



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 8BEF / pdb\_00008bef  
EMDB ID : EMD-16000  
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (CI membrane core)  
Authors : Klusch, N.; Kuehlbrandt, W.  
Deposited on : 2022-10-21  
Resolution : 2.13 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

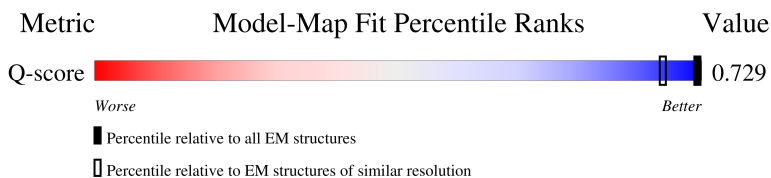
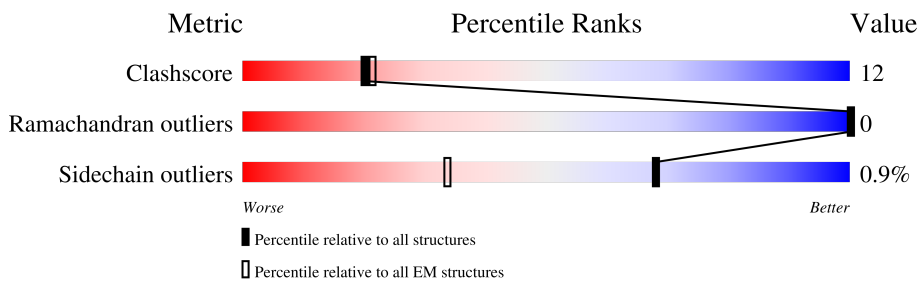
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 2.13 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.




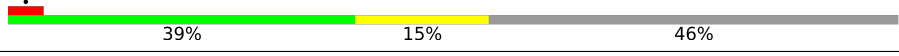
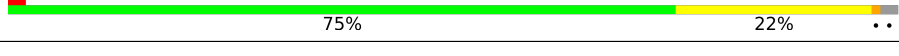
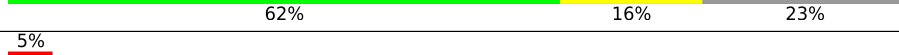
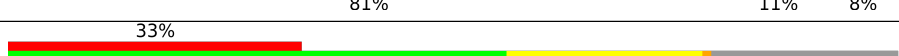
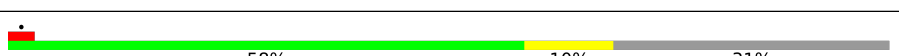
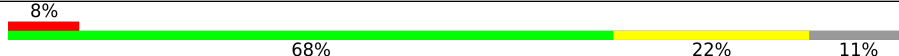








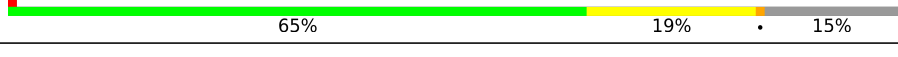


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2439 ( 1.64 - 2.63 )

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	119	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5%      59%      18%      ..      21%</p>
2	H	325	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">.      75%      25%</p>
3	J	205	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">.      63%      21%      15%</p>
4	K	100	<div style="display: flex; align-items: center;"> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">61%      35%      .</p>

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Mol	Chain	Length	Quality of chain
5	L	669	
6	M	495	
7	N	499	
8	O	159	
9	X	106	
10	Y	159	
11	Z	143	
12	a	65	
13	b	65	
14	d	81	
15	e	83	
16	f	106	
17	i	98	
18	u	63	
19	v	113	
20	x	256	
21	y	278	
22	z	275	

## 2 Entry composition i

There are 34 unique types of molecules in this entry. The entry contains 27758 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	94	802	565	110	123	4	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	324	2536	1719	386	416	15	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	174	1399	949	213	228	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	100	784	525	121	131	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	76	623	416	97	107	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	269	2191	1498	328	352	13	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	variant	UNP P93313
M	326	LEU	PRO	variant	UNP P93313
M	383	PHE	SER	variant	UNP P93313

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	488	3839	2587	580	644	28	2	0

- Molecule 8 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	123	963	603	170	186	4	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	X	98	776	486	134	144	12	0	0

- Molecule 10 is a protein called Outer envelope pore protein 16-3, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Y	125	928	596	162	167	3	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	98	Total	C	N	O	S	0	0
			798	514	137	142	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 13 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	43	Total	C	N	O	S	0	0
			315	206	51	55	3		

- Molecule 14 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 16 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	101	Total	C	N	O	S	0	0
			765	491	126	143	5		

- Molecule 17 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	68	Total	C	N	O	S	0	0
			598	376	113	106	3		

- Molecule 18 is a protein called Uncharacterized protein At1g67785.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	u	55	463	298	84	78	3	0	0

- Molecule 19 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	v	29	219	142	38	39	0	0

- Molecule 20 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	x	210	1629	1043	280	301	5	0	0

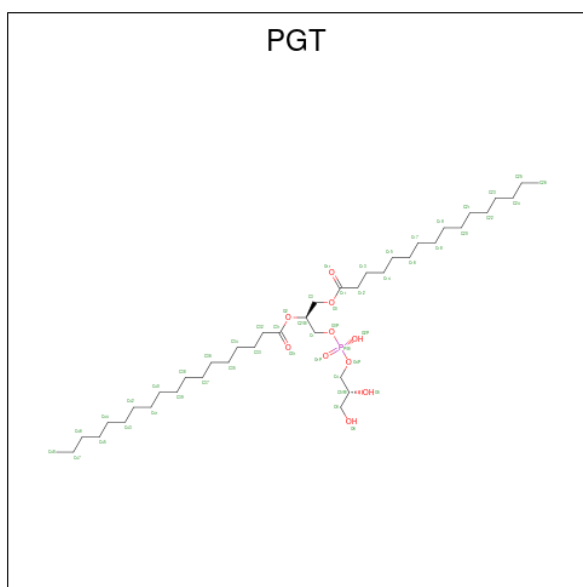
- Molecule 21 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	y	265	2013	1258	359	388	8	0	0

- Molecule 22 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

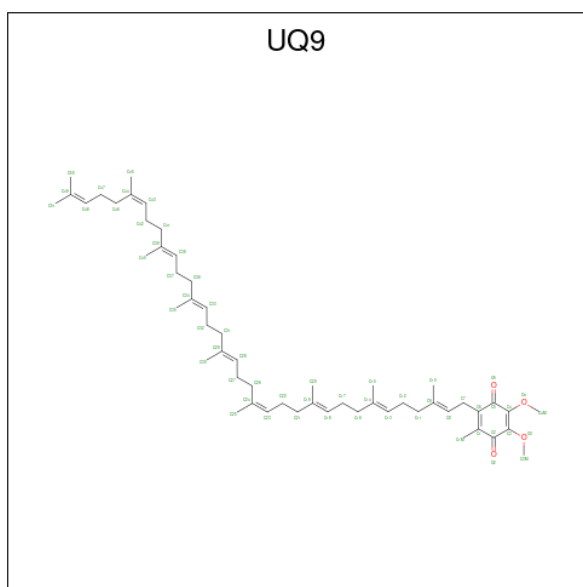
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	z	233	1772	1111	325	330	6	0	0

- Molecule 23 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



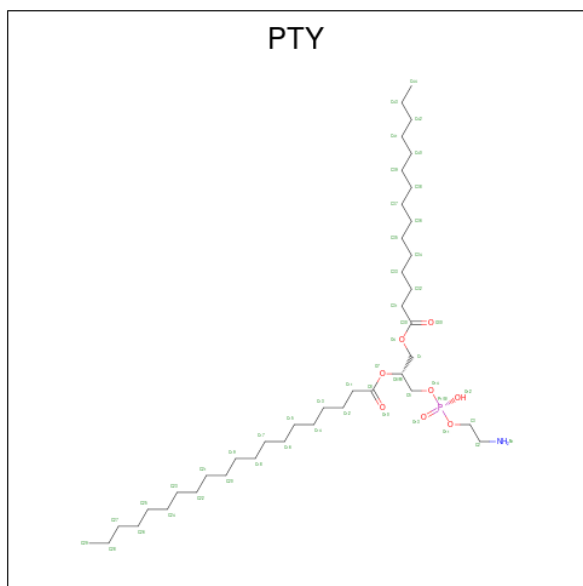
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	A	1	51	40	10	1	0
23	L	1	36	25	10	1	0
23	L	1	51	40	10	1	0
23	M	1	29	18	10	1	0
23	y	1	41	30	10	1	0

- Molecule 24 is Ubiquinone-9 (CCD ID: UQ9) (formula:  $C_{54}H_{82}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	H	1	35	31	4	0

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula:  $C_{40}H_{80}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



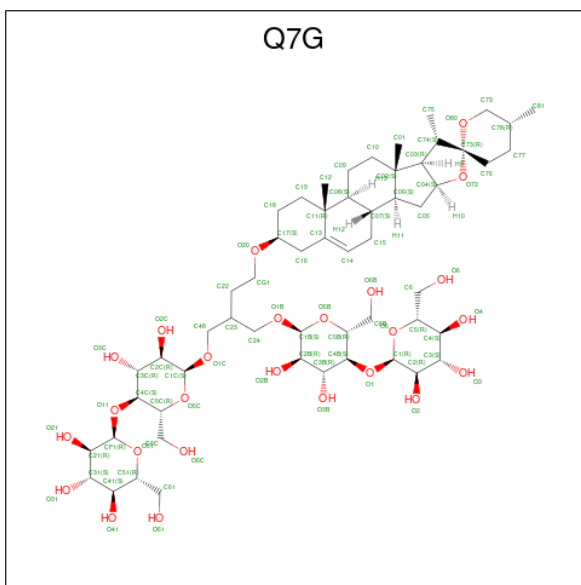
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	H	1	50	40	1	8	1	0
25	L	1	31	21	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
25	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
25	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	N	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	N	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
25	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
25	z	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 26 is 2-[[4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl]oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: C<sub>56</sub>H<sub>92</sub>O<sub>25</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	H	1	Total	C	O	0
			81	56	25	
26	K	1	Total	C	O	0
			81	56	25	

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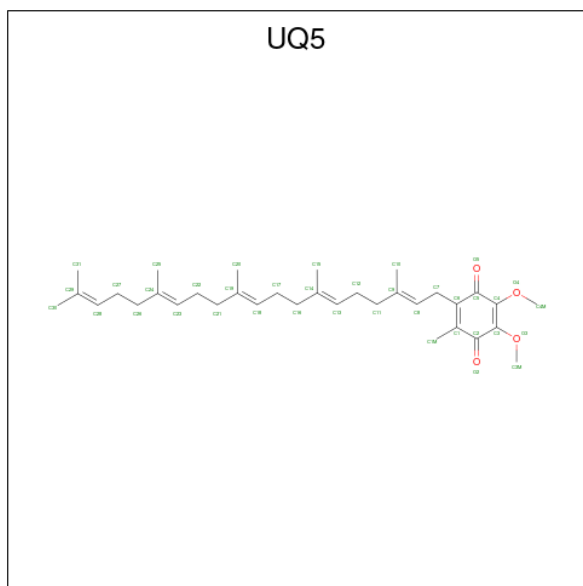
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Mol	Chain	Residues	Atoms			AltConf
26	M	1	Total	C	O	0
			39	34	5	
26	a	1	Total	C	O	0
			39	34	5	

- Molecule 27 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

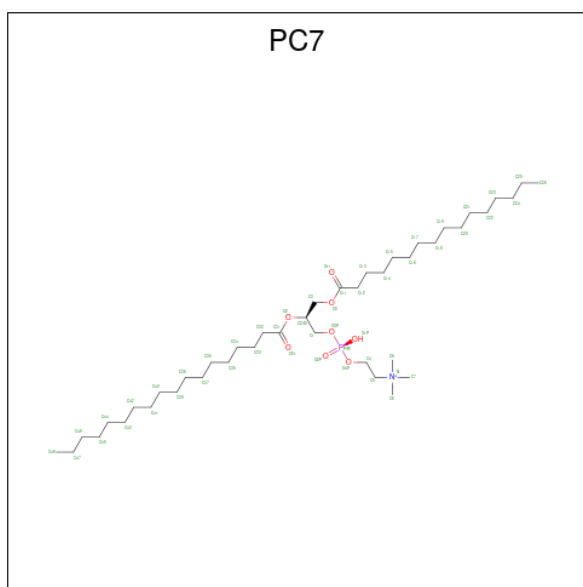
Mol	Chain	Residues	Atoms		AltConf
27	O	1	Total	Fe	0
			1	1	

- Molecule 28 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



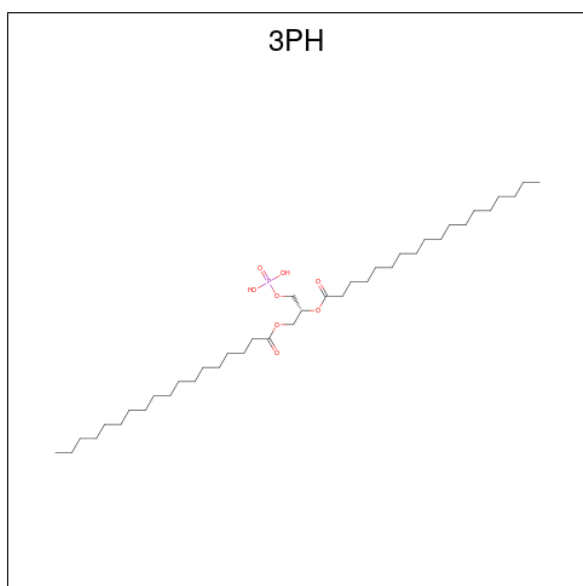
Mol	Chain	Residues	Atoms			AltConf
28	Y	1	Total	C	O	0
			38	34	4	

- Molecule 29 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



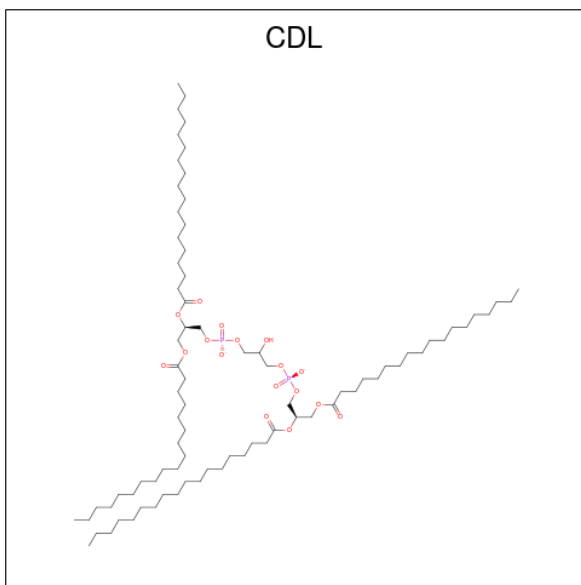
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	d	1	52	42	1	8	1	0
29	f	1	48	38	1	8	1	0
29	v	1	52	42	1	8	1	0

- Molecule 30 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:  $C_{39}H_{77}O_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	f	1	Total	C	O	P	0
			41	32	8	1	
30	f	1	Total	C	O	P	0
			43	34	8	1	

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).

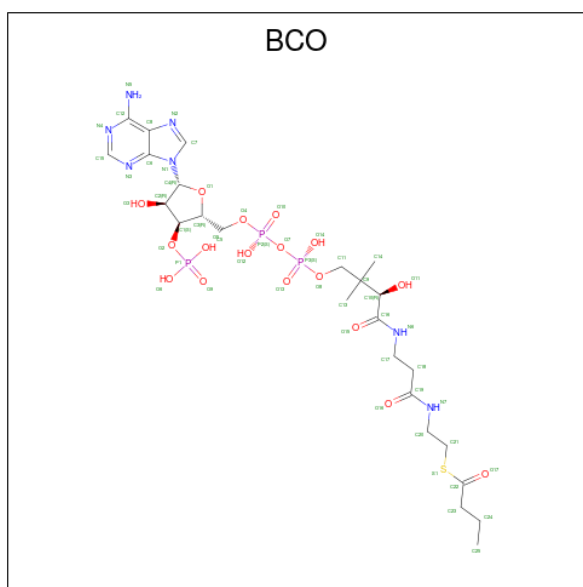


Mol	Chain	Residues	Atoms				AltConf
31	u	1	Total	C	O	P	0
			100	81	17	2	
31	u	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	y	1	Total	Zn	0
			1	1	

- Molecule 33 is Butyryl Coenzyme A (CCD ID: BCO) (formula:  $C_{25}H_{42}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
33	y	1	53	25	7	17	3	1	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	20	Total	O	0
			20	20	
34	H	128	Total	O	0
			128	128	
34	J	63	Total	O	0
			63	63	
34	K	50	Total	O	0
			50	50	
34	L	11	Total	O	0
			11	11	
34	M	30	Total	O	0
			30	30	
34	N	200	Total	O	0
			200	200	
34	O	86	Total	O	0
			86	86	
34	X	19	Total	O	0
			19	19	
34	Y	4	Total	O	0
			4	4	
34	Z	47	Total	O	0
			47	47	

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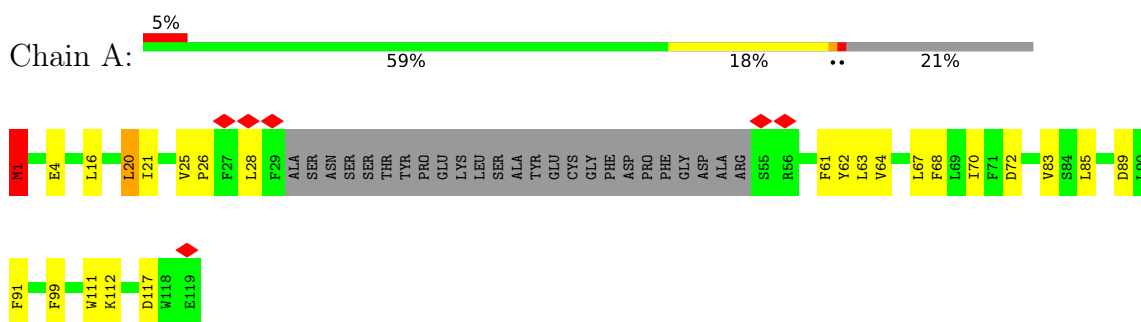
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
34	a	19	Total 19	O 19	0
34	b	2	Total 2	O 2	0
34	d	19	Total 19	O 19	0
34	e	30	Total 30	O 30	0
34	f	49	Total 49	O 49	0
34	i	23	Total 23	O 23	0
34	u	10	Total 10	O 10	0
34	v	10	Total 10	O 10	0
34	x	179	Total 179	O 179	0
34	y	165	Total 165	O 165	0
34	z	120	Total 120	O 120	0

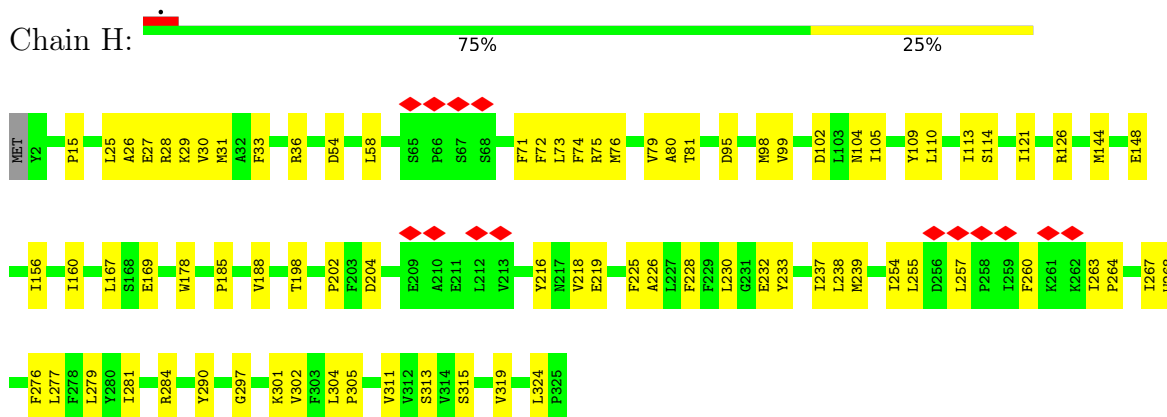
### 3 Residue-property plots [i](#)

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.

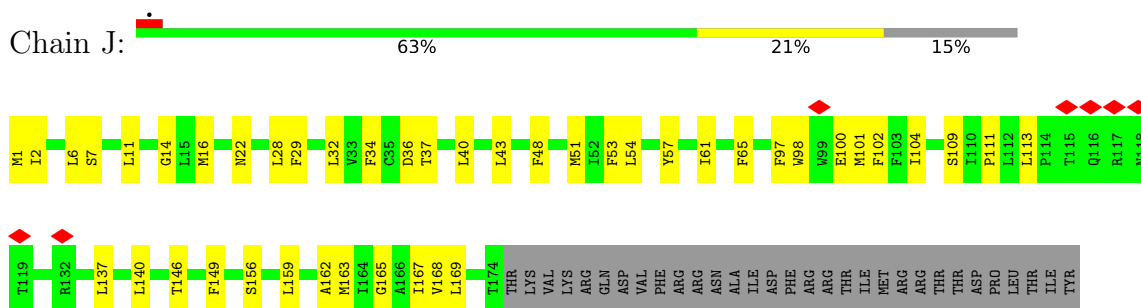
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



- Molecule 2: NADH-ubiquinone oxidoreductase chain 1

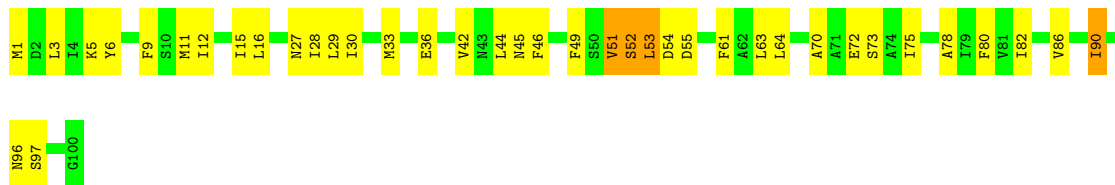


- Molecule 3: NADH-ubiquinone oxidoreductase chain 6



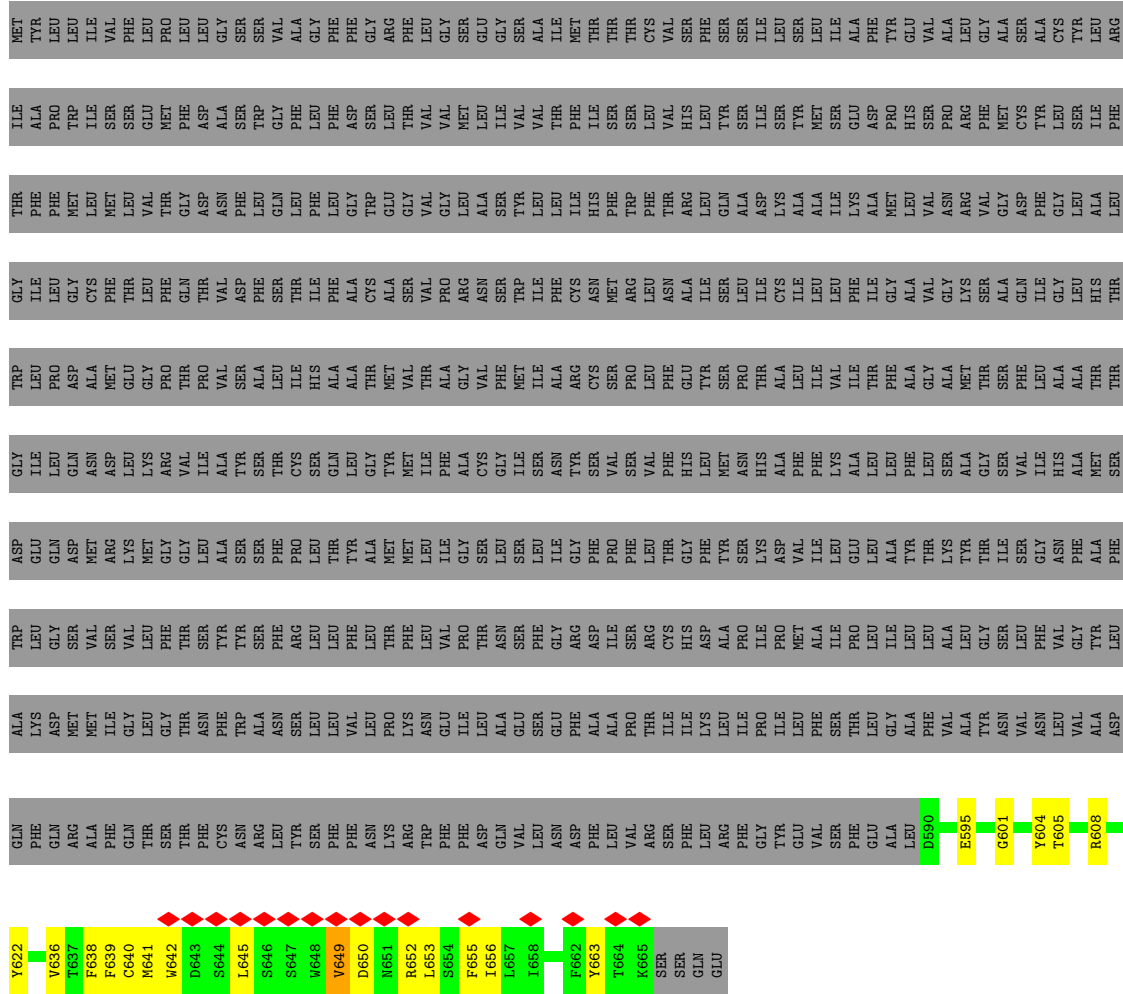
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 

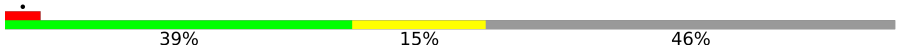


• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

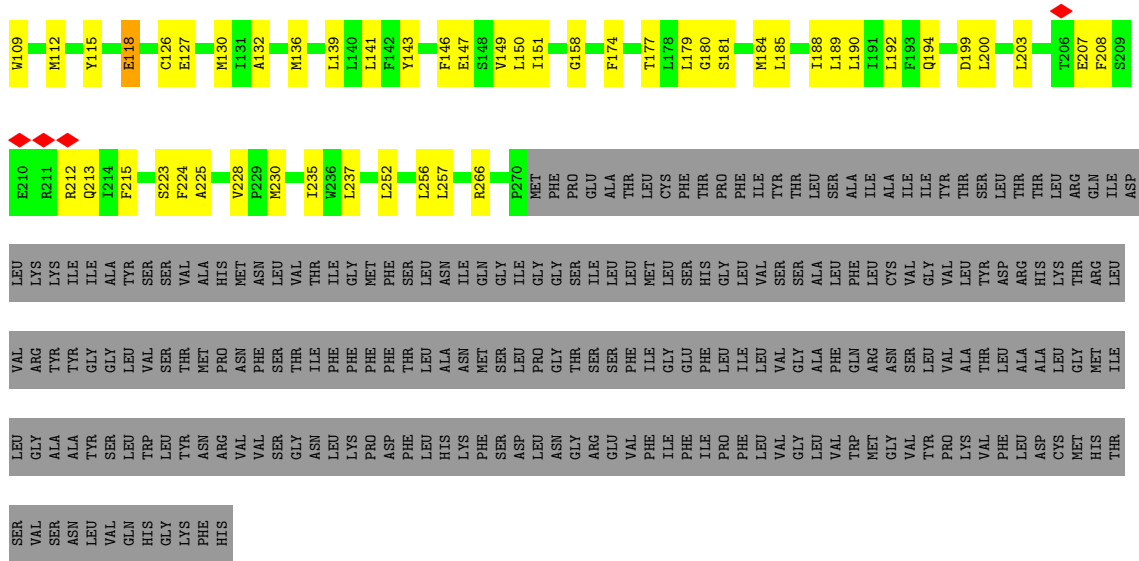
Chain L: 



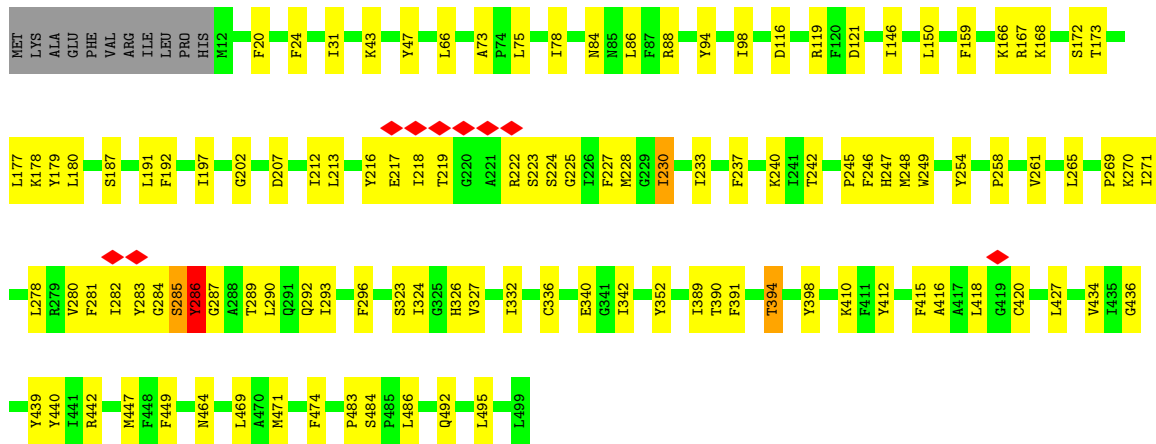
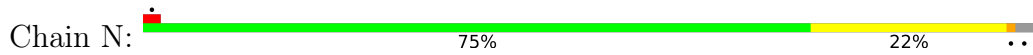
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain M: 

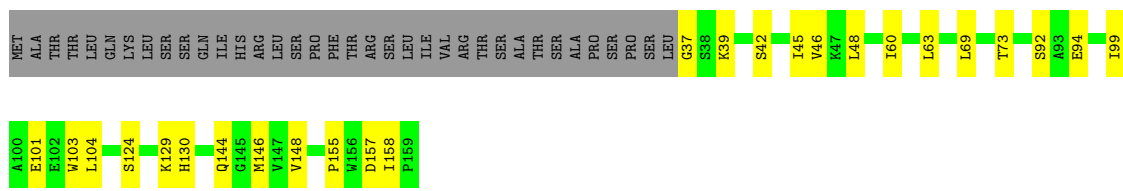




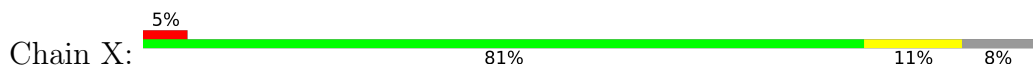
• Molecule 7: NADH-ubiquinone oxidoreductase chain 2



• Molecule 8: AT3G07480.1

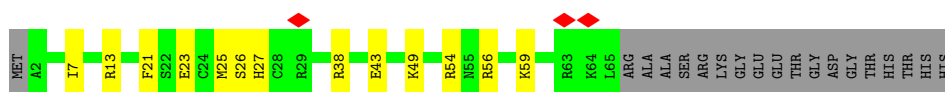


• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

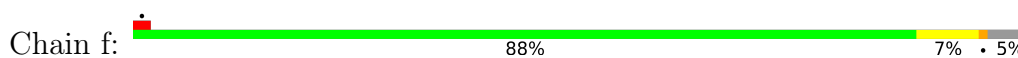




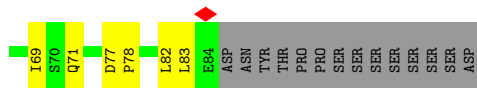
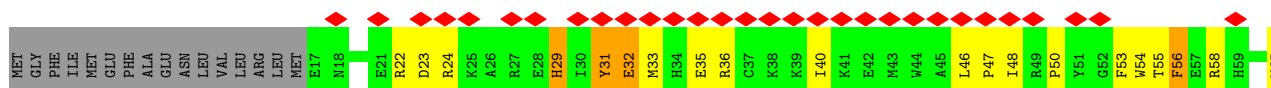
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



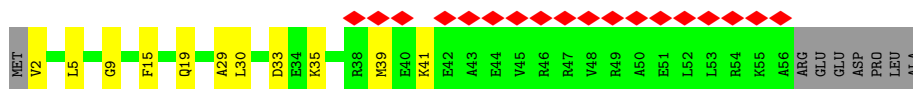
• Molecule 16: At4g16450



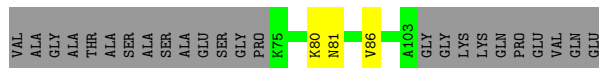
• Molecule 17: P1



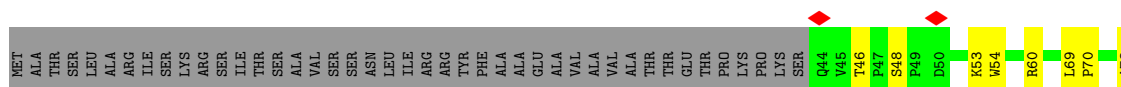
• Molecule 18: Uncharacterized protein At1g67785

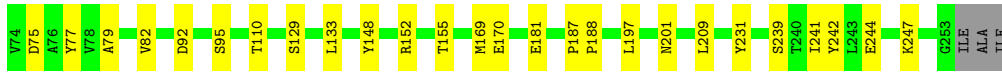


• Molecule 19: Uncharacterized protein At2g27730, mitochondrial

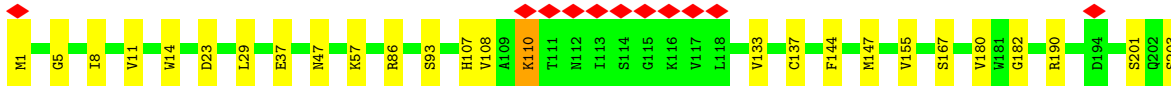
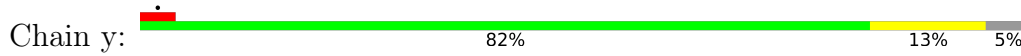


• Molecule 20: Gamma carbonic anhydrase-like 2, mitochondrial

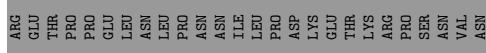




• Molecule 21: Gamma carbonic anhydrase 2, mitochondrial



• Molecule 22: Gamma carbonic anhydrase 1, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	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)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.559	Depositor
Minimum map value	-2.997	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.262	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	169.608, 156.429, 182.787	wwPDB
Map dimensions	319, 273, 296	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	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: 3PH, FME, ZN, Q7G, UQ5, BCO, PC7, CDL, UQ9, PGT, FE, PTY

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	0.19	0/820	0.41	0/1113
2	H	0.19	0/2609	0.39	0/3553
3	J	0.60	0/1435	0.70	0/1957
4	K	1.09	9/785 (1.1%)	1.07	3/1062 (0.3%)
5	L	0.62	2/641 (0.3%)	0.79	2/867 (0.2%)
6	M	0.19	0/2258	0.40	0/3070
7	N	0.66	8/3948 (0.2%)	0.73	6/5360 (0.1%)
8	O	0.60	2/979 (0.2%)	0.64	0/1326
9	X	0.15	0/790	0.36	0/1060
10	Y	0.52	1/944 (0.1%)	0.61	1/1277 (0.1%)
11	Z	0.26	0/820	0.42	0/1108
12	a	0.22	0/481	0.38	0/646
13	b	0.16	0/320	0.40	0/434
14	d	0.62	1/605 (0.2%)	0.69	0/815
15	e	0.69	0/559	0.70	0/745
16	f	0.15	0/771	0.31	0/1042
17	i	0.73	3/616 (0.5%)	1.08	9/830 (1.1%)
18	u	0.13	0/472	0.22	0/632
19	v	0.13	0/222	0.29	0/300
20	x	0.67	3/1669 (0.2%)	0.62	1/2279 (0.0%)
21	y	0.52	0/2046	0.62	2/2772 (0.1%)
22	z	0.59	3/1804 (0.2%)	0.71	3/2441 (0.1%)
All	All	0.53	32/25594 (0.1%)	0.62	27/34689 (0.1%)

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
1	A	0	1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Y	125	ALA	C-O	-8.92	1.13	1.24
20	x	187	PRO	C-O	-8.77	1.14	1.24
5	L	650	ASP	C-O	8.50	1.34	1.23
4	K	53	LEU	C-O	-8.10	1.13	1.24
8	O	42	SER	C-O	-7.71	1.14	1.24

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	32	GLU	CA-C-N	-11.27	101.92	122.09
17	i	32	GLU	C-N-CA	-11.27	101.92	122.09
7	N	286	TYR	N-CA-C	-8.77	102.38	113.43
5	L	650	ASP	CB-CA-C	-8.41	90.89	109.56
10	Y	129	ALA	N-CA-C	-7.74	101.95	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	FME	Mainchain

## 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	802	0	817	21	0
2	H	2536	0	2641	87	0
3	J	1399	0	1472	45	0
4	K	784	0	843	36	0
5	L	623	0	617	28	0
6	M	2191	0	2282	67	0
7	N	3839	0	3943	116	0
8	O	963	0	975	14	0
9	X	776	0	775	13	0
10	Y	928	0	960	38	0
11	Z	798	0	780	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	a	469	0	472	11	0
13	b	315	0	338	3	0
14	d	592	0	610	14	0
15	e	546	0	510	11	0
16	f	765	0	766	8	0
17	i	598	0	567	30	0
18	u	463	0	471	11	0
19	v	219	0	227	8	0
20	x	1629	0	1636	37	0
21	y	2013	0	2024	46	0
22	z	1772	0	1771	59	0
23	A	51	0	78	7	0
23	L	87	0	120	3	0
23	M	29	0	28	4	0
23	y	41	0	52	7	0
24	H	35	0	43	4	0
25	H	50	0	79	6	0
25	L	31	0	35	0	0
25	M	87	0	126	3	0
25	N	174	0	252	16	0
25	Y	50	0	79	3	0
25	z	50	0	79	12	0
26	H	81	0	0	3	0
26	K	81	0	0	1	0
26	M	39	0	0	0	0
26	a	39	0	0	0	0
27	O	1	0	0	0	0
28	Y	38	0	50	9	0
29	d	52	0	84	8	0
29	f	48	0	73	4	0
29	v	52	0	84	7	0
30	f	84	0	120	5	0
31	u	200	0	312	25	0
32	y	1	0	0	0	0
33	y	53	0	40	2	0
34	A	20	0	0	3	0
34	H	128	0	0	35	0
34	J	63	0	0	13	0
34	K	50	0	0	16	0
34	L	11	0	0	3	0
34	M	30	0	0	4	0
34	N	200	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	O	86	0	0	1	0
34	X	19	0	0	1	0
34	Y	4	0	0	0	0
34	Z	47	0	0	2	0
34	a	19	0	0	2	0
34	b	2	0	0	0	0
34	d	19	0	0	2	0
34	e	30	0	0	2	0
34	f	49	0	0	2	0
34	i	23	0	0	5	0
34	u	10	0	0	0	0
34	v	10	0	0	3	0
34	x	179	0	0	13	0
34	y	165	0	0	11	0
34	z	120	0	0	20	0
All	All	27758	0	27231	662	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 12.

The worst 5 of 662 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)
21:y:133:VAL:HG11	22:z:147:MET:CE	1.14	1.57
21:y:133:VAL:CG1	22:z:147:MET:HE1	1.49	1.42
21:y:133:VAL:CG1	22:z:147:MET:CE	2.08	1.24
15:e:56:ARG:HD3	34:e:128:HOH:O	1.35	1.23
7:N:254:TYR:HA	34:N:647:HOH:O	1.38	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	90/119 (76%)	89 (99%)	1 (1%)	0	100	100
2	H	322/325 (99%)	316 (98%)	6 (2%)	0	100	100
3	J	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
4	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
5	L	74/669 (11%)	68 (92%)	6 (8%)	0	100	100
6	M	268/495 (54%)	264 (98%)	4 (2%)	0	100	100
7	N	488/499 (98%)	472 (97%)	16 (3%)	0	100	100
8	O	121/159 (76%)	117 (97%)	4 (3%)	0	100	100
9	X	96/106 (91%)	95 (99%)	1 (1%)	0	100	100
10	Y	123/159 (77%)	116 (94%)	7 (6%)	0	100	100
11	Z	96/143 (67%)	96 (100%)	0	0	100	100
12	a	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
13	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
14	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
15	e	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
16	f	99/106 (93%)	98 (99%)	1 (1%)	0	100	100
17	i	66/98 (67%)	65 (98%)	1 (2%)	0	100	100
18	u	53/63 (84%)	53 (100%)	0	0	100	100
19	v	27/113 (24%)	27 (100%)	0	0	100	100
20	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
21	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
22	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100
All	All	3127/4462 (70%)	3061 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	85/105 (81%)	83 (98%)	2 (2%)	43	45
2	H	271/272 (100%)	271 (100%)	0	100	100
3	J	156/186 (84%)	154 (99%)	2 (1%)	61	67
4	K	85/85 (100%)	84 (99%)	1 (1%)	63	69
5	L	67/568 (12%)	67 (100%)	0	100	100
6	M	240/434 (55%)	238 (99%)	2 (1%)	73	79
7	N	408/416 (98%)	402 (98%)	6 (2%)	57	63
8	O	108/141 (77%)	106 (98%)	2 (2%)	50	55
9	X	88/94 (94%)	88 (100%)	0	100	100
10	Y	92/120 (77%)	91 (99%)	1 (1%)	65	71
11	Z	79/115 (69%)	79 (100%)	0	100	100
12	a	48/53 (91%)	47 (98%)	1 (2%)	47	51
13	b	35/53 (66%)	35 (100%)	0	100	100
14	d	60/66 (91%)	60 (100%)	0	100	100
15	e	59/73 (81%)	59 (100%)	0	100	100
16	f	80/83 (96%)	80 (100%)	0	100	100
17	i	62/90 (69%)	61 (98%)	1 (2%)	55	61
18	u	47/54 (87%)	46 (98%)	1 (2%)	47	51
19	v	22/84 (26%)	22 (100%)	0	100	100
20	x	179/216 (83%)	178 (99%)	1 (1%)	78	84
21	y	221/232 (95%)	220 (100%)	1 (0%)	81	86
22	z	188/228 (82%)	186 (99%)	2 (1%)	65	71
All	All	2680/3768 (71%)	2657 (99%)	23 (1%)	68	77

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	O	158	ILE
17	i	48	ILE
12	a	42	HIS
18	u	33	ASP
6	M	118	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
17	i	60	ASN
21	y	38	HIS
22	z	107	HIS
21	y	47	ASN
6	M	79	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	A	1	1	8,9,10	1.77	1 (12%)	8,9,11	1.58	1 (12%)
4	FME	K	1	4	8,9,10	0.82	0	8,9,11	1.99	3 (37%)
16	FME	f	1	16	8,9,10	1.77	1 (12%)	8,9,11	1.51	1 (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
1	FME	A	1	1	-	0/7/9/11	-
4	FME	K	1	4	-	5/7/9/11	-
16	FME	f	1	16	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	f	1	FME	O-C	4.32	1.36	1.20
1	A	1	FME	O-C	4.29	1.36	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-3.75	115.14	124.77
4	K	1	FME	C-CA-N	3.48	116.22	109.50
16	f	1	FME	O-C-CA	-3.46	115.87	124.77
4	K	1	FME	O-C-CA	-3.02	116.99	124.77
4	K	1	FME	CG-CB-CA	-2.15	106.29	112.87

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	O1-CN-N-CA
4	K	1	FME	N-CA-CB-CG
16	f	1	FME	O1-CN-N-CA
16	f	1	FME	C-CA-CB-CG
16	f	1	FME	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
16	f	1	FME	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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
25	PTY	M	502	-	36,36,49	1.01	4 (11%)	39,41,54	1.13	2 (5%)
33	BCO	y	302	-	53,55,55	4.17	23 (43%)	75,81,81	3.72	24 (32%)
30	3PH	f	202	-	42,42,47	0.67	1 (2%)	45,47,52	0.64	2 (4%)
31	CDL	u	101	-	99,99,99	0.90	7 (7%)	105,111,111	1.08	5 (4%)
25	PTY	z	301	-	49,49,49	0.87	3 (6%)	52,54,54	1.17	3 (5%)
28	UQ5	Y	202	-	38,38,38	0.48	0	48,49,49	1.07	5 (10%)
23	PGT	A	201	-	50,50,50	1.10	4 (8%)	53,56,56	1.09	3 (5%)
26	Q7G	M	504	-	44,44,90	0.78	1 (2%)	64,68,138	1.68	14 (21%)
25	PTY	Y	201	-	49,49,49	0.90	4 (8%)	52,54,54	1.06	2 (3%)
25	PTY	N	503	-	44,44,49	0.95	4 (9%)	47,49,54	1.05	2 (4%)
26	Q7G	a	101	-	44,44,90	0.68	0	64,68,138	1.40	10 (15%)
25	PTY	H	402	-	49,49,49	0.89	4 (8%)	52,54,54	1.03	2 (3%)
24	UQ9	H	401	-	35,35,58	2.53	11 (31%)	43,45,73	2.23	13 (30%)
25	PTY	N	504	-	49,49,49	0.88	4 (8%)	52,54,54	1.10	2 (3%)
23	PGT	y	303	-	40,40,50	1.19	5 (12%)	43,46,56	1.12	2 (4%)
25	PTY	N	501	-	39,39,49	0.98	4 (10%)	42,44,54	1.12	2 (4%)
25	PTY	M	503	-	49,49,49	0.90	4 (8%)	52,54,54	1.21	3 (5%)
26	Q7G	H	403	-	90,90,90	0.71	3 (3%)	134,138,138	1.23	14 (10%)
23	PGT	L	701	-	35,35,50	1.26	4 (11%)	38,41,56	1.11	2 (5%)
29	PC7	d	101	-	51,51,51	0.43	0	57,59,59	0.53	0
31	CDL	u	102	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
26	Q7G	K	201	-	90,90,90	0.80	3 (3%)	134,138,138	1.40	19 (14%)
25	PTY	L	703	-	30,30,49	1.12	4 (13%)	33,35,54	1.17	2 (6%)
25	PTY	N	502	-	38,38,49	0.99	4 (10%)	41,43,54	1.16	2 (4%)
23	PGT	L	702	-	50,50,50	1.10	4 (8%)	53,56,56	1.09	2 (3%)
23	PGT	M	501	-	28,28,50	1.36	4 (14%)	31,34,56	1.22	2 (6%)
29	PC7	f	203	-	47,47,51	1.01	4 (8%)	53,55,59	1.08	2 (3%)
29	PC7	v	201	-	51,51,51	0.99	4 (7%)	57,59,59	1.14	3 (5%)
30	3PH	f	201	-	40,40,47	0.67	1 (2%)	43,45,52	0.74	2 (4%)

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
25	PTY	M	502	-	-	19/40/40/53	-
33	BCO	y	302	-	-	10/54/70/70	0/3/3/3
30	3PH	f	202	-	-	18/44/44/49	-
31	CDL	u	101	-	-	48/110/110/110	-
25	PTY	z	301	-	-	24/53/53/53	-
28	UQ5	Y	202	-	-	11/33/57/57	0/1/1/1
23	PGT	A	201	-	-	25/55/55/55	-
26	Q7G	M	504	-	-	1/12/100/200	0/6/6/10
25	PTY	Y	201	-	-	19/53/53/53	-
25	PTY	N	503	-	-	20/48/48/53	-
26	Q7G	a	101	-	-	3/12/100/200	0/6/6/10
25	PTY	H	402	-	-	17/53/53/53	-
24	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
25	PTY	N	504	-	-	15/53/53/53	-
23	PGT	y	303	-	-	25/45/45/55	-
25	PTY	N	501	-	-	20/43/43/53	-
25	PTY	M	503	-	-	23/53/53/53	-
26	Q7G	H	403	-	-	12/32/200/200	0/10/10/10
23	PGT	L	701	-	-	17/40/40/55	-
29	PC7	d	101	-	-	26/55/55/55	-
31	CDL	u	102	-	-	43/110/110/110	-
26	Q7G	K	201	-	-	6/32/200/200	0/10/10/10
25	PTY	L	703	-	-	18/34/34/53	-
25	PTY	N	502	-	-	18/42/42/53	-
23	PGT	L	702	-	-	25/55/55/55	-
23	PGT	M	501	-	-	18/33/33/55	-
29	PC7	f	203	-	-	23/51/51/55	-
29	PC7	v	201	-	-	23/55/55/55	-
30	3PH	f	201	-	-	15/42/42/49	-

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	y	302	BCO	C15-N4	-15.37	1.06	1.33
33	y	302	BCO	C8-C6	12.70	1.61	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	401	UQ9	C6-C1	9.98	1.53	1.35
33	y	302	BCO	C15-N3	-8.87	1.18	1.33
33	y	302	BCO	C12-N4	-8.10	1.13	1.35

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	y	302	BCO	C8-C6-N3	-13.96	107.50	126.72
33	y	302	BCO	C6-C8-N2	-13.58	95.05	110.58
33	y	302	BCO	C12-C8-N2	13.28	157.70	132.09
33	y	302	BCO	C8-N2-C7	8.48	116.78	103.45
33	y	302	BCO	N3-C6-N1	8.44	141.53	127.17

There are no chirality outliers.

5 of 551 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	201	PGT	C32-C31-O2-C2
23	A	201	PGT	O4P-C4-C5-O5
23	L	702	PGT	C32-C31-O2-C2
23	L	702	PGT	C1-O3P-P-O4P
23	M	501	PGT	C1-O3P-P-O2P

There are no ring outliers.

25 monomers are involved in 122 short contacts:

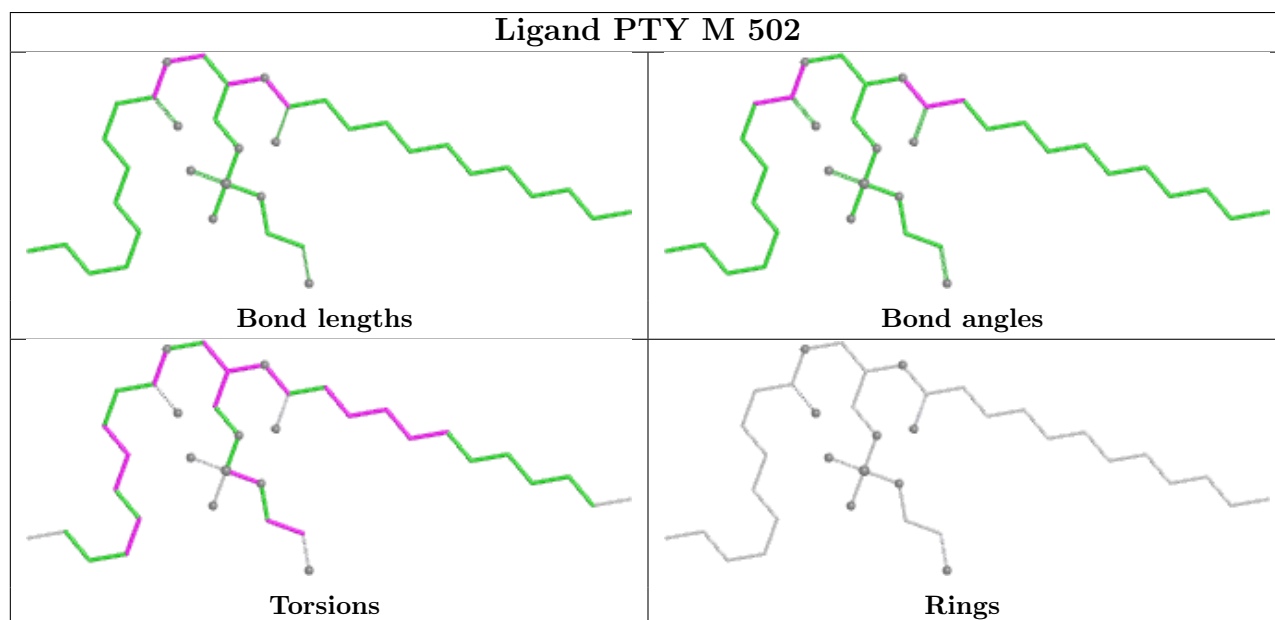
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	y	302	BCO	2	0
30	f	202	3PH	3	0
31	u	101	CDL	12	0
25	z	301	PTY	12	0
28	Y	202	UQ5	9	0
23	A	201	PGT	7	0
25	Y	201	PTY	3	0
25	N	503	PTY	5	0
25	H	402	PTY	6	0
24	H	401	UQ9	4	0
25	N	504	PTY	4	0
23	y	303	PGT	7	0
25	N	501	PTY	5	0
25	M	503	PTY	3	0

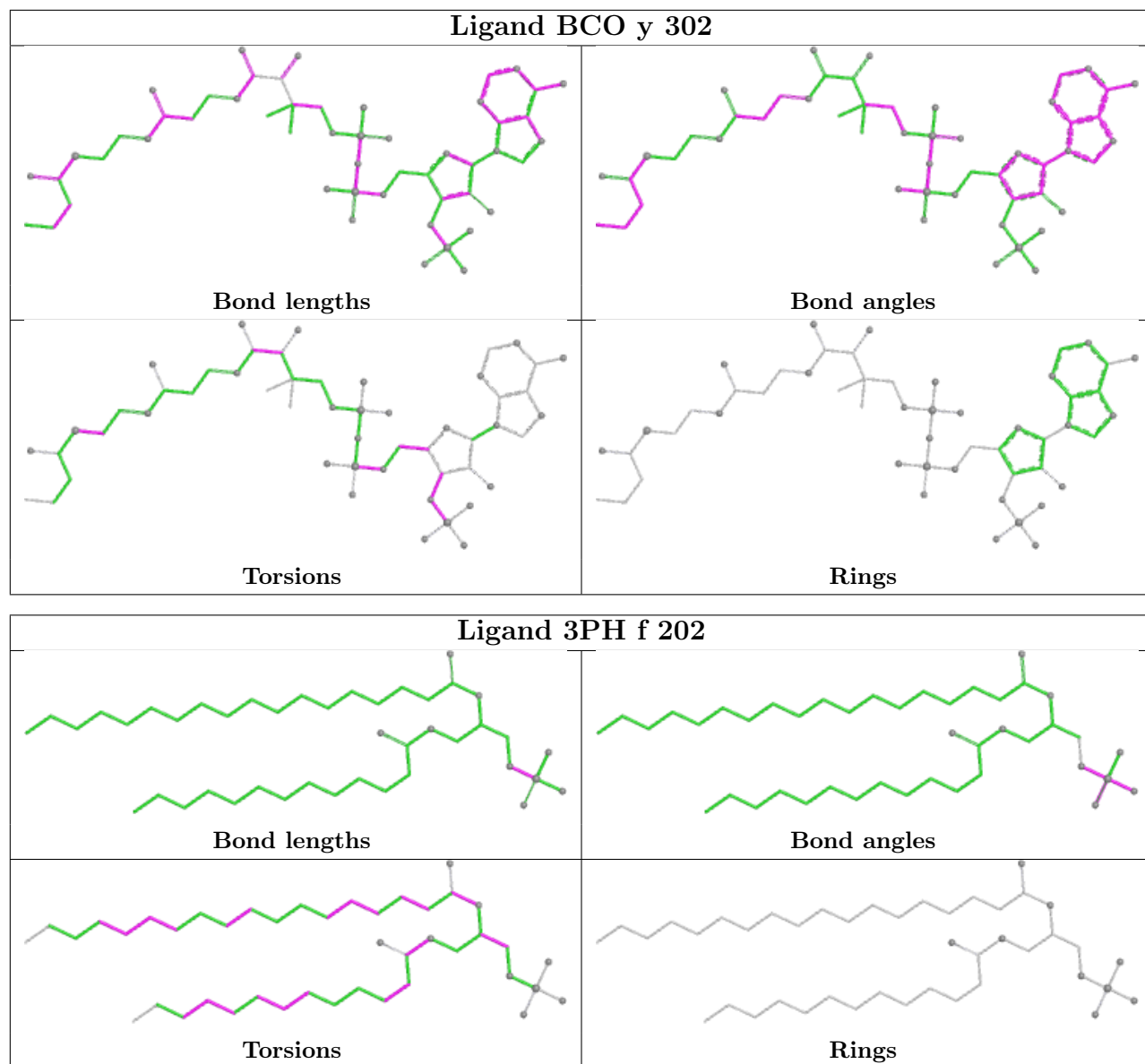
*Continued on next page...*

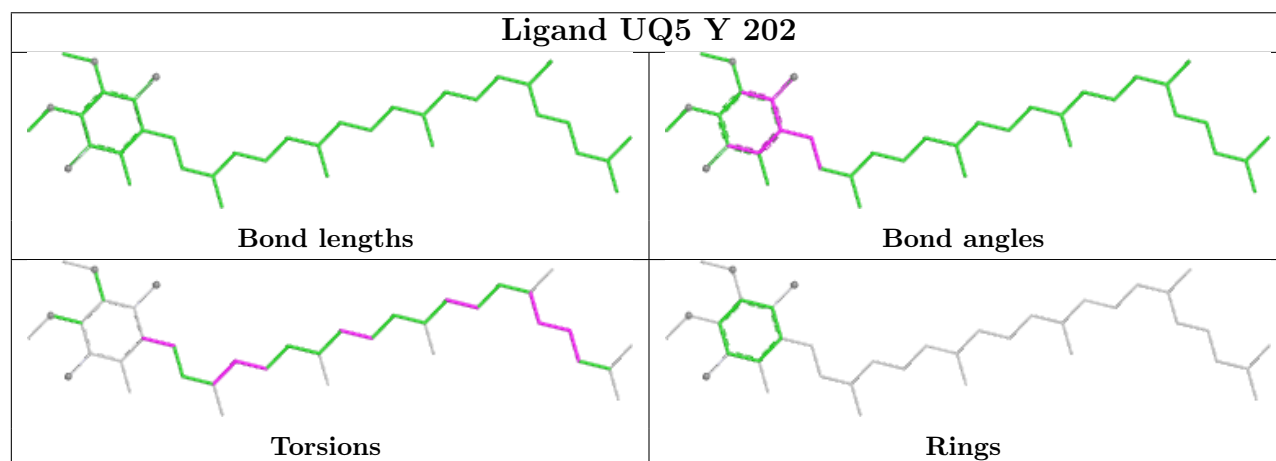
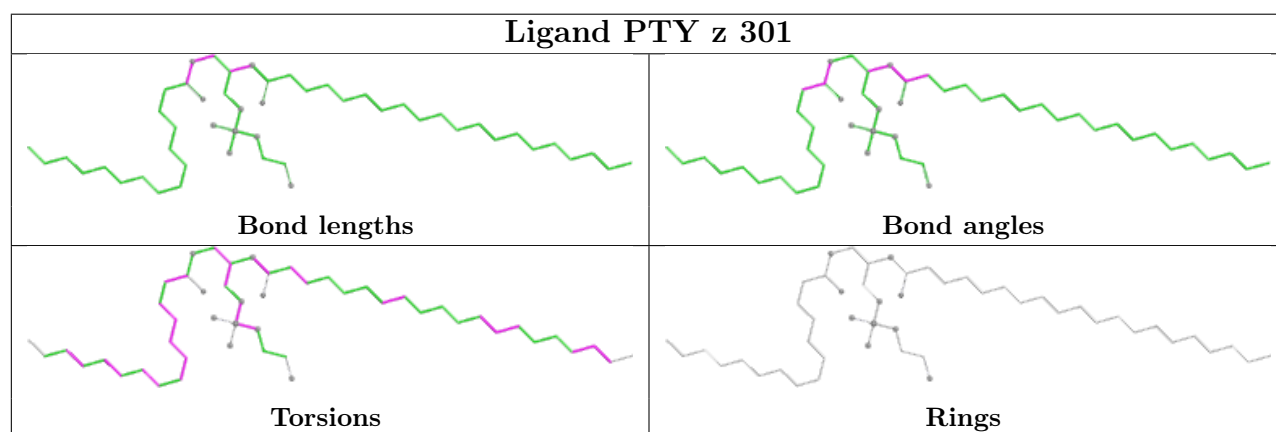
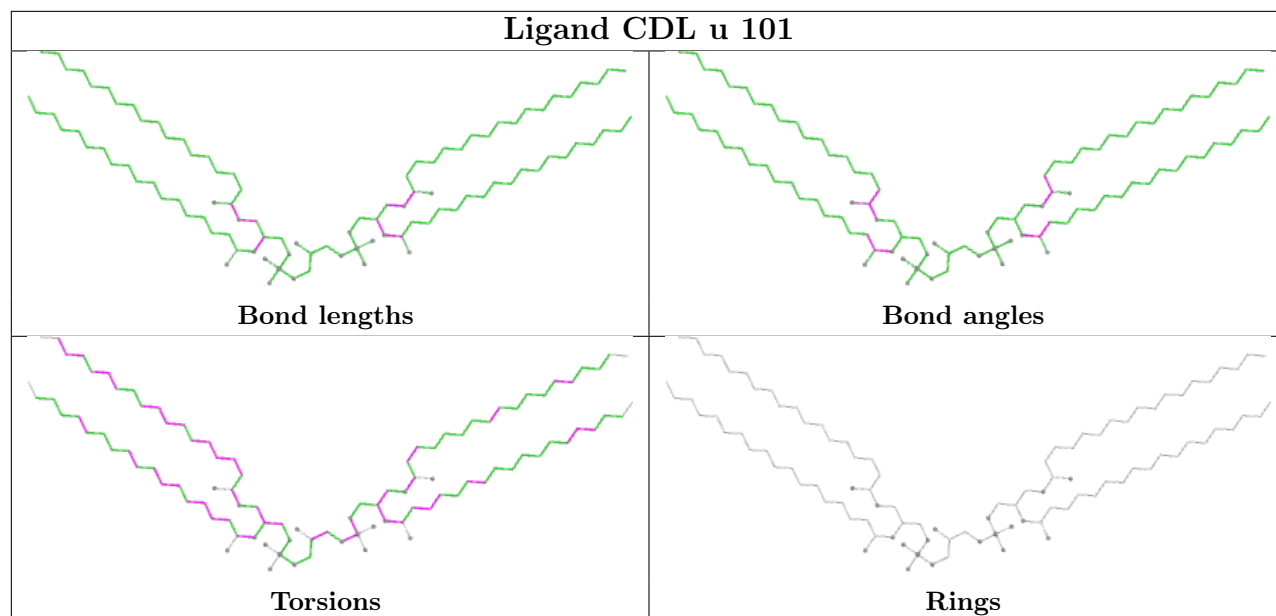
*Continued from previous page...*

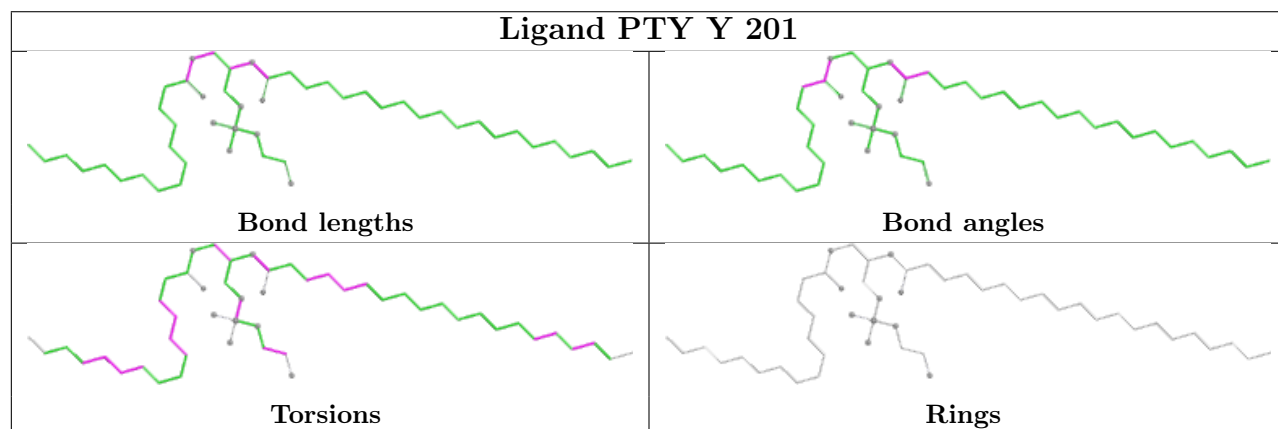
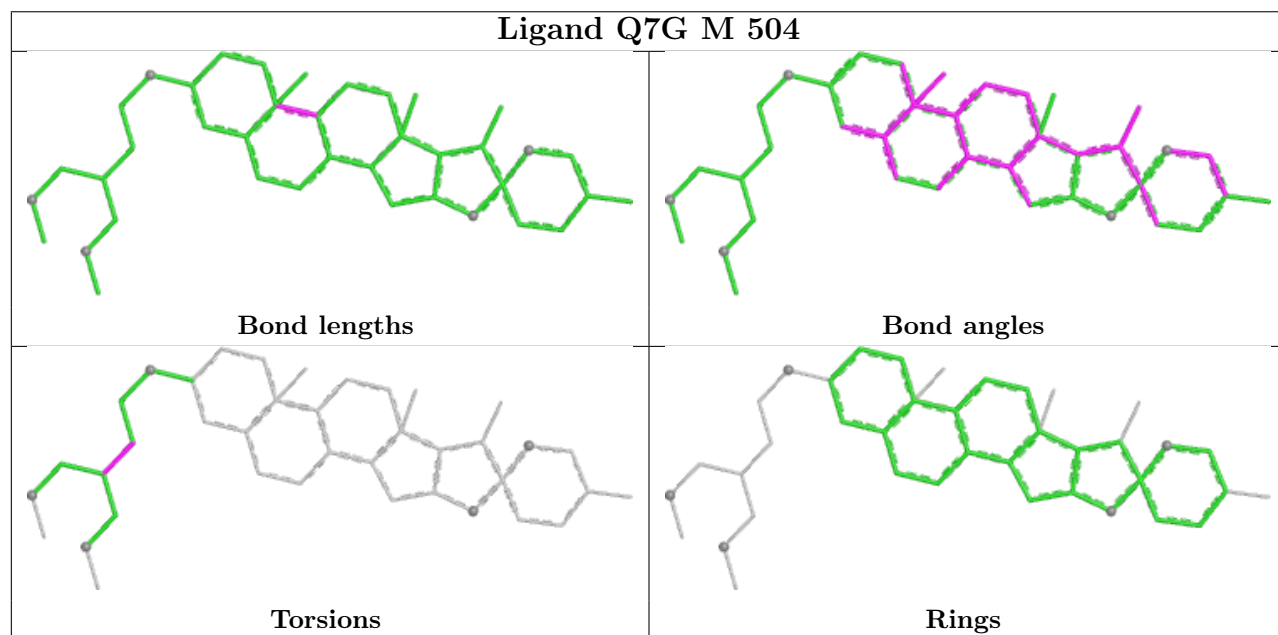
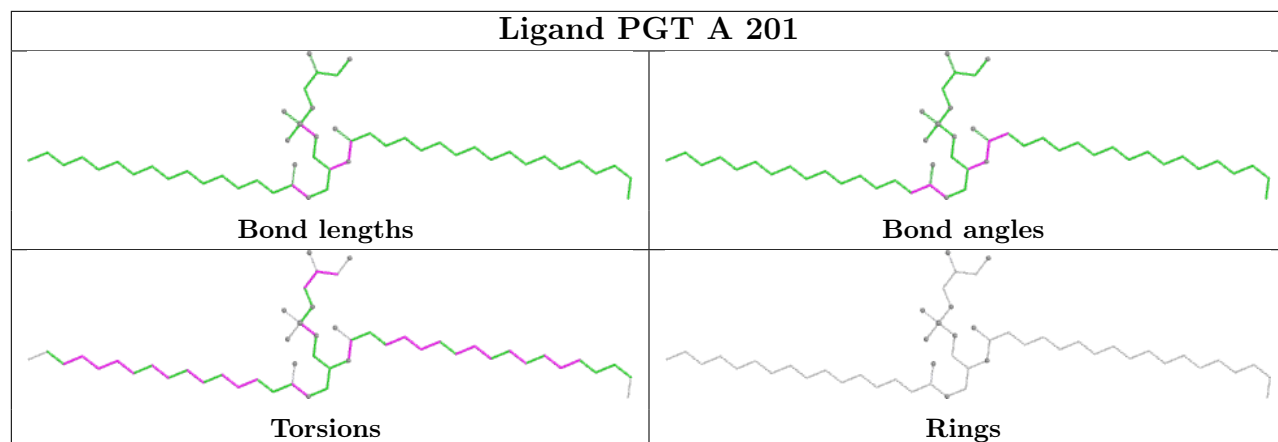
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	H	403	Q7G	3	0
23	L	701	PGT	1	0
29	d	101	PC7	8	0
31	u	102	CDL	13	0
26	K	201	Q7G	1	0
25	N	502	PTY	2	0
23	L	702	PGT	2	0
23	M	501	PGT	4	0
29	f	203	PC7	4	0
29	v	201	PC7	7	0
30	f	201	3PH	2	0

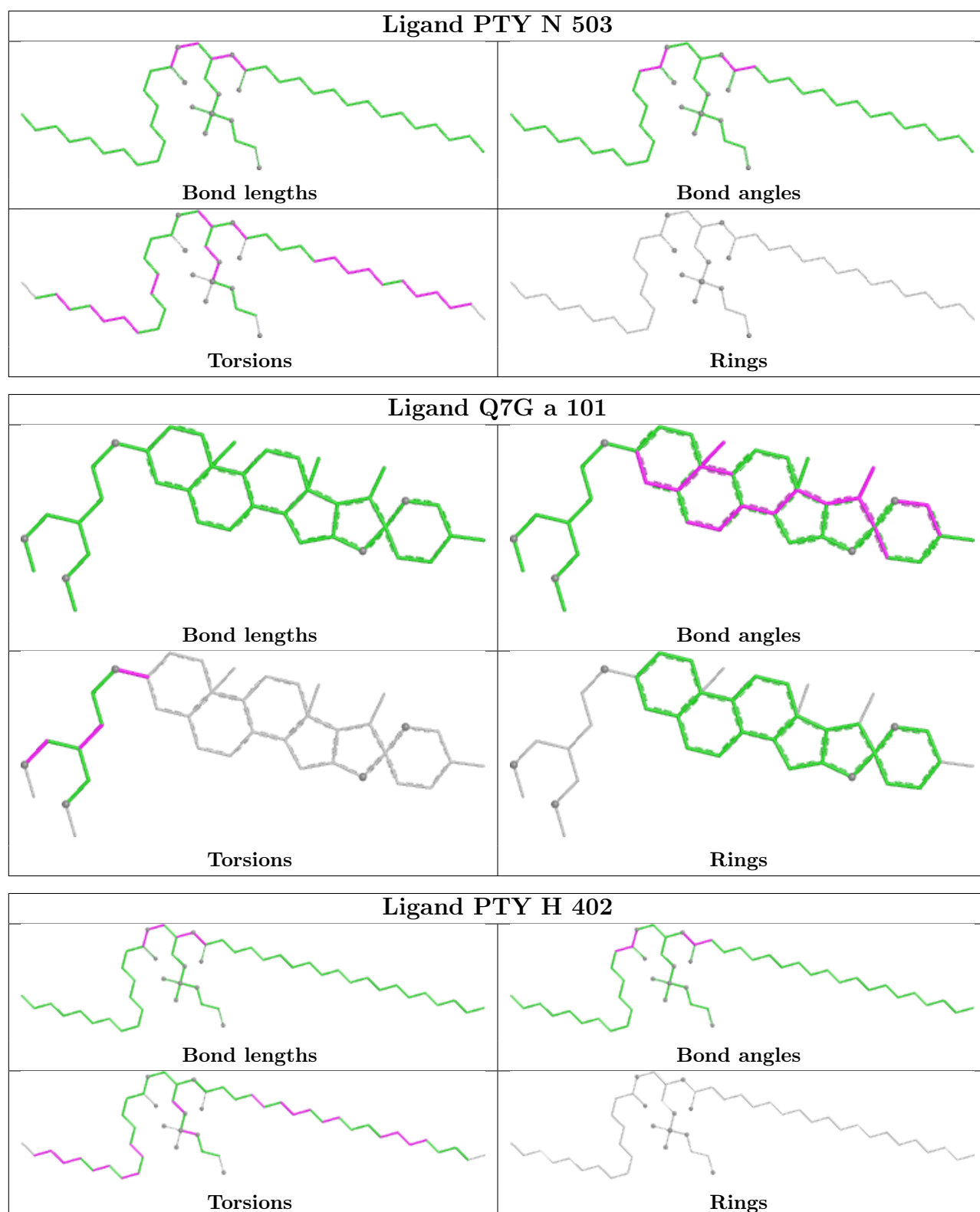
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

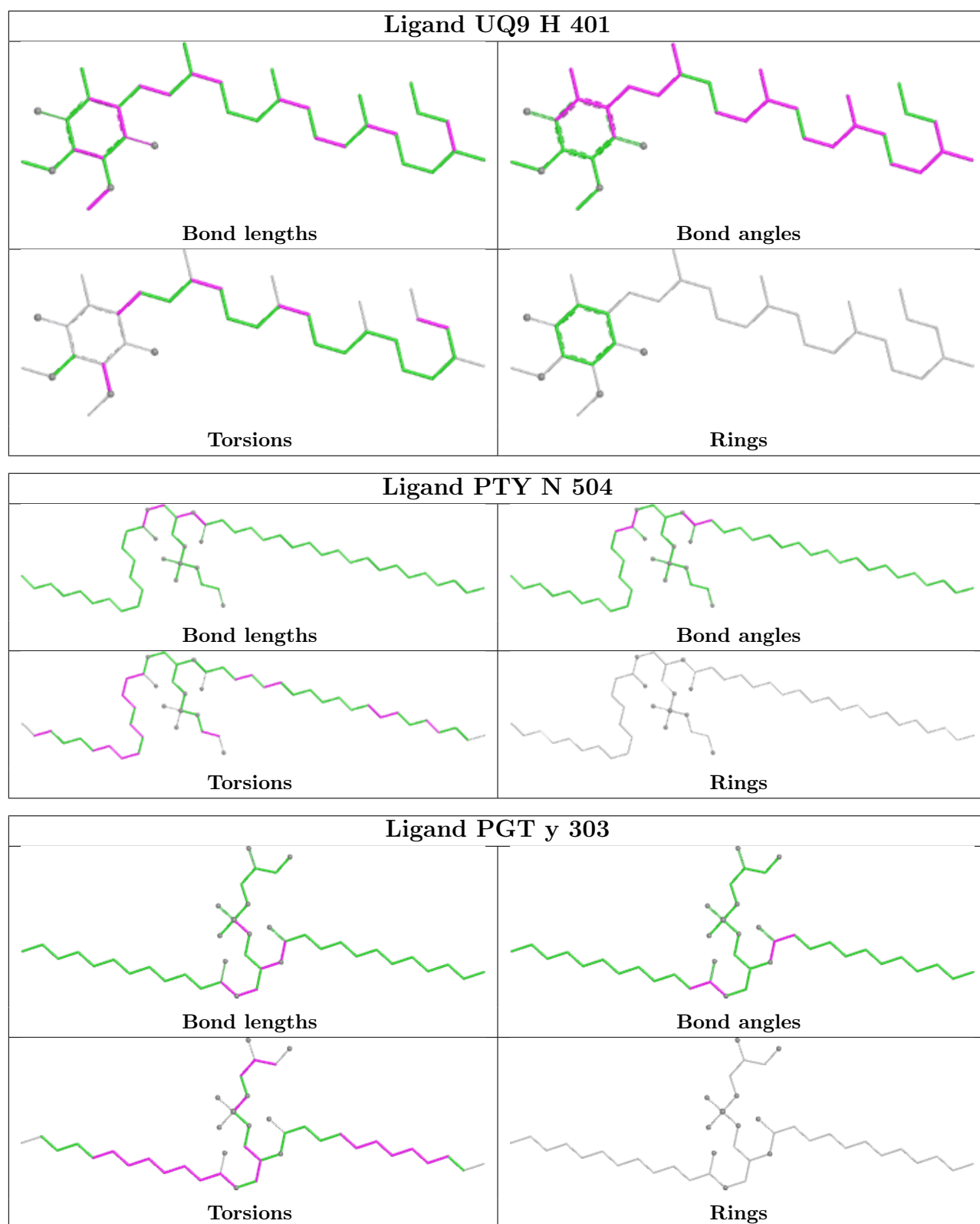


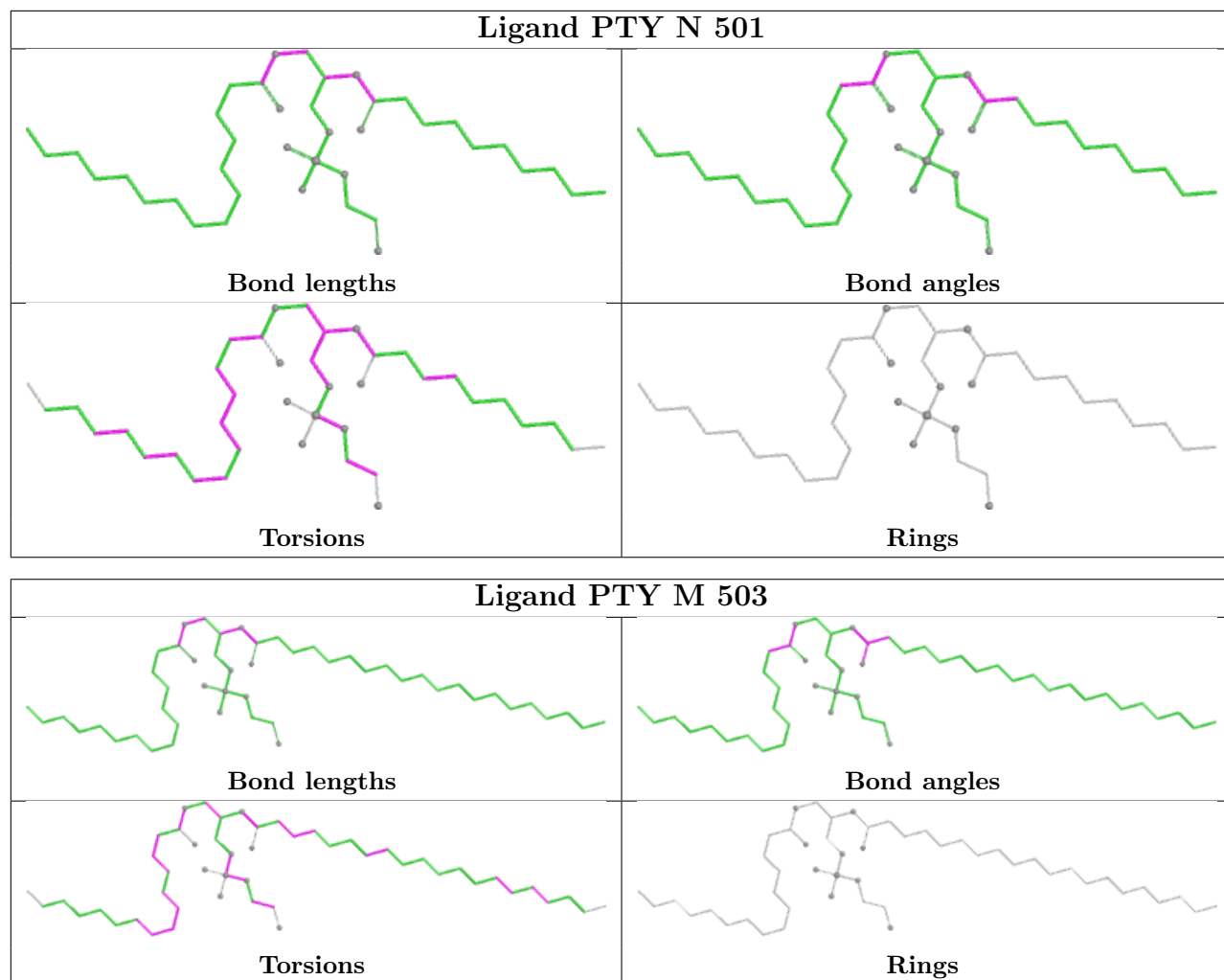


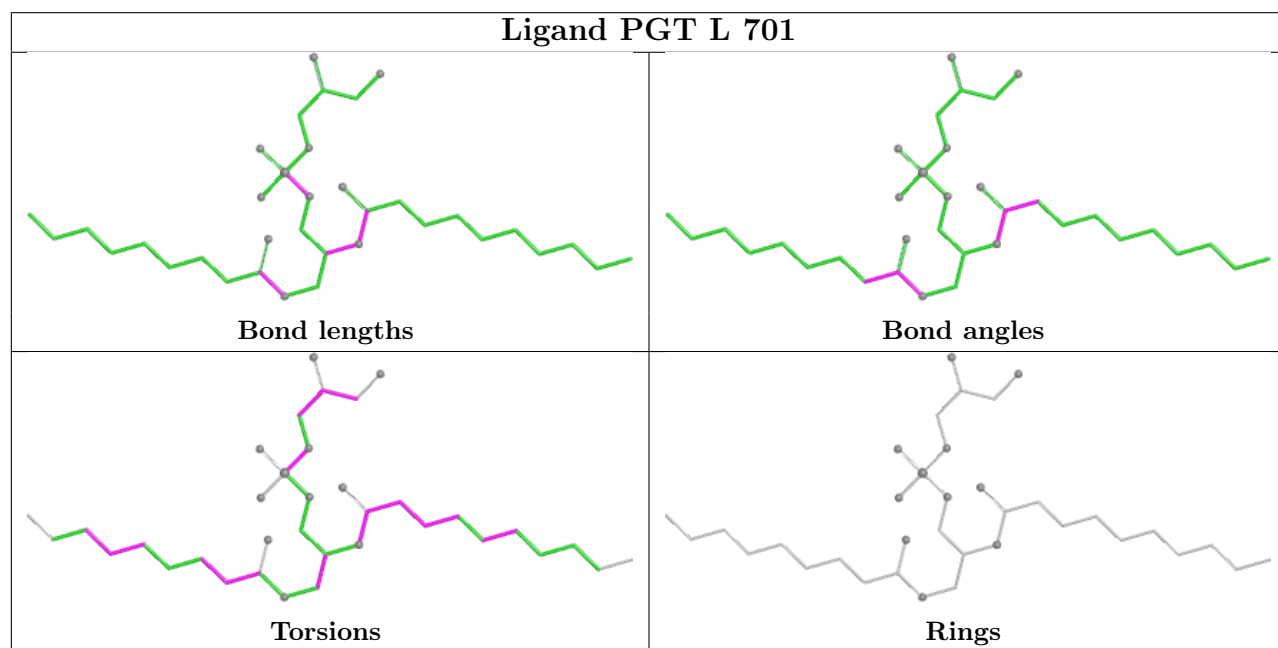
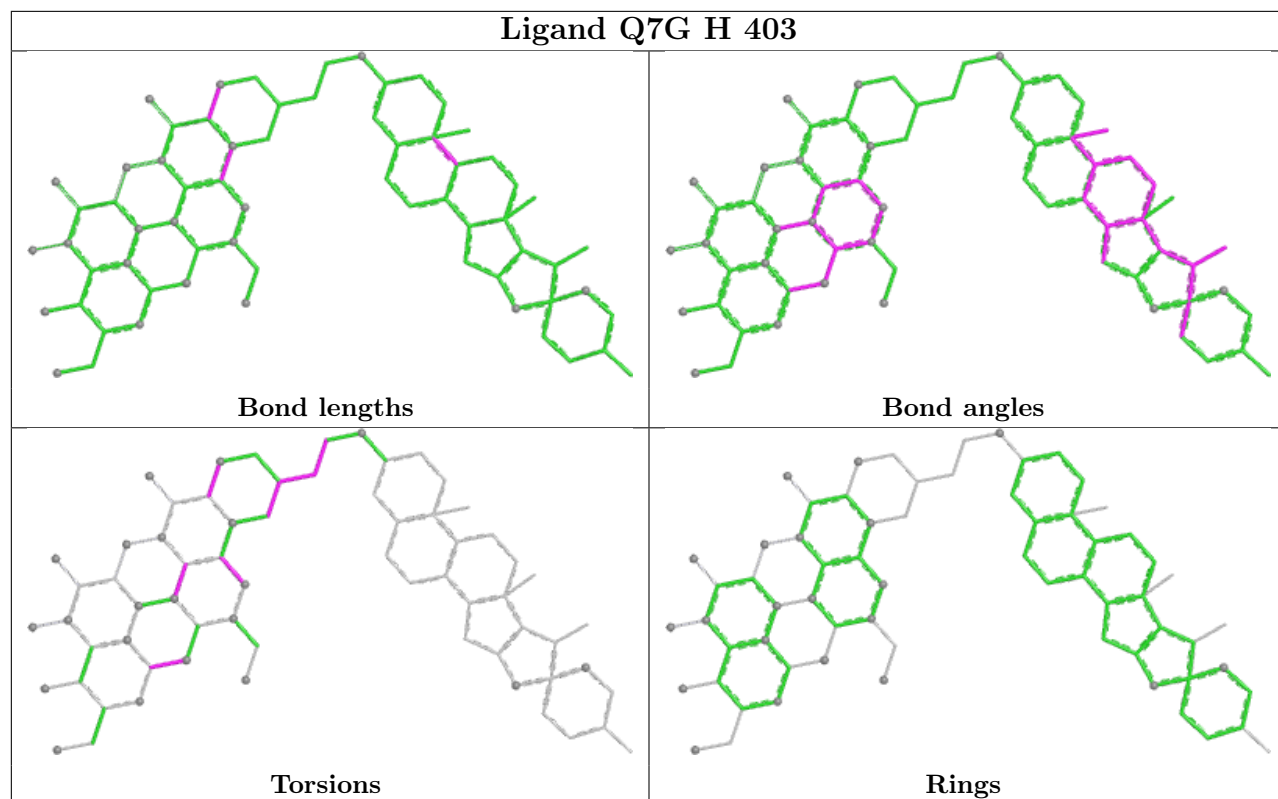


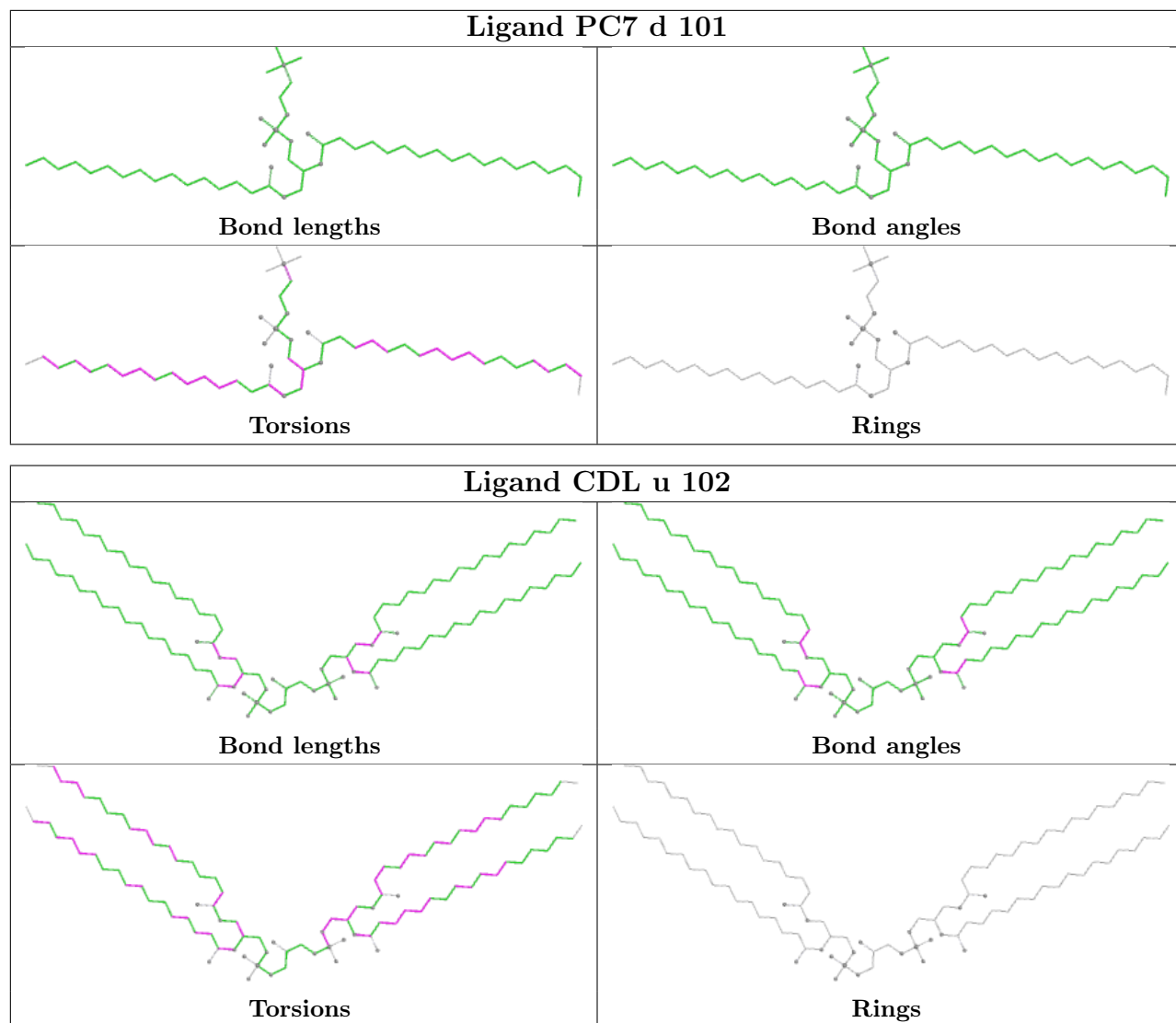


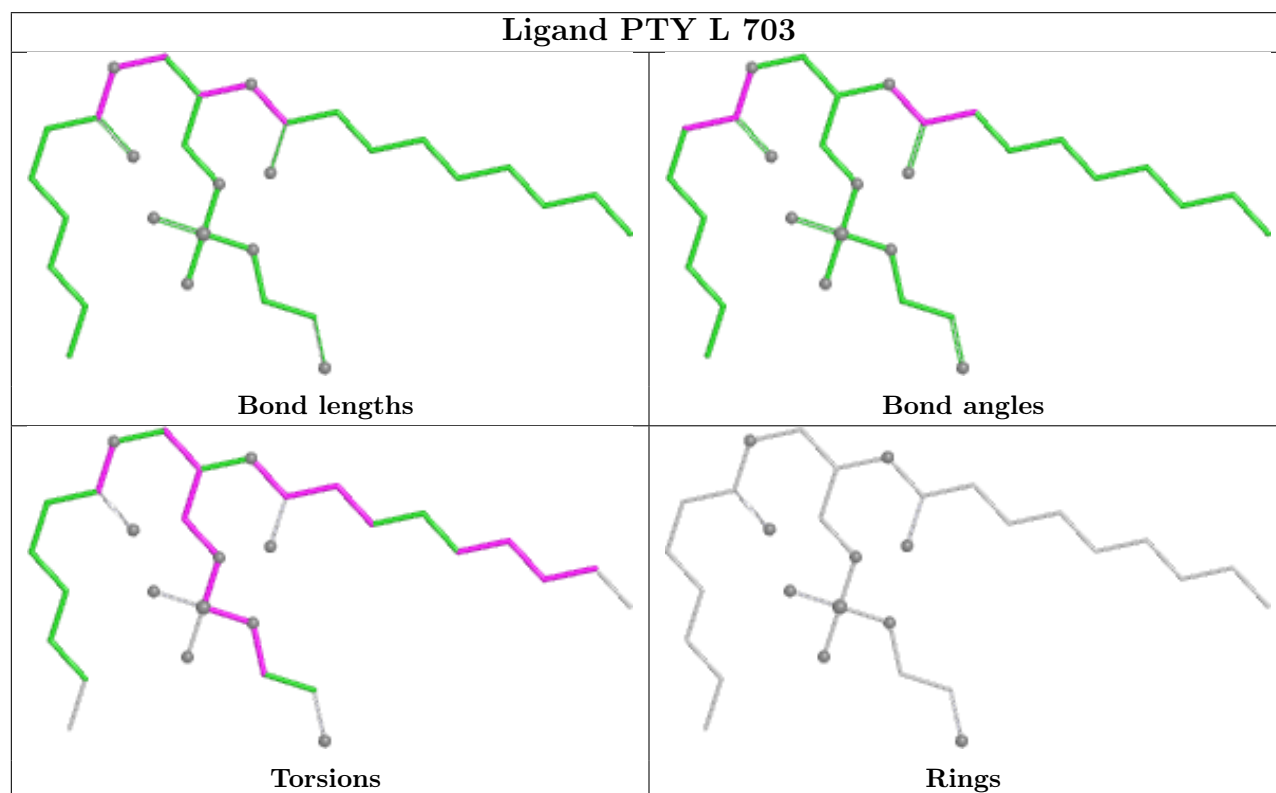
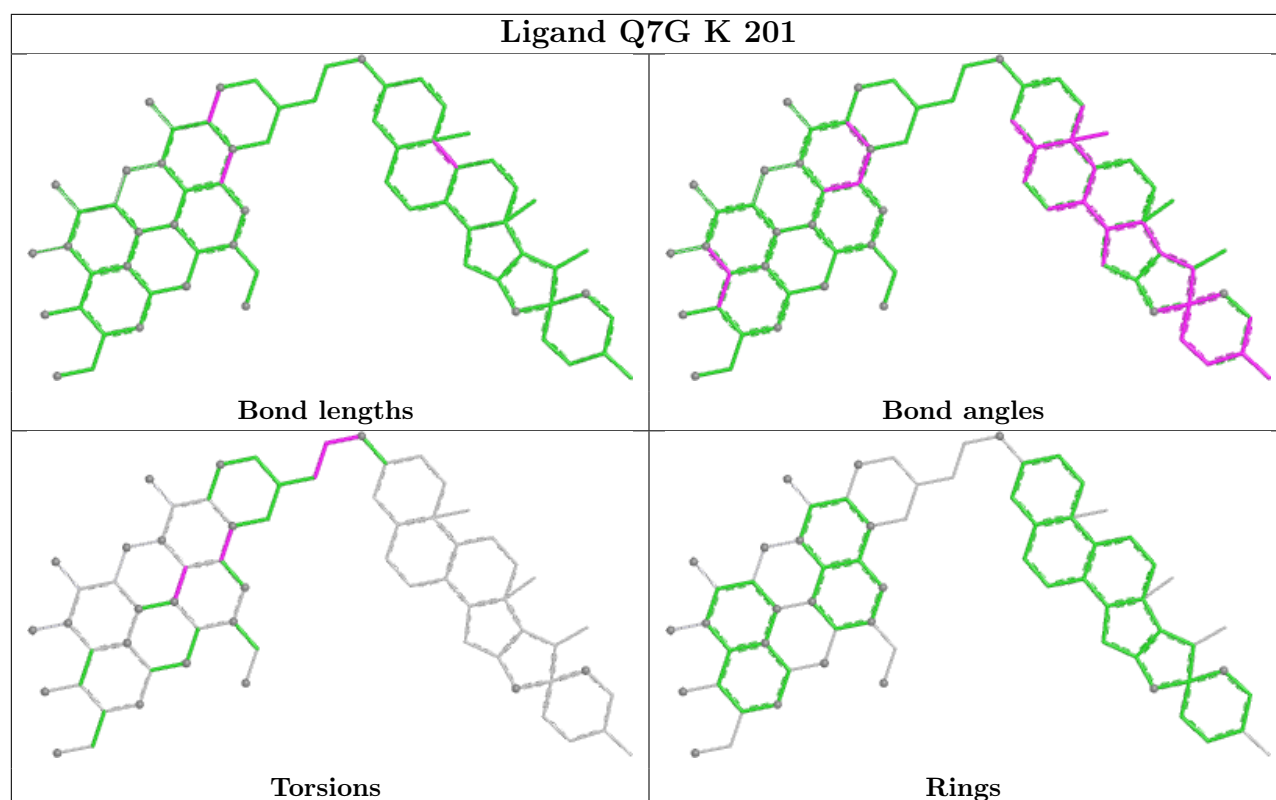


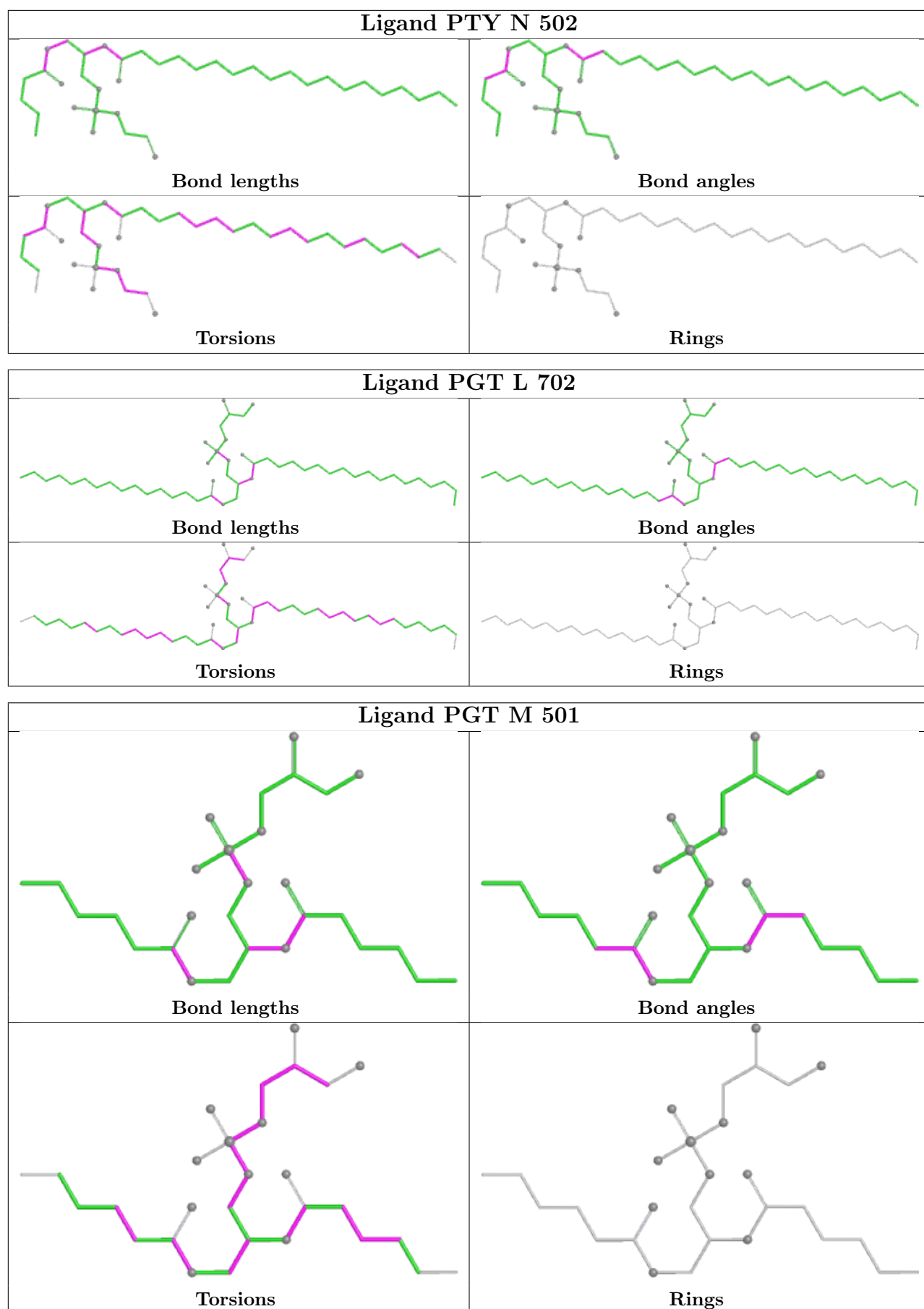


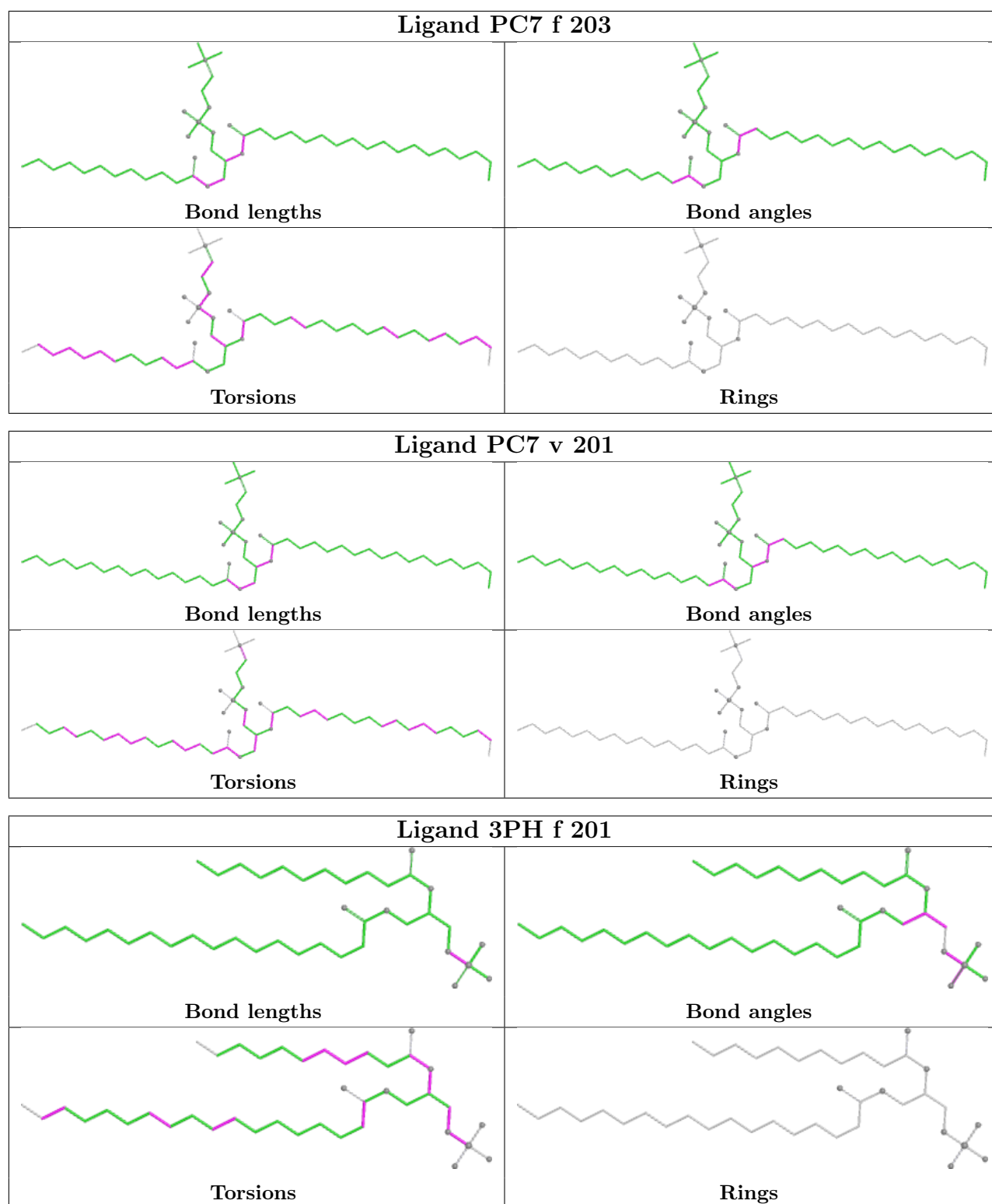












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

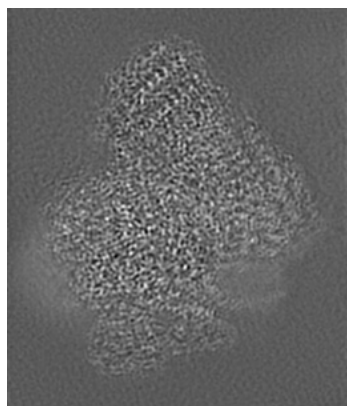
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16000. These allow visual inspection of the internal detail of the map and identification of artifacts.

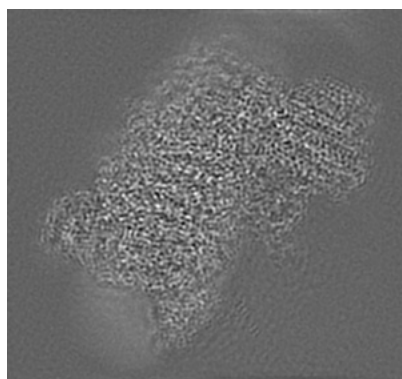
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

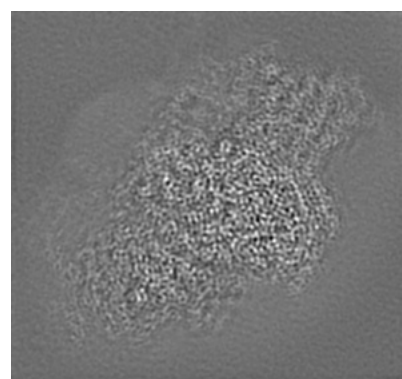
#### 6.1.1 Primary map



X

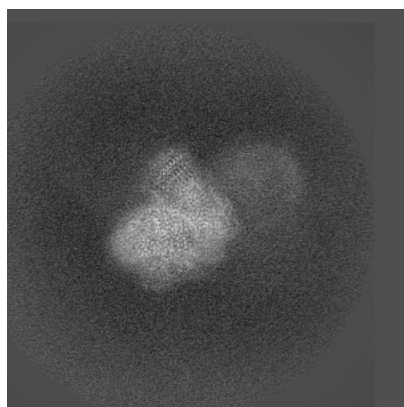


Y

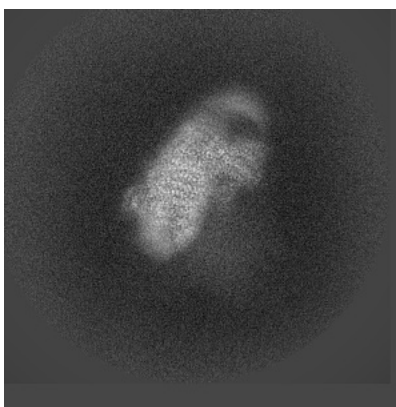


Z

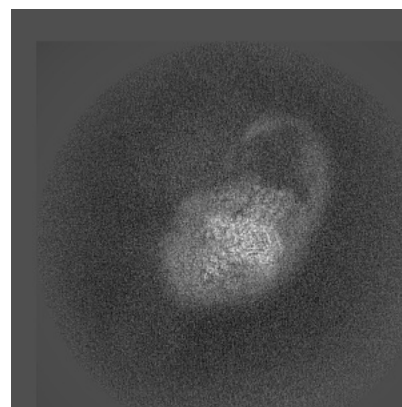
#### 6.1.2 Raw map



X



Y

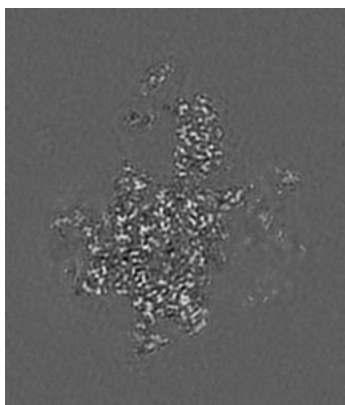


Z

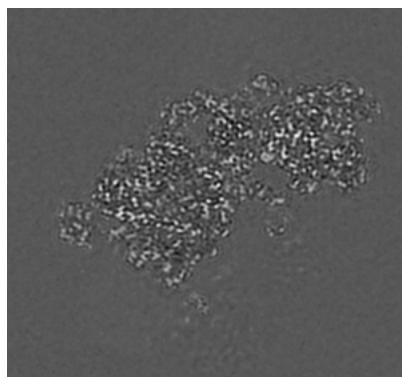
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

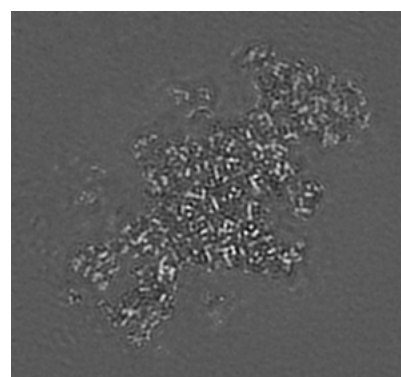
### 6.2.1 Primary map



X Index: 148

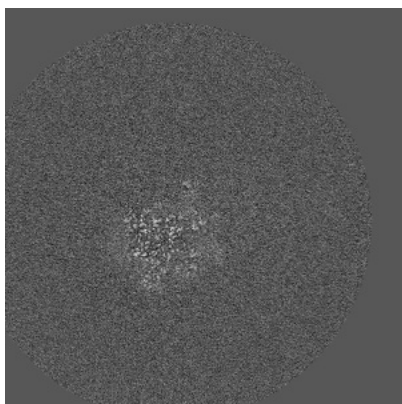


Y Index: 136

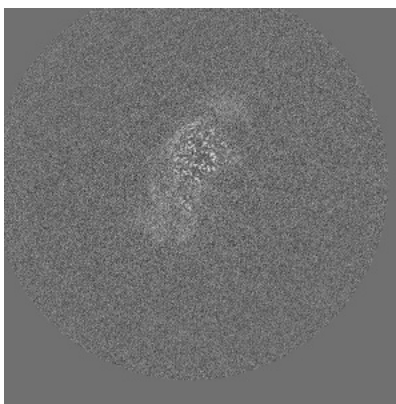


Z Index: 159

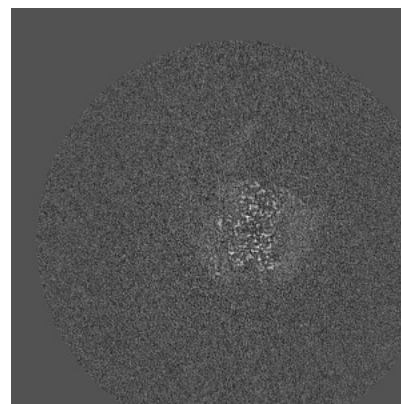
### 6.2.2 Raw map



X Index: 375



Y Index: 375

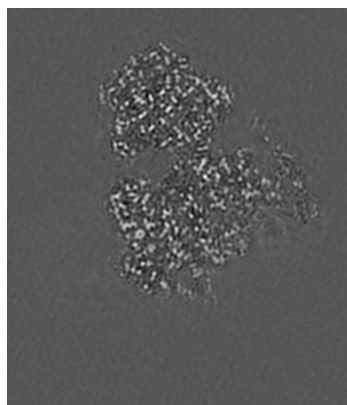


Z Index: 375

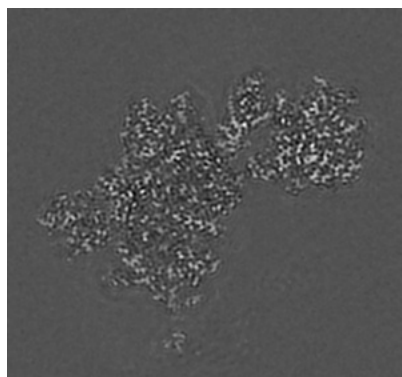
The images above show central slices of the map in three orthogonal directions.

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

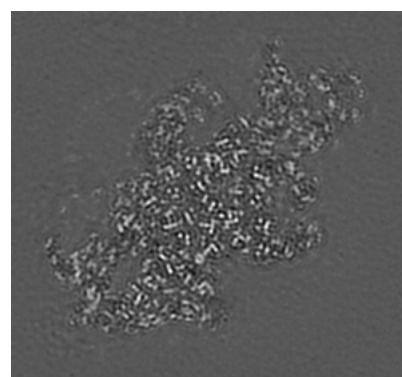
### 6.3.1 Primary map



X Index: 182

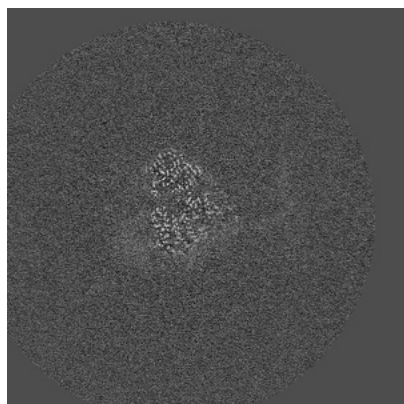


Y Index: 107

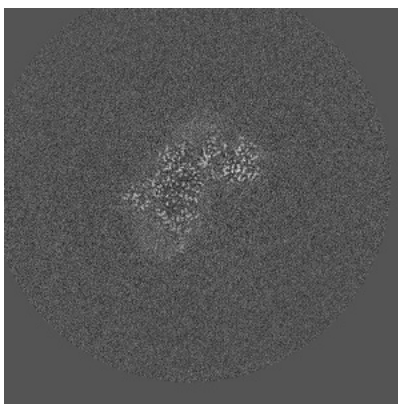


Z Index: 143

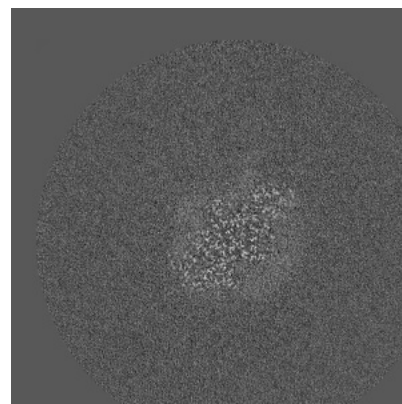
### 6.3.2 Raw map



X Index: 451



Y Index: 293

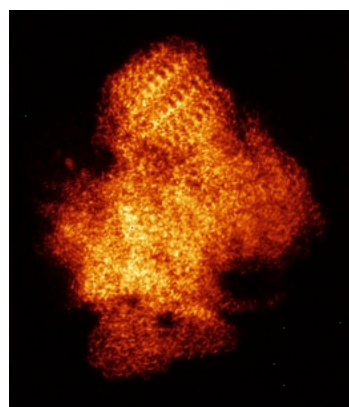


Z Index: 340

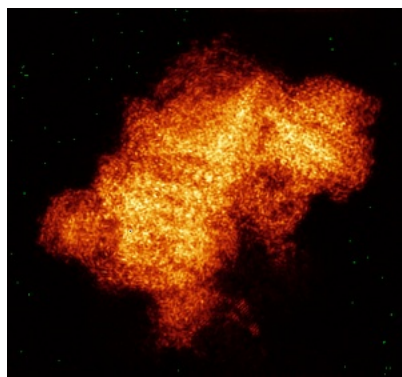
The images above show the largest variance slices of the map in three orthogonal directions.

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

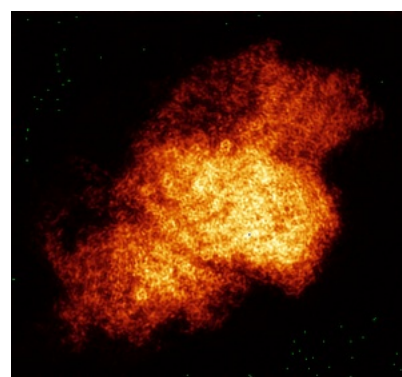
### 6.4.1 Primary map



X

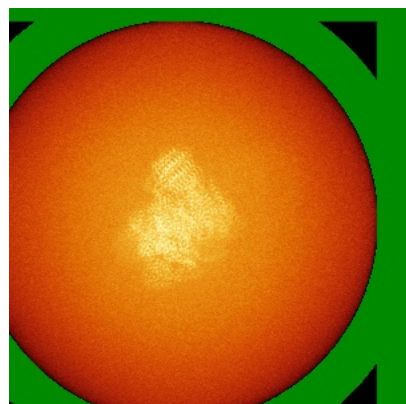


Y

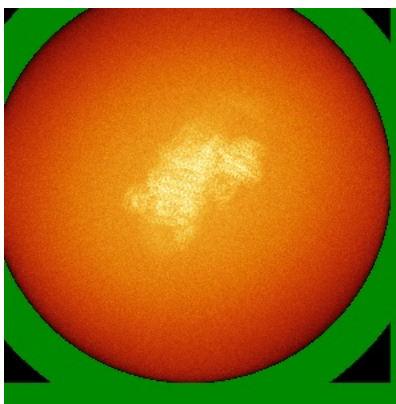


Z

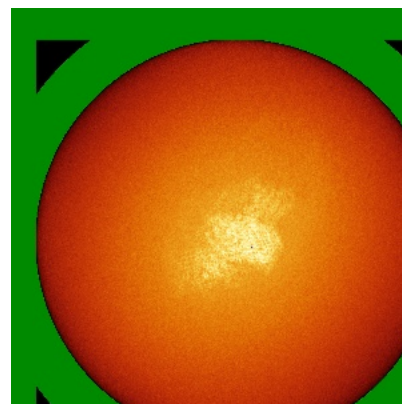
### 6.4.2 Raw map



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 0.6. 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.

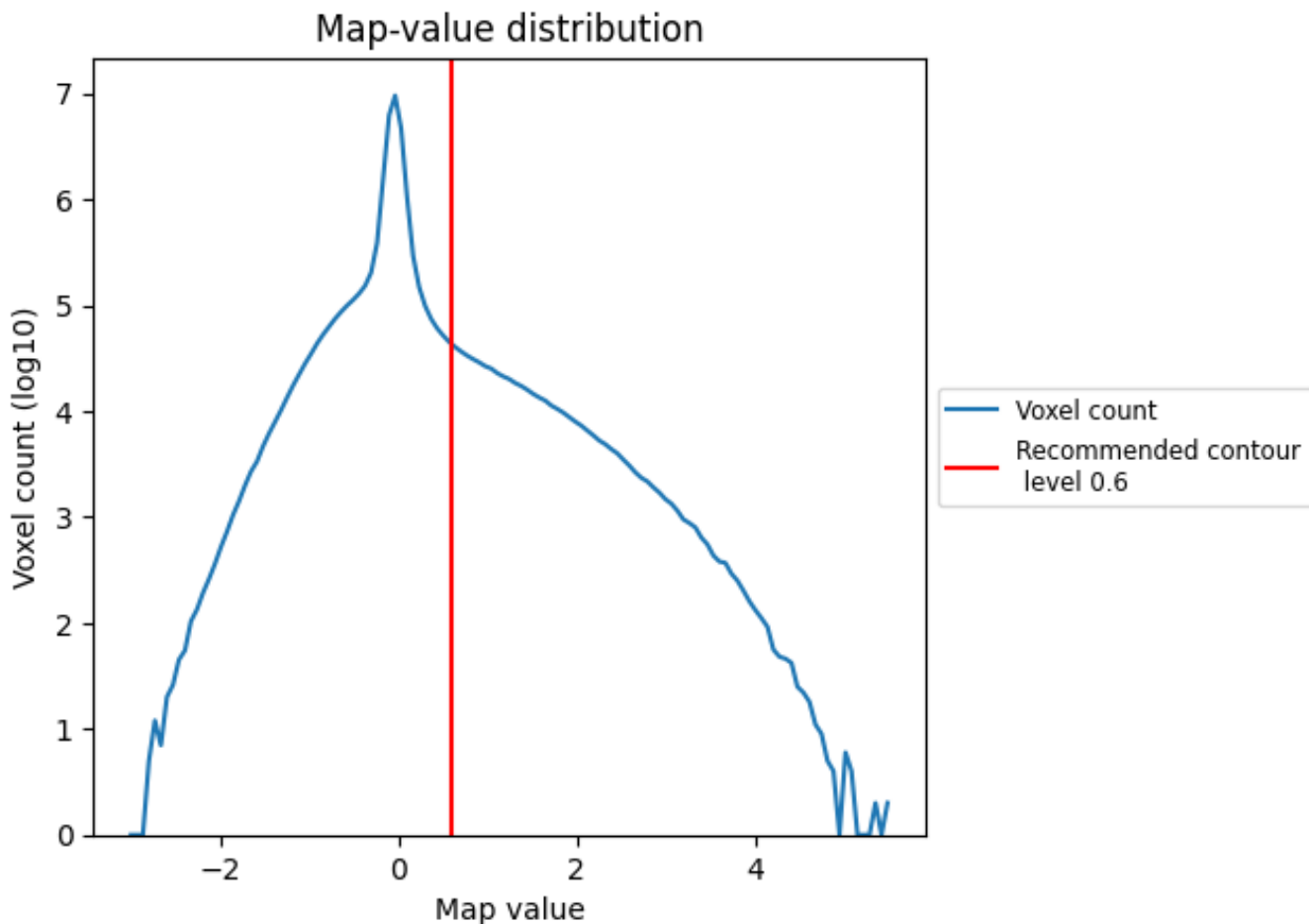
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

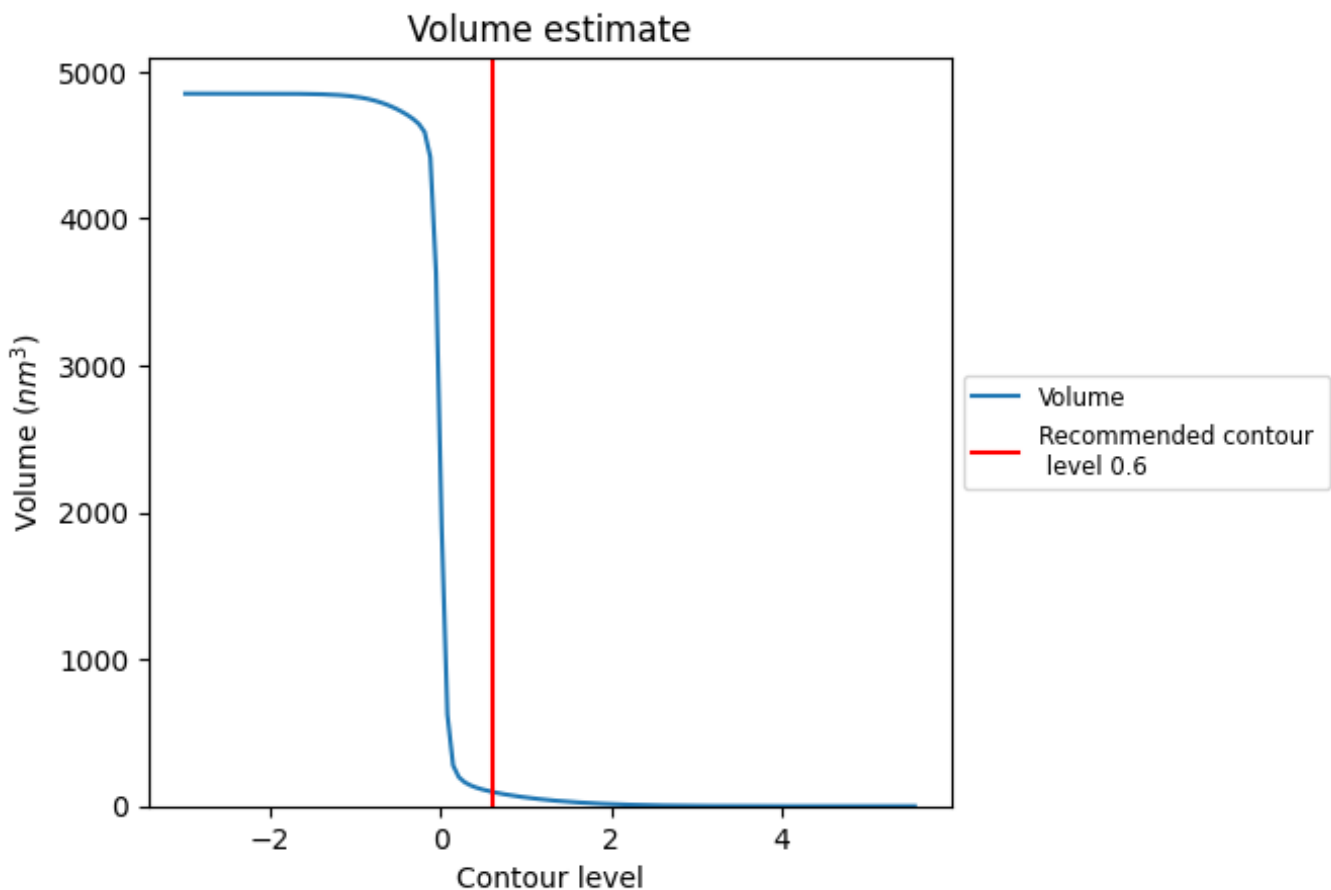
This section contains the results of statistical analysis of the map.

### 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 98 nm<sup>3</sup>; this corresponds to an approximate mass of 88 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.

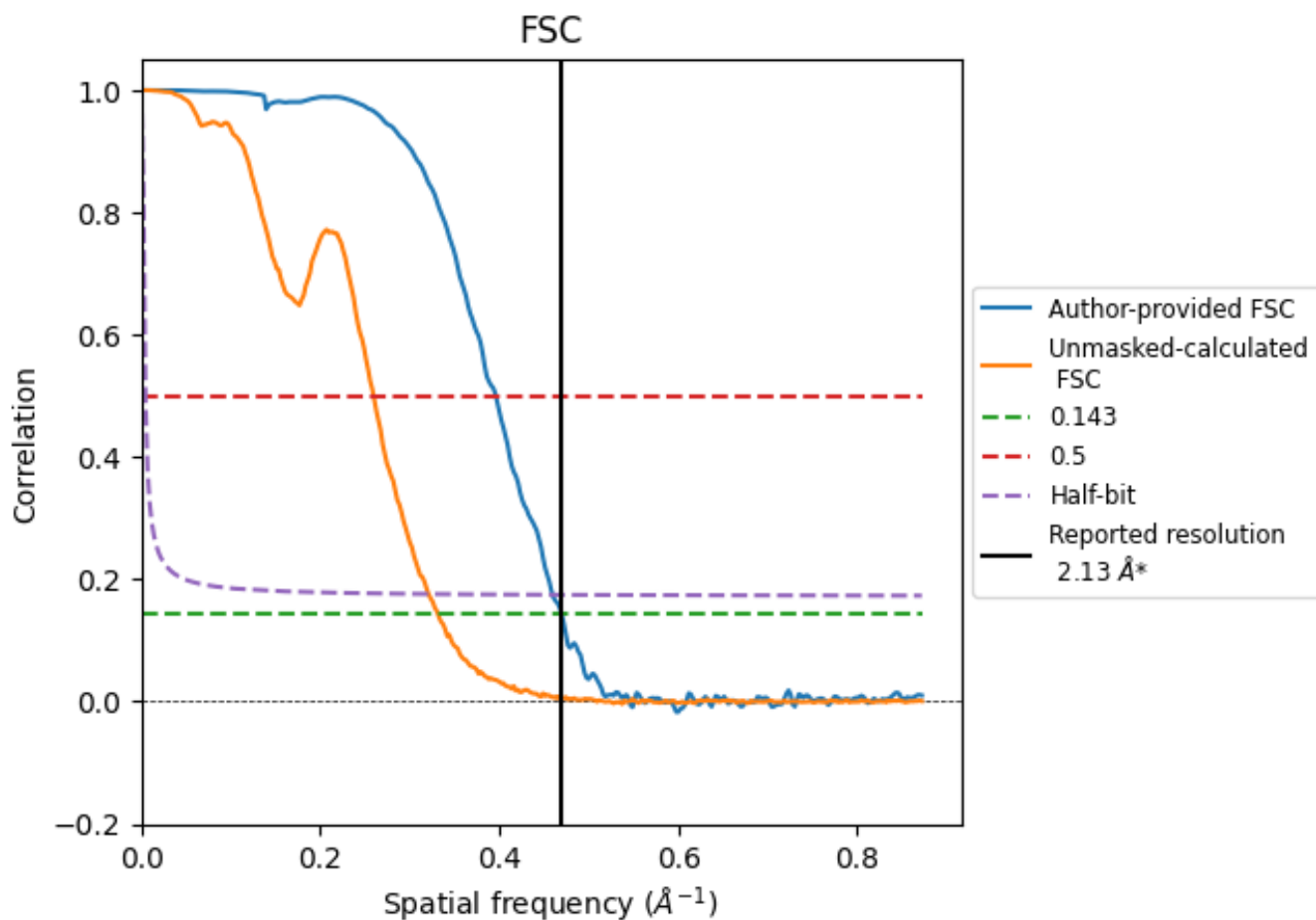
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.469 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

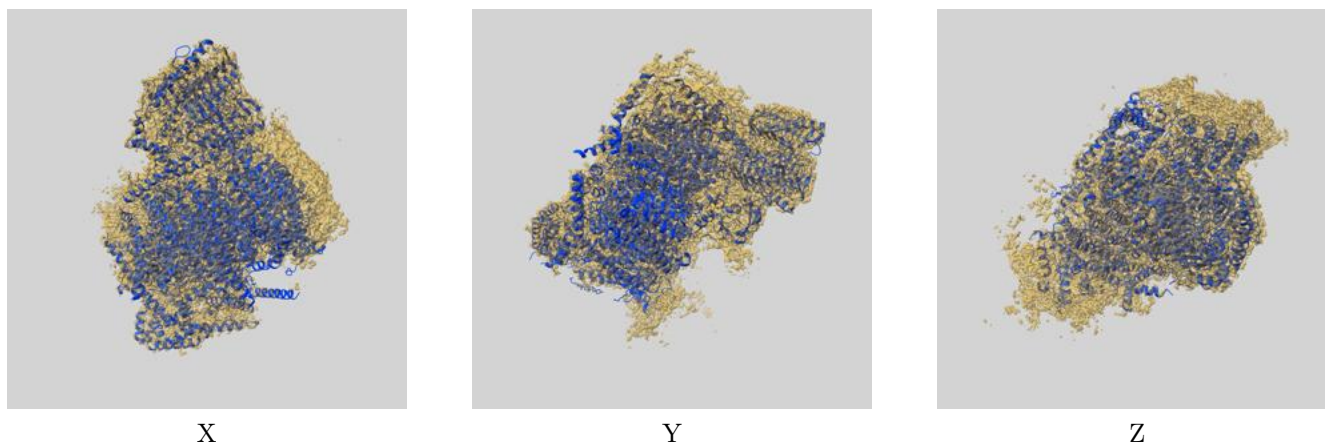
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.52	2.17
Unmasked-calculated*	3.02	3.85	3.11

\*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 3.02 differs from the reported value 2.13 by more than 10 %

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

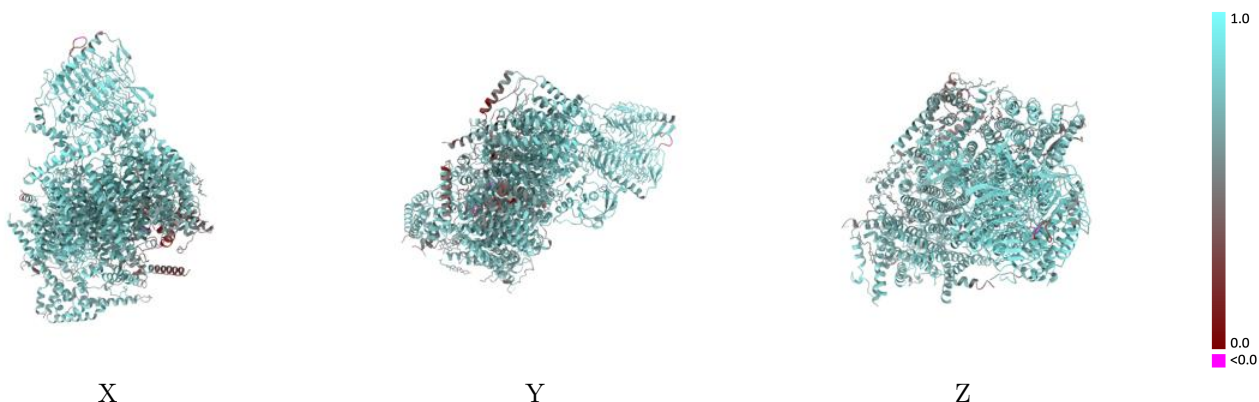
This section contains information regarding the fit between EMDB map EMD-16000 and PDB model 8BEF. Per-residue inclusion information can be found in section 3 on page 16.

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



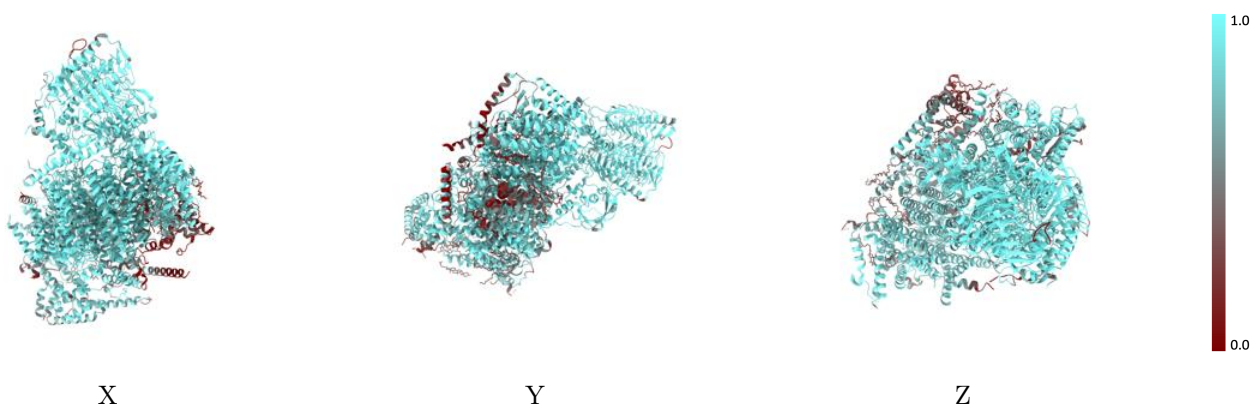
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



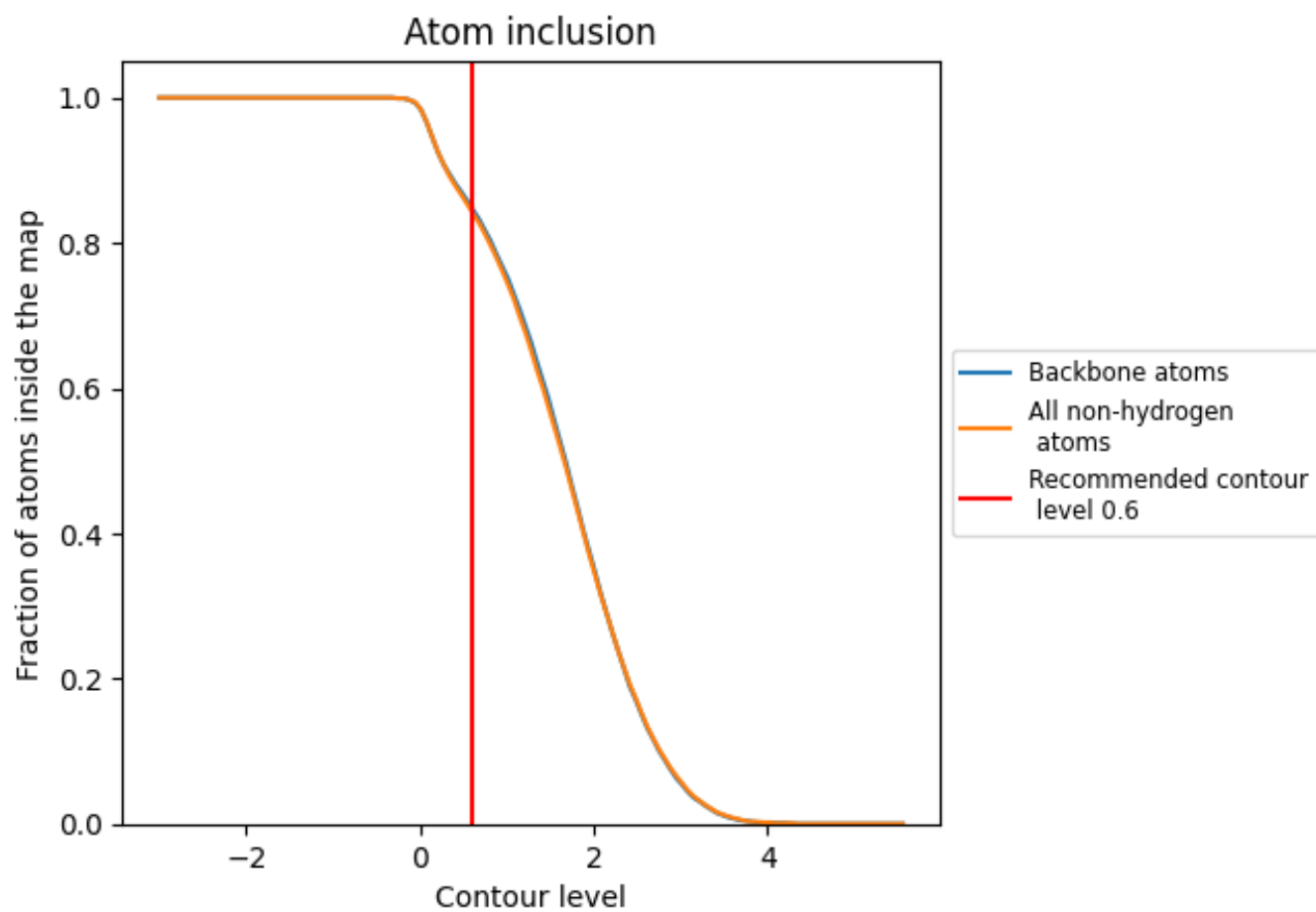
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8430	 0.7290
A	 0.9050	 0.7590
H	 0.8920	 0.7620
J	 0.8890	 0.7460
K	 0.9040	 0.7630
L	 0.6210	 0.6430
M	 0.8000	 0.6770
N	 0.9350	 0.7760
O	 0.9210	 0.7670
X	 0.8060	 0.7000
Y	 0.4590	 0.5610
Z	 0.8770	 0.7350
a	 0.8250	 0.7060
b	 0.7110	 0.6600
d	 0.7930	 0.7010
e	 0.8690	 0.7200
f	 0.8840	 0.7540
i	 0.5020	 0.5450
u	 0.5090	 0.5820
v	 0.8870	 0.7440
x	 0.9600	 0.8020
y	 0.9100	 0.7600
z	 0.9060	 0.7460

