



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:44 AM UTC

PDB ID : 8ZOS / pdb_00008zos
EMDB ID : EMD-60317
Title : Cryo-EM structure of pyraclostrobin-bound porcine bc1 complex
Authors : Wang, Y.X.; Sun, J.Y.; Li, Z.W.; Cui, G.R.; Yang, G.F.
Deposited on : 2024-05-29
Resolution : 2.37 Å (reported)

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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:

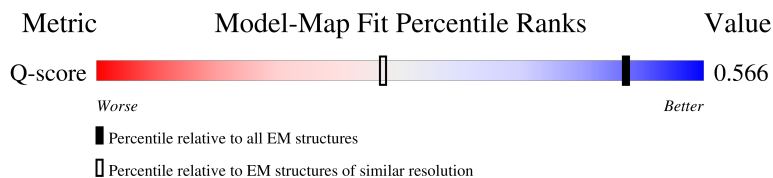
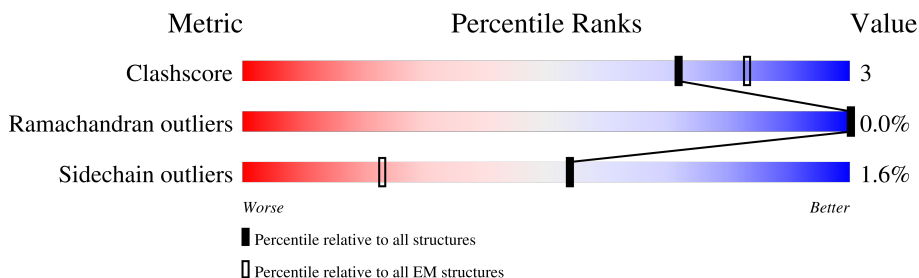
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.37 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	4742 (1.87 - 2.87)

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	A	378	91% 9%
1	a	378	92% 8%
2	B	241	22% 83% 16%
2	b	241	20% 87% 12%

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Mol	Chain	Length	Quality of chain
3	C	196	86% 84% 15% ..
3	c	196	89% 82% 18%
4	D	446	95% .
4	d	446	96% .
5	E	418	94% 6%
5	e	418	93% 7%
6	F	64	48% 84% 12% ..
6	f	64	50% 86% 11% ..
7	G	106	8% 98% .
7	g	106	8% 97% .
8	H	79	8% 90% 10%
8	h	79	15% 91% 9%
9	I	62	68% 71% 24% 5%
9	i	62	69% 65% 29% 6%
10	J	52	94% 75% 19% 6%
10	j	52	98% 83% 15% .
11	K	57	33% 79% 16% 5%
11	k	57	35% 75% 19% 5%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 33531 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	378	Total 3017	C 2026	N 470	O 501	S 20	0	0
1	a	378	Total 3017	C 2026	N 470	O 501	S 20	0	0

- Molecule 2 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	241	Total 1920	C 1225	N 330	O 349	S 16	0	0
2	b	239	Total 1904	C 1214	N 327	O 347	S 16	0	0

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	194	Total 1502	C 946	N 261	O 288	S 7	0	0
3	c	196	Total 1517	C 954	N 265	O 291	S 7	0	0

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	445	Total 3452	C 2157	N 604	O 672	S 19	0	0
4	d	446	Total 3459	C 2161	N 605	O 674	S 19	0	0

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		
5	e	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
6	f	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
7	g	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			608	399	112	95	2		
8	h	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	62	Total	C	N	O	0	0
			507	331	90	86		
9	i	62	Total	C	N	O	0	0
			507	331	90	86		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

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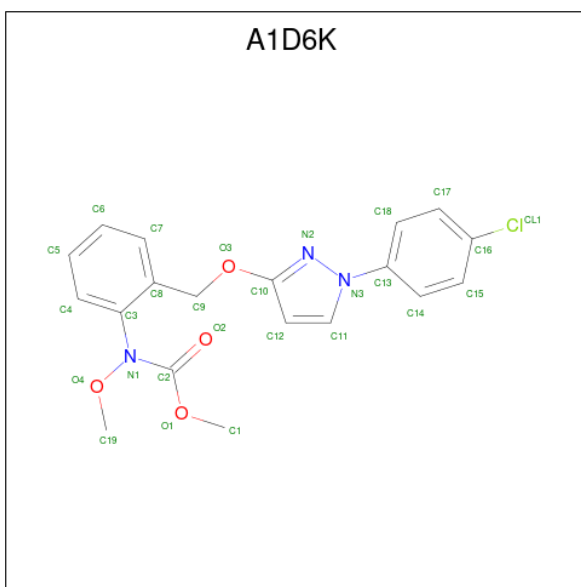
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	51	Total 421	C 281	N 74	O 65	S 1	0	0

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	57	Total 404	C 252	N 74	O 76	S 2	0	0
11	k	57	Total 404	C 252	N 74	O 76	S 2	0	0

- Molecule 12 is methyl {N}-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]phenyl]- {N}-methoxy-carbamate (CCD ID: A1D6K) (formula: C₁₉H₁₈ClN₃O₄) (labeled as "Ligand of Interest" by depositor).

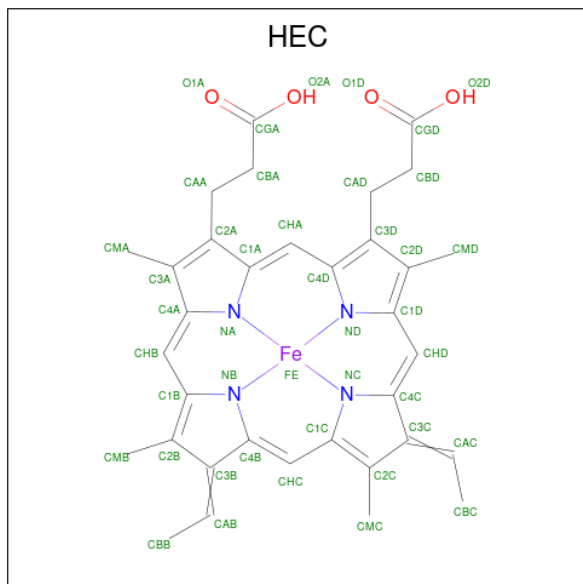


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
12	A	1	Total 27	C 19	Cl 1	N 3	O 4	0
12	a	1	Total 27	C 19	Cl 1	N 3	O 4	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

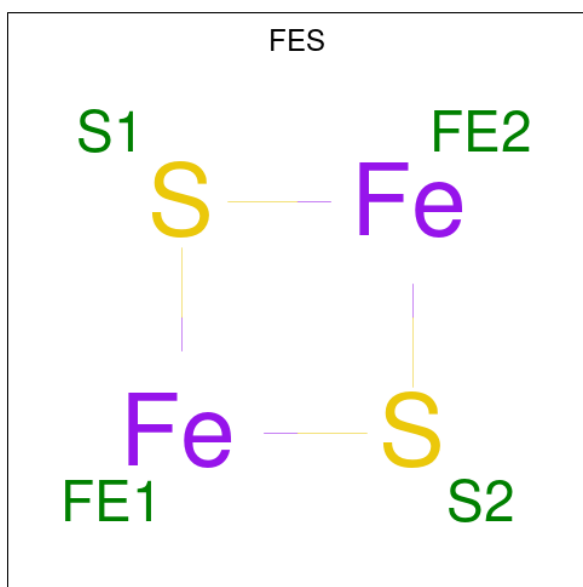
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
14	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



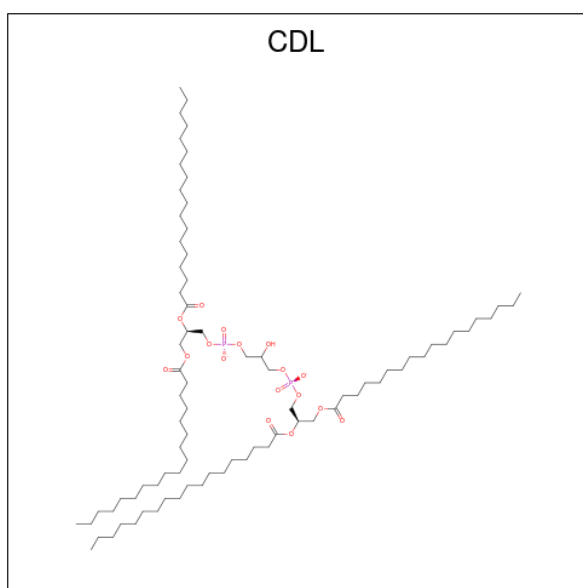
Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	a	1	4	2	2	0
16	c	1	4	2	2	0

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	a	1	64	45	17	2	0
17	a	1	64	45	17	2	0

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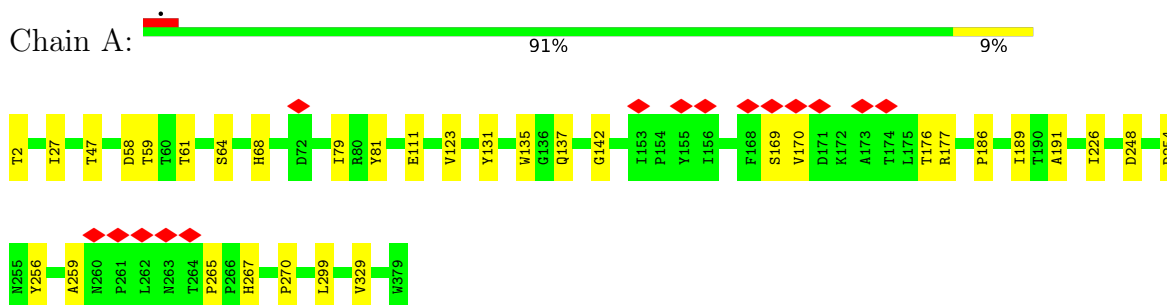
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
17	g	1	64	45	17	2	0

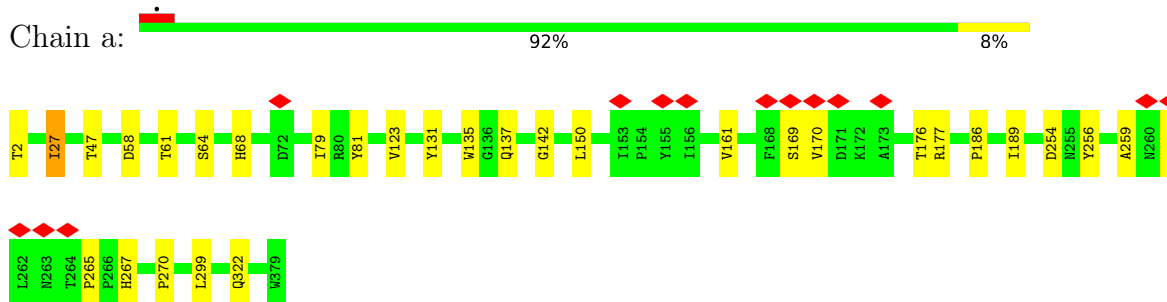
3 Residue-property plots [i](#)

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.

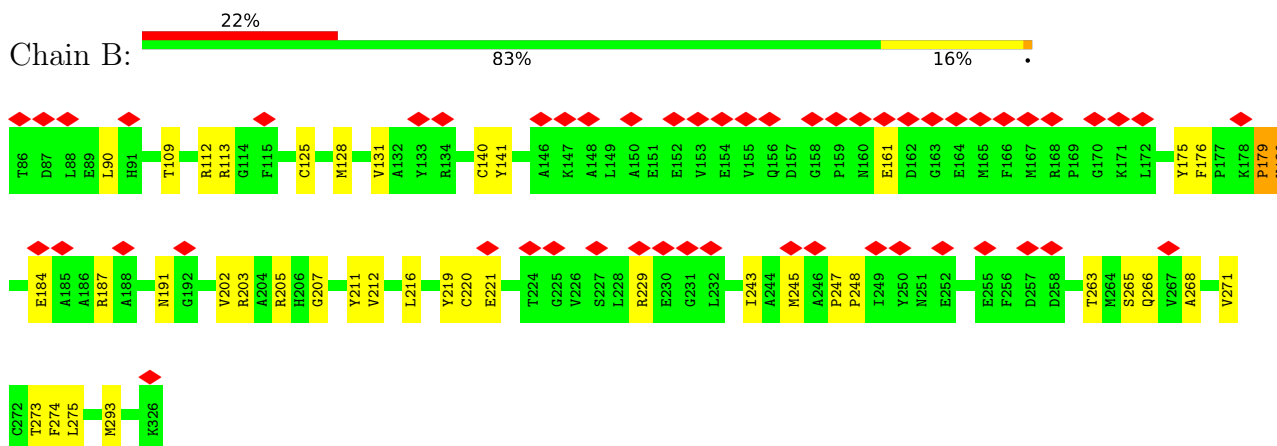
- Molecule 1: Cytochrome b



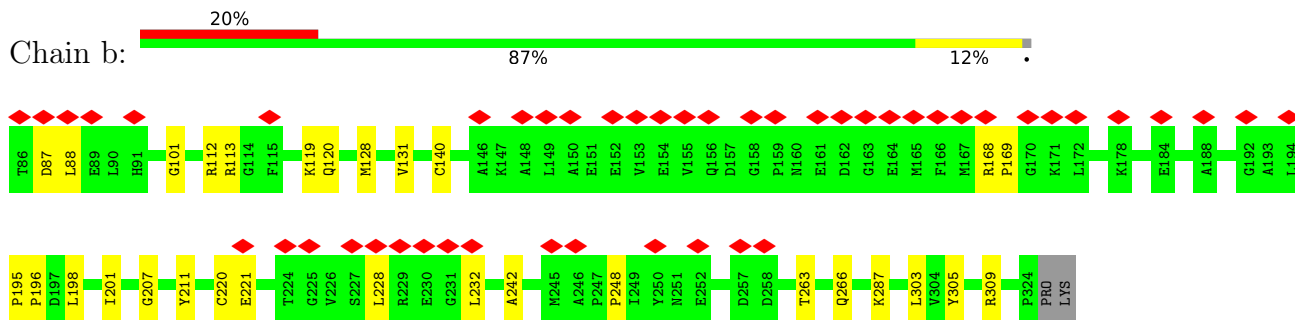
- Molecule 1: Cytochrome b



- Molecule 2: Cytochrome c1, heme protein, mitochondrial



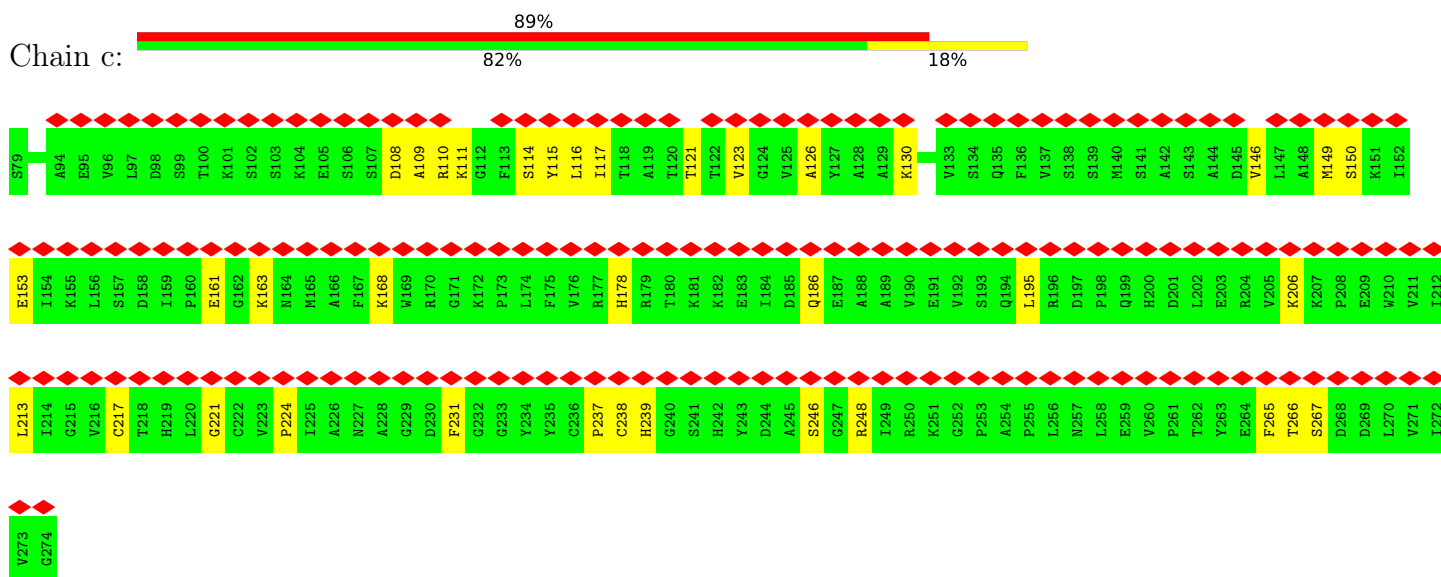
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

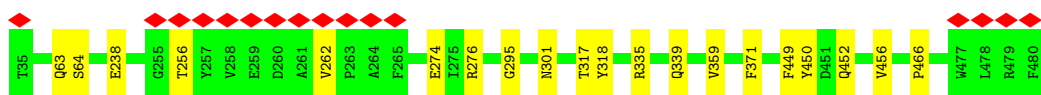


- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial





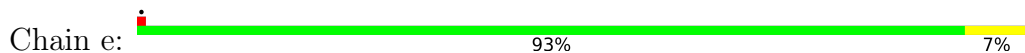
• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial



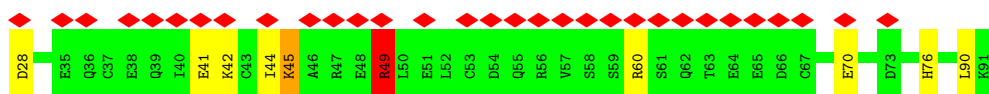
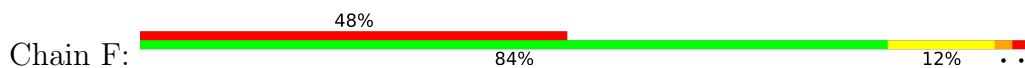
• Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



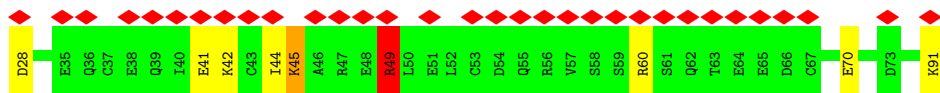
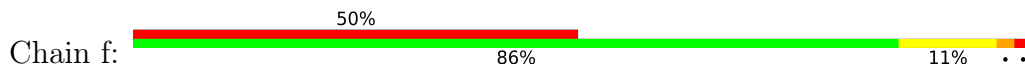
• Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



• Molecule 6: Cytochrome b-c1 complex subunit 6

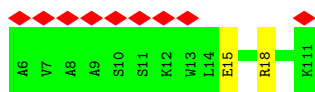


• Molecule 6: Cytochrome b-c1 complex subunit 6

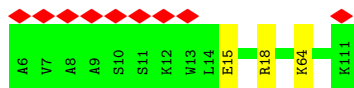


• Molecule 7: Cytochrome b-c1 complex subunit 7

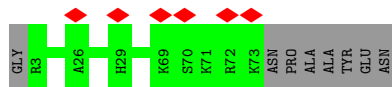
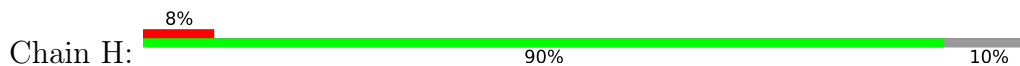




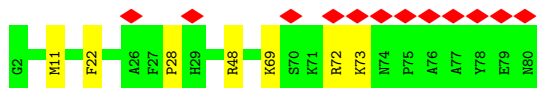
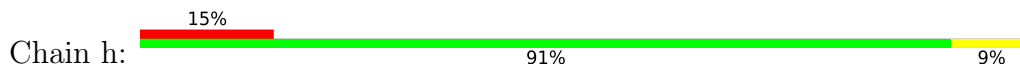
• Molecule 7: Cytochrome b-c1 complex subunit 7



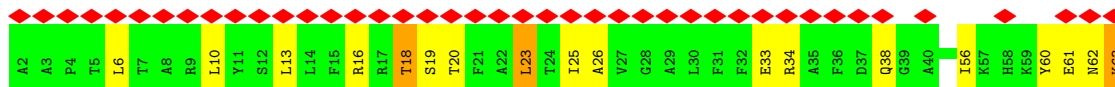
• Molecule 8: Cytochrome b-c1 complex subunit 8



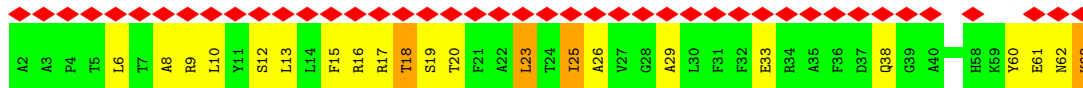
• Molecule 8: Cytochrome b-c1 complex subunit 8



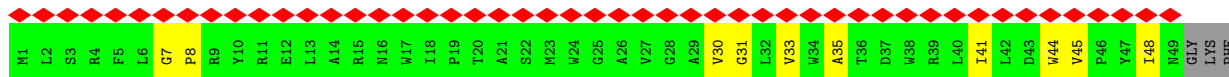
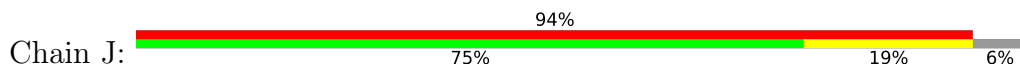
• Molecule 9: Complex III subunit 9



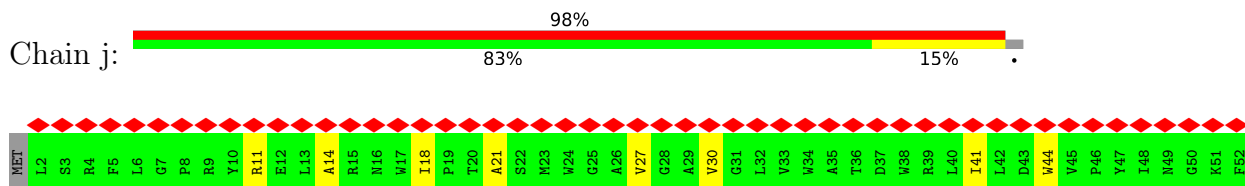
• Molecule 9: Complex III subunit 9



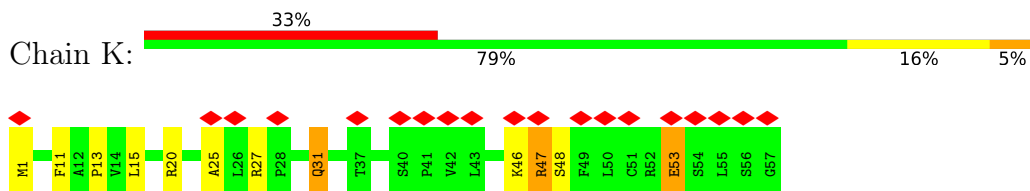
• Molecule 10: Cytochrome b-c1 complex subunit 10



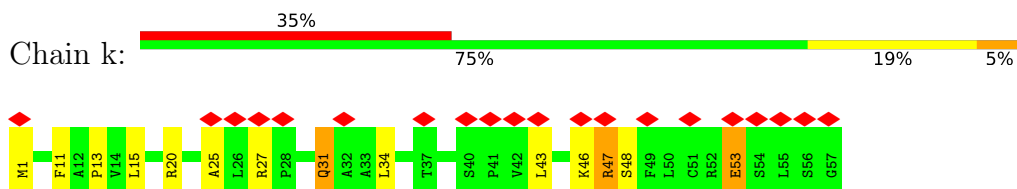
• Molecule 10: Cytochrome b-c1 complex subunit 10



• Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	588793	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 ($e^-/\text{\AA}^2$)	51.68	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.756	Depositor
Minimum map value	-3.095	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.146	Depositor
Recommended contour level	0.543	Depositor
Map size (\AA)	304.0, 304.0, 304.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.95, 0.95, 0.95	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: A1D6K, CDL, HEM, FES, HEC, PEE

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	0.28	0/3115	0.55	0/4259
1	a	0.28	0/3115	0.55	0/4259
2	B	0.28	0/1978	0.73	7/2684 (0.3%)
2	b	0.25	0/1961	0.58	0/2661
3	C	0.30	0/1534	0.77	3/2075 (0.1%)
3	c	0.29	0/1549	0.71	1/2095 (0.0%)
4	D	0.26	0/3524	0.52	2/4783 (0.0%)
4	d	0.26	0/3531	0.54	0/4793
5	E	0.26	0/3187	0.52	0/4314
5	e	0.26	0/3187	0.52	0/4314
6	F	0.26	0/534	0.69	2/714 (0.3%)
6	f	0.26	0/534	0.69	2/714 (0.3%)
7	G	0.24	0/941	0.47	0/1262
7	g	0.24	0/941	0.46	0/1262
8	H	0.31	0/628	0.60	0/848
8	h	0.39	0/688	0.67	0/931
9	I	0.31	0/520	0.77	1/701 (0.1%)
9	i	0.31	0/520	0.77	1/701 (0.1%)
10	J	0.34	0/420	0.73	1/576 (0.2%)
10	j	0.25	0/437	0.63	0/598
11	K	0.37	0/410	0.91	1/556 (0.2%)
11	k	0.36	0/410	0.91	1/556 (0.2%)
All	All	0.28	0/33664	0.60	22/45656 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	c	0	1
4	d	0	2
11	K	0	1
11	k	0	1
All	All	0	11

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	TYR	O-C-N	-11.42	108.18	121.32
3	c	267	SER	N-CA-C	8.46	119.42	108.34
3	C	248	ARG	CA-CB-CG	6.72	127.54	114.10
6	F	49	ARG	CG-CD-NE	5.92	125.02	112.00
6	f	49	ARG	CG-CD-NE	5.92	125.02	112.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	141	TYR	Peptide
2	B	175	TYR	Peptide
2	B	176	PHE	Peptide
2	B	273	THR	Peptide
3	C	200	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	3078	23	0
1	a	3017	0	3078	23	0
2	B	1920	0	1869	27	0
2	b	1904	0	1849	19	0
3	C	1502	0	1490	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	1517	0	1498	23	0
4	D	3452	0	3343	14	0
4	d	3459	0	3350	12	0
5	E	3134	0	3112	17	0
5	e	3134	0	3112	17	0
6	F	528	0	510	8	0
6	f	528	0	510	6	0
7	G	921	0	917	1	0
7	g	921	0	917	2	0
8	H	608	0	616	0	0
8	h	666	0	663	6	0
9	I	507	0	509	7	0
9	i	507	0	509	12	0
10	J	405	0	405	6	0
10	j	421	0	418	4	0
11	K	404	0	425	14	0
11	k	404	0	425	14	0
12	A	27	0	0	6	0
12	a	27	0	0	7	0
13	A	86	0	60	0	0
13	a	86	0	60	0	0
14	A	45	0	67	1	0
14	D	49	0	75	5	0
14	a	49	0	75	0	0
15	B	43	0	32	4	0
15	b	43	0	32	1	0
16	a	4	0	0	0	0
16	c	4	0	0	0	0
17	a	128	0	144	4	0
17	g	64	0	72	2	0
All	All	33531	0	33220	228	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 3.

The worst 5 of 228 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)
2:b:263:THR:HG1	6:f:28:ASP:N	1.66	0.91
2:B:263:THR:HG1	6:F:28:ASP:N	1.71	0.88
1:a:142:GLY:HA3	12:a:401:A1D6K:C5	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLY:HA3	12:A:401:A1D6K:C5	2.22	0.69
2:B:268:ALA:HA	2:B:271:VAL:HG12	1.76	0.68

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	376/378 (100%)	362 (96%)	14 (4%)	0	100	100
1	a	376/378 (100%)	362 (96%)	14 (4%)	0	100	100
2	B	239/241 (99%)	210 (88%)	28 (12%)	1 (0%)	30	40
2	b	237/241 (98%)	211 (89%)	26 (11%)	0	100	100
3	C	192/196 (98%)	158 (82%)	34 (18%)	0	100	100
3	c	194/196 (99%)	158 (81%)	36 (19%)	0	100	100
4	D	443/446 (99%)	430 (97%)	13 (3%)	0	100	100
4	d	444/446 (100%)	428 (96%)	16 (4%)	0	100	100
5	E	416/418 (100%)	403 (97%)	13 (3%)	0	100	100
5	e	416/418 (100%)	403 (97%)	13 (3%)	0	100	100
6	F	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
6	f	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
7	G	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
7	g	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
8	H	69/79 (87%)	65 (94%)	4 (6%)	0	100	100
8	h	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	12
9	I	60/62 (97%)	50 (83%)	10 (17%)	0	100	100
9	i	60/62 (97%)	50 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	47/52 (90%)	41 (87%)	6 (13%)	0	100	100
10	j	49/52 (94%)	43 (88%)	6 (12%)	0	100	100
11	K	55/57 (96%)	49 (89%)	6 (11%)	0	100	100
11	k	55/57 (96%)	49 (89%)	6 (11%)	0	100	100
All	All	4137/4198 (98%)	3864 (93%)	271 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	179	PRO
8	h	28	PRO

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	331/331 (100%)	326 (98%)	5 (2%)	57	75
1	a	331/331 (100%)	326 (98%)	5 (2%)	57	75
2	B	206/206 (100%)	206 (100%)	0	100	100
2	b	204/206 (99%)	204 (100%)	0	100	100
3	C	164/166 (99%)	162 (99%)	2 (1%)	63	79
3	c	165/166 (99%)	165 (100%)	0	100	100
4	D	371/372 (100%)	371 (100%)	0	100	100
4	d	372/372 (100%)	370 (100%)	2 (0%)	81	90
5	E	327/328 (100%)	326 (100%)	1 (0%)	86	93
5	e	327/328 (100%)	326 (100%)	1 (0%)	86	93
6	F	61/61 (100%)	57 (93%)	4 (7%)	15	24
6	f	61/61 (100%)	57 (93%)	4 (7%)	15	24
7	G	95/95 (100%)	95 (100%)	0	100	100
7	g	95/95 (100%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	65/70 (93%)	65 (100%)	0	100	100
8	h	70/70 (100%)	70 (100%)	0	100	100
9	I	50/50 (100%)	38 (76%)	12 (24%)	1	1
9	i	50/50 (100%)	38 (76%)	12 (24%)	1	1
10	J	40/42 (95%)	39 (98%)	1 (2%)	42	61
10	j	41/42 (98%)	41 (100%)	0	100	100
11	K	44/44 (100%)	41 (93%)	3 (7%)	14	23
11	k	44/44 (100%)	41 (93%)	3 (7%)	14	23
All	All	3514/3530 (100%)	3459 (98%)	55 (2%)	54	74

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	27	ILE
5	e	232	GLN
11	k	53	GLU
9	i	61	GLU
1	a	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	345	ASN
4	d	464	GLN
5	e	365	ASN
5	E	155	GLN
5	E	75	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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEM	A	403	1	50,50,50	1.41	8 (16%)	67,82,82	1.67	12 (17%)
15	HEC	b	401	-	46,50,50	1.83	5 (10%)	58,82,82	1.97	5 (8%)
13	HEM	a	402	1	50,50,50	1.35	6 (12%)	67,82,82	1.28	6 (8%)
13	HEM	a	403	1	50,50,50	1.49	7 (14%)	67,82,82	1.16	6 (8%)
17	CDL	g	201	-	63,63,99	1.09	7 (11%)	69,75,111	1.21	5 (7%)
15	HEC	B	401	-	46,50,50	1.85	7 (15%)	58,82,82	1.90	4 (6%)
17	CDL	a	406	-	63,63,99	1.10	8 (12%)	69,75,111	1.13	4 (5%)
16	FES	c	301	-	0,4,4	-	-	-	-	-
13	HEM	A	402	1	50,50,50	1.49	6 (12%)	67,82,82	1.17	6 (8%)
14	PEE	A	404	-	44,44,50	1.59	5 (11%)	47,49,55	1.19	4 (8%)
14	PEE	D	501	-	48,48,50	1.57	7 (14%)	51,53,55	1.23	6 (11%)
16	FES	a	404	-	0,4,4	-	-	-	-	-
12	A1D6K	a	401	-	29,29,29	0.84	1 (3%)	33,39,39	1.37	3 (9%)
14	PEE	a	405	-	48,48,50	1.52	5 (10%)	51,53,55	1.21	4 (7%)
17	CDL	a	407	-	63,63,99	1.10	8 (12%)	69,75,111	1.11	4 (5%)
12	A1D6K	A	401	-	29,29,29	0.83	1 (3%)	33,39,39	1.36	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEM	A	403	1	-	3/14/54/54	-
15	HEC	b	401	-	-	4/14/54/54	-
13	HEM	a	402	1	-	2/14/54/54	-
13	HEM	a	403	1	-	2/14/54/54	-
17	CDL	g	201	-	-	44/74/74/110	-
15	HEC	B	401	-	-	7/14/54/54	-
17	CDL	a	406	-	-	42/74/74/110	-
16	FES	c	301	-	-	-	0/1/1/1
13	HEM	A	402	1	-	2/14/54/54	-
14	PEE	A	404	-	-	18/48/48/54	-
14	PEE	D	501	-	-	31/52/52/54	-
16	FES	a	404	-	-	-	0/1/1/1
12	A1D6K	a	401	-	-	0/21/21/21	0/3/3/3
14	PEE	a	405	-	-	19/52/52/54	-
17	CDL	a	407	-	-	39/74/74/110	-
12	A1D6K	A	401	-	-	0/21/21/21	0/3/3/3

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	401	HEC	CAB-C3B	6.27	1.55	1.35
15	B	401	HEC	CAB-C3B	6.12	1.54	1.35
15	B	401	HEC	CAC-C3C	6.10	1.54	1.35
15	b	401	HEC	CAC-C3C	6.09	1.54	1.35
15	B	401	HEC	C3D-C2D	5.86	1.54	1.38

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	401	HEC	CBC-CAC-C3C	-9.45	108.55	127.43
15	B	401	HEC	CBC-CAC-C3C	-8.98	109.49	127.43
15	b	401	HEC	CBB-CAB-C3B	-7.50	112.44	127.43
15	B	401	HEC	CBB-CAB-C3B	-7.33	112.78	127.43
12	A	401	A1D6K	C19-O4-N1	5.33	115.63	109.98

There are no chirality outliers.

5 of 213 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	403	HEM	C2D-C3D-CAD-CBD

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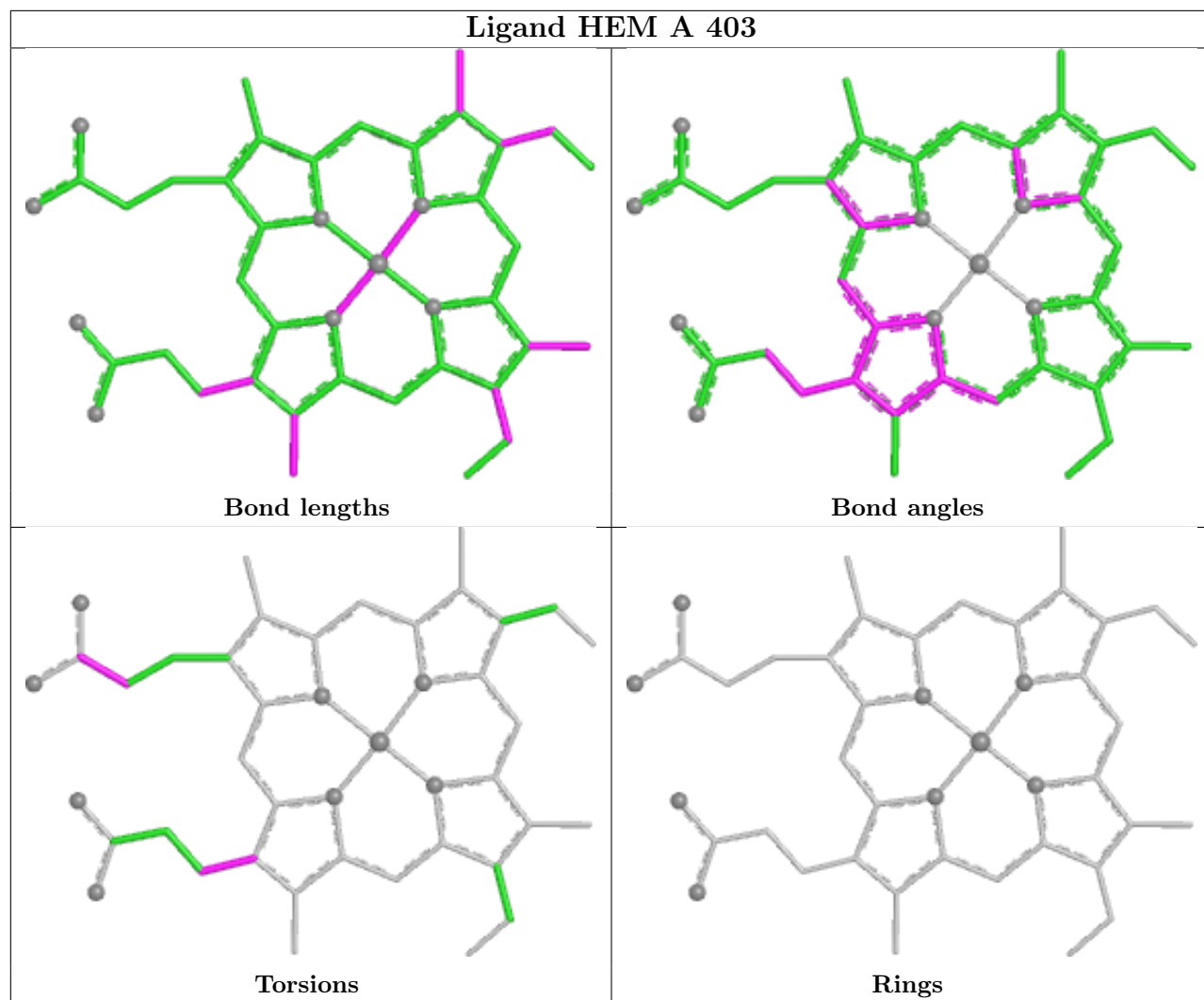
Mol	Chain	Res	Type	Atoms
13	A	403	HEM	C4D-C3D-CAD-CBD
14	A	404	PEE	C1-O3P-P-O1P
14	A	404	PEE	C4-O4P-P-O3P
14	A	404	PEE	C4-O4P-P-O2P

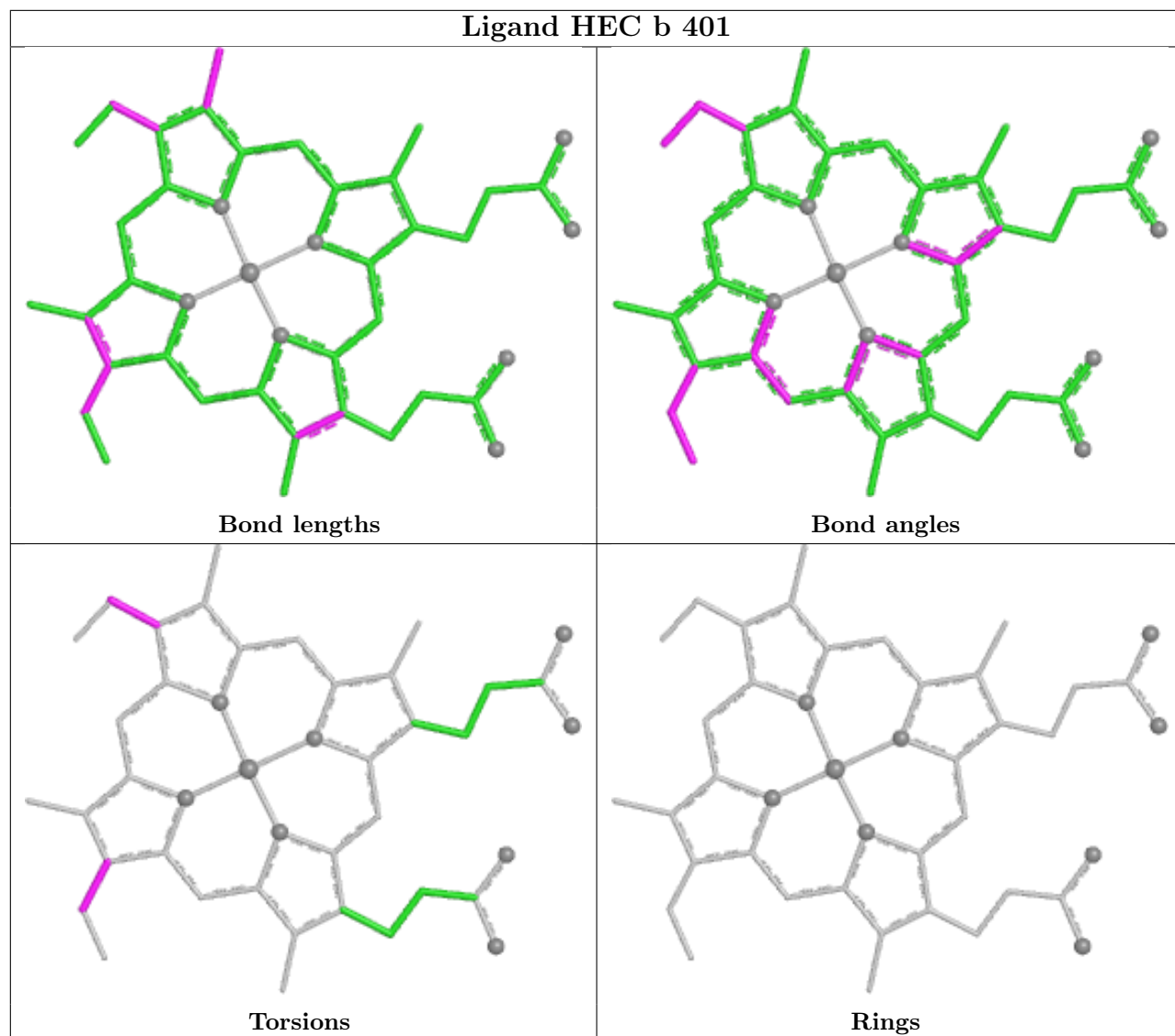
There are no ring outliers.

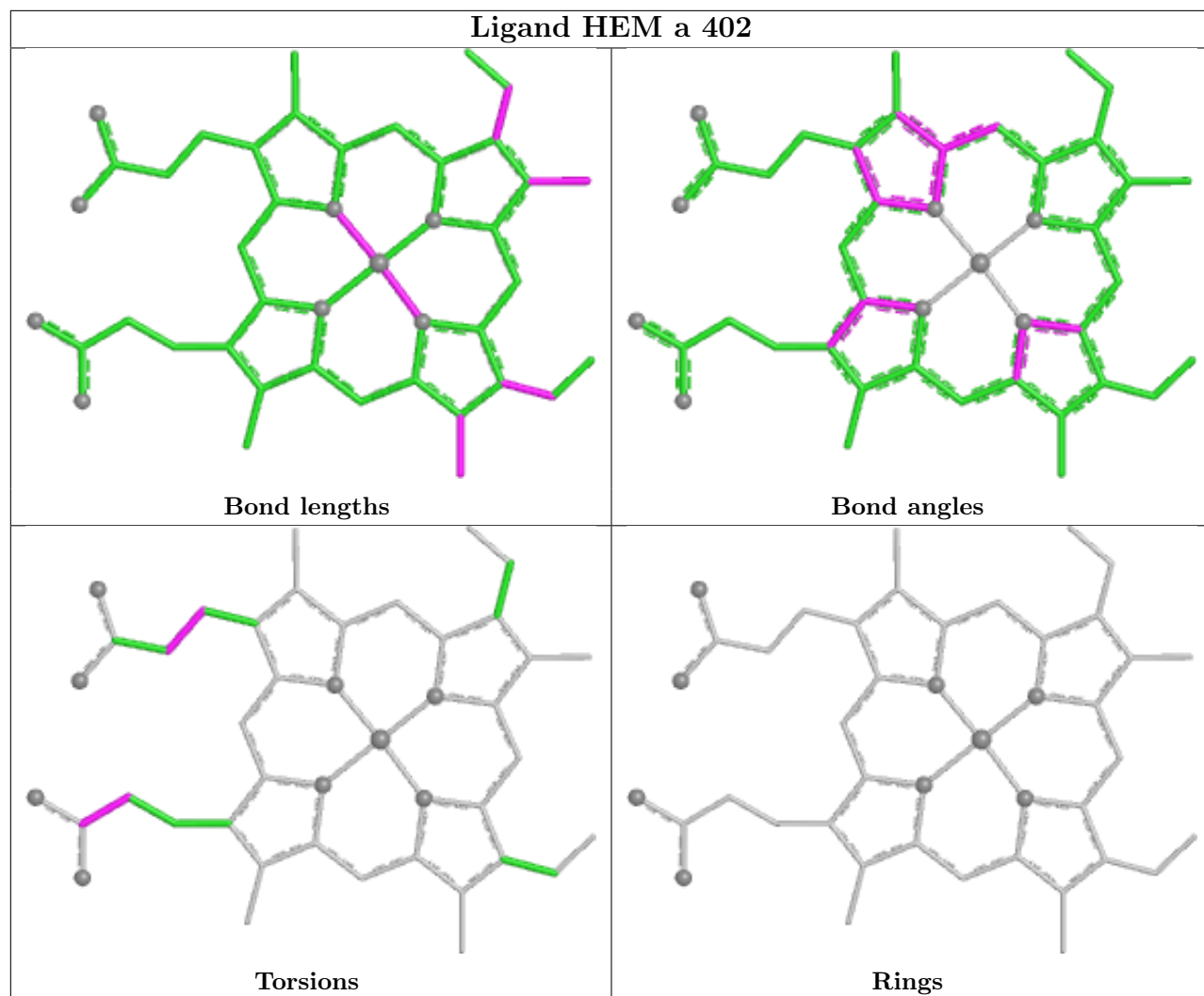
9 monomers are involved in 30 short contacts:

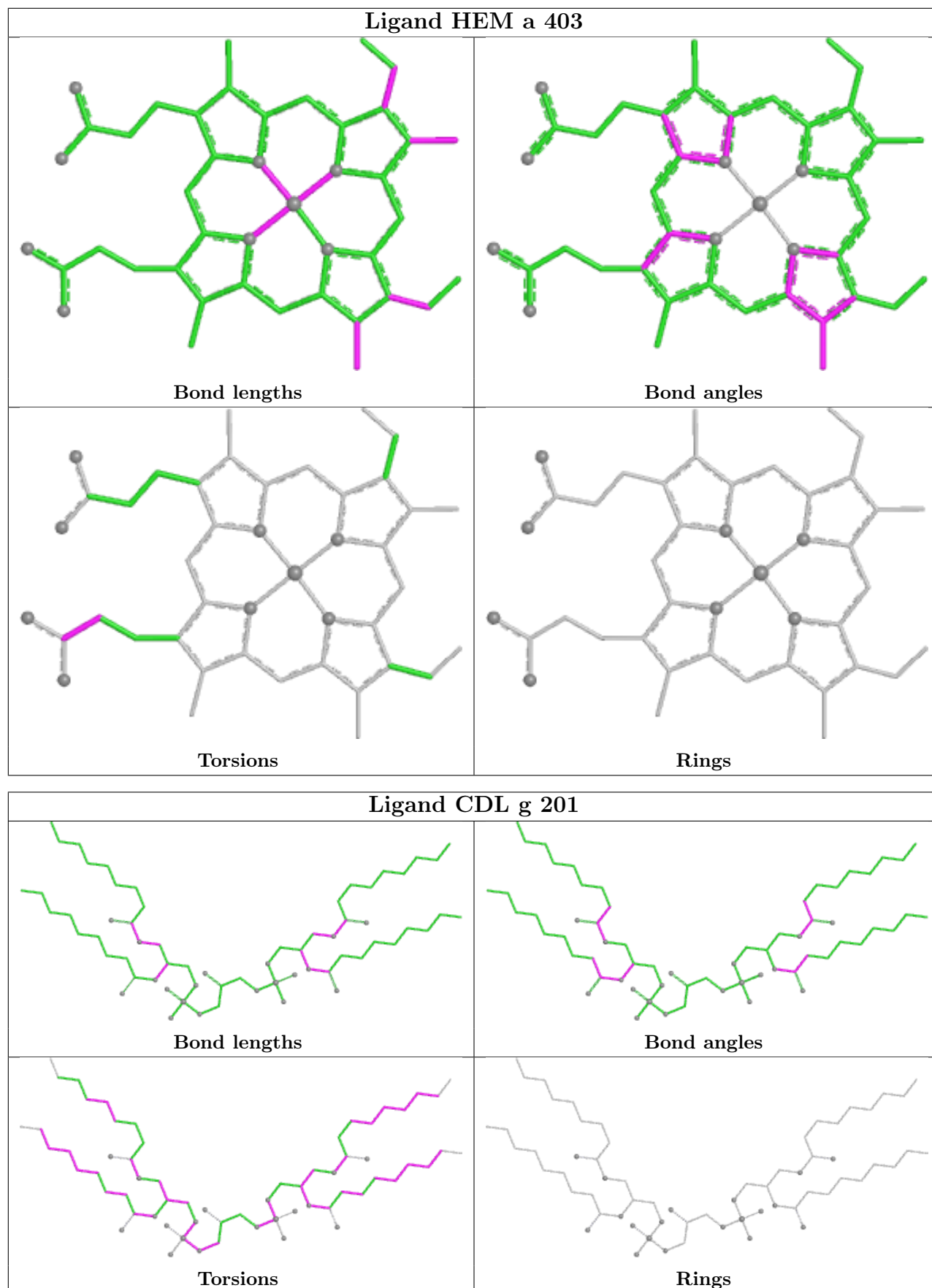
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	401	HEC	1	0
17	g	201	CDL	2	0
15	B	401	HEC	4	0
17	a	406	CDL	2	0
14	A	404	PEE	1	0
14	D	501	PEE	5	0
12	a	401	A1D6K	7	0
17	a	407	CDL	2	0
12	A	401	A1D6K	6	0

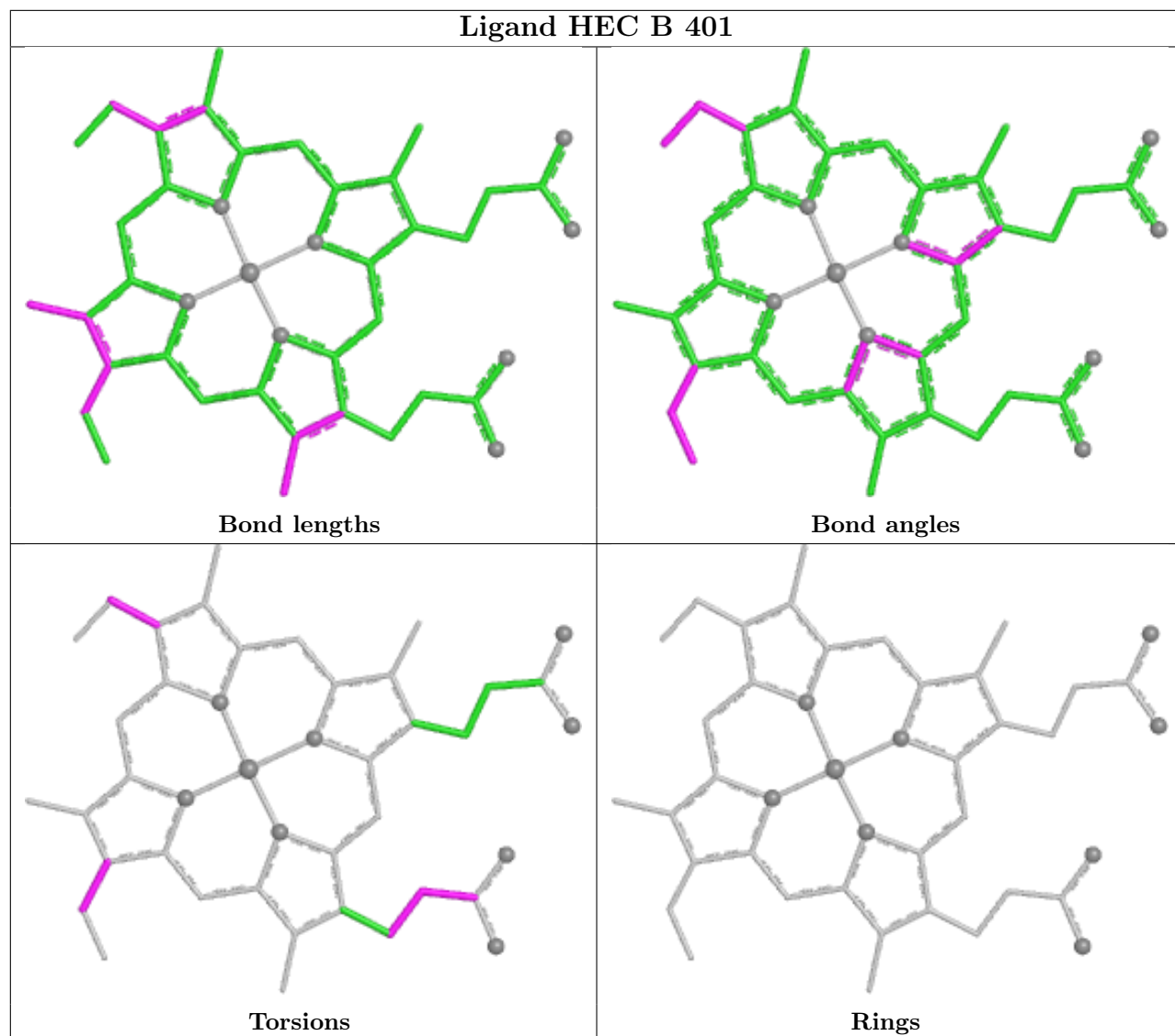
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

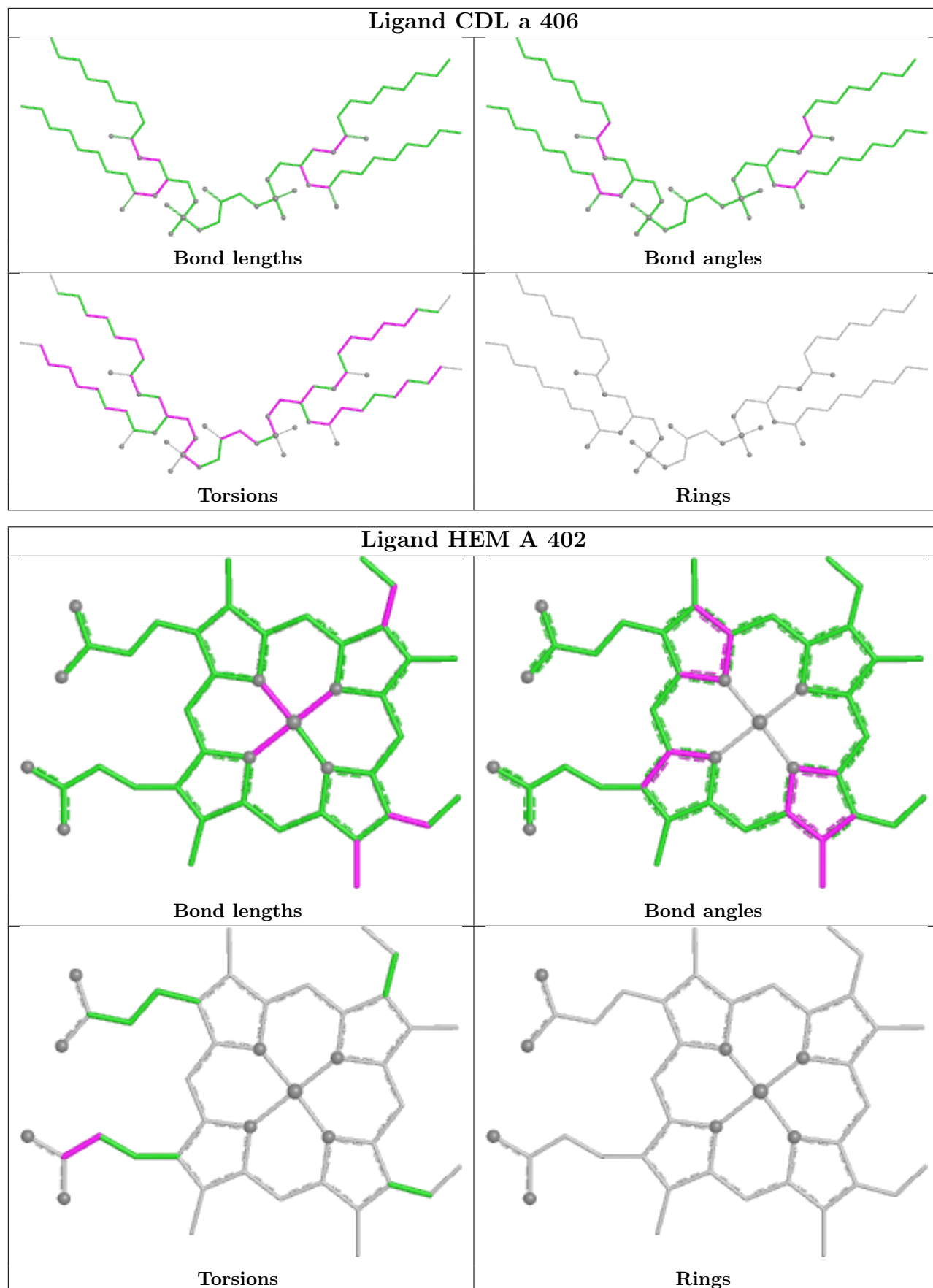


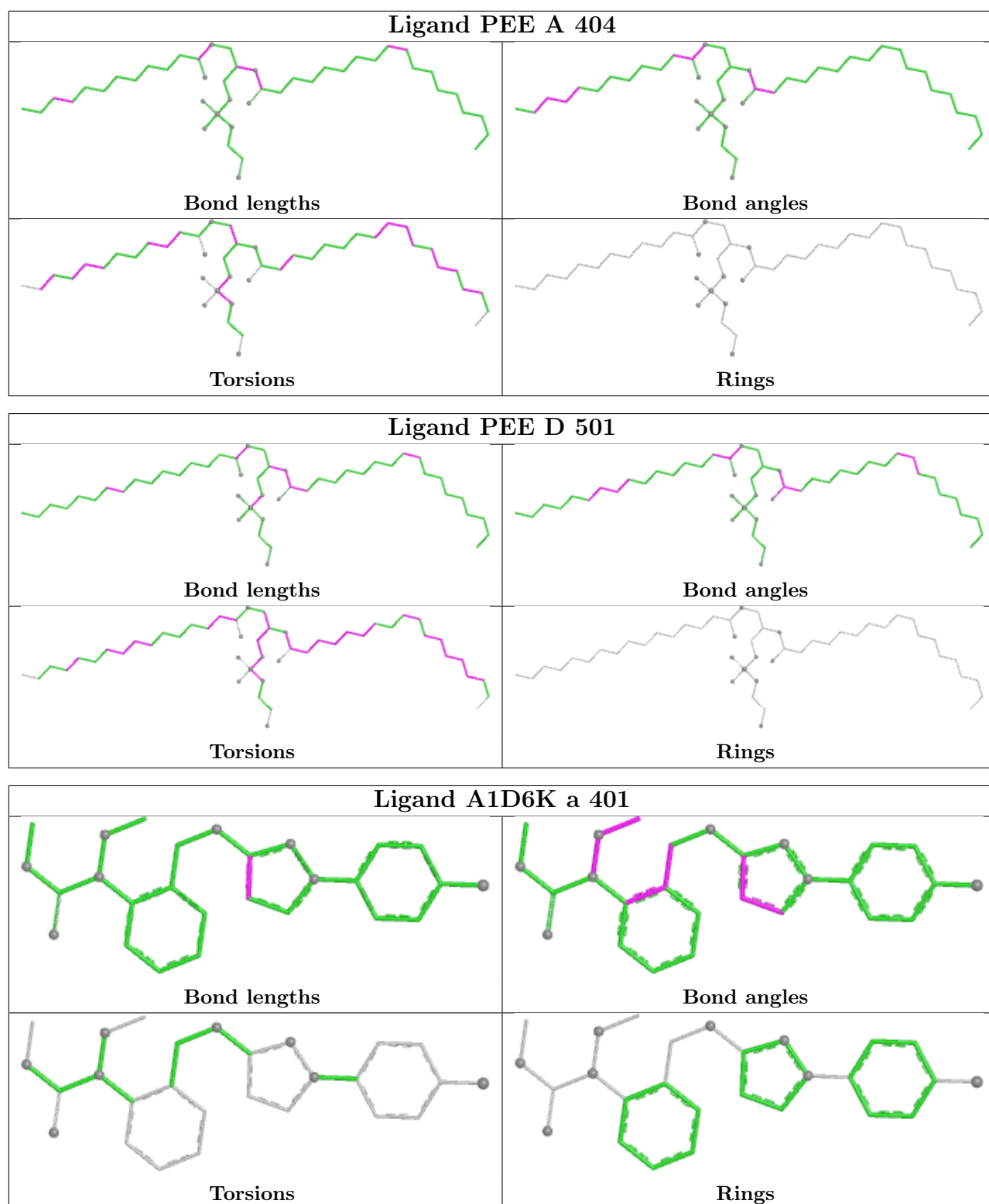


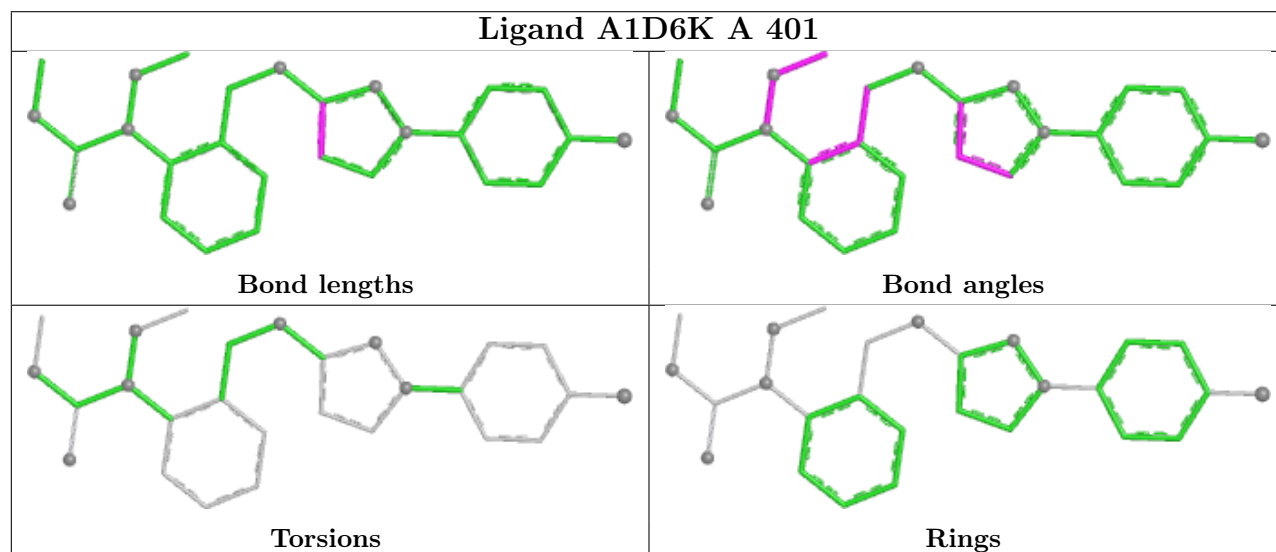
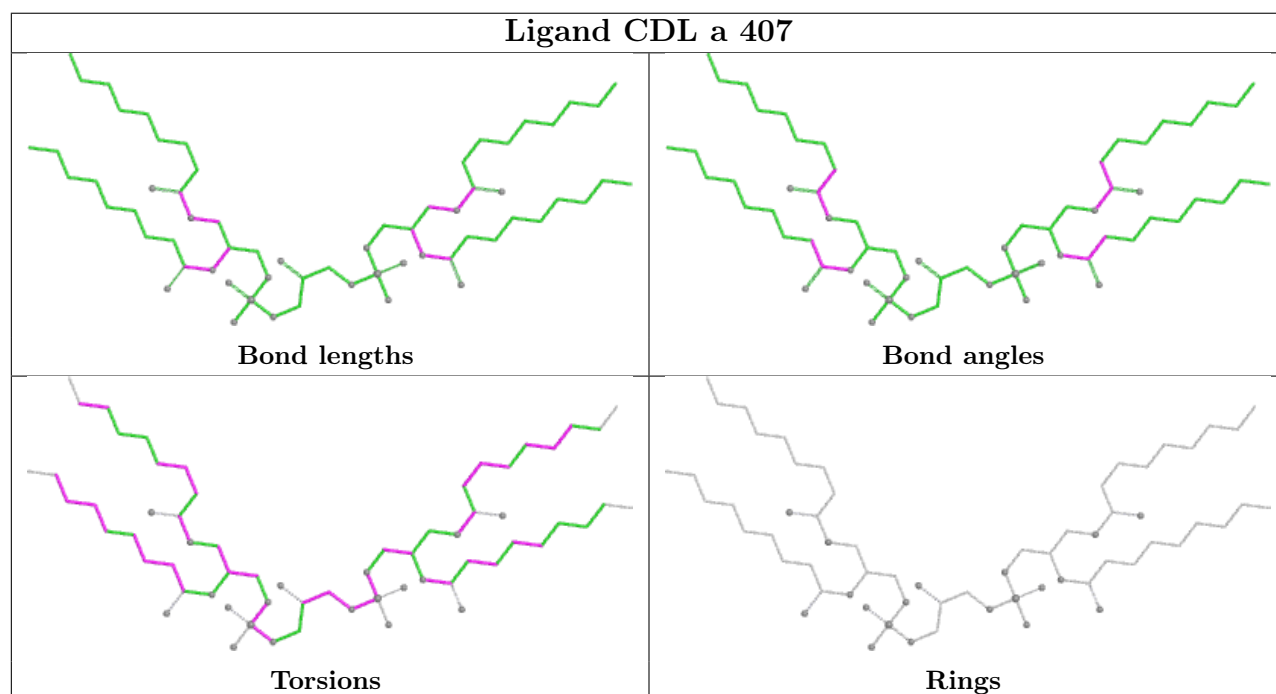
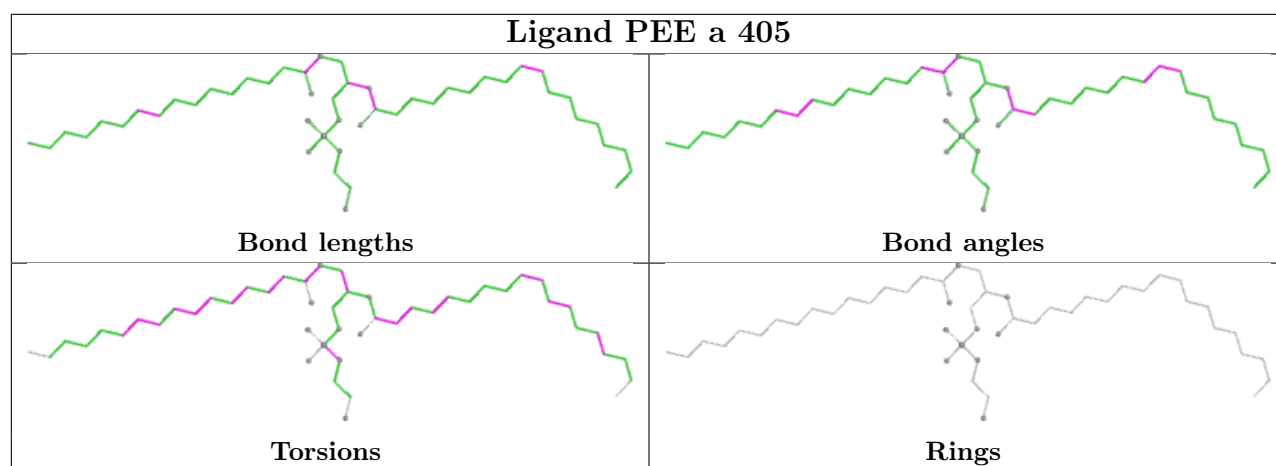












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

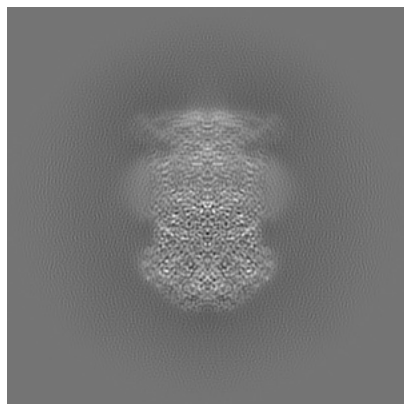
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60317. These allow visual inspection of the internal detail of the map and identification of artifacts.

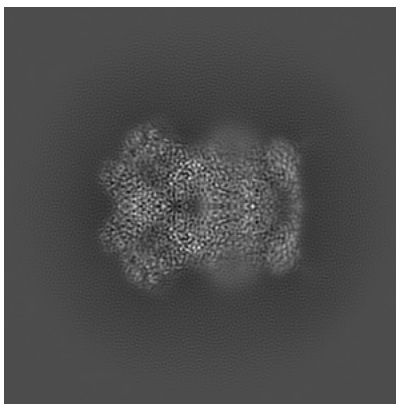
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

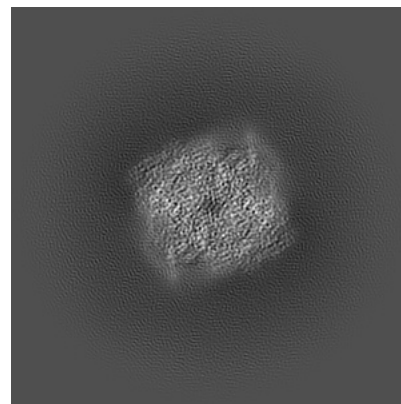
6.1.1 Primary map



X

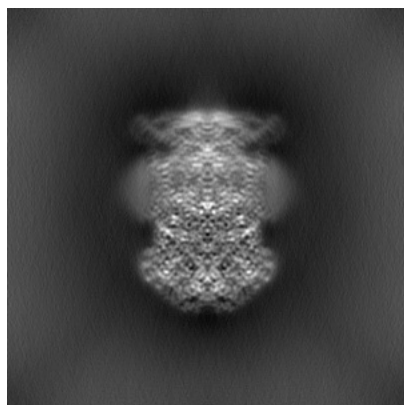


Y

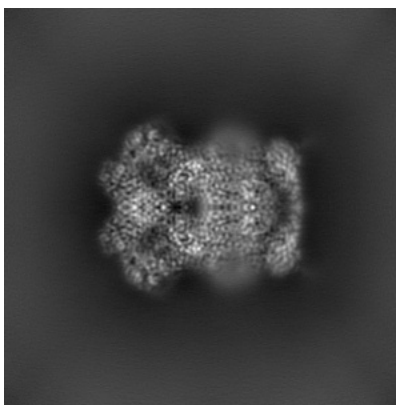


Z

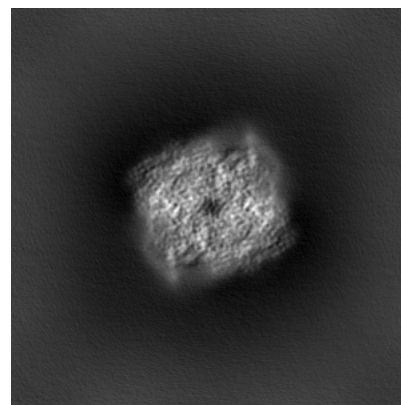
6.1.2 Raw map



X



Y

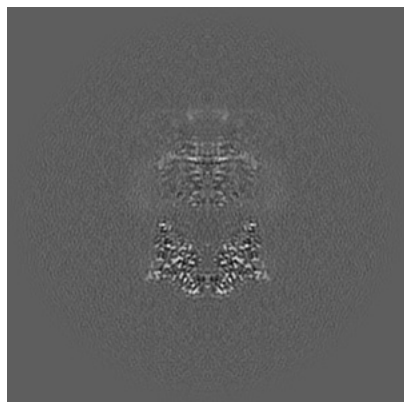


Z

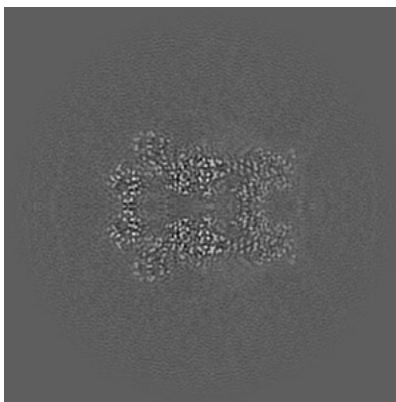
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

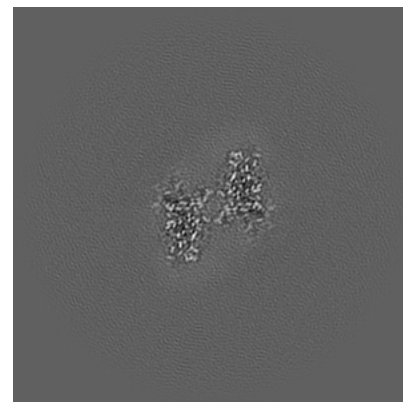
6.2.1 Primary map



X Index: 160

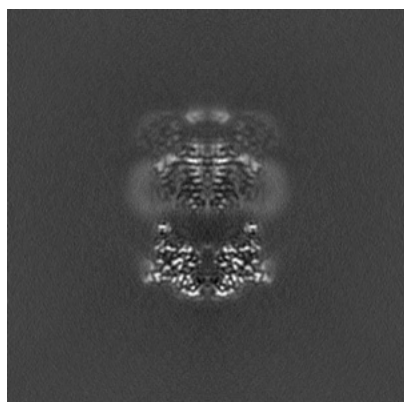


Y Index: 160

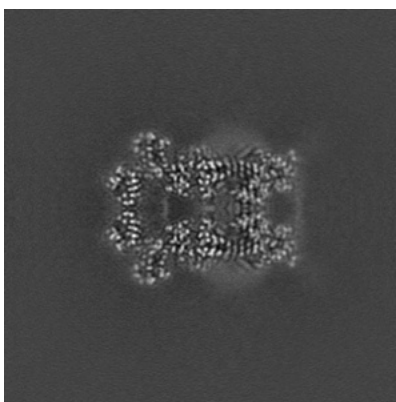


Z Index: 160

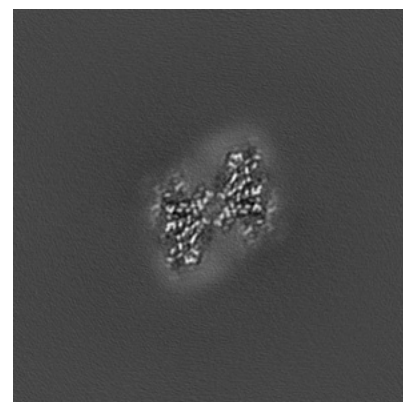
6.2.2 Raw map



X Index: 160



Y Index: 160

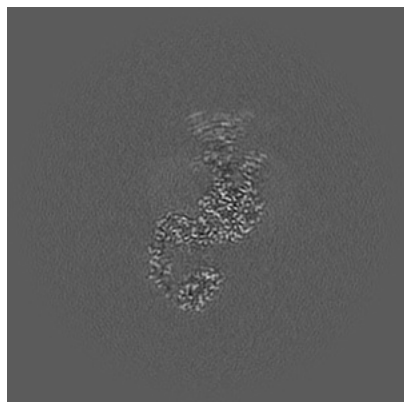


Z Index: 160

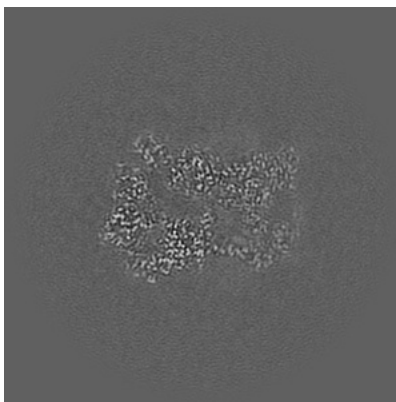
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

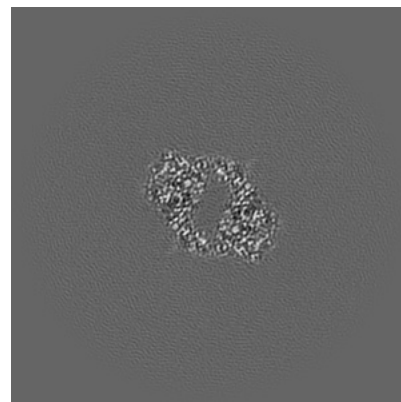
6.3.1 Primary map



X Index: 182

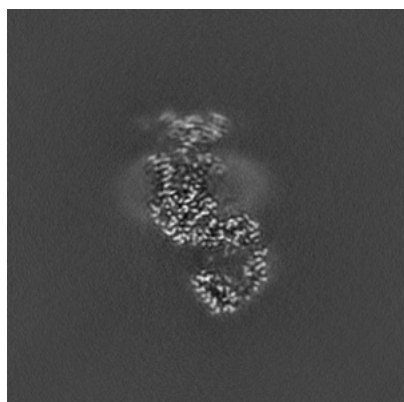


Y Index: 165

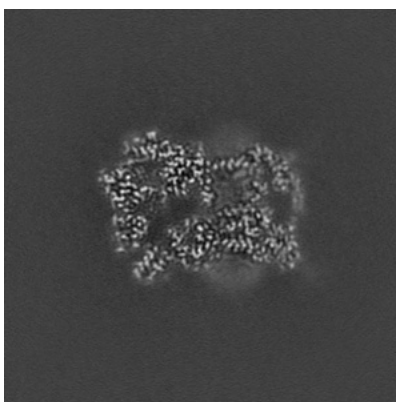


Z Index: 138

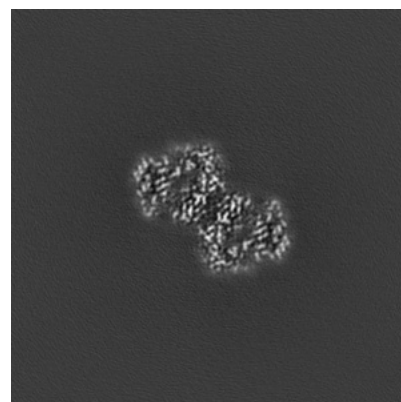
6.3.2 Raw map



X Index: 138



Y Index: 155

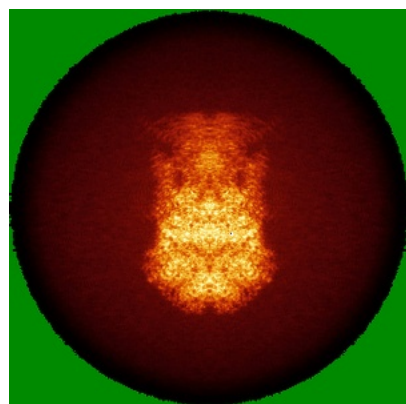


Z Index: 105

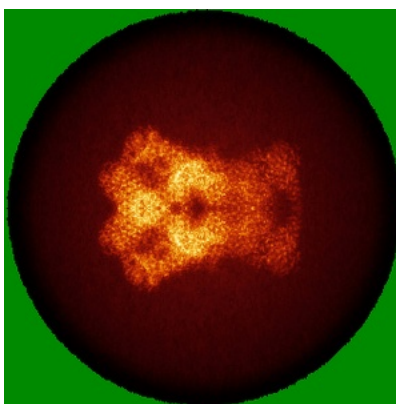
The images above show the largest variance slices of the map in three orthogonal directions.

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

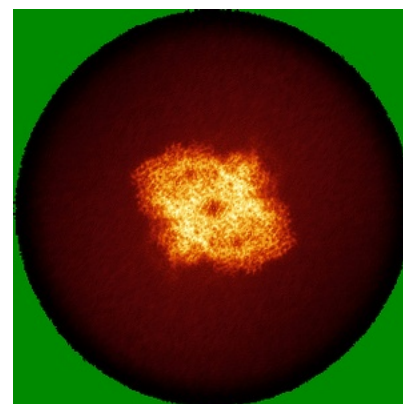
6.4.1 Primary map



X

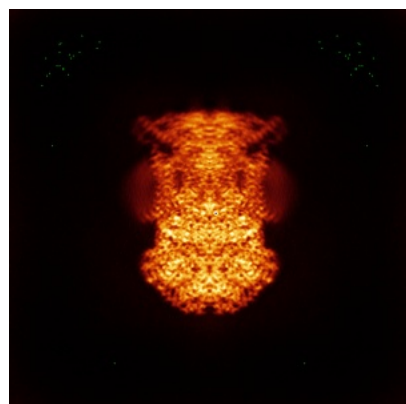


Y

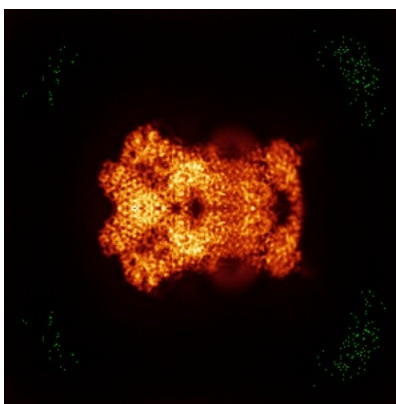


Z

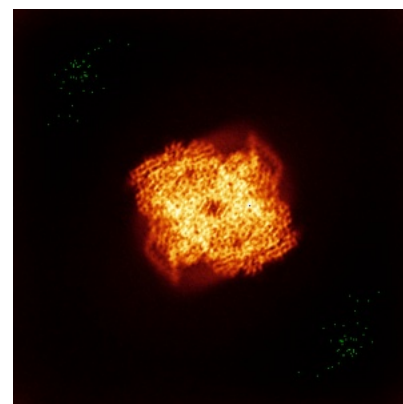
6.4.2 Raw map



X



Y

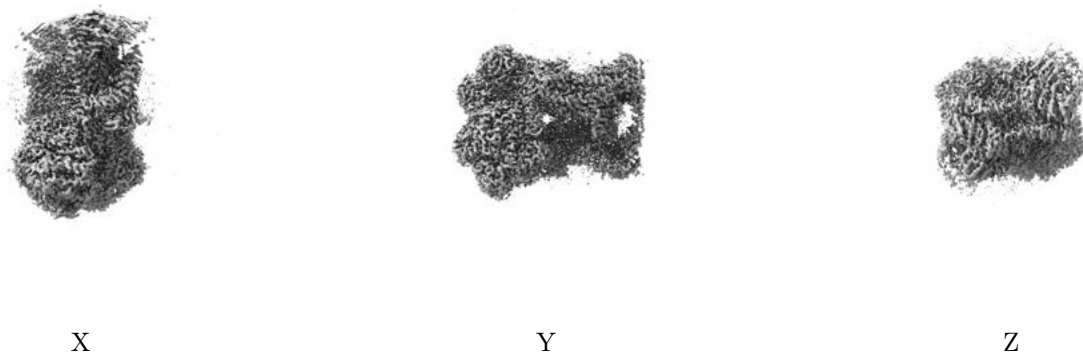


Z

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.

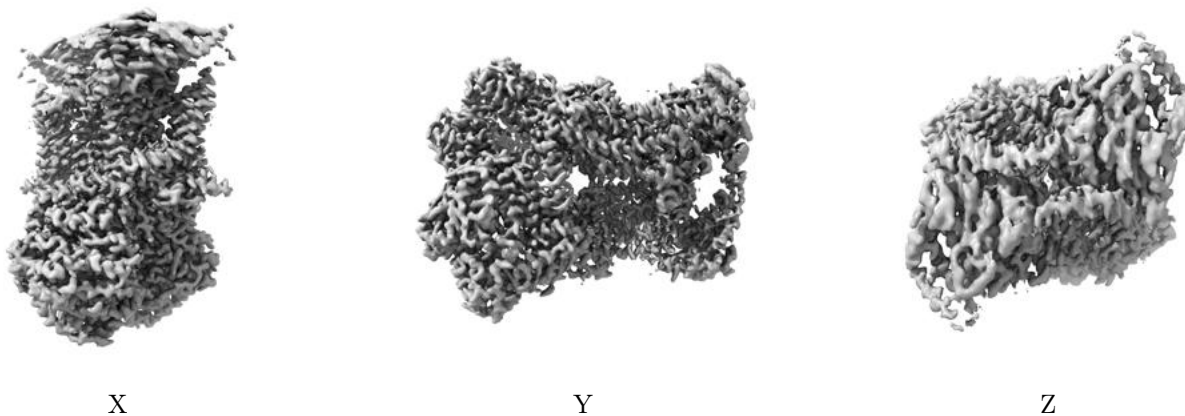
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.543. 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.

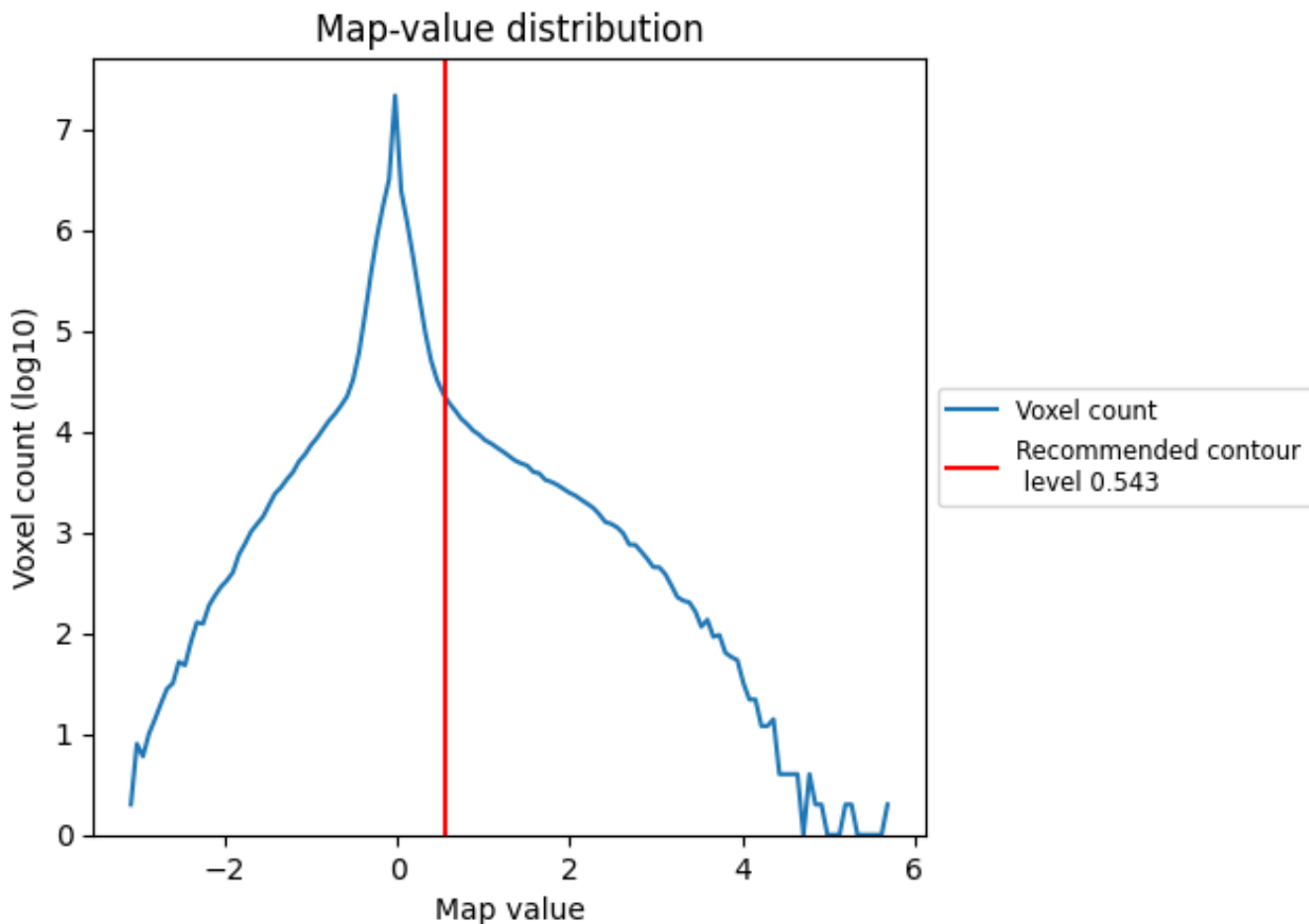
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

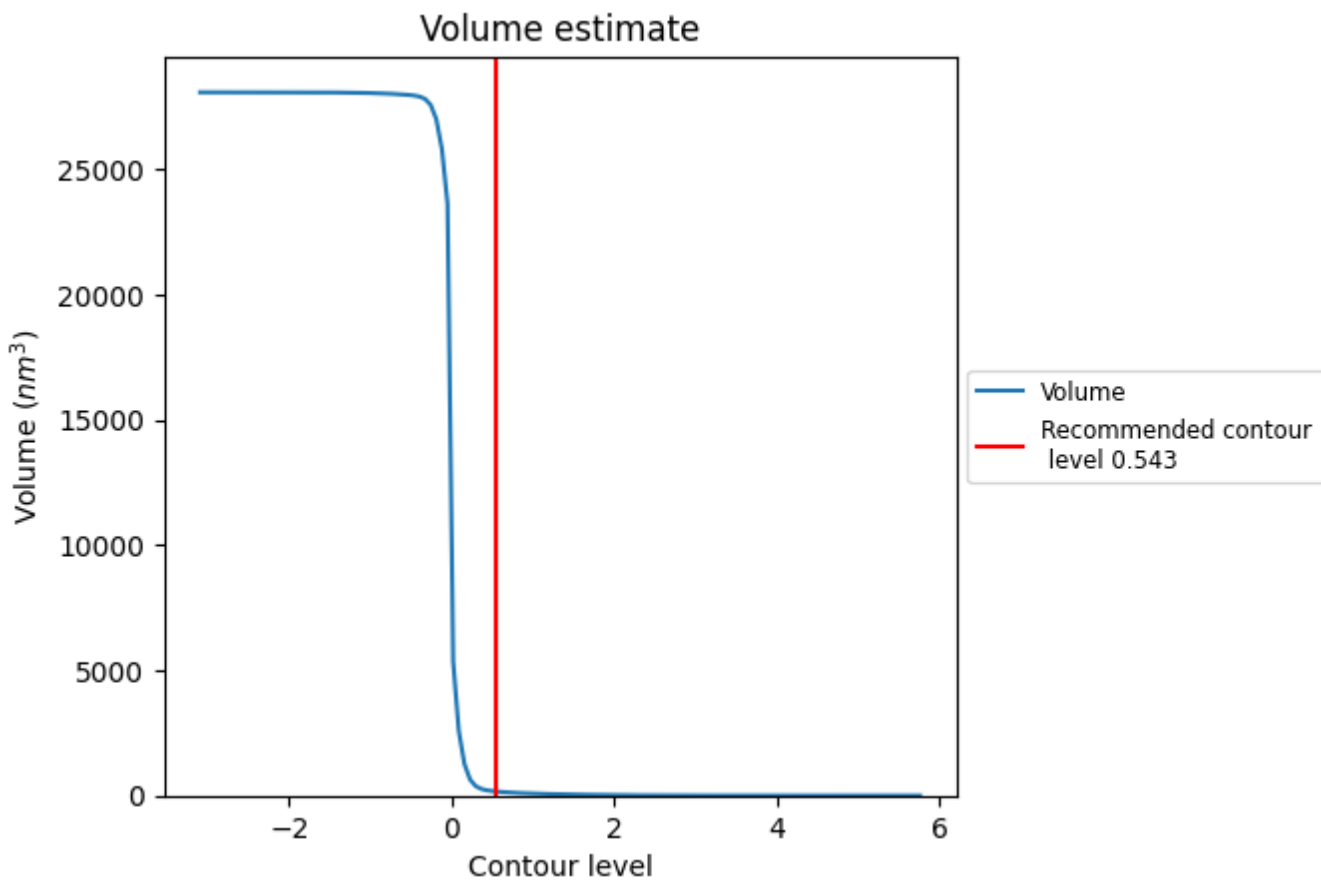
This section contains the results of statistical analysis of the map.

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.

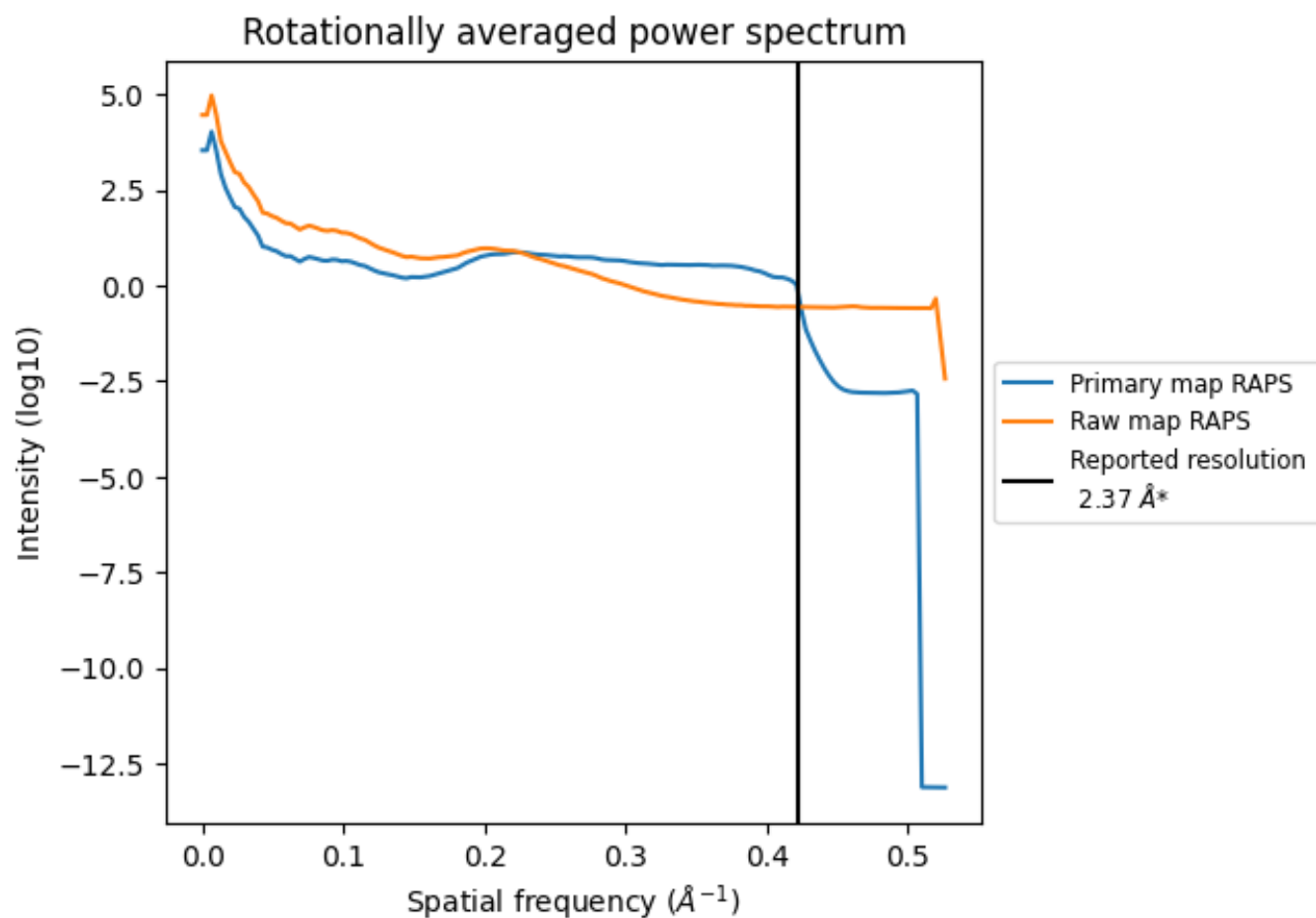
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 164 nm^3 ; this corresponds to an approximate mass of 148 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

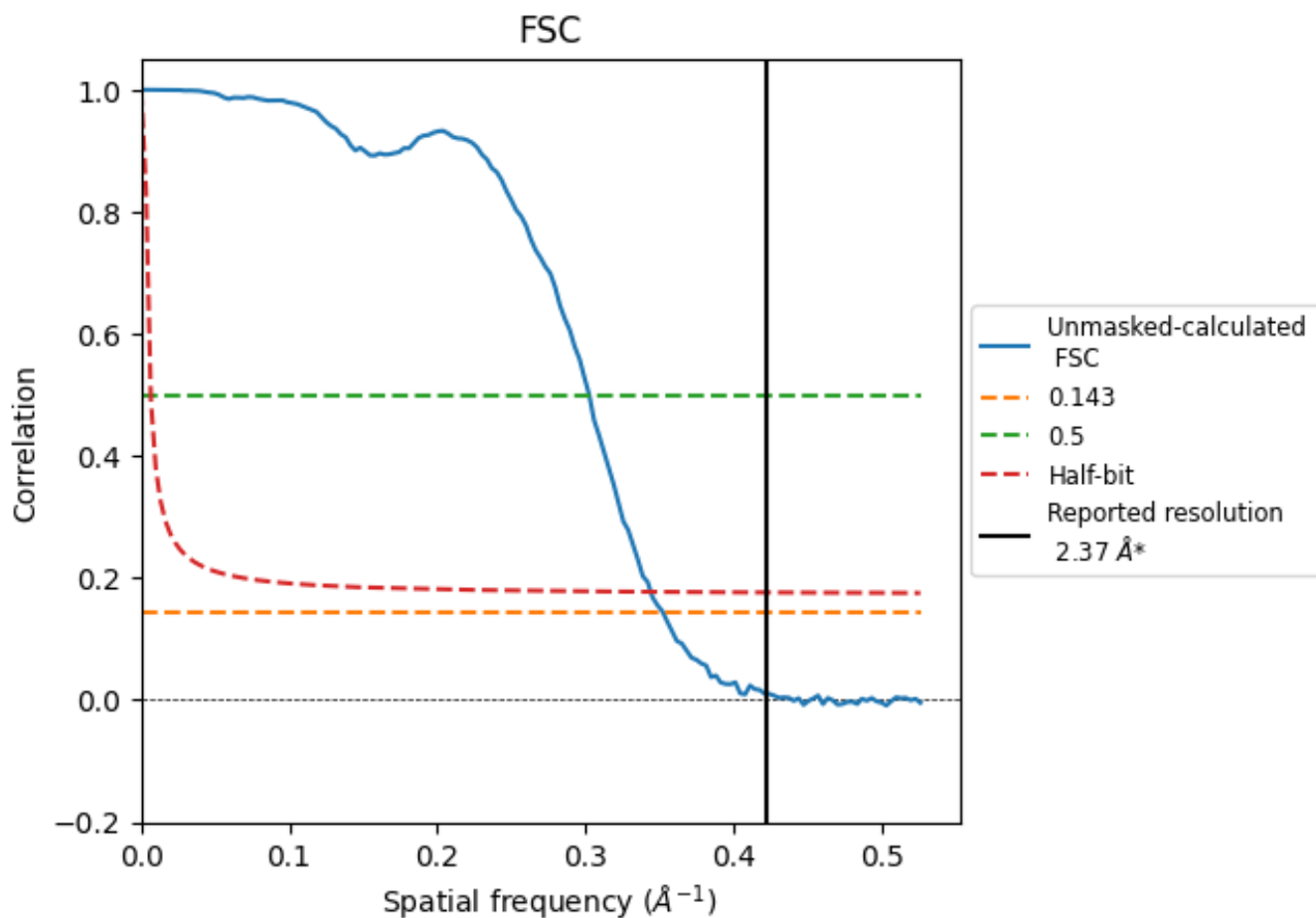


*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

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 0.422 Å⁻¹

8.2 Resolution estimates [i](#)

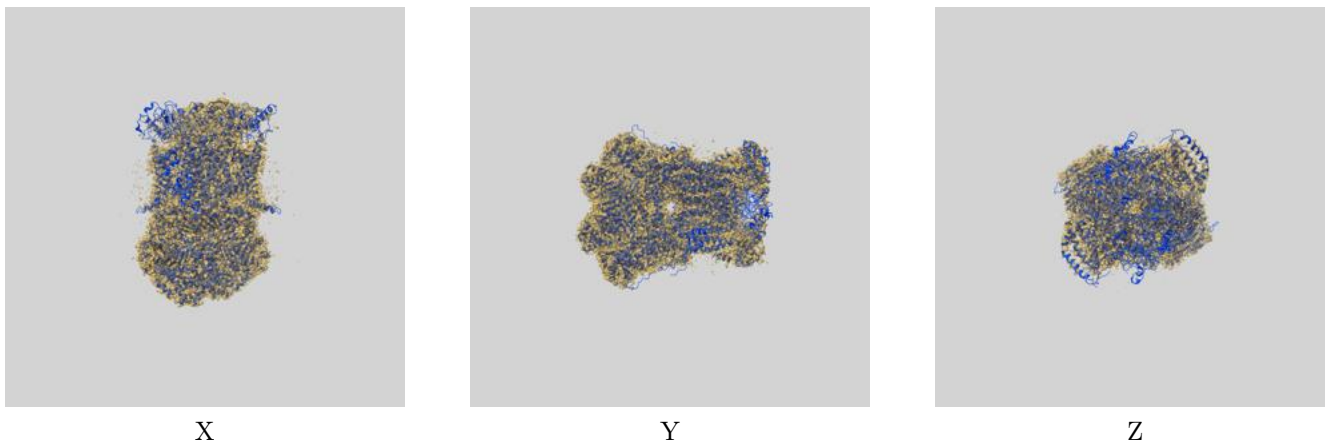
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.30	2.91

*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 2.84 differs from the reported value 2.37 by more than 10 %

9 Map-model fit [i](#)

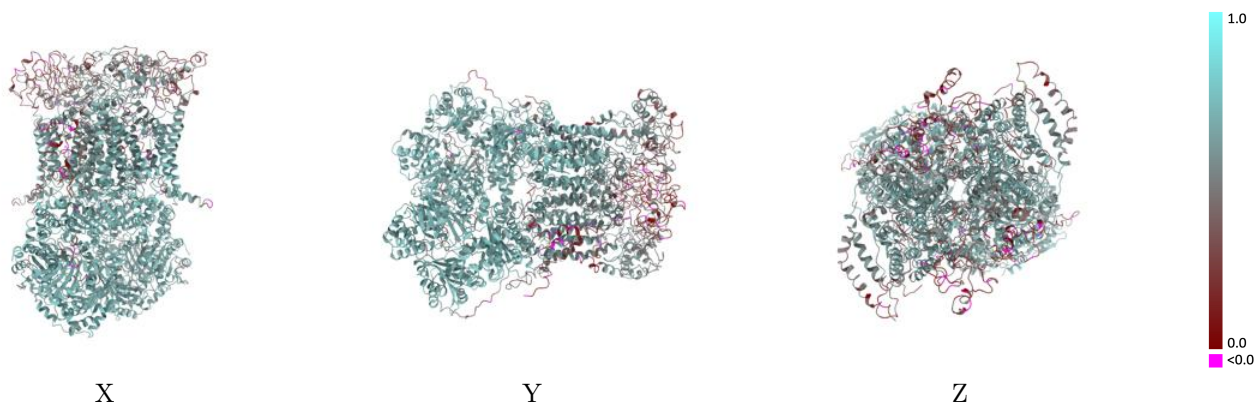
This section contains information regarding the fit between EMDB map EMD-60317 and PDB model 8ZOS. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



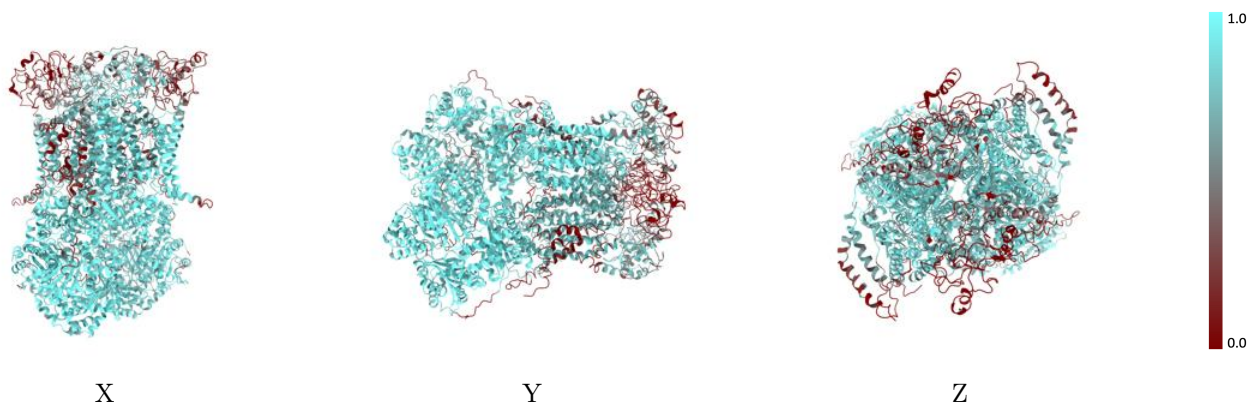
The images above show the 3D surface view of the map at the recommended contour level 0.543 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



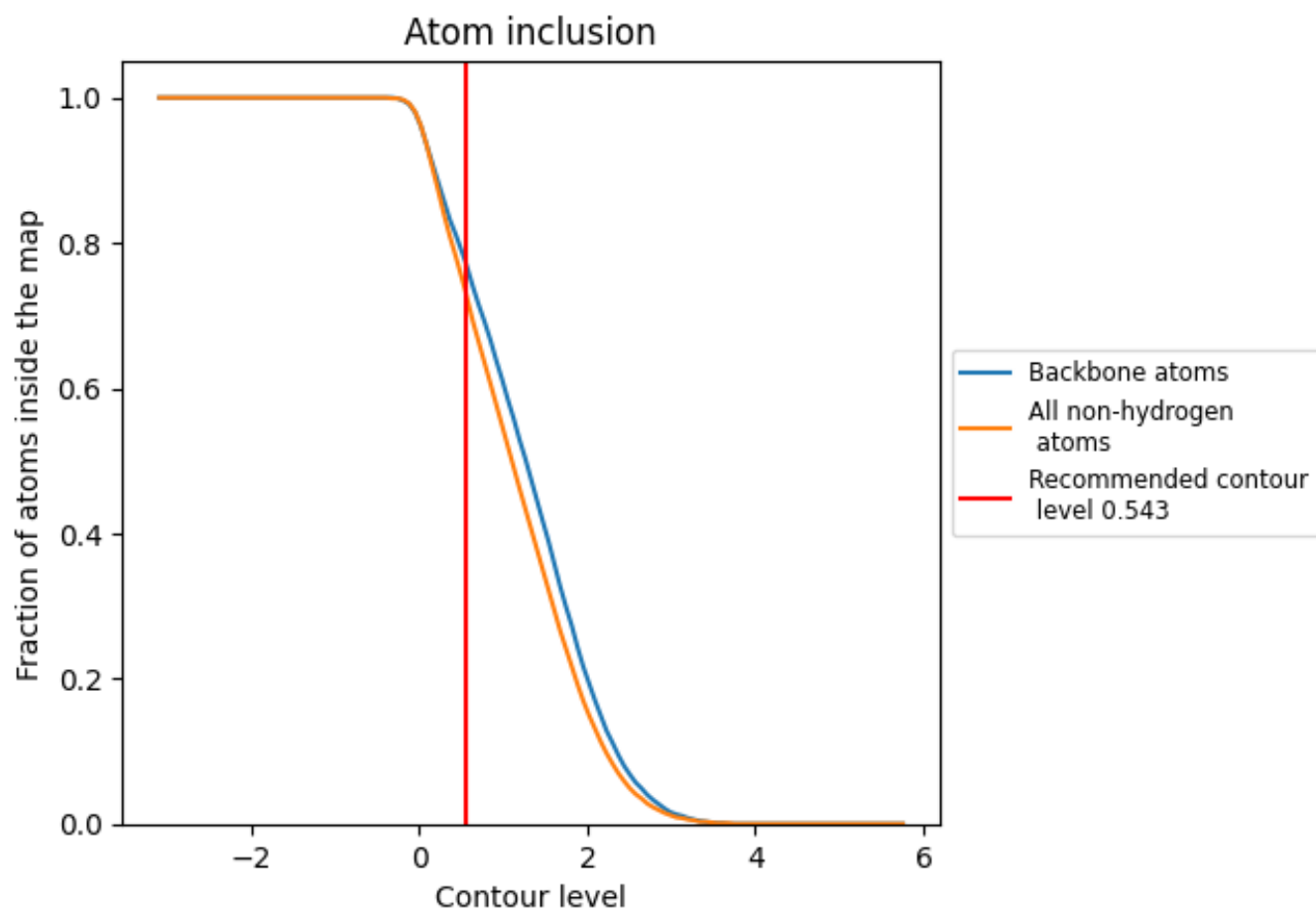
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.543).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 74% 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 (0.543) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7360	 0.5660
A	 0.8760	 0.6200
B	 0.6490	 0.4920
C	 0.1370	 0.3050
D	 0.9080	 0.6570
E	 0.9370	 0.6720
F	 0.4190	 0.4470
G	 0.8810	 0.6570
H	 0.8430	 0.6290
I	 0.2910	 0.3000
J	 0.0030	 0.2290
K	 0.5230	 0.4590
a	 0.8490	 0.6120
b	 0.6800	 0.5050
c	 0.1210	 0.2890
d	 0.9180	 0.6600
e	 0.9360	 0.6730
f	 0.4170	 0.4470
g	 0.8610	 0.6480
h	 0.7740	 0.5910
i	 0.2810	 0.2860
j	 0.0070	 0.1920
k	 0.5200	 0.4590

