



# Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 04:08 PM JST

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

This is a 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:

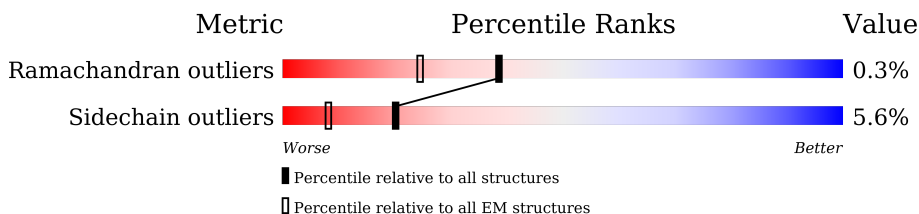
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
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 2.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



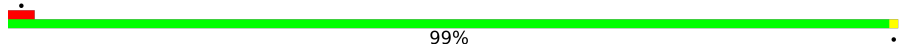


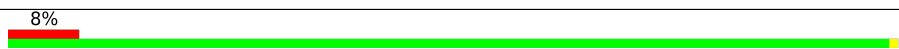
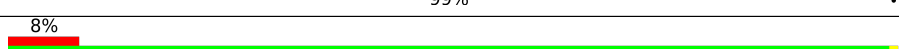
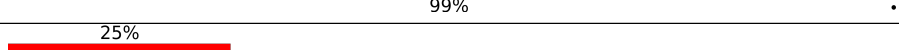
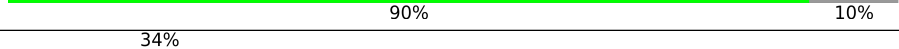
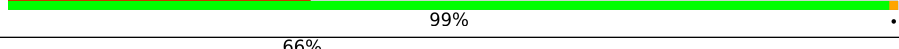



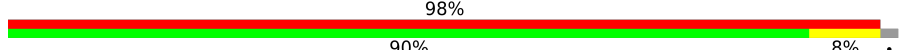

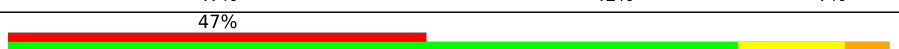
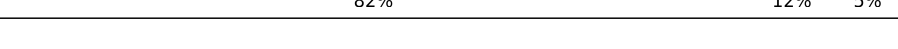














Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	378	97%
1	a	378	97%
2	B	241	15% 96%
2	b	241	14% 93% 5% ..
3	C	196	95% 91% 6% ..
3	c	196	94% 87% 13% ..
4	D	446	97% ..
4	d	446	98% ..
5	E	418	99% ..

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Mol	Chain	Length	Quality of chain
5	e	418	 99%
6	F	64	 61%
6	f	64	 86%
6	f	64	 59%
7	G	106	 84%
7	g	106	 99%
7	g	106	 99%
8	H	79	 25%
8	H	79	 90%
8	h	79	 34%
8	h	79	 99%
9	I	62	 66%
9	I	62	 68%
9	i	62	 69%
9	i	62	 69%
9	i	62	 27%
10	J	52	 94%
10	J	52	 85%
10	j	52	 98%
10	j	52	 90%
10	j	52	 8%
11	K	57	 51%
11	K	57	 47%
11	K	57	 42%
11	K	57	 7%
11	k	57	 47%
11	k	57	 82%
11	k	57	 12%
11	k	57	 5%

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 33477 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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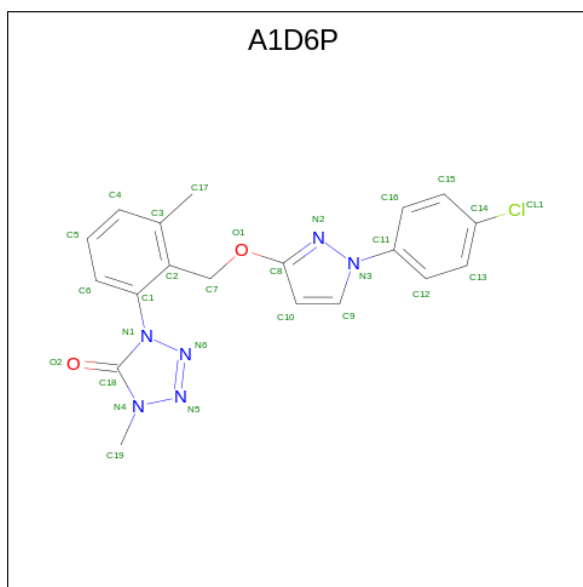
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	51	Total 421	C 281	N 74	O 65	S 1	0	0

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

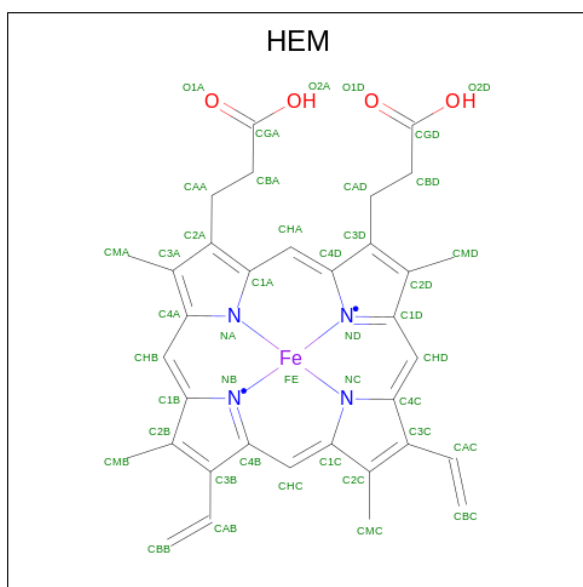
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	57	Total 404	C 252	N 74	O 76	S 2	0	0
11	k	57	Total 404	C 252	N 74	O 76	S 2	0	0

- Molecule 12 is 1-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (three-letter code: A1D6P) (formula: C<sub>19</sub>H<sub>17</sub>ClN<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



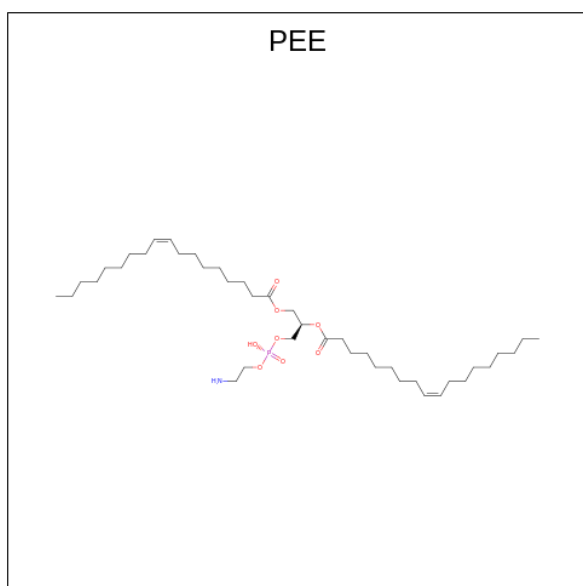
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
12	A	1	Total 28	C 19	Cl 1	N 6	O 2	0
12	A	1	Total 28	C 19	Cl 1	N 6	O 2	0
12	a	1	Total 28	C 19	Cl 1	N 6	O 2	0
12	a	1	Total 28	C 19	Cl 1	N 6	O 2	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



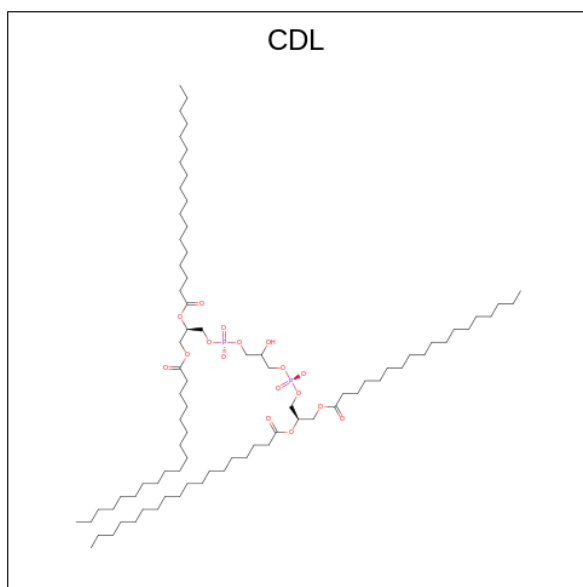
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
13	A	1	43	34	1	4	4	0
13	A	1	43	34	1	4	4	0
13	a	1	43	34	1	4	4	0
13	a	1	43	34	1	4	4	0

- 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	C	N	O	P	0
			45	35	1	8	1	
14	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

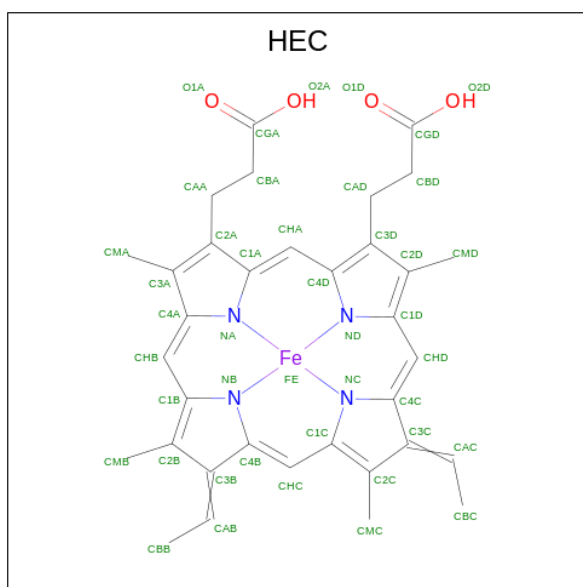
- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

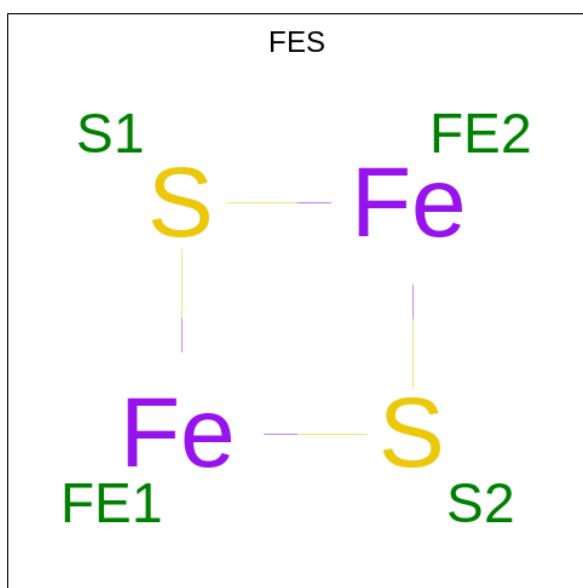
- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).





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

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

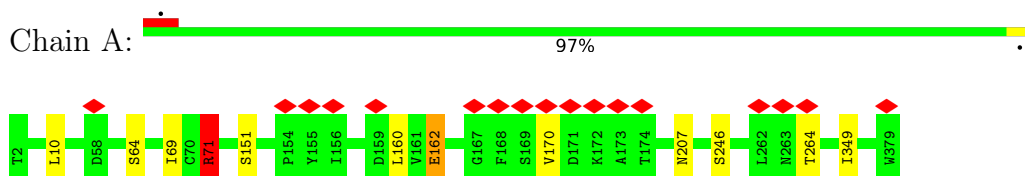


Mol	Chain	Residues	Atoms		AltConf
17	C	1	Total	Fe S	0
			4	2 2	
17	c	1	Total	Fe S	0
			4	2 2	

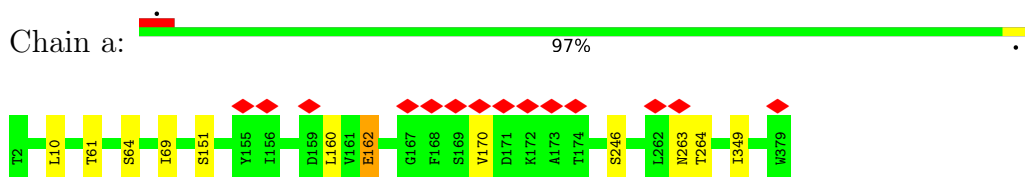
### 3 Residue-property plots [i](#)

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.

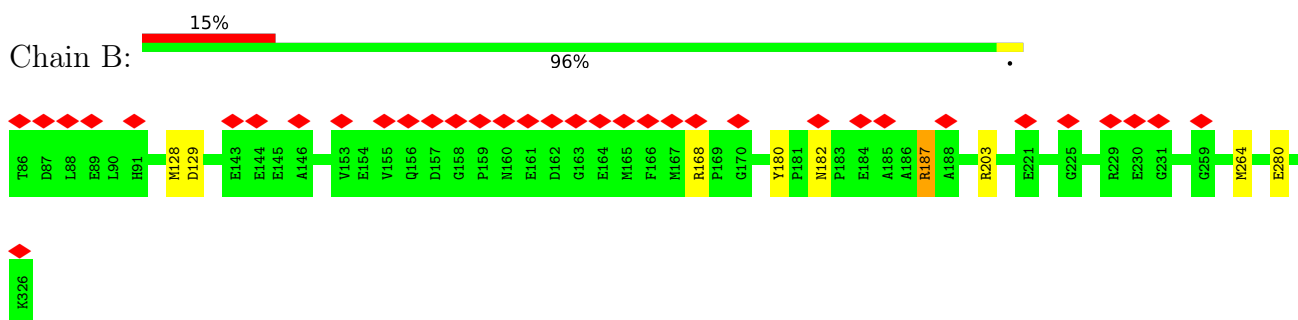
- Molecule 1: Cytochrome b



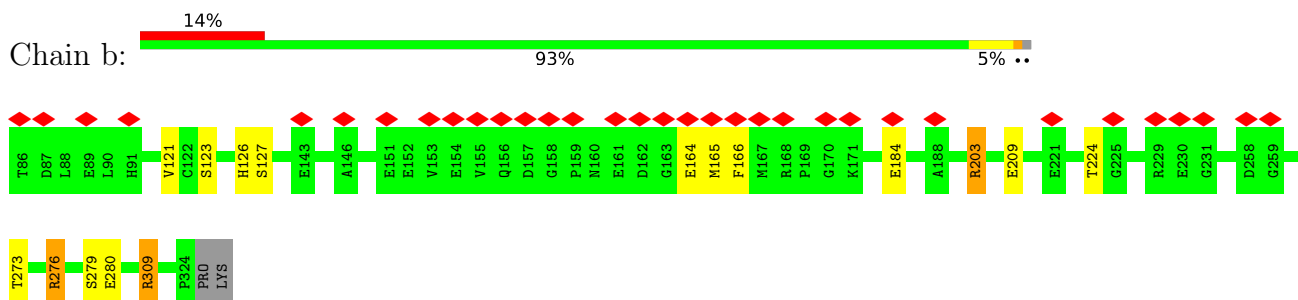
- Molecule 1: Cytochrome b



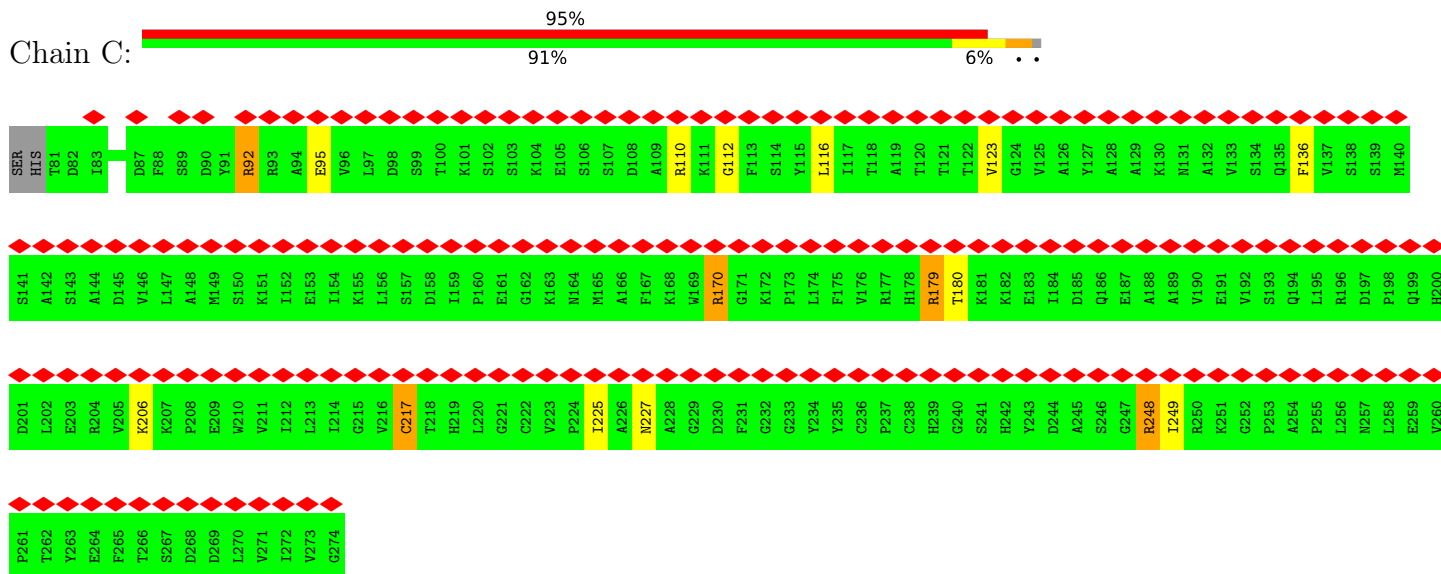
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



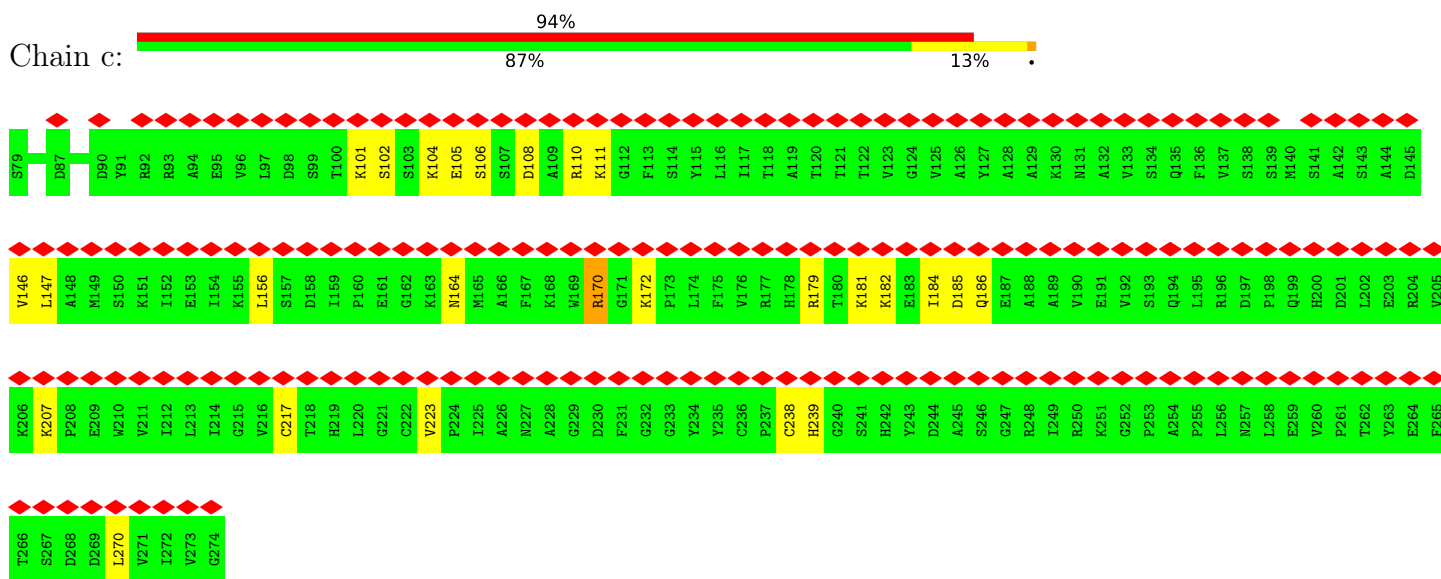
- Molecule 2: Cytochrome c1, heme protein, mitochondrial



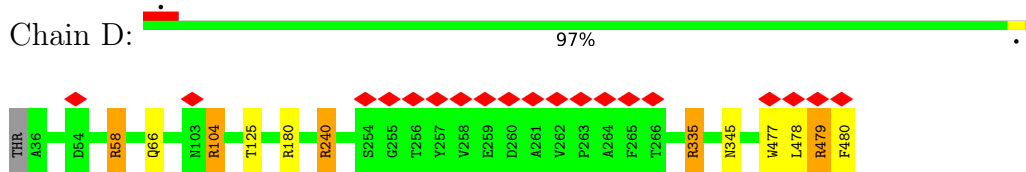
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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

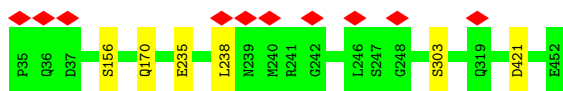


- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

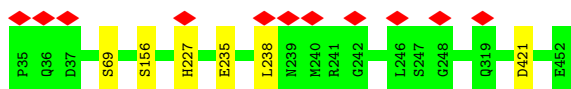




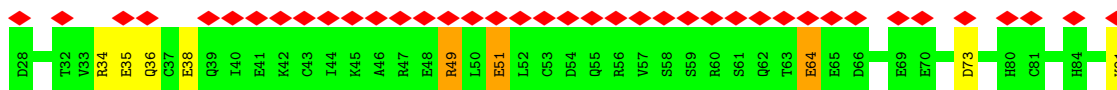
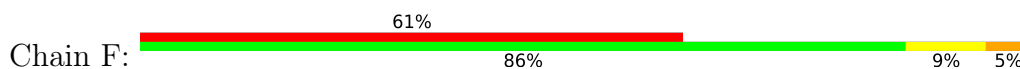
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



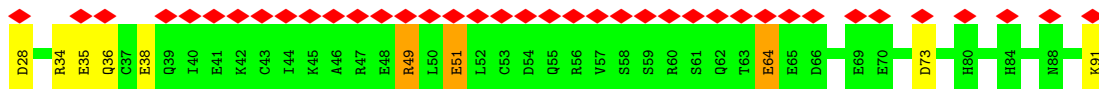
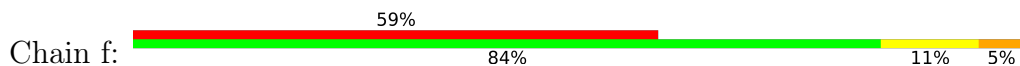
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial



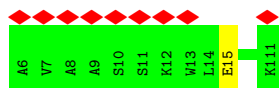
- Molecule 6: Cytochrome b-c1 complex subunit 6



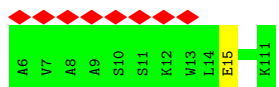
- Molecule 6: Cytochrome b-c1 complex subunit 6



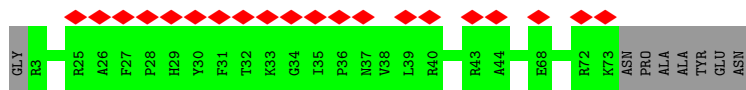
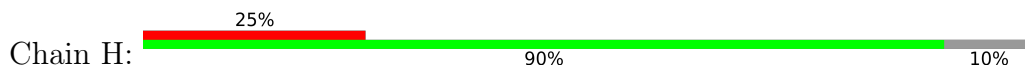
- Molecule 7: Cytochrome b-c1 complex subunit 7



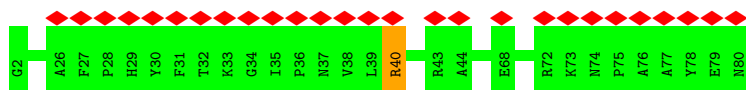
- Molecule 7: Cytochrome b-c1 complex subunit 7



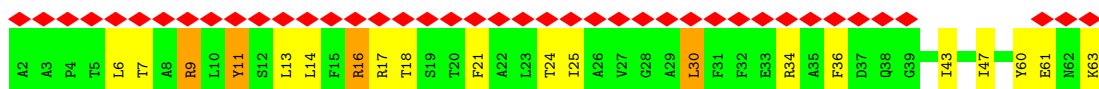
- Molecule 8: Cytochrome b-c1 complex subunit 8



• Molecule 8: Cytochrome b-c1 complex subunit 8



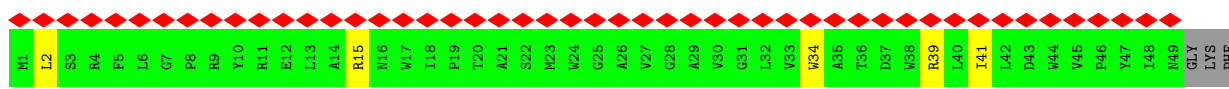
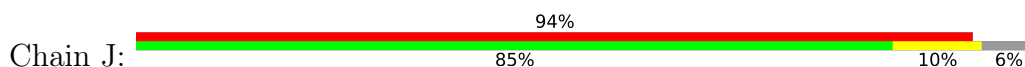
• Molecule 9: Complex III subunit 9



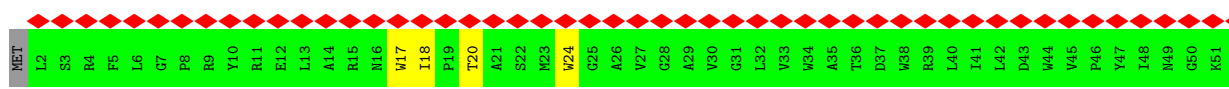
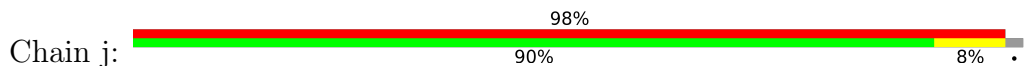
• Molecule 9: Complex III subunit 9



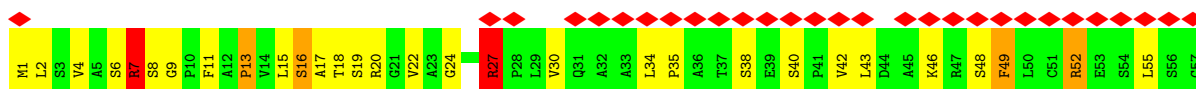
• Molecule 10: Cytochrome b-c1 complex subunit 10




• Molecule 10: Cytochrome b-c1 complex subunit 10

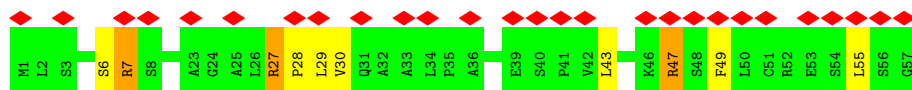


• Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

Chain k: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	411418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.72	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.863	Depositor
Minimum map value	-5.367	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.223	Depositor
Recommended contour level	0.798	Depositor
Map size (Å)	288.0, 288.0, 288.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, HEC, FES, A1D6P, 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	0.44	0/3115	0.62	2/4259 (0.0%)
1	a	0.43	0/3115	0.61	1/4259 (0.0%)
2	B	0.43	0/1978	0.62	0/2684
2	b	0.46	1/1961 (0.1%)	0.69	1/2661 (0.0%)
3	C	0.46	1/1534 (0.1%)	0.78	2/2075 (0.1%)
3	c	0.43	1/1551 (0.1%)	0.73	2/2098 (0.1%)
4	D	0.43	0/3524	0.60	1/4783 (0.0%)
4	d	0.43	1/3531 (0.0%)	0.64	2/4793 (0.0%)
5	E	0.42	0/3187	0.59	0/4314
5	e	0.45	0/3187	0.61	0/4314
6	F	0.42	0/534	0.91	6/714 (0.8%)
6	f	0.43	0/534	0.90	6/714 (0.8%)
7	G	0.46	0/941	0.62	0/1262
7	g	0.46	0/941	0.62	0/1262
8	H	0.42	0/628	0.62	0/848
8	h	0.36	0/688	0.65	0/931
9	I	0.48	0/520	0.89	3/701 (0.4%)
9	i	0.42	0/520	0.93	3/701 (0.4%)
10	J	0.40	0/420	0.76	2/576 (0.3%)
10	j	0.40	0/437	0.77	2/598 (0.3%)
11	K	0.96	0/410	1.28	4/556 (0.7%)
11	k	0.59	0/410	1.06	2/556 (0.4%)
All	All	0.45	4/33666 (0.0%)	0.68	39/45659 (0.1%)

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

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	217	CYS	C-N	8.08	1.52	1.34
2	b	121	VAL	C-N	6.61	1.49	1.34
3	c	111	LYS	C-N	5.18	1.42	1.33
4	d	351	THR	C-O	-5.08	1.13	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	30	LEU	CA-CB-CG	11.00	140.61	115.30
9	i	30	LEU	CA-CB-CG	10.98	140.56	115.30
6	f	49	ARG	NE-CZ-NH2	8.90	124.75	120.30
6	F	49	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	a	162	GLU	CA-CB-CG	8.06	131.12	113.40
1	A	162	GLU	CA-CB-CG	8.04	131.08	113.40
11	k	43	LEU	CA-CB-CG	8.02	133.74	115.30
3	C	116	LEU	CA-CB-CG	7.23	131.93	115.30
11	K	16	SER	CB-CA-C	-6.86	97.07	110.10
6	f	49	ARG	NE-CZ-NH1	-6.81	116.89	120.30
6	F	49	ARG	NE-CZ-NH1	-6.80	116.90	120.30
6	F	49	ARG	CG-CD-NE	6.50	125.45	111.80
6	f	49	ARG	CG-CD-NE	6.49	125.43	111.80
6	F	49	ARG	CD-NE-CZ	6.48	132.67	123.60
6	f	49	ARG	CD-NE-CZ	6.47	132.65	123.60
11	K	7	ARG	N-CA-C	-6.23	94.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	156	LEU	CA-CB-CG	6.22	129.60	115.30
3	C	112	GLY	N-CA-C	6.06	128.26	113.10
11	K	27	ARG	CB-CA-C	-6.05	98.30	110.40
9	I	11	TYR	CB-CA-C	-6.04	98.31	110.40
3	c	270	LEU	CA-CB-CG	5.93	128.94	115.30
10	J	2	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	71	ARG	CB-CA-C	5.76	121.92	110.40
10	j	17	TRP	N-CA-C	-5.52	96.09	111.00
11	K	4	VAL	N-CA-CB	-5.50	99.39	111.50
4	D	478	LEU	CB-CG-CD1	5.41	120.20	111.00
6	f	51	GLU	CA-CB-CG	5.34	125.15	113.40
9	i	11	TYR	CA-CB-CG	5.34	123.54	113.40
6	F	51	GLU	CA-CB-CG	5.32	125.09	113.40
10	j	24	TRP	N-CA-C	-5.30	96.68	111.00
10	J	41	ILE	CG1-CB-CG2	-5.27	99.81	111.40
9	I	30	LEU	CB-CG-CD2	5.25	119.92	111.00
9	i	30	LEU	CB-CG-CD2	5.24	119.91	111.00
2	b	126	HIS	CB-CA-C	5.22	120.84	110.40
4	d	399	LEU	CA-CB-CG	5.19	127.23	115.30
4	d	351	THR	CB-CA-C	-5.16	97.66	111.60
11	k	55	LEU	CA-CB-CG	5.11	127.06	115.30
6	F	64	GLU	CA-CB-CG	5.03	124.47	113.40
6	f	64	GLU	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Sidechain
2	B	180	TYR	Peptide
2	B	187	ARG	Sidechain
3	C	110	ARG	Peptide
3	C	170	ARG	Sidechain
3	C	179	ARG	Sidechain
3	C	206	LYS	Peptide
3	C	248	ARG	Sidechain
3	C	92	ARG	Sidechain
4	D	104	ARG	Sidechain
4	D	240	ARG	Sidechain
4	D	335	ARG	Sidechain
4	D	479	ARG	Sidechain
4	D	58	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	F	34	ARG	Sidechain
9	I	16	ARG	Sidechain
9	I	24	THR	Peptide
9	I	36	PHE	Peptide
9	I	9	ARG	Sidechain
10	J	34	TRP	Peptide
11	K	27	ARG	Sidechain
11	K	52	ARG	Sidechain
11	K	7	ARG	Sidechain
2	b	203	ARG	Sidechain
2	b	273	THR	Peptide
2	b	276	ARG	Sidechain
2	b	309	ARG	Sidechain
3	c	170	ARG	Sidechain
6	f	34	ARG	Sidechain
8	h	40	ARG	Sidechain
9	i	16	ARG	Sidechain
9	i	24	THR	Peptide
9	i	36	PHE	Peptide
11	k	27	ARG	Sidechain
11	k	47	ARG	Sidechain
11	k	6	SER	Mainchain
11	k	7	ARG	Sidechain

## 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	A	376/378 (100%)	362 (96%)	14 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	376/378 (100%)	363 (96%)	13 (4%)	0	100	100
2	B	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30	48
2	b	237/241 (98%)	213 (90%)	24 (10%)	0	100	100
3	C	192/196 (98%)	163 (85%)	29 (15%)	0	100	100
3	c	194/196 (99%)	153 (79%)	41 (21%)	0	100	100
4	D	443/446 (99%)	423 (96%)	20 (4%)	0	100	100
4	d	444/446 (100%)	421 (95%)	23 (5%)	0	100	100
5	E	416/418 (100%)	399 (96%)	17 (4%)	0	100	100
5	e	416/418 (100%)	398 (96%)	18 (4%)	0	100	100
6	F	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
6	f	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
7	G	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
7	g	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
8	H	69/79 (87%)	61 (88%)	8 (12%)	0	100	100
8	h	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
9	I	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
9	i	60/62 (97%)	49 (82%)	11 (18%)	0	100	100
10	J	47/52 (90%)	42 (89%)	5 (11%)	0	100	100
10	j	49/52 (94%)	42 (86%)	6 (12%)	1 (2%)	6	10
11	K	55/57 (96%)	37 (67%)	10 (18%)	8 (14%)	0	0
11	k	55/57 (96%)	43 (78%)	10 (18%)	2 (4%)	3	3
All	All	4137/4198 (98%)	3826 (92%)	299 (7%)	12 (0%)	38	54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	7	ARG
11	K	8	SER
10	j	18	ILE
11	k	27	ARG
11	K	9	GLY
11	K	17	ALA
11	K	49	PHE
2	B	128	MET
11	K	24	GLY

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Mol	Chain	Res	Type
11	K	27	ARG
11	K	13	PRO
11	k	28	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	319 (96%)	12 (4%)	30	53
1	a	331/331 (100%)	319 (96%)	12 (4%)	30	53
2	B	206/206 (100%)	199 (97%)	7 (3%)	32	56
2	b	204/206 (99%)	191 (94%)	13 (6%)	14	28
3	C	164/166 (99%)	152 (93%)	12 (7%)	11	22
3	c	166/166 (100%)	143 (86%)	23 (14%)	3	5
4	D	371/372 (100%)	360 (97%)	11 (3%)	36	61
4	d	372/372 (100%)	365 (98%)	7 (2%)	52	75
5	E	327/328 (100%)	321 (98%)	6 (2%)	54	77
5	e	327/328 (100%)	321 (98%)	6 (2%)	54	77
6	F	61/61 (100%)	53 (87%)	8 (13%)	3	6
6	f	61/61 (100%)	52 (85%)	9 (15%)	2	4
7	G	95/95 (100%)	94 (99%)	1 (1%)	70	86
7	g	95/95 (100%)	94 (99%)	1 (1%)	70	86
8	H	65/70 (93%)	65 (100%)	0	100	100
8	h	70/70 (100%)	69 (99%)	1 (1%)	62	82
9	I	50/50 (100%)	32 (64%)	18 (36%)	0	0
9	i	50/50 (100%)	34 (68%)	16 (32%)	0	0
10	J	40/42 (95%)	38 (95%)	2 (5%)	20	39
10	j	41/42 (98%)	40 (98%)	1 (2%)	44	68
11	K	44/44 (100%)	19 (43%)	25 (57%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	k	44/44 (100%)	39 (89%)	5 (11%)	4	8
All	All	3515/3530 (100%)	3319 (94%)	196 (6%)	20	33

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	64	SER
1	A	69	ILE
1	A	71	ARG
1	A	151	SER
1	A	160	LEU
1	A	162	GLU
1	A	170	VAL
1	A	207	ASN
1	A	246	SER
1	A	264	THR
1	A	349	ILE
2	B	129	ASP
2	B	168	ARG
2	B	182	ASN
2	B	187	ARG
2	B	203	ARG
2	B	264	MET
2	B	280	GLU
3	C	92	ARG
3	C	95	GLU
3	C	123	VAL
3	C	136	PHE
3	C	170	ARG
3	C	179	ARG
3	C	180	THR
3	C	217	CYS
3	C	225	ILE
3	C	227	ASN
3	C	248	ARG
3	C	249	ILE
4	D	58	ARG
4	D	66	GLN
4	D	104	ARG
4	D	125	THR
4	D	180	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	240	ARG
4	D	335	ARG
4	D	345	ASN
4	D	477	TRP
4	D	479	ARG
4	D	480	PHE
5	E	156	SER
5	E	170	GLN
5	E	235	GLU
5	E	238	LEU
5	E	303	SER
5	E	421	ASP
6	F	35	GLU
6	F	36	GLN
6	F	38	GLU
6	F	49	ARG
6	F	51	GLU
6	F	64	GLU
6	F	73	ASP
6	F	91	LYS
7	G	15	GLU
9	I	6	LEU
9	I	7	THR
9	I	9	ARG
9	I	11	TYR
9	I	13	LEU
9	I	14	LEU
9	I	16	ARG
9	I	17	ARG
9	I	18	THR
9	I	21	PHE
9	I	25	ILE
9	I	30	LEU
9	I	34	ARG
9	I	43	ILE
9	I	47	ILE
9	I	60	TYR
9	I	61	GLU
9	I	63	LYS
10	J	15	ARG
10	J	39	ARG
11	K	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	K	2	LEU
11	K	6	SER
11	K	7	ARG
11	K	11	PHE
11	K	13	PRO
11	K	15	LEU
11	K	16	SER
11	K	18	THR
11	K	19	SER
11	K	20	ARG
11	K	22	VAL
11	K	27	ARG
11	K	30	VAL
11	K	34	LEU
11	K	35	PRO
11	K	38	SER
11	K	40	SER
11	K	42	VAL
11	K	43	LEU
11	K	46	LYS
11	K	48	SER
11	K	49	PHE
11	K	52	ARG
11	K	55	LEU
1	a	10	LEU
1	a	61	THR
1	a	64	SER
1	a	69	ILE
1	a	151	SER
1	a	160	LEU
1	a	162	GLU
1	a	170	VAL
1	a	246	SER
1	a	263	ASN
1	a	264	THR
1	a	349	ILE
2	b	123	SER
2	b	127	SER
2	b	164	GLU
2	b	165	MET
2	b	166	PHE
2	b	184	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	b	203	ARG
2	b	209	GLU
2	b	224	THR
2	b	276	ARG
2	b	279	SER
2	b	280	GLU
2	b	309	ARG
3	c	101	LYS
3	c	102	SER
3	c	104	LYS
3	c	105	GLU
3	c	106	SER
3	c	108	ASP
3	c	110	ARG
3	c	146	VAL
3	c	147	LEU
3	c	164	ASN
3	c	170	ARG
3	c	172	LYS
3	c	179	ARG
3	c	181	LYS
3	c	182	LYS
3	c	184	ILE
3	c	185	ASP
3	c	186	GLN
3	c	207	LYS
3	c	217	CYS
3	c	223	VAL
3	c	238	CYS
3	c	239	HIS
4	d	37	THR
4	d	70	THR
4	d	71	VAL
4	d	262	VAL
4	d	269	ARG
4	d	351	THR
4	d	477	TRP
5	e	69	SER
5	e	156	SER
5	e	227	HIS
5	e	235	GLU
5	e	238	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	e	421	ASP
6	f	28	ASP
6	f	35	GLU
6	f	36	GLN
6	f	38	GLU
6	f	49	ARG
6	f	51	GLU
6	f	64	GLU
6	f	73	ASP
6	f	91	LYS
7	g	15	GLU
8	h	40	ARG
9	i	10	LEU
9	i	12	SER
9	i	13	LEU
9	i	16	ARG
9	i	17	ARG
9	i	18	THR
9	i	21	PHE
9	i	25	ILE
9	i	30	LEU
9	i	34	ARG
9	i	43	ILE
9	i	47	ILE
9	i	60	TYR
9	i	61	GLU
9	i	62	ASN
9	i	63	LYS
10	j	20	THR
11	k	7	ARG
11	k	29	LEU
11	k	30	VAL
11	k	47	ARG
11	k	49	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	148	ASN
1	A	207	ASN
1	A	341	GLN
3	C	164	ASN

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Mol	Chain	Res	Type
3	C	219	HIS
4	D	87	ASN
4	D	193	GLN
4	D	305	GLN
4	D	464	GLN
5	E	75	ASN
5	E	155	GLN
5	E	212	HIS
5	E	290	GLN
5	E	399	GLN
5	E	415	GLN
6	F	39	GLN
6	F	80	HIS
10	J	49	ASN
1	a	148	ASN
1	a	341	GLN
2	b	116	GLN
3	c	178	HIS
3	c	200	HIS
4	d	55	ASN
4	d	87	ASN
4	d	193	GLN
4	d	286	HIS
4	d	305	GLN
4	d	345	ASN
4	d	469	ASN
5	e	75	ASN
5	e	155	GLN
5	e	212	HIS
5	e	227	HIS
5	e	290	GLN
5	e	399	GLN
5	e	415	GLN
6	f	39	GLN
8	h	65	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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	A1D6P	a	401	-	30,31,31	1.35	3 (10%)	32,44,44	1.48	5 (15%)
13	HEM	a	404	1	41,50,50	1.49	6 (14%)	45,82,82	1.63	9 (20%)
12	A1D6P	a	402	-	30,31,31	1.40	5 (16%)	32,44,44	1.48	5 (15%)
14	PEE	a	405	-	48,48,50	1.49	5 (10%)	51,53,55	1.31	4 (7%)
12	A1D6P	A	401	-	30,31,31	1.36	4 (13%)	32,44,44	1.48	5 (15%)
15	CDL	a	406	-	63,63,99	1.10	8 (12%)	69,75,111	1.17	4 (5%)
16	HEC	B	401	2	32,50,50	2.22	13 (40%)	24,82,82	2.85	9 (37%)
13	HEM	A	404	1	41,50,50	1.61	7 (17%)	45,82,82	2.23	17 (37%)
16	HEC	b	401	2	32,50,50	2.37	12 (37%)	24,82,82	2.15	5 (20%)
14	PEE	A	405	-	44,44,50	1.54	5 (11%)	46,49,55	1.38	5 (10%)
15	CDL	A	406	-	63,63,99	1.08	8 (12%)	69,75,111	1.14	4 (5%)
17	FES	c	301	3	0,4,4	-	-	-	-	-
13	HEM	a	403	1	41,50,50	1.56	6 (14%)	45,82,82	1.87	13 (28%)
12	A1D6P	A	402	-	30,31,31	1.41	5 (16%)	32,44,44	1.47	5 (15%)
17	FES	C	301	-	0,4,4	-	-	-	-	-
13	HEM	A	403	1	41,50,50	1.51	7 (17%)	45,82,82	1.59	11 (24%)

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
12	A1D6P	a	401	-	-	2/11/13/13	0/4/4/4
13	HEM	a	404	1	-	2/12/54/54	-
12	A1D6P	a	402	-	-	3/11/13/13	0/4/4/4
14	PEE	a	405	-	-	26/52/52/54	-
12	A1D6P	A	401	-	-	2/11/13/13	0/4/4/4
15	CDL	a	406	-	-	37/74/74/110	-
16	HEC	B	401	2	-	4/10/54/54	-
13	HEM	A	404	1	-	4/12/54/54	-
16	HEC	b	401	2	-	3/10/54/54	-
14	PEE	A	405	-	-	28/48/48/54	-
15	CDL	A	406	-	-	44/74/74/110	-
17	FES	c	301	3	-	-	0/1/1/1
13	HEM	a	403	1	-	6/12/54/54	-
12	A1D6P	A	402	-	-	3/11/13/13	0/4/4/4
17	FES	C	301	-	-	-	0/1/1/1
13	HEM	A	403	1	-	2/12/54/54	-

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	401	HEC	C3C-C2C	7.31	1.48	1.40
16	B	401	HEC	C2B-C3B	6.36	1.47	1.40
16	B	401	HEC	C3C-C2C	5.93	1.46	1.40
16	b	401	HEC	C2B-C3B	5.80	1.46	1.40
14	a	405	PEE	C39-C38	4.40	1.57	1.31
13	a	403	HEM	C3C-C2C	-4.36	1.34	1.40
13	A	404	HEM	C3C-C2C	-4.33	1.34	1.40
14	A	405	PEE	C39-C38	4.32	1.56	1.31
14	A	405	PEE	C18-C19	4.16	1.55	1.31
14	a	405	PEE	C18-C19	4.16	1.55	1.31
13	a	404	HEM	C3C-CAC	4.00	1.56	1.47
13	A	403	HEM	C3C-CAC	3.95	1.55	1.47
16	b	401	HEC	C4B-C3B	3.74	1.49	1.43
13	A	403	HEM	C3C-C2C	-3.63	1.35	1.40
13	a	404	HEM	C3C-C2C	-3.50	1.35	1.40
12	a	401	A1D6P	N2-N3	-3.49	1.32	1.39
12	A	401	A1D6P	N2-N3	-3.48	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	403	HEM	C3C-CAC	3.48	1.54	1.47
12	A	402	A1D6P	N2-N3	-3.46	1.32	1.39
12	a	402	A1D6P	N2-N3	-3.45	1.32	1.39
16	b	401	HEC	C2A-C3A	3.36	1.47	1.37
14	a	405	PEE	O3-C30	3.36	1.43	1.33
13	A	404	HEM	C3C-CAC	3.31	1.54	1.47
14	A	405	PEE	O3-C30	3.28	1.42	1.33
16	b	401	HEC	C3D-C2D	3.26	1.47	1.37
13	A	403	HEM	FE-ND	3.20	2.12	1.96
13	a	404	HEM	CAB-C3B	3.16	1.56	1.47
13	A	404	HEM	FE-ND	3.14	2.12	1.96
13	A	403	HEM	CAB-C3B	3.14	1.56	1.47
14	A	405	PEE	O2-C10	3.02	1.42	1.34
16	b	401	HEC	C3C-C4C	3.02	1.48	1.43
13	a	404	HEM	FE-ND	3.02	2.11	1.96
16	B	401	HEC	C3D-C2D	3.00	1.46	1.37
16	B	401	HEC	C2A-C3A	2.97	1.46	1.37
16	B	401	HEC	C3A-C4A	2.97	1.49	1.42
13	a	403	HEM	FE-ND	2.92	2.11	1.96
13	A	404	HEM	FE-NB	2.91	2.11	1.96
12	A	402	A1D6P	C9-C10	2.91	1.42	1.37
14	a	405	PEE	O2-C10	2.90	1.42	1.34
12	a	402	A1D6P	C9-C10	2.88	1.42	1.37
16	B	401	HEC	C2A-C1A	2.88	1.49	1.42
12	A	401	A1D6P	C9-C10	2.85	1.41	1.37
12	a	401	A1D6P	C9-C10	2.82	1.41	1.37
13	a	403	HEM	CAB-C3B	2.72	1.54	1.47
13	A	404	HEM	CAB-C3B	2.67	1.54	1.47
16	b	401	HEC	C2A-C1A	2.64	1.48	1.42
15	A	406	CDL	OB8-CB7	2.61	1.41	1.33
16	B	401	HEC	C4D-CHA	2.54	1.48	1.41
15	a	406	CDL	OA6-CA4	-2.54	1.40	1.46
16	b	401	HEC	C1C-CHC	2.54	1.48	1.41
14	a	405	PEE	O2-C2	-2.51	1.40	1.46
15	A	406	CDL	OA6-CA4	-2.50	1.40	1.46
16	b	401	HEC	C3A-C4A	2.49	1.48	1.42
16	b	401	HEC	C1D-CHD	2.49	1.47	1.41
13	a	403	HEM	FE-NB	2.48	2.09	1.96
16	B	401	HEC	C4B-C3B	2.47	1.47	1.43
12	A	402	A1D6P	O2-C18	-2.44	1.18	1.22
15	a	406	CDL	OA6-CA5	2.43	1.41	1.34
12	A	401	A1D6P	O2-C18	-2.43	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	401	HEC	C4D-CHA	2.41	1.47	1.41
16	B	401	HEC	C1B-CHB	2.41	1.47	1.41
12	a	402	A1D6P	O2-C18	-2.41	1.18	1.22
15	A	406	CDL	OA8-CA7	2.39	1.40	1.33
15	a	406	CDL	OA8-CA7	2.38	1.40	1.33
12	a	401	A1D6P	O2-C18	-2.37	1.18	1.22
15	a	406	CDL	OB8-CB7	2.35	1.40	1.33
15	a	406	CDL	OB6-CB4	-2.33	1.40	1.46
14	A	405	PEE	O2-C2	-2.32	1.40	1.46
15	A	406	CDL	OA8-CA6	-2.29	1.39	1.45
13	A	404	HEM	C3B-C2B	-2.24	1.32	1.37
15	A	406	CDL	OB6-CB4	-2.24	1.41	1.46
15	a	406	CDL	OB8-CB6	-2.22	1.40	1.45
15	a	406	CDL	OB6-CB5	2.22	1.40	1.34
13	A	403	HEM	CAA-C2A	2.20	1.55	1.52
16	b	401	HEC	C1B-CHB	2.20	1.47	1.41
15	A	406	CDL	OA6-CA5	2.20	1.40	1.34
13	a	404	HEM	CAA-C2A	2.19	1.55	1.52
12	a	402	A1D6P	C1-N1	2.18	1.46	1.43
16	B	401	HEC	C1D-CHD	2.18	1.47	1.41
13	a	403	HEM	C3B-C2B	-2.15	1.32	1.37
16	B	401	HEC	C3C-C4C	2.15	1.46	1.43
12	A	402	A1D6P	C1-N1	2.14	1.46	1.43
12	a	402	A1D6P	C8-N2	-2.14	1.31	1.34
15	a	406	CDL	OA8-CA6	-2.14	1.40	1.45
12	A	402	A1D6P	C8-N2	-2.14	1.31	1.34
15	A	406	CDL	OB8-CB6	-2.11	1.40	1.45
15	A	406	CDL	OB6-CB5	2.09	1.40	1.34
13	A	403	HEM	CMB-C2B	2.07	1.55	1.50
16	B	401	HEC	O2D-CGD	-2.06	1.23	1.30
13	A	404	HEM	CAD-C3D	2.05	1.56	1.51
12	A	401	A1D6P	C8-N2	-2.04	1.31	1.34
13	A	403	HEM	CMD-C2D	2.04	1.55	1.50
13	a	404	HEM	CMB-C2B	2.01	1.55	1.50
16	B	401	HEC	O2A-CGA	-2.00	1.24	1.30

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	401	HEC	C1D-C2D-C3D	-7.06	102.08	107.00
16	b	401	HEC	C1D-C2D-C3D	-5.85	102.92	107.00
13	A	404	HEM	CAD-C3D-C4D	5.85	134.88	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	401	HEC	CBD-CAD-C3D	-5.84	102.65	112.62
16	B	401	HEC	CMB-C2B-C3B	5.80	132.64	125.82
16	B	401	HEC	CMC-C2C-C3C	5.50	132.29	125.82
16	b	401	HEC	CMC-C2C-C3C	5.36	132.13	125.82
13	A	404	HEM	CAD-C3D-C2D	-5.18	118.23	127.88
14	A	405	PEE	O2-C10-C11	4.96	122.20	111.50
13	a	403	HEM	CBA-CAA-C2A	-4.76	104.50	112.62
14	a	405	PEE	O2-C10-C11	4.63	121.47	111.50
15	a	406	CDL	OB6-CB5-C51	4.35	120.87	111.50
15	a	406	CDL	OA6-CA5-C11	4.31	120.79	111.50
12	A	401	A1D6P	C19-N4-N5	4.12	128.46	121.14
12	a	401	A1D6P	C19-N4-N5	4.09	128.41	121.14
15	A	406	CDL	OA6-CA5-C11	3.81	119.72	111.50
13	A	404	HEM	CHC-C4B-C3B	3.76	130.32	124.57
13	a	404	HEM	C1B-NB-C4B	3.75	108.94	105.07
13	a	403	HEM	CHC-C4B-C3B	3.74	130.30	124.57
13	A	403	HEM	C1B-NB-C4B	3.70	108.89	105.07
14	A	405	PEE	C3-C2-C1	-3.69	103.06	111.79
12	a	401	A1D6P	C1-N1-N6	3.65	126.99	120.39
12	A	401	A1D6P	C1-N1-N6	3.63	126.94	120.39
15	A	406	CDL	OB6-CB5-C51	3.51	119.06	111.50
13	a	404	HEM	C4C-CHD-C1D	3.49	127.17	122.56
13	a	403	HEM	C1B-NB-C4B	3.47	108.65	105.07
16	B	401	HEC	CBA-CAA-C2A	-3.40	106.88	112.60
13	A	403	HEM	C4D-ND-C1D	3.37	108.55	105.07
13	A	404	HEM	CHA-C4D-C3D	3.32	131.56	125.33
13	a	404	HEM	C4D-ND-C1D	3.30	108.48	105.07
13	A	403	HEM	C4C-CHD-C1D	3.29	126.90	122.56
13	A	404	HEM	C1B-NB-C4B	3.17	108.35	105.07
13	A	404	HEM	C4C-CHD-C1D	3.17	126.74	122.56
13	A	404	HEM	C4D-ND-C1D	3.12	108.30	105.07
16	b	401	HEC	CMB-C2B-C3B	3.10	129.46	125.82
12	a	402	A1D6P	C9-N3-N2	-3.09	109.58	112.72
12	A	402	A1D6P	C9-N3-N2	-3.05	109.62	112.72
12	A	402	A1D6P	C1-N1-N6	3.00	125.80	120.39
12	a	402	A1D6P	C1-N1-N6	2.99	125.79	120.39
13	A	403	HEM	CMB-C2B-C1B	-2.98	120.50	125.04
13	a	403	HEM	C4C-CHD-C1D	2.93	126.43	122.56
13	a	403	HEM	C3B-C2B-C1B	2.93	108.66	106.49
13	A	404	HEM	C3B-C2B-C1B	2.91	108.65	106.49
13	A	404	HEM	CBA-CAA-C2A	-2.91	107.66	112.62
15	A	406	CDL	OB8-CB7-C71	2.90	121.00	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	403	HEM	C4B-CHC-C1C	2.89	126.38	122.56
13	a	404	HEM	CMB-C2B-C1B	-2.85	120.70	125.04
13	A	404	HEM	CHA-C4D-ND	-2.83	120.89	124.38
13	A	404	HEM	CMC-C2C-C3C	2.82	129.95	124.68
13	a	403	HEM	C4D-ND-C1D	2.80	107.97	105.07
13	a	403	HEM	CMC-C2C-C3C	2.75	129.82	124.68
13	A	403	HEM	C4B-CHC-C1C	2.71	126.14	122.56
13	a	404	HEM	C4B-CHC-C1C	2.66	126.07	122.56
13	A	404	HEM	CBD-CAD-C3D	2.62	119.91	112.63
15	A	406	CDL	OA8-CA7-C31	2.62	120.14	111.91
13	A	404	HEM	CAB-C3B-C2B	-2.62	119.97	128.60
15	a	406	CDL	OB8-CB7-C71	2.61	120.11	111.91
13	a	404	HEM	CMC-C2C-C3C	2.59	129.53	124.68
16	b	401	HEC	CMA-C3A-C2A	2.57	129.80	124.94
13	a	403	HEM	CAD-CBD-CGD	-2.57	108.08	113.60
14	a	405	PEE	O3-C30-C31	2.55	119.92	111.91
15	a	406	CDL	OA8-CA7-C31	2.55	119.91	111.91
12	a	402	A1D6P	C10-C8-N2	-2.54	107.77	110.44
14	a	405	PEE	C3-C2-C1	-2.53	105.80	111.79
12	A	402	A1D6P	C10-C8-N2	-2.51	107.80	110.44
13	a	403	HEM	CAB-C3B-C2B	-2.50	120.35	128.60
13	A	404	HEM	C4B-CHC-C1C	2.50	125.86	122.56
12	a	402	A1D6P	C19-N4-N5	2.47	125.53	121.14
12	A	402	A1D6P	C19-N4-N5	2.46	125.51	121.14
16	B	401	HEC	CAA-CBA-CGA	-2.44	106.93	113.76
16	B	401	HEC	CAD-CBD-CGD	-2.42	106.99	113.76
13	A	404	HEM	C3D-C4D-ND	-2.35	107.55	110.17
12	a	401	A1D6P	C9-N3-N2	-2.34	110.34	112.72
12	A	401	A1D6P	C9-N3-N2	-2.33	110.35	112.72
13	A	403	HEM	CMC-C2C-C3C	2.32	129.01	124.68
13	a	404	HEM	C3B-C2B-C1B	2.31	108.20	106.49
13	A	403	HEM	C3B-C2B-C1B	2.27	108.17	106.49
12	a	401	A1D6P	C10-C8-N2	-2.25	108.07	110.44
12	A	401	A1D6P	C10-C8-N2	-2.23	108.09	110.44
16	B	401	HEC	CMD-C2D-C3D	2.21	129.10	124.94
12	A	401	A1D6P	C9-C10-C8	-2.21	103.79	105.54
13	A	403	HEM	C3D-C4D-ND	-2.20	107.71	110.17
12	a	401	A1D6P	C9-C10-C8	-2.18	103.81	105.54
14	A	405	PEE	O3-C30-C31	2.18	118.76	111.91
13	a	403	HEM	C3D-C4D-ND	-2.16	107.76	110.17
16	B	401	HEC	CMA-C3A-C2A	2.16	129.01	124.94
13	A	404	HEM	C1D-C2D-C3D	2.14	109.20	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	403	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
13	a	403	HEM	CAD-C3D-C2D	-2.10	123.96	127.88
13	a	404	HEM	C3D-C4D-ND	-2.10	107.83	110.17
14	a	405	PEE	C17-C18-C19	-2.08	108.74	124.73
12	A	402	A1D6P	C9-C10-C8	-2.08	103.89	105.54
13	a	404	HEM	CHB-C1B-NB	2.06	126.92	124.38
16	b	401	HEC	CBD-CAD-C3D	-2.05	109.12	112.62
14	A	405	PEE	C12-C11-C10	-2.04	106.19	113.62
12	a	402	A1D6P	C9-C10-C8	-2.04	103.92	105.54
13	A	404	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
13	A	403	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
14	A	405	PEE	C17-C18-C19	-2.02	109.26	124.73
13	A	403	HEM	CHB-C1B-NB	2.01	126.86	124.38
13	A	403	HEM	C2D-C1D-ND	-2.00	107.48	109.88

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	401	A1D6P	C12-C11-N3-C9
12	A	401	A1D6P	C16-C11-N3-C9
12	A	402	A1D6P	C16-C11-N3-C9
12	a	401	A1D6P	C12-C11-N3-C9
12	a	401	A1D6P	C16-C11-N3-C9
12	a	402	A1D6P	C16-C11-N3-C9
13	A	404	HEM	C2D-C3D-CAD-CBD
13	A	404	HEM	C4D-C3D-CAD-CBD
14	A	405	PEE	C1-O3P-P-O4P
14	A	405	PEE	C4-O4P-P-O1P
14	A	405	PEE	C5-C4-O4P-P
14	A	405	PEE	O4P-C4-C5-N
14	a	405	PEE	C1-O3P-P-O1P
14	a	405	PEE	C1-O3P-P-O4P
14	a	405	PEE	C5-C4-O4P-P
14	a	405	PEE	O4P-C4-C5-N
15	A	406	CDL	CB2-OB2-PB2-OB3
15	A	406	CDL	CB2-OB2-PB2-OB4
15	A	406	CDL	CB2-OB2-PB2-OB5
15	A	406	CDL	OB9-CB7-OB8-CB6
15	A	406	CDL	C71-CB7-OB8-CB6
15	a	406	CDL	CA2-OA2-PA1-OA3
15	a	406	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
15	a	406	CDL	CA3-OA5-PA1-OA2
15	a	406	CDL	CA3-OA5-PA1-OA3
15	a	406	CDL	CA3-OA5-PA1-OA4
15	a	406	CDL	OB6-CB4-CB6-OB8
15	a	406	CDL	OB7-CB5-OB6-CB4
16	b	401	HEC	C3D-CAD-CBD-CGD
15	A	406	CDL	OA9-CA7-OA8-CA6
15	a	406	CDL	OB9-CB7-OB8-CB6
15	a	406	CDL	C71-CB7-OB8-CB6
14	a	405	PEE	O5-C30-O3-C3
15	A	406	CDL	OB7-CB5-OB6-CB4
14	a	405	PEE	C31-C30-O3-C3
15	A	406	CDL	C31-CA7-OA8-CA6
15	a	406	CDL	C51-CB5-OB6-CB4
14	A	405	PEE	C14-C15-C16-C17
14	A	405	PEE	C37-C38-C39-C40
15	A	406	CDL	O1-C1-CA2-OA2
15	A	406	CDL	O1-C1-CB2-OB2
15	A	406	CDL	C11-CA5-OA6-CA4
15	A	406	CDL	C51-CB5-OB6-CB4
15	A	406	CDL	CB2-C1-CA2-OA2
15	A	406	CDL	OA7-CA5-OA6-CA4
14	a	405	PEE	C14-C15-C16-C17
15	A	406	CDL	CA7-C31-C32-C33
15	A	406	CDL	CA5-C11-C12-C13
14	a	405	PEE	C17-C18-C19-C20
14	A	405	PEE	C4-O4P-P-O3P
14	a	405	PEE	C4-O4P-P-O3P
15	A	406	CDL	CA2-C1-CB2-OB2
15	a	406	CDL	C31-CA7-OA8-CA6
15	A	406	CDL	C31-C32-C33-C34
15	a	406	CDL	C11-CA5-OA6-CA4
14	A	405	PEE	C21-C22-C23-C24
14	a	405	PEE	C12-C13-C14-C15
15	a	406	CDL	C11-C12-C13-C14
15	a	406	CDL	C52-C53-C54-C55
14	A	405	PEE	C33-C34-C35-C36
15	a	406	CDL	OA7-CA5-OA6-CA4
15	A	406	CDL	CB5-C51-C52-C53
15	a	406	CDL	C72-C73-C74-C75
14	a	405	PEE	C22-C23-C24-C25
15	a	406	CDL	OA9-CA7-OA8-CA6

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
15	A	406	CDL	C54-C55-C56-C57
14	A	405	PEE	C12-C13-C14-C15
14	A	405	PEE	C30-C31-C32-C33
14	A	405	PEE	C11-C10-O2-C2
14	a	405	PEE	C11-C10-O2-C2
14	A	405	PEE	O3P-C1-C2-O2
15	A	406	CDL	OA5-CA3-CA4-OA6
15	A	406	CDL	C74-C75-C76-C77
14	A	405	PEE	O4-C10-O2-C2
14	a	405	PEE	O4-C10-O2-C2
14	A	405	PEE	O3P-C1-C2-C3
15	A	406	CDL	OA5-CA3-CA4-CA6
15	A	406	CDL	OB5-CB3-CB4-CB6
15	a	406	CDL	CA4-CA6-OA8-CA7
15	A	406	CDL	CA3-CA4-CA6-OA8
15	a	406	CDL	CB3-CB4-CB6-OB8
15	A	406	CDL	C72-C73-C74-C75
12	A	402	A1D6P	C12-C11-N3-C9
12	a	402	A1D6P	C12-C11-N3-C9
14	a	405	PEE	C42-C43-C44-C45
15	A	406	CDL	CB6-CB4-OB6-CB5
15	A	406	CDL	C33-C34-C35-C36
14	A	405	PEE	C13-C14-C15-C16
15	A	406	CDL	C51-C52-C53-C54
14	a	405	PEE	C37-C38-C39-C40
14	a	405	PEE	C23-C24-C25-C26
15	a	406	CDL	CB5-C51-C52-C53
15	A	406	CDL	C1-CB2-OB2-PB2
13	a	403	HEM	C3D-CAD-CBD-CGD
14	A	405	PEE	C1-C2-C3-O3
14	a	405	PEE	C33-C34-C35-C36
14	A	405	PEE	C10-C11-C12-C13
15	a	406	CDL	OB5-CB3-CB4-OB6
15	a	406	CDL	CB7-C71-C72-C73
15	A	406	CDL	OA6-CA4-CA6-OA8
15	A	406	CDL	OB6-CB4-CB6-OB8
15	a	406	CDL	CA4-CA3-OA5-PA1
14	A	405	PEE	C38-C39-C40-C41
14	a	405	PEE	C11-C12-C13-C14
14	A	405	PEE	C16-C17-C18-C19
14	A	405	PEE	C2-C1-O3P-P
13	A	404	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	A	405	PEE	O2-C2-C3-O3
15	a	406	CDL	CA5-C11-C12-C13
15	A	406	CDL	CA3-OA5-PA1-OA2
14	a	405	PEE	C4-O4P-P-O2P
15	a	406	CDL	C14-C15-C16-C17
15	A	406	CDL	OB5-CB3-CB4-OB6
15	a	406	CDL	C12-C13-C14-C15
12	A	402	A1D6P	C12-C11-N3-N2
12	a	402	A1D6P	C12-C11-N3-N2
15	a	406	CDL	C71-C72-C73-C74
14	a	405	PEE	C32-C33-C34-C35
14	A	405	PEE	C34-C35-C36-C37
15	A	406	CDL	C75-C76-C77-C78
15	A	406	CDL	CA6-CA4-OA6-CA5
15	a	406	CDL	OB5-CB3-CB4-CB6
14	a	405	PEE	C2-C1-O3P-P
15	a	406	CDL	CB3-OB5-PB2-OB2
15	A	406	CDL	CB3-CB4-CB6-OB8
14	a	405	PEE	C38-C39-C40-C41
15	A	406	CDL	C53-C54-C55-C56
15	A	406	CDL	CA4-CA3-OA5-PA1
14	A	405	PEE	C36-C37-C38-C39
15	A	406	CDL	C55-C56-C57-C58
14	a	405	PEE	C13-C14-C15-C16
15	A	406	CDL	C15-C16-C17-C18
14	a	405	PEE	C35-C36-C37-C38
15	a	406	CDL	C54-C55-C56-C57
15	A	406	CDL	C73-C74-C75-C76
14	a	405	PEE	C40-C41-C42-C43
15	a	406	CDL	C13-C14-C15-C16
13	A	403	HEM	CAA-CBA-CGA-O2A
13	a	404	HEM	CAA-CBA-CGA-O2A
15	a	406	CDL	C32-C31-CA7-OA8
13	a	403	HEM	CAA-CBA-CGA-O2A
14	A	405	PEE	C24-C25-C26-C27
15	a	406	CDL	C53-C54-C55-C56
15	A	406	CDL	C11-C12-C13-C14
16	b	401	HEC	CAD-CBD-CGD-O1D
13	a	403	HEM	CAA-CBA-CGA-O1A
13	a	403	HEM	C4B-C3B-CAB-CBB
14	a	405	PEE	C18-C19-C20-C21
15	a	406	CDL	C51-C52-C53-C54

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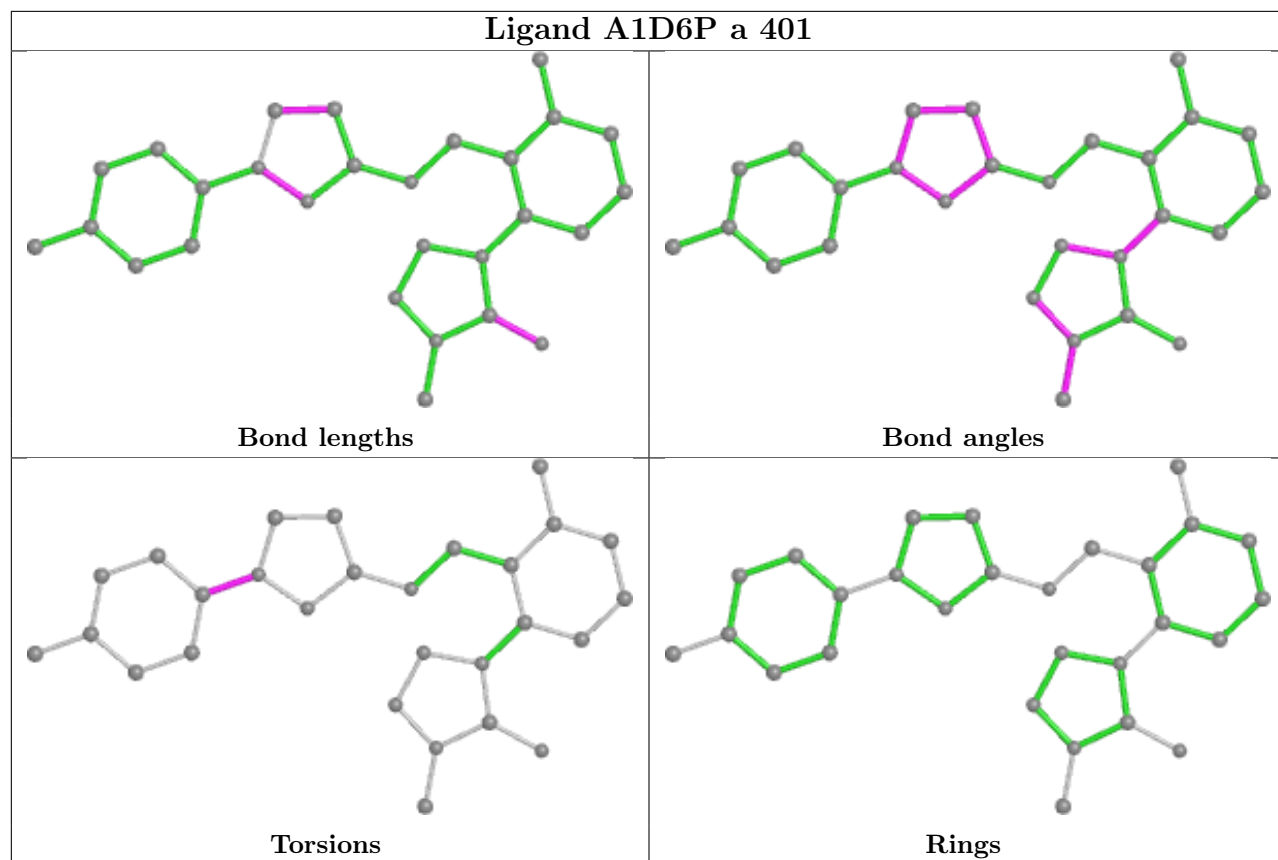
*Continued from previous page...*

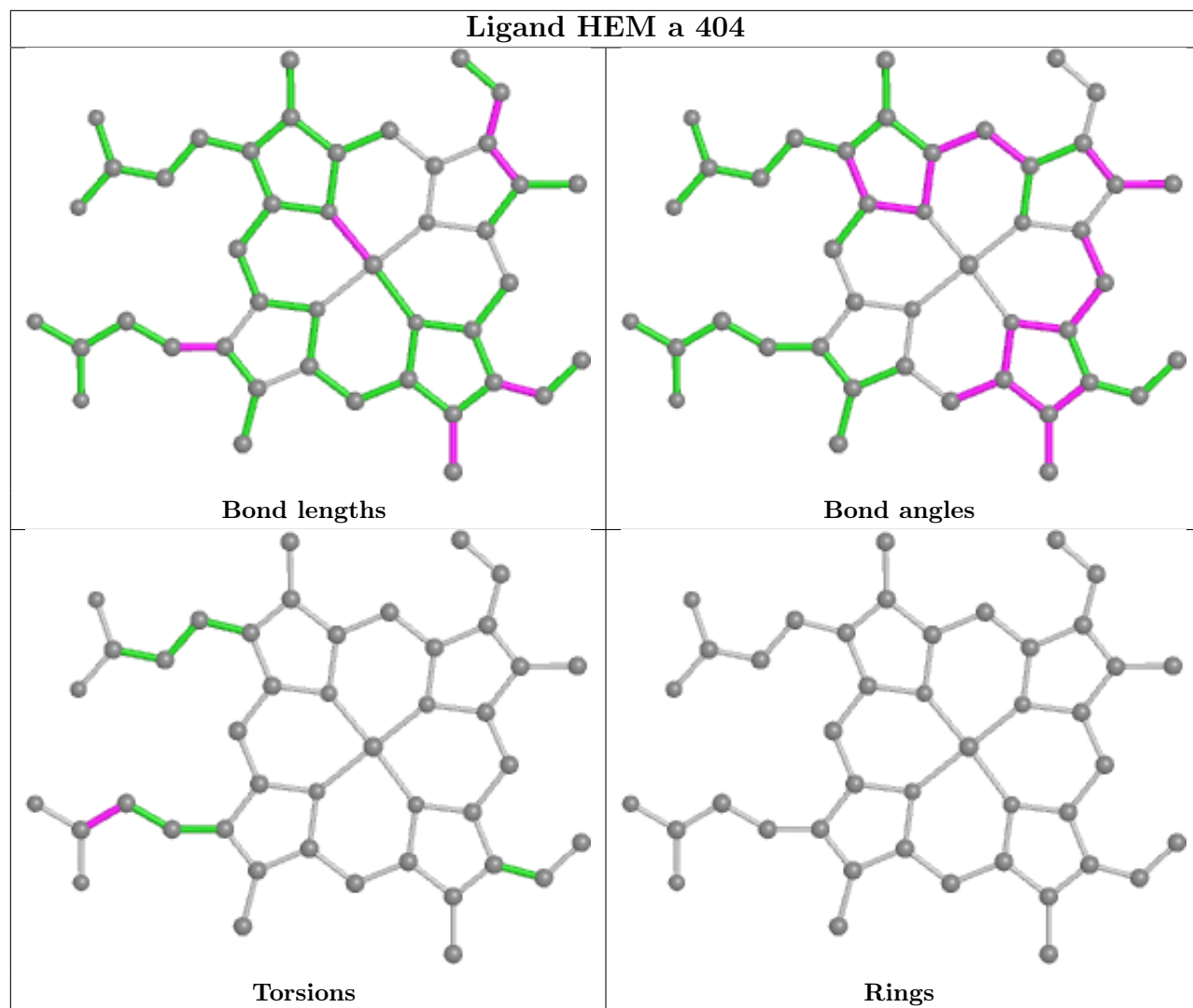
Mol	Chain	Res	Type	Atoms
16	b	401	HEC	CAD-CBD-CGD-O2D
13	a	403	HEM	CAD-CBD-CGD-O1D
13	a	404	HEM	CAA-CBA-CGA-O1A
15	a	406	CDL	C12-C11-CA5-OA6
13	A	403	HEM	CAA-CBA-CGA-O1A
14	A	405	PEE	C22-C23-C24-C25
14	A	405	PEE	C20-C21-C22-C23
15	a	406	CDL	C32-C31-CA7-OA9
16	B	401	HEC	CAA-CBA-CGA-O2A
15	A	406	CDL	CA3-OA5-PA1-OA3
16	B	401	HEC	CAD-CBD-CGD-O2D
16	B	401	HEC	CAA-CBA-CGA-O1A
13	a	403	HEM	CAD-CBD-CGD-O2D
16	B	401	HEC	CAD-CBD-CGD-O1D
13	A	404	HEM	CAA-CBA-CGA-O1A
14	A	405	PEE	O3-C30-C31-C32
15	a	406	CDL	C12-C11-CA5-OA7

There are no ring outliers.

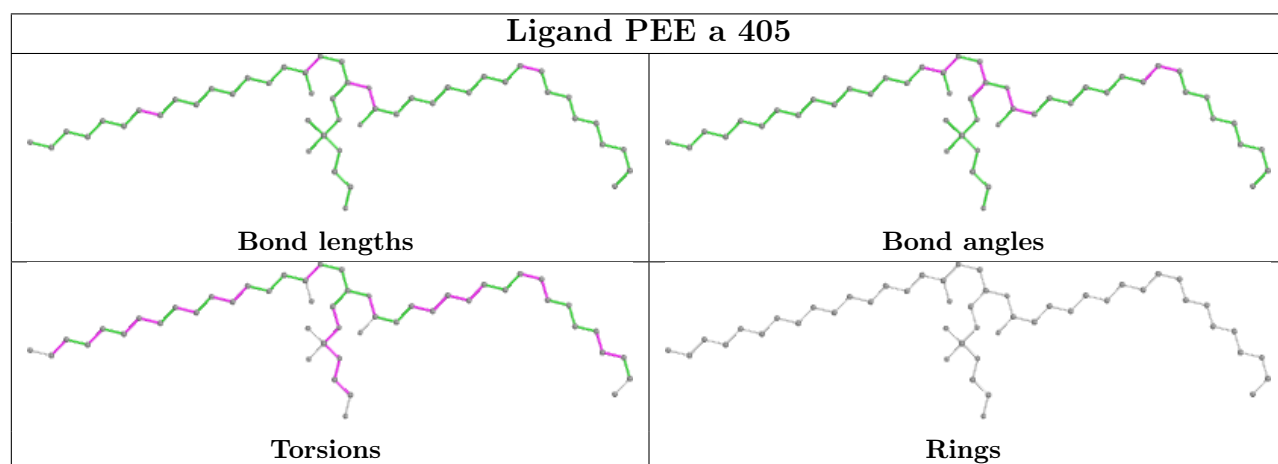
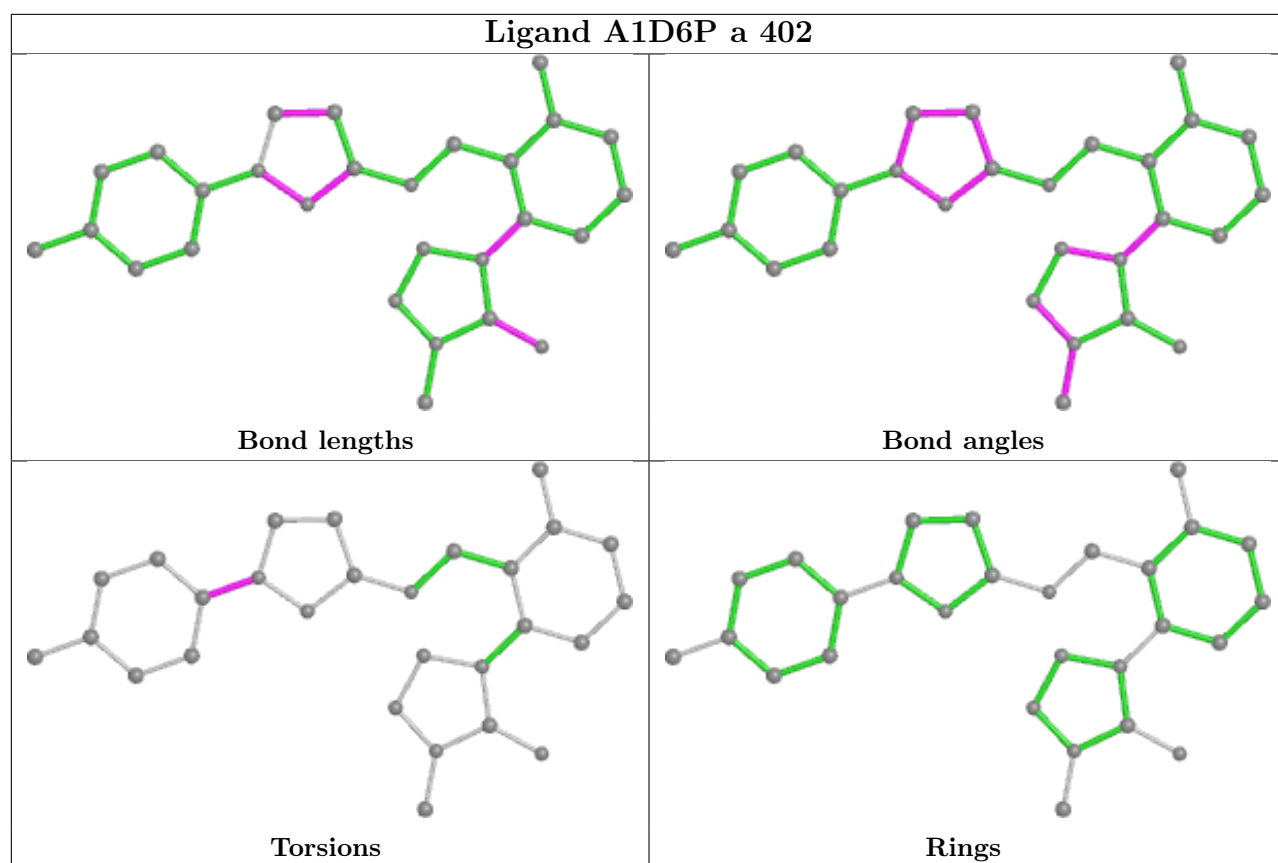
No monomer is involved in short contacts.

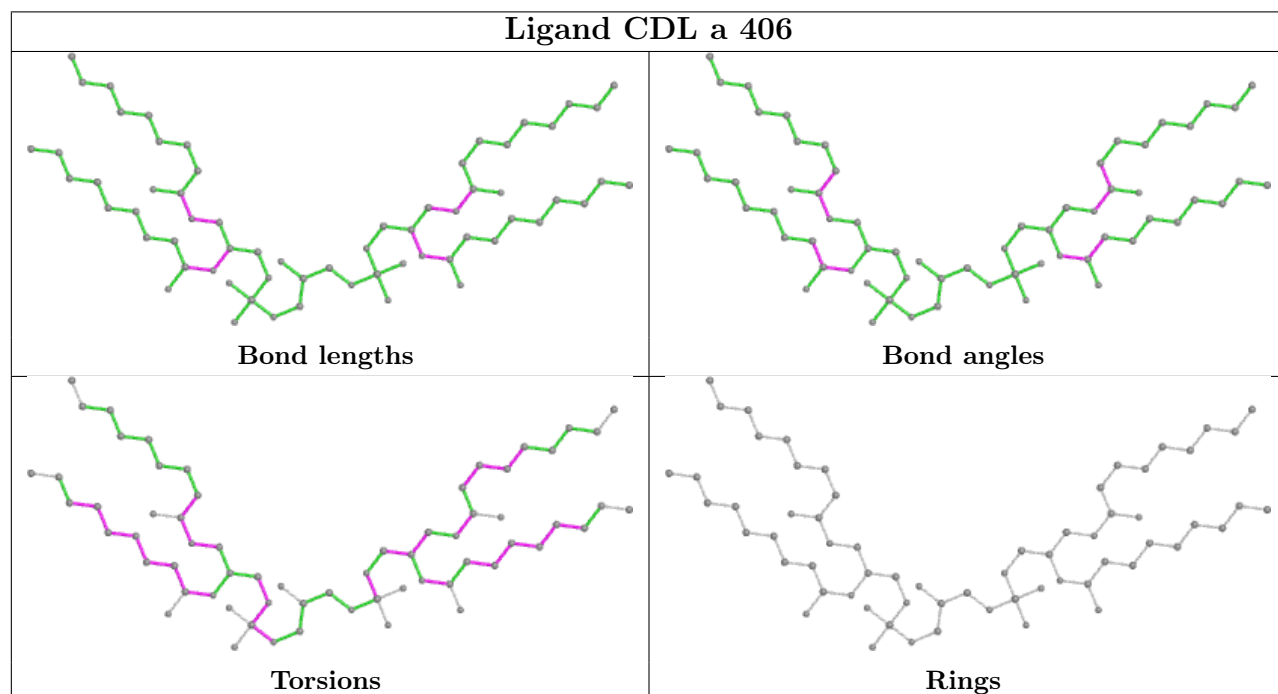
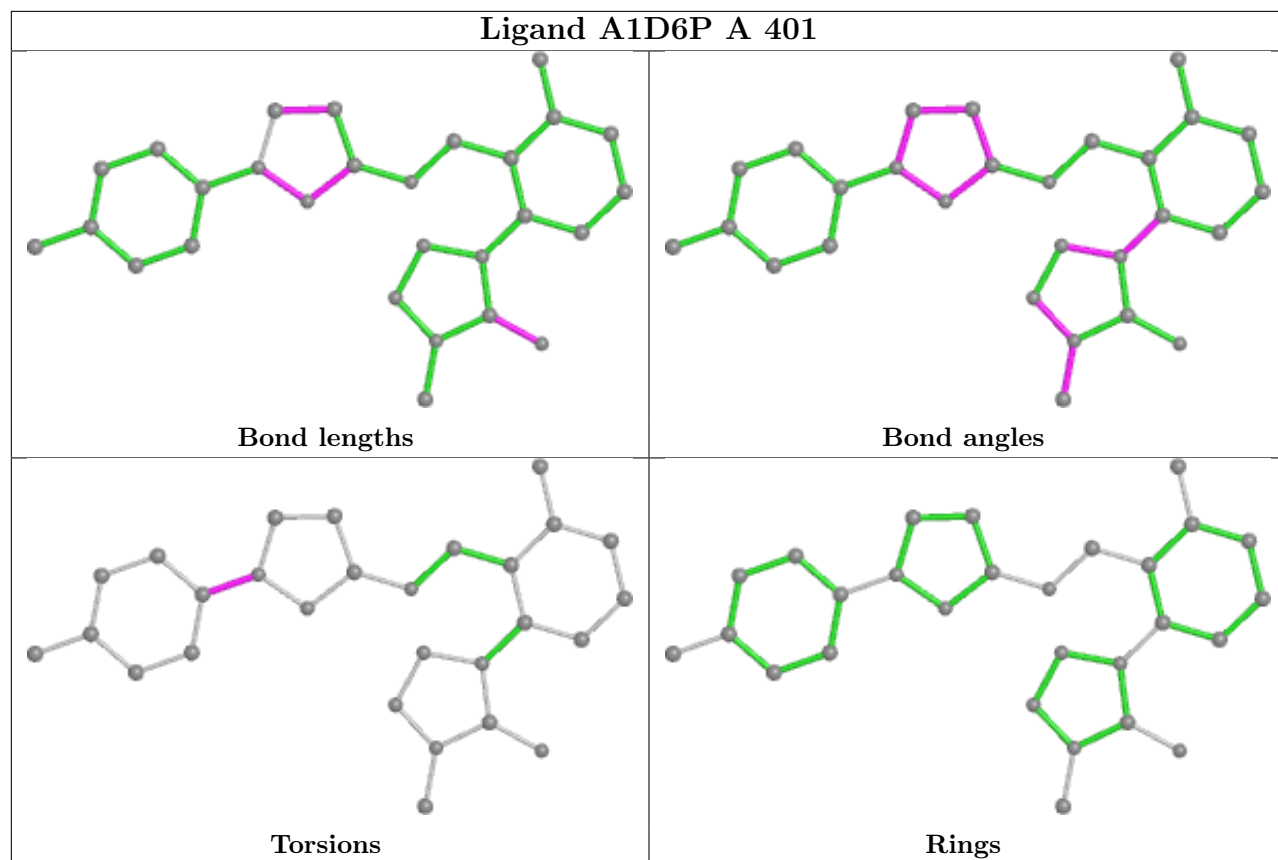
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

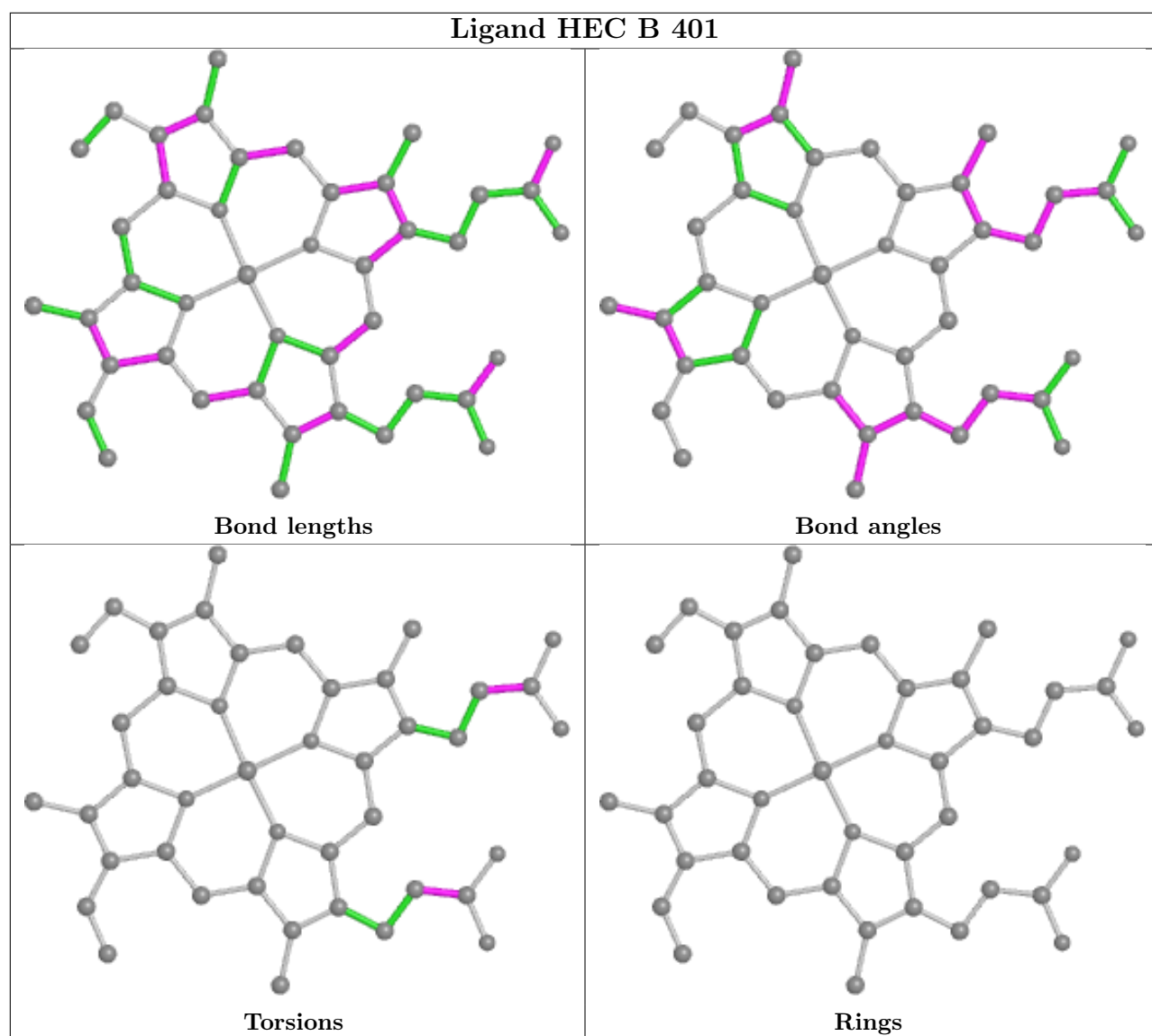


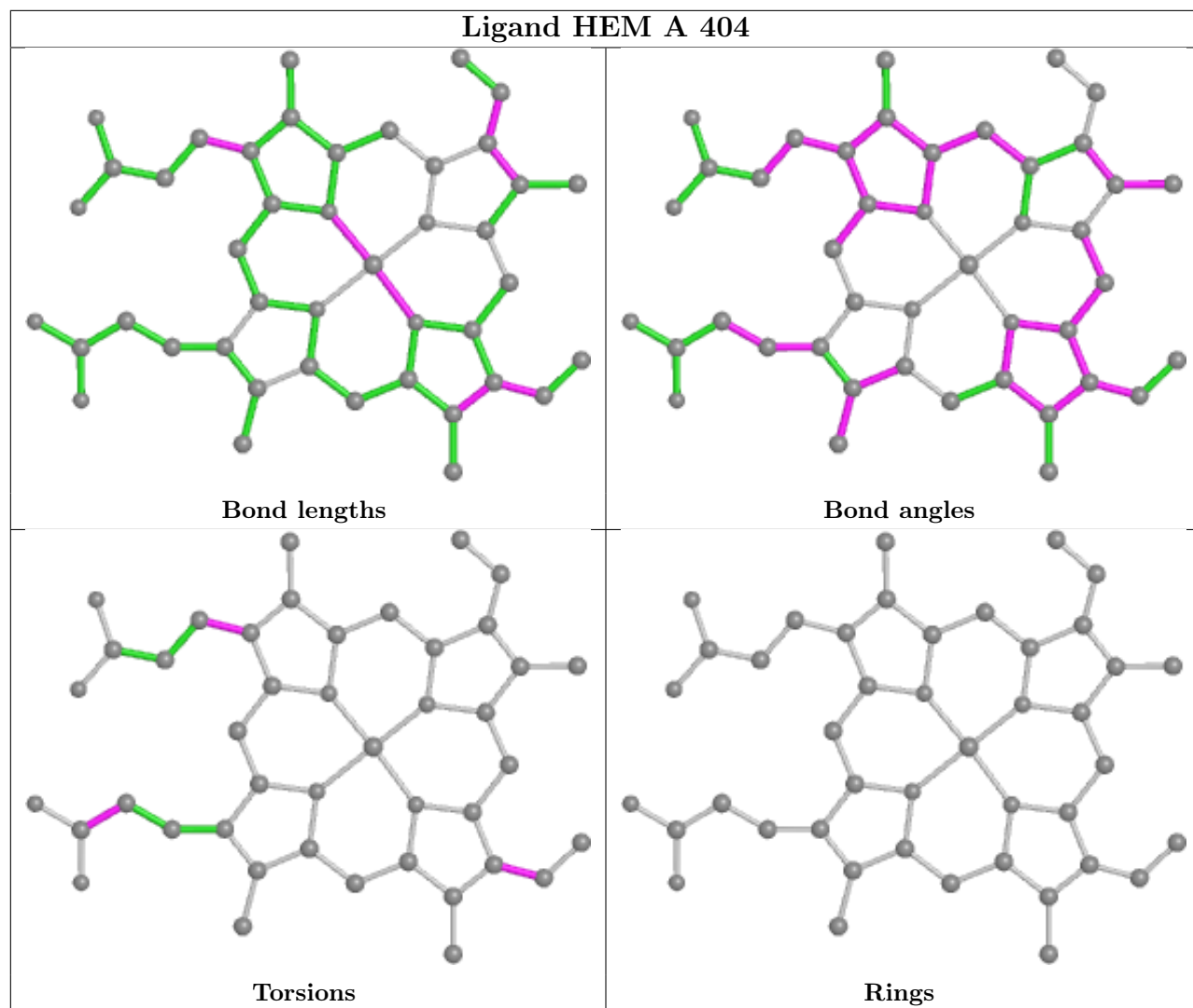


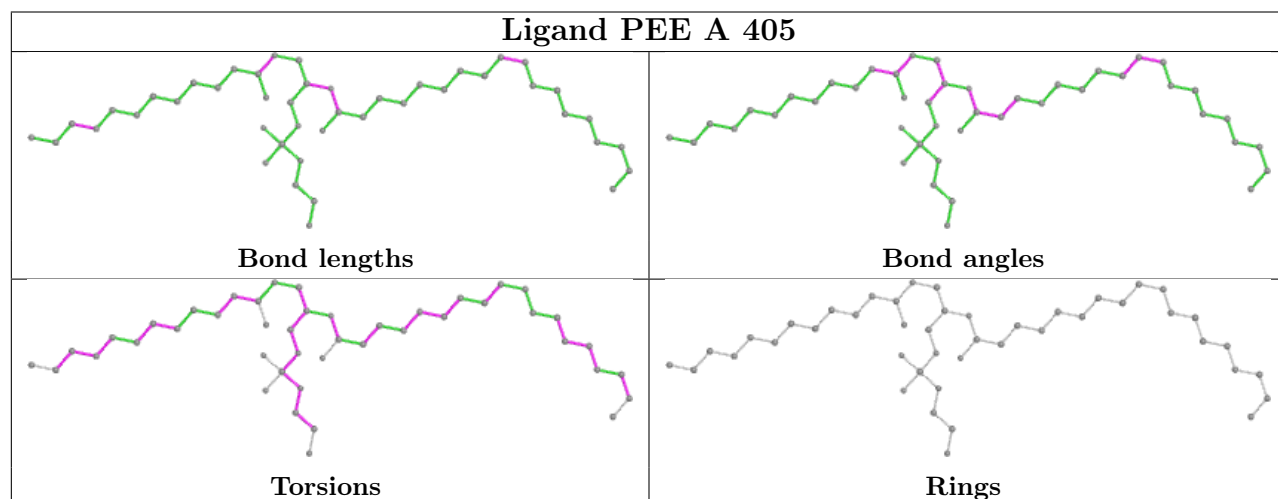
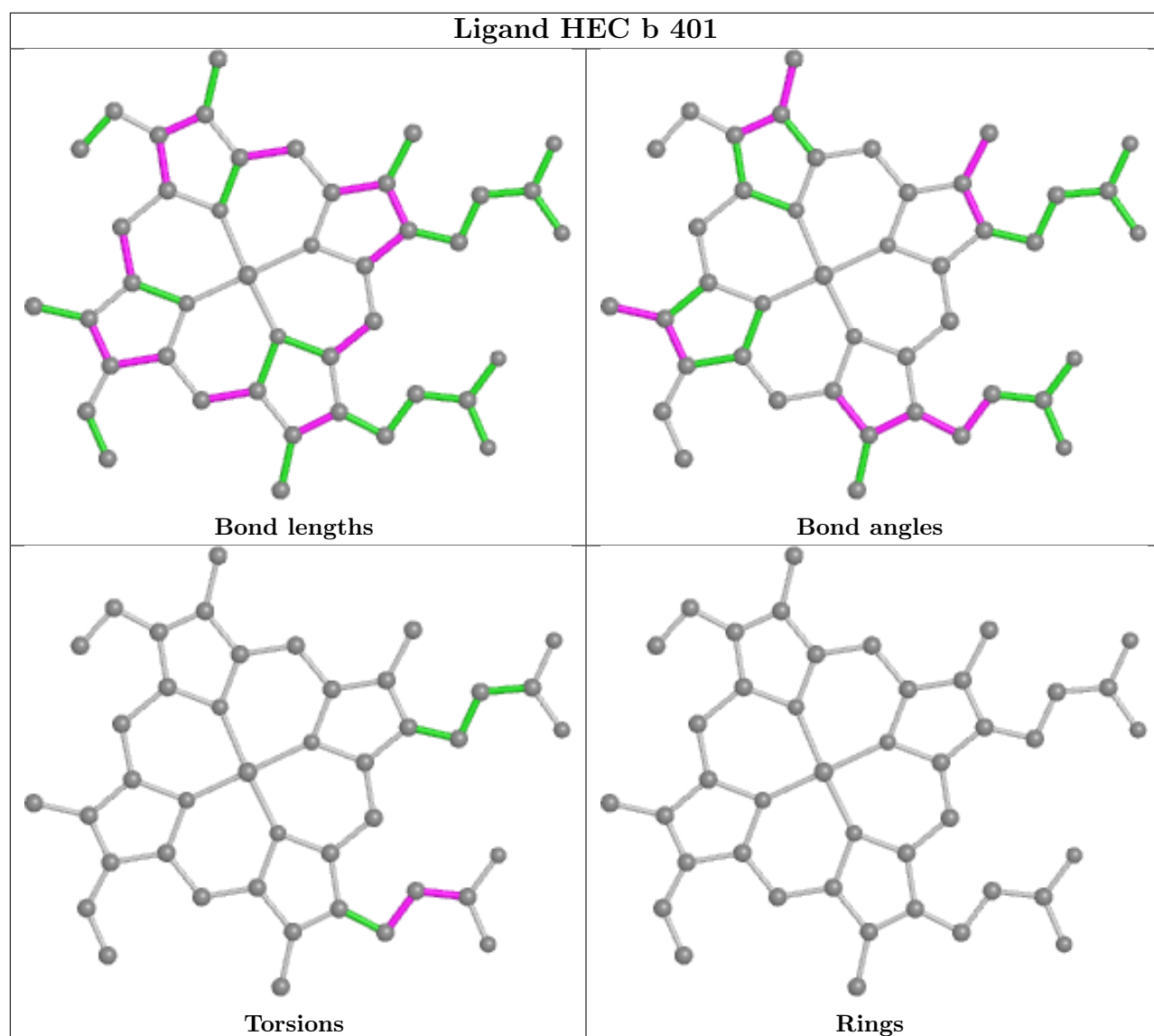


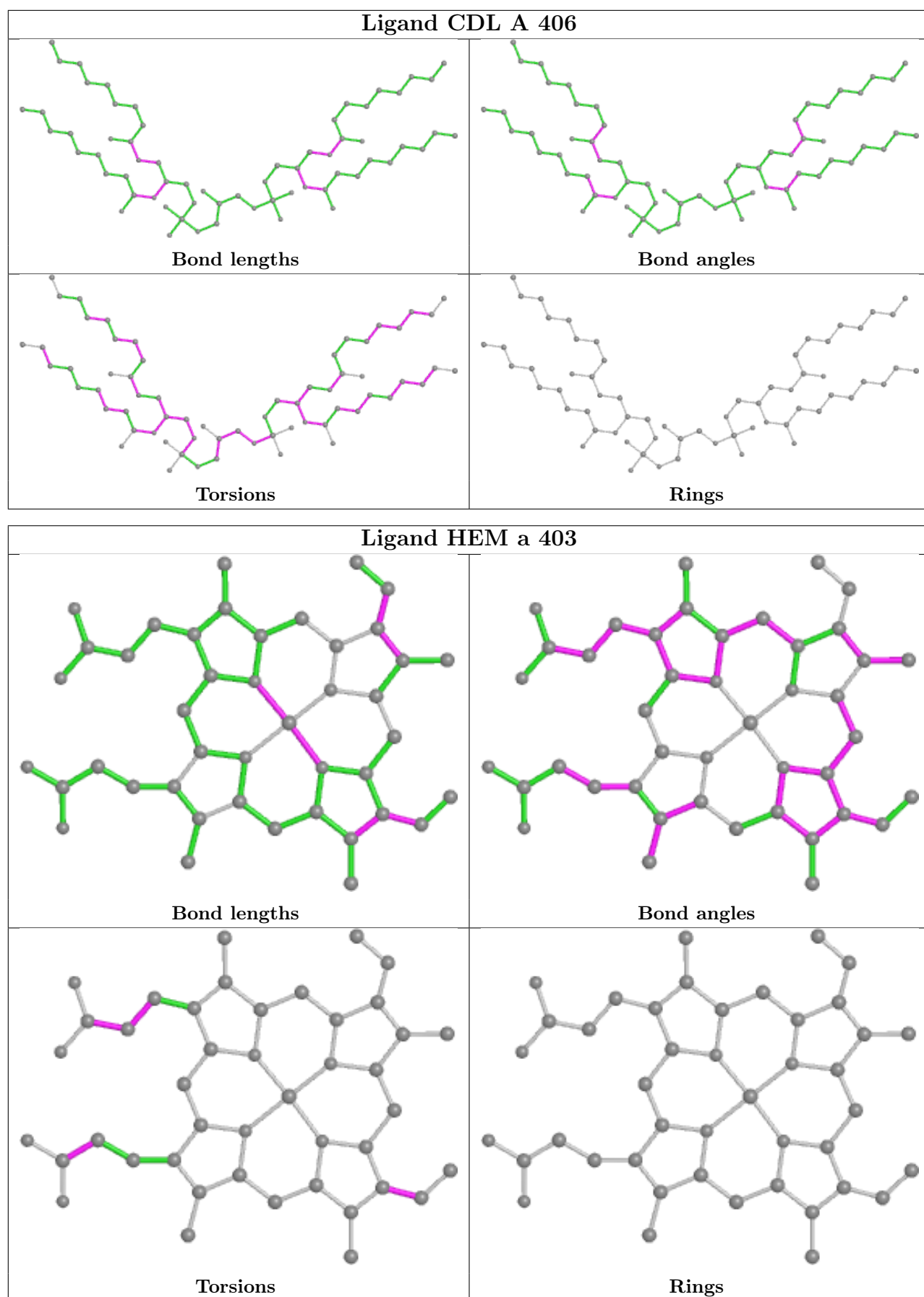


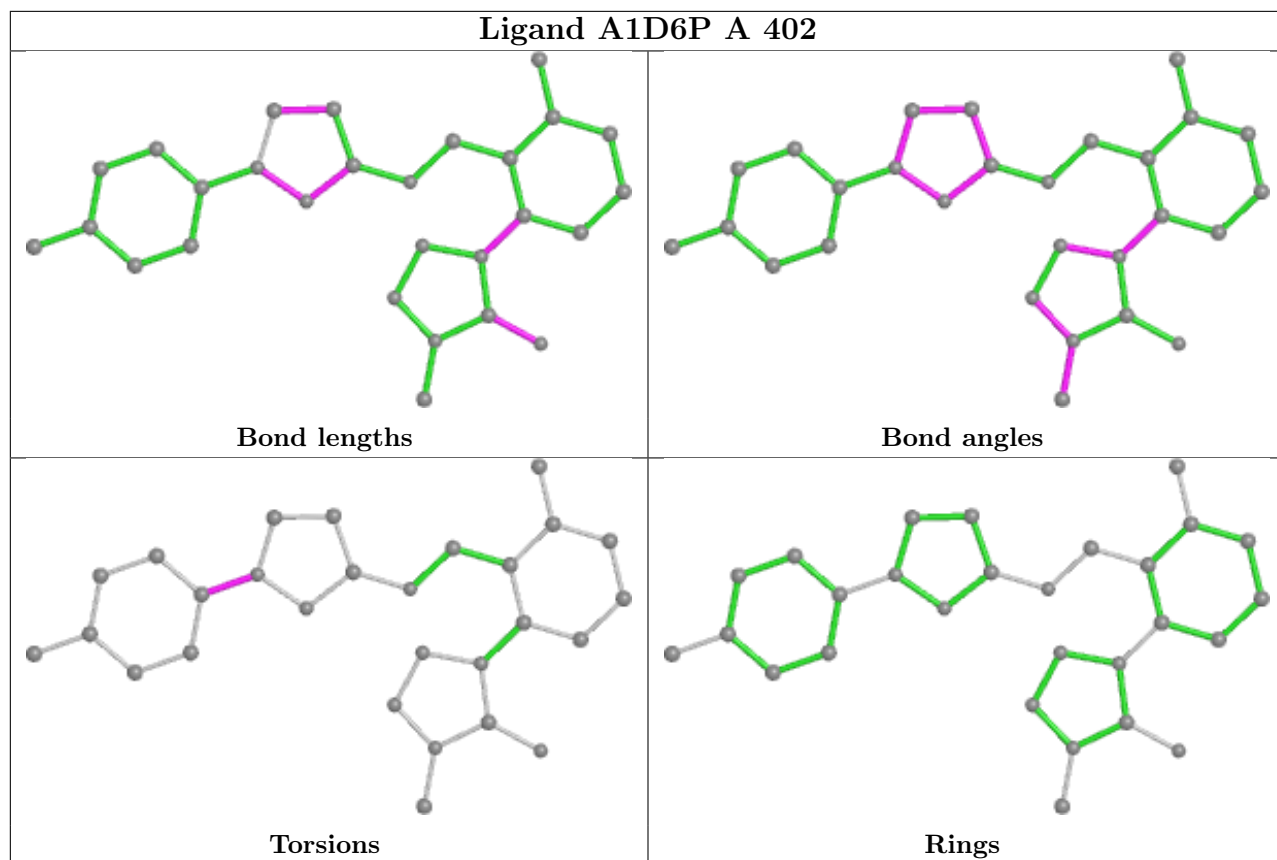


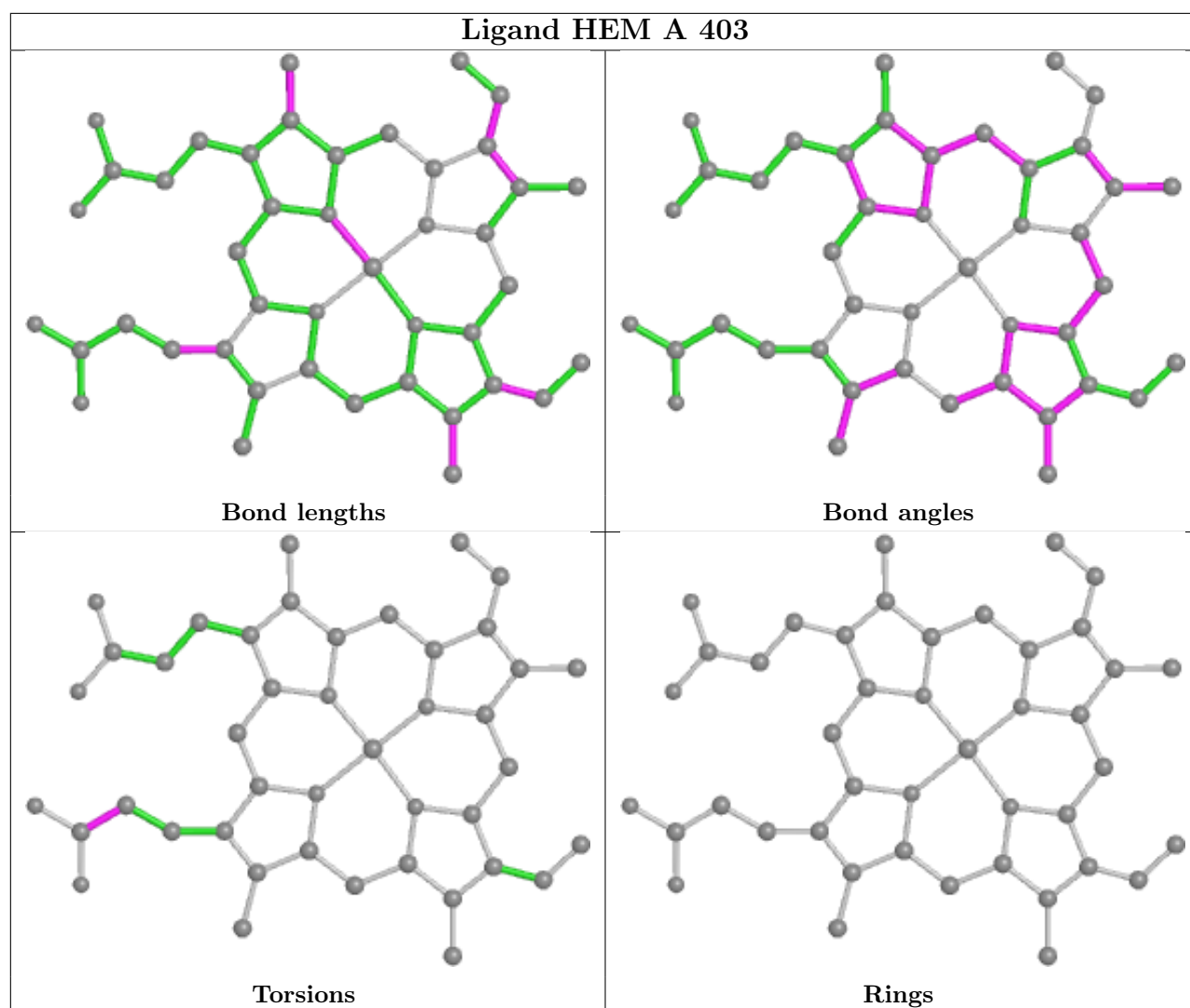












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



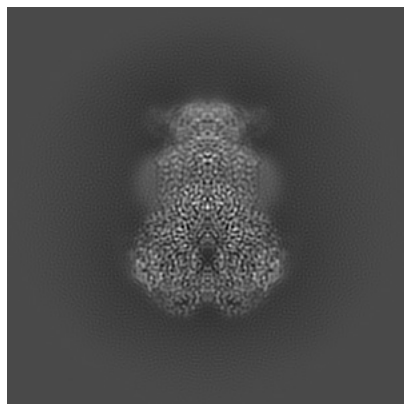
## 6 Map visualisation [i](#)

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

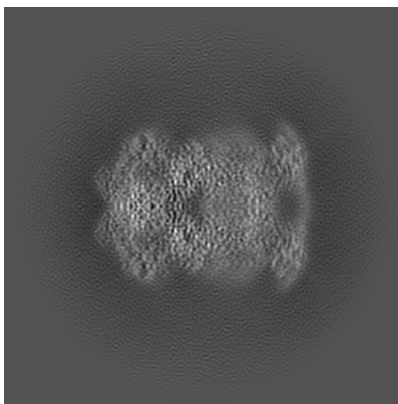
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

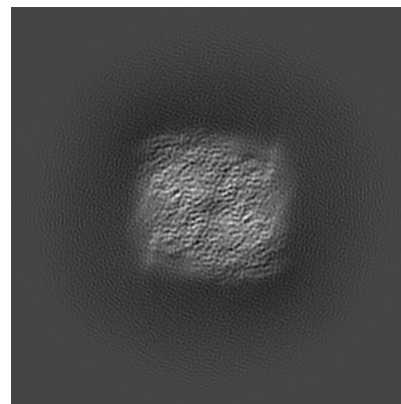
#### 6.1.1 Primary map



X

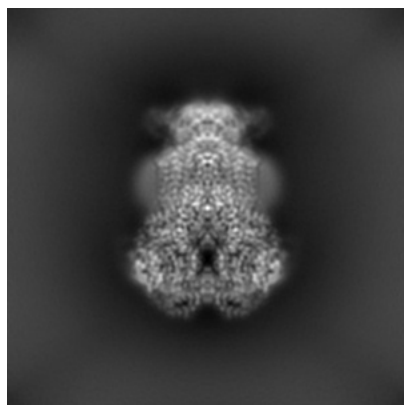


Y

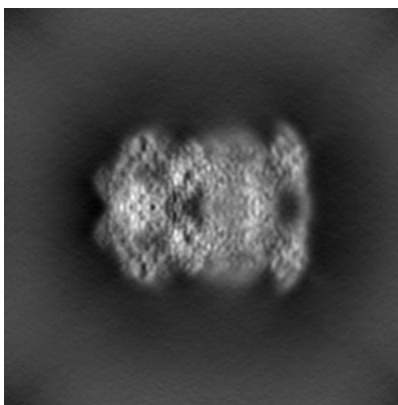


Z

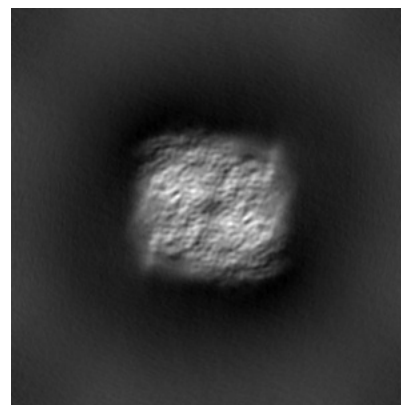
#### 6.1.2 Raw map



X



Y

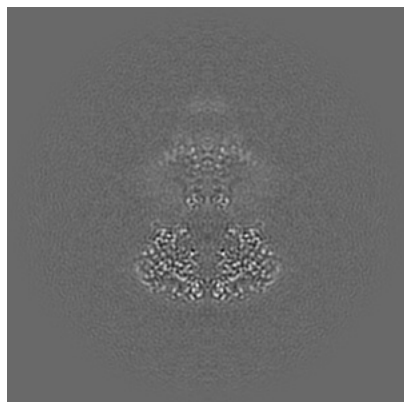


Z

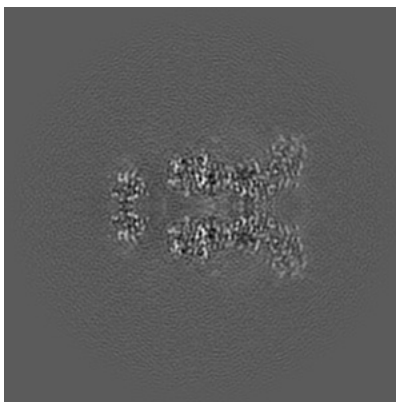
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

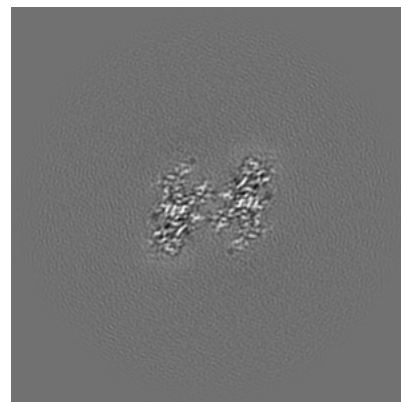
### 6.2.1 Primary map



X Index: 150

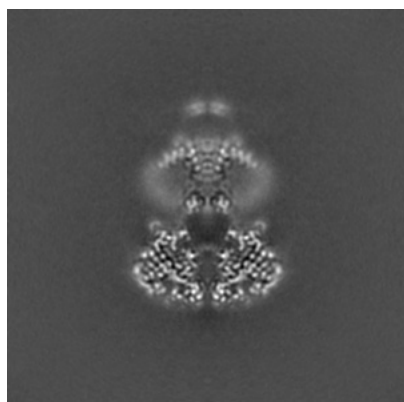


Y Index: 150

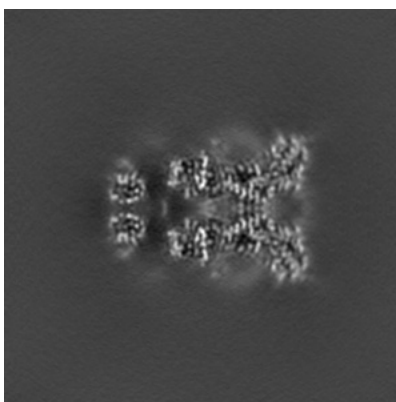


Z Index: 150

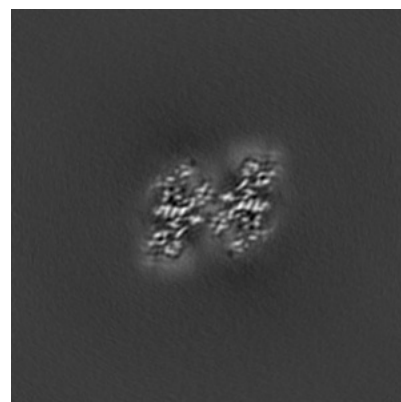
### 6.2.2 Raw map



X Index: 150



Y Index: 150

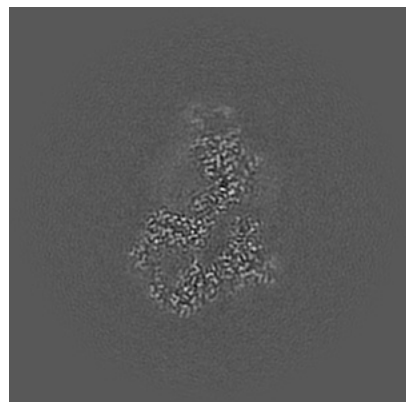


Z Index: 150

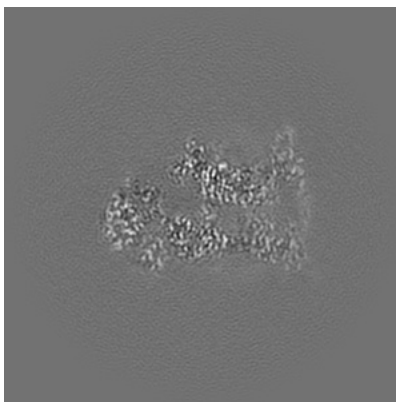
The images above show central slices of the map in three orthogonal directions.

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

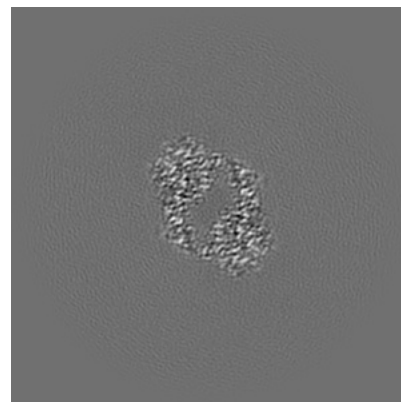
### 6.3.1 Primary map



X Index: 163

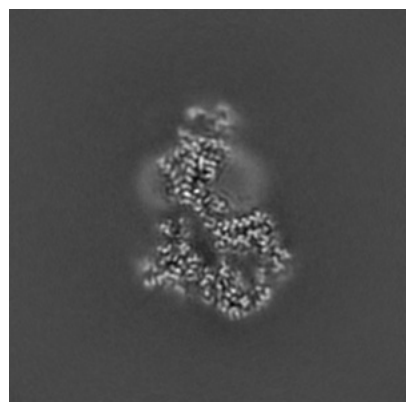


Y Index: 158

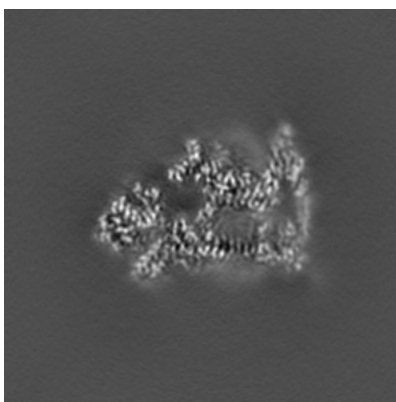


Z Index: 130

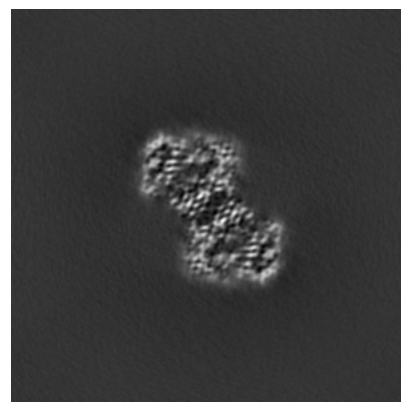
### 6.3.2 Raw map



X Index: 137



Y Index: 161

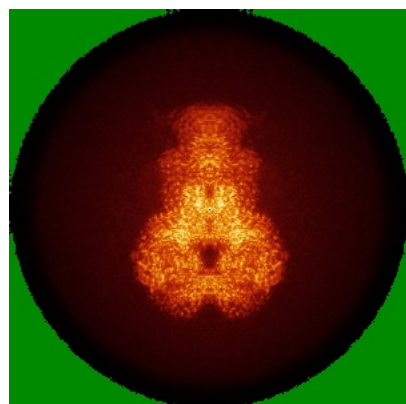


Z Index: 97

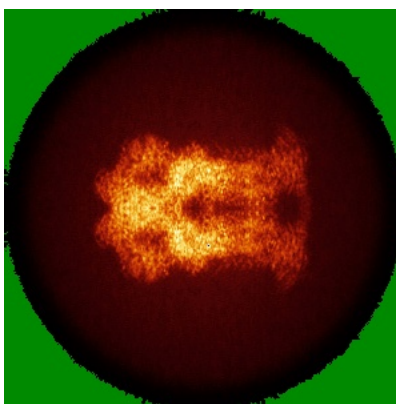
The images above show the largest variance slices of the map in three orthogonal directions.

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

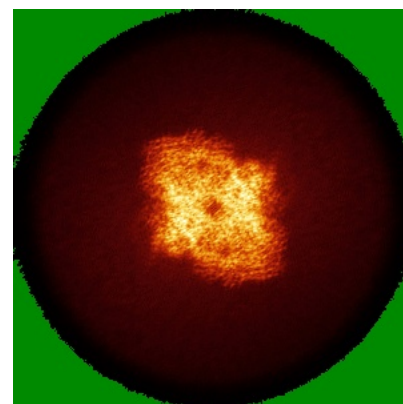
### 6.4.1 Primary map



X

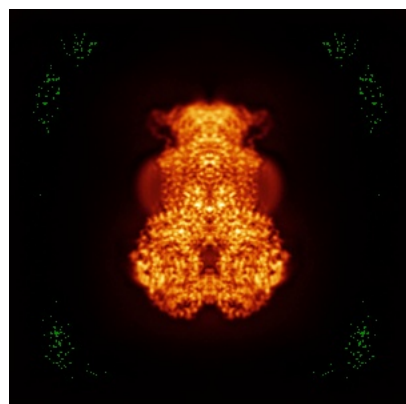


Y

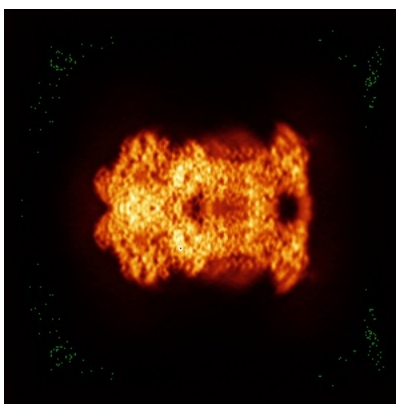


Z

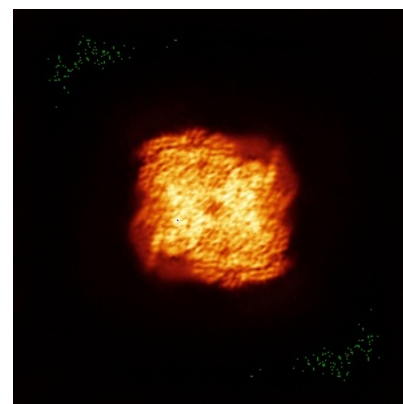
### 6.4.2 Raw map



X



Y

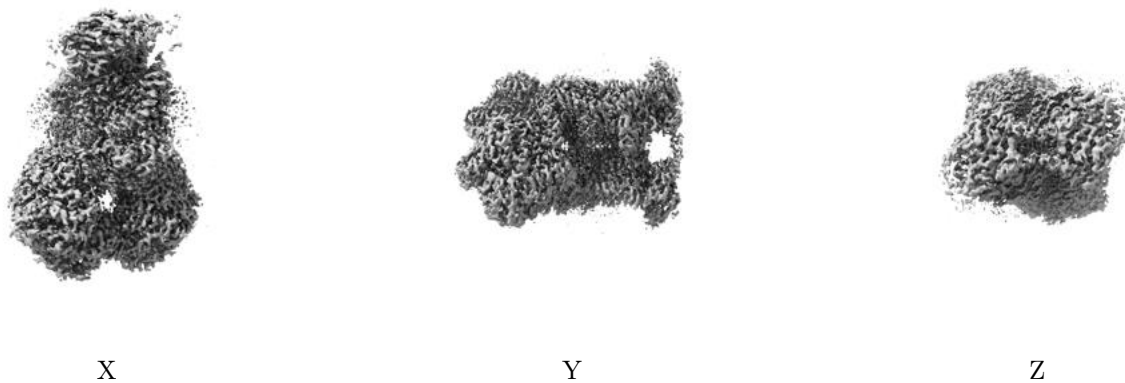


Z

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

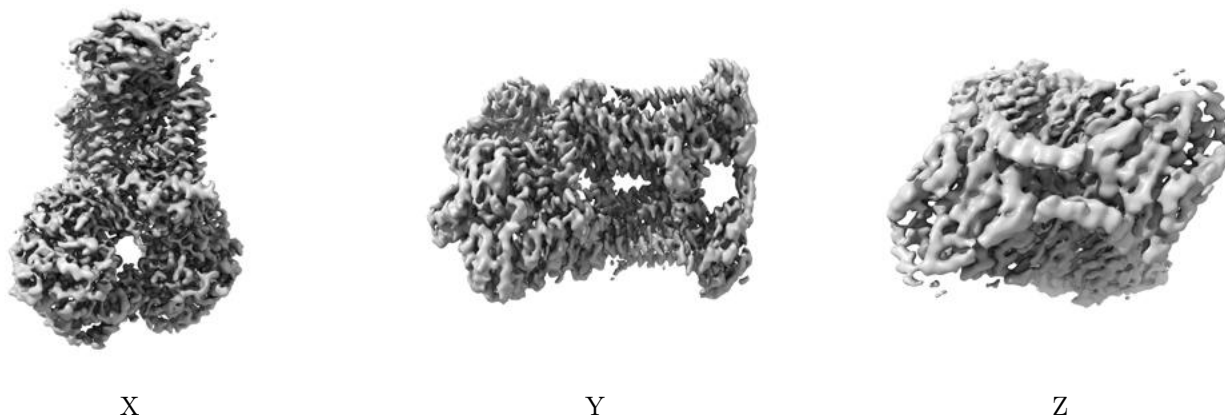
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

### 6.5.2 Raw map



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

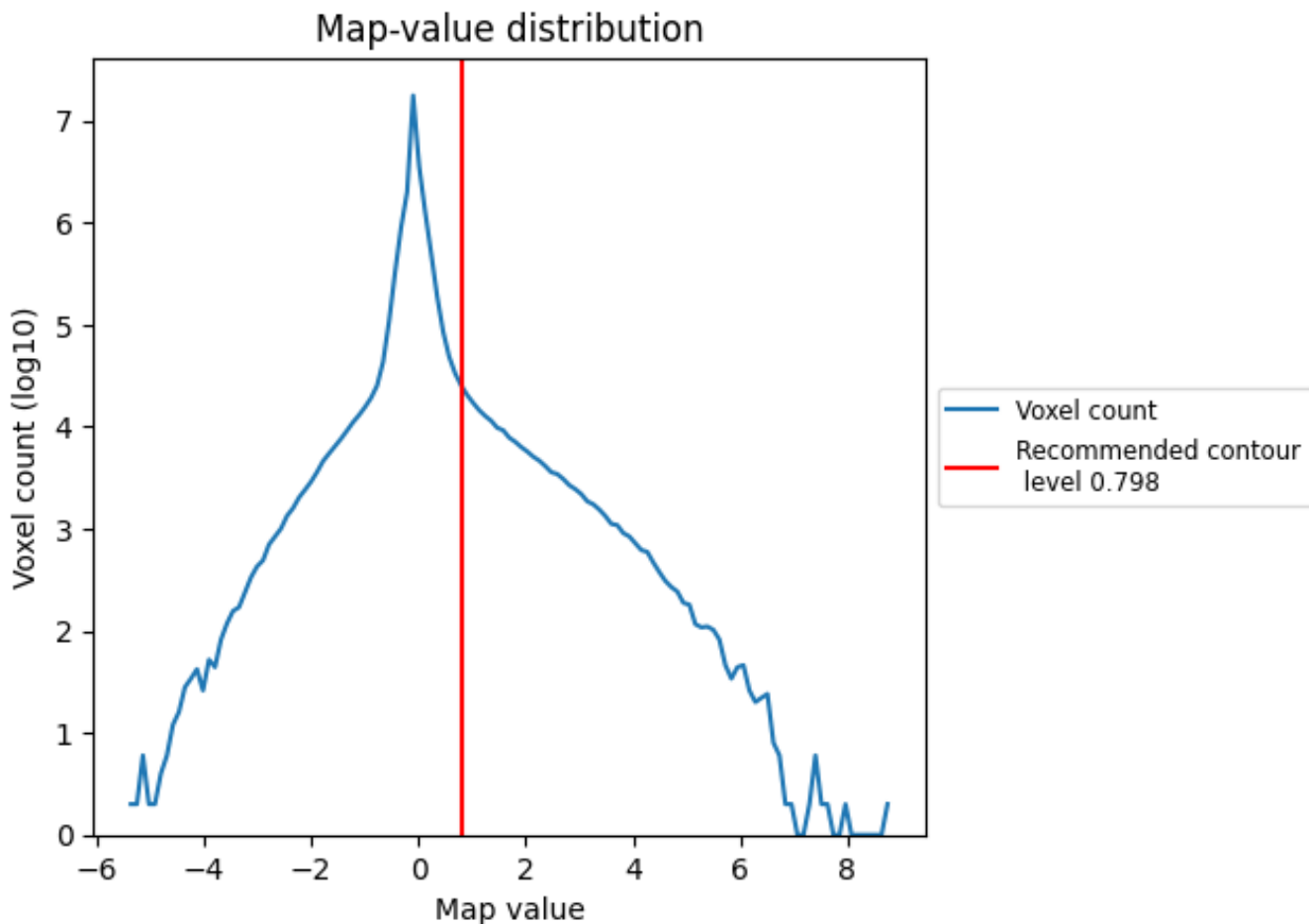
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

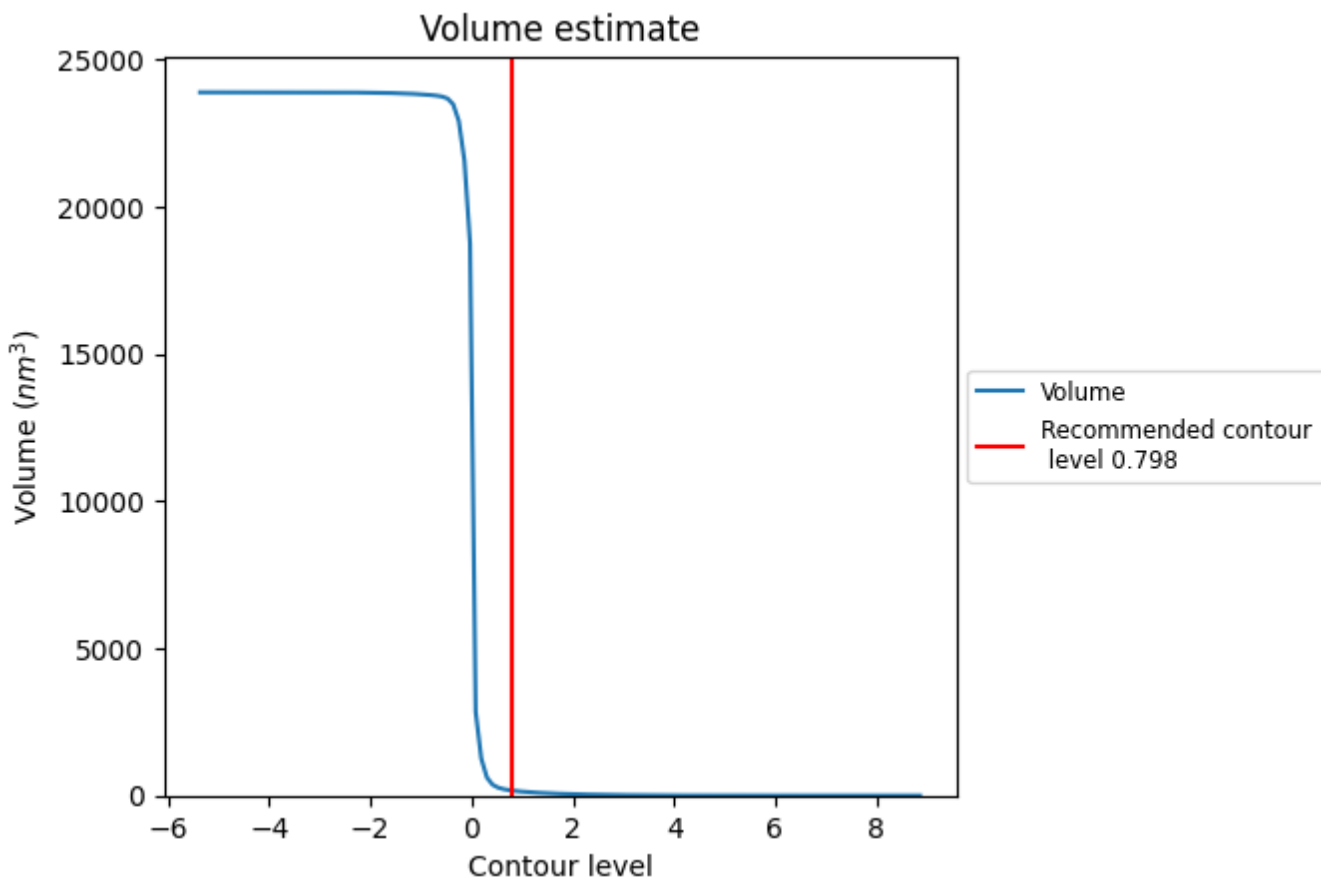
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

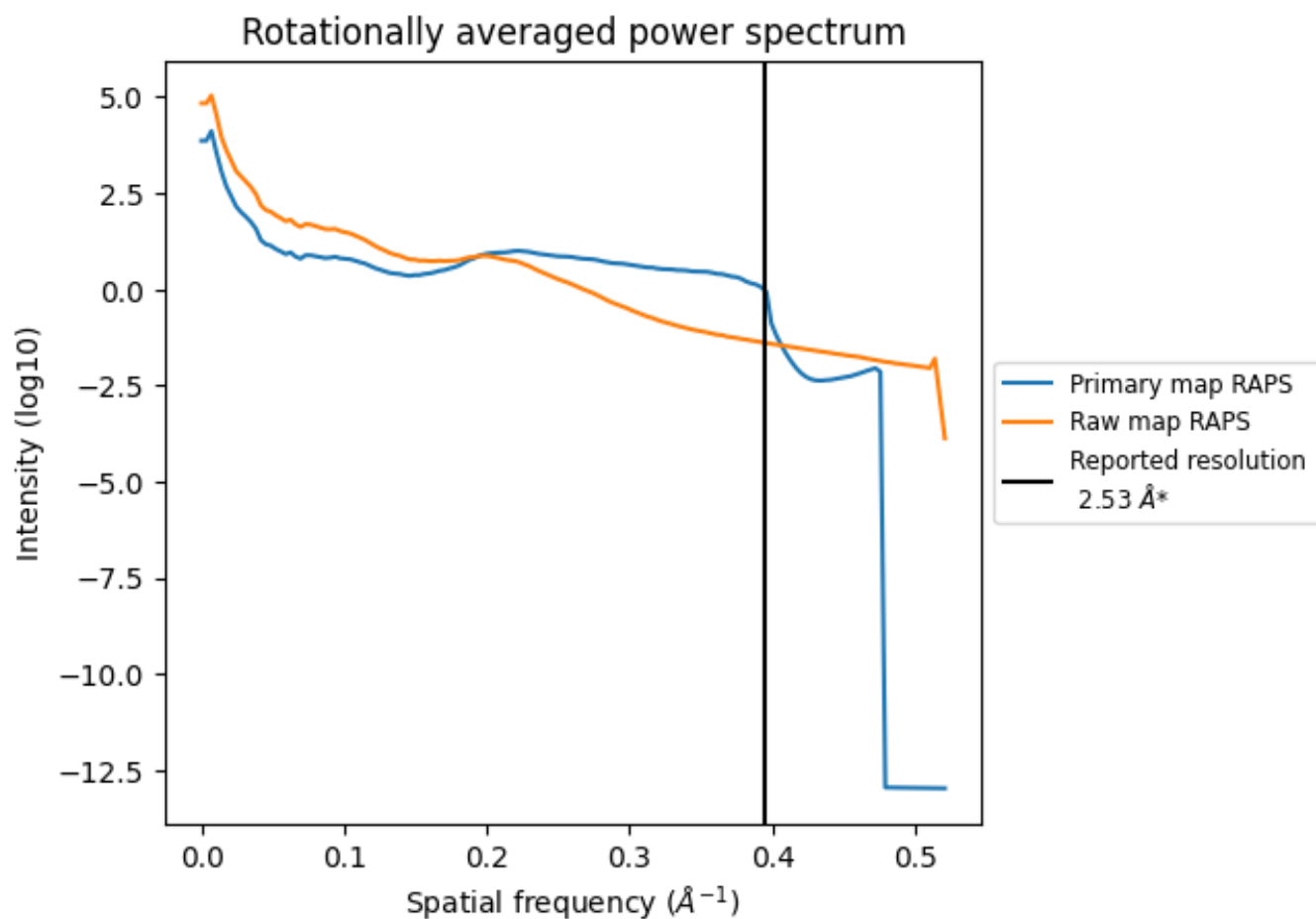
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm<sup>3</sup>; this corresponds to an approximate mass of 155 kDa.

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

### 7.3 Rotationally averaged power spectrum i



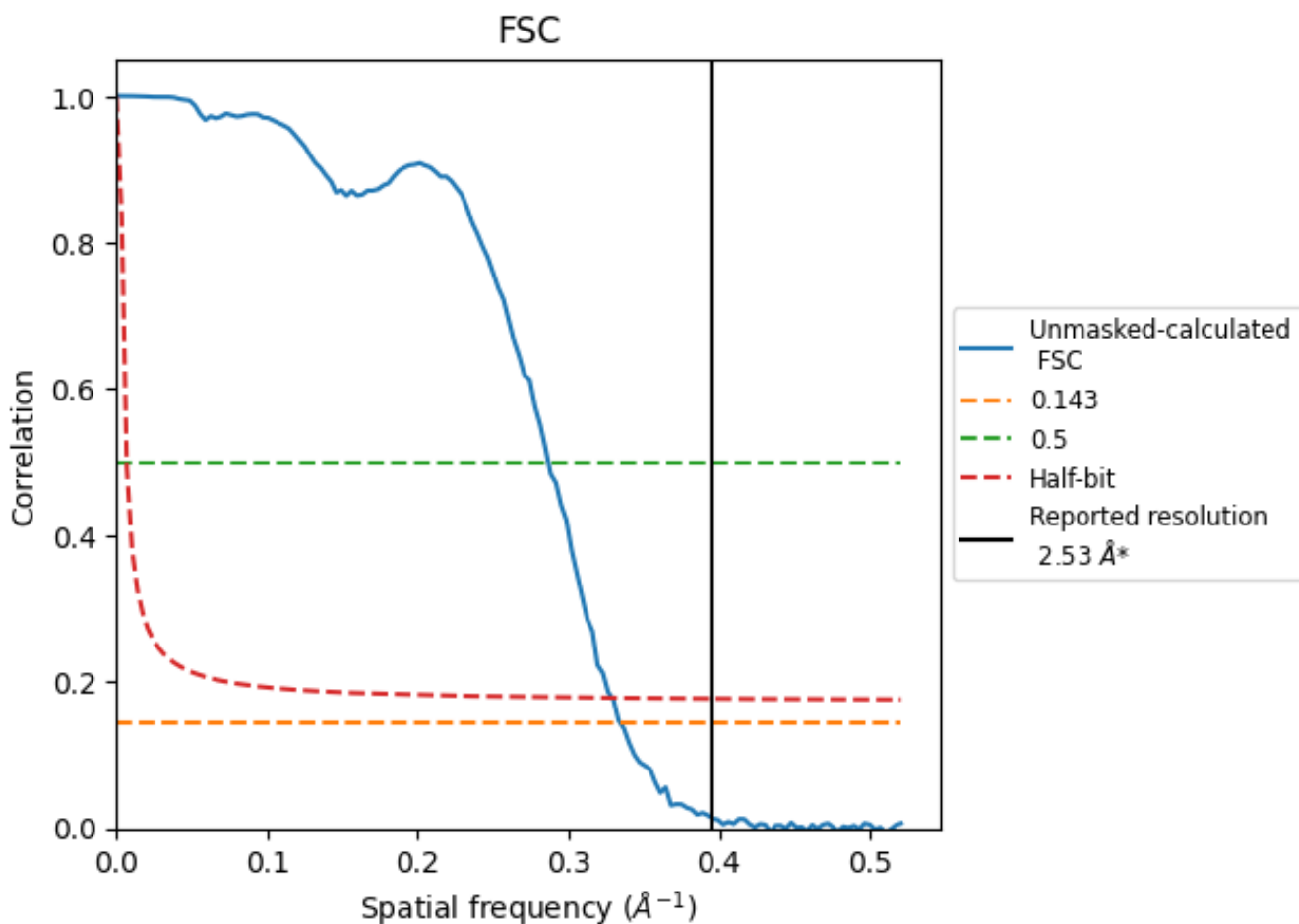
\*Reported resolution corresponds to spatial frequency of 0.395 Å<sup>-1</sup>



## 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  $0.395 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

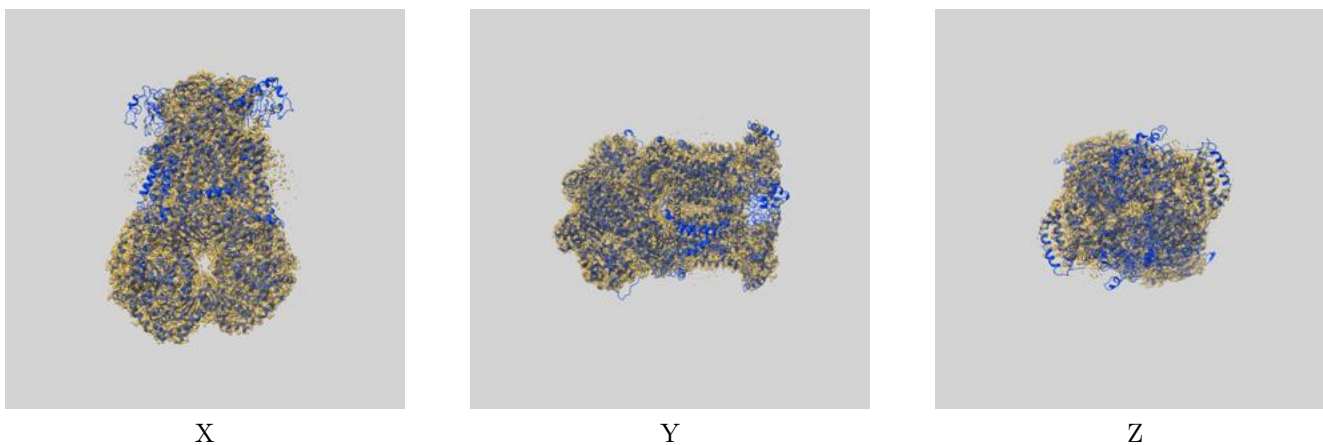
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.49	3.04

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.53 by more than 10 %

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

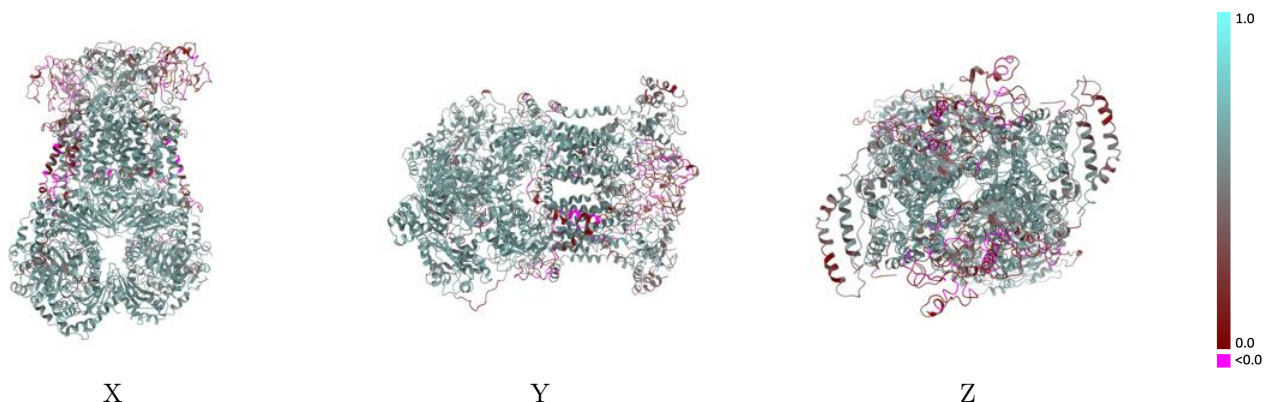
This section contains information regarding the fit between EMDB map EMD-60320 and PDB model 8ZOW. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



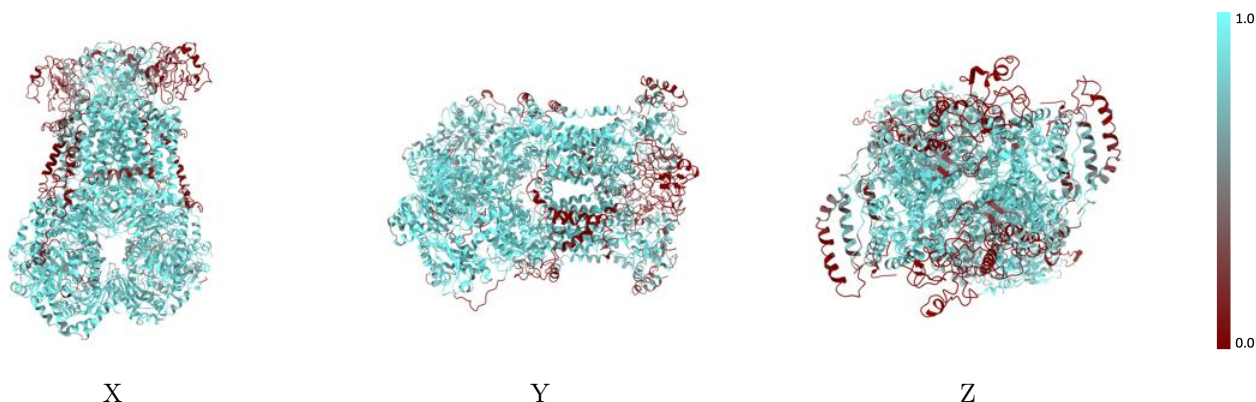
The images above show the 3D surface view of the map at the recommended contour level 0.798 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



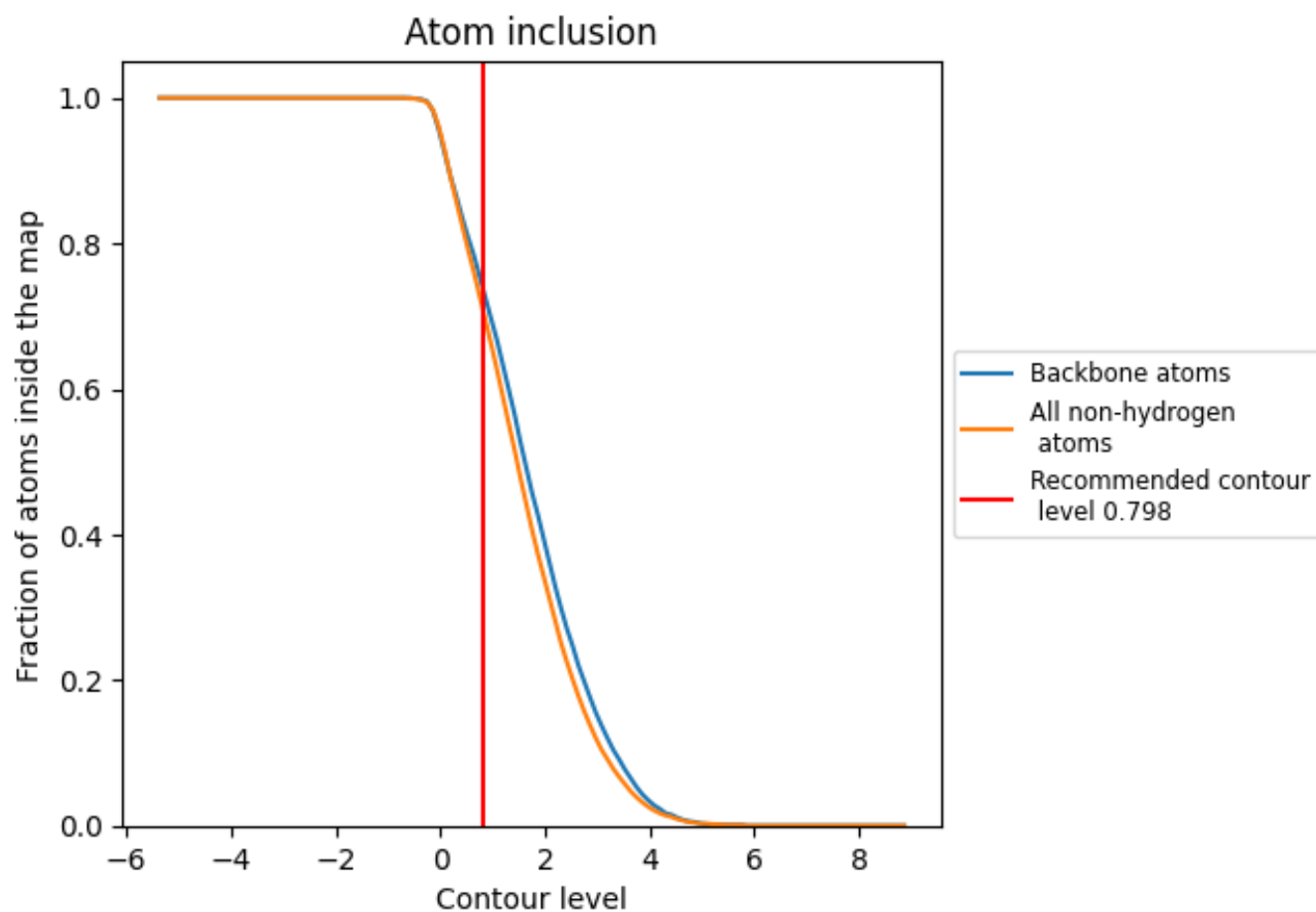
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.798).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.798) and Q-score for the entire model and for each chain.

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

