



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 05:20 PM EDT

PDB ID : 8UGD
EMDB ID : EMD-42221
Title : In-situ complex III, state I
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

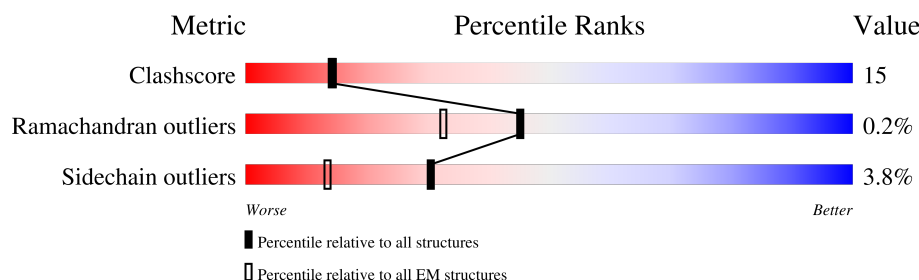
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	3A	480	<div> <div>6%</div> <div>66%</div> <div>24%</div> <div>8%</div> </div>
1	3N	480	<div> <div>67%</div> <div>24%</div> <div>7%</div> </div>
2	3B	453	<div> <div>8%</div> <div>68%</div> <div>23%</div> <div>8%</div> </div>
2	3O	453	<div> <div>5%</div> <div>68%</div> <div>23%</div> <div>8%</div> </div>
3	3C	379	<div> <div>71%</div> <div>27%</div> </div>
3	3P	379	<div> <div>67%</div> <div>32%</div> </div>
4	3D	326	<div> <div>50%</div> <div>22%</div> <div>27%</div> </div>
4	3Q	326	<div> <div>48%</div> <div>24%</div> <div>27%</div> </div>

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Mol	Chain	Length	Quality of chain
5	3E	274	
5	3I	274	
5	3R	274	
5	3V	274	
6	3F	111	
6	3S	111	
7	3G	82	
7	3T	82	
8	3H	91	
8	3U	91	
9	3J	64	
9	3W	64	
10	3X	56	
10	3Y	56	

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
16	FES	3E	301	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33543 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
1	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
2	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
3	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
4	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
5	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
5	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
5	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
6	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
7	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
8	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

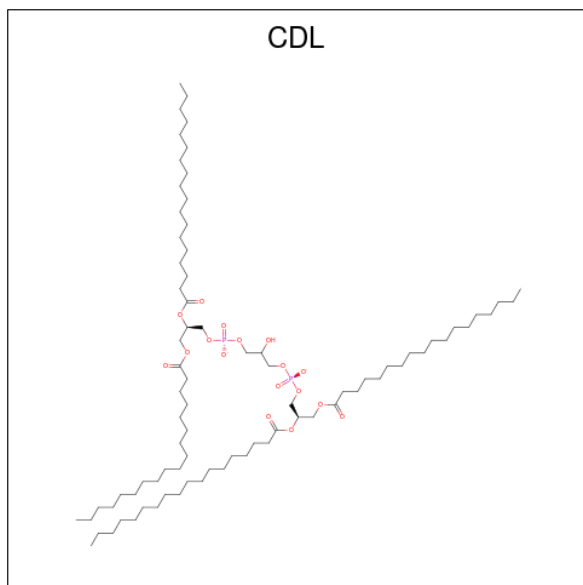
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	3J	56	Total	C	N	O	0	0
			464	305	82	77		
9	3W	56	Total	C	N	O	0	0
			464	305	82	77		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

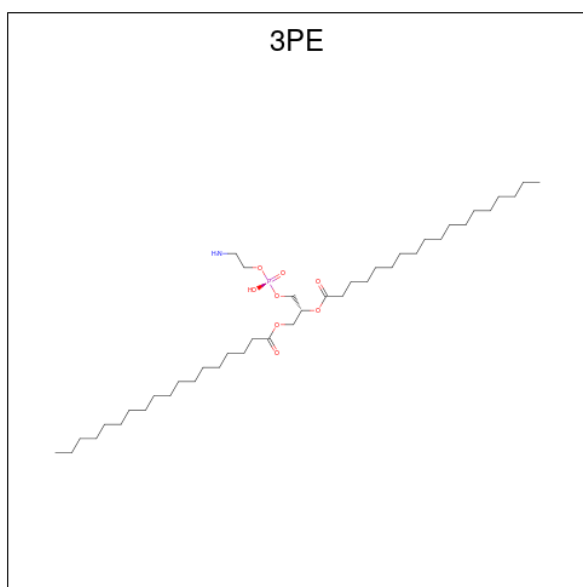
Mol	Chain	Residues	Atoms					AltConf	Trace
10	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
10	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



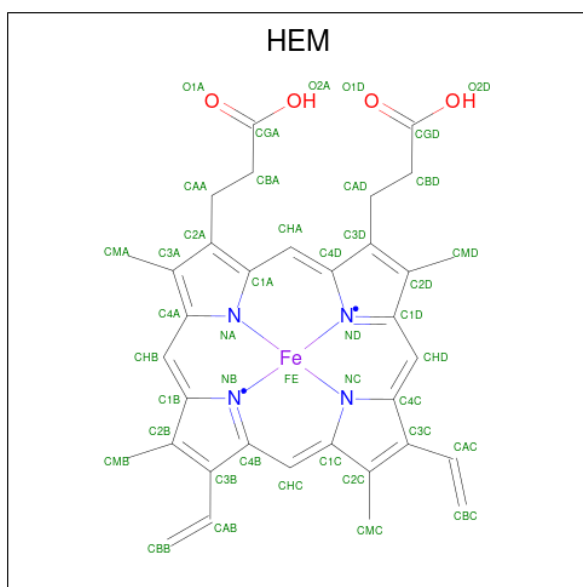
Mol	Chain	Residues	Atoms				AltConf
11	3A	1	Total	C	O	P	0
			58	39	17	2	
11	3C	1	Total	C	O	P	0
			52	33	17	2	
11	3D	1	Total	C	O	P	0
			56	37	17	2	
11	3P	1	Total	C	O	P	0
			56	37	17	2	
11	3P	1	Total	C	O	P	0
			43	24	17	2	
11	3Q	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



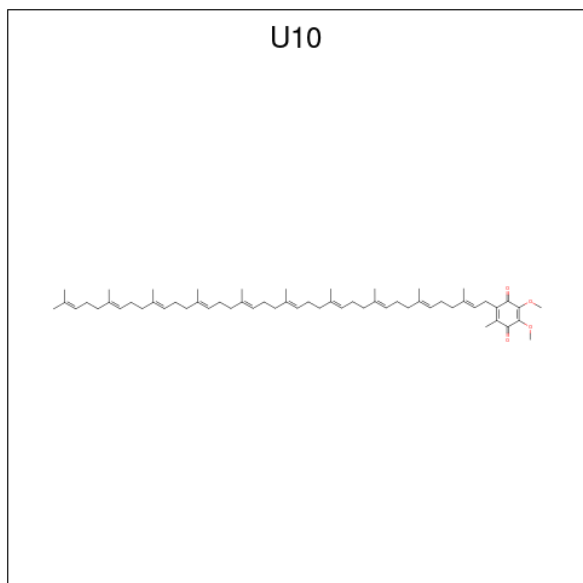
Mol	Chain	Residues	Atoms					AltConf
12	3A	1	Total	C	N	O	P	0
			27	17	1	8	1	
12	3A	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	3D	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3G	1	Total	C	N	O	P	0
			29	19	1	8	1	
12	3N	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3N	1	Total	C	N	O	P	0
			25	15	1	8	1	
12	3P	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
12	3R	1	Total	C	N	O	P	0
			34	24	1	8	1	
12	3Y	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



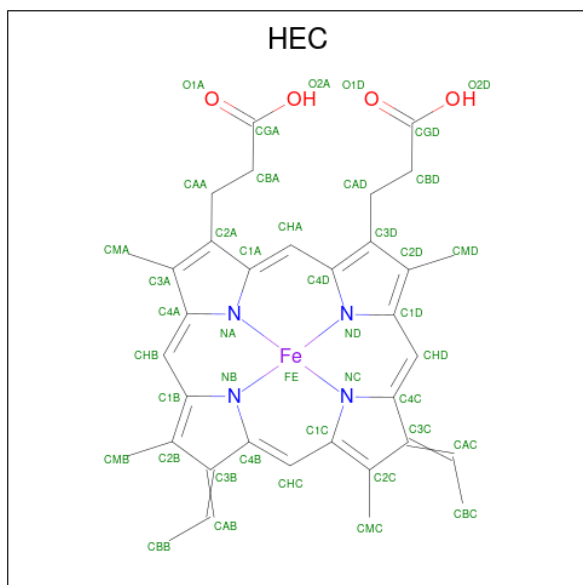
Mol	Chain	Residues	Atoms					AltConf
13	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
14	3C	1	Total	C	O	0
			28	24	4	
14	3C	1	Total	C	O	0
			28	24	4	
14	3P	1	Total	C	O	0
			23	19	4	
14	3P	1	Total	C	O	0
			28	24	4	

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



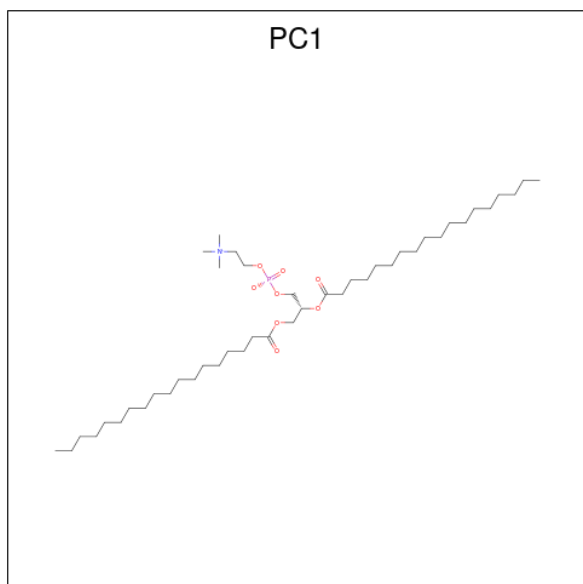
Mol	Chain	Residues	Atoms					AltConf
15	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
15	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
16	3E	1	Total	Fe	S	0
			4	2	2	
16	3R	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
17	3E	1	Total	C	N	O	P	0
			47	37	1	8	1	

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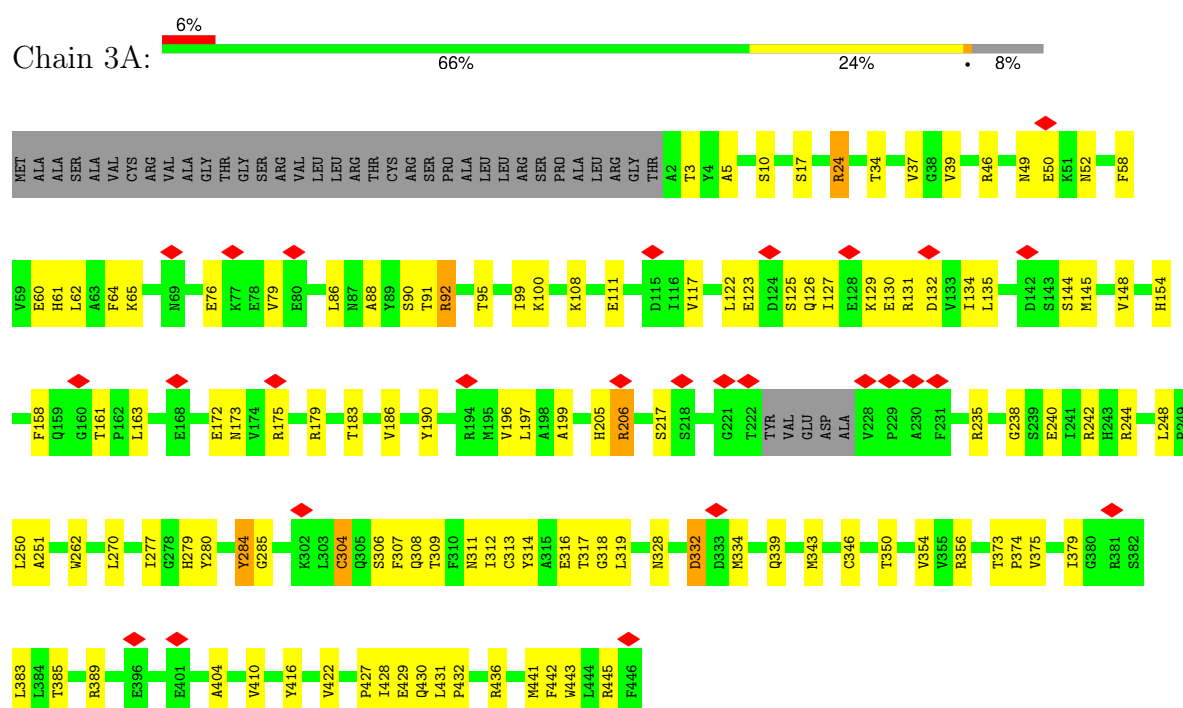
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Mol	Chain	Residues	Atoms					AltConf
17	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
17	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

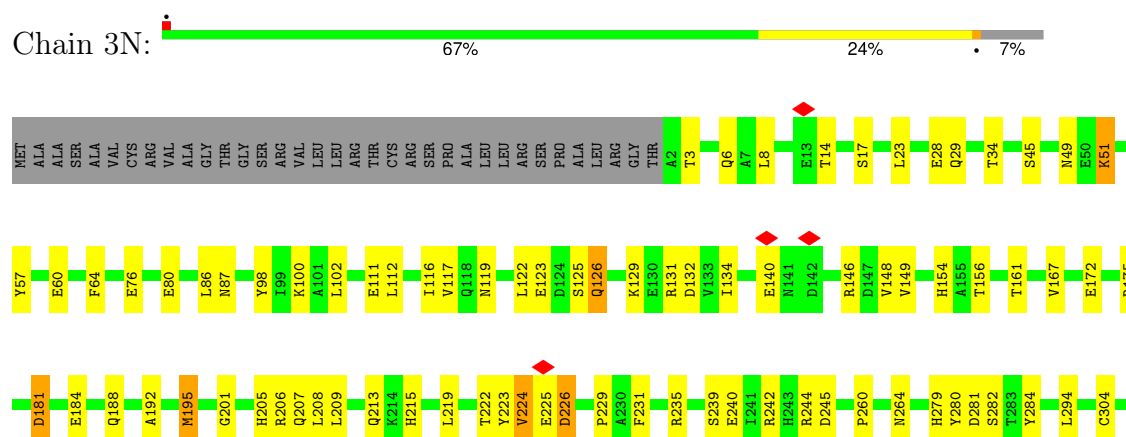
3 Residue-property plots [i](#)

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.

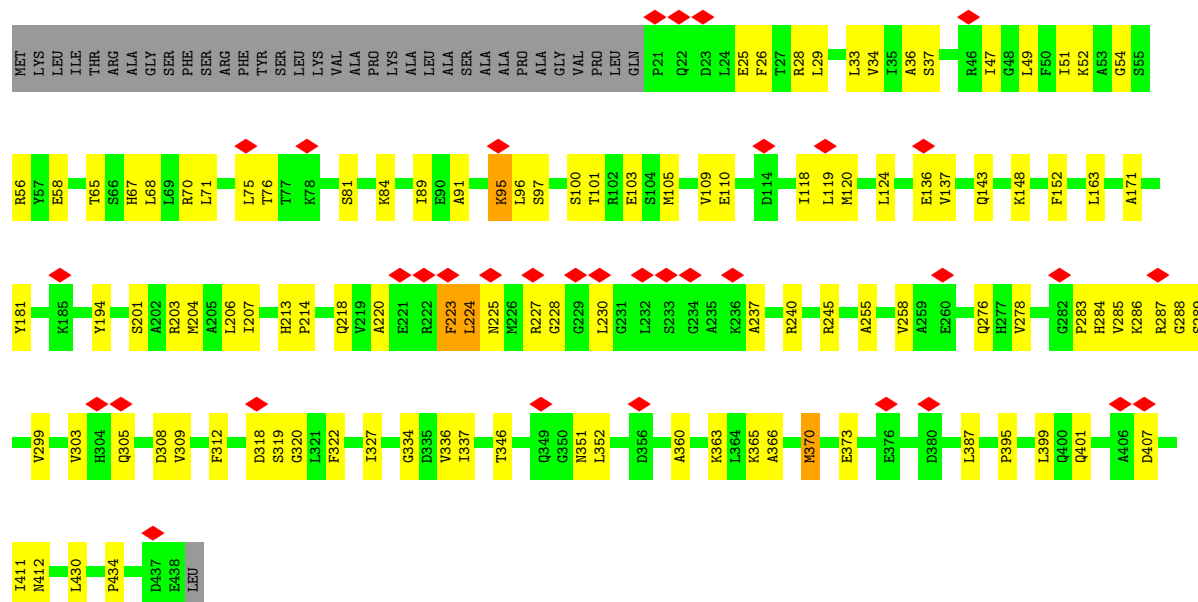
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



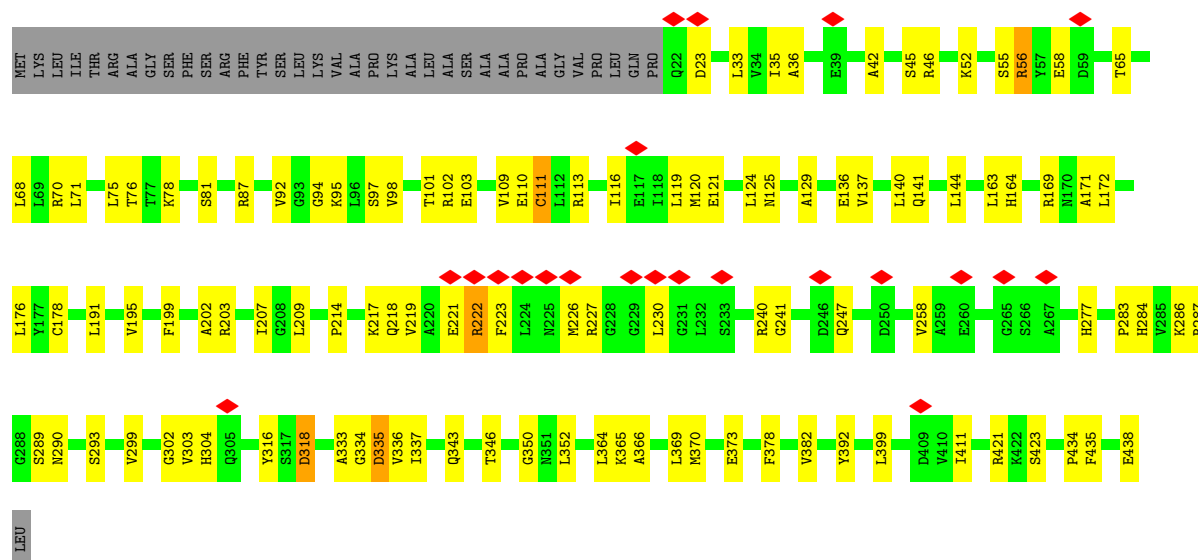
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



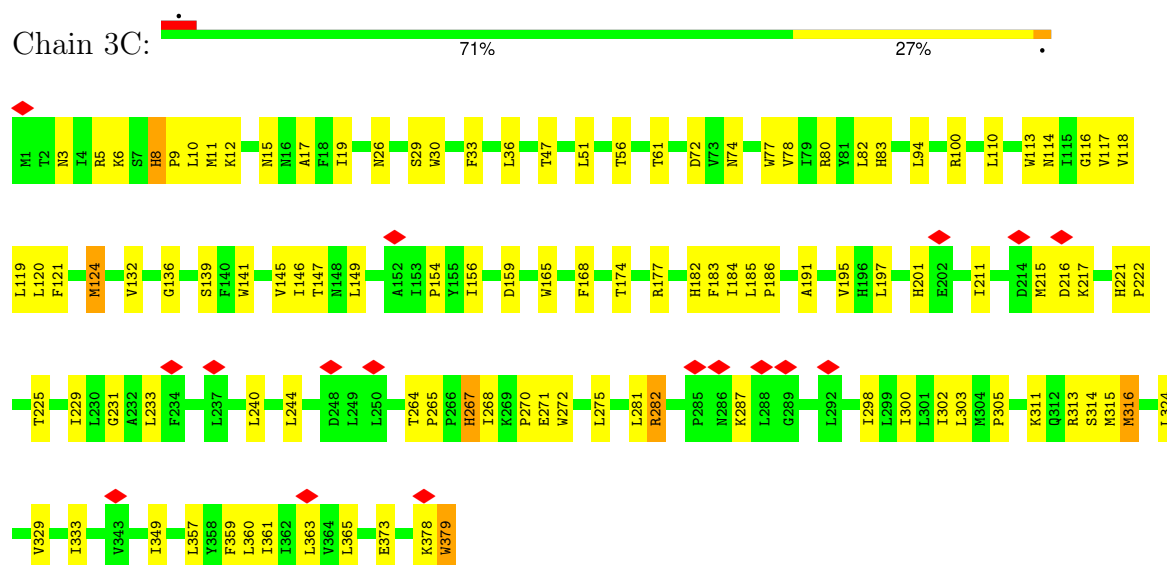
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



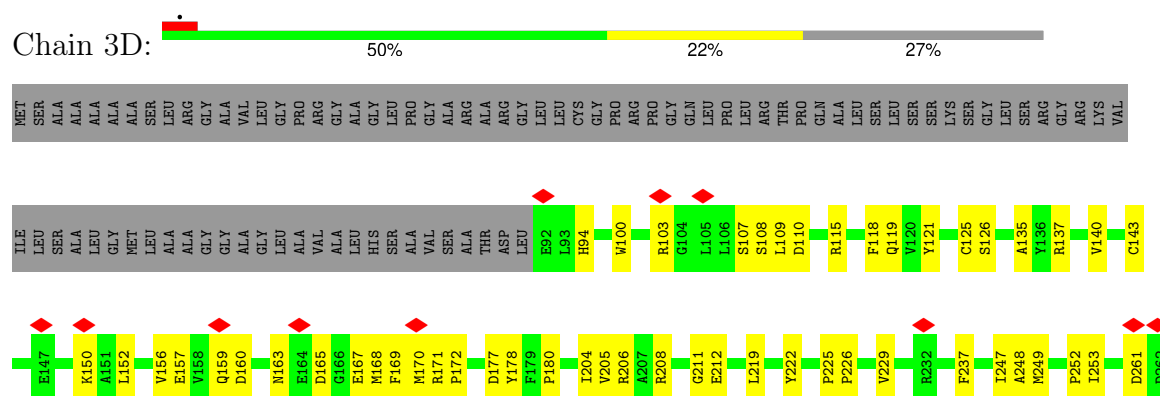
- Molecule 3: Cytochrome b

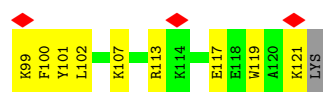


- Molecule 3: Cytochrome b

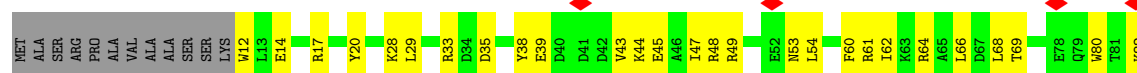


- Molecule 4: Cytochrome c1

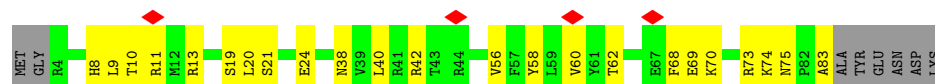




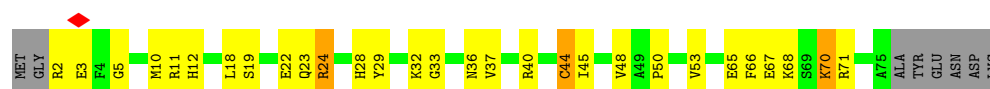
- Molecule 6: Cytochrome b-c1 complex subunit 7



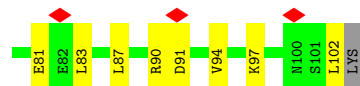
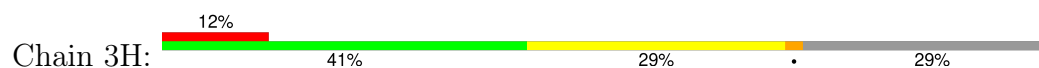
- Molecule 7: Cytochrome b-c1 complex subunit 8



- Molecule 7: Cytochrome b-c1 complex subunit 8



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

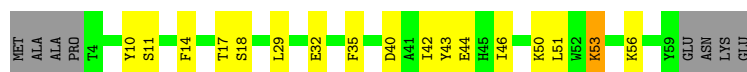




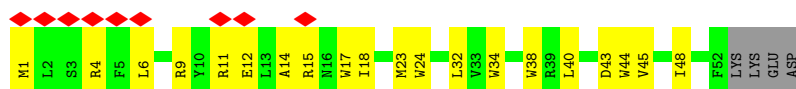
- Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



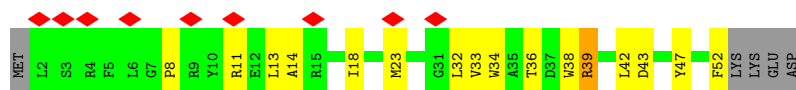
- Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



- Molecule 10: Cytochrome b-c1 complex subunit 10



- Molecule 10: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90000	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)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.210	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CDL, U10, FES, 3PE, HEC, HEM

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	3A	0.29	0/3481	0.51	1/4722 (0.0%)
1	3N	0.29	0/3496	0.50	0/4723
2	3B	0.28	0/3190	0.49	0/4317
2	3O	0.28	0/3175	0.48	0/4292
3	3C	0.31	0/3123	0.45	0/4269
3	3P	0.30	0/3122	0.47	0/4269
4	3D	0.31	0/1946	0.51	0/2641
4	3Q	0.30	0/1962	0.53	1/2663 (0.0%)
5	3E	0.29	0/1551	0.56	0/2098
5	3I	1.63	2/342 (0.6%)	1.54	6/465 (1.3%)
5	3R	0.31	0/1551	0.63	2/2098 (0.1%)
5	3V	0.26	0/225	0.67	0/303
6	3F	0.31	0/888	0.58	0/1193
6	3S	0.28	0/888	0.53	0/1193
7	3G	0.30	0/648	0.57	0/874
7	3T	0.31	0/649	0.63	1/878 (0.1%)
8	3H	0.30	0/538	0.57	0/721
8	3U	0.37	0/539	0.70	1/724 (0.1%)
9	3J	0.28	0/476	0.55	0/641
9	3W	0.29	0/476	0.58	0/641
10	3X	0.29	0/445	0.57	0/608
10	3Y	0.28	0/437	0.57	0/598
All	All	0.34	2/33148 (0.0%)	0.54	12/44931 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	3R	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3I	49	PHE	C-N	27.39	1.97	1.34
5	3I	48	SER	C-N	11.13	1.59	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3I	49	PHE	CA-C-N	-17.88	77.87	117.20
5	3I	48	SER	O-C-N	14.96	146.63	122.70
5	3I	48	SER	CA-C-N	-11.87	91.10	117.20
5	3R	160	PRO	CA-N-CD	-11.37	95.58	111.50
5	3I	49	PHE	C-N-CA	-10.60	95.20	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	3R	163	LYS	Peptide

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	3A	3411	0	3309	85	0
1	3N	3424	0	3350	87	0
2	3B	3138	0	3116	82	0
2	3O	3124	0	3108	77	0
3	3C	3025	0	3090	97	0
3	3P	3024	0	3090	93	0
4	3D	1888	0	1834	64	0
4	3Q	1904	0	1848	68	0
5	3E	1518	0	1498	85	0
5	3I	337	0	346	32	0
5	3R	1518	0	1499	98	0
5	3V	223	0	233	9	0
6	3F	868	0	857	32	0
6	3S	868	0	857	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	3G	628	0	634	19	0
7	3T	628	0	634	36	0
8	3H	533	0	512	20	0
8	3U	533	0	513	28	0
9	3J	464	0	467	59	0
9	3W	464	0	467	20	0
10	3X	429	0	430	13	0
10	3Y	421	0	418	17	0
11	3A	58	0	60	5	0
11	3C	52	0	48	4	0
11	3D	56	0	56	4	0
11	3P	99	0	86	9	0
11	3Q	57	0	58	10	0
12	3A	59	0	66	7	0
12	3C	35	0	44	4	0
12	3D	33	0	40	4	0
12	3G	29	0	32	1	0
12	3N	58	0	62	6	0
12	3P	33	0	40	1	0
12	3Q	47	0	71	7	0
12	3R	34	0	42	3	0
12	3Y	30	0	34	6	0
13	3C	86	0	60	6	0
13	3P	86	0	60	6	0
14	3C	56	0	62	9	0
14	3P	51	0	54	10	0
15	3D	42	0	32	4	0
15	3Q	43	0	32	2	0
16	3E	4	0	0	2	0
16	3R	4	0	0	0	0
17	3E	47	0	68	8	0
17	3R	45	0	64	4	0
17	3X	29	0	32	3	0
All	All	33543	0	33313	1025	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 15.

The worst 5 of 1025 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)
9:3J:53:TRP:CG	9:3J:57:LYS:CE	1.88	1.55
9:3J:53:TRP:CG	9:3J:57:LYS:HE3	1.47	1.45
9:3J:53:TRP:HD1	9:3J:57:LYS:NZ	1.10	1.44
9:3J:53:TRP:CG	9:3J:57:LYS:HE2	1.57	1.27
9:3J:53:TRP:NE1	9:3J:57:LYS:HE2	0.94	1.27

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	3A	436/480 (91%)	410 (94%)	26 (6%)	0	100	100
1	3N	444/480 (92%)	416 (94%)	27 (6%)	1 (0%)	44	75
2	3B	414/453 (91%)	394 (95%)	19 (5%)	1 (0%)	44	75
2	3O	413/453 (91%)	400 (97%)	13 (3%)	0	100	100
3	3C	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
3	3P	377/379 (100%)	361 (96%)	14 (4%)	2 (0%)	25	59
4	3D	235/326 (72%)	214 (91%)	21 (9%)	0	100	100
4	3Q	237/326 (73%)	224 (94%)	12 (5%)	1 (0%)	30	64
5	3E	194/274 (71%)	164 (84%)	29 (15%)	1 (0%)	25	59
5	3I	45/274 (16%)	38 (84%)	6 (13%)	1 (2%)	5	31
5	3R	194/274 (71%)	172 (89%)	22 (11%)	0	100	100
5	3V	29/274 (11%)	29 (100%)	0	0	100	100
6	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
6	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
7	3G	70/82 (85%)	70 (100%)	0	0	100	100
7	3T	72/82 (88%)	72 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	3H	61/91 (67%)	56 (92%)	5 (8%)	0	100	100
8	3U	63/91 (69%)	59 (94%)	4 (6%)	0	100	100
9	3J	54/64 (84%)	51 (94%)	3 (6%)	0	100	100
9	3W	54/64 (84%)	49 (91%)	5 (9%)	0	100	100
10	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
10	3Y	49/56 (88%)	44 (90%)	5 (10%)	0	100	100
All	All	4060/5180 (78%)	3826 (94%)	227 (6%)	7 (0%)	45	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	3E	216	VAL
4	3Q	3	LEU
2	3B	224	LEU
5	3I	50	LEU
3	3P	110	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3A	367/397 (92%)	356 (97%)	11 (3%)	36	63
1	3N	372/397 (94%)	351 (94%)	21 (6%)	17	45
2	3B	328/355 (92%)	321 (98%)	7 (2%)	48	71
2	3O	327/355 (92%)	317 (97%)	10 (3%)	35	63
3	3C	332/332 (100%)	320 (96%)	12 (4%)	30	59
3	3P	332/332 (100%)	321 (97%)	11 (3%)	33	61
4	3D	202/259 (78%)	194 (96%)	8 (4%)	27	56
4	3Q	204/259 (79%)	193 (95%)	11 (5%)	18	46
5	3E	166/225 (74%)	160 (96%)	6 (4%)	30	59
5	3I	36/225 (16%)	34 (94%)	2 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	3R	166/225 (74%)	154 (93%)	12 (7%)	12	37
5	3V	24/225 (11%)	23 (96%)	1 (4%)	25	54
6	3F	90/99 (91%)	88 (98%)	2 (2%)	47	70
6	3S	90/99 (91%)	88 (98%)	2 (2%)	47	70
7	3G	67/73 (92%)	65 (97%)	2 (3%)	36	63
7	3T	67/73 (92%)	65 (97%)	2 (3%)	36	63
8	3H	62/85 (73%)	58 (94%)	4 (6%)	14	41
8	3U	62/85 (73%)	59 (95%)	3 (5%)	21	50
9	3J	46/52 (88%)	46 (100%)	0	100	100
9	3W	46/52 (88%)	45 (98%)	1 (2%)	47	70
10	3X	42/46 (91%)	38 (90%)	4 (10%)	7	28
10	3Y	41/46 (89%)	39 (95%)	2 (5%)	21	50
All	All	3469/4296 (81%)	3335 (96%)	134 (4%)	30	56

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	3R	235	TYR
6	3S	17	ARG
10	3X	43	ASP
8	3H	53	GLU
7	3G	68	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
7	3T	6	HIS
8	3U	26	GLN
5	3I	58	GLN
9	3J	38	GLN
1	3N	9	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 ligands 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
13	HEM	3P	502	3	42,50,50	1.34	7 (16%)	46,82,82	1.74	8 (17%)
12	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.60	0
11	CDL	3P	506	-	55,55,99	0.36	0	61,67,111	0.50	0
17	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.39	0
14	U10	3C	504	-	28,28,63	0.94	3 (10%)	36,37,79	1.35	6 (16%)
14	U10	3P	504	-	28,28,63	0.84	2 (7%)	36,37,79	1.15	5 (13%)
13	HEM	3C	502	3	42,50,50	1.35	7 (16%)	46,82,82	1.78	9 (19%)
12	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.37	0
11	CDL	3Q	502	-	56,56,99	0.35	0	62,68,111	0.48	0
11	CDL	3A	501	-	57,57,99	0.35	0	63,69,111	0.44	0
16	FES	3E	301	5	0,4,4	-	-	-	-	-
12	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.39	0
11	CDL	3D	503	-	55,55,99	0.35	0	61,67,111	0.45	0
17	PC1	3R	302	-	44,44,53	0.31	0	50,52,61	0.38	0
12	3PE	3A	503	-	31,31,50	0.33	0	34,36,55	0.65	1 (2%)
15	HEC	3D	501	4	30,49,50	2.41	12 (40%)	28,80,82	2.19	6 (21%)
12	3PE	3N	502	-	24,24,50	0.38	0	27,29,55	0.65	1 (3%)
14	U10	3C	503	-	28,28,63	0.82	2 (7%)	36,37,79	1.17	5 (13%)
15	HEC	3Q	501	4	32,50,50	2.17	12 (37%)	30,82,82	2.12	7 (23%)
14	U10	3P	503	-	23,23,63	0.99	3 (13%)	30,31,79	1.51	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.65	1 (2%)
12	3PE	3D	502	-	32,32,50	0.34	0	35,37,55	0.43	0
12	3PE	3Q	503	-	46,46,50	0.29	0	49,51,55	0.34	0
12	3PE	3C	506	-	34,34,50	0.32	0	37,39,55	0.44	0
11	CDL	3C	505	-	51,51,99	0.36	0	57,63,111	0.50	0
13	HEM	3C	501	3	42,50,50	1.31	6 (14%)	46,82,82	1.83	10 (21%)
13	HEM	3P	501	3	42,50,50	1.33	7 (16%)	46,82,82	1.84	9 (19%)
17	PC1	3E	302	-	46,46,53	0.30	0	52,54,61	0.30	0
11	CDL	3P	507	-	42,42,99	0.39	0	48,54,111	0.54	0
16	FES	3R	301	5	0,4,4	-	-	-	-	-
12	3PE	3P	505	-	32,32,50	0.35	0	35,37,55	0.51	0
12	3PE	3R	303	-	33,33,50	0.32	0	36,38,55	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEM	3P	502	3	-	6/12/54/54	-
12	3PE	3A	502	-	-	11/30/30/54	-
11	CDL	3P	506	-	-	9/66/66/110	-
17	PC1	3X	101	-	-	11/32/32/57	-
14	U10	3C	504	-	-	5/21/45/87	0/1/1/1
14	U10	3P	504	-	-	3/21/45/87	0/1/1/1
13	HEM	3C	502	3	-	4/12/54/54	-
12	3PE	3Y	101	-	-	10/33/33/54	-
11	CDL	3Q	502	-	-	16/67/67/110	-
11	CDL	3A	501	-	-	8/68/68/110	-
16	FES	3E	301	5	-	-	0/1/1/1
12	3PE	3G	101	-	-	6/32/32/54	-
11	CDL	3D	503	-	-	11/66/66/110	-
17	PC1	3R	302	-	-	6/48/48/57	-
12	3PE	3A	503	-	-	5/35/35/54	-
15	HEC	3D	501	4	-	0/9/53/54	-
12	3PE	3N	502	-	-	7/28/28/54	-
14	U10	3C	503	-	-	7/21/45/87	0/1/1/1
15	HEC	3Q	501	4	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	U10	3P	503	-	-	1/15/39/87	0/1/1/1
12	3PE	3N	501	-	-	6/35/35/54	-
12	3PE	3D	502	-	-	2/36/36/54	-
12	3PE	3Q	503	-	-	5/50/50/54	-
12	3PE	3C	506	-	-	6/38/38/54	-
11	CDL	3C	505	-	-	7/62/62/110	-
13	HEM	3C	501	3	-	3/12/54/54	-
13	HEM	3P	501	3	-	5/12/54/54	-
17	PC1	3E	302	-	-	2/50/50/57	-
11	CDL	3P	507	-	-	10/53/53/110	-
16	FES	3R	301	5	-	-	0/1/1/1
12	3PE	3P	505	-	-	9/36/36/54	-
12	3PE	3R	303	-	-	11/37/37/54	-

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3D	501	HEC	C3C-C2C	6.65	1.48	1.40
15	3D	501	HEC	C2B-C3B	6.59	1.48	1.40
15	3Q	501	HEC	C2B-C3B	6.27	1.47	1.40
15	3Q	501	HEC	C3C-C2C	5.05	1.46	1.40
13	3C	502	HEM	C1B-NB	-3.51	1.34	1.40

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3Q	501	HEC	C1D-C2D-C3D	-6.30	102.62	107.00
15	3D	501	HEC	C1D-C2D-C3D	-5.96	102.85	107.00
15	3Q	501	HEC	CMB-C2B-C3B	5.69	132.51	125.82
15	3D	501	HEC	CMB-C2B-C3B	5.62	132.42	125.82
15	3D	501	HEC	CMC-C2C-C3C	5.16	131.88	125.82

There are no chirality outliers.

5 of 196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	3A	501	CDL	OB9-CB7-OB8-CB6
11	3A	501	CDL	C71-CB7-OB8-CB6
11	3C	505	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
11	3C	505	CDL	CB2-OB2-PB2-OB5
11	3D	503	CDL	CA3-OA5-PA1-OA3

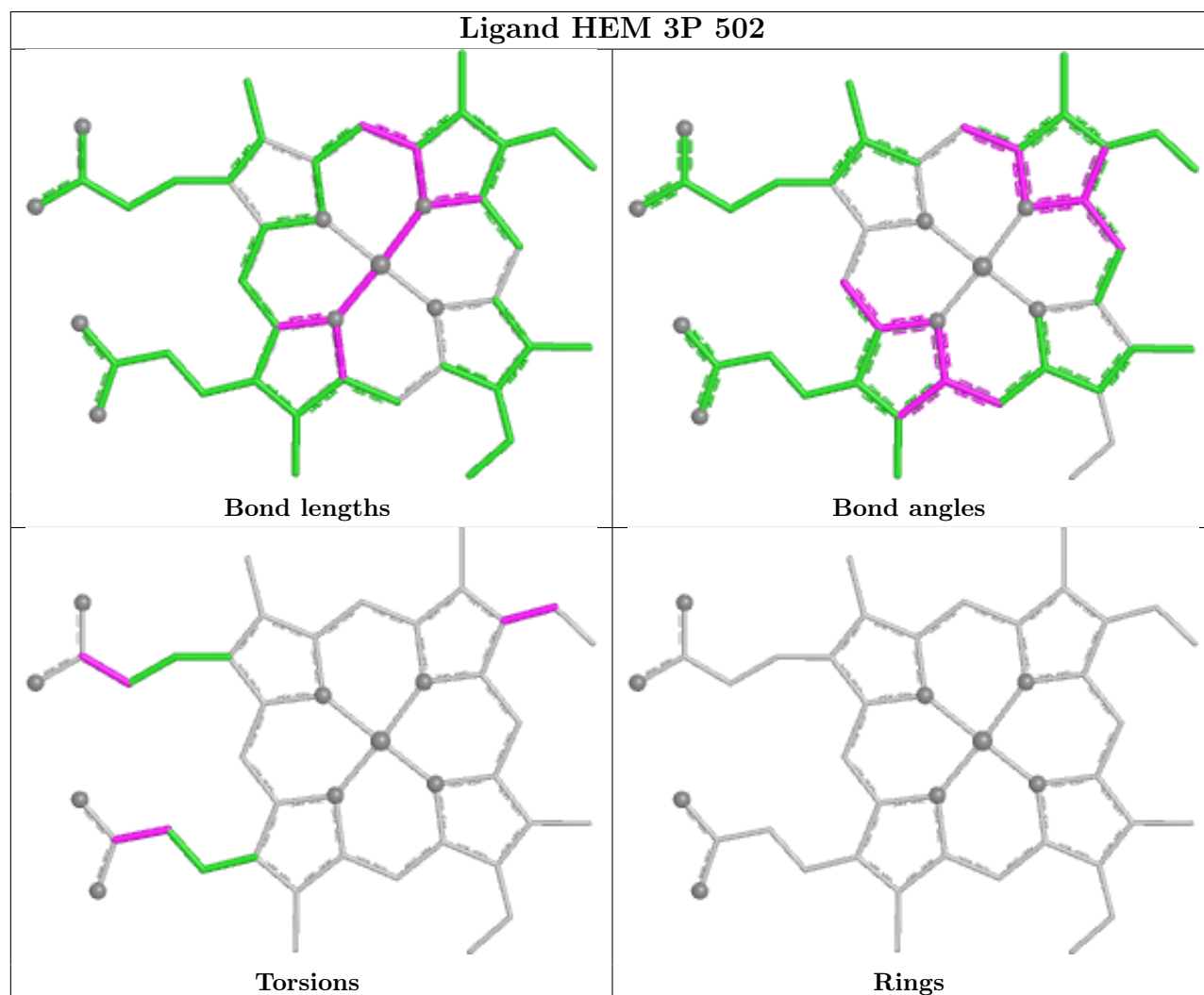
There are no ring outliers.

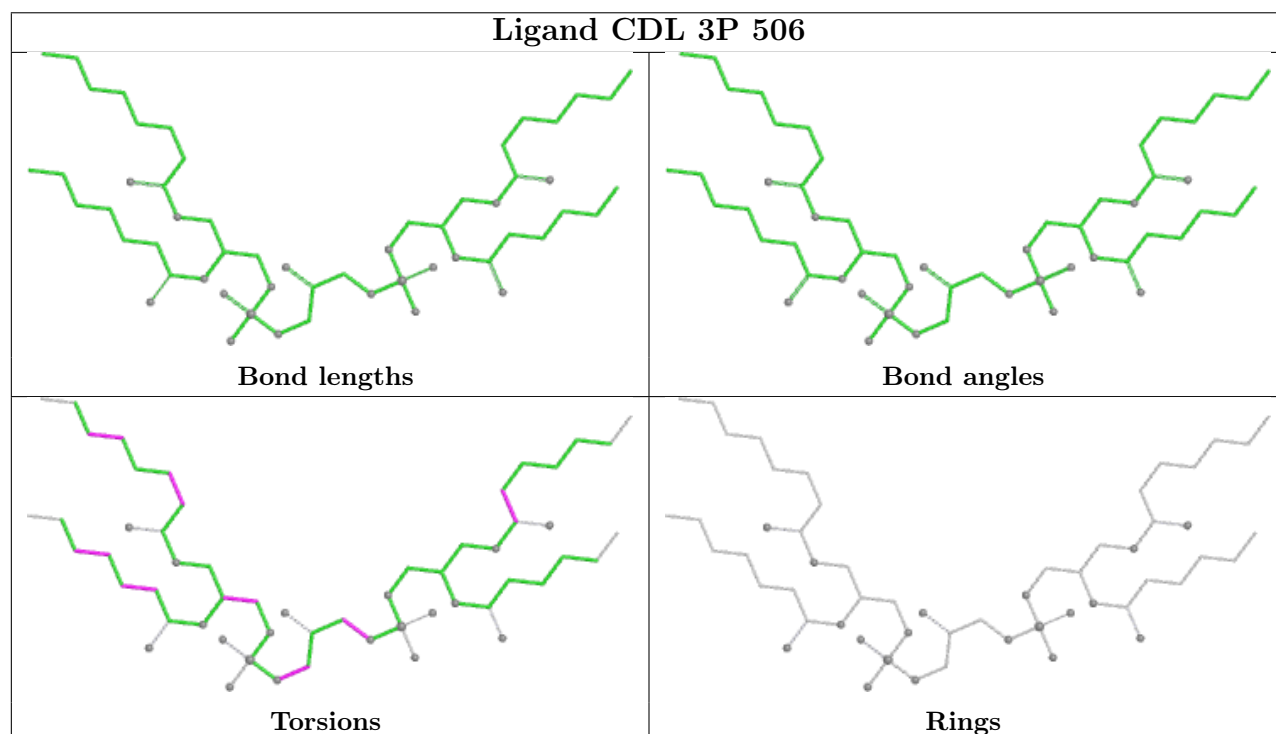
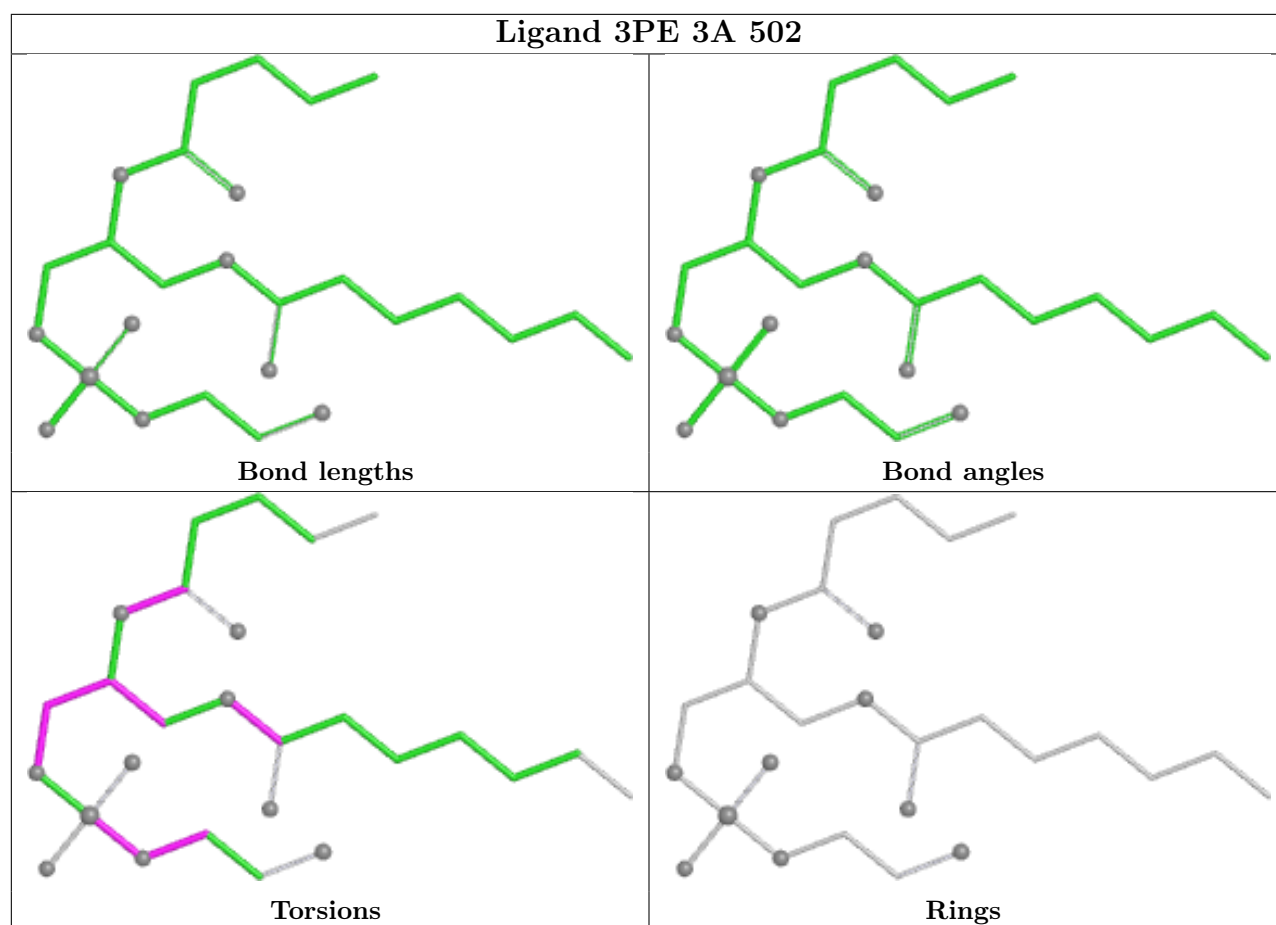
31 monomers are involved in 116 short contacts:

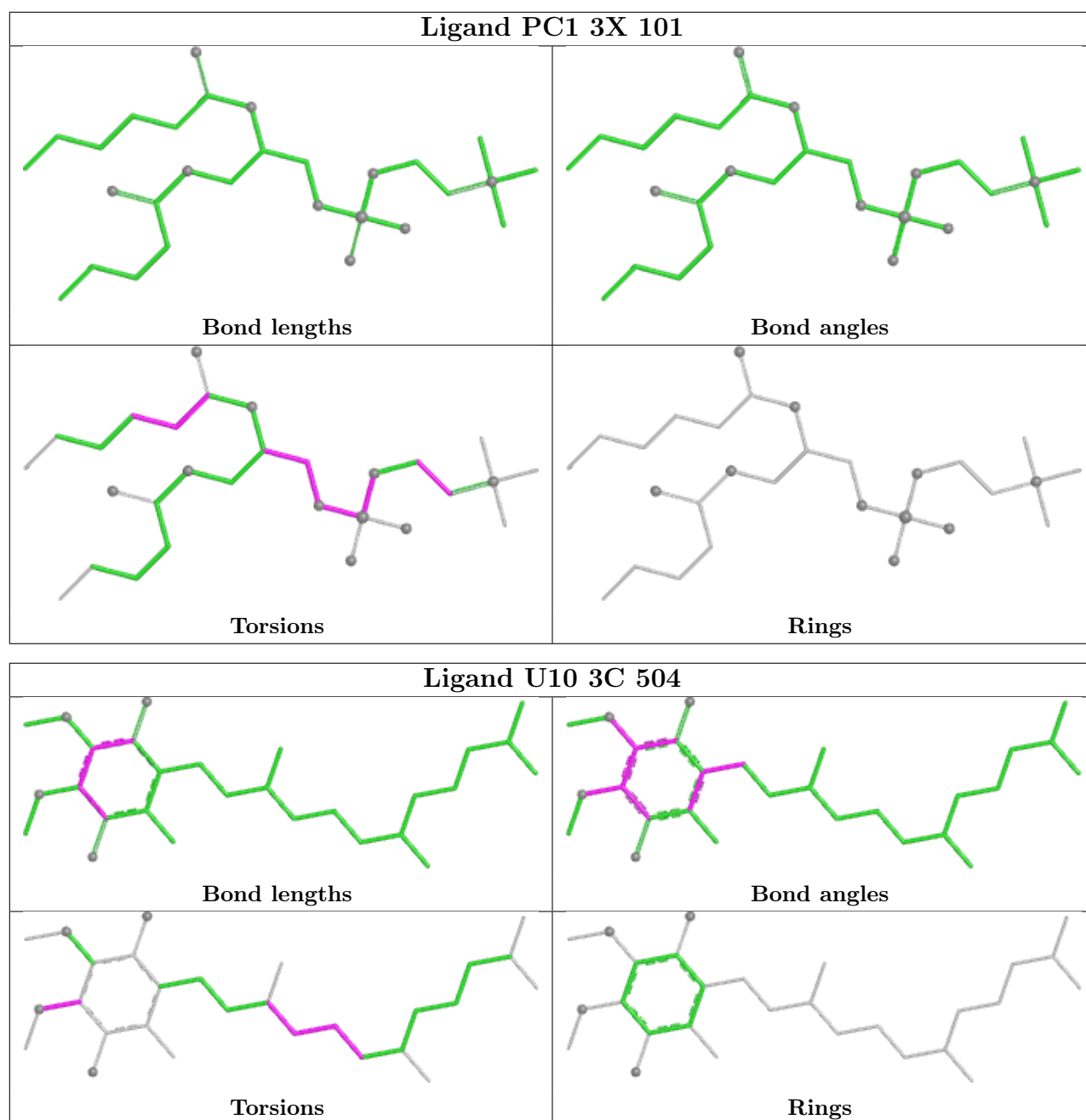
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3P	502	HEM	3	0
12	3A	502	3PE	3	0
11	3P	506	CDL	7	0
17	3X	101	PC1	3	0
14	3C	504	U10	8	0
14	3P	504	U10	3	0
13	3C	502	HEM	2	0
12	3Y	101	3PE	6	0
11	3Q	502	CDL	10	0
11	3A	501	CDL	5	0
16	3E	301	FES	2	0
12	3G	101	3PE	1	0
11	3D	503	CDL	4	0
17	3R	302	PC1	4	0
12	3A	503	3PE	4	0
15	3D	501	HEC	4	0
12	3N	502	3PE	4	0
14	3C	503	U10	1	0
15	3Q	501	HEC	2	0
14	3P	503	U10	7	0
12	3N	501	3PE	2	0
12	3D	502	3PE	4	0
12	3Q	503	3PE	7	0
12	3C	506	3PE	4	0
11	3C	505	CDL	4	0
13	3C	501	HEM	4	0
13	3P	501	HEM	3	0
17	3E	302	PC1	8	0
11	3P	507	CDL	2	0
12	3P	505	3PE	1	0
12	3R	303	3PE	3	0

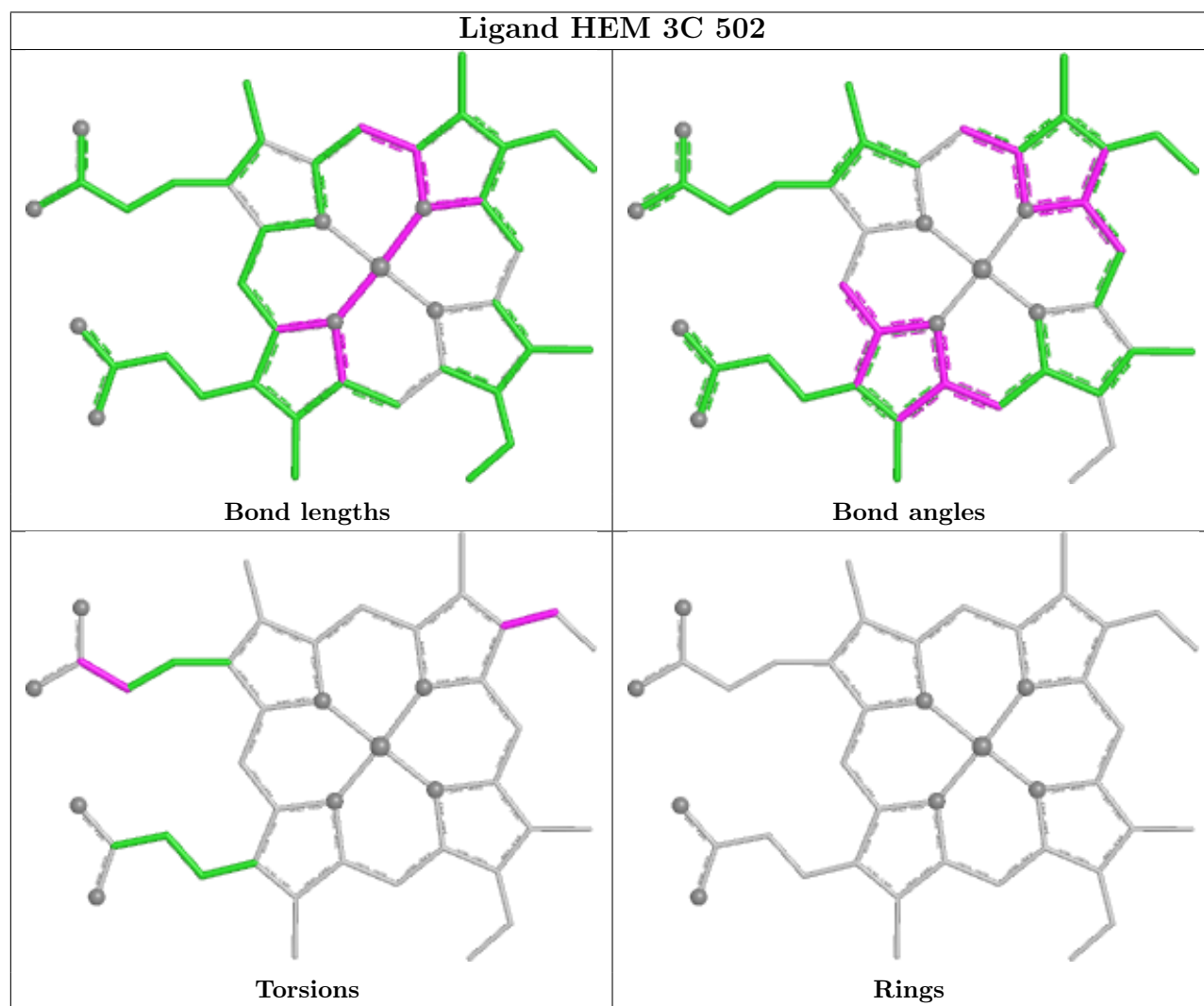
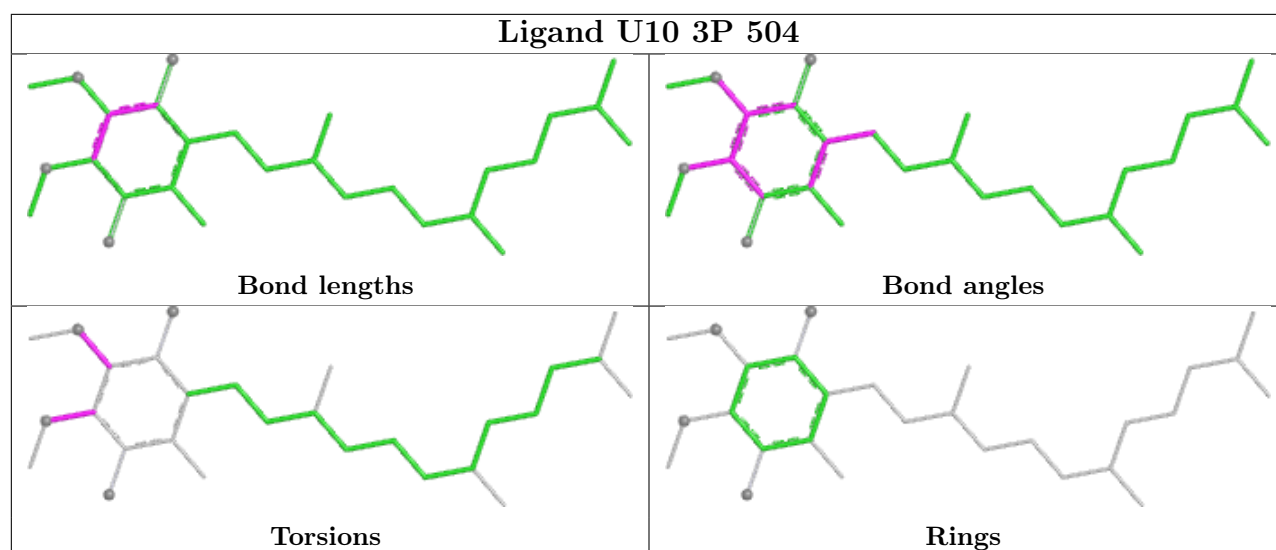
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

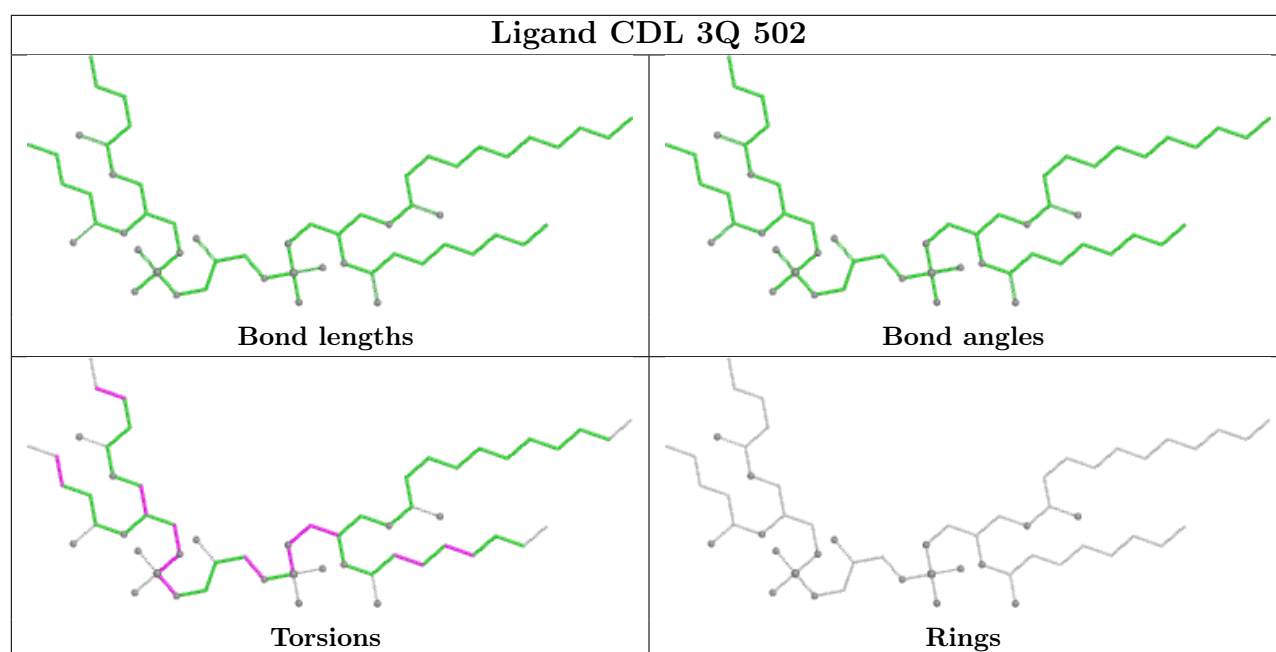
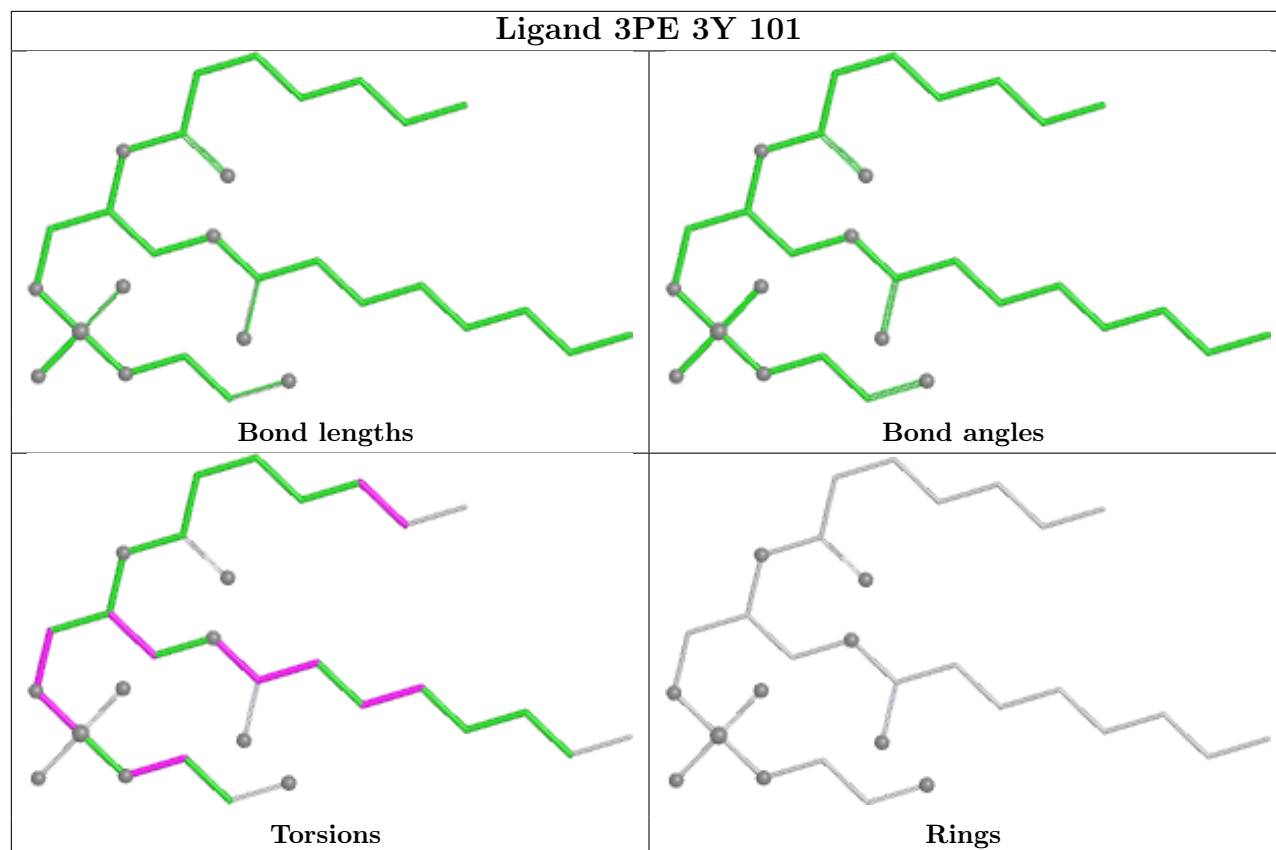
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

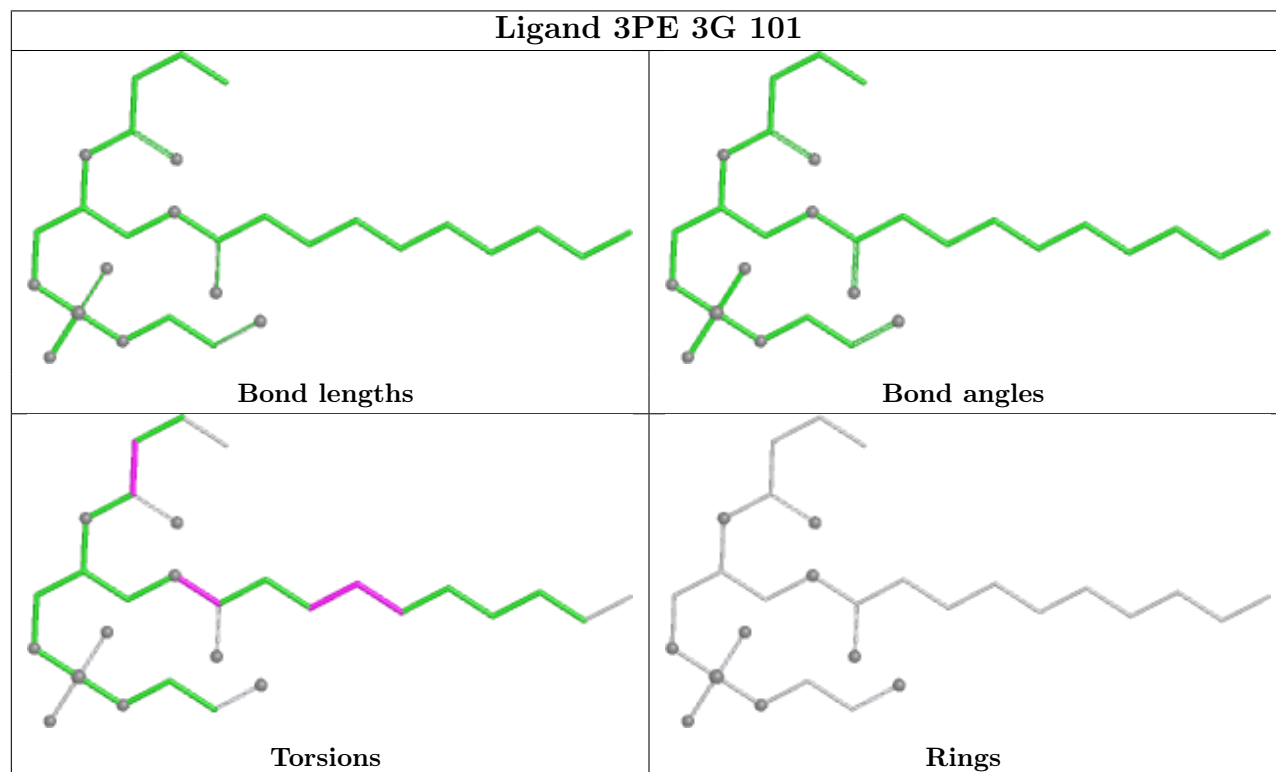
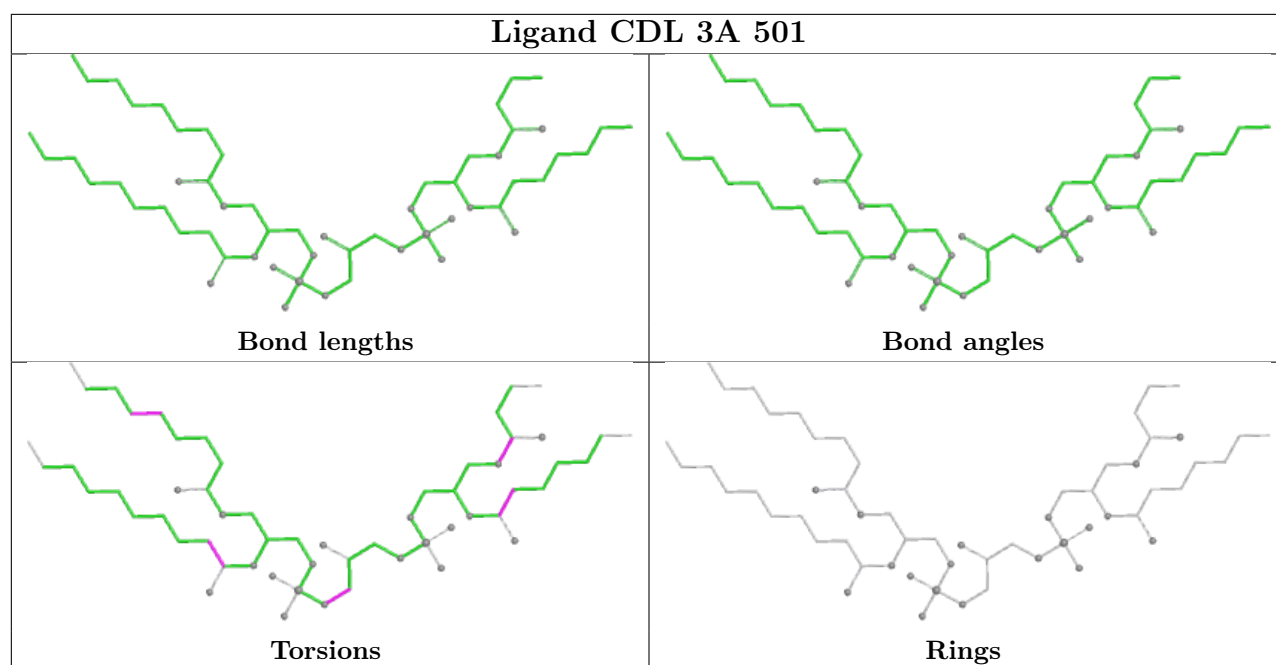


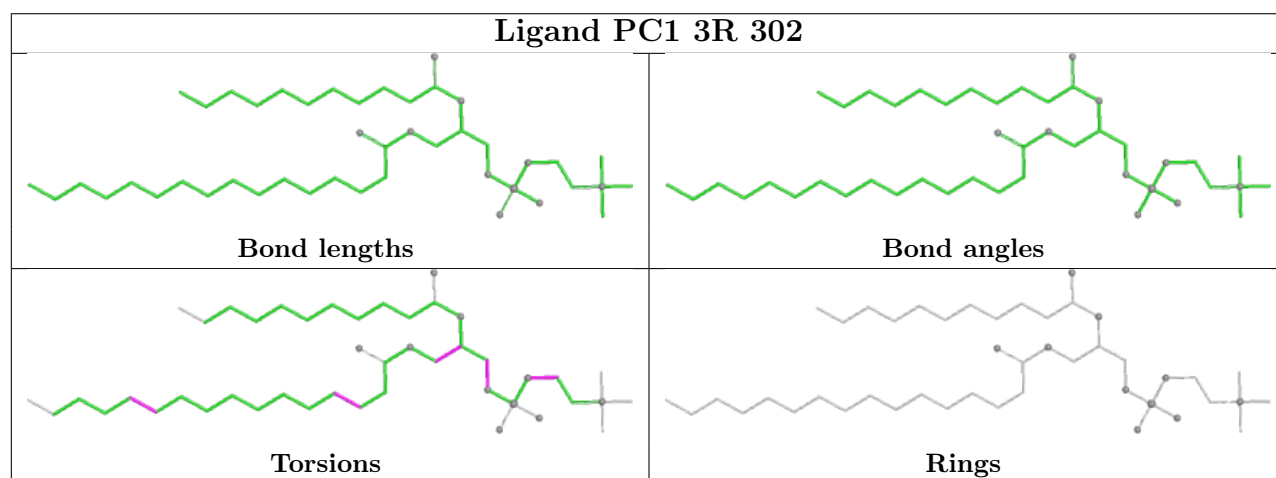
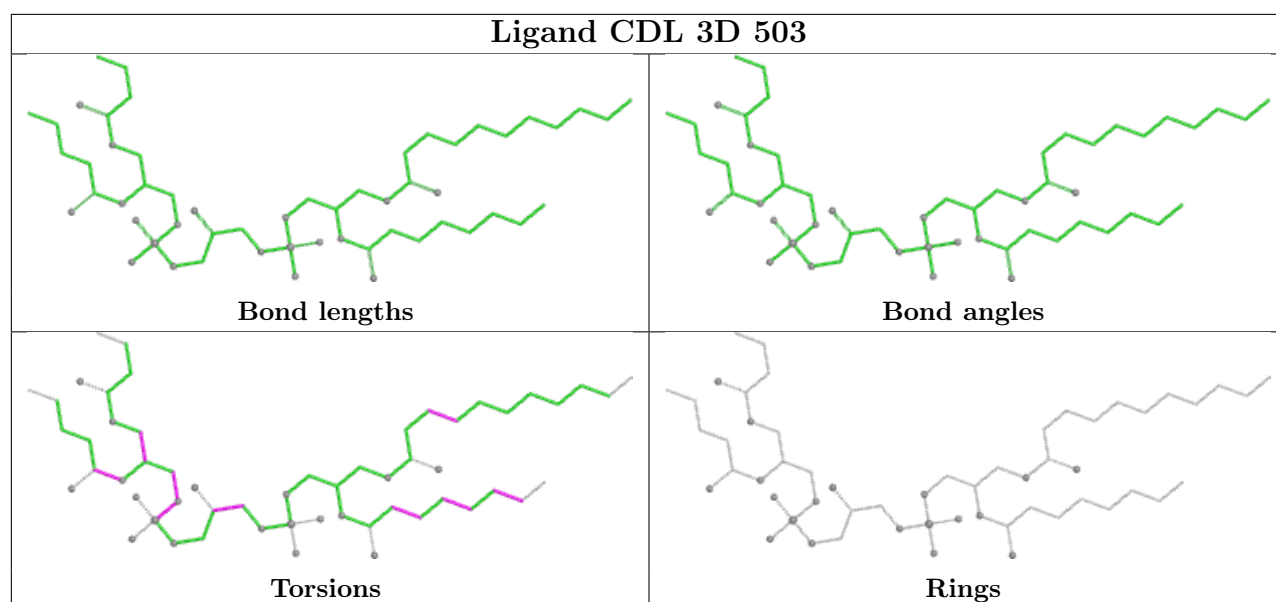


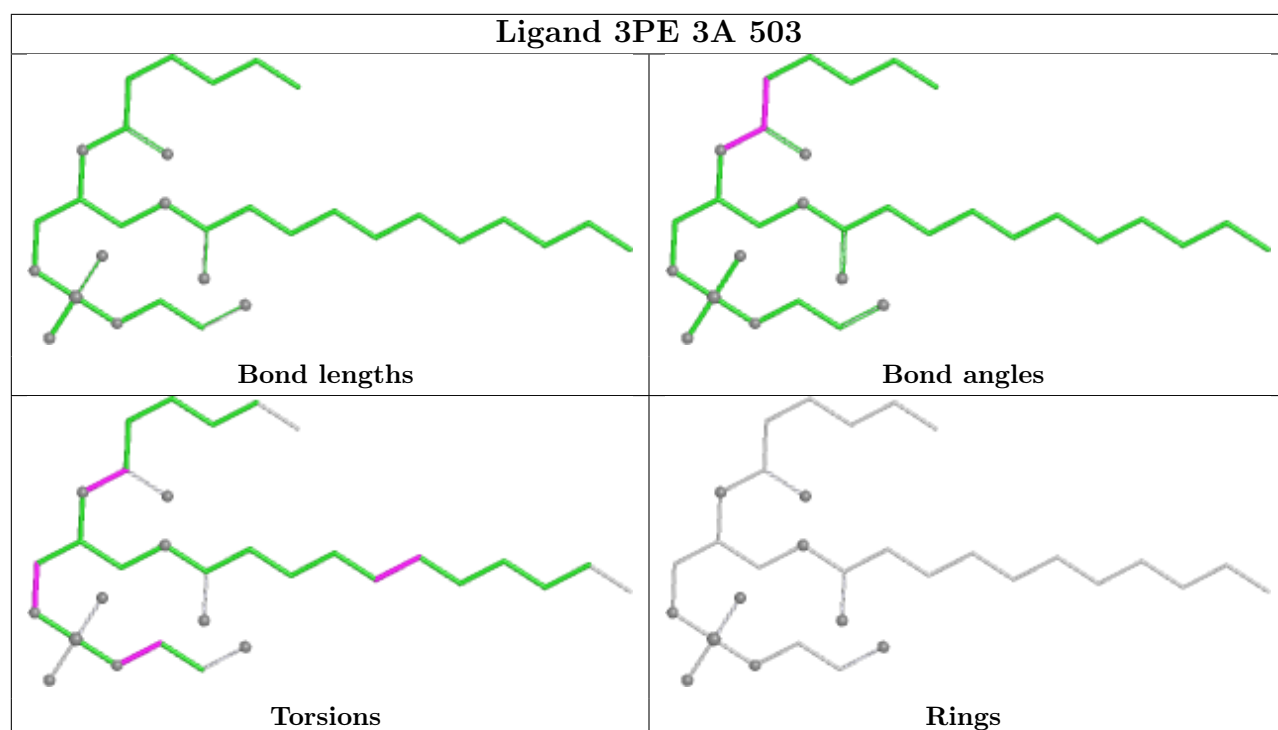


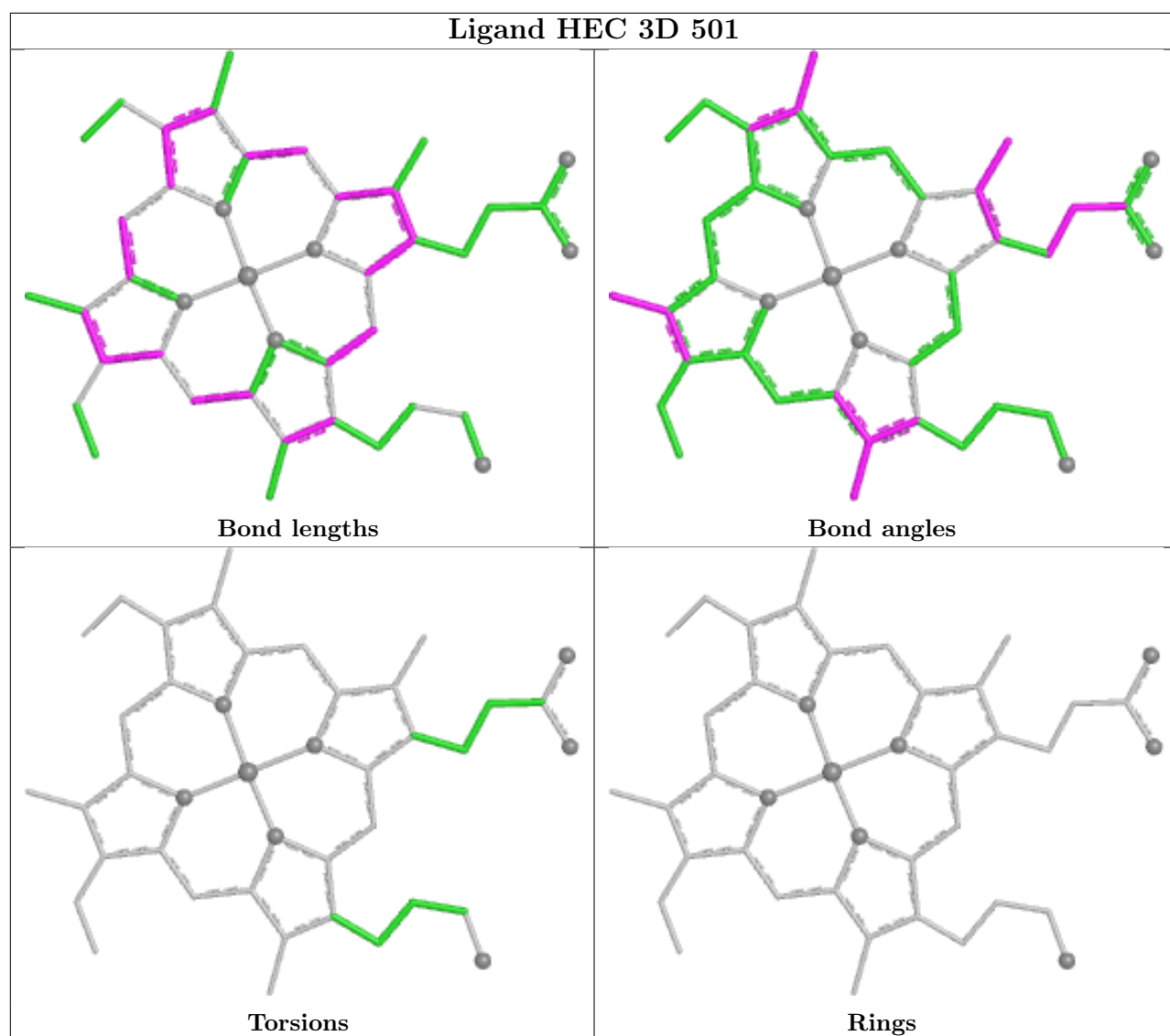


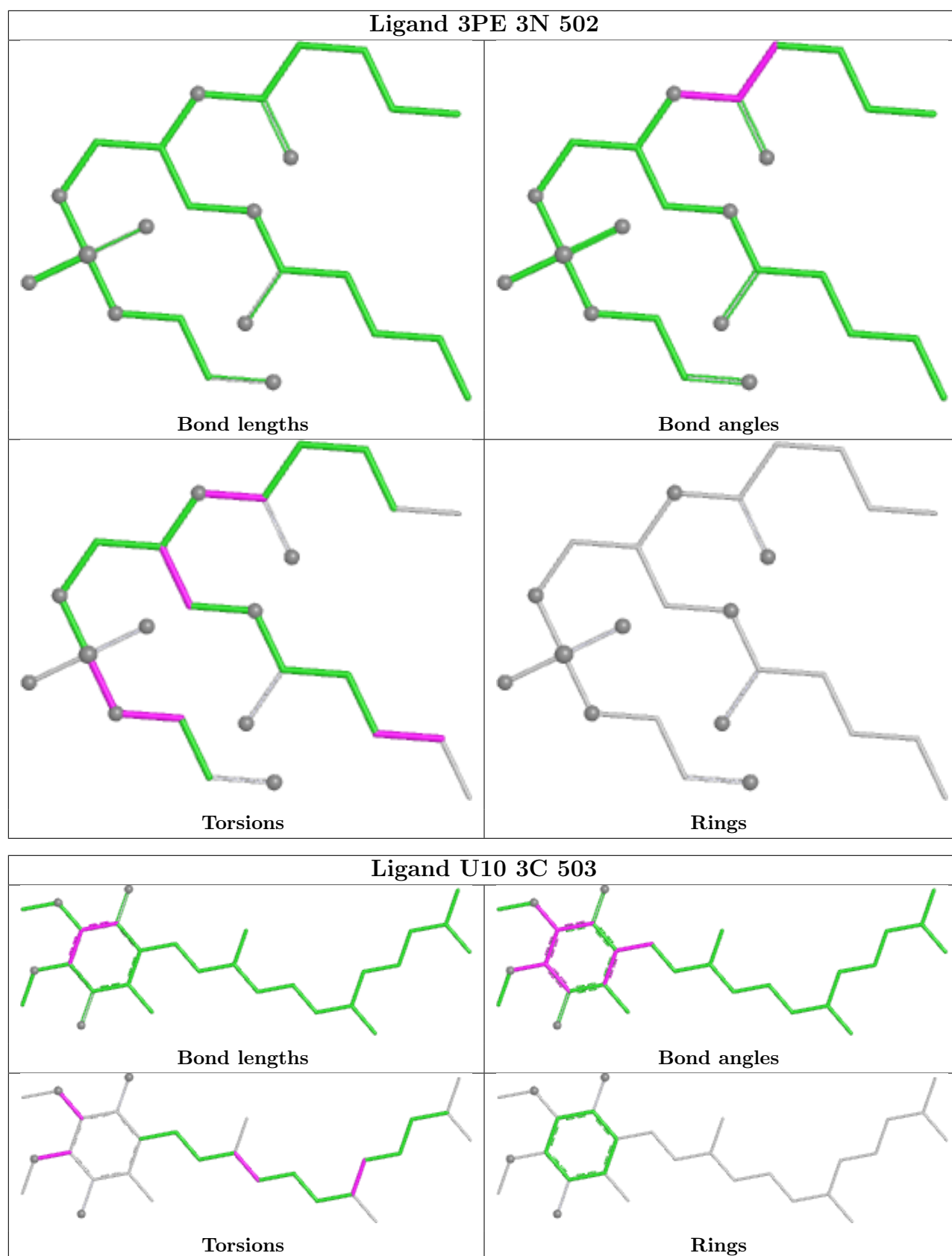




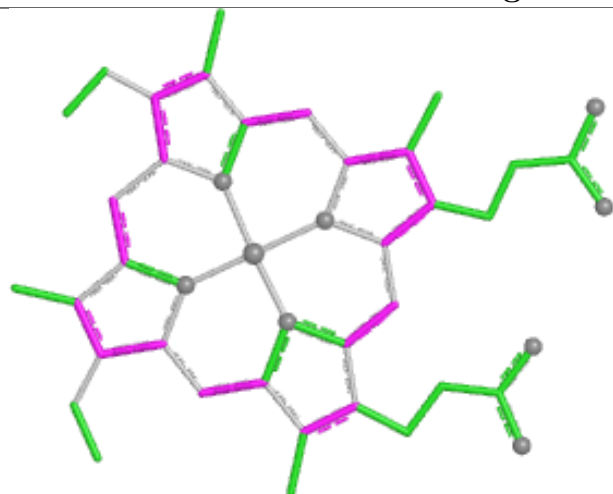




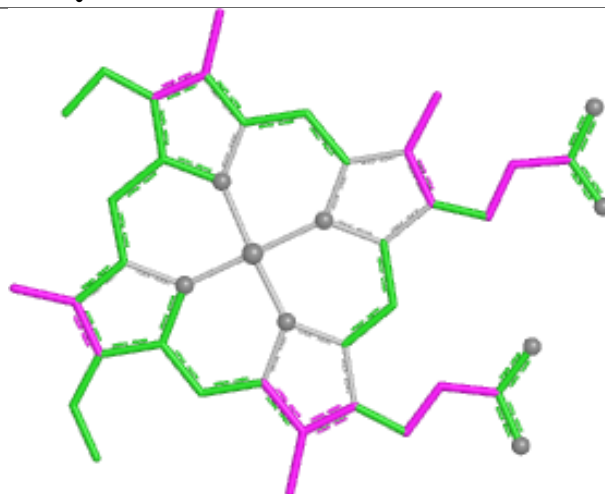




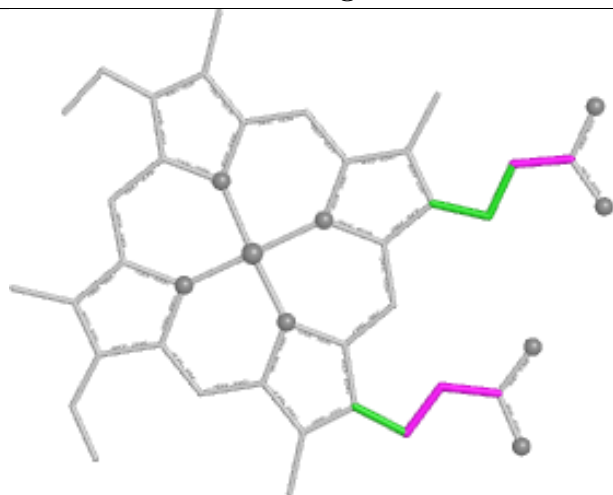
Ligand HEC 3Q 501



Bond lengths



Bond angles

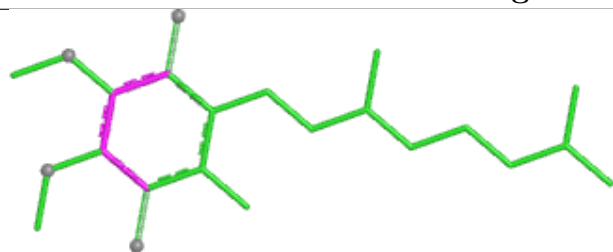


Torsions

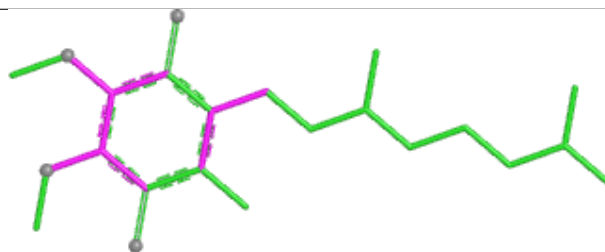


Rings

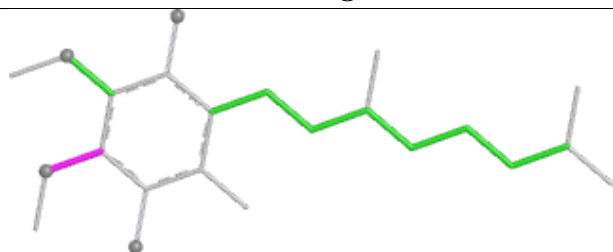
Ligand U10 3P 503



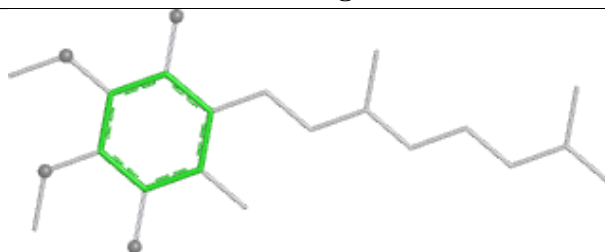
Bond lengths



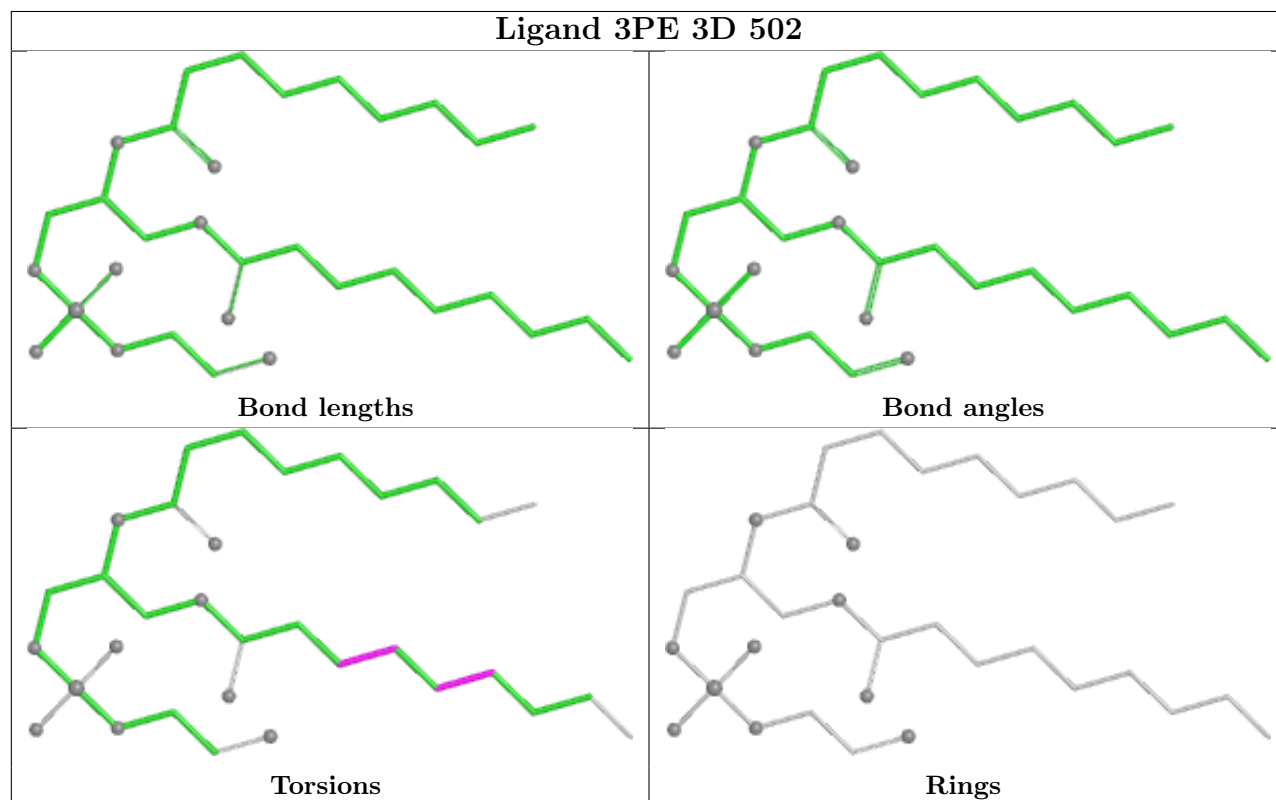
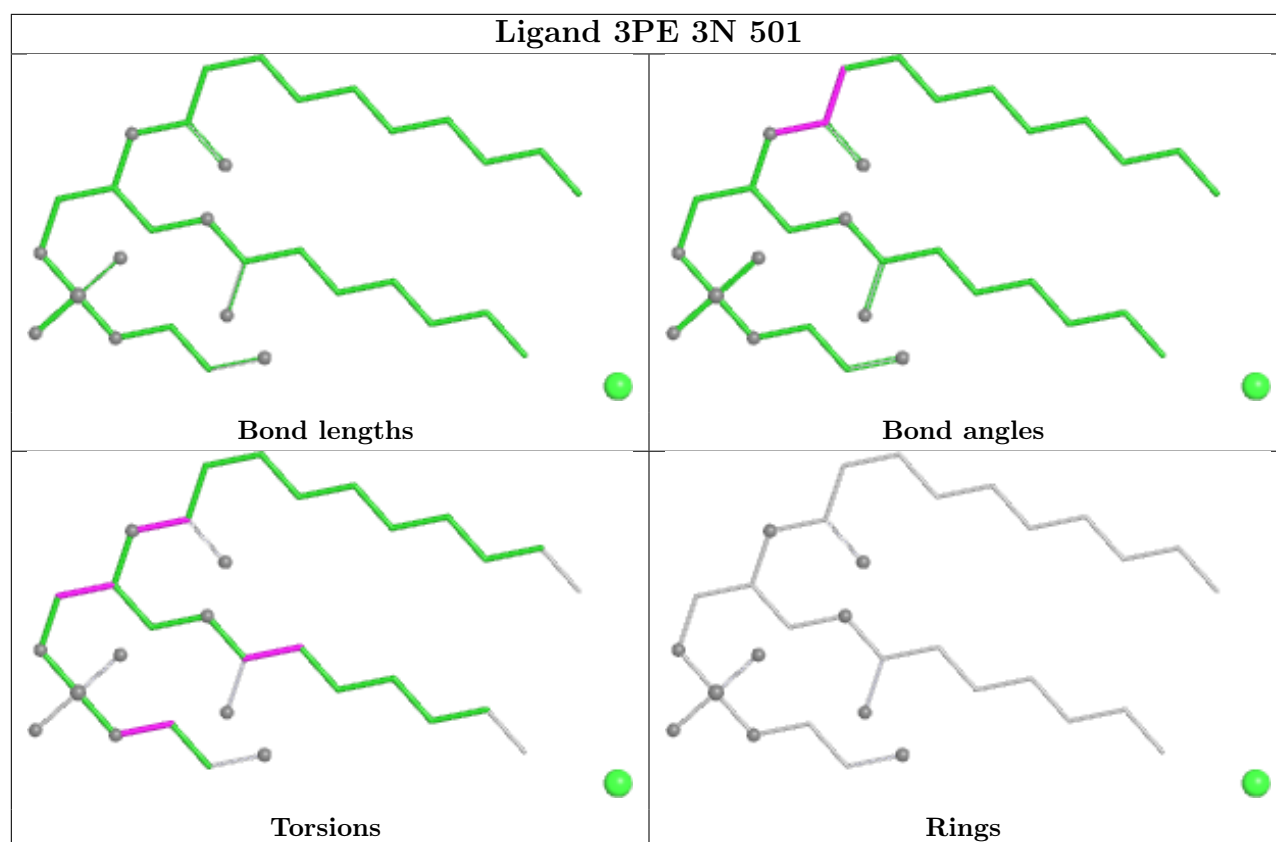
Bond angles

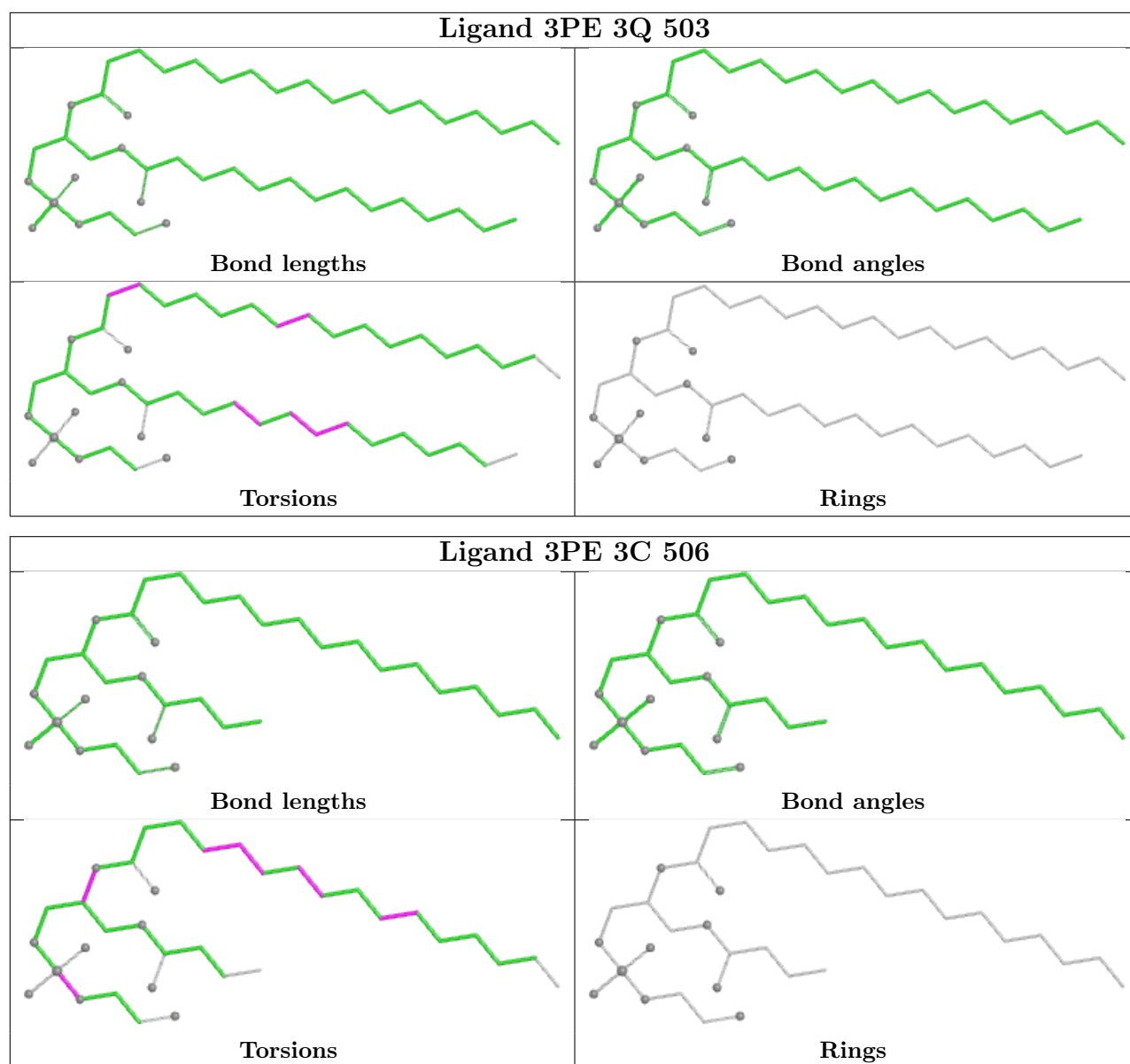


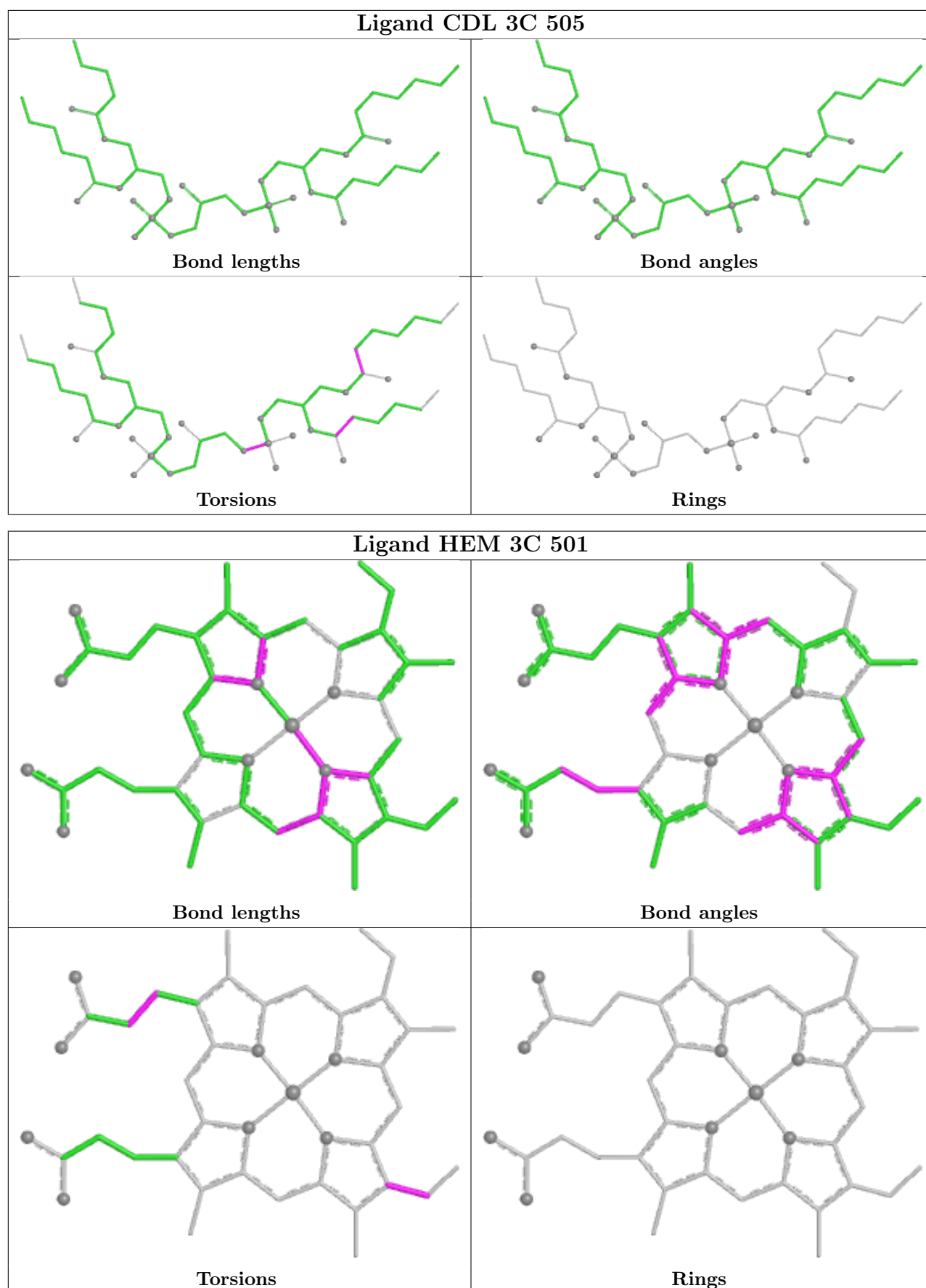
Torsions



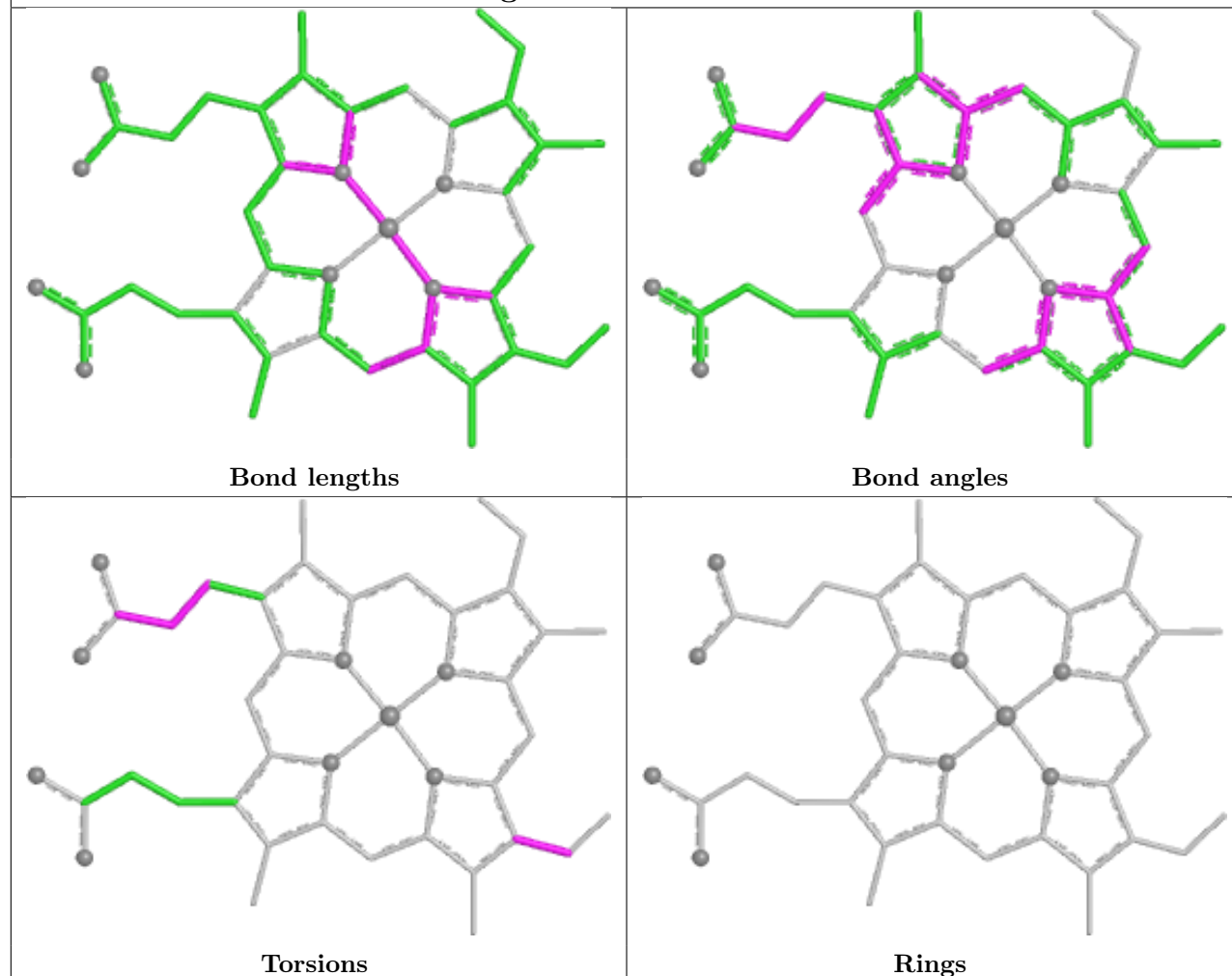
Rings



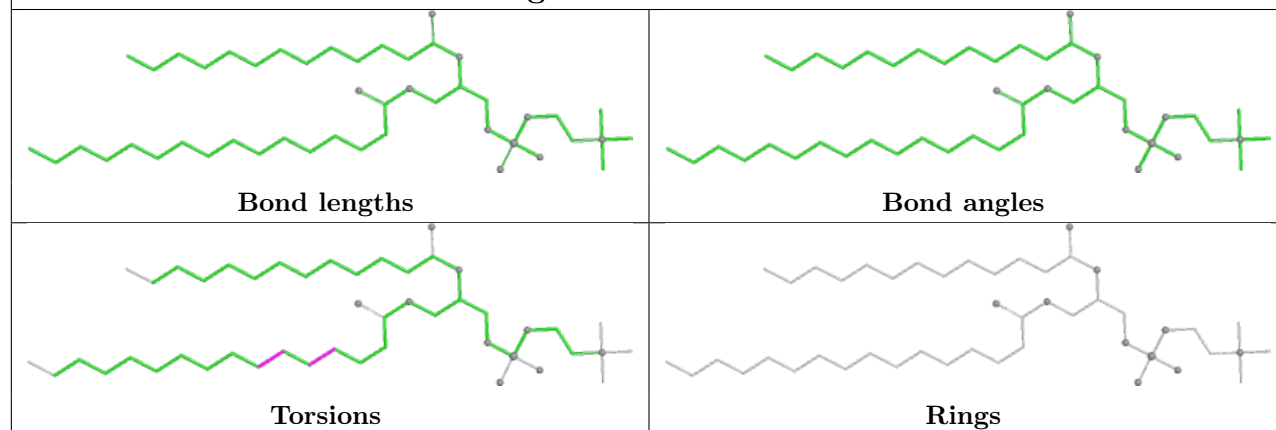


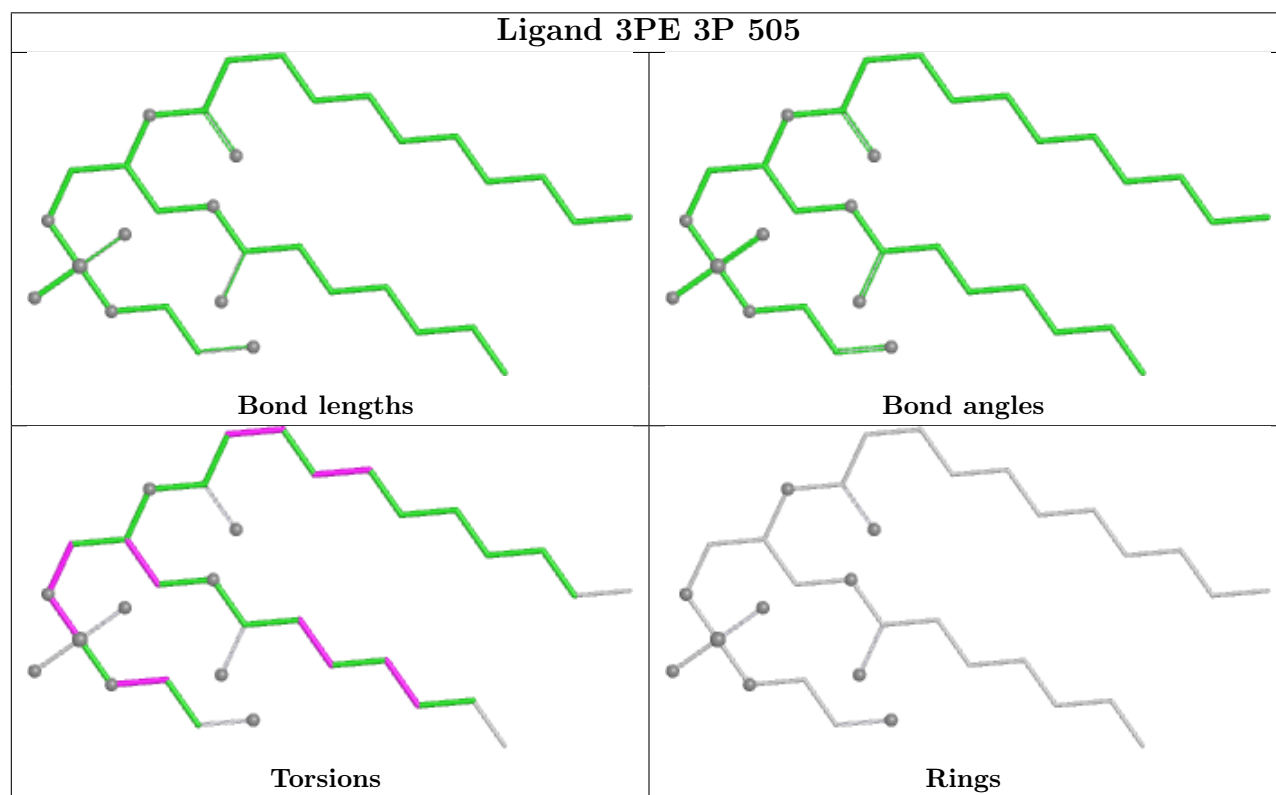
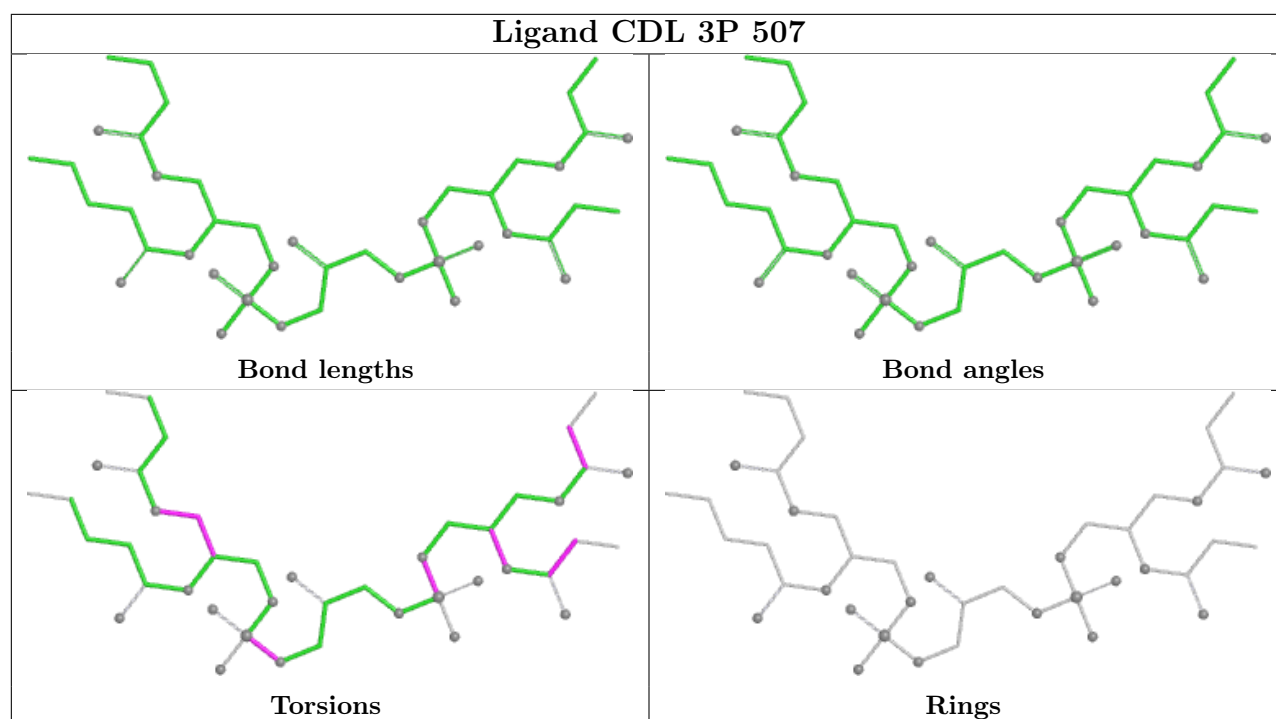


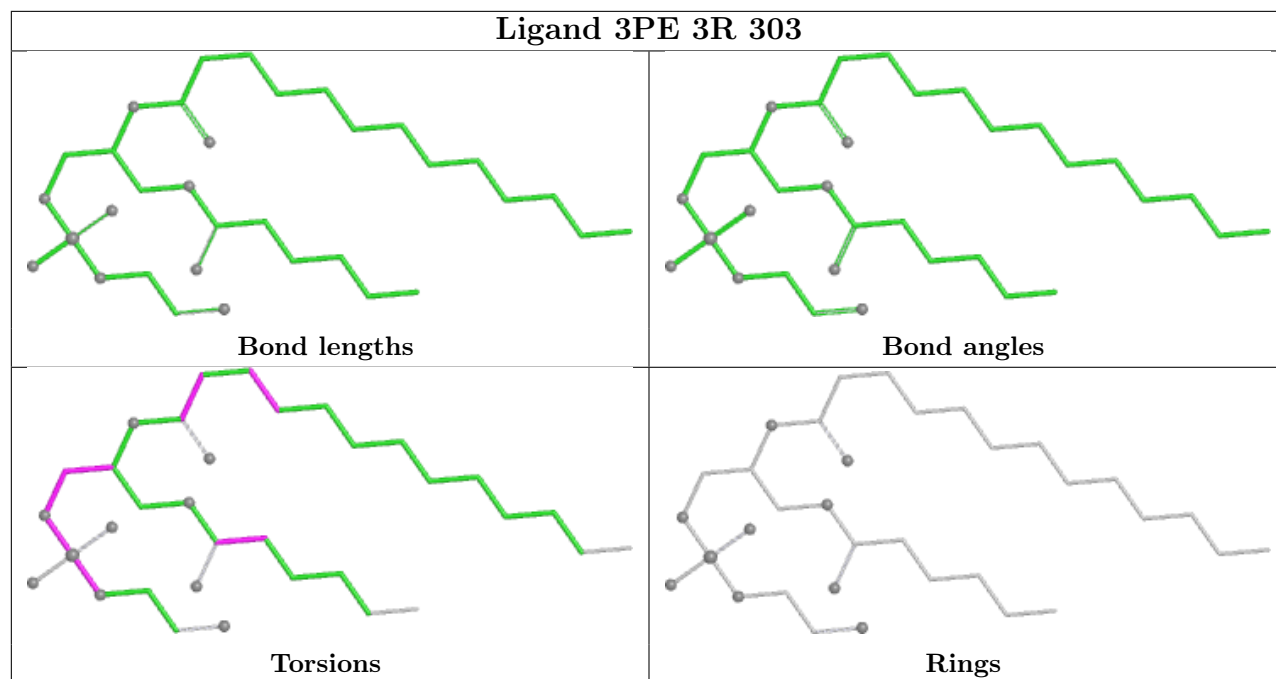
Ligand HEM 3P 501



Ligand PC1 3E 302







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	3G	1
8	3H	1
5	3I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3G	75:ASN	C	82:PRO	N	4.50
1	3H	77:GLU	C	78:ASP	N	3.04
1	3I	49:PHE	C	50:LEU	N	1.97

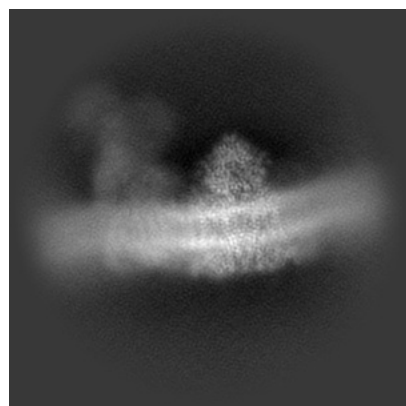
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42221. These allow visual inspection of the internal detail of the map and identification of artifacts.

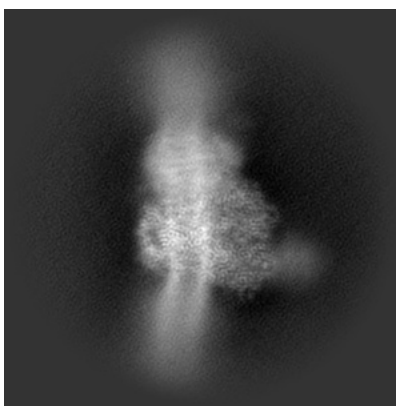
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

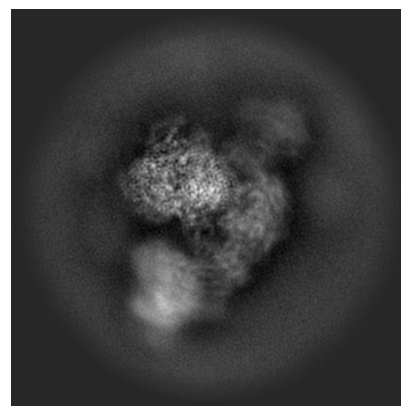
6.1.1 Primary map



X

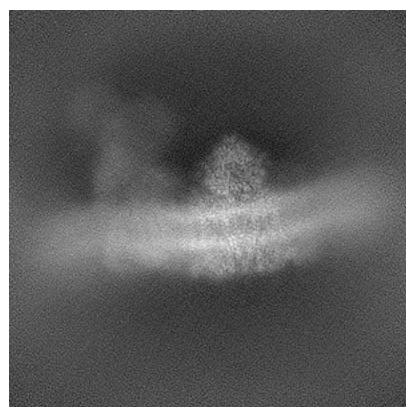


Y

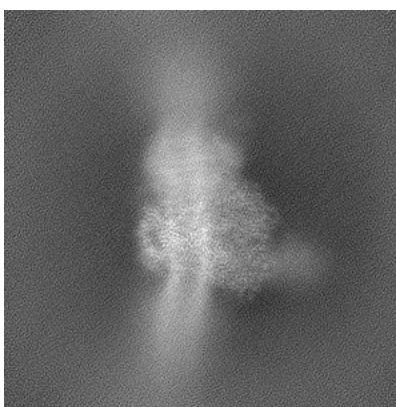


Z

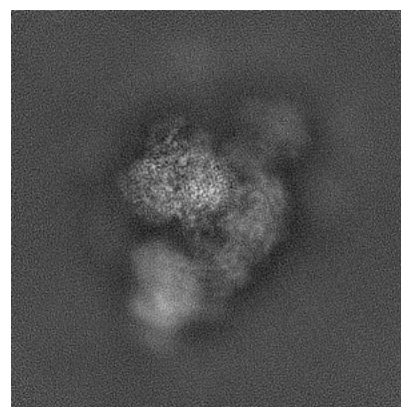
6.1.2 Raw map



X



Y

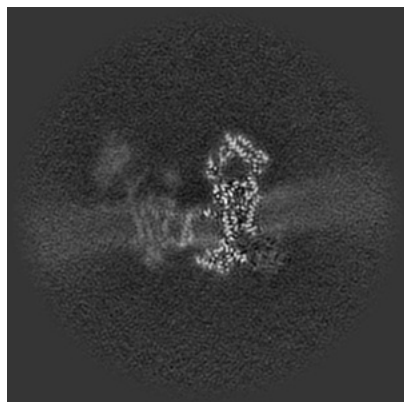


Z

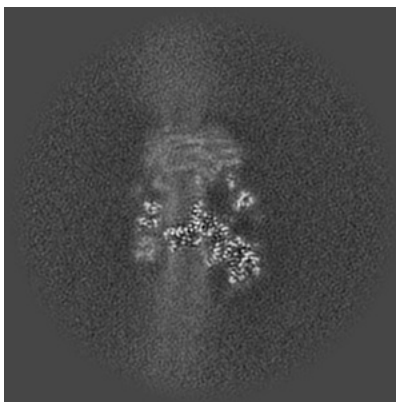
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

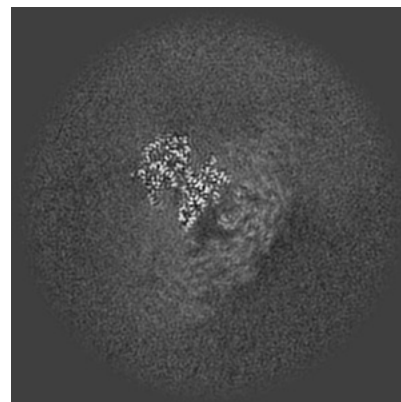
6.2.1 Primary map



X Index: 160

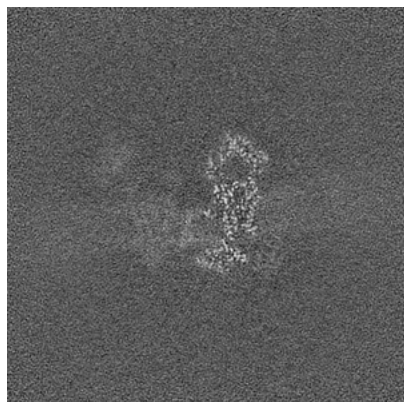


Y Index: 160

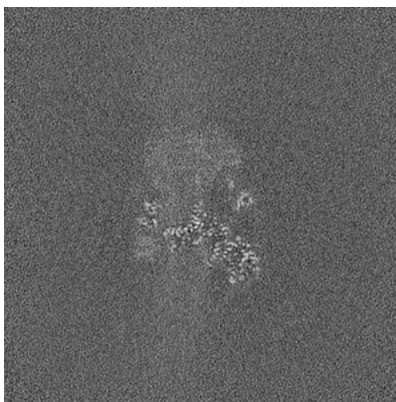


Z Index: 160

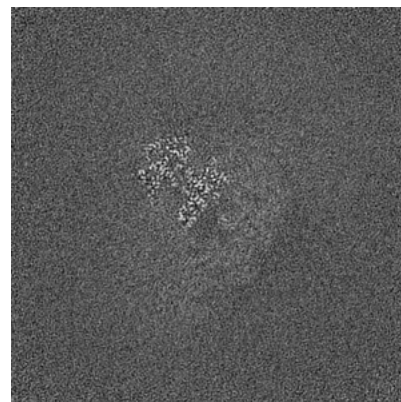
6.2.2 Raw map



X Index: 160



Y Index: 160

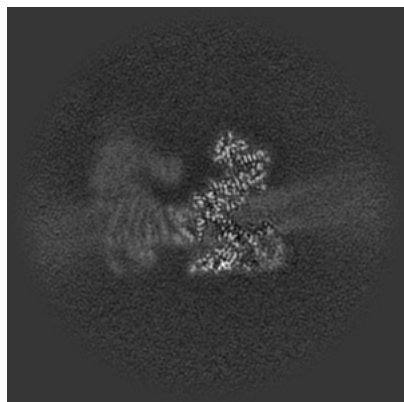


Z Index: 160

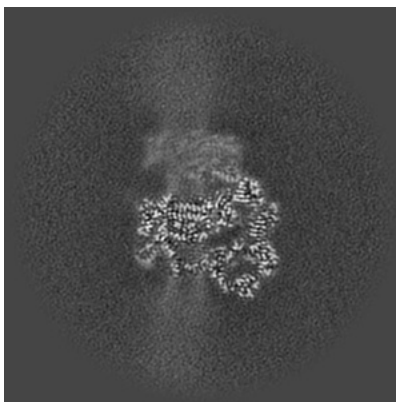
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

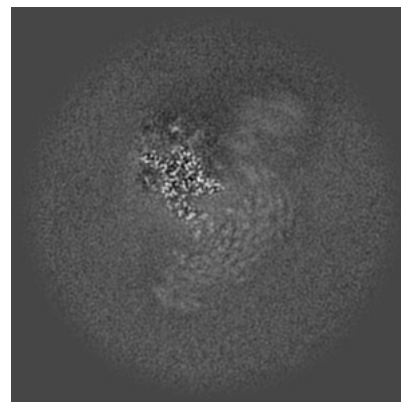
6.3.1 Primary map



X Index: 147

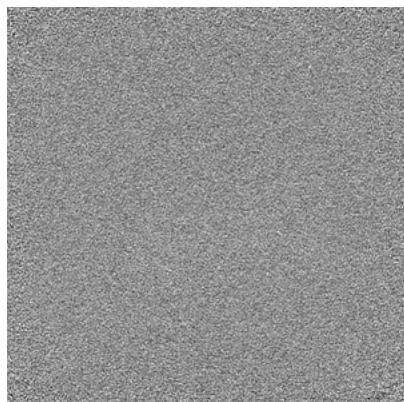


Y Index: 175

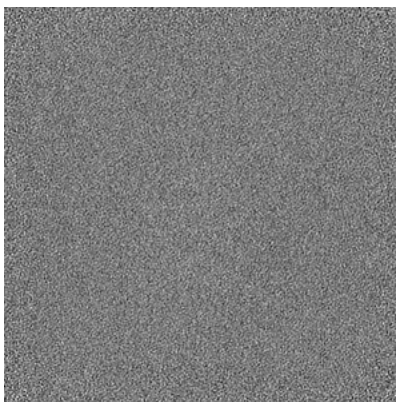


Z Index: 133

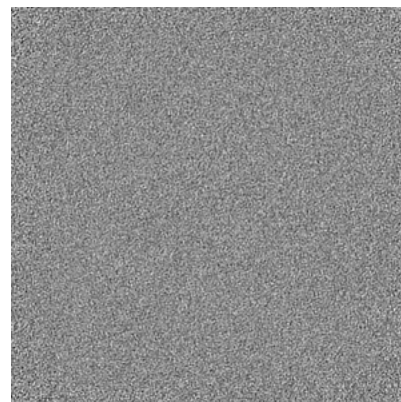
6.3.2 Raw map



X Index: 0



Y Index: 0

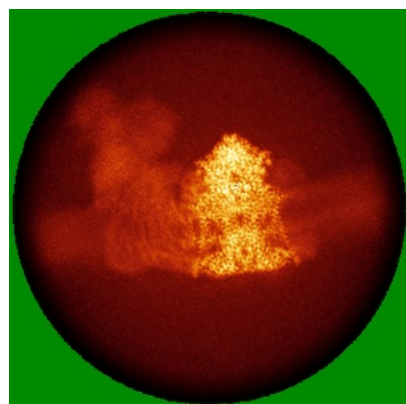


Z Index: 0

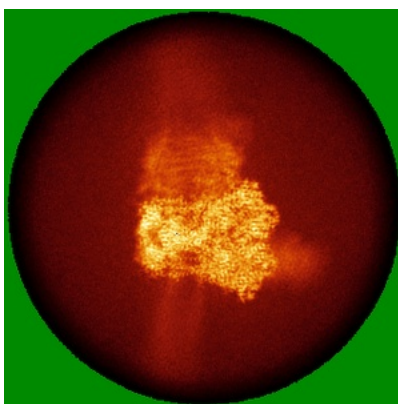
The images above show the largest variance slices of the map in three orthogonal directions.

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

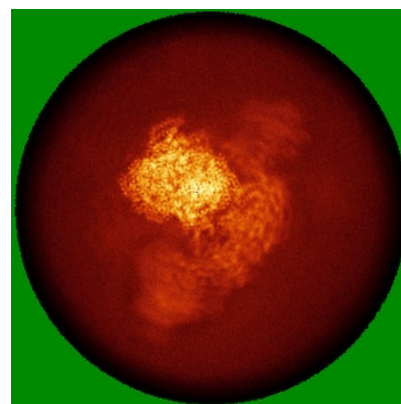
6.4.1 Primary map



X

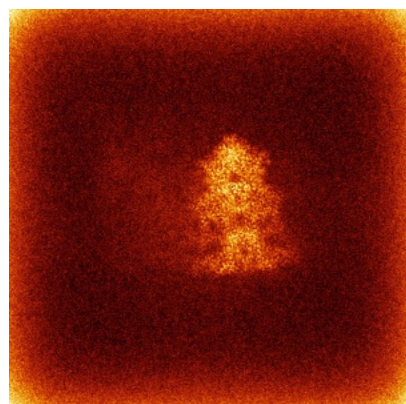


Y

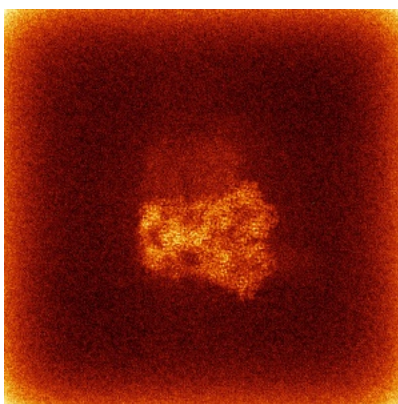


Z

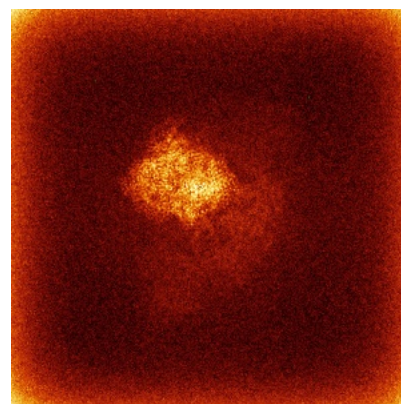
6.4.2 Raw map



X



Y

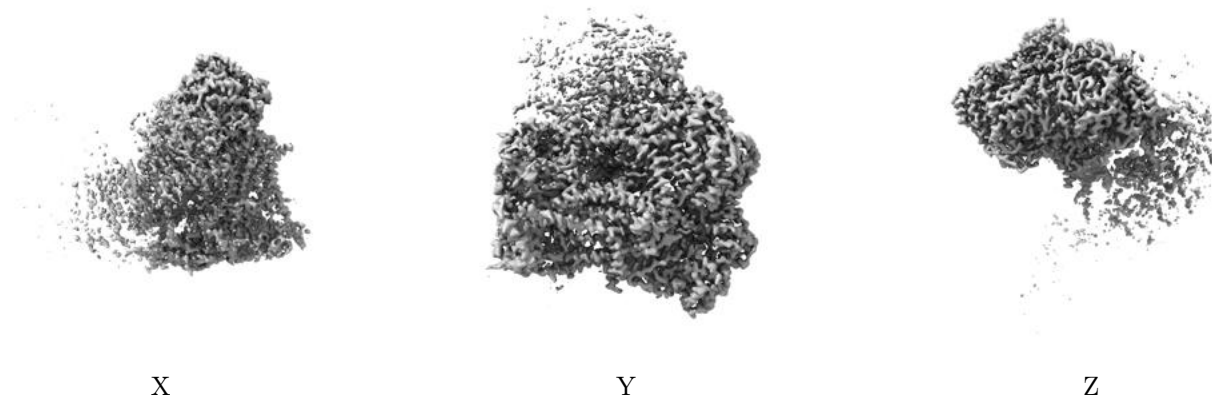


Z

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

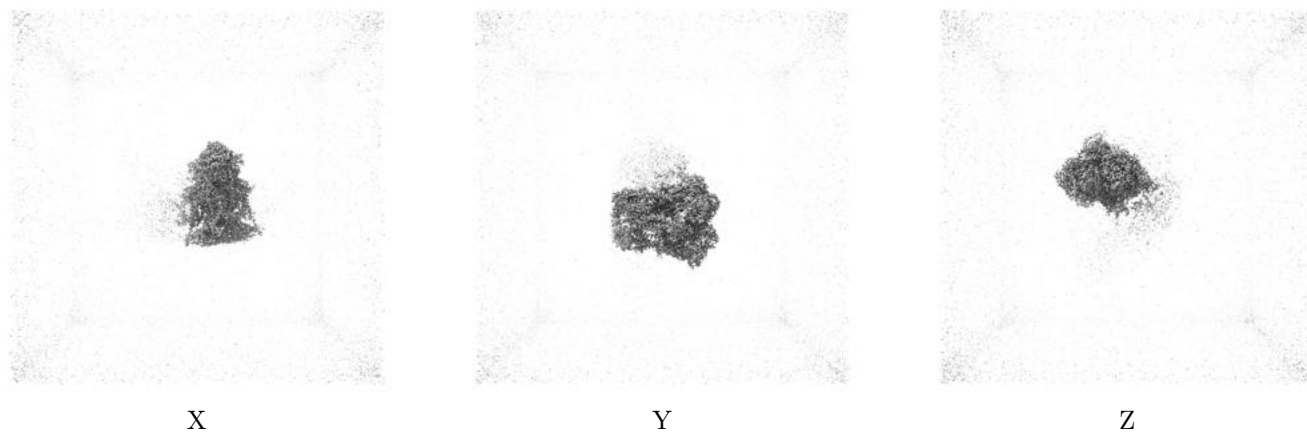
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

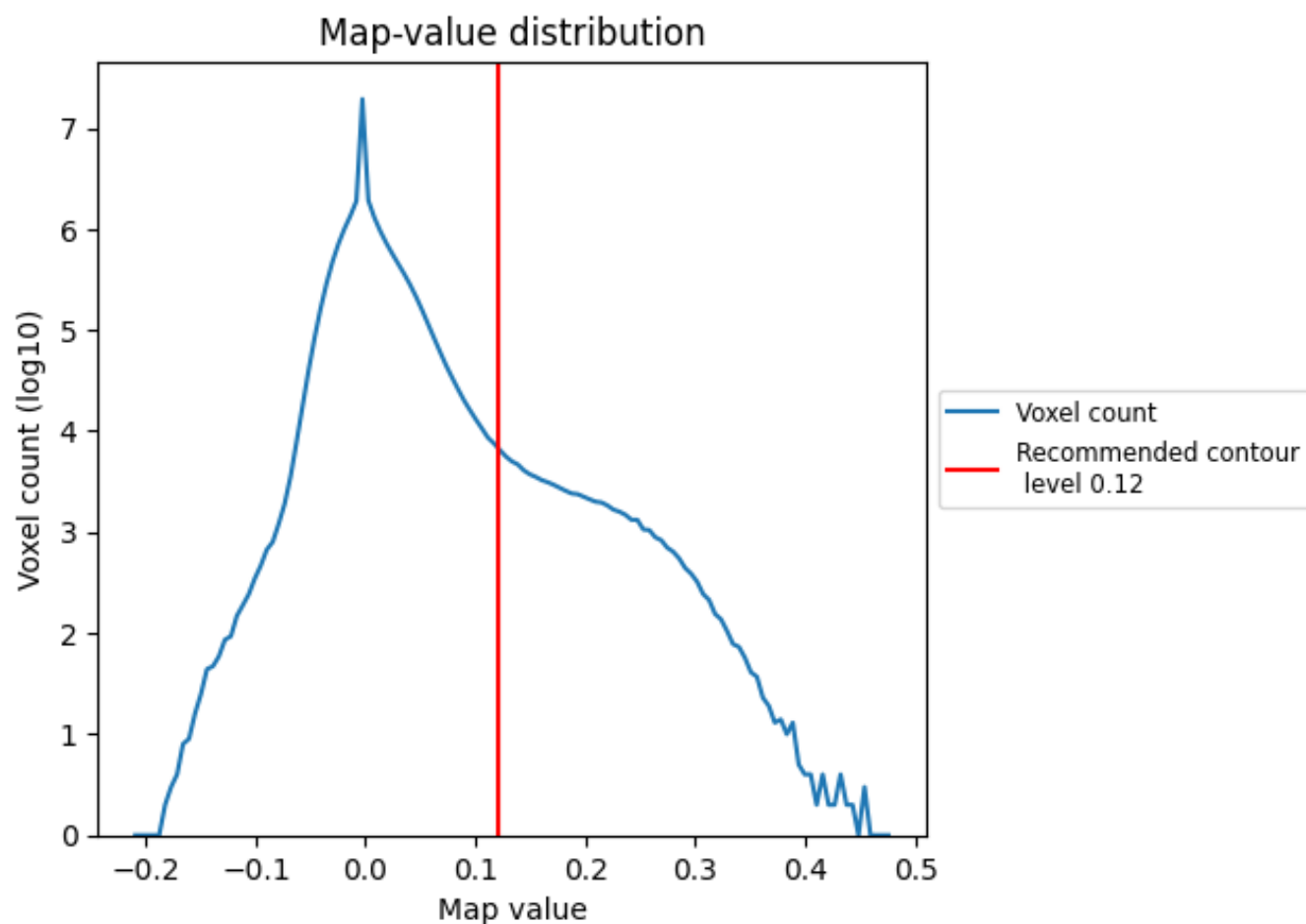
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

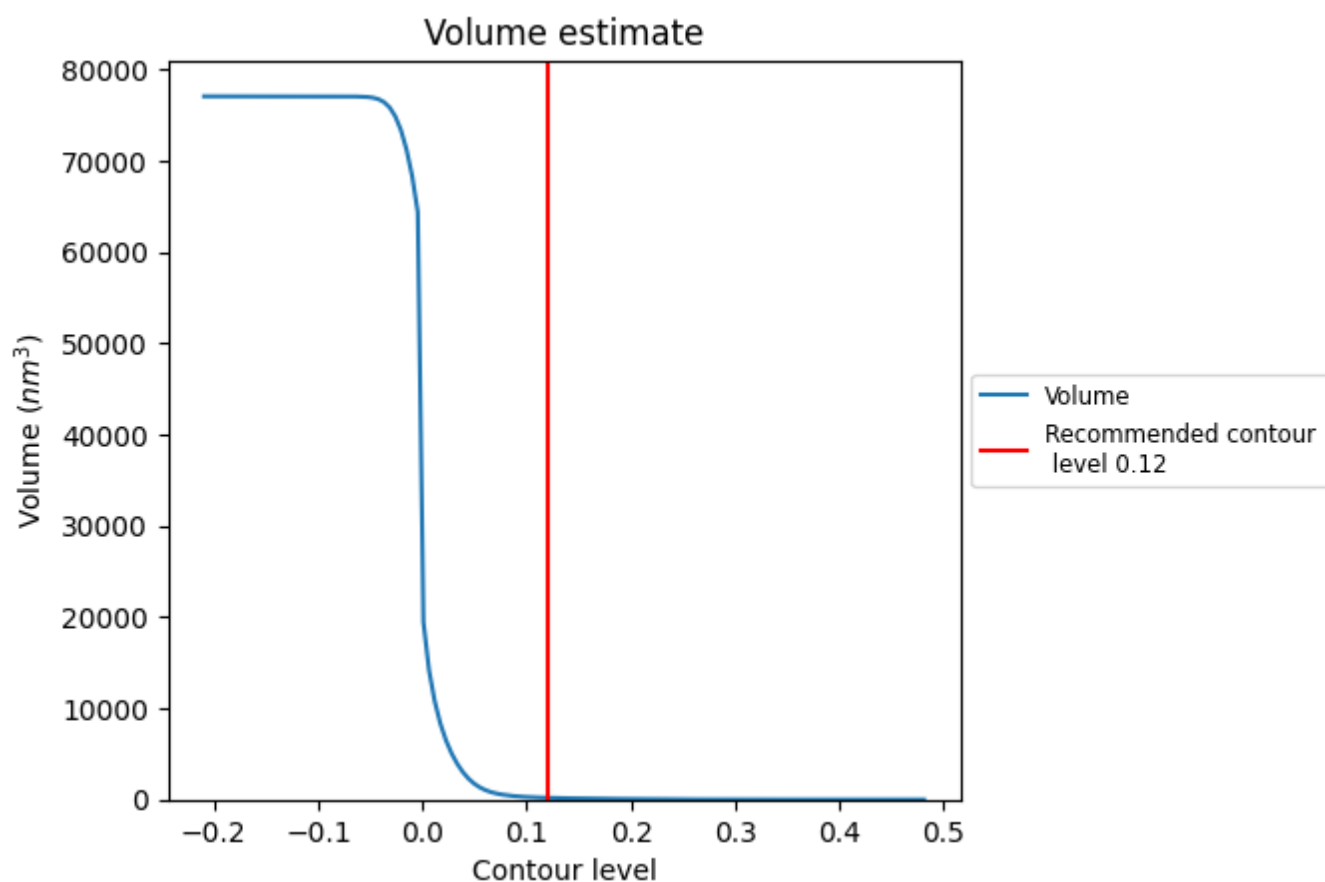
This section contains the results of statistical analysis of the map.

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.

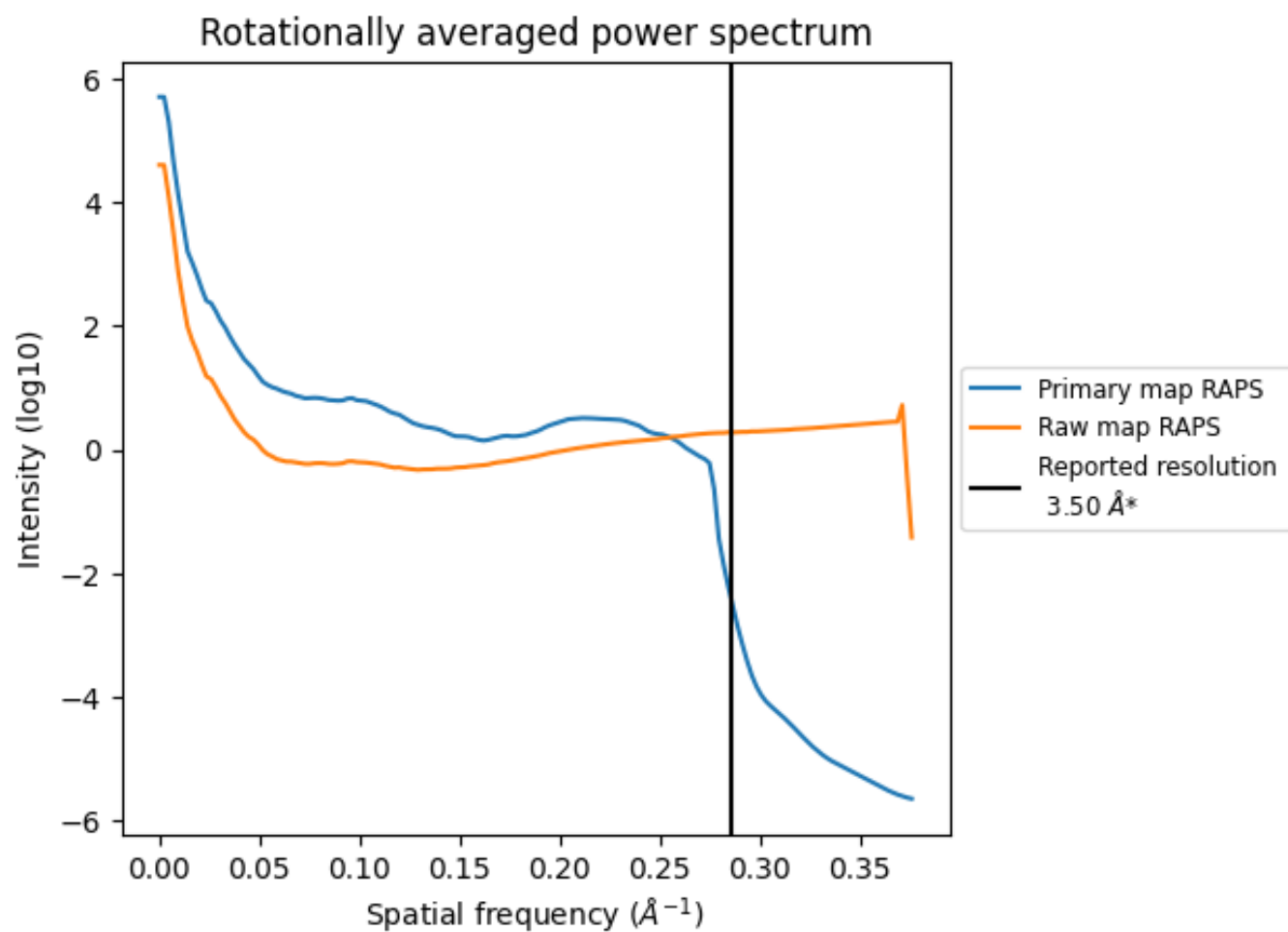
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 172 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

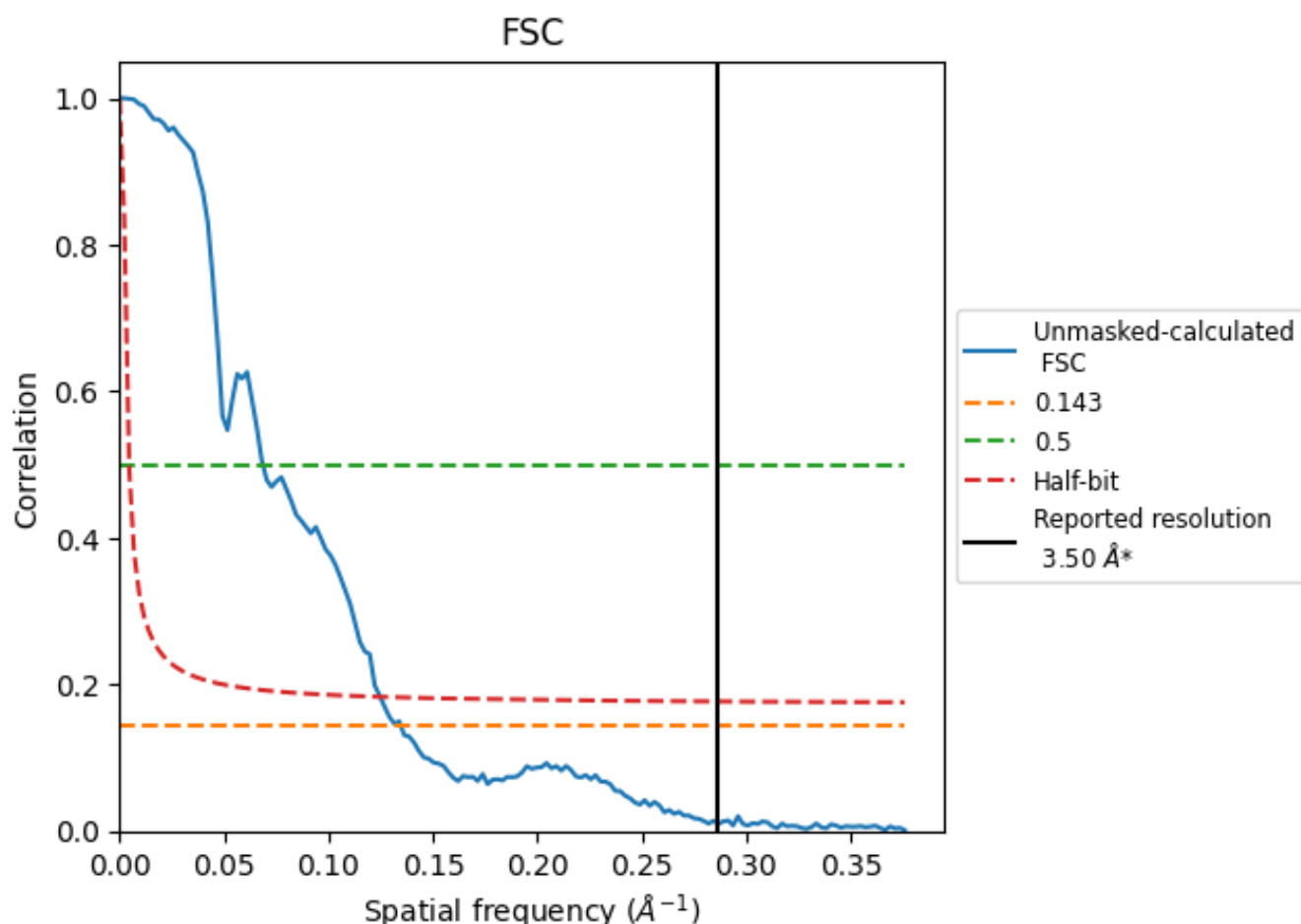


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

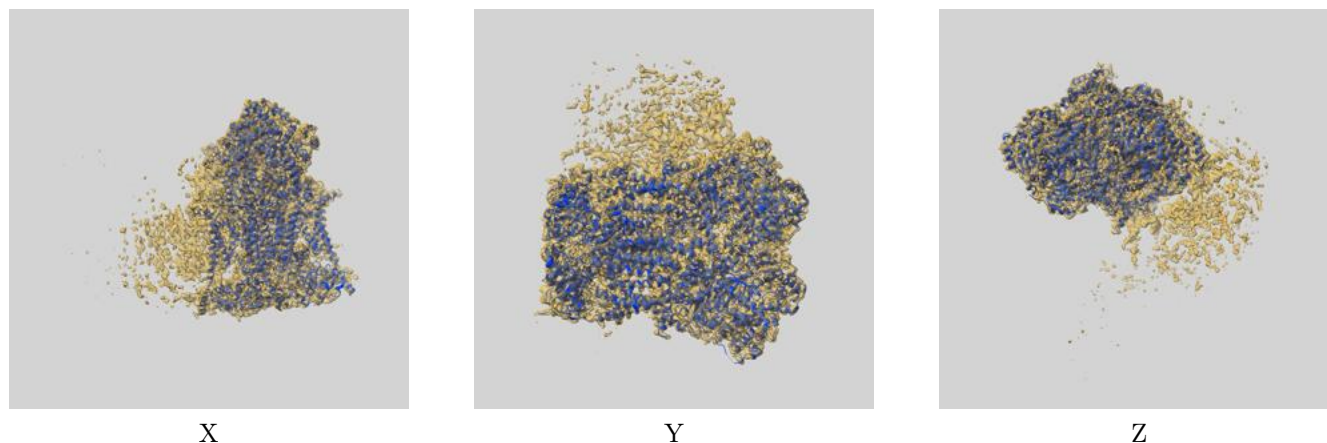
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.42	14.58	8.01

*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 7.42 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

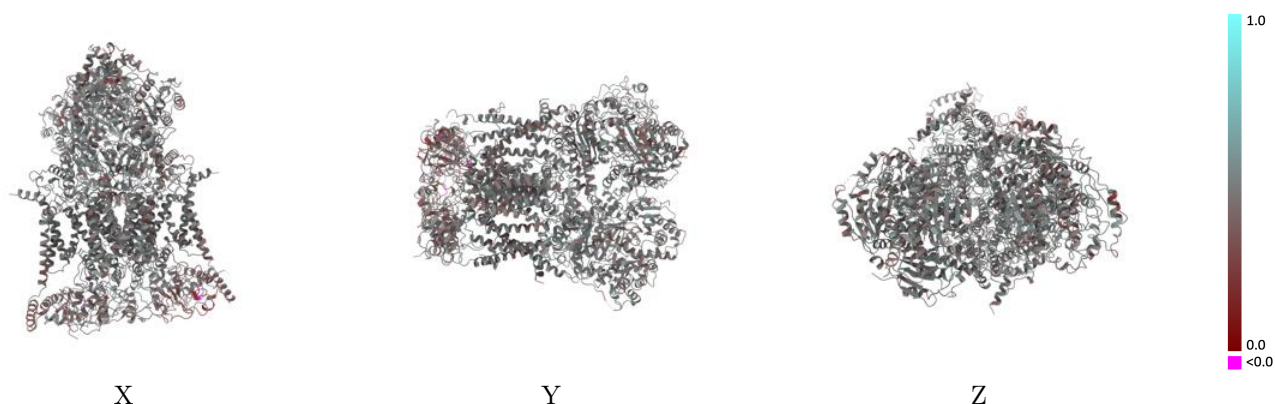
This section contains information regarding the fit between EMDB map EMD-42221 and PDB model 8UGD. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



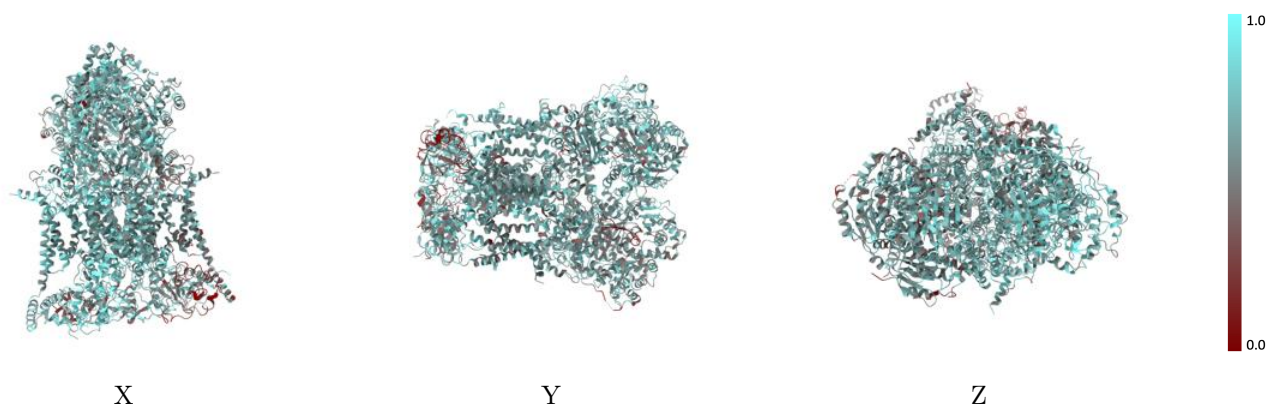
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



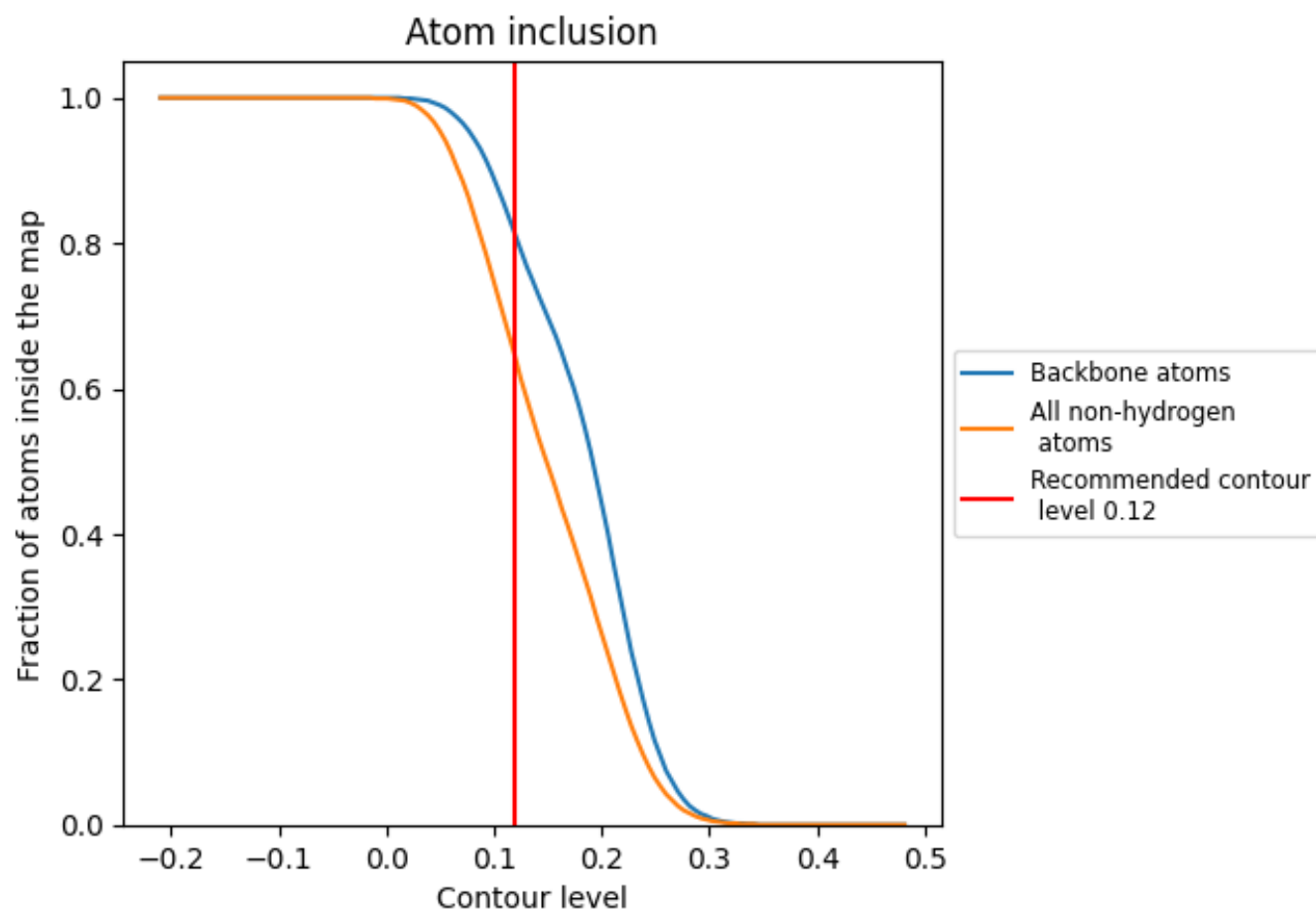
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 64% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6420	 0.4610
3A	 0.6210	 0.4750
3B	 0.6400	 0.4760
3C	 0.6520	 0.4730
3D	 0.6630	 0.4750
3E	 0.4090	 0.3670
3F	 0.6360	 0.4710
3G	 0.6250	 0.4760
3H	 0.5890	 0.4250
3I	 0.1890	 0.3920
3J	 0.6150	 0.4660
3N	 0.7140	 0.4740
3O	 0.6820	 0.4720
3P	 0.7180	 0.4750
3Q	 0.7360	 0.4710
3R	 0.4340	 0.3710
3S	 0.7230	 0.4890
3T	 0.7490	 0.4740
3U	 0.6810	 0.4280
3V	 0.4090	 0.4510
3W	 0.7610	 0.4820
3X	 0.5850	 0.4600
3Y	 0.5230	 0.4530

