wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 04:34 PM JST

PDB ID	:	8ZP0
EMDB ID	:	EMD-60323
Title	:	Cryo-EM structure of YF23694-bound porcine bc1 complex
Authors	:	Wang, Y.X.; Sun, J.Y.; Cui, G.R.; Yang, G.F.
Deposited on	:	2024-05-29
Resolution	:	2.44 Å(reported)

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

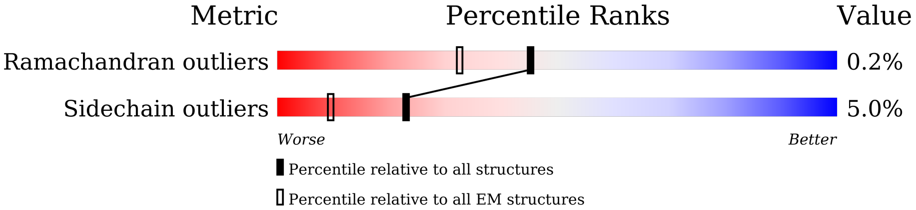
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

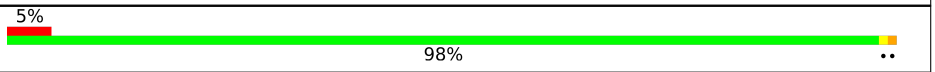
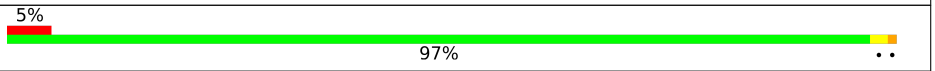
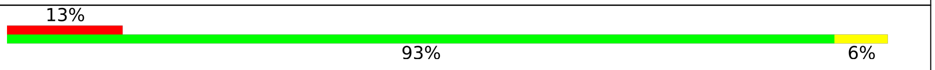
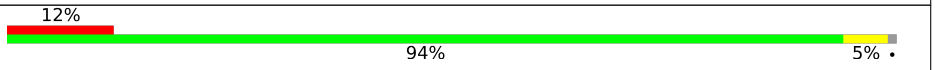
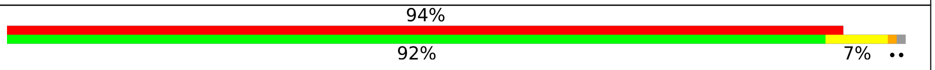
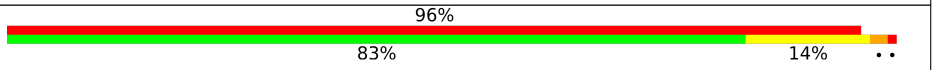
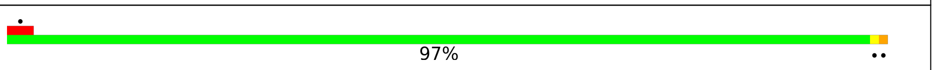
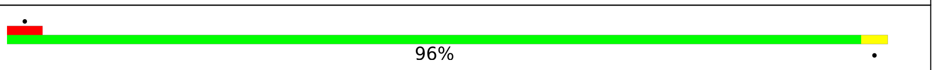
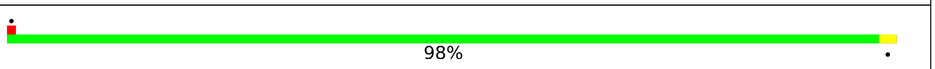
The reported resolution of this entry is 2.44 Å.

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	
1	a	378	
2	B	241	
2	b	241	
3	C	196	
3	c	196	
4	D	446	
4	d	446	
5	E	418	

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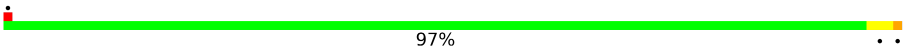
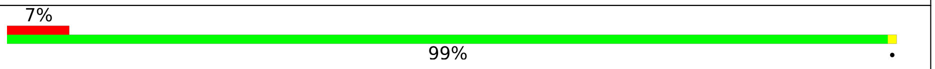
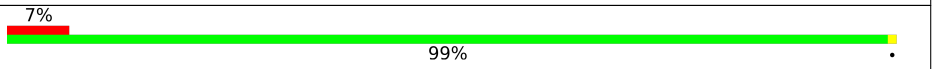
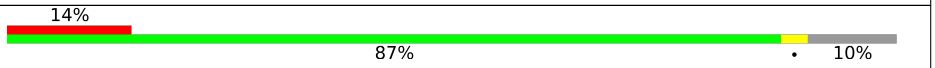
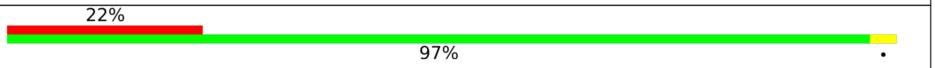
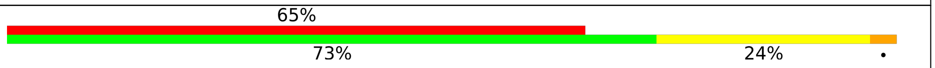
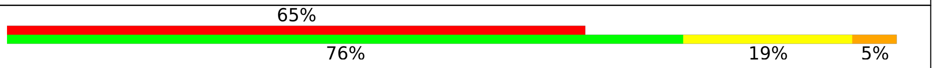
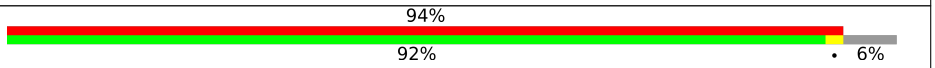
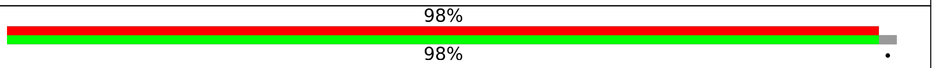
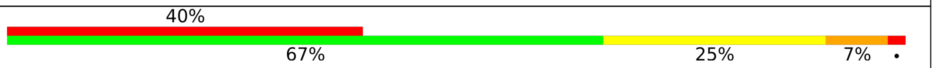
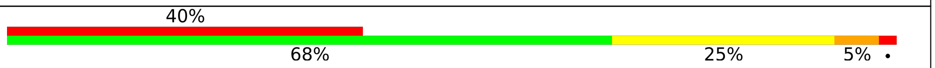
Mol	Chain	Length	Quality of chain
5	e	418	 • 97% • •
6	F	64	 56% 77% 23%
6	f	64	 56% 77% 23%
7	G	106	 7% 99% •
7	g	106	 7% 99% •
8	H	79	 14% 87% • 10%
8	h	79	 22% 97% •
9	I	62	 65% 73% 24% •
9	i	62	 65% 76% 19% 5%
10	J	52	 94% 92% • 6%
10	j	52	 98% 98% •
11	K	57	 40% 67% 25% 7% •
11	k	57	 40% 68% 25% 5% •

2 Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 33585 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 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
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
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
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 3134 1962 556 607 9	0	0
5	e	418	Total C N O S 3134 1962 556 607 9	0	0

- 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 528 320 97 106 5	0	0
6	f	64	Total C N O S 528 320 97 106 5	0	0

- 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 921 589 162 168 2	0	0
7	g	106	Total C N O S 921 589 162 168 2	0	0

- 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 608 399 112 95 2	0	0
8	h	79	Total C N O S 666 434 122 108 2	0	0

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

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

- 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 405 269 71 63 2	0	0

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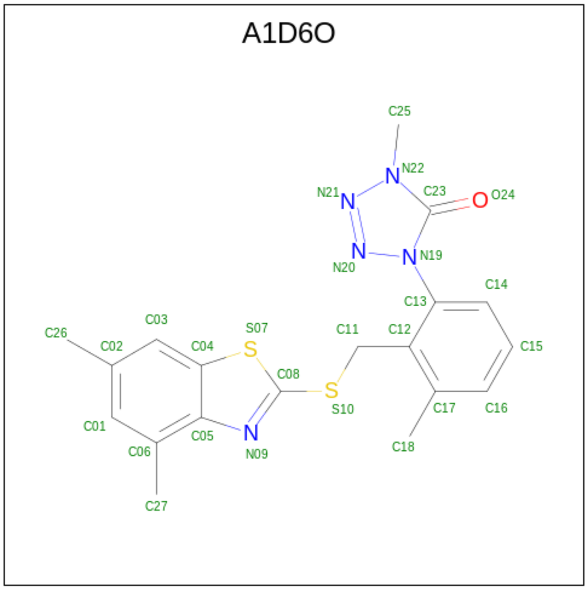
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	51	421	281	74	65	1	0	0

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

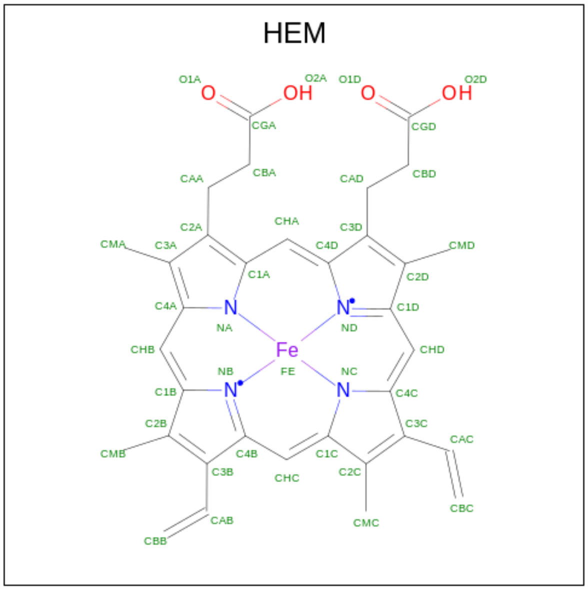
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	57	404	252	74	76	2	0	0
11	k	57	404	252	74	76	2	0	0

- Molecule 12 is 1-[2-[(4,6-dimethyl-1,3-benzothiazol-2-yl)sulfanylmethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (three-letter code: A1D6O) (formula: $C_{19}H_{19}N_5OS_2$) (labeled as "Ligand of Interest" by depositor).



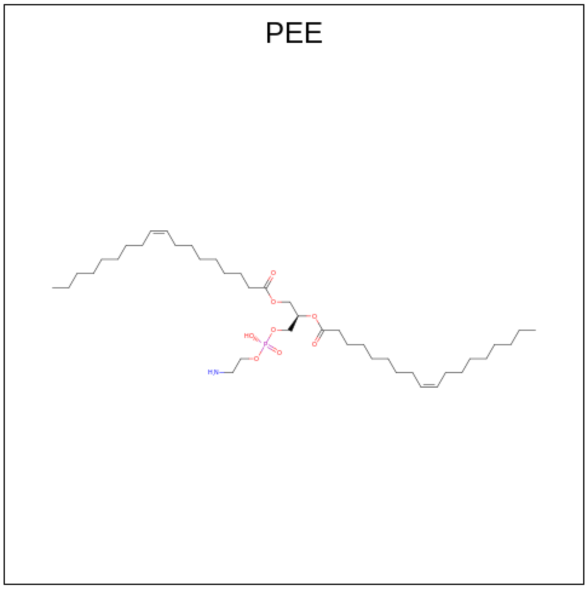
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
12	A	1	27	19	5	1	2	0
12	A	1	27	19	5	1	2	0
12	a	1	27	19	5	1	2	0
12	a	1	27	19	5	1	2	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



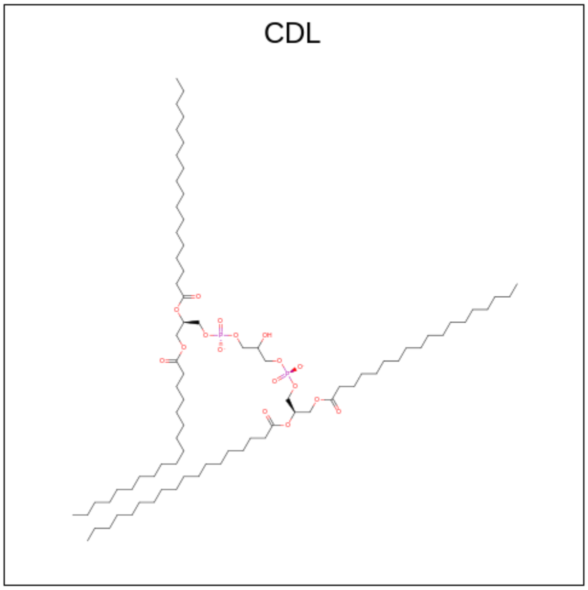
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C Fe N O 43 34 1 4 4	0
13	A	1	Total C Fe N O 43 34 1 4 4	0
13	a	1	Total C Fe N O 43 34 1 4 4	0
13	a	1	Total C Fe N O 43 34 1 4 4	0

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



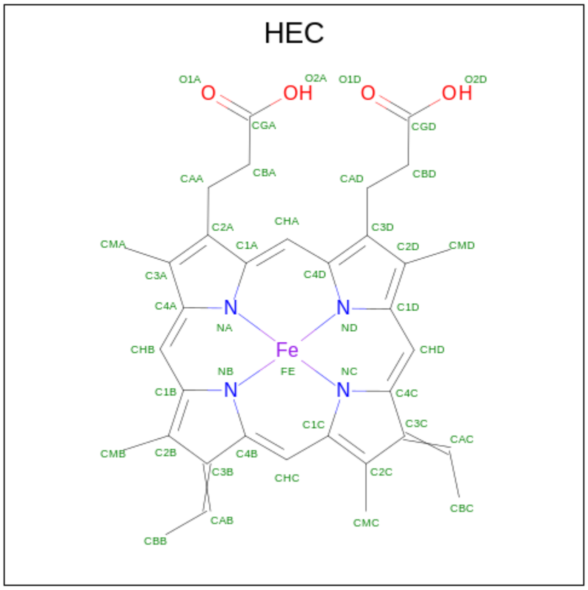
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	N 1	O 8	P 1	0
14	D	1	Total 49	C 39	N 1	O 8	P 1	0
14	a	1	Total 49	C 39	N 1	O 8	P 1	0

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



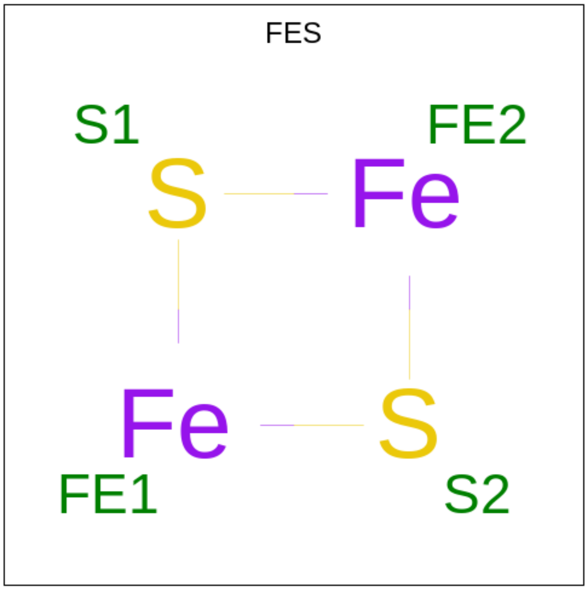
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total 64	C 45	O 17	P 2	0
15	a	1	Total 64	C 45	O 17	P 2	0
15	a	1	Total 64	C 45	O 17	P 2	0

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



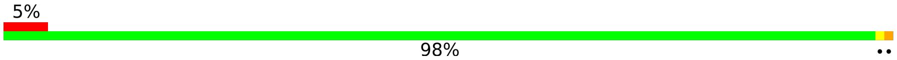
Mol	Chain	Residues	Atoms	AltConf
17	C	1	Total Fe S 4 2 2	0
17	c	1	Total Fe S 4 2 2	0

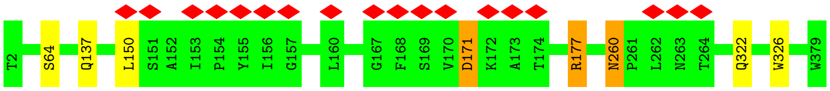
3 Residue-property plots ⓘ

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

- Molecule 1: Cytochrome b

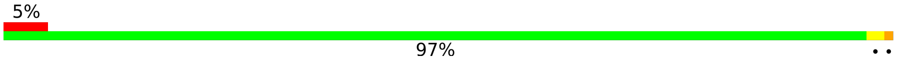
Chain A:

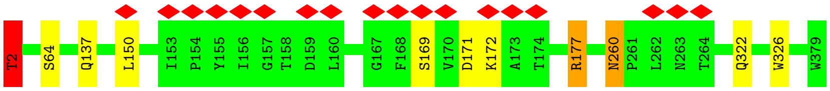




- Molecule 1: Cytochrome b

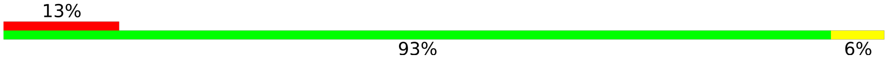
Chain a:

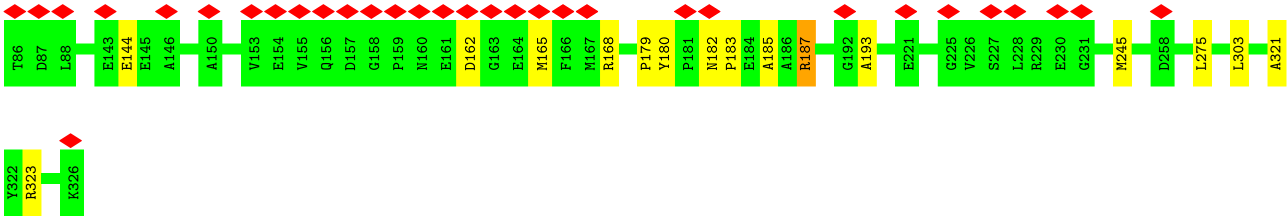




- Molecule 2: Cytochrome c1, heme protein, mitochondrial

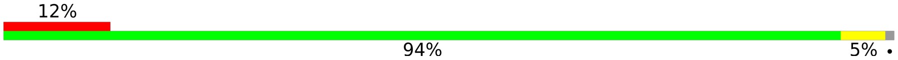
Chain B:

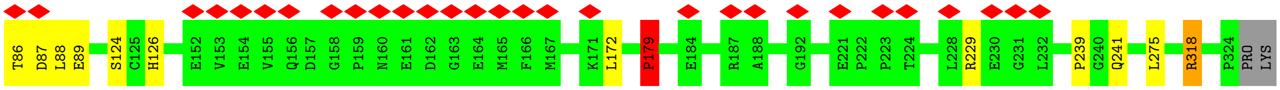




- Molecule 2: Cytochrome c1, heme protein, mitochondrial

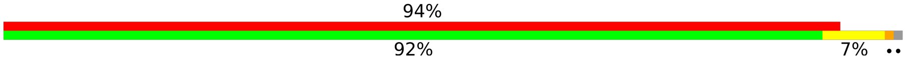
Chain b:

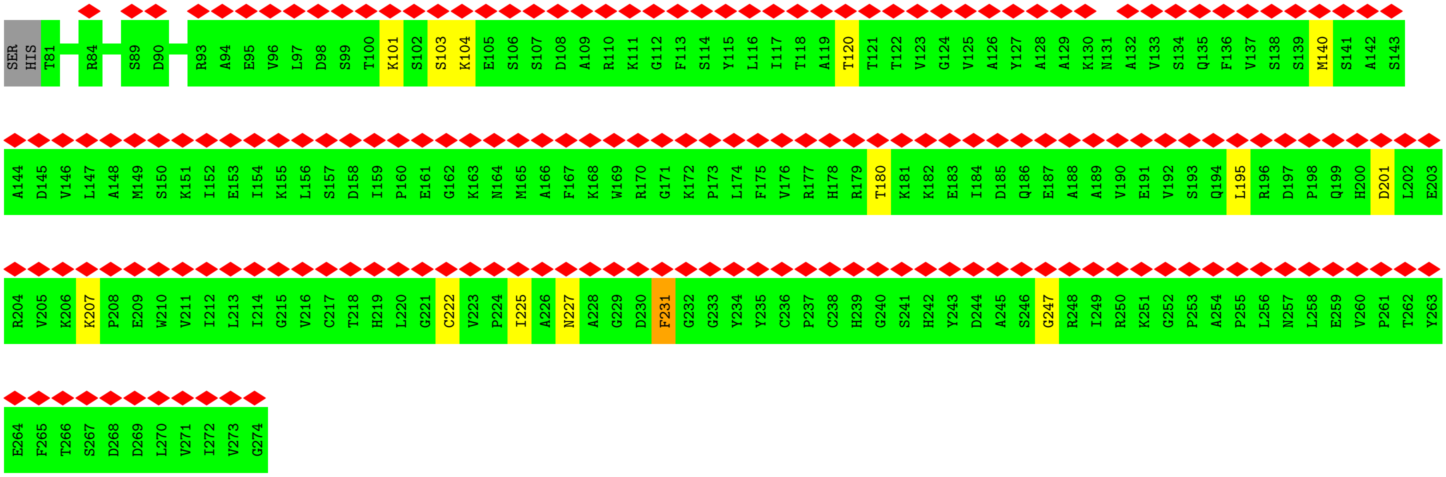




- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

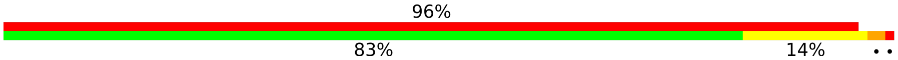
Chain C:

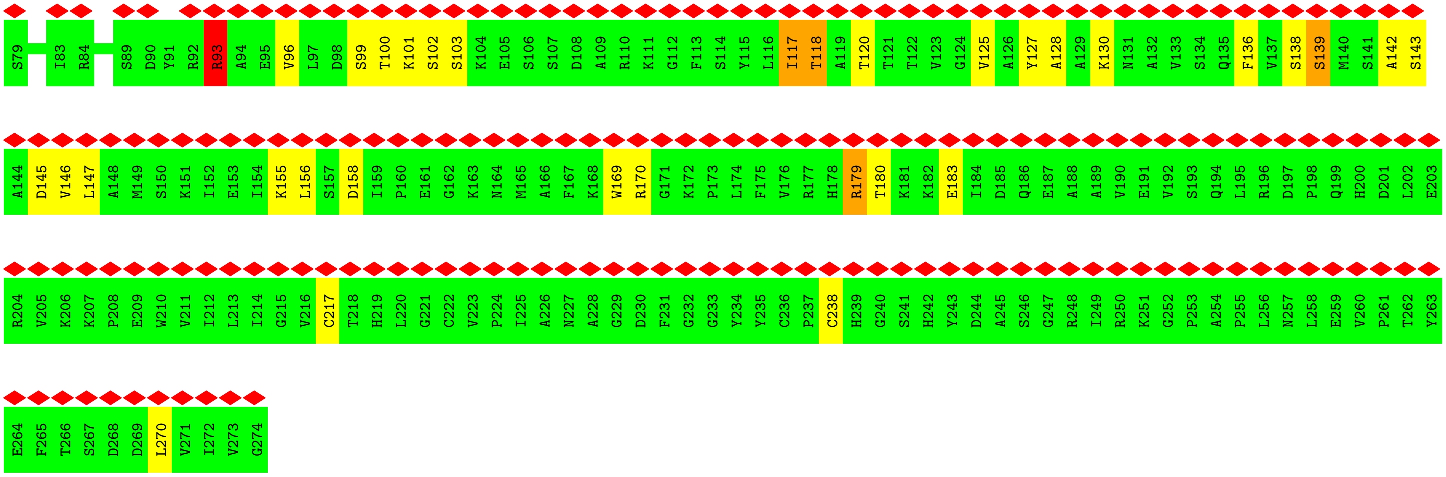




- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

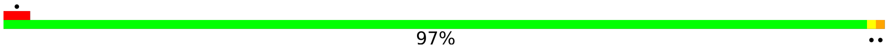
Chain c:

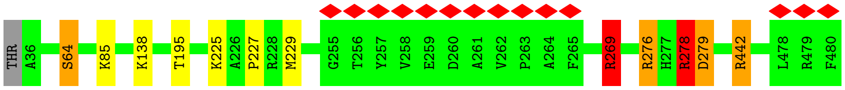




- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

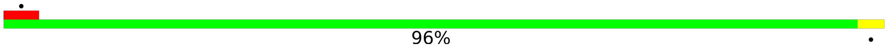
Chain D:

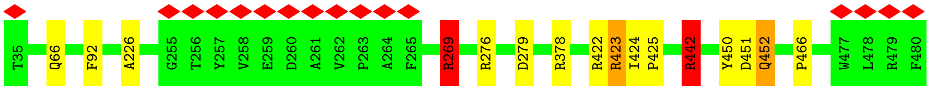




- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

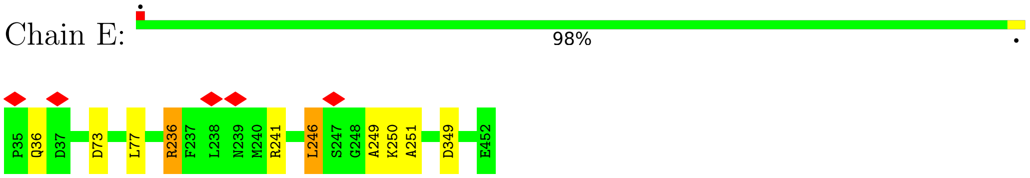
Chain d:





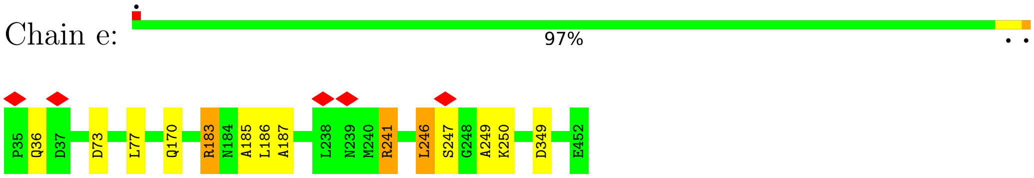
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain E:



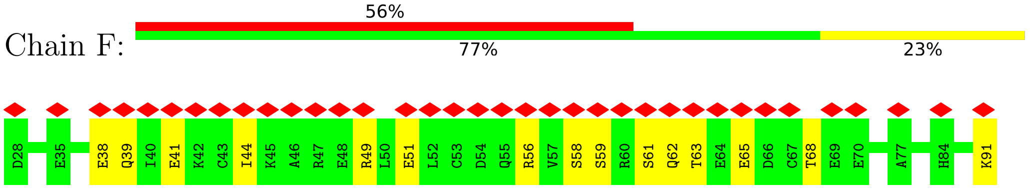
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain e:



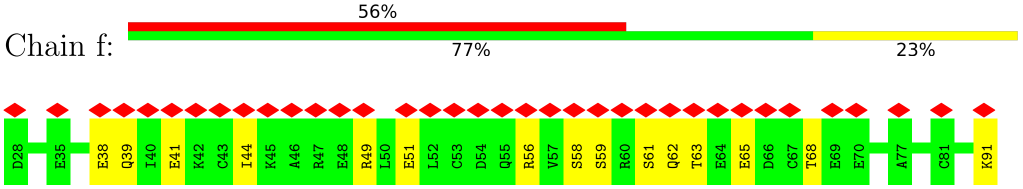
- Molecule 6: Cytochrome b-c1 complex subunit 6

Chain F:



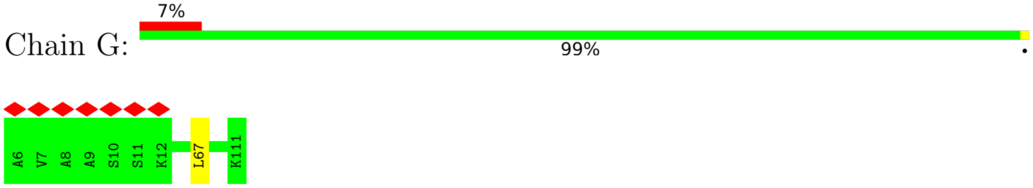
- Molecule 6: Cytochrome b-c1 complex subunit 6

Chain f:



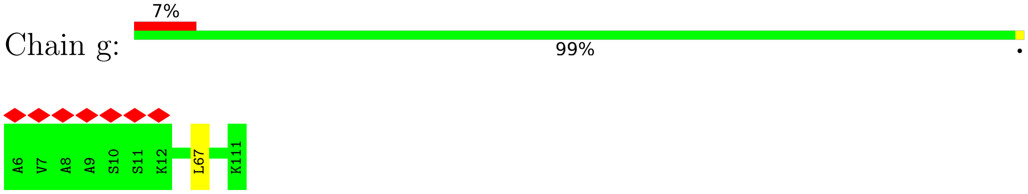
- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain G:



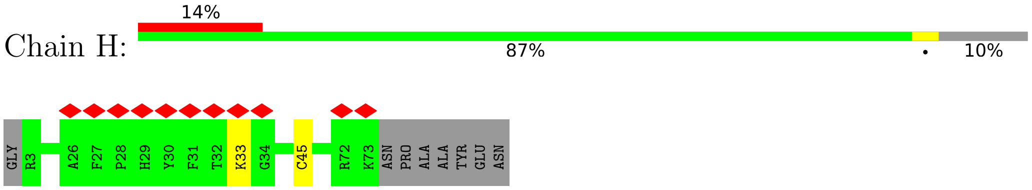
- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain g:



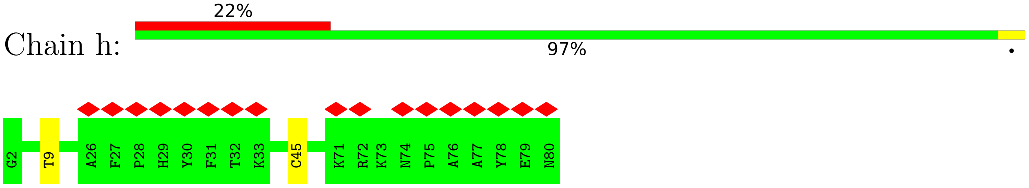
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:



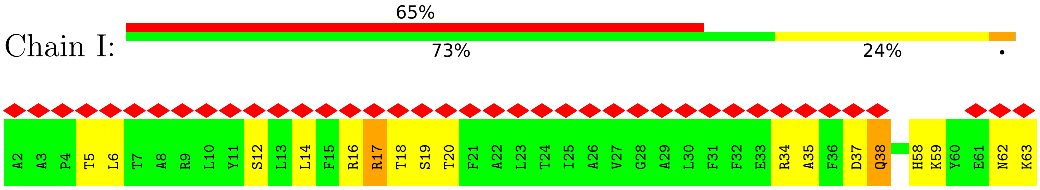
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain h:



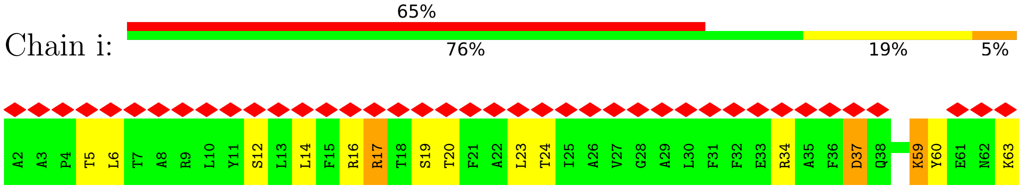
- Molecule 9: Complex III subunit 9

Chain I:



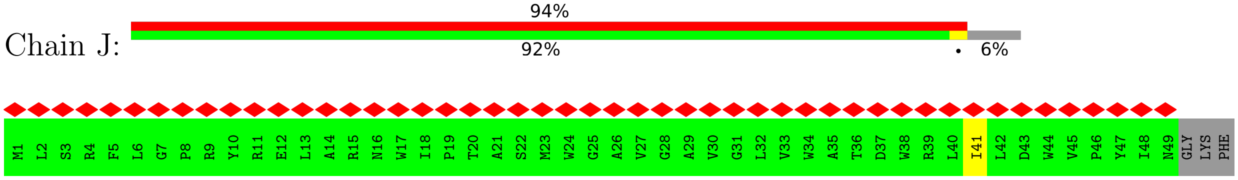
- Molecule 9: Complex III subunit 9

Chain i:



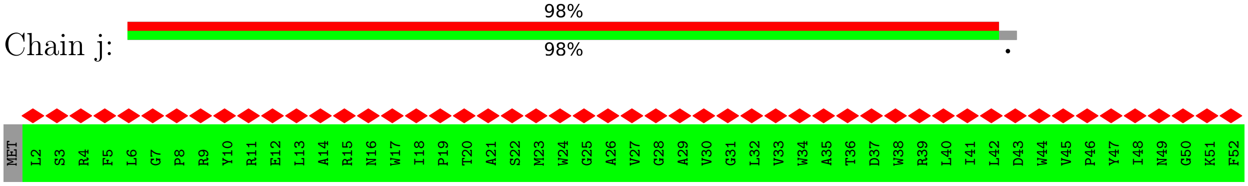
- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J:



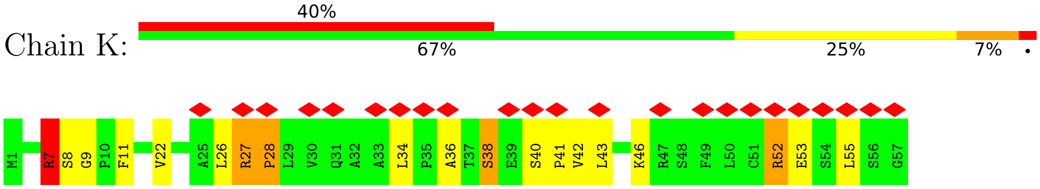
- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain j:



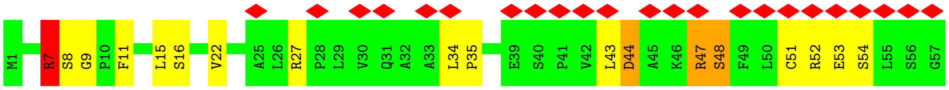
- Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain K:



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

Chain k:


M1
R7
S8
G9
P10
F11
L15
S16
V22
A25
L26
R27
P28
L29
V30
Q31
A32
A33
L34
P35
E39
S40
P41
V42
L43
D44
A45
K46
R47
S48
F49
L50
C51
R52
E53
S54
L55
S56
G57

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	493233	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 ($e^-/\text{Å}^2$)	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	10.253	Depositor
Minimum map value	-6.629	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.286	Depositor
Recommended contour level	1.06	Depositor
Map size (Å)	307.19998, 307.19998, 307.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9599999, 0.9599999, 0.9599999	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: HEM, FES, A1D6O, CDL, PEE, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.45	0/3115	0.68	3/4259 (0.1%)
1	a	0.48	0/3115	0.72	5/4259 (0.1%)
2	B	0.50	0/1978	0.81	9/2684 (0.3%)
2	b	0.52	0/1961	0.81	5/2661 (0.2%)
3	C	0.43	0/1534	0.75	1/2075 (0.0%)
3	c	0.61	3/1549 (0.2%)	0.94	7/2095 (0.3%)
4	D	0.55	6/3524 (0.2%)	0.73	3/4783 (0.1%)
4	d	0.59	6/3531 (0.2%)	0.77	6/4793 (0.1%)
5	E	0.50	1/3187 (0.0%)	0.67	6/4314 (0.1%)
5	e	0.52	3/3187 (0.1%)	0.70	5/4314 (0.1%)
6	F	0.35	0/534	0.62	0/714
6	f	0.38	0/534	0.73	1/714 (0.1%)
7	G	0.45	0/941	0.59	0/1262
7	g	0.45	0/941	0.59	0/1262
8	H	0.45	0/628	0.71	0/848
8	h	0.41	0/688	0.68	0/931
9	I	0.47	0/520	0.92	2/701 (0.3%)
9	i	0.51	1/520 (0.2%)	0.99	3/701 (0.4%)
10	J	0.33	0/420	0.75	1/576 (0.2%)
10	j	0.35	0/437	0.69	0/598
11	K	1.06	3/410 (0.7%)	1.43	8/556 (1.4%)
11	k	1.11	4/410 (1.0%)	1.36	7/556 (1.3%)
All	All	0.53	27/33664 (0.1%)	0.76	72/45656 (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
1	a	0	2
2	B	0	2
2	b	0	2
3	C	0	2
3	c	0	6
4	D	0	4
4	d	0	7
5	E	0	3
5	e	0	4
8	h	0	1
9	I	0	3
9	i	0	1
11	K	0	4
11	k	0	5
All	All	0	47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	46	LYS	C-N	9.61	1.56	1.34
11	k	16	SER	CA-CB	-7.92	1.41	1.52
11	K	9	GLY	C-O	-7.68	1.11	1.23
11	k	9	GLY	C-O	-7.63	1.11	1.23
3	c	102	SER	C-N	6.87	1.49	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	60	TYR	N-CA-CB	-11.63	89.66	110.60
4	D	442	ARG	CB-CG-CD	-11.47	81.77	111.60
3	c	118	THR	CB-CA-C	-10.53	83.16	111.60
4	d	425	PRO	N-CA-CB	-10.39	90.83	103.30
1	a	2	THR	CB-CA-C	-10.18	84.11	111.60

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
2	B	187	ARG	Sidechain
2	B	323	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	231	PHE	Peptide
3	C	247	GLY	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/378 (100%)	370 (98%)	6 (2%)	0	100	100
1	a	376/378 (100%)	368 (98%)	8 (2%)	0	100	100
2	B	239/241 (99%)	209 (87%)	27 (11%)	3 (1%)	10	9
2	b	237/241 (98%)	210 (89%)	24 (10%)	3 (1%)	10	9
3	C	192/196 (98%)	164 (85%)	28 (15%)	0	100	100
3	c	194/196 (99%)	148 (76%)	46 (24%)	0	100	100
4	D	443/446 (99%)	430 (97%)	13 (3%)	0	100	100
4	d	444/446 (100%)	420 (95%)	24 (5%)	0	100	100
5	E	416/418 (100%)	405 (97%)	11 (3%)	0	100	100
5	e	416/418 (100%)	405 (97%)	10 (2%)	1 (0%)	44	53
6	F	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
6	f	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
7	G	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
7	g	104/106 (98%)	103 (99%)	1 (1%)	0	100	100
8	H	69/79 (87%)	66 (96%)	3 (4%)	0	100	100
8	h	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
9	I	60/62 (97%)	47 (78%)	13 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	60/62 (97%)	48 (80%)	12 (20%)	0	100	100
10	J	47/52 (90%)	44 (94%)	3 (6%)	0	100	100
10	j	49/52 (94%)	45 (92%)	4 (8%)	0	100	100
11	K	55/57 (96%)	42 (76%)	13 (24%)	0	100	100
11	k	55/57 (96%)	40 (73%)	15 (27%)	0	100	100
All	All	4137/4198 (98%)	3856 (93%)	274 (7%)	7 (0%)	45	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	241	GLN
2	B	179	PRO
2	B	185	ALA
5	e	185	ALA
2	b	239	PRO

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%)	324 (98%)	7 (2%)	48	62
1	a	331/331 (100%)	322 (97%)	9 (3%)	40	52
2	B	206/206 (100%)	200 (97%)	6 (3%)	37	49
2	b	204/206 (99%)	197 (97%)	7 (3%)	32	43
3	C	164/166 (99%)	152 (93%)	12 (7%)	11	13
3	c	165/166 (99%)	140 (85%)	25 (15%)	2	1
4	D	371/372 (100%)	362 (98%)	9 (2%)	44	57
4	d	372/372 (100%)	366 (98%)	6 (2%)	58	71
5	E	327/328 (100%)	324 (99%)	3 (1%)	75	85
5	e	327/328 (100%)	322 (98%)	5 (2%)	60	73
6	F	61/61 (100%)	46 (75%)	15 (25%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	61/61 (100%)	47 (77%)	14 (23%)	0	0
7	G	95/95 (100%)	94 (99%)	1 (1%)	70	80
7	g	95/95 (100%)	94 (99%)	1 (1%)	70	80
8	H	65/70 (93%)	63 (97%)	2 (3%)	35	47
8	h	70/70 (100%)	69 (99%)	1 (1%)	62	75
9	I	50/50 (100%)	36 (72%)	14 (28%)	0	0
9	i	50/50 (100%)	36 (72%)	14 (28%)	0	0
10	J	40/42 (95%)	40 (100%)	0	100	100
10	j	41/42 (98%)	41 (100%)	0	100	100
11	K	44/44 (100%)	31 (70%)	13 (30%)	0	0
11	k	44/44 (100%)	33 (75%)	11 (25%)	0	0
All	All	3514/3530 (100%)	3339 (95%)	175 (5%)	23	28

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	156	LEU
6	f	61	SER
3	c	180	THR
5	e	186	LEU
9	i	5	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	222	GLN
5	e	170	GLN
4	d	286	HIS
5	e	75	ASN
5	e	290	GLN

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

18 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	41,50,50	1.48	7 (17%)	45,82,82	1.59	8 (17%)
14	PEE	D	501	-	48,48,50	0.42	0	51,53,55	0.60	1 (1%)
12	A1D6O	A	402	-	27,30,30	1.28	3 (11%)	27,44,44	2.90	9 (33%)
15	CDL	A	406	-	63,63,99	1.09	8 (12%)	69,75,111	1.09	4 (5%)
15	CDL	a	406	-	63,63,99	1.10	6 (9%)	69,75,111	1.07	4 (5%)
13	HEM	a	403	1	41,50,50	1.56	6 (14%)	45,82,82	1.52	10 (22%)
16	HEC	B	401	2	32,50,50	2.12	11 (34%)	24,82,82	3.03	10 (41%)
17	FES	C	301	-	0,4,4	-	-	-		
15	CDL	a	407	-	63,63,99	1.07	6 (9%)	69,75,111	1.12	6 (8%)
17	FES	c	301	-	0,4,4	-	-	-		
14	PEE	A	405	-	44,44,50	0.79	2 (4%)	46,49,55	0.84	2 (4%)
12	A1D6O	a	401	-	27,30,30	1.45	4 (14%)	27,44,44	3.47	12 (44%)
16	HEC	b	401	2	32,50,50	2.10	10 (31%)	24,82,82	3.06	10 (41%)
13	HEM	A	404	1	41,50,50	1.61	5 (12%)	45,82,82	2.04	16 (35%)
14	PEE	a	405	-	48,48,50	0.81	2 (4%)	51,53,55	0.85	2 (3%)
13	HEM	A	403	1	41,50,50	1.47	7 (17%)	45,82,82	1.58	8 (17%)
12	A1D6O	A	401	-	27,30,30	1.45	3 (11%)	27,44,44	3.47	12 (44%)
12	A1D6O	a	402	-	27,30,30	1.28	3 (11%)	27,44,44	2.90	9 (33%)

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	-	2/12/54/54	-
14	PEE	D	501	-	-	34/52/52/54	-
12	A1D6O	A	402	-	-	0/7/9/9	0/4/4/4
15	CDL	A	406	-	-	33/74/74/110	-
15	CDL	a	406	-	-	46/74/74/110	-
13	HEM	a	403	1	-	5/12/54/54	-
16	HEC	B	401	2	-	0/10/54/54	-
17	FES	C	301	-	-	-	0/1/1/1
15	CDL	a	407	-	-	44/74/74/110	-
17	FES	c	301	-	-	-	0/1/1/1
14	PEE	A	405	-	-	23/48/48/54	-
12	A1D6O	a	401	-	-	1/7/9/9	0/4/4/4
16	HEC	b	401	2	-	0/10/54/54	-
13	HEM	A	404	1	-	6/12/54/54	-
14	PEE	a	405	-	-	27/52/52/54	-
13	HEM	A	403	1	-	2/12/54/54	-
12	A1D6O	A	401	-	-	1/7/9/9	0/4/4/4
12	A1D6O	a	402	-	-	0/7/9/9	0/4/4/4

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	401	HEC	C2B-C3B	6.22	1.47	1.40
16	B	401	HEC	C2B-C3B	6.20	1.47	1.40
16	B	401	HEC	C3C-C2C	5.38	1.46	1.40
16	b	401	HEC	C3C-C2C	5.19	1.46	1.40
12	A	401	A1D6O	C08-S10	4.53	1.83	1.74

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	401	A1D6O	C11-S10-C08	12.77	112.14	101.20
12	a	401	A1D6O	C11-S10-C08	12.77	112.14	101.20
16	b	401	HEC	CBD-CAD-C3D	-7.83	99.26	112.62
16	B	401	HEC	CBD-CAD-C3D	-7.74	99.40	112.62
12	a	402	A1D6O	C11-S10-C08	7.23	107.39	101.20

There are no chirality outliers.

5 of 224 torsion outliers are listed below:

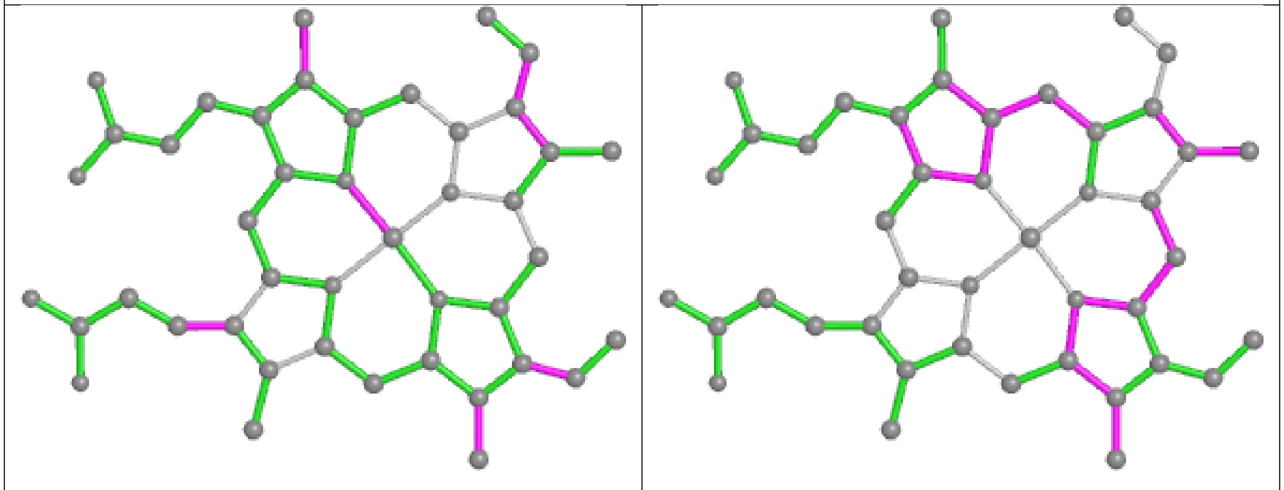
Mol	Chain	Res	Type	Atoms
13	A	404	HEM	C2D-C3D-CAD-CBD
13	A	404	HEM	C4D-C3D-CAD-CBD
14	A	405	PEE	C1-O3P-P-O1P
14	A	405	PEE	C4-O4P-P-O2P
14	A	405	PEE	C4-O4P-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

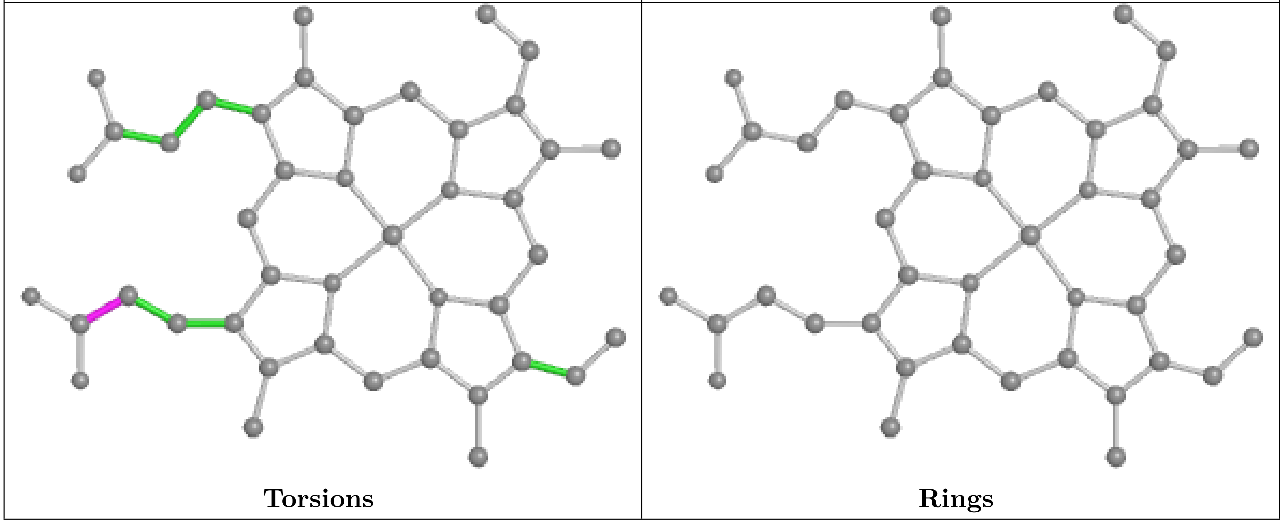
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand HEM a 404



Bond lengths

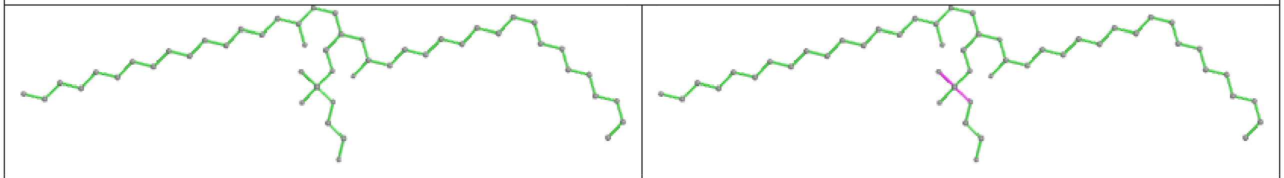
Bond angles



Torsions

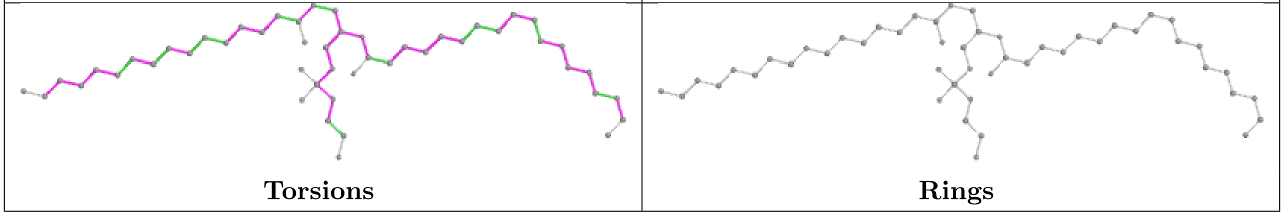
Rings

Ligand PEE D 501



Bond lengths

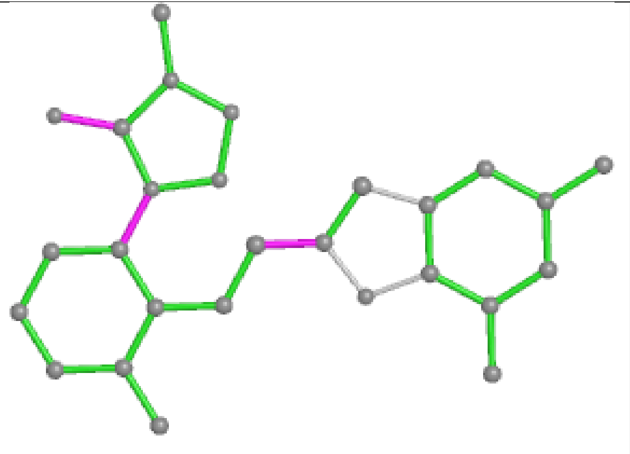
Bond angles



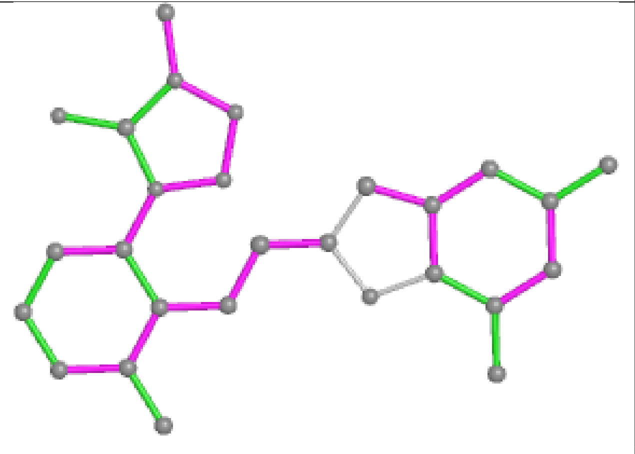
Torsions

Rings

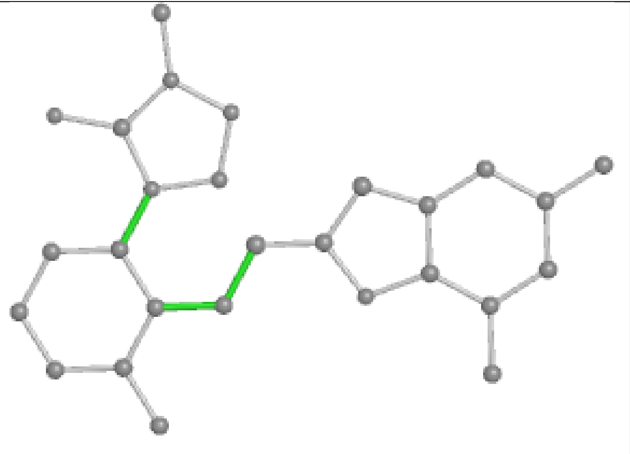
Ligand A1D6O A 402



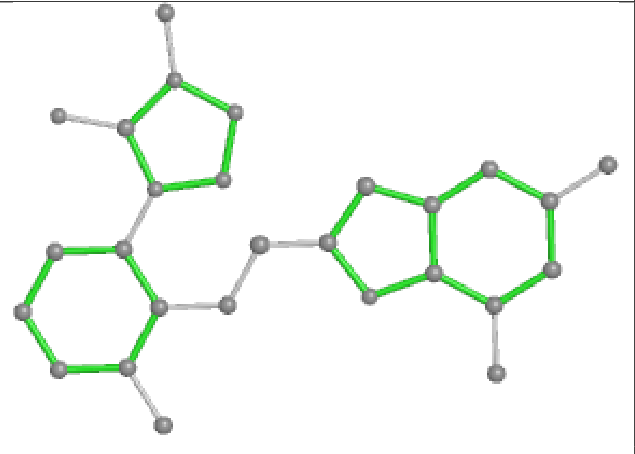
Bond lengths



Bond angles

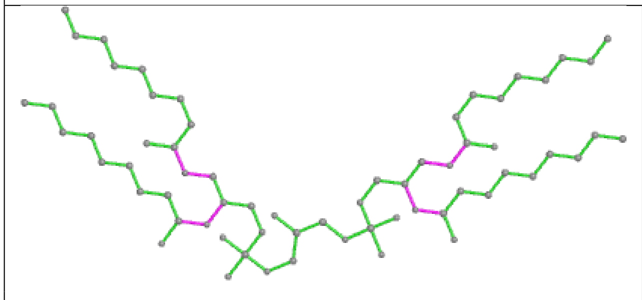


Torsions

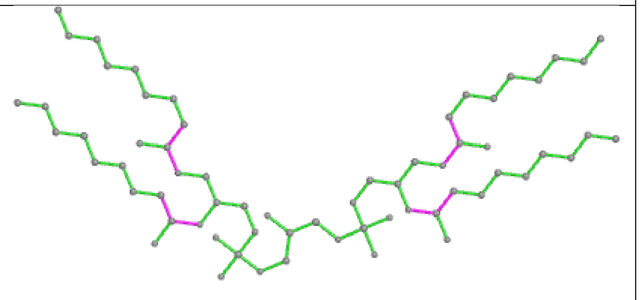


Rings

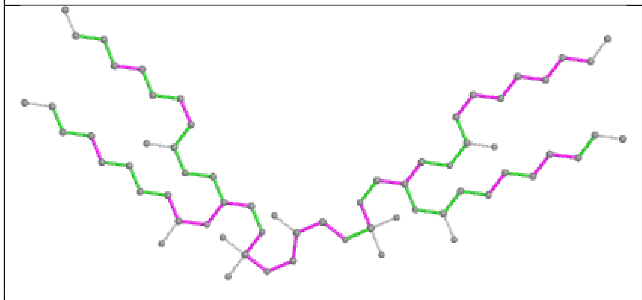
Ligand CDL A 406



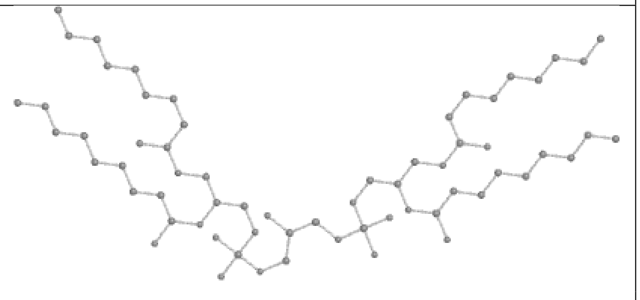
Bond lengths



Bond angles

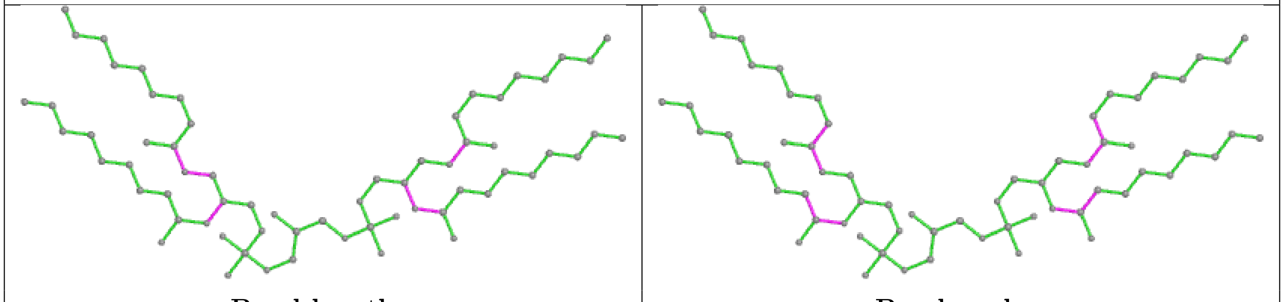


Torsions



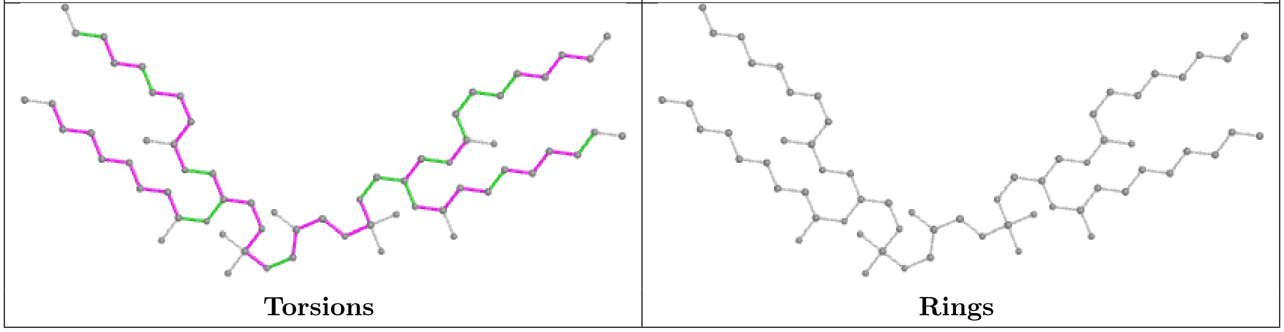
Rings

Ligand CDL a 406



Bond lengths

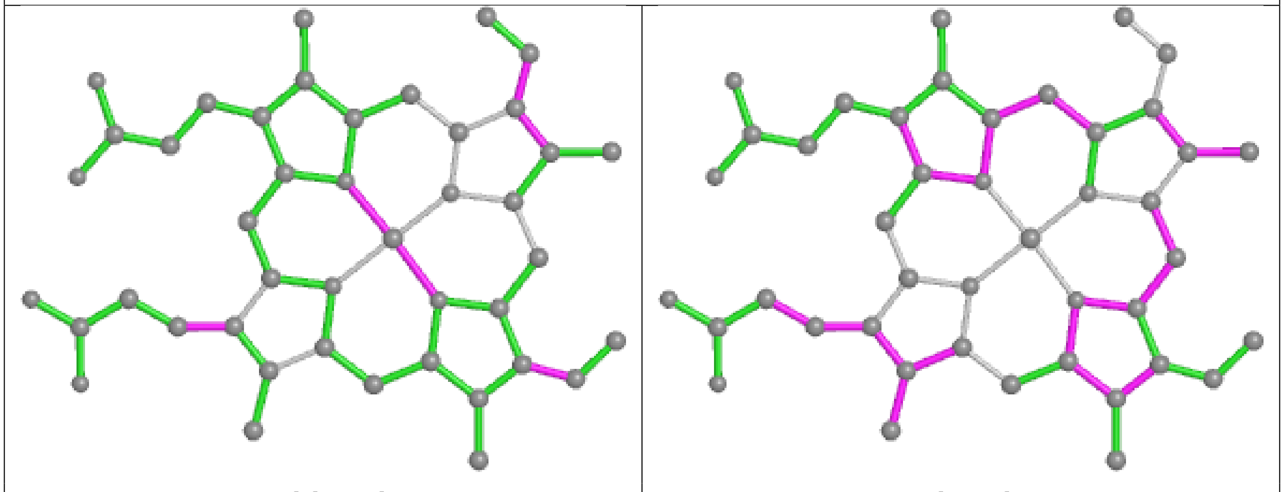
Bond angles



Torsions

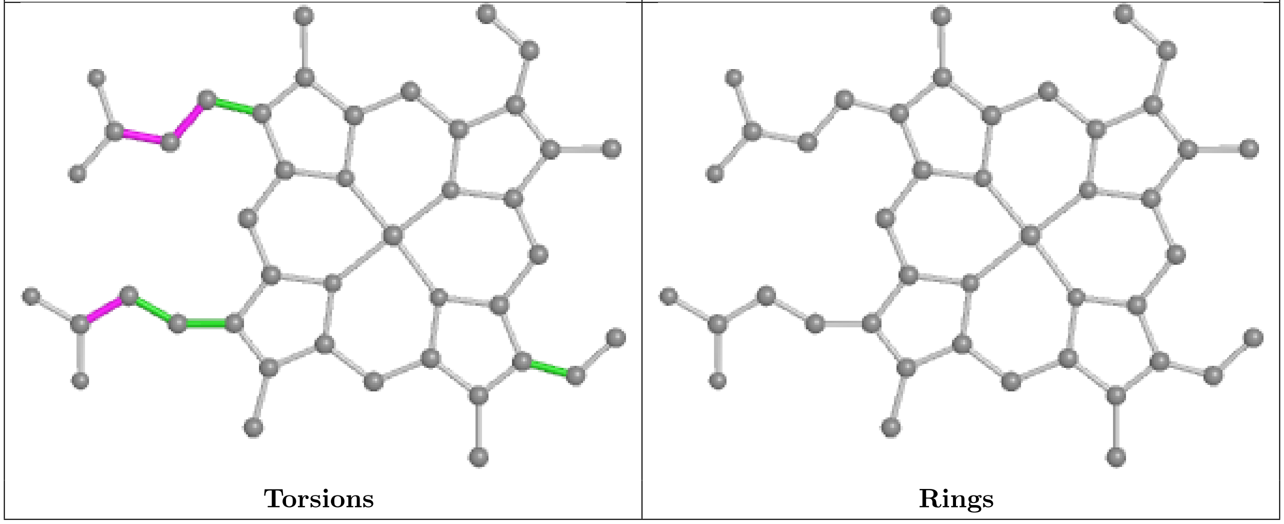
Rings

Ligand HEM a 403



Bond lengths

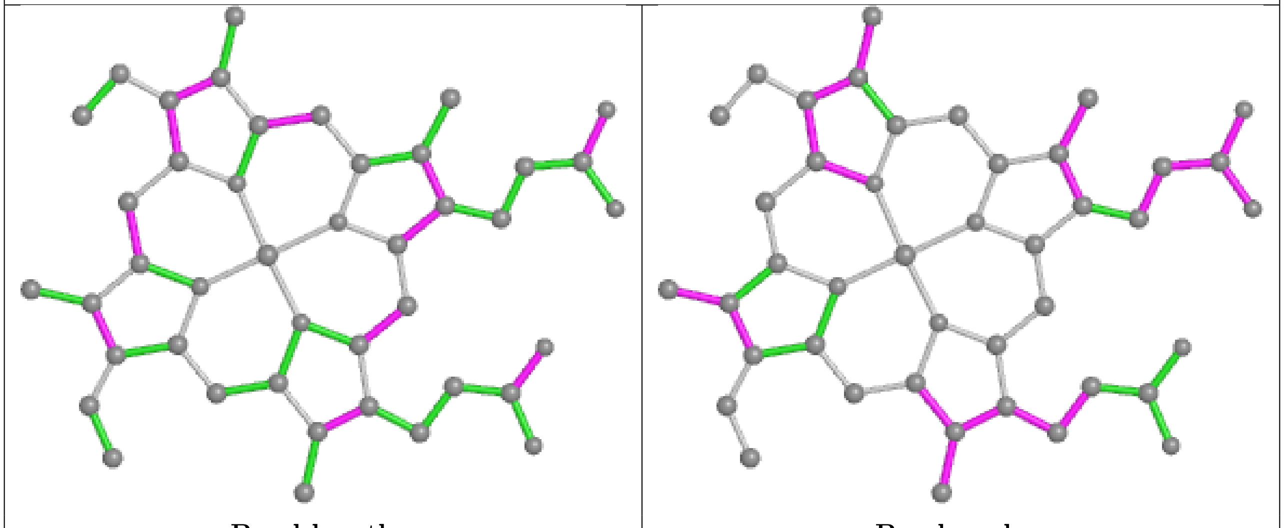
Bond angles



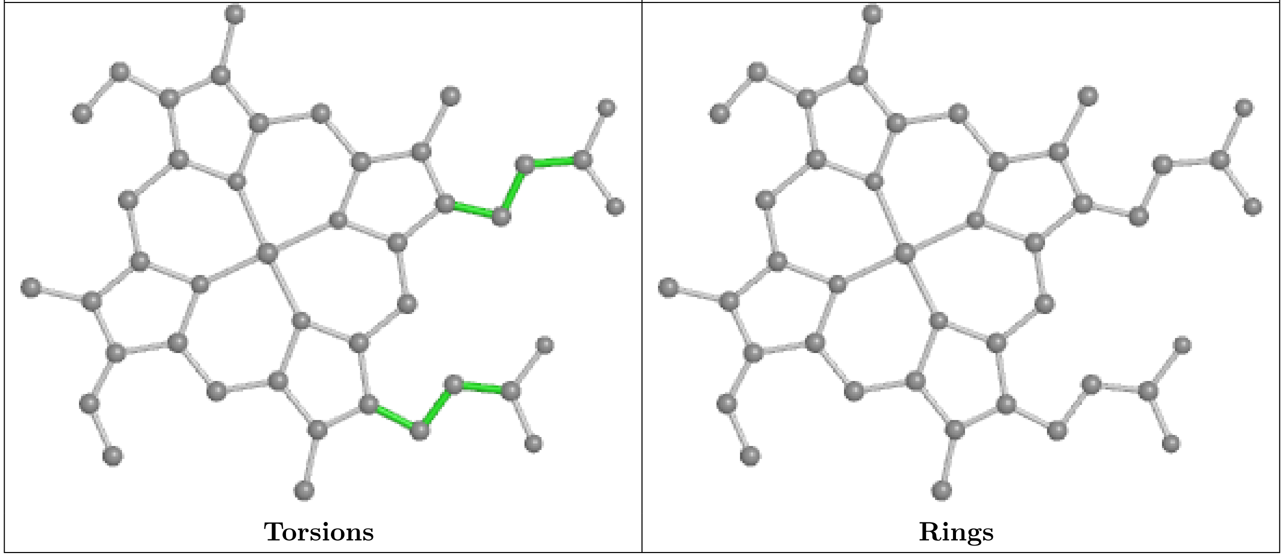
Torsions

Rings

Ligand HEC B 401

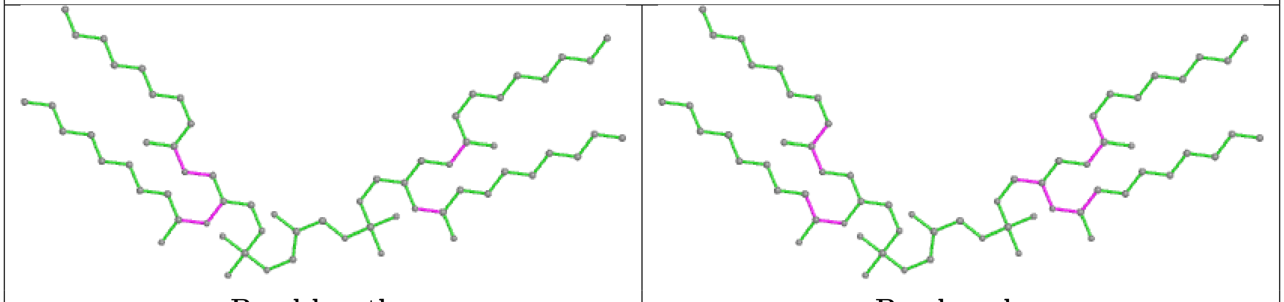


Bond lengths **Bond angles**



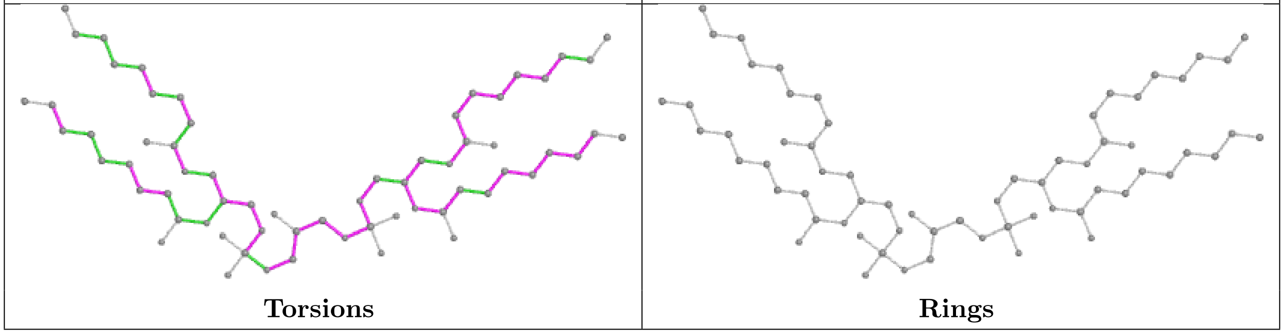
Torsions **Rings**

Ligand CDL a 407



Bond lengths

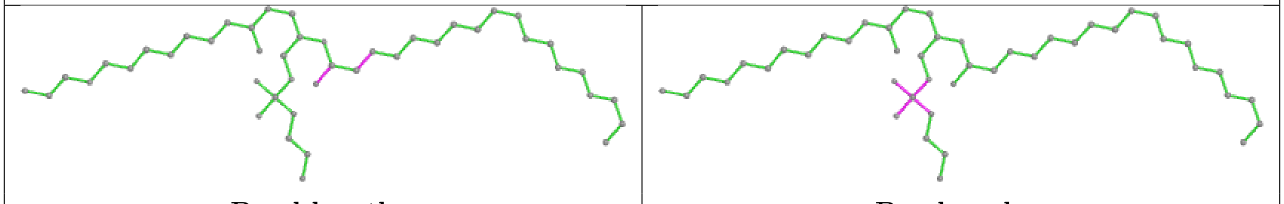
Bond angles



Torsions

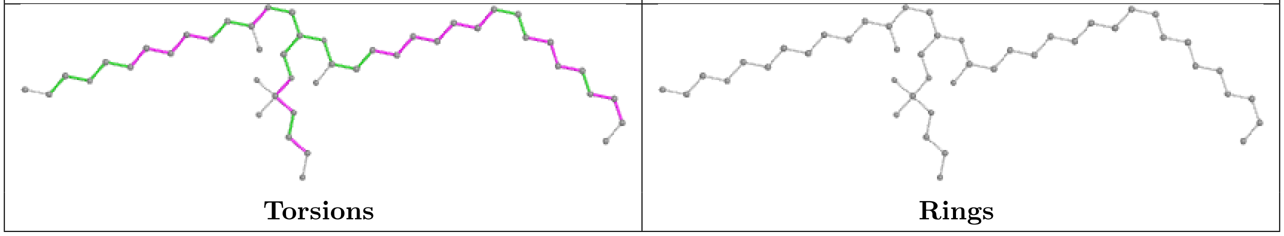
Rings

Ligand PEE A 405



Bond lengths

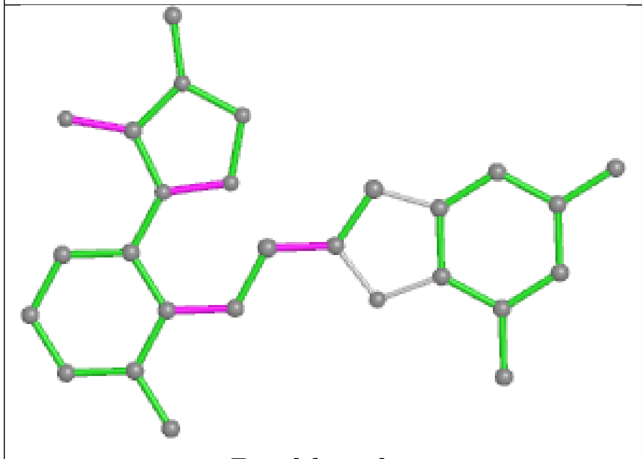
Bond angles



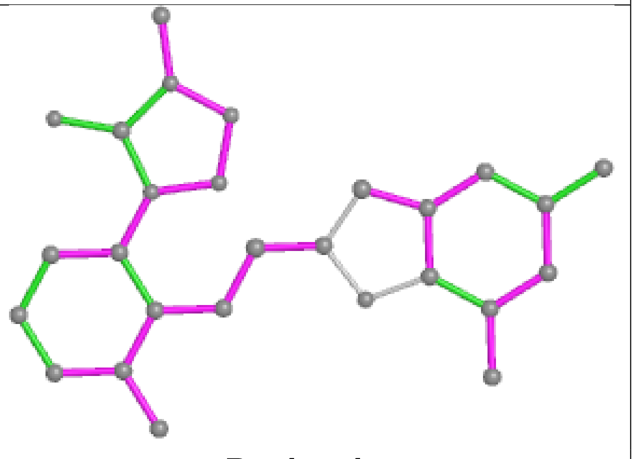
Torsions

Rings

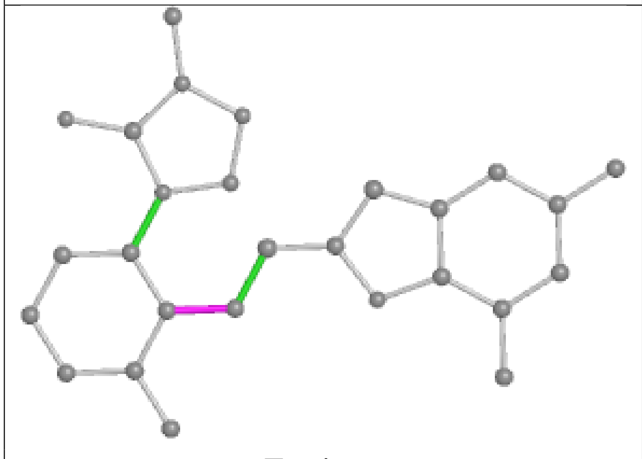
Ligand A1D6O a 401



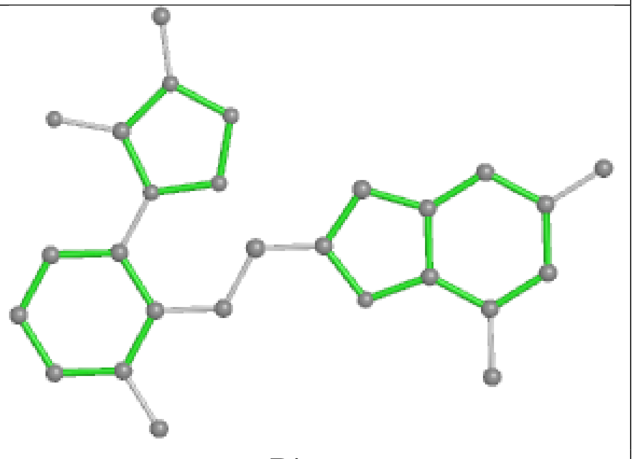
Bond lengths



Bond angles

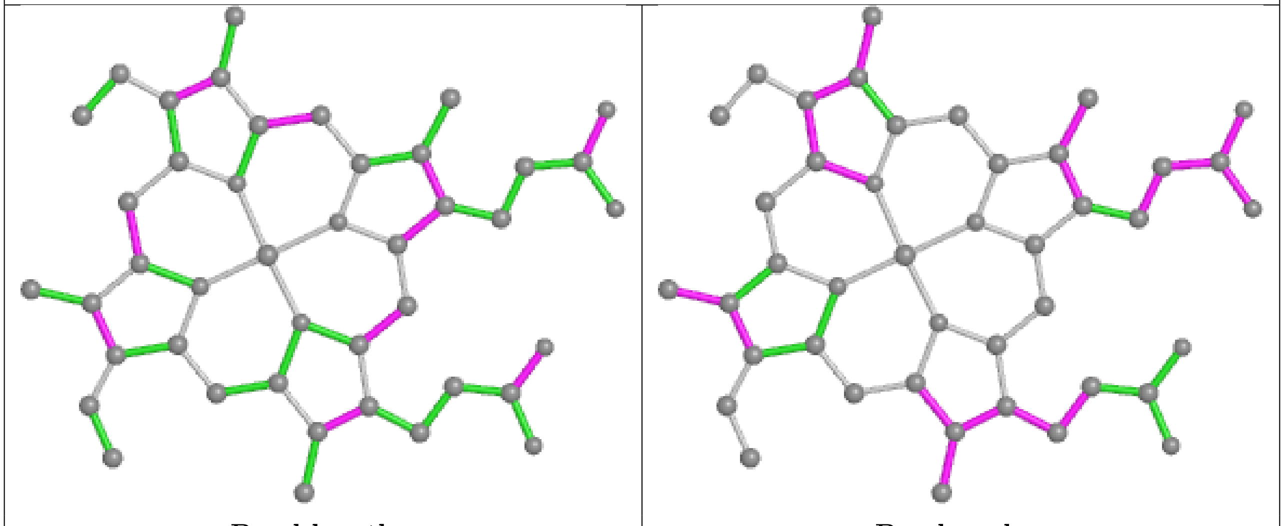


Torsions



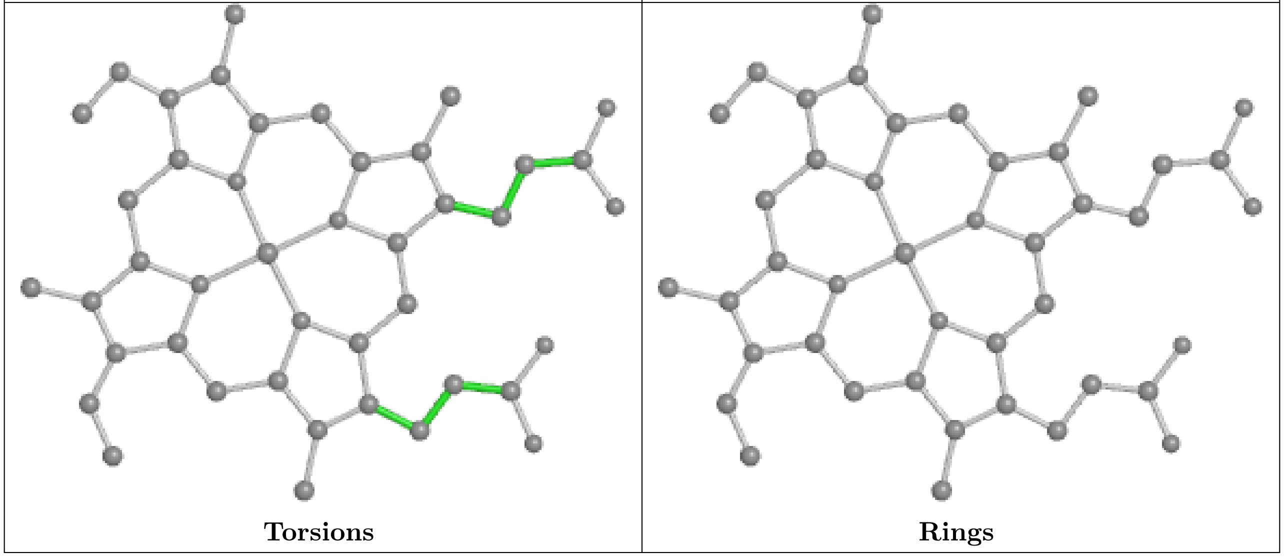
Rings

Ligand HEC b 401



Bond lengths

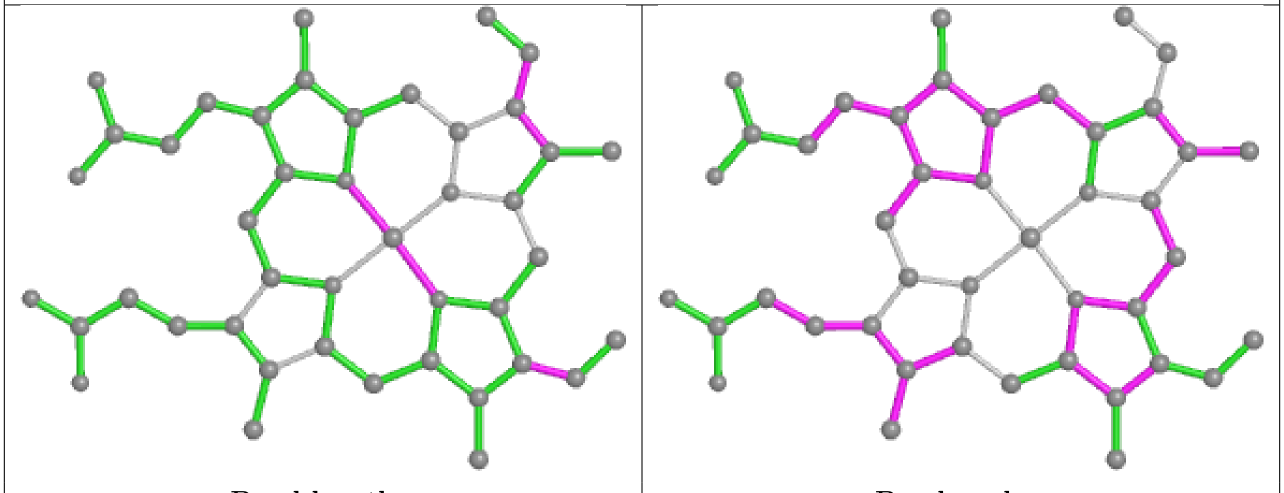
Bond angles



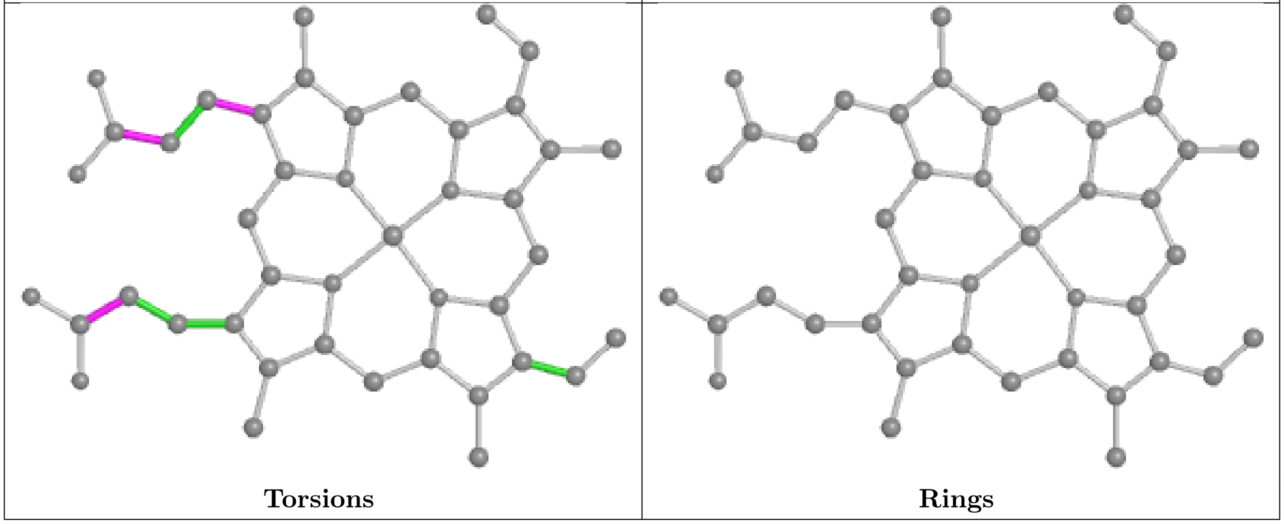
Torsions

Rings

Ligand HEM A 404

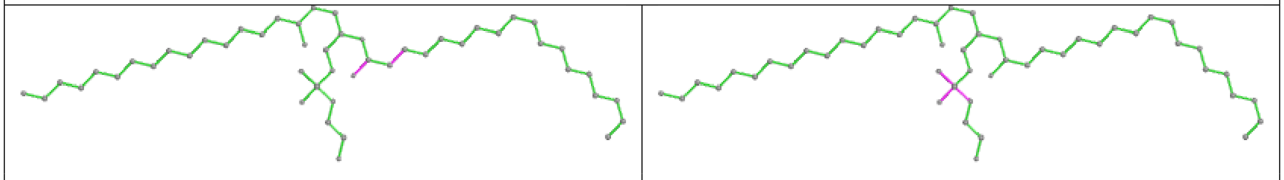


Bond lengths Bond angles

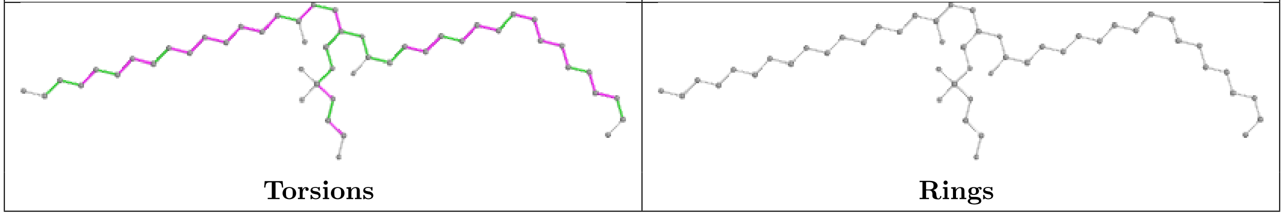


Torsions Rings

Ligand PEE a 405

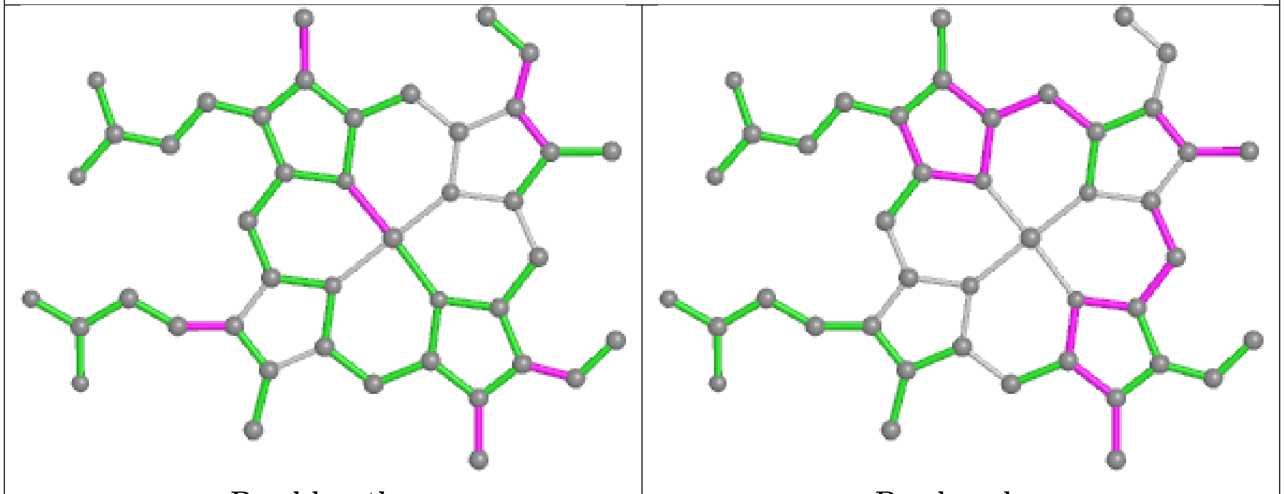


Bond lengths Bond angles

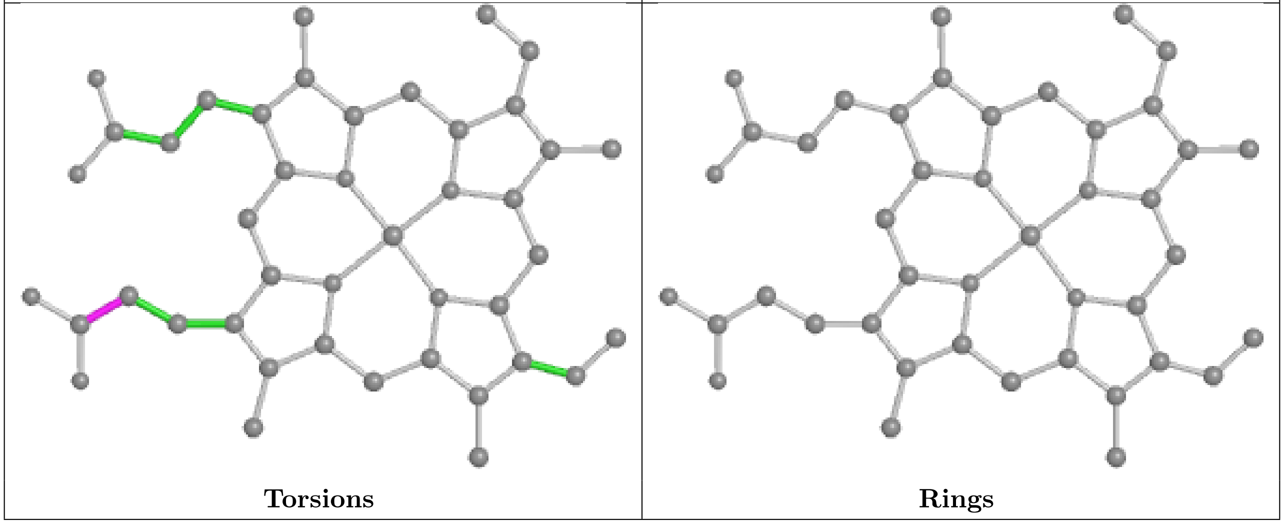


Torsions Rings

Ligand HEM A 403

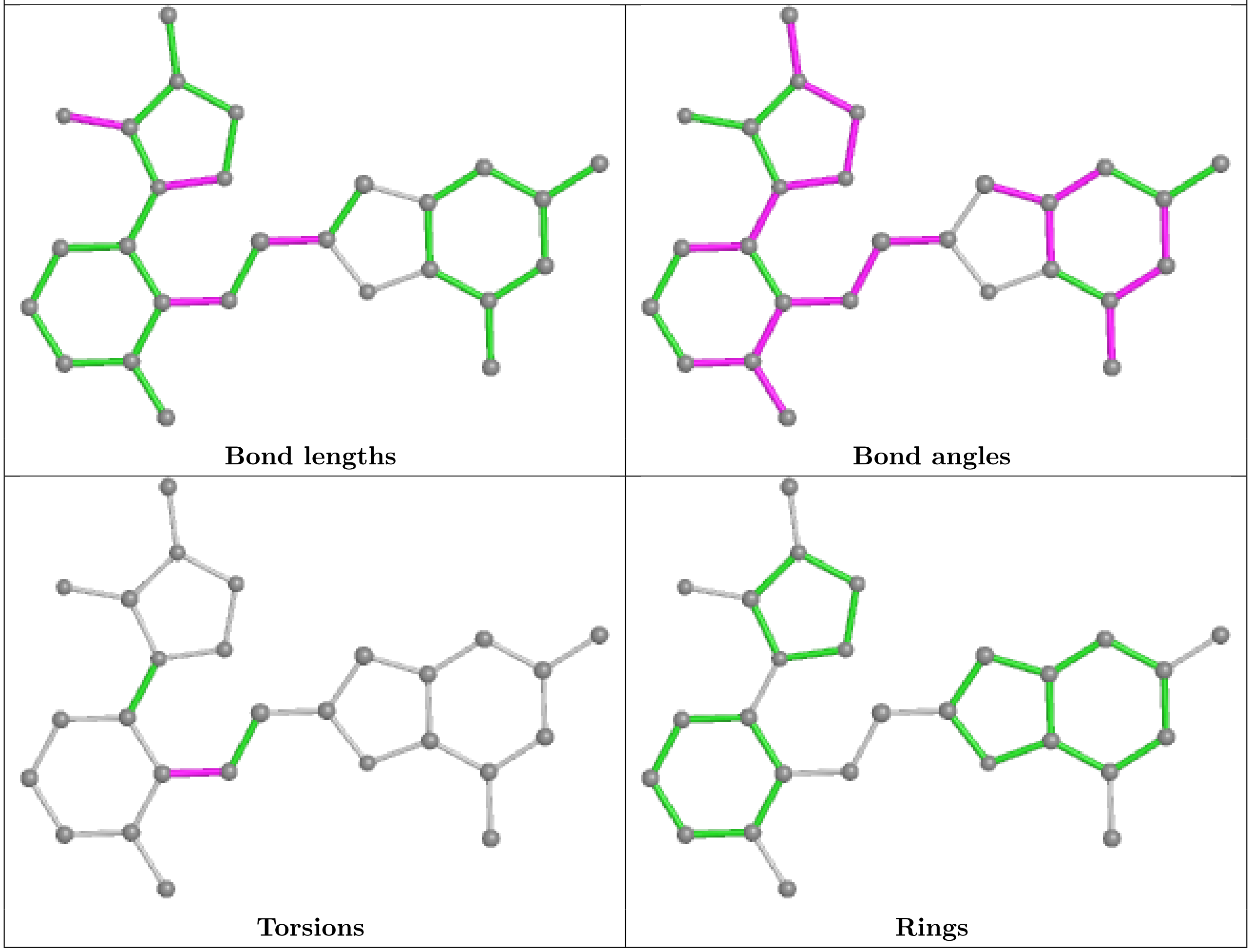


Bond lengths **Bond angles**



Torsions **Rings**

Ligand A1D6O A 401



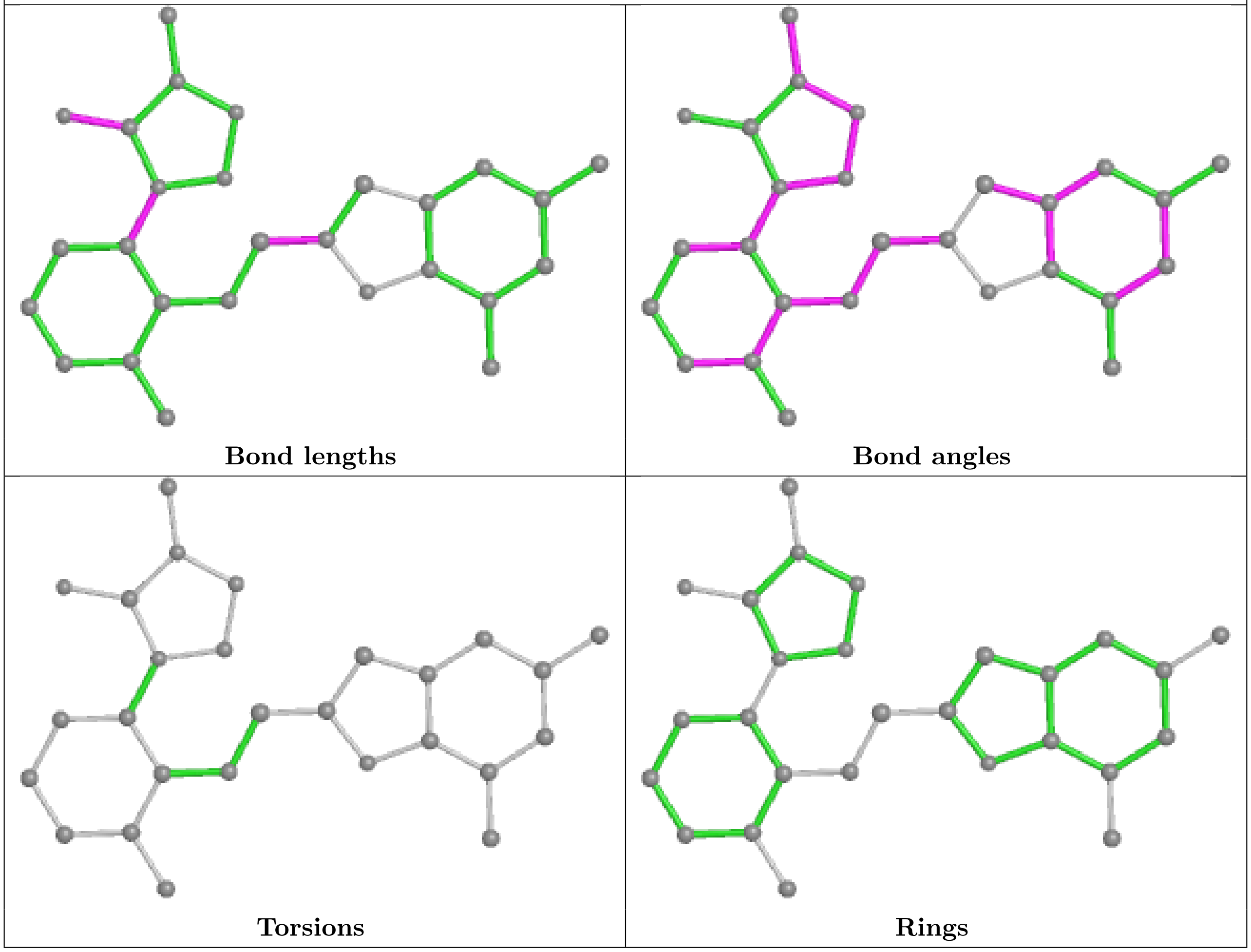
Bond lengths

Bond angles

Torsions

Rings

Ligand A1D6O a 402



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.

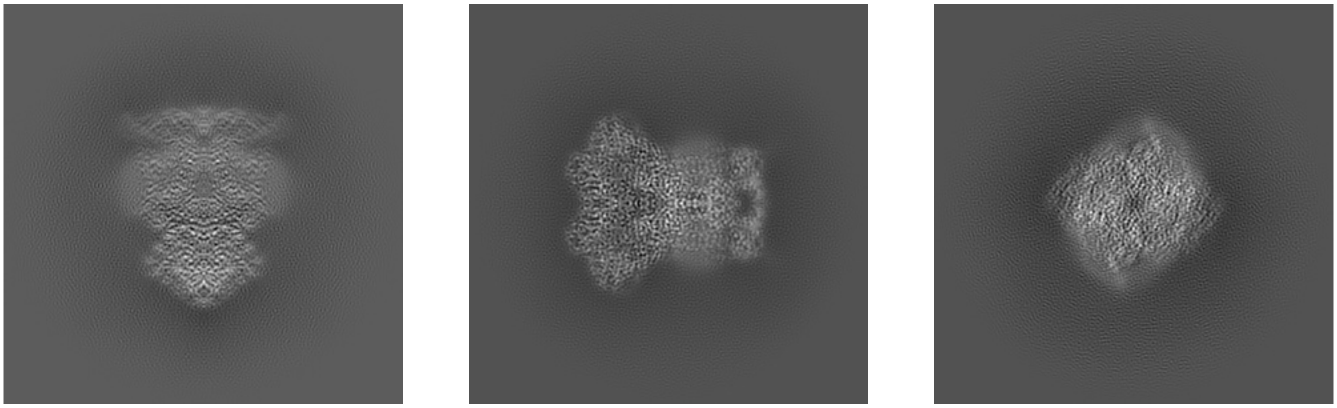
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-60323. 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.

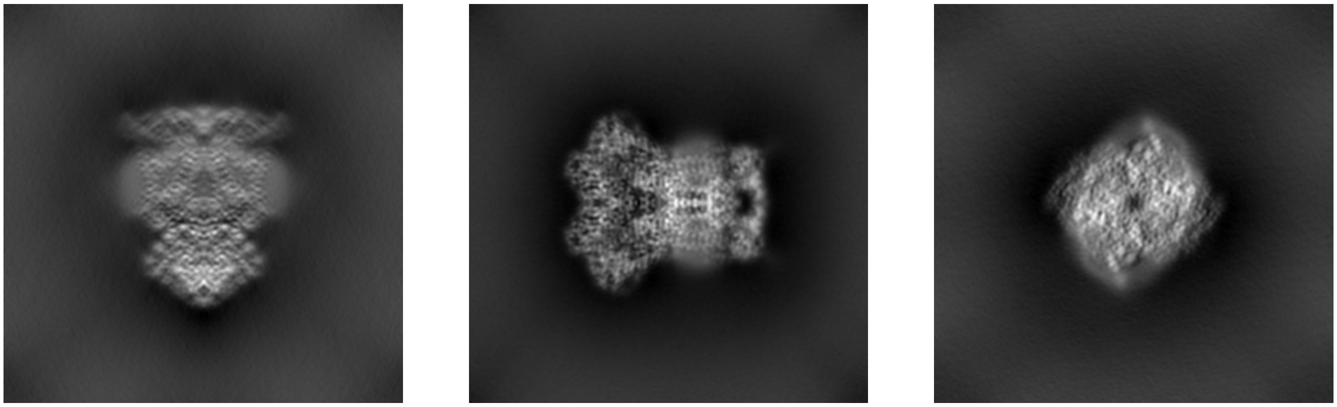
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

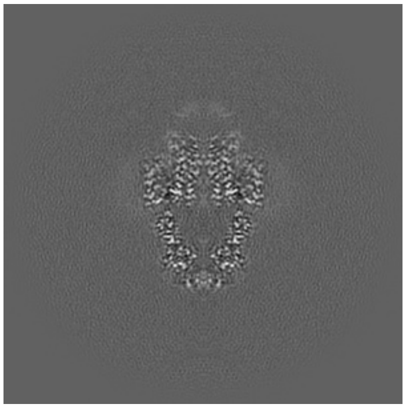


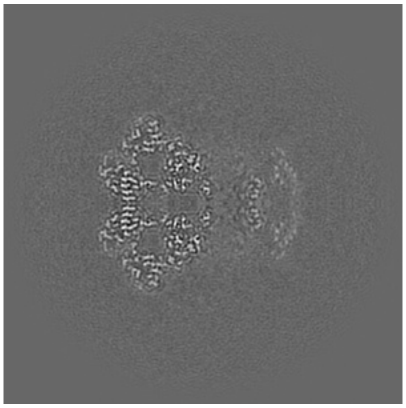
X Y Z

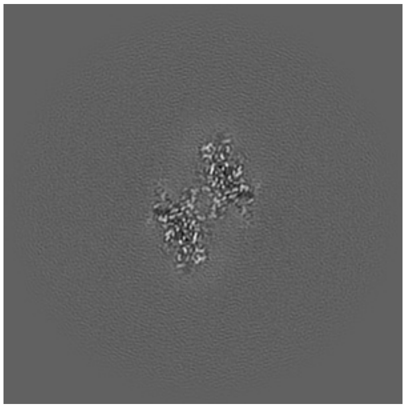
The images above show the map projected in three orthogonal directions.

6.2 Central slices

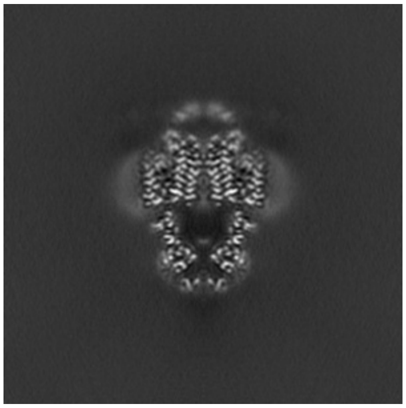
6.2.1 Primary map

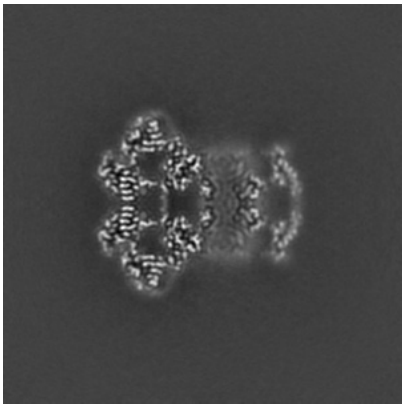

X Index: 160

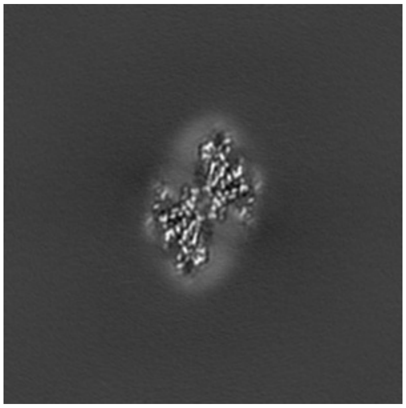

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

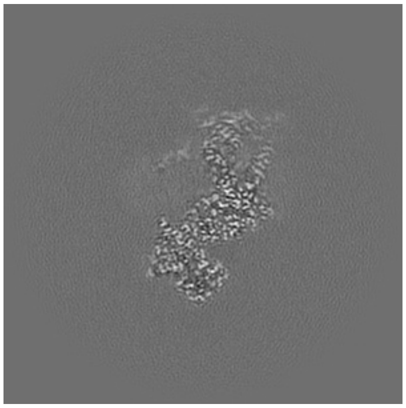

Y Index: 160


Z Index: 160

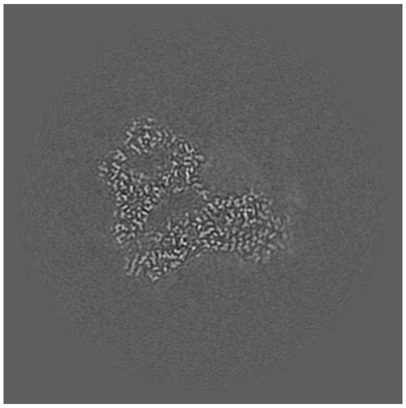
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

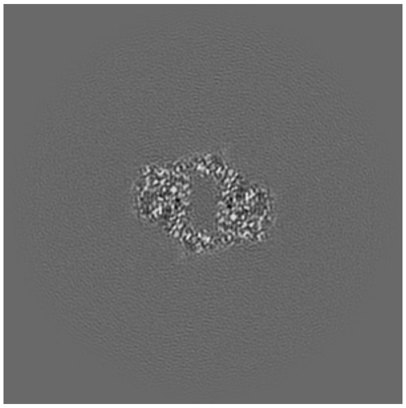
6.3.1 Primary map



X Index: 176

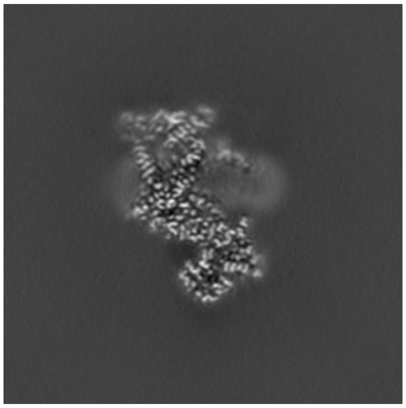


Y Index: 150

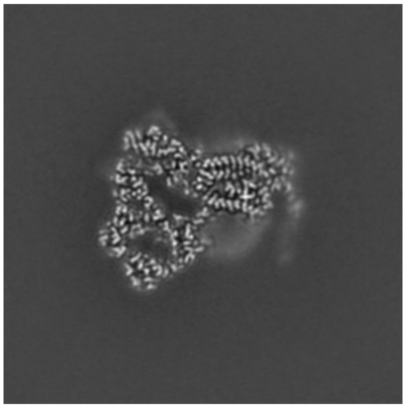


Z Index: 138

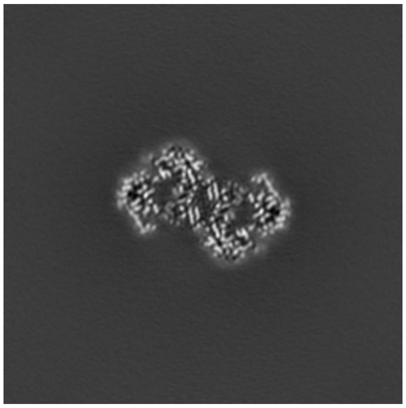
6.3.2 Raw map



X Index: 144



Y Index: 170

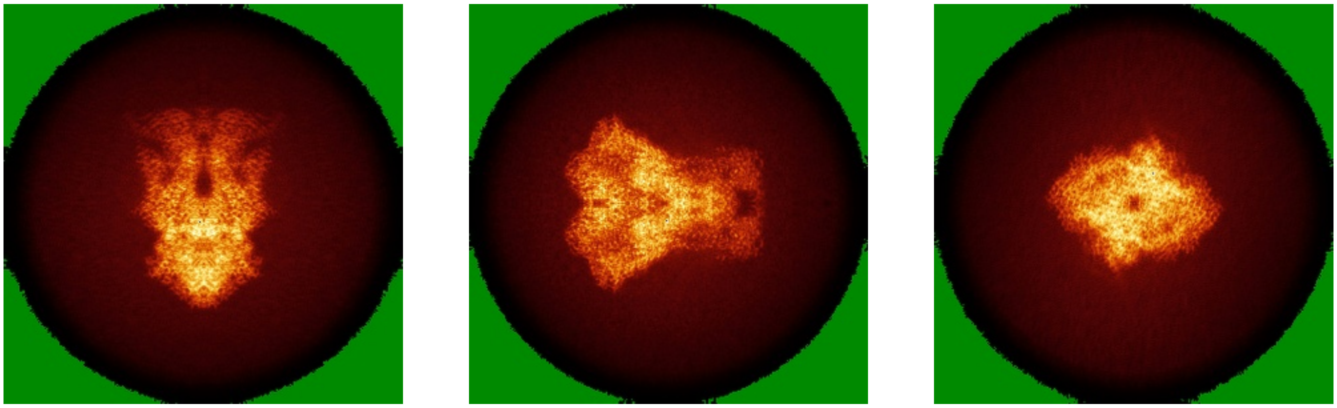


Z Index: 108

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

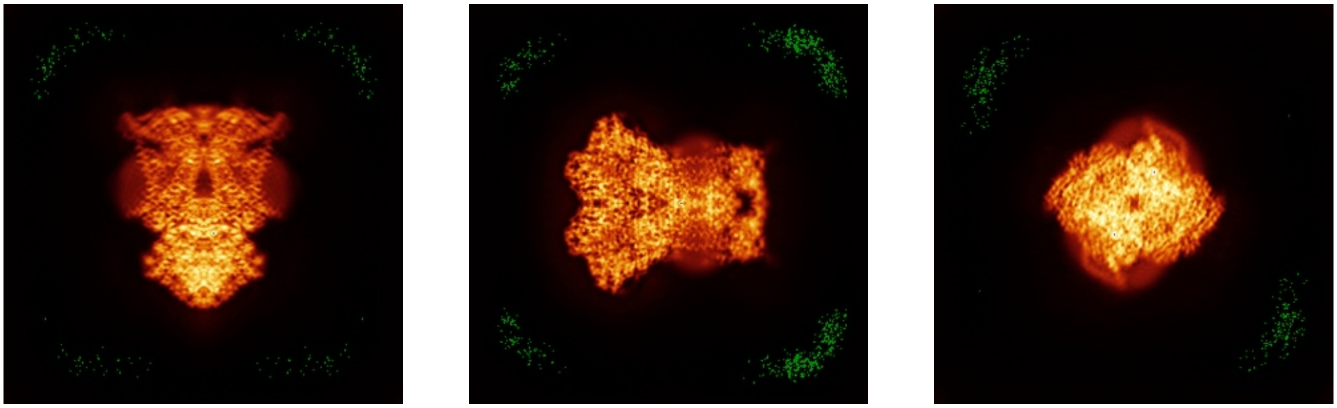
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

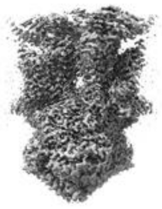


X Y Z

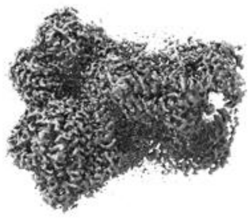
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

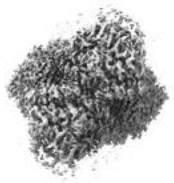
6.5.1 Primary map



X



Y

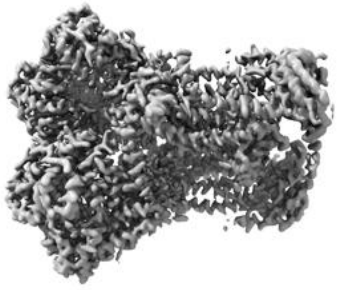


Z

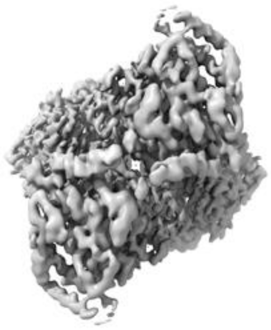
The images above show the 3D surface view of the map at the recommended contour level 1.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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.

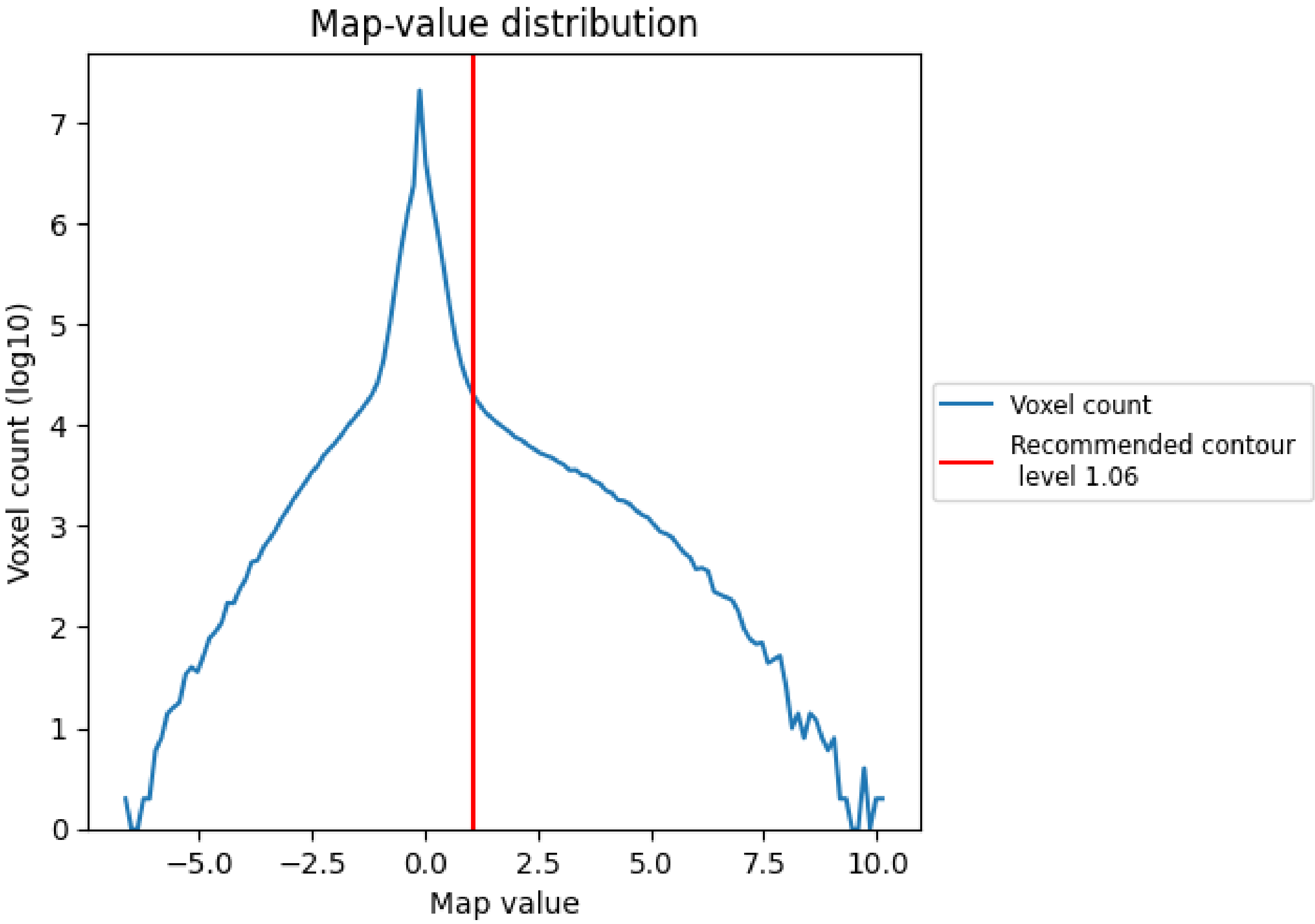
6.6 Mask visualisation

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

7 Map analysis ⓘ

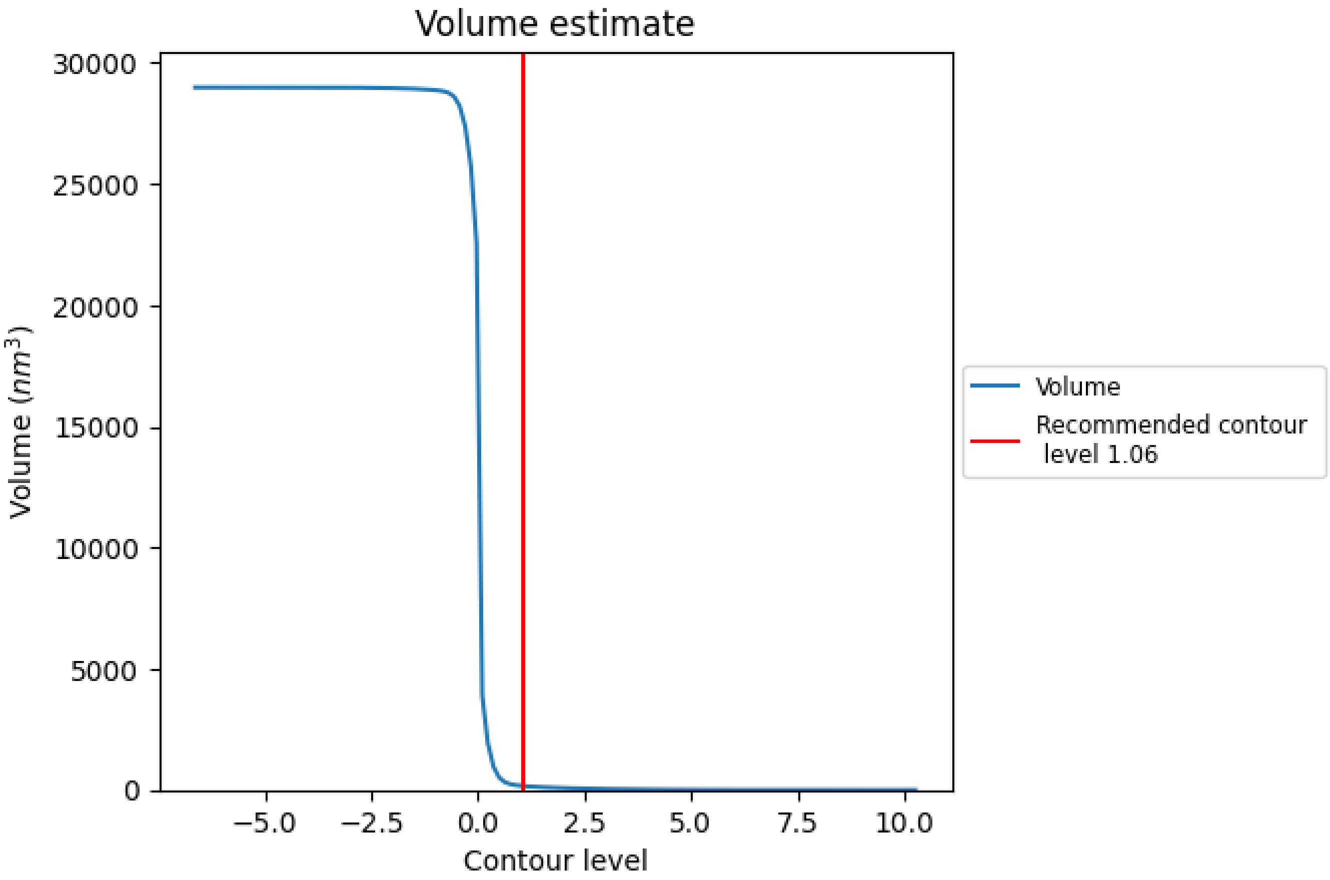
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

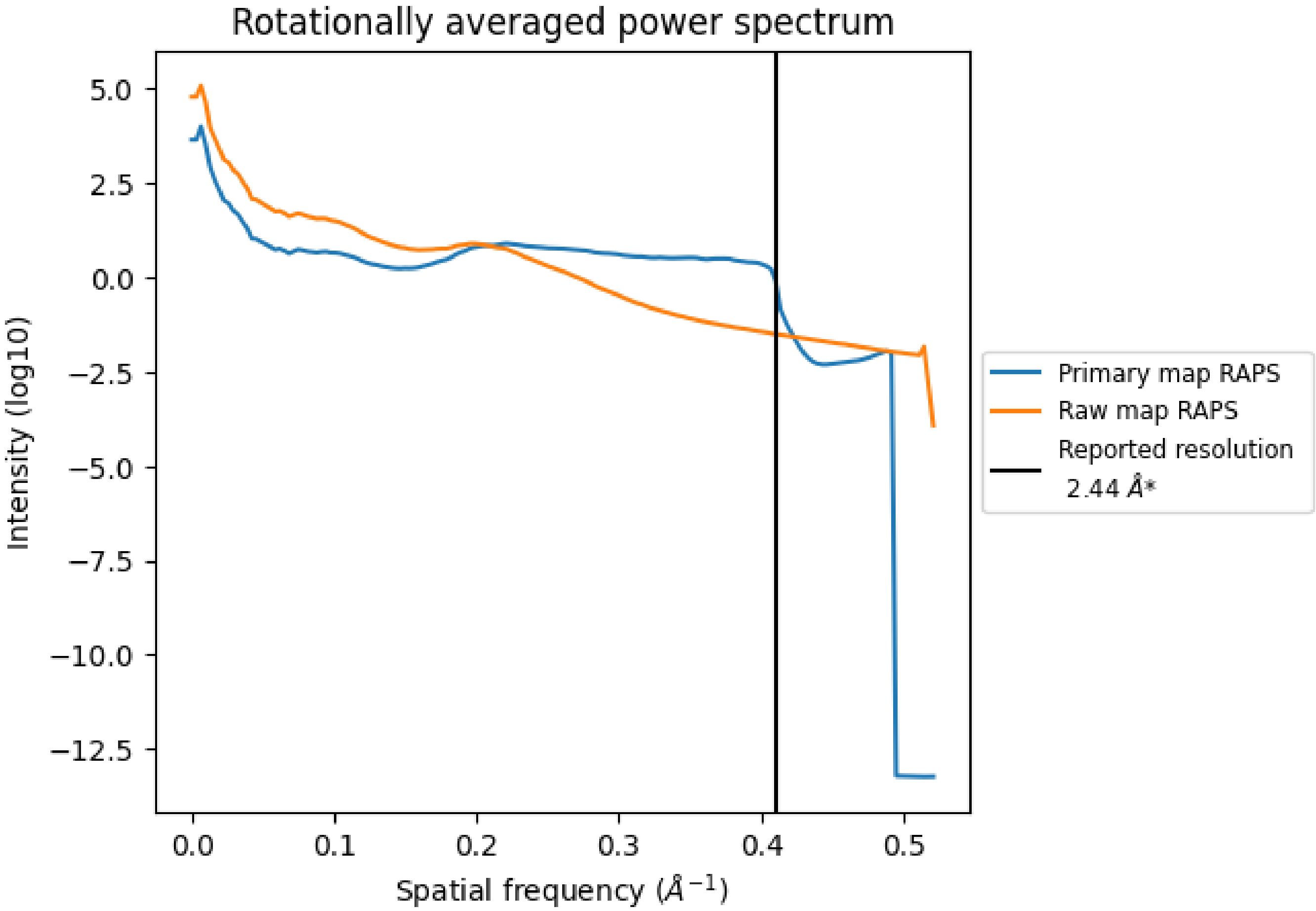
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 147 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

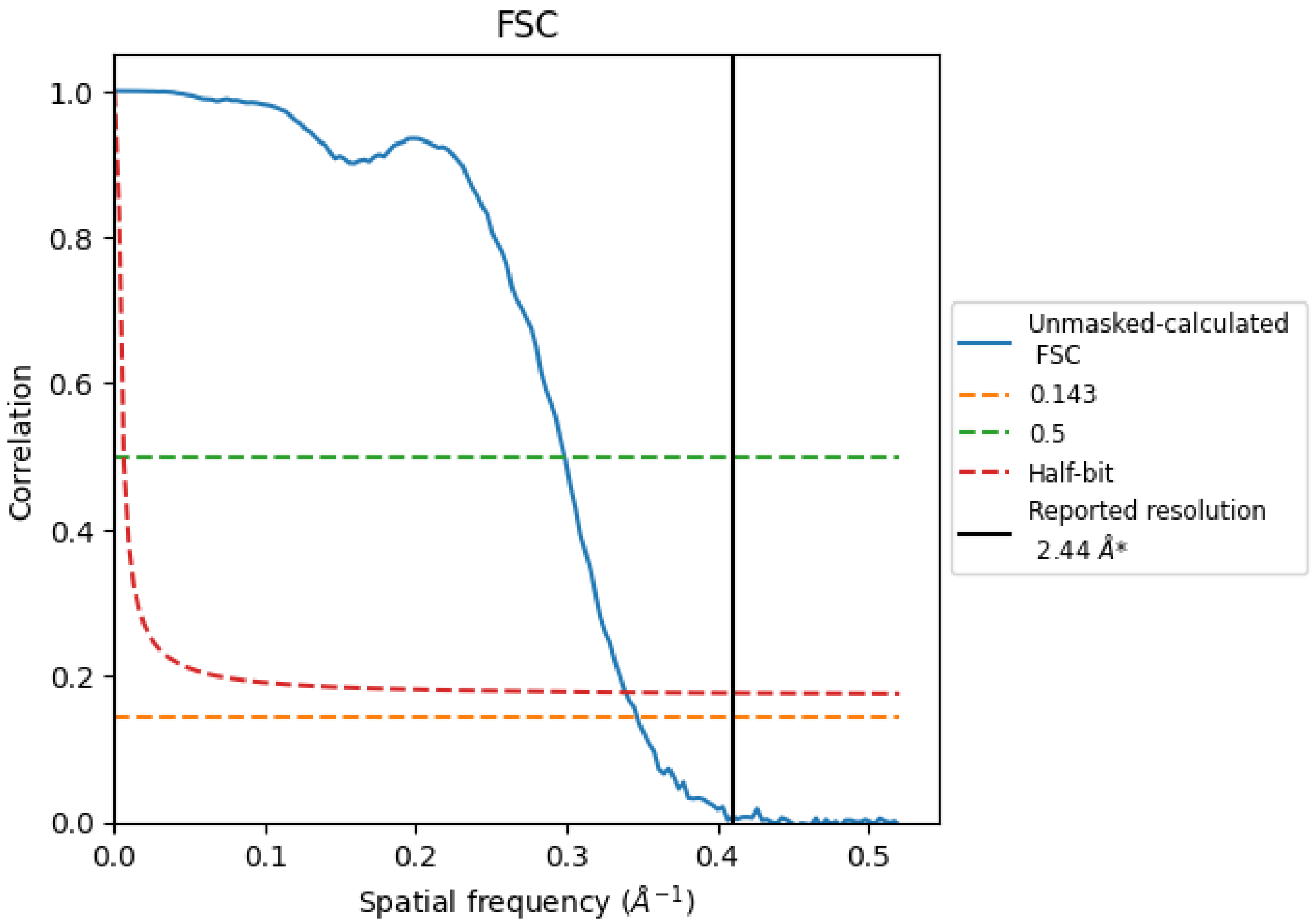


*Reported resolution corresponds to spatial frequency of 0.410 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.410 $Å^{-1}$

8.2 Resolution estimates ⓘ

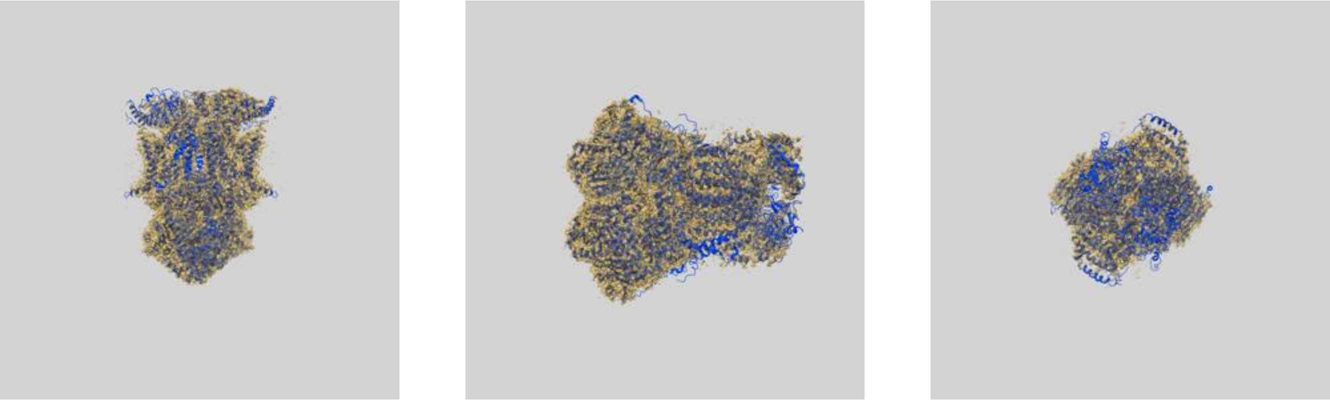
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.35	2.95

*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 2.88 differs from the reported value 2.44 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-60323 and PDB model 8ZP0. Per-residue inclusion information can be found in section 3 on page 10.

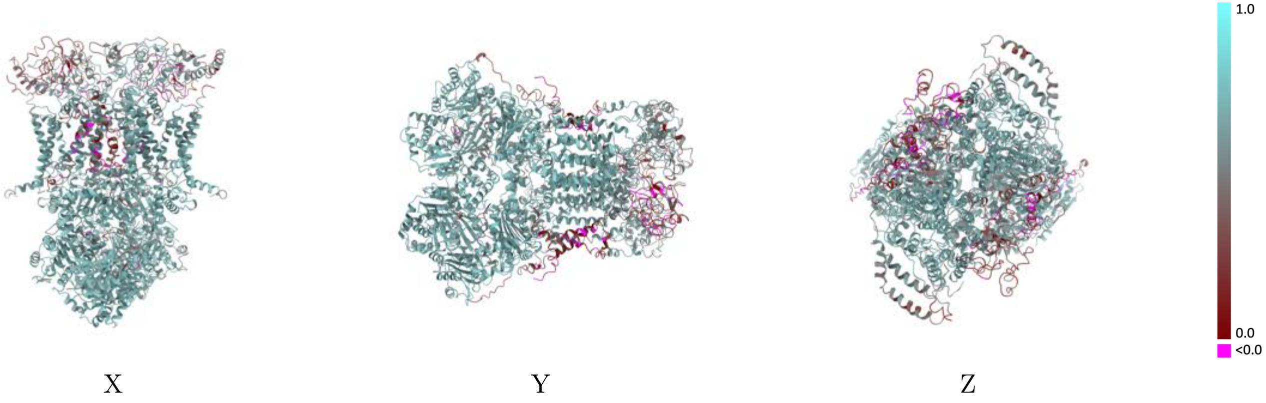
9.1 Map-model overlay ⓘ



X Y Z

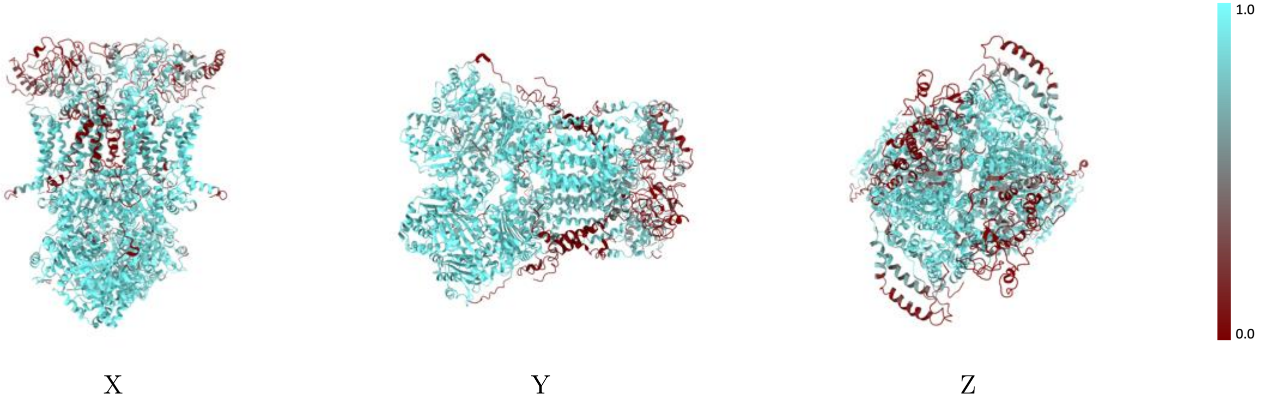
The images above show the 3D surface view of the map at the recommended contour level 1.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



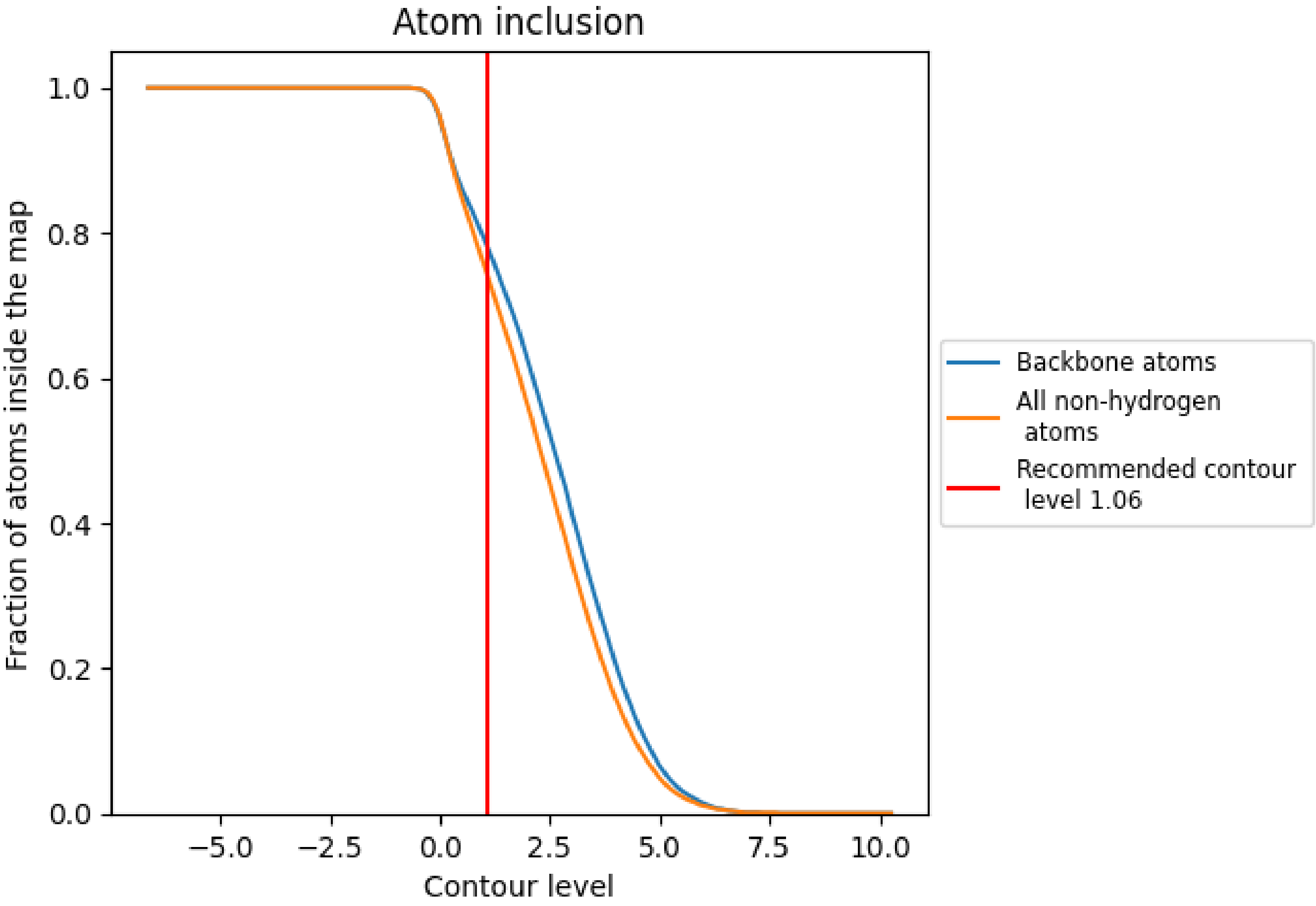
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



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 (1.06).

9.4 Atom inclusion ⓘ



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 (1.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.5780
A	0.8930	0.6450
B	0.7460	0.5820
C	0.0530	0.2900
D	0.9110	0.6610
E	0.9440	0.6680
F	0.3820	0.4860
G	0.8940	0.6630
H	0.7760	0.6080
I	0.3170	0.3120
J	0.0050	0.1980
K	0.4870	0.4200
a	0.8860	0.6430
b	0.7610	0.5910
c	0.0600	0.2220
d	0.9160	0.6620
e	0.9450	0.6690
f	0.3900	0.4780
g	0.8930	0.6630
h	0.7240	0.5740
i	0.3190	0.2970
j	0.0030	0.1840
k	0.5000	0.4250