



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 12:02 PM EST

PDB ID : 6XKZ  
EMDB ID : EMD-22230  
Title : R. capsulatus CIII2CIV tripartite super-complex, conformation B (SC-1B)  
Authors : Steimle, S.; Van Eeuwen, T.; Ozturk, Y.; Kim, H.J.; Braitbard, M.; Selamoglu, N.; Garcia, B.A.; Schneidman-Duhovny, D.; Murakami, K.; Daldal, F.  
Deposited on : 2020-06-27  
Resolution : 7.20 Å(reported)  
Based on initial model : 6XI0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

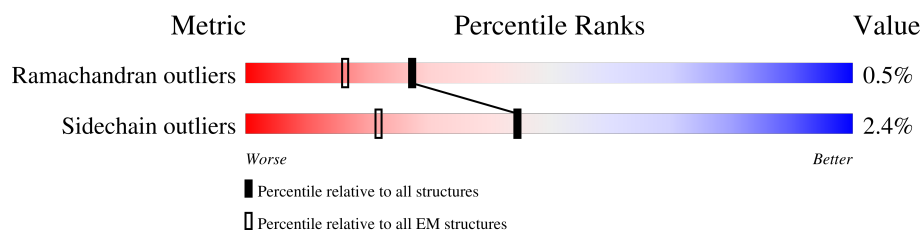
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 7.20 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  $\geq 3$ , 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	E	191	<div> <div>67%</div> <div>94%</div> <div>5%</div> </div>
1	R	191	<div> <div>79%</div> <div>93%</div> <div>5%</div> </div>
2	C	437	<div> <div>27%</div> <div>96%</div> <div>.</div> </div>
2	P	437	<div> <div>17%</div> <div>97%</div> <div>.</div> </div>
3	D	279	<div> <div>32%</div> <div>84%</div> <div>16%</div> </div>
3	Q	279	<div> <div>14%</div> <div>84%</div> <div>16%</div> </div>
4	n	532	<div> <div>22%</div> <div>82%</div> <div>6%</div> <div>11%</div> </div>
5	o	242	<div> <div>17%</div> <div>74%</div> <div>.</div> <div>21%</div> </div>
6	p	474	<div> <div>19%</div> <div>49%</div> <div>5%</div> <div>46%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20406 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 Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	181	Total	C	N	O	S	0	0
			1365	855	246	256	8		
1	R	181	Total	C	N	O	S	0	0
			1365	855	246	256	8		

- Molecule 2 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	423	Total	C	N	O	S	0	0
			3244	2186	519	525	14		
2	P	423	Total	C	N	O	S	0	0
			3244	2186	519	525	14		

- Molecule 3 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	235	Total	C	N	O	S	0	0
			1801	1148	301	337	15		
3	Q	235	Total	C	N	O	S	0	0
			1794	1144	300	335	15		

- Molecule 4 is a protein called Cytochrome c oxidase, Cbb3-type, subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	471	Total	C	N	O	S	0	0
			3711	2481	598	609	23		

- Molecule 5 is a protein called Cytochrome c oxidase, Cbb3-type, subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	o	190	Total	C	N	O	S	0	0
			1498	960	244	284	10		

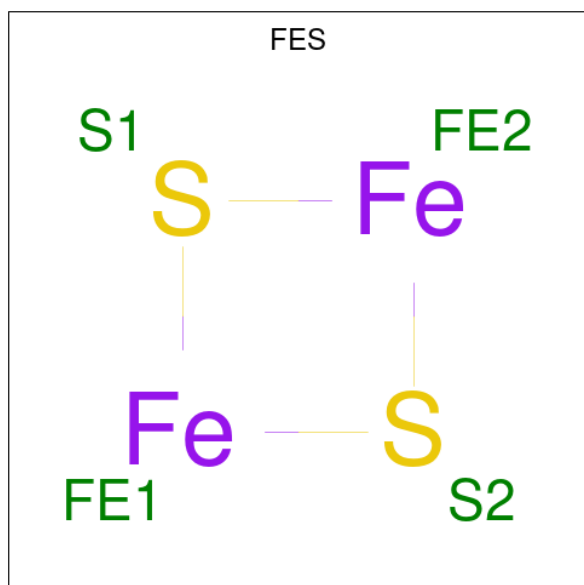
- Molecule 6 is a protein called Cbb3-type cytochrome c oxidase subunit CcoP,Cytochrome c-type cyt cy.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	p	254	Total	C	N	O	S	0	0
			1902	1203	322	367	10		

There are 8 discrepancies between the modelled and reference sequences:

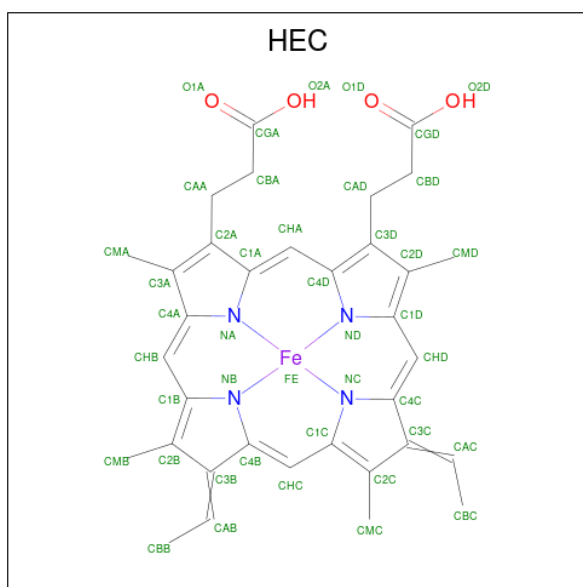
Chain	Residue	Modelled	Actual	Comment	Reference
p	467	ASP	-	expression tag	UNP Q05389
p	468	TYR	-	expression tag	UNP Q05389
p	469	LYS	-	expression tag	UNP Q05389
p	470	ASP	-	expression tag	UNP Q05389
p	471	ASP	-	expression tag	UNP Q05389
p	472	ASP	-	expression tag	UNP Q05389
p	473	ASP	-	expression tag	UNP Q05389
p	474	LYS	-	expression tag	UNP Q05389

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
7	E	1	Total	Fe	S	0
			4	2	2	
7	R	1	Total	Fe	S	0
			4	2	2	

- Molecule 8 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	n	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	n	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	o	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	p	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	p	1	Total 43	C 34	Fe 1	N 4	O 4	0

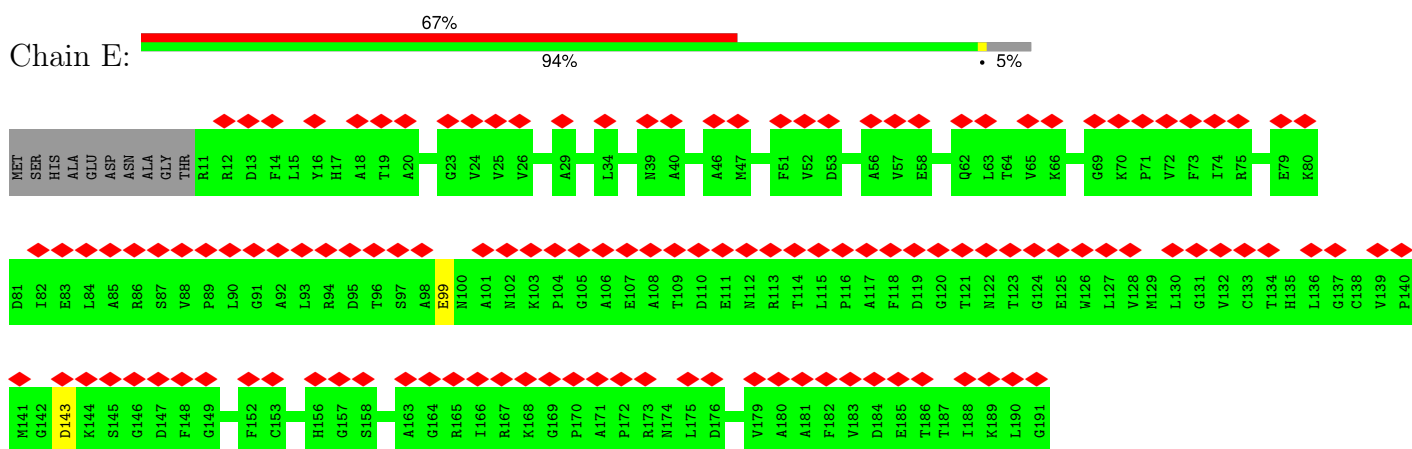
- Molecule 9 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
9	n	1	Total	Cu	0
			1	1	

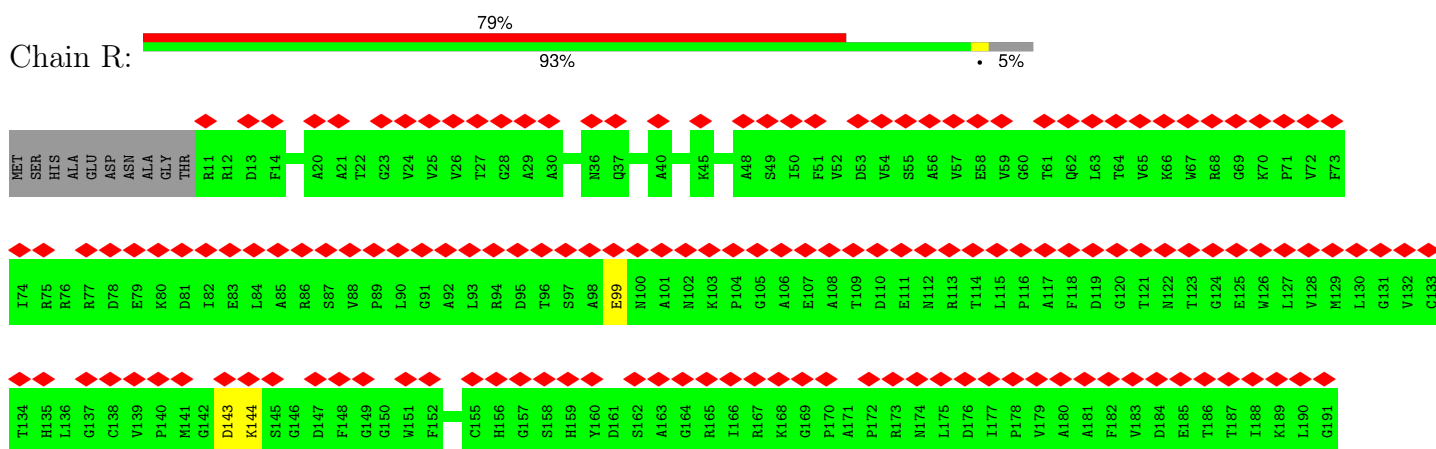
### 3 Residue-property plots

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.

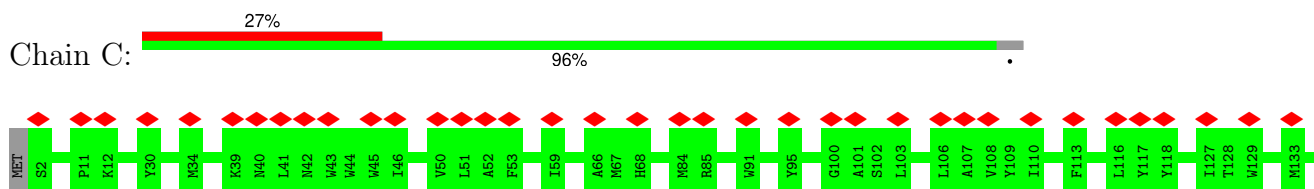
- Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

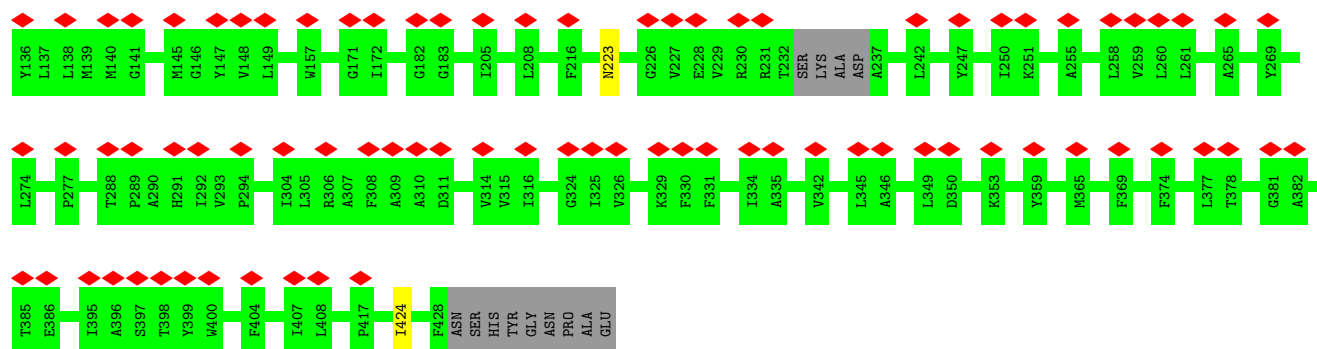


- Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

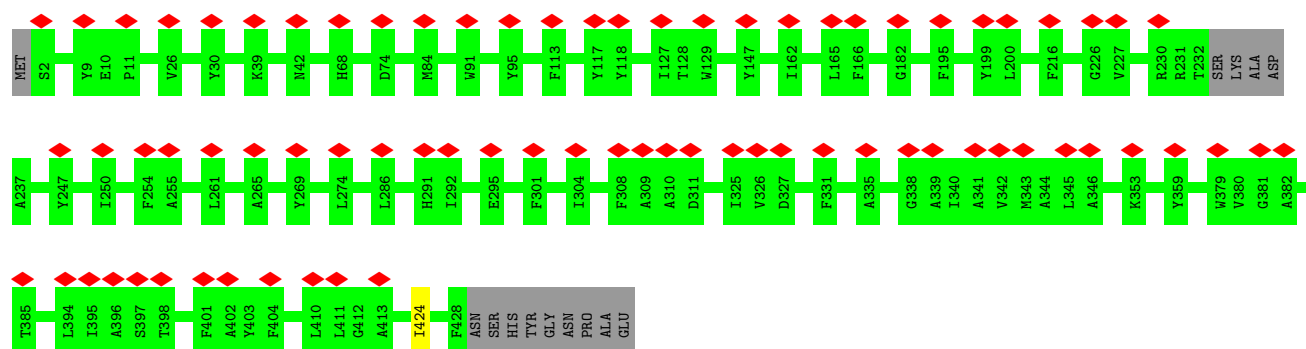


- Molecule 2: Cytochrome b

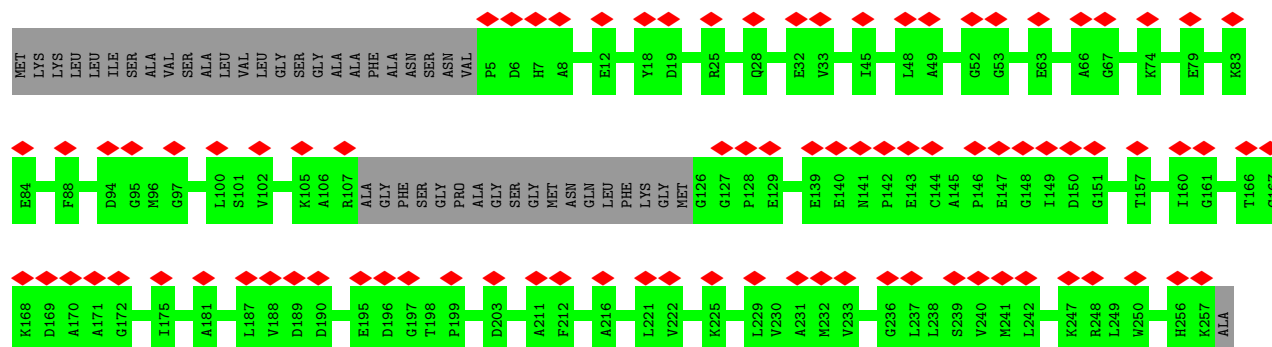
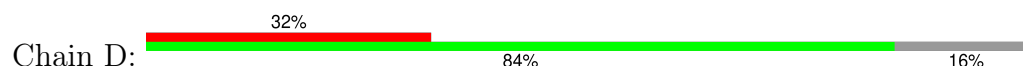




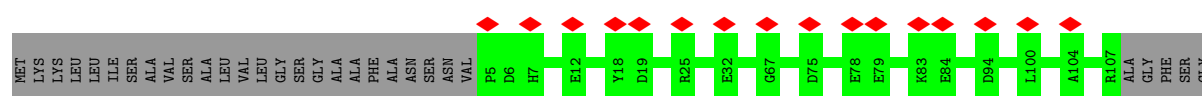
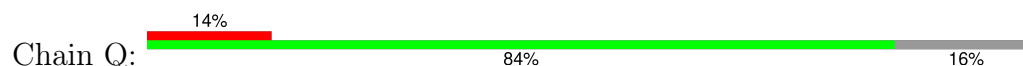
• Molecule 2: Cytochrome b

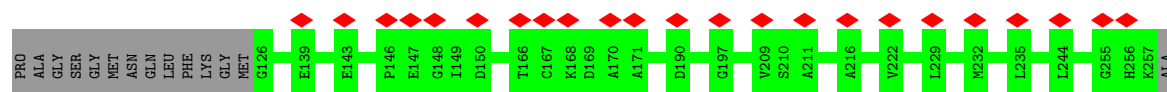


• Molecule 3: Cytochrome c1

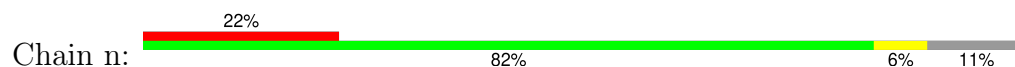


• Molecule 3: Cytochrome c1

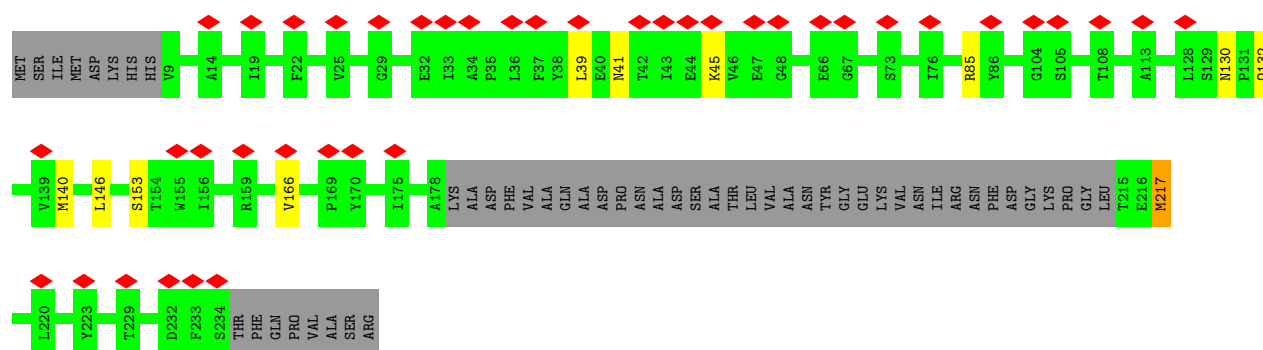




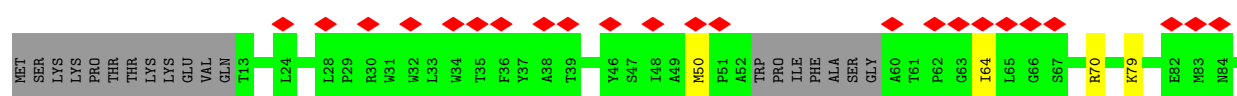
• Molecule 4: Cytochrome c oxidase, Cbb3-type, subunit I



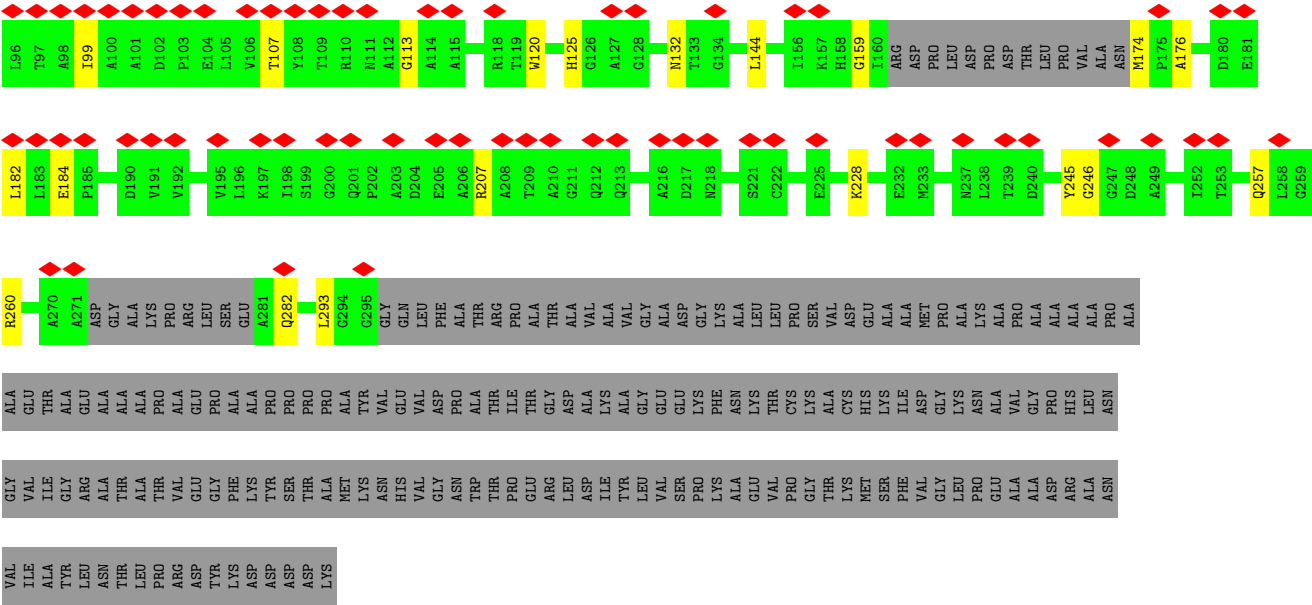
• Molecule 5: Cytochrome c oxidase, Cbb3-type, subunit II



• Molecule 6: Cbb3-type cytochrome c oxidase subunit CcoP, Cytochrome c-type cyt cy







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87026	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size ( $\text{\AA}$ )	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CU, 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	E	0.31	0/1395	0.56	1/1895 (0.1%)
1	R	0.31	0/1395	0.56	1/1895 (0.1%)
2	C	0.40	0/3363	0.48	0/4617
2	P	0.40	0/3363	0.48	0/4617
3	D	0.34	0/1846	0.49	0/2500
3	Q	0.33	0/1839	0.49	0/2492
4	n	0.89	0/3836	1.15	8/5232 (0.2%)
5	o	0.92	0/1535	1.10	3/2092 (0.1%)
6	p	0.87	0/1948	1.21	8/2660 (0.3%)
All	All	0.61	0/20520	0.80	21/28000 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	p	107	THR	N-CA-CB	7.23	124.03	110.30
6	p	125	HIS	O-C-N	-6.05	112.92	123.20
5	o	153	SER	N-CA-CB	5.97	119.45	110.50
4	n	286	GLN	CB-CA-C	-5.94	98.51	110.40
6	p	257	GLN	CB-CA-C	-5.79	98.82	110.40
4	n	293	SER	CB-CA-C	-5.74	99.20	110.10
6	p	174	MET	CG-SD-CE	-5.72	91.04	100.20
6	p	159	GLY	C-N-CA	5.66	135.85	121.70
4	n	292	TYR	CB-CG-CD2	5.58	124.34	121.00
6	p	113	GLY	N-CA-C	-5.58	99.16	113.10
6	p	120	TRP	O-C-N	-5.54	113.84	122.70
4	n	244	THR	C-N-CA	-5.38	108.24	121.70
1	E	143	ASP	CB-CG-OD2	5.32	123.08	118.30
4	n	104	MET	CG-SD-CE	-5.27	91.77	100.20
1	R	143	ASP	CB-CG-OD2	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	p	70	ARG	C-N-CA	5.20	134.69	121.70
5	o	140	MET	CG-SD-CE	-5.13	92.00	100.20
4	n	429	ARG	CB-CA-C	-5.08	100.23	110.40
5	o	217	MET	CG-SD-CE	-5.08	92.07	100.20
4	n	520	PRO	N-CA-C	-5.08	98.90	112.10
4	n	293	SER	N-CA-CB	5.03	118.05	110.50

There are no chirality outliers.

There are no planarity outliers.

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

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

## 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	E	179/191 (94%)	141 (79%)	37 (21%)	1 (1%)	22	60
1	R	179/191 (94%)	141 (79%)	36 (20%)	2 (1%)	12	47
2	C	419/437 (96%)	352 (84%)	65 (16%)	2 (0%)	25	64
2	P	419/437 (96%)	352 (84%)	66 (16%)	1 (0%)	44	78
3	D	231/279 (83%)	198 (86%)	33 (14%)	0	100	100
3	Q	231/279 (83%)	197 (85%)	34 (15%)	0	100	100
4	n	469/532 (88%)	458 (98%)	9 (2%)	2 (0%)	30	68
5	o	186/242 (77%)	177 (95%)	9 (5%)	0	100	100
6	p	246/474 (52%)	225 (92%)	16 (6%)	5 (2%)	6	32
All	All	2559/3062 (84%)	2241 (88%)	305 (12%)	13 (0%)	27	64

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	n	289	ARG
6	p	176	ALA
1	E	99	GLU
1	R	99	GLU
6	p	182	LEU
6	p	184	GLU
6	p	246	GLY
4	n	291	VAL
6	p	50	MET
1	R	144	LYS
2	C	223	ASN
2	C	424	ILE
2	P	424	ILE

### 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	E	142/149 (95%)	142 (100%)	0	100	100
1	R	142/149 (95%)	142 (100%)	0	100	100
2	C	300/360 (83%)	300 (100%)	0	100	100
2	P	300/360 (83%)	300 (100%)	0	100	100
3	D	184/220 (84%)	184 (100%)	0	100	100
3	Q	182/220 (83%)	182 (100%)	0	100	100
4	n	376/421 (89%)	349 (93%)	27 (7%)	12	32
5	o	163/205 (80%)	154 (94%)	9 (6%)	18	39
6	p	192/357 (54%)	181 (94%)	11 (6%)	17	38
All	All	1981/2441 (81%)	1934 (98%)	47 (2%)	45	62

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	n	58	LYS
4	n	82	LEU

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Mol	Chain	Res	Type
4	n	106	ASN
4	n	109	ARG
4	n	125	ASN
4	n	161	ILE
4	n	182	ASN
4	n	197	LEU
4	n	222	PHE
4	n	228	MET
4	n	245	LYS
4	n	257	MET
4	n	272	THR
4	n	291	VAL
4	n	298	ILE
4	n	300	HIS
4	n	305	ILE
4	n	308	TYR
4	n	338	MET
4	n	358	LEU
4	n	371	ILE
4	n	387	LYS
4	n	400	ILE
4	n	414	ILE
4	n	447	ILE
4	n	487	LYS
4	n	511	ASN
5	o	39	LEU
5	o	41	ASN
5	o	45	LYS
5	o	85	ARG
5	o	130	ASN
5	o	132	GLN
5	o	146	LEU
5	o	166	VAL
5	o	217	MET
6	p	64	ILE
6	p	79	LYS
6	p	99	ILE
6	p	132	ASN
6	p	144	LEU
6	p	207	ARG
6	p	228	LYS
6	p	245	TYR

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Mol	Chain	Res	Type
6	p	260	ARG
6	p	282	GLN
6	p	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	17	HIS
1	E	122	ASN
2	C	68	HIS
2	C	222	ASN
3	D	31	ASN
3	D	177	HIS
2	P	68	HIS
2	P	222	ASN
3	Q	31	ASN
3	Q	177	HIS
1	R	17	HIS
1	R	122	ASN
4	n	106	ASN
4	n	230	HIS
4	n	233	ASN
4	n	248	GLN
4	n	300	HIS
5	o	41	ASN
5	o	124	HIS
5	o	130	ASN
5	o	148	ASN
5	o	225	GLN
6	p	16	HIS
6	p	84	ASN
6	p	155	ASN
6	p	212	GLN
6	p	237	ASN
6	p	282	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](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

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$
8	HEC	C	502	2	32,50,50	1.95	5 (15%)	30,82,82	1.63	6 (20%)
8	HEC	o	301	5	32,50,50	2.34	4 (12%)	30,82,82	2.77	6 (20%)
8	HEC	p	501	6	32,50,50	2.27	6 (18%)	30,82,82	2.51	7 (23%)
8	HEC	D	501	3	32,50,50	2.00	3 (9%)	30,82,82	2.12	5 (16%)
8	HEC	P	502	2	32,50,50	1.94	4 (12%)	30,82,82	1.63	6 (20%)
8	HEC	n	602	4	32,50,50	2.54	5 (15%)	30,82,82	1.47	4 (13%)
8	HEC	P	501	2	32,50,50	2.00	4 (12%)	30,82,82	1.71	9 (30%)
8	HEC	n	601	4	32,50,50	2.30	6 (18%)	30,82,82	1.73	6 (20%)
7	FES	R	501	1	0,4,4	-	-	-	-	-
8	HEC	Q	501	3	32,50,50	2.00	3 (9%)	30,82,82	2.12	5 (16%)
7	FES	E	501	1	0,4,4	-	-	-	-	-
8	HEC	p	502	6	32,50,50	2.14	3 (9%)	30,82,82	2.70	12 (40%)
8	HEC	C	501	2	32,50,50	2.00	4 (12%)	30,82,82	1.70	9 (30%)

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
8	HEC	C	502	2	-	5/10/54/54	-
8	HEC	o	301	5	-	4/10/54/54	-
8	HEC	p	501	6	-	2/10/54/54	-
8	HEC	D	501	3	-	2/10/54/54	-
8	HEC	P	502	2	-	5/10/54/54	-
8	HEC	n	602	4	-	2/10/54/54	-
8	HEC	P	501	2	-	4/10/54/54	-
8	HEC	n	601	4	-	4/10/54/54	-
7	FES	R	501	1	-	-	0/1/1/1
8	HEC	Q	501	3	-	2/10/54/54	-
7	FES	E	501	1	-	-	0/1/1/1
8	HEC	p	502	6	-	2/10/54/54	-
8	HEC	C	501	2	-	4/10/54/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	o	301	HEC	C3C-C2C	-8.21	1.31	1.40
8	n	602	HEC	C3C-C2C	-7.19	1.32	1.40
8	p	501	HEC	C2B-C3B	-7.11	1.32	1.40
8	p	502	HEC	C3C-C2C	-7.06	1.32	1.40
8	n	602	HEC	C2B-C3B	-6.84	1.33	1.40
8	o	301	HEC	C2B-C3B	-6.79	1.33	1.40
8	n	601	HEC	C3C-C2C	-6.33	1.33	1.40
8	p	502	HEC	C2B-C3B	-6.17	1.33	1.40
8	D	501	HEC	C2B-C3B	-5.81	1.34	1.40
8	Q	501	HEC	C2B-C3B	-5.76	1.34	1.40
8	p	501	HEC	C3C-C2C	-5.76	1.34	1.40
8	Q	501	HEC	C3D-C2D	5.33	1.53	1.37
8	C	501	HEC	C3C-C2C	-5.32	1.34	1.40
8	D	501	HEC	C3D-C2D	5.30	1.53	1.37
8	n	601	HEC	C2B-C3B	-5.30	1.34	1.40
8	n	601	HEC	C3D-C2D	5.28	1.53	1.37
8	P	501	HEC	C3C-C2C	-5.26	1.34	1.40
8	n	602	HEC	C3D-C2D	5.25	1.53	1.37
8	p	501	HEC	C3D-C2D	5.03	1.52	1.37
8	P	501	HEC	C2B-C3B	-4.99	1.35	1.40
8	C	501	HEC	C2B-C3B	-4.95	1.35	1.40
8	C	502	HEC	C2B-C3B	-4.91	1.35	1.40
8	P	502	HEC	C2B-C3B	-4.88	1.35	1.40
8	C	502	HEC	C3C-C2C	-4.84	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	501	HEC	C3C-C2C	-4.82	1.35	1.40
8	D	501	HEC	C3C-C2C	-4.77	1.35	1.40
8	P	502	HEC	C3C-C2C	-4.73	1.35	1.40
8	C	501	HEC	CBC-CAC	-4.50	1.32	1.49
8	P	501	HEC	CBC-CAC	-4.47	1.32	1.49
8	p	502	HEC	C3D-C2D	4.43	1.50	1.37
8	o	301	HEC	C3D-C2D	4.41	1.50	1.37
8	P	501	HEC	CBB-CAB	-4.19	1.34	1.49
8	n	602	HEC	CBC-CAC	-4.19	1.34	1.49
8	n	602	HEC	CBB-CAB	-4.19	1.34	1.49
8	C	501	HEC	CBB-CAB	-4.14	1.34	1.49
8	n	601	HEC	CBC-CAC	-4.14	1.34	1.49
8	C	502	HEC	CBC-CAC	-4.09	1.34	1.49
8	P	502	HEC	CBC-CAC	-4.06	1.34	1.49
8	C	502	HEC	CBB-CAB	-4.05	1.34	1.49
8	P	502	HEC	CBB-CAB	-4.05	1.34	1.49
8	n	601	HEC	CBB-CAB	-4.05	1.34	1.49
8	p	501	HEC	C3C-C4C	3.02	1.48	1.43
8	n	601	HEC	C4D-ND	2.22	1.40	1.36
8	p	501	HEC	C4D-CHA	-2.10	1.35	1.41
8	C	502	HEC	CAA-C2A	2.06	1.55	1.52
8	o	301	HEC	C1B-CHB	-2.03	1.35	1.41
8	p	501	HEC	C1B-CHB	-2.02	1.35	1.41

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	o	301	HEC	CBB-CAB-C3B	-9.62	104.97	127.49
8	p	501	HEC	CBB-CAB-C3B	-7.31	110.39	127.49
8	p	502	HEC	CBC-CAC-C3C	-7.28	110.44	127.49
8	p	502	HEC	CBB-CAB-C3B	-6.84	111.48	127.49
8	Q	501	HEC	CBB-CAB-C3B	-6.61	112.02	127.49
8	D	501	HEC	CBB-CAB-C3B	-6.59	112.07	127.49
8	o	301	HEC	CBC-CAC-C3C	-6.19	113.01	127.49
8	p	501	HEC	CBC-CAC-C3C	-5.56	114.48	127.49
8	Q	501	HEC	CBC-CAC-C3C	-5.46	114.72	127.49
8	D	501	HEC	CBC-CAC-C3C	-5.43	114.78	127.49
8	p	501	HEC	CBD-CAD-C3D	-5.40	103.46	112.54
8	o	301	HEC	CMC-C2C-C3C	-5.31	119.58	125.82
8	p	501	HEC	CMC-C2C-C1C	-4.70	121.57	128.46
8	p	502	HEC	CMC-C2C-C3C	-4.54	120.48	125.82
8	p	502	HEC	CMC-C2C-C1C	-4.41	121.99	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	o	301	HEC	CBA-CAA-C2A	-4.27	105.51	112.55
8	p	501	HEC	CAA-CBA-CGA	-4.13	102.70	113.83
8	n	601	HEC	CMB-C2B-C1B	-4.07	122.50	128.46
8	p	502	HEC	CBD-CAD-C3D	-4.01	105.79	112.54
8	Q	501	HEC	CMC-C2C-C1C	-4.01	122.59	128.46
8	D	501	HEC	CMC-C2C-C1C	-4.00	122.60	128.46
8	C	502	HEC	CMC-C2C-C1C	-3.86	122.81	128.46
8	P	502	HEC	CMC-C2C-C1C	-3.85	122.82	128.46
8	P	501	HEC	CMB-C2B-C1B	-3.64	123.13	128.46
8	C	501	HEC	CMB-C2B-C1B	-3.60	123.17	128.46
8	n	601	HEC	CMB-C2B-C3B	3.59	130.04	125.82
8	o	301	HEC	CMC-C2C-C1C	-3.53	123.28	128.46
8	n	602	HEC	CBA-CAA-C2A	-3.40	106.95	112.55
8	n	601	HEC	CAD-CBD-CGD	-3.21	105.18	113.83
8	P	502	HEC	CMB-C2B-C1B	-3.19	123.79	128.46
8	C	502	HEC	CMB-C2B-C1B	-3.18	123.80	128.46
8	p	502	HEC	CAA-CBA-CGA	-3.01	105.73	113.83
8	C	502	HEC	CMC-C2C-C3C	2.99	129.33	125.82
8	P	502	HEC	CMC-C2C-C3C	2.94	129.27	125.82
8	P	502	HEC	CMD-C2D-C1D	-2.91	124.19	128.46
8	p	502	HEC	CBA-CAA-C2A	-2.90	107.78	112.55
8	C	502	HEC	CMD-C2D-C1D	-2.89	124.22	128.46
8	P	501	HEC	CMB-C2B-C3B	2.89	129.22	125.82
8	D	501	HEC	CBD-CAD-C3D	-2.88	107.70	112.54
8	C	501	HEC	CMB-C2B-C3B	2.84	129.16	125.82
8	Q	501	HEC	CBD-CAD-C3D	-2.83	107.79	112.54
8	p	501	HEC	CMB-C2B-C3B	2.82	129.13	125.82
8	P	501	HEC	CBA-CAA-C2A	-2.74	108.04	112.55
8	C	501	HEC	CBA-CAA-C2A	-2.73	108.05	112.55
8	p	501	HEC	CMB-C2B-C1B	-2.70	124.49	128.46
8	n	601	HEC	CBC-CAC-C3C	-2.65	121.29	127.49
8	p	502	HEC	O1A-CGA-CBA	-2.63	114.74	123.09
8	P	501	HEC	CMD-C2D-C1D	-2.52	124.76	128.46
8	C	501	HEC	CMD-C2D-C1D	-2.51	124.78	128.46
8	p	502	HEC	O1D-CGD-CBD	-2.50	115.17	123.09
8	o	301	HEC	O1A-CGA-CBA	-2.41	115.45	123.09
8	n	601	HEC	O1A-CGA-CBA	-2.37	115.58	123.09
8	P	501	HEC	CMC-C2C-C1C	-2.35	125.01	128.46
8	C	501	HEC	CMC-C2C-C1C	-2.32	125.06	128.46
8	P	502	HEC	CMB-C2B-C3B	2.28	128.50	125.82
8	C	501	HEC	CBD-CAD-C3D	-2.27	108.73	112.54
8	C	502	HEC	CMB-C2B-C3B	2.26	128.48	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	501	HEC	CBD-CAD-C3D	-2.26	108.75	112.54
8	n	601	HEC	CAA-CBA-CGA	-2.26	107.76	113.83
8	p	502	HEC	C1D-C2D-C3D	-2.21	105.46	107.00
8	P	502	HEC	CBD-CAD-C3D	-2.20	108.83	112.54
8	p	502	HEC	CMB-C2B-C1B	-2.19	125.25	128.46
8	C	502	HEC	CBD-CAD-C3D	-2.18	108.87	112.54
8	C	501	HEC	C4C-C3C-C2C	2.18	108.70	106.35
8	p	502	HEC	CAD-CBD-CGD	-2.17	107.98	113.83
8	n	602	HEC	O1A-CGA-CBA	-2.17	116.22	123.09
8	D	501	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
8	C	501	HEC	CBB-CAB-C3B	-2.16	122.44	127.49
8	P	501	HEC	CBB-CAB-C3B	-2.14	122.48	127.49
8	Q	501	HEC	C1D-C2D-C3D	-2.10	105.53	107.00
8	P	501	HEC	C4C-C3C-C2C	2.09	108.61	106.35
8	C	501	HEC	CBC-CAC-C3C	-2.08	122.63	127.49
8	n	602	HEC	CBC-CAC-C3C	-2.07	122.65	127.49
8	P	501	HEC	CBC-CAC-C3C	-2.06	122.67	127.49
8	n	602	HEC	CBB-CAB-C3B	-2.02	122.76	127.49

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	502	HEC	C2A-CAA-CBA-CGA
8	P	502	HEC	C2A-CAA-CBA-CGA
8	C	502	HEC	C3A-C2A-CAA-CBA
8	P	502	HEC	C3A-C2A-CAA-CBA
8	C	502	HEC	C1A-C2A-CAA-CBA
8	P	502	HEC	C1A-C2A-CAA-CBA
8	n	601	HEC	CAD-CBD-CGD-O1D
8	n	601	HEC	CAD-CBD-CGD-O2D
8	p	501	HEC	CAA-CBA-CGA-O1A
8	o	301	HEC	CAA-CBA-CGA-O1A
8	p	502	HEC	CAD-CBD-CGD-O2D
8	o	301	HEC	CAD-CBD-CGD-O1D
8	p	502	HEC	CAD-CBD-CGD-O1D
8	o	301	HEC	CAA-CBA-CGA-O2A
8	n	602	HEC	CAD-CBD-CGD-O2D
8	o	301	HEC	CAD-CBD-CGD-O2D
8	C	502	HEC	CAA-CBA-CGA-O2A
8	P	502	HEC	CAA-CBA-CGA-O2A
8	p	501	HEC	CAA-CBA-CGA-O2A

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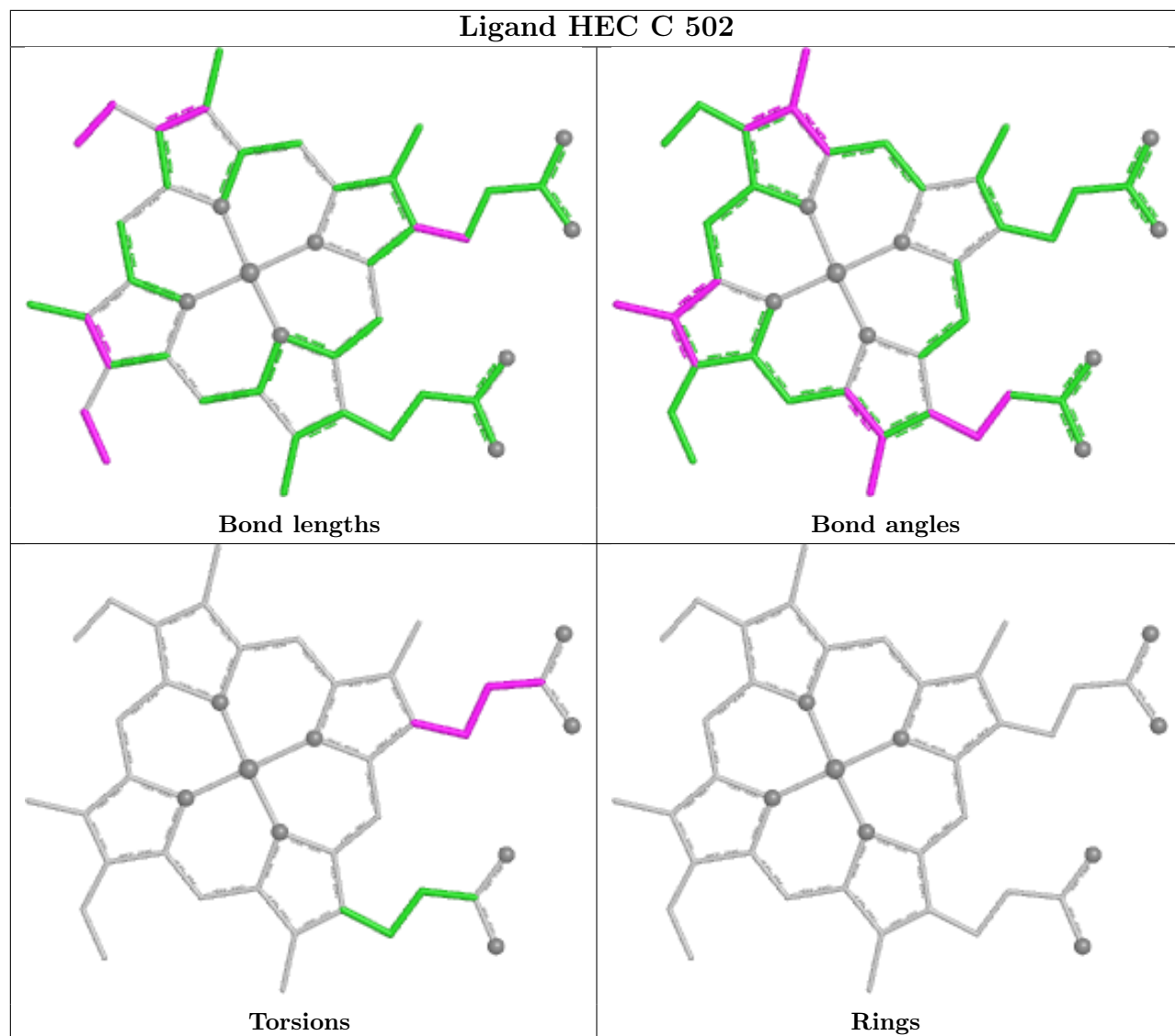
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Mol	Chain	Res	Type	Atoms
8	n	602	HEC	CAD-CBD-CGD-O1D
8	C	502	HEC	CAA-CBA-CGA-O1A
8	P	502	HEC	CAA-CBA-CGA-O1A
8	C	501	HEC	CAD-CBD-CGD-O1D
8	P	501	HEC	CAD-CBD-CGD-O1D
8	n	601	HEC	CAA-CBA-CGA-O2A
8	D	501	HEC	CAA-CBA-CGA-O2A
8	Q	501	HEC	CAA-CBA-CGA-O2A
8	C	501	HEC	CAD-CBD-CGD-O2D
8	P	501	HEC	CAD-CBD-CGD-O2D
8	n	601	HEC	CAA-CBA-CGA-O1A
8	C	501	HEC	CAA-CBA-CGA-O2A
8	P	501	HEC	CAA-CBA-CGA-O2A
8	D	501	HEC	CAA-CBA-CGA-O1A
8	Q	501	HEC	CAA-CBA-CGA-O1A
8	C	501	HEC	CAA-CBA-CGA-O1A
8	P	501	HEC	CAA-CBA-CGA-O1A

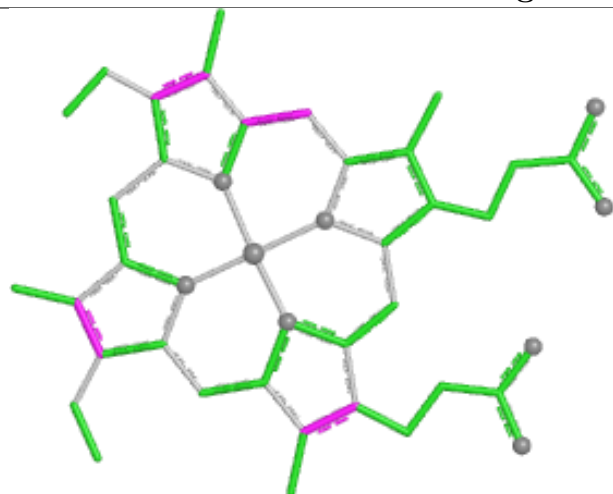
There are no ring outliers.

No monomer is involved in short contacts.

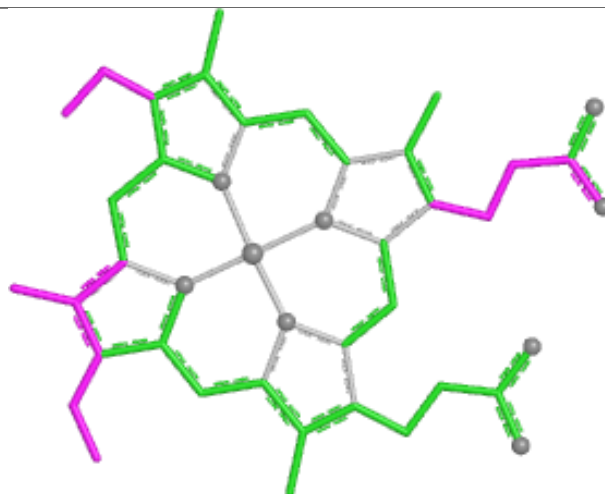
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



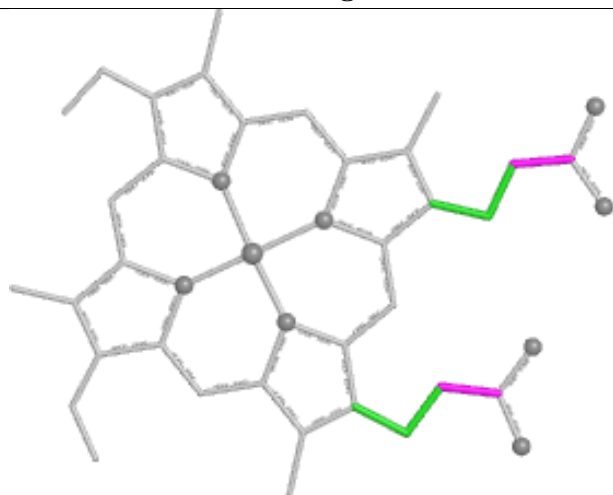
## Ligand HEC o 301



Bond lengths



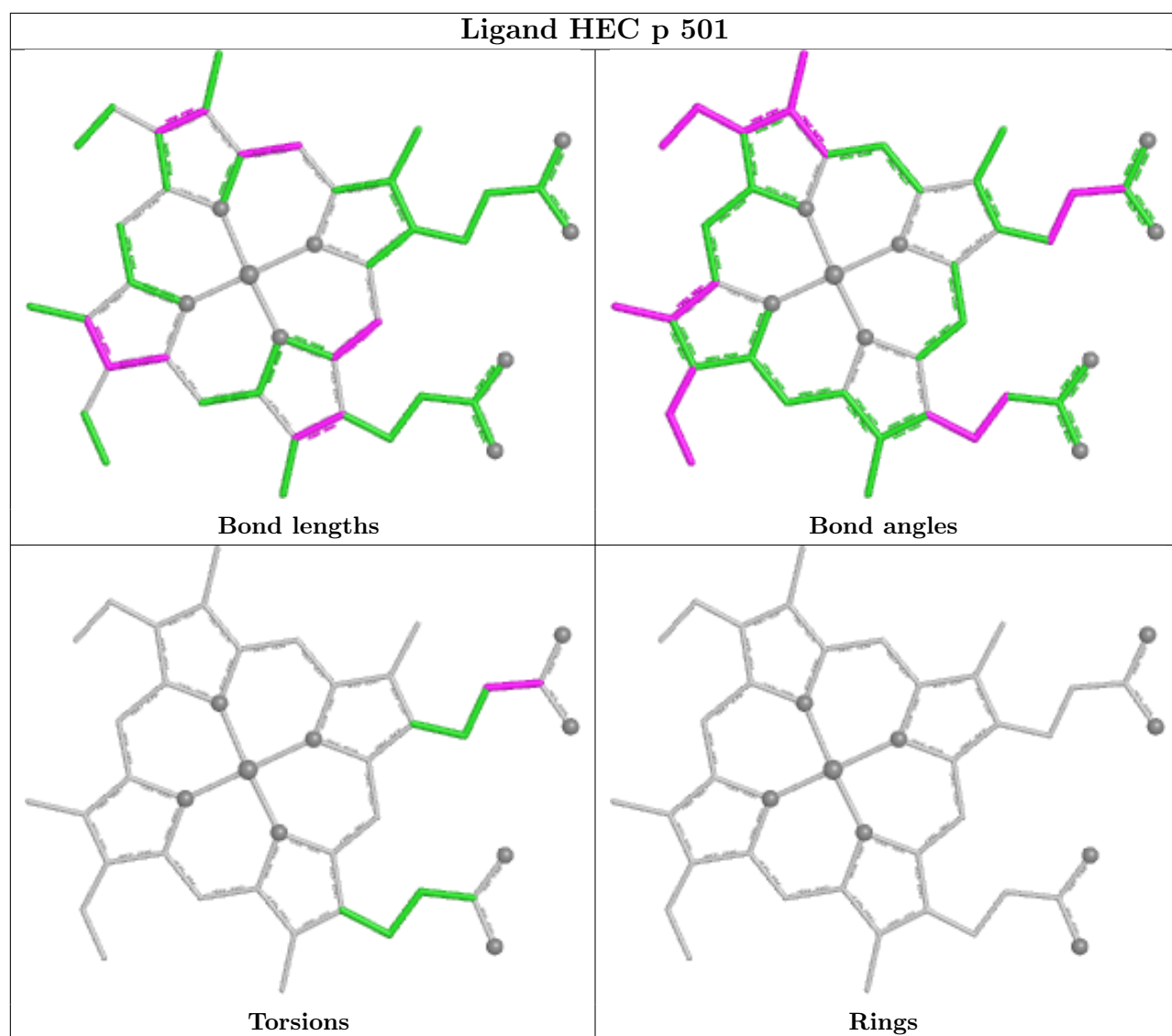
Bond angles



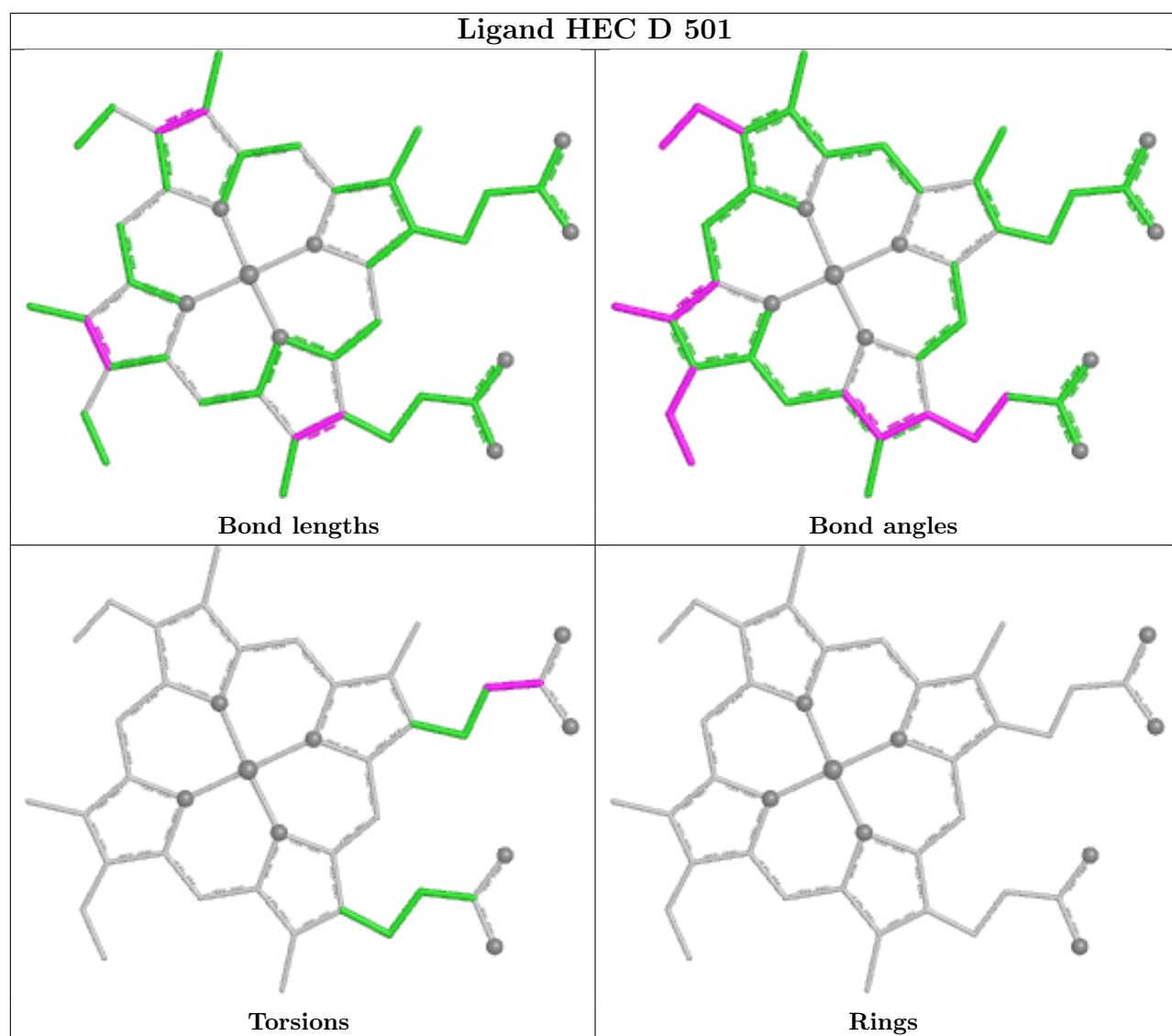
Torsions



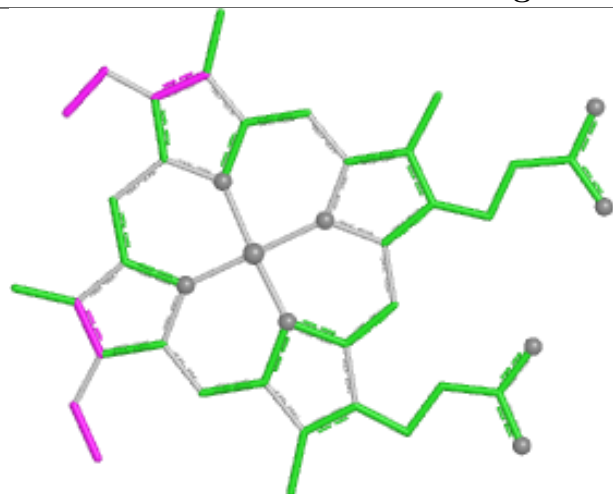
Rings



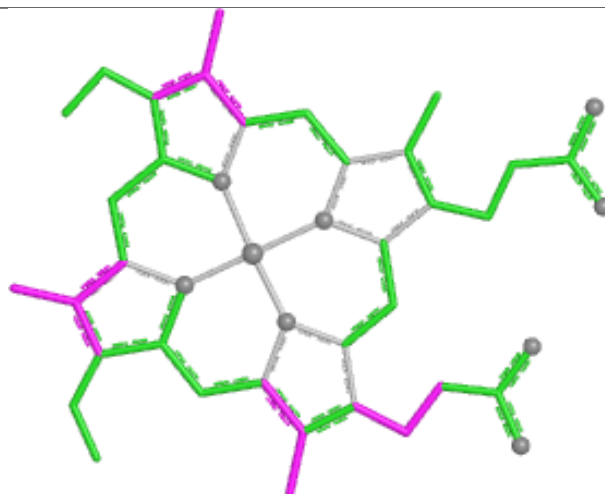




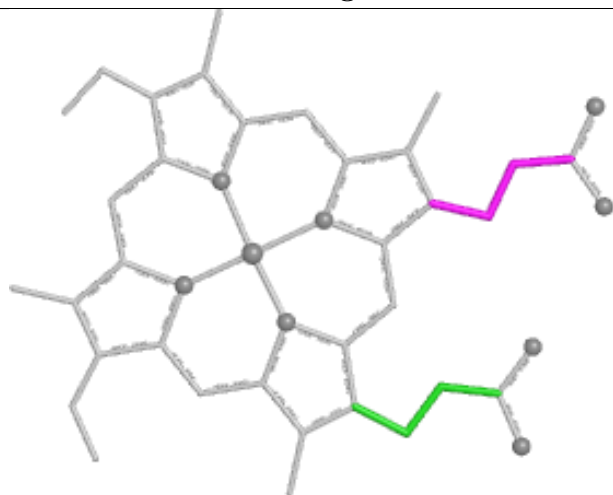
## Ligand HEC P 502



Bond lengths



Bond angles

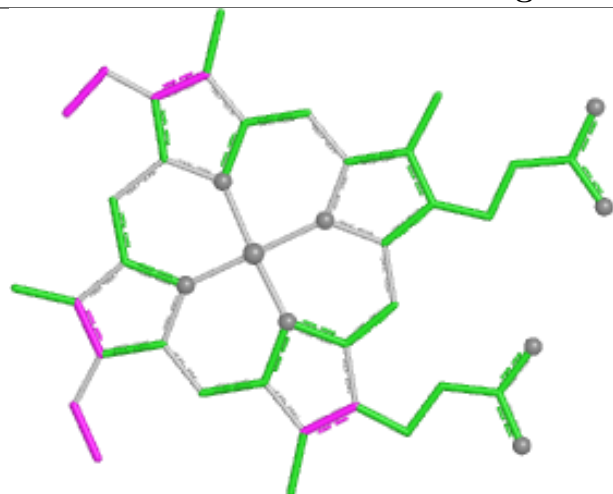


Torsions

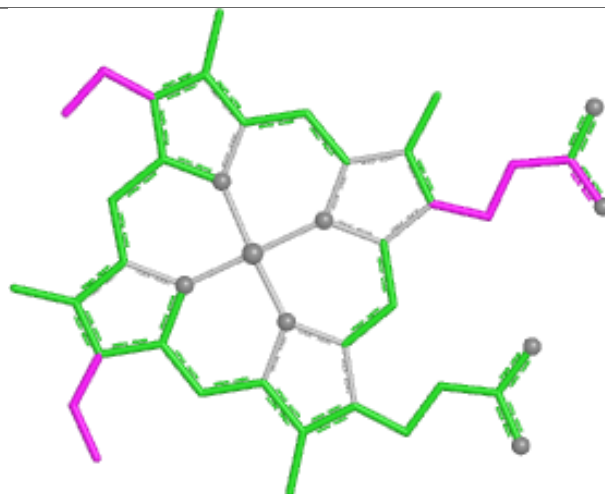


Rings

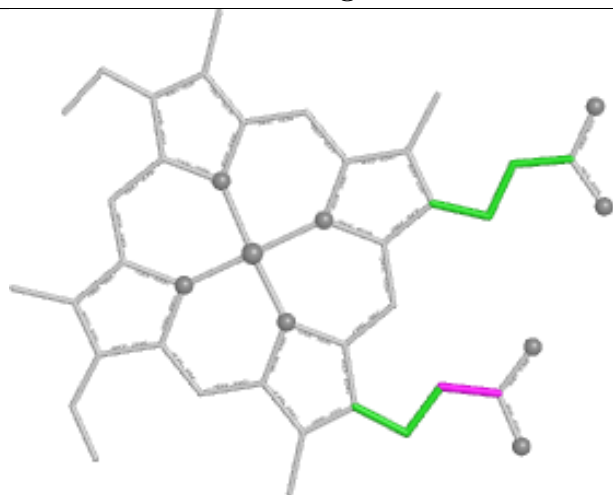
## Ligand HEC n 602



Bond lengths



Bond angles

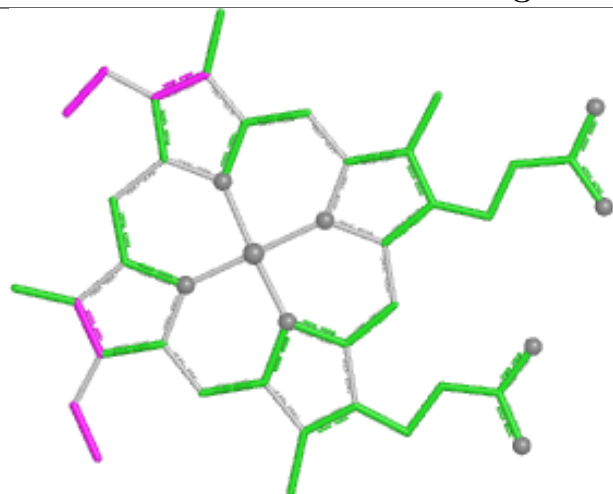


Torsions

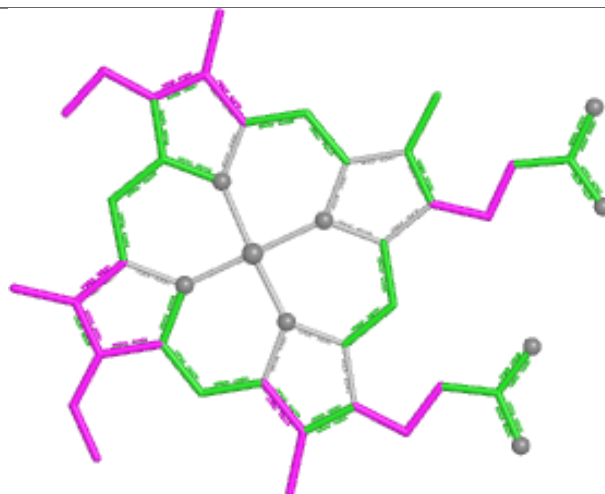


Rings

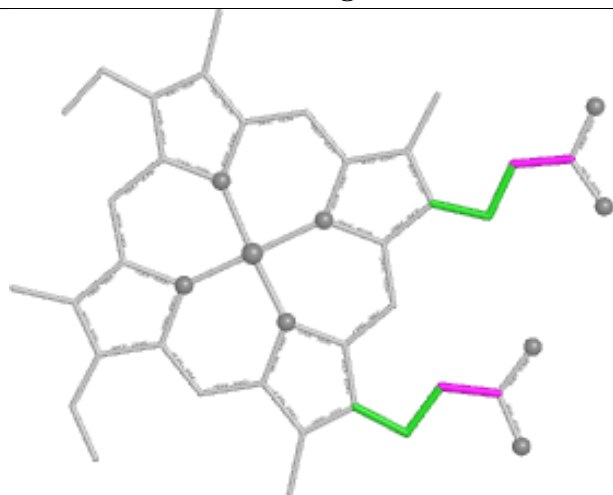
## Ligand HEC P 501



Bond lengths



Bond angles

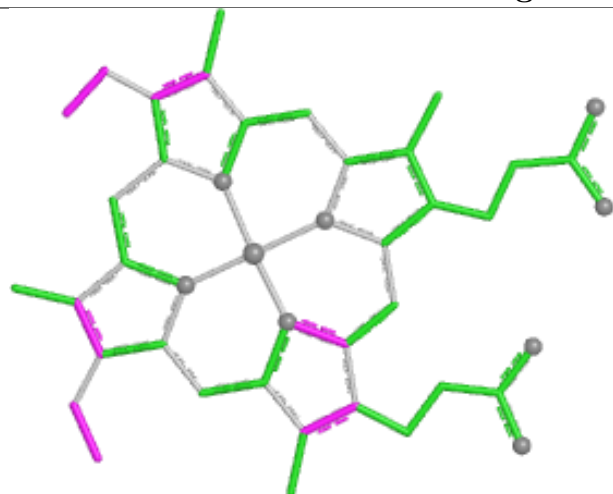


Torsions

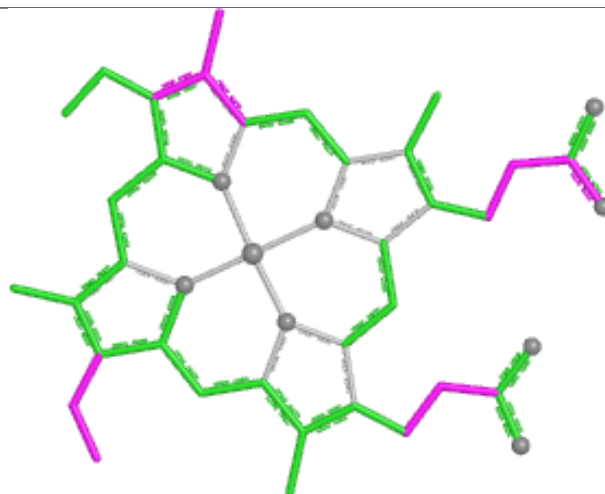


Rings

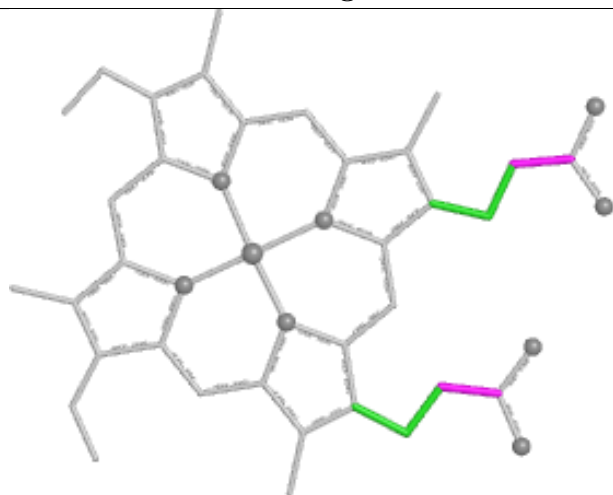
## Ligand HEC n 601



Bond lengths



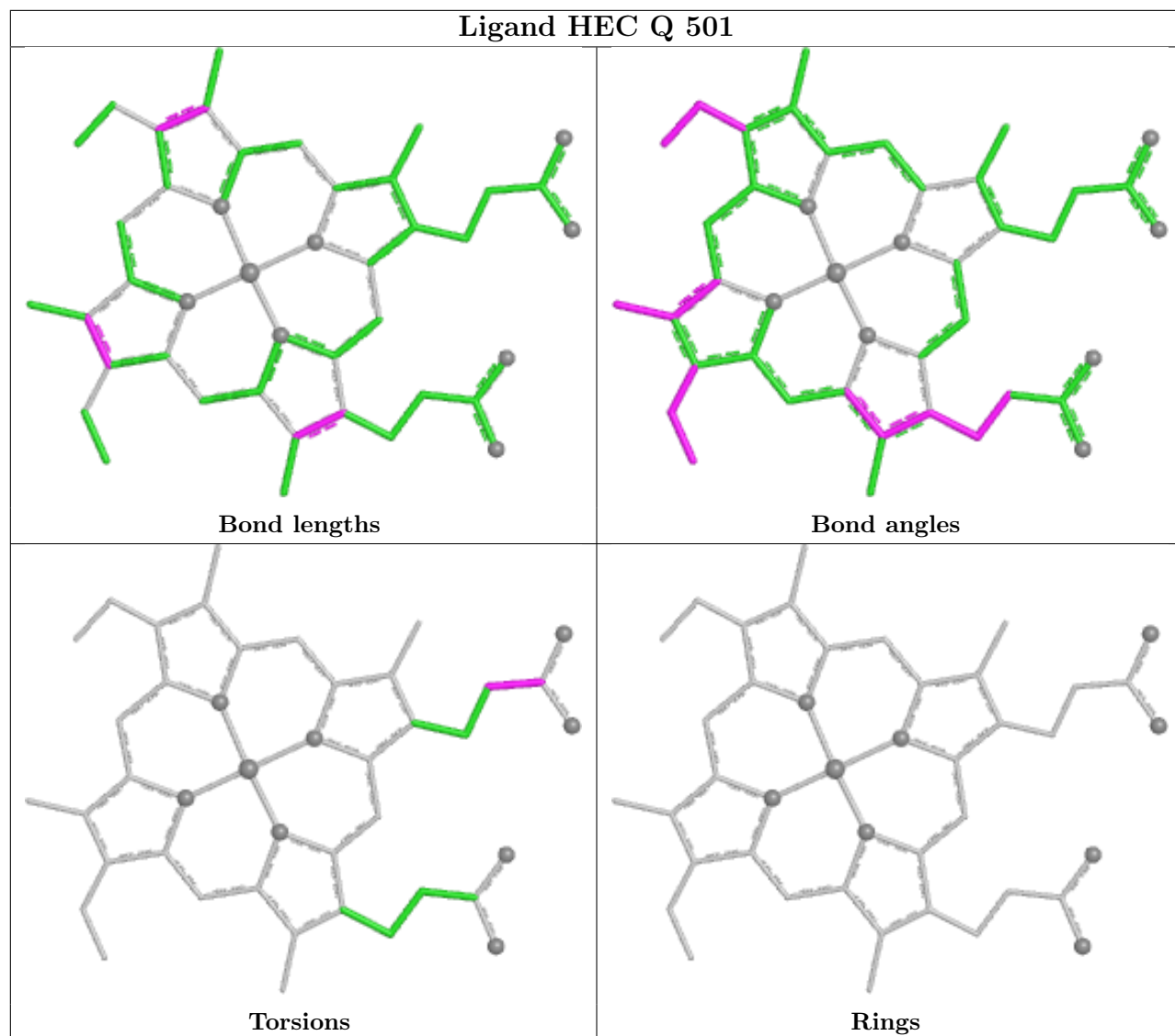
Bond angles



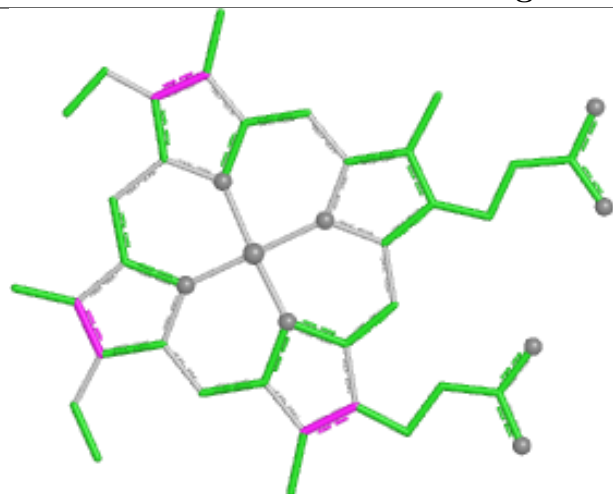
Torsions



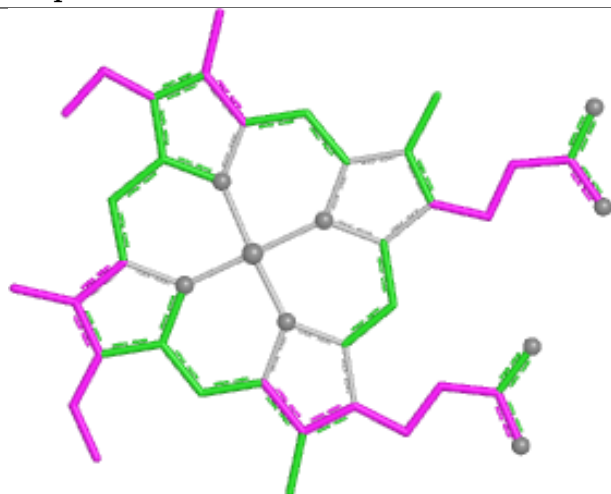
Rings



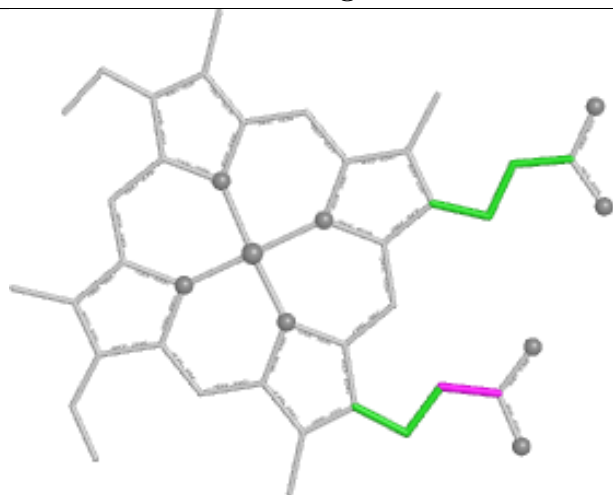
## Ligand HEC p 502



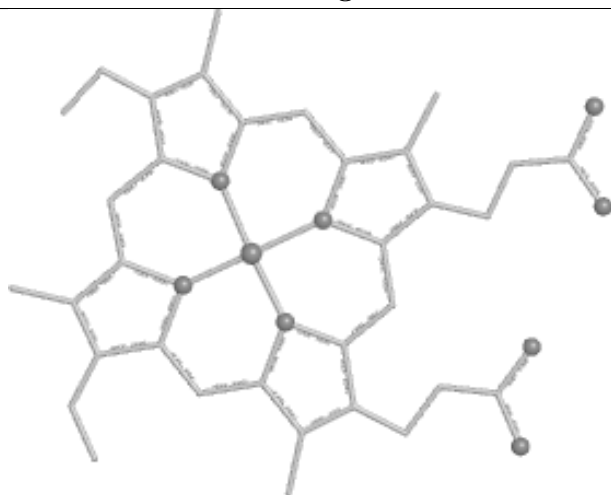
Bond lengths



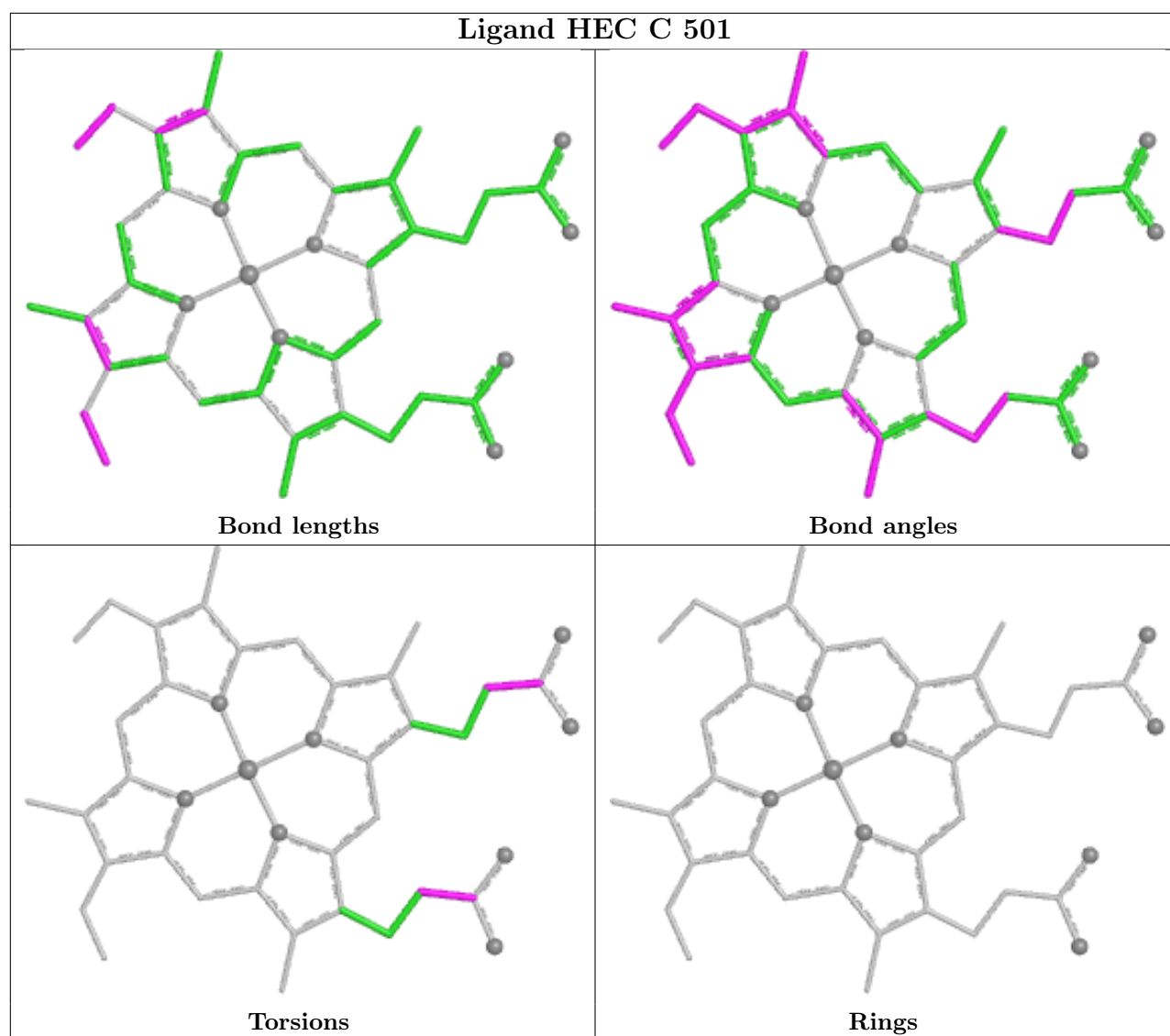
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



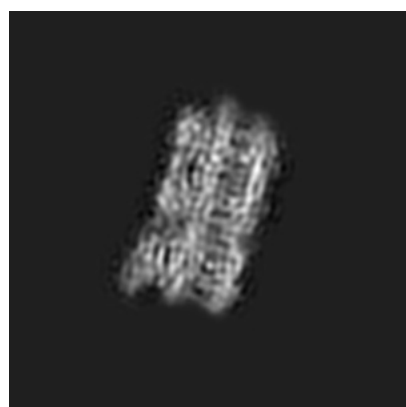
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22230. These allow visual inspection of the internal detail of the map and identification of artifacts.

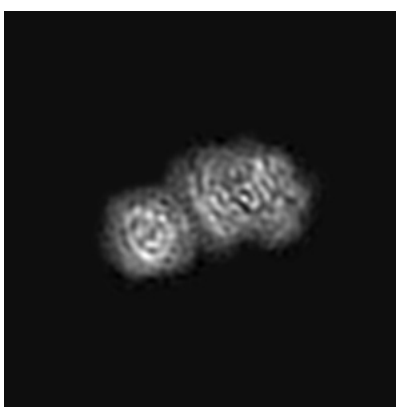
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

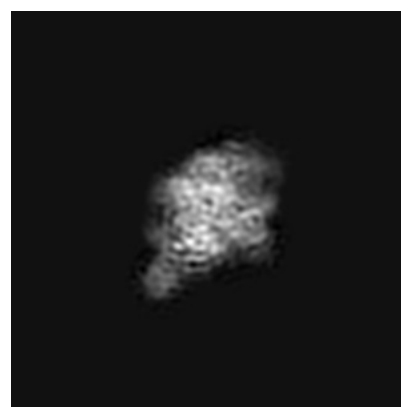
#### 6.1.1 Primary map



X



Y



Z

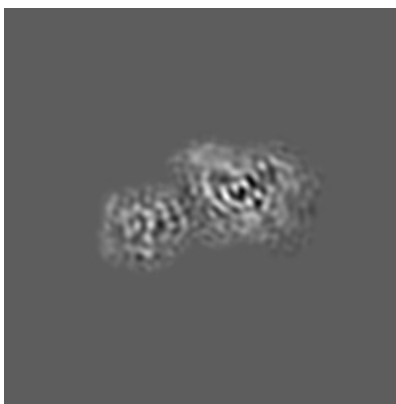
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

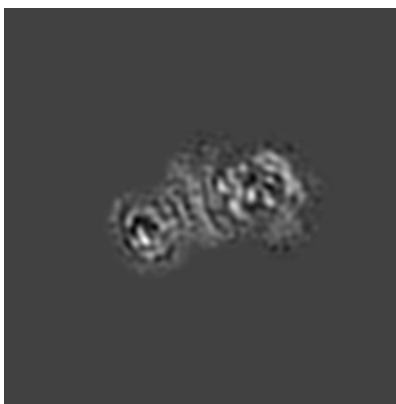
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 122



Y Index: 112

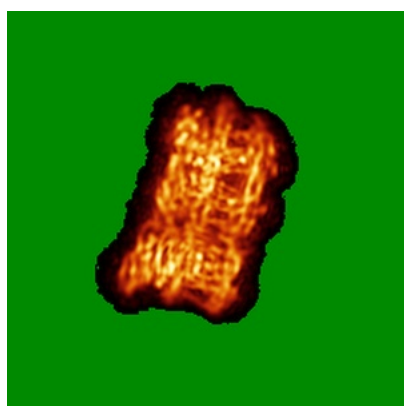


Z Index: 86

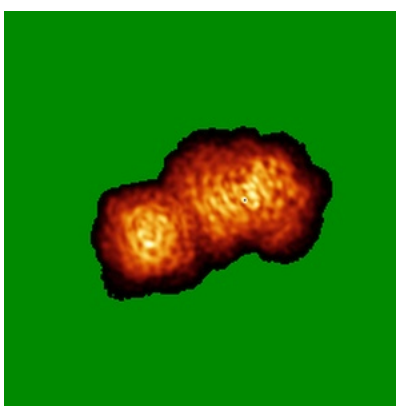
The images above show the largest variance slices of the map in three orthogonal directions.

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

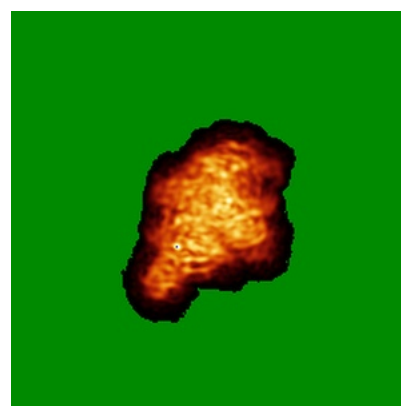
### 6.4.1 Primary map



X



Y



Z

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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

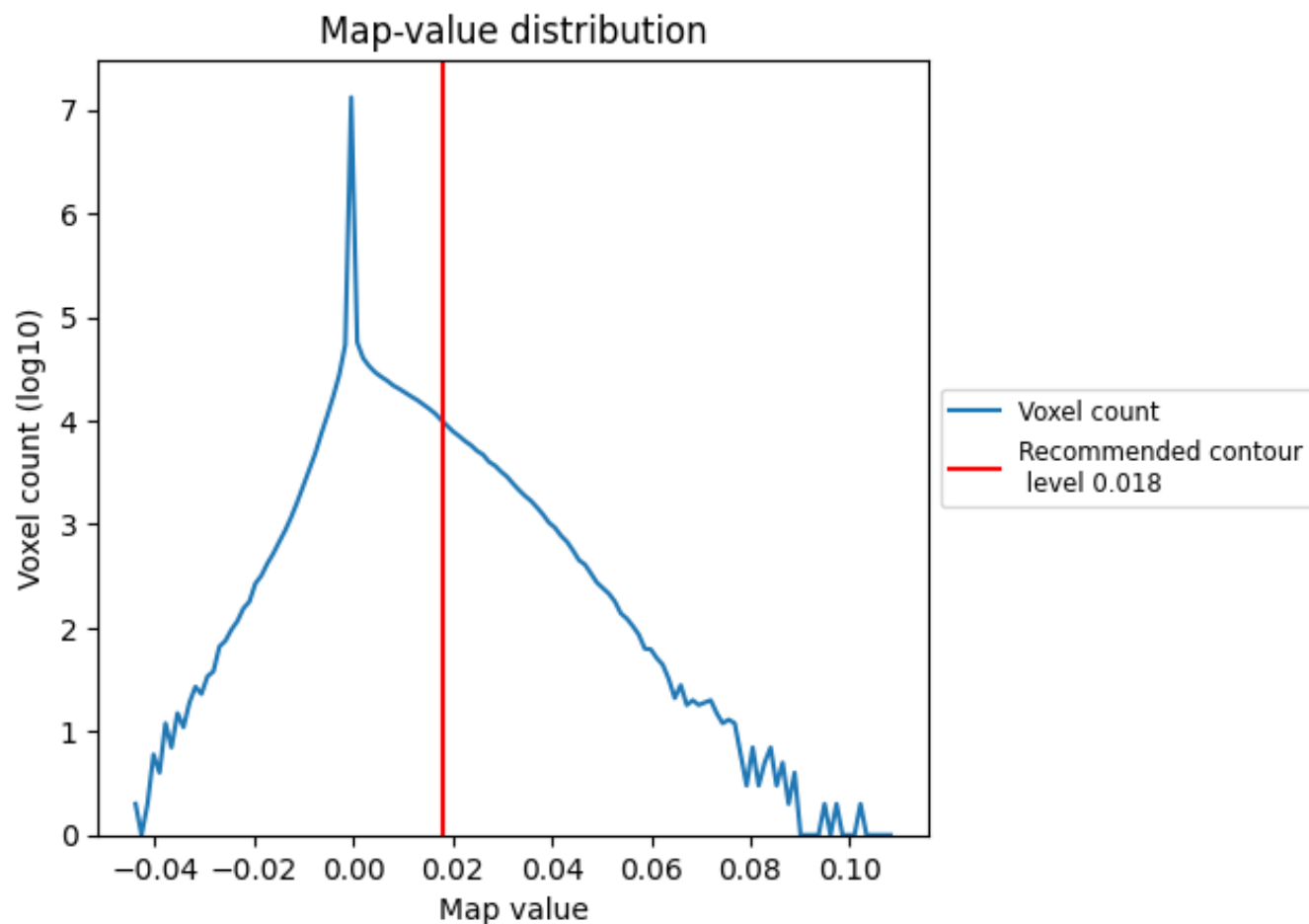
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

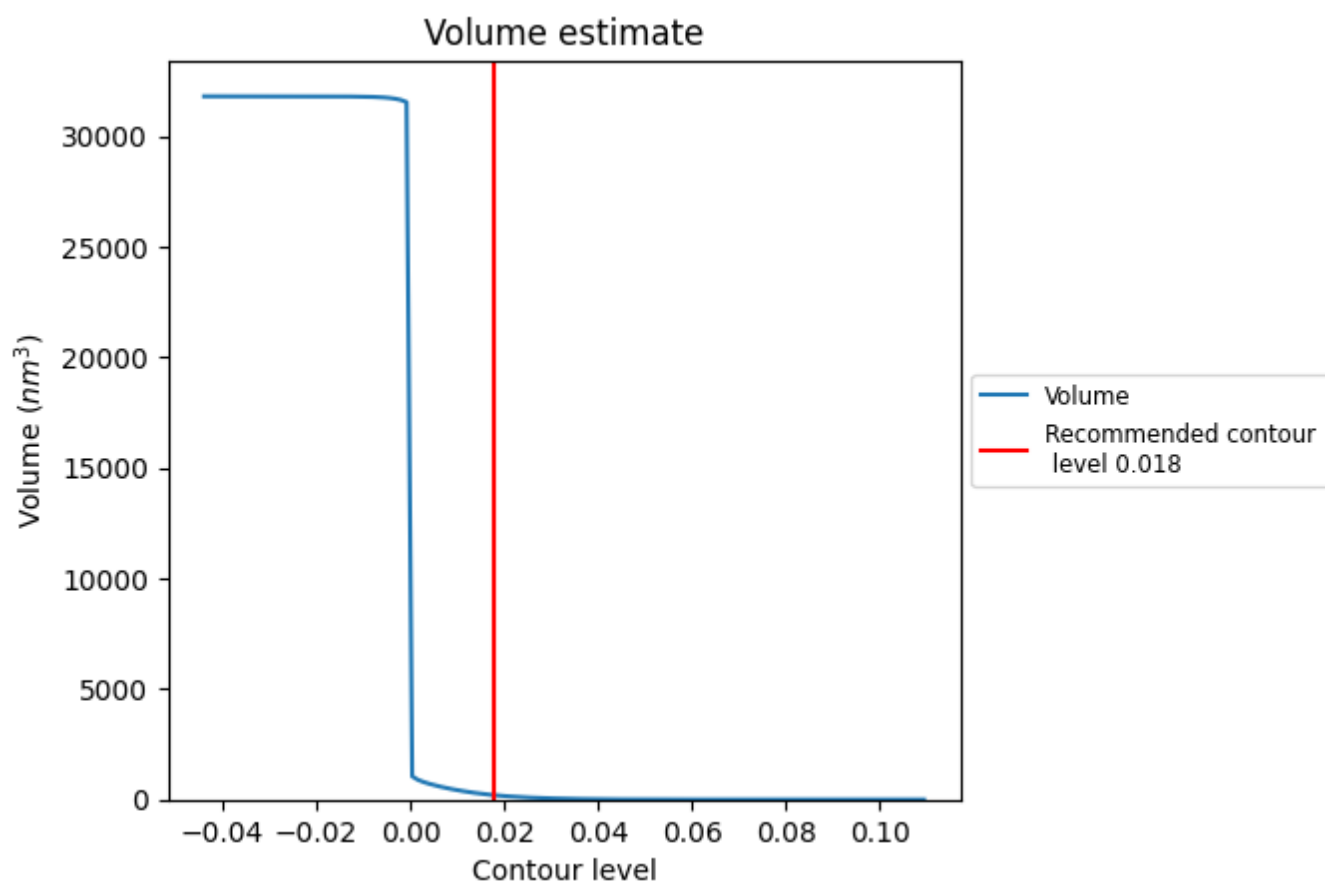
This section contains the results of statistical analysis of the map.

### 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.

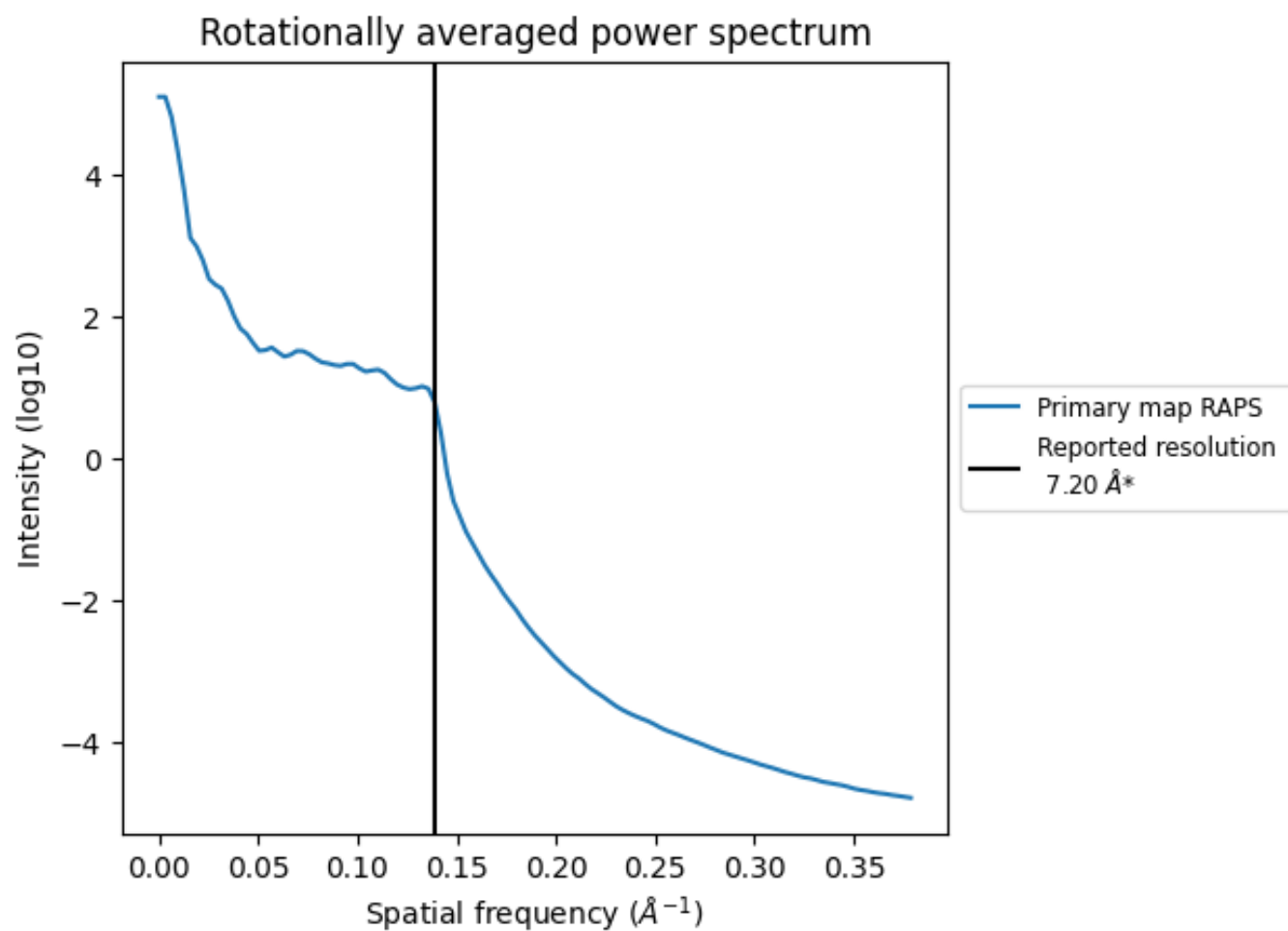
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196  $\text{nm}^3$ ; 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 ⓘ

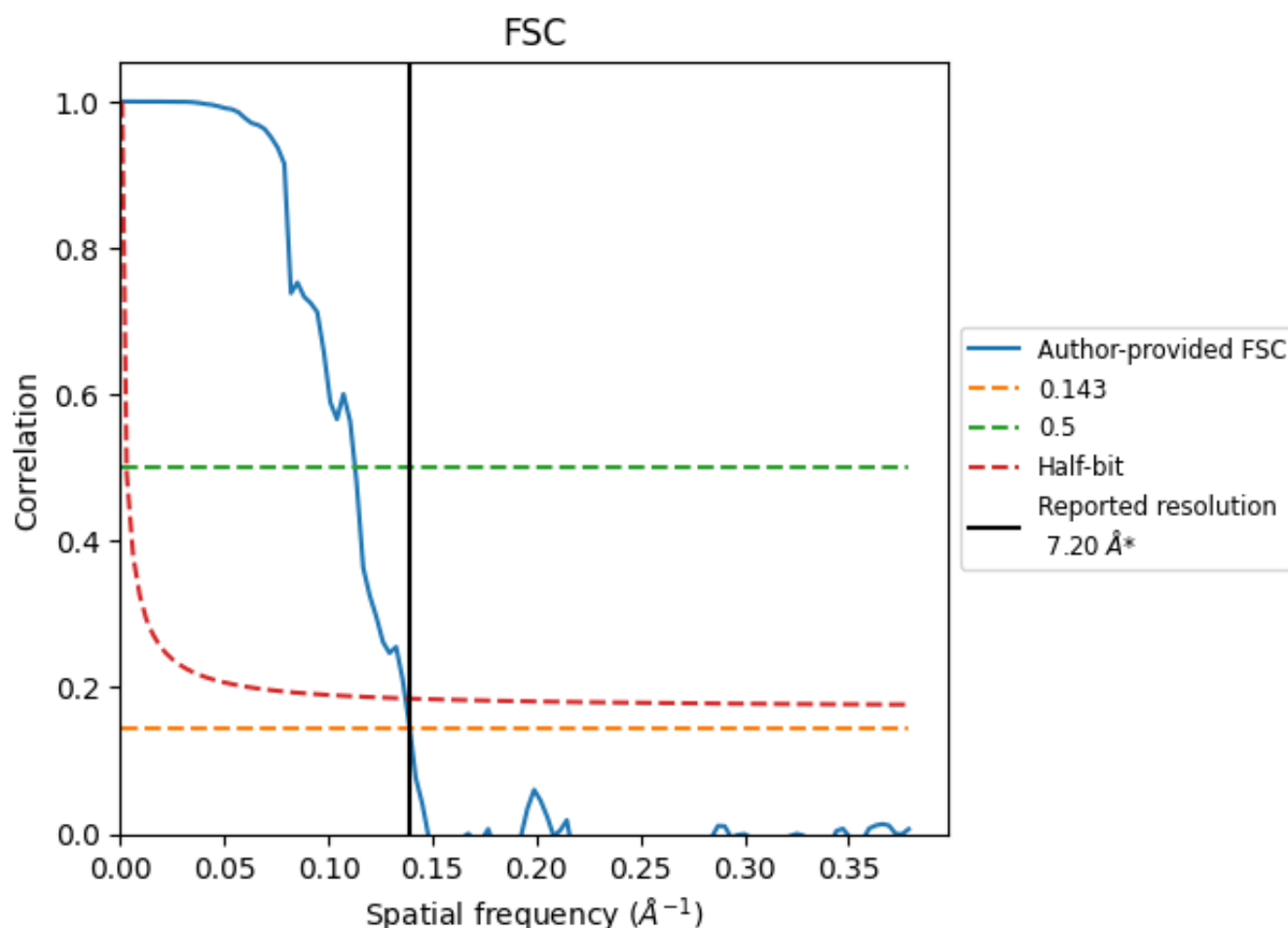


\*Reported resolution corresponds to spatial frequency of 0.139 Å<sup>-1</sup>

## 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 0.139  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.18	8.86	7.29
Unmasked-calculated*	-	-	-

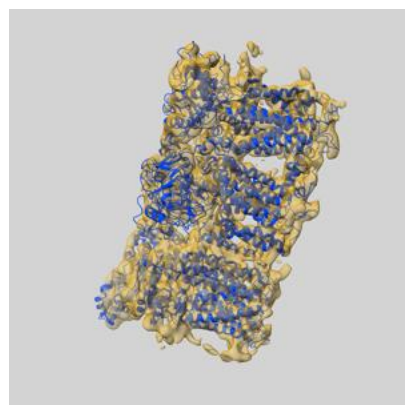
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



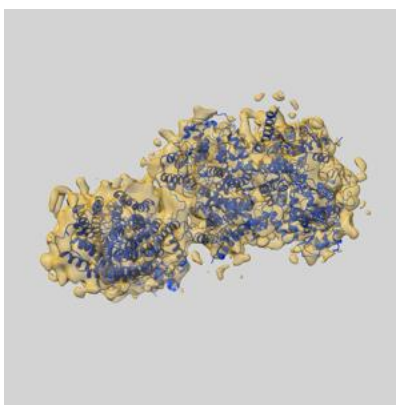
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22230 and PDB model 6XKZ. Per-residue inclusion information can be found in section 3 on page 6.

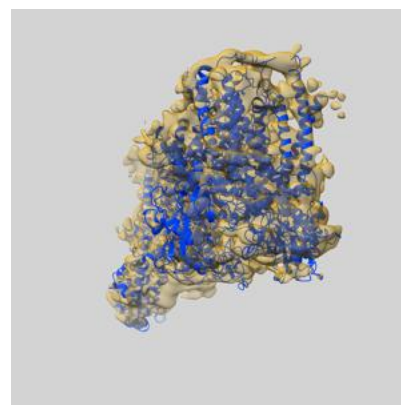
### 9.1 Map-model overlay [i](#)



X



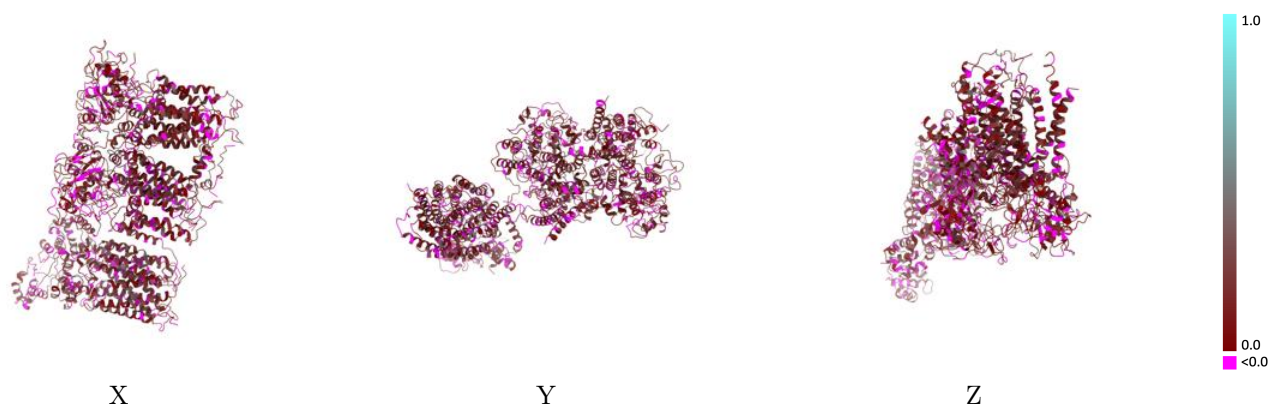
Y



Z

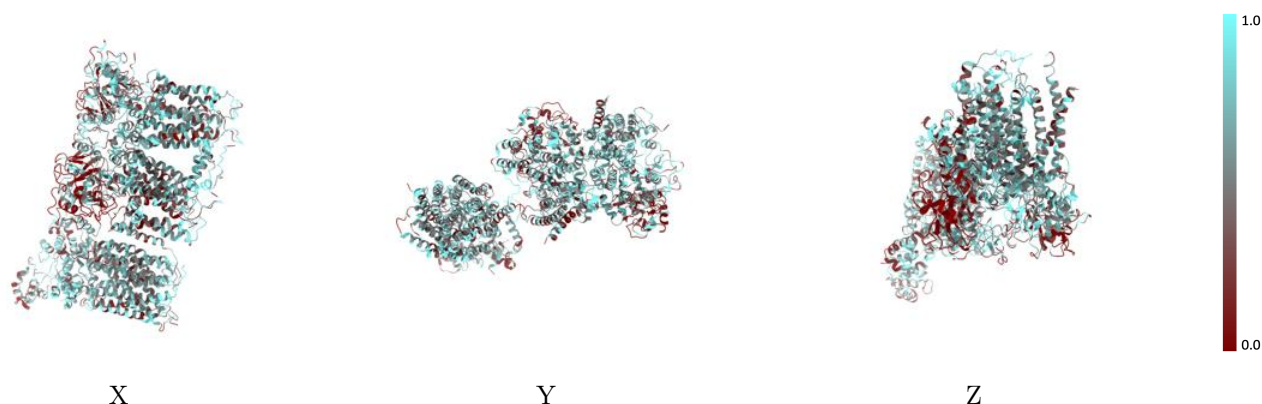
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



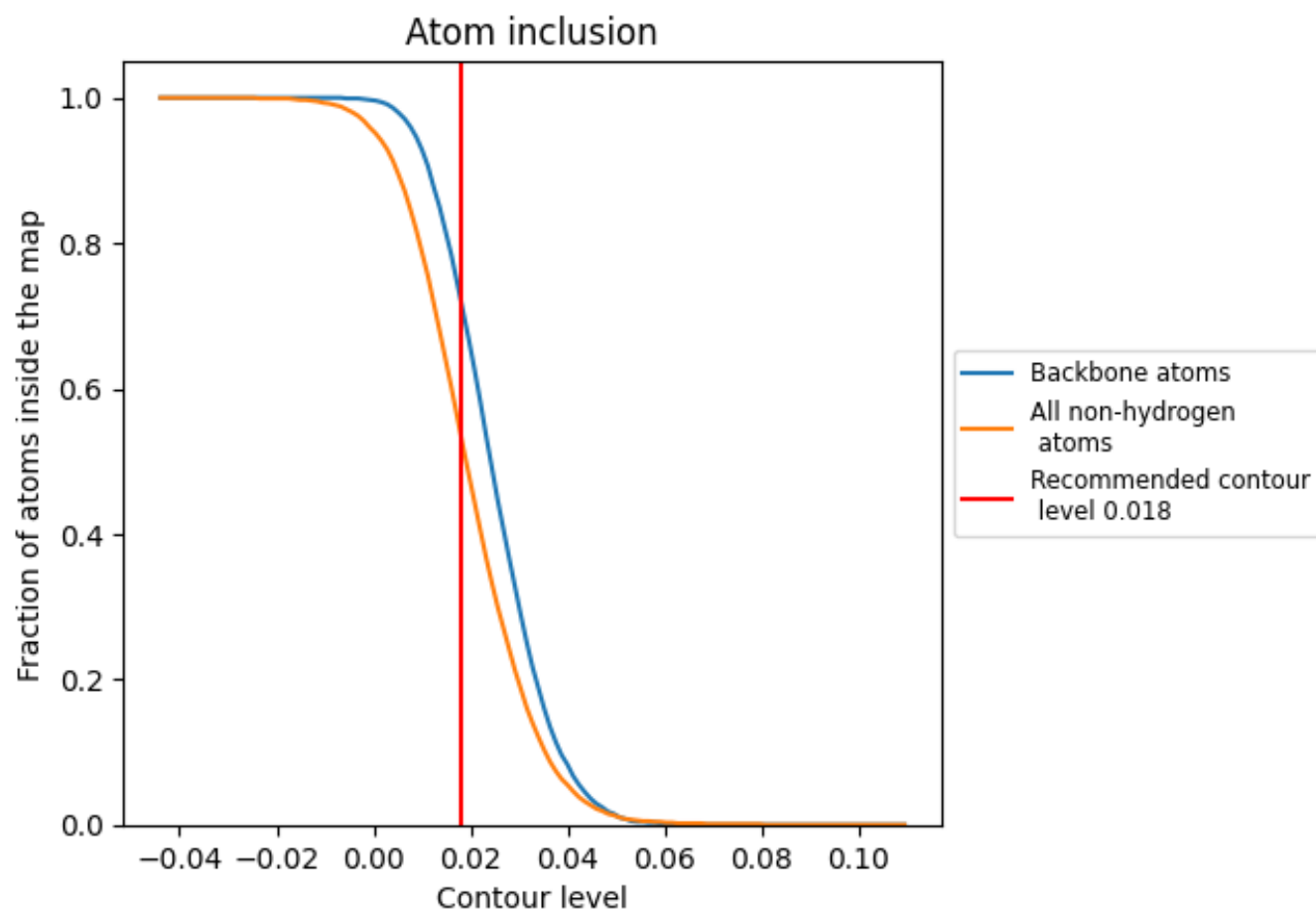
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 54% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5350	<div><div></div></div> 0.1220
C	<div><div></div></div> 0.5710	<div><div></div></div> 0.1350
D	<div><div></div></div> 0.5330	<div><div></div></div> 0.1100
E	<div><div></div></div> 0.2610	<div><div></div></div> 0.1020
P	<div><div></div></div> 0.6150	<div><div></div></div> 0.1410
Q	<div><div></div></div> 0.6450	<div><div></div></div> 0.1470
R	<div><div></div></div> 0.1600	<div><div></div></div> 0.0670
n	<div><div></div></div> 0.5930	<div><div></div></div> 0.1270
o	<div><div></div></div> 0.6080	<div><div></div></div> 0.1290
p	<div><div></div></div> 0.5260	<div><div></div></div> 0.0890

1.0

0.0

<0.0