



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 8IOG / pdb_00008iog
EMDB ID : EMD-35618
Title : Cryo-EM structure of porcine bc1 complex in isolated state
Authors : Wang, Y.X.; Dong, J.Q.; Yang, G.F.
Deposited on : 2023-03-11
Resolution : 2.88 Å (reported)
Based on initial model : 5GUP

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

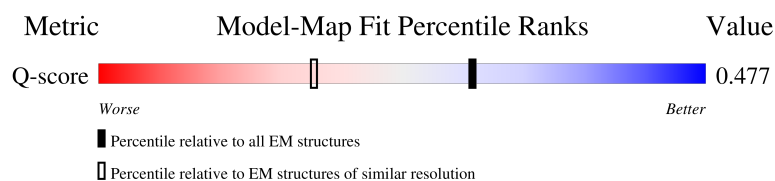
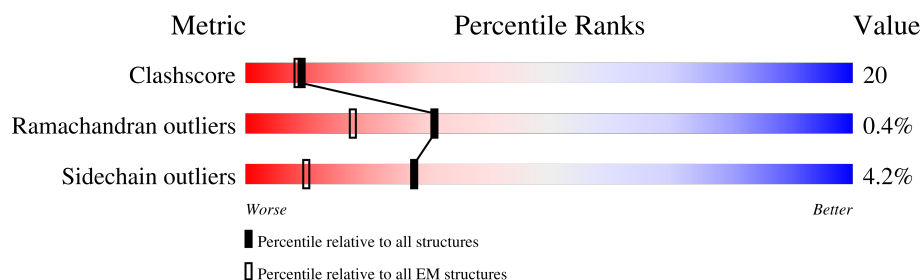
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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	379	
1	a	379	
2	B	326	
2	b	326	

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Mol	Chain	Length	Quality of chain
3	C	196	
3	c	196	
4	D	480	
4	d	480	
5	E	453	
5	e	453	
6	F	91	
6	f	91	
7	G	111	
7	g	111	
8	H	82	
8	h	82	
9	I	64	
9	i	64	
10	J	56	
10	j	56	
11	K	78	
11	k	78	

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
15	FES	C	301	-	-	X	-
15	FES	c	301	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 33413 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		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	SER	GLY	variant	UNP P24964
a	314	SER	GLY	variant	UNP P24964

- 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
			1517	954	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		

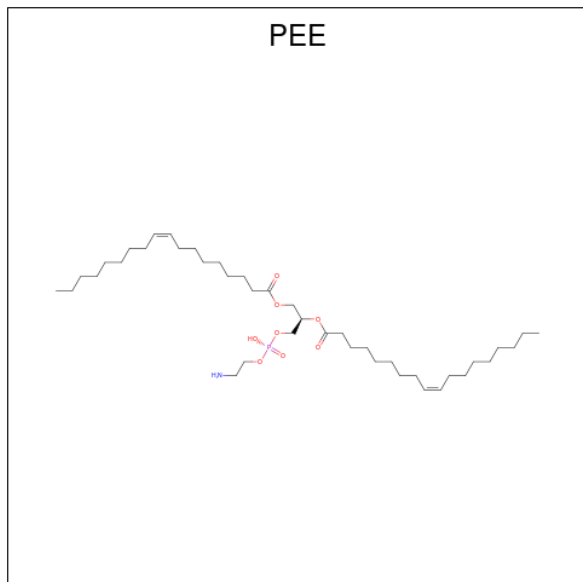
- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 10 | J | 49 | Total
405 | C
269 | N
71 | O
63 | S
2 | 0 | 0 |
| 10 | j | 51 | Total
421 | C
281 | N
74 | O
65 | S
1 | 0 | 0 |

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

- [illegible]

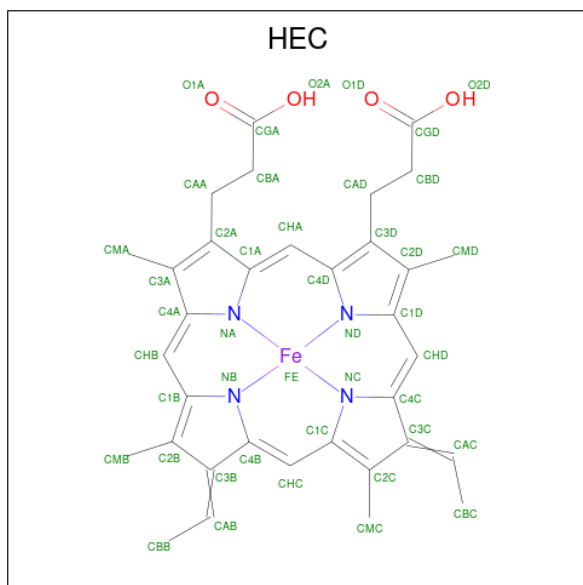
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
12	a	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



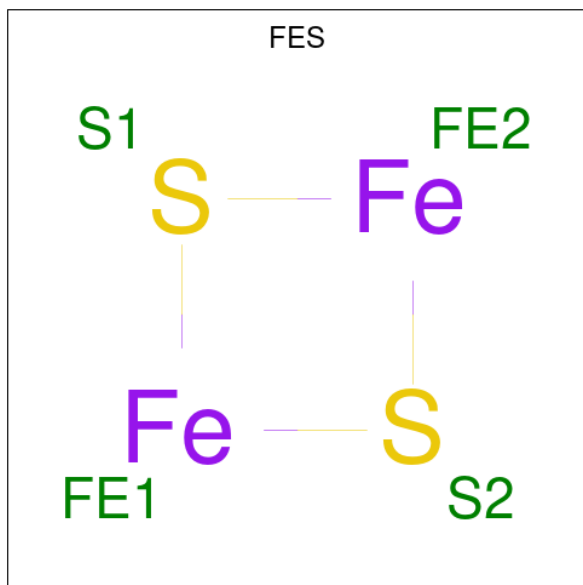
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	D	1	Total	C	N	O	P	0
			49	39	1	8	1	
13	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



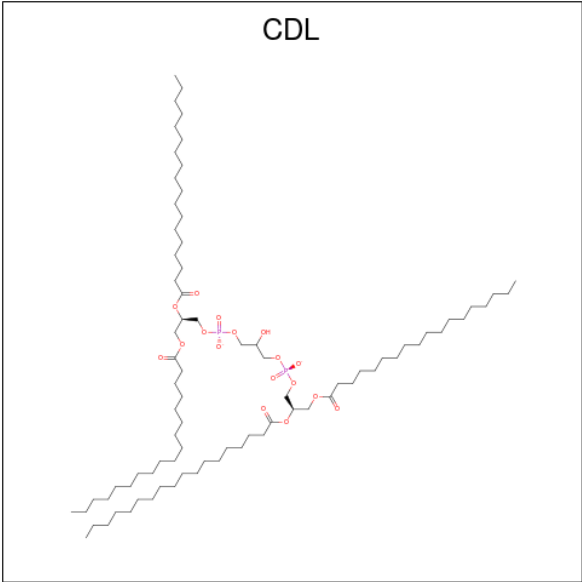
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).

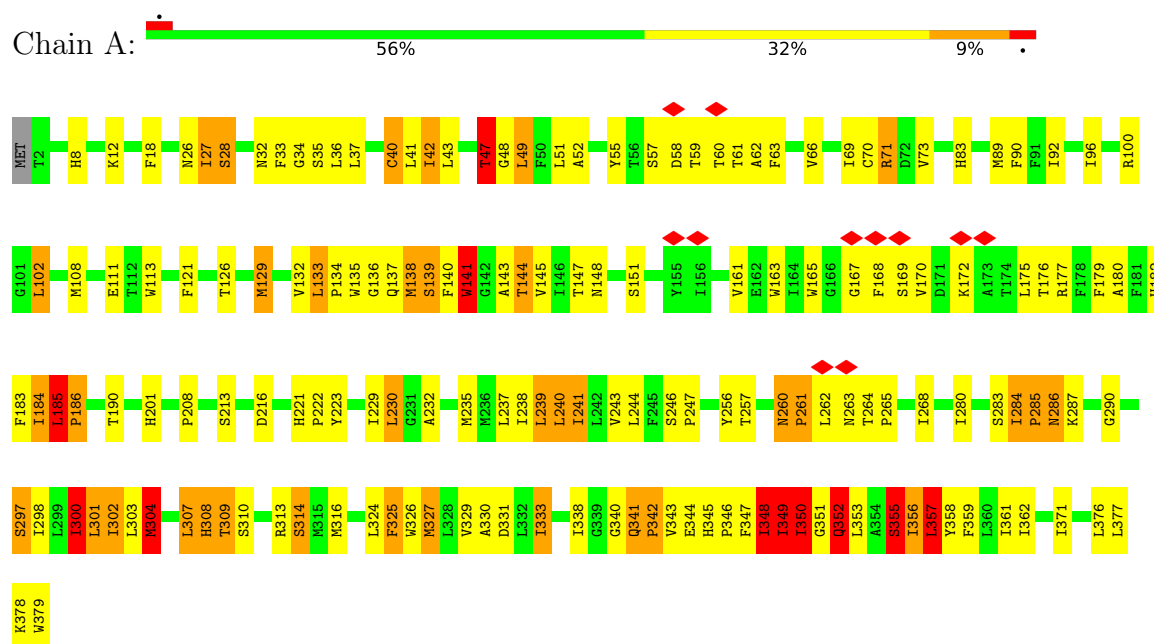


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	D	1	64	45	17	2	0
16	a	1	64	45	17	2	0

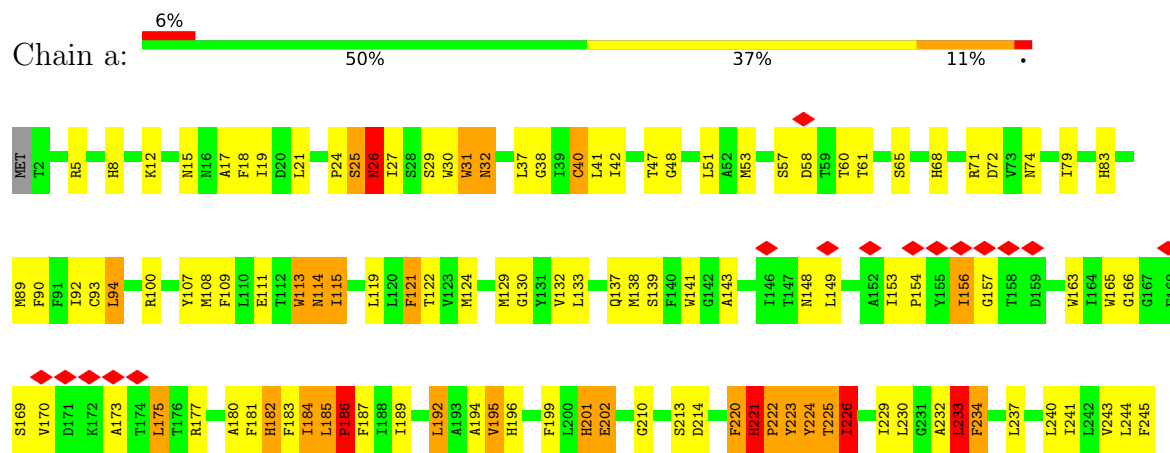
3 Residue-property plots [i](#)

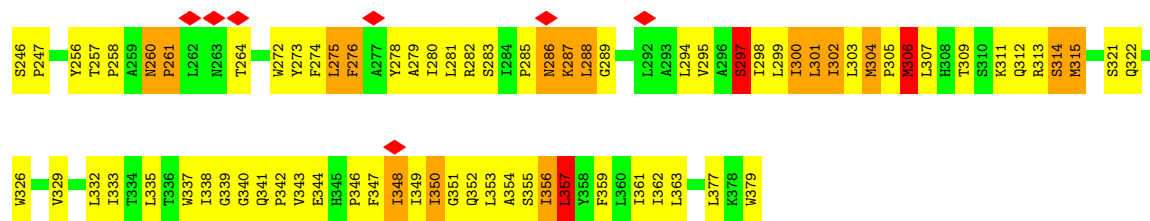
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Cytochrome b

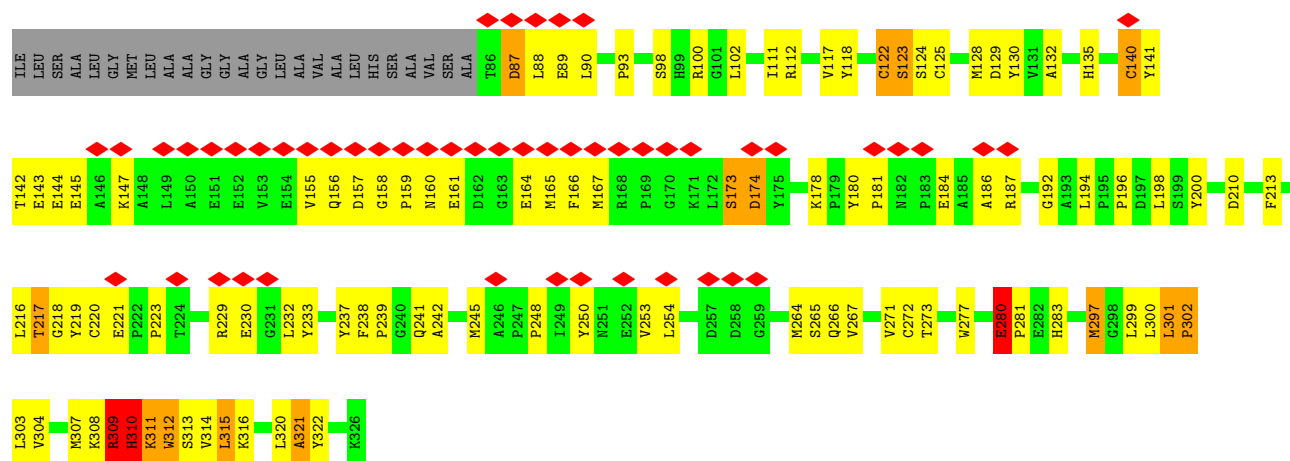
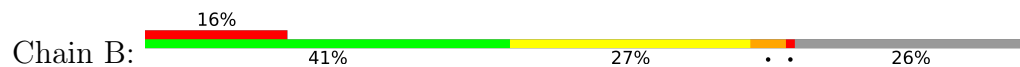


• Molecule 1: Cytochrome b

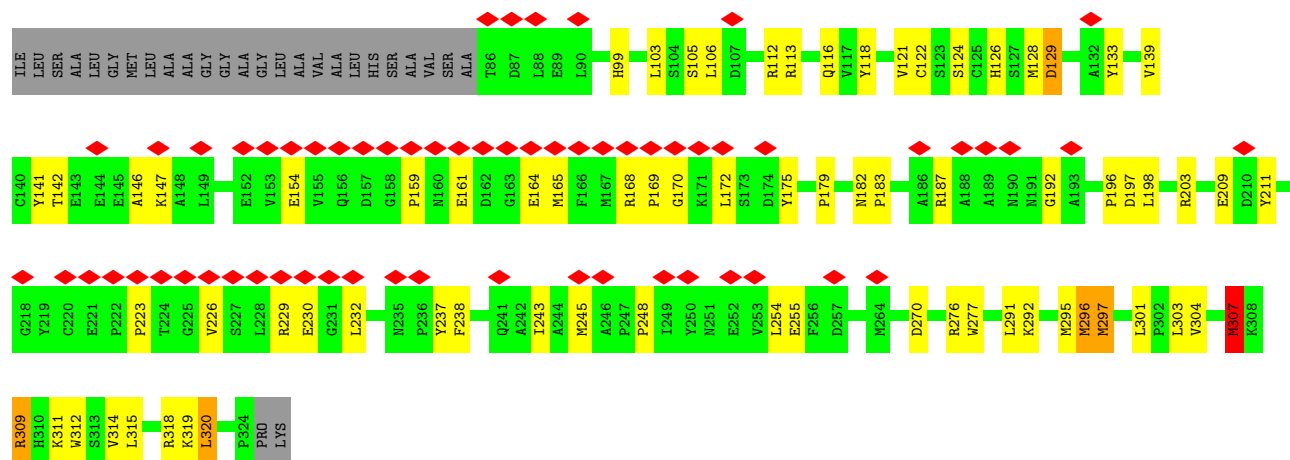




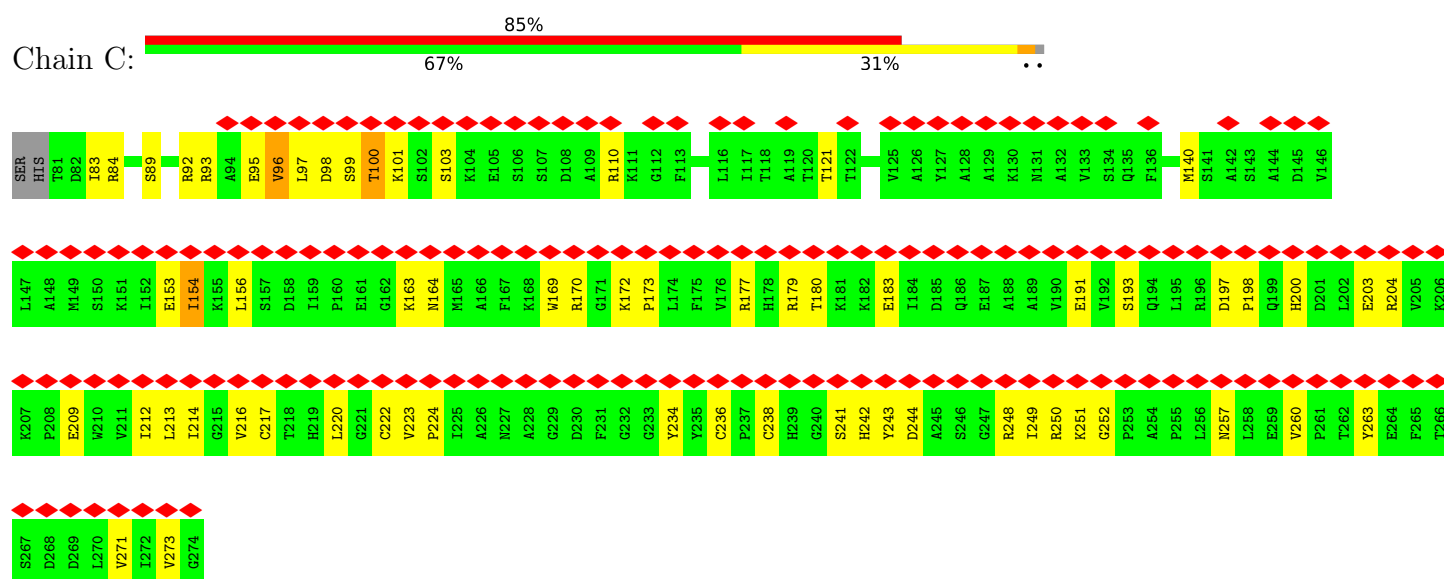
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



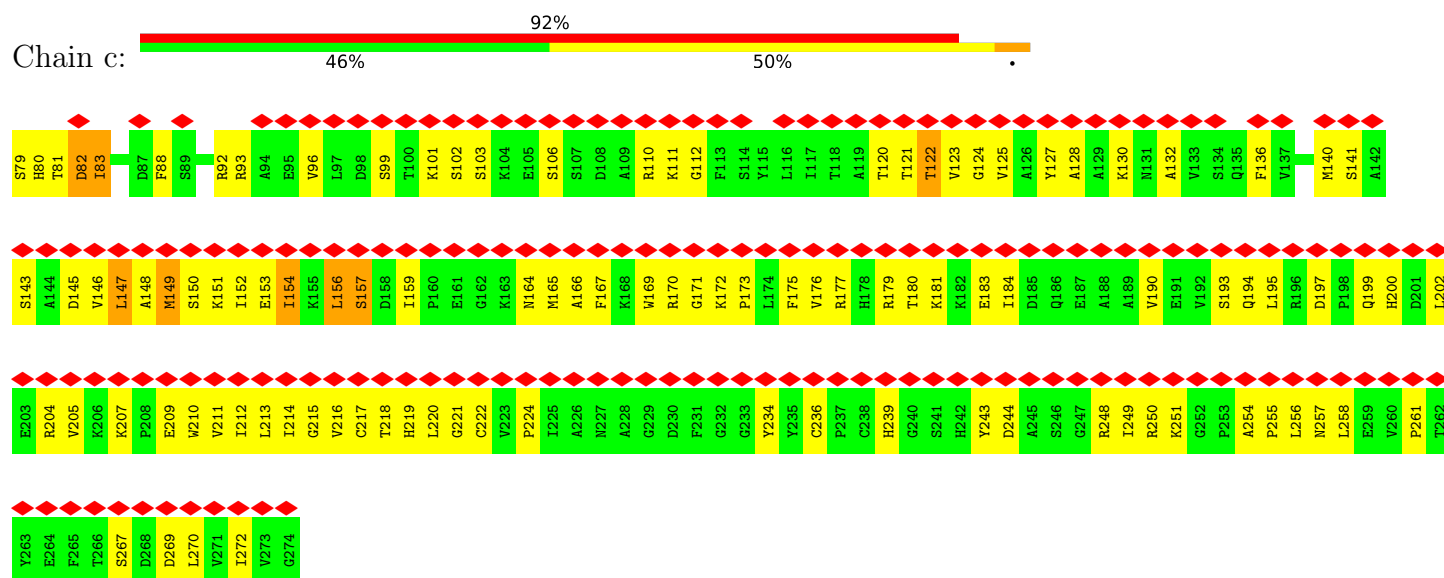
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



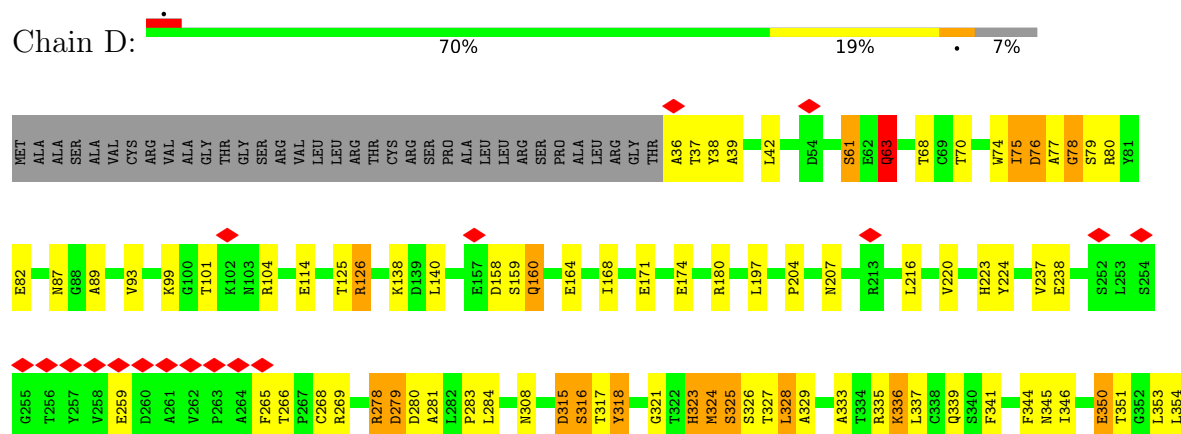
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

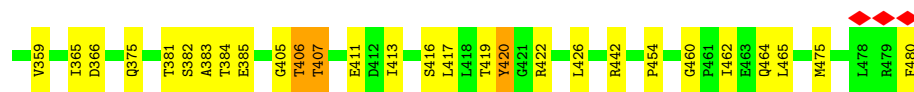


- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

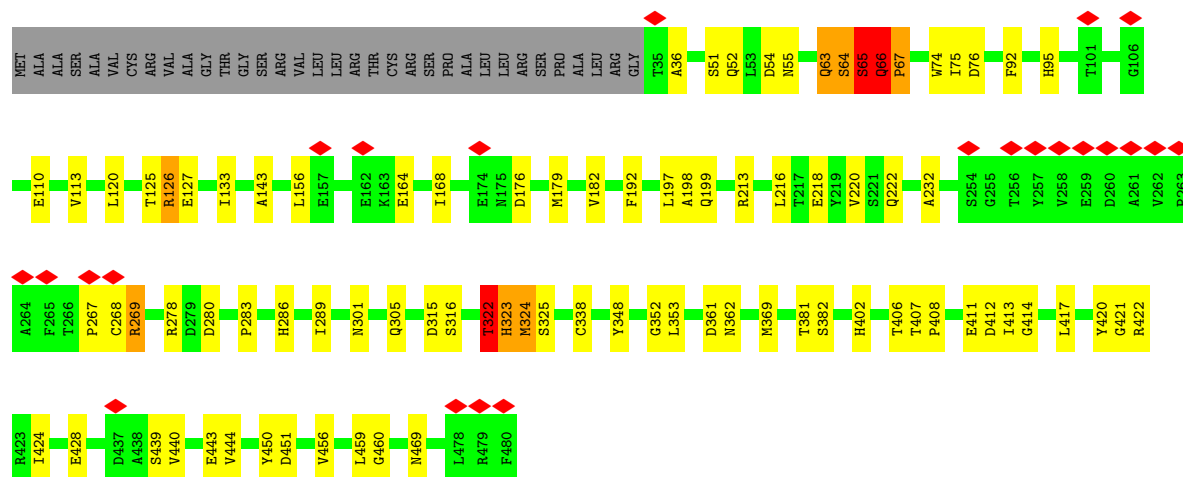
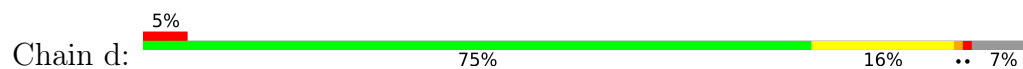


- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

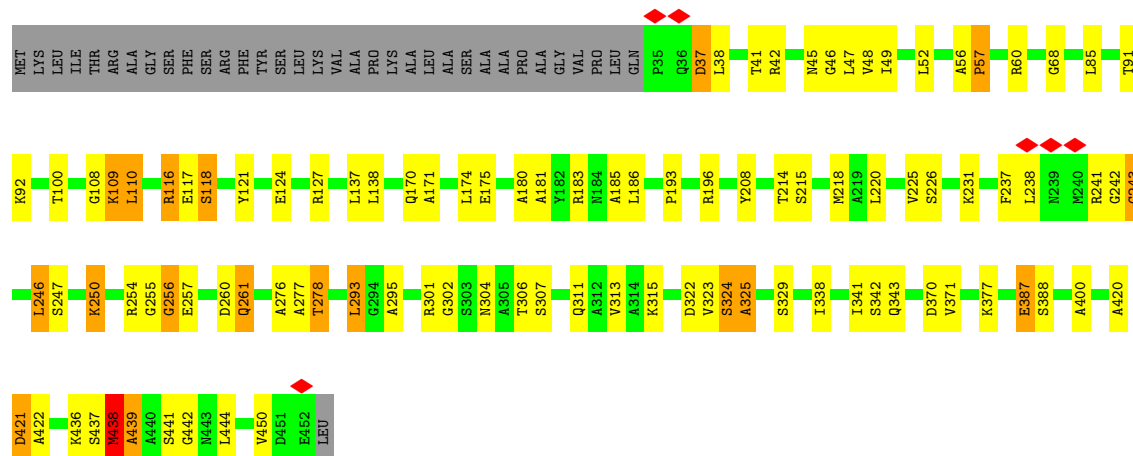




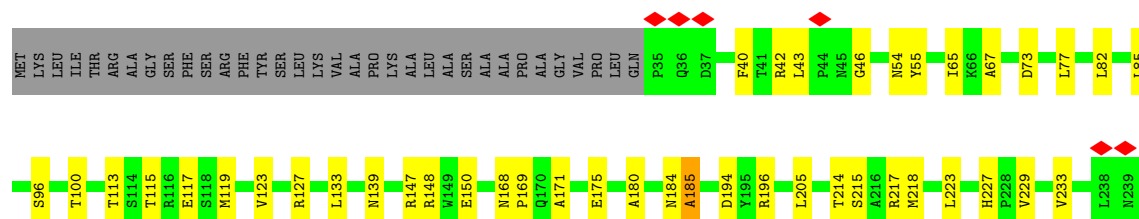
- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial



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

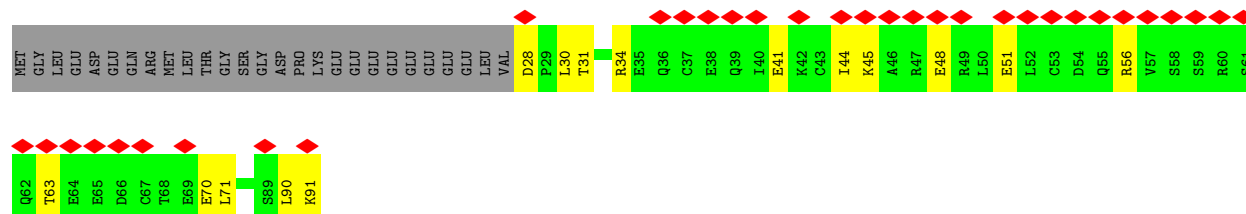


- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

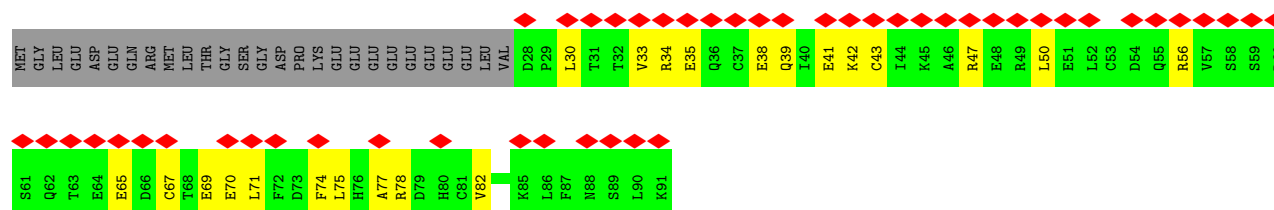




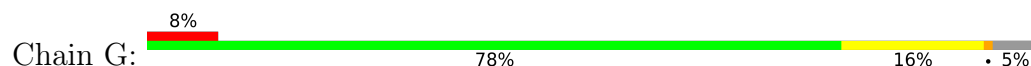
• Molecule 6: Cytochrome b-c1 complex subunit 6



• Molecule 6: Cytochrome b-c1 complex subunit 6



• Molecule 7: Cytochrome b-c1 complex subunit 7

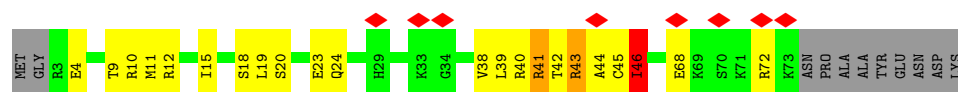


• Molecule 7: Cytochrome b-c1 complex subunit 7

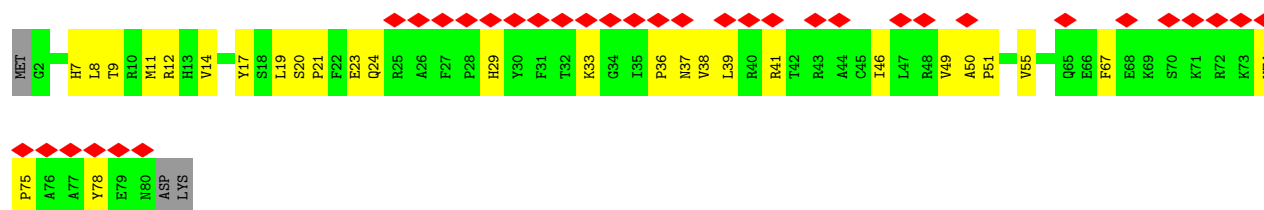
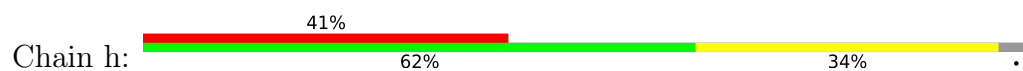


• Molecule 8: Cytochrome b-c1 complex subunit 8

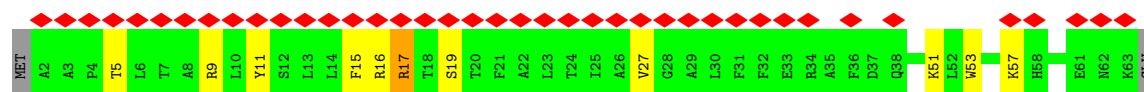




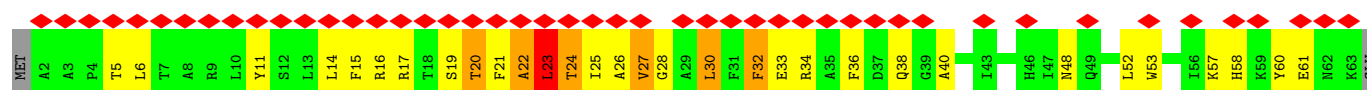
- Molecule 8: Cytochrome b-c1 complex subunit 8



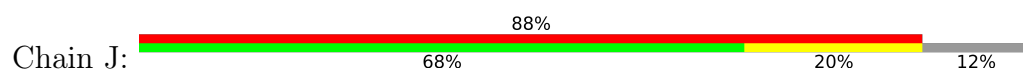
- Molecule 9: Complex III subunit 9



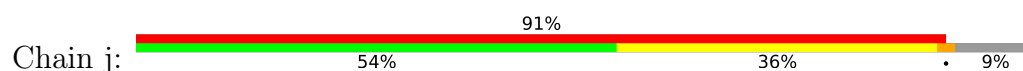
- Molecule 9: Complex III subunit 9



- Molecule 10: Cytochrome b-c1 complex subunit 10

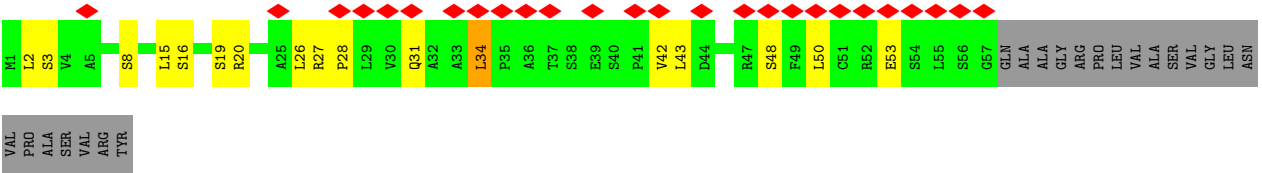


- Molecule 10: Cytochrome b-c1 complex subunit 10



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





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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98300	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 ($e^-/\text{\AA}^2$)	49.21	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.627	Depositor
Minimum map value	-2.368	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	240.8, 240.8, 240.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, PEE, FES, HEM, 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	1.11	41/3115 (1.3%)	1.23	49/4259 (1.2%)
1	a	1.06	36/3115 (1.2%)	1.19	52/4259 (1.2%)
2	B	0.98	16/1978 (0.8%)	1.00	19/2684 (0.7%)
2	b	0.52	2/1961 (0.1%)	0.68	3/2661 (0.1%)
3	C	0.22	0/1534	0.61	2/2075 (0.1%)
3	c	0.22	0/1549	0.57	1/2095 (0.0%)
4	D	0.65	7/3524 (0.2%)	0.82	16/4783 (0.3%)
4	d	0.57	7/3531 (0.2%)	0.73	8/4793 (0.2%)
5	E	0.80	14/3187 (0.4%)	0.96	22/4314 (0.5%)
5	e	0.64	9/3187 (0.3%)	0.88	17/4314 (0.4%)
6	F	0.15	0/534	0.41	0/714
6	f	0.17	0/534	0.44	0/714
7	G	0.38	0/941	0.60	0/1262
7	g	0.66	2/941 (0.2%)	0.77	4/1262 (0.3%)
8	H	0.54	0/628	0.88	1/848 (0.1%)
8	h	0.28	0/688	0.62	0/931
9	I	0.18	0/520	0.51	0/701
9	i	0.52	1/520 (0.2%)	0.87	3/701 (0.4%)
10	J	0.16	0/420	0.44	0/576
10	j	0.18	0/437	0.54	1/598 (0.2%)
11	K	0.31	0/410	0.88	1/556 (0.2%)
11	k	0.28	0/410	0.83	1/556 (0.2%)
All	All	0.71	135/33664 (0.4%)	0.88	200/45656 (0.4%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
4	D	0	2
4	d	0	3
8	h	0	1
9	I	0	1
11	K	0	2
All	All	0	14

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	311	LYS	C-O	-13.89	1.05	1.24
2	B	308	LYS	C-O	-13.68	1.07	1.24
1	a	196	HIS	C-O	-11.92	1.10	1.24
5	e	438	MET	CA-C	10.99	1.67	1.52
1	a	195	VAL	C-O	-10.41	1.12	1.24

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	440	ALA	N-CA-C	-14.98	86.76	107.88
1	a	297	SER	N-CA-C	14.41	126.70	111.14
5	e	245	GLY	N-CA-C	14.23	129.01	112.50
1	A	304	MET	N-CA-C	13.42	130.66	112.55
5	e	242	GLY	N-CA-C	13.16	129.62	112.77

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	GLN	Peptide
1	A	141	TRP	Peptide
4	D	160	GLN	Peptide
4	D	420	TYR	Peptide
9	I	17	ARG	Peptide

5.2 Too-close contacts [\(i\)](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	3078	235	0
1	a	3017	0	3078	261	0
2	B	1920	0	1869	104	0
2	b	1904	0	1849	99	0
3	C	1502	0	1488	71	0
3	c	1517	0	1495	219	0
4	D	3452	0	3343	116	0
4	d	3459	0	3350	84	0
5	E	3134	0	3112	79	0
5	e	3134	0	3112	70	0
6	F	528	0	510	11	0
6	f	528	0	510	18	0
7	G	921	0	917	15	0
7	g	921	0	917	21	0
8	H	608	0	616	17	0
8	h	666	0	663	25	0
9	I	507	0	509	11	0
9	i	507	0	509	51	0
10	J	405	0	405	11	0
10	j	421	0	418	18	0
11	K	404	0	425	17	0
11	k	404	0	425	18	0
12	A	86	0	60	8	0
12	a	86	0	60	12	0
13	A	45	0	67	2	0
13	D	49	0	75	1	0
13	a	49	0	75	3	0
14	B	43	0	32	3	0
14	b	43	0	32	7	0
15	C	4	0	0	2	0
15	c	4	0	0	5	0
16	D	64	0	72	3	0
16	a	64	0	72	4	0
All	All	33413	0	33143	1358	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 20.

The worst 5 of 1358 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:122:CYS:CB	14:b:401:HEC:HAB	1.38	1.48
4:D:327:THR:HG21	4:D:375:GLN:NE2	1.32	1.39
3:c:80:HIS:NE2	4:d:182:VAL:HG12	1.39	1.33
3:c:82:ASP:O	3:c:83:ILE:HG23	1.14	1.31
3:C:220:LEU:HB2	15:C:301:FES:S2	1.72	1.28

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	376/379 (99%)	352 (94%)	22 (6%)	2 (0%)	24	51
1	a	376/379 (99%)	340 (90%)	32 (8%)	4 (1%)	11	33
2	B	239/326 (73%)	215 (90%)	20 (8%)	4 (2%)	7	23
2	b	237/326 (73%)	217 (92%)	20 (8%)	0	100	100
3	C	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
3	c	194/196 (99%)	177 (91%)	16 (8%)	1 (0%)	24	51
4	D	443/480 (92%)	424 (96%)	19 (4%)	0	100	100
4	d	444/480 (92%)	400 (90%)	42 (10%)	2 (0%)	24	51
5	E	416/453 (92%)	387 (93%)	28 (7%)	1 (0%)	43	70
5	e	416/453 (92%)	375 (90%)	40 (10%)	1 (0%)	43	70
6	F	62/91 (68%)	59 (95%)	3 (5%)	0	100	100
6	f	62/91 (68%)	59 (95%)	3 (5%)	0	100	100
7	G	104/111 (94%)	95 (91%)	9 (9%)	0	100	100
7	g	104/111 (94%)	90 (86%)	14 (14%)	0	100	100
8	H	69/82 (84%)	56 (81%)	11 (16%)	2 (3%)	3	13
8	h	77/82 (94%)	64 (83%)	13 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	60/64 (94%)	49 (82%)	11 (18%)	0	100	100
9	i	60/64 (94%)	57 (95%)	3 (5%)	0	100	100
10	J	47/56 (84%)	47 (100%)	0	0	100	100
10	j	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
11	K	55/78 (70%)	33 (60%)	22 (40%)	0	100	100
11	k	55/78 (70%)	34 (62%)	21 (38%)	0	100	100
All	All	4137/4632 (89%)	3763 (91%)	357 (9%)	17 (0%)	31	56

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	PRO
1	a	221	HIS
3	c	83	ILE
4	d	66	GLN
4	d	67	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	331/332 (100%)	299 (90%)	32 (10%)	8	23
1	a	331/332 (100%)	305 (92%)	26 (8%)	11	32
2	B	206/259 (80%)	193 (94%)	13 (6%)	16	42
2	b	204/259 (79%)	199 (98%)	5 (2%)	42	72
3	C	164/166 (99%)	161 (98%)	3 (2%)	51	78
3	c	165/166 (99%)	158 (96%)	7 (4%)	26	58
4	D	371/397 (94%)	356 (96%)	15 (4%)	28	60
4	d	372/397 (94%)	362 (97%)	10 (3%)	39	70
5	E	327/354 (92%)	316 (97%)	11 (3%)	32	64
5	e	327/354 (92%)	320 (98%)	7 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	61/85 (72%)	61 (100%)	0	100	100
6	f	61/85 (72%)	61 (100%)	0	100	100
7	G	95/99 (96%)	94 (99%)	1 (1%)	65	86
7	g	95/99 (96%)	91 (96%)	4 (4%)	26	58
8	H	65/73 (89%)	58 (89%)	7 (11%)	6	19
8	h	70/73 (96%)	70 (100%)	0	100	100
9	I	50/52 (96%)	50 (100%)	0	100	100
9	i	50/52 (96%)	44 (88%)	6 (12%)	5	14
10	J	40/46 (87%)	40 (100%)	0	100	100
10	j	41/46 (89%)	41 (100%)	0	100	100
11	K	44/59 (75%)	44 (100%)	0	100	100
11	k	44/59 (75%)	44 (100%)	0	100	100
All	All	3514/3844 (91%)	3367 (96%)	147 (4%)	28	58

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	122	THR
9	i	24	THR
3	c	157	SER
5	e	241	ARG
4	D	61	SER

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	63	GLN
5	e	170	GLN
4	d	160	GLN
4	d	286	HIS
6	f	55	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	PEE	D	502	-	48,48,50	1.62	8 (16%)	51,53,55	1.22	3 (5%)
15	FES	c	301	-	0,4,4	-	-	-		
13	PEE	a	403	-	48,48,50	1.56	6 (12%)	51,53,55	1.18	4 (7%)
12	HEM	a	402	1	50,50,50	1.52	9 (18%)	67,82,82	1.31	11 (16%)
16	CDL	a	404	-	63,63,99	1.11	8 (12%)	69,75,111	1.14	4 (5%)
14	HEC	b	401	2	46,50,50	1.85	7 (15%)	58,82,82	1.97	5 (8%)
12	HEM	a	401	1	50,50,50	1.34	5 (10%)	67,82,82	1.18	5 (7%)
16	CDL	D	501	-	63,63,99	1.10	8 (12%)	69,75,111	1.22	5 (7%)
12	HEM	A	402	1	50,50,50	1.42	8 (16%)	67,82,82	1.66	18 (26%)
14	HEC	B	401	2	46,50,50	1.86	6 (13%)	58,82,82	2.01	8 (13%)
15	FES	C	301	3	0,4,4	-	-	-		
12	HEM	A	401	1	50,50,50	1.49	8 (16%)	67,82,82	1.74	18 (26%)
13	PEE	A	403	-	44,44,50	1.59	7 (15%)	47,49,55	1.32	6 (12%)

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	PEE	D	502	-	-	17/52/52/54	-
15	FES	c	301	-	-	-	0/1/1/1
13	PEE	a	403	-	-	23/52/52/54	-
12	HEM	a	402	1	-	4/14/54/54	-
16	CDL	a	404	-	-	34/74/74/110	-
14	HEC	b	401	2	-	7/14/54/54	-
12	HEM	a	401	1	-	4/14/54/54	-
16	CDL	D	501	-	-	35/74/74/110	-
12	HEM	A	402	1	-	9/14/54/54	-
14	HEC	B	401	2	-	6/14/54/54	-
15	FES	C	301	3	-	-	0/1/1/1
12	HEM	A	401	1	-	8/14/54/54	-
13	PEE	A	403	-	-	23/48/48/54	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	401	HEC	CAB-C3B	6.14	1.54	1.35
14	B	401	HEC	CAC-C3C	6.12	1.54	1.35
14	b	401	HEC	CAC-C3C	6.12	1.54	1.35
14	B	401	HEC	CAB-C3B	6.07	1.54	1.35
14	B	401	HEC	C3D-C2D	6.00	1.54	1.38

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	401	HEC	CBC-CAC-C3C	-9.34	108.76	127.43
14	B	401	HEC	CBB-CAB-C3B	-8.84	109.77	127.43
14	b	401	HEC	CBB-CAB-C3B	-8.72	110.01	127.43
14	B	401	HEC	CBC-CAC-C3C	-8.33	110.79	127.43
12	A	402	HEM	CAD-C3D-C4D	5.11	133.60	124.70

There are no chirality outliers.

5 of 170 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	402	HEM	C1A-C2A-CAA-CBA
12	A	402	HEM	C2D-C3D-CAD-CBD
12	A	402	HEM	C4D-C3D-CAD-CBD
12	a	401	HEM	C1A-C2A-CAA-CBA

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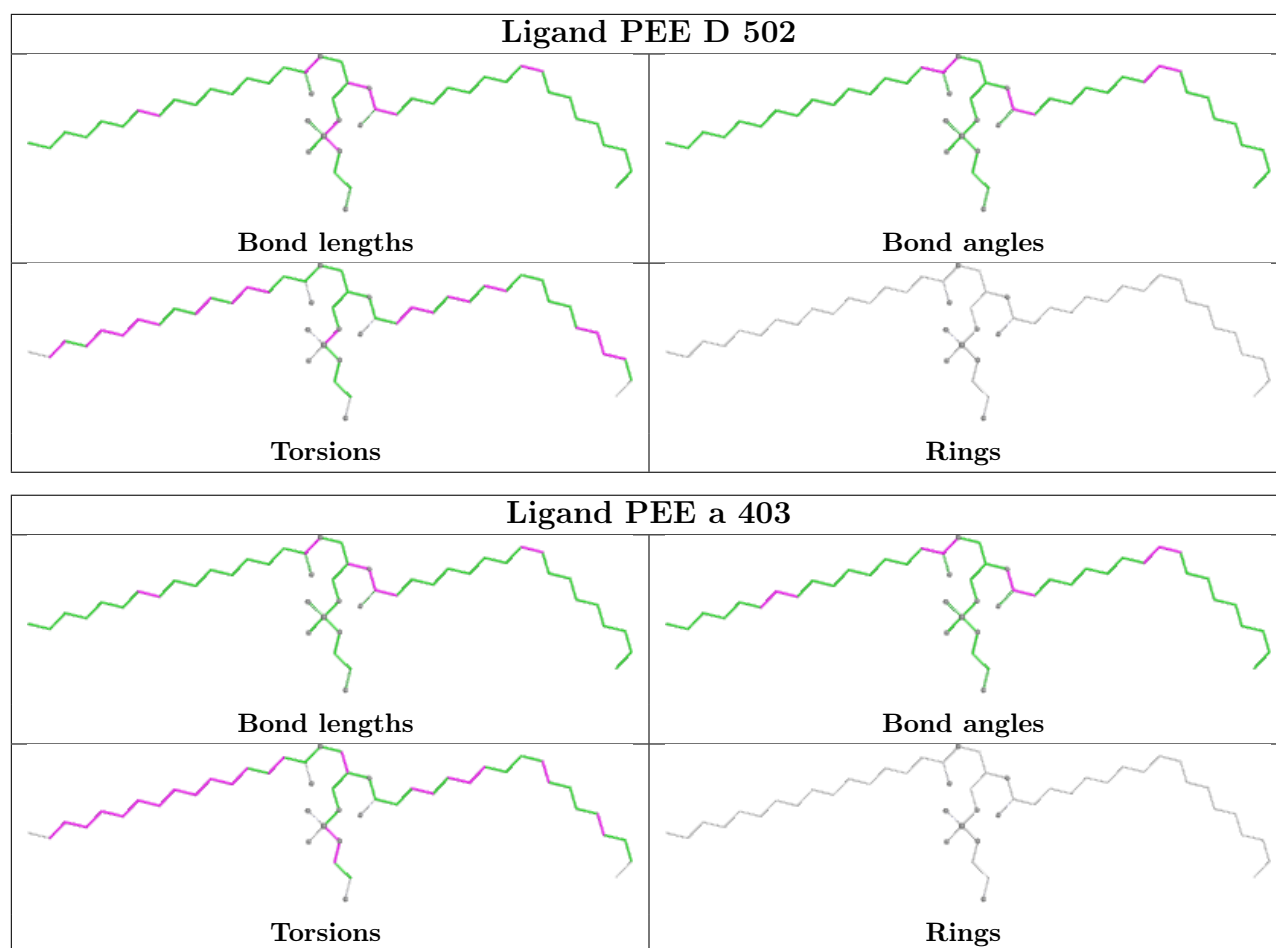
Mol	Chain	Res	Type	Atoms
12	a	401	HEM	C3D-CAD-CBD-CGD

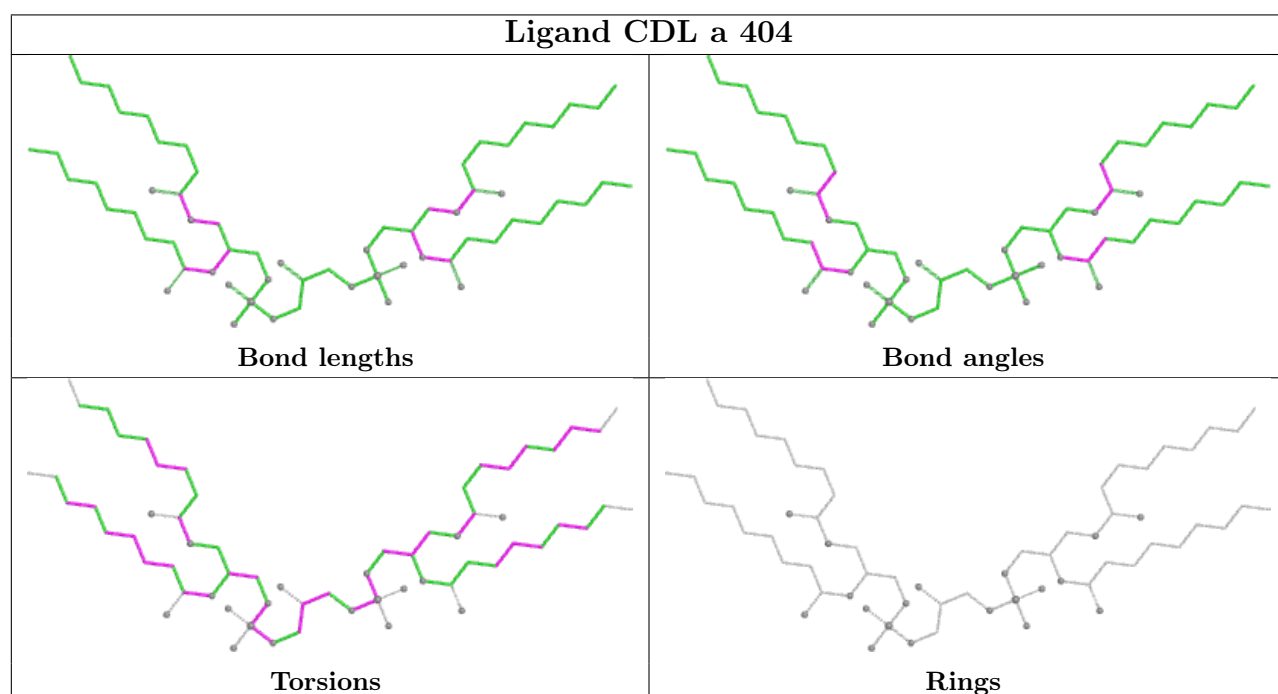
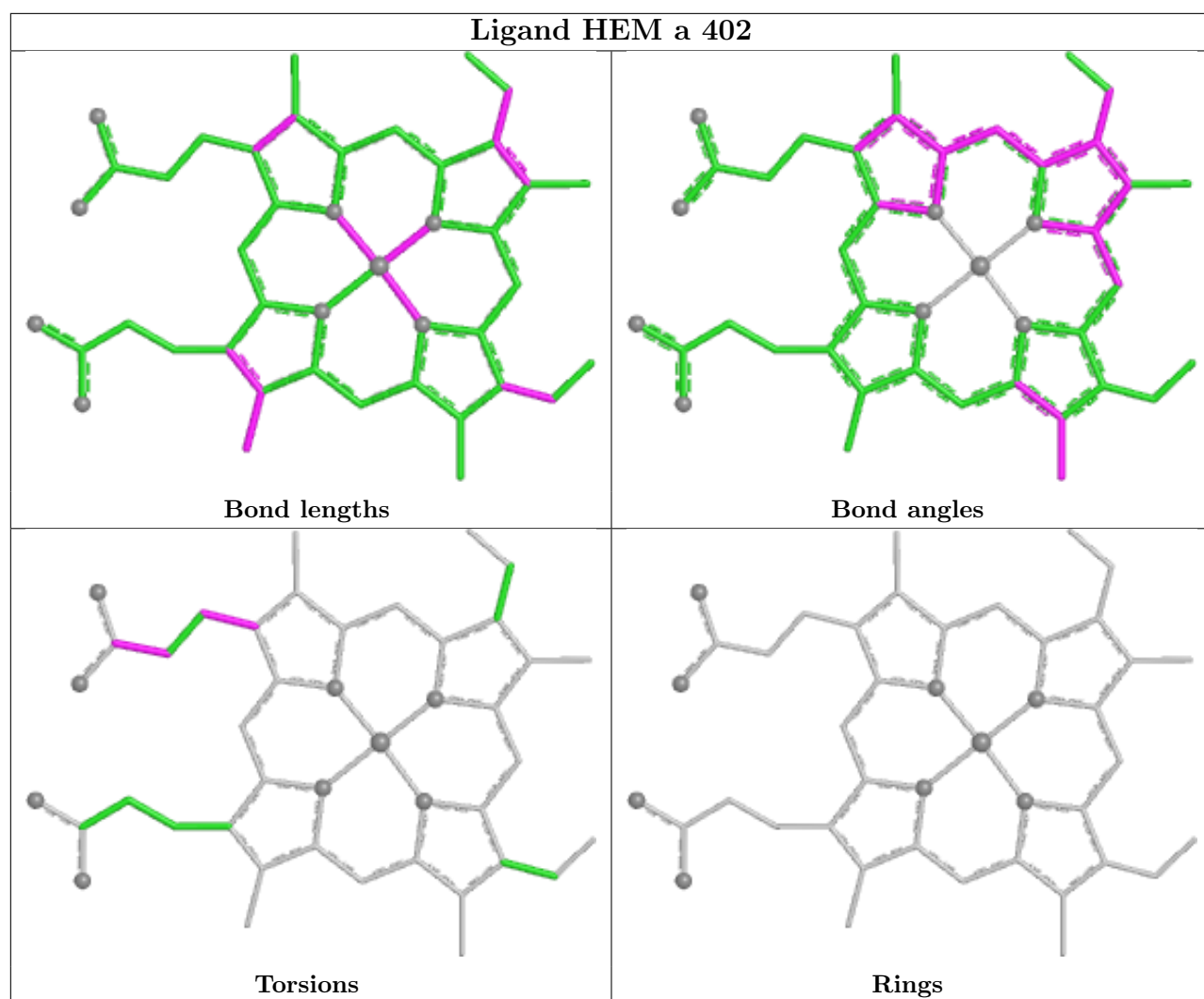
There are no ring outliers.

13 monomers are involved in 48 short contacts:

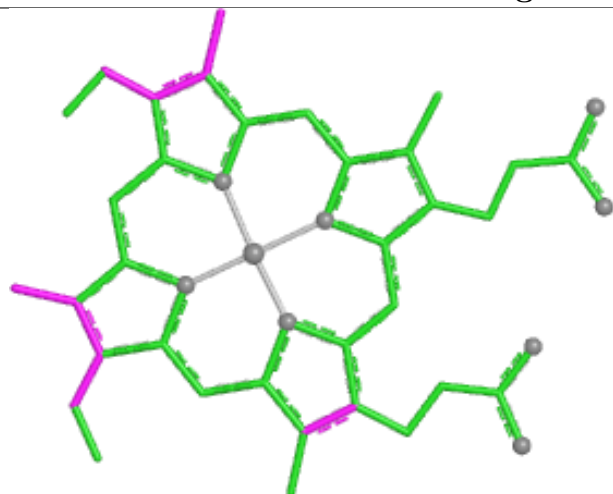
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	502	PEE	1	0
15	c	301	FES	5	0
13	a	403	PEE	3	0
12	a	402	HEM	5	0
16	a	404	CDL	4	0
14	b	401	HEC	7	0
12	a	401	HEM	7	0
16	D	501	CDL	3	0
12	A	402	HEM	5	0
14	B	401	HEC	3	0
15	C	301	FES	2	0
12	A	401	HEM	3	0
13	A	403	PEE	2	0

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.

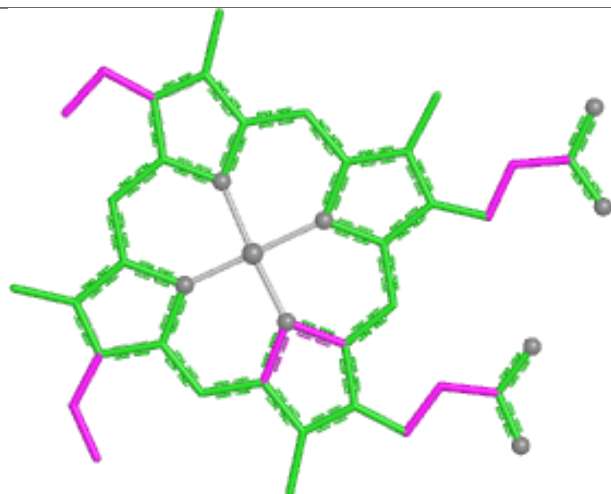




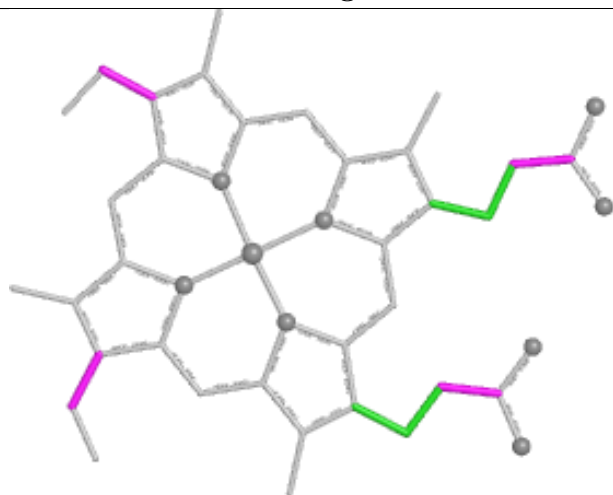
Ligand HEC b 401



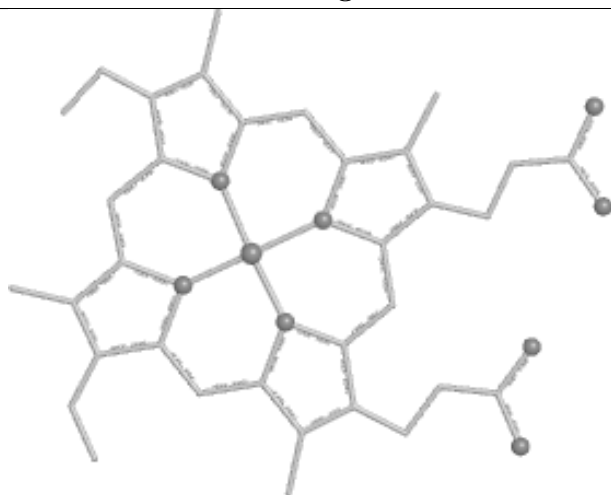
Bond lengths



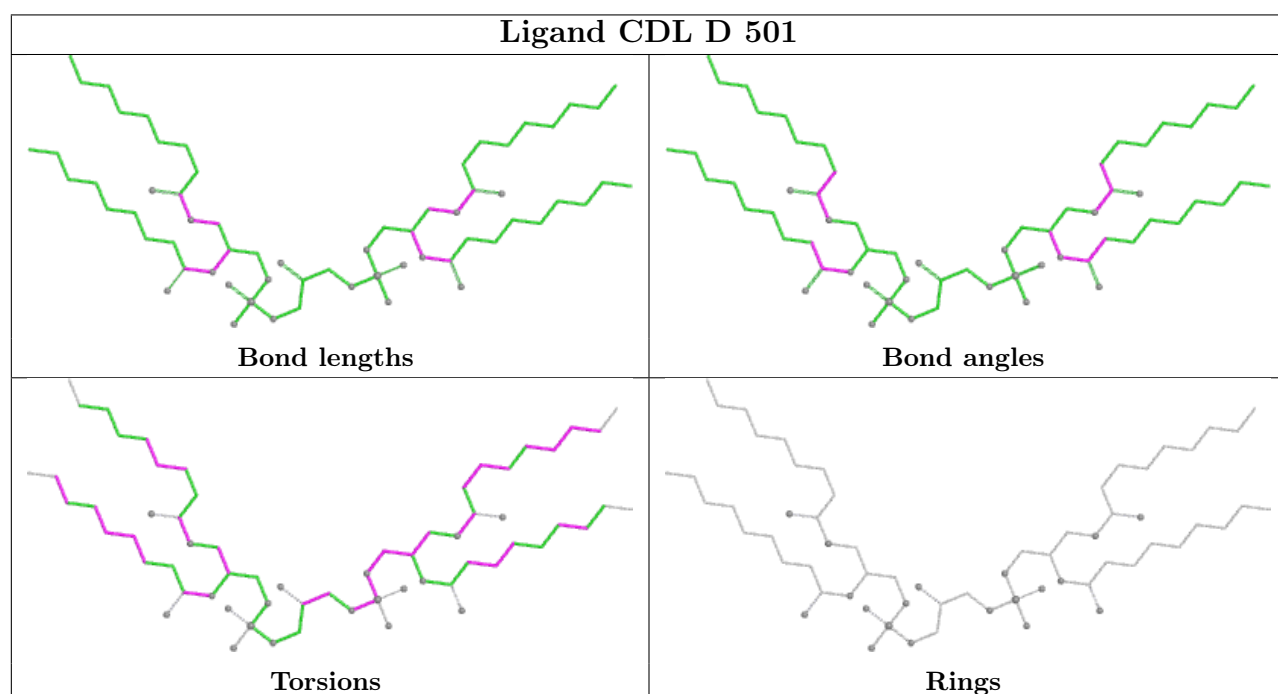
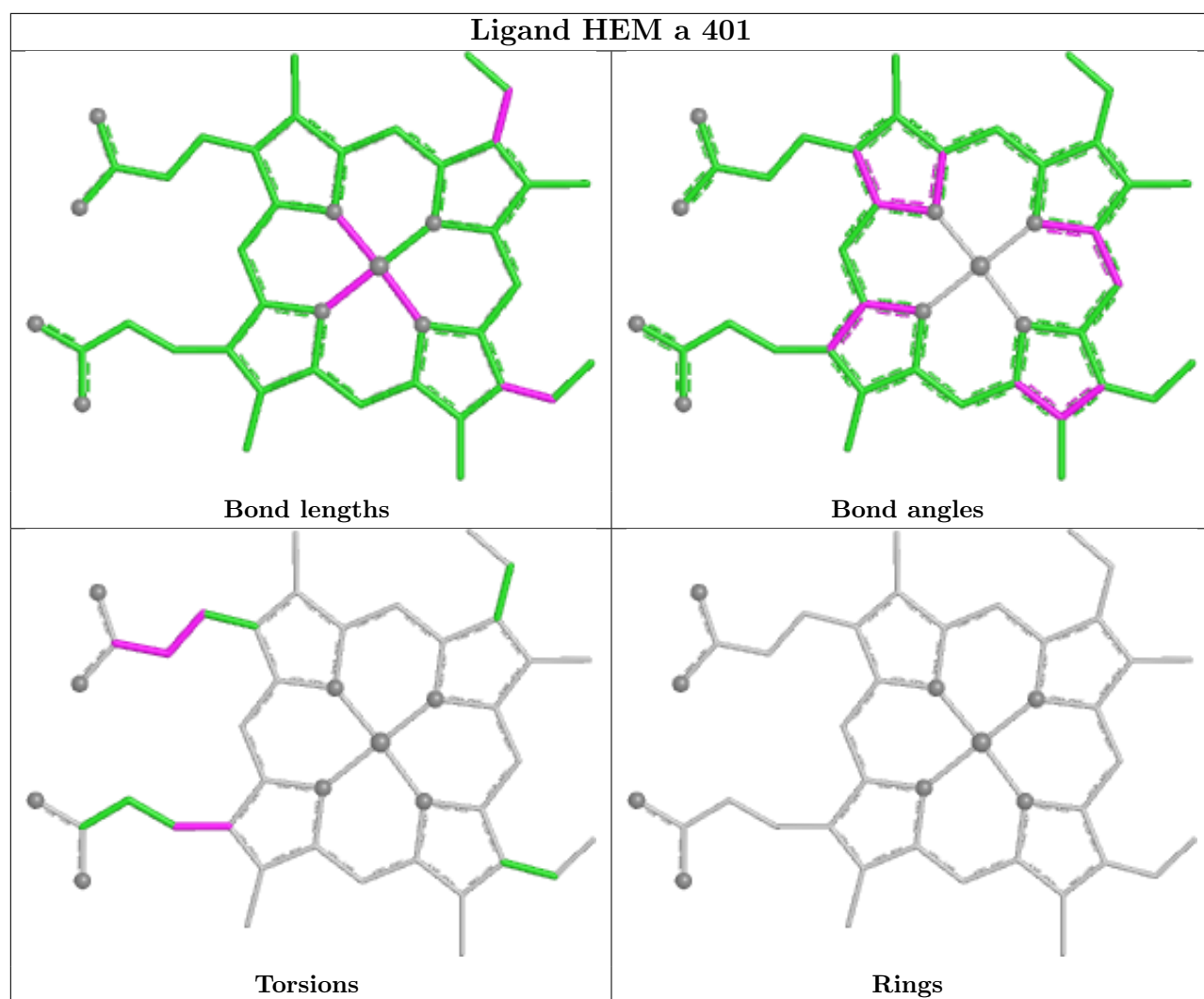
Bond angles

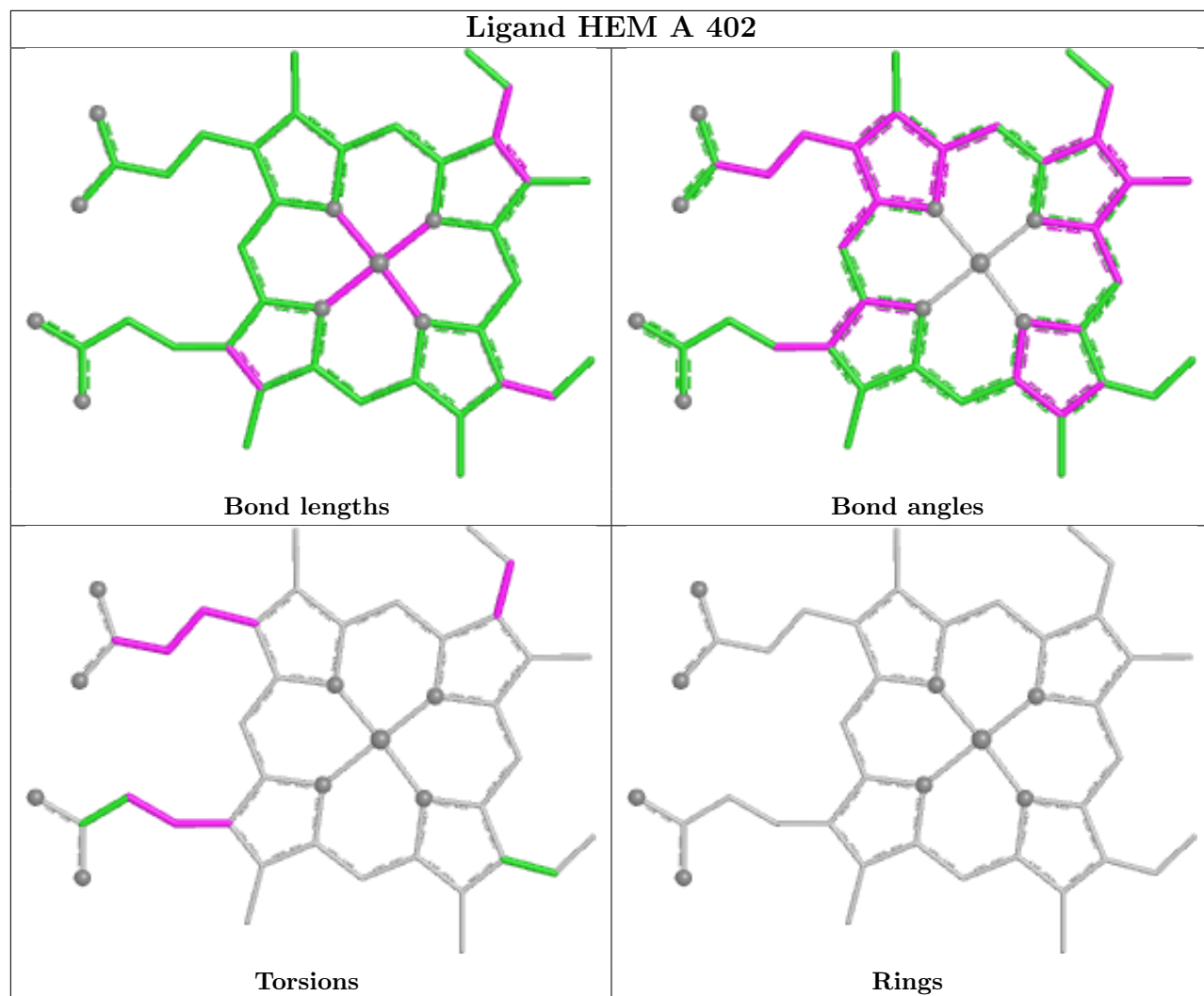


Torsions

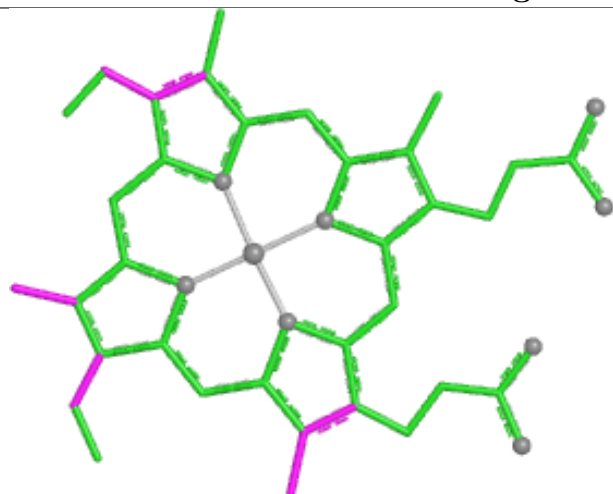


Rings

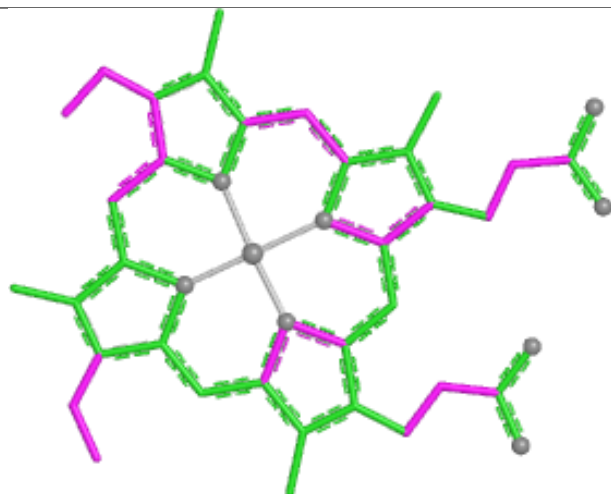




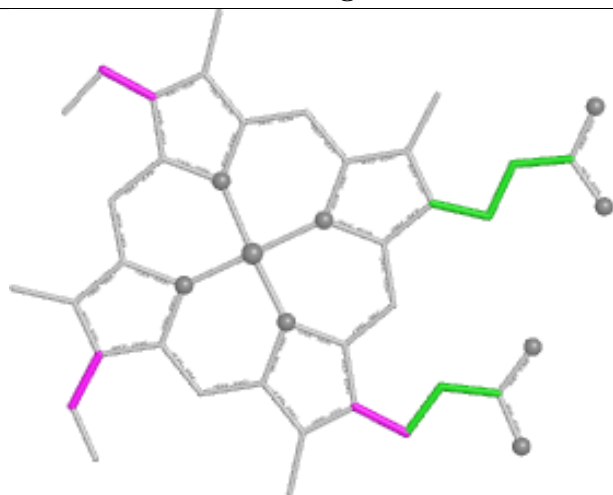
Ligand HEC B 401



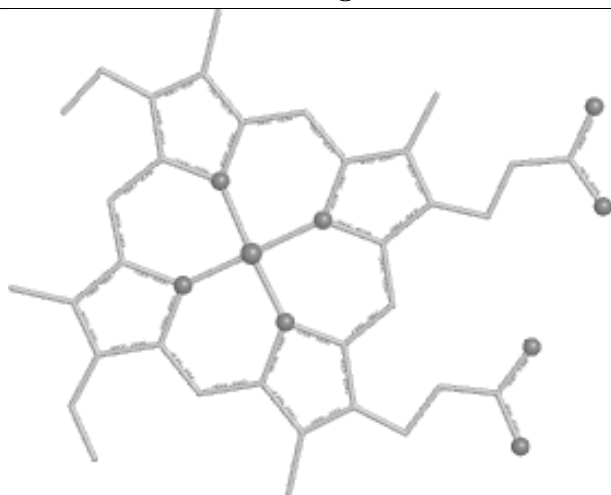
Bond lengths



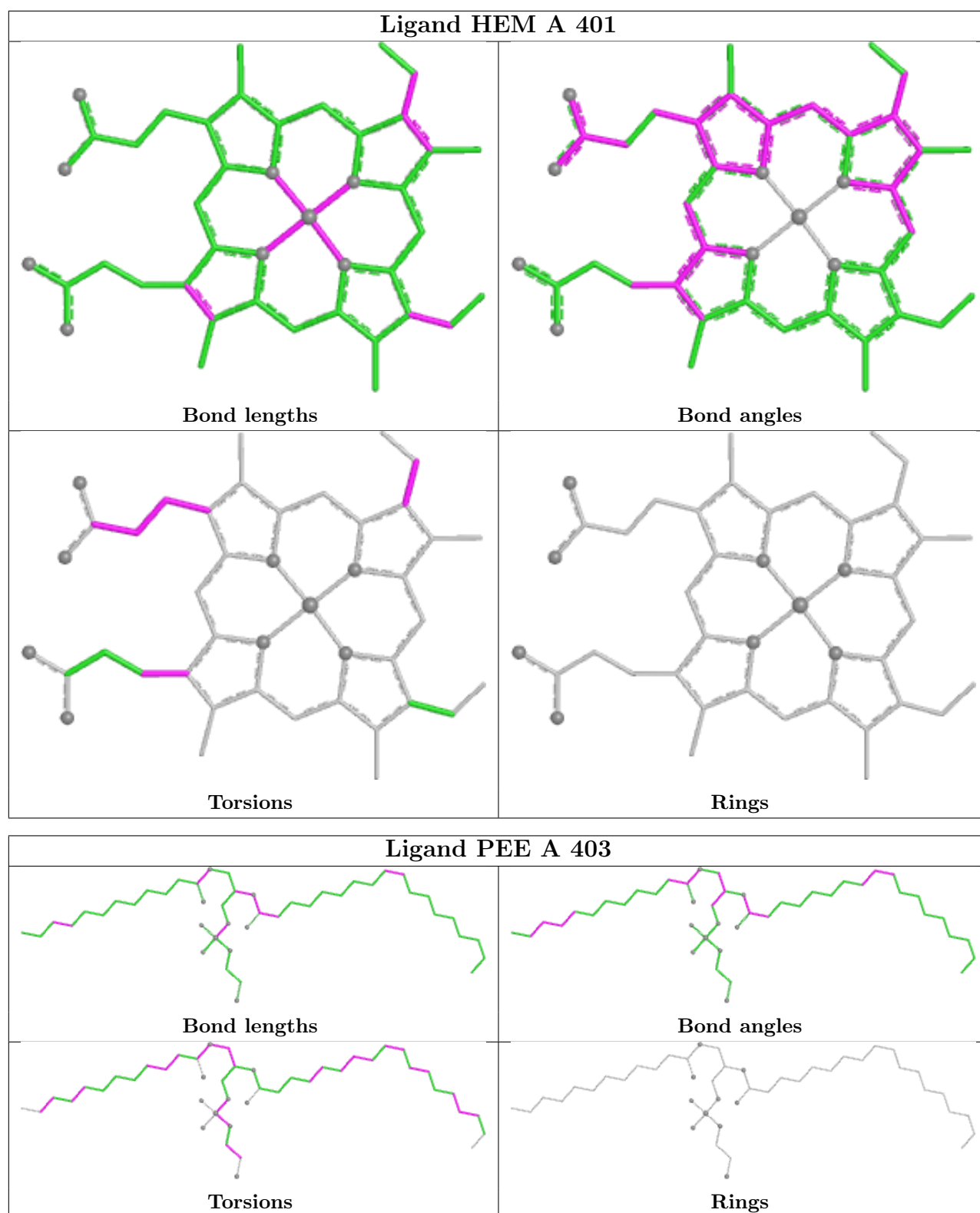
Bond angles



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.

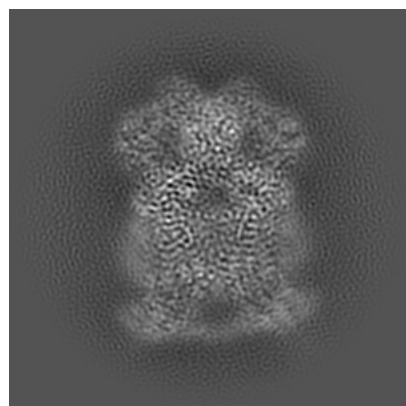
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35618. These allow visual inspection of the internal detail of the map and identification of artifacts.

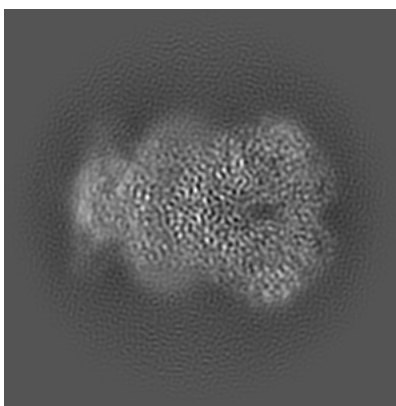
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

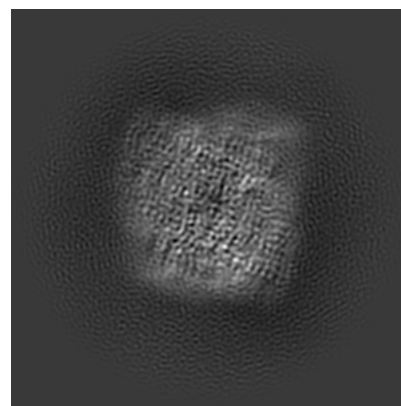
6.1.1 Primary map



X

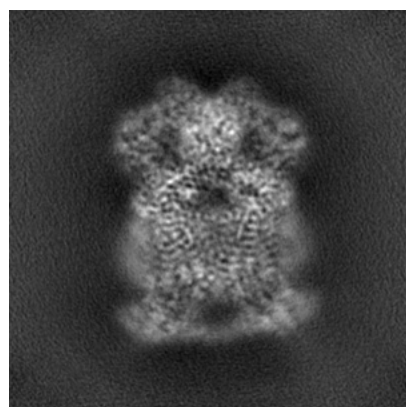


Y

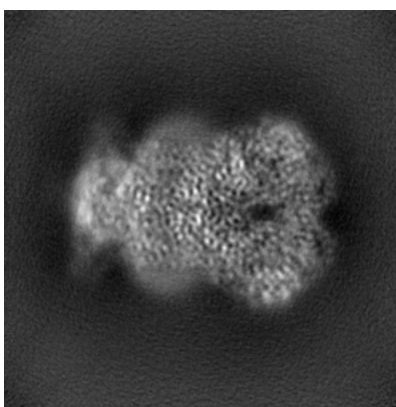


Z

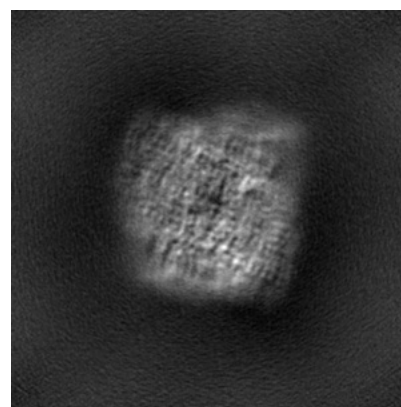
6.1.2 Raw map



X



Y

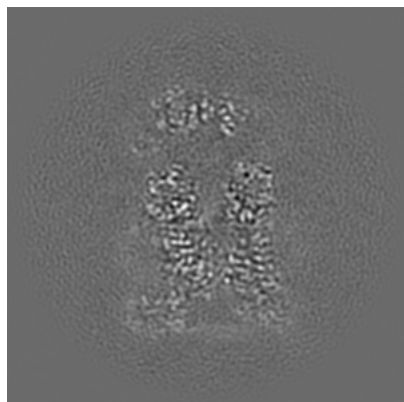


Z

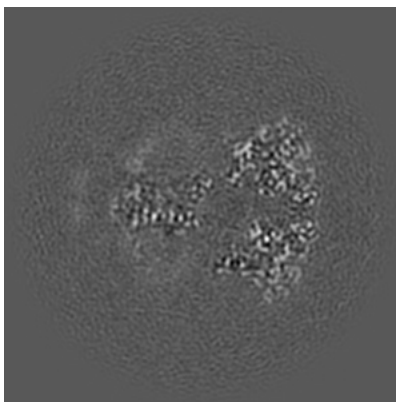
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

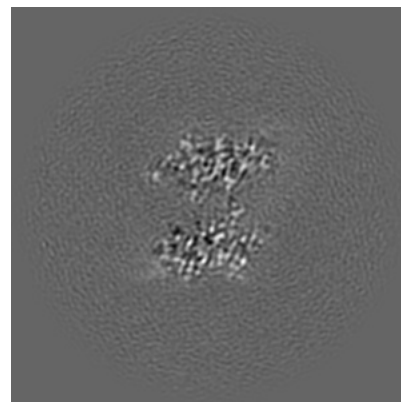
6.2.1 Primary map



X Index: 140

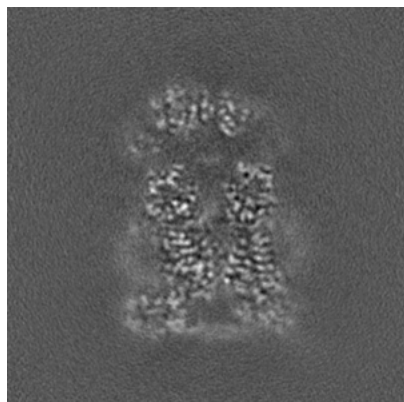


Y Index: 140

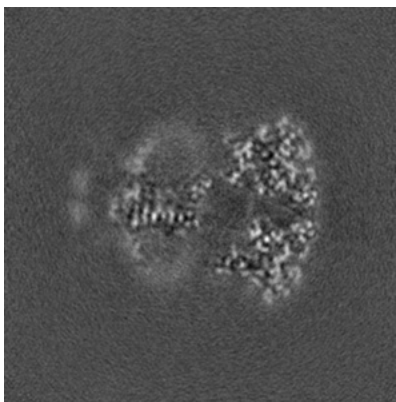


Z Index: 140

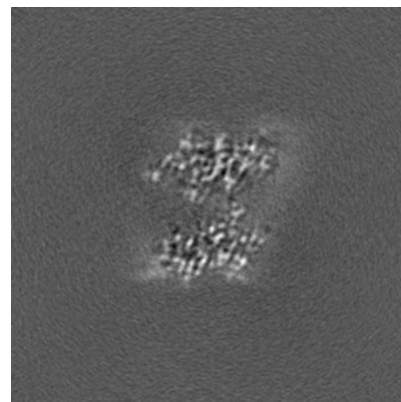
6.2.2 Raw map



X Index: 140



Y Index: 140

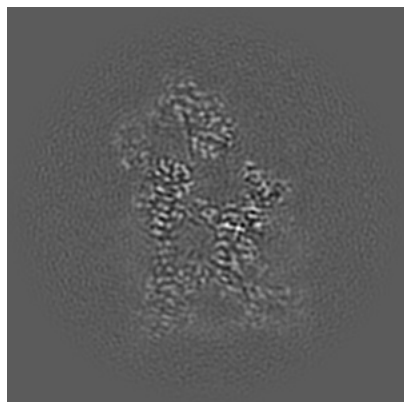


Z Index: 140

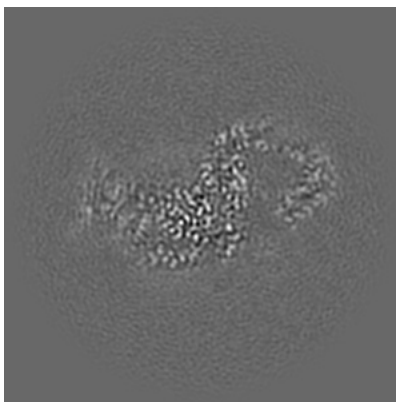
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

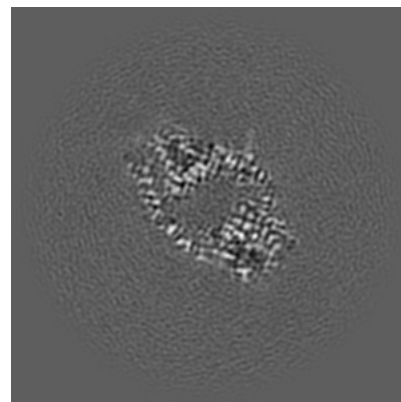
6.3.1 Primary map



X Index: 153

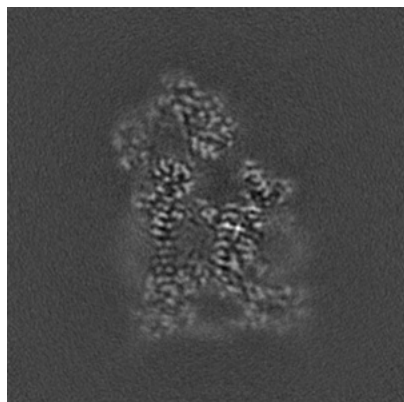


Y Index: 117

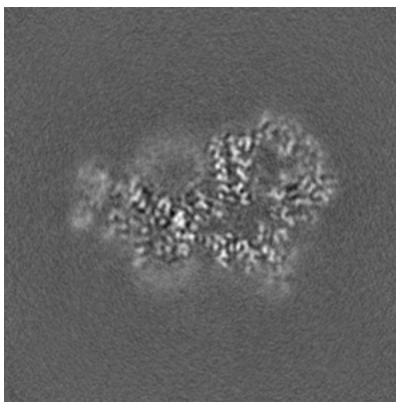


Z Index: 164

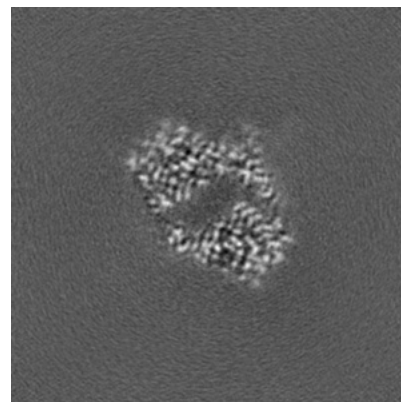
6.3.2 Raw map



X Index: 153



Y Index: 125

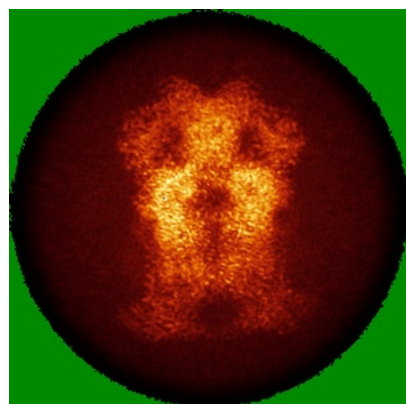


Z Index: 160

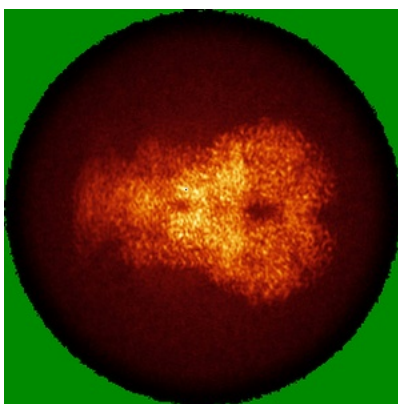
The images above show the largest variance slices of the map in three orthogonal directions.

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

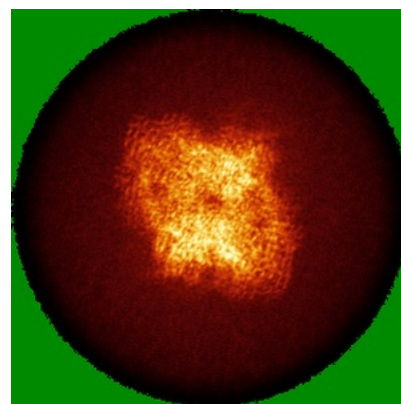
6.4.1 Primary map



X

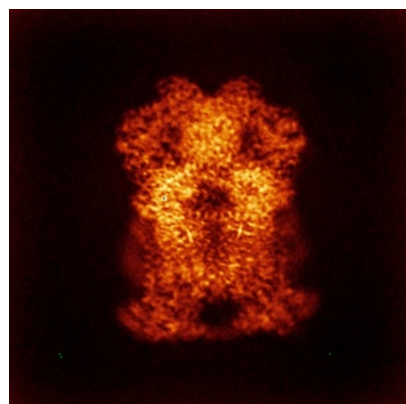


Y

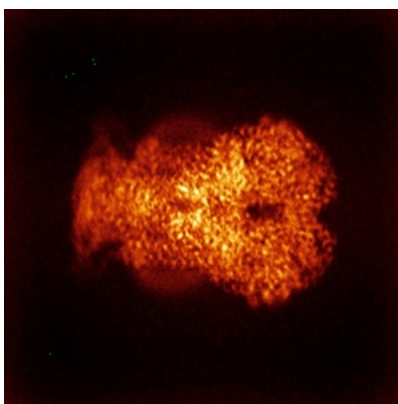


Z

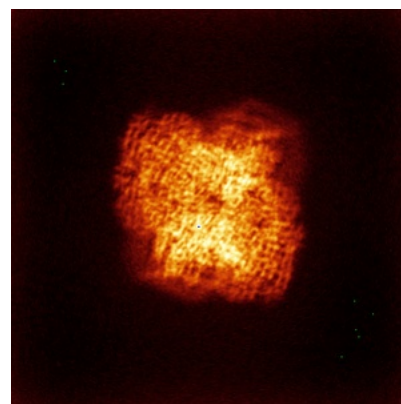
6.4.2 Raw map



X



Y

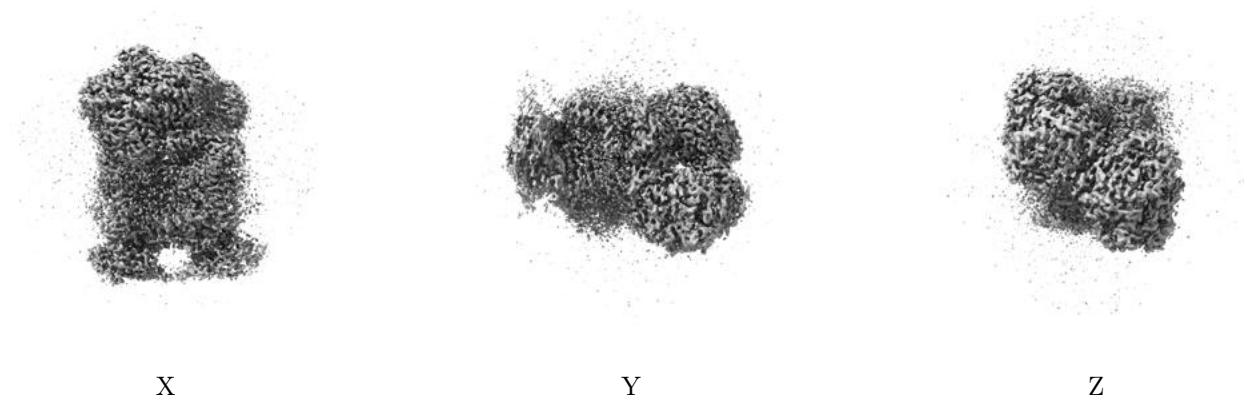


Z

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

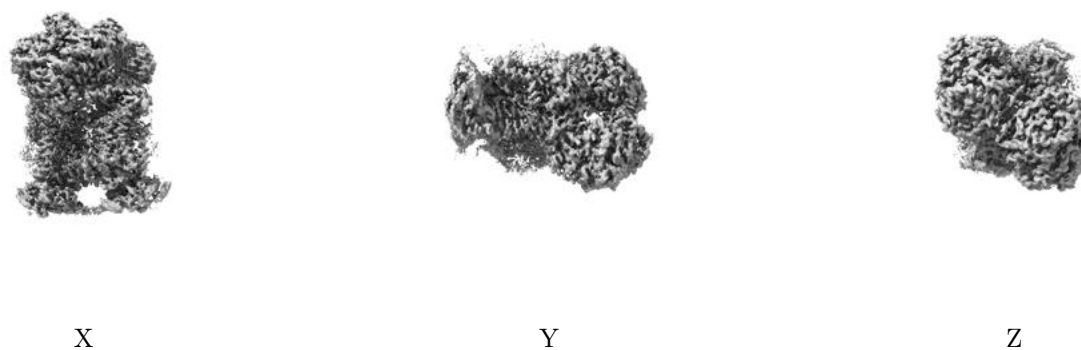
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

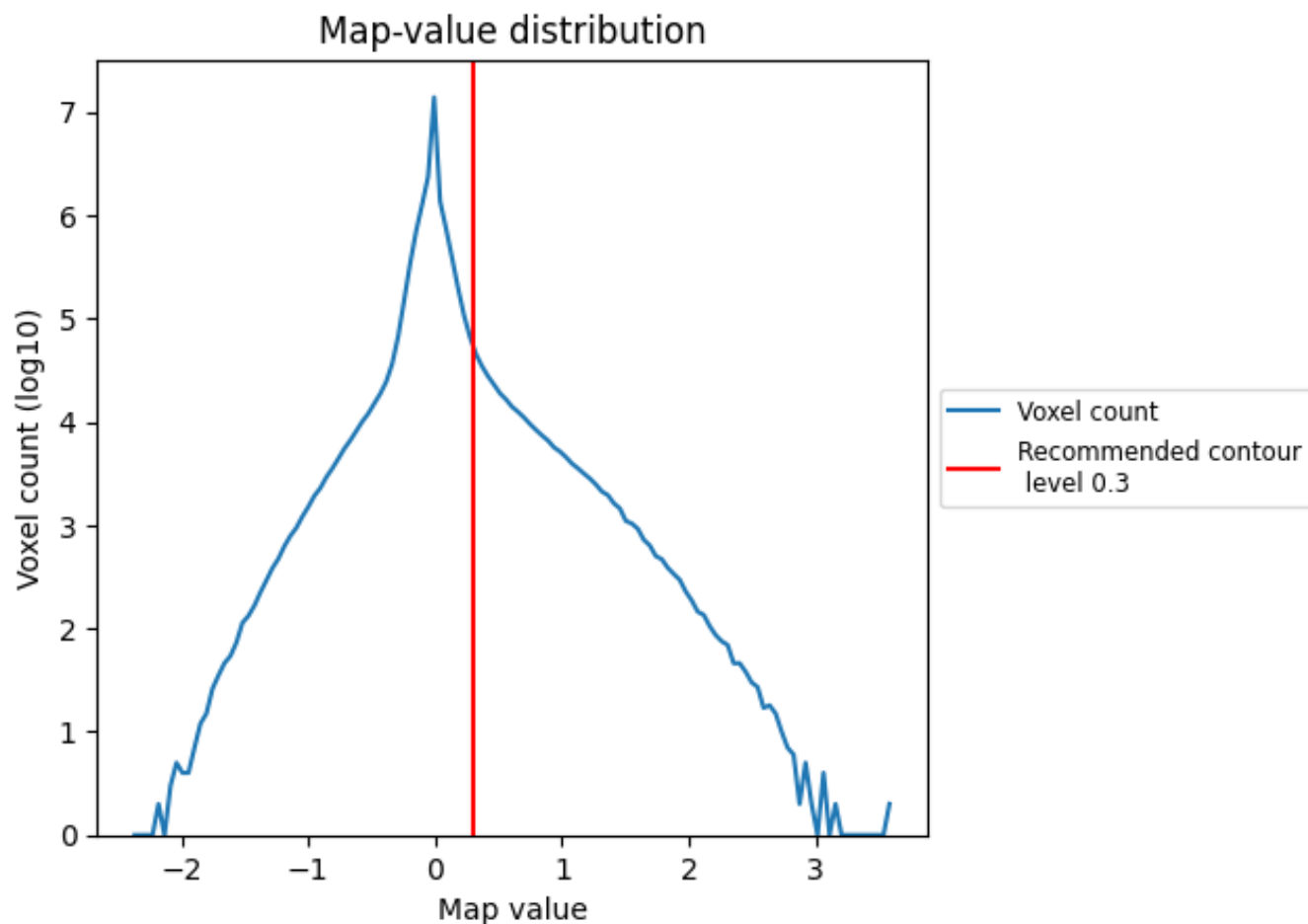
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

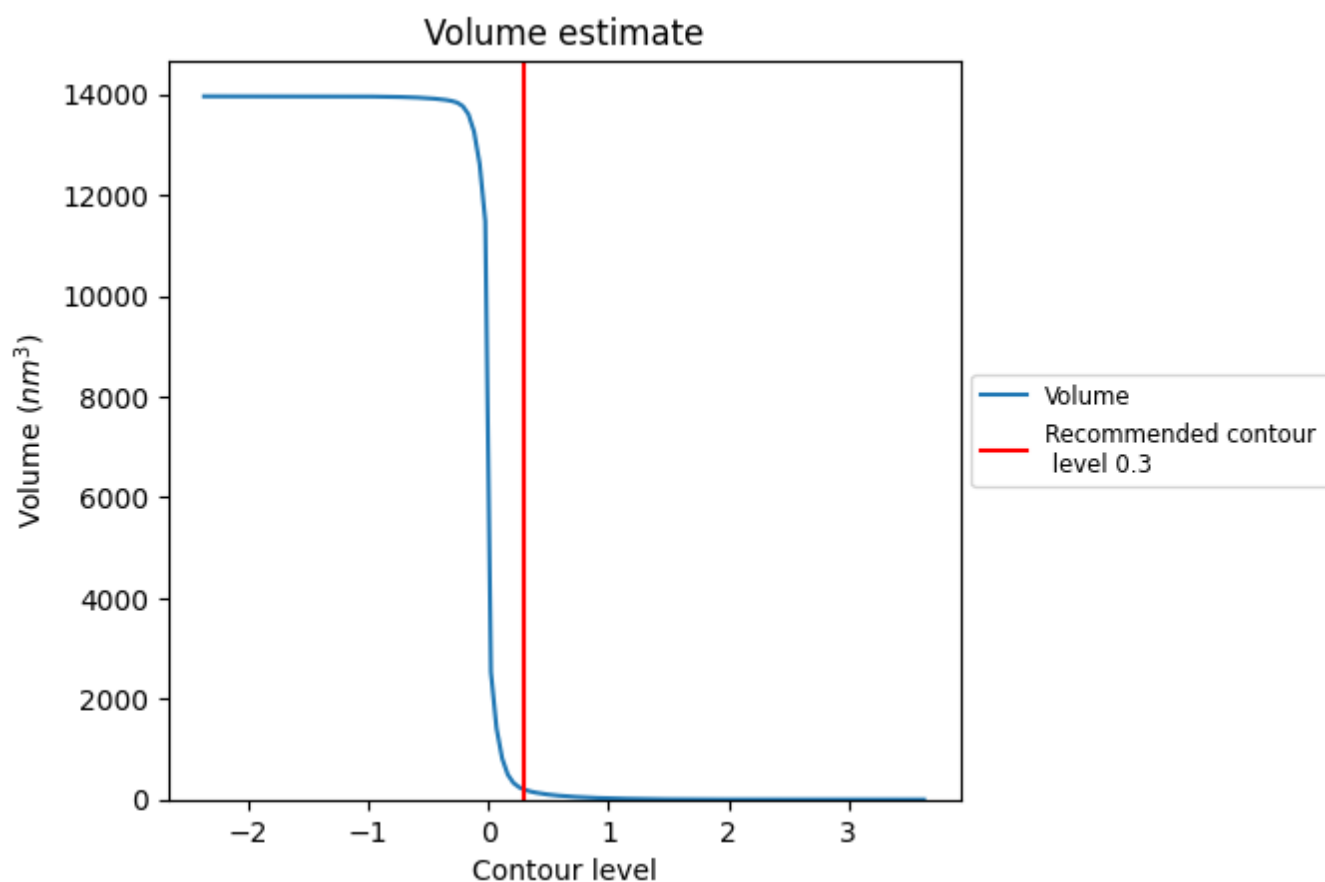
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

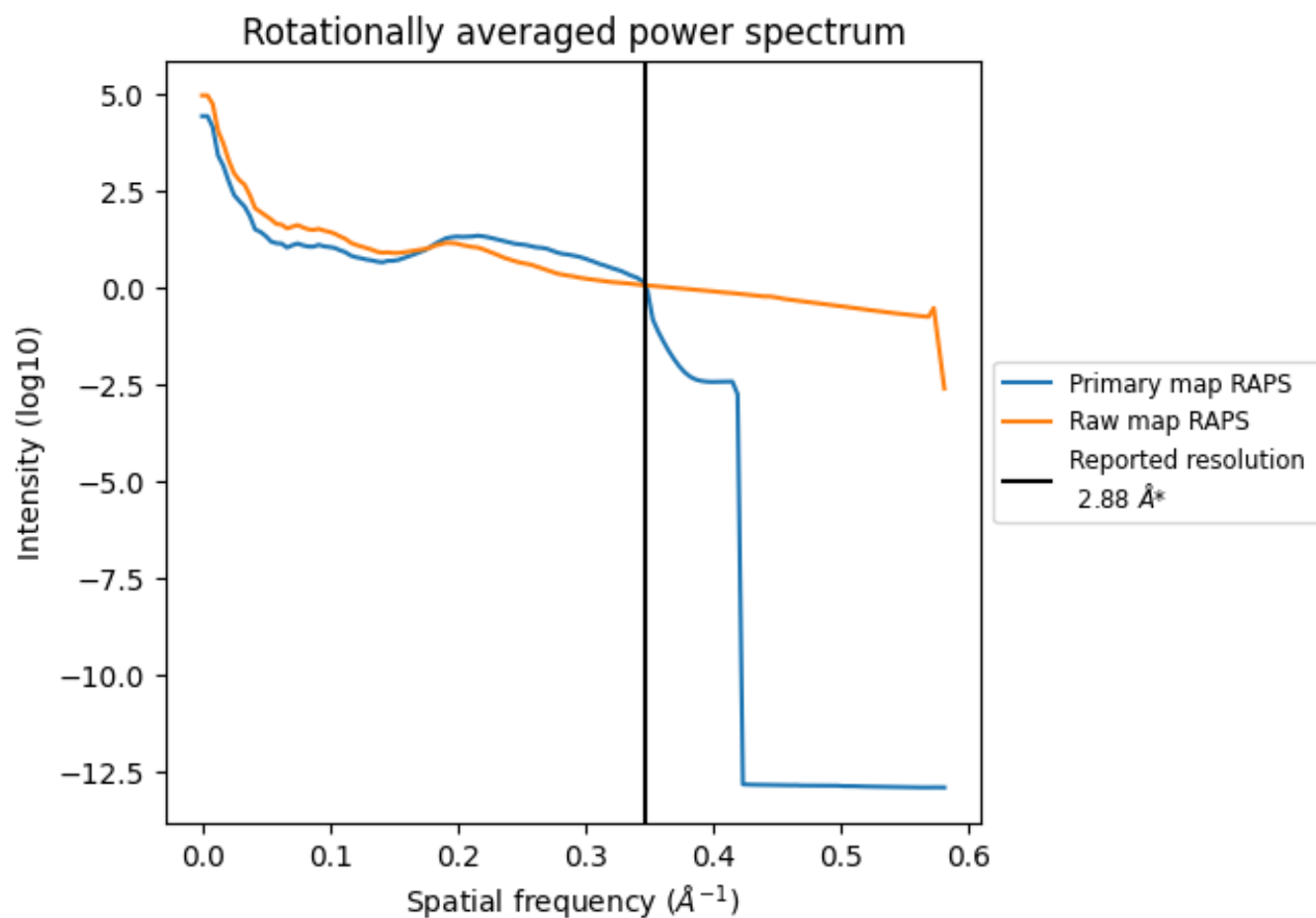
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm^3 ; this corresponds to an approximate mass of 177 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 ⓘ

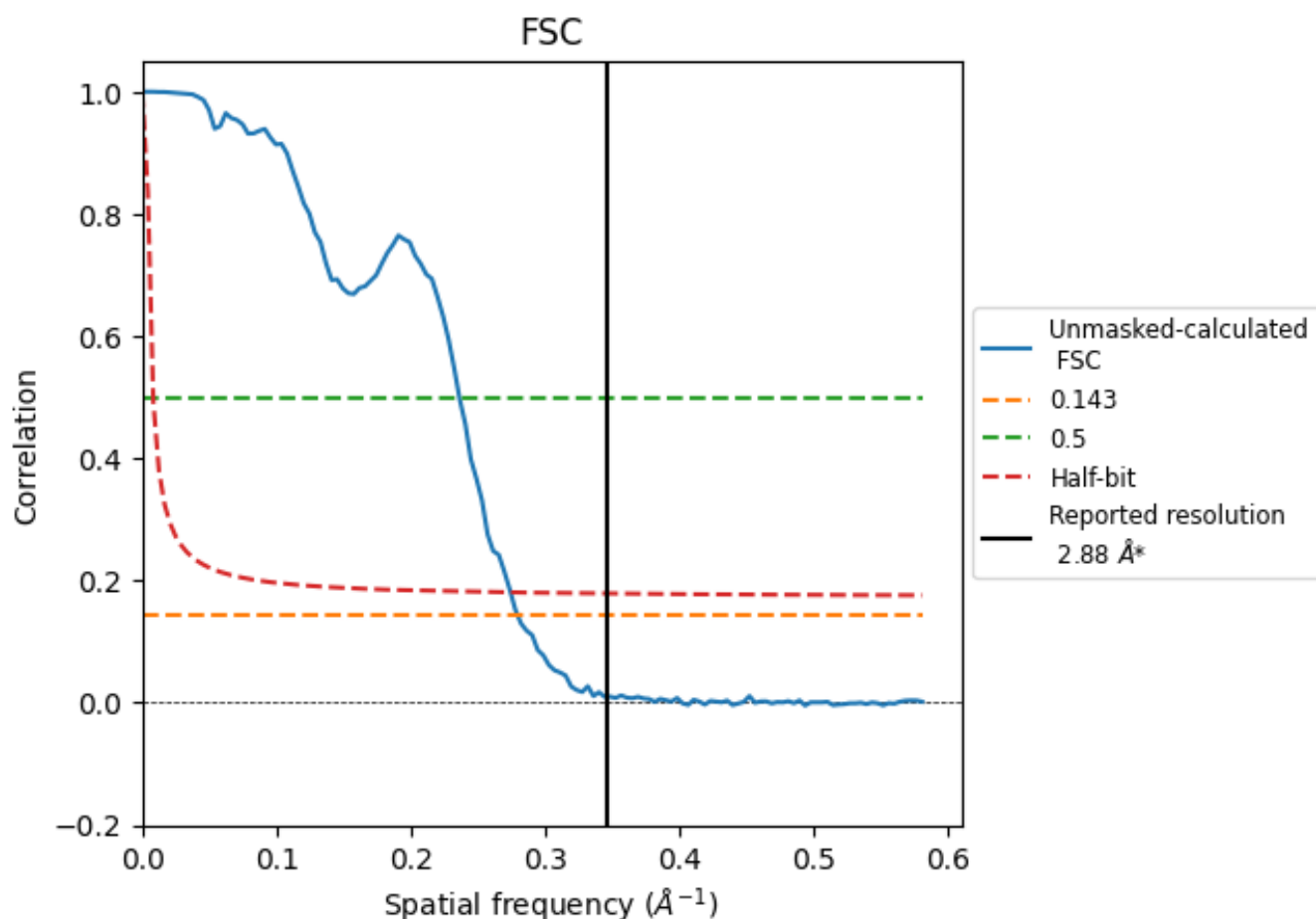


*Reported resolution corresponds to spatial frequency of 0.347 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

8.2 Resolution estimates [i](#)

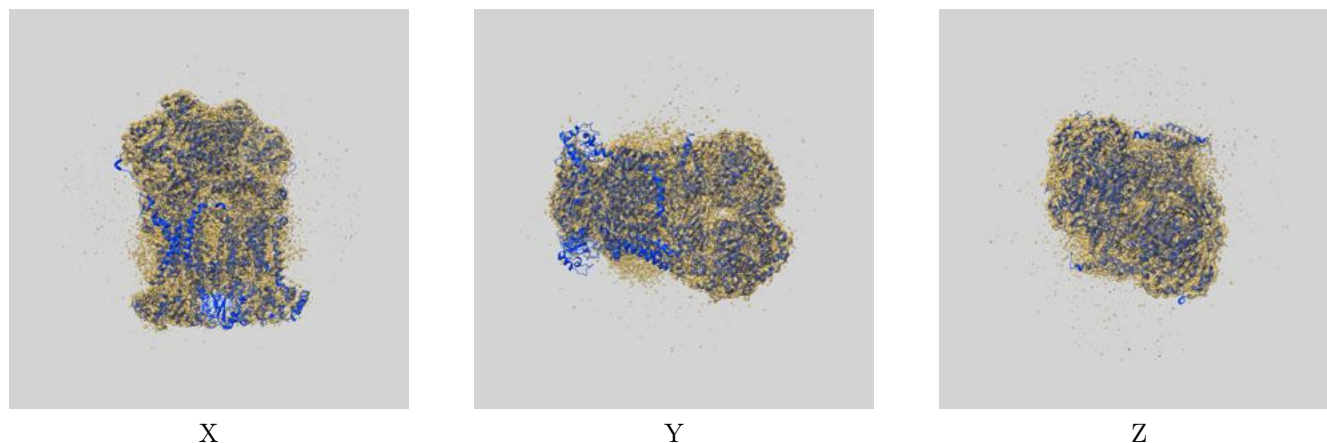
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.23	3.64

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

9 Map-model fit [i](#)

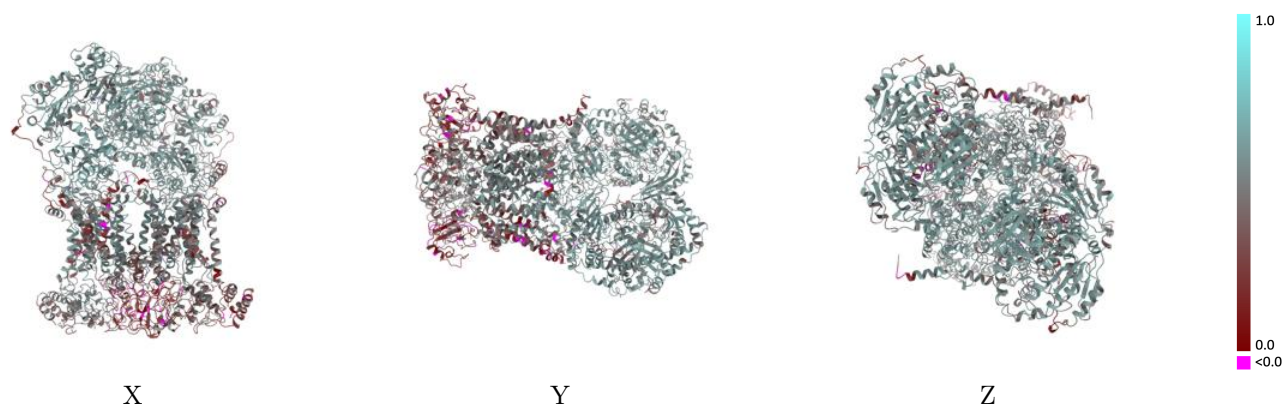
This section contains information regarding the fit between EMDB map EMD-35618 and PDB model 8IOG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 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](#)

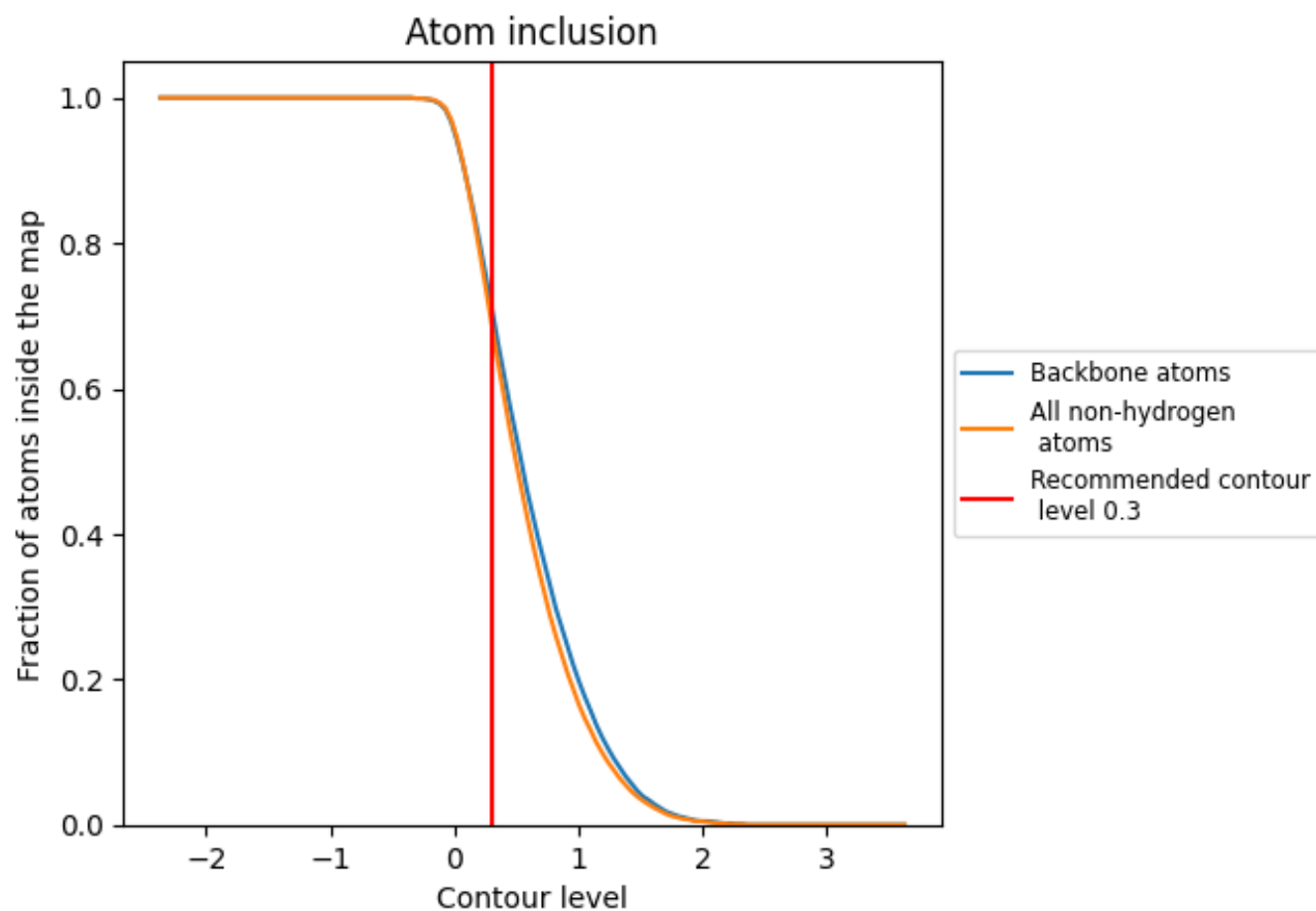


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 69% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.4770
A	 0.8720	 0.5310
B	 0.6660	 0.4620
C	 0.1280	 0.2640
D	 0.8340	 0.5480
E	 0.8810	 0.5630
F	 0.4340	 0.3910
G	 0.8770	 0.5590
H	 0.7710	 0.5100
I	 0.3130	 0.3820
J	 0.0360	 0.2290
K	 0.4540	 0.3630
a	 0.8170	 0.5000
b	 0.6050	 0.4310
c	 0.0930	 0.2300
d	 0.8480	 0.5490
e	 0.8870	 0.5660
f	 0.2460	 0.3040
g	 0.8050	 0.5230
h	 0.4910	 0.4020
i	 0.2080	 0.3260
j	 0.0250	 0.1960
k	 0.4090	 0.3600

