



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 11:55 PM UTC

PDB ID : 8IBG / pdb_00008ibg
EMDB ID : EMD-35343
Title : Respiratory complex CIII2, focus-refined of type II, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 3.80 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:

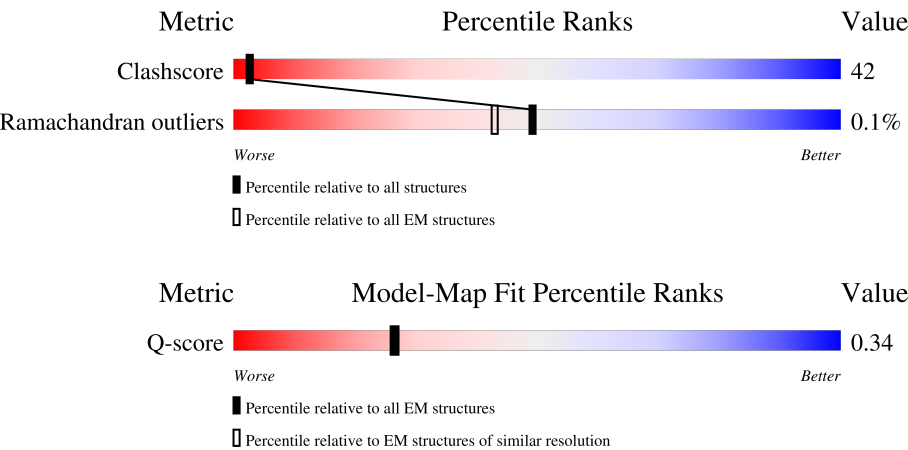
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	45% 36% 18%
1	Aa	480	5% 42% 38% 18%
2	AB	453	5% 62% 29% 8%
2	Ab	453	6% 50% 40% 8%
3	AC	381	21% 53% 44% ..

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Mol	Chain	Length	Quality of chain
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
16	3PH	Ad	402	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 30396 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	395	Total	C	N	O	S	0	0
			3077	1918	545	598	16		
1	Aa	394	Total	C	N	O	S	0	0
			3076	1923	545	592	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	418	Total	C	N	O	S	0	0
			3137	1970	552	606	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	236	Total	C	N	O	S	0	0
			1878	1200	323	341	14		
4	Ad	239	Total	C	N	O	S	0	0
			1903	1215	326	348	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	109	Total	C	N	O	S	0	0
			830	525	152	147	6		
5	AI	28	Total	C	N	O		0	0
			200	129	37	34			
5	Ae	188	Total	C	N	O	S	0	0
			1451	916	254	274	7		
5	Ai	28	Total	C	N	O		0	0
			204	130	40	34			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	97	Total	C	N	O	S	0	0
			855	546	152	154	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	74	Total	C	N	O	S	0	0
			622	404	114	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	64	Total	C	N	O	S	0	0
			527	321	98	103	5		
8	Ah	62	Total	C	N	O	S	0	0
			512	316	93	98	5		

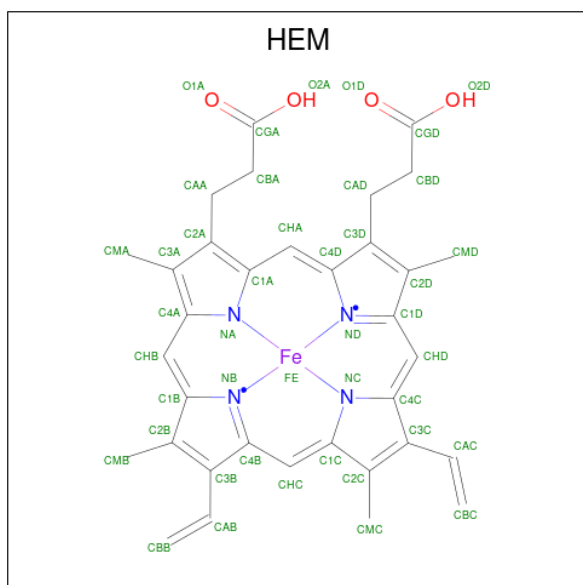
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AJ	21	Total	C	N	O	0	0
			165	109	27	29		
9	Aj	43	Total	C	N	O	0	0
			345	223	59	63		

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

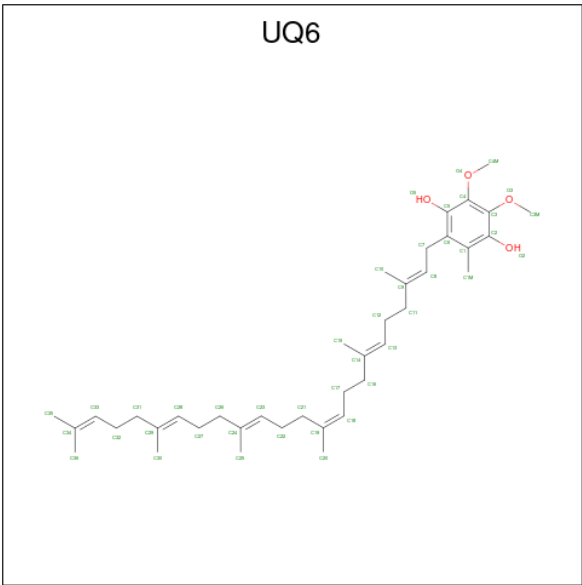
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	17	Total	C	N	O	S	0	0
			118	77	19	21	1		
10	AK	38	Total	C	N	O	S	0	0
			309	202	58	48	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



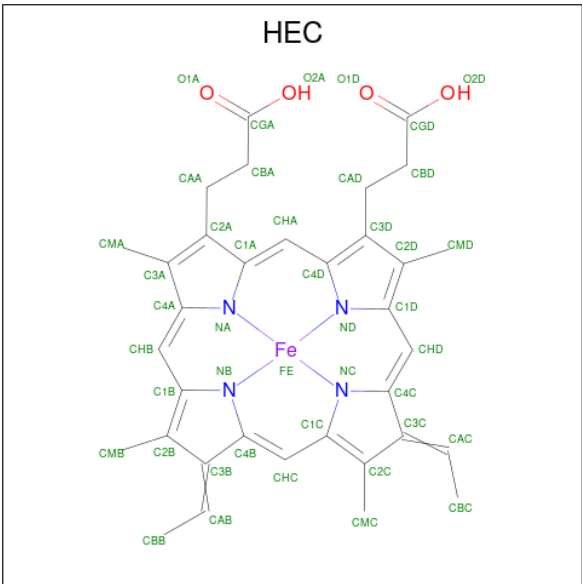
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 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
12	AC	1	Total	C	O	0
			28	24	4	
12	Ac	1	Total	C	O	0
			28	24	4	

- Molecule 13 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



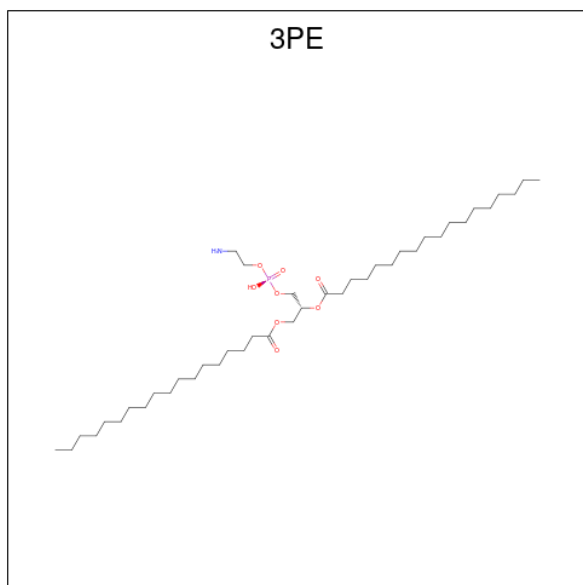
Mol	Chain	Residues	Atoms					AltConf
13	AD	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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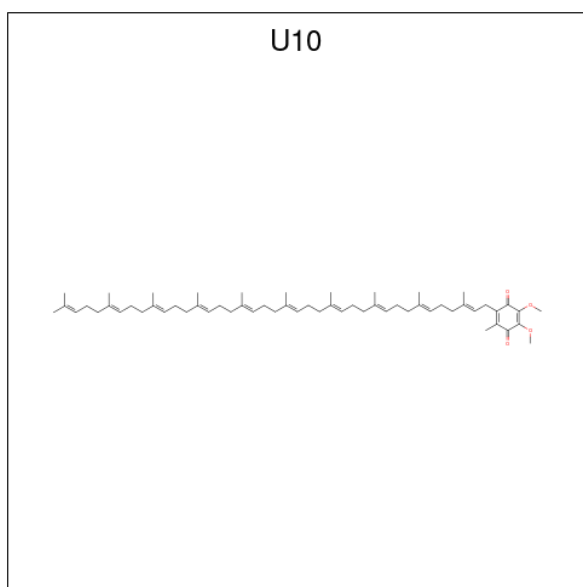
Mol	Chain	Residues	Atoms					AltConf
13	Ad	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



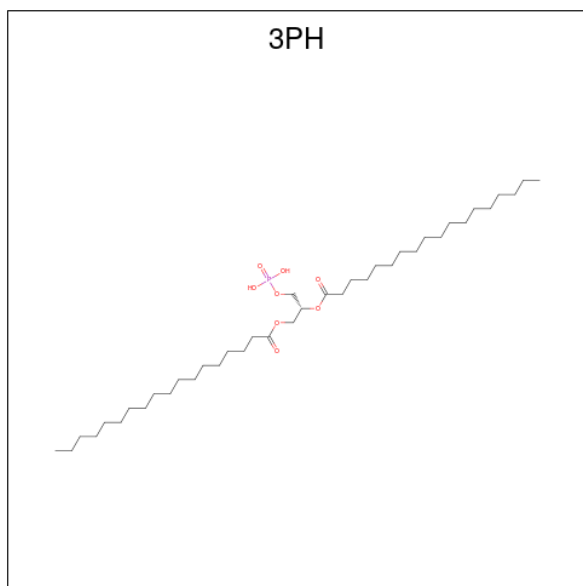
Mol	Chain	Residues	Atoms					AltConf
14	Aa	1	Total	C	N	O	P	0
			23	13	1	8	1	
14	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
14	Ag	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 15 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



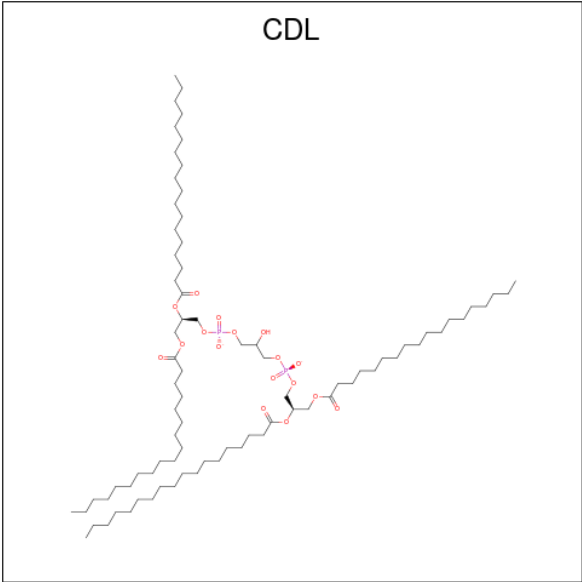
Mol	Chain	Residues	Atoms			AltConf
15	Ac	1	Total	C	O	0
			23	19	4	

- Molecule 16 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
16	Ad	1	Total	C	O	P	0
			36	27	8	1	

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

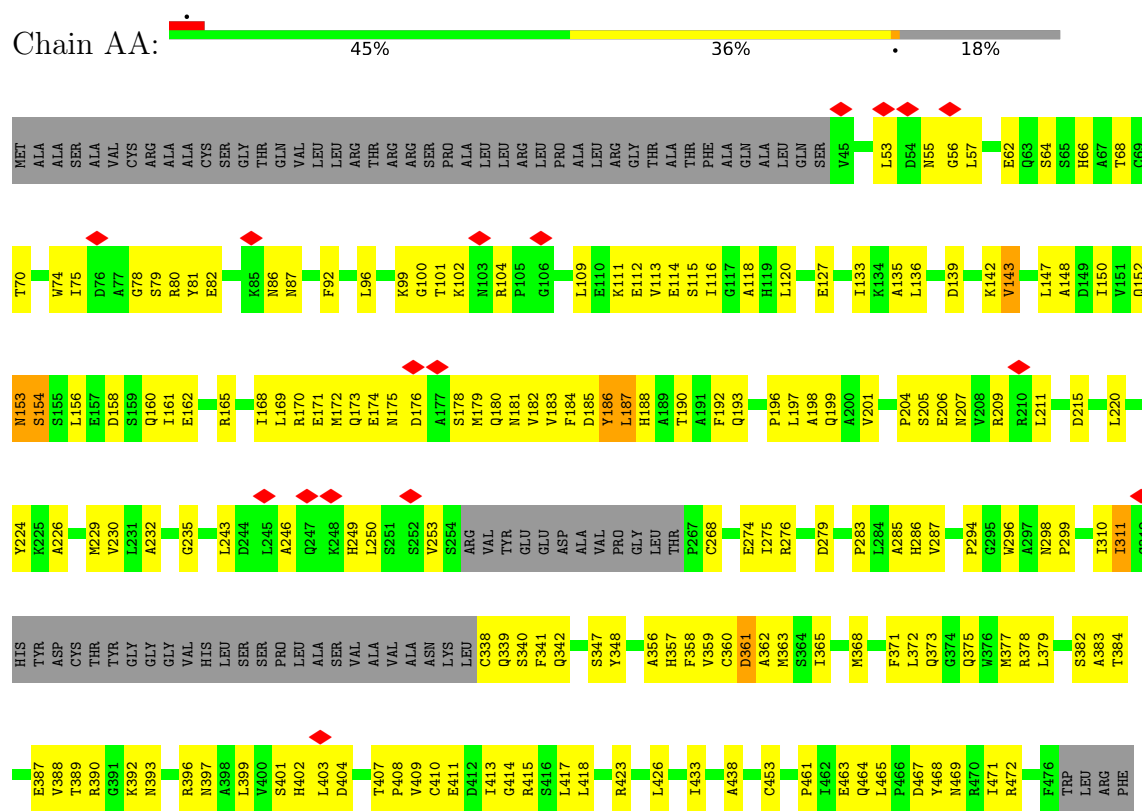


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	Ag	1	42	23	17	2	0
17	Ag	1	56	37	17	2	0

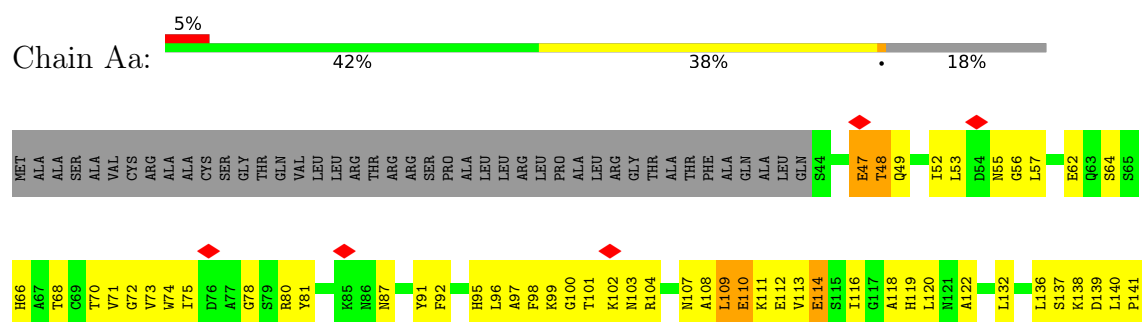
3 Residue-property plots [i](#)

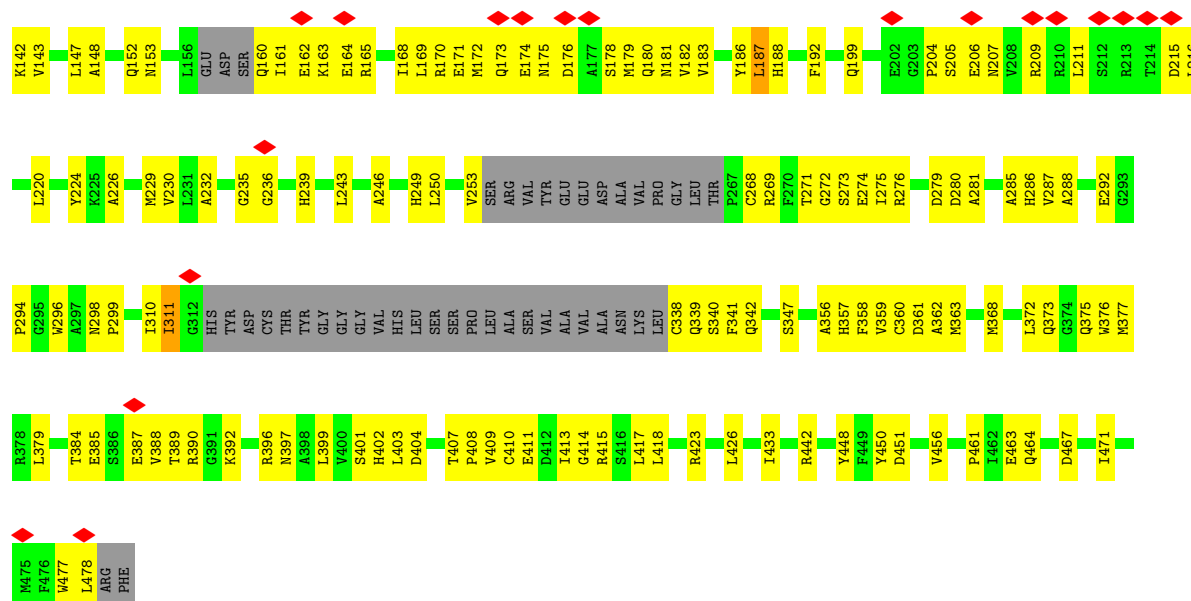
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

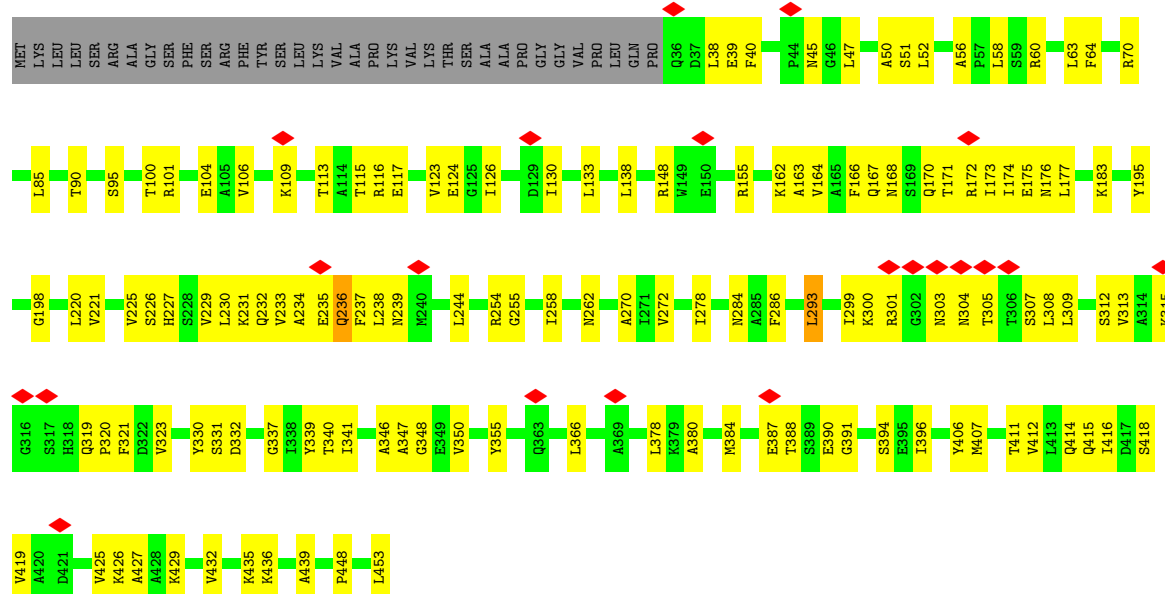


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

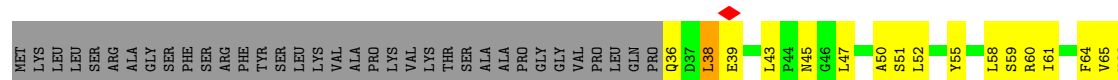


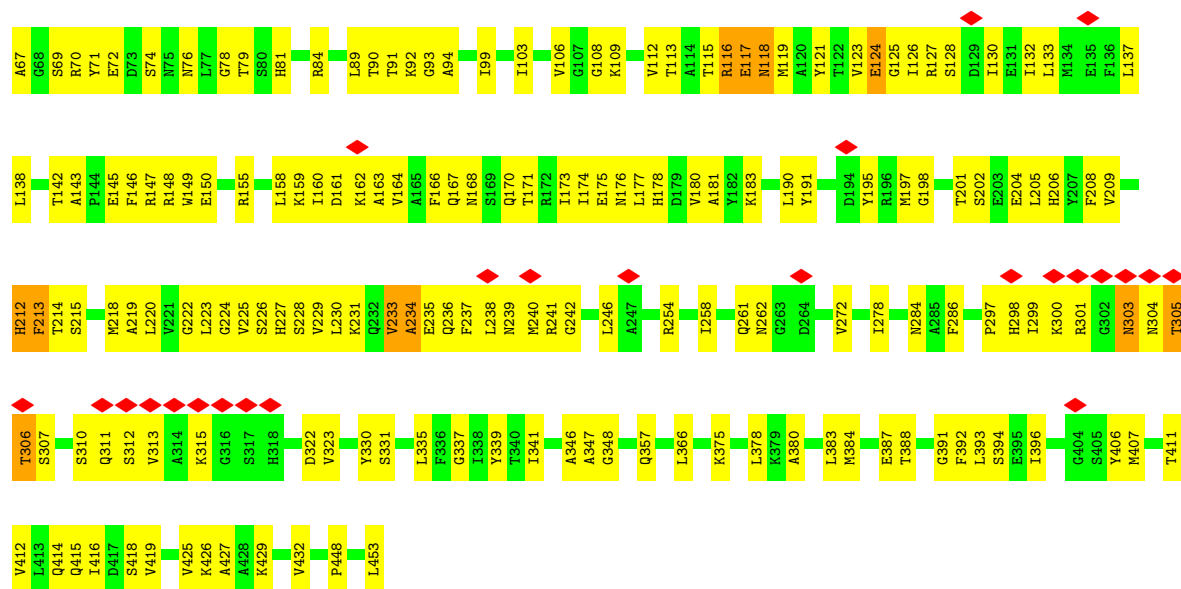


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

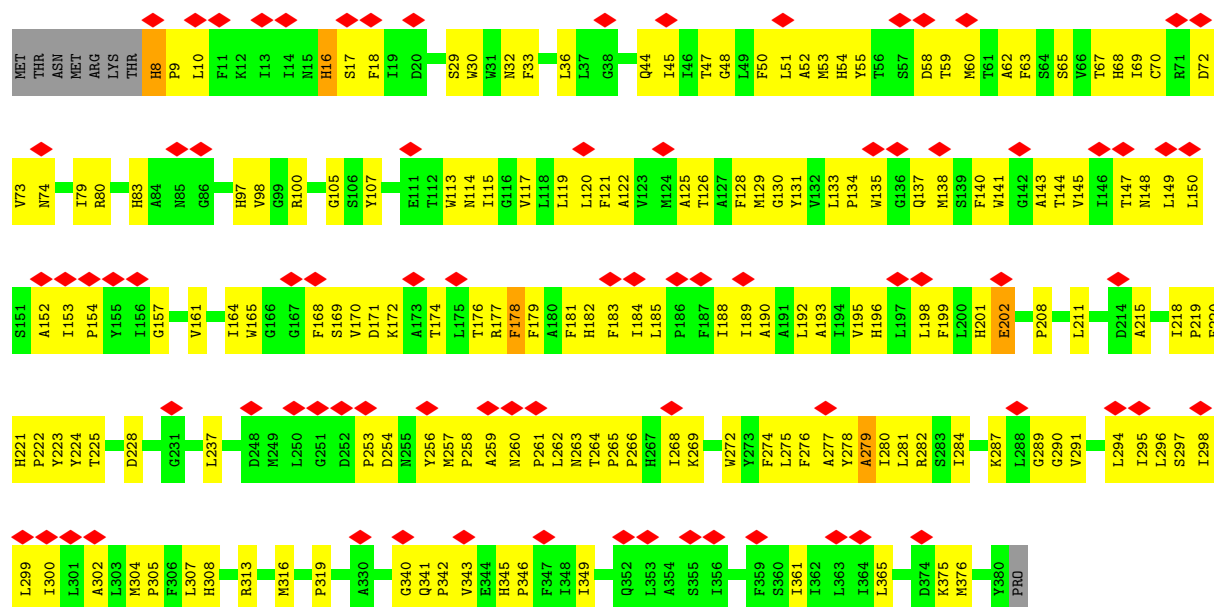


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

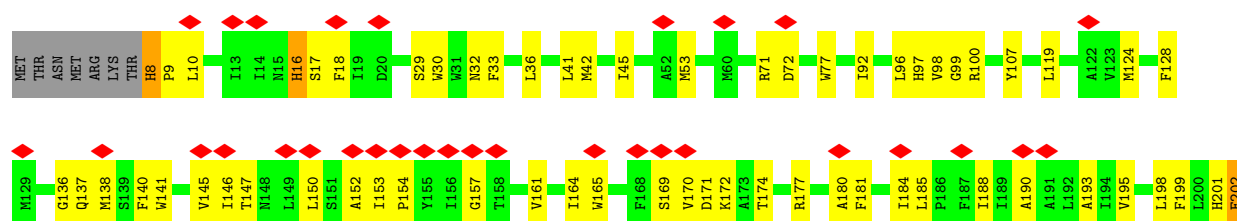


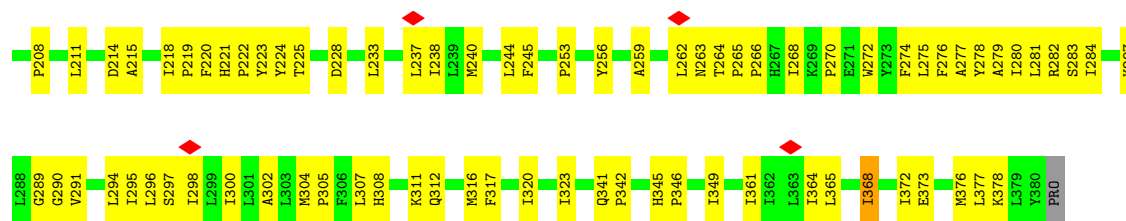


• Molecule 3: Cytochrome b

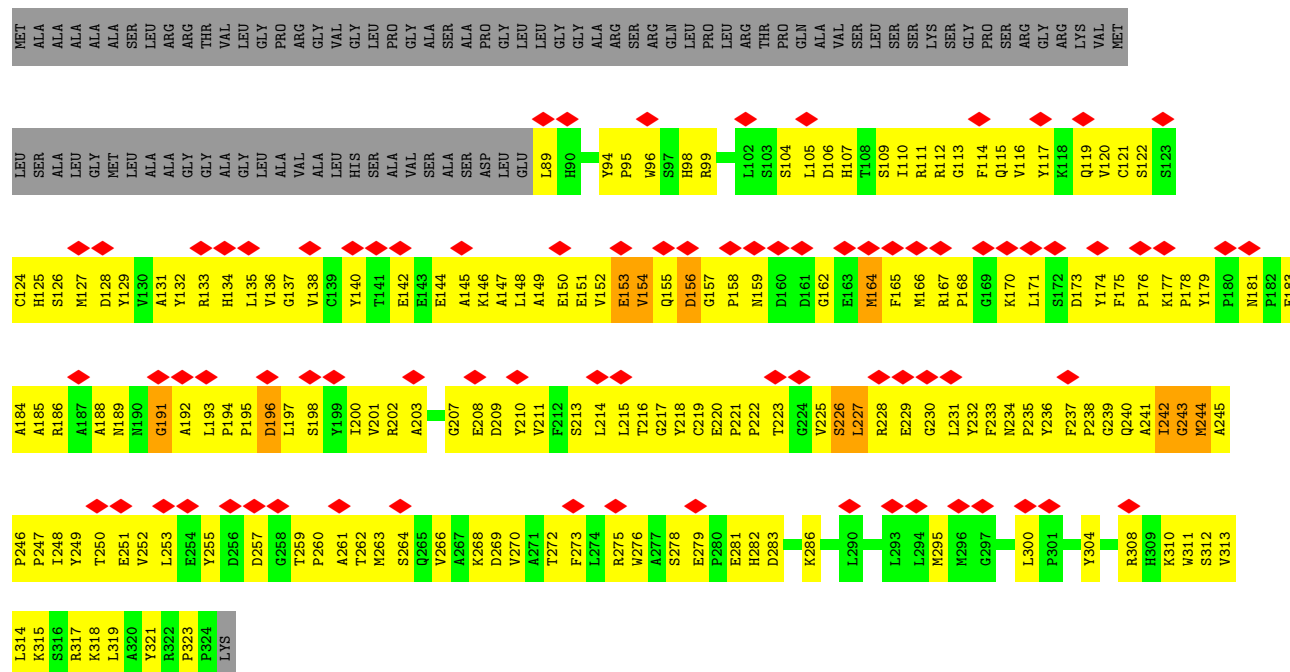
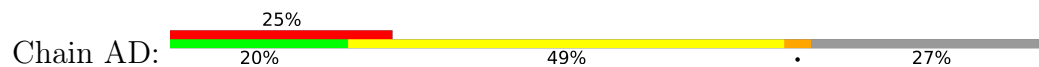


• Molecule 3: Cytochrome b

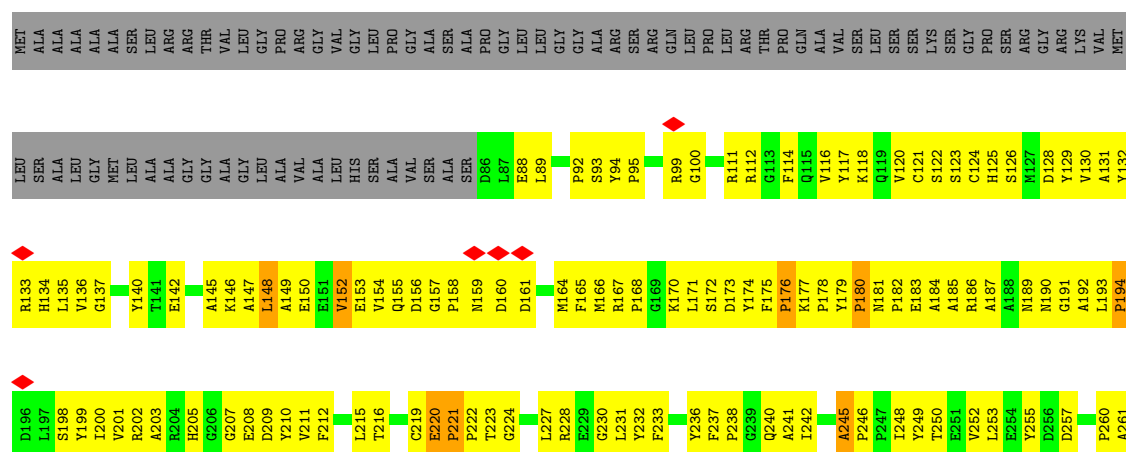


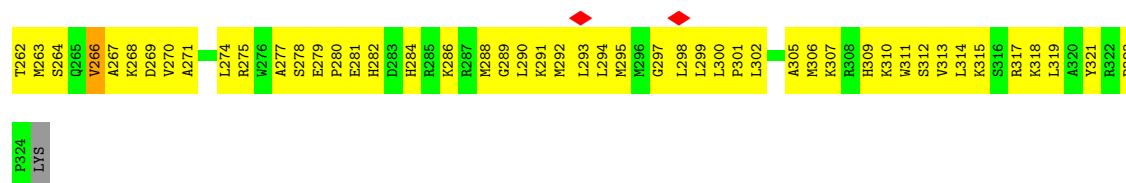


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

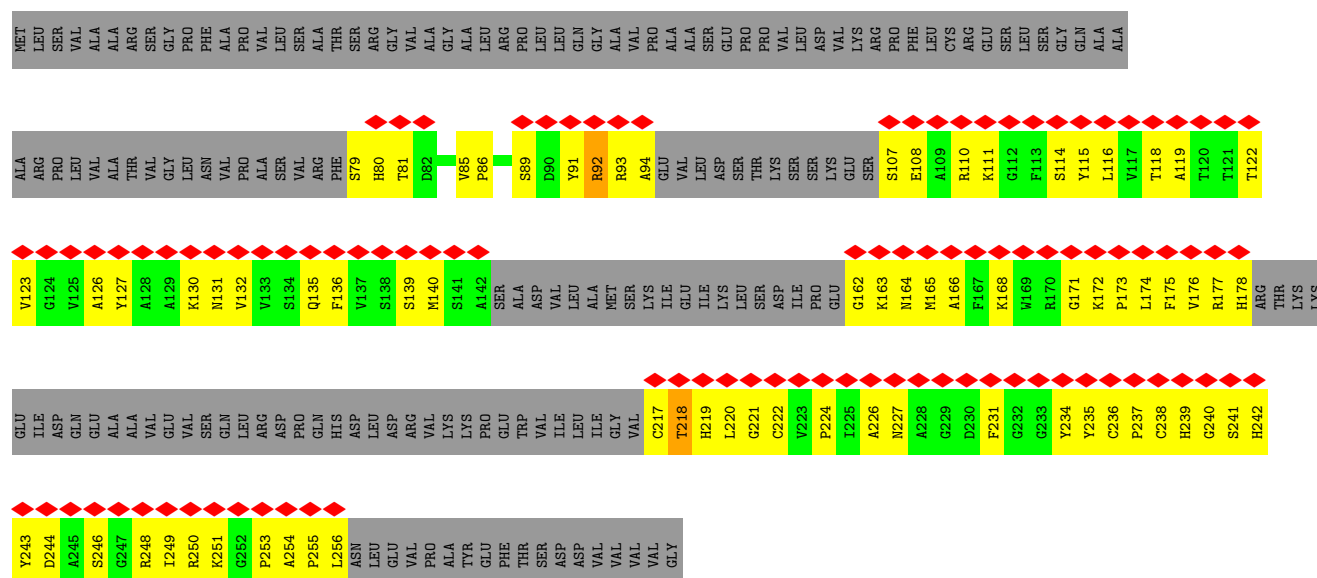


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

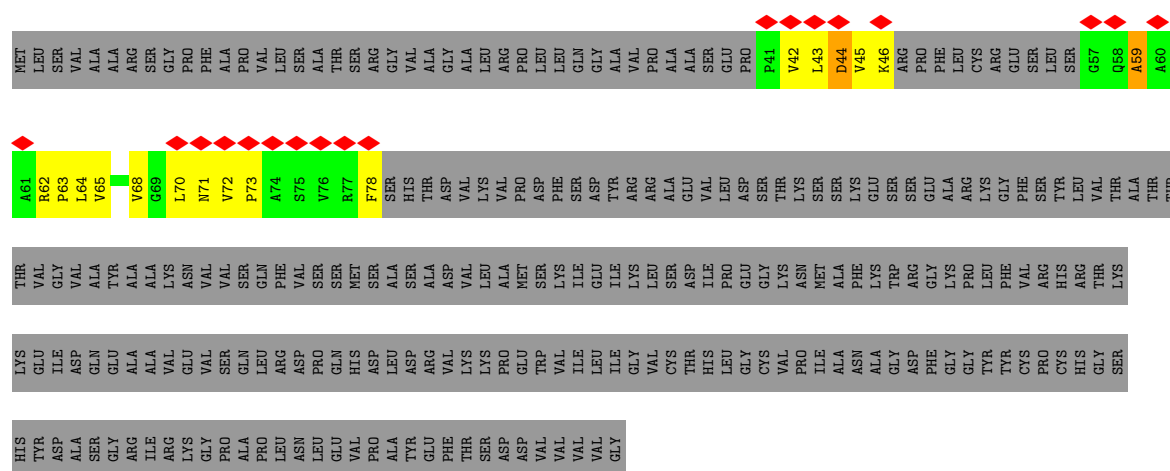




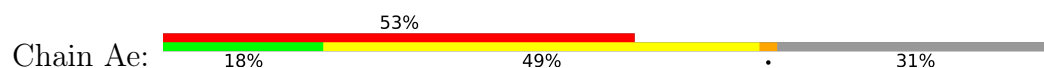
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

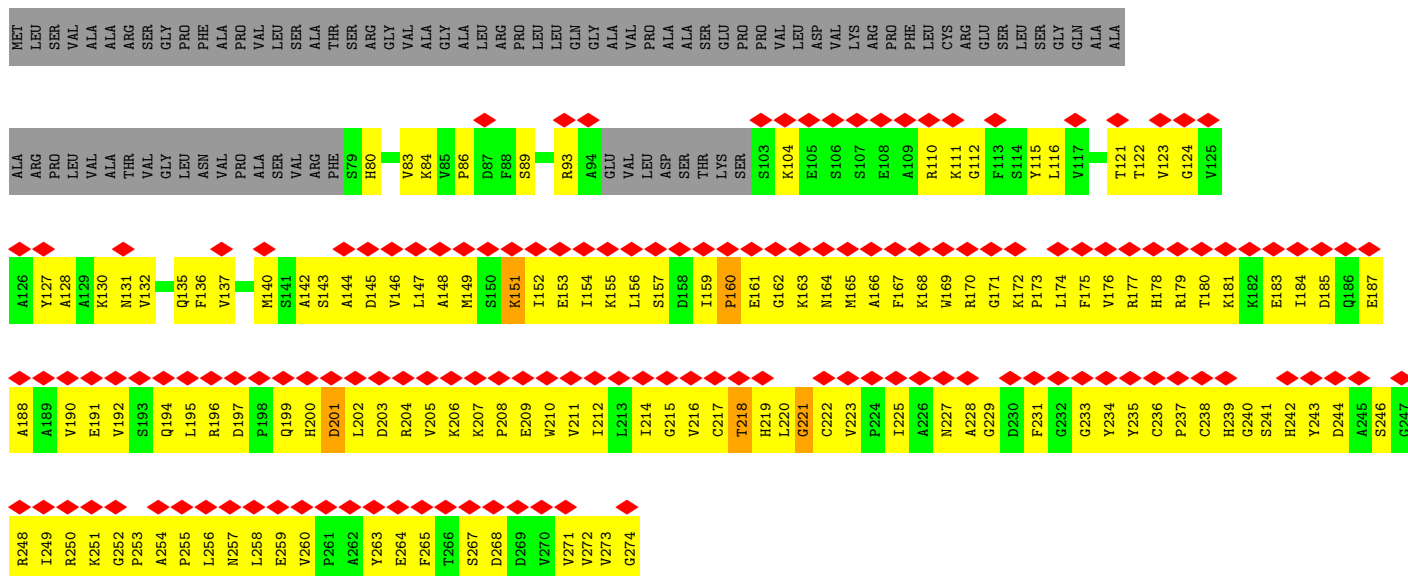


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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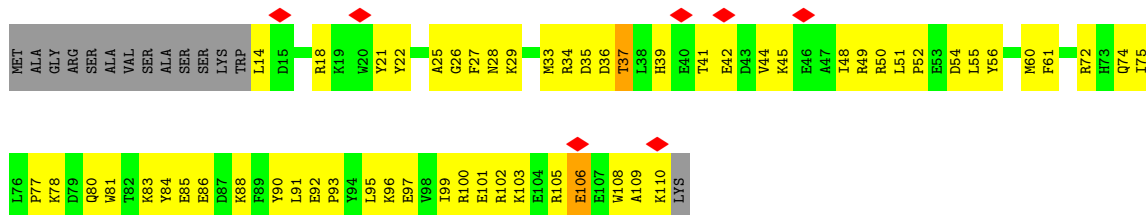




- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

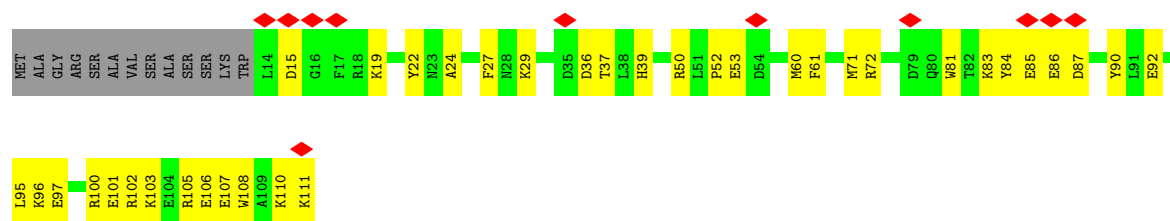


- Molecule 6: Cytochrome b-c1 complex subunit 7

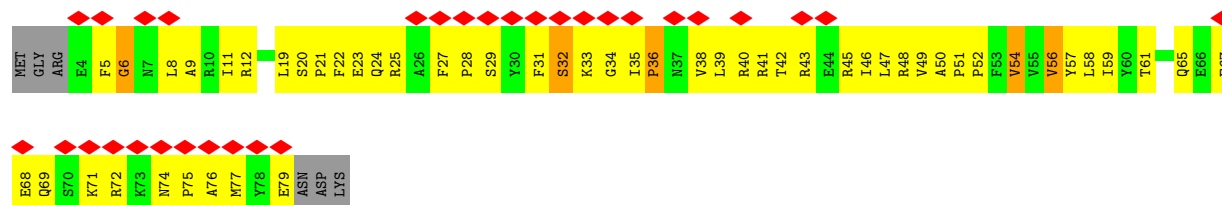


- Molecule 6: Cytochrome b-c1 complex subunit 7

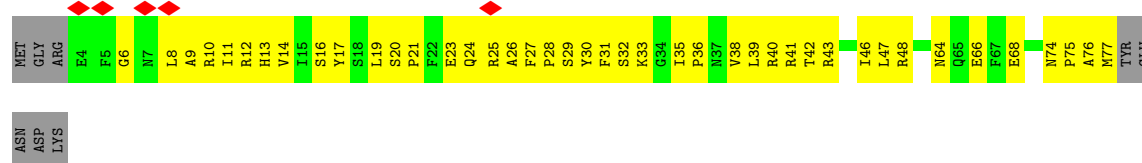
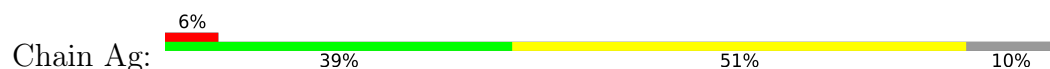




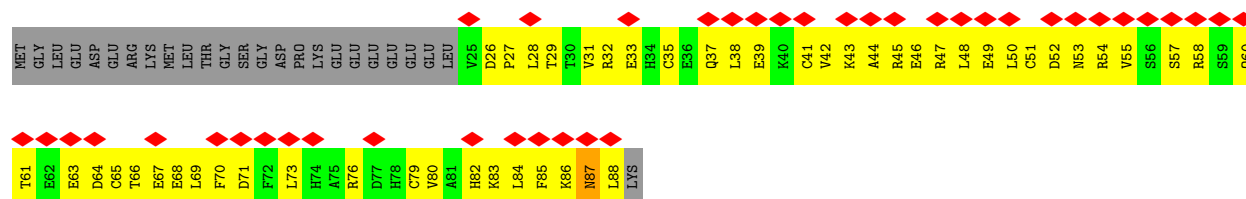
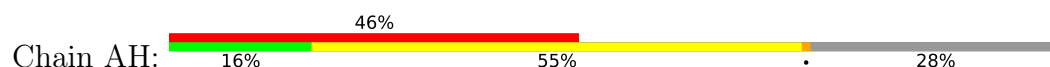
• Molecule 7: Cytochrome b-c1 complex subunit 8



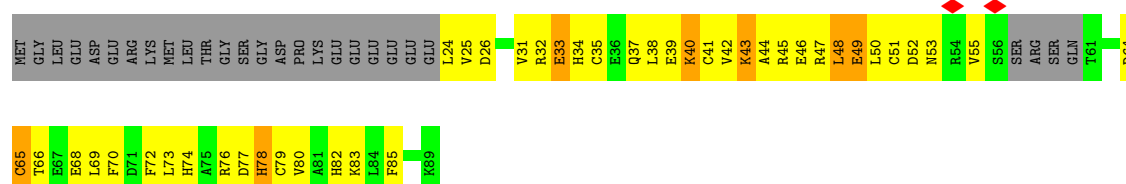
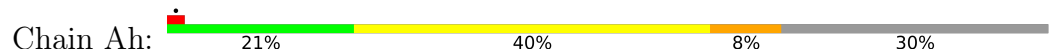
• Molecule 7: Cytochrome b-c1 complex subunit 8



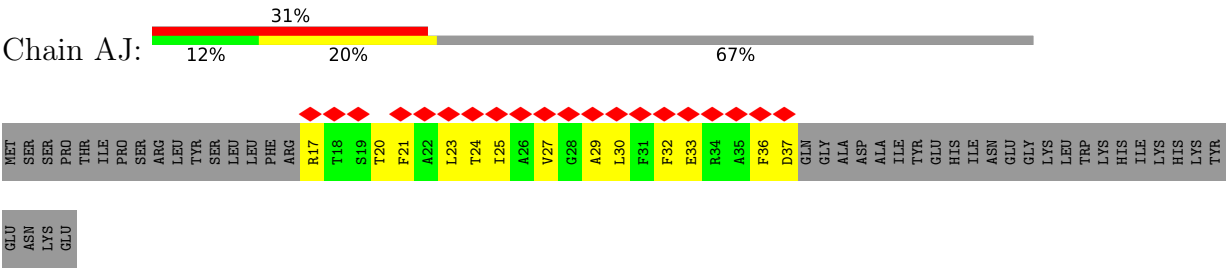
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



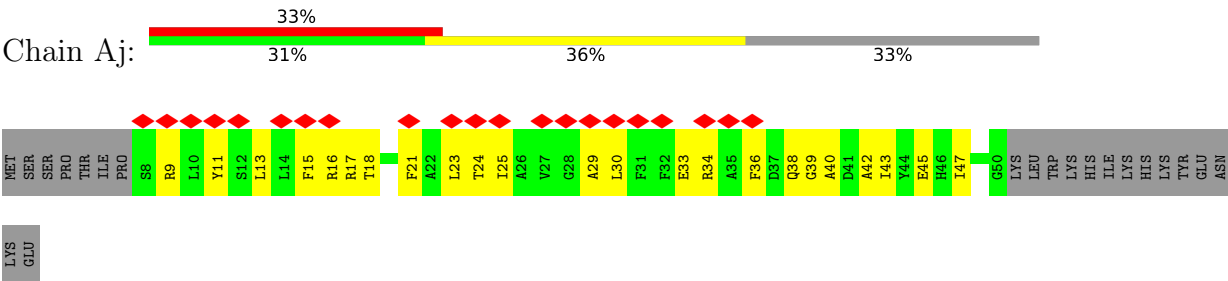
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



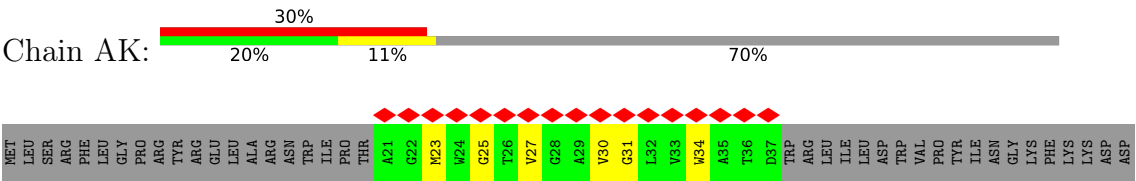
• Molecule 9: Cytochrome b-c1 complex subunit 9



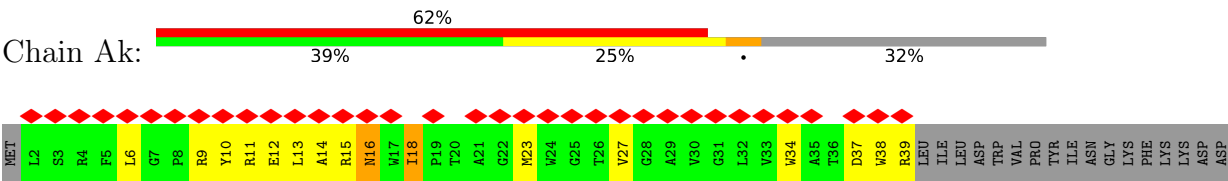
• Molecule 9: Cytochrome b-c1 complex subunit 9



• 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	177076	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 ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.293	Depositor
Minimum map value	-1.374	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.35	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, HEM, U10, UQ6, CDL, 3PH, HEC

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	0.62	2/3134 (0.1%)	0.89	11/4248 (0.3%)
1	Aa	0.58	1/3134 (0.0%)	0.89	14/4248 (0.3%)
2	AB	0.44	0/3187	0.65	3/4308 (0.1%)
2	Ab	0.58	1/3187 (0.0%)	0.91	18/4308 (0.4%)
3	AC	0.51	0/3089	0.84	10/4221 (0.2%)
3	Ac	0.45	0/3089	0.73	7/4221 (0.2%)
4	AD	0.54	0/1937	0.97	11/2632 (0.4%)
4	Ad	0.85	3/1962 (0.2%)	1.07	17/2666 (0.6%)
5	AE	0.47	0/851	0.94	3/1146 (0.3%)
5	AI	1.86	2/202 (1.0%)	1.43	4/274 (1.5%)
5	Ae	0.63	0/1483	1.10	7/2007 (0.3%)
5	Ai	1.87	2/205 (1.0%)	1.49	5/277 (1.8%)
6	AF	0.64	0/875	0.90	6/1173 (0.5%)
6	Af	0.38	0/884	0.52	0/1184
7	AG	0.57	1/662 (0.2%)	1.10	5/895 (0.6%)
7	Ag	0.55	0/640	0.93	1/865 (0.1%)
8	AH	0.53	0/534	0.84	2/717 (0.3%)
8	Ah	0.76	0/518	1.14	7/694 (1.0%)
9	AJ	0.41	0/168	0.62	0/226
9	Aj	0.59	0/352	0.78	0/474
10	AK	0.47	0/121	0.84	1/166 (0.6%)
10	Ak	0.52	0/320	1.14	6/437 (1.4%)
All	All	0.60	12/30534 (0.0%)	0.89	138/41387 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	44	ASP	C-N	20.17	1.52	1.33
5	Ai	44	ASP	C-N	19.98	1.52	1.33
4	Ad	221	PRO	N-CD	18.51	1.73	1.47
5	Ai	45	VAL	C-N	15.71	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AI	45	VAL	C-N	14.48	1.53	1.33

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	115	ILE	N-CA-C	-11.23	99.16	110.62
10	AK	38	TRP	N-CA-C	10.76	126.05	110.24
2	Ab	303	ASN	N-CA-C	-9.85	100.17	112.88
2	Ab	306	THR	N-CA-C	9.83	123.22	111.33
1	Aa	187	LEU	N-CA-C	-9.79	100.43	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3077	0	2996	199	0
1	Aa	3076	0	3001	230	0
2	AB	3137	0	3143	153	0
2	Ab	3137	0	3143	252	0
3	AC	2988	0	3045	294	0
3	Ac	2988	0	3045	216	0
4	AD	1878	0	1827	294	0
4	Ad	1903	0	1848	279	0
5	AE	830	0	802	136	0
5	AI	200	0	216	32	0
5	Ae	1451	0	1433	264	0
5	Ai	204	0	221	34	0
6	AF	855	0	841	64	0
6	Af	864	0	854	38	0
7	AG	643	0	643	88	0
7	Ag	622	0	628	54	0
8	AH	527	0	507	76	0
8	Ah	512	0	497	84	0
9	AJ	165	0	162	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Aj	345	0	333	37	0
10	AK	118	0	111	39	0
10	Ak	309	0	304	27	0
11	AC	86	0	60	27	0
11	Ac	86	0	60	11	0
12	AC	28	0	31	11	0
12	Ac	28	0	31	15	0
13	AD	43	0	32	18	0
13	Ad	43	0	32	12	0
14	Aa	23	0	20	3	0
14	Ac	35	0	44	7	0
14	Ag	38	0	53	9	0
15	Ac	23	0	23	20	0
16	Ad	36	0	45	39	0
17	Ag	98	0	84	9	0
All	All	30396	0	30115	2519	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 42.

The worst 5 of 2519 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)
5:Ae:239:HIS:ND1	5:Ae:253:PRO:HG3	1.39	1.37
2:Ab:212:HIS:CE1	2:Ab:246:LEU:HD23	1.63	1.32
4:Ad:221:PRO:CD	4:Ad:221:PRO:N	1.73	1.32
3:AC:268:ILE:HD12	5:Ae:238:CYS:SG	1.67	1.31
2:Ab:297:PRO:CG	2:Ab:304:ASN:HD21	1.43	1.31

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	AA	389/480 (81%)	372 (96%)	17 (4%)	0	100	100
1	Aa	350/480 (73%)	334 (95%)	16 (5%)	0	100	100
2	AB	416/453 (92%)	408 (98%)	8 (2%)	0	100	100
2	Ab	307/453 (68%)	290 (94%)	17 (6%)	0	100	100
3	AC	371/381 (97%)	361 (97%)	10 (3%)	0	100	100
3	Ac	190/381 (50%)	188 (99%)	2 (1%)	0	100	100
4	AD	234/325 (72%)	213 (91%)	21 (9%)	0	100	100
4	Ad	237/325 (73%)	224 (94%)	12 (5%)	1 (0%)	30	62
5	AE	101/274 (37%)	95 (94%)	6 (6%)	0	100	100
5	AI	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
5	Ae	184/274 (67%)	168 (91%)	15 (8%)	1 (0%)	24	57
5	Ai	24/274 (9%)	22 (92%)	2 (8%)	0	100	100
6	AF	95/111 (86%)	94 (99%)	1 (1%)	0	100	100
6	Af	96/111 (86%)	96 (100%)	0	0	100	100
7	AG	74/82 (90%)	70 (95%)	4 (5%)	0	100	100
7	Ag	72/82 (88%)	72 (100%)	0	0	100	100
8	AH	62/89 (70%)	61 (98%)	1 (2%)	0	100	100
8	Ah	58/89 (65%)	55 (95%)	3 (5%)	0	100	100
9	AJ	19/64 (30%)	19 (100%)	0	0	100	100
9	Aj	41/64 (64%)	40 (98%)	1 (2%)	0	100	100
10	AK	15/56 (27%)	15 (100%)	0	0	100	100
10	Ak	36/56 (64%)	34 (94%)	2 (6%)	0	100	100
All	All	3395/5178 (66%)	3253 (96%)	140 (4%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Ae	160	PRO
4	Ad	194	PRO

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	HEC	AD	401	4	46,50,50	2.53	23 (50%)	58,82,82	2.10	21 (36%)
14	3PE	Ac	403	-	34,34,50	1.09	2 (5%)	37,39,55	1.16	3 (8%)
17	CDL	Ag	101	-	41,41,99	1.40	4 (9%)	47,53,111	1.37	7 (14%)
16	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	38,40,52	1.29	4 (10%)
11	HEM	Ac	401	3	50,50,50	1.31	8 (16%)	67,82,82	1.60	12 (17%)
11	HEM	Ac	402	3	50,50,50	1.61	8 (16%)	67,82,82	1.86	16 (23%)
14	3PE	Aa	501	-	22,22,50	1.36	2 (9%)	25,27,55	1.15	3 (12%)
12	UQ6	Ac	405	-	28,28,43	2.54	6 (21%)	36,37,55	1.49	6 (16%)
15	U10	Ac	404	-	23,23,63	1.29	4 (17%)	30,31,79	2.06	7 (23%)
11	HEM	AC	401	3	50,50,50	1.55	6 (12%)	67,82,82	1.70	11 (16%)
11	HEM	AC	402	3	50,50,50	1.60	9 (18%)	67,82,82	1.75	15 (22%)
17	CDL	Ag	102	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	8 (13%)
14	3PE	Ag	103	-	37,37,50	1.06	2 (5%)	40,42,55	1.22	3 (7%)
13	HEC	Ad	401	4	46,50,50	1.81	5 (10%)	58,82,82	1.92	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	UQ6	AC	403	-	28,28,43	2.52	6 (21%)	36,37,55	1.61	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEC	AD	401	4	-	3/14/54/54	-
14	3PE	Ac	403	-	-	2/38/38/54	-
17	CDL	Ag	101	-	-	11/52/52/110	-
16	3PH	Ad	402	-	-	9/37/37/49	-
11	HEM	Ac	401	3	-	9/14/54/54	-
11	HEM	Ac	402	3	-	7/14/54/54	-
14	3PE	Aa	501	-	-	5/26/26/54	-
12	UQ6	Ac	405	-	-	5/21/21/39	0/1/1/1
15	U10	Ac	404	-	-	6/15/39/87	0/1/1/1
11	HEM	AC	401	3	-	9/14/54/54	-
11	HEM	AC	402	3	-	6/14/54/54	-
17	CDL	Ag	102	-	-	18/66/66/110	-
14	3PE	Ag	103	-	-	8/41/41/54	-
13	HEC	Ad	401	4	-	4/14/54/54	-
12	UQ6	AC	403	-	-	4/21/21/39	0/1/1/1

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Ac	405	UQ6	C5-C6	6.25	1.49	1.40
13	Ad	401	HEC	CAC-C3C	6.07	1.54	1.35
12	AC	403	UQ6	C5-C6	6.06	1.48	1.40
13	Ad	401	HEC	CAB-C3B	6.04	1.54	1.35
12	AC	403	UQ6	C5-C4	5.99	1.49	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Ad	401	HEC	CBC-CAC-C3C	-8.55	110.34	127.43
13	Ad	401	HEC	CBB-CAB-C3B	-8.34	110.77	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Ac	404	U10	C6-C1-C2	7.81	125.33	119.17
11	Ac	402	HEM	CHC-C4B-NB	6.13	131.03	124.42
11	AC	402	HEM	CHC-C4B-NB	5.81	130.67	124.42

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	401	HEM	C2B-C3B-CAB-CBB
11	AC	401	HEM	C2C-C3C-CAC-CBC
11	AC	401	HEM	C4C-C3C-CAC-CBC
11	AC	402	HEM	C2B-C3B-CAB-CBB
11	AC	402	HEM	C2C-C3C-CAC-CBC

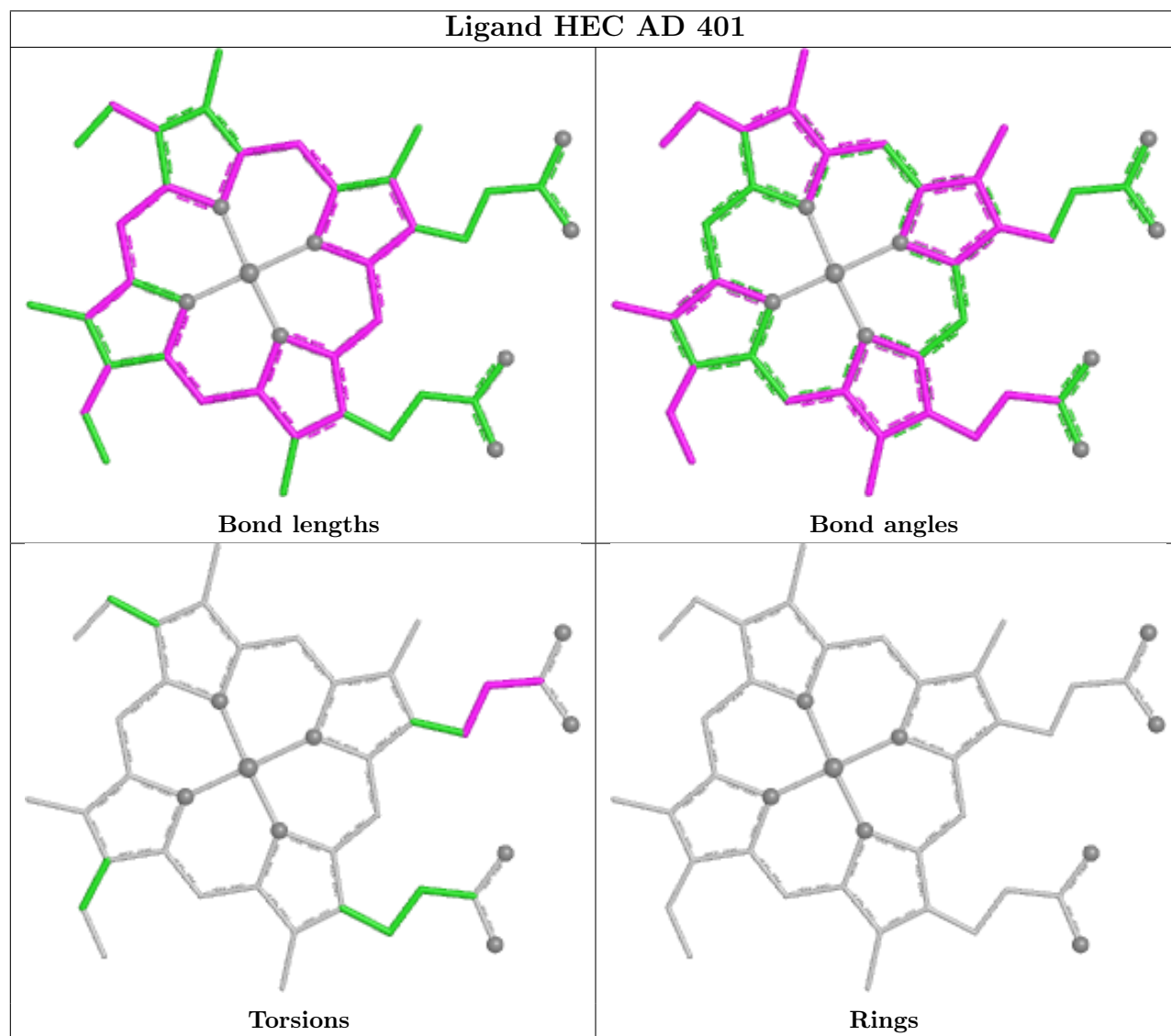
There are no ring outliers.

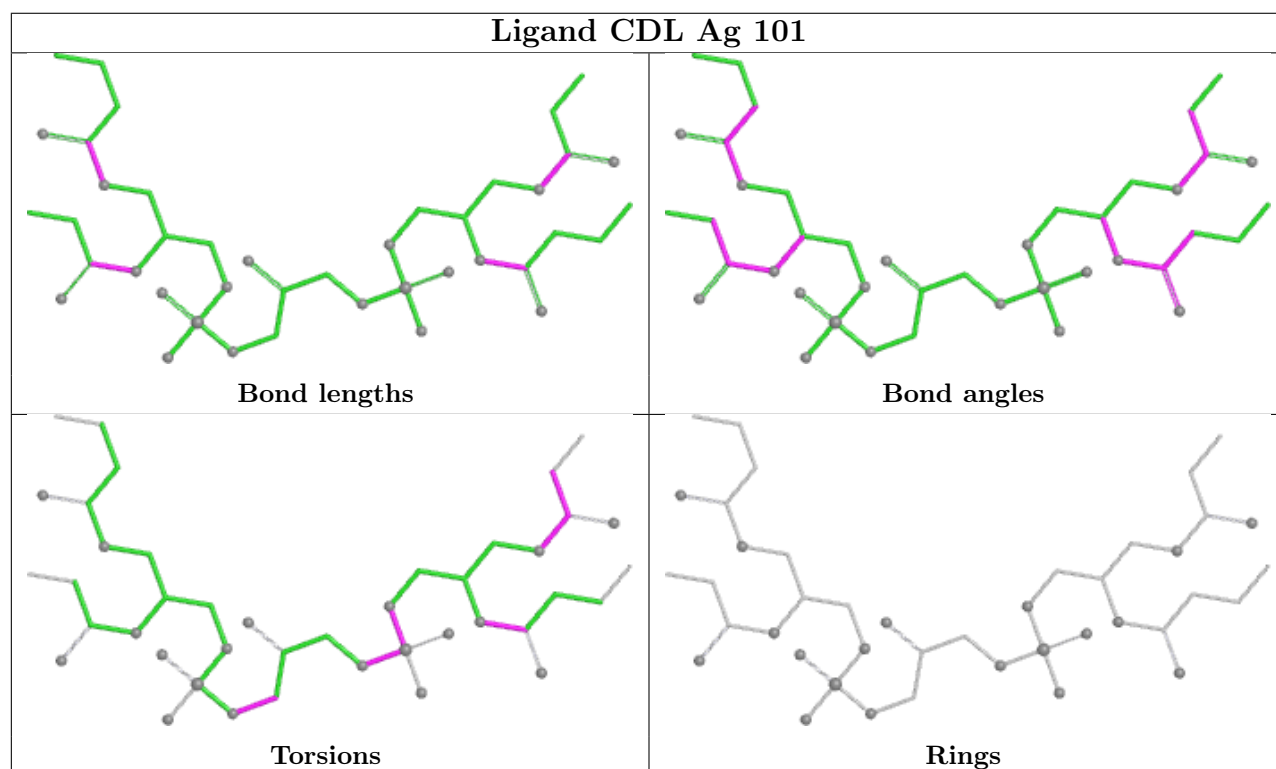
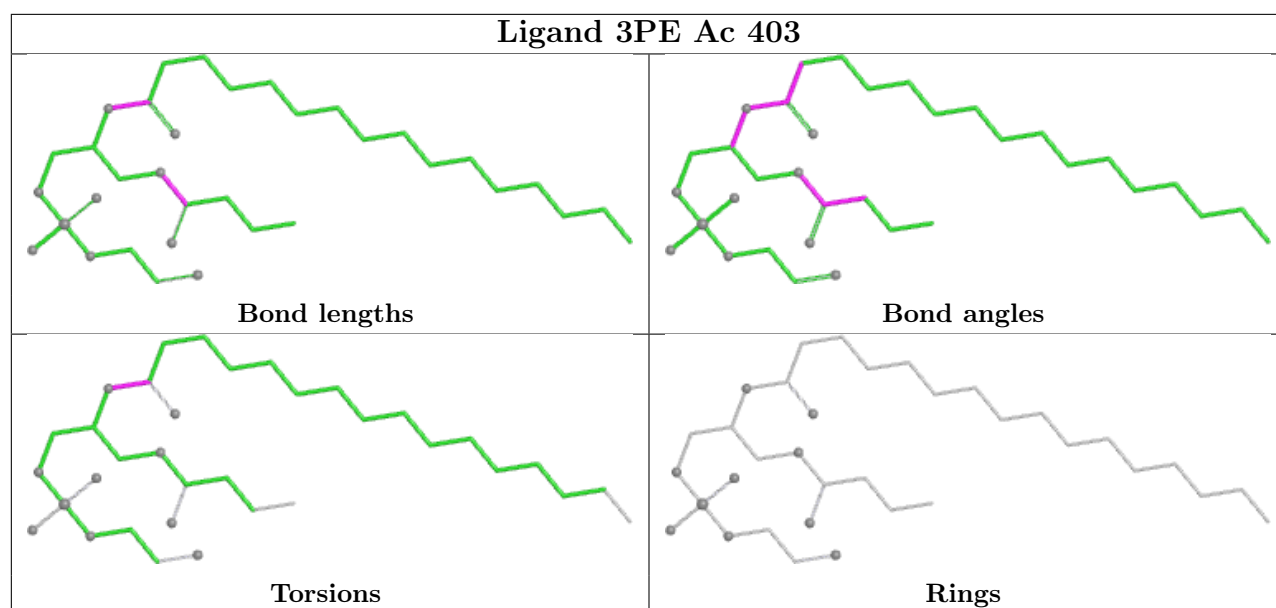
15 monomers are involved in 174 short contacts:

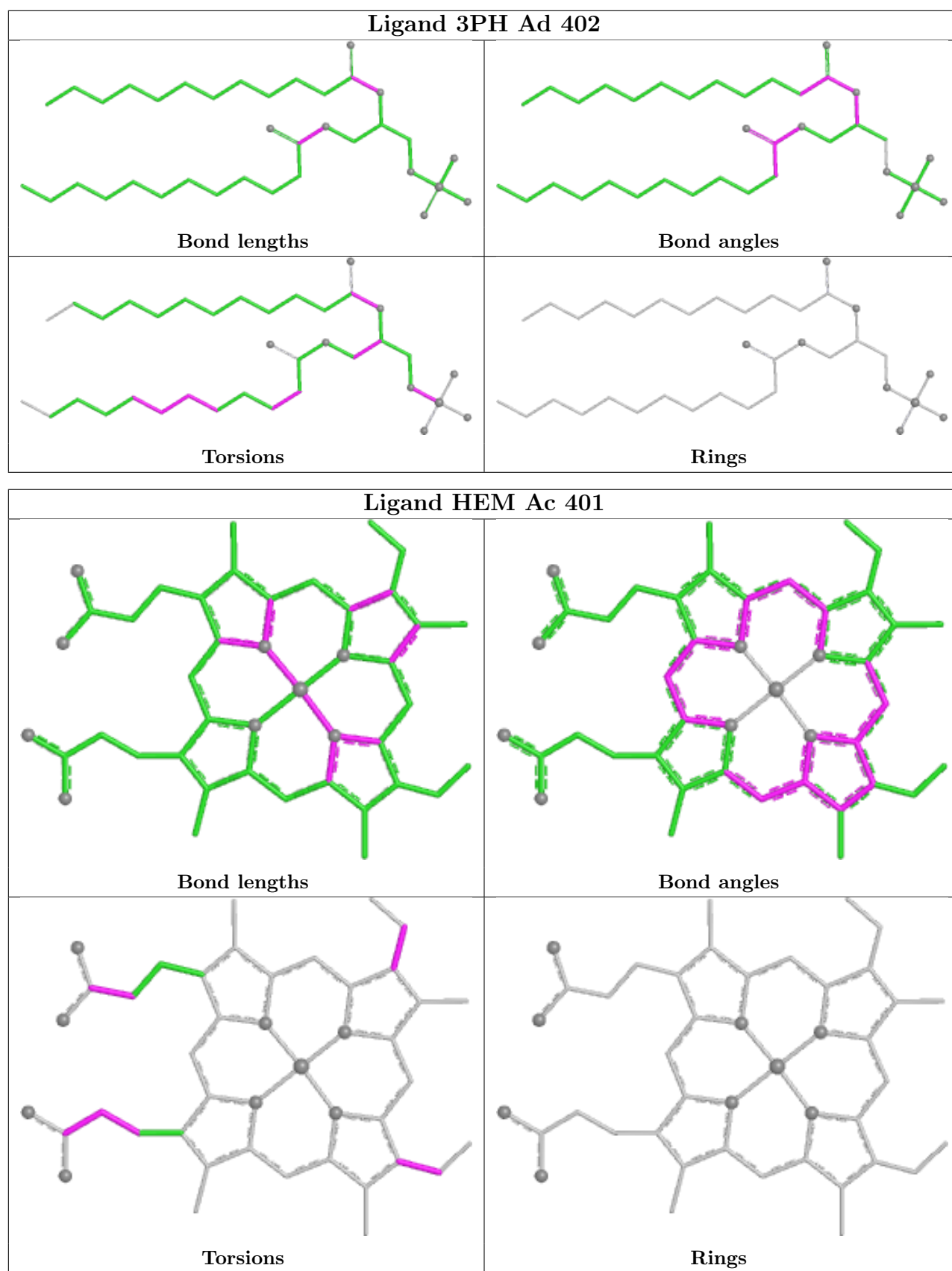
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	AD	401	HEC	18	0
14	Ac	403	3PE	7	0
17	Ag	101	CDL	5	0
16	Ad	402	3PH	39	0
11	Ac	401	HEM	1	0
11	Ac	402	HEM	10	0
14	Aa	501	3PE	3	0
12	Ac	405	UQ6	15	0
15	Ac	404	U10	20	0
11	AC	401	HEM	18	0
11	AC	402	HEM	9	0
17	Ag	102	CDL	4	0
14	Ag	103	3PE	9	0
13	Ad	401	HEC	12	0
12	AC	403	UQ6	11	0

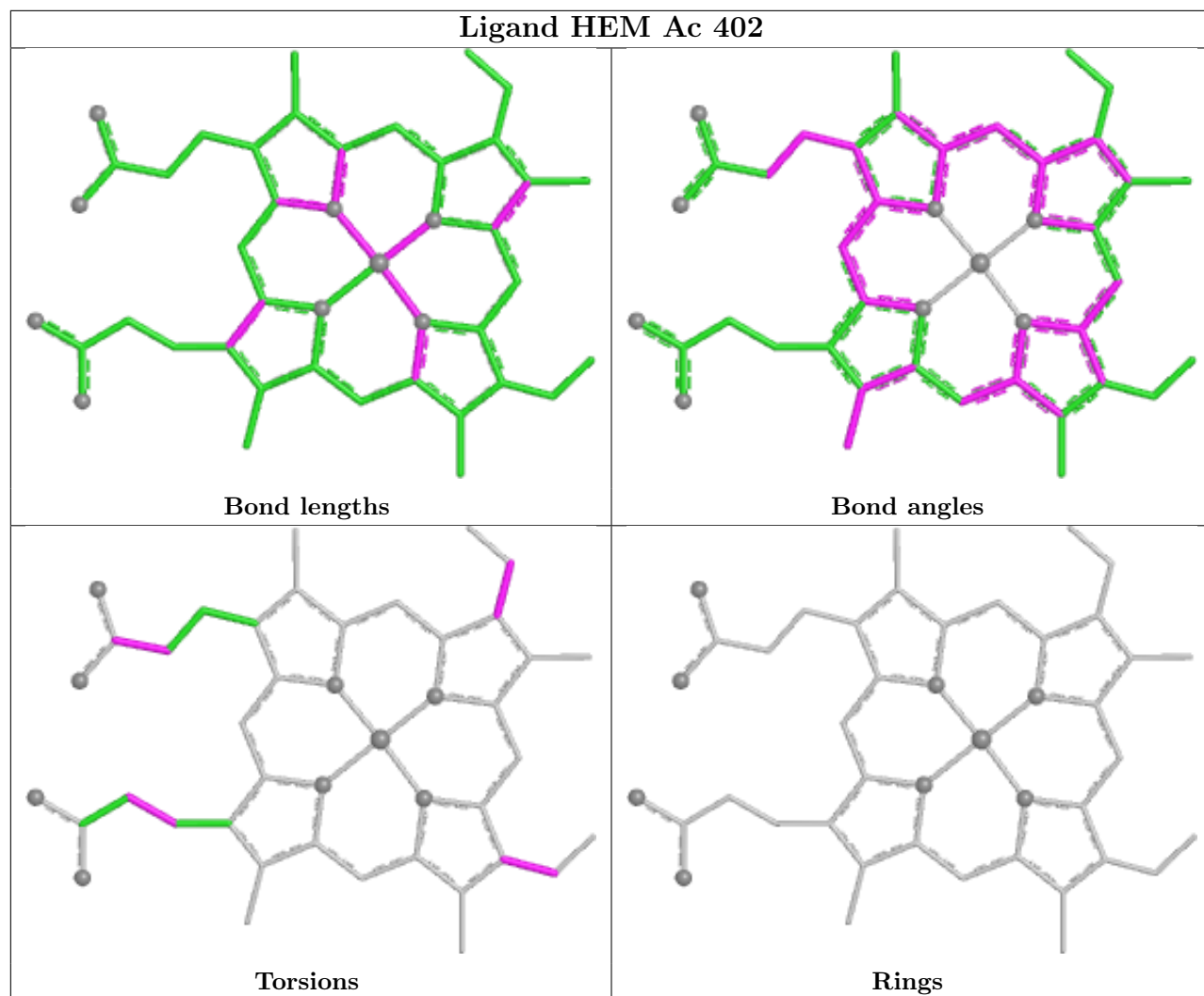
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

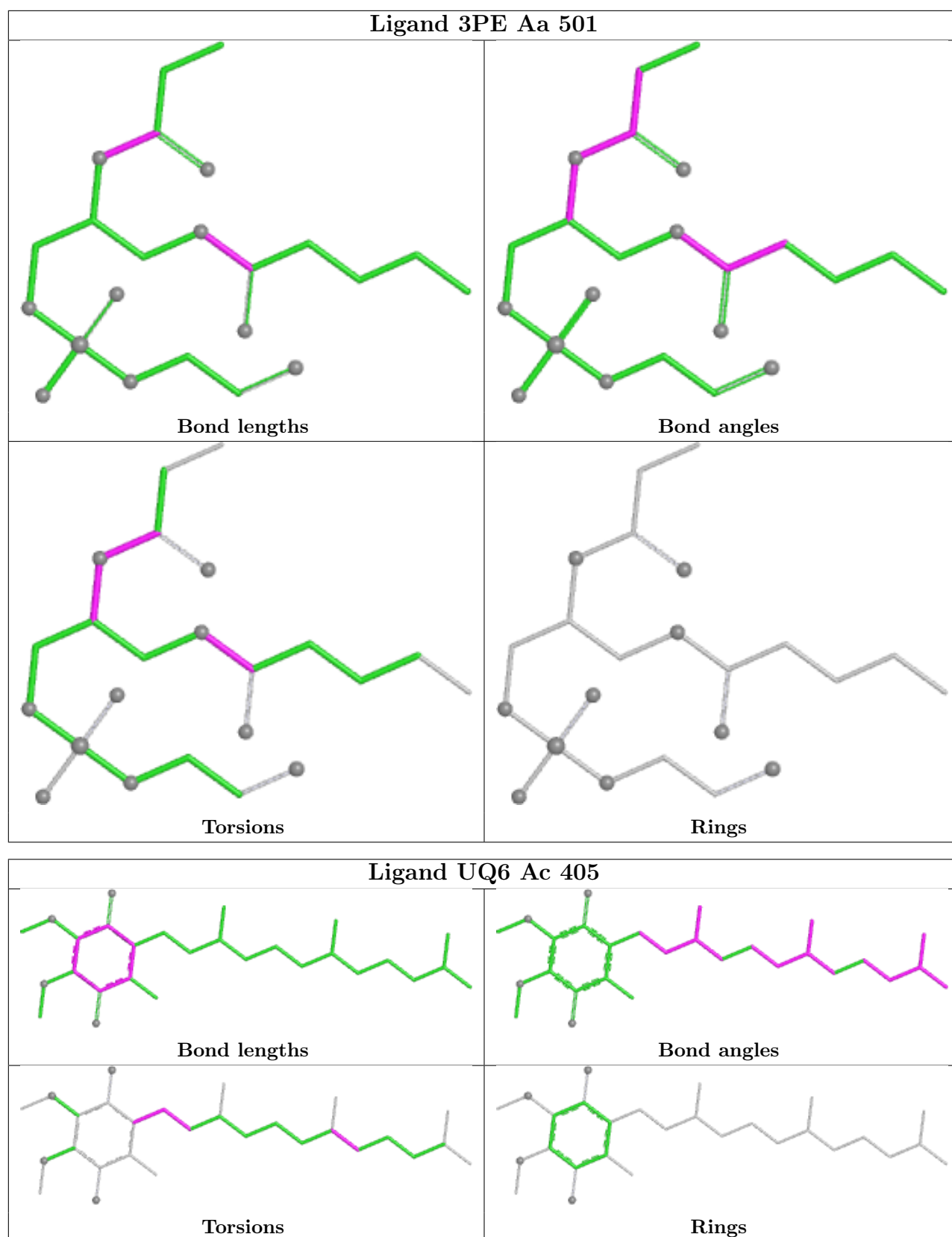
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

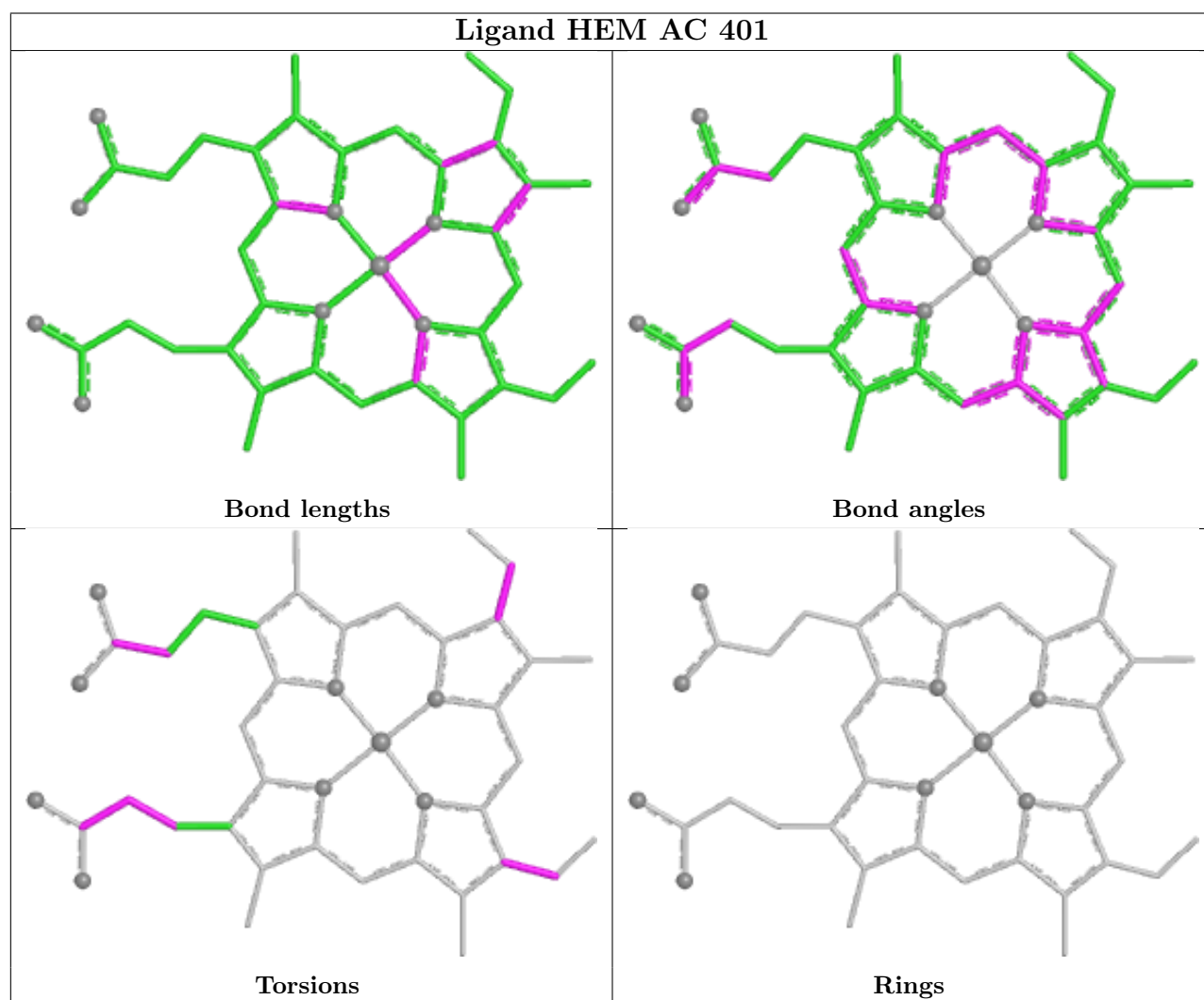
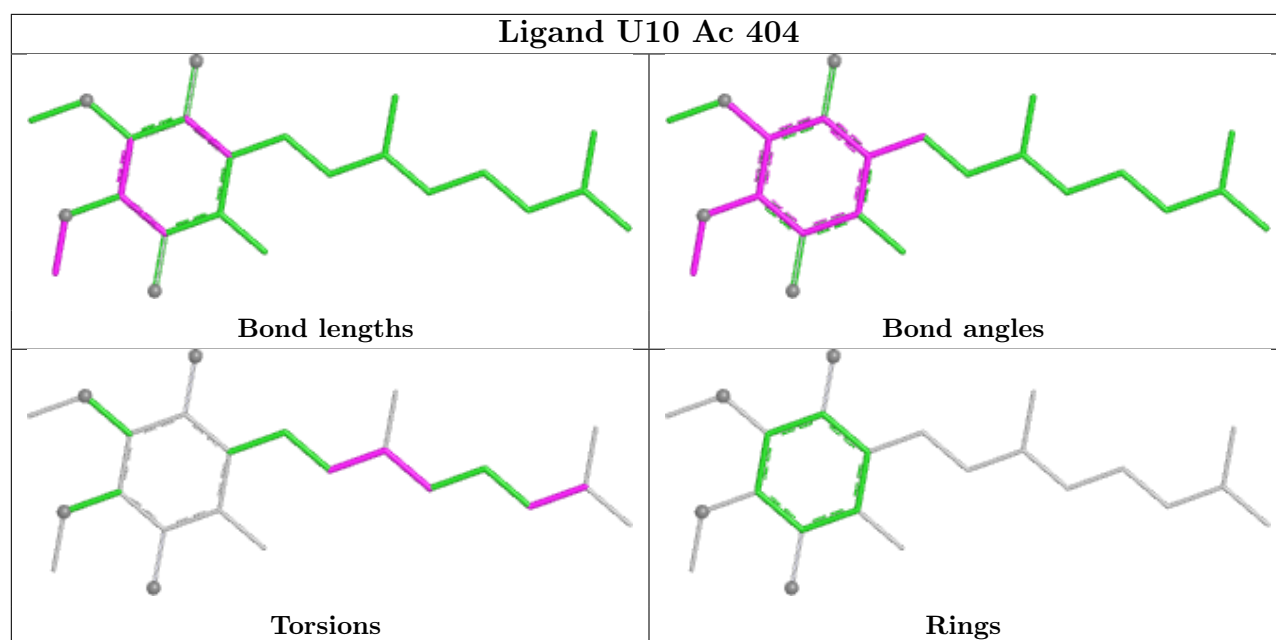




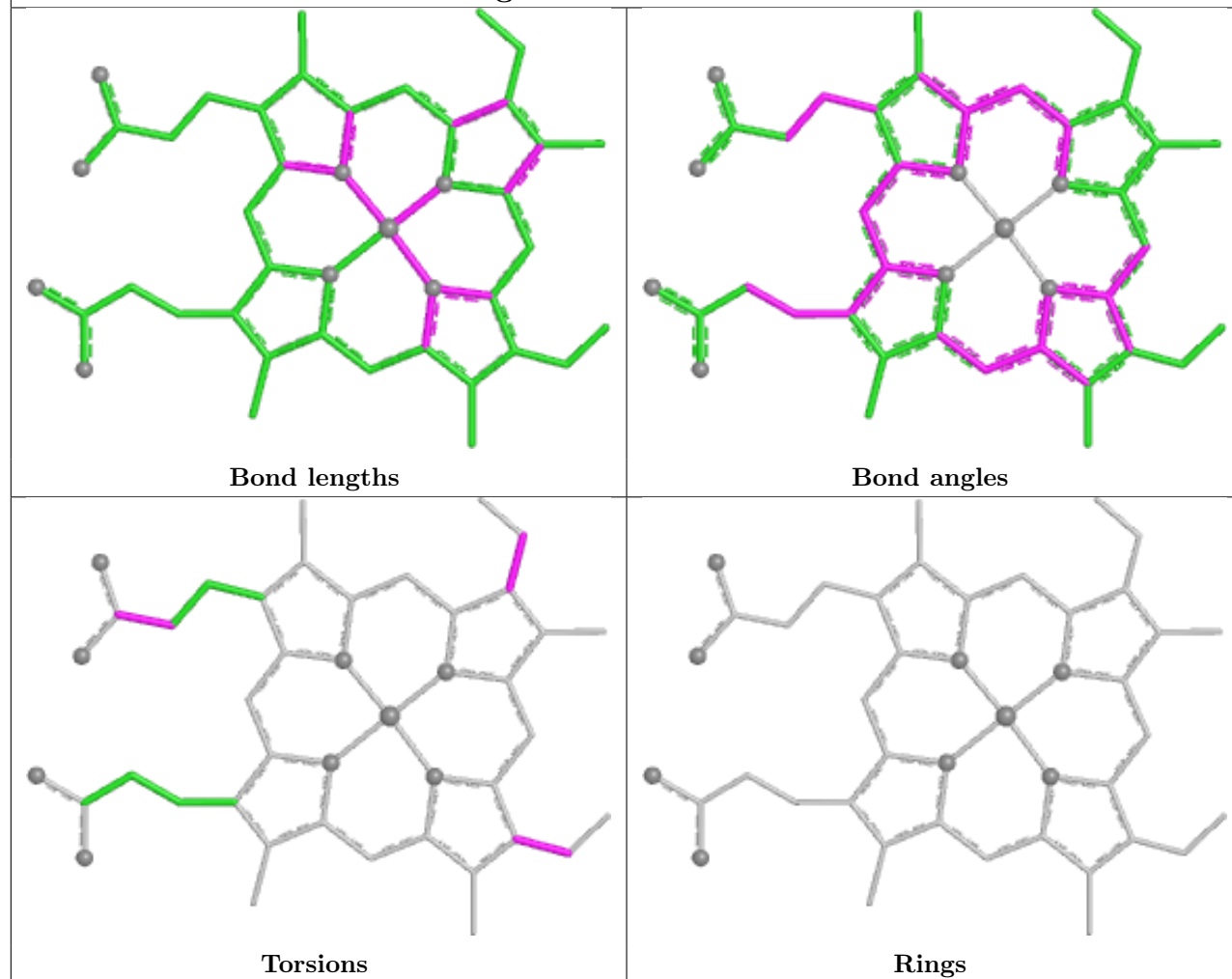




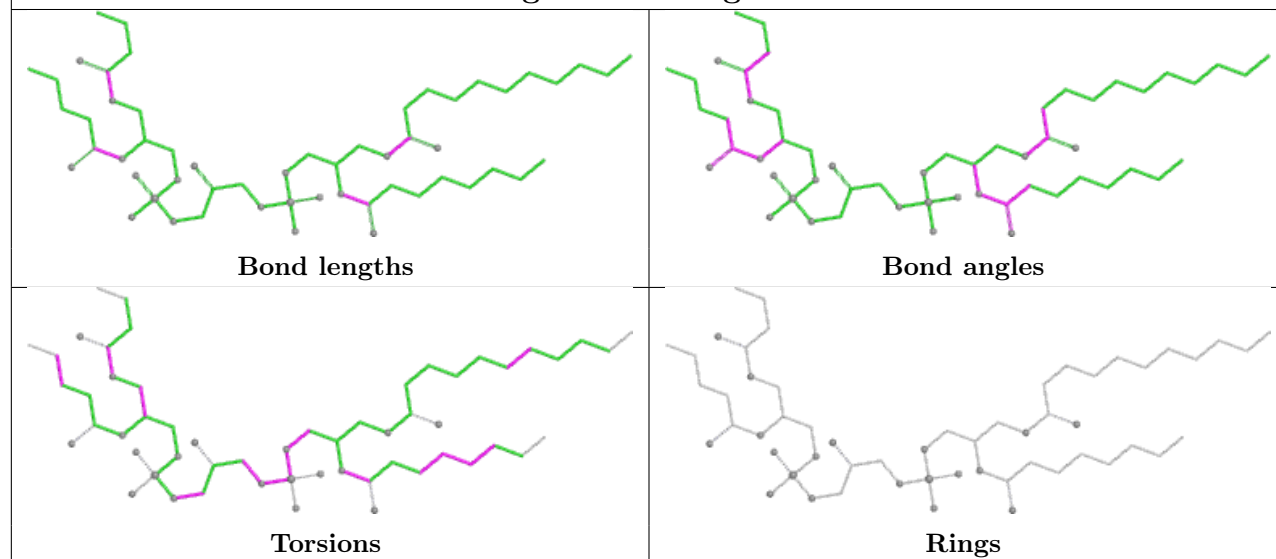


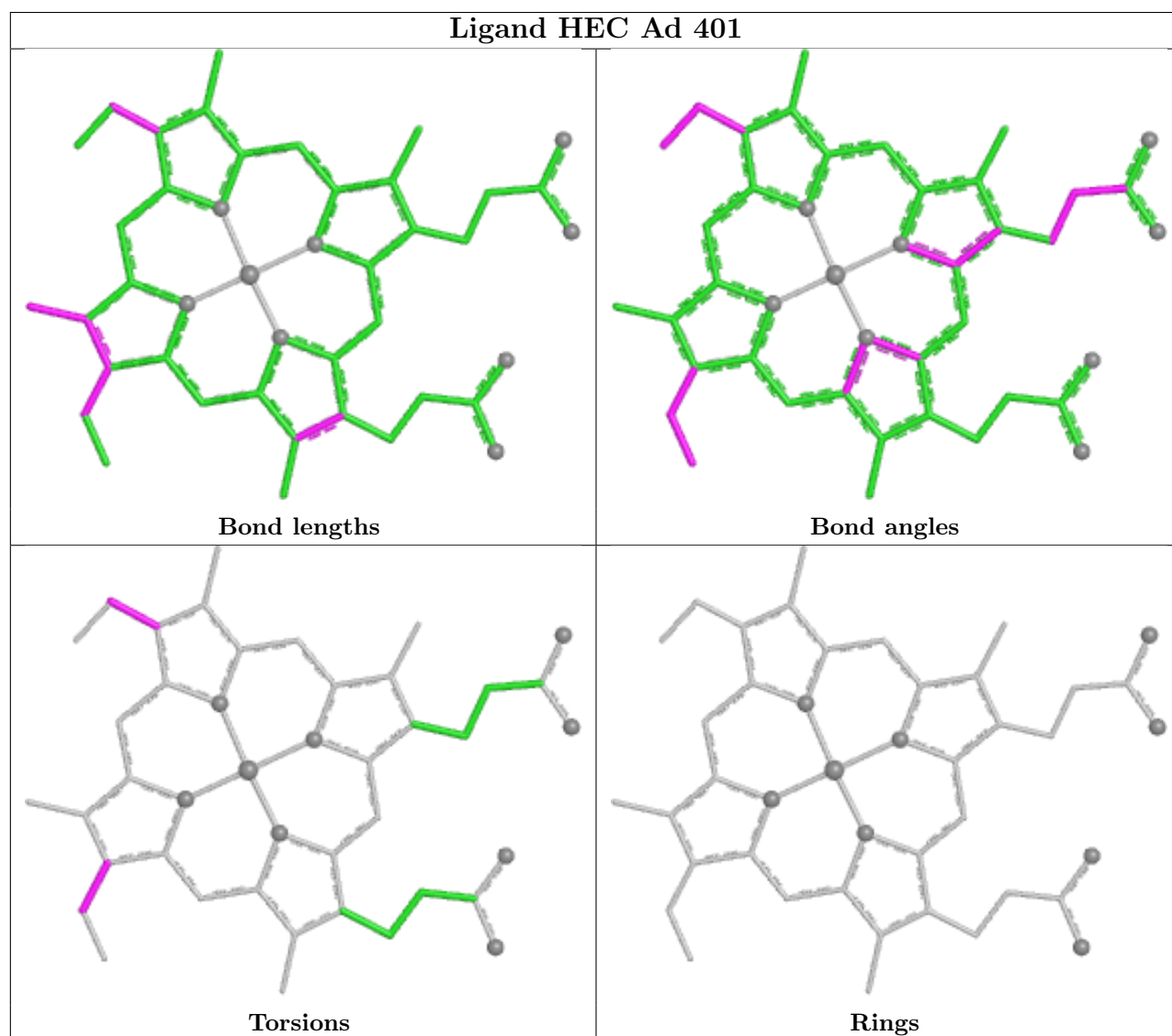
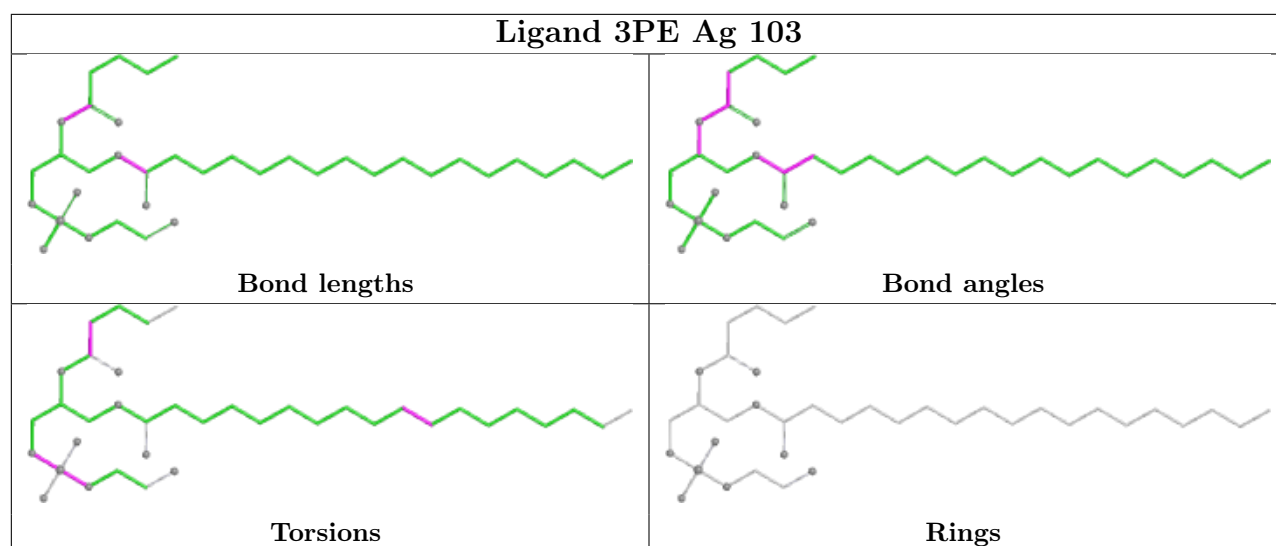


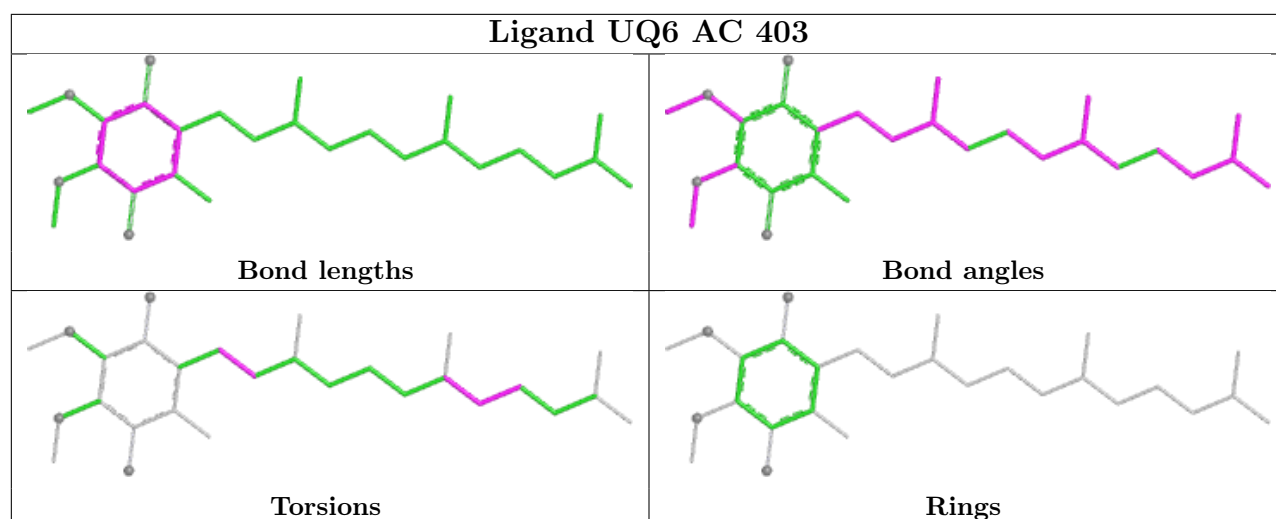
Ligand HEM AC 402



Ligand CDL Ag 102







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.

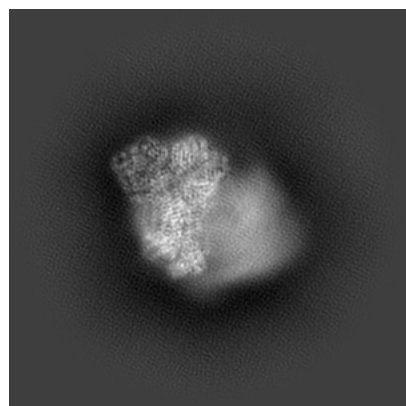
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35343. These allow visual inspection of the internal detail of the map and identification of artifacts.

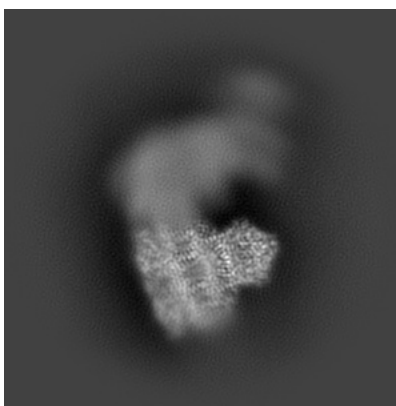
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

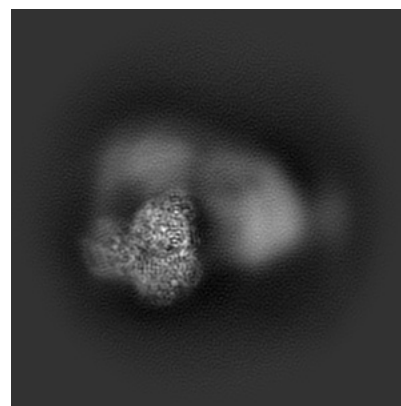
6.1.1 Primary map



X

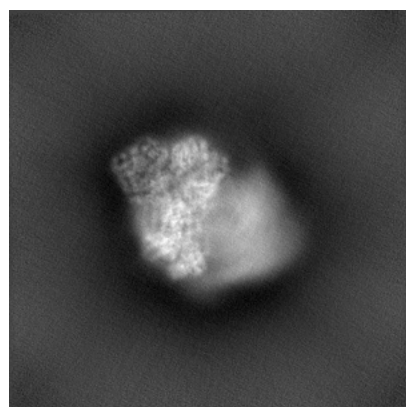


Y

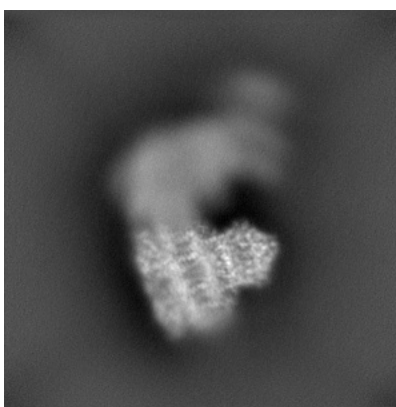


Z

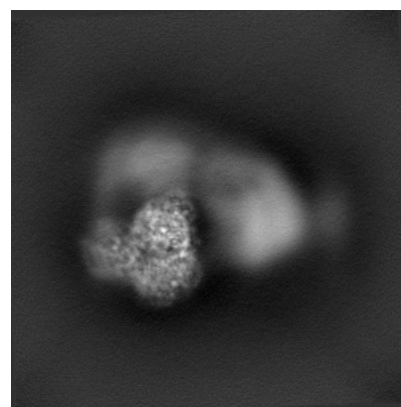
6.1.2 Raw map



X



Y

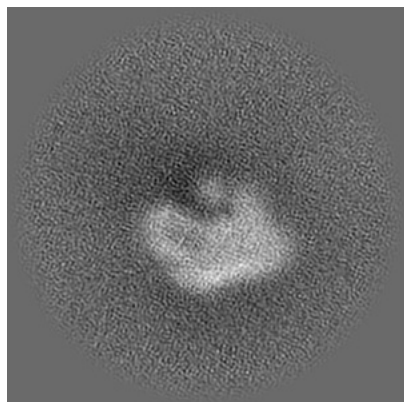


Z

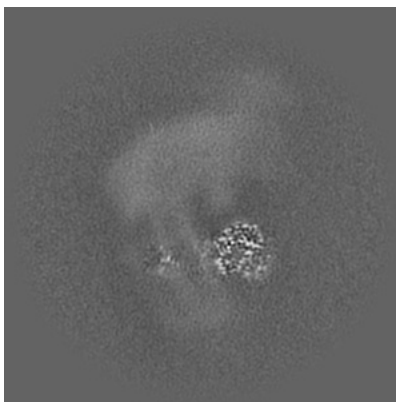
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

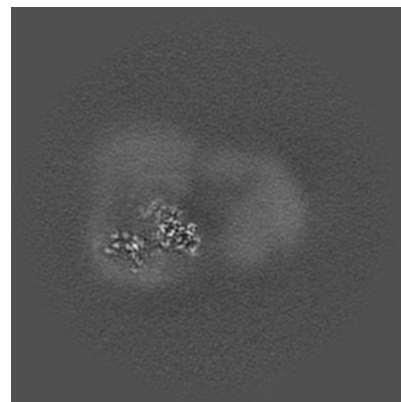
6.2.1 Primary map



X Index: 192

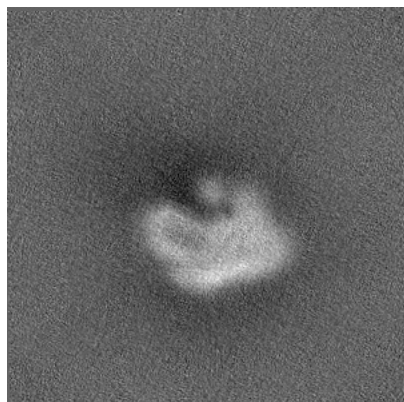


Y Index: 192

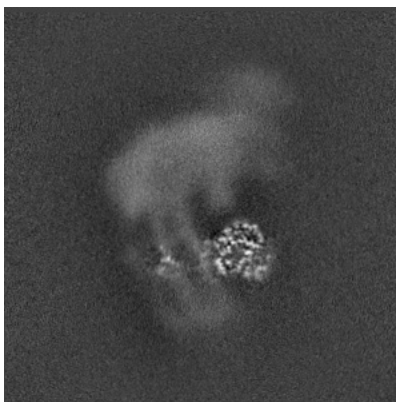


Z Index: 192

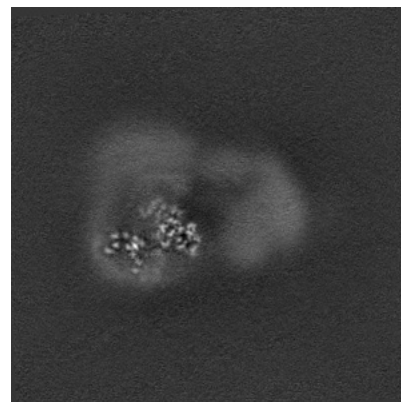
6.2.2 Raw map



X Index: 192



Y Index: 192

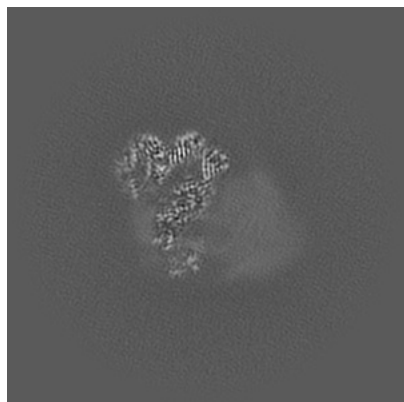


Z Index: 192

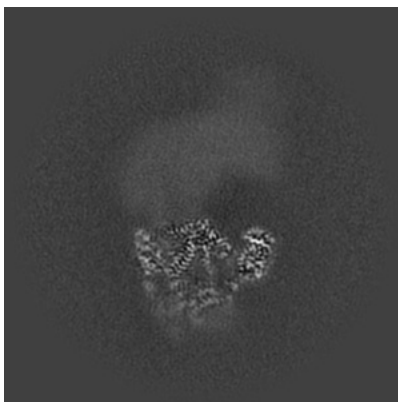
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

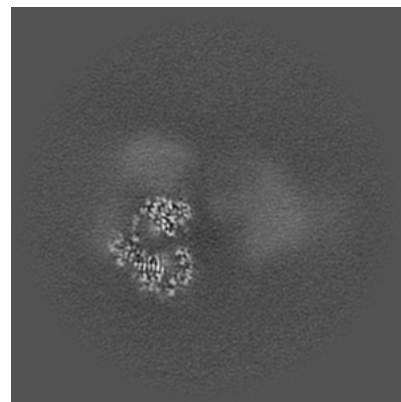
6.3.1 Primary map



X Index: 158

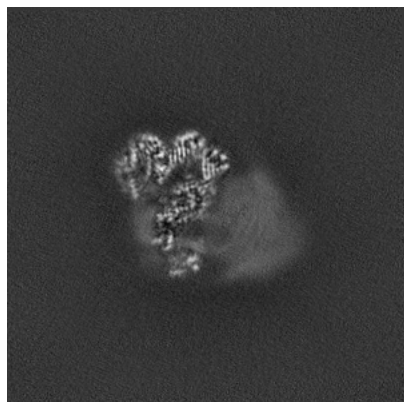


Y Index: 165

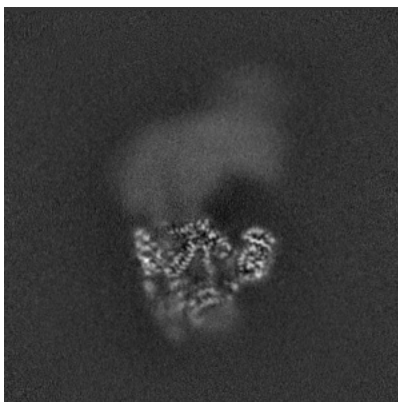


Z Index: 215

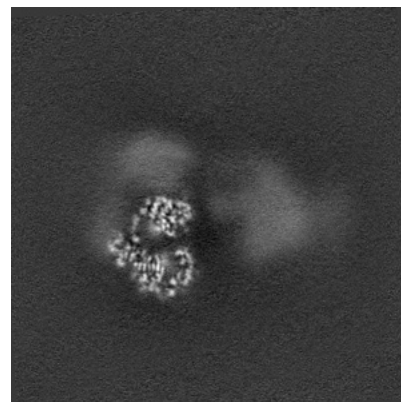
6.3.2 Raw map



X Index: 158



Y Index: 165

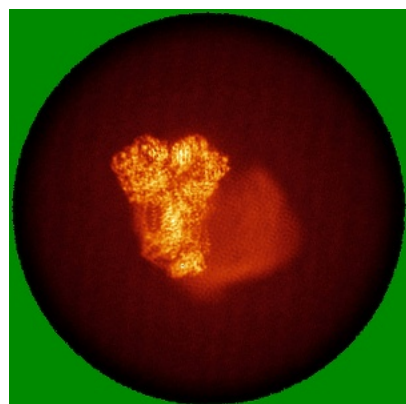


Z Index: 215

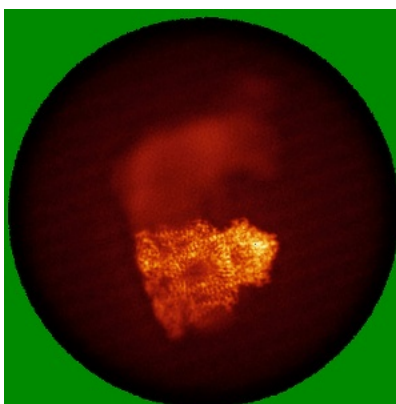
The images above show the largest variance slices of the map in three orthogonal directions.

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

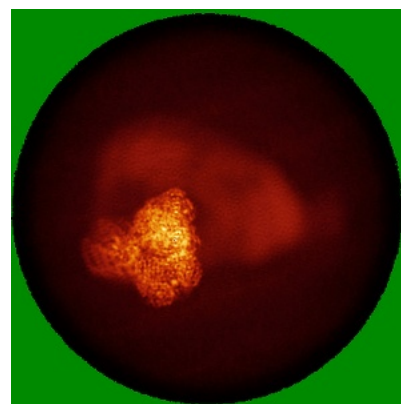
6.4.1 Primary map



X

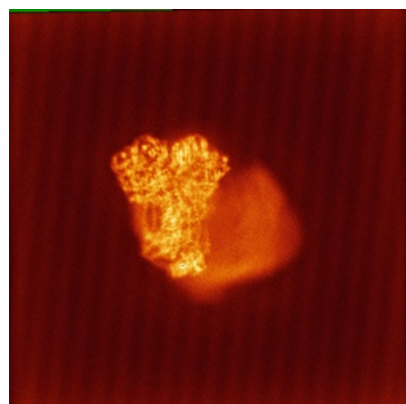


Y

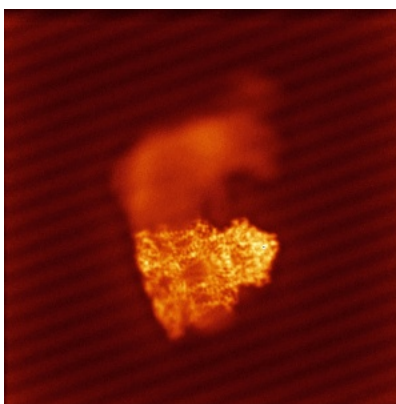


Z

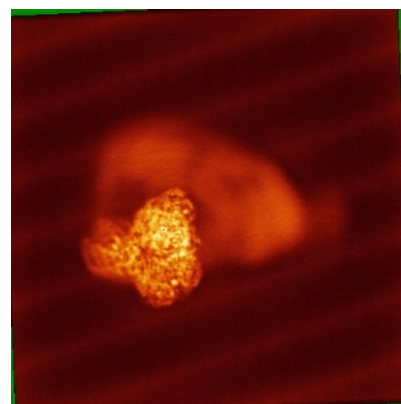
6.4.2 Raw map



X



Y

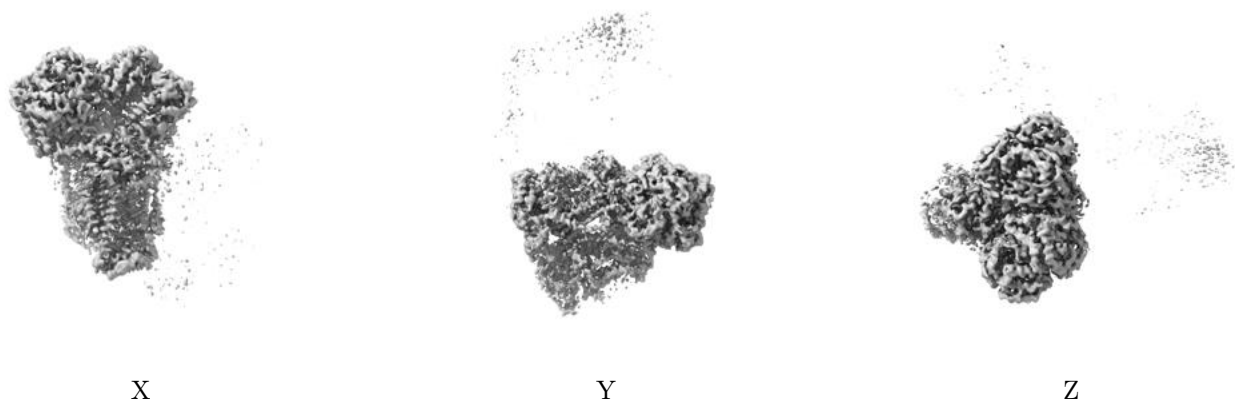


Z

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.

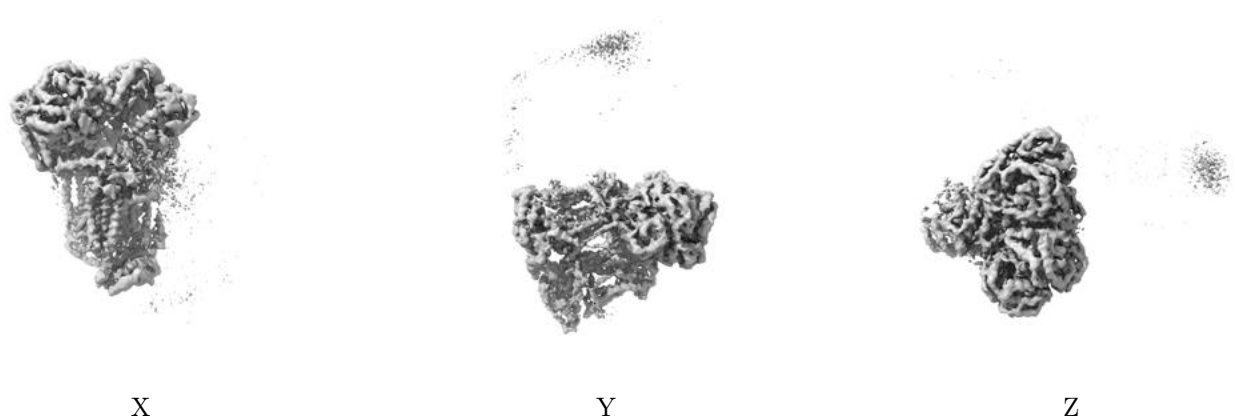
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

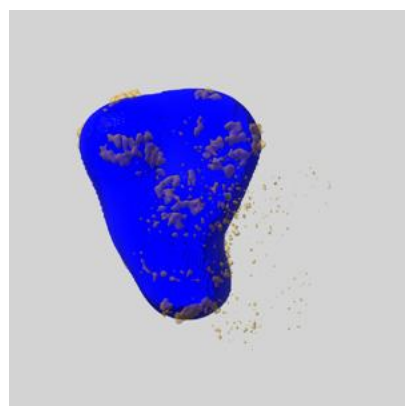
6.6 Mask visualisation [i](#)

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

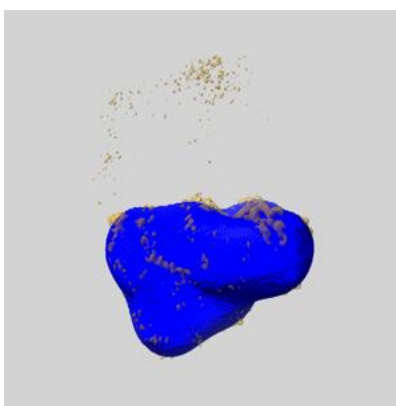
A mask typically either:

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

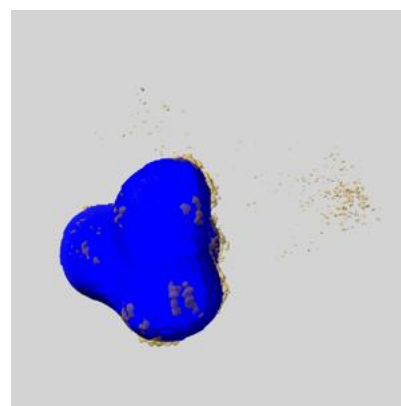
6.6.1 emd_35343_msk_1.map [i](#)



X



Y

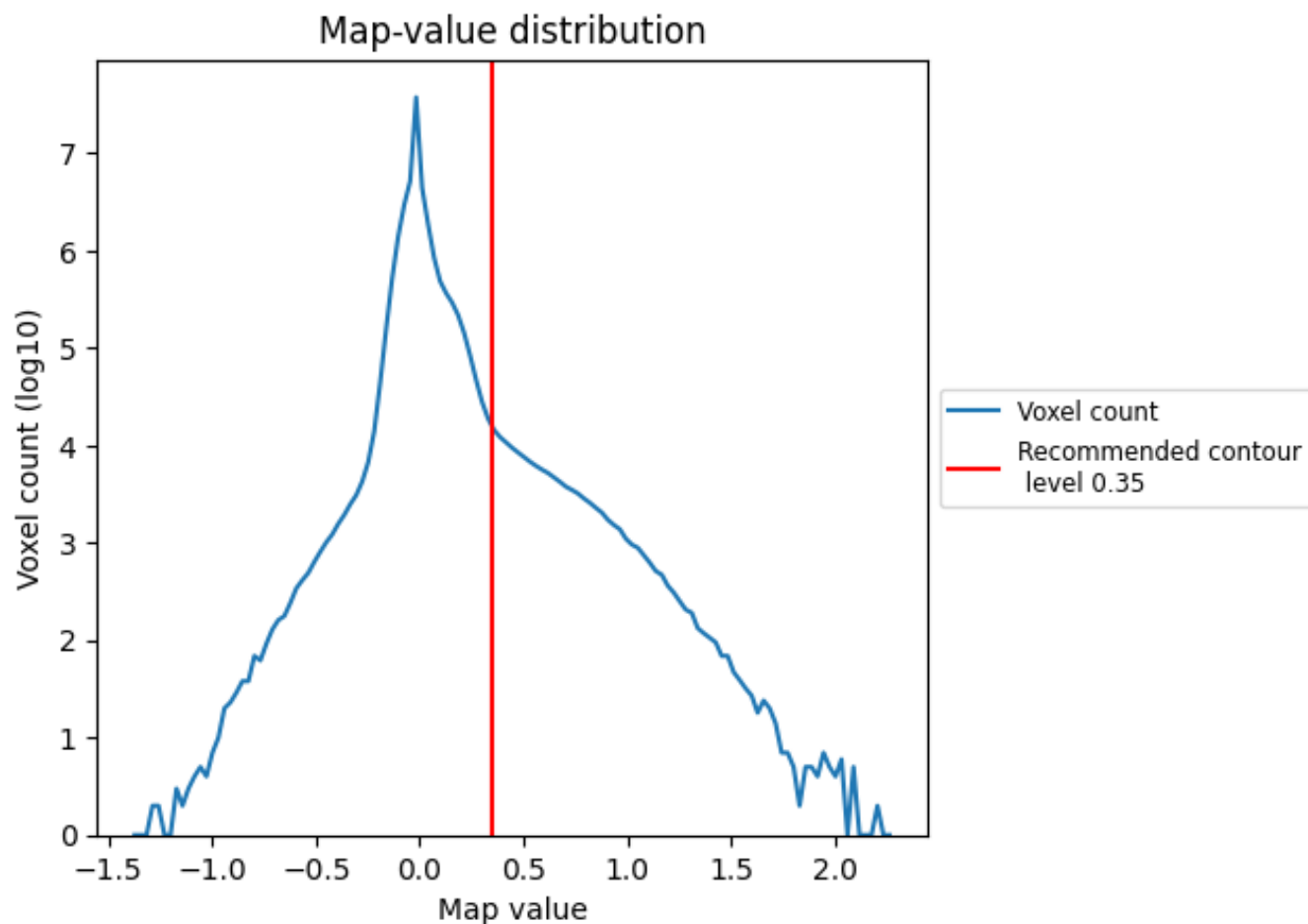


Z

7 Map analysis [i](#)

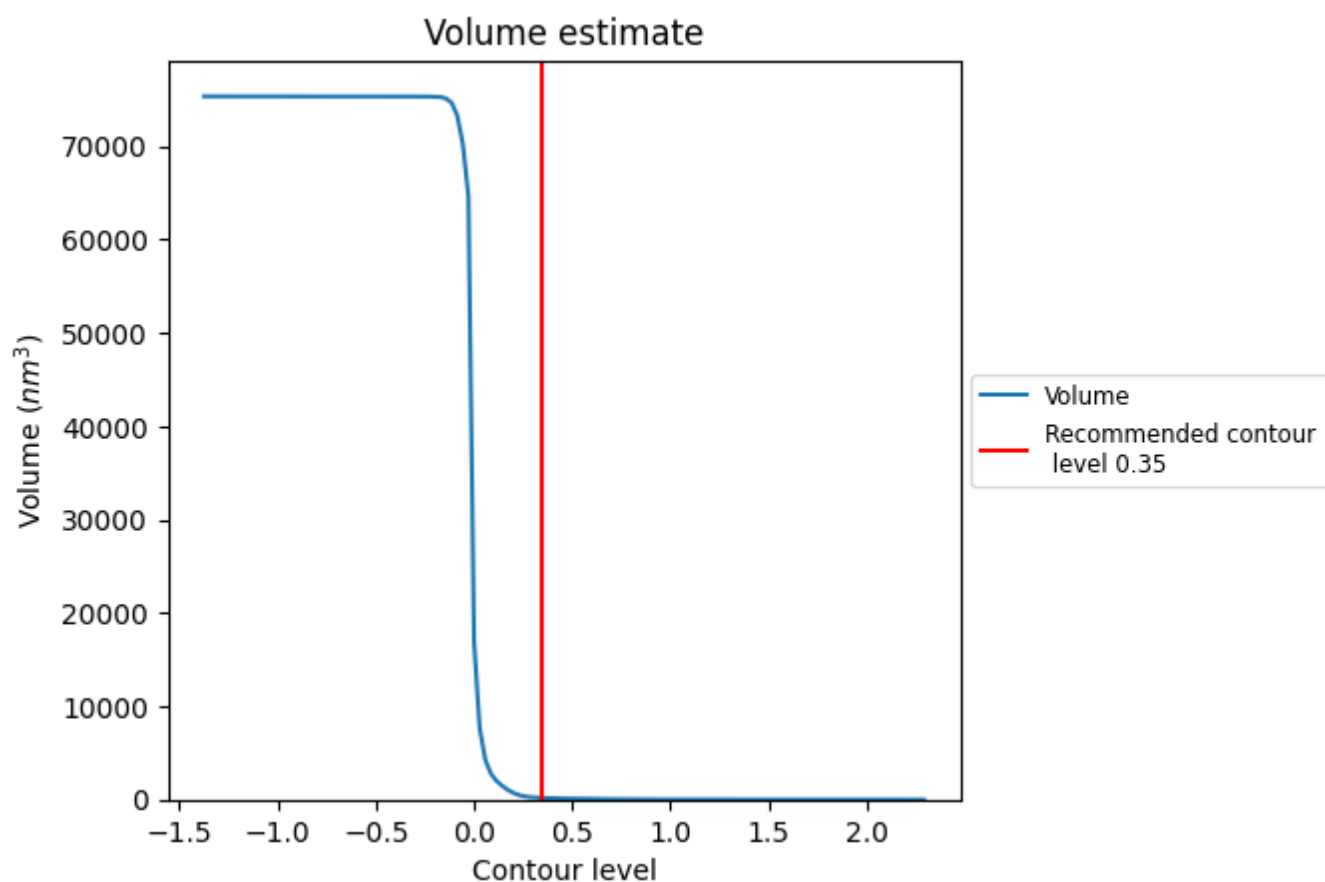
This section contains the results of statistical analysis of the map.

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.

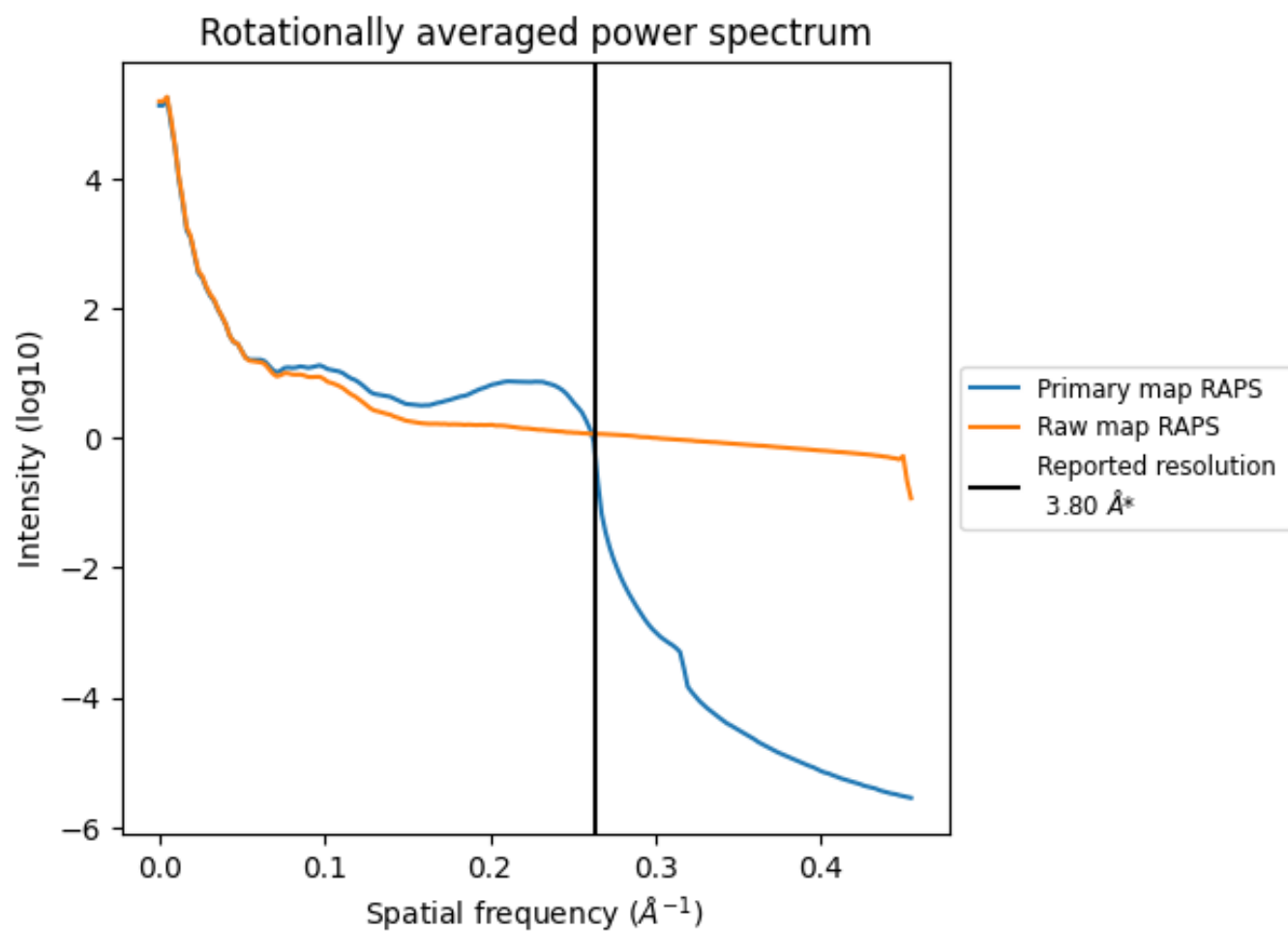
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

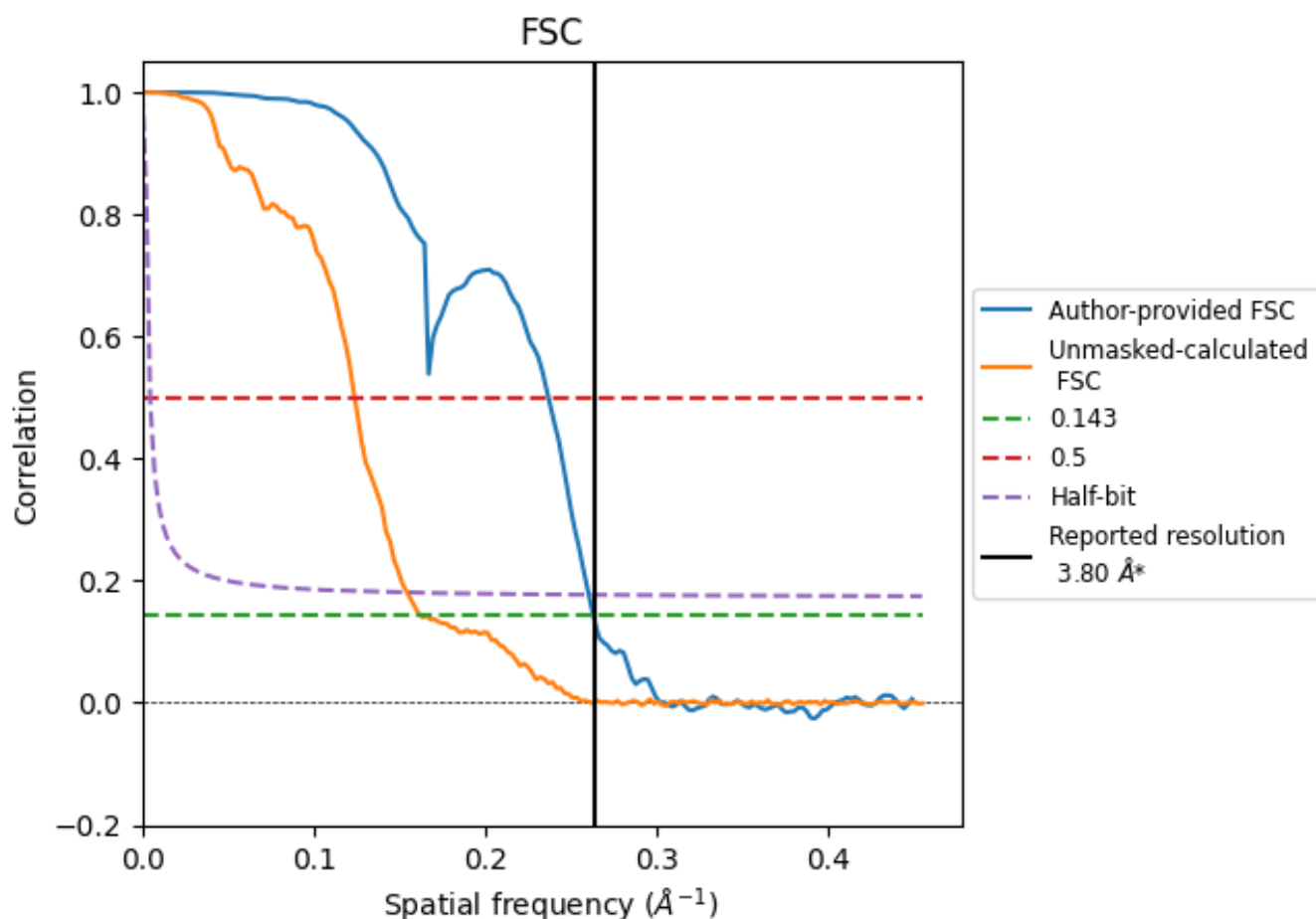


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

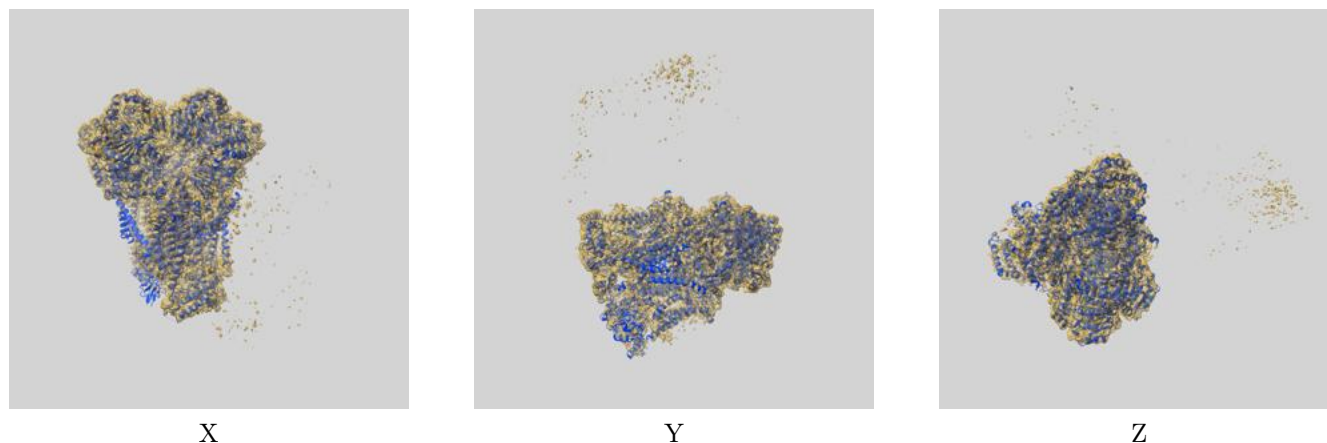
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.22	3.84
Unmasked-calculated*	6.17	8.08	6.48

*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 6.17 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

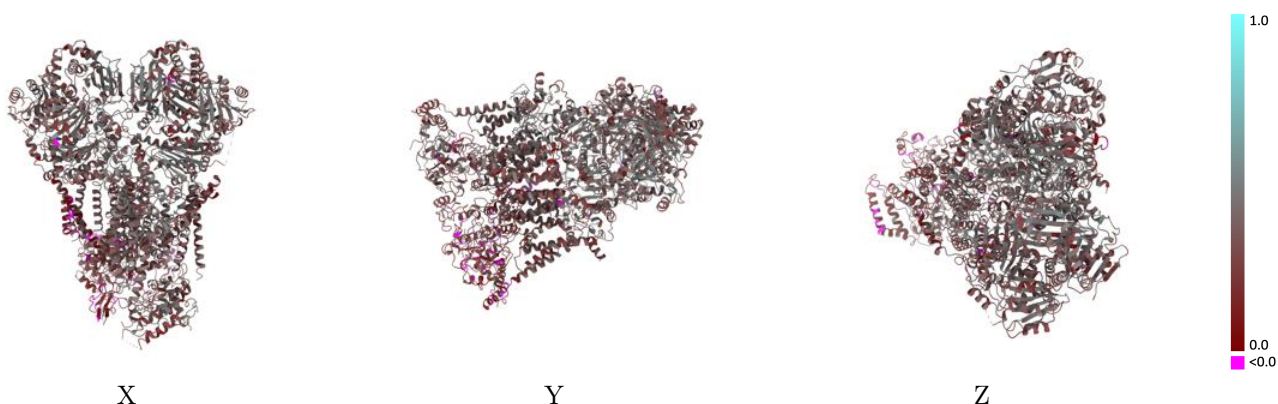
This section contains information regarding the fit between EMDB map EMD-35343 and PDB model 8IBG. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



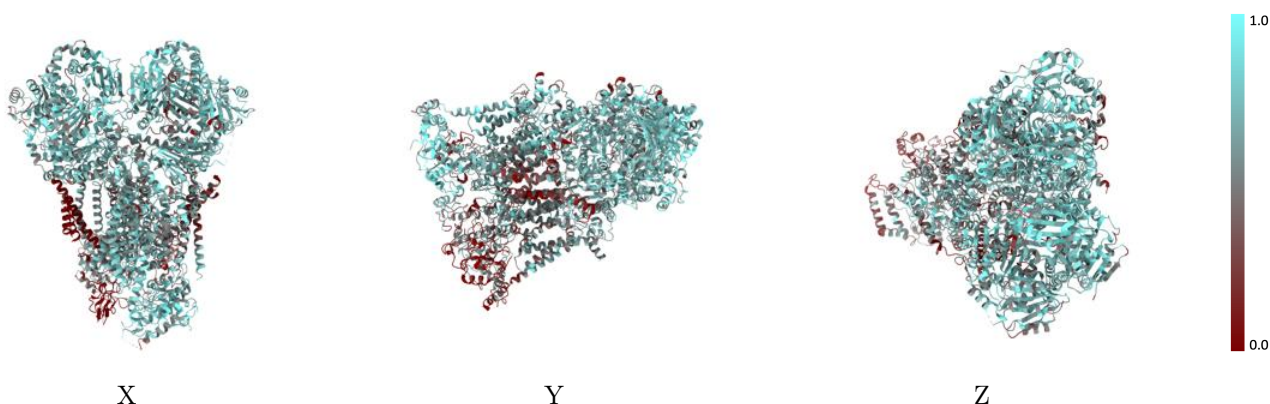
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



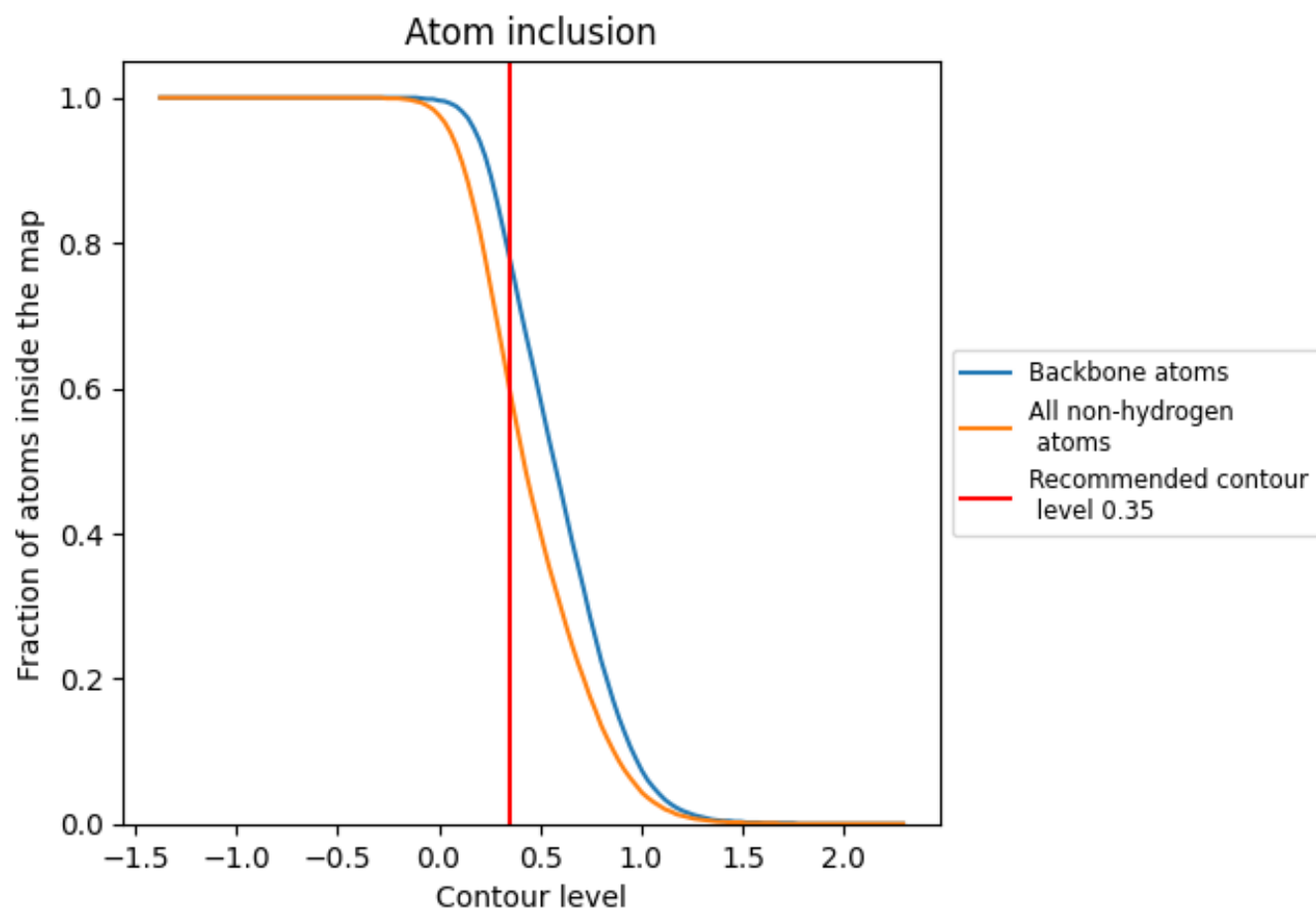
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5980	 0.3400
AA	 0.6840	 0.3720
AB	 0.7140	 0.3880
AC	 0.5610	 0.3140
AD	 0.5090	 0.2460
AE	 0.0830	 0.1740
AF	 0.6650	 0.3680
AG	 0.4360	 0.3030
AH	 0.3090	 0.1520
AI	 0.3780	 0.2840
AJ	 0.0190	 0.1070
AK	 0.0090	 0.1800
Aa	 0.6980	 0.3920
Ab	 0.7300	 0.3910
Ac	 0.6500	 0.3660
Ad	 0.7240	 0.3610
Ae	 0.2010	 0.2350
Af	 0.6820	 0.3860
Ag	 0.6460	 0.4020
Ah	 0.6730	 0.3020
Ai	 0.3890	 0.2640
Aj	 0.4180	 0.2910
Ak	 0.1460	 0.2830

