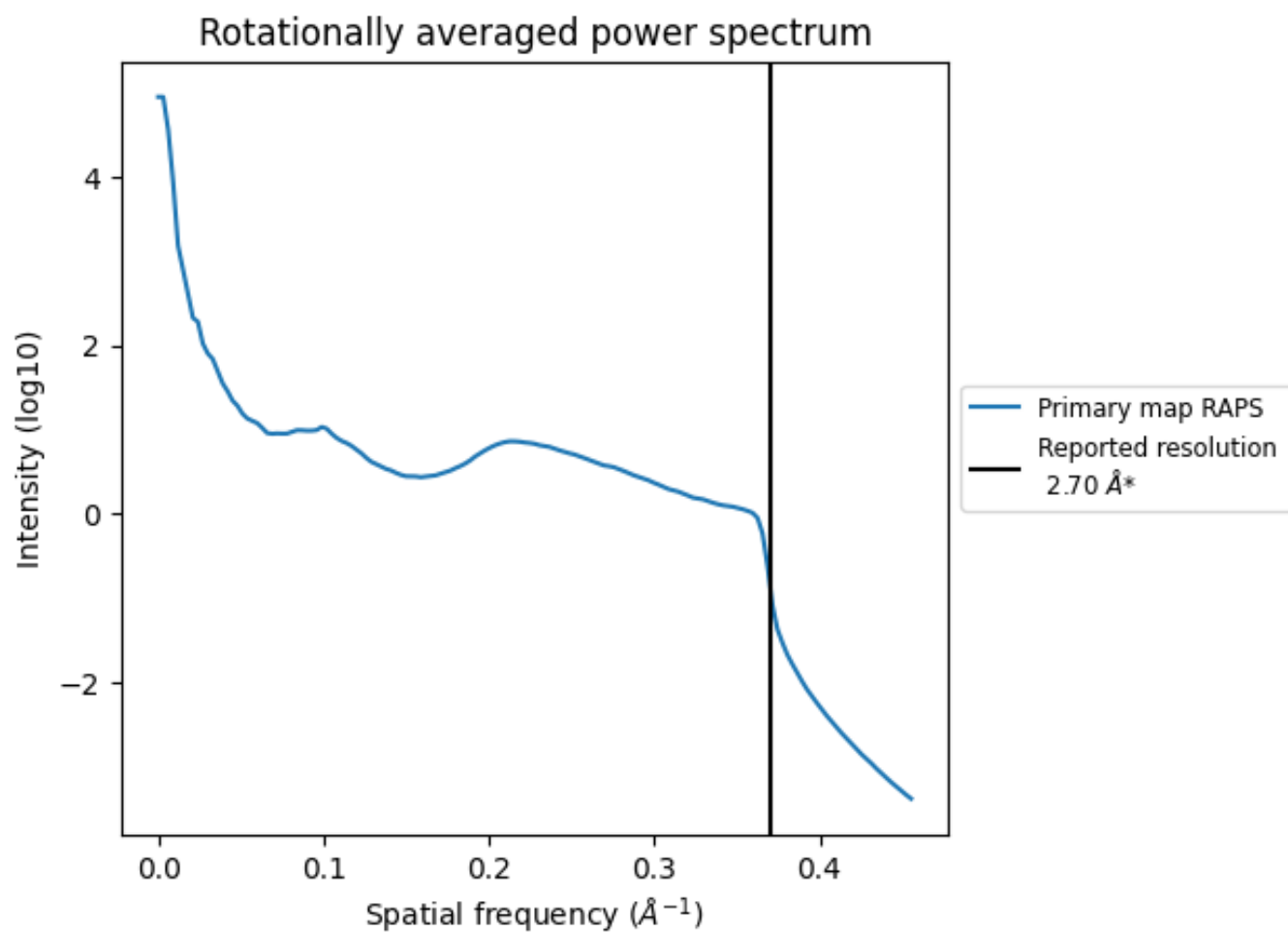
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 373 nm<sup>3</sup>; this corresponds to an approximate mass of 337 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  $0.370 \text{\AA}^{-1}$

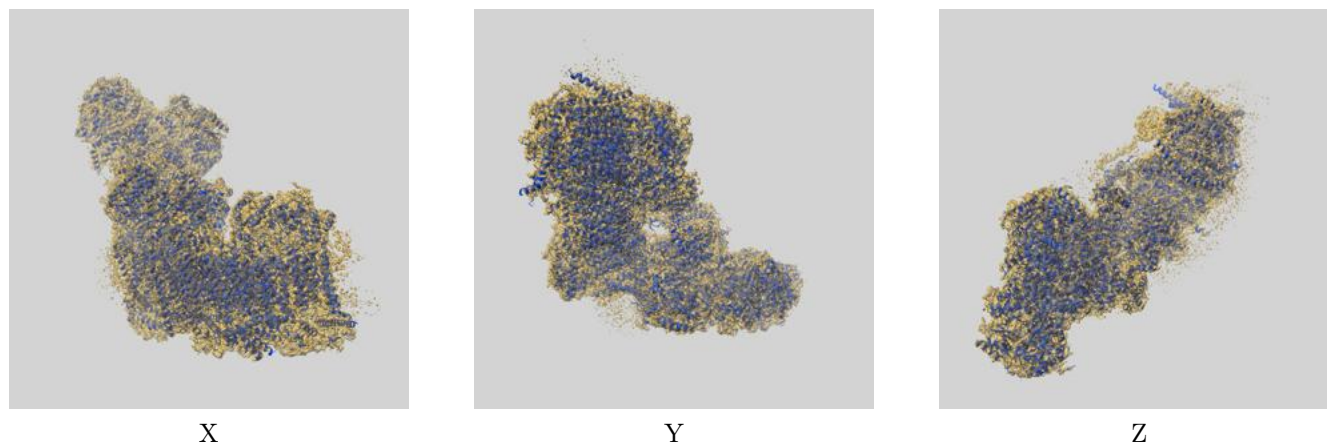
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

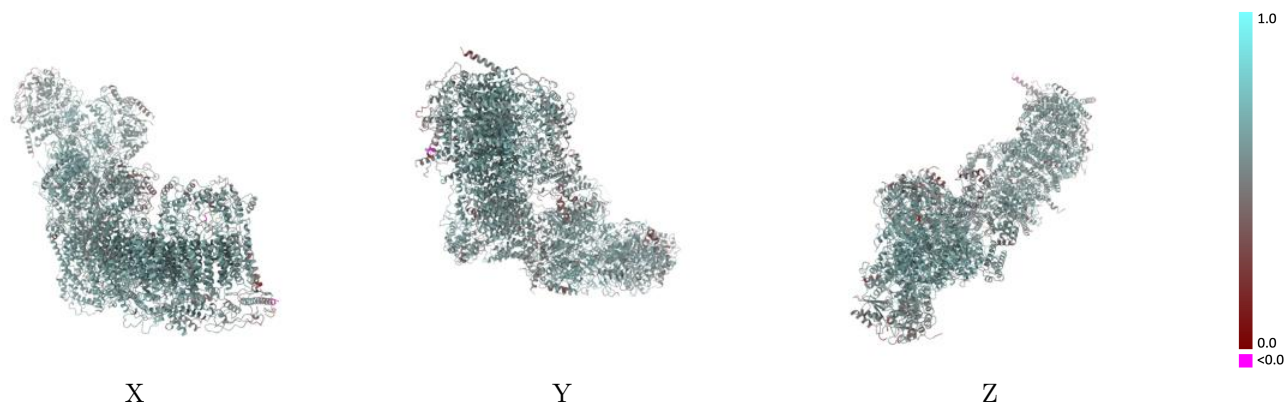
This section contains information regarding the fit between EMDB map EMD-31648 and PDB model 7V30. Per-residue inclusion information can be found in section 3 on page 20.

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



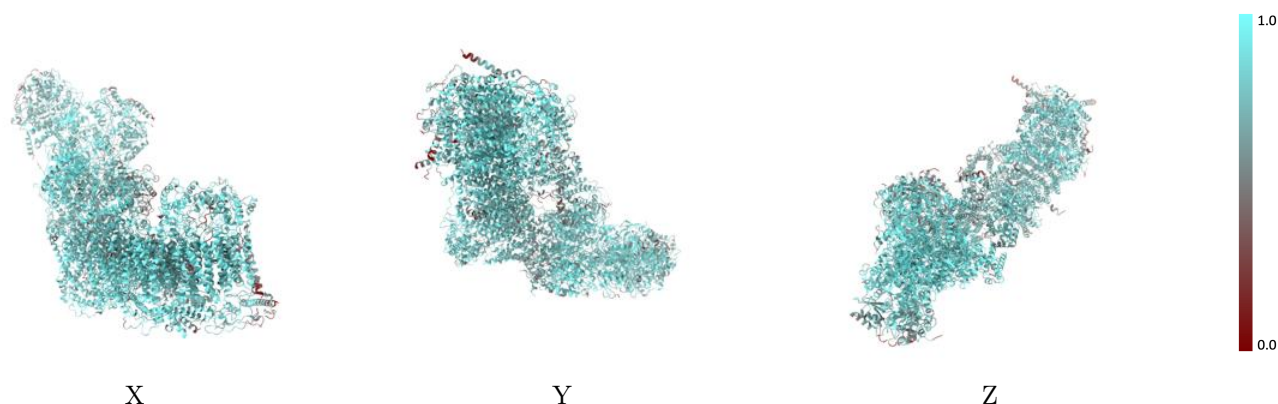
The images above show the 3D surface view of the map at the recommended contour level 0.0239 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



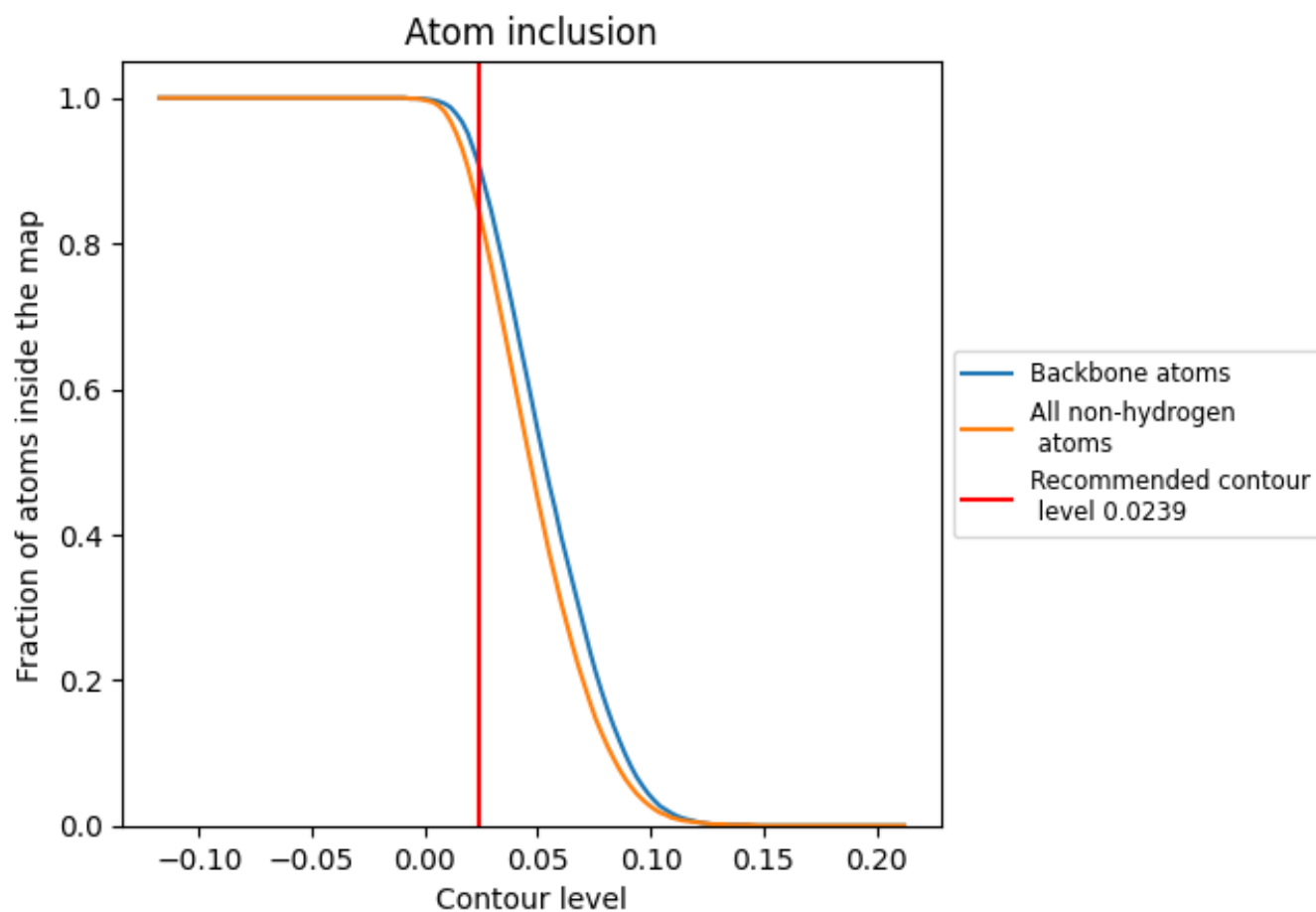
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0239).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.0239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.5900
A	 0.7820	 0.5530
B	 0.9630	 0.6490
C	 0.9040	 0.6250
E	 0.8270	 0.5820
F	 0.6840	 0.4920
G	 0.5430	 0.4230
H	 0.8470	 0.5700
I	 0.8470	 0.6050
J	 0.7910	 0.5600
K	 0.6830	 0.5150
L	 0.8890	 0.6180
M	 0.8810	 0.6020
N	 0.8800	 0.6180
O	 0.7300	 0.5270
P	 0.9450	 0.6450
Q	 0.9390	 0.6410
S	 0.9350	 0.6190
T	 0.8700	 0.6080
U	 0.8600	 0.5900
V	 0.6560	 0.5400
W	 0.8900	 0.6020
X	 0.7630	 0.5410
Y	 0.7130	 0.5230
Z	 0.6170	 0.4920
a	 0.8600	 0.6070
b	 0.7460	 0.5380
c	 0.8300	 0.5810
d	 0.8060	 0.5690
e	 0.7830	 0.5630
f	 0.7340	 0.5300
g	 0.9080	 0.6160
h	 0.8700	 0.6010
i	 0.9360	 0.6340
j	 0.7800	 0.5660



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
k	 0.8500	 0.5950
l	 0.8740	 0.6130
m	 0.8270	 0.5820
n	 0.7210	 0.5620
o	 0.8310	 0.5870
p	 0.8270	 0.5710
r	 0.9410	 0.6370
s	 0.9110	 0.6190
u	 0.8790	 0.6000
v	 0.6930	 0.4900
w	 0.8110	 0.5660