Full wwPDB EM Validation Report ⓘ

Sep 10, 2024 – 04:24 PM JST

PDB ID	:	8IB7
EMDB ID	:	EMD-35334
Title	:	Respiratory complex CIII2, focus-refined of type IA, Wild type mouse under cold temperature
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-02-09
Resolution	:	3.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

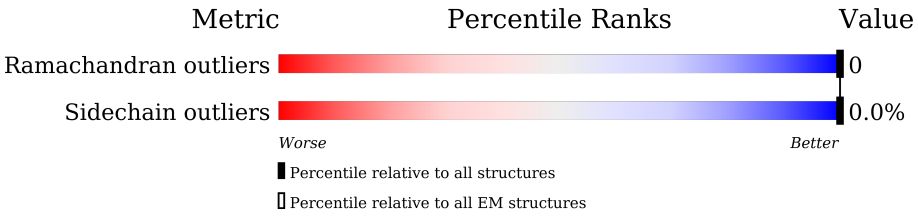
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	480	83% 17%
1	Aa	480	86% 14%
2	AB	453	92% 8%
2	Ab	453	92% 8%
3	AC	381	98%
3	Ac	381	98%
4	AD	325	5% 73% 27%
4	Ad	325	73% 27%
5	AE	274	39% 67% 32%

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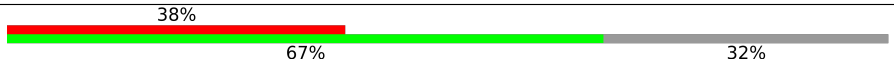
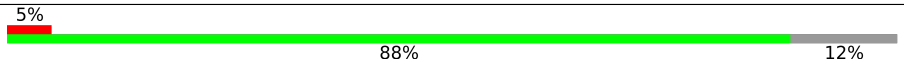
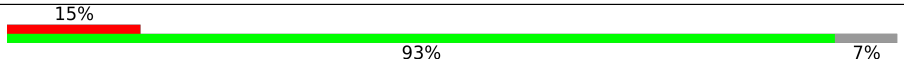
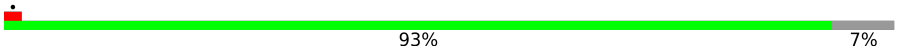
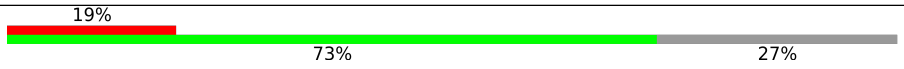
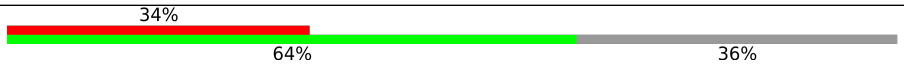
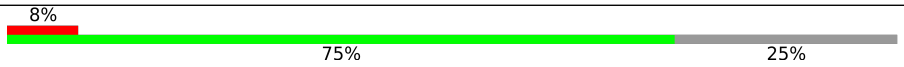
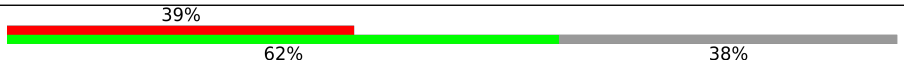
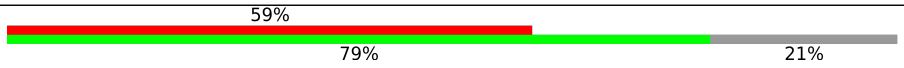
Mol	Chain	Length	Quality of chain
5	AI	274	
5	Ae	274	
6	AF	111	
6	Af	111	
7	AG	82	
7	Ag	82	
8	AH	89	
8	Ah	89	
9	AJ	64	
9	Aj	64	
10	AK	56	
10	Ak	56	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 31874 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-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	400	Total	C	N	O	S	0	0
			3128	1952	557	603	16		
1	Aa	412	Total	C	N	O	S	0	0
			3225	2016	569	624	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		
2	Ab	418	Total	C	N	O	S	0	0
			3137	1970	552	606	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
3	Ac	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
4	Ad	238	Total	C	N	O	S	0	0
			1895	1211	325	345	14		

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

Mol	Chain	Residues	Atoms	AltConf	Trace
5	AE	185	Total C N O S 1427 902 250 268 7	0	0
5	AI	51	Total C N O 345 221 64 60	0	0
5	Ae	185	Total C N O S 1432 905 250 270 7	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	AF	98	Total C N O S 864 552 154 155 3	0	0
6	Af	98	Total C N O S 864 552 154 155 3	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	AG	76	Total C N O S 643 418 116 108 1	0	0
7	Ag	76	Total C N O S 643 418 116 108 1	0	0

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	AH	65	Total C N O S 535 327 99 104 5	0	0
8	Ah	66	Total C N O S 544 333 101 105 5	0	0

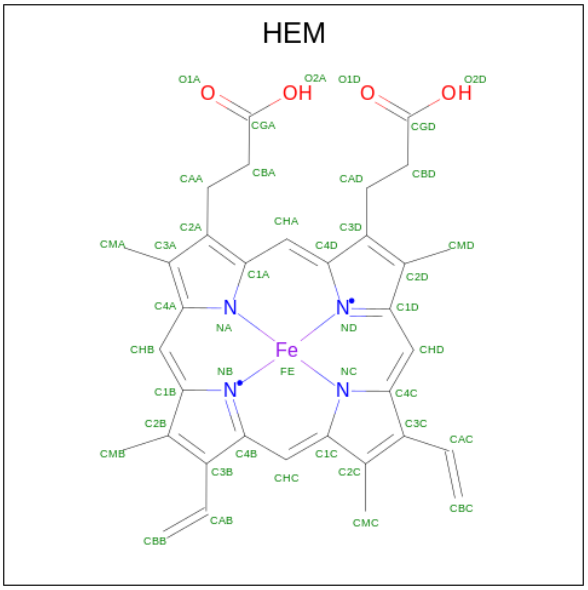
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	AJ	41	Total C N O 332 216 57 59	0	0
9	Aj	48	Total C N O 392 257 67 68	0	0

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

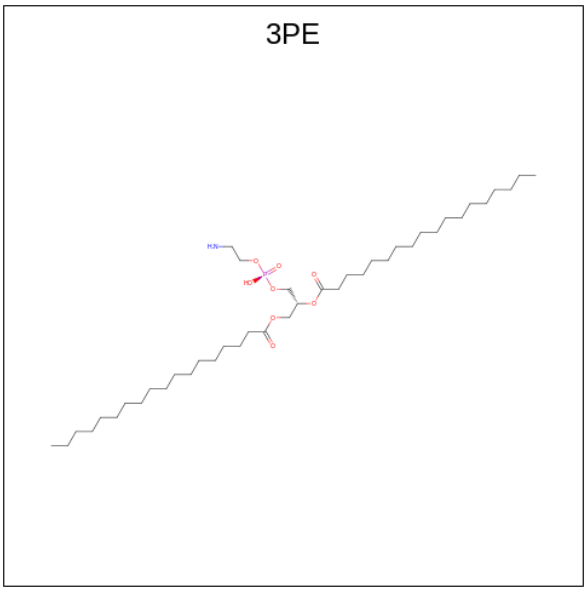
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	35	Total	C	N	O	S	0	0
			281	184	52	44	1		
10	Ak	44	Total	C	N	O	S	0	0
			357	236	63	57	1		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



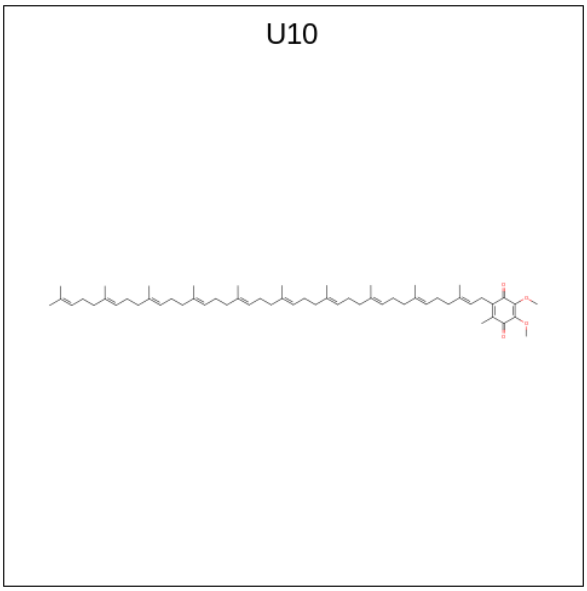
Mol	Chain	Residues	Atoms					AltConf
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	Ac	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



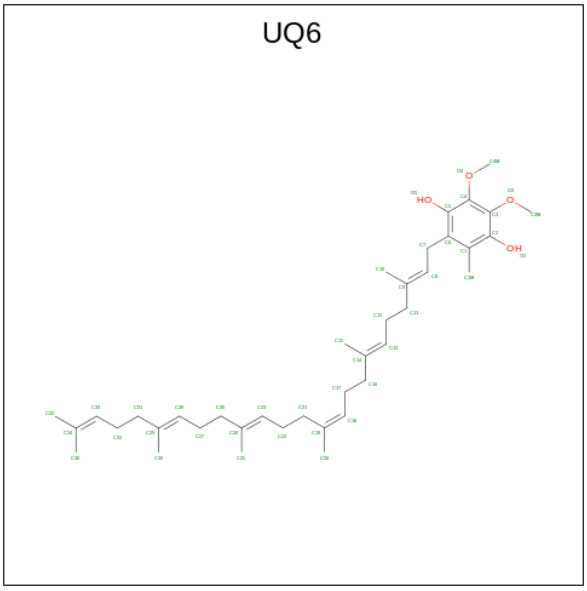
Mol	Chain	Residues	Atoms					AltConf
12	AC	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	AF	1	Total	C	N	O	P	0
			42	32	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	
12	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	Ag	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	AC	1	Total	C	O	0
			23	19	4	
13	Ac	1	Total	C	O	0
			38	34	4	

- Molecule 14 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	AC	1	Total	C	O	0
			28	24	4	

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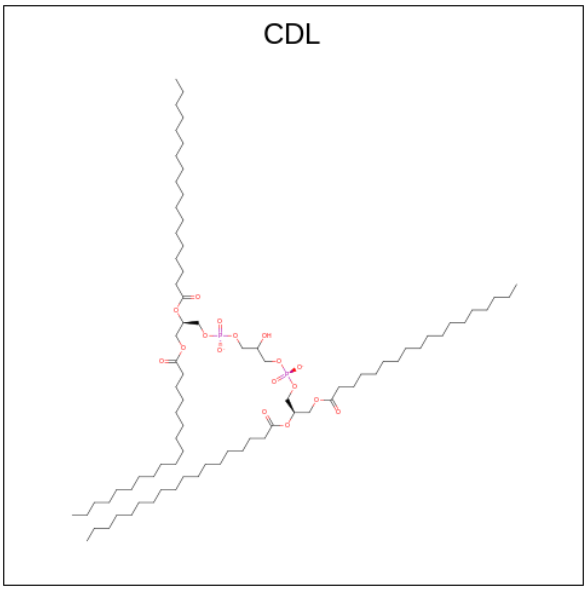
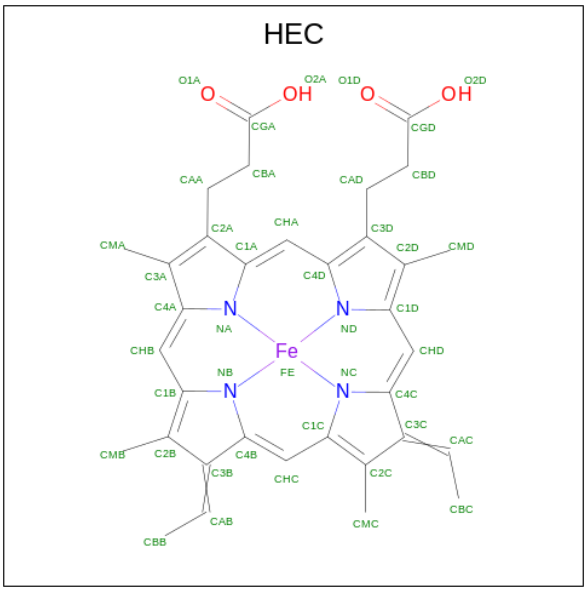
Mol	Chain	Residues	Atoms			AltConf
14	Ac	1	Total 28	C 24	O 4	0

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



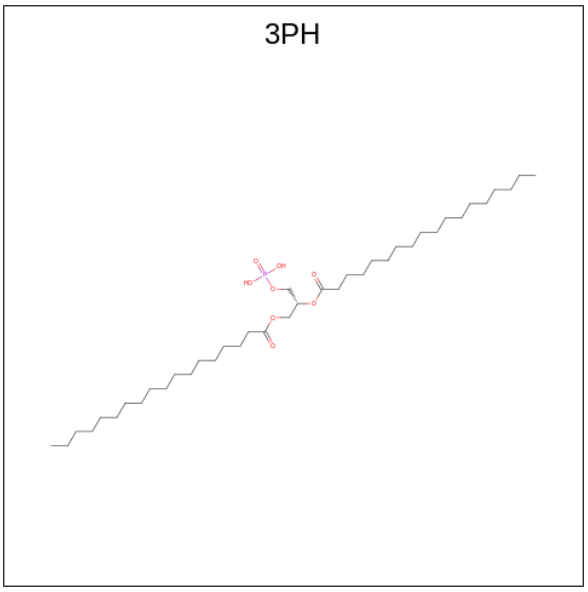
Mol	Chain	Residues	Atoms				AltConf
15	AC	1	Total 56	C 37	O 17	P 2	0
15	Aa	1	Total 46	C 27	O 17	P 2	0
15	Ac	1	Total 42	C 23	O 17	P 2	0
15	Ag	1	Total 56	C 37	O 17	P 2	0

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
17	AD	1	Total	C	O	P	0
			36	27	8	1	

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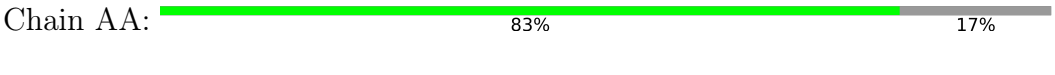
Mol	Chain	Residues	Atoms				AltConf
17	Ad	1	Total	C	O	P	0
			36	27	8	1	

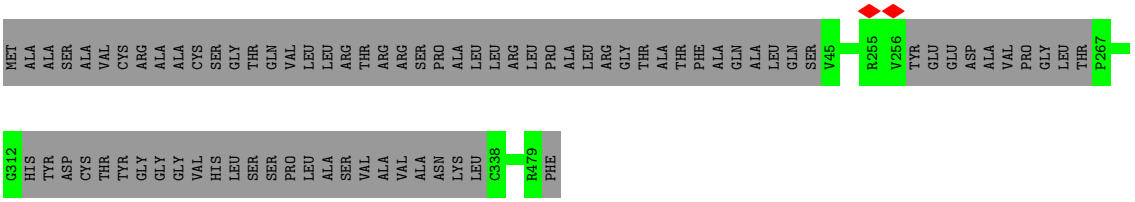
3 Residue-property plots (i)

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-c1 complex subunit 1, mitochondrial

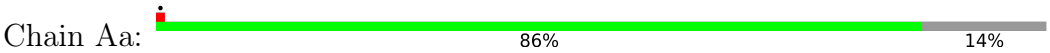
Chain AA:

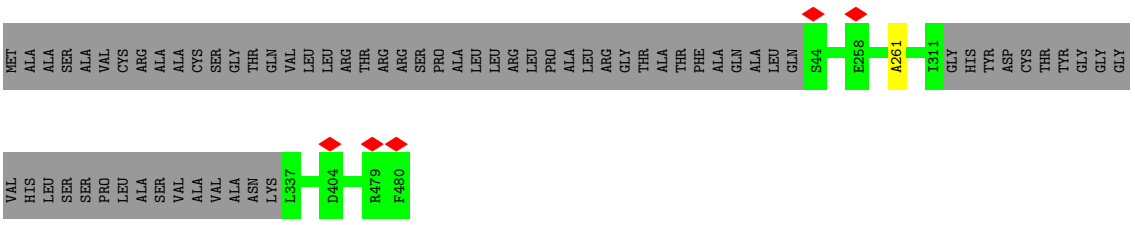




• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

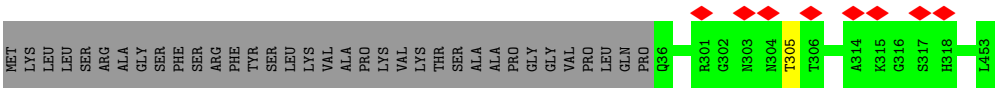
Chain Aa:





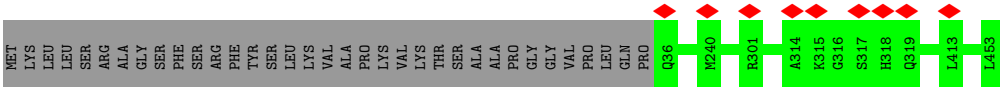
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AB:



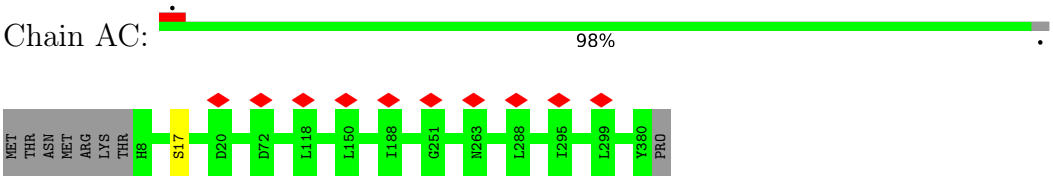
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Ab:



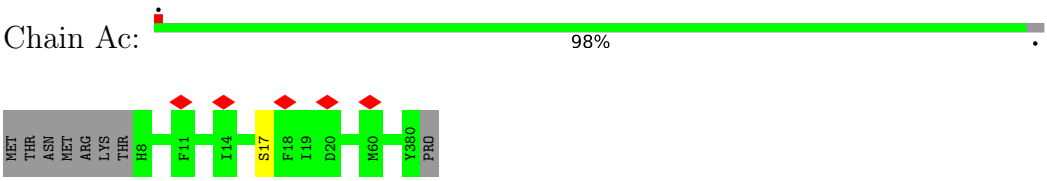
• Molecule 3: Cytochrome b

Chain AC:



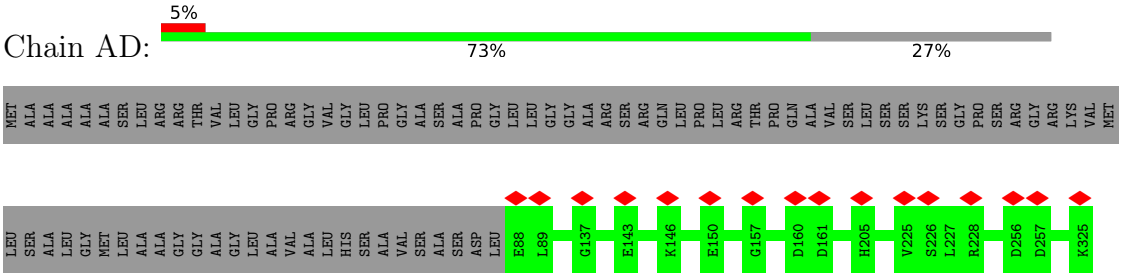
• Molecule 3: Cytochrome b

Chain Ac:



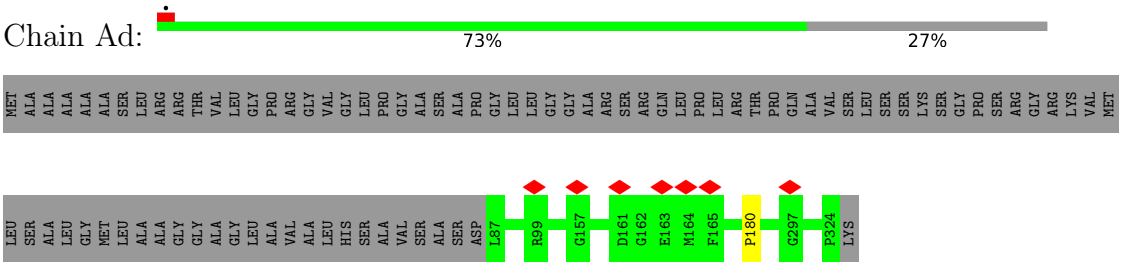
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain AD:



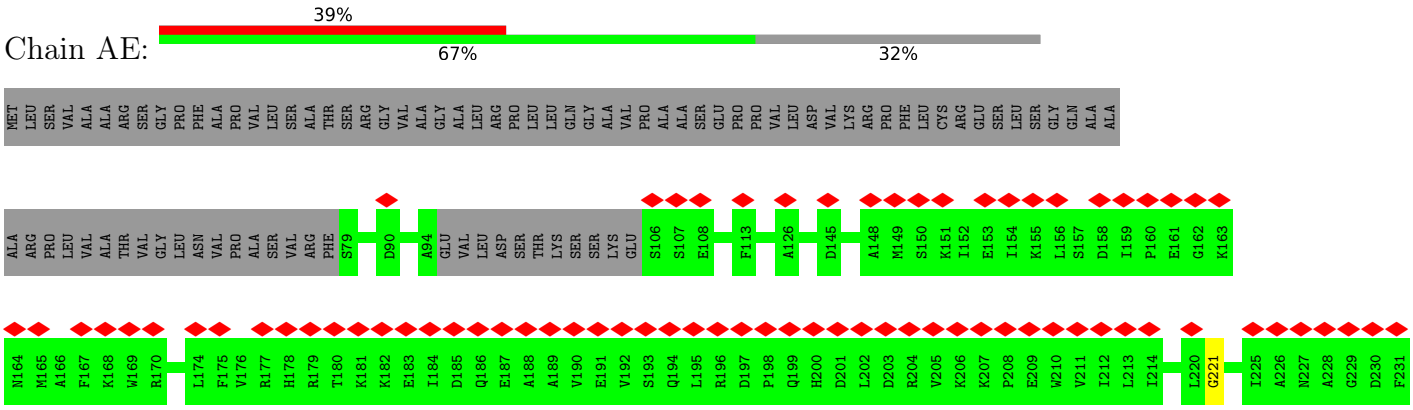
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

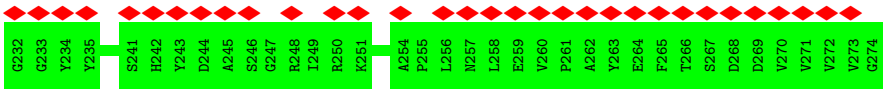
Chain Ad:



• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

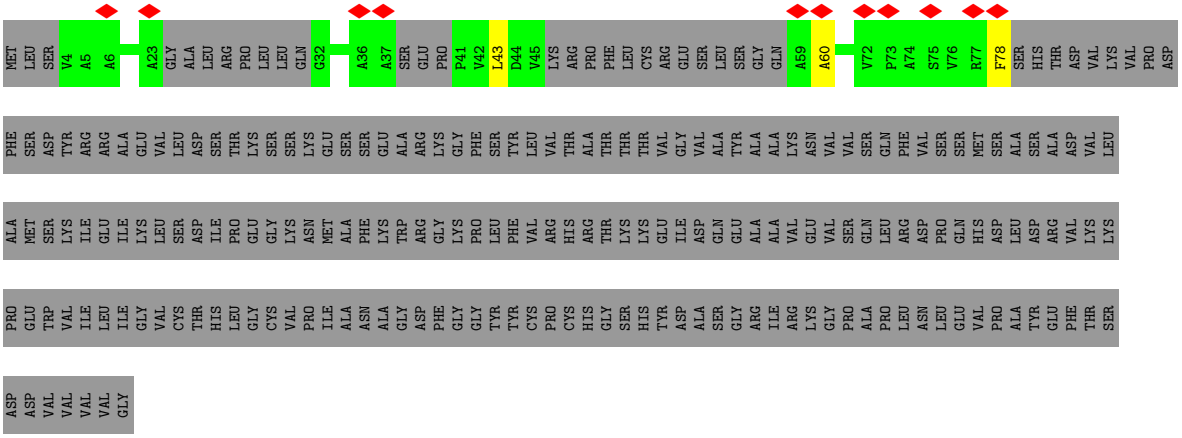
Chain AE:





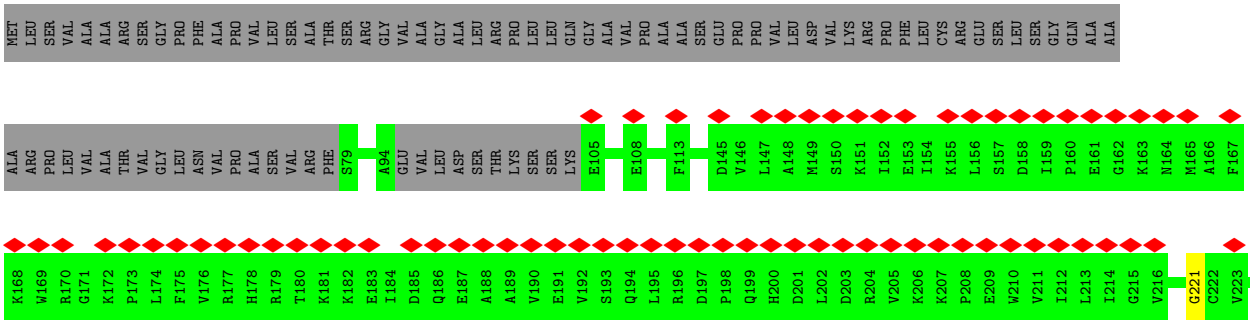
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain AI:



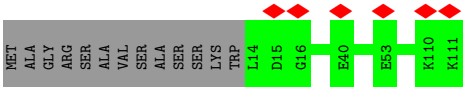
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain Ae:



• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain AF:

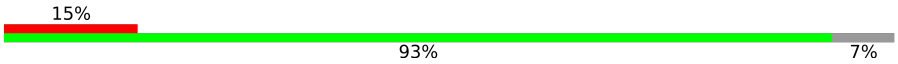


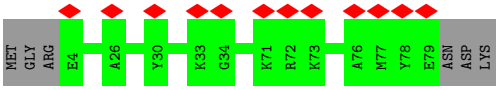
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain Af:

• Molecule 7: Cytochrome b-c1 complex subunit 8

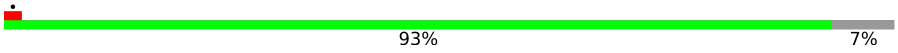
Chain AG:

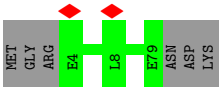




• Molecule 7: Cytochrome b-c1 complex subunit 8

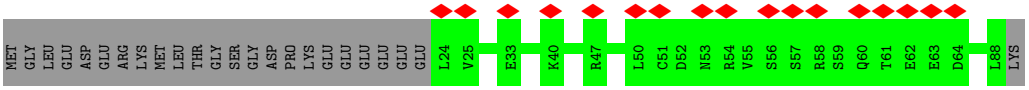
Chain Ag:





• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain AH:

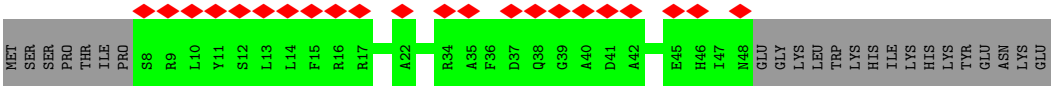


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain Ah:

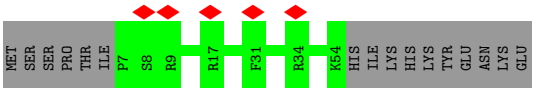
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain AJ:



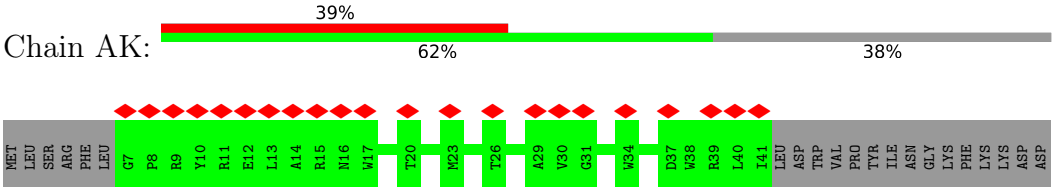
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain Aj:



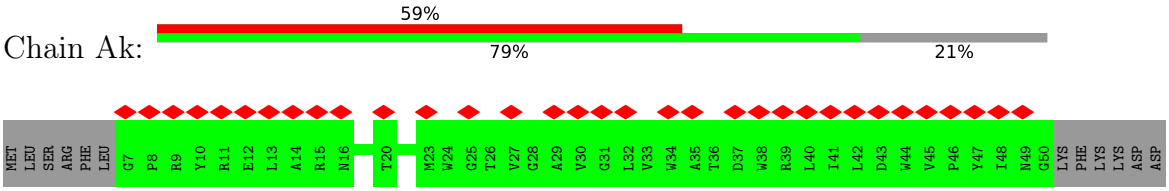
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain AK:



• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.856	Depositor
Minimum map value	-1.742	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, 3PE, 3PH, UQ6, U10, HEC, HEM

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	AA	0.41	0/3187	0.61	0/4320
1	Aa	0.42	0/3288	0.61	1/4462 (0.0%)
2	AB	0.35	0/3187	0.58	1/4308 (0.0%)
2	Ab	0.36	0/3187	0.56	0/4308
3	AC	0.35	0/3089	0.55	1/4221 (0.0%)
3	Ac	0.36	0/3089	0.56	1/4221 (0.0%)
4	AD	0.38	0/1955	0.53	0/2655
4	Ad	0.44	1/1954 (0.1%)	0.55	0/2655
5	AE	0.47	0/1459	0.63	1/1976 (0.1%)
5	AI	0.47	0/349	0.73	3/476 (0.6%)
5	Ae	0.47	0/1464	0.63	1/1983 (0.1%)
6	AF	0.32	0/884	0.50	0/1184
6	Af	0.32	0/884	0.50	0/1184
7	AG	0.37	0/662	0.55	0/895
7	Ag	0.42	0/662	0.53	0/895
8	AH	0.34	0/542	0.61	0/728
8	Ah	0.44	0/551	0.60	0/739
9	AJ	0.35	0/339	0.48	0/457
9	Aj	0.42	0/402	0.61	0/541
10	AK	0.31	0/291	0.49	0/399
10	Ak	0.41	0/371	0.55	0/511
All	All	0.39	1/31796 (0.0%)	0.57	9/43118 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Ad	180	PRO	N-CD	-8.24	1.36	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aa	261	ALA	N-CA-C	-5.85	95.20	111.00
5	AI	60	ALA	N-CA-CB	-5.83	101.94	110.10
3	Ac	17	SER	N-CA-CB	-5.66	102.01	110.50
3	AC	17	SER	N-CA-CB	-5.61	102.09	110.50
5	Ae	221	GLY	N-CA-C	5.51	126.87	113.10
5	AE	221	GLY	N-CA-C	5.50	126.85	113.10
5	AI	60	ALA	N-CA-C	5.37	125.51	111.00
2	AB	305	THR	N-CA-CB	-5.23	100.36	110.30
5	AI	43	LEU	CB-CG-CD1	-5.05	102.41	111.00

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	AA	394/480 (82%)	381 (97%)	13 (3%)	0	100	100
1	Aa	408/480 (85%)	388 (95%)	20 (5%)	0	100	100
2	AB	416/453 (92%)	404 (97%)	12 (3%)	0	100	100
2	Ab	416/453 (92%)	405 (97%)	11 (3%)	0	100	100
3	AC	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
3	Ac	371/381 (97%)	367 (99%)	4 (1%)	0	100	100
4	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
4	Ad	236/325 (73%)	220 (93%)	16 (7%)	0	100	100
5	AE	181/274 (66%)	169 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AI	43/274 (16%)	39 (91%)	4 (9%)	0	100	100
5	Ae	181/274 (66%)	166 (92%)	15 (8%)	0	100	100
6	AF	96/111 (86%)	96 (100%)	0	0	100	100
6	Af	96/111 (86%)	96 (100%)	0	0	100	100
7	AG	74/82 (90%)	74 (100%)	0	0	100	100
7	Ag	74/82 (90%)	73 (99%)	1 (1%)	0	100	100
8	AH	63/89 (71%)	62 (98%)	1 (2%)	0	100	100
8	Ah	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
9	AJ	39/64 (61%)	39 (100%)	0	0	100	100
9	Aj	46/64 (72%)	44 (96%)	2 (4%)	0	100	100
10	AK	33/56 (59%)	33 (100%)	0	0	100	100
10	Ak	42/56 (75%)	40 (95%)	2 (5%)	0	100	100
All	All	3880/4904 (79%)	3755 (97%)	125 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	338/398 (85%)	338 (100%)	0	100	100
1	Aa	349/398 (88%)	349 (100%)	0	100	100
2	AB	328/356 (92%)	328 (100%)	0	100	100
2	Ab	328/356 (92%)	328 (100%)	0	100	100
3	AC	325/333 (98%)	325 (100%)	0	100	100
3	Ac	325/333 (98%)	325 (100%)	0	100	100
4	AD	203/260 (78%)	203 (100%)	0	100	100
4	Ad	203/260 (78%)	203 (100%)	0	100	100
5	AE	155/224 (69%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	AI	34/224 (15%)	33 (97%)	1 (3%)	37 61
5	Ae	156/224 (70%)	156 (100%)	0	100 100
6	AF	90/99 (91%)	90 (100%)	0	100 100
6	Af	90/99 (91%)	90 (100%)	0	100 100
7	AG	69/74 (93%)	69 (100%)	0	100 100
7	Ag	69/74 (93%)	69 (100%)	0	100 100
8	AH	62/83 (75%)	62 (100%)	0	100 100
8	Ah	63/83 (76%)	63 (100%)	0	100 100
9	AJ	33/55 (60%)	33 (100%)	0	100 100
9	Aj	39/55 (71%)	39 (100%)	0	100 100
10	AK	26/46 (56%)	26 (100%)	0	100 100
10	Ak	34/46 (74%)	34 (100%)	0	100 100
All	All	3319/4080 (81%)	3318 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	AI	78	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	87	ASN
1	AA	103	ASN
1	AA	173	GLN
1	AA	207	ASN
1	AA	286	HIS
1	AA	342	GLN
1	AA	397	ASN
1	AA	402	HIS
2	AB	167	GLN
2	AB	304	ASN
2	AB	415	GLN
3	AC	201	HIS
3	AC	341	GLN
4	AD	189	ASN
4	AD	190	ASN

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Mol	Chain	Res	Type
5	AE	131	ASN
5	AE	135	GLN
5	AE	242	HIS
10	AK	16	ASN
1	Aa	87	ASN
1	Aa	103	ASN
1	Aa	119	HIS
1	Aa	173	GLN
1	Aa	181	ASN
1	Aa	207	ASN
2	Ab	284	ASN
2	Ab	290	GLN
2	Ab	291	HIS
2	Ab	304	ASN
2	Ab	415	GLN
3	Ac	148	ASN
3	Ac	312	GLN
3	Ac	341	GLN
4	Ad	115	GLN
4	Ad	155	GLN
4	Ad	190	ASN
5	Ae	131	ASN
5	Ae	135	GLN
5	Ae	242	HIS
7	Ag	24	GLN
8	Ah	60	GLN
8	Ah	82	HIS
9	Aj	48	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
11	HEM	Ac	403	3	41,50,50	1.42	6 (14%)	45,82,82	1.84	11 (24%)
16	HEC	Ad	401	4	32,50,50	2.18	11 (34%)	24,82,82	2.45	6 (25%)
14	UQ6	AC	405	-	28,28,43	2.49	6 (21%)	33,37,55	1.80	10 (30%)
14	UQ6	Ac	406	-	28,28,43	2.51	6 (21%)	33,37,55	1.59	9 (27%)
11	HEM	Ac	402	3	41,50,50	1.42	6 (14%)	45,82,82	2.15	11 (24%)
17	3PH	Ad	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.13	3 (7%)
15	CDL	AC	406	-	55,55,99	1.21	4 (7%)	61,67,111	1.20	6 (9%)
17	3PH	AD	402	-	35,35,47	1.08	2 (5%)	39,40,52	1.21	3 (7%)
16	HEC	AD	401	4	32,50,50	2.16	10 (31%)	24,82,82	2.57	6 (25%)
13	U10	AC	404	-	23,23,63	1.78	2 (8%)	28,31,79	1.49	5 (17%)
12	3PE	Ac	404	-	34,34,50	1.09	2 (5%)	37,39,55	1.23	4 (10%)
11	HEM	AC	402	3	41,50,50	1.47	8 (19%)	45,82,82	2.43	16 (35%)
11	HEM	AC	401	3	41,50,50	1.36	5 (12%)	45,82,82	1.88	10 (22%)
15	CDL	Aa	501	-	45,45,99	0.36	0	51,57,111	0.42	0
15	CDL	Ag	101	-	55,55,99	1.21	4 (7%)	61,67,111	1.26	6 (9%)
12	3PE	AC	403	-	34,34,50	1.10	2 (5%)	37,39,55	1.18	3 (8%)
12	3PE	Ag	102	-	38,38,50	1.04	2 (5%)	41,43,55	1.13	4 (9%)
13	U10	Ac	405	-	38,38,63	1.37	2 (5%)	46,49,79	1.71	12 (26%)
12	3PE	AF	201	-	41,41,50	1.00	2 (4%)	44,46,55	0.98	2 (4%)
15	CDL	Ac	407	-	41,41,99	1.40	4 (9%)	47,53,111	1.40	7 (14%)
12	3PE	Ac	401	-	22,22,50	0.38	0	25,27,55	0.48	0

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
11	HEM	Ac	403	3	-	8/12/54/54	-
16	HEC	Ad	401	4	-	2/10/54/54	-
14	UQ6	AC	405	-	-	3/21/21/39	0/1/1/1
14	UQ6	Ac	406	-	-	7/21/21/39	0/1/1/1
11	HEM	Ac	402	3	-	3/12/54/54	-
17	3PH	Ad	402	-	-	8/37/37/49	-
15	CDL	AC	406	-	-	18/66/66/110	-
17	3PH	AD	402	-	-	8/37/37/49	-
16	HEC	AD	401	4	-	3/10/54/54	-
13	U10	AC	404	-	-	0/15/39/87	0/1/1/1
12	3PE	Ac	404	-	-	8/38/38/54	-
11	HEM	AC	402	3	-	4/12/54/54	-
11	HEM	AC	401	3	-	6/12/54/54	-
15	CDL	Aa	501	-	-	16/56/56/110	-
15	CDL	Ag	101	-	-	12/66/66/110	-
12	3PE	AC	403	-	-	12/38/38/54	-
12	3PE	Ag	102	-	-	5/42/42/54	-
13	U10	Ac	405	-	-	9/33/57/87	0/1/1/1
12	3PE	AF	201	-	-	9/45/45/54	-
15	CDL	Ac	407	-	-	11/52/52/110	-
12	3PE	Ac	401	-	-	10/26/26/54	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	AC	404	U10	C6-C1	7.59	1.49	1.35
13	Ac	405	U10	C6-C1	7.42	1.48	1.35
16	Ad	401	HEC	C3C-C2C	6.23	1.47	1.40
14	AC	405	UQ6	C2-C3	5.95	1.49	1.39
14	Ac	406	UQ6	C2-C3	5.90	1.49	1.39
14	Ac	406	UQ6	C5-C4	5.87	1.48	1.39
14	Ac	406	UQ6	C5-C6	5.87	1.49	1.40
16	AD	401	HEC	C2B-C3B	5.76	1.46	1.40
14	AC	405	UQ6	C5-C4	5.67	1.48	1.39
16	Ad	401	HEC	C2B-C3B	5.65	1.46	1.40
14	AC	405	UQ6	C5-C6	5.60	1.48	1.40
14	AC	405	UQ6	C6-C1	5.57	1.49	1.40
14	Ac	406	UQ6	C6-C1	5.46	1.49	1.40
16	AD	401	HEC	C3C-C2C	5.42	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Ac	406	UQ6	C4-C3	4.68	1.49	1.39
14	AC	405	UQ6	C4-C3	4.53	1.48	1.39
14	AC	405	UQ6	C2-C1	4.40	1.49	1.40
15	AC	406	CDL	OB8-CB7	4.34	1.46	1.33
15	Ag	101	CDL	OB8-CB7	4.27	1.45	1.33
15	Ac	407	CDL	OA8-CA7	4.26	1.45	1.33
15	Ac	407	CDL	OB8-CB7	4.26	1.45	1.33
14	Ac	406	UQ6	C2-C1	4.25	1.48	1.40
17	AD	402	3PH	O31-C31	4.24	1.45	1.33
17	Ad	402	3PH	O31-C31	4.23	1.45	1.33
12	Ag	102	3PE	O31-C31	4.22	1.45	1.33
12	Ac	404	3PE	O31-C31	4.20	1.45	1.33
12	AF	201	3PE	O31-C31	4.18	1.45	1.33
12	AC	403	3PE	O31-C31	4.15	1.45	1.33
15	AC	406	CDL	OA8-CA7	4.09	1.45	1.33
12	AF	201	3PE	O21-C21	4.05	1.45	1.34
15	AC	406	CDL	OB6-CB5	4.04	1.45	1.34
15	Ag	101	CDL	OA8-CA7	4.04	1.45	1.33
15	Ag	101	CDL	OB6-CB5	4.04	1.45	1.34
15	Ac	407	CDL	OA6-CA5	4.03	1.45	1.34
12	AC	403	3PE	O21-C21	4.01	1.45	1.34
12	Ag	102	3PE	O21-C21	4.00	1.45	1.34
11	Ac	403	HEM	C1B-NB	-3.95	1.33	1.40
15	Ag	101	CDL	OA6-CA5	3.95	1.45	1.34
15	Ac	407	CDL	OB6-CB5	3.93	1.45	1.34
17	AD	402	3PH	O21-C21	3.91	1.45	1.34
11	AC	402	HEM	C1B-NB	-3.91	1.33	1.40
17	Ad	402	3PH	O21-C21	3.91	1.45	1.34
12	Ac	404	3PE	O21-C21	3.89	1.45	1.34
15	AC	406	CDL	OA6-CA5	3.89	1.45	1.34
11	Ac	402	HEM	C1B-NB	-3.80	1.33	1.40
11	Ac	403	HEM	C4D-ND	-3.66	1.34	1.40
11	AC	402	HEM	C4D-ND	-3.55	1.34	1.40
11	AC	401	HEM	C4D-ND	-3.44	1.34	1.40
11	AC	401	HEM	C1B-NB	-3.43	1.34	1.40
11	Ac	402	HEM	C4D-ND	-3.39	1.34	1.40
16	AD	401	HEC	C2A-C3A	3.26	1.47	1.37
16	Ad	401	HEC	C2A-C3A	3.23	1.47	1.37
16	AD	401	HEC	C3D-C2D	3.22	1.47	1.37
16	Ad	401	HEC	C3D-C2D	3.15	1.47	1.37
11	Ac	402	HEM	FE-NB	3.14	2.12	1.96
13	AC	404	U10	C4-C3	3.08	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Ac	405	U10	C4-C3	3.04	1.48	1.36
16	AD	401	HEC	C3C-C4C	3.03	1.48	1.43
16	AD	401	HEC	C2A-C1A	3.01	1.49	1.42
11	AC	402	HEM	C4B-NB	-2.98	1.32	1.38
11	AC	402	HEM	C1B-C2B	-2.94	1.38	1.44
16	AD	401	HEC	C4B-C3B	2.85	1.48	1.43
11	AC	401	HEM	FE-NB	2.84	2.10	1.96
16	Ad	401	HEC	C3C-C4C	2.83	1.48	1.43
11	Ac	403	HEM	FE-NB	2.78	2.10	1.96
16	Ad	401	HEC	C3A-C4A	2.75	1.48	1.42
11	Ac	402	HEM	CHB-C1B	2.71	1.41	1.35
16	AD	401	HEC	C3A-C4A	2.71	1.48	1.42
16	Ad	401	HEC	C2A-C1A	2.70	1.48	1.42
16	AD	401	HEC	C1D-CHD	2.53	1.48	1.41
11	AC	402	HEM	FE-NB	2.47	2.09	1.96
16	Ad	401	HEC	C1B-CHB	2.46	1.47	1.41
16	Ad	401	HEC	C4B-C3B	2.39	1.47	1.43
11	Ac	403	HEM	C4B-NB	-2.36	1.33	1.38
16	AD	401	HEC	C4D-CHA	2.36	1.47	1.41
11	AC	402	HEM	C1D-ND	-2.29	1.34	1.38
16	Ad	401	HEC	C4D-CHA	2.27	1.47	1.41
11	Ac	402	HEM	C1D-ND	-2.22	1.34	1.38
11	Ac	403	HEM	C1D-ND	-2.20	1.34	1.38
11	AC	402	HEM	FE-ND	-2.14	1.86	1.96
11	Ac	402	HEM	C3B-C4B	2.14	1.49	1.44
11	AC	401	HEM	C4B-NB	-2.13	1.34	1.38
11	AC	402	HEM	C3B-C2B	-2.11	1.33	1.37
16	Ad	401	HEC	C1C-CHC	2.08	1.46	1.41
11	AC	401	HEM	C1D-ND	-2.06	1.34	1.38
11	Ac	403	HEM	FE-ND	-2.04	1.86	1.96

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AD	401	HEC	CMC-C2C-C3C	7.21	134.30	125.82
11	Ac	402	HEM	C4B-C3B-C2B	-6.98	101.57	107.11
16	Ad	401	HEC	C1D-C2D-C3D	-6.40	102.54	107.00
11	AC	402	HEM	CHC-C4B-NB	6.27	131.24	124.43
16	AD	401	HEC	C1D-C2D-C3D	-6.03	102.80	107.00
14	AC	405	UQ6	C7-C8-C9	-5.55	118.63	127.24
11	AC	401	HEM	CHC-C4B-NB	5.47	130.37	124.43
16	Ad	401	HEC	CBD-CAD-C3D	-5.09	103.93	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Ac	402	HEM	C3B-C2B-C1B	4.83	110.07	106.49
11	AC	402	HEM	CHD-C1D-ND	4.79	129.63	124.43
11	AC	402	HEM	C3B-C2B-C1B	-4.70	103.00	106.49
11	AC	402	HEM	CHB-C1B-NB	4.65	130.13	124.38
11	AC	401	HEM	CHD-C1D-ND	4.54	129.36	124.43
16	Ad	401	HEC	CMC-C2C-C3C	4.47	131.08	125.82
11	Ac	403	HEM	CHC-C4B-NB	4.42	129.23	124.43
11	Ac	402	HEM	CHD-C1D-ND	4.42	129.23	124.43
11	AC	402	HEM	C4B-C3B-C2B	4.35	110.57	107.11
11	Ac	403	HEM	CHD-C1D-ND	4.30	129.11	124.43
12	Ac	404	3PE	O21-C21-C22	4.22	120.61	111.50
16	AD	401	HEC	CMB-C2B-C3B	4.15	130.70	125.82
12	Ag	102	3PE	O21-C21-C22	4.11	120.36	111.50
11	Ac	403	HEM	CHA-C4D-ND	4.06	129.39	124.38
11	Ac	402	HEM	CHC-C4B-NB	4.05	128.83	124.43
13	AC	404	U10	C7-C8-C9	-4.04	120.07	126.79
15	Ag	101	CDL	OA6-CA5-C11	4.02	120.17	111.50
15	Ac	407	CDL	OB6-CB5-C51	4.00	120.12	111.50
15	Ag	101	CDL	OB6-CB5-C51	3.95	120.01	111.50
11	AC	402	HEM	CHA-C4D-ND	3.92	129.23	124.38
11	AC	401	HEM	CHA-C4D-ND	3.84	129.12	124.38
12	AC	403	3PE	O21-C21-C22	3.84	119.77	111.50
11	AC	402	HEM	CMA-C3A-C4A	-3.80	122.63	128.46
15	AC	406	CDL	OA6-CA5-C11	3.76	119.61	111.50
13	Ac	405	U10	C22-C23-C24	-3.74	118.65	127.66
16	Ad	401	HEC	CMD-C2D-C3D	3.74	131.99	124.94
11	AC	401	HEM	C1B-NB-C4B	3.72	108.92	105.07
15	AC	406	CDL	OB6-CB5-C51	3.72	119.52	111.50
13	Ac	405	U10	C12-C13-C14	-3.71	118.72	127.66
11	AC	401	HEM	CHB-C1B-NB	3.67	128.91	124.38
11	AC	402	HEM	CHB-C1B-C2B	-3.65	116.61	126.72
14	AC	405	UQ6	C15-C14-C16	3.60	121.33	115.27
11	Ac	403	HEM	CHB-C1B-NB	3.55	128.77	124.38
17	AD	402	3PH	O21-C21-C22	3.54	119.13	111.50
11	Ac	402	HEM	CHA-C4D-ND	3.54	128.76	124.38
16	AD	401	HEC	CBD-CAD-C3D	-3.50	106.65	112.62
17	Ad	402	3PH	O21-C21-C22	3.44	118.91	111.50
15	Ac	407	CDL	OA6-CA5-C11	3.41	120.31	110.80
14	Ac	406	UQ6	C7-C8-C9	-3.40	121.97	127.24
15	Ac	407	CDL	OB8-CB7-C71	3.38	120.24	111.38
11	Ac	403	HEM	C1B-NB-C4B	3.34	108.53	105.07
12	AF	201	3PE	O21-C21-C22	3.33	118.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Ad	401	HEC	CMB-C2B-C3B	3.21	129.59	125.82
11	AC	402	HEM	C1B-NB-C4B	3.17	108.35	105.07
16	AD	401	HEC	CMC-C2C-C1C	-3.17	123.59	128.46
13	Ac	405	U10	C15-C14-C16	3.11	120.51	115.27
13	AC	404	U10	C10-C9-C11	3.11	120.50	115.27
11	Ac	402	HEM	C1B-NB-C4B	3.05	108.22	105.07
13	Ac	405	U10	C10-C9-C11	3.04	120.39	115.27
11	Ac	402	HEM	CHD-C1D-C2D	-3.04	120.23	124.98
11	AC	402	HEM	C4D-ND-C1D	3.03	108.20	105.07
15	Ag	101	CDL	CA4-OA6-CA5	-3.02	110.37	117.79
12	Ac	404	3PE	C2-O21-C21	-3.00	110.40	117.79
13	Ac	405	U10	C20-C19-C21	2.96	120.25	115.27
11	Ac	402	HEM	CHC-C4B-C3B	-2.94	120.07	124.57
13	Ac	405	U10	C1M-C1-C6	-2.92	119.63	124.40
11	AC	402	HEM	C2B-C1B-NB	2.89	113.26	109.84
12	Ag	102	3PE	O31-C31-C32	2.86	120.89	111.91
13	Ac	405	U10	C17-C18-C19	-2.85	120.80	127.66
14	AC	405	UQ6	C10-C9-C11	2.85	120.06	115.27
12	AC	403	3PE	C2-O21-C21	-2.82	110.85	117.79
17	AD	402	3PH	O31-C31-C32	2.81	120.74	111.91
15	Ac	407	CDL	CA4-OA6-CA5	-2.77	110.97	117.79
14	Ac	406	UQ6	C10-C9-C11	2.77	119.92	115.27
14	Ac	406	UQ6	C4M-O4-C4	2.76	122.35	114.78
15	Ac	407	CDL	CB4-OB6-CB5	-2.75	111.01	117.79
14	AC	405	UQ6	C12-C13-C14	-2.75	121.03	127.66
11	AC	402	HEM	CHD-C1D-C2D	-2.74	120.69	124.98
11	Ac	403	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
11	AC	402	HEM	CBD-CAD-C3D	-2.69	105.15	112.63
17	Ad	402	3PH	C2-O21-C21	-2.68	111.19	117.79
14	Ac	406	UQ6	C6-C7-C8	-2.65	107.97	112.17
15	AC	406	CDL	OB8-CB7-C71	2.62	120.13	111.91
11	Ac	403	HEM	CBD-CAD-C3D	-2.60	105.41	112.63
12	AC	403	3PE	O31-C31-C32	2.58	119.99	111.91
11	AC	401	HEM	C4D-ND-C1D	2.57	107.73	105.07
11	Ac	403	HEM	CHA-C4D-C3D	-2.56	120.52	125.33
11	AC	402	HEM	CBA-CAA-C2A	-2.56	108.26	112.62
11	Ac	403	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
14	Ac	406	UQ6	C17-C18-C19	-2.55	119.05	127.75
12	Ac	404	3PE	O31-C31-C32	2.54	119.88	111.91
14	Ac	406	UQ6	C21-C19-C20	2.54	120.22	114.60
15	Ag	101	CDL	OA8-CA7-C31	2.54	119.87	111.91
15	Ag	101	CDL	CB4-OB6-CB5	-2.52	111.59	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Ad	402	3PH	O31-C31-C32	2.52	119.81	111.91
12	AF	201	3PE	O31-C31-C32	2.49	119.73	111.91
13	Ac	405	U10	C27-C28-C29	-2.48	119.27	127.75
14	AC	405	UQ6	C21-C19-C20	2.47	120.06	114.60
11	AC	401	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
13	AC	404	U10	C16-C14-C15	2.45	120.02	114.60
15	Ag	101	CDL	OB8-CB7-C71	2.45	119.59	111.91
15	Ac	407	CDL	OA8-CA7-C31	2.45	119.59	111.91
13	AC	404	U10	C1M-C1-C6	-2.38	120.52	124.40
17	AD	402	3PH	C2-O21-C21	-2.37	111.94	117.79
15	AC	406	CDL	OA8-CA7-C31	2.37	119.34	111.91
11	AC	401	HEM	CHA-C4D-C3D	-2.37	120.88	125.33
14	AC	405	UQ6	C4M-O4-C4	2.36	121.25	114.78
11	Ac	403	HEM	CHB-C1B-C2B	-2.32	120.29	126.72
15	AC	406	CDL	CB4-OB6-CB5	-2.32	112.07	117.79
11	Ac	402	HEM	C4A-C3A-C2A	2.32	108.61	107.00
11	Ac	402	HEM	CHA-C4D-C3D	-2.32	120.97	125.33
11	Ac	402	HEM	CHB-C1B-NB	2.30	127.23	124.38
14	AC	405	UQ6	C7-C6-C5	-2.30	117.80	120.82
13	Ac	405	U10	C31-C29-C30	2.30	119.68	114.60
11	Ac	403	HEM	C4D-ND-C1D	2.28	107.43	105.07
13	AC	404	U10	C12-C13-C14	-2.23	120.11	127.75
14	AC	405	UQ6	C17-C18-C19	-2.23	120.11	127.75
11	AC	402	HEM	CMA-C3A-C2A	2.21	129.10	124.94
11	AC	401	HEM	CHB-C1B-C2B	-2.17	120.71	126.72
16	AD	401	HEC	C3B-C4B-NB	2.15	115.00	110.94
15	AC	406	CDL	CA4-OA6-CA5	-2.14	112.52	117.79
16	Ad	401	HEC	CAA-CBA-CGA	-2.14	107.76	113.76
14	AC	405	UQ6	C1M-C1-C6	-2.11	117.37	120.42
15	Ac	407	CDL	OB6-CB5-OB7	-2.10	118.62	123.70
12	Ag	102	3PE	C2-O21-C21	-2.09	112.63	117.79
13	Ac	405	U10	C7-C6-C5	2.09	121.00	118.48
13	Ac	405	U10	C25-C24-C26	2.09	118.78	115.27
14	AC	405	UQ6	C1M-C1-C2	2.08	124.03	120.50
14	Ac	406	UQ6	C7-C6-C5	-2.08	118.09	120.82
11	AC	402	HEM	CMB-C2B-C1B	2.08	128.20	125.04
12	Ac	404	3PE	O21-C21-O22	-2.06	118.73	123.70
14	Ac	406	UQ6	C3M-O3-C3	2.04	120.38	114.78
14	Ac	406	UQ6	C17-C16-C14	-2.04	106.26	112.98
13	Ac	405	U10	C7-C8-C9	-2.04	123.40	126.79
11	AC	401	HEM	CAA-CBA-CGA	-2.03	108.07	113.76
12	Ag	102	3PE	O31-C31-O32	-2.01	118.52	123.59

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AC	402	HEM	C2B-C3B-CAB-CBB
11	AC	402	HEM	C4B-C3B-CAB-CBB
11	Ac	403	HEM	C2B-C3B-CAB-CBB
11	Ac	403	HEM	C4B-C3B-CAB-CBB
12	AC	403	3PE	C1-O11-P-O12
12	AC	403	3PE	C1-O11-P-O13
12	AC	403	3PE	C1-O11-P-O14
12	AC	403	3PE	C11-O13-P-O12
12	AC	403	3PE	C11-O13-P-O14
12	Ac	401	3PE	C1-O11-P-O12
12	Ac	401	3PE	C22-C21-O21-C2
12	Ag	102	3PE	C11-O13-P-O11
12	Ag	102	3PE	C11-O13-P-O12
12	Ag	102	3PE	C11-O13-P-O14
13	Ac	405	U10	C5-C6-C7-C8
14	AC	405	UQ6	C13-C14-C16-C17
14	AC	405	UQ6	C15-C14-C16-C17
14	Ac	406	UQ6	C1-C6-C7-C8
14	Ac	406	UQ6	C13-C14-C16-C17
14	Ac	406	UQ6	C15-C14-C16-C17
15	AC	406	CDL	CA2-OA2-PA1-OA4
15	AC	406	CDL	CA3-OA5-PA1-OA3
15	AC	406	CDL	CA3-OA5-PA1-OA4
15	AC	406	CDL	C31-CA7-OA8-CA6
15	Aa	501	CDL	CA3-OA5-PA1-OA2
15	Aa	501	CDL	CB4-CB3-OB5-PB2
15	Ac	407	CDL	CB2-OB2-PB2-OB3
15	Ac	407	CDL	CB2-OB2-PB2-OB4
15	Ac	407	CDL	CB2-OB2-PB2-OB5
15	Ac	407	CDL	CB3-OB5-PB2-OB3
15	Ag	101	CDL	C1-CB2-OB2-PB2
15	Ag	101	CDL	CB2-OB2-PB2-OB5
15	Ag	101	CDL	CB3-OB5-PB2-OB2
15	Ag	101	CDL	CB3-OB5-PB2-OB3
15	Ag	101	CDL	CB3-OB5-PB2-OB4
16	AD	401	HEC	C1A-C2A-CAA-CBA
17	Ad	402	3PH	C22-C21-O21-C2
15	AC	406	CDL	OA9-CA7-OA8-CA6
12	AF	201	3PE	O32-C31-O31-C3
12	Ac	401	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
15	AC	406	CDL	OA7-CA5-OA6-CA4
17	Ad	402	3PH	O22-C21-O21-C2
13	Ac	405	U10	C25-C24-C26-C27
12	AF	201	3PE	C32-C31-O31-C3
12	AC	403	3PE	O32-C31-O31-C3
12	AC	403	3PE	C32-C31-O31-C3
15	AC	406	CDL	C11-CA5-OA6-CA4
15	Ag	101	CDL	CB4-CB3-OB5-PB2
15	AC	406	CDL	OB9-CB7-OB8-CB6
15	AC	406	CDL	C71-CB7-OB8-CB6
15	Aa	501	CDL	CA2-C1-CB2-OB2
15	Aa	501	CDL	O1-C1-CB2-OB2
17	AD	402	3PH	O21-C2-C3-O31
11	Ac	402	HEM	C2A-CAA-CBA-CGA
11	Ac	403	HEM	C2A-CAA-CBA-CGA
16	AD	401	HEC	C2A-CAA-CBA-CGA
15	Ag	101	CDL	C31-CA7-OA8-CA6
11	Ac	403	HEM	C3D-CAD-CBD-CGD
14	Ac	406	UQ6	C9-C11-C12-C13
15	Ag	101	CDL	OA9-CA7-OA8-CA6
12	AC	403	3PE	C11-O13-P-O11
12	AF	201	3PE	C1-O11-P-O13
12	AF	201	3PE	C11-O13-P-O11
15	AC	406	CDL	CA2-OA2-PA1-OA5
15	AC	406	CDL	CA3-OA5-PA1-OA2
15	AC	406	CDL	CB2-OB2-PB2-OB5
15	Ac	407	CDL	CB3-OB5-PB2-OB2
13	Ac	405	U10	C23-C24-C26-C27
15	Aa	501	CDL	C11-CA5-OA6-CA4
12	AF	201	3PE	C34-C35-C36-C37
15	Aa	501	CDL	OA7-CA5-OA6-CA4
13	Ac	405	U10	C12-C11-C9-C10
13	Ac	405	U10	C20-C19-C21-C22
13	Ac	405	U10	C12-C11-C9-C8
15	Ag	101	CDL	C74-C75-C76-C77
13	Ac	405	U10	C18-C19-C21-C22
12	Ac	401	3PE	O21-C21-C22-C23
15	Aa	501	CDL	C72-C71-CB7-OB8
12	Ac	404	3PE	C32-C31-O31-C3
15	AC	406	CDL	OB6-CB4-CB6-OB8
17	Ad	402	3PH	C25-C26-C27-C28
12	AC	403	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
12	Ac	404	3PE	C22-C21-O21-C2
12	AC	403	3PE	C22-C23-C24-C25
17	AD	402	3PH	C1-C2-C3-O31
17	Ad	402	3PH	C1-C2-C3-O31
13	Ac	405	U10	C1-C6-C7-C8
12	Ac	404	3PE	O32-C31-O31-C3
15	AC	406	CDL	CA6-CA4-OA6-CA5
12	AC	403	3PE	O22-C21-O21-C2
17	AD	402	3PH	C32-C31-O31-C3
15	AC	406	CDL	CB3-CB4-CB6-OB8
12	Ag	102	3PE	C32-C31-O31-C3
17	Ad	402	3PH	O21-C2-C3-O31
12	Ac	404	3PE	O22-C21-O21-C2
15	Aa	501	CDL	C1-CB2-OB2-PB2
14	Ac	406	UQ6	C5-C6-C7-C8
15	Ac	407	CDL	C51-CB5-OB6-CB4
16	Ad	401	HEC	C3D-CAD-CBD-CGD
11	AC	401	HEM	C2B-C3B-CAB-CBB
17	AD	402	3PH	O32-C31-O31-C3
12	Ag	102	3PE	O32-C31-O31-C3
15	Ac	407	CDL	OB7-CB5-OB6-CB4
12	Ac	404	3PE	C23-C24-C25-C26
17	Ad	402	3PH	C2-C3-O31-C31
12	Ac	401	3PE	C1-O11-P-O13
15	AC	406	CDL	CA4-CA3-OA5-PA1
12	AF	201	3PE	C1-O11-P-O14
12	AF	201	3PE	C11-O13-P-O12
12	AF	201	3PE	C11-O13-P-O14
12	Ac	401	3PE	C1-O11-P-O14
15	AC	406	CDL	CB2-OB2-PB2-OB3
15	Aa	501	CDL	CA3-OA5-PA1-OA4
15	Ac	407	CDL	CB3-OB5-PB2-OB4
15	Ag	101	CDL	CB2-OB2-PB2-OB4
15	Ag	101	CDL	C54-C55-C56-C57
16	AD	401	HEC	C3A-C2A-CAA-CBA
12	AF	201	3PE	C35-C36-C37-C38
12	Ac	401	3PE	C2-C1-O11-P
14	Ac	406	UQ6	C3-C4-O4-C4M
17	AD	402	3PH	C2-C3-O31-C31
15	AC	406	CDL	CB4-CB3-OB5-PB2
15	Ac	407	CDL	C1-CA2-OA2-PA1
11	Ac	403	HEM	CAD-CBD-CGD-O1D

Continued on next page...

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Mol	Chain	Res	Type	Atoms
17	AD	402	3PH	C25-C26-C27-C28
15	Aa	501	CDL	CA4-CA6-OA8-CA7
11	AC	401	HEM	CAD-CBD-CGD-O2D
11	AC	401	HEM	CAD-CBD-CGD-O1D
15	Aa	501	CDL	C33-C34-C35-C36
12	AC	403	3PE	C24-C25-C26-C27
11	AC	402	HEM	CAD-CBD-CGD-O2D
11	Ac	402	HEM	CAD-CBD-CGD-O1D
15	Aa	501	CDL	CA6-CA4-OA6-CA5
11	AC	401	HEM	CAA-CBA-CGA-O1A
11	AC	402	HEM	CAD-CBD-CGD-O1D
11	AC	401	HEM	CAA-CBA-CGA-O2A
11	Ac	403	HEM	CAD-CBD-CGD-O2D
17	Ad	402	3PH	C37-C38-C39-C3A
11	Ac	402	HEM	CAD-CBD-CGD-O2D
15	Ag	101	CDL	C11-C12-C13-C14
17	AD	402	3PH	C1-O11-P-O13
12	Ac	401	3PE	C1-C2-O21-C21
13	Ac	405	U10	C5-C4-O4-C4M
14	AC	405	UQ6	C14-C16-C17-C18
17	AD	402	3PH	O22-C21-O21-C2
12	Ac	404	3PE	O21-C21-C22-C23
11	AC	401	HEM	C4B-C3B-CAB-CBB
11	Ac	403	HEM	CAA-CBA-CGA-O1A
15	Aa	501	CDL	C72-C71-CB7-OB9
11	Ac	403	HEM	CAA-CBA-CGA-O2A
14	Ac	406	UQ6	C5-C4-O4-C4M
12	Ac	404	3PE	O22-C21-C22-C23
12	Ac	401	3PE	O22-C21-C22-C23
15	Ac	407	CDL	C71-CB7-OB8-CB6
15	Aa	501	CDL	O1-C1-CA2-OA2
12	Ac	404	3PE	C2-C3-O31-C31
15	Aa	501	CDL	CB3-OB5-PB2-OB3
12	Ac	401	3PE	C3-C2-O21-C21
17	Ad	402	3PH	C23-C24-C25-C26
15	Ac	407	CDL	OB9-CB7-OB8-CB6
16	Ad	401	HEC	CAA-CBA-CGA-O2A
15	Aa	501	CDL	C12-C11-CA5-OA6

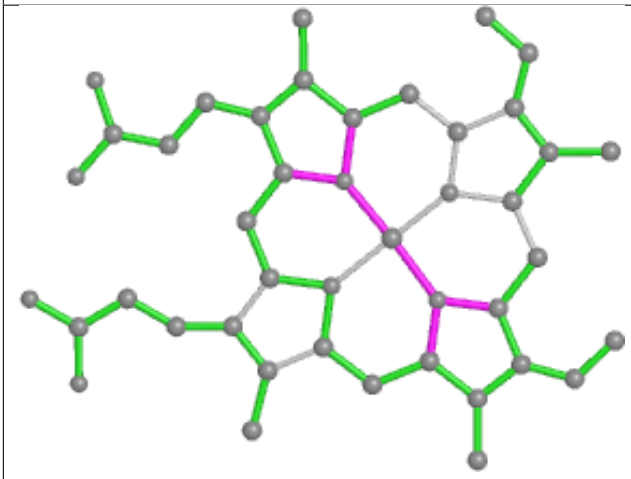
There are no ring outliers.

No monomer is involved in short contacts.

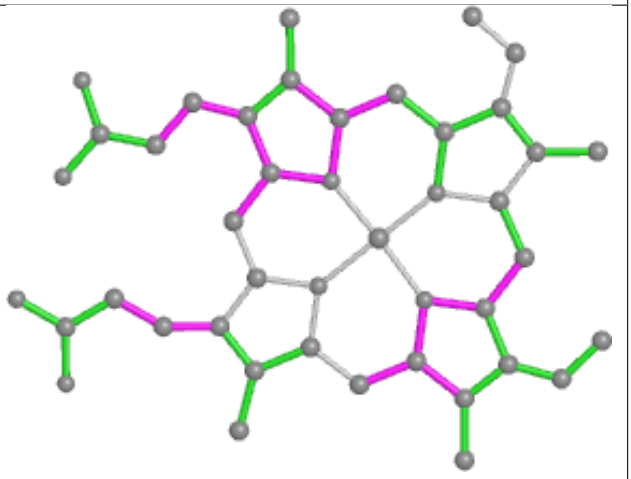
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

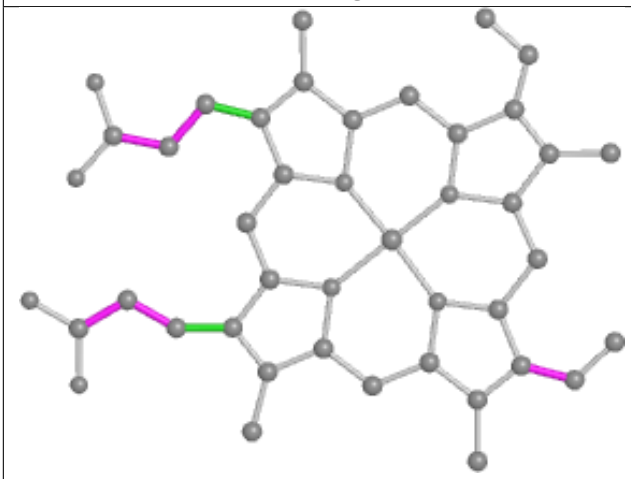
Ligand HEM Ac 403



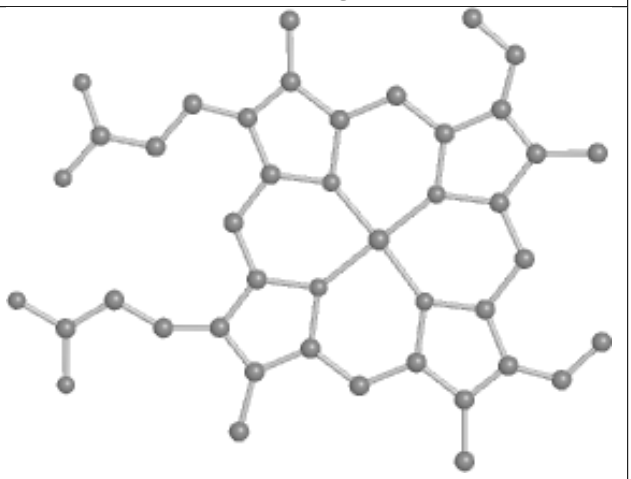
Bond lengths



Bond angles

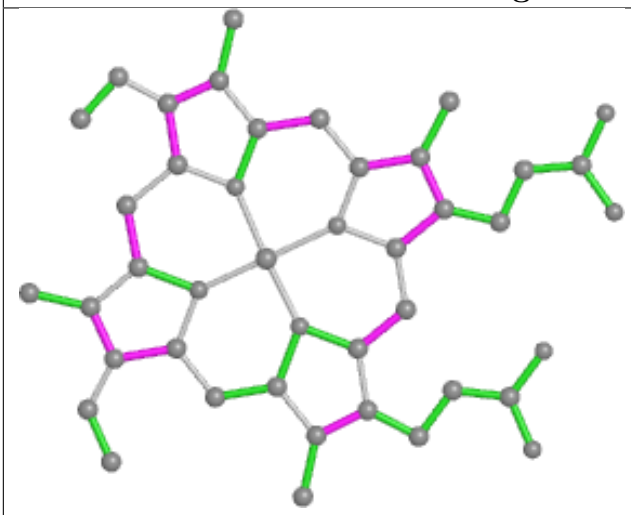


Torsions

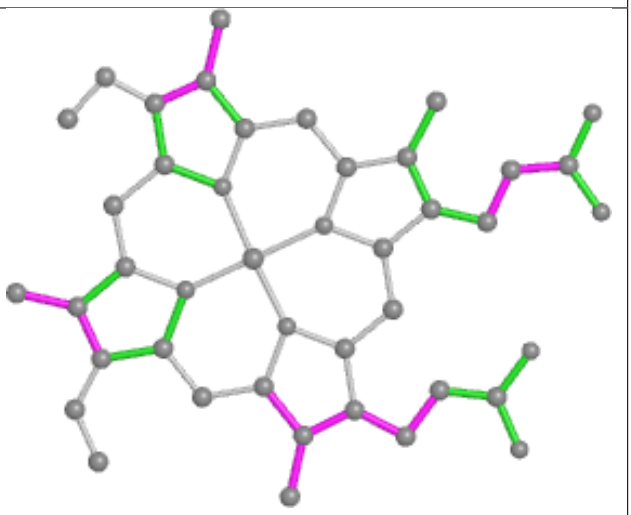


Rings

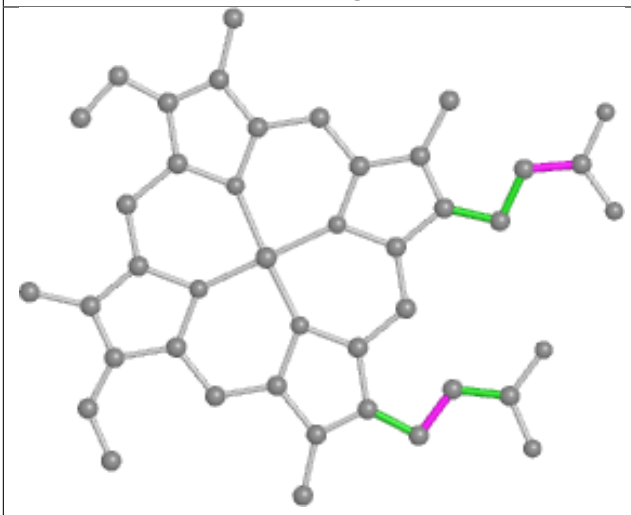
Ligand HEC Ad 401



Bond lengths



Bond angles



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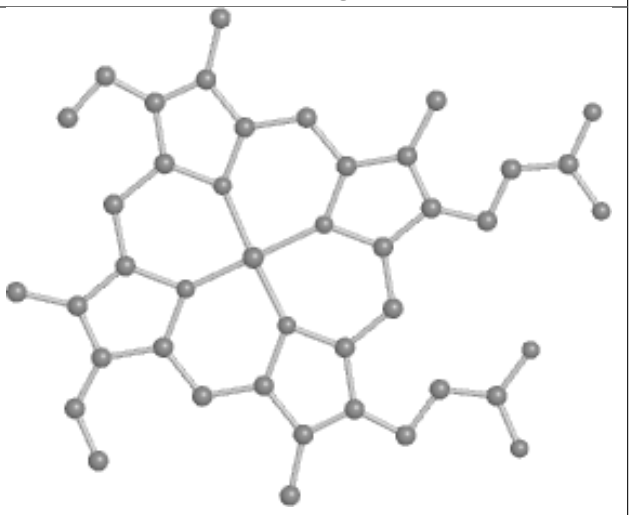
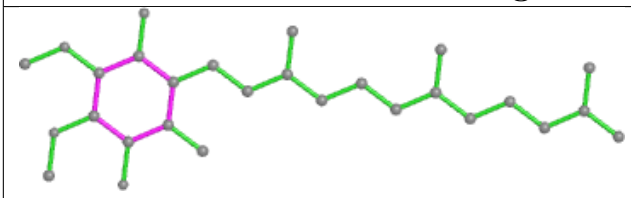
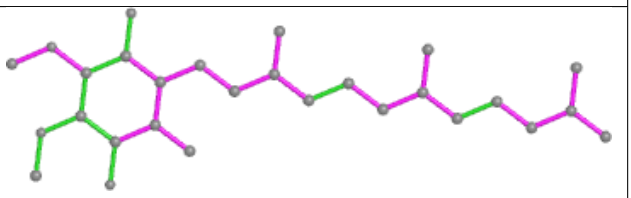


Rings

Ligand UQ6 AC 405



Bond lengths



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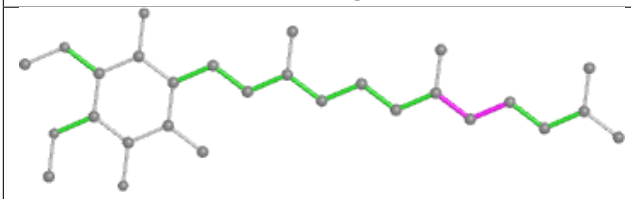
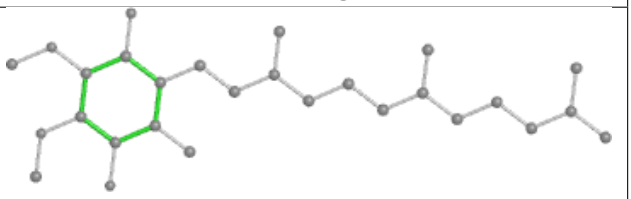
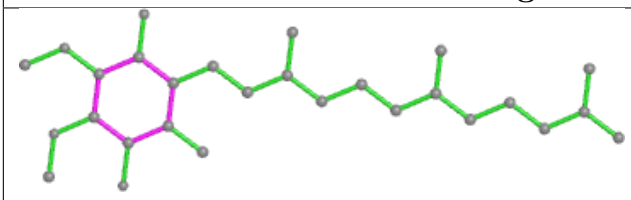


Torsions

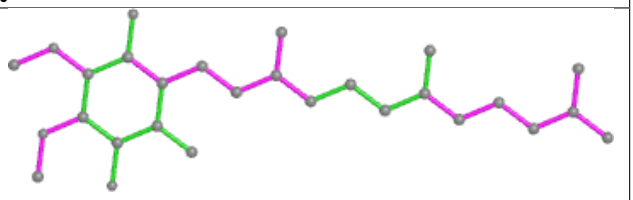


Rings

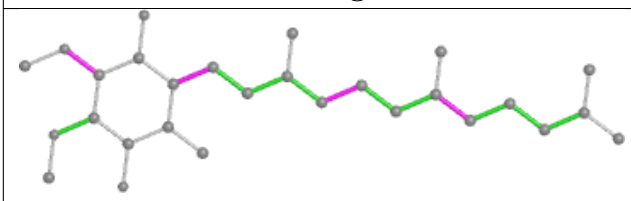
Ligand UQ6 Ac 406



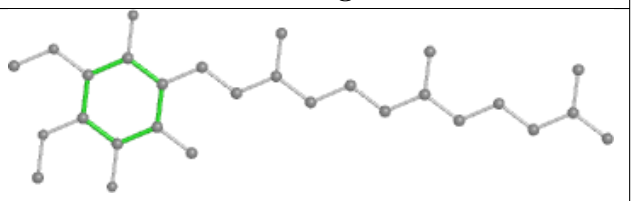
Bond lengths



Bond angles

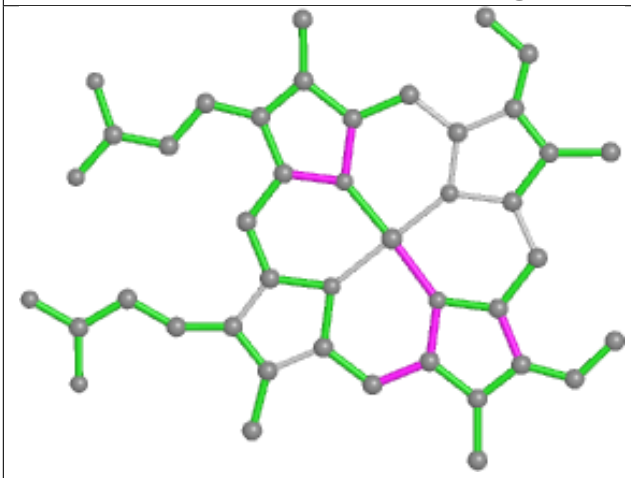


Torsions



Rings

Ligand HEM Ac 402



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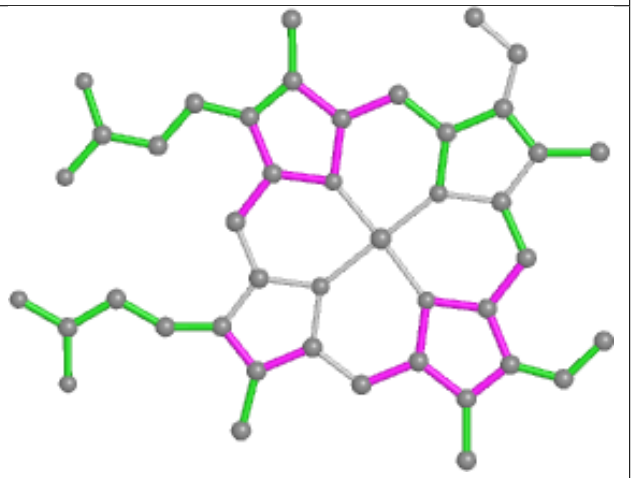
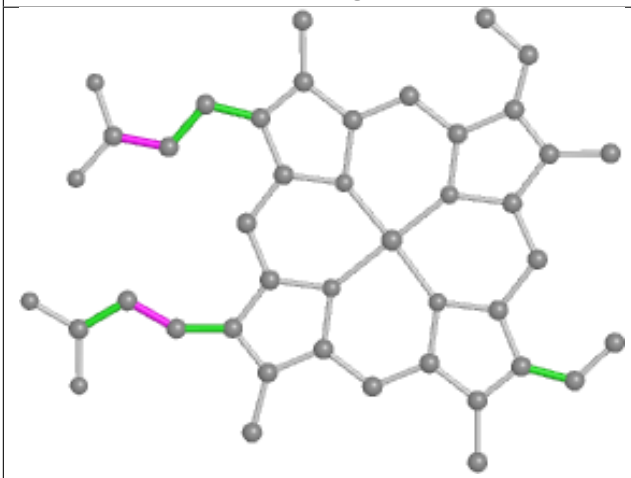


Bond angles



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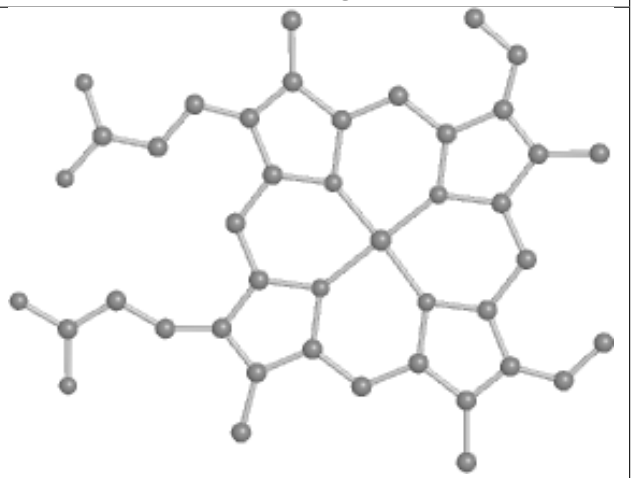
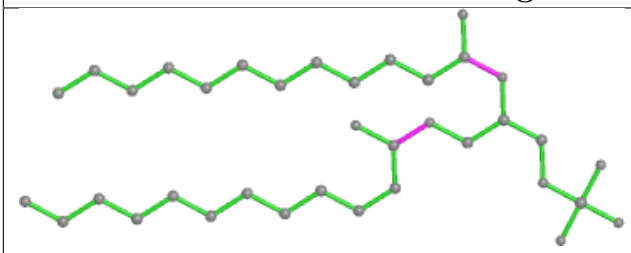


Rings

Ligand 3PH Ad 402



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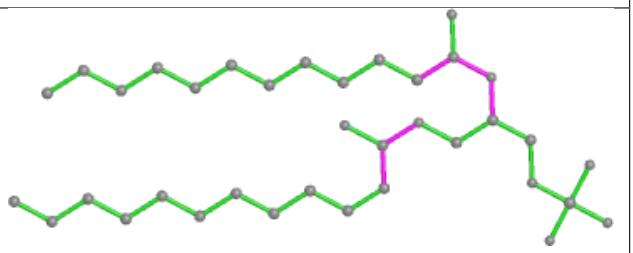

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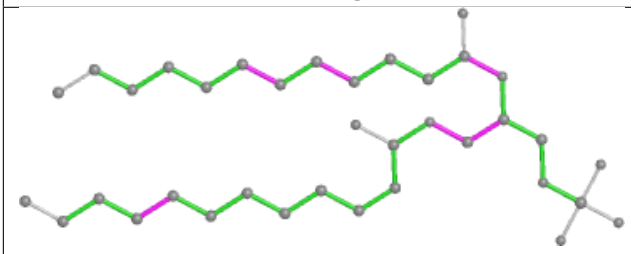
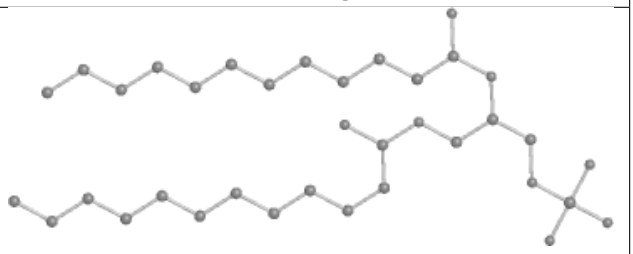
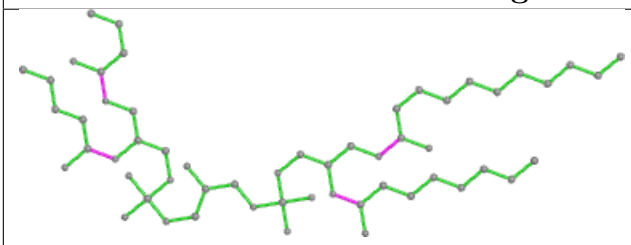


Torsions



Rings

Ligand CDL AC 406



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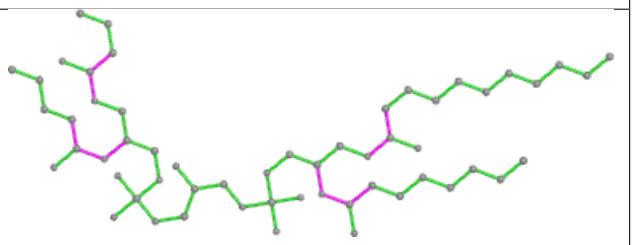
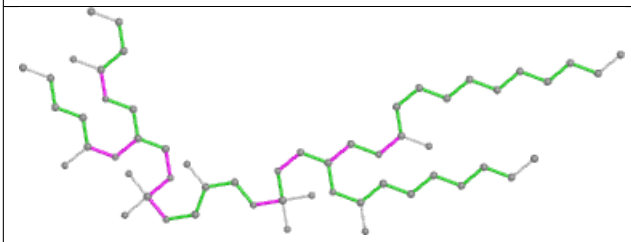


Bond angles



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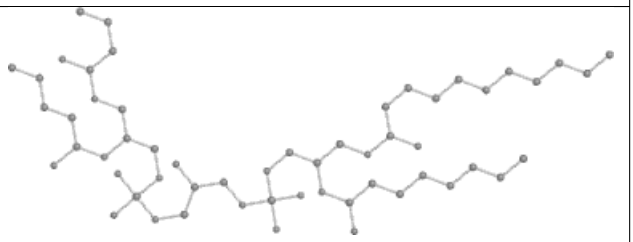
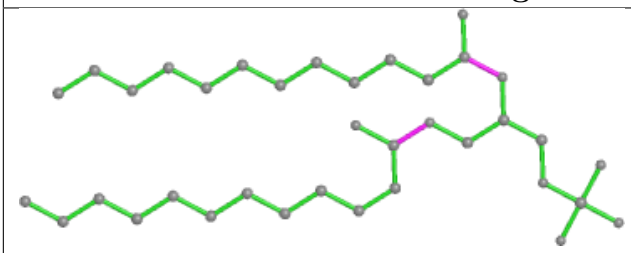


Rings

Ligand 3PH AD 402



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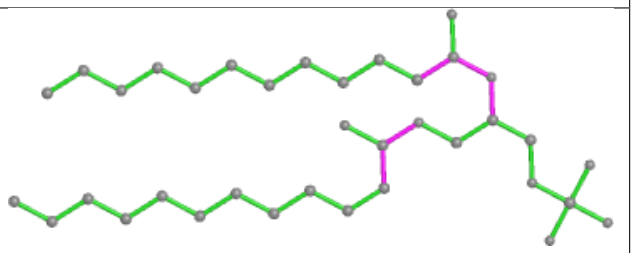
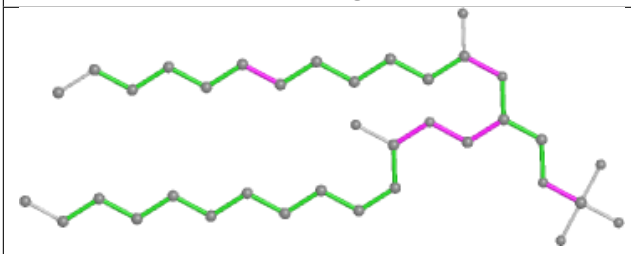
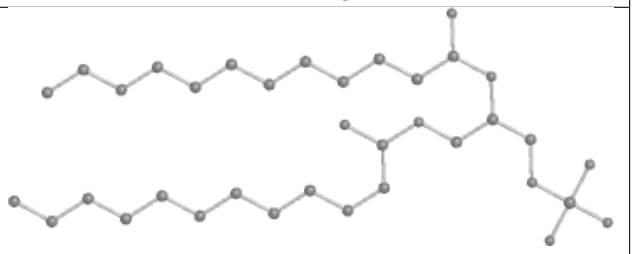


Bond angles

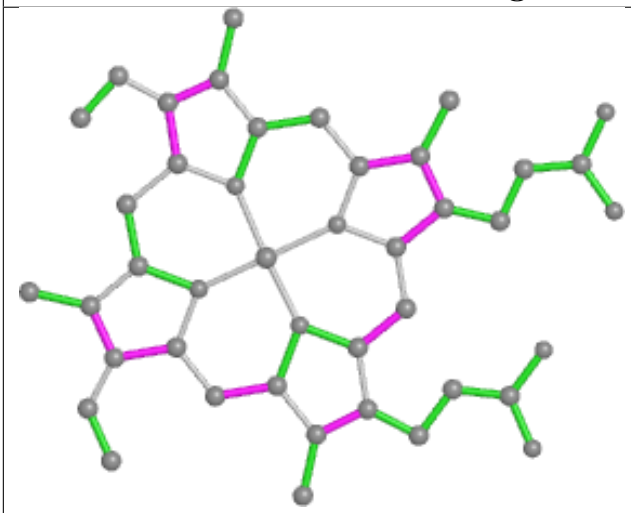


Torsions

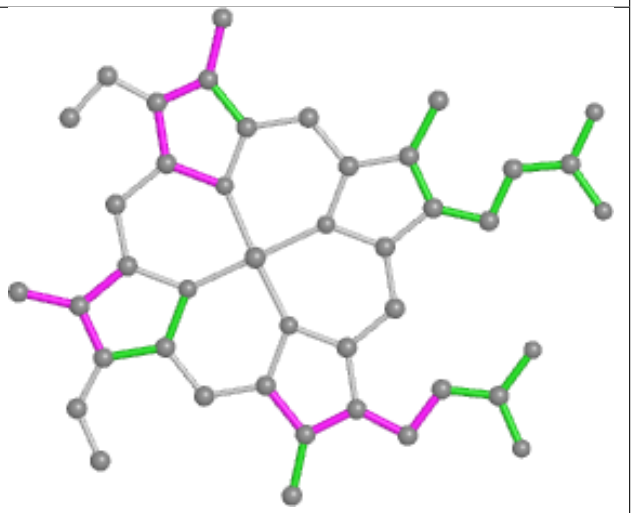


Rings

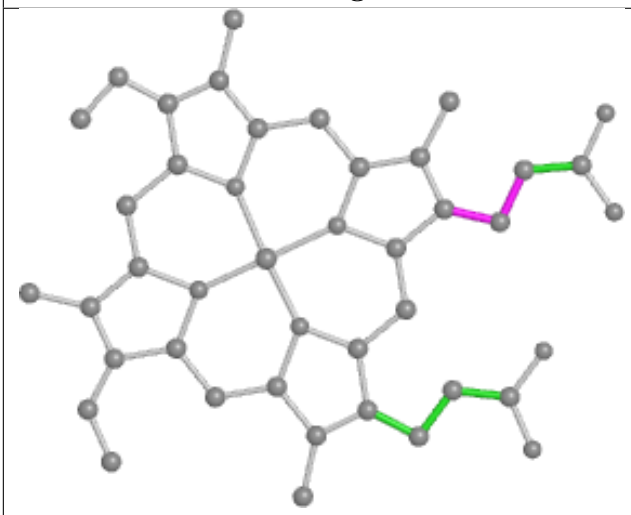
Ligand HEC AD 401



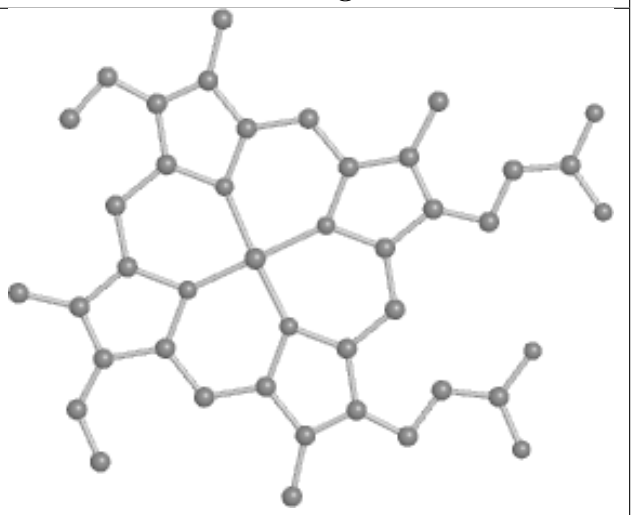
Bond lengths



Bond angles

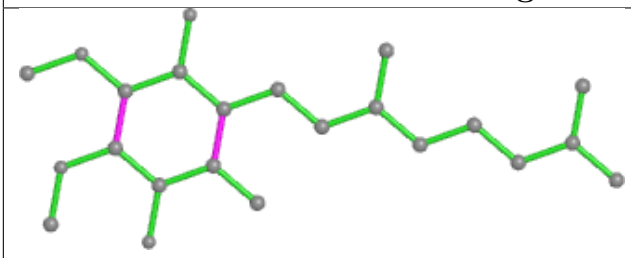


Torsions



Rings

Ligand U10 AC 404



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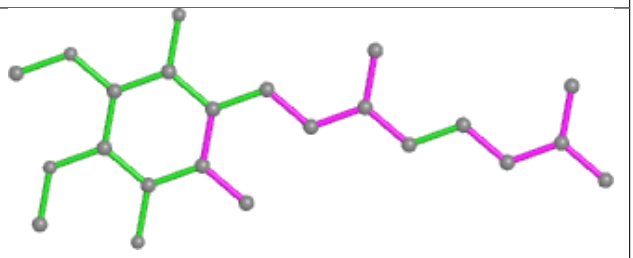
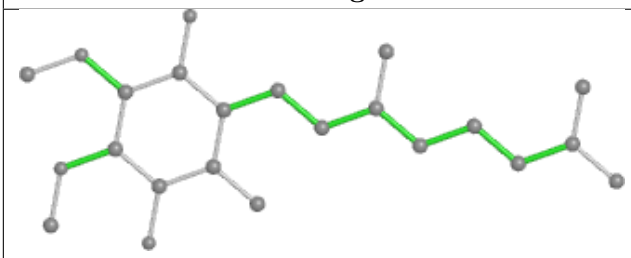


Bond angles



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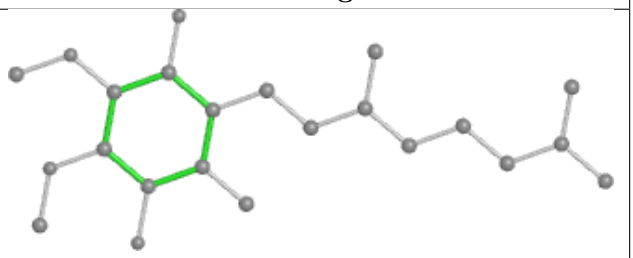
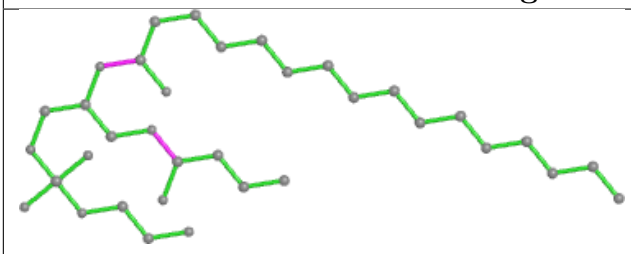
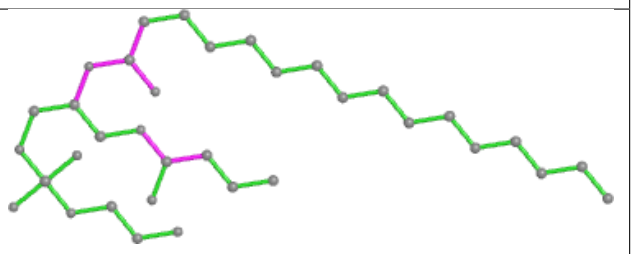


Rings

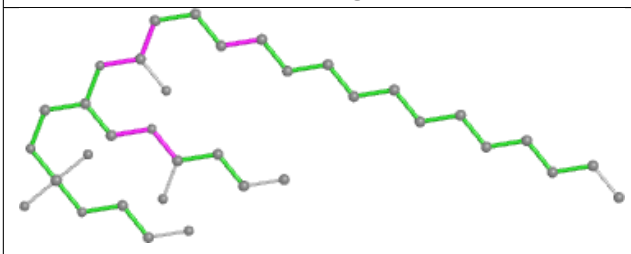
Ligand 3PE Ac 404



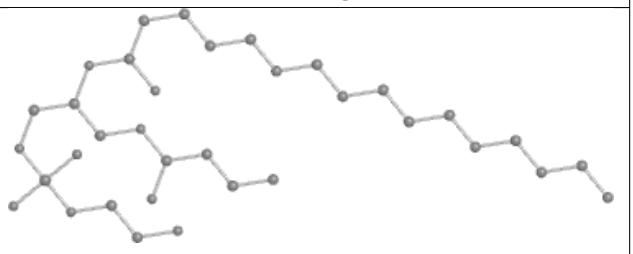
Bond lengths



Bond angles

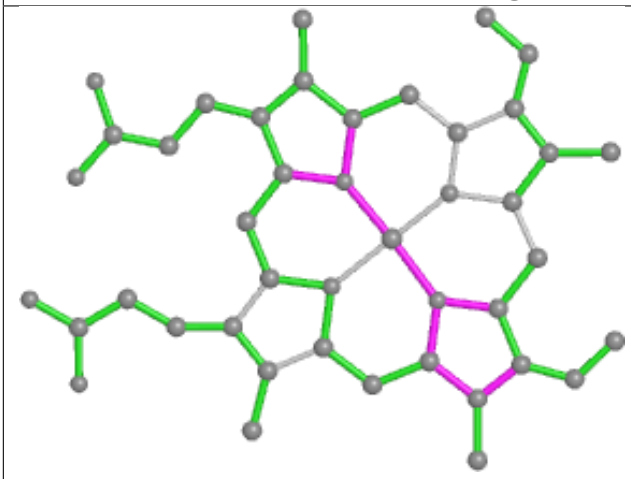


Torsions

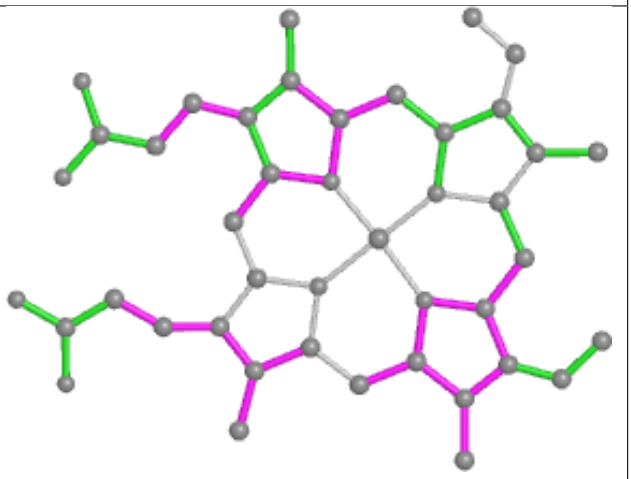


Rings

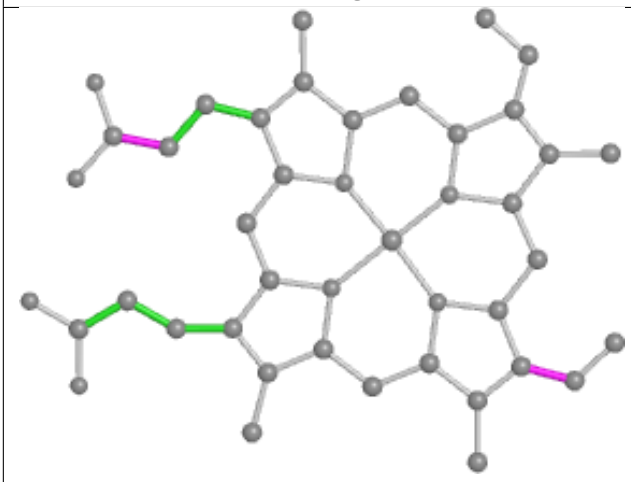
Ligand HEM AC 402



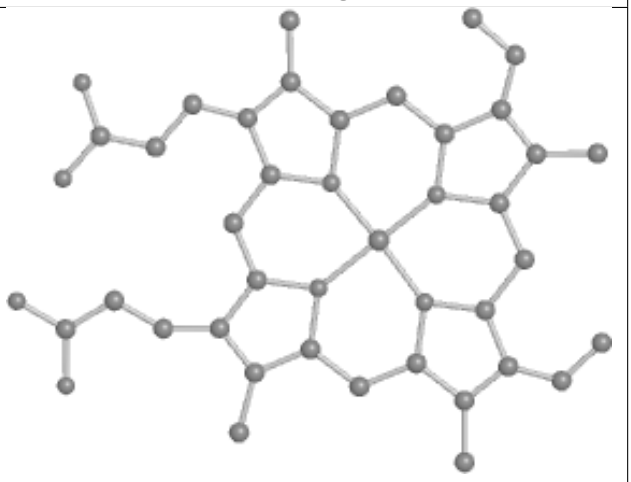
Bond lengths



Bond angles

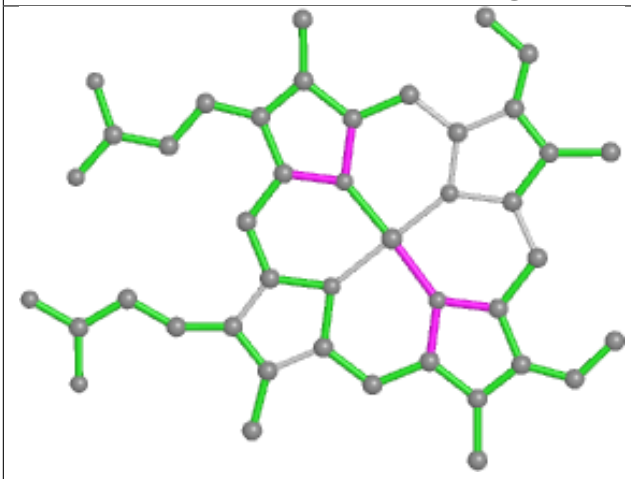


Torsions

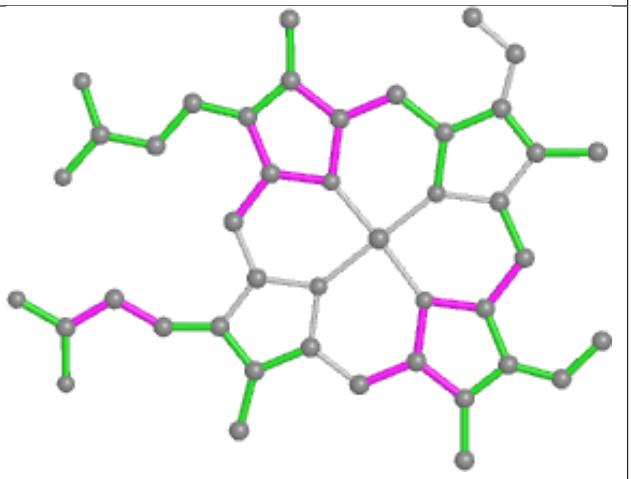


Rings

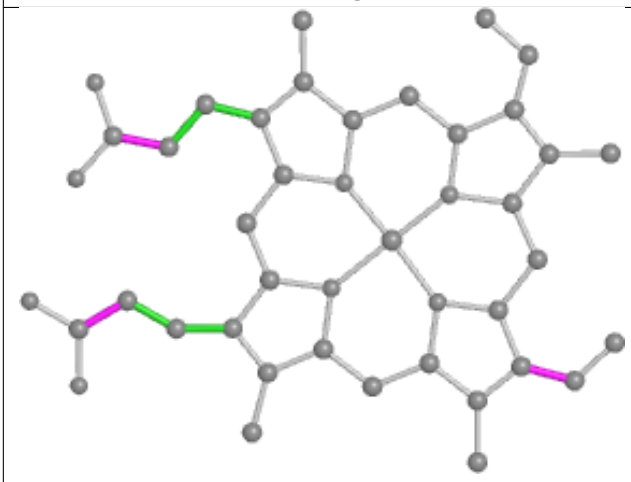
Ligand HEM AC 401



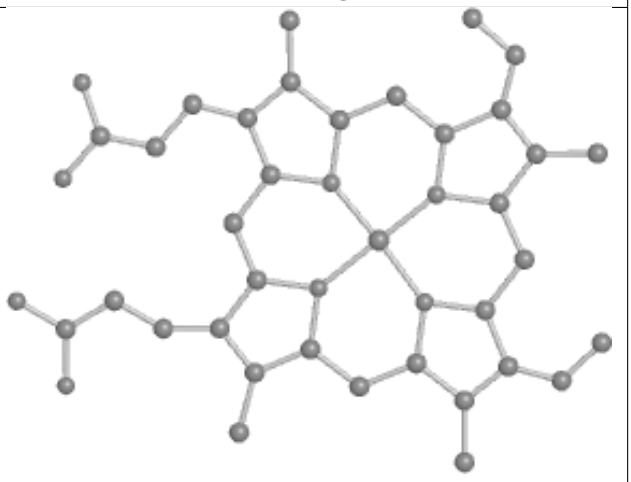
Bond lengths



Bond angles

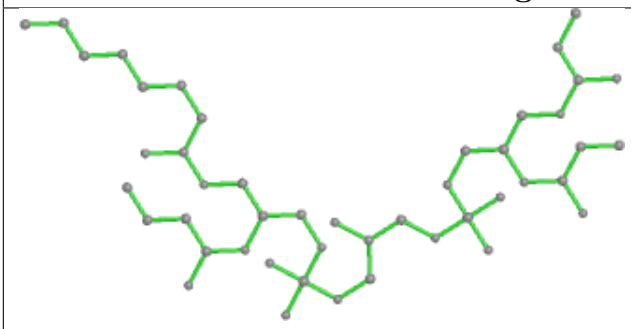


Torsions

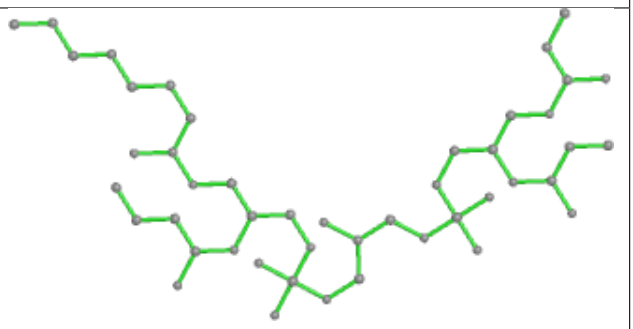


Rings

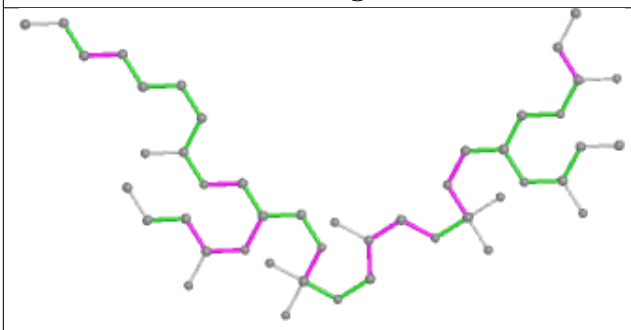
Ligand CDL Aa 501



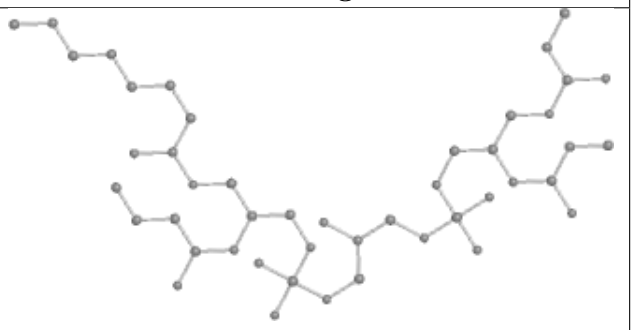
Bond lengths



Bond angles

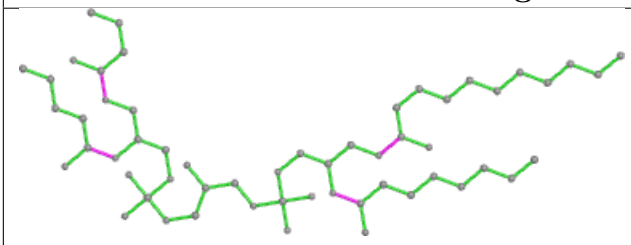


Torsions

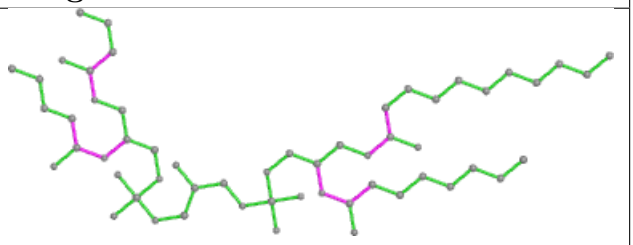


Rings

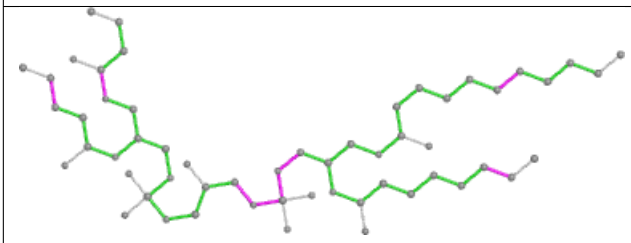
Ligand CDL Ag 101



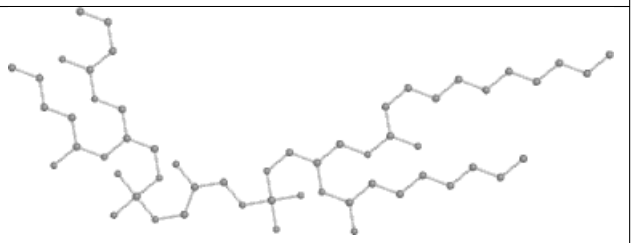
Bond lengths



Bond angles

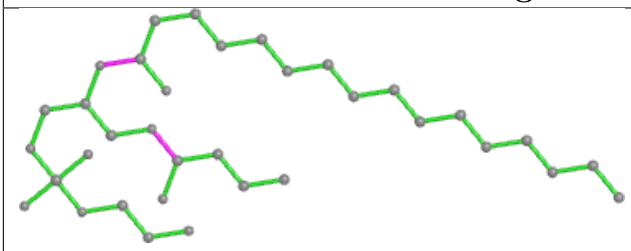


Torsions

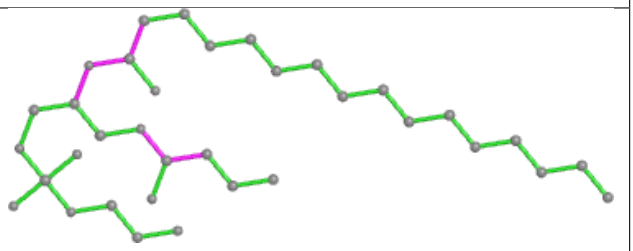


Rings

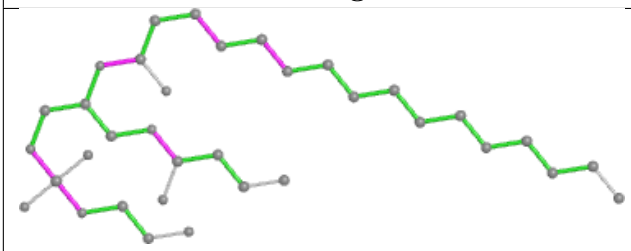
Ligand 3PE AC 403



Bond lengths



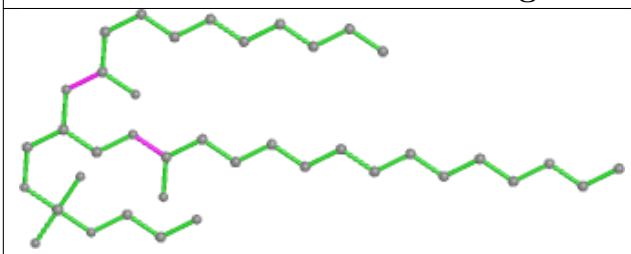
Bond angles



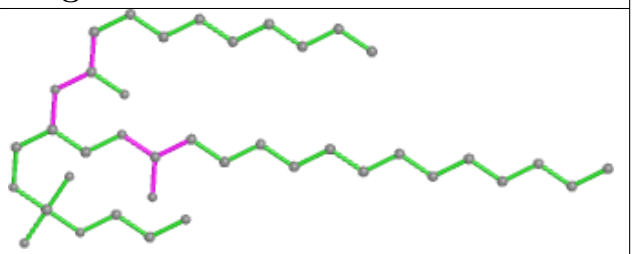
Torsions

Rings

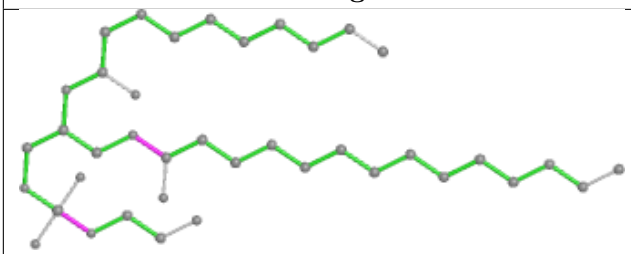
Ligand 3PE Ag 102



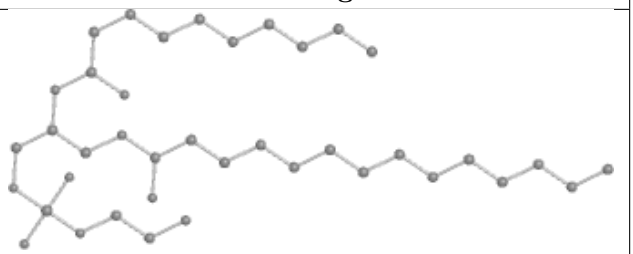
Bond lengths



Bond angles

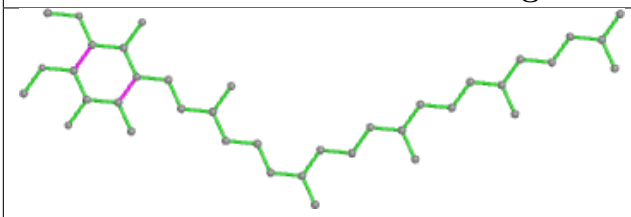


Torsions

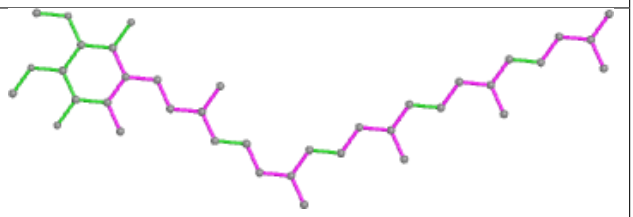


Rings

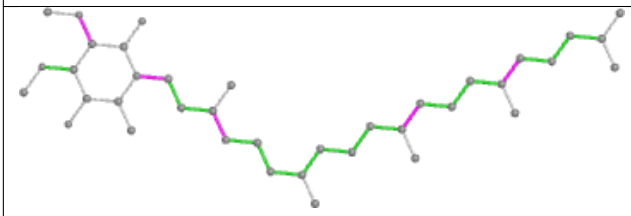
Ligand U10 Ac 405



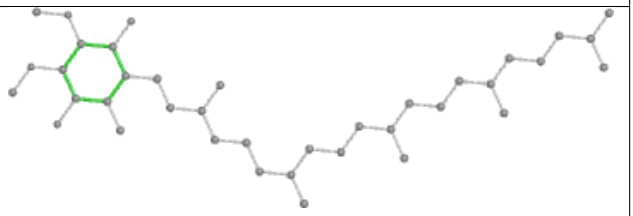
Bond lengths



Bond angles

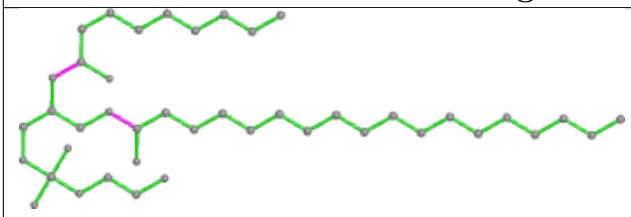


Torsions

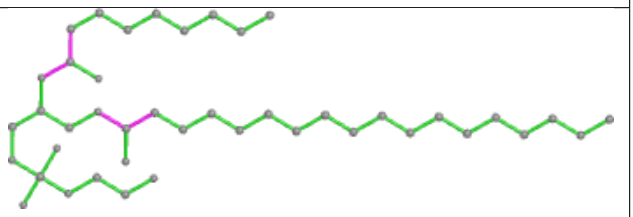


Rings

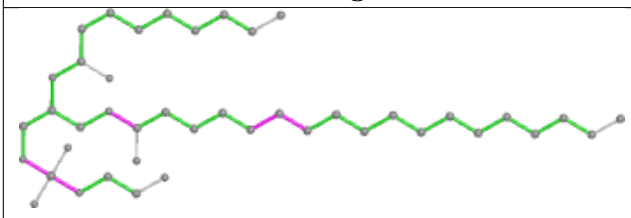
Ligand 3PE AF 201



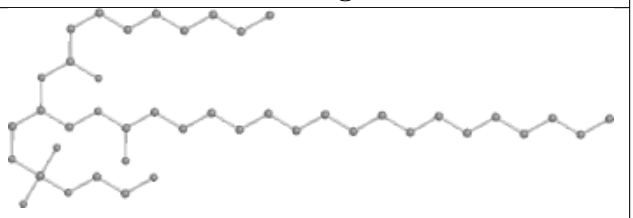
Bond lengths



Bond angles

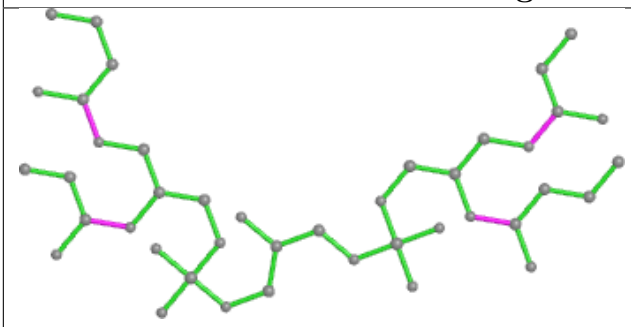


Torsions

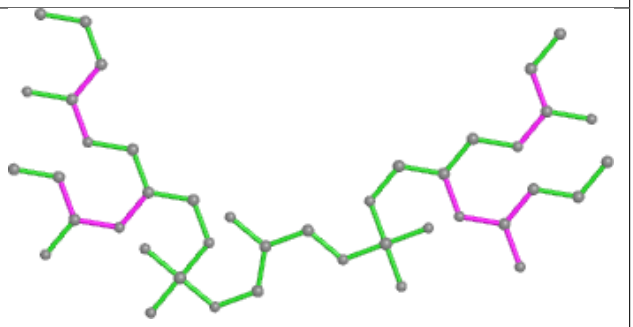


Rings

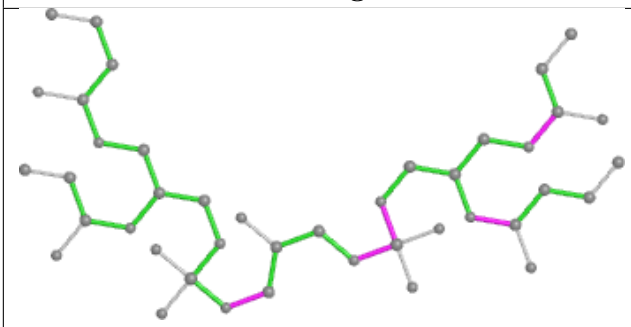
Ligand CDL Ac 407



Bond lengths



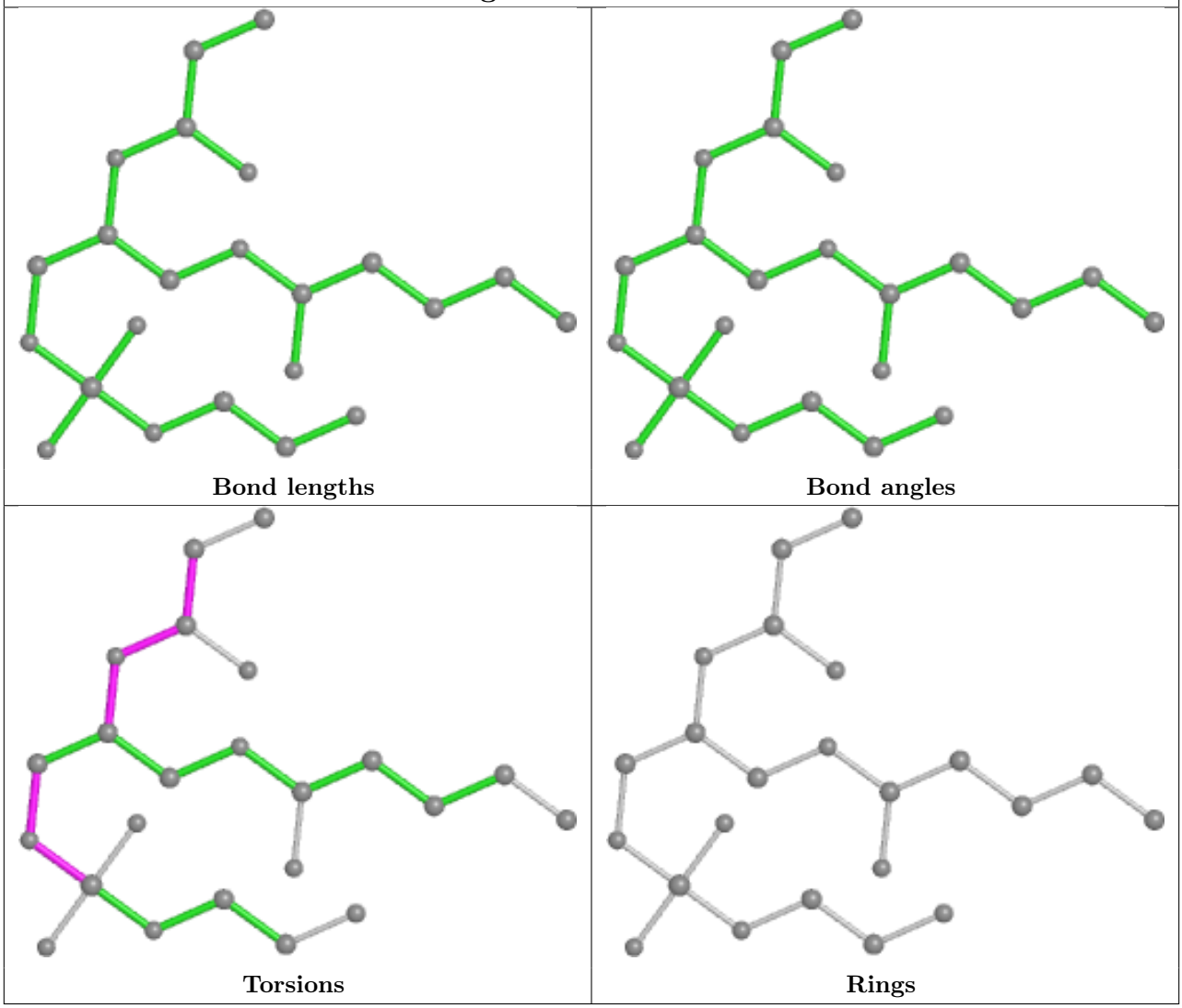
Bond angles



Torsions

Rings

Ligand 3PE Ac 401



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.

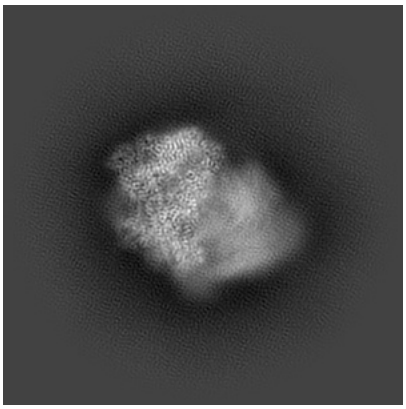
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35334. These allow visual inspection of the internal detail of the map and identification of artifacts.

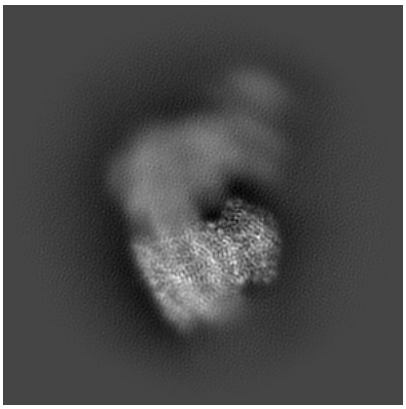
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

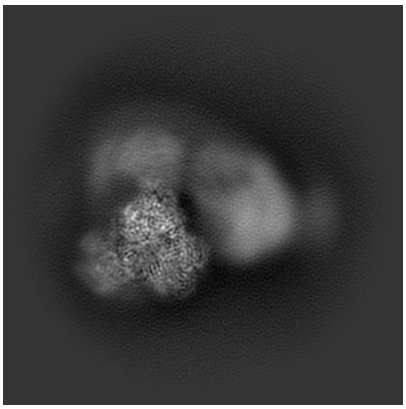
6.1.1 Primary map



X

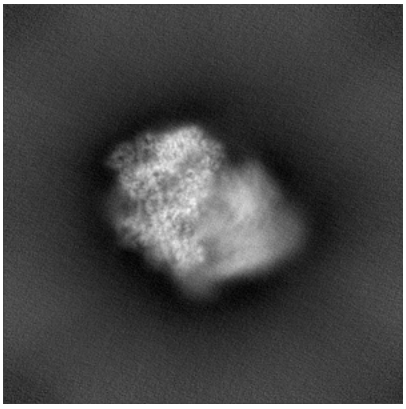


Y

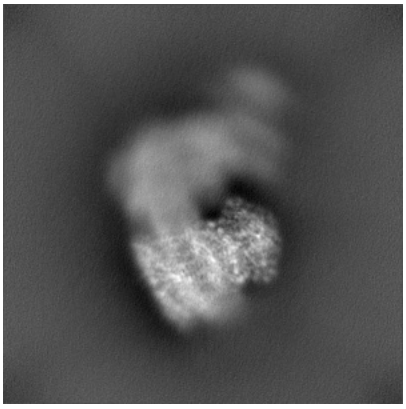


Z

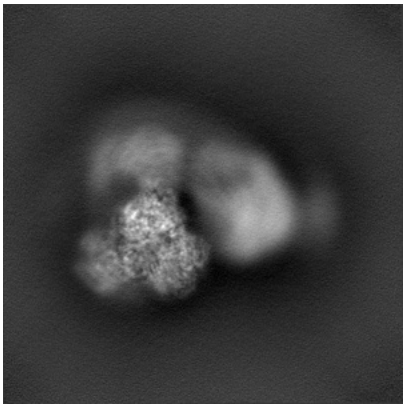
6.1.2 Raw map



X



Y

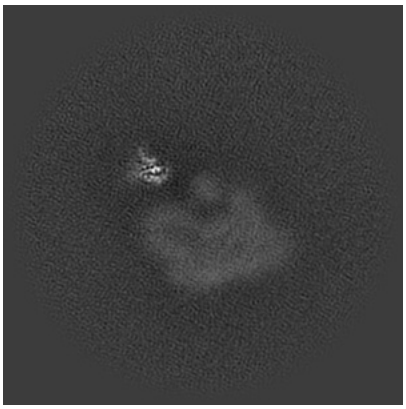


Z

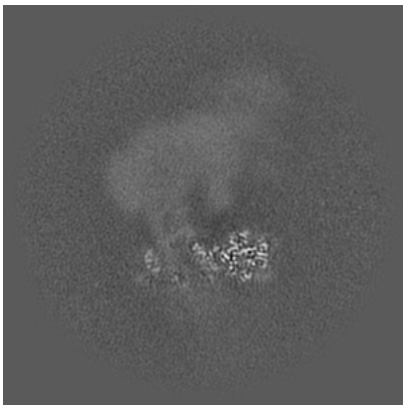
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

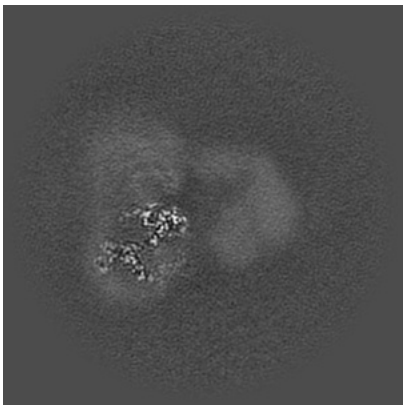
6.2.1 Primary map



X Index: 192

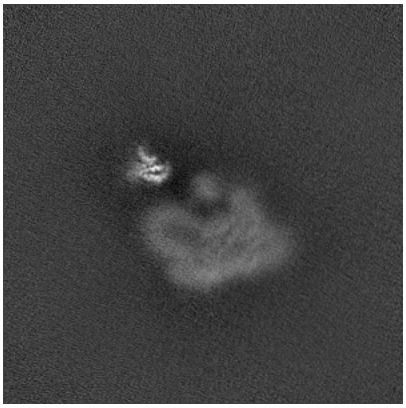


Y Index: 192

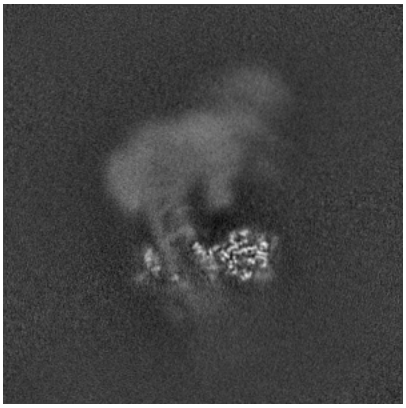


Z Index: 192

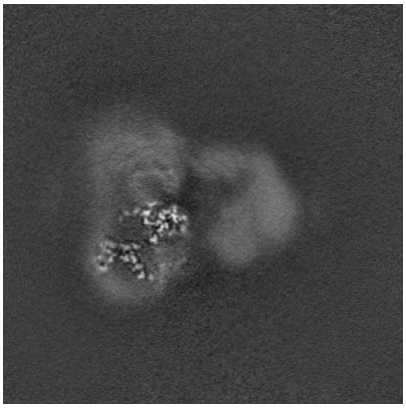
6.2.2 Raw map



X Index: 192



Y Index: 192

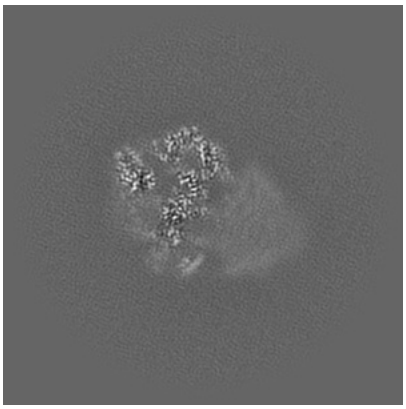


Z Index: 192

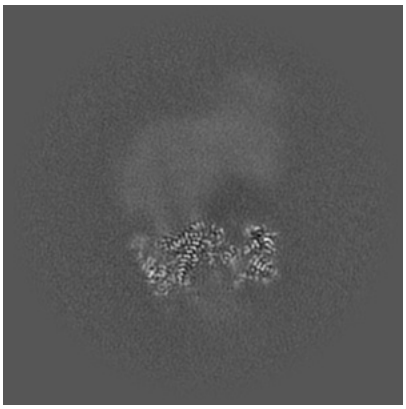
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

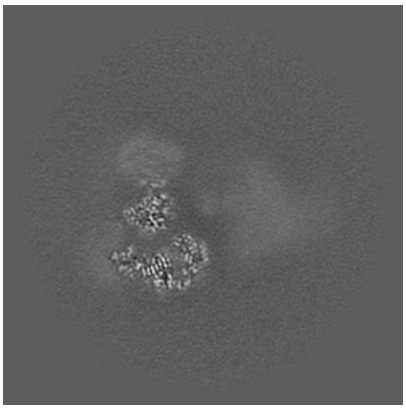
6.3.1 Primary map



X Index: 149

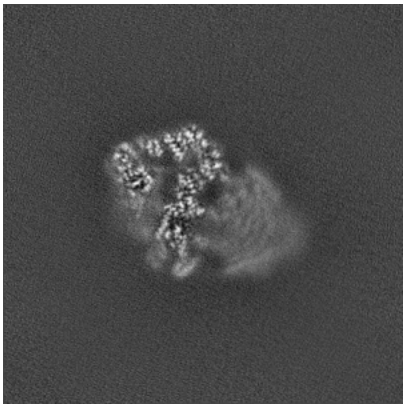


Y Index: 168

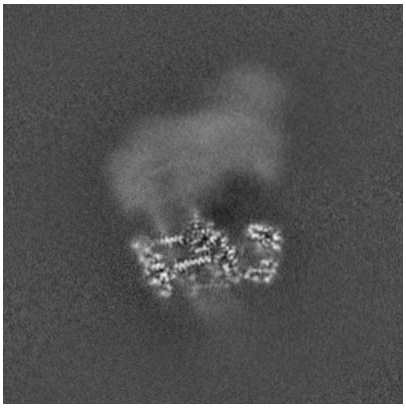


Z Index: 217

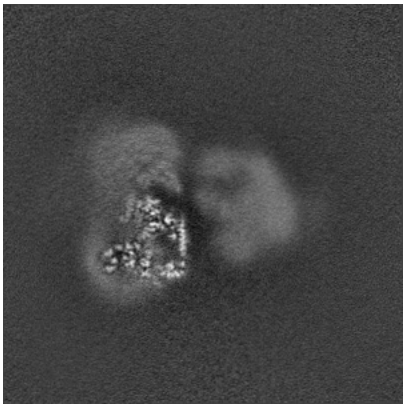
6.3.2 Raw map



X Index: 153



Y Index: 175

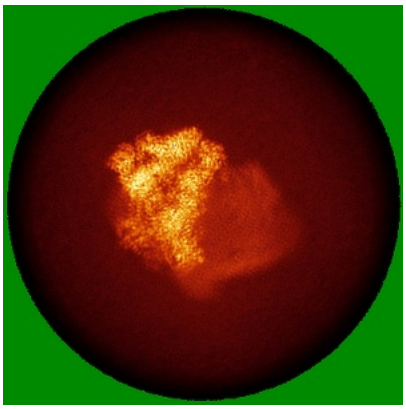


Z Index: 200

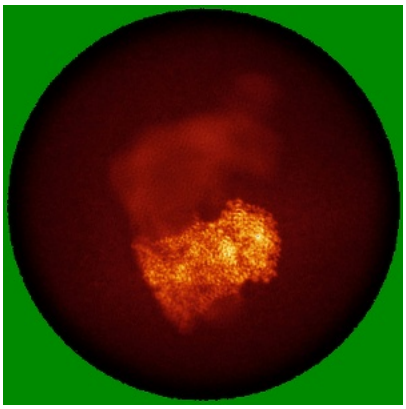
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

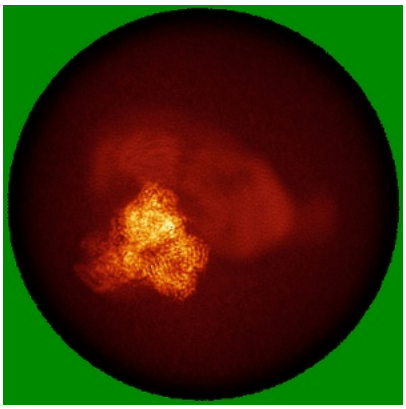
6.4.1 Primary map



X

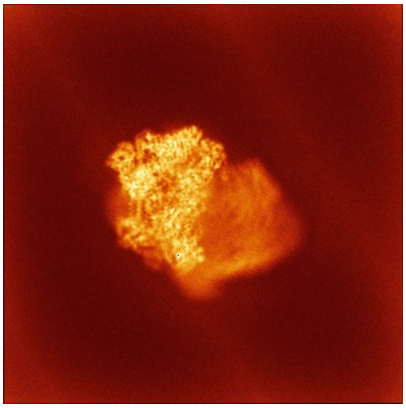


Y

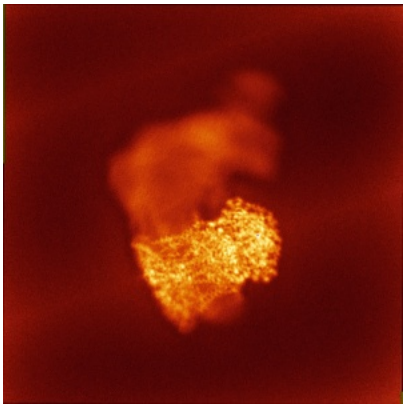


Z

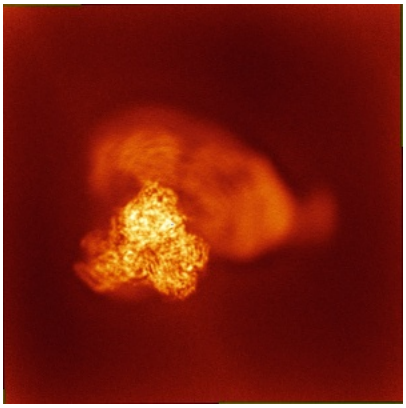
6.4.2 Raw map



X



Y



Z

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

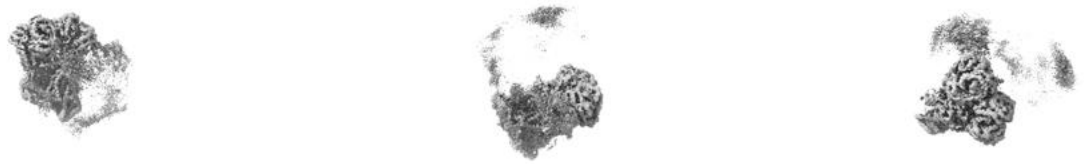
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

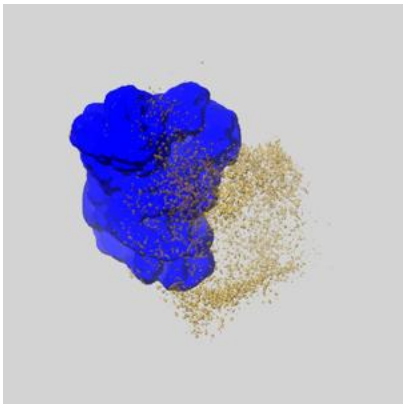
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

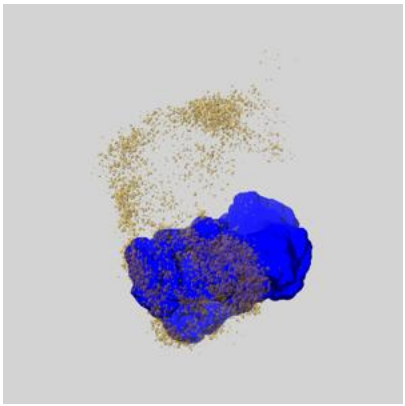
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

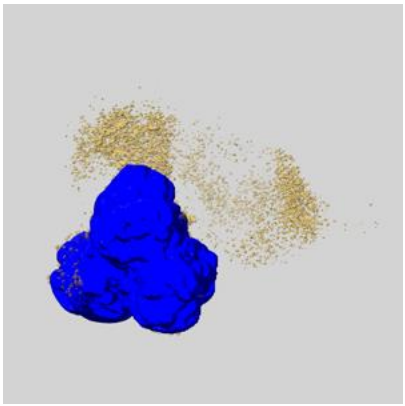
6.6.1 emd_35334_msk_1.map (i)



X



Y

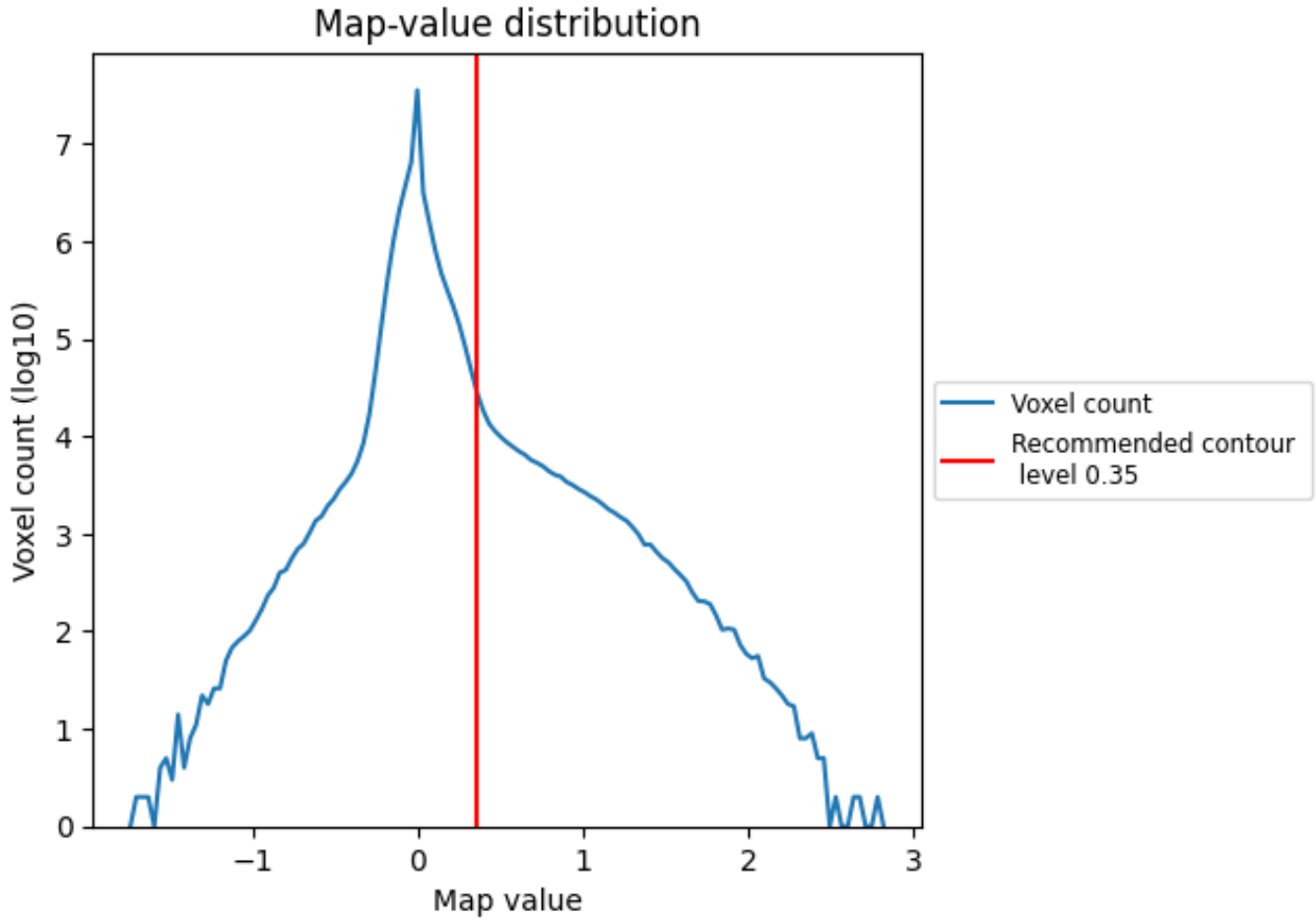


Z

7 Map analysis

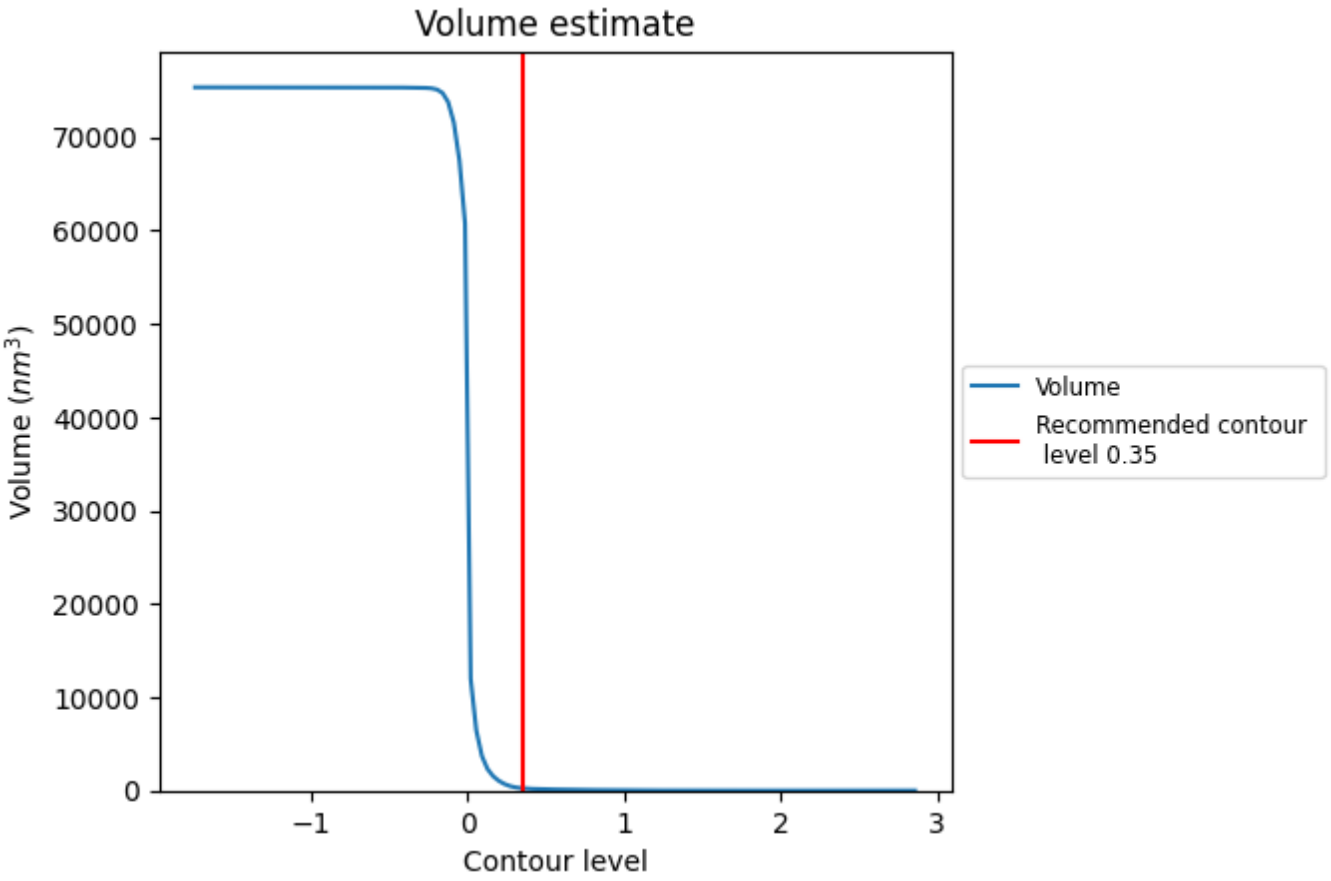
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

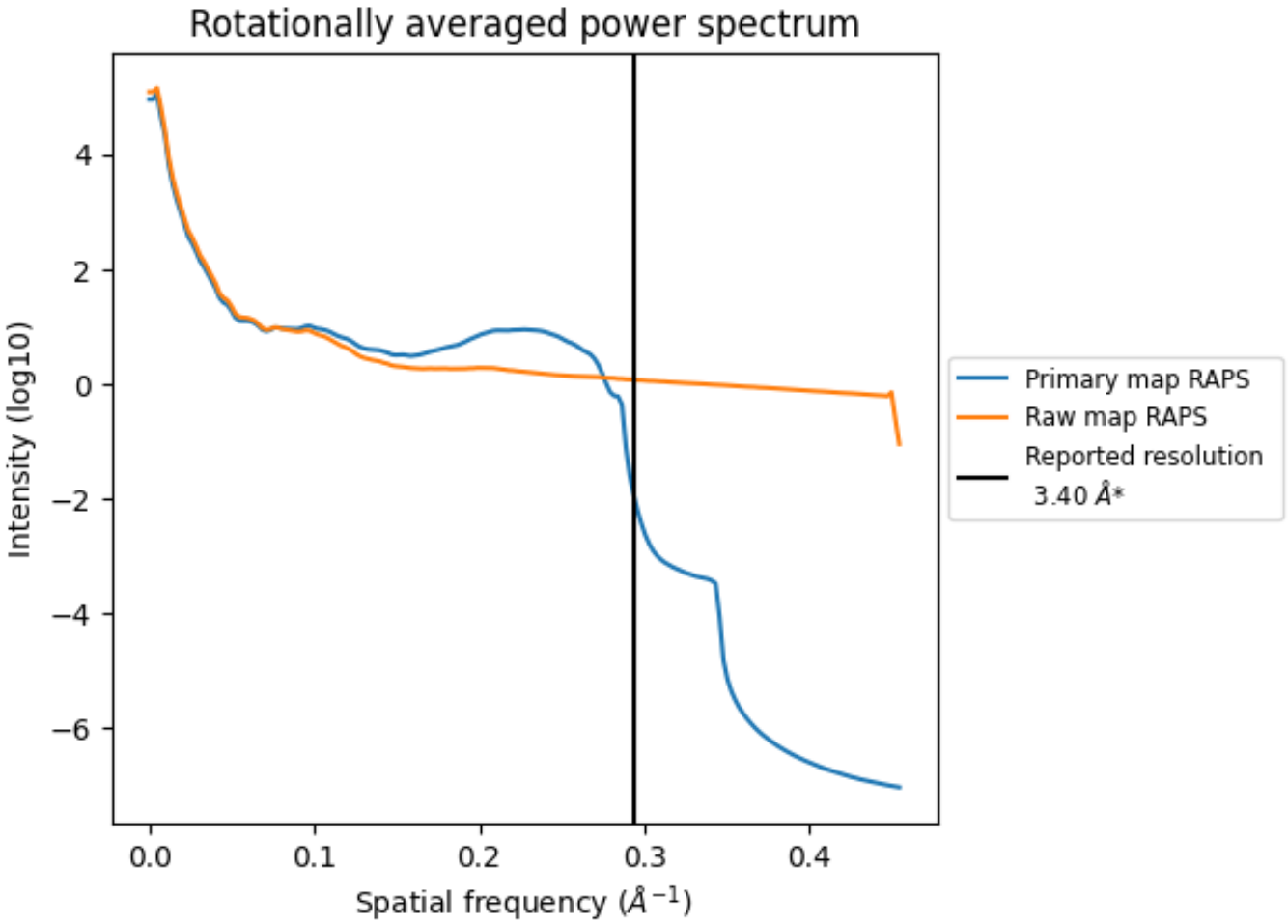
7.2 Volume estimate



The volume at the recommended contour level is 244 nm^3; this corresponds to an approximate mass of 220 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)

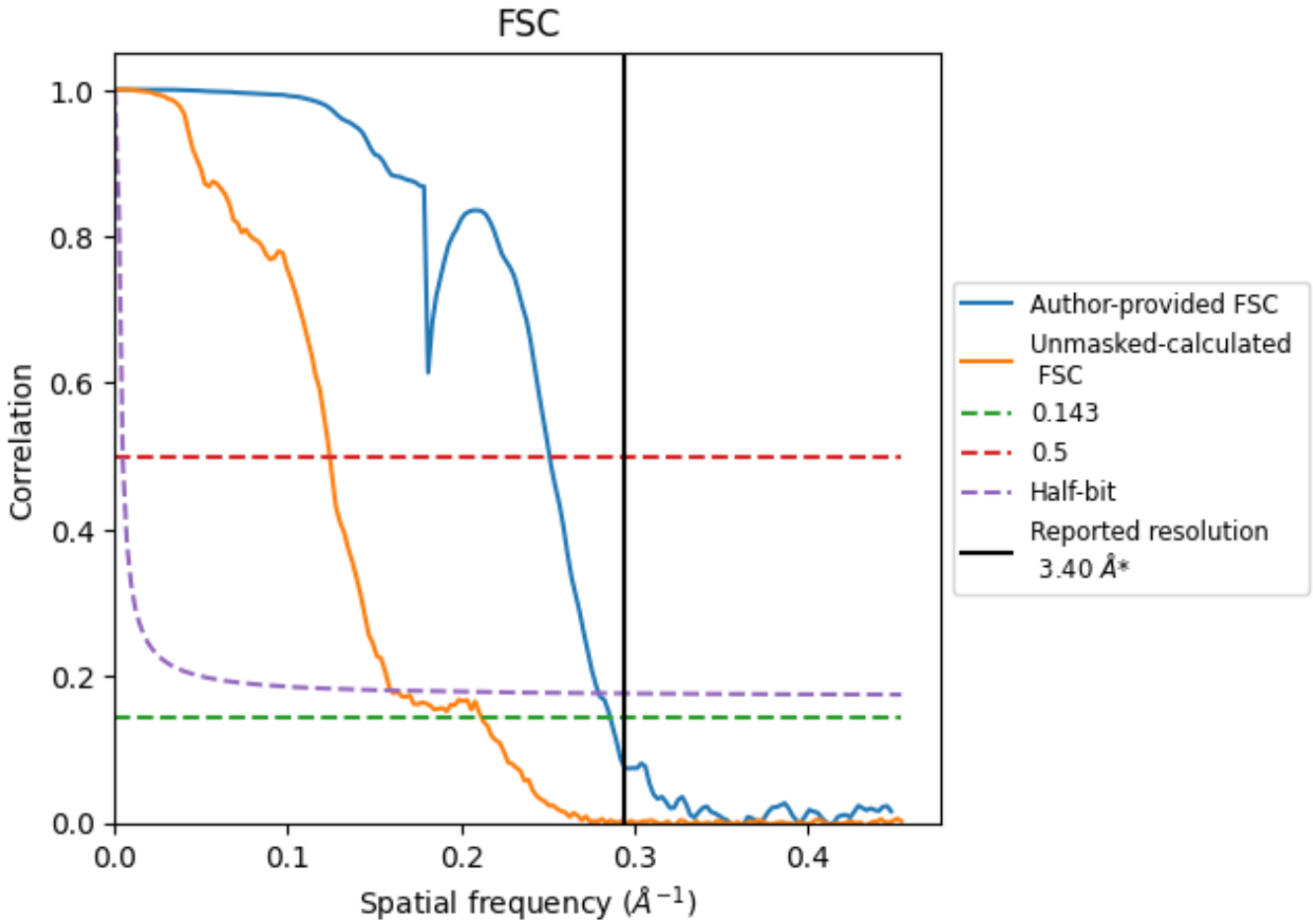


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

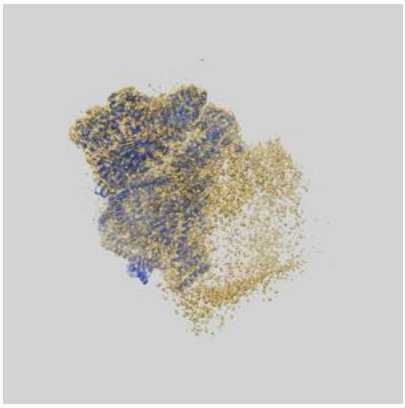
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.49	3.98	3.58
Unmasked-calculated*	4.72	8.05	6.25

*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 4.72 differs from the reported value 3.4 by more than 10 %

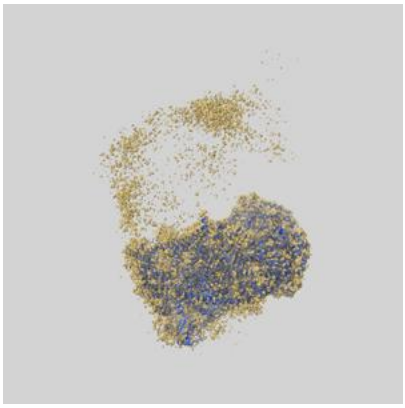
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35334 and PDB model 8IB7. Per-residue inclusion information can be found in section 3 on page 12.

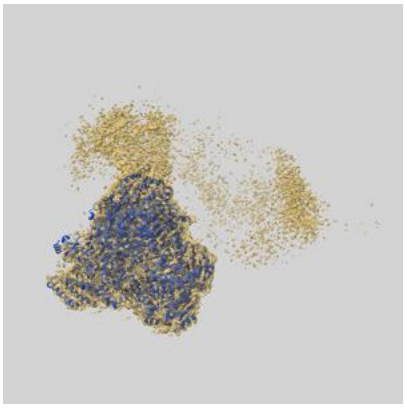
9.1 Map-model overlay



X



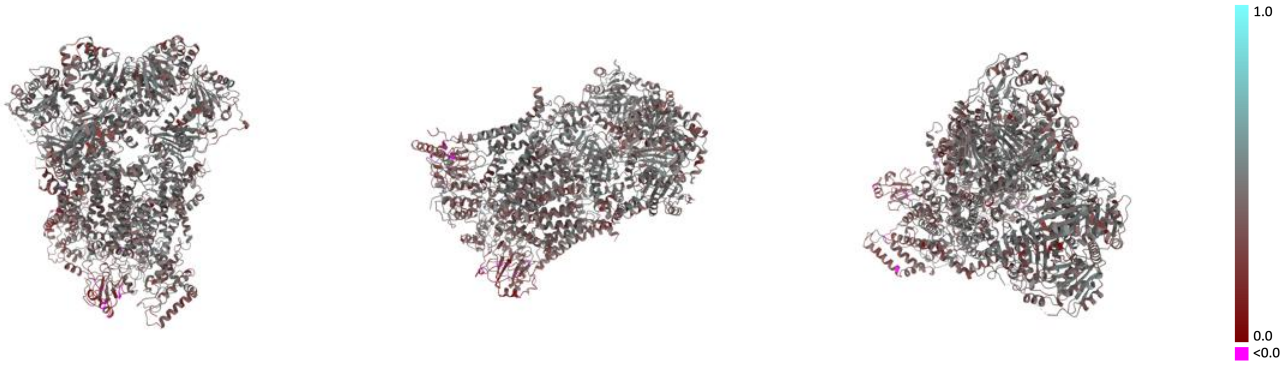
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

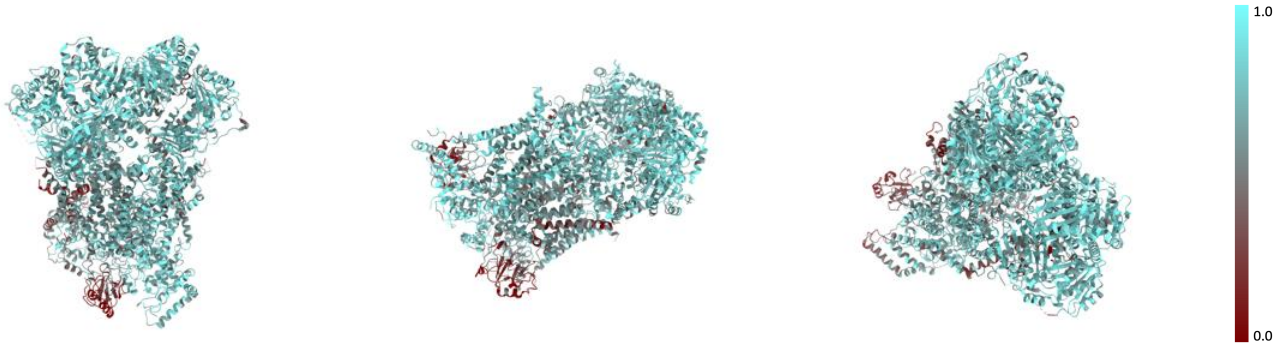
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

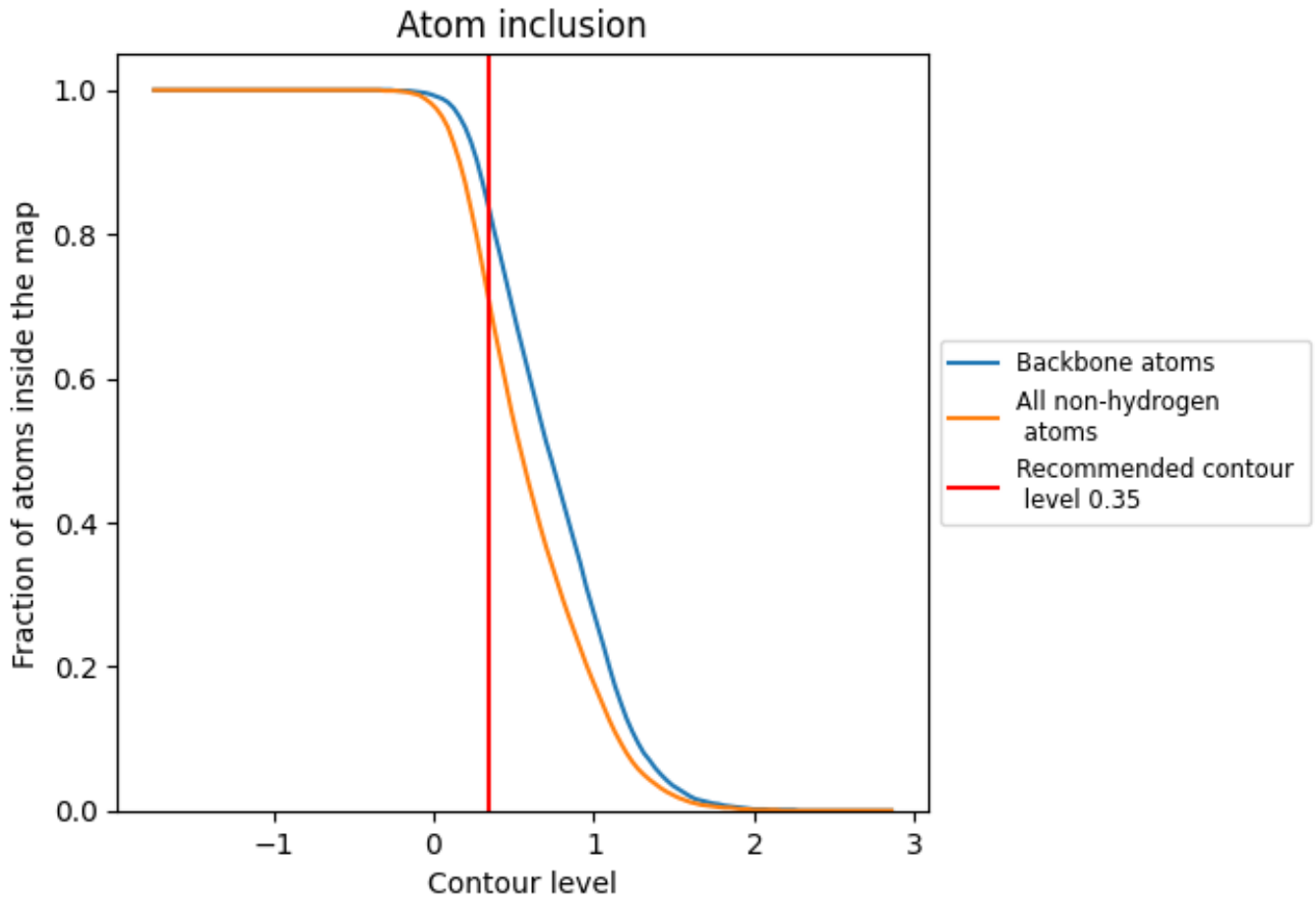
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4070
AA	0.7960	0.4360
AB	0.7840	0.4260
AC	0.7000	0.4210
AD	0.7040	0.3820
AE	0.3450	0.2790
AF	0.7160	0.4100
AG	0.6480	0.3710
AH	0.5430	0.2770
AI	0.5790	0.4280
AJ	0.3540	0.2930
AK	0.3360	0.3550
Aa	0.7780	0.4360
Ab	0.7910	0.4330
Ac	0.7620	0.4450
Ad	0.7940	0.4150
Ae	0.3540	0.2940
Af	0.7660	0.4520
Ag	0.7480	0.4470
Ah	0.7740	0.3640
Aj	0.6120	0.3990
Ak	0.2570	0.3700