



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 12:40 PM JST

PDB ID : 8ZOW / pdb_00008zow
EMDB ID : EMD-60320
Title : Cryo-EM structure of Metyltetraprole-bound porcine bc1 complex
Authors : Wang, Y.X.; Sun, J.Y.; Cui, G.R.; Yang, G.F.
Deposited on : 2024-05-29
Resolution : 2.53 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:

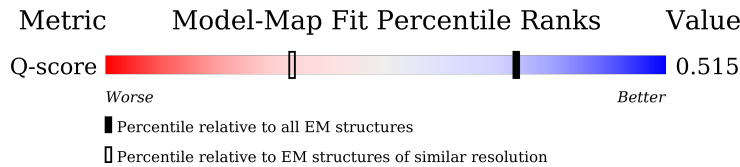
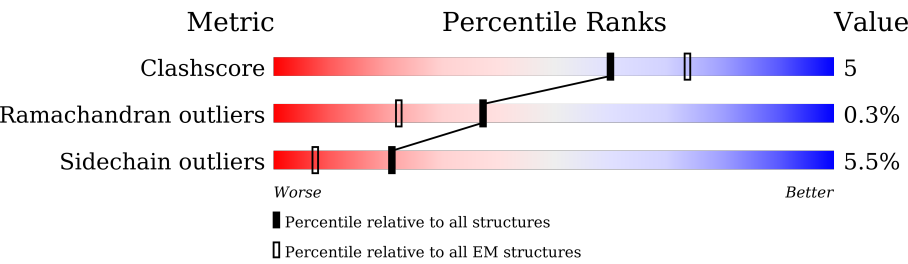
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 2.53 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	7309 (2.03 - 3.03)

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	90%9%
1	a	378	92%7%
2	B	241	15%89%10%
2	b	241	14%82%14%

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Mol	Chain	Length	Quality of chain
3	C	196	95% 74% 20% • •
3	c	196	94% 72% 20% 7% •
4	D	446	93% 6% •
4	d	446	93% 6% •
5	E	418	90% 9%
5	e	418	90% 9%
6	F	64	61% 73% 20% 5% •
6	f	64	59% 75% 17% 6% •
7	G	106	8% 97% • •
7	g	106	8% 95% • •
8	H	79	25% 87% • 10%
8	h	79	34% 92% 6% •
9	I	62	66% 52% 32% 11% 5%
9	i	62	69% 58% 24% 16% •
10	J	52	94% 73% 19% • 6%
10	j	52	98% 79% 15% • •
11	K	57	51% 25% 30% 33% 12%
11	k	57	47% 60% 30% 5% 5%

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	HEC	B	401	X	-	-	-
16	HEC	b	401	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33477 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
1	A	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
1	a	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1502	946	261	288	7		
3	c	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		

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

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

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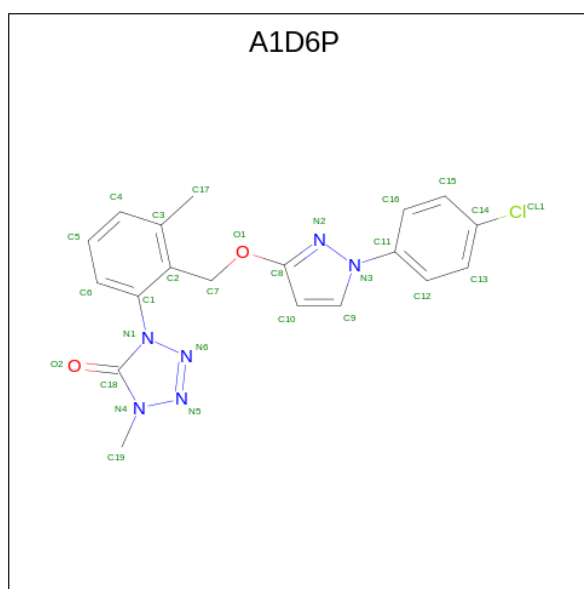
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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

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

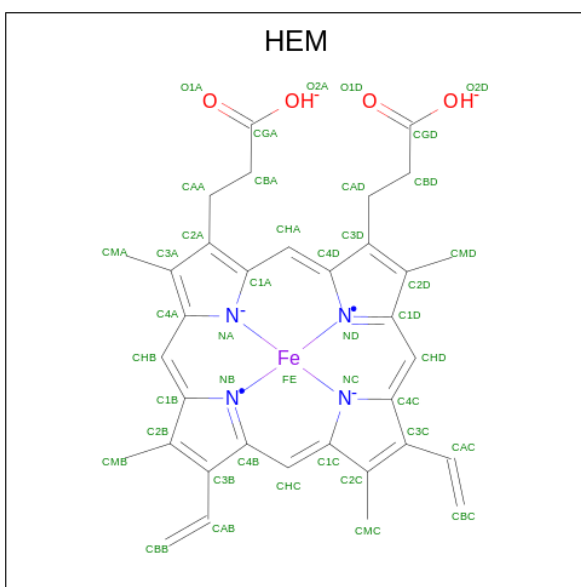
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total	C	N	O	S	0	0
			404	252	74	76	2		
11	k	57	Total	C	N	O	S	0	0
			404	252	74	76	2		

- Molecule 12 is 1-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (CCD ID: A1D6P) (formula: C₁₉H₁₇ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



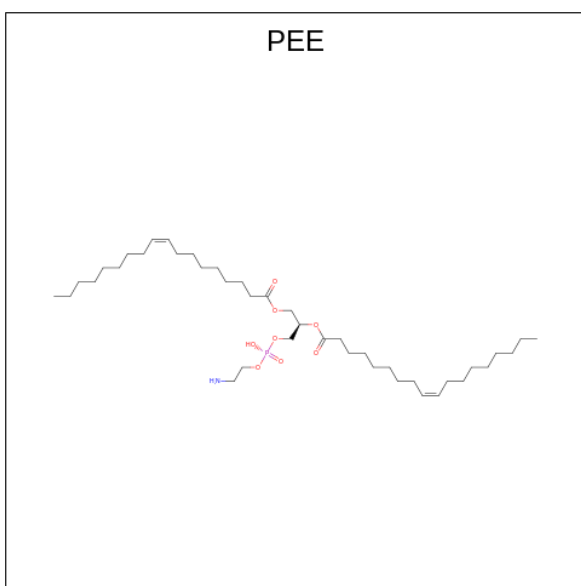
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
12	A	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
12	a	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
12	a	1	Total	C	Cl	N	O	0
			28	19	1	6	2	

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



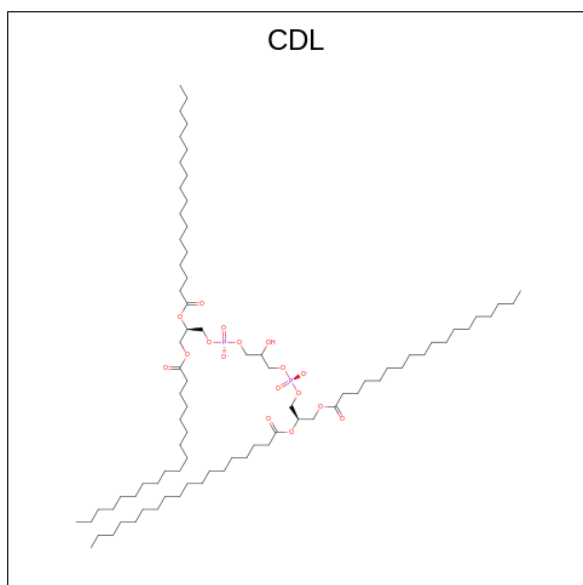
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



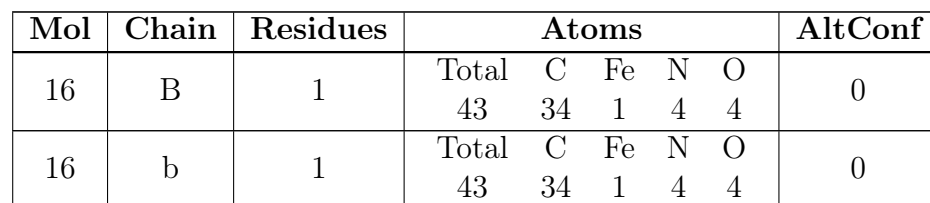
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 15 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
15	A	1	Total	C	O	P	0
			64	45	17	2	
15	a	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



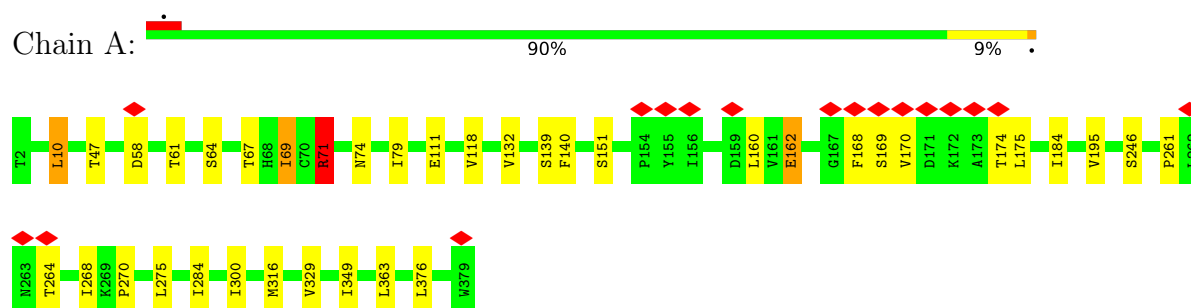
- FES
-
- S1
- S⁻²
- FE2
- Fe
- Fe
- S⁻²
- FE1
- S2

Mol	Chain	Residues	Atoms			AltConf
17	C	1	Total 4	Fe 2	S 2	0
17	c	1	Total 4	Fe 2	S 2	0

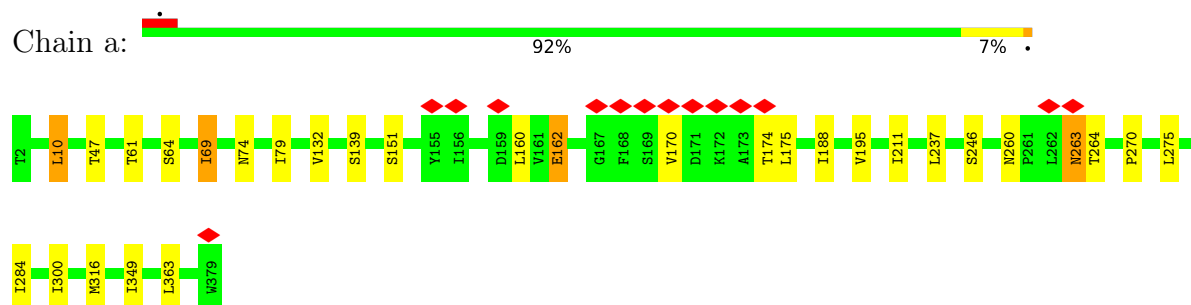
3 Residue-property plots [i](#)

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.

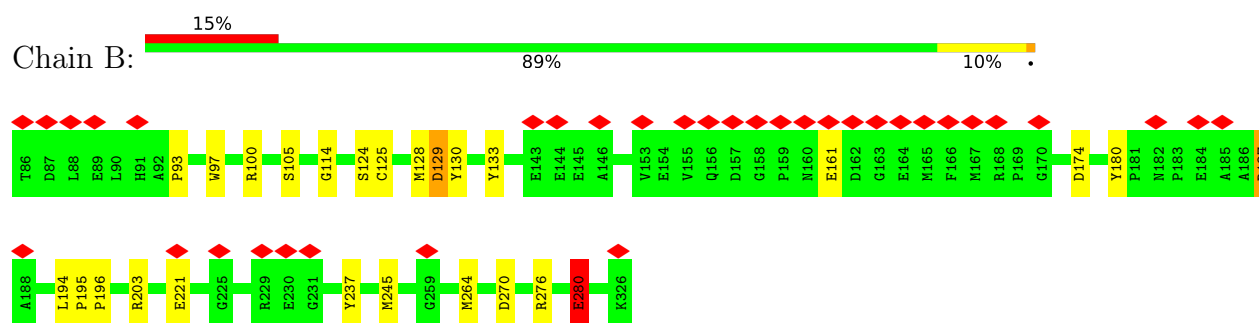
- Molecule 1: Cytochrome b



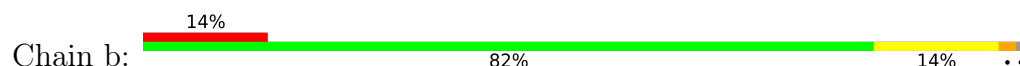
- Molecule 1: Cytochrome b

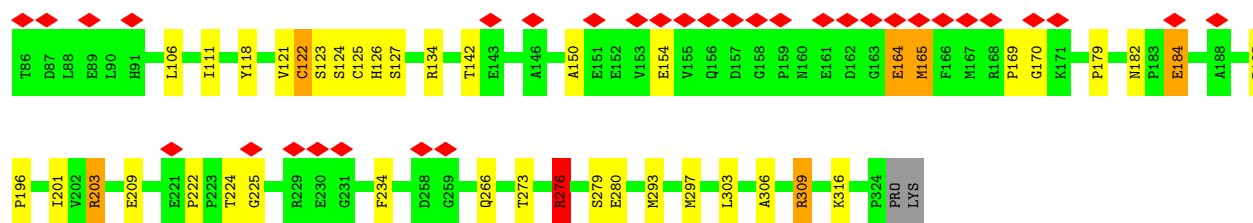


- Molecule 2: Cytochrome c1, heme protein, mitochondrial

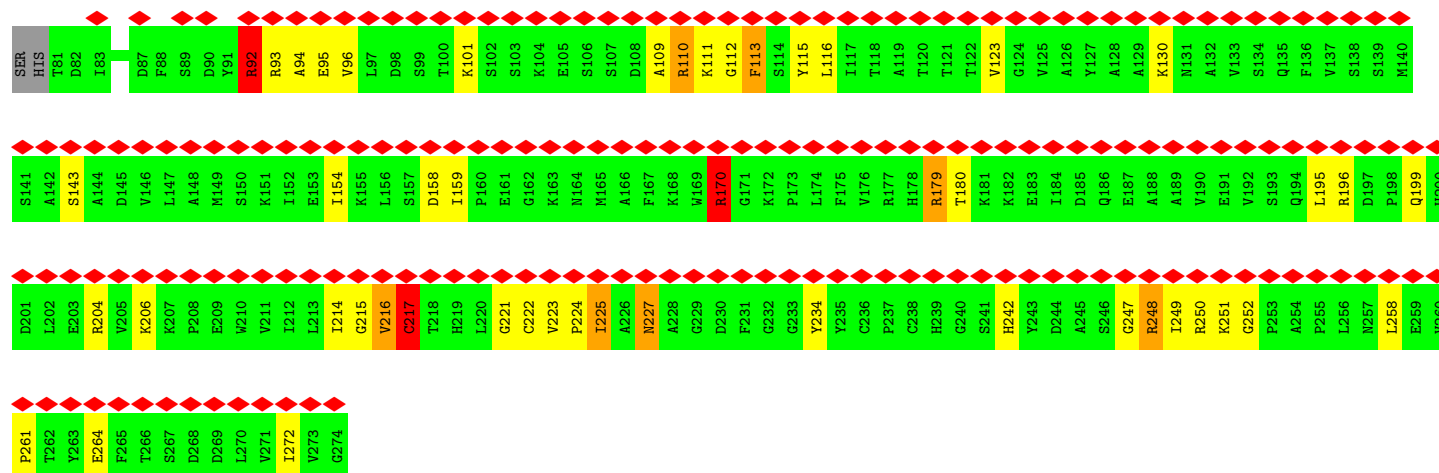
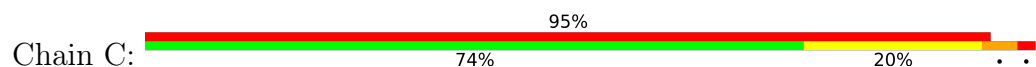


- Molecule 2: Cytochrome c1, heme protein, mitochondrial

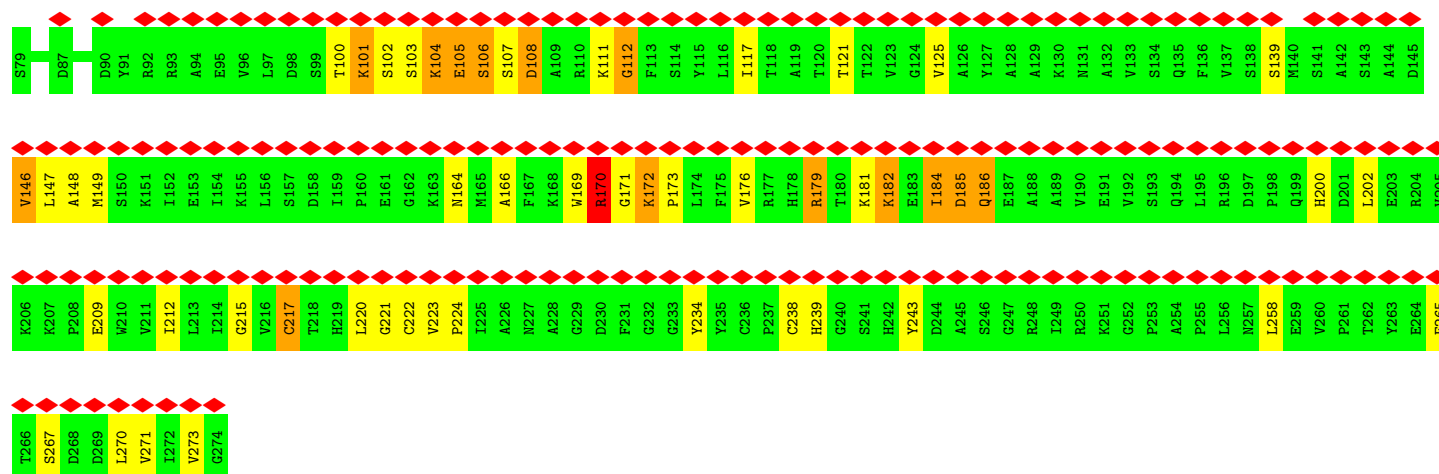
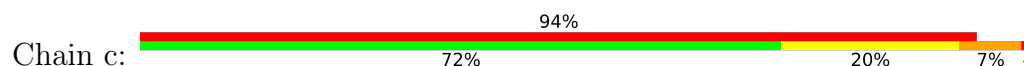




• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

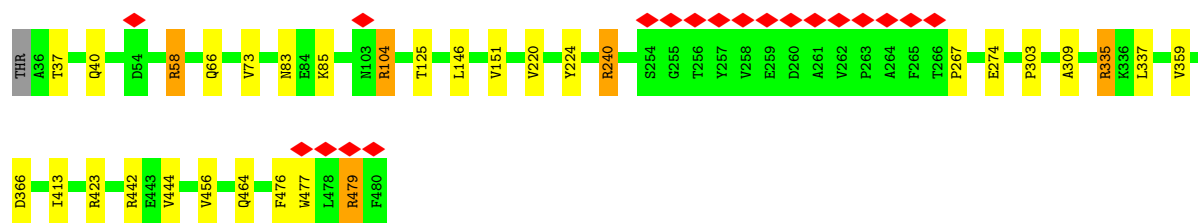


• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



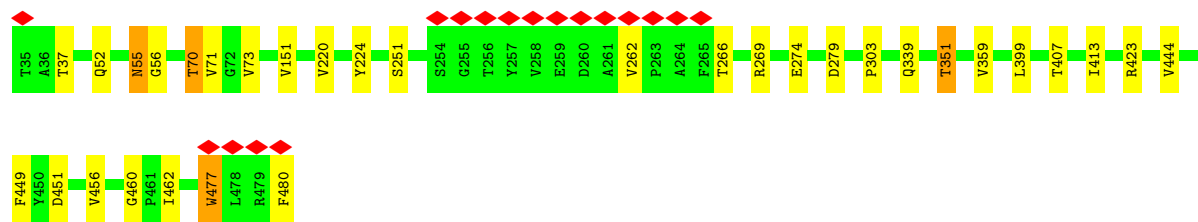
• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial





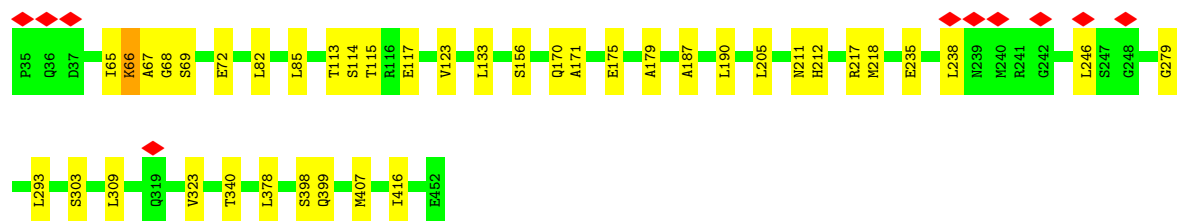
- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain d: 93% 6%



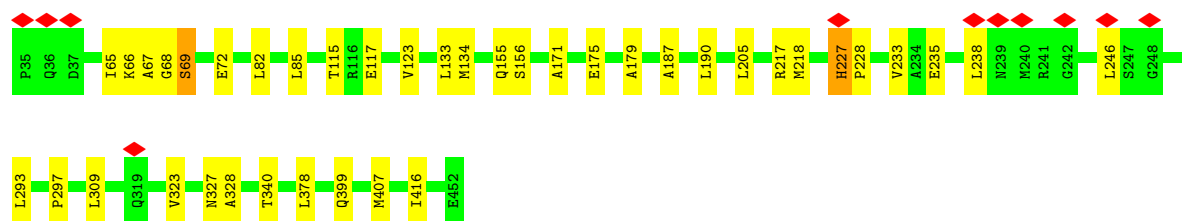
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain E: 90% 9%



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

Chain e: 90% 9%

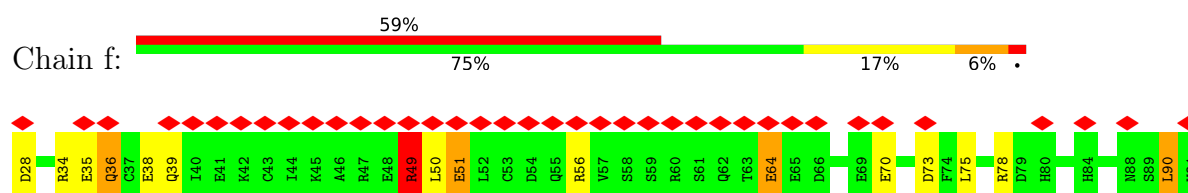


- Molecule 6: Cytochrome b-c1 complex subunit 6

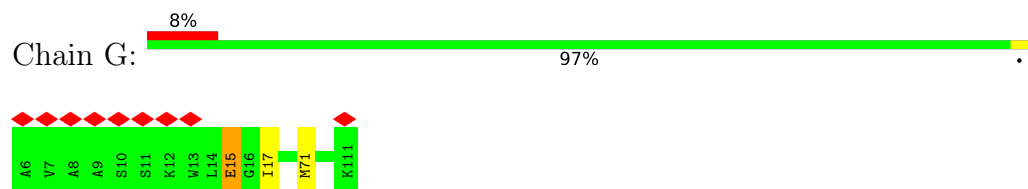
Chain F: 61% 73% 20% 5%



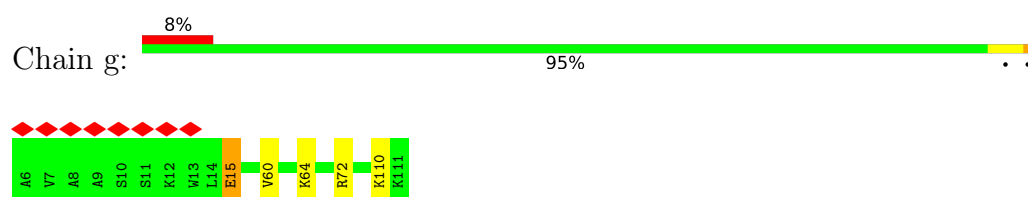
- Molecule 6: Cytochrome b-c1 complex subunit 6



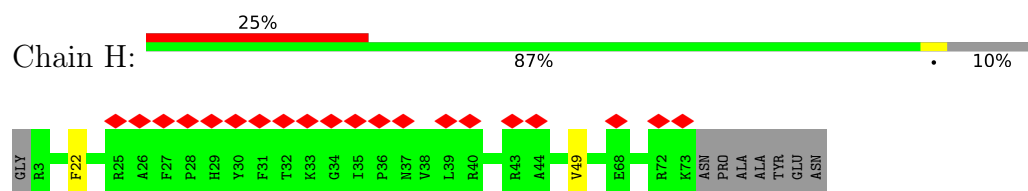
• Molecule 7: Cytochrome b-c1 complex subunit 7



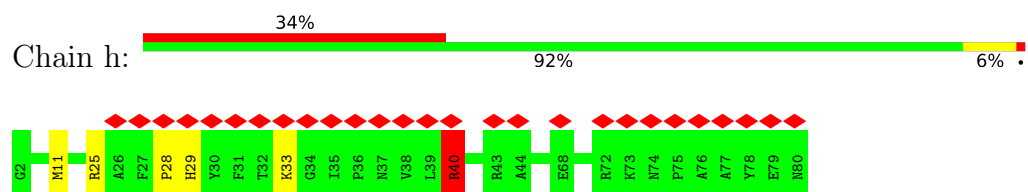
• Molecule 7: Cytochrome b-c1 complex subunit 7



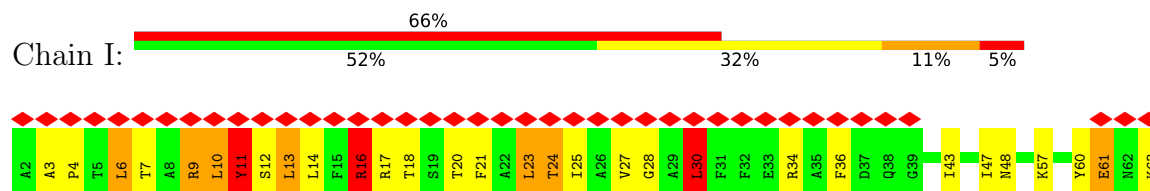
• Molecule 8: Cytochrome b-c1 complex subunit 8



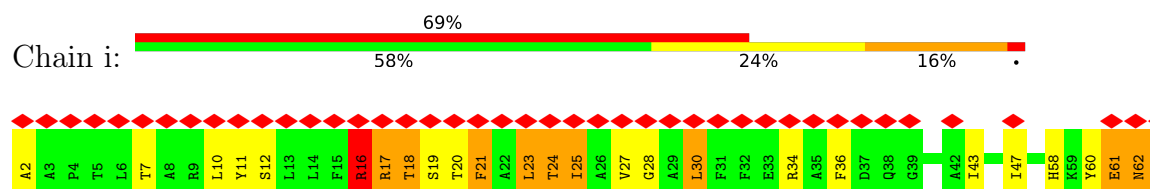
• Molecule 8: Cytochrome b-c1 complex subunit 8



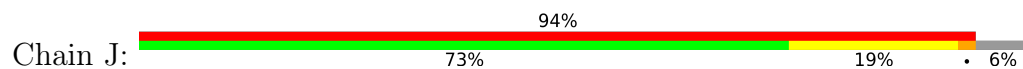
• Molecule 9: Complex III subunit 9



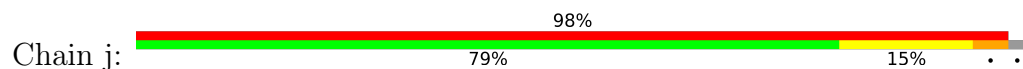
• Molecule 9: Complex III subunit 9



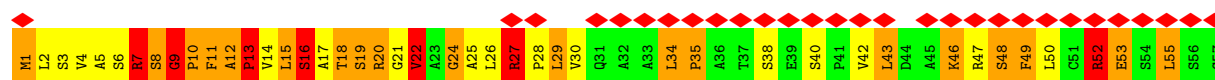
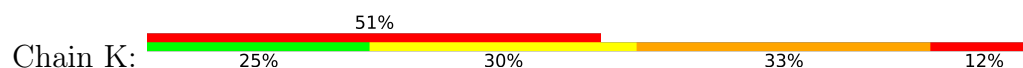
- Molecule 10: Cytochrome b-c1 complex subunit 10



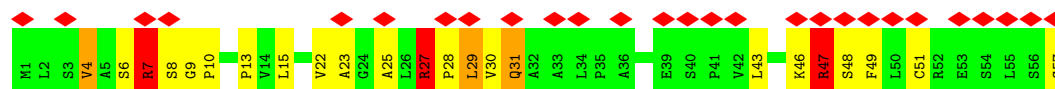
- Molecule 10: Cytochrome b-c1 complex subunit 10



- 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	411418	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 ($e^-/\text{\AA}^2$)	49.72	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.863	Depositor
Minimum map value	-5.367	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.223	Depositor
Recommended contour level	0.798	Depositor
Map size (Å)	288.0, 288.0, 288.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, HEM, FES, HEC, A1D6P, CDL

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	0.43	0/3115	0.66	3/4259 (0.1%)
1	a	0.42	0/3115	0.64	2/4259 (0.0%)
2	B	0.48	0/1978	0.79	6/2684 (0.2%)
2	b	0.55	1/1961 (0.1%)	0.89	8/2661 (0.3%)
3	C	0.59	1/1534 (0.1%)	0.88	6/2075 (0.3%)
3	c	0.51	1/1551 (0.1%)	0.90	2/2098 (0.1%)
4	D	0.42	0/3524	0.63	0/4783
4	d	0.48	2/3531 (0.1%)	0.72	6/4793 (0.1%)
5	E	0.45	2/3187 (0.1%)	0.63	1/4314 (0.0%)
5	e	0.48	2/3187 (0.1%)	0.67	4/4314 (0.1%)
6	F	0.35	0/534	0.91	6/714 (0.8%)
6	f	0.38	0/534	0.90	6/714 (0.8%)
7	G	0.39	0/941	0.64	1/1262 (0.1%)
7	g	0.39	0/941	0.64	1/1262 (0.1%)
8	H	0.38	0/628	0.71	0/848
8	h	0.34	0/688	0.75	0/931
9	I	0.66	0/520	1.17	3/701 (0.4%)
9	i	0.49	0/520	1.15	3/701 (0.4%)
10	J	0.40	0/420	0.87	1/576 (0.2%)
10	j	0.49	0/437	1.03	4/598 (0.7%)
11	K	1.42	4/410 (1.0%)	1.87	10/556 (1.8%)
11	k	0.73	0/410	1.34	3/556 (0.5%)
All	All	0.49	13/33666 (0.0%)	0.78	76/45659 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	b	0	4
3	C	0	6
3	c	0	1
4	D	0	5
6	F	0	1
6	f	0	1
8	h	0	1
9	I	0	4
9	i	0	3
10	J	0	1
11	K	0	3
11	k	0	4
All	All	0	37

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	217	CYS	C-N	13.54	1.52	1.33
2	b	121	VAL	C-N	9.97	1.49	1.33
4	d	351	THR	C-O	-9.46	1.13	1.23
5	e	67	ALA	C-O	-8.54	1.14	1.23
5	E	67	ALA	C-N	-8.49	1.25	1.32

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	VAL	N-CA-CB	-11.65	99.39	112.21
9	i	19	SER	N-CA-C	-11.05	99.93	113.41
10	j	17	TRP	N-CA-C	-10.00	96.09	110.59
4	d	451	ASP	CA-CB-CG	9.42	122.02	112.60
11	K	16	SER	N-CA-C	9.21	124.14	108.02

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Sidechain
2	B	180	TYR	Peptide
2	B	187	ARG	Sidechain
3	C	110	ARG	Peptide

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Mol	Chain	Res	Type	Group
3	C	92	ARG	Sidechain

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	A	3017	0	3078	22	0
1	a	3017	0	3078	14	0
2	B	1920	0	1869	17	0
2	b	1904	0	1849	24	0
3	C	1502	0	1490	30	0
3	c	1518	0	1501	43	0
4	D	3452	0	3343	16	0
4	d	3459	0	3350	16	0
5	E	3134	0	3112	25	0
5	e	3134	0	3112	21	0
6	F	528	0	510	8	0
6	f	528	0	510	5	0
7	G	921	0	917	2	0
7	g	921	0	917	5	0
8	H	608	0	616	2	0
8	h	666	0	663	5	0
9	I	507	0	509	11	0
9	i	507	0	509	12	0
10	J	405	0	405	9	0
10	j	421	0	418	4	0
11	K	404	0	425	48	0
11	k	404	0	425	19	0
12	A	56	0	0	0	0
12	a	56	0	0	0	0
13	A	86	0	60	0	0
13	a	86	0	60	0	0
14	A	45	0	67	4	0
14	a	49	0	75	3	0
15	A	64	0	72	2	0
15	a	64	0	72	2	0
16	B	43	0	32	5	0
16	b	43	0	32	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	4	0	0	0	0
17	c	4	0	0	0	0
All	All	33477	0	33076	300	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 5.

The worst 5 of 300 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:125:CYS:SG	16:B:401:HEC:HBC3	1.86	1.16
1:A:169:SER:HB2	3:c:171:GLY:HA3	1.45	0.95
2:b:125:CYS:SG	16:b:401:HEC:CAC	2.55	0.95
5:e:328:ALA:HA	11:k:8:SER:HB2	1.46	0.94
2:B:125:CYS:SG	16:B:401:HEC:CBC	2.54	0.94

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%)	363 (96%)	13 (4%)	0	100	100
2	B	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30	47
2	b	237/241 (98%)	213 (90%)	24 (10%)	0	100	100
3	C	192/196 (98%)	163 (85%)	29 (15%)	0	100	100
3	c	194/196 (99%)	153 (79%)	41 (21%)	0	100	100
4	D	443/446 (99%)	423 (96%)	20 (4%)	0	100	100
4	d	444/446 (100%)	421 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	416/418 (100%)	399 (96%)	17 (4%)	0	100	100
5	e	416/418 (100%)	398 (96%)	18 (4%)	0	100	100
6	F	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
6	f	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
7	G	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
7	g	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
8	H	69/79 (87%)	61 (88%)	8 (12%)	0	100	100
8	h	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
9	I	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
9	i	60/62 (97%)	49 (82%)	11 (18%)	0	100	100
10	J	47/52 (90%)	42 (89%)	5 (11%)	0	100	100
10	j	49/52 (94%)	42 (86%)	6 (12%)	1 (2%)	6	9
11	K	55/57 (96%)	37 (67%)	10 (18%)	8 (14%)	0	0
11	k	55/57 (96%)	43 (78%)	10 (18%)	2 (4%)	2	3
All	All	4137/4198 (98%)	3826 (92%)	299 (7%)	12 (0%)	37	53

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	7	ARG
11	K	8	SER
10	j	18	ILE
11	k	27	ARG
11	K	9	GLY

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	A	331/331 (100%)	319 (96%)	12 (4%)	31	55
1	a	331/331 (100%)	318 (96%)	13 (4%)	28	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	206/206 (100%)	201 (98%)	5 (2%)	43	69
2	b	204/206 (99%)	191 (94%)	13 (6%)	16	31
3	C	164/166 (99%)	151 (92%)	13 (8%)	11	22
3	c	166/166 (100%)	144 (87%)	22 (13%)	4	7
4	D	371/372 (100%)	365 (98%)	6 (2%)	55	78
4	d	372/372 (100%)	366 (98%)	6 (2%)	55	78
5	E	327/328 (100%)	323 (99%)	4 (1%)	63	82
5	e	327/328 (100%)	322 (98%)	5 (2%)	57	79
6	F	61/61 (100%)	52 (85%)	9 (15%)	3	5
6	f	61/61 (100%)	51 (84%)	10 (16%)	2	4
7	G	95/95 (100%)	94 (99%)	1 (1%)	65	83
7	g	95/95 (100%)	94 (99%)	1 (1%)	65	83
8	H	65/70 (93%)	65 (100%)	0	100	100
8	h	70/70 (100%)	69 (99%)	1 (1%)	59	80
9	I	50/50 (100%)	29 (58%)	21 (42%)	0	0
9	i	50/50 (100%)	33 (66%)	17 (34%)	0	0
10	J	40/42 (95%)	39 (98%)	1 (2%)	42	67
10	j	41/42 (98%)	39 (95%)	2 (5%)	22	43
11	K	44/44 (100%)	18 (41%)	26 (59%)	0	0
11	k	44/44 (100%)	38 (86%)	6 (14%)	3	7
All	All	3515/3530 (100%)	3321 (94%)	194 (6%)	21	38

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	165	MET
3	c	238	CYS
2	b	224	THR
3	c	146	VAL
4	d	351	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	148	ASN
8	h	65	GLN
3	c	239	HIS
6	f	62	GLN
5	e	227	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	404	1	50,50,50	1.58	7 (14%)	66,82,82	1.40	10 (15%)
16	HEC	b	401	2	50,50,50	2.86	26 (52%)	68,82,82	2.50	26 (38%)
17	FES	c	301	3	0,4,4	-	-	-	-	-
12	A1D6P	a	402	-	31,31,31	1.70	7 (22%)	34,44,44	1.92	6 (17%)
15	CDL	A	406	-	63,63,99	1.08	8 (12%)	69,75,111	1.14	4 (5%)
12	A1D6P	a	401	-	31,31,31	1.65	5 (16%)	34,44,44	1.92	4 (11%)
14	PEE	a	405	-	48,48,50	1.49	5 (10%)	51,53,55	1.31	4 (7%)
13	HEM	A	404	1	50,50,50	1.62	7 (14%)	66,82,82	1.94	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	FES	C	301	-	0,4,4	-	-	-		
13	HEM	A	403	1	50,50,50	1.62	7 (14%)	66,82,82	1.36	10 (15%)
12	A1D6P	A	402	-	31,31,31	1.71	7 (22%)	34,44,44	1.91	6 (17%)
16	HEC	B	401	2	50,50,50	2.76	28 (56%)	68,82,82	2.62	32 (47%)
12	A1D6P	A	401	-	31,31,31	1.65	6 (19%)	34,44,44	1.92	4 (11%)
15	CDL	a	406	-	63,63,99	1.10	8 (12%)	69,75,111	1.17	4 (5%)
13	HEM	a	403	1	50,50,50	1.53	6 (12%)	66,82,82	1.62	17 (25%)
14	PEE	A	405	-	44,44,50	1.54	5 (11%)	46,49,55	1.38	5 (10%)

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	404	1	-	2/14/54/54	-
16	HEC	b	401	2	1/1/3/7	8/14/54/54	-
17	FES	c	301	3	-	-	0/1/1/1
12	A1D6P	a	402	-	-	2/13/13/13	0/4/4/4
15	CDL	A	406	-	-	44/74/74/110	-
12	A1D6P	a	401	-	-	2/13/13/13	0/4/4/4
14	PEE	a	405	-	-	26/52/52/54	-
13	HEM	A	404	1	-	4/14/54/54	-
17	FES	C	301	-	-	-	0/1/1/1
12	A1D6P	A	402	-	-	2/13/13/13	0/4/4/4
13	HEM	A	403	1	-	2/14/54/54	-
16	HEC	B	401	2	1/1/3/7	8/14/54/54	-
12	A1D6P	A	401	-	-	2/13/13/13	0/4/4/4
15	CDL	a	406	-	-	37/74/74/110	-
13	HEM	a	403	1	-	6/14/54/54	-
14	PEE	A	405	-	-	28/48/48/54	-

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	403	HEM	FE-ND	5.76	2.12	1.94
13	A	404	HEM	FE-ND	5.67	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	404	HEM	FE-ND	5.46	2.11	1.94
13	a	403	HEM	FE-ND	5.31	2.11	1.94
13	A	404	HEM	FE-NB	5.30	2.11	1.94

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	402	A1D6P	C10-C8-N2	-7.59	107.77	113.53
12	A	402	A1D6P	C10-C8-N2	-7.54	107.80	113.53
12	a	401	A1D6P	C10-C8-N2	-7.19	108.07	113.53
12	A	401	A1D6P	C10-C8-N2	-7.16	108.09	113.53
16	b	401	HEC	CAB-C3B-C4B	5.89	132.45	124.81

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	B	401	HEC	NA
16	b	401	HEC	NA

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	401	A1D6P	C10-C8-O1-C7
12	A	402	A1D6P	C10-C8-O1-C7
12	A	402	A1D6P	N2-C8-O1-C7
12	a	401	A1D6P	C10-C8-O1-C7
12	a	402	A1D6P	C10-C8-O1-C7

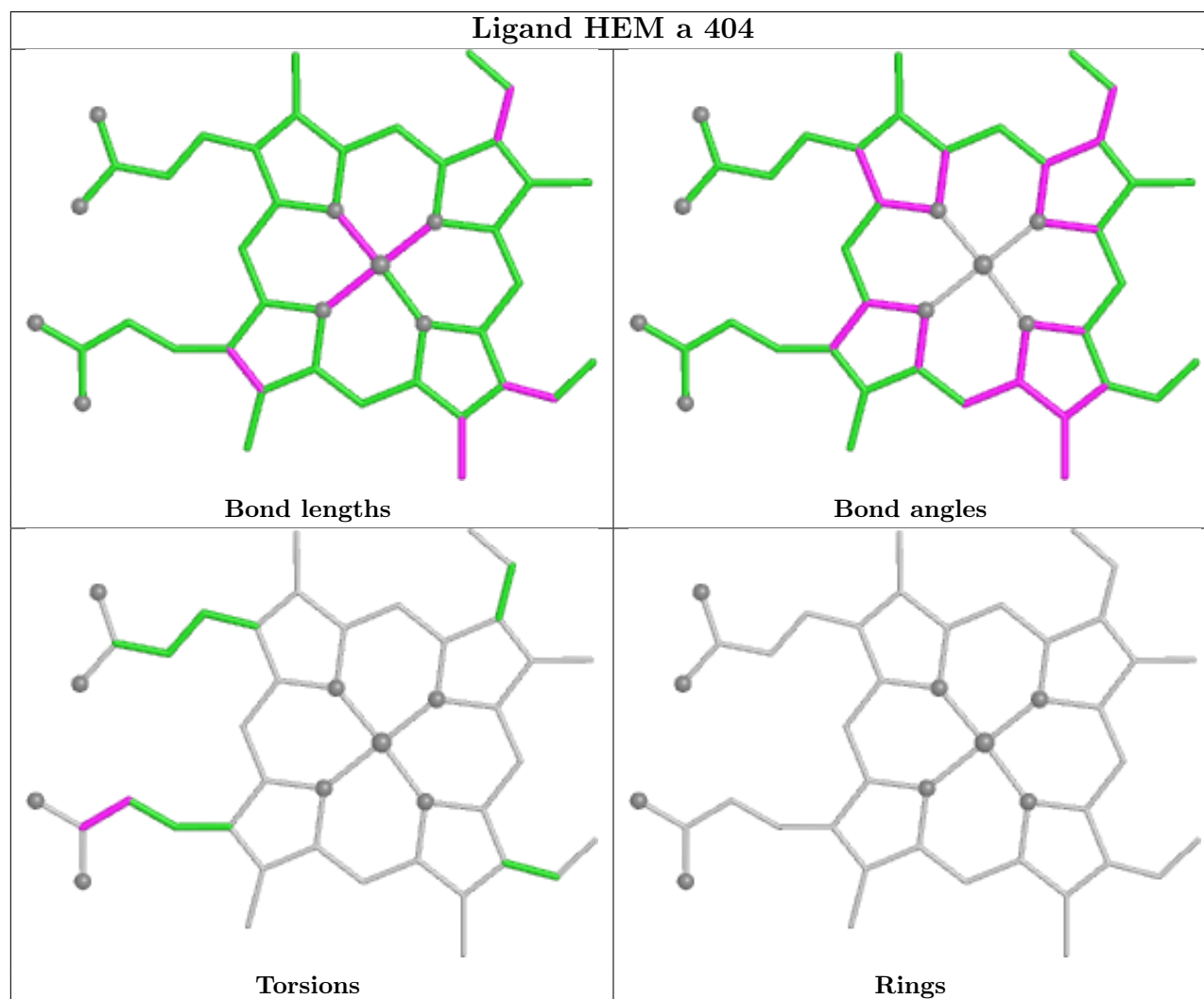
There are no ring outliers.

6 monomers are involved in 20 short contacts:

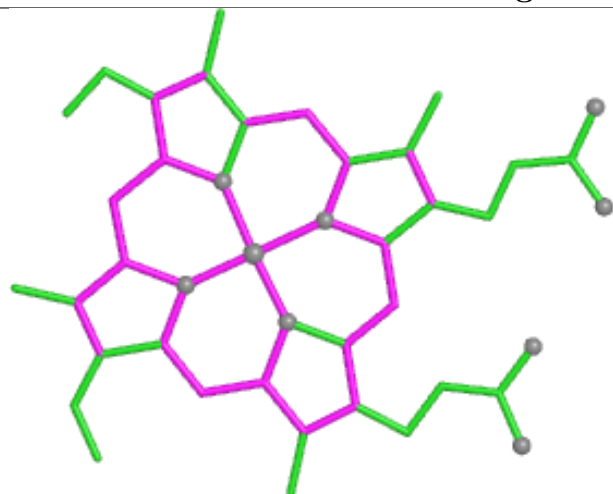
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	401	HEC	4	0
15	A	406	CDL	2	0
14	a	405	PEE	3	0
16	B	401	HEC	5	0
15	a	406	CDL	2	0
14	A	405	PEE	4	0

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

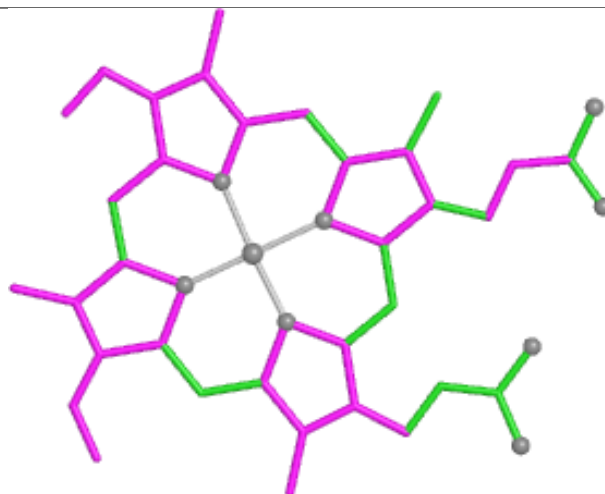
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



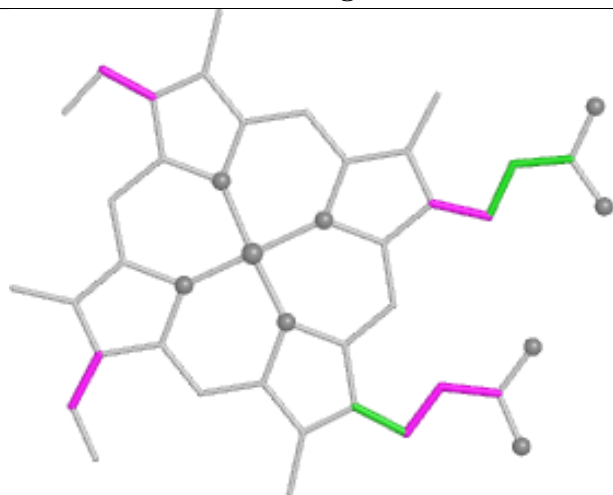
Ligand HEC b 401



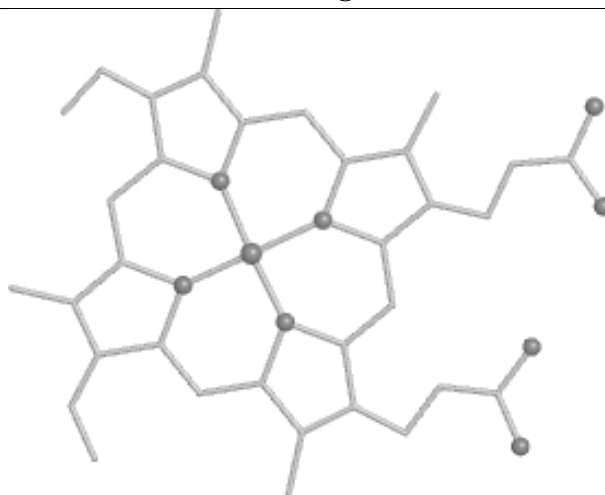
Bond lengths



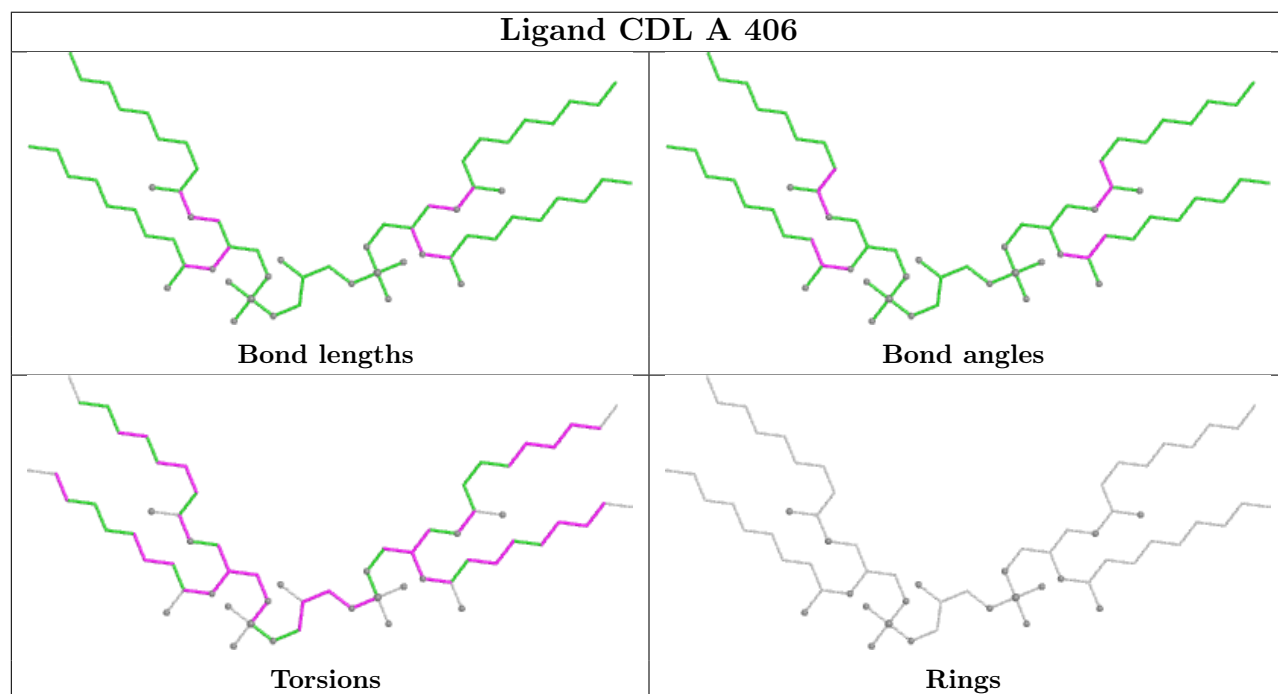
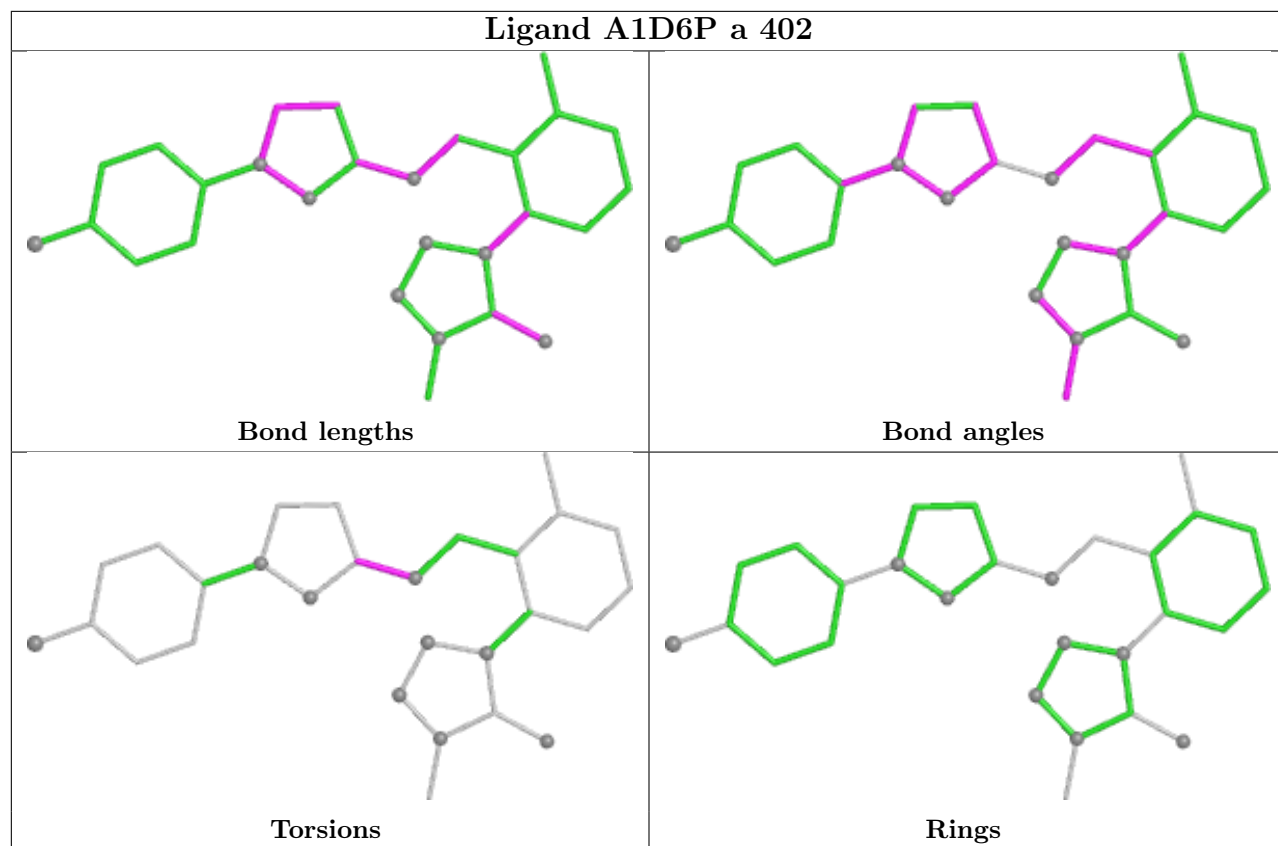
Bond angles

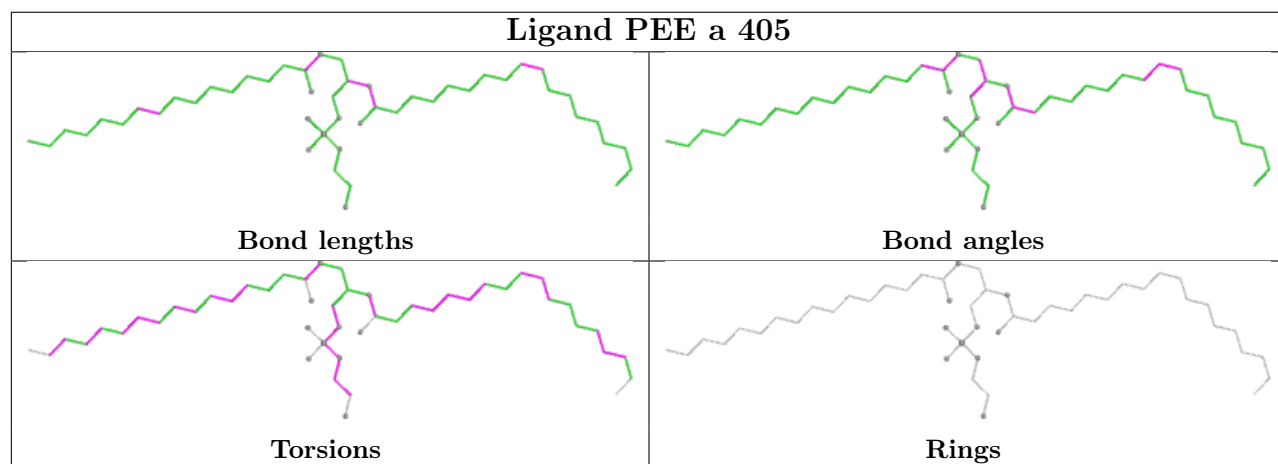
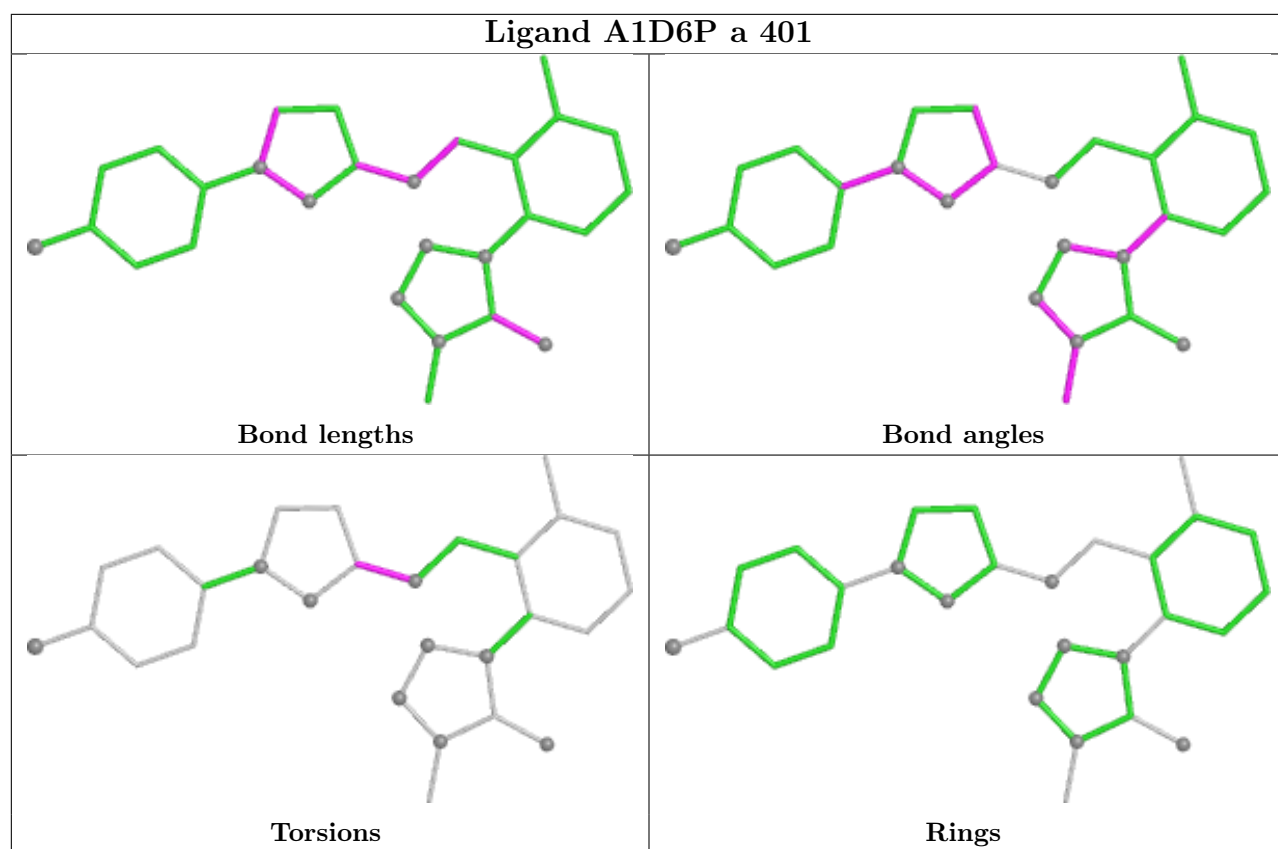


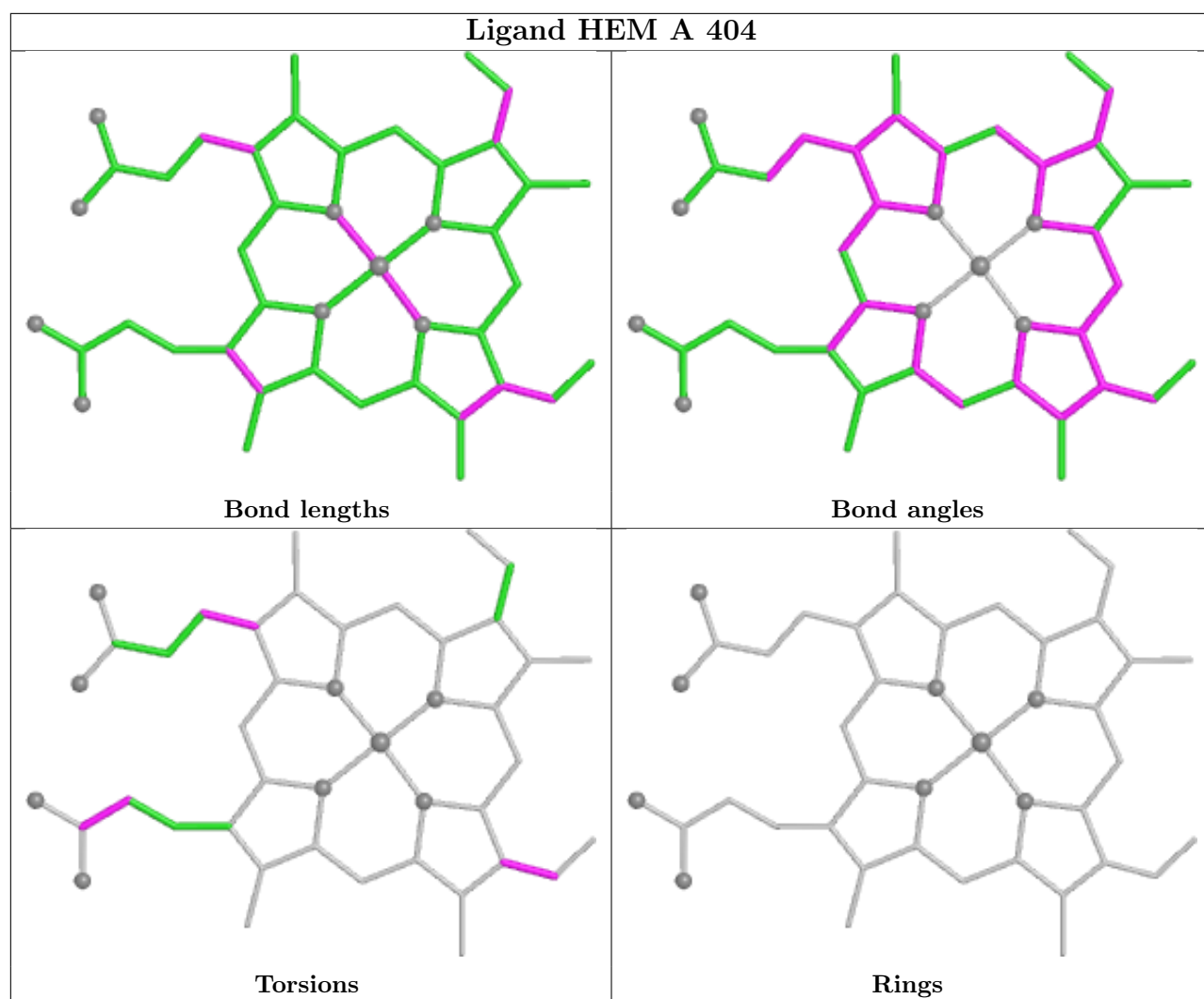
Torsions

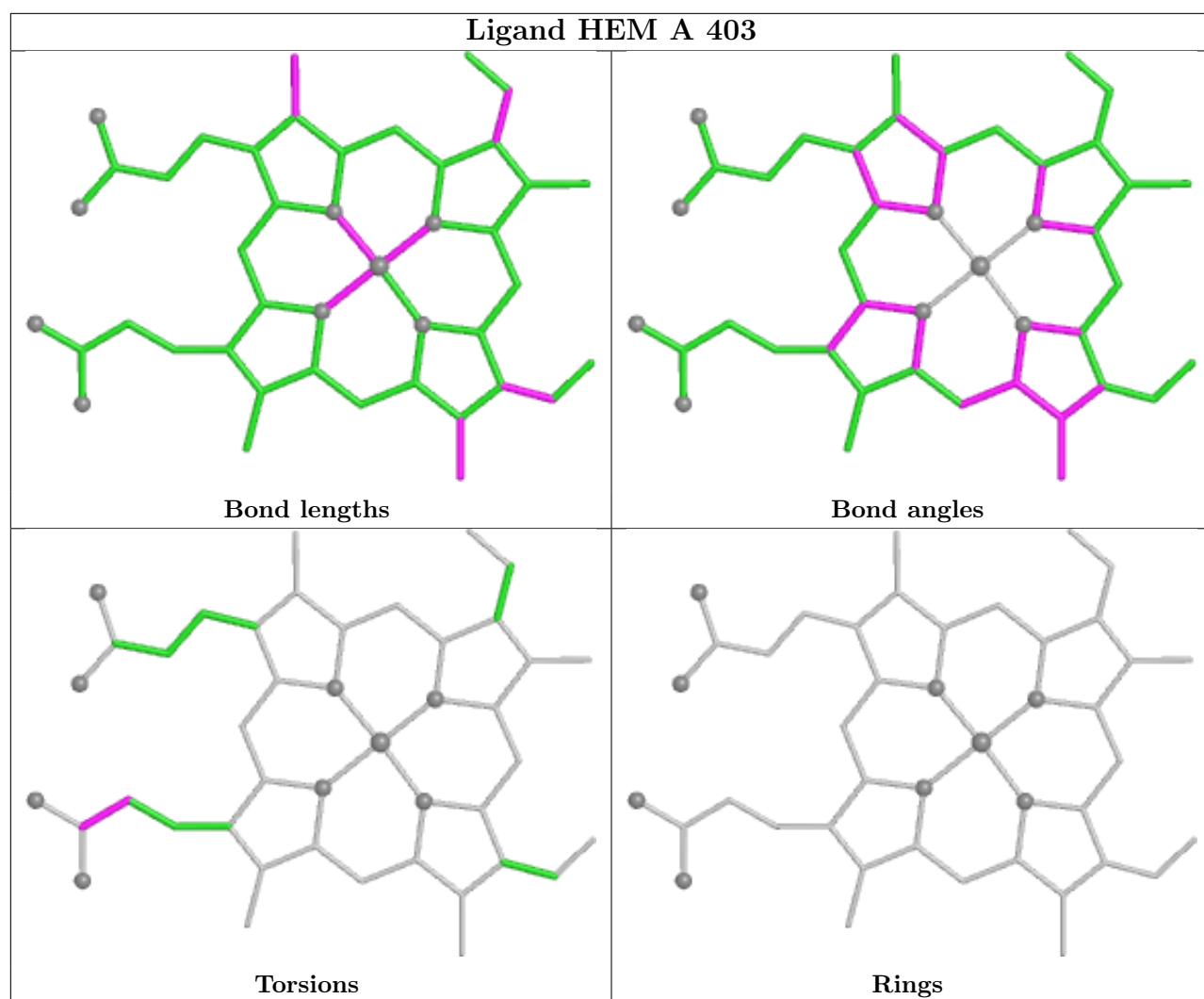


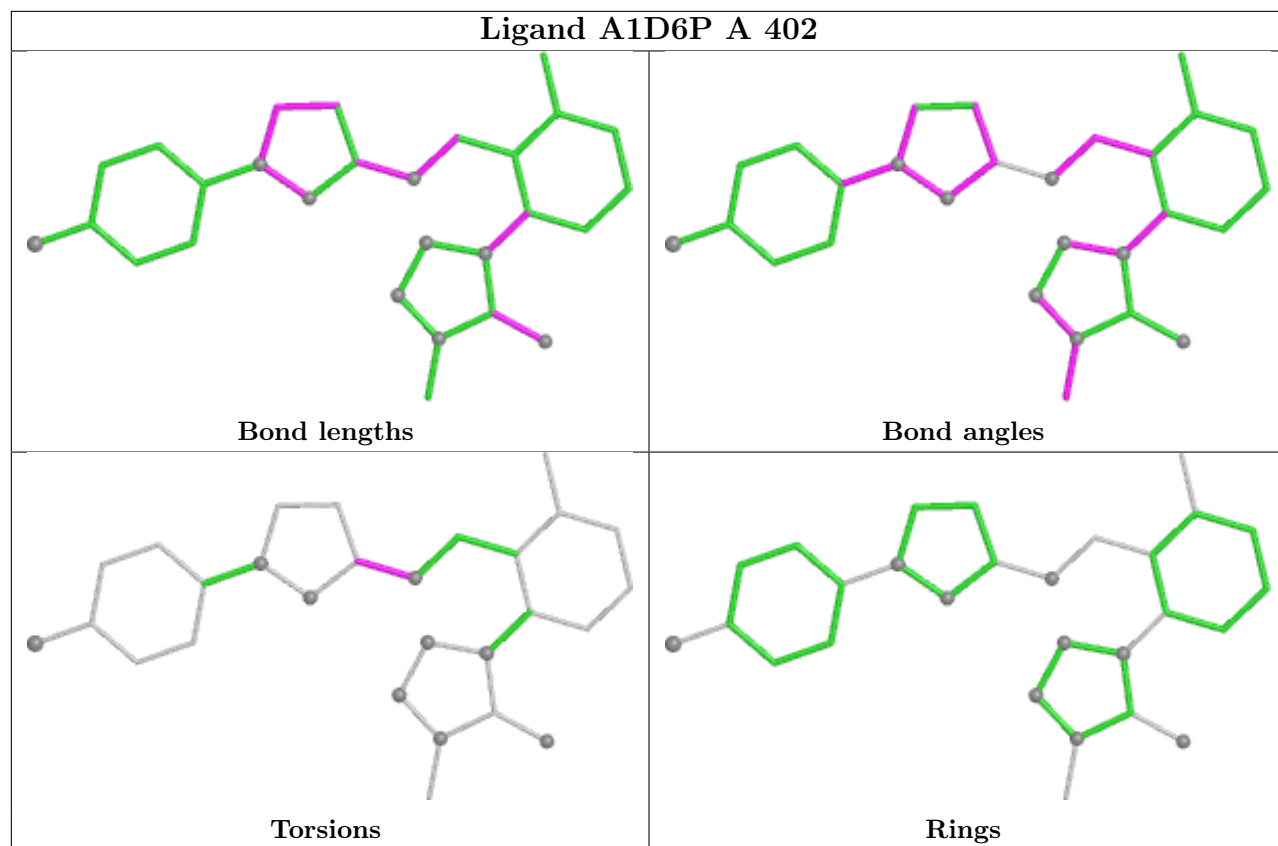
Rings

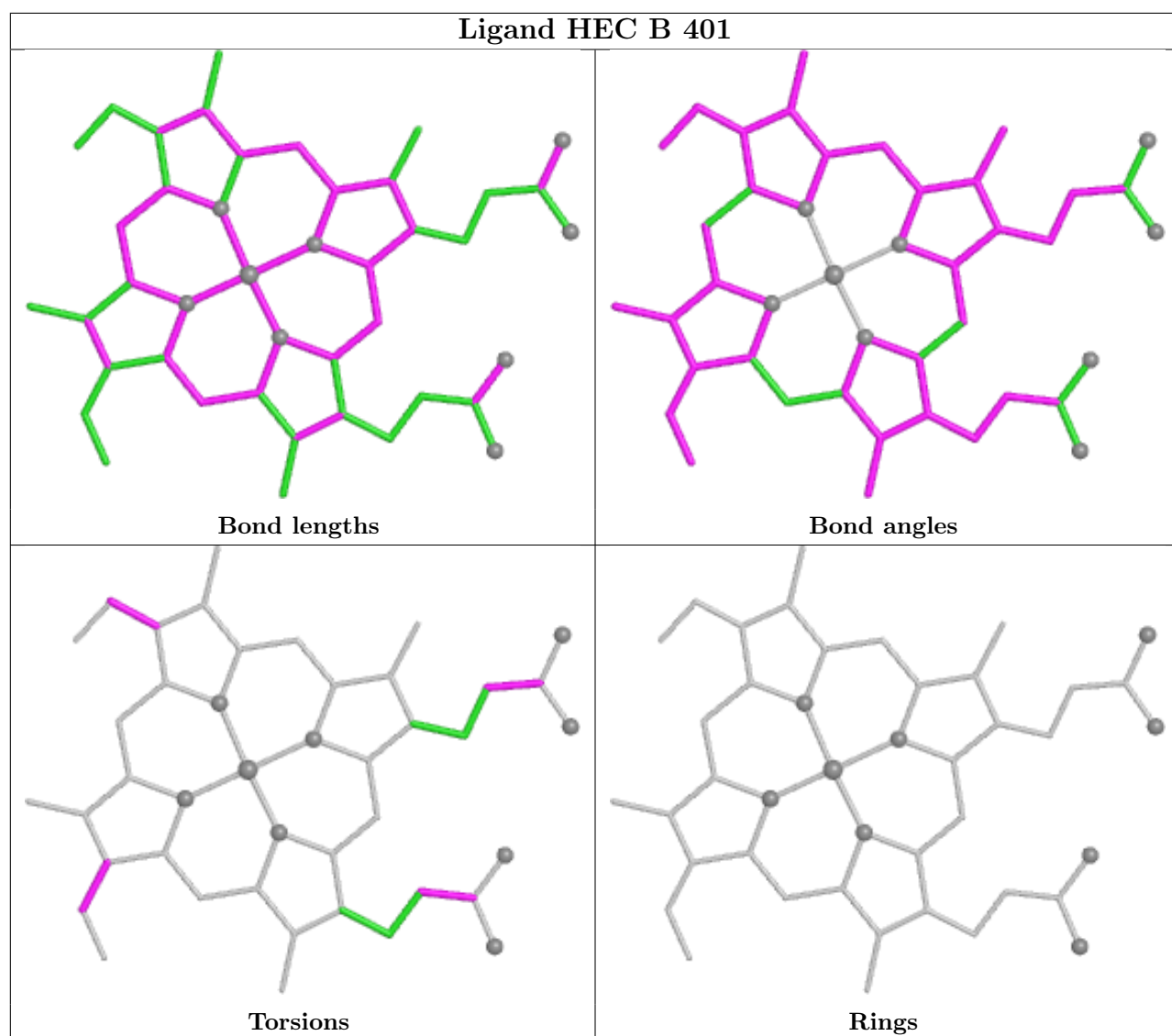


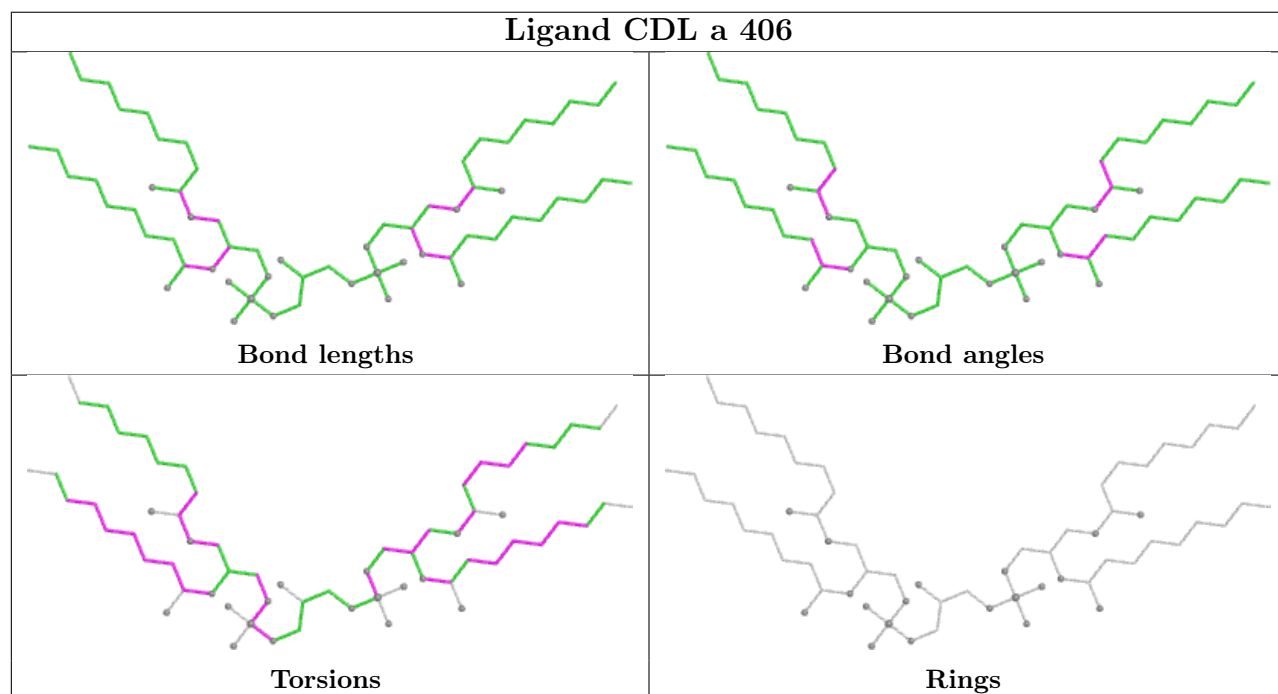
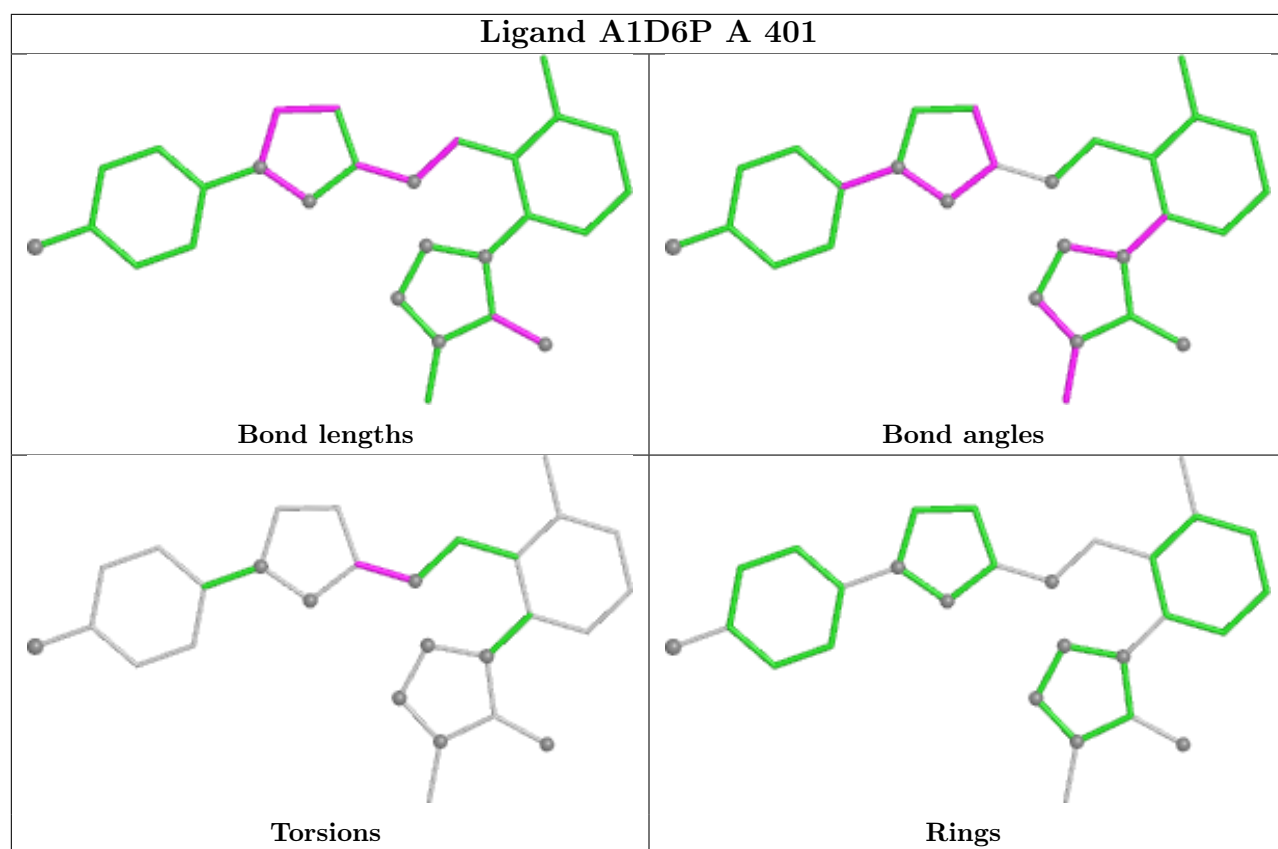


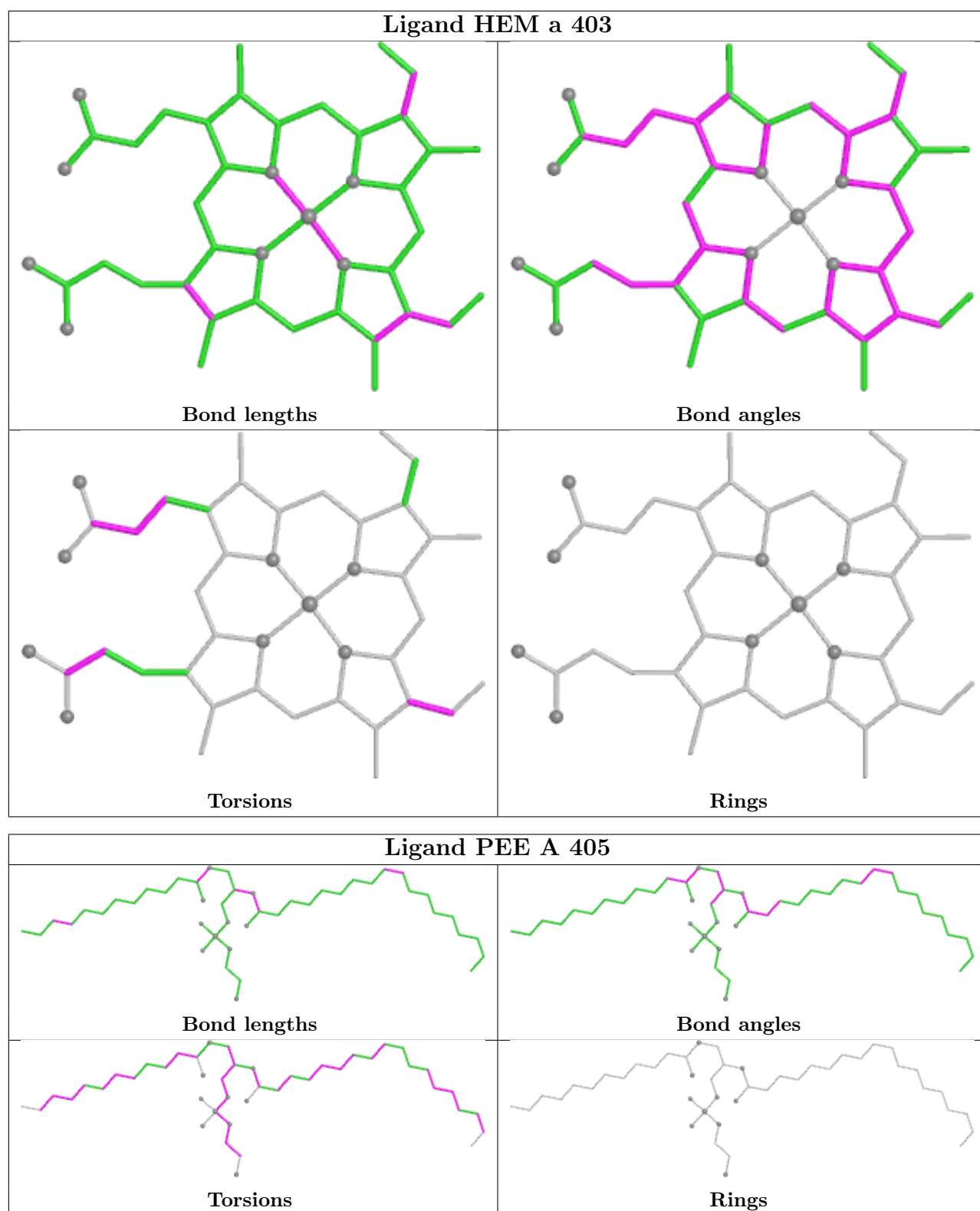












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

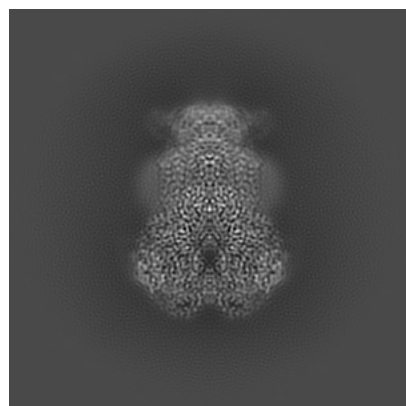
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60320. These allow visual inspection of the internal detail of the map and identification of artifacts.

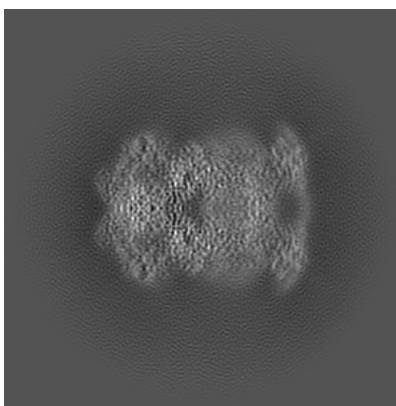
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

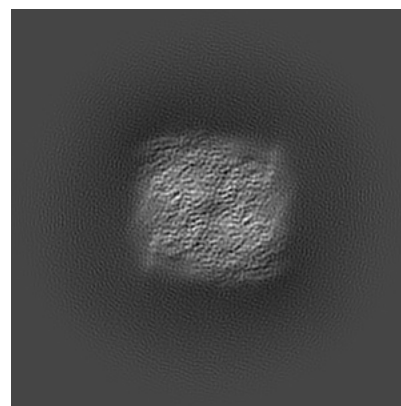
6.1.1 Primary map



X

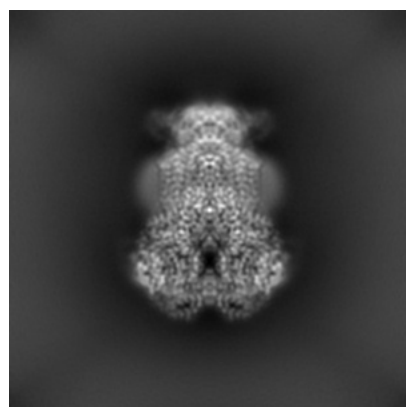


Y

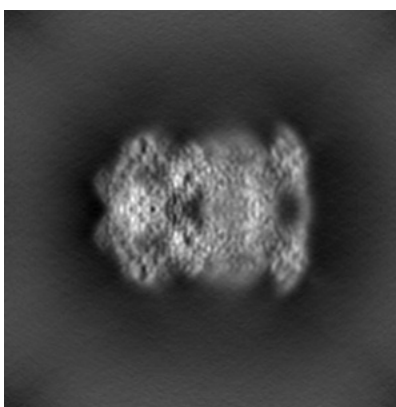


Z

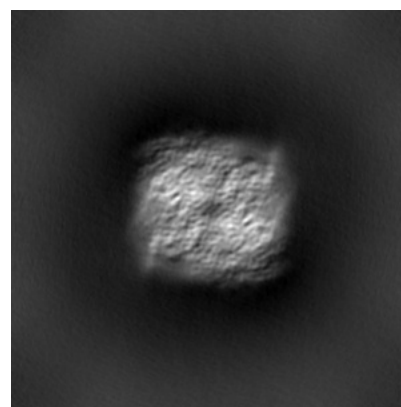
6.1.2 Raw map



X



Y

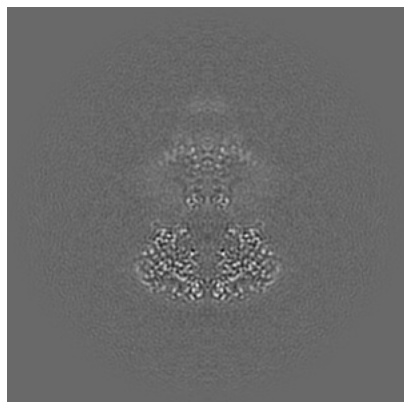


Z

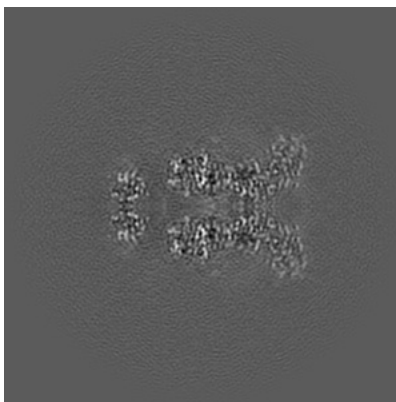
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

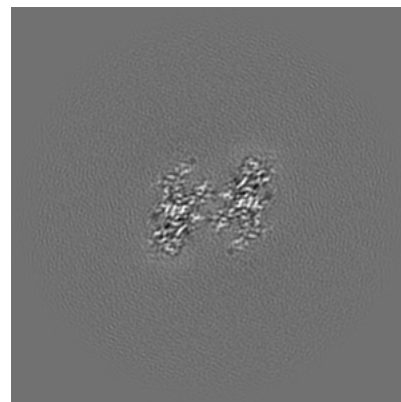
6.2.1 Primary map



X Index: 150

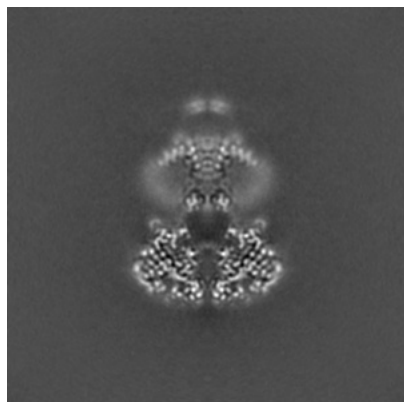


Y Index: 150

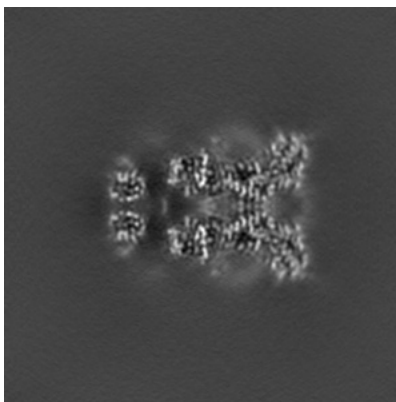


Z Index: 150

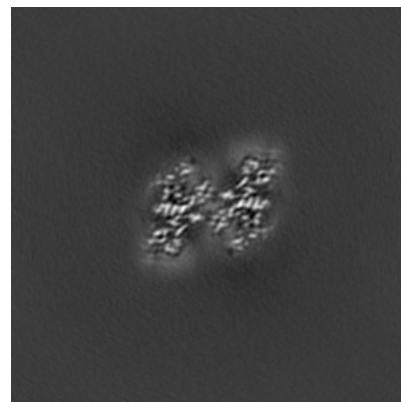
6.2.2 Raw map



X Index: 150



Y Index: 150

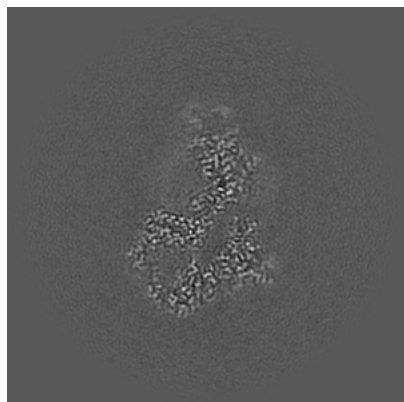


Z Index: 150

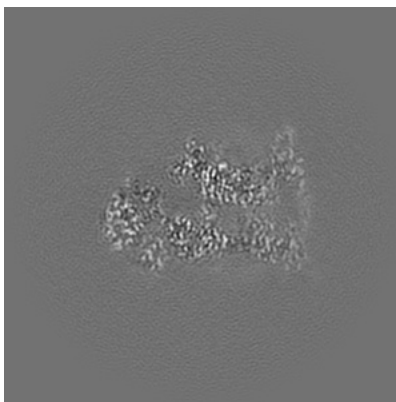
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

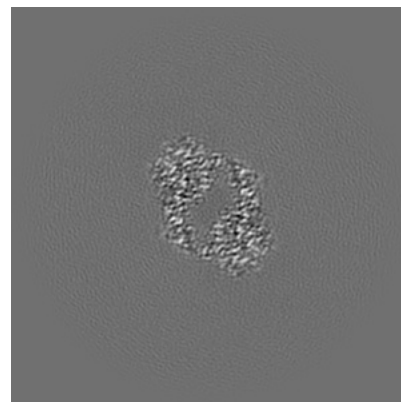
6.3.1 Primary map



X Index: 163

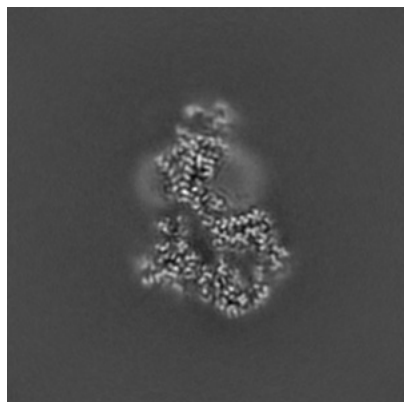


Y Index: 158

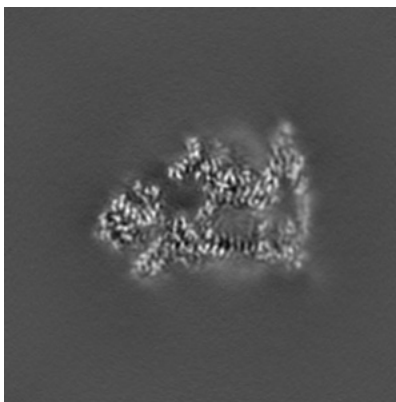


Z Index: 130

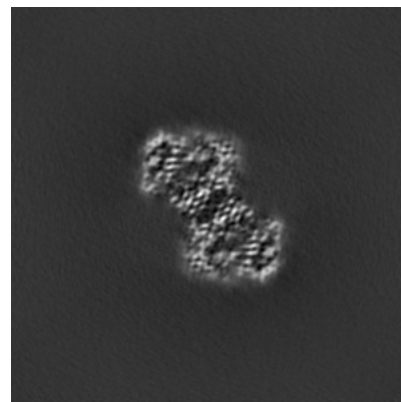
6.3.2 Raw map



X Index: 137



Y Index: 161

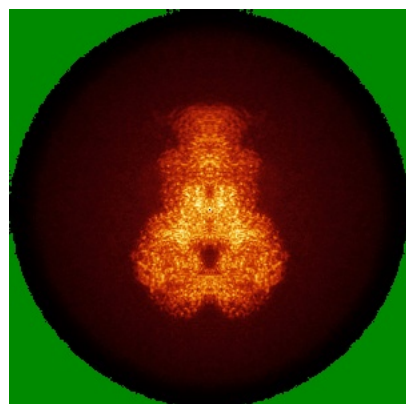


Z Index: 97

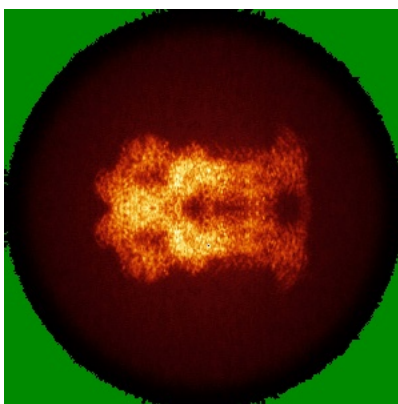
The images above show the largest variance slices of the map in three orthogonal directions.

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

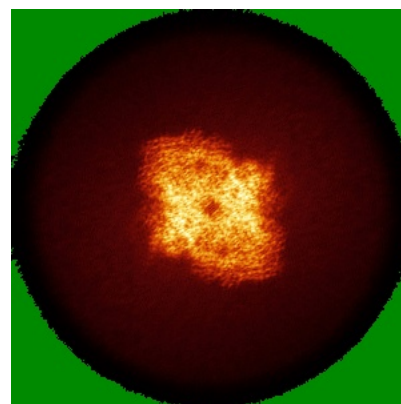
6.4.1 Primary map



X

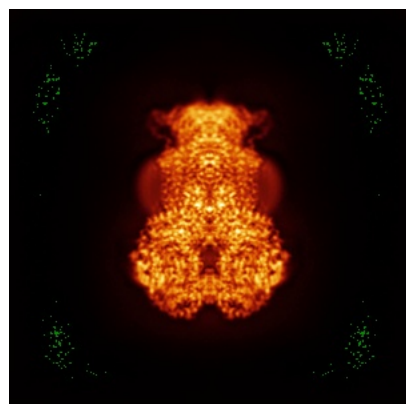


Y

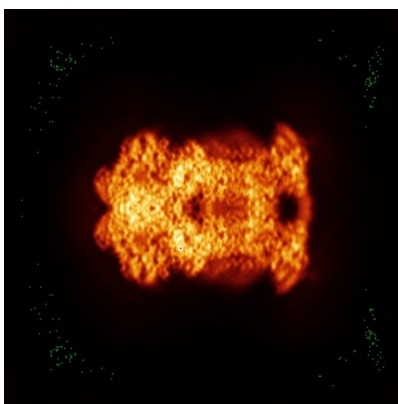


Z

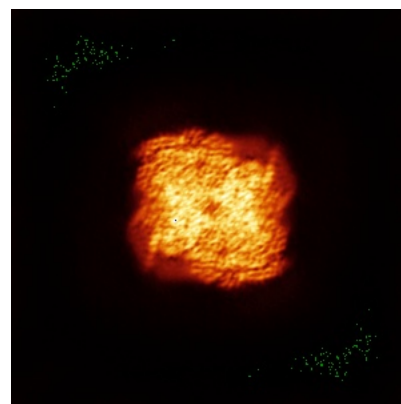
6.4.2 Raw map



X



Y



Z

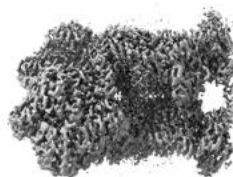
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



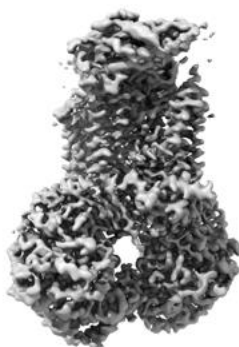
Y



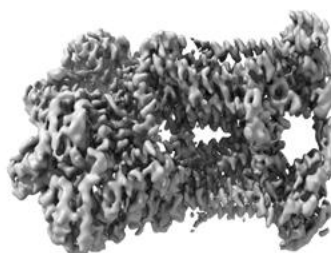
Z

The images above show the 3D surface view of the map at the recommended contour level 0.798. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

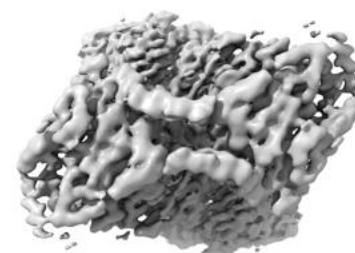
6.5.2 Raw map



X



Y



Z

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.

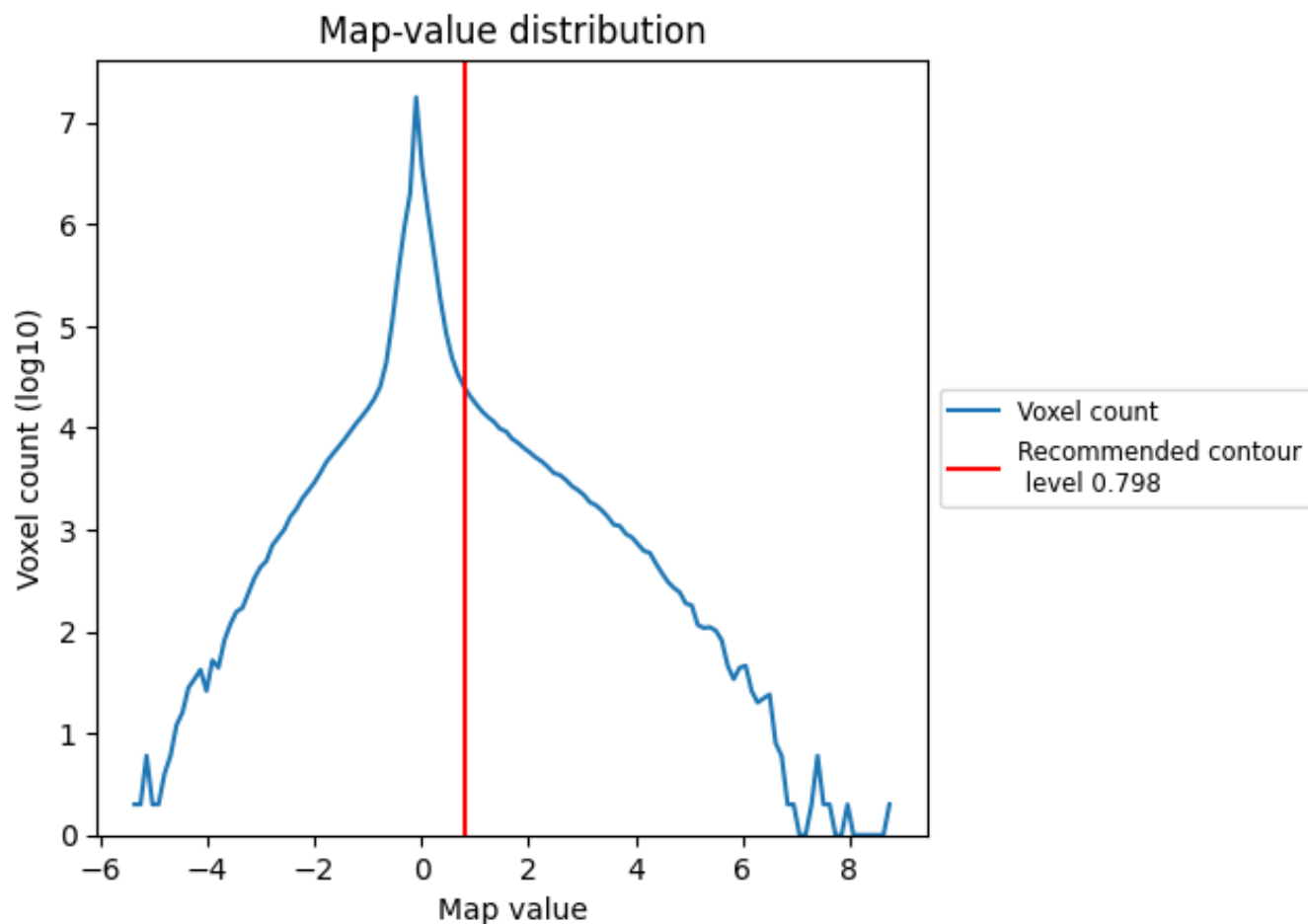
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

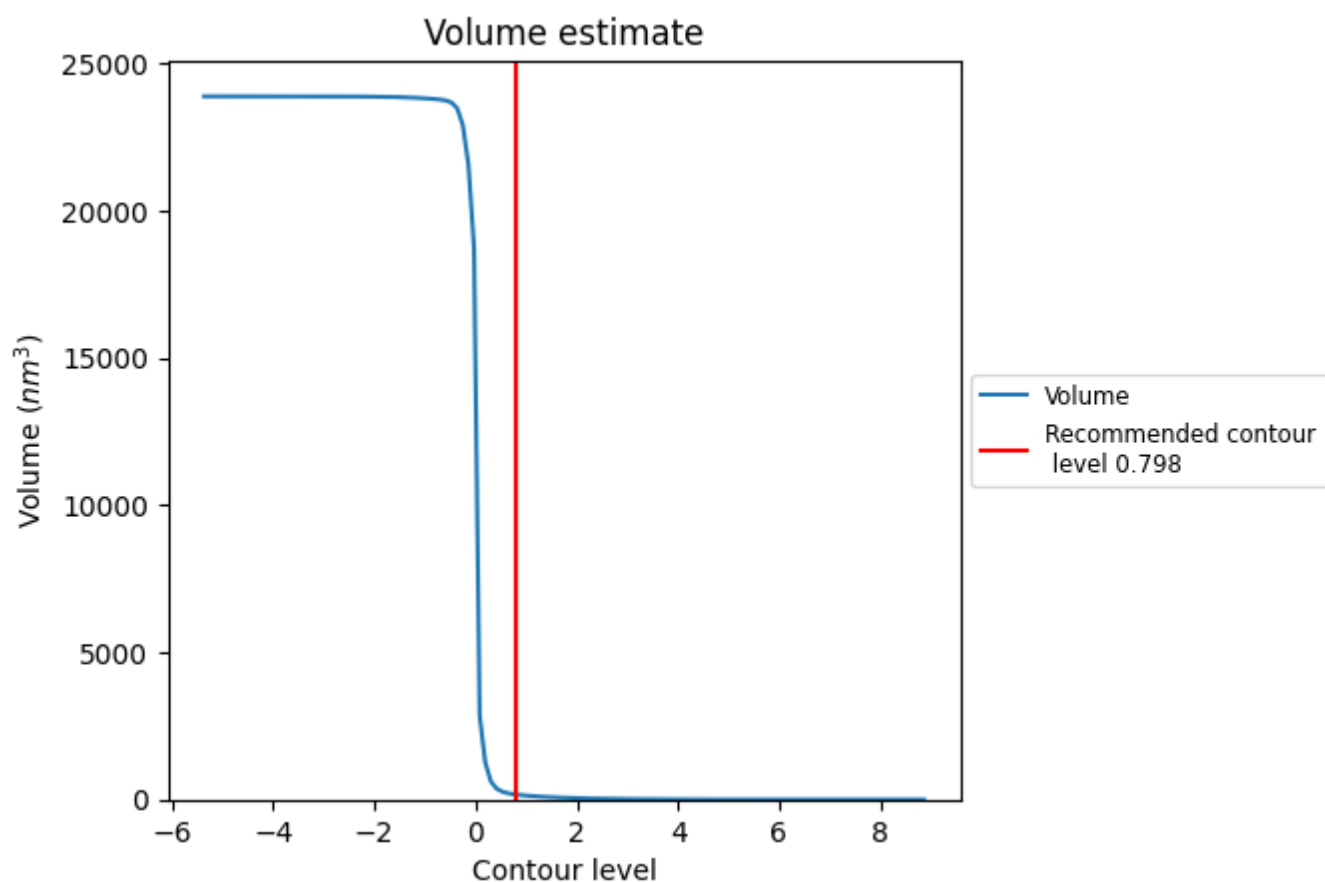
This section contains the results of statistical analysis of the map.

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.

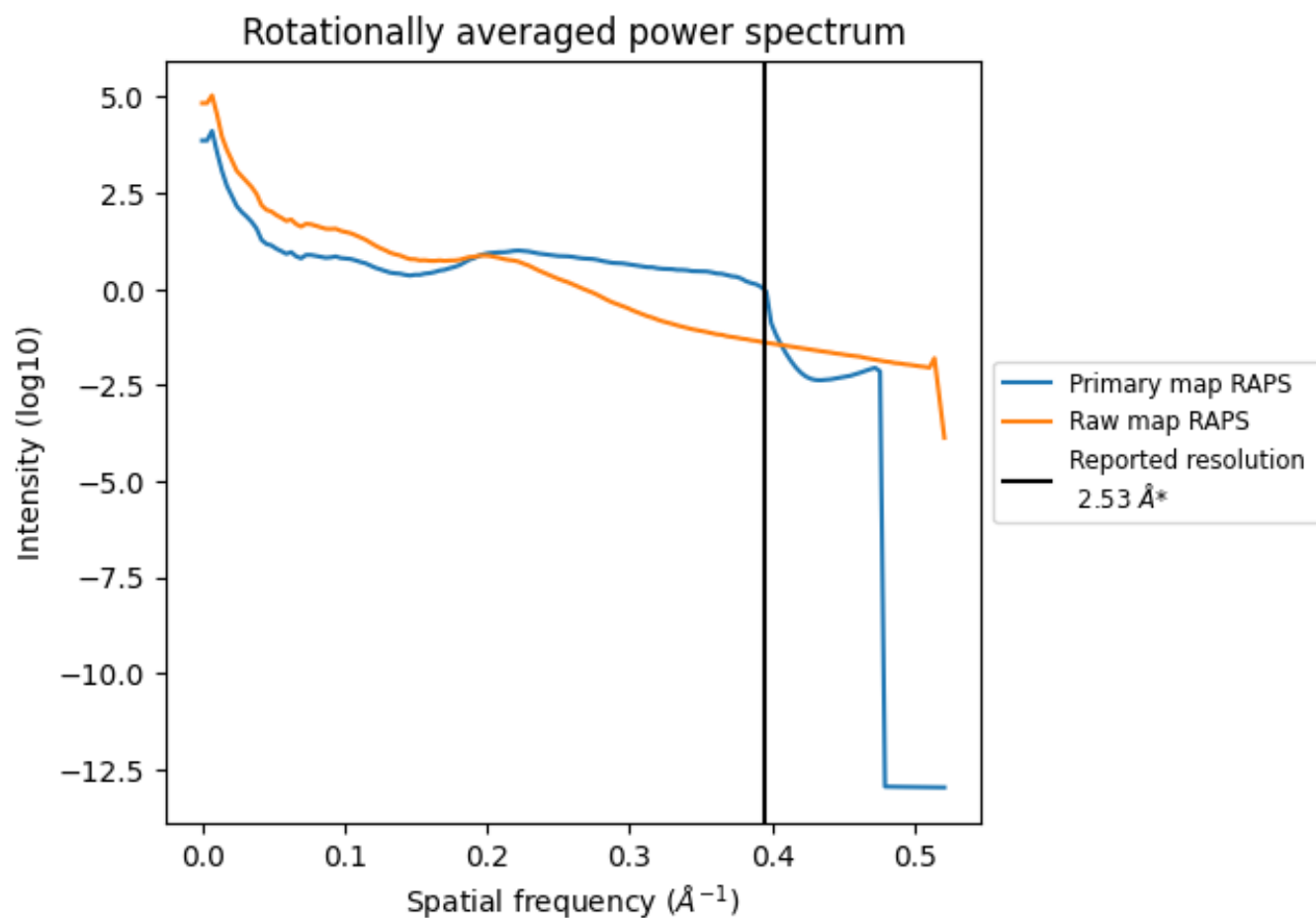
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 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 ⓘ

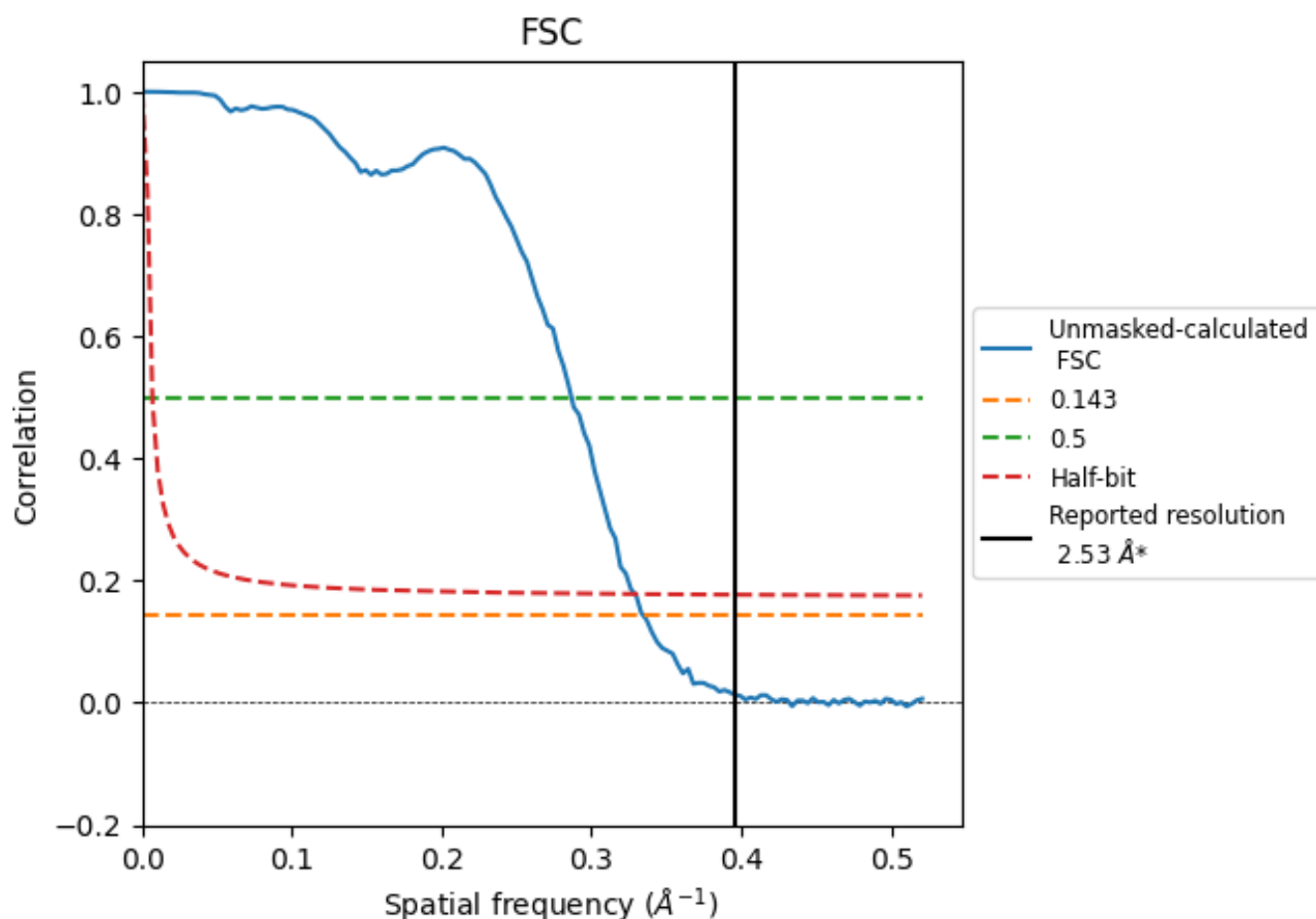


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

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 0.395 Å⁻¹

8.2 Resolution estimates [i](#)

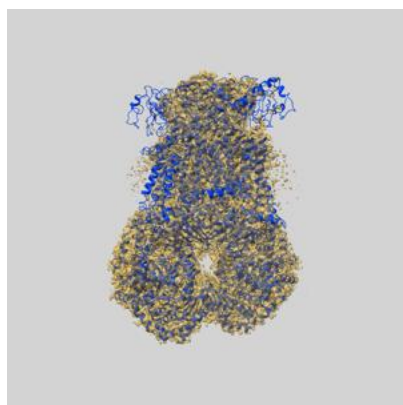
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.49	3.04

*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 2.99 differs from the reported value 2.53 by more than 10 %

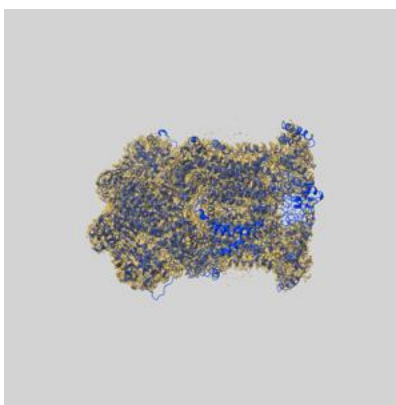
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60320 and PDB model 8ZOW. Per-residue inclusion information can be found in section [3](#) on page [10](#).

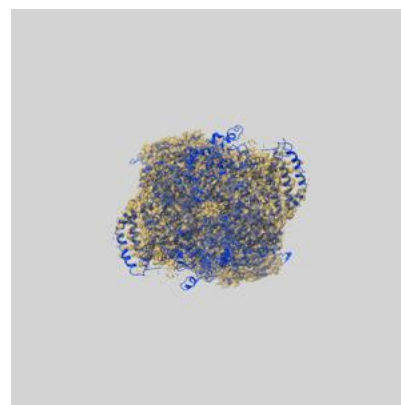
9.1 Map-model overlay [i](#)



X



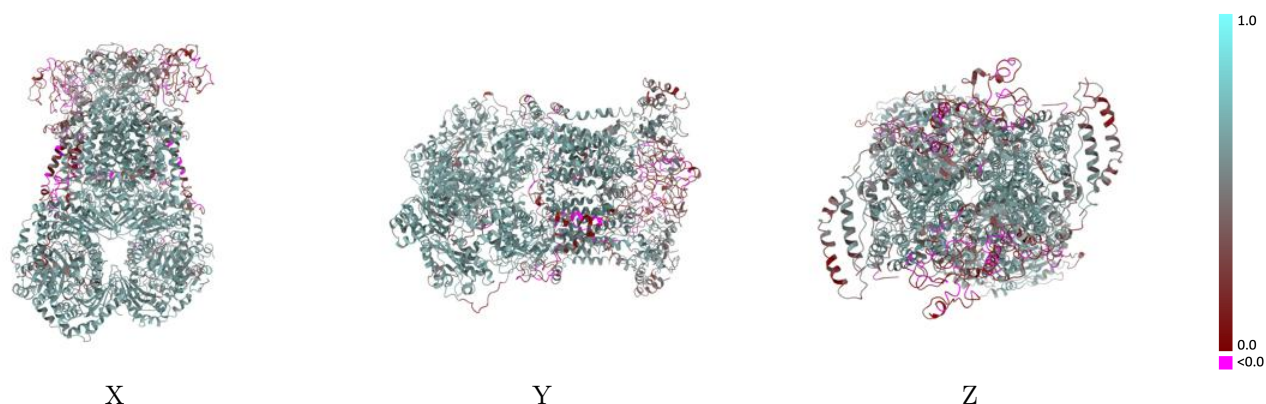
Y



Z

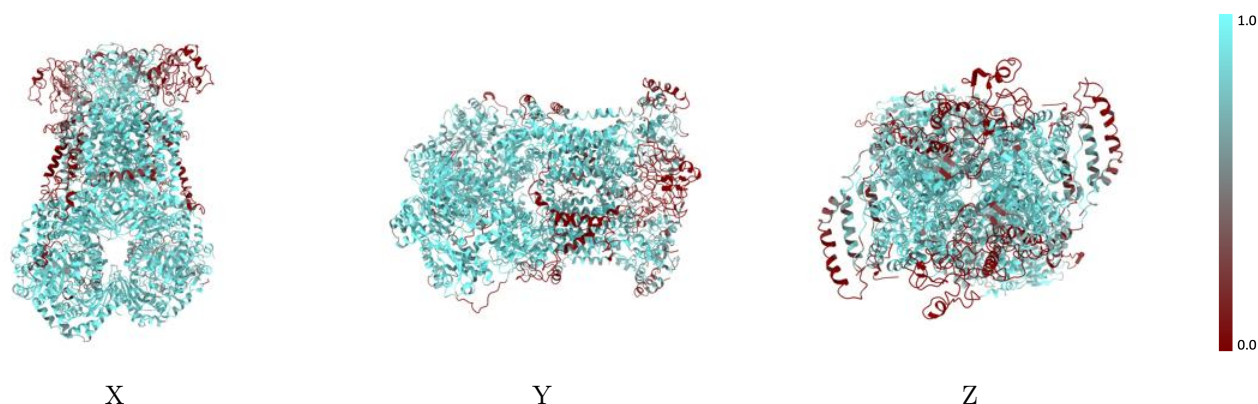
The images above show the 3D surface view of the map at the recommended contour level 0.798 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



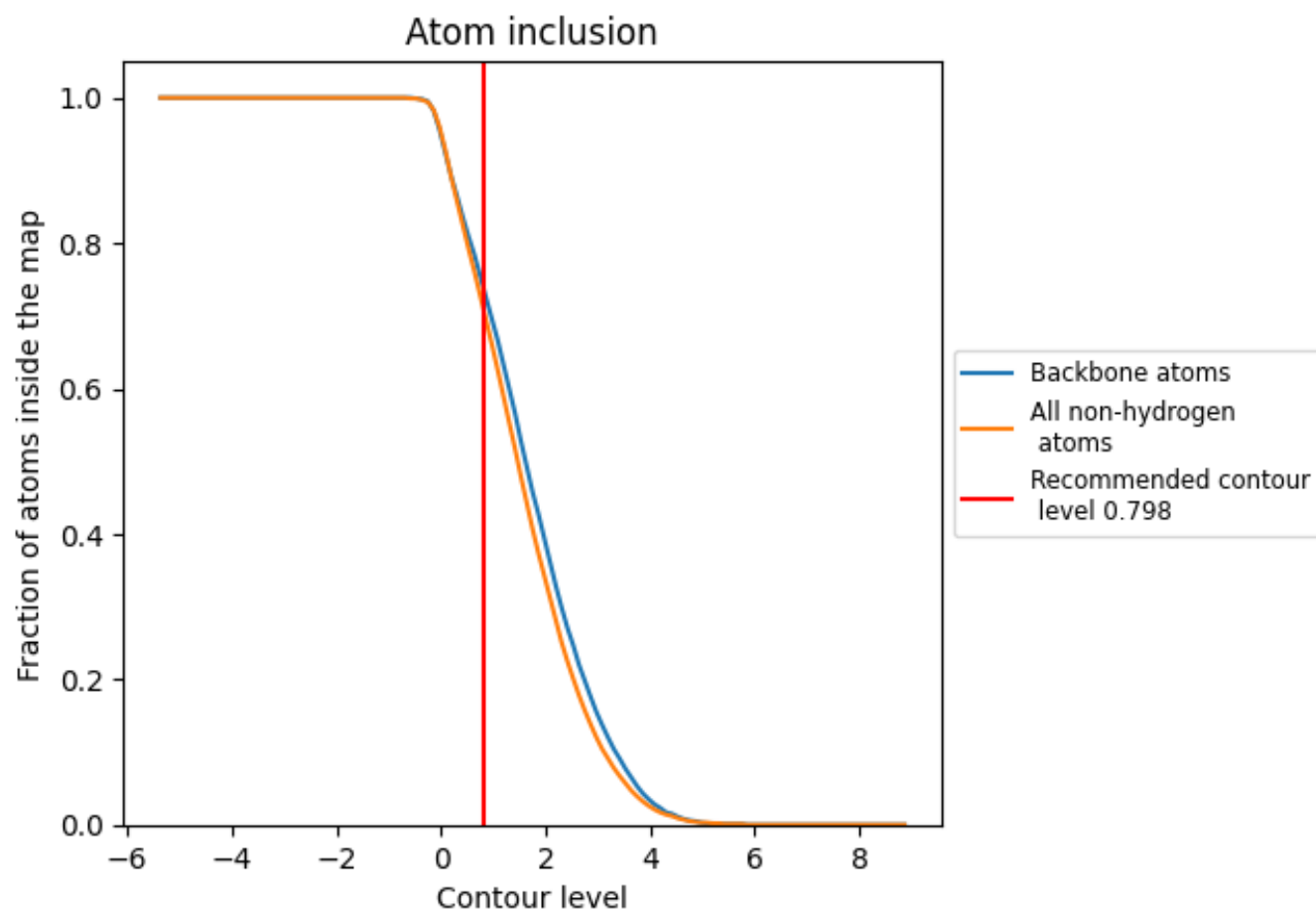
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.798).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (0.798) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.5150
A	 0.8860	 0.5960
B	 0.7420	 0.5260
C	 0.0430	 0.1950
D	 0.8730	 0.5880
E	 0.8970	 0.6100
F	 0.3680	 0.4050
G	 0.8720	 0.5920
H	 0.6290	 0.5160
I	 0.2610	 0.2550
J	 0.0000	 0.1600
K	 0.3930	 0.2910
a	 0.8860	 0.5960
b	 0.7450	 0.5280
c	 0.0580	 0.1690
d	 0.8780	 0.5940
e	 0.8910	 0.6070
f	 0.3660	 0.4100
g	 0.8620	 0.5960
h	 0.5720	 0.4890
i	 0.2590	 0.2290
j	 0.0050	 0.1600
k	 0.4470	 0.3970

