



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:02 PM JST

PDB ID : 8IAR / pdb_00008iar
EMDB ID : EMD-35316
Title : Respiratory complex CIII2, focus-refined of type I, Wild type mouse under thermoneutral temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 3.40 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:

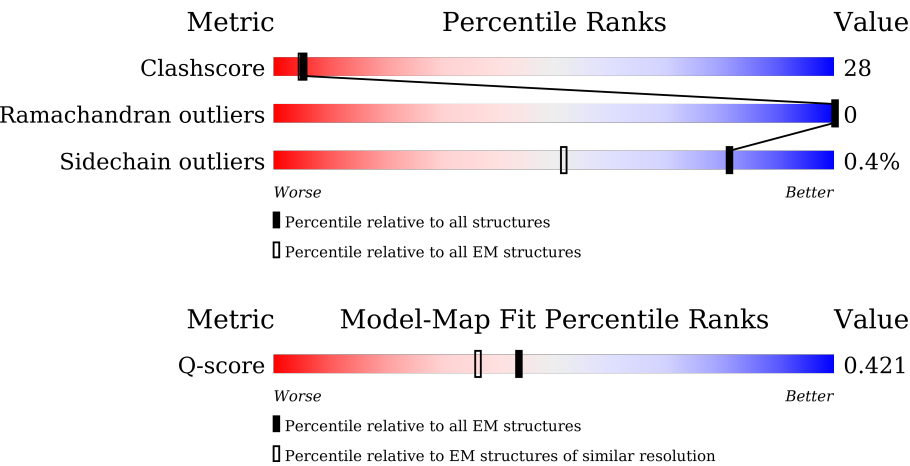
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 3.40 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	14717 (2.90 - 3.90)

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	AA	480	
1	Aa	480	
2	AB	453	
2	Ab	453	

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Mol	Chain	Length	Quality of chain
3	AC	381	
3	Ac	381	
4	AD	325	
4	Ad	325	
5	AE	274	
5	AI	274	
5	Ae	274	
5	Ai	274	
6	AF	111	
6	Af	111	
7	AG	82	
7	Ag	82	
8	AH	89	
8	Ah	89	
9	AJ	64	
9	Aj	64	
10	AK	56	
10	Ak	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
13	U10	Ac	404	-	-	X	-
14	UQ6	AC	406	-	-	X	-
15	HEC	AD	401	X	-	-	-
15	HEC	Ad	401	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32253 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	AA	403	Total	C	N	O	S	0	0
			3153	1970	560	607	16		
1	Aa	412	Total	C	N	O	S	0	0
			3225	2016	569	624	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
2	Ab	412	Total	C	N	O	S	0	0
			3094	1945	542	598	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
3	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		
4	Ad	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
5	AI	30	Total	C	N	O		0	0
			217	138	42	37			
5	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
5	Ai	28	Total	C	N	O		0	0
			207	133	40	34			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	98	Total	C	N	O	S	0	0
			864	552	154	155	3		
6	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	76	Total	C	N	O	S	0	0
			643	418	116	108	1		
7	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	68	Total	C	N	O	S	0	0
			562	343	103	111	5		
8	Ah	68	Total	C	N	O	S	0	0
			562	343	103	111	5		

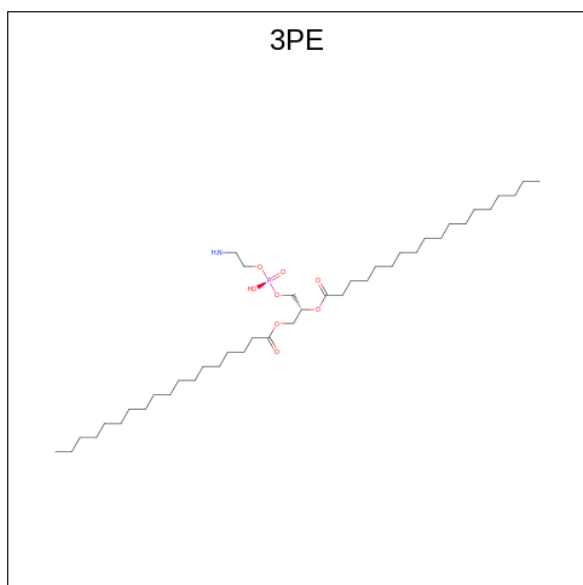
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AJ	41	Total	C	N	O	0	0
			332	216	57	59		
9	Aj	48	Total	C	N	O	0	0
			391	257	66	68		

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

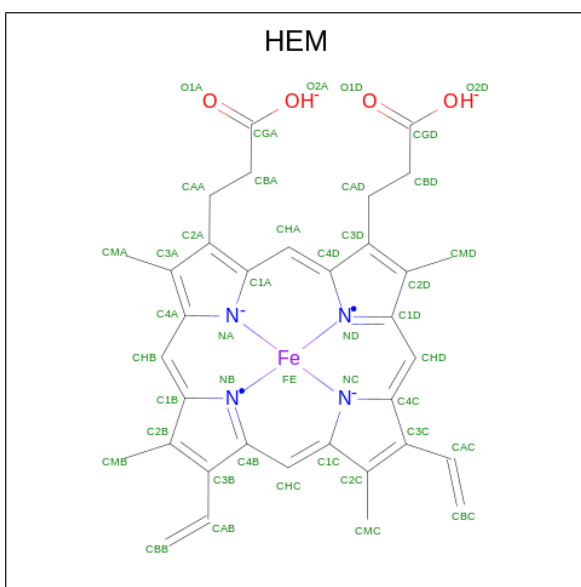
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	49	Total	C	N	O	S	0	0
			401	266	71	63	1		
10	AK	49	Total	C	N	O	S	0	0
			401	266	71	63	1		

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



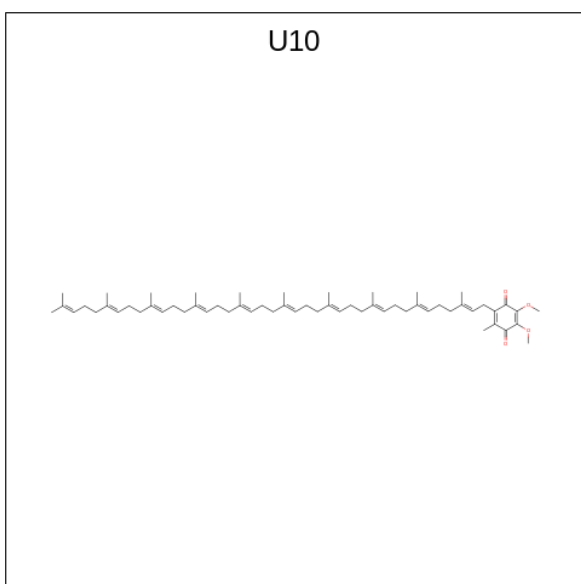
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	N	O	P	0
			23	13	1	8	1	
11	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
11	AG	1	Total	C	N	O	P	0
			51	41	1	8	1	
11	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
11	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
11	Ag	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



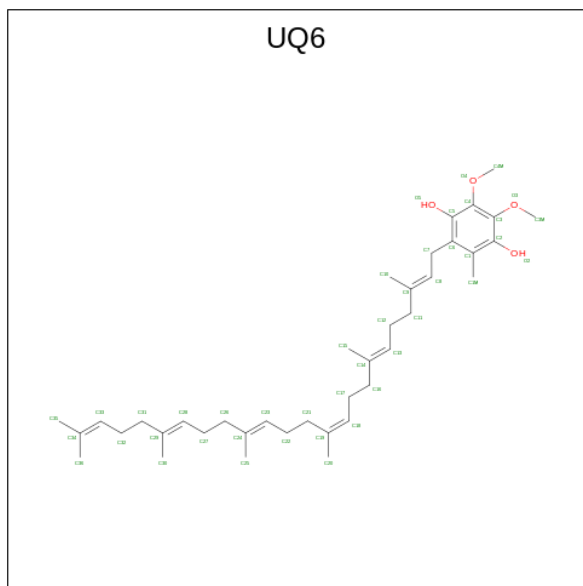
Mol	Chain	Residues	Atoms					AltConf
12	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



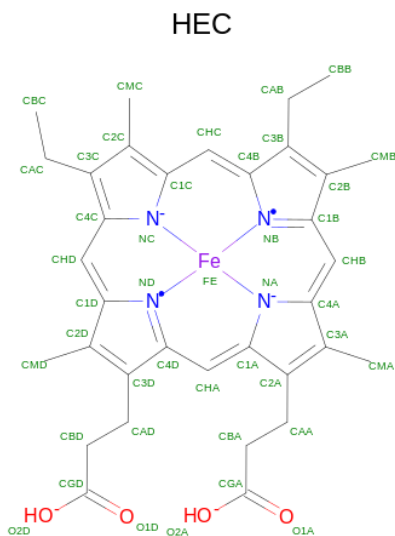
Mol	Chain	Residues	Atoms			AltConf
13	AC	1	Total	C	O	0
			23	19	4	
13	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



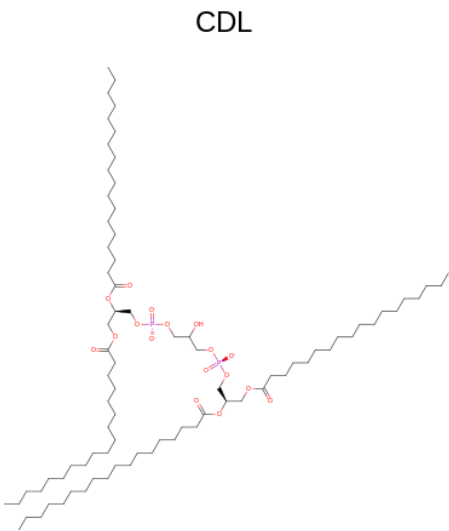
Mol	Chain	Residues	Atoms			AltConf
14	AC	1	Total	C	O	0
			28	24	4	
14	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	AD	1	Total 43	C 34	Fe 1	N 4	O 4	0
15	Ad	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



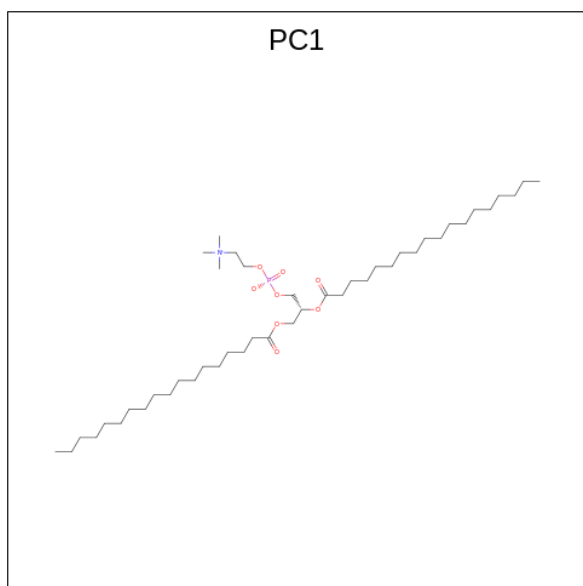
Mol	Chain	Residues	Atoms				AltConf
16	AG	1	Total	C	O	P	0
			42	23	17	2	

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Mol	Chain	Residues	Atoms				AltConf
16	AG	1	Total	C	O	P	0
			56	37	17	2	
16	Aa	1	Total	C	O	P	0
			46	27	17	2	
16	Ag	1	Total	C	O	P	0
			42	23	17	2	
16	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).

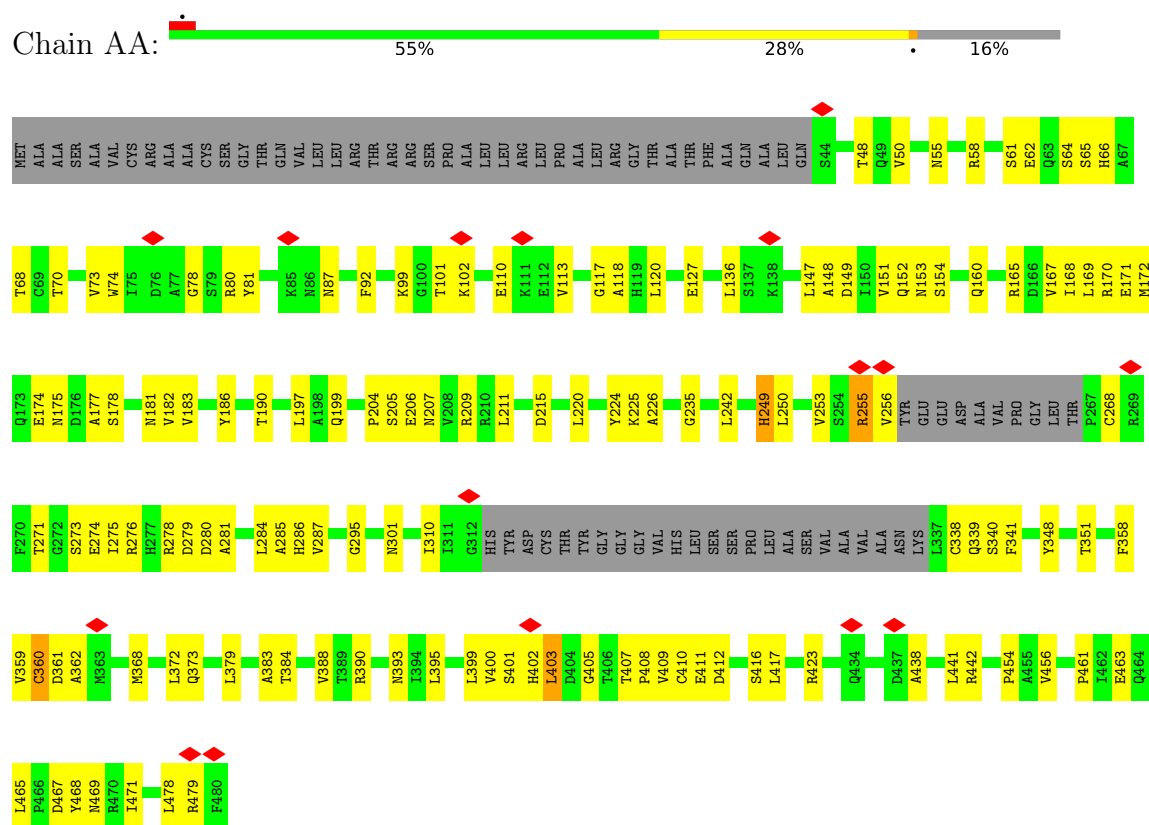


Mol	Chain	Residues	Atoms					AltConf
17	Ae	1	Total	C	N	O	P	0
			35	25	1	8	1	

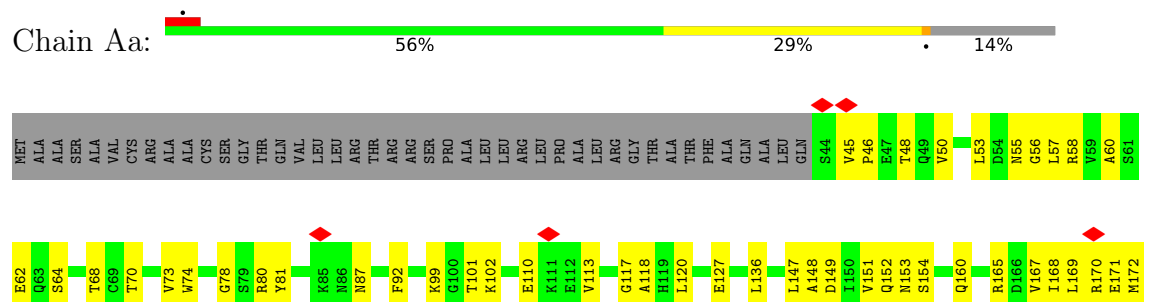
3 Residue-property plots

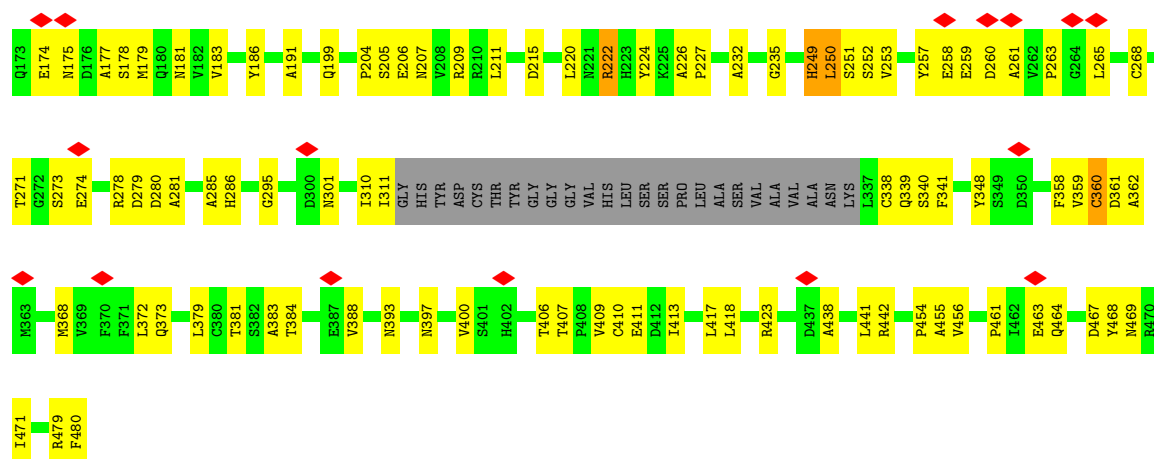
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

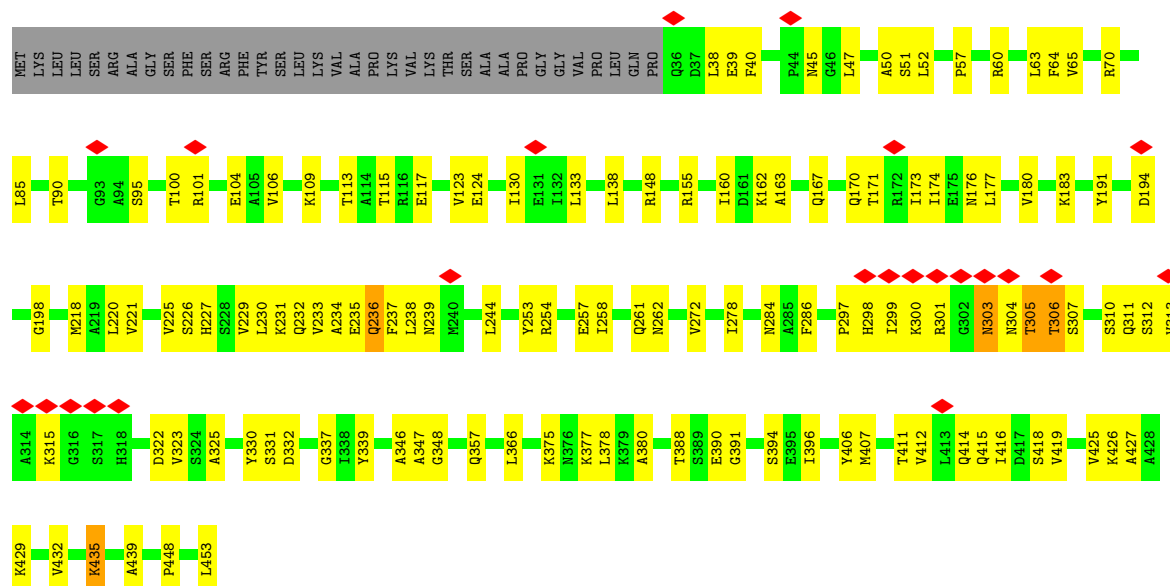


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

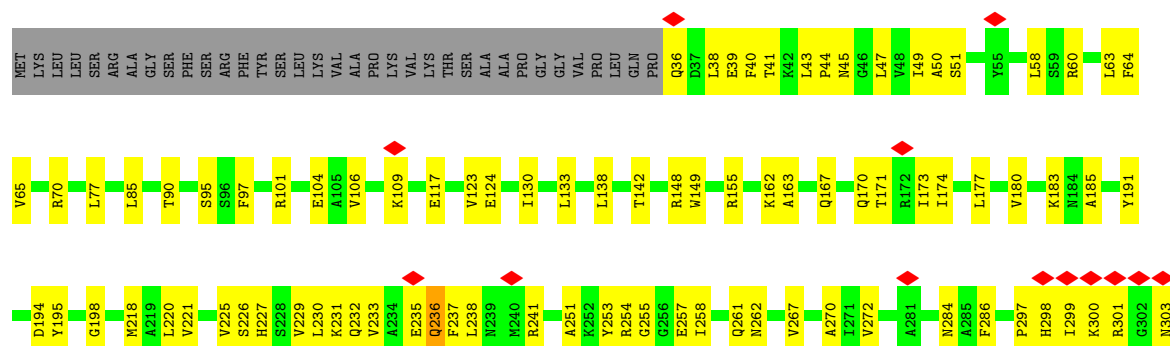




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

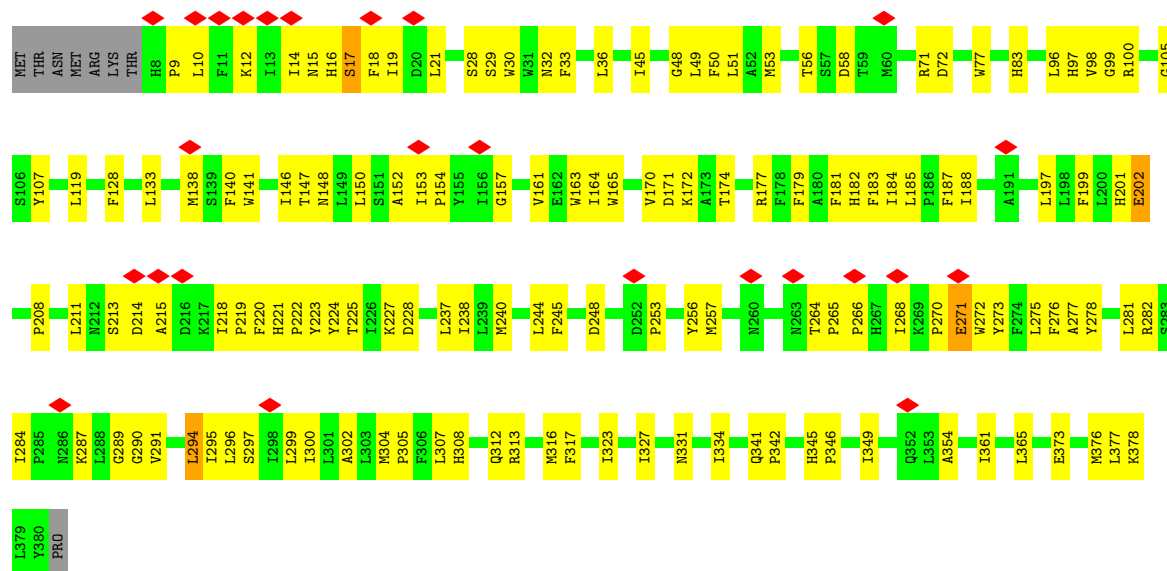


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

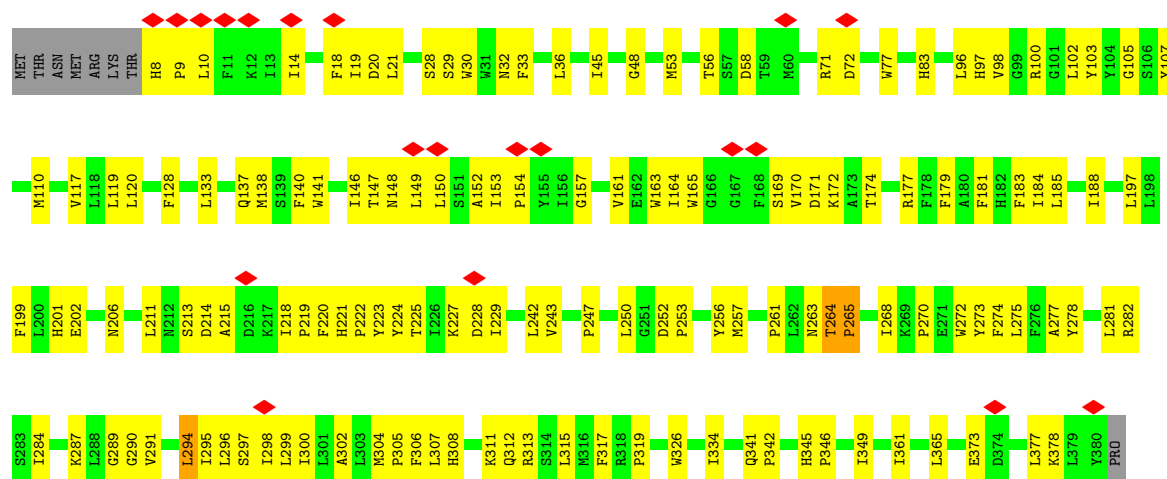




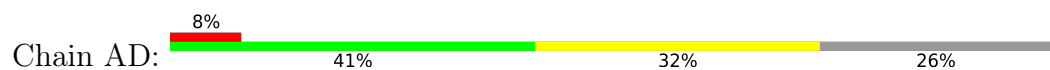
• Molecule 3: Cytochrome b

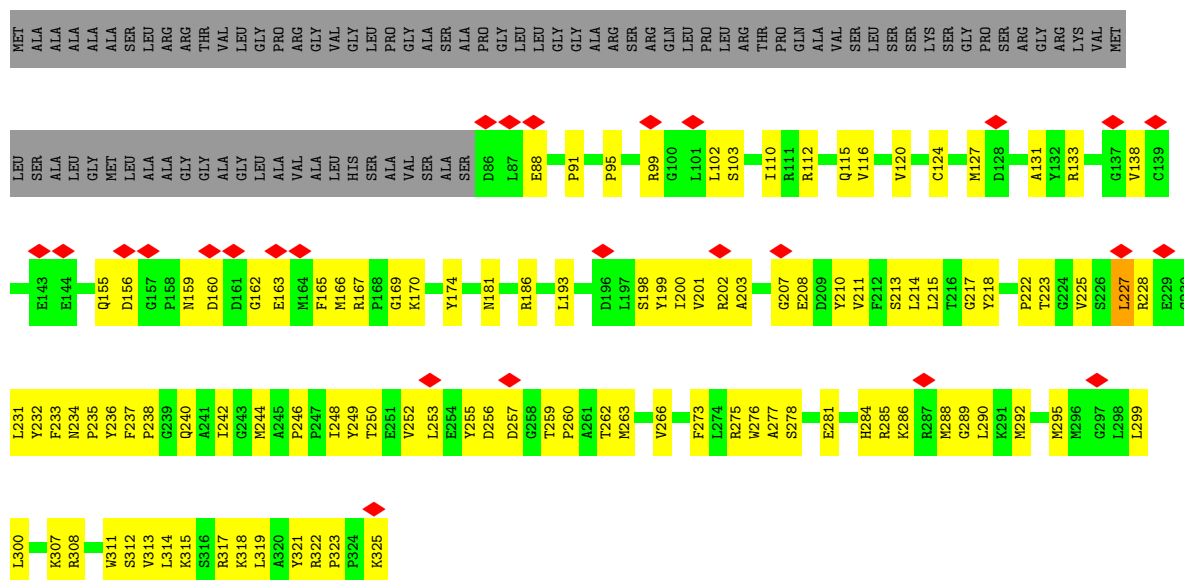


• Molecule 3: Cytochrome b

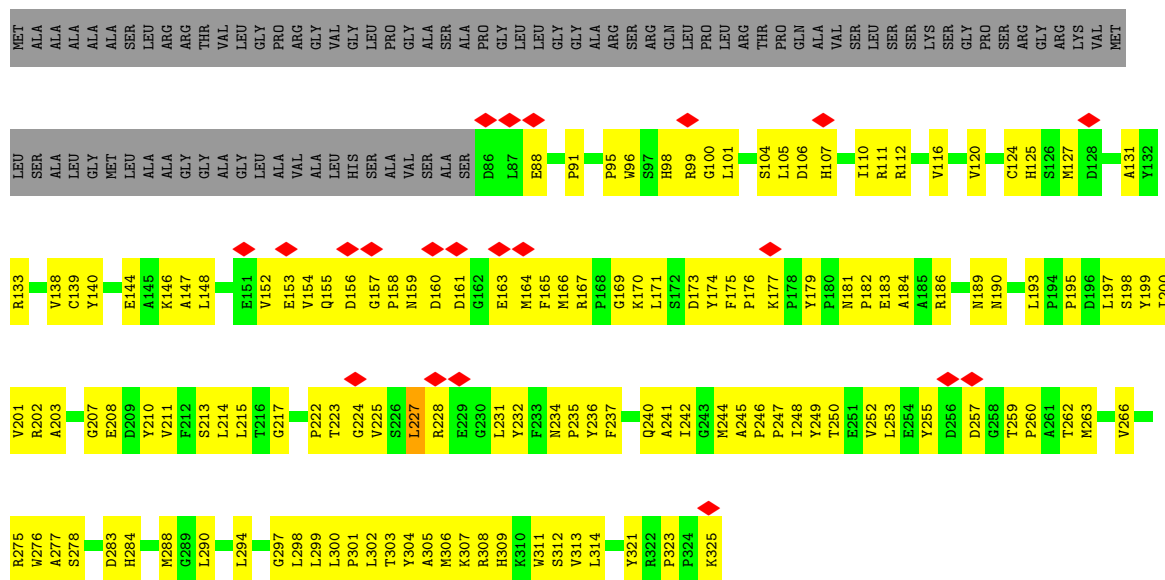


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

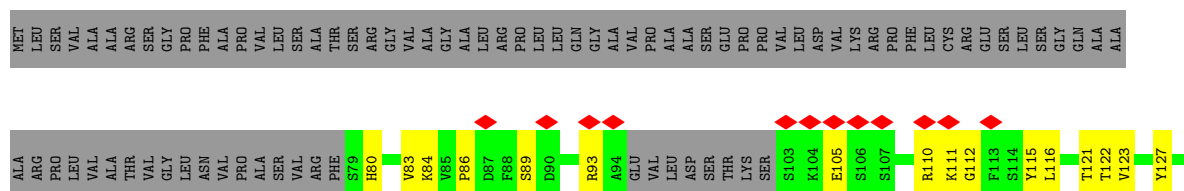




• Molecule 4: Cytochrome c1, heme protein, mitochondrial

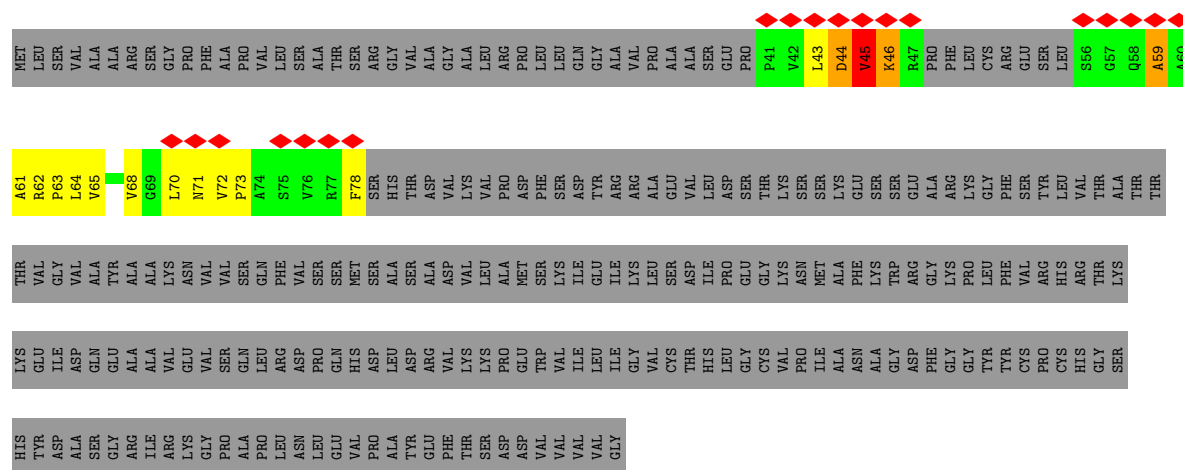


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

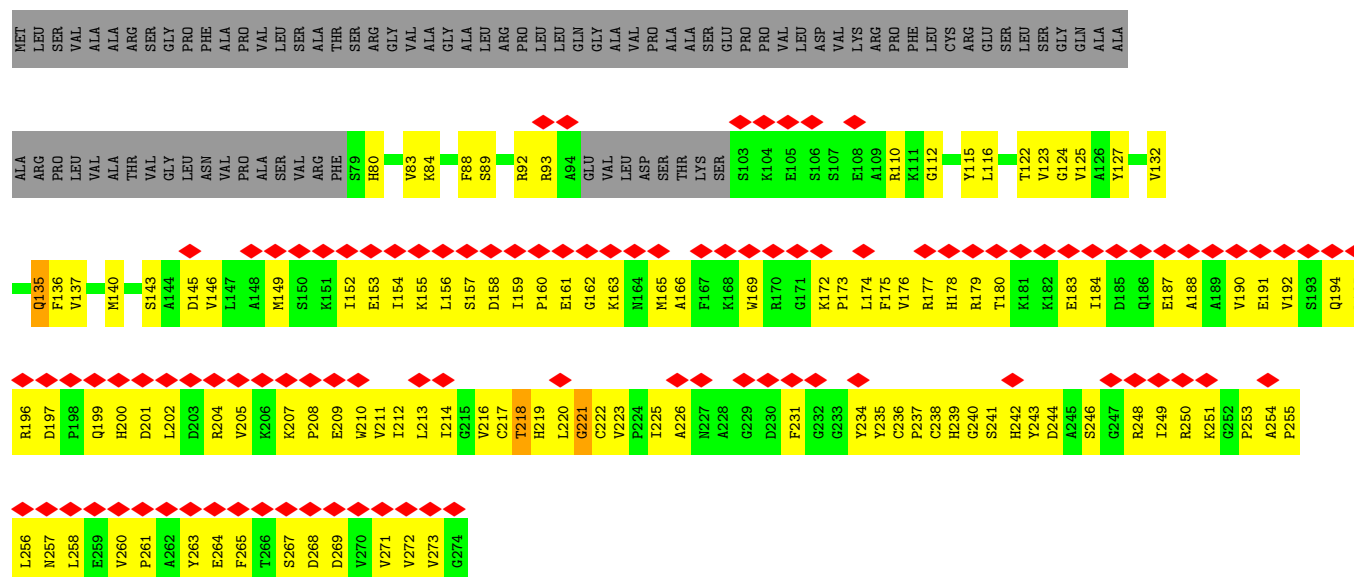




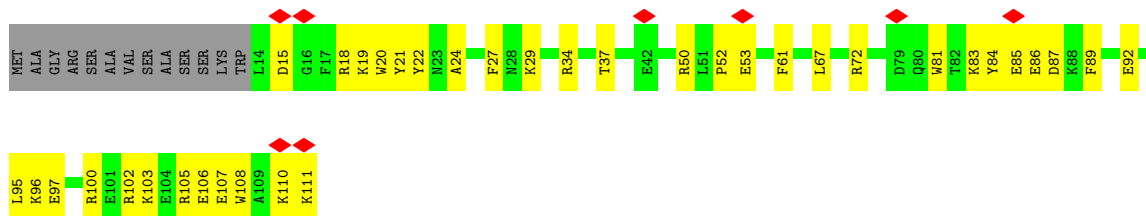
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



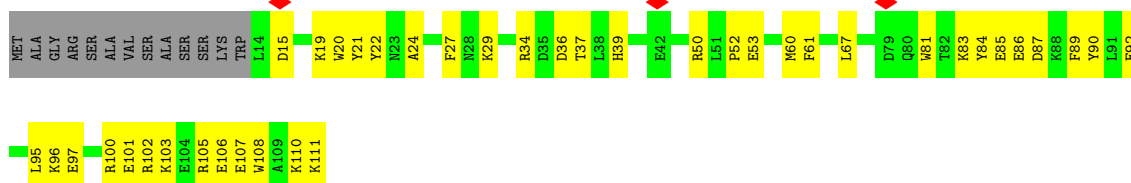
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



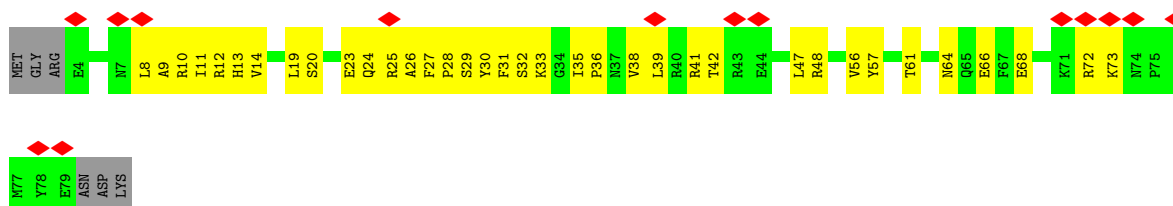
Chain Ai: 7% 5% 90%



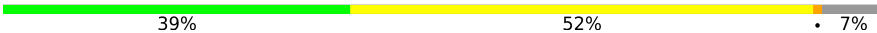
Chain Af: 52% 36% 12%

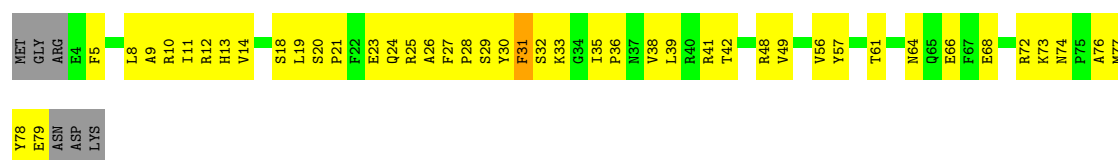


Chain AG:



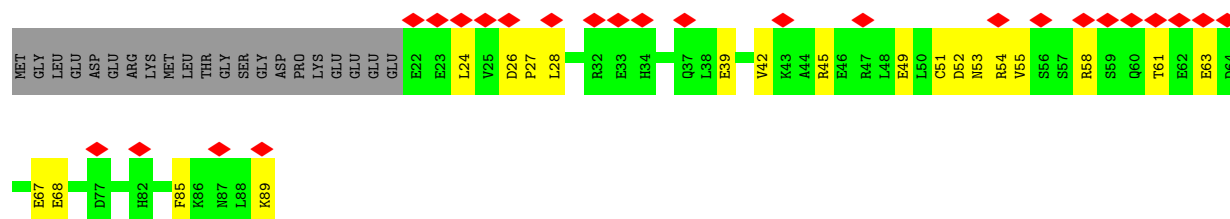
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain Ag: 



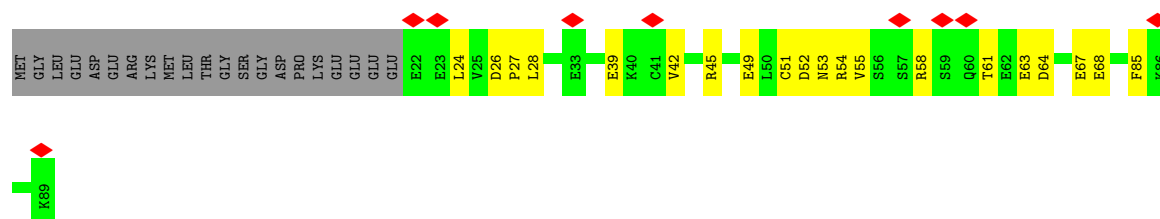
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH: 

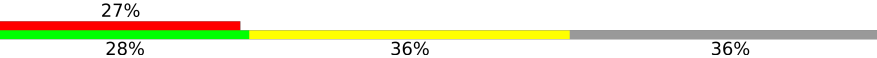


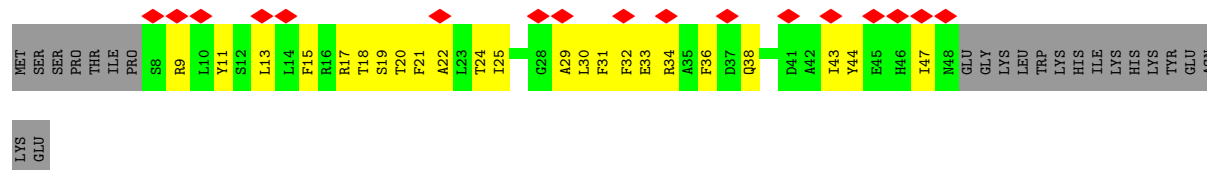
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah: 



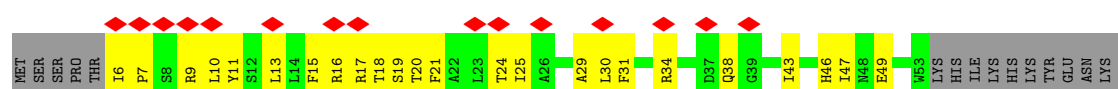
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain AJ: 

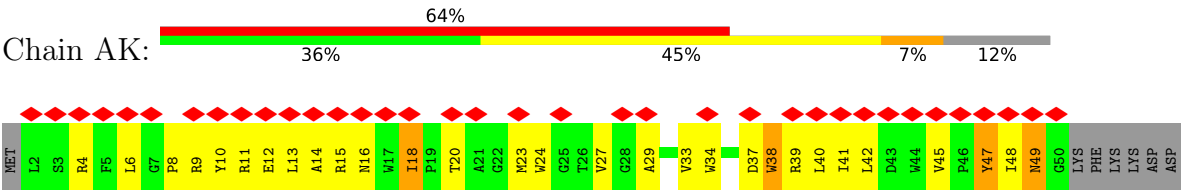


- Molecule 9: Cytochrome b-c1 complex subunit 9

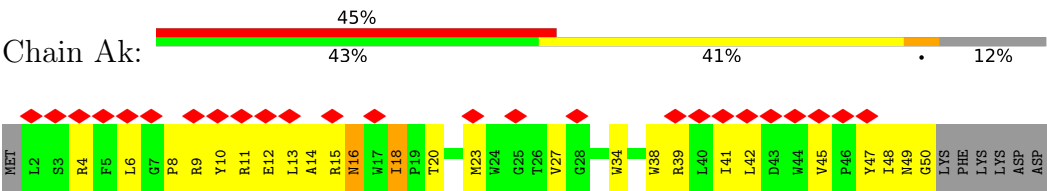
Chain Aj: 



● 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	85845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.363	Depositor
Minimum map value	-1.370	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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: HEC, PC1, HEM, CDL, U10, 3PE, UQ6

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	AA	0.38	0/3213	0.69	5/4355 (0.1%)
1	Aa	0.50	1/3288 (0.0%)	0.69	3/4462 (0.1%)
2	AB	0.36	0/3187	0.64	5/4308 (0.1%)
2	Ab	0.43	0/3142	0.68	4/4246 (0.1%)
3	AC	0.48	1/3089 (0.0%)	0.68	3/4221 (0.1%)
3	Ac	0.46	1/3089 (0.0%)	0.73	7/4221 (0.2%)
4	AD	0.41	0/1971	0.70	3/2677 (0.1%)
4	Ad	0.54	0/1971	0.81	5/2677 (0.2%)
5	AE	0.63	0/1483	1.03	3/2007 (0.1%)
5	AI	1.83	2/219 (0.9%)	1.48	5/296 (1.7%)
5	Ae	0.63	0/1483	1.03	3/2007 (0.1%)
5	Ai	1.51	1/209 (0.5%)	1.16	1/283 (0.4%)
6	AF	0.38	0/884	0.52	0/1184
6	Af	0.38	0/884	0.52	0/1184
7	AG	0.49	0/662	0.87	1/895 (0.1%)
7	Ag	0.50	0/662	0.89	1/895 (0.1%)
8	AH	0.38	0/569	0.68	0/763
8	Ah	0.38	0/569	0.68	0/763
9	AJ	0.53	0/339	0.71	0/457
9	Aj	0.55	0/401	0.71	0/542
10	AK	0.53	0/416	0.97	5/571 (0.9%)
10	Ak	0.53	0/416	0.81	2/571 (0.4%)
All	All	0.50	6/32146 (0.0%)	0.75	56/43585 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Ai	44	ASP	C-N	20.05	1.52	1.33
5	AI	44	ASP	C-N	20.05	1.52	1.33
1	Aa	250	LEU	C-N	19.52	1.58	1.33
5	AI	45	VAL	C-N	15.63	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AC	271	GLU	C-N	13.65	1.52	1.34

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	306	THR	N-CA-C	9.96	123.38	111.33
2	Ab	306	THR	N-CA-C	9.92	123.33	111.33
2	AB	303	ASN	N-CA-C	-9.88	100.14	112.88
2	Ab	303	ASN	N-CA-C	-9.85	100.17	112.88
1	Aa	250	LEU	O-C-N	-9.83	112.22	121.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3153	0	3077	144	0
1	Aa	3225	0	3141	160	0
2	AB	3137	0	3143	170	0
2	Ab	3094	0	3102	176	0
3	AC	2988	0	3045	214	0
3	Ac	2988	0	3045	188	0
4	AD	1912	0	1860	141	0
4	Ad	1912	0	1860	150	0
5	AE	1451	0	1433	160	0
5	AI	217	0	234	41	0
5	Ae	1451	0	1433	162	0
5	Ai	207	0	226	37	0
6	AF	864	0	854	54	0
6	Af	864	0	854	47	0
7	AG	643	0	643	50	0
7	Ag	643	0	643	64	0
8	AH	562	0	543	24	0
8	Ah	562	0	543	26	0
9	AJ	332	0	324	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Aj	391	0	385	25	0
10	AK	401	0	396	46	0
10	Ak	401	0	396	46	0
11	AC	58	0	64	8	0
11	AG	51	0	82	16	0
11	Aa	23	0	20	7	0
11	Ac	35	0	44	4	0
11	Ag	51	0	82	1	0
12	AC	86	0	60	15	0
12	Ac	86	0	60	12	0
13	AC	23	0	23	19	0
13	Ac	23	0	23	21	0
14	AC	28	0	31	27	0
14	Ac	28	0	31	12	0
15	AD	43	0	31	12	0
15	Ad	43	0	31	11	0
16	AG	98	0	84	16	0
16	Aa	46	0	36	4	0
16	Ag	98	0	84	9	0
17	Ae	35	0	44	6	0
All	All	32253	0	32010	1809	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 28.

The worst 5 of 1809 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)
4:AD:124:CYS:SG	15:AD:401:HEC:HAC	1.40	1.60
2:AB:297:PRO:CG	2:AB:304:ASN:HD21	1.43	1.29
2:Ab:297:PRO:CG	2:Ab:304:ASN:HD21	1.43	1.28
3:AC:21:LEU:HD22	14:AC:406:UQ6:C3M	1.66	1.24
4:AD:124:CYS:SG	15:AD:401:HEC:CAC	2.28	1.21

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	397/480 (83%)	388 (98%)	9 (2%)	0	100	100
1	Aa	408/480 (85%)	395 (97%)	13 (3%)	0	100	100
2	AB	416/453 (92%)	406 (98%)	10 (2%)	0	100	100
2	Ab	408/453 (90%)	396 (97%)	12 (3%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	368 (99%)	3 (1%)	0	100	100
4	AD	238/325 (73%)	230 (97%)	8 (3%)	0	100	100
4	Ad	238/325 (73%)	225 (94%)	13 (6%)	0	100	100
5	AE	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
5	AI	26/274 (10%)	23 (88%)	3 (12%)	0	100	100
5	Ae	184/274 (67%)	171 (93%)	13 (7%)	0	100	100
5	Ai	24/274 (9%)	23 (96%)	1 (4%)	0	100	100
6	AF	96/111 (86%)	96 (100%)	0	0	100	100
6	Af	96/111 (86%)	96 (100%)	0	0	100	100
7	AG	74/82 (90%)	74 (100%)	0	0	100	100
7	Ag	74/82 (90%)	74 (100%)	0	0	100	100
8	AH	66/89 (74%)	66 (100%)	0	0	100	100
8	Ah	66/89 (74%)	66 (100%)	0	0	100	100
9	AJ	39/64 (61%)	39 (100%)	0	0	100	100
9	Aj	46/64 (72%)	46 (100%)	0	0	100	100
10	AK	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
10	Ak	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
All	All	3916/5178 (76%)	3811 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	341/398 (86%)	339 (99%)	2 (1%)	78	80
1	Aa	349/398 (88%)	347 (99%)	2 (1%)	78	80
2	AB	328/356 (92%)	327 (100%)	1 (0%)	86	84
2	Ab	324/356 (91%)	323 (100%)	1 (0%)	86	84
3	AC	325/333 (98%)	324 (100%)	1 (0%)	86	84
3	Ac	325/333 (98%)	324 (100%)	1 (0%)	86	84
4	AD	205/260 (79%)	205 (100%)	0	100	100
4	Ad	205/260 (79%)	205 (100%)	0	100	100
5	AE	158/224 (70%)	157 (99%)	1 (1%)	78	80
5	AI	23/224 (10%)	22 (96%)	1 (4%)	26	51
5	Ae	158/224 (70%)	157 (99%)	1 (1%)	78	80
5	Ai	22/224 (10%)	20 (91%)	2 (9%)	9	30
6	AF	90/99 (91%)	90 (100%)	0	100	100
6	Af	90/99 (91%)	90 (100%)	0	100	100
7	AG	69/74 (93%)	69 (100%)	0	100	100
7	Ag	69/74 (93%)	69 (100%)	0	100	100
8	AH	65/83 (78%)	65 (100%)	0	100	100
8	Ah	65/83 (78%)	65 (100%)	0	100	100
9	AJ	33/55 (60%)	33 (100%)	0	100	100
9	Aj	39/55 (71%)	39 (100%)	0	100	100
10	AK	39/46 (85%)	39 (100%)	0	100	100
10	Ak	39/46 (85%)	39 (100%)	0	100	100
All	All	3361/4304 (78%)	3348 (100%)	13 (0%)	81	83

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	249	HIS
2	Ab	435	LYS
5	Ai	64	LEU
5	Ae	135	GLN
5	Ai	45	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	55	ASN
10	Ak	16	ASN
1	Aa	240	GLN
7	Ag	65	GLN
4	Ad	190	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](#)

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](#)

22 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
14	UQ6	AC	406	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
11	3PE	Aa	501	-	22,22,50	1.37	2 (9%)	25,27,55	1.20	2 (8%)
16	CDL	AG	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.33	6 (12%)
11	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.21	3 (8%)
12	HEM	AC	403	3	50,50,50	1.34	6 (12%)	66,82,82	1.66	16 (24%)
12	HEM	Ac	402	3	50,50,50	1.32	5 (10%)	66,82,82	1.66	16 (24%)
15	HEC	AD	401	4	50,50,50	1.72	5 (10%)	68,82,82	1.35	7 (10%)
12	HEM	AC	402	3	50,50,50	1.31	7 (14%)	66,82,82	1.68	15 (22%)
16	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.35	6 (12%)
11	3PE	AG	103	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
13	U10	Ac	404	-	23,23,63	1.24	3 (13%)	28,31,79	2.08	7 (25%)
13	U10	AC	405	-	23,23,63	1.24	3 (13%)	28,31,79	2.10	7 (25%)
15	HEC	Ad	401	4	50,50,50	1.73	5 (10%)	68,82,82	1.36	8 (11%)
17	PC1	Ae	301	-	34,34,53	1.17	2 (5%)	40,42,61	1.18	4 (10%)
11	3PE	AC	401	-	22,22,50	0.47	0	25,27,55	0.73	1 (4%)
16	CDL	Aa	502	-	45,45,99	1.34	4 (8%)	51,57,111	1.36	6 (11%)
11	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.29	0
14	UQ6	Ac	405	-	28,28,43	0.81	1 (3%)	33,37,55	0.75	0
11	3PE	AC	404	-	34,34,50	1.10	2 (5%)	37,39,55	1.14	3 (8%)
16	CDL	AG	102	-	55,55,99	1.20	4 (7%)	61,67,111	1.25	6 (9%)
16	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
12	HEM	Ac	401	3	50,50,50	1.30	7 (14%)	66,82,82	1.67	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	UQ6	AC	406	-	-	13/21/21/39	0/1/1/1
11	3PE	Aa	501	-	-	7/26/26/54	-
16	CDL	AG	101	-	-	8/52/52/110	-
11	3PE	Ac	403	-	-	3/38/38/54	-
12	HEM	AC	403	3	-	8/14/54/54	-
15	HEC	AD	401	4	1/1/3/7	0/14/54/54	-
12	HEM	Ac	402	3	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	AC	402	3	-	9/14/54/54	-
16	CDL	Ag	101	-	-	7/52/52/110	-
11	3PE	AG	103	-	-	9/54/54/54	-
13	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
13	U10	AC	405	-	-	6/15/39/87	0/1/1/1
15	HEC	Ad	401	4	1/1/3/7	0/14/54/54	-
17	PC1	Ae	301	-	-	7/38/38/57	-
11	3PE	AC	401	-	-	7/26/26/54	-
16	CDL	Aa	502	-	-	13/56/56/110	-
11	3PE	Ag	103	-	-	10/54/54/54	-
14	UQ6	Ac	405	-	-	13/21/21/39	0/1/1/1
11	3PE	AC	404	-	-	1/38/38/54	-
16	CDL	AG	102	-	-	15/66/66/110	-
16	CDL	Ag	102	-	-	13/66/66/110	-
12	HEM	Ac	401	3	-	9/14/54/54	-

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Ad	401	HEC	C3D-C2D	8.07	1.53	1.36
15	AD	401	HEC	C3D-C2D	7.98	1.53	1.36
17	Ae	301	PC1	O31-C31	4.33	1.46	1.33
16	Aa	502	CDL	OA8-CA7	4.24	1.45	1.33
16	Aa	502	CDL	OB8-CB7	4.24	1.45	1.33

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AC	405	U10	C6-C1-C2	7.80	125.35	119.18
13	Ac	404	U10	C6-C1-C2	7.71	125.28	119.18
15	Ad	401	HEC	C1D-ND-C4D	6.43	111.71	105.07
15	AD	401	HEC	C1D-ND-C4D	6.42	111.70	105.07
12	AC	402	HEM	CHC-C4B-NB	4.75	129.58	124.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	AD	401	HEC	NA
15	Ad	401	HEC	NA

5 of 172 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	401	3PE	C11-O13-P-O12
11	AC	401	3PE	O13-C11-C12-N
11	AG	103	3PE	C1-O11-P-O12
11	AG	103	3PE	C1-O11-P-O13
11	AG	103	3PE	C1-O11-P-O14

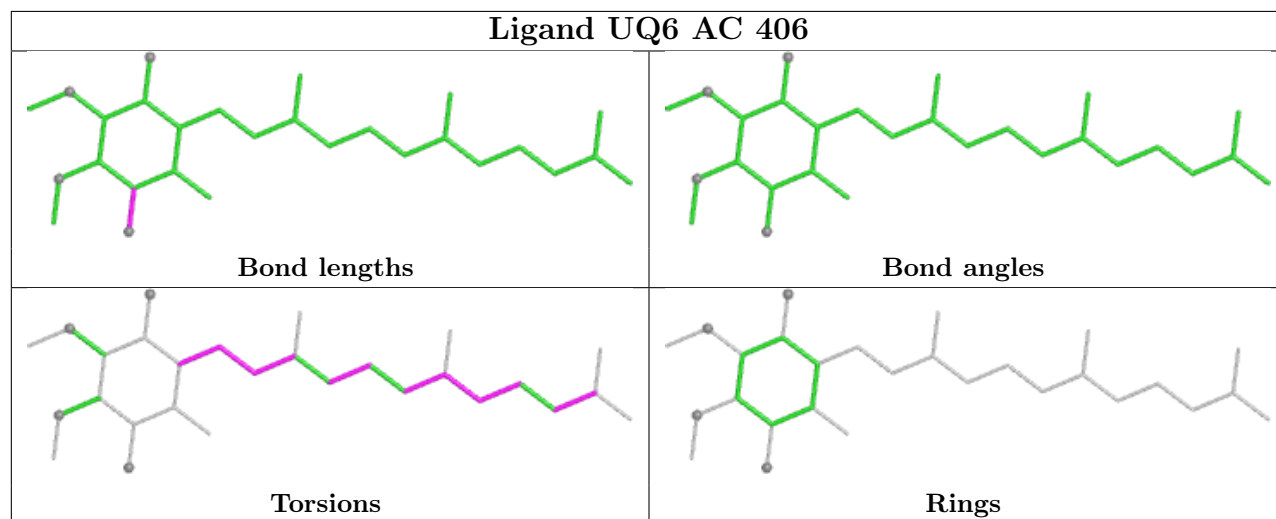
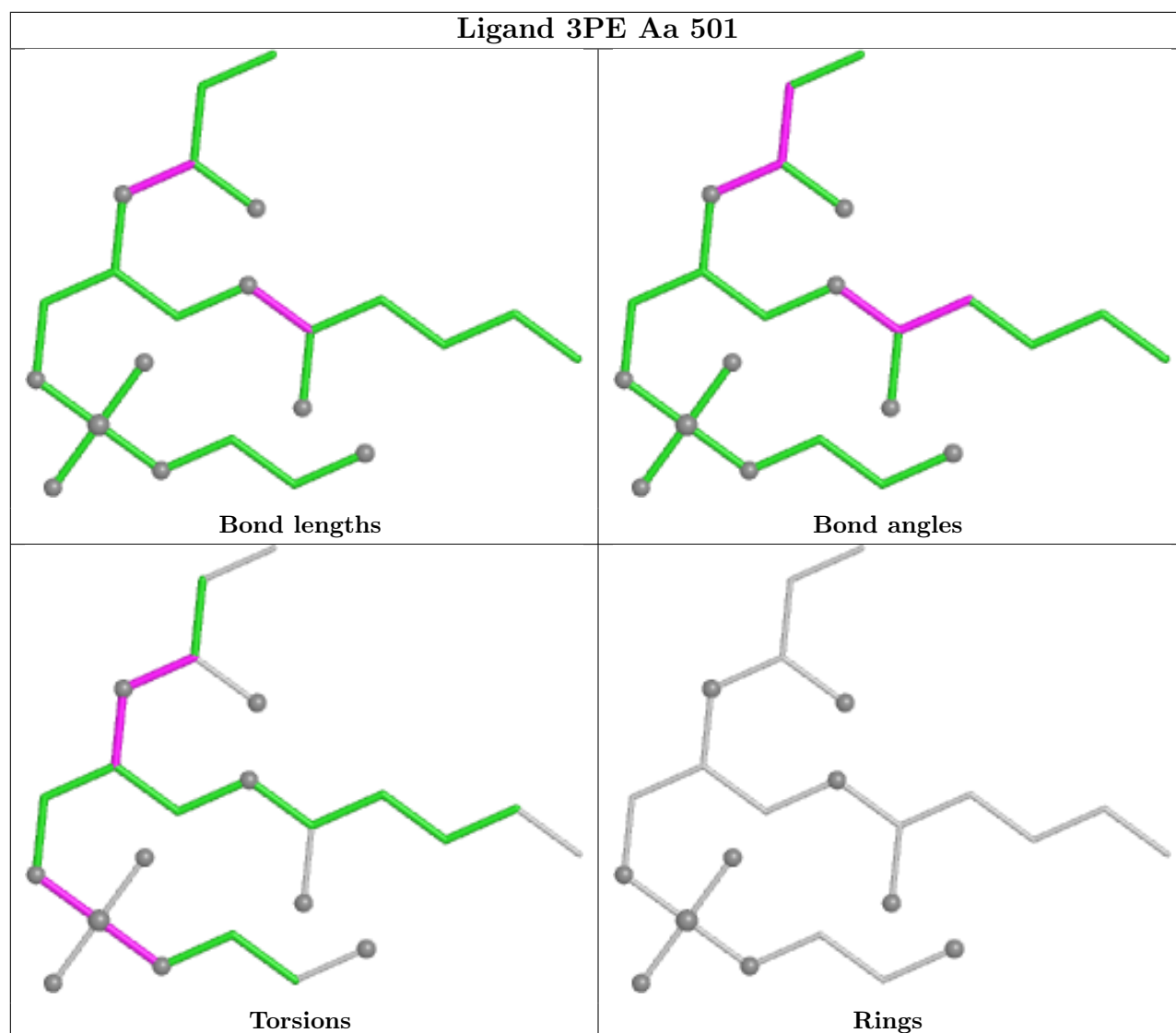
There are no ring outliers.

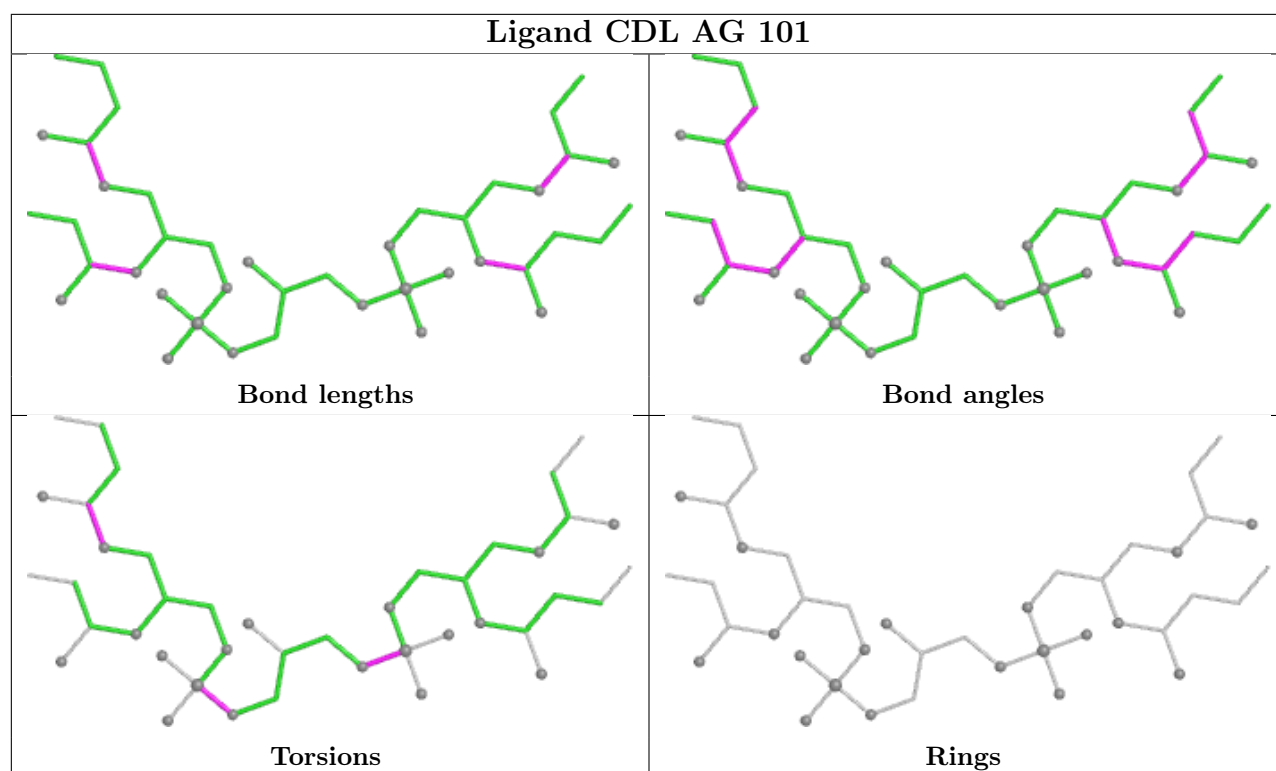
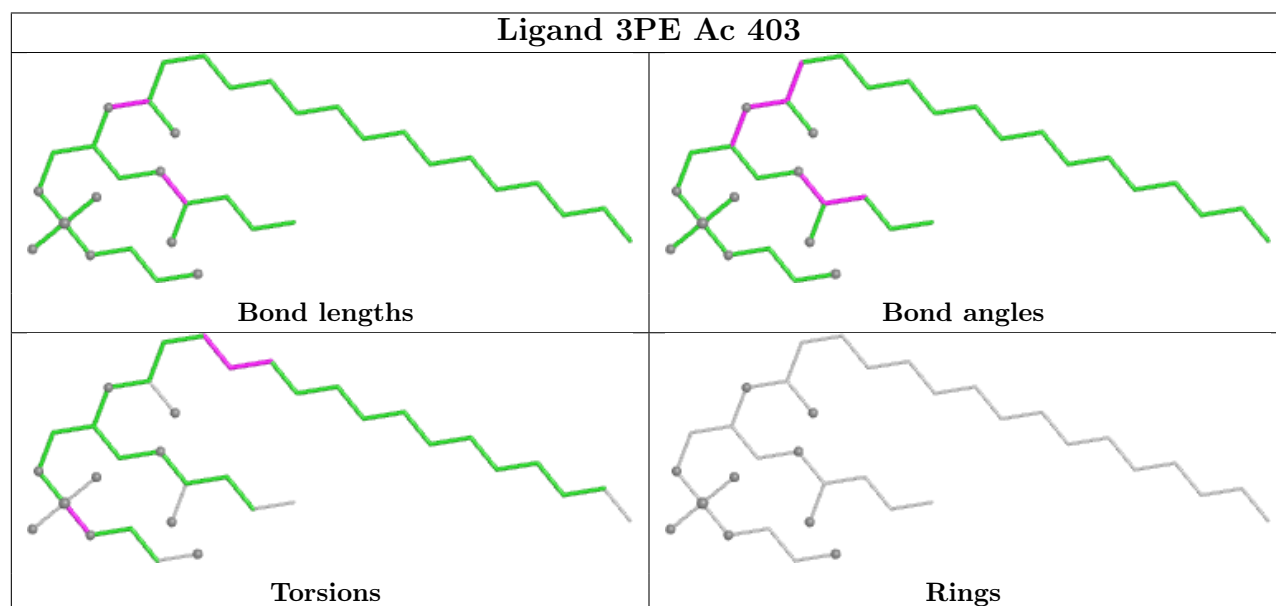
22 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	AC	406	UQ6	27	0
11	Aa	501	3PE	7	0
16	AG	101	CDL	8	0
11	Ac	403	3PE	4	0
12	AC	403	HEM	8	0
12	Ac	402	HEM	9	0
15	AD	401	HEC	12	0
12	AC	402	HEM	7	0
16	Ag	101	CDL	4	0
11	AG	103	3PE	16	0
13	Ac	404	U10	21	0
13	AC	405	U10	19	0
15	Ad	401	HEC	11	0
17	Ae	301	PC1	6	0
11	AC	401	3PE	2	0
16	Aa	502	CDL	4	0
11	Ag	103	3PE	1	0
14	Ac	405	UQ6	12	0
11	AC	404	3PE	6	0
16	AG	102	CDL	8	0
16	Ag	102	CDL	5	0
12	Ac	401	HEM	3	0

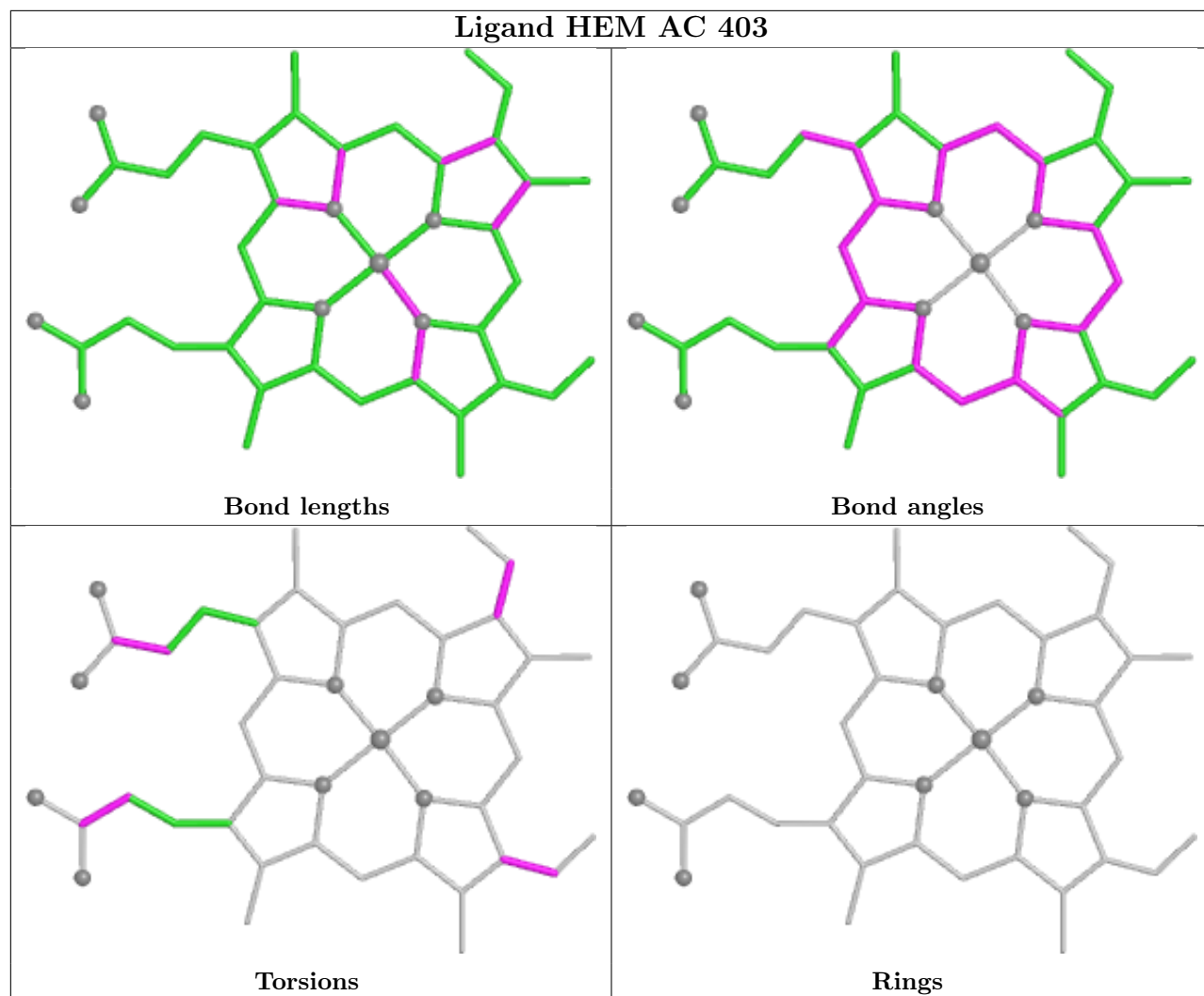
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

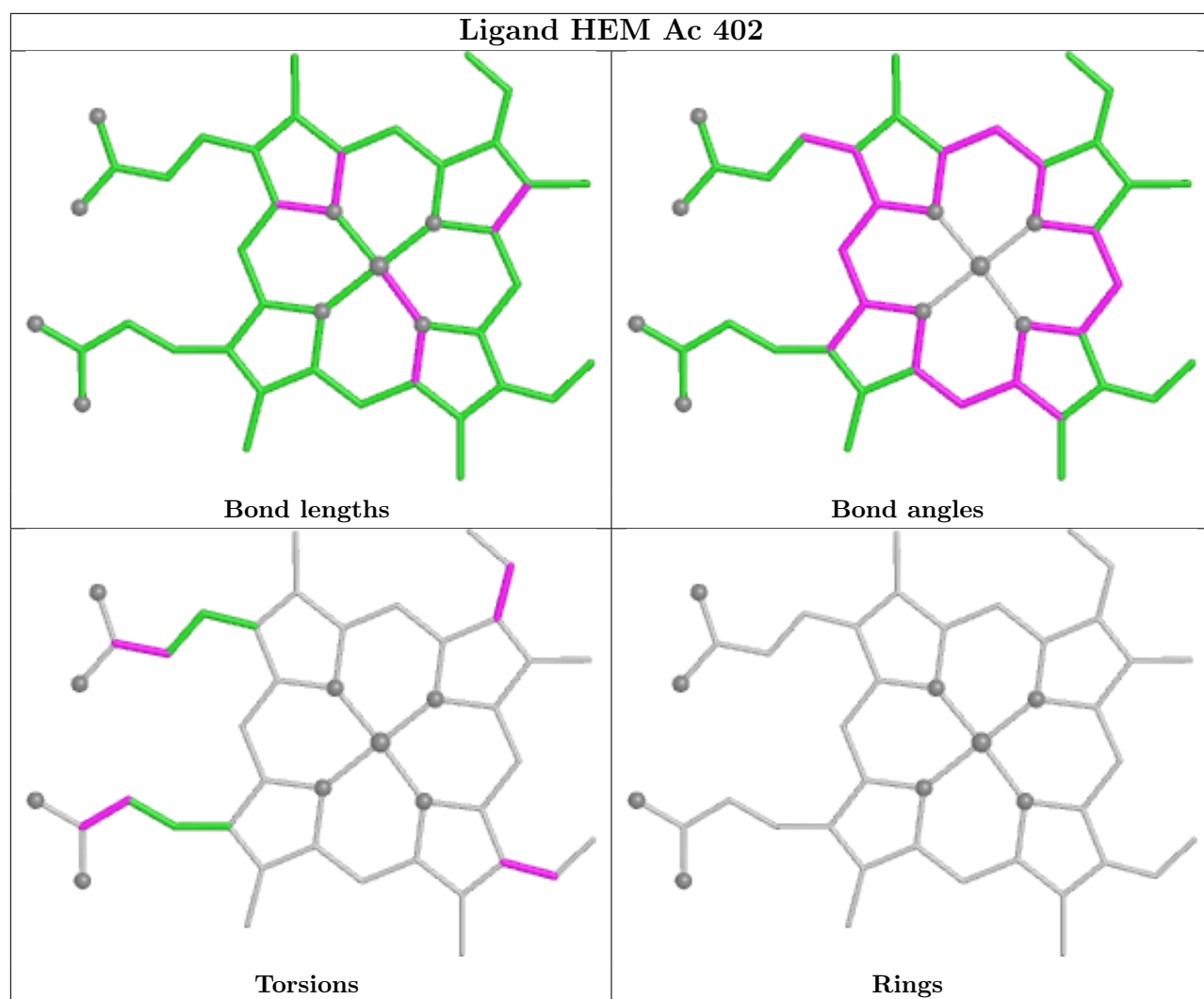
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



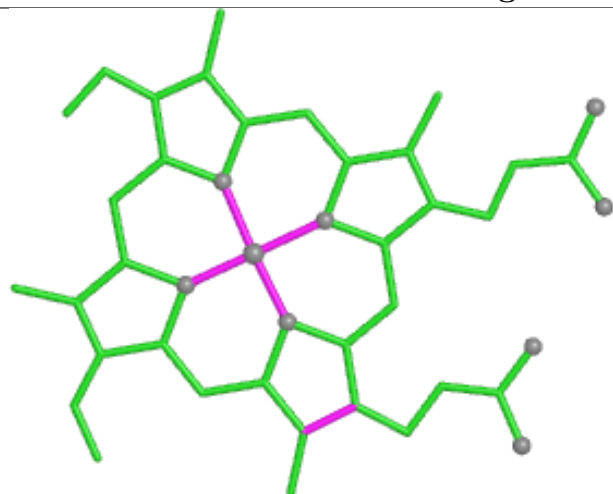


Ligand HEM AC 403

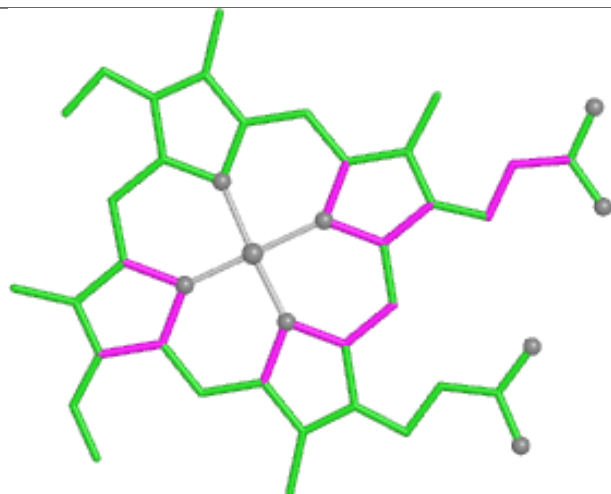




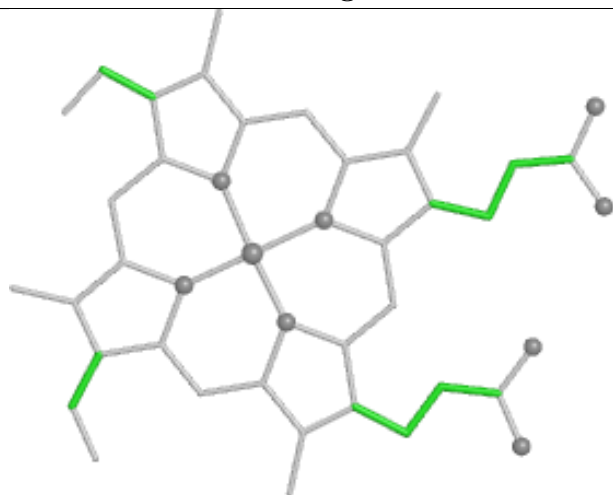
Ligand HEC AD 401



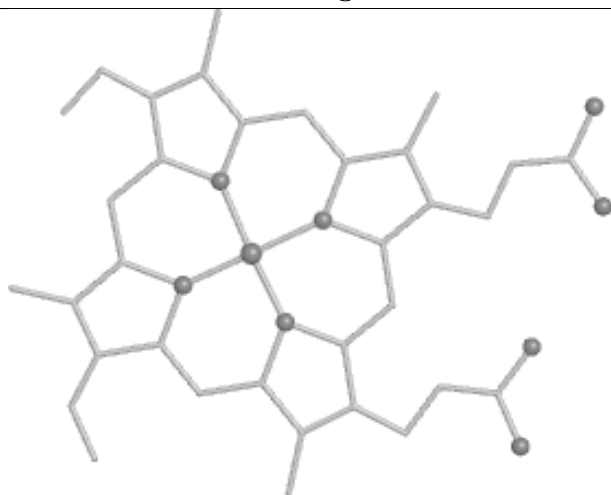
Bond lengths



Bond angles

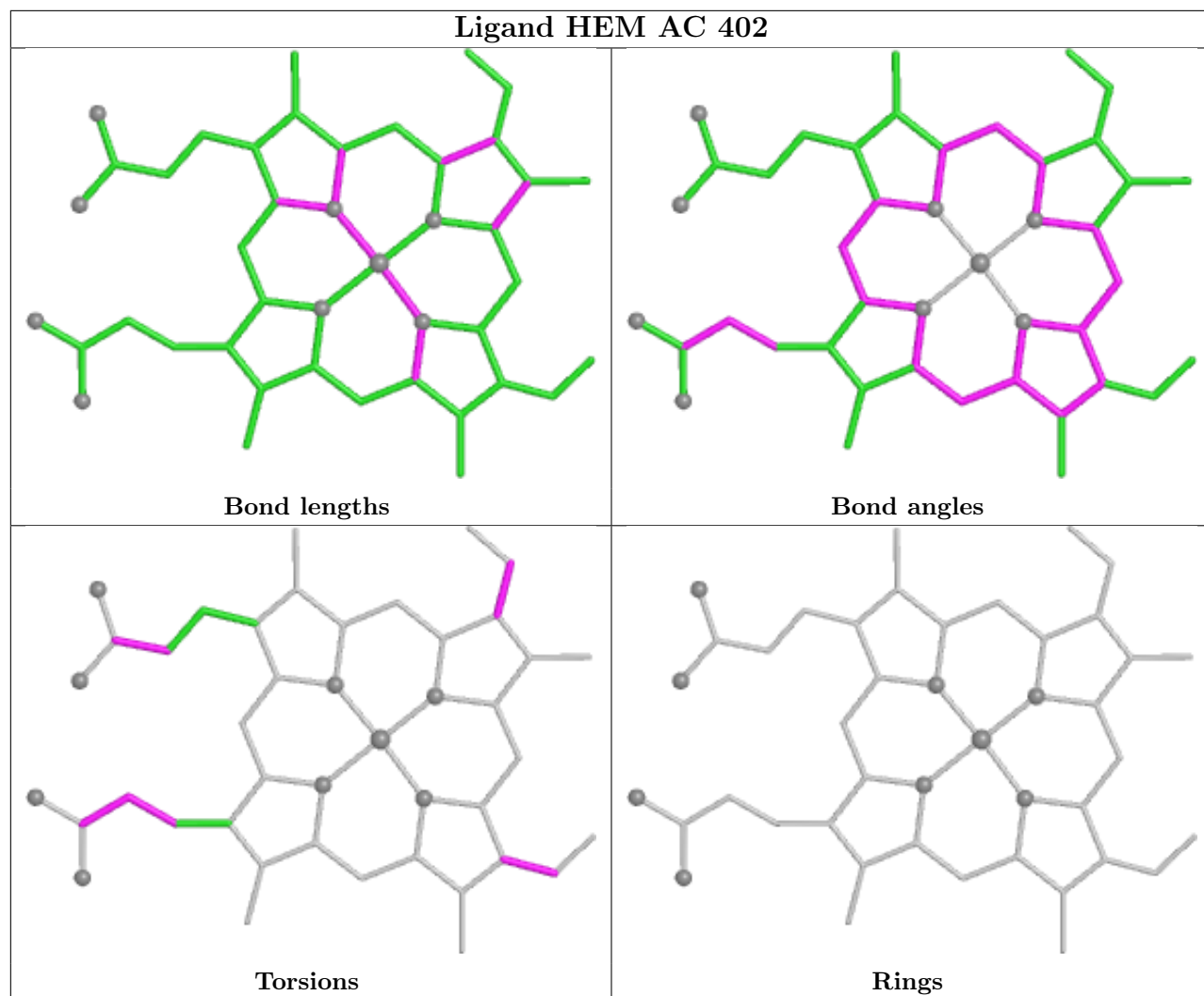


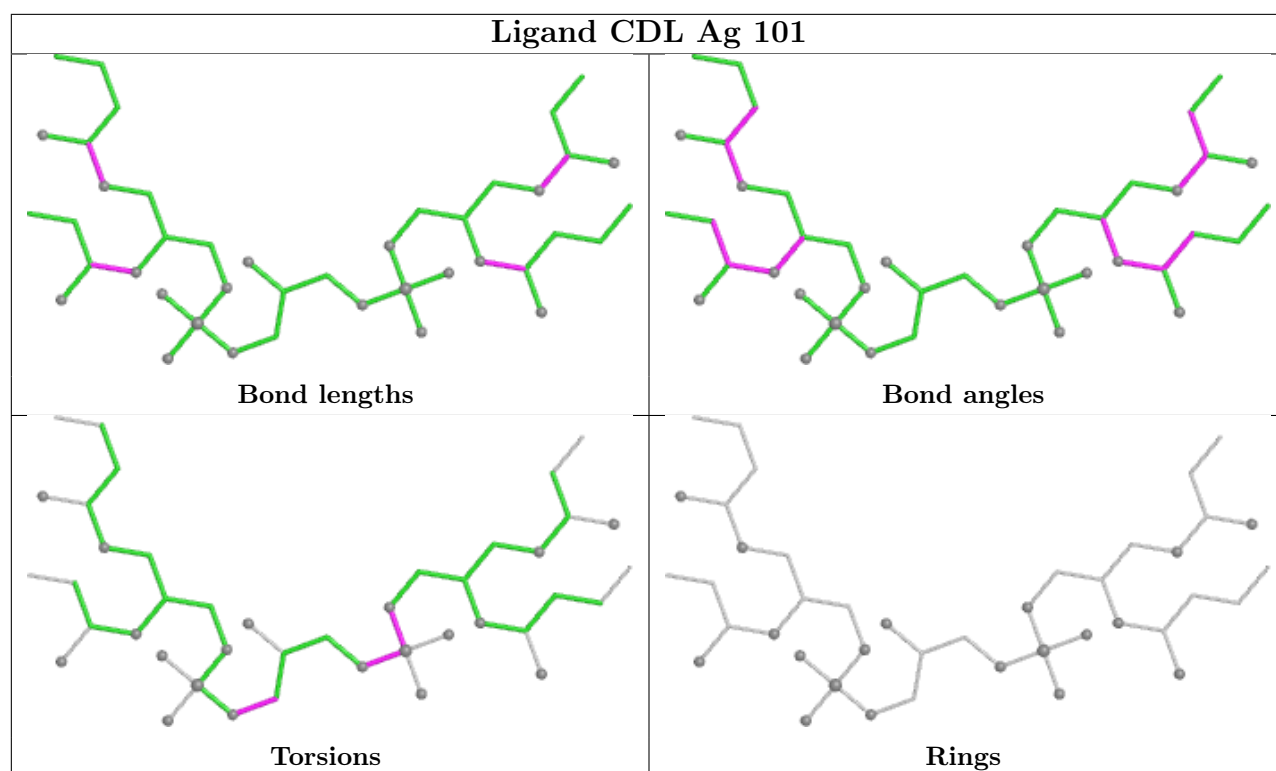
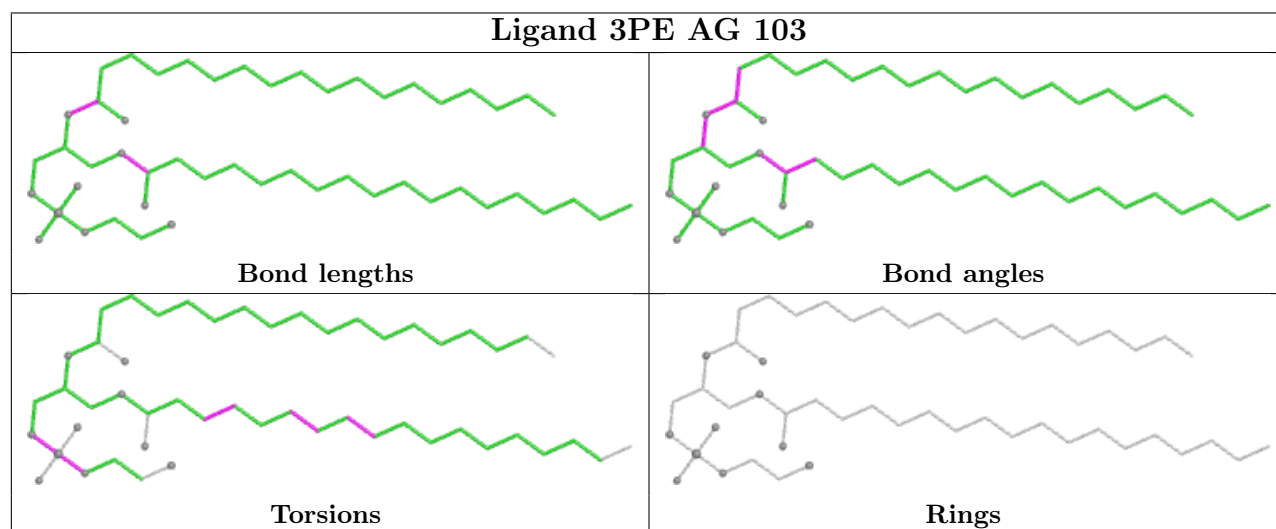
Torsions

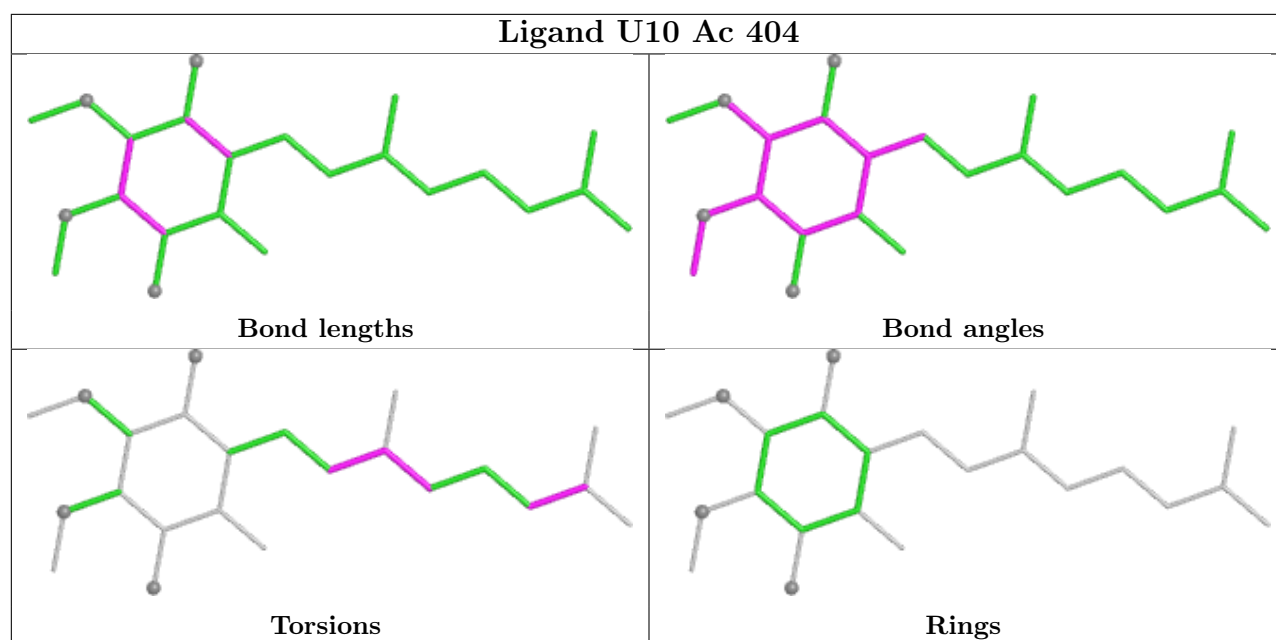
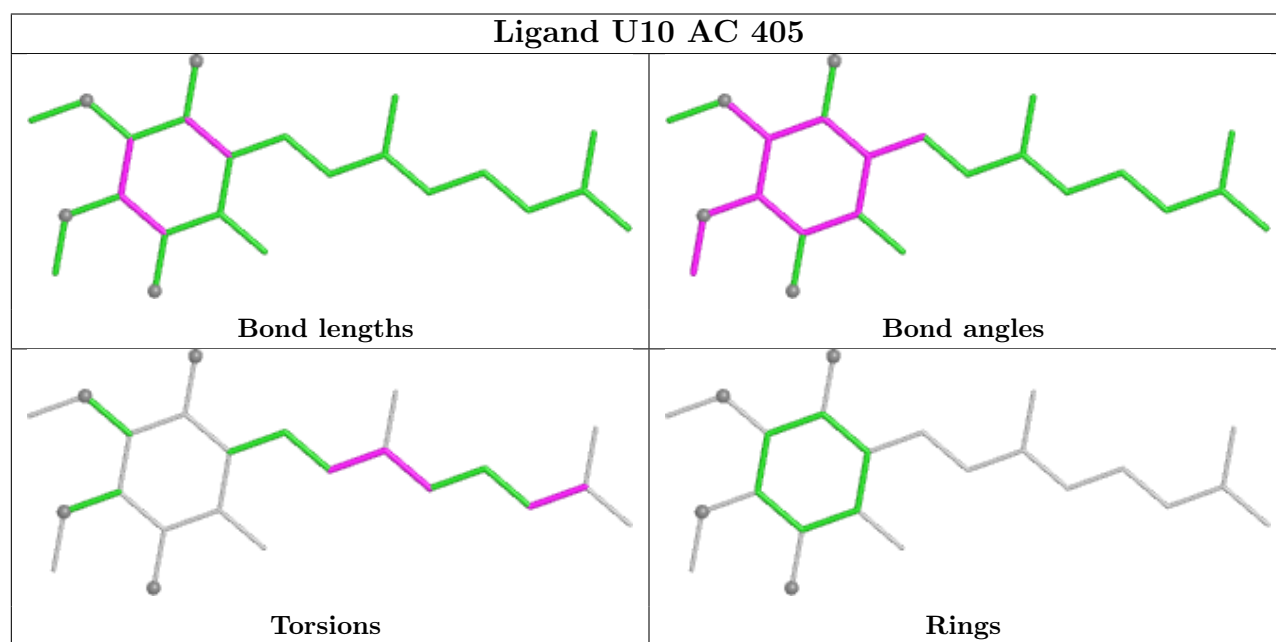


Rings

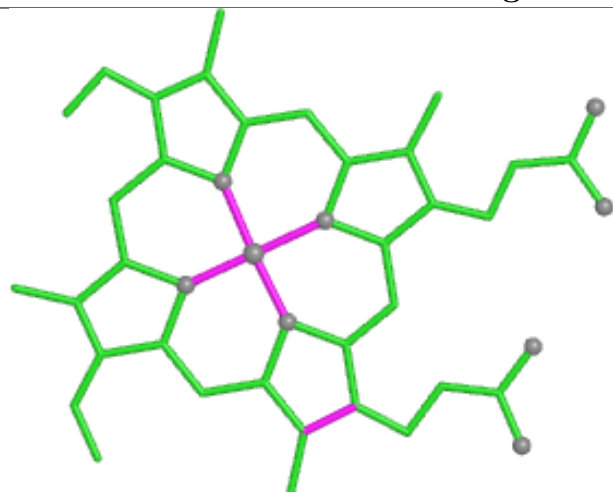
Ligand HEM AC 402



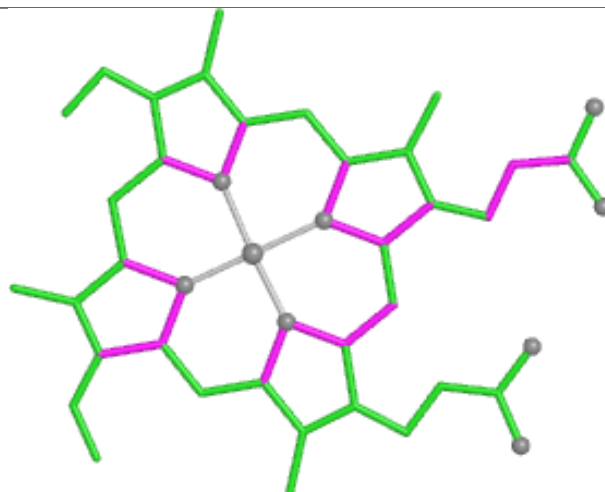




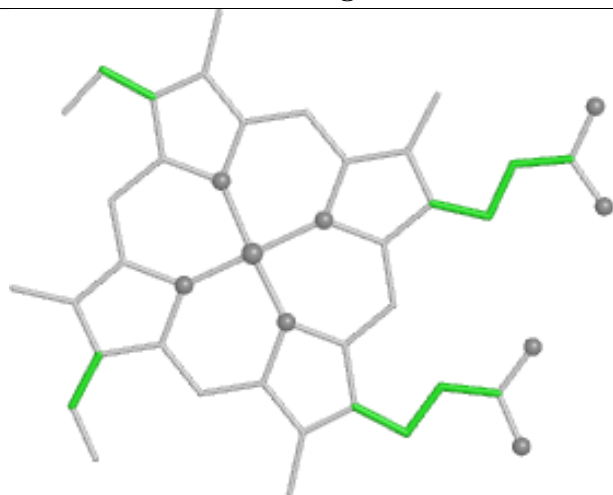
Ligand HEC Ad 401



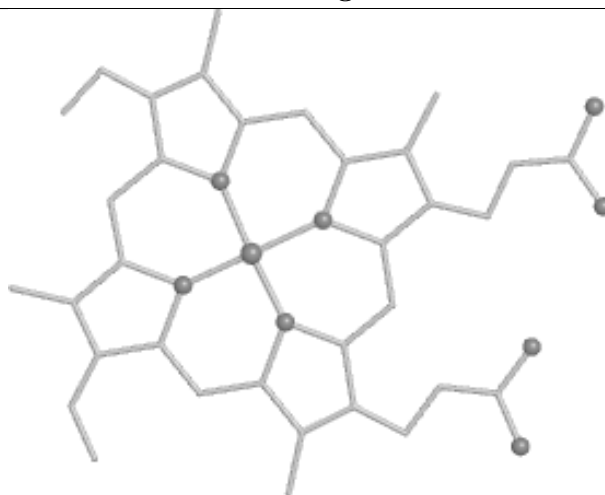
Bond lengths



Bond angles

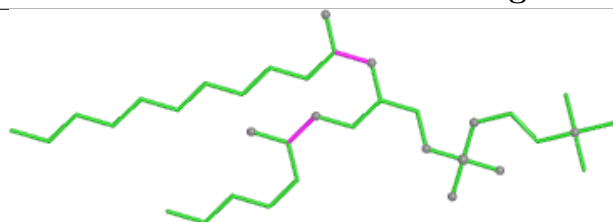


Torsions

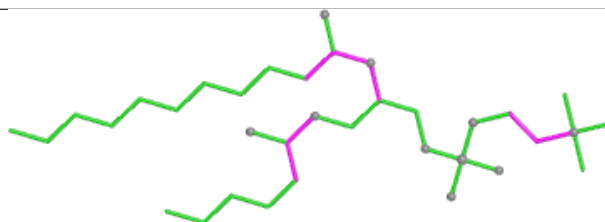


Rings

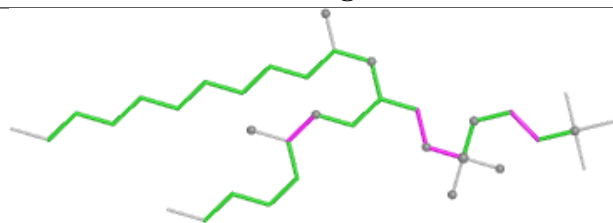
Ligand PC1 Ae 301



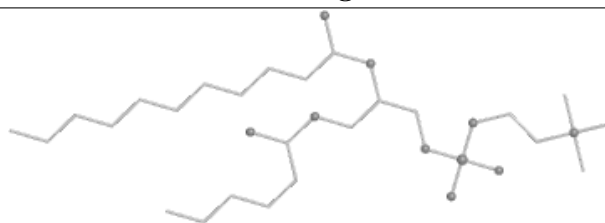
Bond lengths



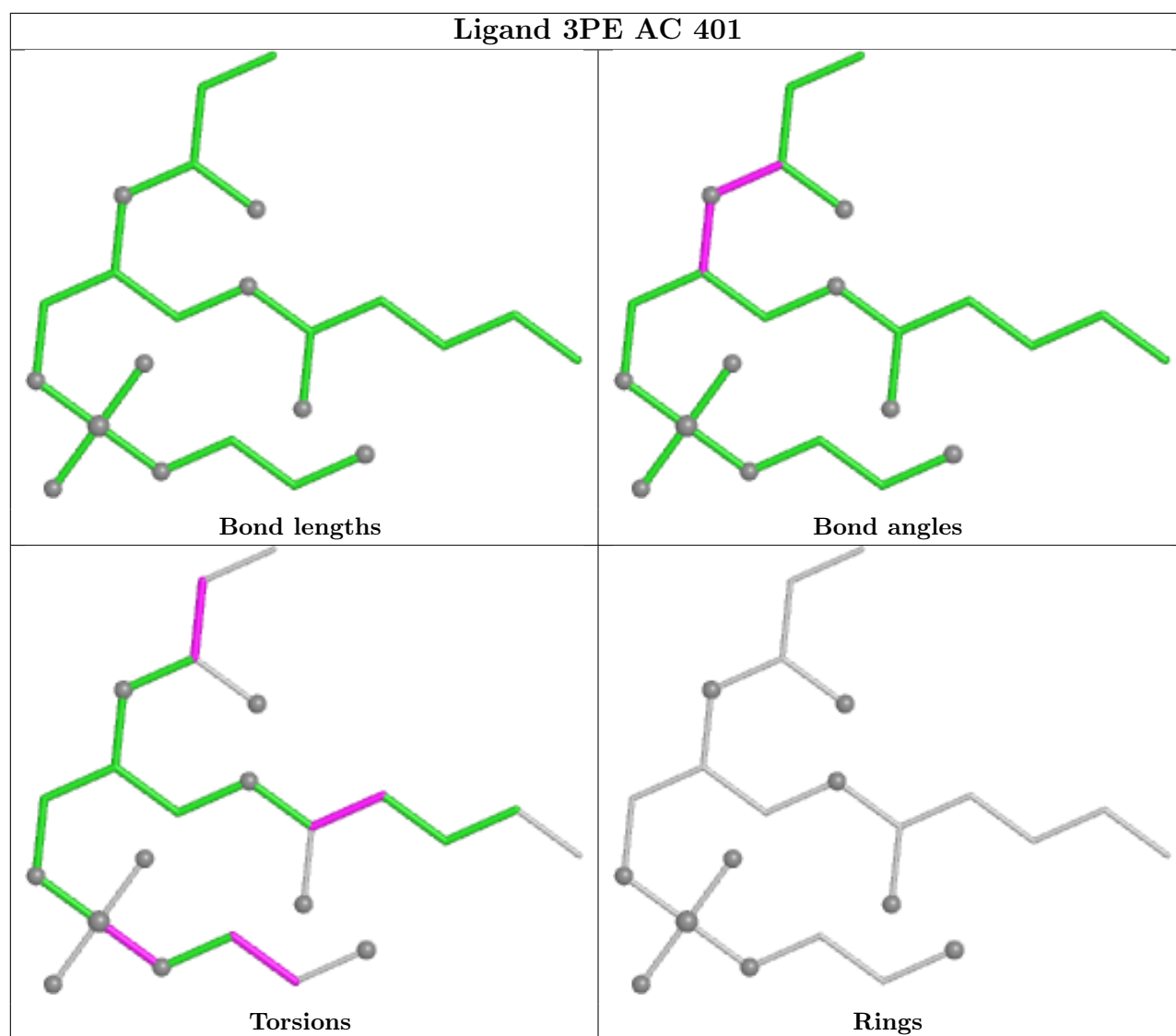
Bond angles

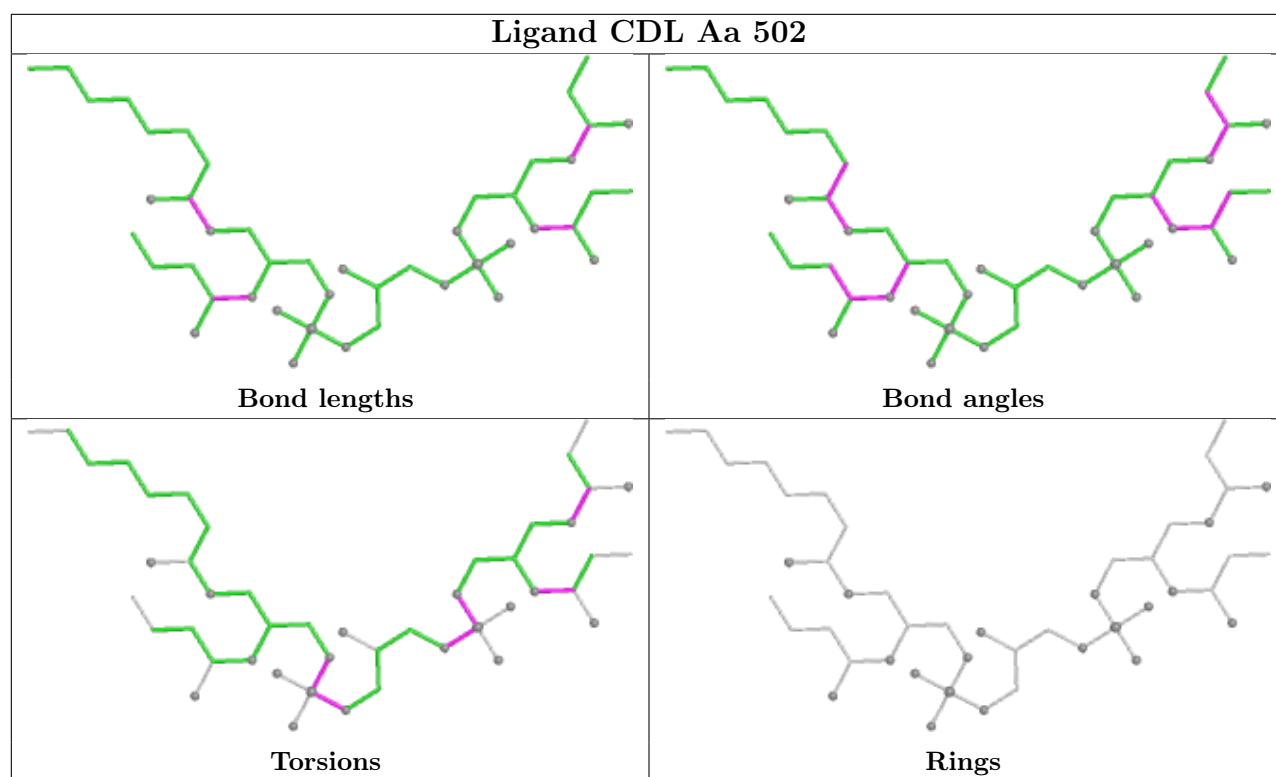
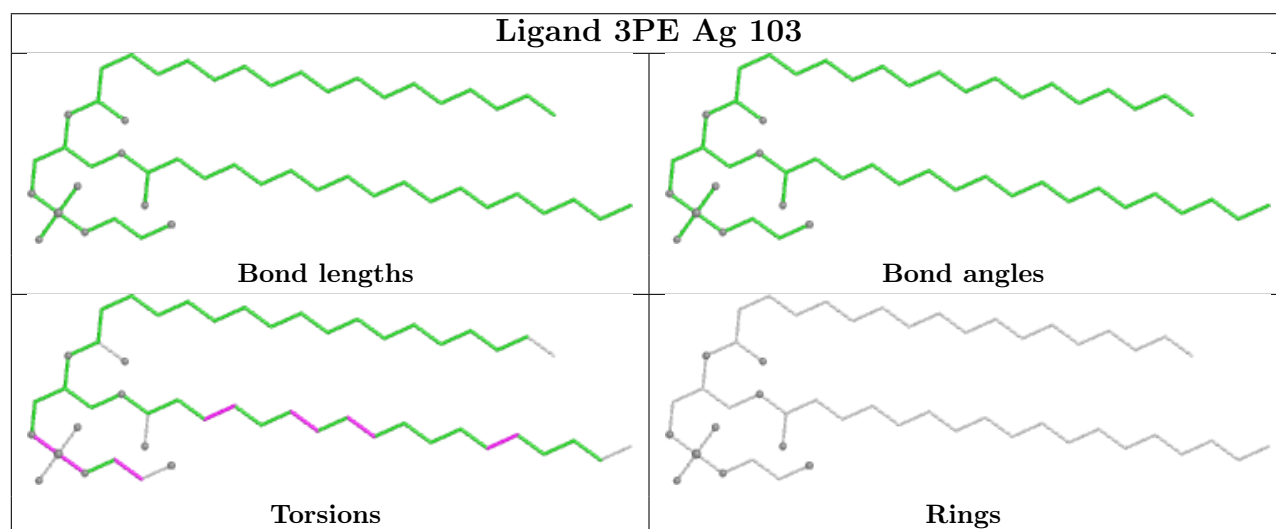


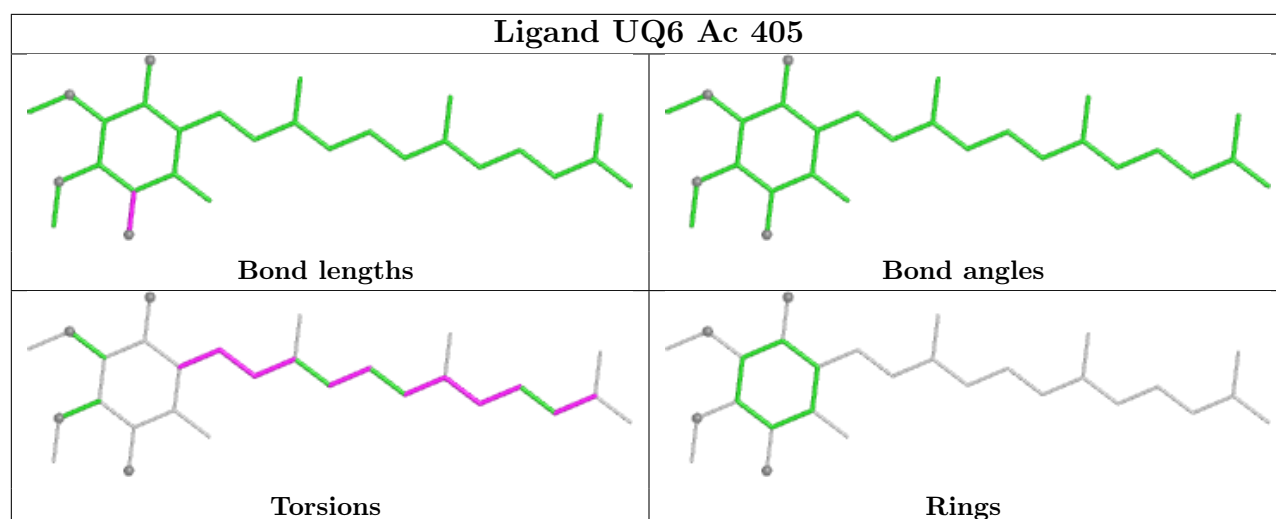
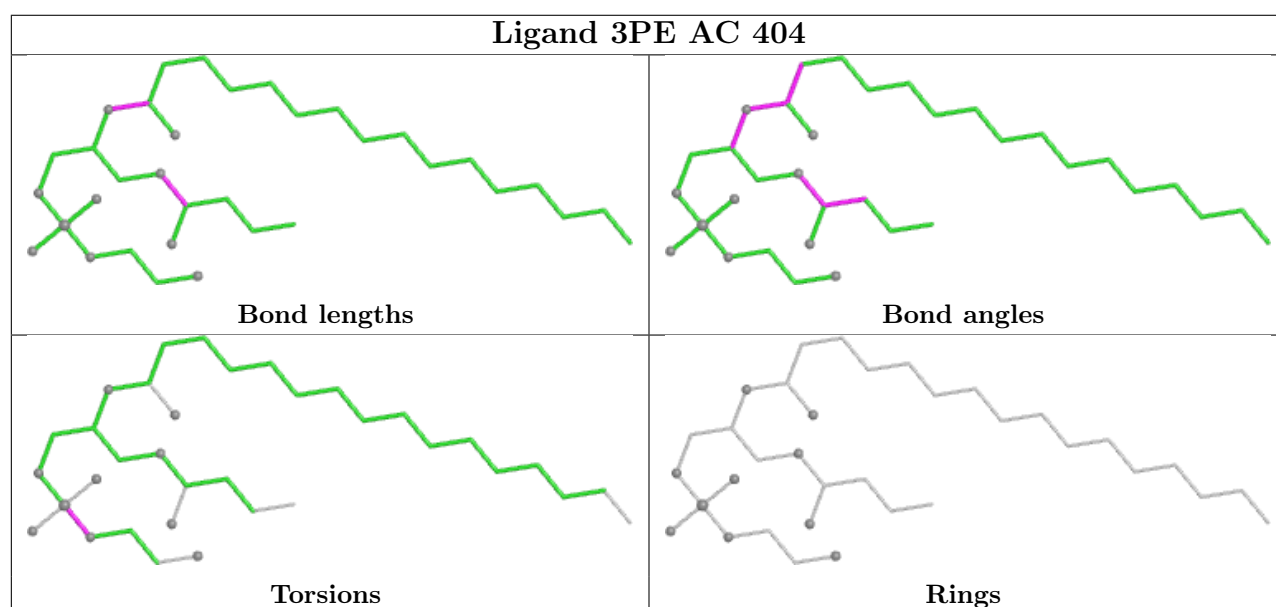
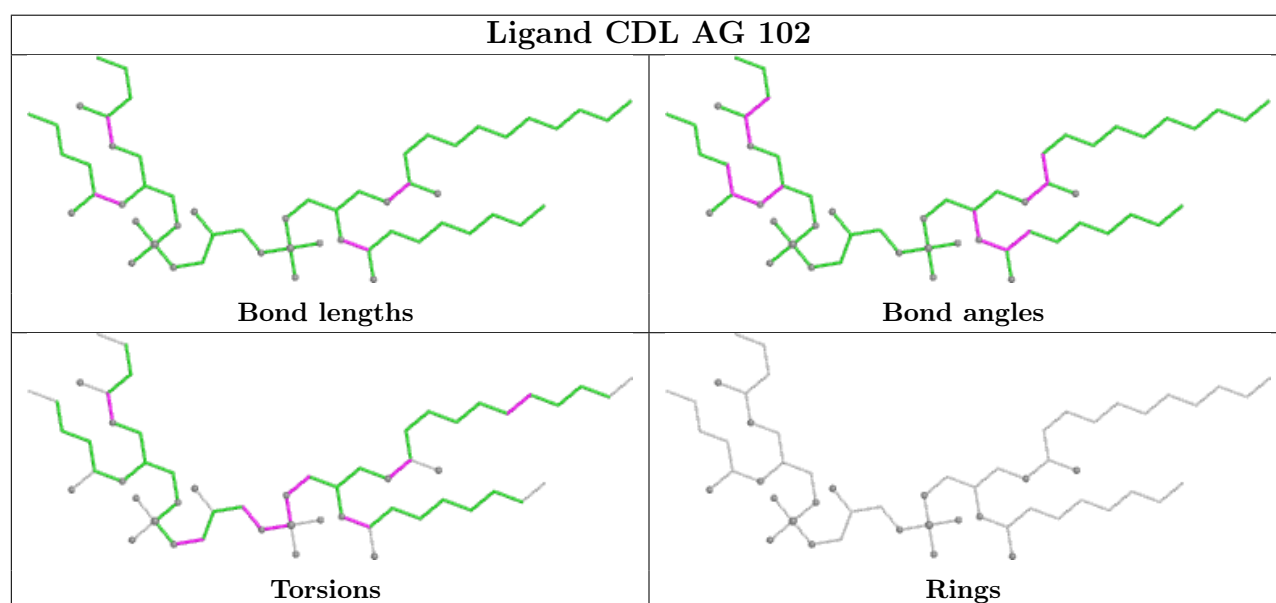
Torsions

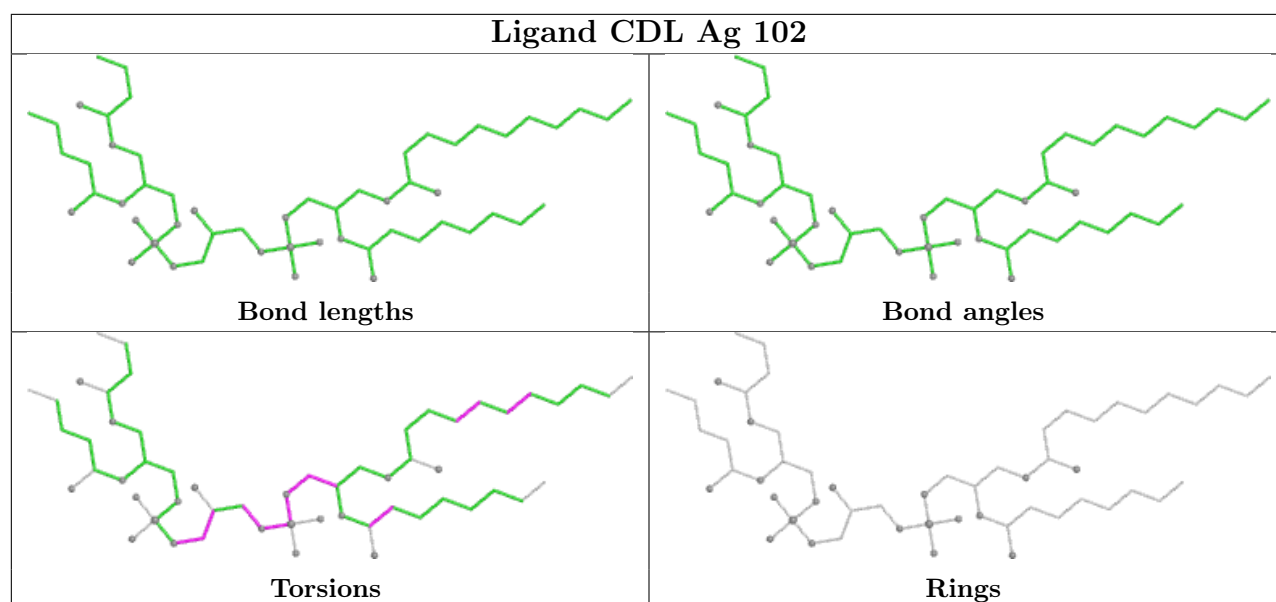
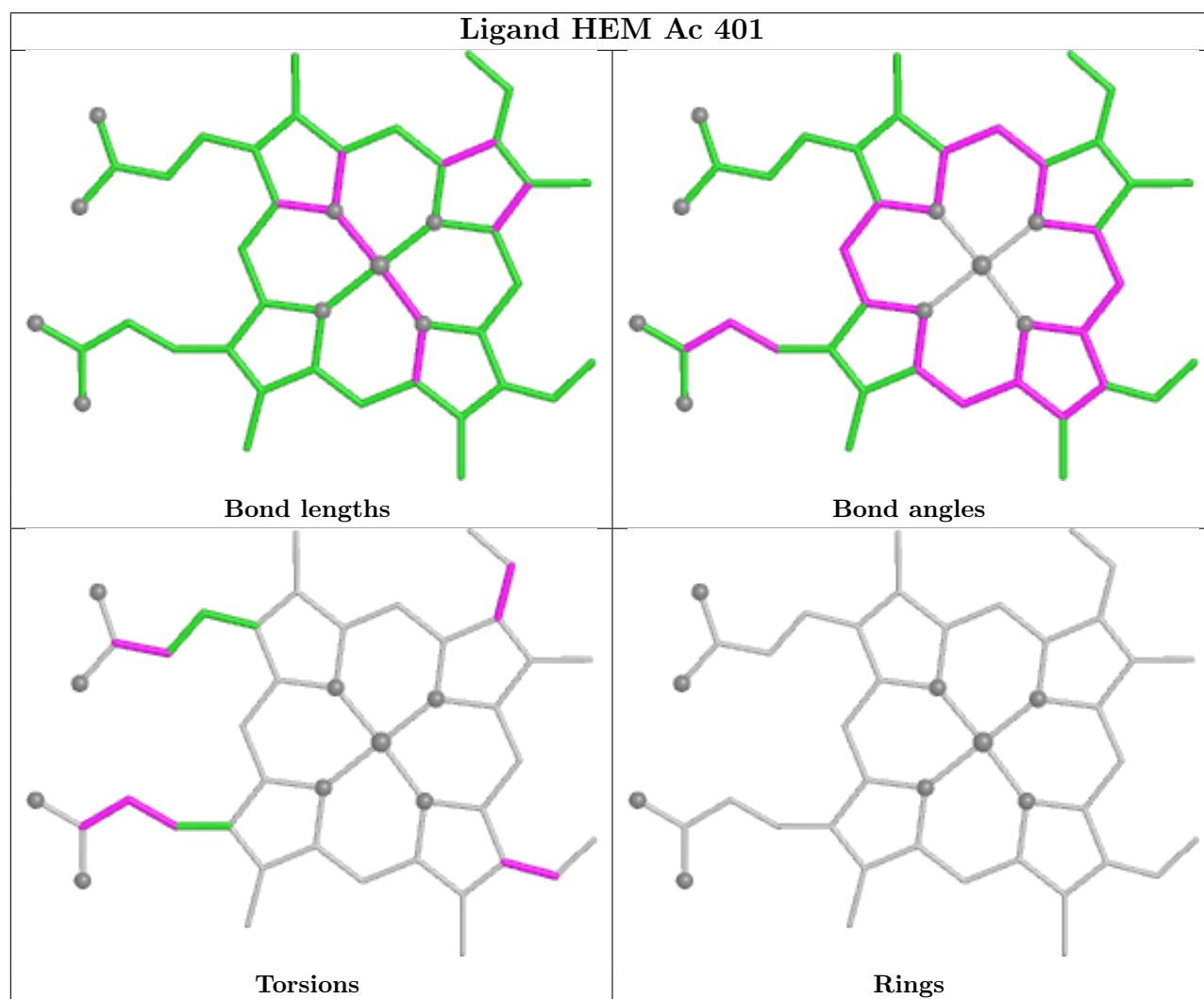


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

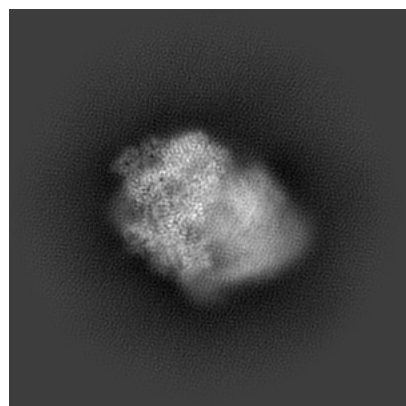
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35316. These allow visual inspection of the internal detail of the map and identification of artifacts.

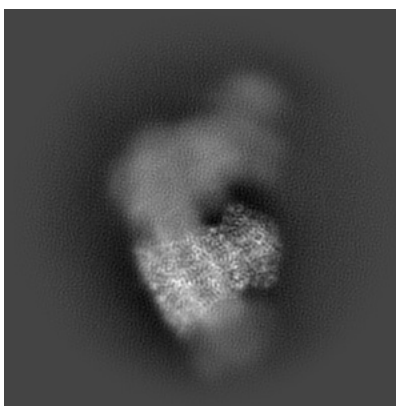
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

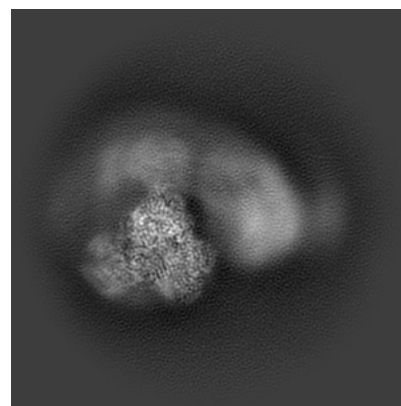
6.1.1 Primary map



X

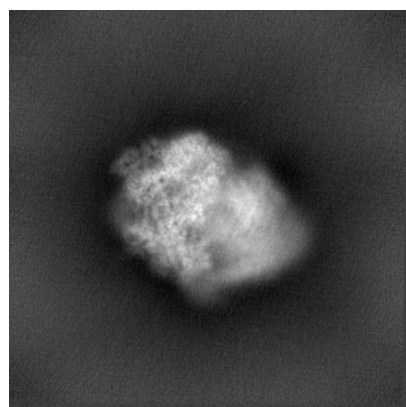


Y

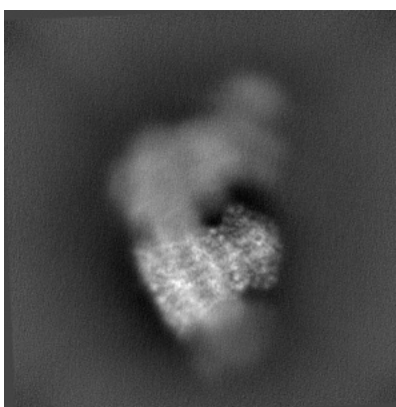


Z

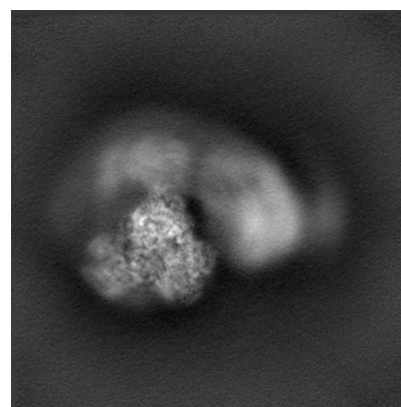
6.1.2 Raw map



X



Y

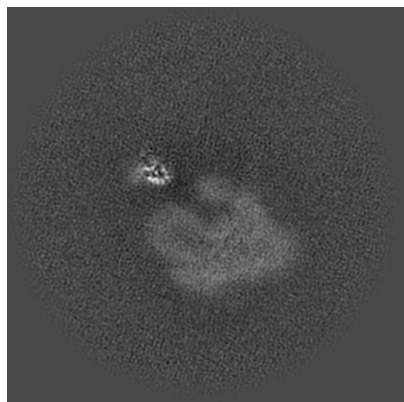


Z

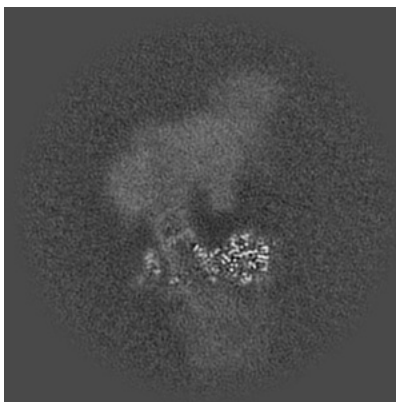
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

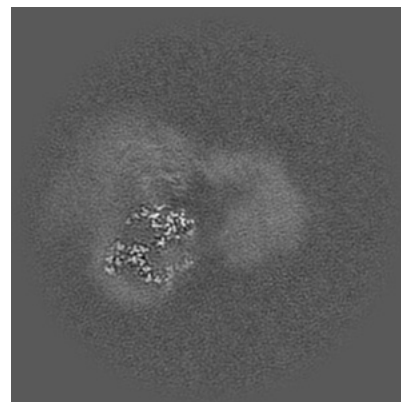
6.2.1 Primary map



X Index: 192

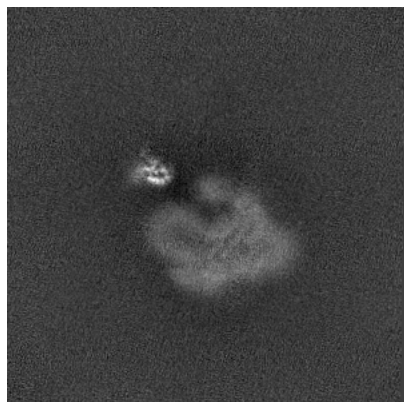


Y Index: 192

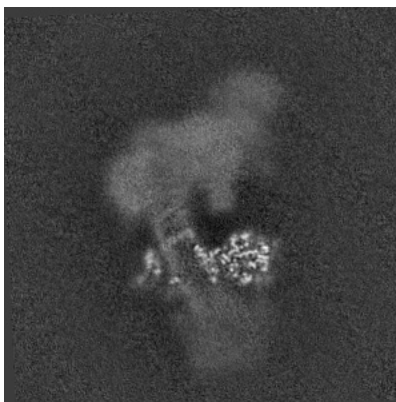


Z Index: 192

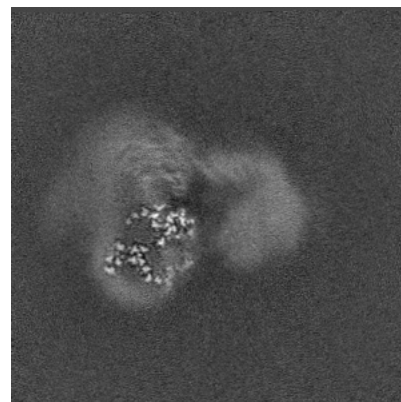
6.2.2 Raw map



X Index: 192



Y Index: 192

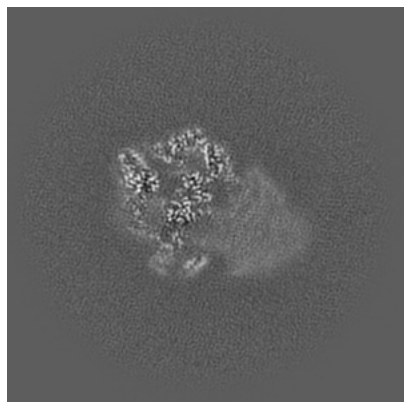


Z Index: 192

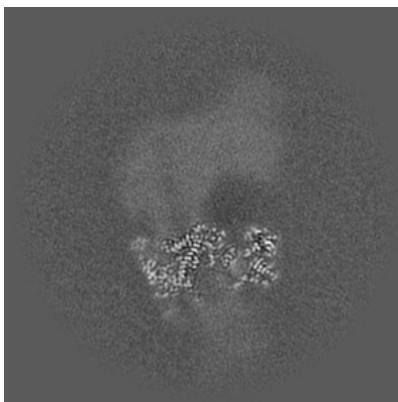
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

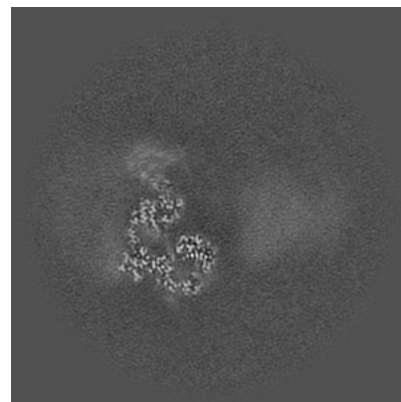
6.3.1 Primary map



X Index: 148

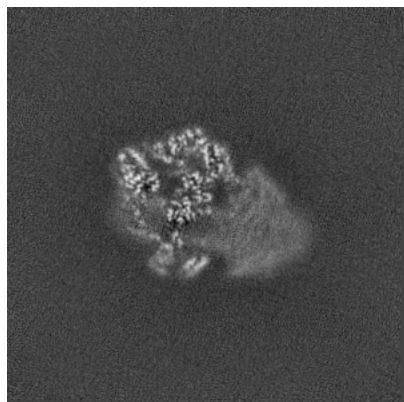


Y Index: 168

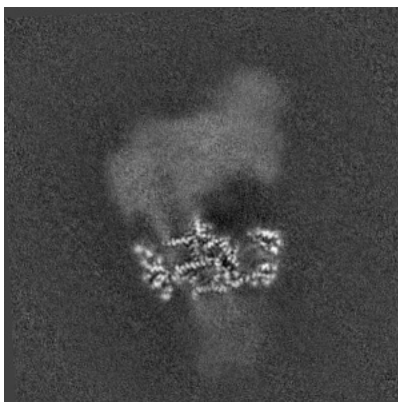


Z Index: 223

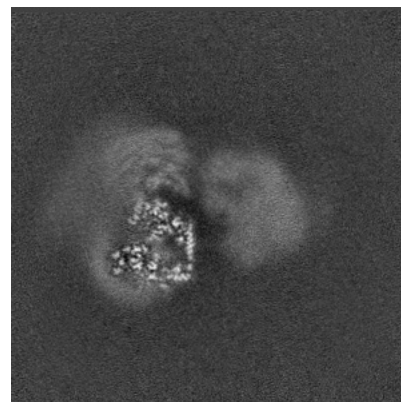
6.3.2 Raw map



X Index: 148



Y Index: 177

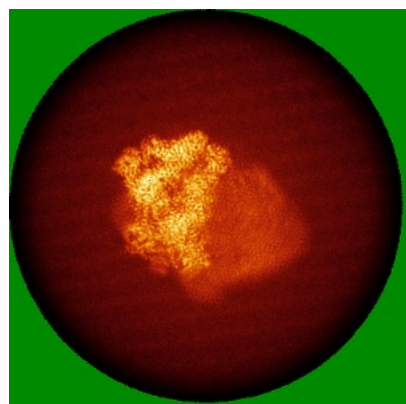


Z Index: 200

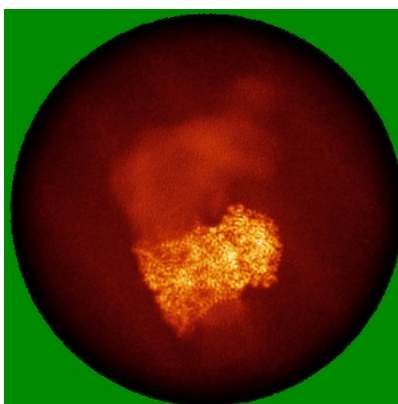
The images above show the largest variance slices of the map in three orthogonal directions.

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

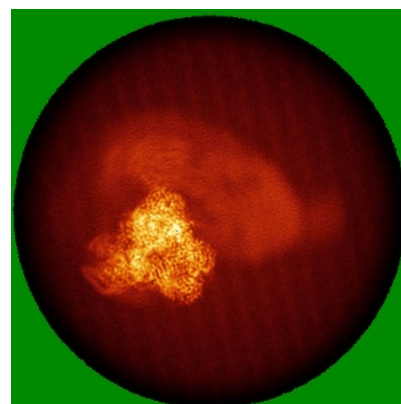
6.4.1 Primary map



X

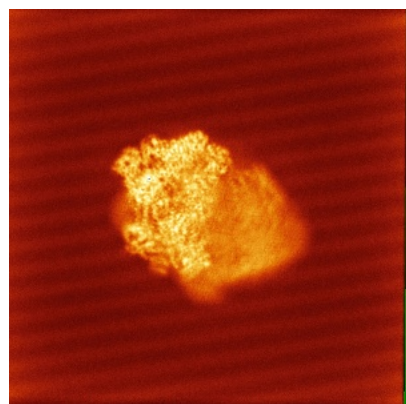


Y

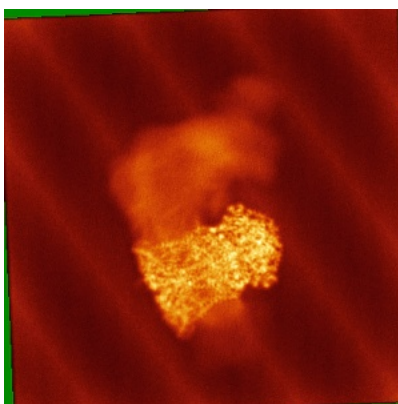


Z

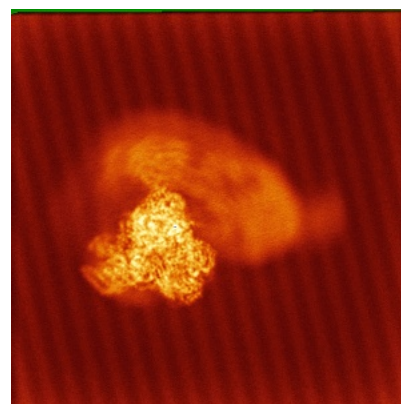
6.4.2 Raw map



X



Y

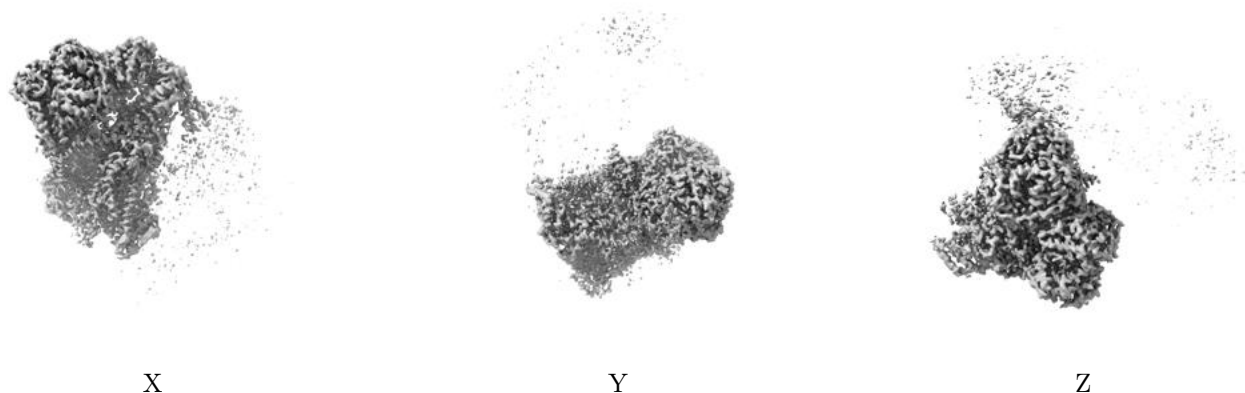


Z

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.

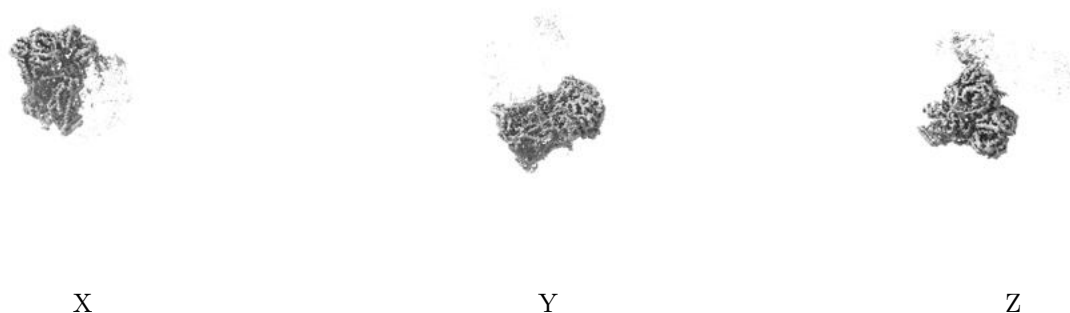
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

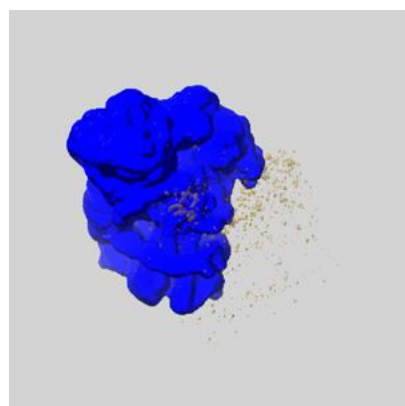
6.6 Mask visualisation [i](#)

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

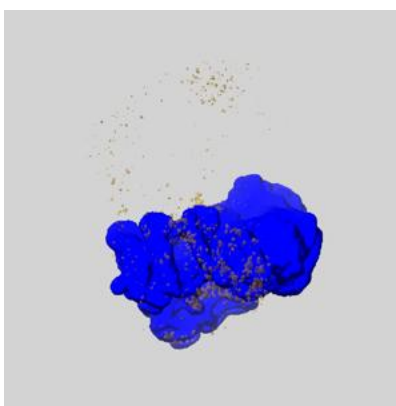
A mask typically either:

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

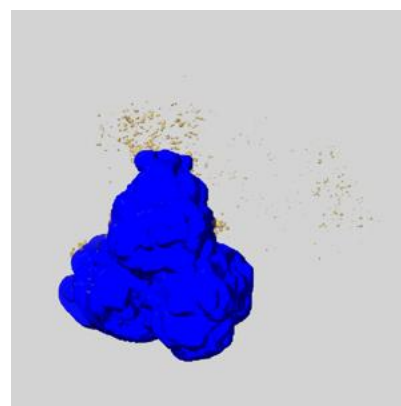
6.6.1 emd_35316_msk_1.map [i](#)



X



Y

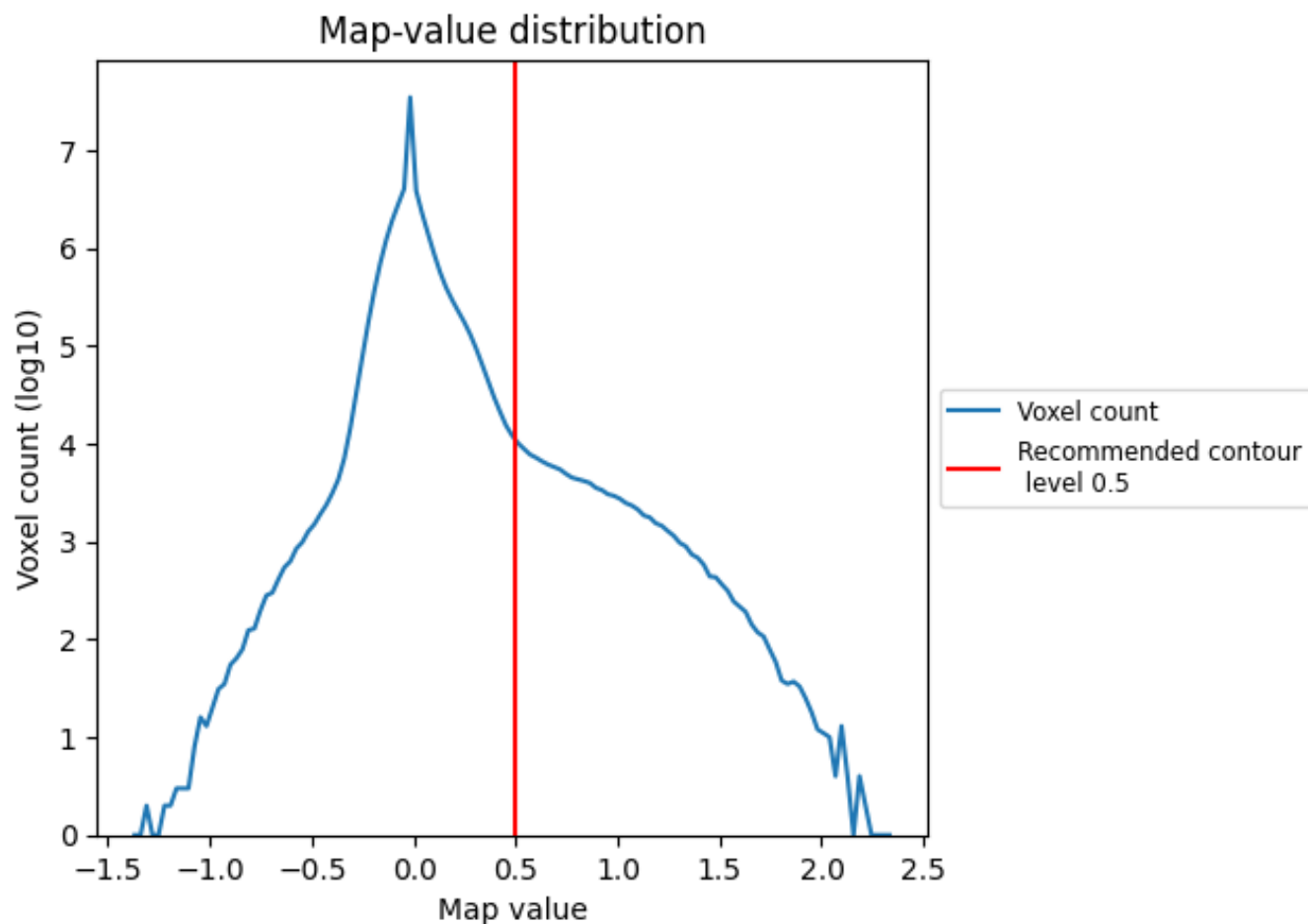


Z

7 Map analysis [i](#)

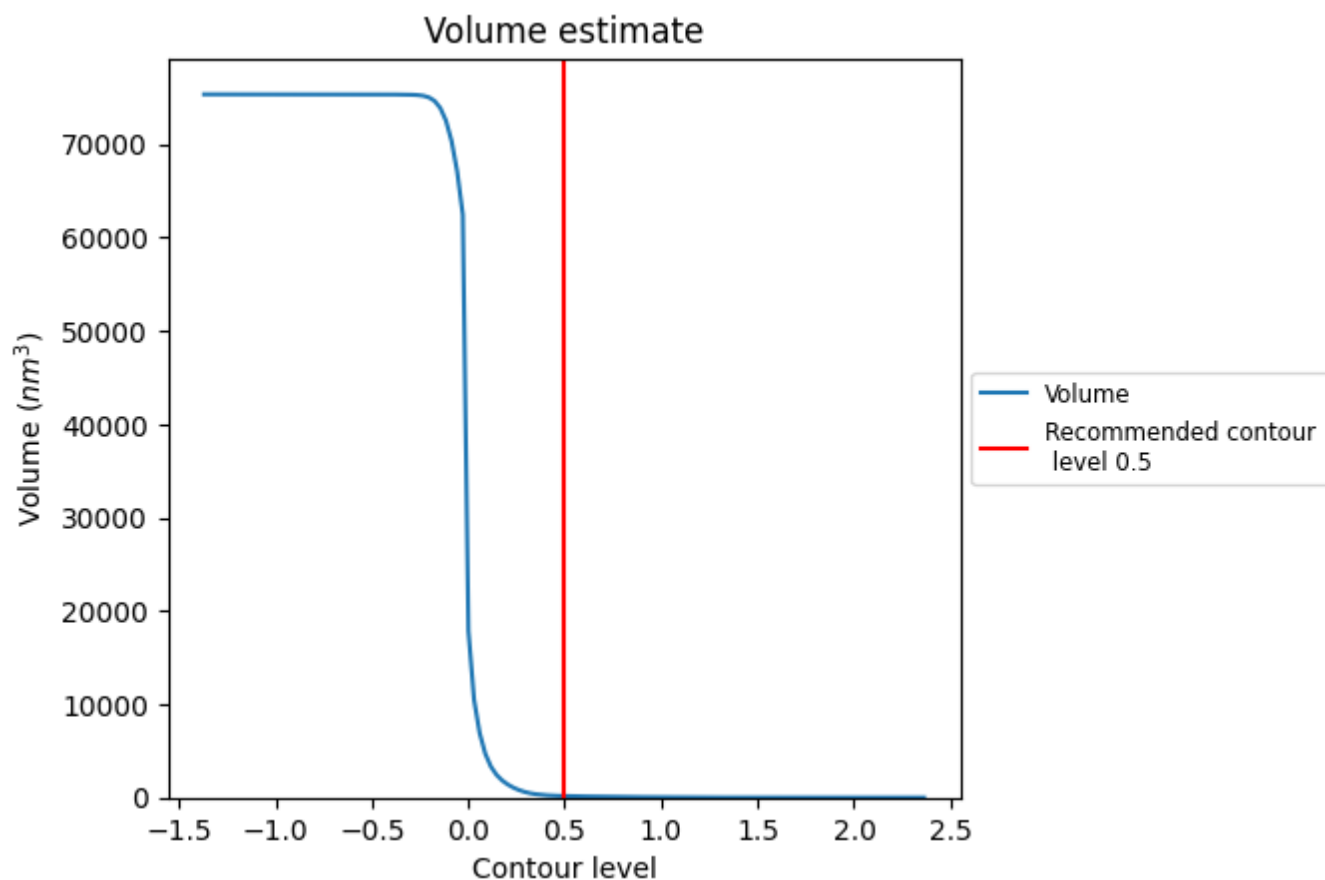
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

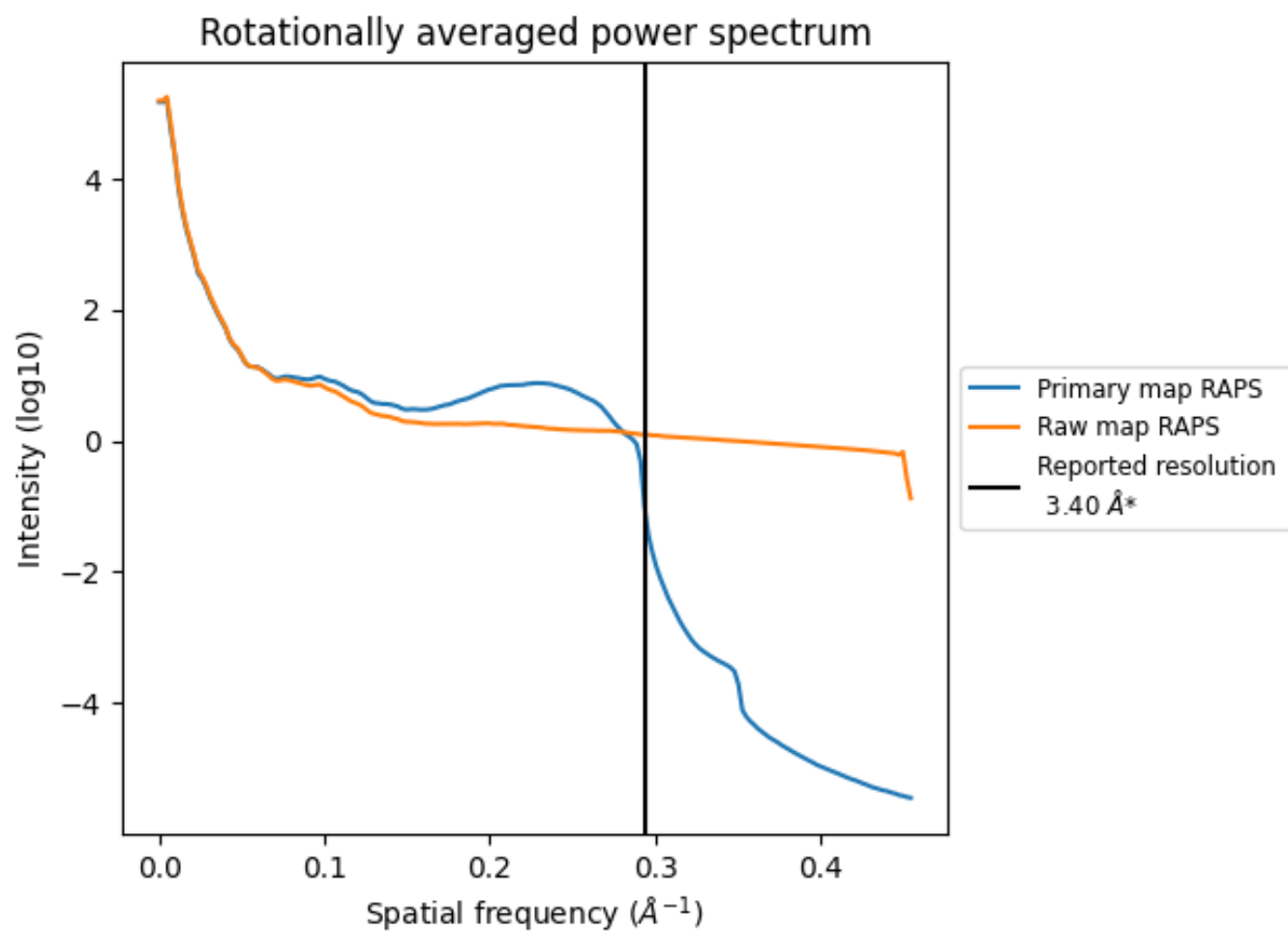
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm³; this corresponds to an approximate mass of 147 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 ⓘ

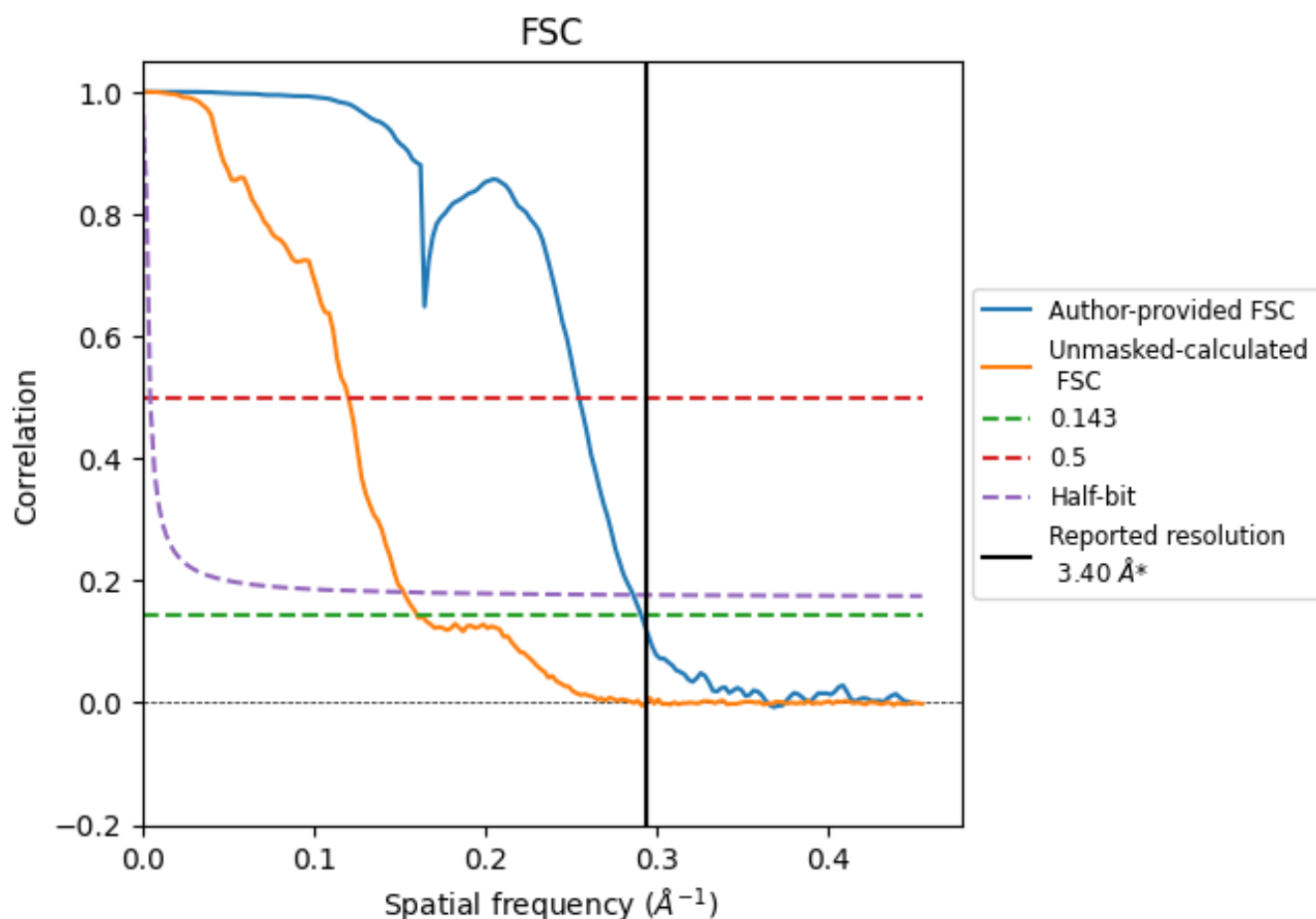


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

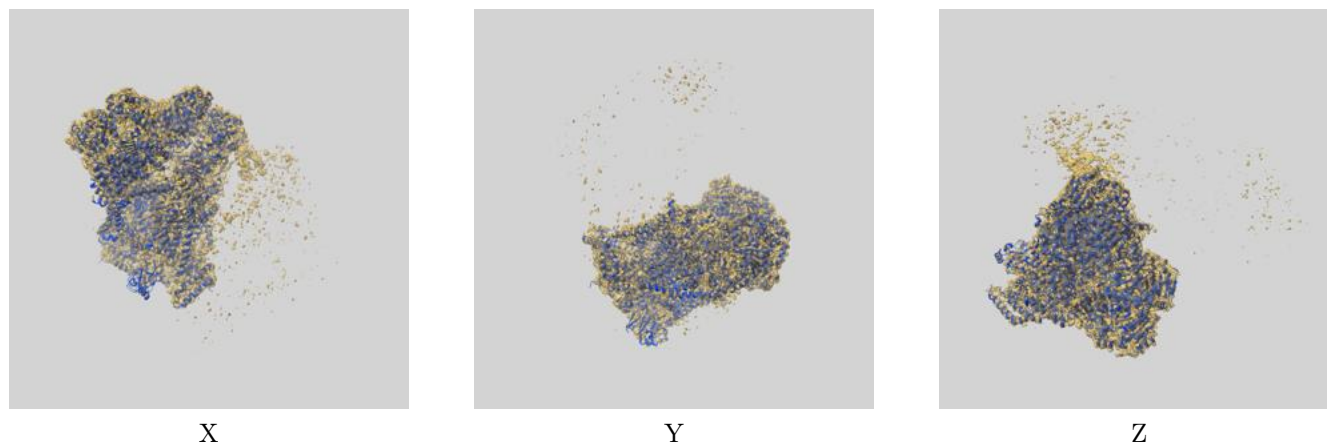
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.44	3.93	3.50
Unmasked-calculated*	6.24	8.33	6.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.24 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

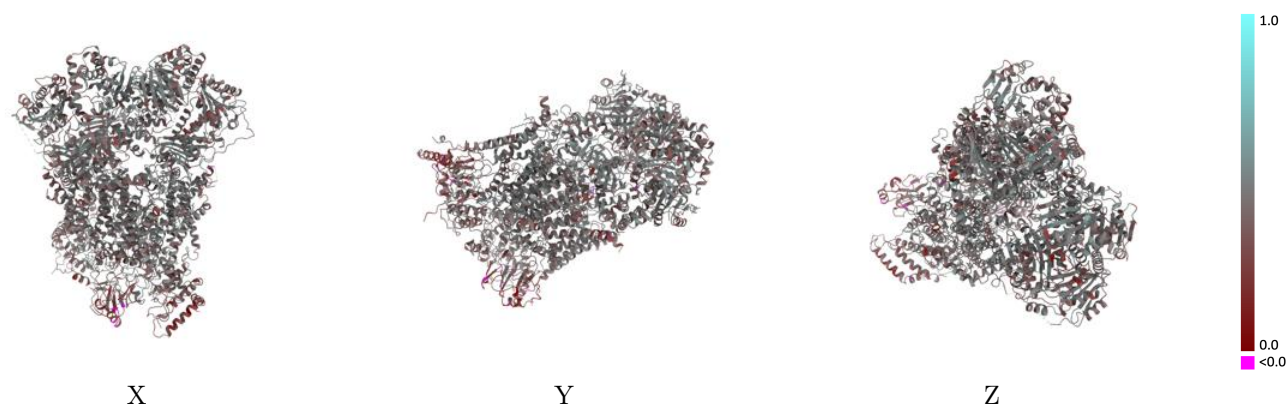
This section contains information regarding the fit between EMDB map EMD-35316 and PDB model 8IAR. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



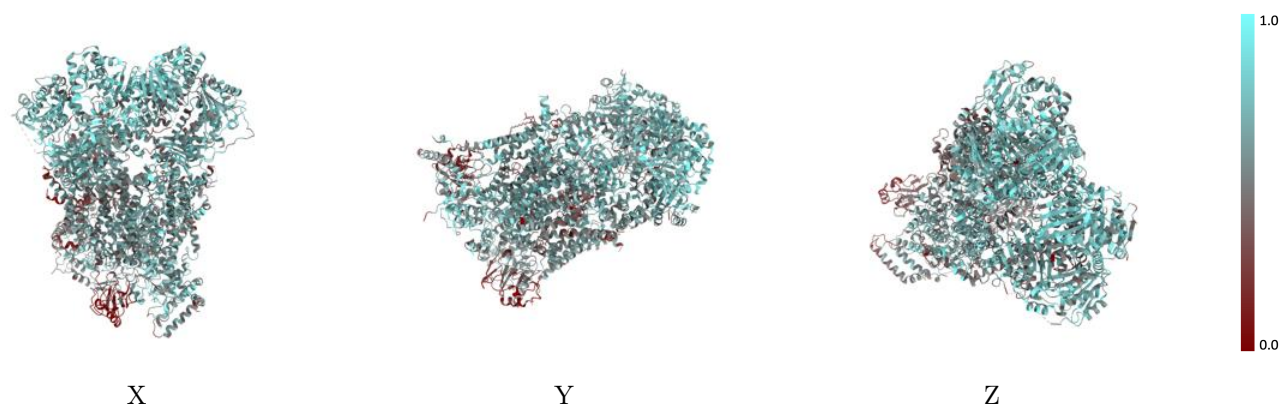
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



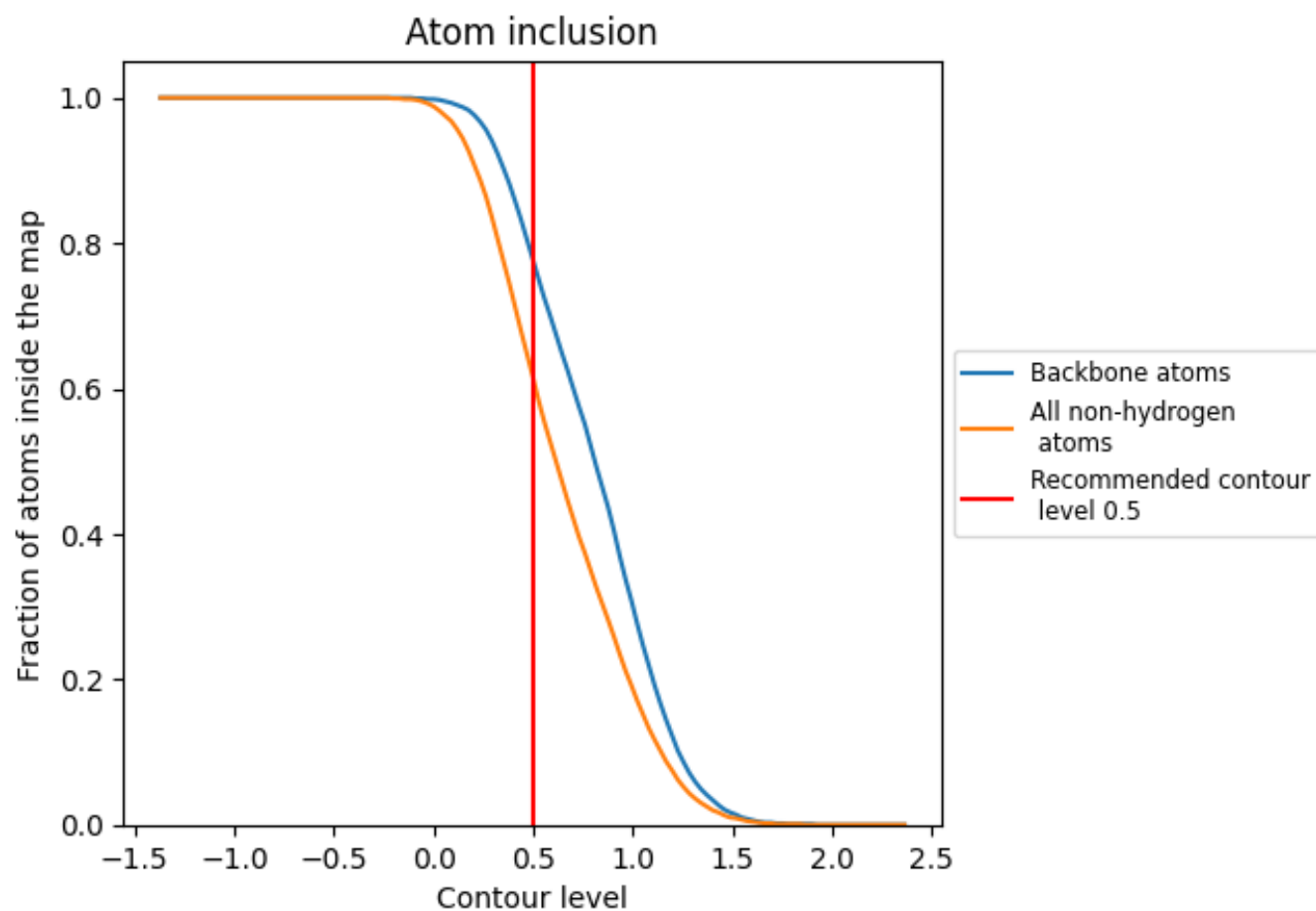
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 61% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.4210
AA	 0.6930	 0.4360
AB	 0.6970	 0.4430
AC	 0.6340	 0.4390
AD	 0.6420	 0.4110
AE	 0.3000	 0.3300
AF	 0.6890	 0.4360
AG	 0.5460	 0.4300
AH	 0.4600	 0.3000
AI	 0.2990	 0.4200
AJ	 0.4040	 0.4060
AK	 0.2680	 0.4070
Aa	 0.6650	 0.4410
Ab	 0.7140	 0.4410
Ac	 0.6520	 0.4510
Ad	 0.6810	 0.4290
Ae	 0.3660	 0.3230
Af	 0.6890	 0.4560
Ag	 0.6160	 0.4490
Ah	 0.5440	 0.3010
Ai	 0.2490	 0.3150
Aj	 0.4970	 0.3930
Ak	 0.3720	 0.3750

